Linear Conjugated Molecular Wires:

Organic Materials and Single-Molecule Electronics

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Abstract

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In this work, the synthesis and properties of different families of molecule wires are described. These families are made up of collections of linear conjugated oligomers, such as oligoenes and phenylenevinylenes and their derivatives. The bulk properties of each system were examined in order to establish structure-performance relationship between the intrinsic molecular properties of the bridging organic wire and the performance of their single-molecule junctions. The electrical as well as mechanical characteristics of single-molecular junctions were measured using the scanning tunneling-based break junction (STM-BJ) and atomic force microscope-based break junction (AFM-BJ) techniques. In addition, stilbene molecular wires and their derivatives are ideal model compounds for both of these oligomeric families and have helped to isolate and quantify some of the factors that govern charge transport through linear conjugated molecules.

After an introduction of molecular electronics, a highly tunable class of oligoenes, the α,ω-diphenyl–μ,ν-dicyano-oligoenes (DPDC) is described in the second chapter. They range from three to eleven linear C=C double bonds in length. Their synthesis is reported while their bulk solution properties show novel electronic structures, as well as broad optical absorptions and high extinction coefficients. Theoretical investigation using DFT calculations as well as strategies for functionalizing DPDCs are described. We have found that functionalization of these intractable materials has opened new doors for their

material applications. We envisioned functionalized oligoenes as molecular building blocks (i.e. conducting wires or rigid connectors) in the bottom up construction of new materials and devices.

Their prototypical structure and variable length would make DPDCs ideal candidates for molecular wires especially in the field of single-molecule electronics. Molecular junctions of the form metal-oligoene-metal were formed using the STM-BJ method and their charge transport characteristics were quantified in Chapter 2. In addition, we utilize long DPDC oligomers ($n > 5$) as variable resistance single-molecule potentiometers.

In chapter 3, we synthesize and employ our oligoene model compounds, the stilbenes, to differentiate the mechanical from electrical properties in molecular junctions. This enabled the development of new tools for uncovering the transport mechanisms in other molecules. One example is demonstrated in chapter 4, where stilbenes proved useful as mono-functionalized molecular wires. Together with extended oligoenes, stilbene molecular wires helped us to understand how current flows through a conjugated scaffold having only one electrode binding functional group (chapter 5). We observed a π-Au interaction that is weak, however strong enough to couple electronically to the electrode and complete the molecular circuit.

In the last chapter, we showcase a variety of new chemical structures that were prepared to probe the IV characteristics of organic single-molecule wires. A series of end-functionalized (p-phenylenevinylene) (PPV) oligomers and DPDC molecular wires were prepared. Exotic end-groups were important modifications for PPV's, since they increase oligomer solubility; the singe-molecule STM-BJ measurements would not be

possible on these otherwise insoluble compounds. PPV materials are very stable and can be further functionalized along their main-chains, however due to shorter effective conjugations lengths (smaller than that of the oligoenes), the range of electronic tunability is smaller in these materials. In addition to this family of symmetric molecules other asymmetric oligoene molecules were synthesized as candidates for single-molecule rectification. These molecules allow different electronic coupling to the right and left electrodes, which may modulate their IV characteristics.

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Acknowledgements

Prof. Colin Nuckolls has been instrumental to my academic and experimental career. His informal advising style has given me the opportunity to find my own interests in organic materials, empowering me to launch into new research directions, especially when they involve collaborations with scientists outside my field.

Of these, I especially thank Prof. Latha Venkataraman for her patience in teaching a synthetic chemist a little bit about applied physics. There have been many students in her group that I've had the pleasure of working with and learning from, such as Masha Kamenetska, Eek Huisman, Sriharsha Aradhya, Arunabh Batra, Jonathan Widawsky, and Radha Parameswaran. These scientists are responsible for the measurements and data analysis of much of the STM and AFM-BJ experiments in this dissertation.

Other collaborators have been essential to my projects in the last five years; Darcy Peterka, Prof. William Wilson, and Prof. Rafa Yuste for their interest in tailoring oligoene SHG properties as voltage sensors. Also, Prof. Christopher Murray and Jun Chan for collaborations in oligoene self-assembly and ligand exchange on metal oxide surfaces, as well as Luis Campos for his genuine insights in polymeric materials.

The members of the Nuckolls group have been an ongoing source of ideas and input, of the many I especially acknowledge Danielle Sedbrook, Matthew Carnes, Noah Tremblay, Kyle Plunkett, Tracy Chen, Seokhoon Ahn, Bryce Boardman and two undergraduate researchers, Markrete Krikorian and Carmen del Valle. Michael Steigerwald has been a unique influence. Often I've thought of him as my second advisor, who has the enchanting ability to turn devastating result into the fitting answer for a different, nonetheless exciting, question. His "lemons-to-lemonade" trick is evidence of his vast understanding and childlike amazement of the world around us.

Lastly, I recognize the many individuals outside of the world of science that have all made lasting impressions throughout my time at Columbia. They are my parents, Teresa and Dwight Meisner, my grandparents, Donna and Robert Colclesser, my sisters, Laurie and Merry, and my friends Andress Barnes, Joseph Parks, Bryan Handyside, Nili Ostrov, Jamison Heldrich, Andy Miller, Uma, Bella, Cassandra Simon, Alain Rostain, Carolyn Morrison, Jennifer Glenn, Janet Linnell, Petra Ornstein, Courtny Hopen, Grady Turner, NY Tribe, Brandon Robinson, Shea, Hacienda Group, Evan Kushin and Andrew Cray.

This work is dedicated to Donna and Robert Colclesser, my grandparents.

Preface

Before beginning, it is important that the reader is informed that much of the work in this dissertation was collaborative and many of the concepts, experiments and analysis carried out by others. The most influential collaboration has been that with the Venkataraman group here in Columbia's Applied Engineering and Mathematics Department. Many graduate and undergraduate students, post-docs and Prof. Venkataraman herself have guided my understanding of single-molecule electronics and preformed the STM and AFM-BJ experiments for Chapters 3 through 5. Following is a chapter-by-chapter account describing how each individual contributed to the work in this dissertation.

In chapter 2, Danielle F. Sedbrook, and I synthesized all oligoene compounds, with assistance from Markrete Krikorian, while collaborators at University of Pennsylvania synthesized and characterized the nanoparticles. Danielle Sedbrook prepared monolayer devices and preformed SEM studies. Michael Steigerwald ran and analyzed the DFT calculations. Aaron Sattler in the Parkin Group, carried out single-crystal X-ray diffraction characterization on the oligoene molecules.

The molecules in chapter 3 were synthesized by myself with the assistance of Markrete Krikorian and the single-molecule STM-BJ measurements were preformed by Maria Kamenetska. DFT calculations were preformed by Michael Steigerwald.

In chapter 4, the synthesis was carried out by Markrete Krikorian and myself, while the STM-BJ measurements were preformed by Seokhoon Ahn, Radha Parameswaran and Sriharsha Aradhya. AFM-BJ studies were preformed by Sriharsha Aradhya. DFT calculations were run and analyzed by Michael Steigerwald.

STM-BJ measurements in chapter 5 were also preformed by Seokhoon Ahn with the assistance of Radha Parameswaran and Sriharsha Aradhya. AFM-BJ studies and analysis were done by Sriharsha Aradhya. Both Sri and Seokhoon are responsible for the

statistical analysis of variation. Molecules were synthesized by Markrete Krikorian and myself. Michael Steigerwald and myself ran the DFT calculations.

Finally in chapter 6, all molecules were synthesized by myself, while physical investigations were performed by Eek Huisman, Jonathan Widawsky and Arun Batra. Collaborators from University of California Berkeley in Prof. Jeff Neaton's group, Pierre Darancet are responsible for modeling and calculations. Other DFT calculations were run by Michael Steigerwald and myself.

Chapter 1. Introduction on Molecular Electonics

1.1. Introduction

This dissertation is centered on the construction and design of organic molecules that when placed in metal-molecule-metal junctions provide insight into the molecular effects that govern junction behavior. In other words, the focus is on the "molecule" portion of these single-molecule junctions. Here, the charge transport through molecular junctions is understood, and ultimately controlled, by making rational modifications to the chemical structure of the bridging molecule. Changes in their atomically defined structures lead to differences in junction performance and character. Identifying such effects enable us to outline structure-performance relationships that guide the design and fabrication of functional devices with tailored or enhanced properties. In this chapter, we will inspect a few reports in the literature to contextualize what types of molecules have been studied since the introduction of modern single-molecular measurement techniques, of which the most relevant is the break junction method.

There are many factors that govern the charge transport properties through a molecular junction. Some of these factors are: the length of the conductance path; Fermi energy (E_F) of the electrode materials; as well as the alignment of the E_F with the molecular orbitals of the bridging molecule;[8] and the strength of the metal-molecule contact. To no surprise, the way in which molecules contact the electrode surface is critical. Not only does this contact determine electronic coupling between the molecule and electrodes but also plays major roles in the mechanical dynamics of the junction. In

the following chapters, several systems of molecules are showcased that enable the decoupling of these two factors including the novel systems having multiple conductance pathways, variable resistivity, quantum interference pathways and asymmetric chemical structures. These results, combined with those already present in the literature, paint a clear picture showing that inside a metal-molecule-metal junction, the molecule is not simply "just a molecule," but may instead be a critical component be used to control the transport properties of the junction.

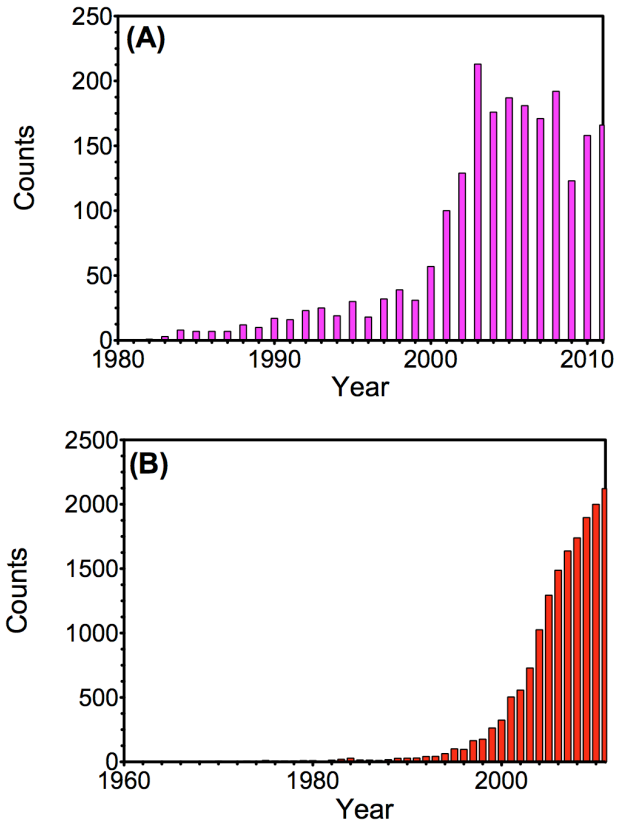


Figure 1.1: The increase in the number of publications containing the phrase (A) "molecular electronics" and (B) "single-molecule."

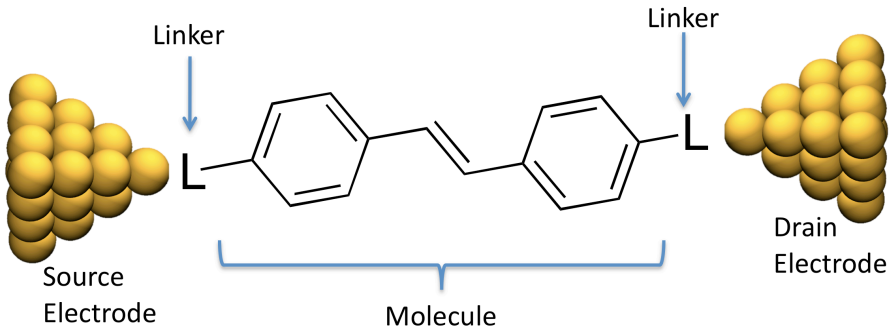
1.2. Molecular Electronics

Molecular electronics is a highly interdisciplinary field drawing from many natural and applied disciplines, such as engineering, physics, materials science and chemistry. Together they pursue a common interest to develop and utilize molecular-sized components in the fabrication of electrical devices. The essential goal is to control charge transport across atomically precise systems. This is an appealing goal not only because of the small size of such devices, but also because the great diversity of chemical structure that is available through synthetic chemistry can be used to tailor junction properties for specific applications. In fact, the term "molecular electronics" itself is poorly defined. Some authors include "molecular-based" materials referring to thin-film and liquid crystalline-based devices. Others define it more specifically to mean strictly single-molecule-based or single-molecule-thick applications, such is the type found in molecular wires or arrays of self-assembling monolayers. Here, the latter is accepted, since this work discusses the electronic properties of single metal-molecule-metal junctions (Figure 1.2).

Until a few decades ago tools to study systems at the single-molecule level were unavailable and thus fabrication of molecular-sized and single-molecule devices were unrealistic. Since then the amount of scientific research in this area has burgeoned. For historical context Figure 2 illustrates the number of peer-reviewed articles and patents published on this topic.[1] In order to progress the field, knowledge of how to make, handle and study molecular-scaled devices is required.

1.3. Measuring Single-molecular Properties

Special techniques are needed in order to measure the transport characteristics of a single molecule, of which a handful of strategies have been developed. Most take advantage of the ability for molecules to self-assemble on metal surfaces or into molecular-sized gaps. For example, self-assembled monolayers (SAMs)[2] on conductive surfaces, such as silver or gold, orient molecular wires away from the substrate. Since these molecules are bound to the conductive substrate they are already attached to the bottom contact of a device. To make a second contact, another electrode is either deposited or brought into contact with the top of the monolayer.[3] One popular method utilizes a gold conducting probe atomic force microscope (CP-AFM) tip and gold substrate as the source and drain electrodes.[4] Even though this method does not usually measure the charge transport through a single molecules it is worth mentioning since many accomplishments in molecular electronics have been made employing the SAM-based method.



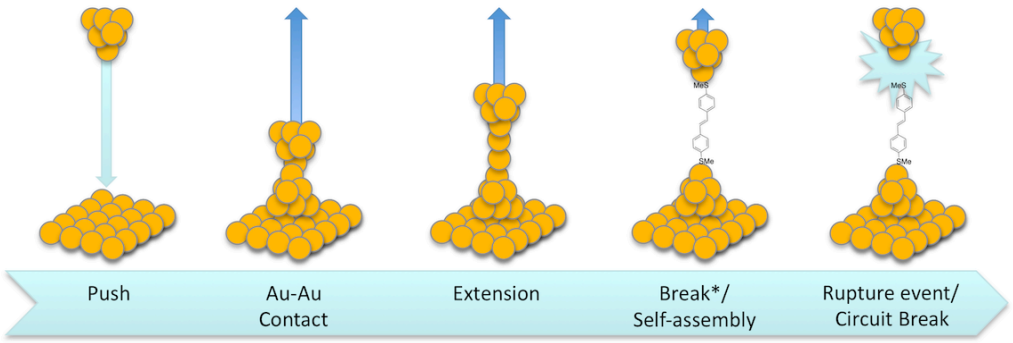


Figure 1.2: (top) A single-molecule junction. (bottom) Procedure for forming junctions using the STM-BJ method.

Another method that is more relevant to this dissertation relies on the mechanical stretching of nanometer-sized gold wires, and is called the mechanical break junction (BJ) technique. When stretched, the gold wire extends in length while thinning down to an atomically thick string of atoms before breaking. When preformed in solutions of molecular wires, the bridging molecules self-assemble between the insipient nanoscale gap. Here, each end of the gap functions as the source and drain electrodes. Variations upon this principal have been made that utilize substrate bending[5] and electromigration.[6] A breakthrough was pioneered by Tao and coworkers that utilized a scanning tunneling microscope (STM) with a gold tip and gold substrate.[7] This method, the STM-BJ method, has grown in popularity since thousands of reliable measurements to be carried out in a matter of hours. The tip may be repeatedly smashed into the gold surface and drawn away each time making fresh electrodes, from which a new molecule junction may be formed and measured. This process is depicted in the bottom of Figure 1.2. Due to the quantity of measurements, statistical interpretations on the conductance of molecular junctions are therefore possible. To compare different molecular systems we primarily use this method

in the following chapters to quantify the charge transport through oligoene and oligo-phenylenevinylene molecules.

1.4. Single-molecule Devices

The simplest single-molecule device can be seen in Figure 1.2. Comprised of a molecule bound between two electrodes, it represents a metal-molecule-metal junction. Gold is a popular electrode material owing to its oxidative stability and malleability. Electrodes are an important consideration, since the work function differences will effect the alignment of the Fermi energy (E_F) with the molecular levels.[8]

Molecules of many different types may be bound into the device. This is the most varied portion of the junction in the literature. Changes in atomic constitution determine the intrinsic attributes of the bridging molecule, such as the level of conjugation, energy of the molecular orbitals, strength and character of molecule-electrode interactions, even the length of the molecule. Each of these plays major roles in device performance. For instance, the conductance of unsaturated vs. saturated molecular junctions, such as 1,4-diminobutane and 1,4-diamiobenzene, has been compared.[9,11] Both are linked through primary amines and are four carbons in length, but perform very differently. The aromatic molecule has a significantly lower HOMO-LUMO difference and its frontier orbitals align more closely with the E_F of the electrodes. Thus, conductance of the benzene derivative (6.4×10^{-3} G_0) is higher than the alkane (1×10^{-3} G_0).

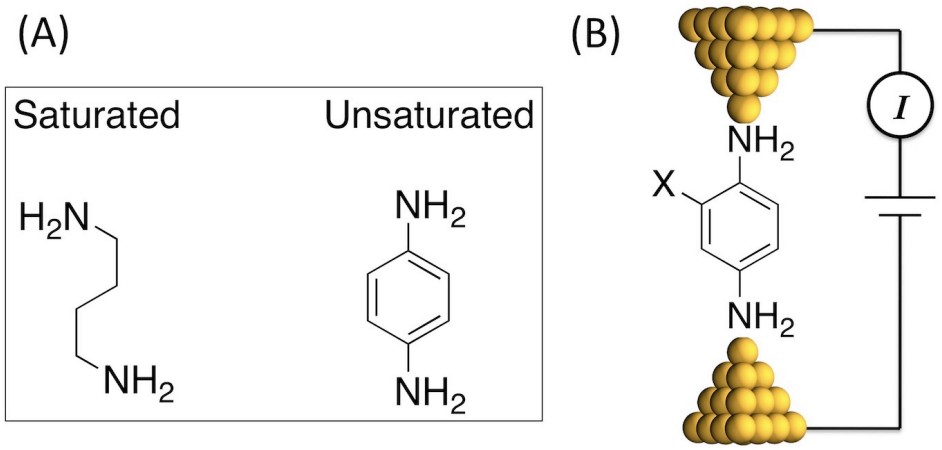


Figure 1.3: The atomic constitution of the molecule in molecular junction can modulate the junction conductance. (A) Saturated alkanes are less conductive than aromatic molecules of similar length. (B) Slight changes in the electronic structure of aromatic molecules through installation of chemical substituents affects junction conductance.

Molecular structures can be further modified by decoration functional groups. In 2007 functionalized 1,4-diaminobenzene, with electron-donating and electron-withdrawing groups.[9] A schematic of these junctions are given in Figure 1.3. Both the number and type of substituents were varied. Here in conjugated molecule such effects are easier to see since they are less resistive than aliphatic molecules. Similarly, our group has previously demonstrated how functionalization of biphenyls controls the conformational twist about the aryl-aryl bond. The bulkier the substituent, the more twisted the molecule becomes, thus changing the degree conjugation and ultimately the molecular conductance.

In summary, there is interplay between electrode material, chemical structure and linker constitution. Together they determine the charge transport properties of the

junction. However, the greatest possibility for variation belongs to the molecular portion. Here a wide variety of structure can be made with a variety of properties and functions, such as the level of conjugation, energy of the molecular orbitals, strength and character of molecule-electrode interactions, even the simple length of the molecule. Each of these plays major roles in device performance.

In order to deconvolute the many factors mentioned above, and quantify them individually, it is necessary to use sets of rationally designed molecular architectures that allow for simple comparisons and deductions to be made. These "molecular toolboxes" would contain sets of atomically precise molecular variations, each of which would be tailored to modulate one (or a few) of the many contributing factors. Since organic synthetic chemistry possesses the know-how to synthesize new molecules and their variations, it is central to overcoming these challenges in molecular electronics.

1.5. Linker effects

A design requirement for single-molecule electrical devices is that the molecule must be both structurally and electrically connected to the metallic electrodes, even if only weakly so. Therefore, just as much emphasis is placed on the functional groups that attach the bridging molecules to the electrodes as the design of their interiors. We name the chemical functional groups that anchor the molecules into the molecular junction as linkers. Since gold leads are used in our STM-BJ setup, aurophilic functional groups are used to form Au-molecule-Au junctions. To date many different linkers have been employed, such as -SH,[6,10] -NH_2, -SMe, -PR_2, -COOH, -SCN, -NO_2, and others.[11,12] Even

strained aromatic groups act as linkers, such as in oligo(para[2.2]cyclophanes)[13] and buckminsterfullerene.[14]

Linker choice is very important, since linkers affect the level of electronic coupling between the molecule and the electrode, as well as junction mechanics. Each of these factors attenuates the junction performance (see Figure 1.4A). Other junction properties can also be affected by the type of linker, such as conductance step-lengths and rupture forces.[15] For example, Vekataraman and coworkers measured three analogous series of alkanes functionalized at each end with a linker group (either primary amines, methylsulfides, or dimethylphosphines).[12] Each series was systematically elongated and measured using the STM-BJ method. Fitting the conductance vs. length data (Figure 1.4B) gave similar decay constants for each series, which is expected since the atomic constitution of the molecular backbone was identical. Although the decay parameters were identical, the overall resistivity between each series varied. This was the result of differences in the effective contact resistance, or the resistivity attributed to the metal-molecule interfaces. It was found to depend systematically on the linker type and ranged from 370 kΩ for amines to 270 kΩ and 130 kΩ for the methylsulfides and phosphines, respectively.

Linker groups also result in differences in the molecular conductance step lengths, called step lengths for short. As the electrodes are pulled apart, the step-length is the distance between electrodes just before the circuit breaks. It is the maximal junction length and correlates to the molecular length. Figure 1.4C, shows how dramatic linker effects are in the step length of difunctionalized n-butane molecules. For NH_2 linkers

(green line) a step-length of ~0.8 Å is observed, while for SMe (red line) and PMe_2 (blue line) step-lengths are 1.7 Å and 3.2 Å.

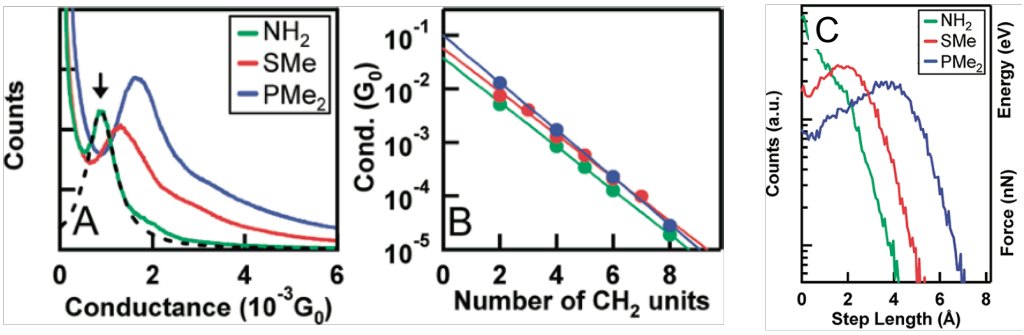


Figure 1: Linker effects in oligo-alkanes. (A) Step-length differences in a set of three butane molecules each functionalized with different linkers. Figures were adapted from a previously published article.[12]

1.6. Challenges and Frontiers

Despite the many accomplishments in single-molecular electronics, future goals seek to harness molecular components in molecule-based integrated circuitry; these goals are far from met. First, expansion into measurements on more exotic molecular designs will push our current understanding of molecular electronics. Such materials present many obstacles (i.e. low band gap and photoxidative materials), since they are more difficult to synthesize, store and measure. More complex structures may also establish bridging components with multiple conductance pathways, which will inevitably convolute their analysis. Secondly, there is more to make than simple resistors; the most well understood property of organic single-molecule wires is their resistivity. How do we use that to make devices with higher functions? Lastly, conductance is the primary means

of understanding single-molecular junctions. Therefore, it is difficult to quantify junction performance in low and non-conductive systems. Such molecules include cross-conjugated and quantum interfered systems or molecules of sufficient length to conduct below the sensitivity of our instrumentation. In these cases, it is difficult to quantify the electron transport through these structures, let alone prove that a junction has formed at all. Only systems that are electrically conductive within our detection limits can be measured properly. Therefore it is necessary to enable the measure of alternative quantities (such as force). This would open established techniques to molecules of greater length and even polymeric materials, cross-conjugated molecules and systems having pathways dominated by quantum interference.

1.7. Addressing Future Challenges

In this dissertation we seek to meet these challenges by synthesizing novel molecular tools, such as those discussed in chapter 2 and 6, to expand our understanding of the role that intrinsic molecular properties play in the transport of single-molecule junctions. In chapter 4 we use a new technique, developed by the Venkataraman Group, to measure simple systems exhibiting quantum interference; a phenomenon that up until now could not be studied with previous single-molecular methods. We target not only the electronic performance of rationally designed molecules, but also investigate the interplay between mechanical factors and charge transport (chapter 5). In chapter 6 we describe the unusual IV and mechanical characteristics of a family of conjugated oligomers. In doing so we have gone beyond the simple resistor to create new electrical

components, such as potentiometers (chapter 3) and rectifiers (chapter 7), on the molecular scale.

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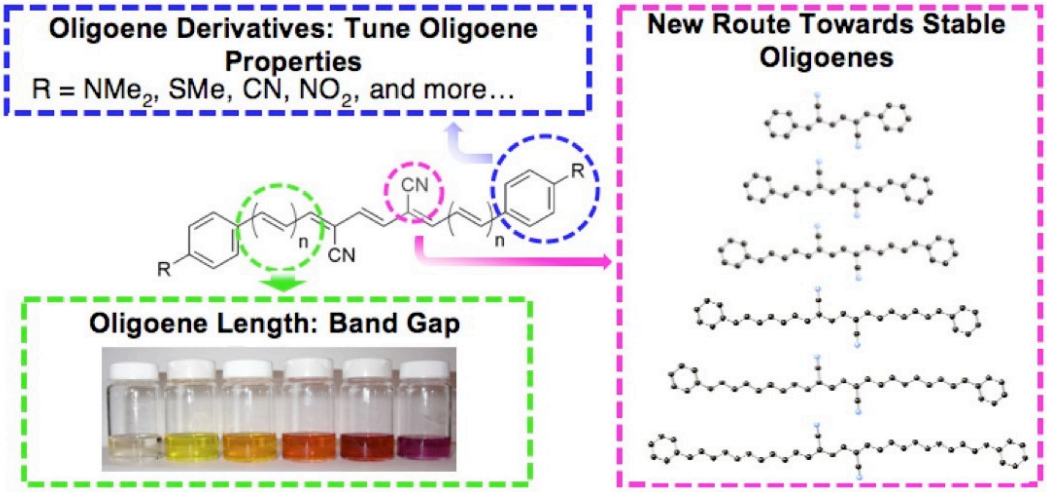
Chapter 2. Functionalizing Molecular Wires: A Tunable Class of α,ω-diphenyl-μ,ν-dicyano-oligoenes[†]

All molecules in Chapter 2 were synthesized by Danielle Sedbrook and I with assistance from Markrete Krikorian. Our collaborators at University of Pennsylvania synthesized and characterized the nanoparticles. Danielle Sedbrook did the SEM studies. Michael Steigerwald with assistance from myself ran the DFT calculations.



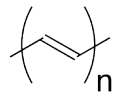
2.1. Motivations

Molecules with linear conjugated structures are ideal candidates as molecular wires and connectors in molecular-sized devices. Oligomers having well defined, atomically precise fragments enable the systematic study of their length-dependent properties and yield insight into the assembly and electronics of their polymer analogues. In this chapter we explore the electronic and physical properties of a new class of oligoene materials and their derivatives.

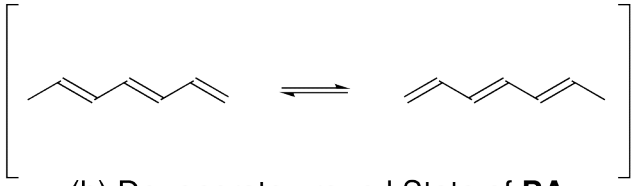
[†]Parts of Chapter 2 were reproduced or adapted with permission from the authors: Meisner, J. S.; Sedbrook, D. F.; Krikorian, M.; Chen, J.; Sattler, A.; Carnes, M. E.; Murray, C. B.; Steigerwald, M.L.; Nuckolls, C., *Chem. Sci.*, **2012**, 3, 1007–1014. Copyright 2012 Royal Chemical Society.

2.1.1. From Polyacetylene to Oligoenes

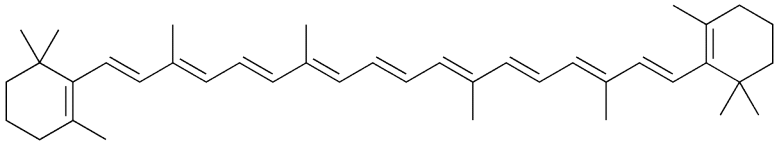
Of the many classes of conjugated materials, oligo-olefins are of particular importance owing to their prototypical chemical structure; they are monodisperse vinylogues of the classic electronic polymer, polyacetylene (PA, Figure 2.1a). The simplest conjugated hydrocarbon polymer, PA is made up of alternating C-C single and C=C double bonds. Its ground electronic state is doubly degenerate (Figure 2.1b) allowing for delocalization of the π-electrons along the conjugated backbone. It is a semiconductor, however, is highly conductive when doped.[1] In fact, depending on the type and concentration of the dopant, the conductivity of PA may be increased by over eight orders of magnitude (I_2 doping) reaching conductivity values similar to silver metal. Additionally, PA has a low band gap and shows large nonlinear optical susceptibilities.[2] Since the fully conjugated high polymer is electrically conductive, we believe that well-defined oligomers, hereafter referred to as oligoenes, should be useful molecular conductors in nanoscale situations. In addition, naturally occurring terpenoid-based oligoenes, such as carotenoids (Figure 2.1c), have been made into electrical devices and are known to have useful optical properties.[3] Although, nature provides a limited number of structures that are often difficult to functionalize further, thus preventing their use in widespread applications.



(a) Polyaetylene (**PA**)



(b) Degenerate ground State of **PA**



(c) β-carotene

Figure 2.1: Structure of Polyacetylene (**PA**). **PA** has a doubly-degenerate ground state. (c) carotenoids are tetreterpenoids that naturally occurring oligoenes. β-carotene is a widely known example of a carotenoid.

The synthesis and study of conjugated oligomers has flourished over the past 20 years, however oligoene systems remain understudied. Three major challenges have hampered the development of oligoenes as electronic materials: (1) The most thoroughly studied examples of PA oligomers have been obtained inefficiently through the painstaking isolation of individual oligomers from polymerization reactions terminated at low monomer conversion.[4] (2) Previous preparative methods have not supported diverse functionalization to incorporate them into electronic devices. (3) Oligomers of PA are chemically impractical because they are nearly insoluble and oxidatively unstable. Using the new synthetic strategy detailed below for the α,ω-diphenyl-μ,ν-dicyanooligoenes.[5]

(DPDC, Figure 2.2b) we have overcome these challenges. The key to this synthesis is the use of sterically innocent yet electronically stabilizing cyano groups bound directly to the oligoene chain while protecting the reactive terminal olefins with bulky phenyl groups.[6] These phenyl end-groups can easily be modified with a diverse range of functional groups to reveal a wide variety of compounds that can be produced through our synthetic method. We also highlight the versatility and adaptability of these new electronic materials by using appropriately functionalized oligoenes as electrical conduits that connect magnetic nanoparticles to a semiconductor surface.

Other methods have been used to stabilize oligoenes. Several approaches protect the highly reactive terminal olefins with bulky end-groups such as phenyl (DPO, Figure 2.2a)[6] or *tert*-butyl.[7,8] Other than such hydrocarbon-end-capped oligoenes, however, there are few other examples of non-terpenoid α,ω-disubstituted oligoenes longer than pentaenes.[9,10]

2.1.2. Naturally Occurring Oligoenes

Nature provides its own methods of oligoene stabilization: terpenoid-based biomolecules such as carotenoids (Figure 2.1c). Carotenoids are the most studied class of oligoenes, of which the most well-known member is β-carotene. They play essential roles in many biological processes such as vision (retinal), cell differentiation (retinol) and photosynthesis and pigmentaion.[11] Built from terpene subunits, methyl groups decorate the oligoene backbones and contribute to both the solubility and stability. However, they also create allylic-1,3-strain along the poly-olefin backbone, which cause the molecules to bend. Torsional distortions reduce the conjugation and increase the energy difference

between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), and shifts the electronic absorptions to higher energies.

2.1.3. Rational Design Toward Cyano-functionalized Oligoenes

In order to use oligoenes in optical devices, it is desirable to have a family of light-harvesters that cover the entire visible and near-infrared spectral regions. Therefore, we sought small and synthetically available substituents that could confer stability while maintaining the bathochromic absorption shifts expected for longer oligoenes. Cyano groups, shown in Figure 2.3, fulfill these requirements: they are π-electron withdrawing groups with a linear geometry and are not bulky enough to disrupt molecular planarity. The A-value of s cyano group has been determined to be 0.19 kcal/mol in contrast to that of a bulkier methyl group (1.74 Kcal/mol).[12] They have been used to alter the band gaps of a variety of aromatic molecules and conjugated polymer materials.[13] Cyano groups are known as strong electron-withdrawing groups as evidenced by their high Hammett substituent coefficient (σ_p = 0.66)[14] and because of their electron-withdrawing ability they are expected to lower the energies of the frontier orbitals, thus stabilizing the system toward oxidative decomposition. As an ultimate benefit they are easily installed and enable an economical synthesis that allows for diverse end-group functionalization.

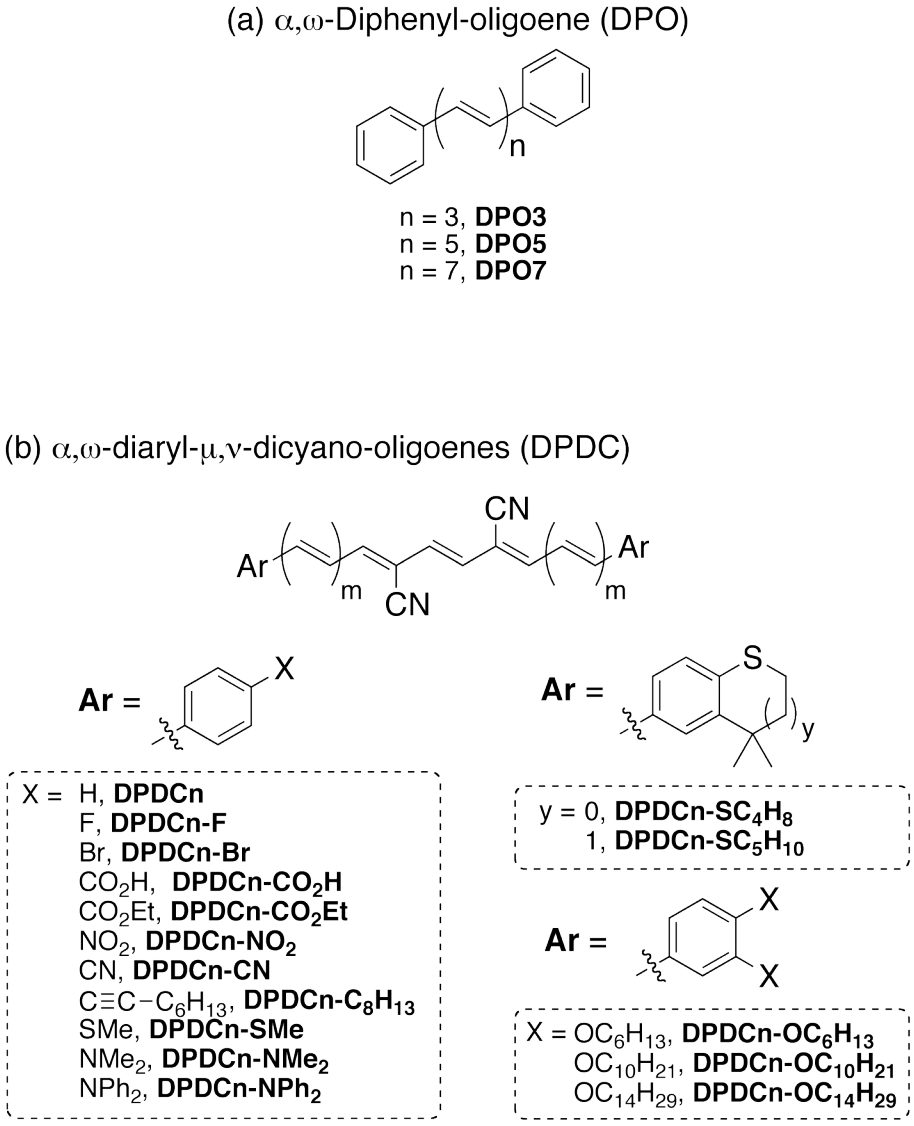


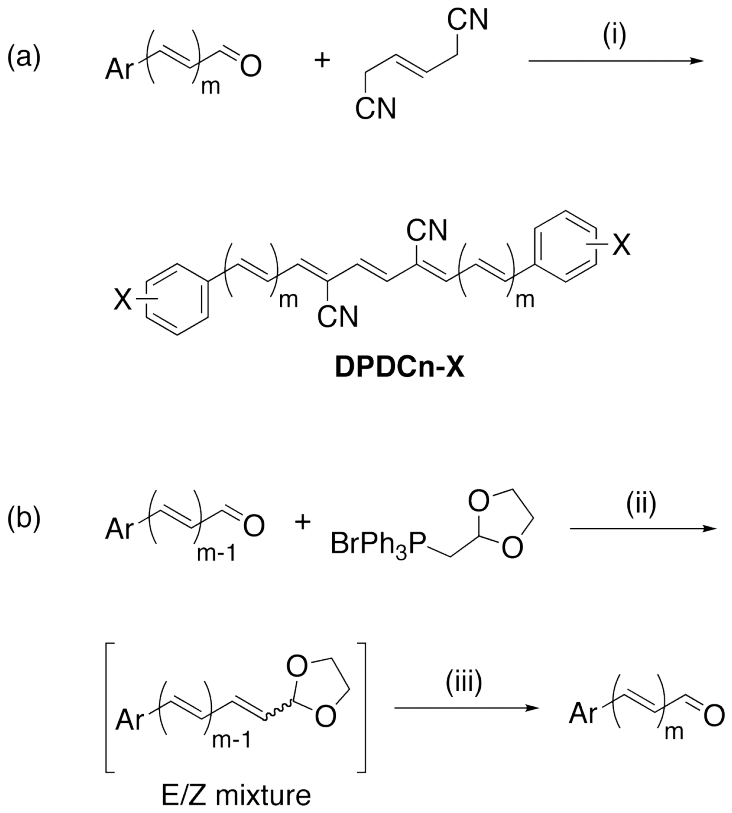
Figure 2.2: (top) Structure of α,ω-diphenyl-oligoenes (DPO), which we regard as control molecules for comparison with (bottom) cyano-functionalized α,ω-diphenyl-oligoenes (DPDC). We identify the oligoene molecules according to the length of their linear conjugated backbone (**n**) and aryl end-group (**X**), **DPDCn-X**. For instance, 1,10-di-(4-bromophenyl)-4,7-dicyano-deca-1,3,5,7,9-pentaene is denoted as **DPDC5-Br**. See Appendix A for a complete list of molecules.

2.2. α,ω-diphenyl-μ,ν-dicyano-oligoenes

2.2.1. Synthetic Approach

A convergent synthetic pathway was necessary to allow easy access to multiple oligomeric lengths while avoiding unique synthetic routes to each individual member of the series. The Knoevenagel condensation reaction was first published in 1898,[15] where one equivalent of benzaldehyde reacted with malonic acid under basic conditions. A bronsted base first deprotonates the acidic α-proton, subsequently attacking the electrophilic carbonyl center on the aldehyde. From the tetrahedral intermediate proton transfer to the incipient hydroxyl generates a good leaving group, water.

The key step in our synthesis, a double Knoevenagel condensation between 1,4-dicyano-2-butene and two equivalents of the appropriate aryl-enal (Scheme 2.1a) sews together the oligoene backbone while simultaneously installing two central cyano groups. We prepare the aryl-oligoenals starting from the analogous benzaldehyde or *trans*-cinnamaldehyde via iterative Wittig homologations[16] and subsequent acidic hydrolysis of the intermediate acetal. The conditions for both reactions tolerate a wide variety of functionality and give access to a range of derivatives. Figure 2.2b shows those derivatives that we prepared for this study via this method. They are made in a small number of steps from commercially available starting materials.



Scheme 2.1: Synthesis of DPDCs via (a) Double-Knoevanegel condensation reaction and (b) Wittig reaction. (i) DBU, MeOH, 25º C, 6-12 h, (60-10%, for **DPDCn** series; from m = 0 to 5); (ii) LiOMe, THF, 75º C, 12-24 h. (iii); 10% aq. HCl, 25º C, 2 h (70-98%). For instance, if m = 1, then the intermediate acetal leads to the product (2*E*,4*E*)-5-phenylpenta-2,4-dienal. A list of all compounds is provided in Appendix A.

In general, the Knoevenagel condensations give moderate yields, which decease with increasing molecular length producing the **DPDCn** series in 10–60% isolated yields, shown in Table 2.1. Despite moderate yields, the condensation reaction is operationally simple: (1) A common base, such as sodium methoxide (NaOMe) or the non-nucleophilic organic base 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU), is the only reagent, of which the later can be stored under normal laboratory conditions; (2) anhydrous solvents are not necessary and (3) isolation does not require chromatography. This reaction joins two

fragments together; more than doubling the length of the starting aryl-oligoenals. The products precipitate from the reaction mixture and are easily isolated by filtration. When necessary the crude products are purified by recrystallization from CH_2Cl_2 by adding MeOH. With this approach, the synthesis of **DPDC13** (one of the longest oligoenes prepared to date) is straightforward and involves only five steps. It is also important to mention that the sequence shown in Scheme 2.1 is scalable; we tested members of the **DPDCn** series on the gram-scale with no loss in their isolated yields.

Table 2.1: Double Knoevenagel Condensation Yields for the **DPDCn** Series.

Oligoene	Oligomeric	Isolated Yield (%)
DPDC3	3	55
DPDC5	5	60
DPDC7	7	54
DPDC9	9	45
DPDC11	11	40
DPDC13	13	10

All of the compounds have exclusively *trans*-stereochemistry in their double bonds. The stereochemistry of the double bonds in the each aryl-oligoenal starting material can be identified by the coupling constants of the olefinic doublet of doublets near 6.5 ppm (this signal belongs to the β-proton of the aryl-enal). This resonance is coupled to the aldehyde and a *trans*-olefin (-CH=) proton, and resides in an isolated region of the spectra allowing for stereochemical characterization throughout the growth of the aryl-oligoenals.

Wittig conditions (Scheme 2.1b) produce an *E*/*Z*-mixture of stereoisomers, however acid hydrolysis of the intermediate acetals exclusively produces the *trans*-product. Cleavage of the acetal is carried out before separation, however to further understand our method we tracked the stereoisomeric transformations throughout the extension of *trans*-cinnamaldehyde to (2*E*,4*E*)-5-phenylpenta-2,4-dienal. In this case performing the Wittig reaction on *trans*-cinnamaldehyde produces the (*E*)- and (*Z*)-4-phenylpenta-2,4-dienyl acetals in 16% and 60% yield, respectively. We separated each product by column chromatography; coupling constants from ^{1}H-NMR spectra identified each stereoisomer. Acid hydrolysis of either stereoisomer, *E* or *Z*, by addition of 10% aq. hydrochloric acid to a solution of acetal in tetrahydrofuran generates the same product, (2*E*,4*E*)-5-phenylpenta-2,4-dienal, in quantitative yields.

Many Wittig homologations are carried out with potassium or sodium *tert*-butoxide (i.e. ^{t}BuOK), however significant reduction in the yields of our aryl-oligoenals were observed with these bases. The difference in yield is due to the base-induce disproportionation of the aldehyde starting material. First reported in 1853 by Stanislao Cannizzaro this reaction is called the Cannizzaro reaction.[17] In the Wittig homologation starting from *trans*-cinnamldehyde and instead using potassium *tert*-butoxide the cinnamyl alcohol was isolated in 20% yield.

2.2.2. Solid-state Structure

We have grown crystals of each member of the **DPDCn** family (from n = 3 to 13) and determined the molecular structure of each crystallographically. Shown in Figure 2.3, each oligoene occurs exclusively in the all-*trans* form. **DPDC13** is the longest oligoene

thus far characterized by XRD, longer even than the natural product, rhodopin glucoside,[18] which contains 11 linear conjugated C=C bonds. Although some of the shorter vinylogues have been previously reported in the resin dye patent literature,[19] a systematic characterization has been heretofore unavailable. Only a few non-terpenoid structures having more than six conjugated C=C bonds have been previously reported, and none having more than nine.[20]

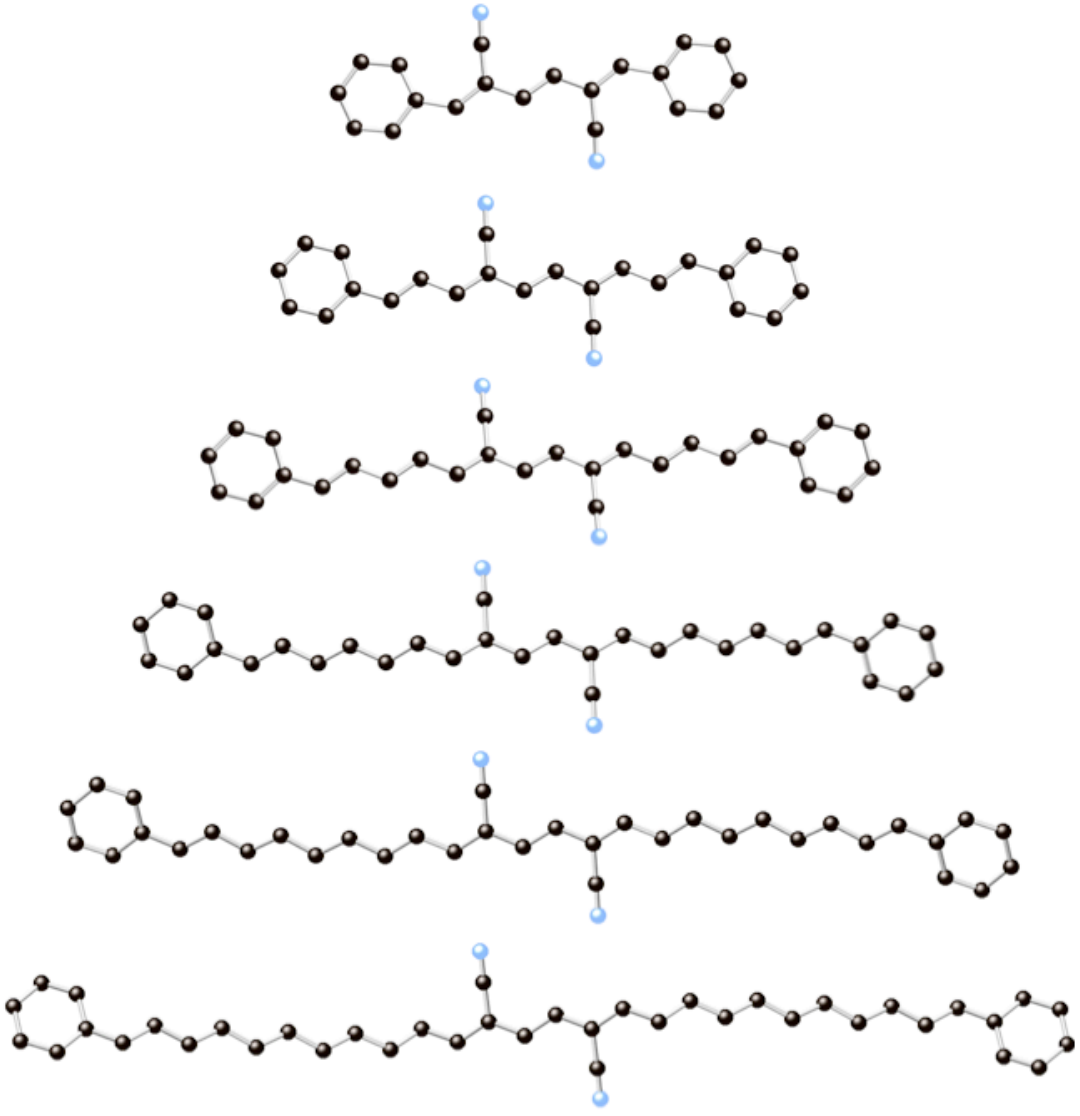


Figure 2.3: Crystal structures of **DPDCn** series were determined by single crystal X-ray diffraction.

We observe different packing structures within the parent series of **DPDCn** oligomers. The shortest vinylogues, **DPDC3** and **DPDC5**, are planar and stack in a herringbone pattern, indicating that the cyano groups do not significantly interact with allylic hydrogens (Figure 2.4). The longer oligomers, **DPDC7-DPDC13**, co-crystallize with one solvent molecule per unit cell and are not fully planar. The central dicyano-butene moiety is planar and to either side out-of-plane bending of the conjugated backbone is accompanied by a slight twist. DFT calculations at the B3LYP/6-31G** level predict fully planar conformations, however the incorporation of solvent as well as bending is common in crystal structures of oligoenes having more than six C=C bonds.[7,8]

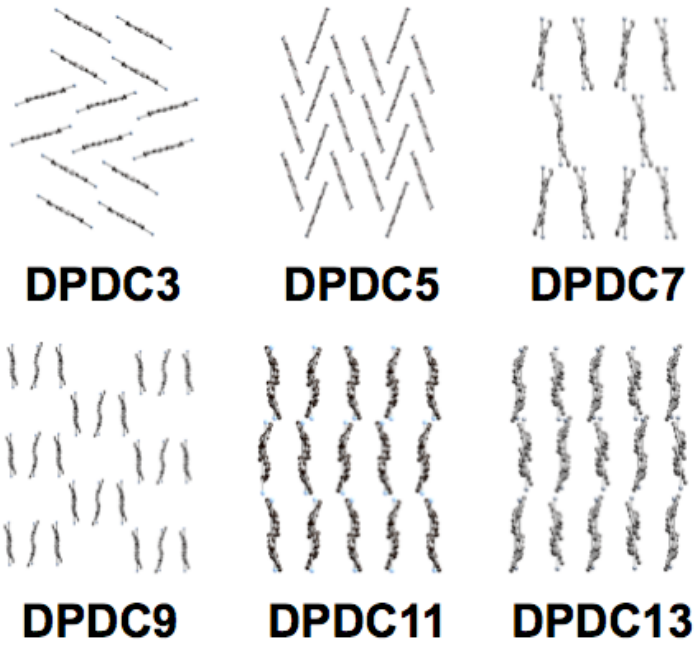


Figure 2.4: Packing structures of **DPDC3-DPDC13**. Solid-state packing morphs from herringbone-type to aligned stacks of oligoenes as oligoene length increases. For **DPDC7-DPDC13** solvent molecules were omitted for clarity.

There exists a dearth of solid-state structural information on oligoenes especially for those having more than 5 linear conjugated C=C bonds. For instance, the Cambridge Structural Database (CSD) provides only two non-terpenoid (such as carotenoids) oligoene structures containing 9 or more linear conjugated C=C double bonds. Both structures belong to the cyclic oligomer, [18]-annulene.[20] Other search results show: 6 structures for n = 8; 10 for n = 7; and 13 for n = 6.

We were concerned that the cyano groups would disturb the local structure of the oligoene backbone and minimize the degree of conjugation. Despite the observed bending, the central alkene unit (that having doubly allylic cyano groups) remains planar for each member of the series with a dihedral angle of 180.0°. This suggests that deviations from planarity may be attributed to co-crystallization with solvent molecules and not the result of cyano-functionalization.

2.2.3. Control Group: α,ω-diphenyl-oligoenes (DPO)

In order to verify the practical value of cyano substitution, we have also prepared the unsubstituted α,ω-diphenyl-oligoenes (DPO) of the corresponding lengths, **DPO3**, **DPO5** and **DPO7**. We synthesized these molecules lacking the cyano groups via the Horner-Wadsworth-Emmons reaction[21] as described by Spangler and coworkers.[10] Dicyano-oligoenes are less reactive toward ambient oxidation, intermolecular oligomerization or intramolecular decomposition than their unsubstituted relatives; we can conveniently study them under normal aerobic laboratory conditions for extended periods.[22] The thermal stability of these dicyano-oligoenes (**DPDC3-DPDC13**) is similar to that of the α,α,ω,ω–tetrakis-*t*-butyl-functionalized oligoenes reported by Hopf and

coworkers[8] and far higher than that of the methyl and unfunctionalized analogs.[23] Differential scanning calorimetry shows that under an inert atmosphere all members of the parent series **DPDC3-DPDC13** are thermally stable up to ~250° C. For a direct comparison between cyano-functionalized and unfunctionalized oligoenes, we photooxidatively decomposed both **DPO5** and **DPDC5** in a side-by-side experiment. We monitored the oligoene starting materials with UV-vis spectroscopy and found that the unsubstituted material decomposes four times faster than the cyano-functionalized material.[24]

2.2.4. Band-gap Modulation

In order to realize what kind of effect the cyano groups have on the electronic properties we first consider the derivatives that have unsubstituted phenyl groups, the parent **DPDCn** series. Despite providing stabilization to the oligoene core, the cyano groups do not fundamentally alter the "polyacetylene-like" electronic behavior of oligoenes in the sense that the HOMO-LUMO gap decreases as the length of the oligoene increases, which is typical of other vinylogous series.[25] The optical absorptions of the **DPDCn** series for n between 3 and 13 span the entire visible spectrum (Figure 2.5a). The absorptions are also quite intense with molar extinction coefficients (ε) that exceed 10^5 $M^{-1}cm^{-1}$. We estimate the solution-phase optical band gap (E_{og}) for **DPDC11** and **DPDC13** to be 1.81 eV and 1.77 eV, respectively. These values approach the band gap observed for PA itself.[26] Similarly, we can analyze this series using the quantum mechanical “particle in a box” model, which is often used to describe optical absorptions in one-dimensional systems. This model holds that the excitation energies in a simple

system vary with the inverse square of the dimensional length. Fitting the excitation energies in the **DPDCn** series with such an inverse-square expression (see Figure 2.5c) leads to an effective mass of 2.15 x 10^{-45} kg. Extrapolation of the wavelength for the strongest absorption (λ_{max}) and optical band gap (E_{og}) to an infinite "box" length estimates values of 577 nm and 1.59 eV, respectively. This is within the reported range of band gaps (1.4-1.6 eV) for *trans*-PA.[1,26] Our extrapolations were carried out as simple linear regression analyses; the Meier correction[27] didn't provide any benefit in this case because the effective conjugation length (ECL) of the series had not been reached. The ECL of oligoenes is higher than other poly-conjugated systems[25] and has been estimated to lie between 15 and 20 repeat units.[4,28] We estimate the ECL of the **DPDCn** series by selecting the point in our three extrapolations where a change in oligomeric length of one repeat unit corresponds to a negligible energy difference of less than 0.01 eV. In each case, the emergence of size-independent electronic properties (λ_{max}, E_{og} and E_{cv}) is predicted to occur at lengths ≥ 19 alkene repeat unites.

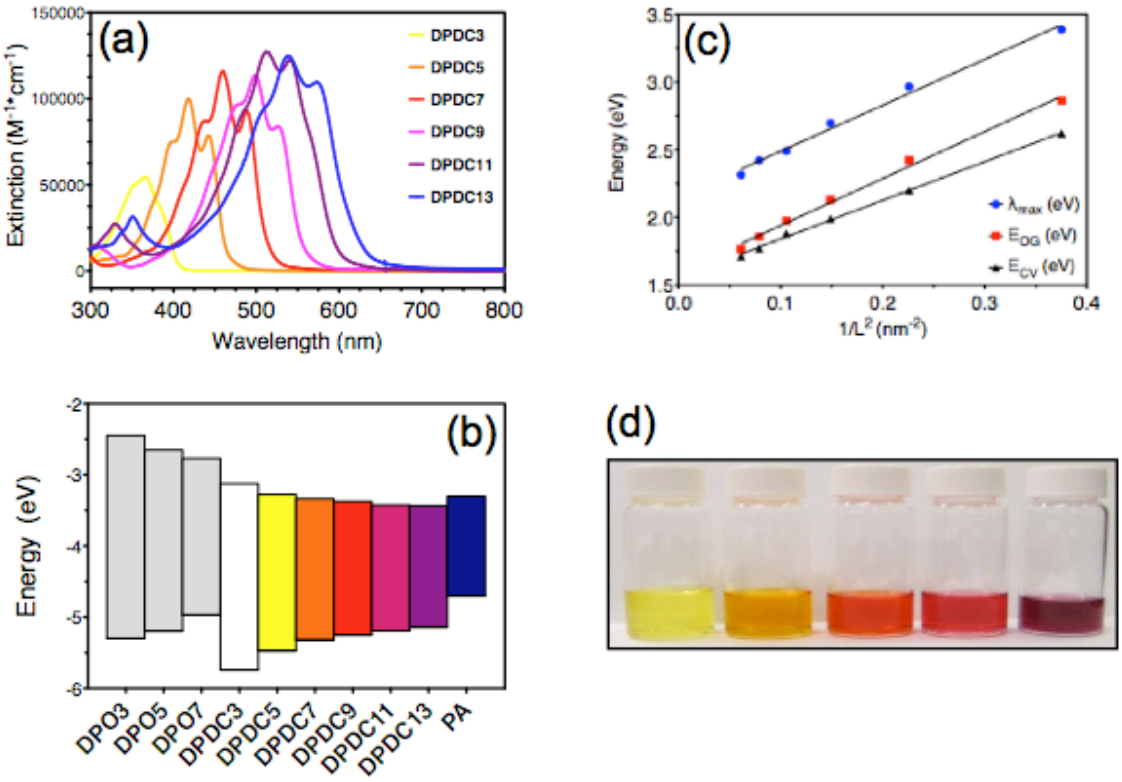


Figure 2.5: (a) UV-vis absorption spectra of the parent oligoene series (**DPDCn**) in CH_2Cl_2. The wavelength of strongest absorption, λ_{max}, (from left to right) at 363, 418, 459, 499, 513, and 536 nm; increasing the oligomeric length tunes the optical absorptions over a range of 350 nm. (b) Effect of the cyano groups on the HOMO and LUMO energies of diphenyl-oligoenes determined by cyclic voltammetry (CV). Redox gap of **DPO3**, **DPO5**, **DPO7** (grey) and the cyano-functionalized series, **DPDCn**. CVs were obtained in DMF solution with 0.1 M $(n\text{-}Bu)_4N^+ \bullet PF_6^-$. Ferrocene was used as an internal standard for electrochemical measurements. Experimentally determined values for PA (blue) are included for reference.[26] (c) λ_{max}, the optical band gap (E_{og}) and the redox band gap (E_{cv}) for the **DPDCn** series are fit using "particle in a box" energies. Extrapolative analysis estimates the analogous values for an oligomer of infinite length (polymer) of 577 nm, 1.59 eV and 1.55 eV, respectively. Predicted values agree with experimentally determined values for PA.

2.2.5. Electrochemical Studies

Since cyano groups are strongly electron withdrawing, their presence should lower the energies of the frontier orbitals with respect to those of the unfunctionalized DPOs. The redox potentials determined by cyclic voltammetry were used to estimate the energies of the HOMOs and LUMOs of the **DPDCn** series. We found that installation of two cyano groups onto the oligoene core stabilizes the HOMO and LUMO by as much as 0.44 eV and 0.68 eV with respect to the corresponding unsubstituted **DPOn** molecules (Figure 2.5b). This is consistent with UV-vis absorption spectroscopy, in which we observe a bathochromic shift of up to 35 nm between **DPOn** and **DPDCn** series. The electrochemically determined energy gap, E_{cv}, for **DPDCn** molecules can also be extrapolated to predict the band gap of the homologous polymer. In Figure 2.5c we again use simple "particle in a box" energies to predict the band gap for the polymer to be 1.55 eV. Both the E_{cv} and the E_{og} converge to similar values.

2.2.6. Theoretical Band Gap

To gain further insight into the electronic structure of the parent **DPDCn** series, as well as the **DPOn** series, we preformed density functional theory (DFT) calculations on each member of the series. All electronic structure calculations used Jaguar (version 7.7, Schrodinger LLC, New York, NY, 2010) using the B3LYP hybrid functional and the 6-31G** basis sets. The geometries of **DPDCn** and **DPOn** were fully optimized before calculation of its molecular orbitals. The final geometries, total energies, bond angles, bond distances and molecular orbital energies can be found in Appendix A.

DFT was used as an a third way to estimate the band gap of the **DPDCn** series. In Figure 2.6, DFT band gaps are smaller than those found by solution-based techniques, however as oligomeric length increases the various methods converge to similar values.

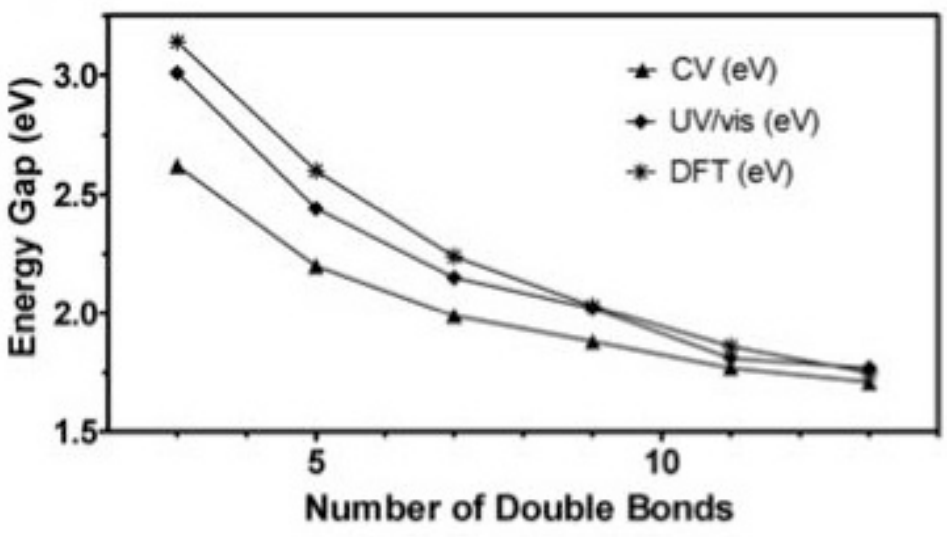


Figure 2.6: Comparison of band gap estimations from CV, UV-Vis and DFT. Greater variation between methods is seen for the shorter oligomers while values converge as molecular length increases.

2.3. End-functionalized DPDC Derivatives.

Substitution on the terminal phenyl groups offers another opportunity to tailor the electrical and physical properties of oligoenes. We synthesized a family of derivatives of **DPDC5** (Table 2.2), whose phenyl-substituents varied from strongly electron-withdrawing (NO_2) to electron-donating (NMe_2). We found *para*-substitution to be most effective, apparently since it is strongly resonance-coupled to the oligoene backbone and at the same time sterically remote (Appendix A). Spangler and coworkers reported

similar results for non-cyano DPOs having the *para*-substituents NO_2, Cl, SMe, OMe, and NMe_2.[9] Examples of the effect of aryl-functionalization on the optical absorption are displayed in Figure 2.7a.

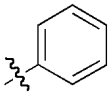
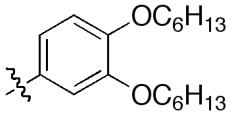
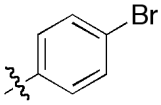
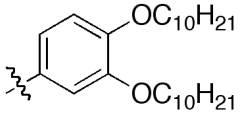
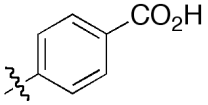
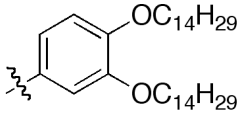
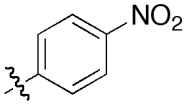
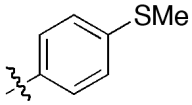
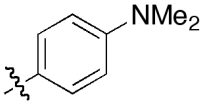
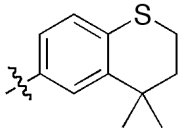
entry	R group	λ_{max} (nm/eV)[a]	entry	R group	λ_{max} (nm/eV)[a]
1	 **DPDC5**	418/2.97	6	 **DPDC5-OC_6H_{13}**	454/2.73
2	 **DPDC5-Br**	426/2.91	7	 **DPDC5-$OC_{10}H_{21}$**	453/2.74
3	 **DPDC5-CO_2H**	426[b]/2.91	8	 **DPDC5-$OC_{14}H_{29}$**	455/2.73
4	 **DPDC5-NO_2**	449/2.76	9	 **DPDC5-SMe**	453/2.74
5	 **DPDC5-NMe_2**	523/2.37	10	 **DPDC5-SC_5H_{10}**	465/2.67

Table 2.2: Comparison of selected **DPDC5** derivatives and their UV-vis strongest-wavelength absorptions. [a]The strongest wavelength absorption is taken at the global λ_{max} and is not indicative of HOMO-LUMO gap energies, E_{og}.

2.3.1. Tuning the Solid-state Assembly through End-functionalization

Strong electron-donating groups give the largest bathochromic shifts and broadened absorption peaks. Functionalization of the **DPDC5** scaffold with *p*-NMe_2 groups shifts the longest-wavelength absorption from 490 nm to 640 nm, and this shift is accompanied by the loss of vibronic fine-structure.[29] These electronic differences indicate topological changes in the frontier orbitals due to a transformation from an oligoene π-π* excitation to a "push-pull" n-π* transition; giving rise to an intramolecular charge transfer (ICT).[30] We performed time-dependent density functional theory (TD-DFT)[31] calculations at the B3LYP/6-31** level on **DPDC5** and **DPDC5-NMe_2** to investigate their excited states and the topologies of relevant molecular orbitals. In each case we found that the lowest-energy excitation is predominantly promotion of an electron from the HOMO to the LUMO, and in each case this transition is strongly allowed. We show these frontier orbitals for each molecule in Figure 2.7c and 2.7d, respectively. The LUMOs of **DPDC5** and **DPDC5-NMe_2** are remarkably similar: each is primarily the expected, lowest-energy π*-orbital of a conjugated polyene. However, the HOMOs of the two molecules differ. While the HOMO of **DPDC5** is primarily the expected, highest-energy π-orbital of the polyene, in **DPDC5-NMe_2** there is significant electron density on the terminal aryl groups and the nitrogen lone pairs. A similar trend in the frontier orbitals is predicted even when the cyano groups are removed from the oligoene core (see Appendix A) implying that the cyano groups contribute less to the intramolecular charge transfer (ICT) than do the NMe_2 groups. Thus while the HOMO-LUMO excitation in **DPDC5** is largely π–π*, that in **DPDC5-NMe_2** has a significant component of n-π* character. This may be considered ICT.[29]

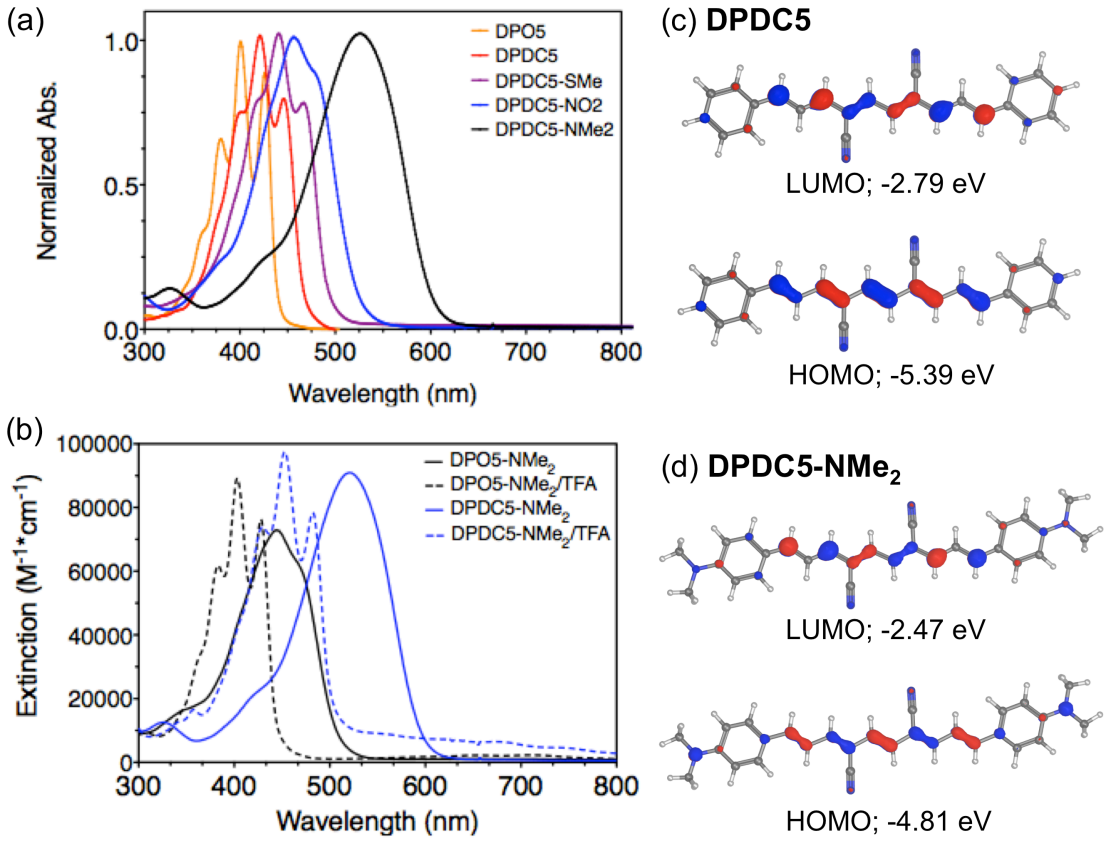


Figure 2.7: (a) UV-vis absorption spectra of oligoene derivatives in CH_2Cl_2; **DPO5** (orange), **DPDC5** (red), **DPDC5-SMe** (purple), **DPDC5-NO$_2$** (blue) and **DPDC5-NMe$_2$** (black). For easy comparison absorptions have been normalized to 1. (b) Absorption spectra of protonated (solid line) and deprotonated (dashed line) forms of **DPDC5-NMe$_2$** (black) and **DPO5-NMe$_2$** (blue) in CH_2Cl_2. TD-DFT calculations compare the LUMO and HOMO of (c) **DPDC5** and (d) **DPDC5-NMe$_2$**.

Since the HOMO-LUMO transition in **DPDC5-NMe$_2$** is due, at least in part, to n-π* promotion, protonation of the nitrogens should remove the nitrogen lone pair from participation in the HOMO and therefore quench any ICT, leaving behind the π–π* absorptions of the oligoene. Indeed, addition of trifluoracetic acid to solutions of **DPDC5-NMe$_2$** and **DPO5-NMe$_2$** resulted in a hypsochromic shift and resolution of the

vibronic fine-structure as seen in Figure 2.7b. The effect is reversible; when we neutralize the erstwhile acidic solutions with triethylamine, absorption is again shifted to the red and the vibronic structure is lost.

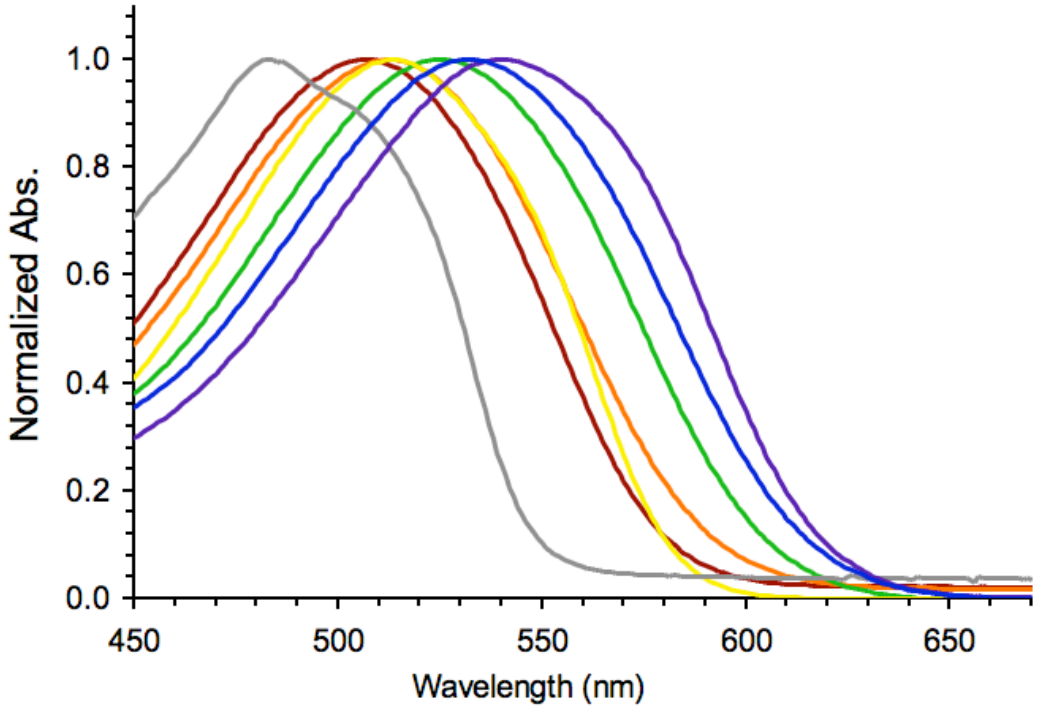


Figure 2.8. Salvotochromic behavior of **DPDC5-NMe$_2$** selected solvents; heptane (grey) ethyl acetate (red), acetone (orange), toluene (yellow), chlorobenzene (green), DMSO (blue), and nitrobenzene (purple). Spectra are normalized to 1.0 abs. Absorption data from 15 different solvents is tabulated in Appendix A.

Solvatochromism may be used to assess the amount of ICT behavior in conjugated push-pull systems, since the polarizability of π-electrons partially depends on the environment provided by the solvent, such as solvent polarizability and cavity size.[29] The absorption behavior of **DPDC5-NMe$_2$** was surveyed throughout fifteen organic

solvents. In figure 2.8, the λ_{max} was observed to shift 55 nm from solutions of heptane to nitrobenzene, while the longest-wavelength absorption shifted 70 nm from heptane to dimethyl sulfoxide (DMSO). Absorption data for all solvents has been placed in Appendix A.

2.3.2. Solubility Enhancements

The rigid structure of conjugated oligoenes leaves them sparingly soluble in organic solvents and hinders solution-based processing techniques such as spin-casting or inkjet printing. This is an important obstacle for promising organic electronic materials to overcome for application in film-based technologies. Again, we take advantage of the facile functionalization of phenyl end-groups in order to enhance oligoene solubility. Long alkoxy groups and bulky thioethers (Table 2.2, entries 6-10) tune the solubility over a wide range while maintaining consonant electronic properties (based on UV-vis absorption, as well as ^{1}H- and ^{13}C-NMR spectra; Appendix A). For example, **DPDC5-$OC_{14}H_{29}$** and **DPDC5-SC_5H_{10}** reach molarities up to ~0.10 M in chloroform at room temperature; increasing the solubility from ~10^{-4} M for **DPDC5**. These derivatives are also soluble in other common organic solvents such as toluene, tetrahydrofuran, and benzene. Using this synthetic approach, longer alkoxy chains or even polymeric attachments are presumed to be possible.

2.3.3. Tuning the Solid-state Assembly through End-functionalization

The molecular organization in the solid state changes when we functionalize the DPDCs with carboxylate groups. Unlike the pentaene of the parent series (**DPDC5**),

crystals of **DPDC5-CO_2H** contain two molecules of solvent, dimethylformamide (DMF), per oligoene and do not organize in a herringbone structure. In Figure 2.9c we show that hydrogen bonding with DMF facilitates the assembly of the carboxylic acids into π-stacked sheets of oligoenes. The lack of solvent between oligoenes allows for the intermolecular distances to decrease to 3.38 Å between π-faces of neighboring molecules. These values approach the interplanar distances found for the classic carbon allotrope, graphite; 3.35 Å.[33] **DPDC5-CO_2H** stacks in an oblique alignment with six close neighbors oriented in a hexagonal pattern when viewed down the length of the molecule.[34] All molecules in the crystal are aligned in the same direction and overlap with neighboring molecules through π-stacking interactions. This is an ideal geometry for charge transport through a single crystal.

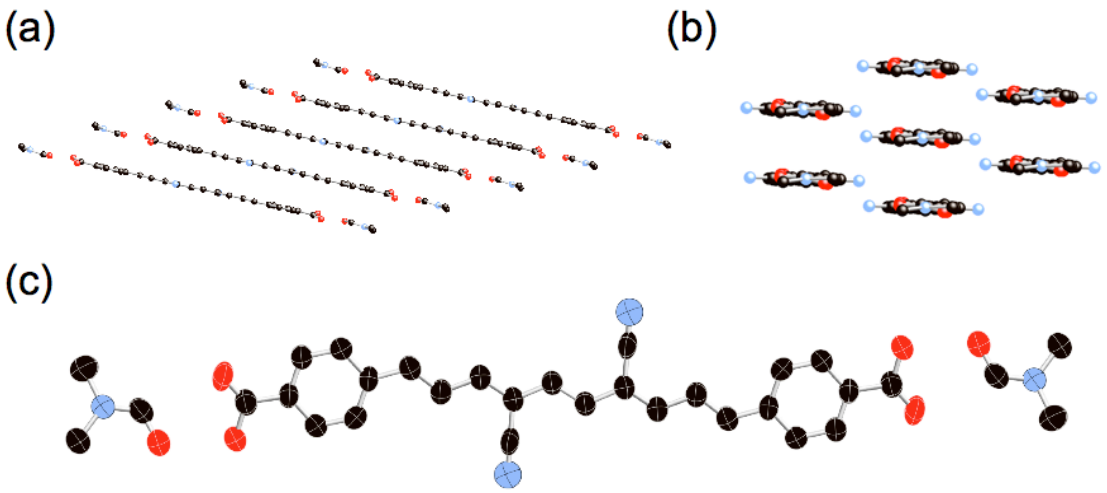


Figure 2.9: Packing structure of **DPDC5-CO_2H•2DMF** (a) viewed from the side and (b) down the length of oligoene chain. (c) Ellipsoids represent 50% probability levels. Hydrogen atoms have been omitted.

2.4. Material Applications

Despite the unique electronic properties of oligoenes, such as large extinction coefficients, broad absorptions and low band gaps, they have not made particularly useful electronic materials. Not only has solubility and instability, but other factors, such as control over their assembly, have hindered applications as thin-film materials in organic photovoltaics (OPV's) and organic field-effect transistors (OFET's) and also in liguid crystalline arrays. However, oligoenes are not predicted to be usefull as organic light-emitting diodes (OLED's), since they have low fluorescent quantum yields.

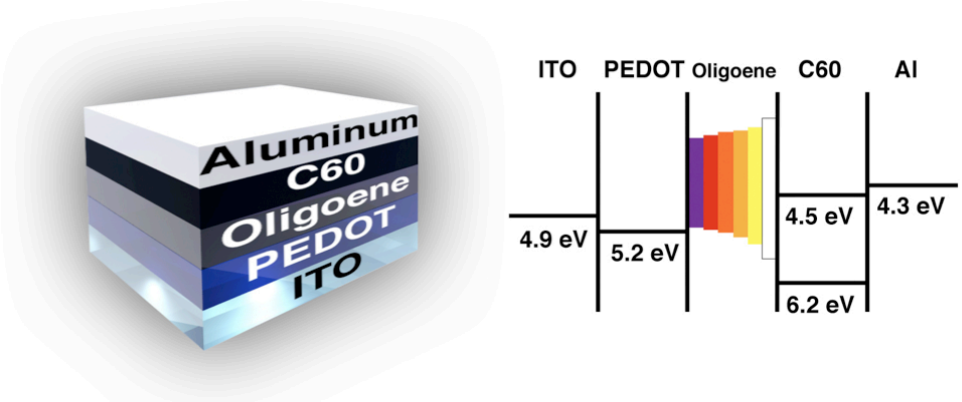


Figure 2.10: OPV device architecture. (left) Donor-acceptor bilayer device using indium tin oxide (ITO) as the transparent cathode and thermally deposited aluminum as the anode. (right) Band gap alignment diagram, demonstrates how to tune the energies of the MO's to align with other elements of the device (i.e. the work functions of the metal electrodes and the orbitals of the acceptor material) simply by changing the lengh of the oligoene donor.

To investigate potential in photovoltaics, bilayer OPV's of **DPDC5-DPDC9** were prepared by thermal deposition of the donor layer (oligoene) atop an acceptor (C_{60}) layer over ITO/PEDOT. The schematic of the device architecture is displayed in Figure 2.10.

Efficiencies for these devices were low, reaching ~0.5% under 1 sun (AM1.5G) standard solar illumination in air for **DPDC9**. Similarly, OFET devices constructed by spin-coating hot soultions of **DPDC11** in THF onto silicon oxide surfaces yielded devices with low performance. Even though device performance was poor, conductanece values doubled after devices were exposed to iodine vapor for twenty minutes and could be the result of I_2-doped oligoene films.

2.4.1. Self-assembly of Oligoenes on Semiconducting Sufaces

As a demonstration of how end-functionalized oligoenes allow for their incorporation as molecular wires into molecular architectures, we used carboxylic acid-functionalized oligoenes (**DPDC3-CO_2H**) to assemble monolayers of magnetic nanoparticles on GaAs substrates. It has been shown previously that carboxylic acids bind to GaAs[35] and Fe_3O_4 through known ligand exchange procedures.[36] In fact, preliminary ligand exchange studies found that the addition of **DPDC3-CO_2H** solutions to solutions of 10-nm and 5-nm magnetite nanoparticles in DMF lead to the immediate formation of an insoluble dark grey solid, which could not be characterized. Therefore, we presumed that our carboxylates readily undergo ligand exchange at the nanoparticle surface.

To form a self-assembled monolayers (SAMs) atop a GaAr surface, the native oxide layer of the GaAs substrates were removed through submersion in aqueous ammonium hydroxide (NH_4OH). After rinsing with ethanol they were submerged in a 1.5 mM solution of oligoene (**DPDC3-CO_2H)** in DMSO. They were then removed from solution, again rinsed with ethanol, and submerged for 1 hour in a solution of 10-nm

Fe_2O_4 nanoparticles in DMF. Scanning electron microscopy (SEM) analysis of these films shows clear formation of nanoparticle monolayers as shown in Figure 2.11a. At low concentration of oligoene coverage was complete; yielding a compact monolayer of nanoparticles that coats the entire surface with long-range uniformity. Nanoparticle coverage was found to be dependent upon the concentration (1.5 mM, 3.0 mM, or 6.0 mM) of the oligoene solution. When solutions of 3.0 mM (Figure 2.11b) and higher were used, multilayer coverage was observed. As a control, no monolayer formation was observed when only DMSO without oligoene was used or upon the direct submersion of the GaAs substrate into the nanoparticle solution (see Appendix A).

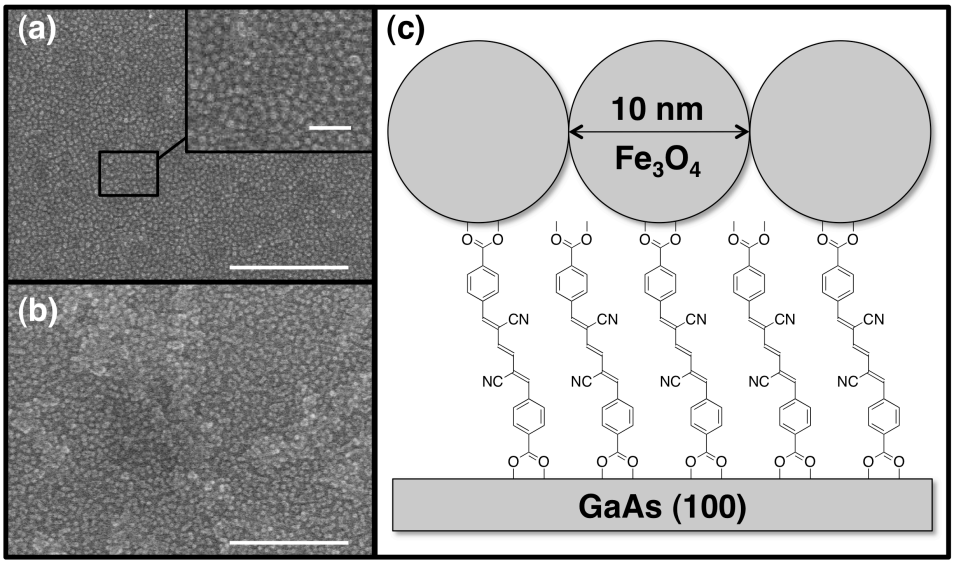


Figure 2.11: Scanning electron micrographs (SEM) of 10-nm Fe_3O_4 nanoparticle SAMs made using (a) 1.5 mM and (b) 3.0 mM solution of **DPDC3-CO_2H**, show monolayer coverage at low concentrations and the presence of multilayers at higher concentration. Scale bars are set to 500 nm, while insert scale bar is set to 50 nm. (c) Schematic of oligoene-Fe_3O_4 composite monolayer.

2.5. Conclusions and Future Outlook

We have developed a new method to synthesize cyano-substituted oligoenes with up to thirteen all-*trans* conjugated C=C bonds, and have demonstrated its utility in the synthesis of a wide variety of aryl-functionalized oligoenes. These materials are highly tunable summarized in Figure 2.12. Cyano groups decrease the band gap of oligoenes and stabilize them for study under normal laboratory conditions while preserving the conjugation along the poly-olefin backbone. Derivatization of the terminal phenyl groups allows us to fine-tune the electronic structure and physical properties. We can access practically any energy within the visible spectral region by pairing the appropriate oligoene length with the appropriate aryl end-group.

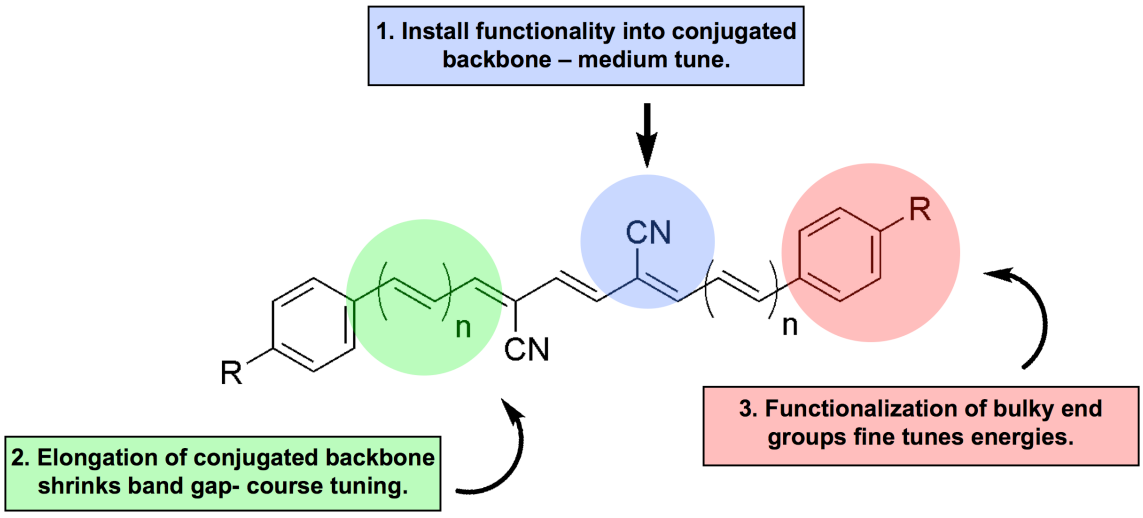


Figure 2.12: Three ways to tune the band gap of oligoene materials: (1) main-chain cyano groups lower the energies of the frontier orbitals relative to unfunctionalized conjugated backbones; (2) the length-dependent properties greatly effect the band gap, while (3) end-functionalization can fine-tune the gap amongst each oligomeric length.

Functionalized oligoenes are ideal structures for nanoscale electronic and structural components and can be used to guide oligoene self-assembly and the construction of heterogeneous materials. Furthermore, the utility of these materials in photovoltaics is an obvious application since their band gaps are easily tuned, their absorptions are broad and cover the visible spectrum, and their extinctions coefficients are large. DPDC molecules are also predicted to be useful in singlet fission,[37] since their first excited triplet state is (T_1) is well positioned (energetically) to undergo such a process. We are currently building devices that utilized singlet-fission for use in photodetection and photovoltaics.

2.6. References and Footnotes

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5. The symbols, μ and ν, are used to designate central positions along the oligoene main chain, because they are the middle letters in the Greek alphabet. This nomenclature is unprecedented, but serves to distinguish central locations from the terminal locations, α and ω.

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17. The Cannizarro reaction is a Aldehyde disproportionation reaction beginning with nucleophilic attack on the electrophilic carbonyl center from a hydroxide anion, therefore forming the tetrahedral intermediate. Hydride transfer occurs as the newly charged species attack a second aldehyde forming an alkoxide and acid anion, which exchange a final proton, resulting in an alcohol and carboxylate. See, Cannizzaro, S., *Liebigs Annalen*, **1853**, *88*, 129–130.
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22. Stability of **DPDCn series** was observed by ^{1}H-NMR and thin layer chromatography over the duration of 6 months. When stored at 0° C in the absence of light **DPDCn** and **DPOn** series showed no signs of degradation. When stored on the bench top in ambient conditions **DPDC3**-**DPDC7** also did not degrade. However, the degradation of **DPDC9**-**DPDC13** were observed and increased with increased molecular length. Broadened peaks were found in their ^{1}H-NMR spectra and **DPDC13** was observed to lighten in color. At short lengths (n = 3 to 7) **DPDCn** and **DPOn** series are stable in ambient conditions. Further comparisons between the each series were limited, since we were unable to synthesize/characterize longer **DPOn** molecules due to very low solubility.
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24. Dilute solutions (~10^{-4} M) of **DPO5** and **DPDC5** were prepared and irradiated with a 450 W ACE mercury lamp (#7825-34) at room temperature. This procedure was

carried out under both aerobic and anaerobic conditions. We observed degradation of **DPO5** and **DPDC5** through the loss of their longest-wavelength absorbance by UV-vis spectrometry.

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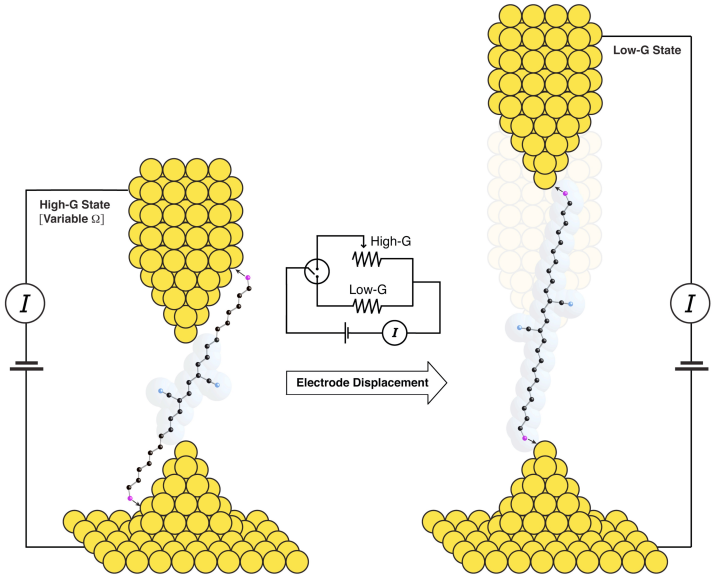
Chapter 3. Oligoenes in Single-molecule Electronics†

The molecules in Chapter 3 were synthesized by myself with the assistance of Markrete Krikorian. The single-molecule STM-BJ measurements were preformed by Maria Kamenetska. DFT calculations were preformed by Michael Steigerwald.



3.1. Motivations

Understanding and controlling charge transport through molecular devices is critical, not only to the realization of molecular sized devices, but also in advancing the performance of organic based electronics.[1,2] For such devices, it is insufficient simply to ascertain that certain molecular backbones can conduct; one must predict, and ultimately control, molecular conductance. In this chapter a new type of single-molecule electronic device is described, which we are able to predictably adjust the conductance of the individual molecular circuit over a well-defined range.[3] In doing so, the length-dependent

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charge-transport properties through a series systematically elongated oligoenes (**An** and **Bn**) that have been end-functionalized were quantified.

3.1.1. Oligoene Single-molecule Wires

Very few reports of molecular junctions formed form oligoenes has been reported. Oligoenes that require specific end-functionalizations can be difficult to synthesize. Also, STM-BJ measurements are often carried out in air under normal conditions, which may lead to oligoene decomposition, especially in terminal oligoenes. The first reported oligoene single-molecular junction appeared in 2003, where Lindsay and coworkers[4] synthesized a terpenoid-based linear nonaene terminated with benzyl thiols. Known to interact strongly with gold, the dithiol was embedding into a docosanyl thiol monolayer, from which a bottom chemicontact to a gold substrate was established. Steric congestion oriented the molecule like the dososanes and away from the surface. Gold nanoparticles where bound to the second thiol and used as top contacts. Electrical measurements were then made by contacting those nanoparticles with a gold-coated AFM probe tip. Because only one compound was measured they were unable to obtain information about the electrical decay constants (β). It was not until their later reports, where two similar families of oligo-terpenoids we measured: (1) a series of three pyridyl and (2) four benzyl thiol end-functionalized carotenoids.[5] Differences in the effective contact resistance due to atomic constitution of the electrode binding groups (pyridyl vs. $ArCH_2SH$) can be observed between each series. The decay constants, however, were in closer agreement with one another ($\beta_{pyr} = 0.17 \pm 0.03$ Å^{-1} and $\beta_{thiol} = 0.22 \pm 0.04$ Å^{-1}).

Outside of the conducting probe AFM/nanoparticle technique oligoenes have not been studied further, nor have any non-terpenoid oligoenes, which are predicted to be better suited for electronic transport because they do not contain main-chain methyl groups that distort the planar structure due to allylic-1,3-strain.[6] Here, we investigate the charge transport properties of two families of non-terpenoid oligoenes using the STM-BJ technique. Each family contains five oligomeric vinylogues that range from the triene to the undecene.

3.1.2. Scanning Tunneling Microscope Break Junctions (STM-BJ's)

Using a custom-built STM, cut or etched gold STM tips and Au (011) surfaces are used as the macroscopic bottom and top contacts. Current is continually measured allowing us to monitor junction formation and rupture processes, as well as record the current that flows through single-molecule junctions. A step-by-step schematic of this process is given in Figure 3.1A. The STM begins in the open position with the tip-displaced from the surface. Then each is brought into contact via piezoelectric controls forming Au-Au bonds. Next, the tip is displaced from the surface and, as this occurs, the Au-Au chemicontacts begin thinning down until the bridging metal becomes as thick as a single Au atom. These pre-electrodes are referred to as gold atomic point-contacts, which have a conductance equal to the quantum of conductance ($G_0 = 2e^2/h$) and is highlighted by a dashed arrow in Figure 3.1B. Further displacement ruptures the point contacts, breaking the circuit and leaving under-coordinated Au-atoms at the surface of the tip and substrate. When these point contacts are broken in a solution of molecular wires, we are able to trap individual molecules (sometimes multiple molecules) between the electrodes.

Three sample traces are shown in Figure 3.1B. Point contact rupture is clearly visible by a large drop in conductance (after the dashed arrow), to a lower conductance plateau (solid arrow) signifying the formation of a molecular junction. When we elongate further, the junction ruptures and conductance ceases.

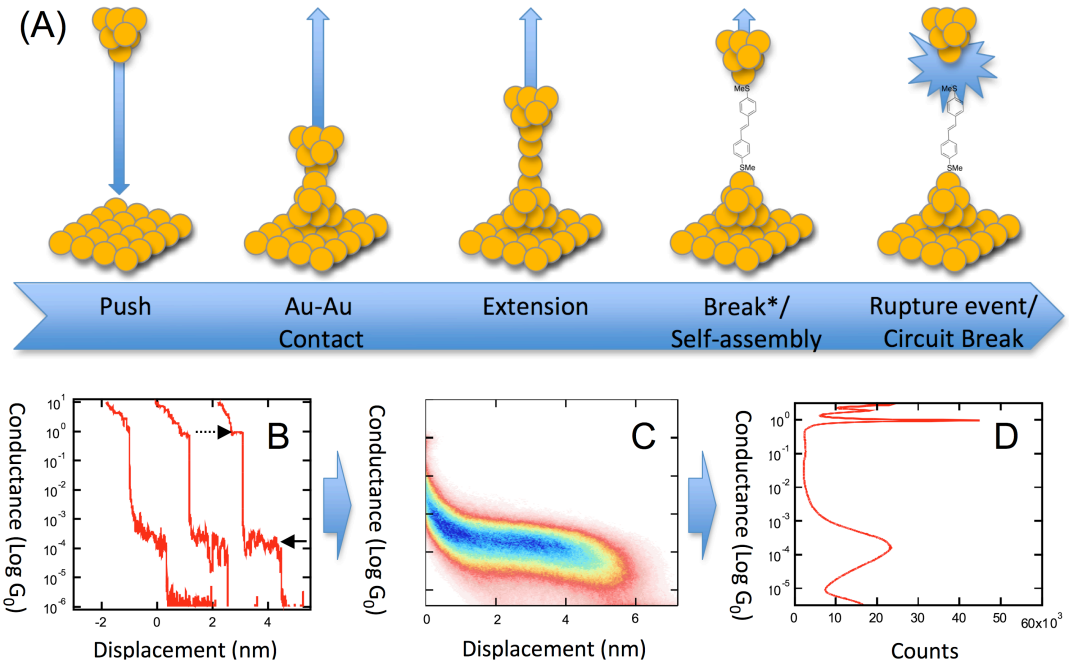


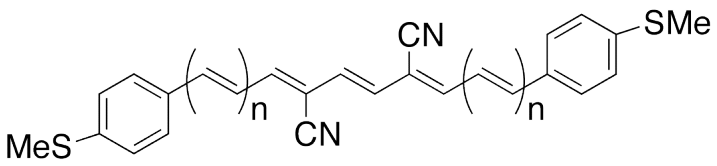
Figure 3.1: STM-BJ method. (A) Step-by-step visualization of STM-BJ formation and rupture. (B) Examples of individual conductance-displacement traces measured from a single-molecule junction using the STM-BJ technique. By combining thousands of these traces together histographical analysis containing statistically relevant data can be viewed as (C) 2D conductance-displacement or (D) 1D conductance histograms.

Junction-to-junction variance is observed when measuring single-molecules. Therefore, we run thousands of measurement and generate thousands of traces, which we compile into histograms giving statistically relevant data. Generally, we use unselected

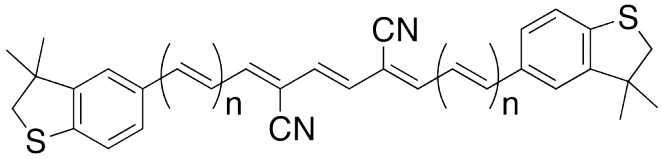
data to construct our histograms without the refinement of choice data to give an accurate account of our junctions.

3.1.3. End-Functionalized DPDC Molecular Wires

The design of the molecular wires is shown in Figure 3.1A. They are α,ω-diphenyl-μ,ν-dicyano-oligoenes (DPDC), which have been end-functionalized with methylsulfide (Ar-SMe)[7] or cyclic alkylsulfide (Ar-SR, where R completes a 3,3-dimethyl-2,3-dihydrobenzo[*b*]thiophene) end-group. These end-groups are localized, two-electron donor and are aurephilic, meaning that they readily interact with Au (aurophilic), forming dynamic donor-acceptor bonds. These end-groups are important and referred to as linkers, since they act as terminal contacts, which serves as the physical anchor linking the molecule to the electrodes in a molecular junction. Secondly, the electrical variable-contact is the set of alternating π-bonds that form the conjugated π-space of a linear oligoene. During the conductance measurement, electronic coupling of the electrodes to the terminal contacts results in a low fixed junction conductance, while additional direct coupling through the π-space leads to higher tunable junction conductance. Basically, as the contact moves along the molecular π-space (over a distance of more than 1 nm), the device conductance changes continuously. This sampled distance can be controlled easily via our piezoelectronic cantilever controls. Thus, the conductance for the molecule can be *a priori* simply by selecting the appropriate inter-electrode spacing. These experiments form the basis for a new type of tunable molecular electronic device, a single-molecule potentiometer.



An; n = 0, 1, 2, 3, & 4



Bn, n = 0, 1, 2, 3, & 4

Figure 3.2: Chemical structure of oligoene molecular wires, **An** and **Bn**. Each series is composed of systematically elongated members ranging in length from 3 to 11 C=C double bonds. Oligoenes are end-functionalized with (**An**) methylsulfide or (**Bn**) cyclic alkylsulfide linkers.

For this study, we designed and synthesized two series of molecular wires that are atomically defined segments of polyacetylene,[8,9] each with different terminal anchor groups (**An** and **Bn** in Figure 3.2). A simple synthesis was developed that affords molecules longer than 4 nm. This synthesis also tolerates a diversity of end-groups while the cyano-groups on the molecular backbone enhance molecular stability due to lowered HOMO and LUMO energies relative to vacuum (see Appendix B). The crystallographically determined molecular structures of the parent series oligomers (**DPDCn** series) show an ideal path of conjugation with alternating single and double bonds exclusively in the *trans* configuration (see Ch.2, Figure 2.3). In each series above, the color of these compounds is a strong function of the molecular length, indicating that

the HOMO-LUMO gap in these molecules decreases with increasing molecular length (see Appendix B and Ch. 2, Figure 2.5B).

3.2. Charge-transport Properties

We first demonstrate that these oligoenes behave as molecular wires by measuring their electrical properties using a STM-BJ method.[10] STM-BJ's are formed in dilute solutions of oligoene (10 mM in 1,2,4-trichlorobenzene), allowing for effective trapping of individual oligoenes between the electrodes.[11] We apply a constant bias voltage (between 200 and 750 mV)[12] and measure the current that passes between the electrodes. When oligoenes bridge the broken point-contacts we measure the conductance of these metal-oligoene-metal junctions as a function of the distance between the two electrodes. The data are recorded in the form of individual conductance traces, of which thousands are measured and compiled into histograms without any data selection to reveal statistically significant conductance values.

Oligoenes that bind to under-coordinated Au though their alkylsulfide linkers. Differences are observed between the two oligoene series (**An** and **Bn)**; **An** is functionalized with methylsulfide linkers and shows a broader conductance distribution than the cyclic analogues, **Bn**.[12] This difference is due to the rotational freedom around the aryl-sulfur bond in the former set, which broadens the electronic coupling between the electrode and p-orbital. However, the general trends within and between the two sets are similar – incorporation of the linking sulfur atom into the five-membered ring does not significantly alter the fundamental physics, however it does simplify the analysis.

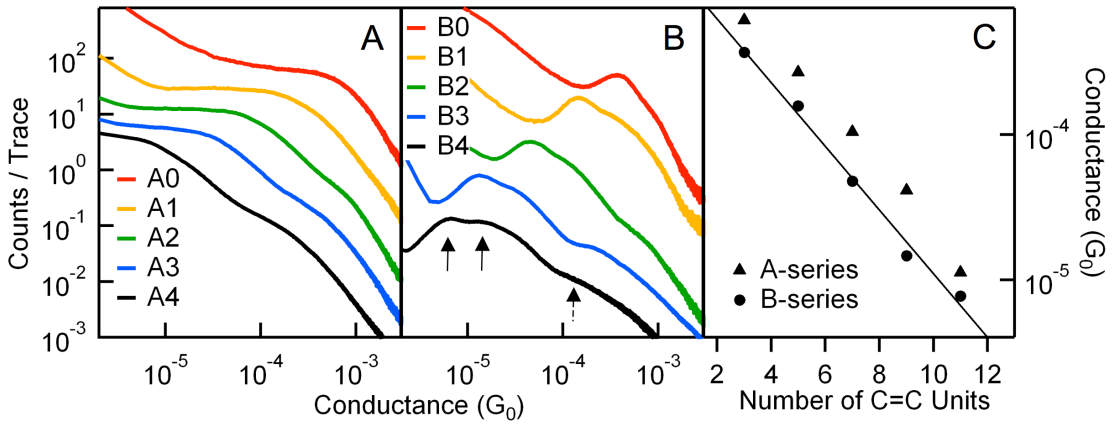


Figure 3.3: Linear histograms generated without data selection from >5000 conductance traces collected in the presence of each of the (A) **An** and (B) **Bn** molecules. The **Bn** series show clear peaks at molecule-specific conductance values, indicated by the solid arrow for **B4**. In the longer molecules, a shoulder at higher conductance is visible, indicated by the dashed arrow for **B4**. (C) Peak positions of the single-molecule conductance peaks observed for the **An** and **Bn** series as a function of the total number of oligoene units. For the **An** series the peak position was taken from the logarithmic histograms (see Appendix B). A linear fit to the data on the semi-log plots reveals that in both cases, conductance decays exponentially with a decay factor, $\beta = 0.22/\text{Å}$.

3.2.1. Conductance Histograms

Within each series, the peak in the conductance histograms (Figure 3.3A and 2.3B) decays exponentially with increasing length, following the expected relation, $G \sim e^{-\beta n}$ (Figure 3.3C). Fitting the conductance data in accordance with this relationship allows us to extract the non-resonant tunneling decay constant, β. The decay constant was determined to be $\beta = 0.22/\text{Å}$ for the **Bn** series, in agreement with previously published values for conjugated molecules.[5] Typically, histograms show a single conductance peak; however, for **n** > **1** in **An** and **Bn,** in addition to the conductance peaks indicated by

arrows in Figure 3.3B, we see a second broad increase in counts at significantly higher conductance values (dashed arrow).

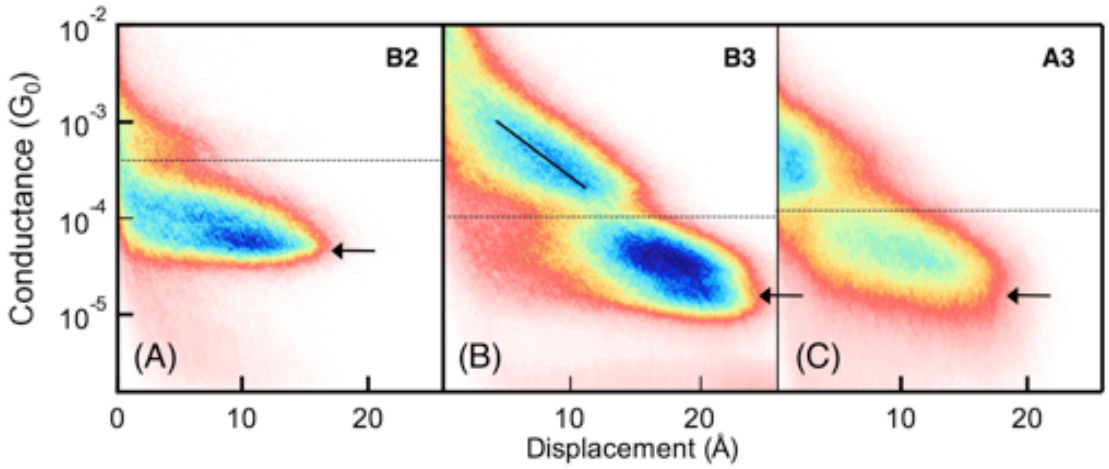


Figure 3.4: 2D conductance-displacement histograms preserve displacement information for (A) **B2**, (B) **B3** and (C) **A3** respectively. Comparing (A) and (B), within the same linker-family, longer molecules are able to sustain more junction elongation while remaining bound in the junction. All three molecules show a higher conductance shoulder in the region above the dashed line, corresponding to a junction geometry that forms immediately after rupture of the Au point contact. The average slope of this high conductance shoulder (solid line) reveals that conductance in this geometry decays with $\beta \sim 0.2$/Å as the junction is stretched, in agreement with the decay constant shown in Figure 3.3C. Arrows indicate the corresponding peak conductance positions appearing in the 1D conductance histograms in Figure 3.3B.

3.2.2. Conductance-Displacement Histograms

To elucidate the two conductance regions found in the 1D histograms, we examined two-dimensional conductance histograms[14,15] that preserve displacement information during junction elongation. In Figure 3.4, we show 2D conductance-displacement histograms for **B2**, **B3** and **A3,** where two regions with increased counts are clearly seen, a high- and low-conductance regime (separated by the dashed line for clarity). The higher region forms immediately following the breaking of the Au point contact (at zero-displacement in this 2D histogram). The extent to which this high-conductance state persists as the junction extends depends on **n,** as well as the terminal group (see Appendix B). In Figure 3.4B, we see also that the high-conductance value decreases almost exponentially as the gap widens. Furthermore, this high-conductance region is absent in the shortest molecules.

One possibility for the two different conductance regimes is that these all-*trans* oligoenes may access two different conformations: the s-*cis* and s-*trans*. As the junction is elongated, oligoenes undergo rotations around the C-C single bonds. However, the two conformers are expected to have similar conductance; thus, rotational isomerization cannot explain this finding.[16]

We postulate instead that there are two independent conductance pathways. In the higher conductance state the tunneling path originates at one electrode, passes directly to the olefin backbone, thence via the sulfide to the second electrode, as illustrated in Figure 3.5A. In the lower conductance state, which occurs only when inter-electrode distances are sufficiently large, the tunneling path switches from electrode-olefin-sulfide-electrode to the more typical electrode-sulfide-olefin-sulfide-electrode.

For the shortest molecules in our study, the length of the olefin chain is comparable to the distance between electrodes upon Au-Au point-contact rupture (6-7 Å).[17,18] Thus, direct contact between the electrode and the backbone is rarely accommodated. As a result, no clear high-conductance peak is seen in the 1D conductance histograms of Figure 3.3A and 3.3B (see Appendix B). Other factors such as steric hindrance and the electron-withdrawing properties of the nitriles may result in only one conductance value.

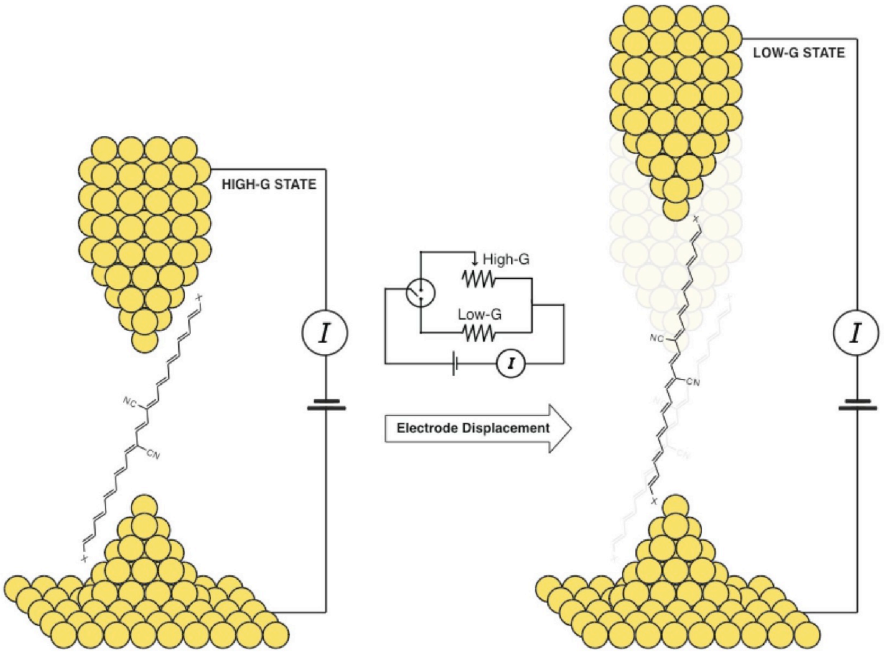


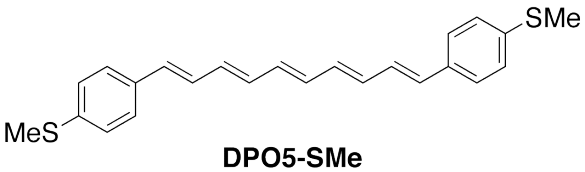
Figure 3.5: Schematic depiction of an oligoene break junction. Both the polyolefin chain and the end-groups, X, may act as electrical contacts. Oligoenes behave as a resistive potentiometer as the tip displaces along the olefin backbone, while the alkylthio end-groups stabilize the junction.

For the longer molecules, the initial electrode separation distance is significantly shorter than the length of our oligoenes. Although both terminal alkylthio groups anchor the oligoene to the electrodes, close proximity of the electrode to the olefin backbone results in a low-resistance pathway directly from the electrode to the olefin backbone (Figure 3.5A). As the junction is extended further, it slides up the backbone until an abrupt change in conductance is observed. Once fully extended, the oligoene is bound at the apex of each electrode, where Au atoms are no longer in proximity to the polyolefin chain, and the high-conductance state turns off. The lower conductance at this stage corresponds to the conductance through the entire molecule, and follows an exponential decay with increasing molecule length. Extending the junction further breaks the molecular circuit, and conductance is lost.

3.2.3. Control Molecules

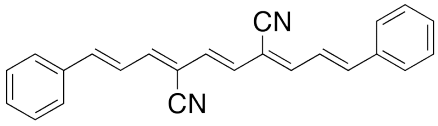
One group has reported the use of nitriles as linker groups to gold electrodes.[19] In order to dismiss the possibility that cyano groups in the DPDC's were establishing an electrical contact to the electrode, we synthesized an oligoene analogous to **A1**, but lacking nitriles. For this molecule we observe the two-conductance states as well, indicating that the nitriles are not responsible for this two-state behavior (see Appendix B). In fact, the enhanced high-conductance state in this molecule compared to **A1** suggests that the absence of cyano groups facilitates greater coupling of the olefin to the electrode by removing some steric hindrance, as well as making the olefin more electron rich. Other dinitriles were also measured, such as the central dinitrile moiety of the **An**

and **Bn**, 1,4-dicyano-2-butene and the unfunctionalized **DPDCn** series, also do not conduct.

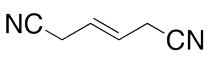


DPO5-SMe

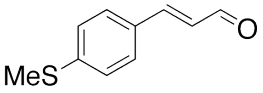
1,10-di-(4-methylthio)phenyl-deca-1,2,5,7,9-pentaene



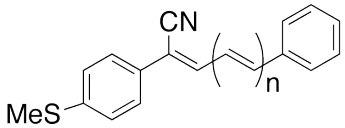
DPDC5



1,4-dicyano-2-butene



(*E*)-(4-(methylthio)cinnamaldehyde



Cn, n = 0, 1, 2, 3, & 4

Figure 3.6: (A) Control molecules (from top to bottom) **DPO5-SMe**, **DPDC5**, as well as the starting materials for the Knoevenagel condensation in the preparation of **A1**, 1,4-dicyano-2-butene and (*E*)-(4-methylthio)cinnamaldehyde. Asymmetric oligoenes (bottom) containing only one linker group were synthesized.

While both S-Au and olefin-Au bonds form, it is clear that the former is stronger than the latter. We demonstrate the importance of this with a series of asymmetric

oligoenes, each having only one methylsulfide (**Cn**), and with the parent DPDC series that lacks sulfides entirely (**DPDCn**) (see Appendix B). None of the **DPDCn** examples that we tested showed a measureable conductance, while the **Cn** series showed measurable conductance, albeit quite low. Moreover, the absolute height of the peak in the conductance histogram for **Cn** is quite low, suggesting that the formation of an Au-**Cn**-Au junction is a lower probability event. Thus, the π-complex is not strong enough to hold the mechanical circuit together alone, but if the molecule is held in the junction by at least one strong structural element, the π-complex link is strong enough to complete the electrical circuit.

3.2.4. Theoretical investigations

To further explore this unusual mode of electrode-molecule coupling, we turned to computation. Density functional theory (DFT) calculations (B3LYP/6-31G**) on **A1** allowed us to clearly visualize the molecular orbitals (MO's) pertinent to molecular junction formation (see Appendix B).[20] We modeled this as a two-step process; the molecule first binds to one electrode, and then this electrode-molecule complex binds to the second electrode. This model helps us to understand junction formation, after the first terminal has been contacted and elucidates the different binding modes to the second electrode that are available to the molecule as the gap between the two electrodes changes. For conceptual, as well as computational simplicity, we chose to model the Au electrode with a homonuclear diatomic gold cluster. The Au_2 is the simplest model and offers the empty orbital space (Lewis acidity), into which the S-lone pair can delocalize, to form the donor-acceptor bond that initiates the molecular-bridge-forming process. This

avoids many of the pitfalls of using atomic Au since it contains one unpaired s-electron, further complicating the analysis. The Los Alamos core valence potential (LACVP) basis set was used for calculations on complexes containing Au_2 clusters, since 6-31G basis set isn't large enough to accommodate the additional orbitals in gold.

In Figure 3.7A, we show the HOMO of Au_2-**A1,** in which the Au_2 unit is bound to one of the terminal sulfides. Examination of these MO's suggests that oligoenes contain two potential electrode-binding locations; not only at the distal sulfurs, but also along to the π-system of the polyolefin backbone. Both binding locations have ample precedent in homogeneous organometallic chemistry[21] and would result in different electron tunneling pathways. Thus these calculations are consistent with our observations that **An** and **Bn** show two conductance channels. Previous reports reveal that it is common for transition metals to interact with oligoenes. In addition to the numerous weak and dynamic interactions between transition metals and alkenes, stable inorganic complexes have been isolated, in which Pd and Ru interact directly with oligoenes through the π-system.[22-24]

For comparison, in Figure 3.7B we show the HOMO for Au_2-**C4**. This orbital is entirely localized in the π-space of the oligoene. Thus the channel for electrical conduction is present in **C4**, and it is quite similar to the channel in the **An** and **Bn** series. The difference in the conductances of **A1** (and **B1**) versus **C4** lies in the capability of the alkylsulfide linker to mechanically stabilize the oligoene close to the electrode surface, rather than in the electronic structure of the molecular conductor.

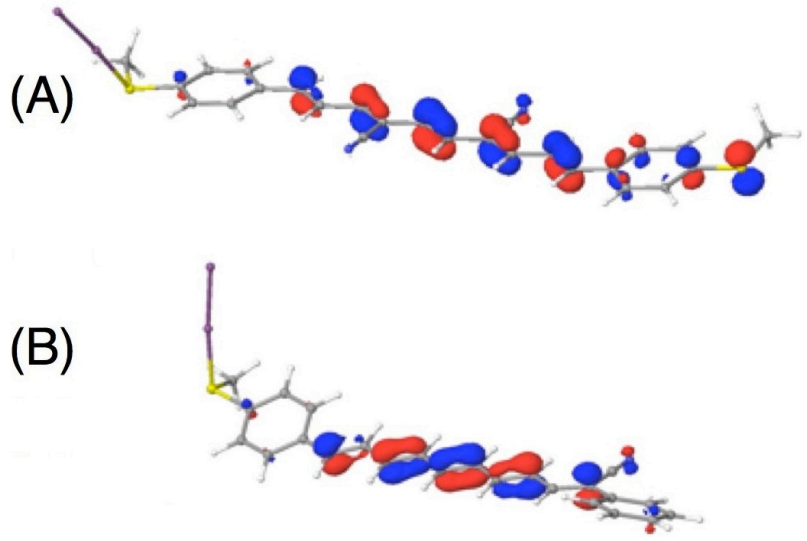


Figure 3.7: DFT calculations produce the HOMO of (A) Au_2-**A1** and (B) Au_2-**C4** complexes. The HOMO shows significant electron density both along the polyolefin chain and at the terminal methylsulfide functional group, we consider both spots to be available for interactions with the Au electrodes.

3.3. Single-molecule Potentiometer

3.3.1. Variable And Reversible Resistance

If we indeed have a direct conduction path from the electrode through the olefin backbone, it should be possible to change the conductance by modulating the electrode position and generating a single-molecule circuit that functions as a potentiometer. This is shown in Figure 3.8. Here, conductance is measured in a solution of **B4** while applying a modified ramp to our piezoelectric actuator, which controls the substrate position relative to the fixed tip[25] (dashed trace in Figure 3.8A). Of the 3000 traces measured with this ram**p**, over 50% of the traces show a molecule in the high conductance regime at the start of the zigzag ramp, as determined by an automated algorithm. A sample of selected

traces is shown in Figure 3.8A, and all selected traces were used to construct the 2D conductance-time histogram on a semi-log scale, shown in Figure 3.8B.

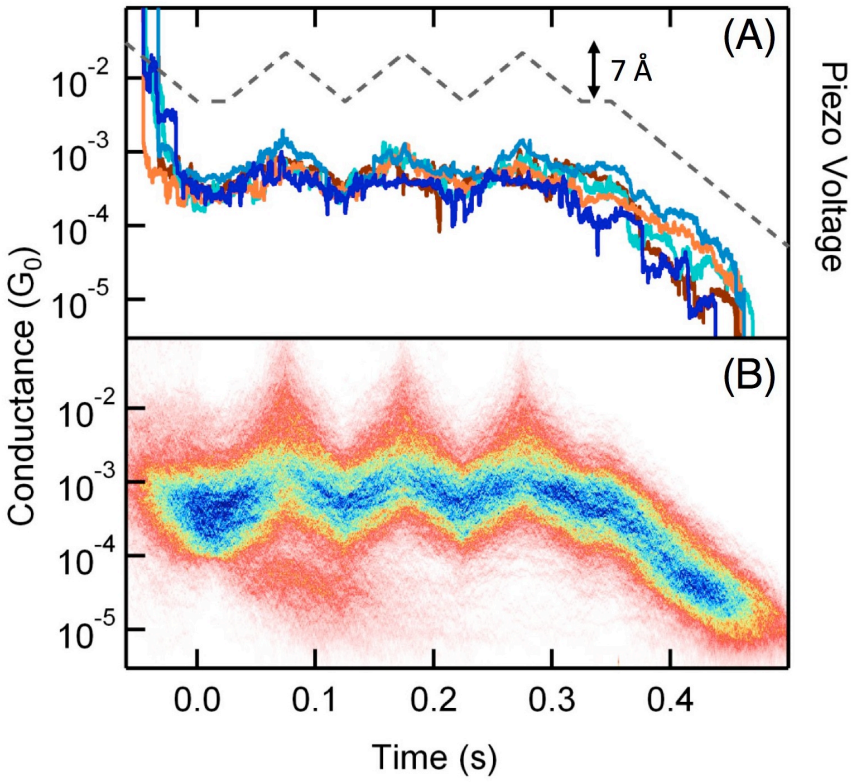


Figure 3.8: (A) Sample traces collected in the presence of **B4**, showing conductance changing continuously and reversibly as piezo voltage is modulated along the dashed line repeatedly stretching and compressing the junction. (B) 2D histogram constructed from selected traces, for which the average conductance during the initial hold section fell within the high-conductance range; > 50% of the 3000 traces collected met the selection criteria. Fitting the average slope of the different sections of the ramp shows that the conductance grows and decays exponentially with a factor of 0.2/Å throughout the measurement, emphasizing the reproducibility of the potentiometer behavior.

The conductance follows a zigzag pattern, as the tip-sample distance is modulated by 7 Å, with an average change in conductance from ~4 × 10^{-4} G_0 to ~2 × 10^{-3} G_0. This range is similar to that of the high conductance peak for this molecule, and has an exponential dependence on separation ($e^{-0.2/Å}$; β = 0.2 $Å^{-1}$). This exponential dependence of conductance on electrode distance suggests that, while the contact resistance does not change, the length of the backbone through which transport occurs varies as the junction is compressed or elongated.

3.3.2. Controls Experiments

Control experiments with alkanes show no modulation of conductance (see Appendix B for 1D conductance histograms). Throughout the zigzag ramp traces collected in pure solvent show changes in conductance between 10^{-6} G_0 to 10^{-1} G_0. These intense changes would be expected for tunneling through a gap without molecules. The ability to change the conductance of the junction continuously in this high-conductance state with an exponential decay of 0.2/Å can only be explained if the contact to the molecule is through direct π-coupling to the electrodes.

3.4. Conclusion

In conclusion, we experimentally demonstrate transport through single-molecule junctions where direct electronic coupling between the molecular π-conjugated backbone and Au electrode is achieved. Furthermore, this coupling is enabled by an auxiliary terminal chemical linker that provides mechanical support for the junction. Conductance through the molecular backbone can be tuned continuously and reversibly by changing

the electrode separation. Thus, this system provides a new class of molecular scale devices that perform as a resistive potentiometer.

3.5. References and Footnotes

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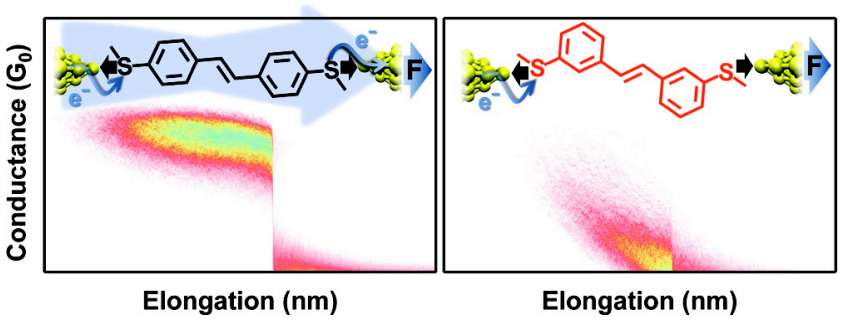
Chapter 4. Stilbene Single-molecule Wires: Dissecting the Electrical and Mechanical Contributions in Molecular Junctions †

In Chapter 4, the synthesis was carried out by myself with the assistance of Markrete Krikorian. STM-BJ measurements were preformed by Seokhoon Ahn and Radha Parameswaran. AFM-BJ studies and analysis were done by Sriharsha Aradhya. DFT calculations were run and analyzed by Michael Stiegerwald.



4.1. Background and Motivations

Understanding and controlling the electronic properties of molecular wires is fundamentally important for molecular electronics.[1,2] The scanning tunneling microscope (STM) based break junction approach gives a deep insight into the structure-conductance relationship in single-molecule junctions because it provides a statistical interpretation over an ensemble of measurements.[3-5] However, in these studies only one physical property, the junction conductance, is measured. This limits the interpretation of the results in junctions where the conductance is either very small or ill-defined. Theory predicts that there will be large modulations in single molecule conductance for systems

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exhibiting quantum interference, such as variously substituted aromatic molecules and cross-conjugated molecular wires.[6-12] For example, theoretical calculations have predicted that a benzene ring bound to metal electrodes with linker groups at the 1 and 3 positions (meta to each other) should have a conductance that is five orders of magnitude lower than that of a 1,4-linked benzene.[6] To determine, from low-bias conductance measurements alone, whether such effects are present is difficult because the conductance of the *meta*-substituted molecules is often below the experimental noise limit of the instruments. At high biases, non-equilibrium effects, junction heating, and inelastic processes cannot be ruled out.[13-15] Furthermore, a statistical approach is needed to demonstrate the robustness of interference phenomenon by rigorously accounting for experimental details such as junction formation probability, binding strength, junction-to-junction variation and junction structure.

In this manuscript, we overcome these critical challenges by simultaneously measuring force and conductance across single molecule junctions using a conducting atomic force microscope setup.[16,17] We study three molecular backbones: 4,4′-di(methylthio)stilbene (**1**), 1,2-bis(4-(methylthio)phenyl)ethane (**2**), and 3,3′-di(methylthio)stilbene (**3**). These molecules are chosen for three reasons: (1) stilbenes are model compounds for understanding single-molecule electronic properties of longer extended oligoenes; (2) since the longer stilbene backbones, rather than benzene backbones discussed above, form molecular junctions more frequently and (3) the thiomethyl (SMe) terminal groups provide reliable mechanical and electrical contacts to the Au electrodes.[18,19] We exploit the high binding probabilities and reliable contact properties to acquire and analyze large data sets comprised of thousands of individual

junctions to probe the robustness of interference effects, in each case. The *para*-positioned linker groups in **1** effectively couple across the π-system and provide a conducting single-molecule junction. In **2**, the mechanical linkages between the metal and the molecule are the same as in **1**, but conjugation is broken due to the saturated bridge, which results in lower junction conductance. In **3**, the mechanical linkers are moved to the *meta*-positions but the conjugated bridge is retained, as in **1**. There is no measurable single-molecule conductance feature in **3**. We use the simultaneously measured force data to independently obtain signatures of junction formation and rupture. We quantitatively determine the elongation length and rupture force for each of the three molecules, irrespective of their conductance. In contrast to the conductance, we find that the rupture force is insensitive to the linker group placement. We are able to demonstrate, for the first time, that the meta-substituted **3** forms mechanically stable Au–molecule–Au junctions but does not show a measurable conductance, and theoretical calculations point to quantum mechanical interference as the origin of this behavior. These measurements enable us not only to investigate junctions of non-conducting molecules, but more generally allow us to deconvolute electronic effects from mechanical evolution in single-molecule junctions.

4.2 Independent Measure of Force and Conductance

Simultaneous measurements of single-molecule conductance and force are carried out using a custom-built conductive atomic force microscope (AFM), which has been described in detail previously.[17] Molecular junctions are formed between an Au-coated AFM cantilever and an Au-on-mica substrate schematically represented in Figure 4.1a.

Conductance is determined by measuring current through the junction at an applied bias of 75 mV. Simultaneous measurements of cantilever deflection relate to the force applied across the junction. The AFM is operated in ambient conditions at room temperature. Dilute solutions (0.1 mM) of the target molecules (**1**–**3**, Figure 4.1b) in 1,2,4-trichlorobenzene are deposited on the substrate. For each measurement, the tip is brought into contact with the substrate until a conductance greater than 5 G_0 ($G_0 = 2e^2/h$, the quantum of conductance) is achieved and then retracted at a constant velocity of 18 nm/s while both conductance and cantilever deflection are continuously recorded. During this elongation, the Au contact thins down to a single atom point contact, clearly identified by a conductance plateau of 1 G_0. In the absence of molecules the Au contact ruptures to a broken junction when elongated further. However, in a solution of molecules, molecular junctions are frequently formed after the rupture of the 1 G_0 plateau.

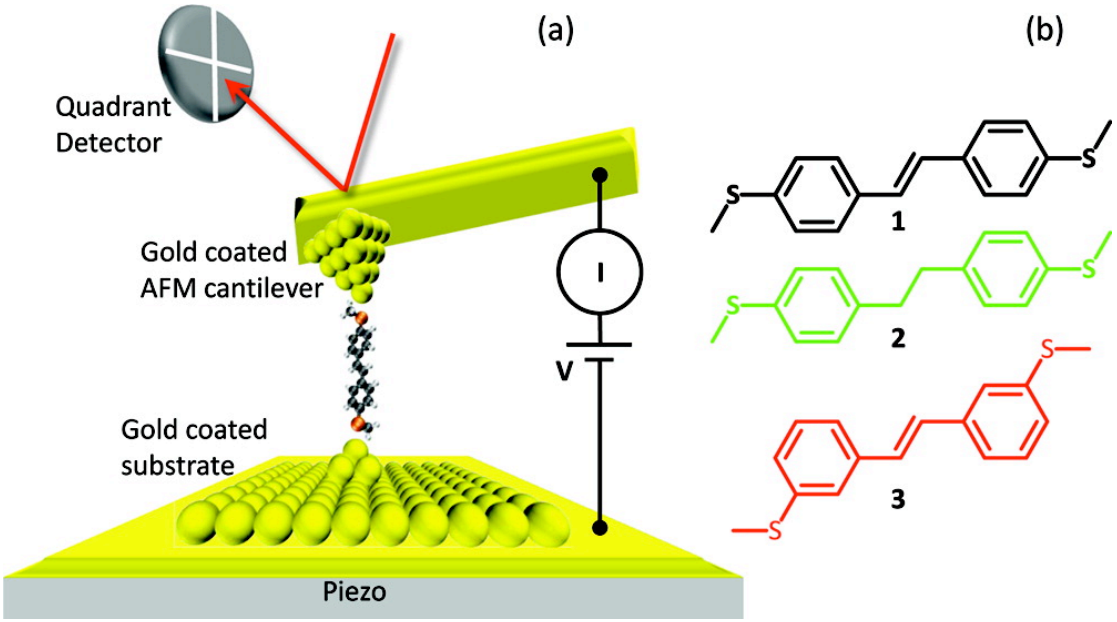

Figure 4.1: (a) Schematic of AFM apparatus and (b) chemical structures of molecules **1**–**3**.

Figure 4.2 displays simultaneously measured force and conductance traces obtained while breaking Au point contacts without molecules (Figure 4.2a) or with **1** and **3** (Figure 4.2b and 4.2c, respectively). We see a stepwise decrease in conductance (red) while the simultaneously measured force (blue) has a characteristic sawtooth pattern with alternating linear ramps (elastic loading) and abrupt drops (structural rearrangement or bond rupture) in force.[17,20] After the rupture of the Au single-atom contact in the absence of molecules (identified by its characteristic 1 G_0 conductance plateau), no further features are seen in either conductance or force. The conductance drops below the measurable level ($\sim 10^{-5} G_0$), and the force stays constant because there is no more a load on the cantilever, as seen in Figure 4.2a. When an Au point contact is broken in the presence of **1** or **2**, a single-molecule junction with a characteristic conductance feature is formed ~90% of the time.[18,19] This additional plateau is seen in the conductance traces immediately following the rupture of the Au contact, as illustrated in Figure 4.2b (red trace) for an individual measurement with **1**. The simultaneously acquired force traces (blue) also show additional sawtooth features. In this trace, we see that the 1 G_0 ruptures at ~0.5 nm along the displacement axis and the molecular junction ruptures after an additional elongation of about 0.6 nm. Once this molecular junction has ruptured, no more conductance or force features are seen in measurements with **1** or **2**. In contrast, measurements with **3** do not exhibit any well-defined conductance plateau, however a majority of the measured traces show multiple force features after the rupture of the Au-contact as illustrated in Figure 4.2c. Such force features are similar in magnitude to those seen in measurements of **1** and **2**.

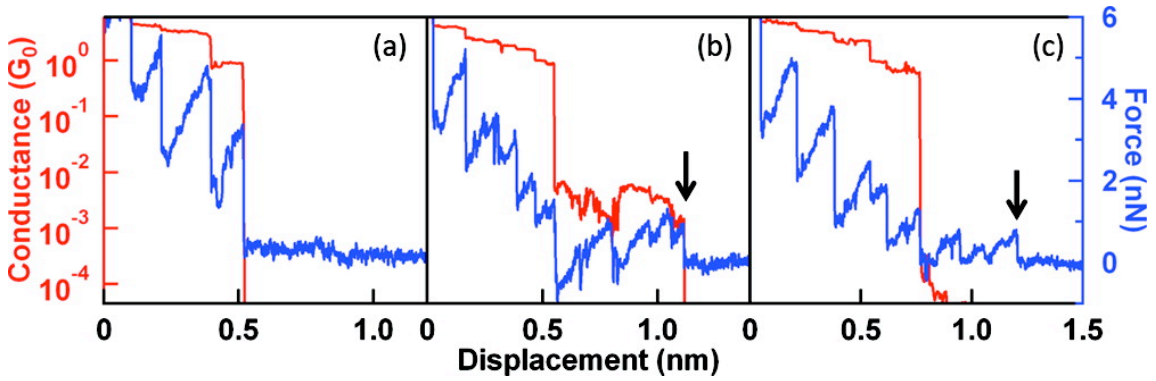

Figure 4.2: Sample traces of simultaneously measured conductance (red, left axis) and force (blue, right axis) for (a) Au–Au junctions (b) Au–**1**–Au and (c) Au–**3**–Au single molecule junctions. Downward arrows indicate the final force event identifying junction rupture.

4.3. Data Analysis

For each molecule (**1**–**3**), we analyze 7000 simultaneously measured conductance and force traces using an automated algorithm detailed in the Appendix C document. We use these large data sets to obtain statistically significant information because the atomic-scale structure varies from junction to junction. We begin by locating the displacement when the Au point contact ruptures in the conductance traces. This is the point in the trace when conductance drops below 1 G_0. Focusing on the simultaneously acquired force trace, we analyze a 1 nm long segment of this trace (~S–S distance for the three molecules) beyond the 1 G_0 rupture point to locate the final junction rupture event, that is, the last abrupt force drop. The distance between the 1 G_0 rupture location and this final force event defines the molecular junction elongation length. For conducting molecules (Figure 4.2b), we observe that molecular junctions form immediately after the rupture of the Au point contacts and therefore junction elongation length is equivalent to the conductance plateau length, which has been used in previous studies to characterize

single-molecule junction mechanics.[16,18,21] It is important to note that we are able to identify molecular junction rupture events through force data and do not require a well-defined conductance plateau to obtain the elongation length.

Two-dimensional conductance and force histograms are now generated using the location of the final force event as the origin along the displacement axis.[18] For conductance, individual traces are offset laterally such that the rupture location is the origin of the displacement axis. The 2D conductance histograms have linear bins along the displacement axis (*x*-axis, 500 bins/nm) and logarithmic bins along the conductance axis (*y*-axis, 200 bins/decade).[22] For force data, individual traces are offset both laterally as above and vertically such that the force value at the origin is zero. The 2D force histograms have linear bins along displacement (*x*, 500 bins/nm) and force (*y*, 12.5 bins/nN) axes. Every vertical section of this 2D force histogram is fit with a Gaussian and its peak is used to determine a statistically averaged force profile for the entire data set.[17] Since there is no selection based on conductance, every trace with a significant force event after Au rupture (>85% of measured traces in each case) is analyzed.

4.4. Stilbene Molecular Junctions

In Figure 4.2b, we display a sample force and conductance measurement with **1**. We see a clear conductance plateau after the rupture of Au point contacts. The simultaneously acquired force traces shows several sawtooth features indicating multiple structural changes in the junction; ultimately rupturing after ~0.6 nm of elongation.[23] The final force event (downward arrow in Figure 4.2b) occurs at exactly the same displacement as the conductance drop. Figure 4.3a shows the 2D conductance histogram

for **1** representing 6788 of the 7000 individual traces for which a significant force event was found after 1 G_0 rupture. Although only force data was used to identify and set the zero displacement at the molecular junction rupture point, we observe that the conductance also drops sharply to the instrument noise level at zero-displacement, demonstrating the reliability of this force-based alignment procedure. A conductance profile of this histogram shows a clear peak at $1.3 \times 10^{-3} G_0$ (Figure 4.3d, black trace), which compares well with the 1D conductance histograms created from all the measured traces (see Appendix C). We see that the para-linked molecule **1** forms junctions with relatively high, well-defined conductance, as observed for other fully conjugated molecular wires. The 2D force histogram created from the simultaneously acquired force traces is shown in Figure 4.4, along with the statistically averaged force profile. This force profile shows an abrupt drop of 0.5 nN at zero displacement, corresponding to the force required to rupture this junction.[17]

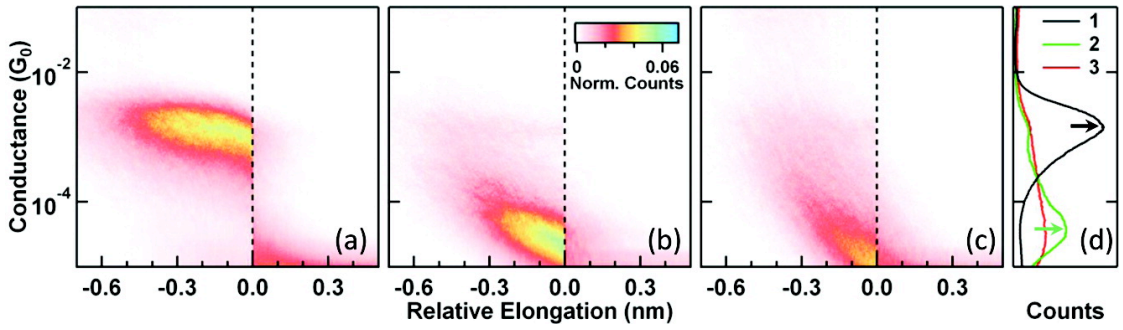

Figure 4.3: Displacement-preserving 2D conductance histograms (a, b, c) for **1**, **2**, and **3**, respectively, and profiles of conductance before rupture (d). The histograms represent more than 85% of the 7000 measured traces that show a significant force event beyond Au rupture in each case. The abrupt jump in conductance at the displacement origin (dashed vertical lines provided as a visual guide) for **1** and **2** shows that bond rupture

coincides with conductance drops. Arrows indicate the most frequently measured conductance value from the conductance profiles of **1** and **2**.

Molecule **2** shows similar behavior in conductance and force. The 2D conductance histogram (Figure 4.3b, from > 6000 traces) shows a clear conductance feature at a significantly lower value of $3.2 \times 10^{-5} G_0$. This result is intuitively understood as arising from the lowered communication between the aromatic rings due to the ethane bridge at the center, even though the para-positions of the linkers is identical to **1**. The 2D force histogram created from the simultaneously acquired force traces is shown in Appendix C. From the statistically averaged force profile (inset, Figure 4.4, green trace), we find that these junctions also rupture at a force of 0.5 nN and show a loading and rupture behavior similar to **1**.

Qualitatively different behavior is found in junctions of **3**. We do not see clear conductance plateaus in individual traces, as shown in Figure 4.2c. Individual force traces, however, do show sawtooth signatures typical of junction structure evolution and bond rupture and are analogous to force measurements of **1** and **2**. This is representative of the loading and rupture event of the molecular junction in individual traces. The 2D conductance histogram (Figure 4.3c), constructed from all traces that show a clear bond rupture event in the force data, shows a broad conductance feature slightly above the noise level as seen in the profile in Figure 4.3d (red trace). This can be ascribed to the small, but nonzero contribution to conductance from the sigma channel, through-space tunneling between the electrodes and possibly dispersive interactions between the molecular π-orbitals and the Au electrodes.[9,24] The 2D force histogram for this molecule is shown in Appendix C. The averaged force profile centered at the rupture event

generated from 5965 traces is shown in the inset of Figure 4.4 (red trace). Clearly, there are a statistically significant number of traces that have rupture events after the G_0 plateau, a fraction similar to **1** and **2**, which could not be identified by conductance data alone. The bond rupture force for these junctions is also 0.5 nN. Therefore, we conclude that single-molecule junctions of **3** are formed but do not show clear conductance plateaus and have a significantly lower conductance, confirming the theoretical predictions of a low conductance due to interference effects. It is important to note that the character of the conductance we observe for **3** is qualitatively very different from that seen in **1** or **2**, as is further evidenced in the conventional linear and log binned 1D conductance histograms shown in Appendix C.

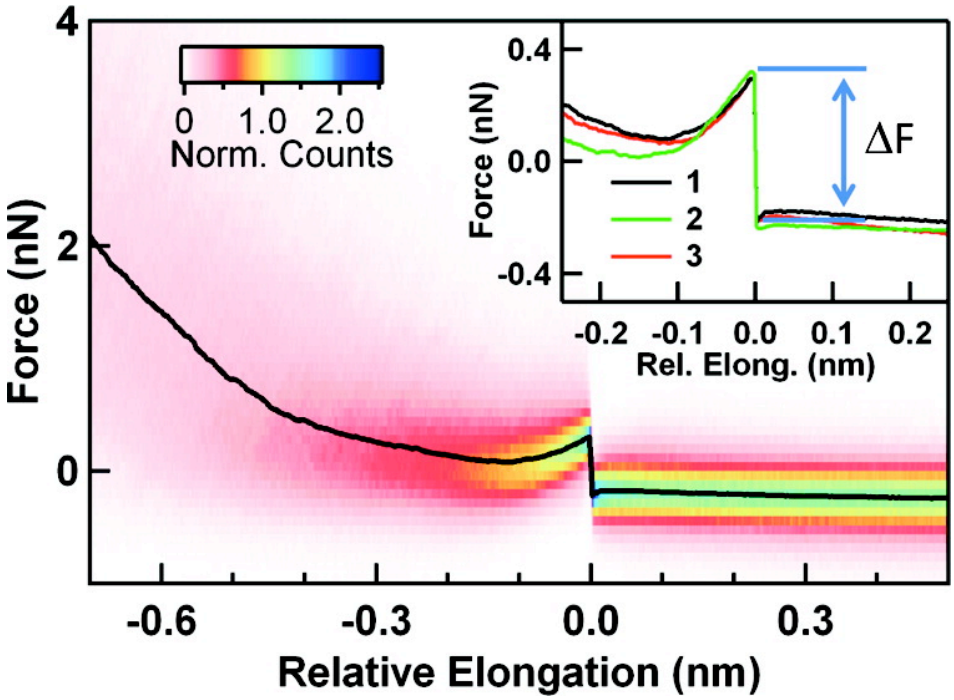

Figure 4.4: The 2D force histogram for molecule **1** with the averaged force profile overlaid. (Inset) Statistically averaged force profiles for molecular junctions of **1**, **2**, and **3** in black, green, and red, respectively.

Taken together, the force profiles for **1**, **2**, and **3** illustrate that bond rupture forces are approximately the same for all three molecular junctions, independent of the linker position. The rupture force depends on the specific interaction of the Au-SMe donor–acceptor bond in each molecule, and the apparent insensitivity of the rupture force to the linker position, within our experimental resolution, can be explained by the similar local structure near the Au-SMe bonds for **1**–**3**.

The independent analysis of force and conductance allows us to study the mechanical aspects of junction evolution even in the absence of conductance plateaus. In particular, the amount of elongation sustained by the junction before rupture, the junction elongation length, gives information about the geometry of the Au–molecule–Au junction. In general, the molecule in the junction can sample multiple binding sites during elongation before achieving the idealized vertical Au–molecule–Au junction geometry.[18] The junction elongation length scales with the molecular S–S distance but is smaller than the molecule length, because of a nonzero gap that is opened when the Au point contact is broken.[22] Histograms of elongation lengths are constructed from individual traces and have a Gaussian distribution (Appendix C). The peak values obtained from these distributions for **1**–**3** are presented in Table 4.1. The plateau lengths of **1** and **3** are in accordance with their respective S–S distances. However, a relatively smaller plateau length is observed for **2**. This could be due to nonplanar configurations accessible to the ethane bridge in **2**, which are not allowed in either **1** or **3** due to the central C═C double bond. These measured elongation lengths give us further confirmation of the junction formation, independent of conductance.[3,25]

Table 4.1. Conductance, Elongation Length, and Rupture Force for Single Molecule Junctions with Molecules **1**–**3.**

	experimental measurements				**DFT**
molecule	**conductance (G_0)**	**elongation (nm)**	**length**	**rupture force (nN)**	**S–Sdistance (nm)[a]**
1	1.3×10^{-3}	0.42		0.5	1.31
2	3.2×10^{-5}	0.32		0.5	1.29
3[b]		0.31		0.5	1.17

[a]B3LYP/6-31G** level of theory.
[b]Nonconductive molecule did not show well-defined peak in conductance profiles.

Having established the similar mechanical stability for **1**–**3**, we are able to make direct comparisons between the chemical structures and the corresponding conductance values. We can unambiguously conclude that **2** is less conducting than **1** due to broken conjugation, while **3** forms mechanically stable yet electrically insulating junctions. Molecular backbones **1** and **3** are essentially planar structures with all sp^2-carbon atoms and with similar molecular lengths; however, the meta-positioned linker groups effectively turn off the conductance.

4.5. Theoretical Analysis

To better understand these results, we have examined the electronic structures of the organic molecules bonded to an Au dimer (which represents one of the Au electrodes) through an Au–S donor–acceptor bond. We use a dimer of Au atoms to avoid

complications attendant to the unpaired spin occupying the valence 6s orbital of a single Au atom. We attach the candidate organic molecule to just one "electrode" in order to appreciate what the second electrode sees as it encounters the metal-bound organic. In effect, this is a simplified model for the chemical state of the system prior to the charge transfer. We performed DFT calculations of the electronic structures of these model systems at the B3LYP/6-31G** level.[26] The highest occupied molecular orbital (HOMO) from the geometry-optimized structures, Au_2-**1**, Au_2-**2**, and Au_2-**3**, are shown in Figure 4.5. The HOMO of **1** extends across the entire π-space of the molecule in contrast to that of **2** and **3**. Significantly, in **1** the HOMO connects both the terminal sulfur atoms and provides a clear electronic conduit between the sulfur groups. In contrast, in **2** one side of the molecule does not communicate with the other, which is a direct result of the saturated ethane bridge. In addition, rotation around these sp^3-carbons increases the conformational freedom in the molecular junction. Therefore, a broad peak is expected in the conductance histograms without retarding the rupture force. In **3**, we observe that although the HOMO extends across the bridge, it does not have significant amplitude on the sulfur atom at the meta-position. This finding is consistent with observations from various related approaches, such as organic reaction kinetics,[27,28] Hammett coefficients,[29] and even classic organic arrow-pushing conventions, which predict a node at the meta-position.[30] For direct experimental evidence, Daub and co-workers electrochemically quantified the charge-transport kinetics between meta- and para-(styryl)stilbenes.[31] However, this area has recently received more theoretical attention due to the possibility of studying these effects at the single-molecule level.[6-12]

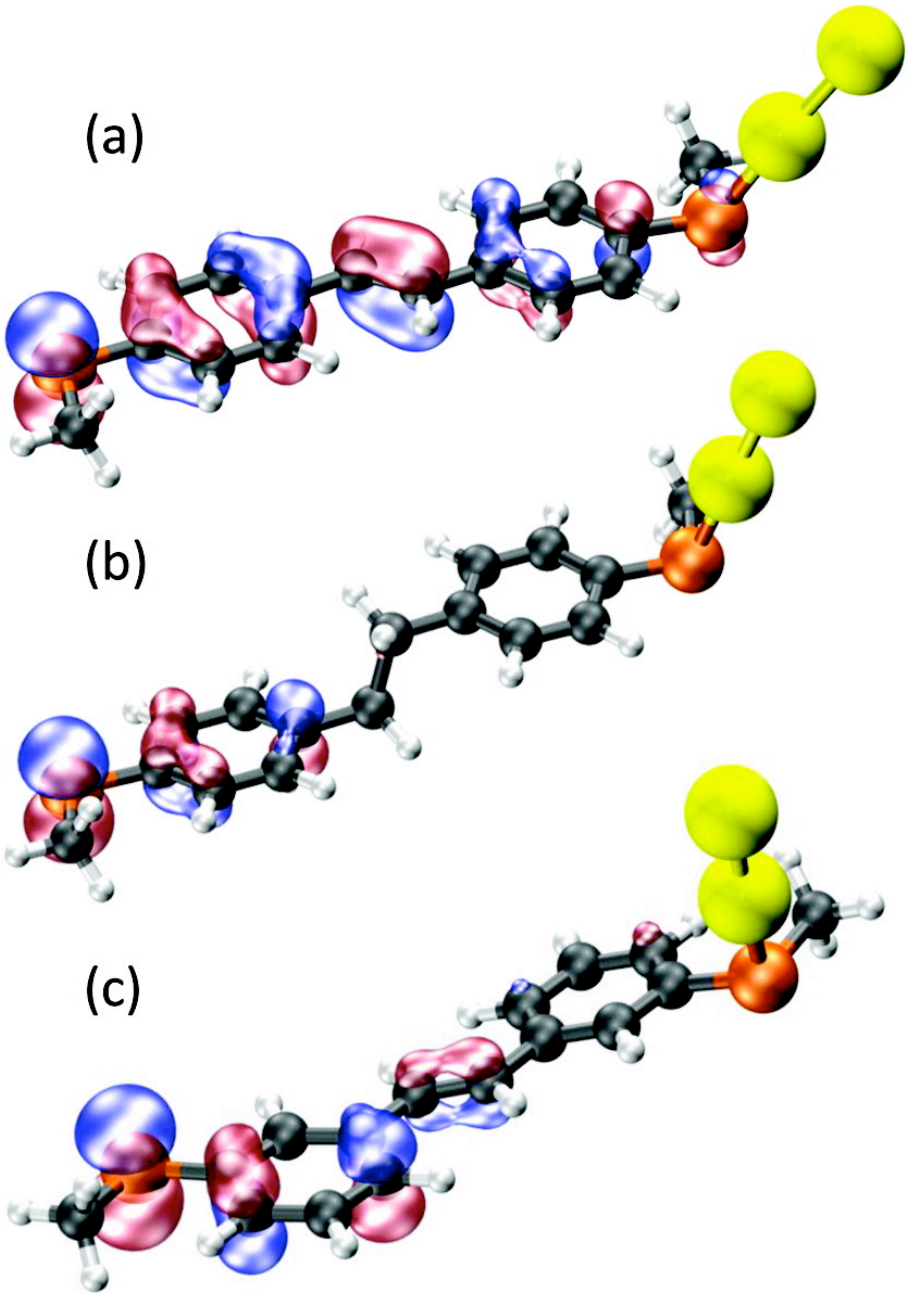

Figure 4.5. DFT optimized structures and isosurface plots of the HOMO of (a) Au_2-**1**, (b) Au_2-**2**, and (c) Au_2-**3**.

4.6. Conclusions

Single-molecule junctions of stilbene derivates with para and meta-linked stilbenes have been formed using a conducting-AFM approach that allows for

measurements of single-molecule mechanics through force, independent of conductance. We have found that despite great differences in their conductance values, each molecule assembles into single-molecule junctions that are mechanically stable. Our results show that both para- and meta-linkers provide similar mechanical stability to the junctions yet radically change the conductance. For these reasons the para-linker groups behave as typical electro-mechano contacts, while meta-linkers disrupt the conduction acting primarily as mechanical contacts. By quantitatively accounting for the contact mechanics, these results represent the first direct proof that quantum interference is an inherent property arising from the molecular structure and is not quenched by microscopic junction-to-junction variations. This two-property measurement capability extends our understanding of single-molecule junction properties to such low-conductive and insulating systems as simple molecular connectors and dielectrics materials. Moreover, this approach provides a means to design and study new molecular switches and devices that utilize quantum interference.

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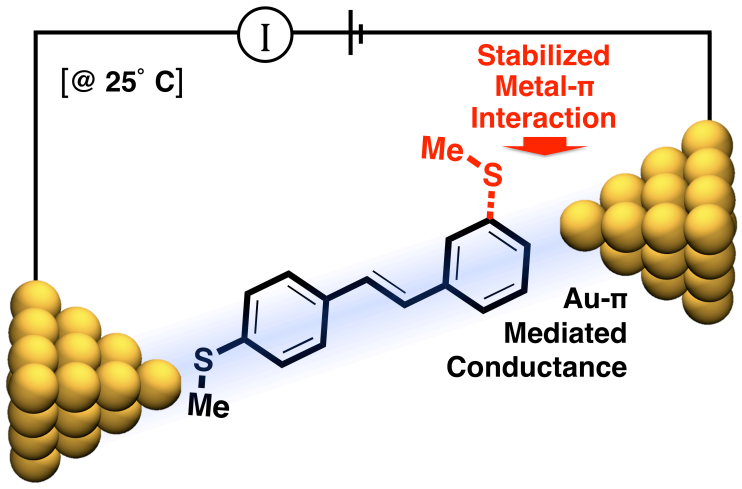
Chapter 5. Direct Metal-π Bonding in Conjugated Single-molecule Junctions[†]

STM-BJ measurements in Chapter 5 were preformed by Seokhoon Ahn with the assistance of Radha Parameswaran. AFM-BJ studies and analysis were done by Sriharsha Aradhya. Molecules were synthesized by Markrete Krikorian and myself. DFT calculations were run by Michael Steigerwald and myself.



5.1. Introduction

This study describes the mechanism of conduction through asymmetric molecular junctions containing conjugated molecules having only one electrode-binding "linker" group.[1] Linker groups are aurophilic functional groups that bind the molecule between Au electrodes, such as thiols (-SH), primary amines ($-NH_2$) and methylsulfides (-SMe).[2] Typical molecules employed in single-molecule electronics are conjugated or short aliphatic molecules that are functionalized at each end with linker groups. Here,

[†] Chapter 5 was reproduced with permission from the authors: Meisner, J. S.; Ahn, S.; Aradhya, S. V.; Krikorian, M.; Parameswaran, R.; Steigerwald, M. L.; Venkataraman, L.; Nuckolls, C.; *J. Am. Chem. Soc.*, **2012**, Accepted on Nov. 21, 2012. Copyright 2012 American Chemical Society.

conjugated olefins of varying lengths are end-functionalized with methylsulfide and amine linkers at one or both terminal phenyl rings. To explore quantum mechanical effects[3] we vary the position of these linkers between the *meta* or *para* positions. The conductance and rupture forces of single-molecule junctions formed from these molecules are measured using the break-junction (BJ) technique with a scanning tunneling microscope (STM)[2a] and an atomic force microscope (AFM).[4] We find that for measurable conductivity to occur, at least one of the rings must have a linker *para* to the olefin providing strong electronic coupling to the electrode. We measure both the highest conductivity and the narrowest distribution of conductance for olefins with two *para* linkers. When one of these *para* linkers is replaced with a *meta* linker, the conductance decreases by almost an order of magnitude, due to a reduction in the Au-molecule-Au coupling. If this mechanical contact, the *meta* linker, is removed leaving only a single *para* linker, the conductance decreases even further. We show that the conductance of our molecular wires that have at least one *para* linker decay exponentially with increasing oligomeric length and that they have step lengths corresponding to their molecular length. Both of these results indicate that we are probing the conductance of single-molecule junctions, as opposed to junctions formed by overlapping or interdigitated molecular dyads. That is, these measurements allow us to conclude that mono-functionalized stilbene molecules do not readily form junctions where molecules conduct via intermolecular carrier transfer (i.e. π-π-stacking interactions).[5]

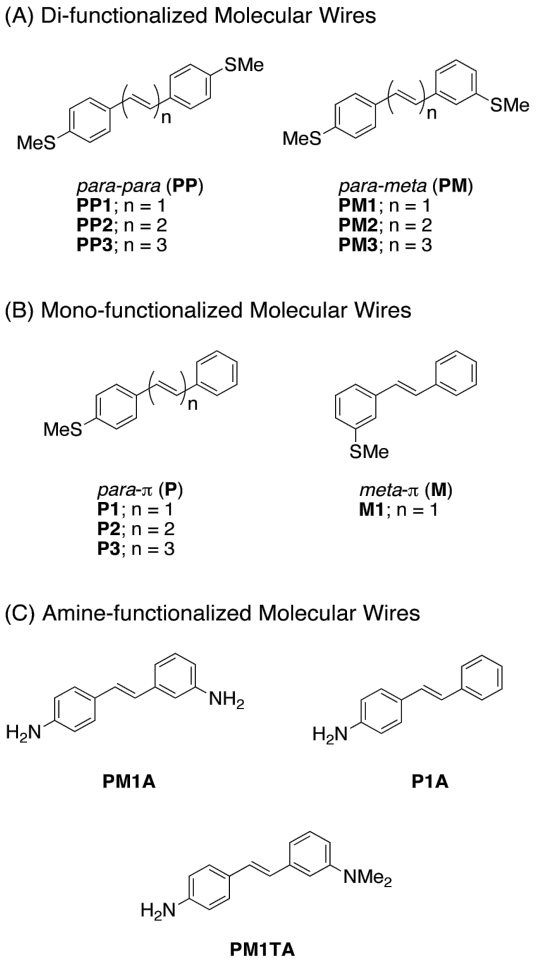


Figure 5.1: Chemical structures of *trans*-stilbene and all-*trans*-oligoene molecular wires: (A) difunctionalized series, having only *para*-positioned linker groups (**PPn**) or a mixture of *para* and *meta* linkers (**PMn**); (B) mono-functionalized wires **Pn** and **M1** contain either one *meta* or one *para* linker. (C) Stilbene derivatives end-functionalized with primary and tertiary amines.

5.2. Experimental Methods

5.2.1. Molecular Wire Synthesis. For this study we synthesized three different vinylogous series of methylsulfide functionalized *trans*-α,ω-diphenyl-oligoenes as well as 3-(methylthio)stilbene. Each series ranges in length from the stilbene (n = 1) to the triene (n = 3) and is displayed in Figure 5.1A and 5.1B. Convenient shorthand is used to

name these compounds (**PPn**, **PMn**, **Pn**, and **M1**), which includes the linker substitution (P = *para*, M = *meta*) and the length of the oligomer (n). As examples, **PP2** denotes *para-para'*-dithiomethyl-diphenylbutadiene and **PM3** denotes *para-meta'*-dithiomethyl-diphenylhexatriene. Both difunctionalized (**PPn** and **PMn**) and mono-functionalized (**Pn** and **M1**) molecules were synthesized through Wittig[6] and Horner-Wadsworth-Emmons reactions (see Appendix D for synthetic details and characterization).[7]

A set of three additional stilbene derivatives bearing amine linkers were synthesized in order to deconvolute the electronic and mechanical contributions in molecular junctions; (*E*)-3,4'-diaminostilbene (**PM1A**) and (*E*)-4-amino-stilbene (**P1A**) as analogous compounds to the conducting (*E*)-(methylthio)stilbenes above, as well as (*E*)-3-dimethylamino-4'-aminostilbene (**PM1TA**); where A = amine and TA = tertiary amine.

5.2.2. STM and AFM-BJ Measurements. STM-BJ measurements[2a,2b] were performed in dilute solutions (1 ± 0.1 mM in 1,2,4-trichlorobenzene) of molecular wires using a gold-on-mica substrate and a gold STM tip (cut Au wire, 0.25 mm diameter, 99.998%, Alfa Aesar). Gold atomic point contacts were repeatedly formed and broken in the solution of molecules under a 500 mV voltage applied to the junction with a 100 kΩ resistor in series. As the point contacts are broken, one or a few molecules may bind to bridge the gap between the broken Au contact, thereby forming molecular junctions. The electrodes are then pulled farther apart until the junction is broken. Conductance (current/voltage) is measured as a function of piezo displacement yielding individual conductance traces. In doing so, our STM-BJ method does not take consecutive measurements on a single junction. Instead, at the end of each measurement the junction is destroyed. Then, before forming a new junction the tip and substrate are smashed

together and pulled apart forming fresh electrodes and thus a new junction. For each molecule, over 5000 traces are collected and analyzed by creating one-dimensional (1D) conductance and two-dimensional (2D) conductance-displacement histograms[2d,8] that reveal statistically relevant information on junction conductance, as well its evolution under junction elongation.

Molecular conductance step lengths[9] and the slopes of the conductance features ($ß_S$) in the 2D histograms were determined by fitting the average conductance profile; both procedures are outlined in detail in Appendix D.

Simultaneous conductance and force measurements were obtained using a custom built conducting AFM set-up.[4a] Single-molecule junctions were formed between a gold-coated commercial AFM cantilever (NanoAndMore, Inc) and a gold-on-mica substrate. Conductance is measured across the tip/sample junction at a bias of 75 mV. The force is measured simultaneously by monitoring the deflection of a laser focused on the back of the cantilever. AFM-BJ measurements are carried out on **PP1**, **PM1** and **P1**. In each case 2D force-displacement histograms are constructed from measurements on over 8000 junctions.

5.2.3. Theoretical Methods. Density functional theory (DFT) electronic structure calculations examined shape and energy differences amongst the most relevant molecular orbitals (MO's) for molecular conductance. All calculations were preformed using Jaguar[10] with the B3LYP hybrid functional and the 6-31G** basis sets. The molecular geometries were fully optimized. The final geometries, total energies and MO energies for each molecule in this study are given provided in the Appendix D.

5.3. Results and Discussion

5.3.1. Single-molecule Conductance: General Substitution Effects. We begin by comparing the conductance and rupture forces of molecular junctions of four stilbene derivatives having either one or two methylsulfide linkers in either the *meta* or *para* positions (**PP1**, **PM1**, **P1**, and **M1**). Their 1D logarithmically binned conductance histograms are obtained from STM-BJ measurements and are compared in Figure 5.2A. The histogram for **PP1** shows a clear molecular conductance peak, indicating that reproducible single-molecule junctions are formed throughout thousands of measurements. The sharpest peak at 10^{-3} G_0 is characteristic of a conjugated stilbene having two *para*-linkers, as has been show before.[3d,11] A characteristic conductance signature (peak in the histogram) appears for **P1** even though it contains only one linker. The peak conductance for **P1** is almost two orders of magnitude lower than that for **PP1**, therefore electronic coupling across the **P1** junction is weaker than with **PP1**. From the width of the peak, we conclude that the junction conductance varies significantly more than in the case of **PP1**, which has two linkers. We quantify the peak width for all junctions in Table 5.1 using the half width at half-maximum. We next compare **P1** with **M1**, which also has only one linker, but now at the *meta*-position; we see no peak in this histogram indicating that junctions with a conductance above our instrument noise (~10^{-7} G_0) are not formed with **M1**. This trend is expected since *meta*-linkers do not provide strong electronic coupling into the π-system.[3a] Nonetheless, they do provide a mechanical link as we have previously shown.[3d] Indeed, we see with **PM1** that the additional mechanical stability provided by the *meta* linker yields both a higher conductance and a

narrower distribution compared with **P1**. Conductance values for each compound are given in Table 5.1.

5.3.2. Single-molecule Rupture Forces: General Substitution Effects. We confirm the mechanical enhancement provided by the *meta* linker by measuring force in AFM-BJ's of **PP1**, **PM1** and **P1**. The rupture forces are measured by pulling the junction apart until it breaks and (to a first order approximation) establish an upper limit on the strength of the weakest Au-molecule interaction. Stilbenes with two methylsulfide linkers (regardless of their position on the phenyl rings) are stabilized in the junction and give rupture forces of 0.5 nN, as is the case with **PP1**[3d] and **PM1** (Figure 5.2C). In contrast, we found that the rupture force for **P1** is smaller than 0.3 nN (twice the instrumental noise). Our rupture force results for each stilbene are overlaid in Figure 5.2C (inset). Consequently, the interaction between the Au electrode and unsubstituted phenyl ring does not contribute much to the mechanical stability of the junction at room temperature. Since linkers in the *meta*-position behave as typical mechanical contacts (albeit without providing electrical coupling), we postulate that the conductance modulation found between the **PMn** and **Pn** series is the result of a strengthened Au-π interaction, where the tunneling pathway is coupling directly into the π-space of the second ring while the *meta*-linker secures that end to the electrode surface. Similar metal-π (Pt or Ag) interactions have been used to rationalize the conductance mechanism through symmetric metal-benzene-metal junctions at low temperature,[12] as well as molecular junctions of C_{60} and stacked oligomers of paracyclophane using Au electrodes at room temperature.[13]

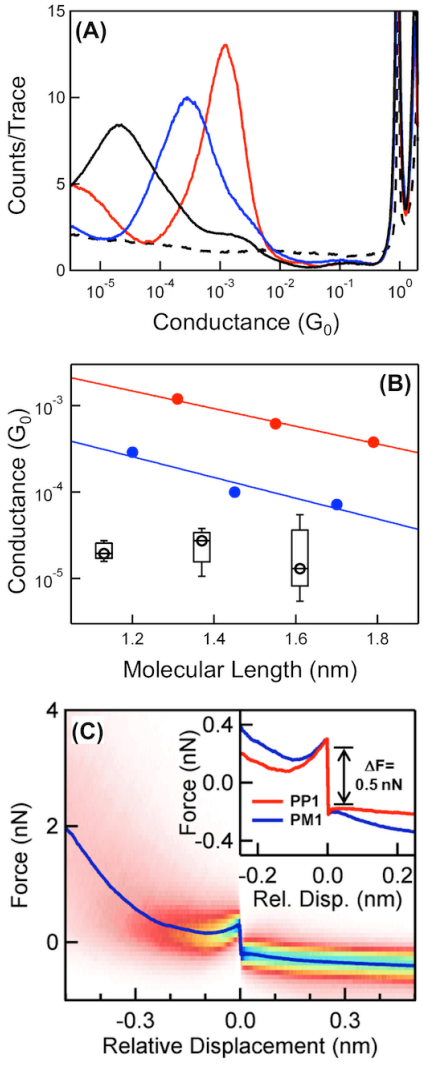


Figure 5.2: (A) 1D conductance histograms constructed using logarithm bins for junctions of **PP1** (red), **PM1** (blue), **P1** (black) and **M1** (dashed). **M1** does not form conductive junctions. Histograms were generated from over 5000 traces without data selection, using 100 bins/decade. (B) Plot of molecular length vs. conductance for *para-para* series (**PPn**; red) and *para-meta* series (**PMn**; blue). Exponential decay constants were found to be ß = 0.23 ± 0.03 $Å^{-1}$ and 0.27 ± 0.08 $Å^{-1}$, respectively. The effective contact resistance for **PPn** is 520 kW and for **PMn** is 1820 kW. Conductance for **Pn** (black) is represented with the mean peak conductance (black circles) within a distribution of the inner 50th percentile (black boxes) and the inner 80th percentile (bars). Due to junction-to-junction variations larger samples sizes were used for **Pn** (over 30,000 individual conductance traces). (C) The 2D force histogram of **PM1** junctions compiled

from ~8000 traces. Colored contours represent the normalized histographical counts. (Inset): Average force profiles of **PP1** and **PM1** are overlaid yielding rupture forces of 0.5 nN for each.

5.3.3. Length-dependent Molecular Conductance. To understand the conduction mechanism in greater detail it is necessary to verify that conductance occurs through the molecular backbone of a single molecule. Therefore, we measured the length-dependence of conductance through a series of oligomers **PPn**, **PMn** and **Pn,** with n = 1, 2, and 3. The peak conductance of each oligomer is given in Table 5.1. In Figure 5.2B, we plot the conductance histogram peaks against the molecular length for each series. The *para-para* bound series, **PPn**, is especially useful as a control group representing typical linear α,ω-diphenyl-oligoenes.[14] The decay constant (ß), which describes the exponential decrease of conductance with increasing molecular length is found to be ß = 0.23 ± 0.02 $Å^{-1}$, in good agreement with published results.[15] For the **PMn** series, we also find an exponentially decreasing conductance with a decay constant of ß = 0.27 ± 0.08 $Å^{-1}$, which is similar to that of **PPn**. This indicates that conduction is through the π-system of a single molecule and not by any other mechanism, such as π-π-stacking between dimers.[5] When measuring conductance of the **Pn** series, we found that conductance peak values shifted within half of an order of magnitude over the course of the experiment (thousands of consecutive traces). This junction-to-junction variation in conductance is illustrated by the error bars in Figure 5.2B. The variability increased with molecular length (**P1** < **P2** < **P3**) making it impossible to determine a decay constant with precision.[16] Outside of the mono-substituted **Pn** series, the variation during and between different experimental runs (changing tip and substrate) caused insignificant variations in

the most frequently measured conductance. This is typically the result obtained with methylsulfide linkers.[17]

5.3.4. Molecular Junction Evolution. In order to further understand junction evolution, we show how the conductance changes during elongation. By constructing 2D conductance-displacement histograms, we can determine the maximal junction length, or step length, as well as trends in the molecule-electrode coupling. Figure 5.3A-C displays the 2D histograms[18] of the stilbenes junctions, **PP1**, **PM1** and **P1** (all others are given in Appendix D). Their molecular conductance features extend about 0.6 nm. The step lengths are summarized in Table 5.1. We note that they are ~0.7 nm shorter than the molecular lengths, which is common in STM-BJ's due to snapback relaxations at the Au electrodes.[19] The fact that all three molecules have step lengths corresponding to their molecular length indicates that in each case molecular junctions are formed with a single molecule. We quantify the step length for each molecule as detailed in Appendix D and summarize them in Table 5.1. For each oligomeric series, the step length increases linearly with molecular backbone length (Figure 5.3D).[2c] The step lengths of **Pn** are slightly longer (0.02-0.04 nm) than those of **PPn**. We attribute the difference to changes in the linker group[2c] (*para*-SMe vs. Au-π) and not the formation of π-π-stacked dimers, since significantly larger step lengths would then be expected.

The 2D histograms also show that the slope of the conductance-versus-displacement curves change significantly between each series in the order, **PPn > PMn** > **Pn**. The white lines overlaid in Figure 5.3A-C represent the statistically averaged decreasing conductance, whose slopes are tabulated in Table 5.1 for all our molecules. Steeper

slopes correspond to junctions that are more sensitive to elongation. For example, the largest change in slope is observed between **PPn** and **PMn** and can be attributed to more geometrically demanding coupling in the **PMn** and **Pn** series. Since the *meta*-SMe linker improves the mechanical stabilization of the junction, the slope of **PMn** is shallower than **Pn**. It is important to note that the numerical value of the slope depends on several factors, such as mechanical stability, structural evolution during pulling, and competing tunneling current. Therefore, while our systematic approach allows us to qualitatively understand the differences between each series at this point, quantitative comparisons will require further, more-detailed experiments combined with significant theoretical efforts.

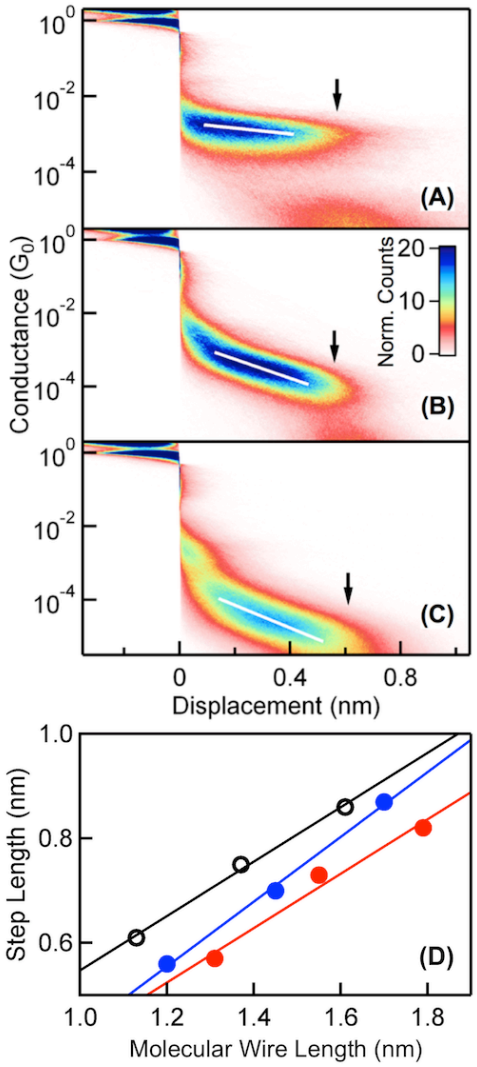


Figure 5.3: 2D conductance-displacement histograms are generated from over 5000 individual measurements on (A) **PP1**, (B) **PM1** and (C) **P1** single-molecule junctions. Colored contour represents the number of counts x 1000. Step lengths are marked by black arrows, representing the 90th percentile of conductance, at 0.57, 0.56 and 0.61 nm, respectively. (D) Plot of the step lengths vs. molecular wire lengths of **PPn** (red), **PMn** (blue) and **Pn** (black) series, with slopes of 0.52, 0.62 and 0.52, respectively. Molecular wire lengths were determined by DFT calculations.

Table 5.1: Tabulation of Conductance Parameters from STM-BJ Measurements.

Molecule	1D Conductance Peak (G_0)	Conductance Peak Width[e]	Slope β_s ($Å^{-1}$)	Step Length (nm)	Molecule Length[a] (nm)
PP1	1.2×10^{-3}	0.42	0.18	0.57	1.31[c]
PP2	6.2×10^{-4}	0.44	0.12	0.73	1.55[c]
PP3	3.8×10^{-4}	0.44	0.12	0.82	1.79[c]
PM1	2.9×10^{-4}	0.63	0.58	0.56	1.20[c]
PM2	1.0×10^{-4}	0.69	0.35	0.70	1.45[c]
PM3	7.2×10^{-5}	0.74	0.35	0.87	1.70[c]
P1	2.1×10^{-5}	0.90	0.67	0.61	1.13[d]
P2	2.6×10^{-5}	0.94	0.54	0.75	1.37[d]
P3	1.7×10^{-5}	1.02	0.46	0.86	1.61[d]
M1	n/a[b]	n/a[b]	n/a[b]	n/a[b]	1.00[d]
PM1A	2.2×10^{-4}	0.83	0.67	0.63	1.14[c]
P1A	2.8×10^{-5}	0.98	0.70	0.67	1.09[d]
PM1TA	2.8×10^{-5}	1.03	0.89	0.66	1.09[d]

[a]Molecular length is taken from DFT optimized structures. [b]Molecules do not form conductive junctions. [c]Length refers to the through-space distance between terminal linker group heteroatoms. [d]Length refers to the through-space distance from the *para*-linker group heteroatom to most distant carbon atom. [e]Conductance peak widths are determined using the half width at half-maximum on the high-conductance side of the peak, since low-conductance half-maxima are sometimes lost in the experimental noise.

5.3.5. Deciphering Electronic from Mechanical Contributions Using Amine Derivatives. Since the conductance of the **PPn** series is systematically higher than the

corresponding **PMn** series, and since *meta*-substitution appears to be non-conductive, our data suggest that conduction in **PMn** junctions occurs through the combination of an Au-S interaction in the *para*-substituted ring and a direct Au-π interaction in the *meta*-substituted ring. To verify these effects, we employed a series of amine-terminated stilbenes where, in contrast to the methylsulfide stilbenes, we are able to retain electronic effects while disrupting the mechanical coupling at the *meta*-linker (**PM1A** and **PM1TA** from Figure 5.1C). Molecules terminated with primary amines (RNH_2) bind to the Au electrodes forming molecular junctions in the STM-BJ set-up. However, when primary amines are methylated to form tertiary amines ($RNMe_2$), they do not bind to Au.[2b] In this way, the linker group's electron-donating contributions to the MO's are preserved, while arresting additional mechanical stabilization**.**

Conductance histograms of **PM1A**, **P1A** and P**M1TA** junctions are compared in Figure 5.4. The conductance peak for the *para-meta* bound junction (**PM1A**) is almost an order of magnitude higher than that of the *para*-π bound junction (**P1A)**, similar to what was observed for the methylsulfide analogues (**PM1** vs. **P1**). However, when the *meta*-NH_2 of **PM1A** is replaced by *meta*-NMe_2, the conductance of the resulting **PM1TA** drops by an order of magnitude, overlapping the conductance of mono-functionalized **P1A**. With these direct structural comparisons we conclude that the electrical pathway in the *para-meta*-bound series is through an Au-π interaction and that the *meta* linker serves as a mechanical stabilizer that enhances the electronic coupling between the terminal phenyl group and Au electrode.

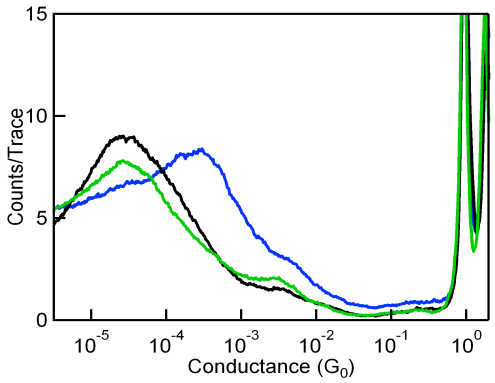


Figure 5.4: Log-binned conductance histograms of amine-functionalized stilbene molecular wires: *para-meta* **PM1A** (blue), *para*-π **P1A** (green), and methylated *para-meta* **PM1TA** (black) were generated from 5000 individual conductance traces.

5.4. Theoretical Analysis

To gain insight into the electronic structure of our molecular junctions, DFT calculations were carried out to examine the shape of MO's. The methylsulfide-functionalized stilbenes (**PP1**, **PM1**, and **P1**) are considered. The most relevant MOs are those nearest to the Fermi level of the electrodes. Since these junctions are generally HOMO conducting,[20] we examine the HOMO, HOMO-1 and HOMO-2 of **PP1** and **PM1**, which contain the p-π orbitals of sulfur and the olefin (C=C), as well as the HOMO and HOMO-1 for compounds **P1**. Since other MO's are much lower in energy their contributions become negligible.

First, we inspect the results of the *para-para* case (**PP1**), which are shown in Figure 5.5A. We see that the orbitals are strongly coupled across the molecular backbone and include both sulfur lone pairs (S_{LP}). In contrast, the two S_{LP}'s in the *para-meta* compound (**PM1**; Figure 5.5B) are decoupled. In fact, the energy cost to mix these orbitals and establish a conduction pathway (through each S_{LP}) is roughly equal to the energetic cost (~0.85 eV) required to disrupt that in the previous case (**PP1**). In light of this, it would be

reasonable to expect **PM1** to not conduct at all. However, upon deeper inspection we find density located on the phenyl ring opposite the *para*-linker and purpose this as an alternative conduction pathway. This secondary path is also predicted to exist in **PP1**; however, since it is expected to be more resistive, it may not be experimentally distinguishable in **PP1**. In the special case of **PM1,** the secondary path may be the only available conductance pathway.

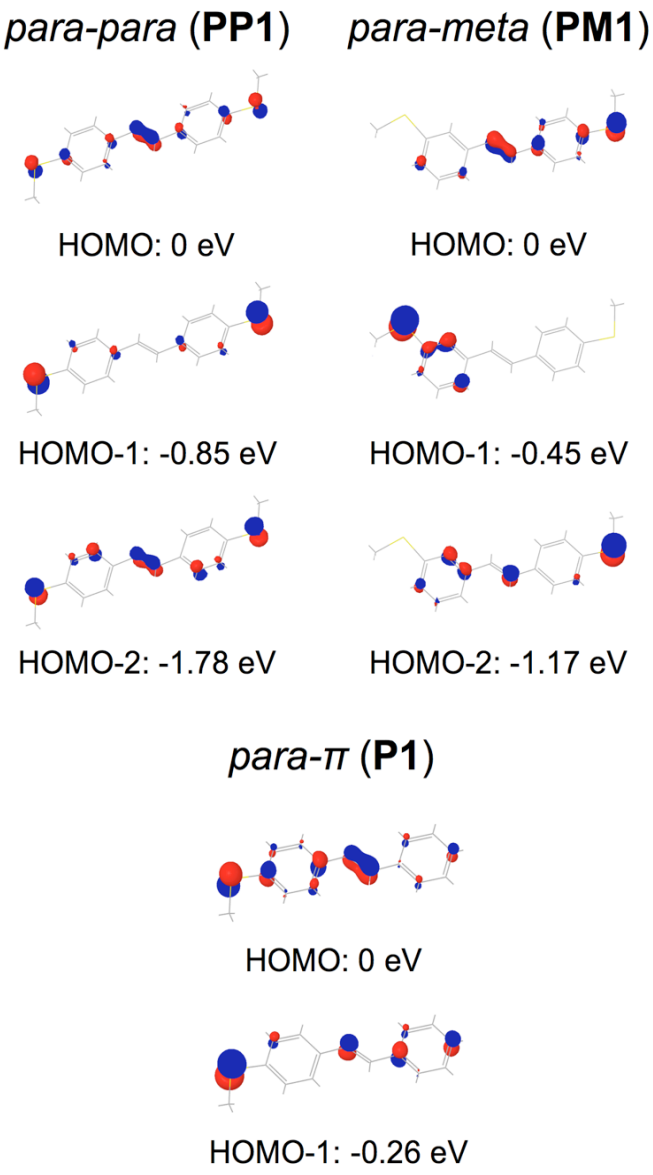


Figure 5.5: DFT calculated isosurfaces of MO's relevant in single-molecule conductance. Geometries of **PP1**, **PM1** and **P1** were optimized and MOs calculated at the B3LYP/6-31** level of theory in the gas phase. HOMO energies were normalized to 0 eV for easy comparison. Contour values set at 0.75.

For the *para*-π bound molecule (**P1**; Figure 5.5C) the ring systems and S_{LP} are strongly coupled to one another. Due to the lack of a second linker, a single conductance pathway

exists in **P1**, which closely resembles that of the secondary path found in **PM1**, leading to conducting junctions, despite lacking in the mechanical stability provided by a second linker. This MO interpretation helps to identify relationships linking the intrinsic properties of the bridging molecule with the conductance mechanism and overall device performance. Further studies that include the mapping of the density of states and couplings of the Au electrodes are beyond the scope of this study. Our theoretical results agree with our experimental findings and give weight to a dominant secondary pathway in **PM1** that is similar to that found in **P1**.

5.5. Conclusion

The mechanism of conductance through mono-functionalized single-molecule wires was determined by measuring the electrical and mechanical properties in single-molecule junctions. By using a combination of rational molecular design, STM- and AFM-BJ techniques, we showed that mono and difunctionalized molecular wires conduct through the backbone of a single molecule rather than though π-π-stacked dimers. The conductance mechanism differs between the *para-para* bound (**PPn**) and *para*-π bound molecules (**Pn**, **P1A** and **P1TA**). Since the **Pn** series is functionalized with only one linker, a mechanically weak, yet electronically coupled, Au-π interaction completes the molecular circuit. The limited strength of this new interaction causes significant variability in junction-to-junction conductance. However, installing a second linker at the *meta* position stabilizes this interaction by securing the terminal phenyl group to the electrode surface, such as for the *para-meta* compounds (**PMn** and **PM1A**). *Meta* linkers result in quantum electronic interference effects, but the position of the linkers (*meta* vs.

para) does not significantly alter their mechanical attachment to the Au electrodes. By exploiting this attribute we strengthen a direct molecule-metal interaction that dominates in the charge transport of mono-functionalized molecular junctions, in turn enabling us to quantify the charge transport properties arising from Au-π interactions. This strategy may prove useful in future molecular-scale device architectures for the positioning of molecules onto electrode surfaces while mediating their electronic couplings, such as is needed for advancement in single-molecule rectification.[21]

5.6. References and Footnotes

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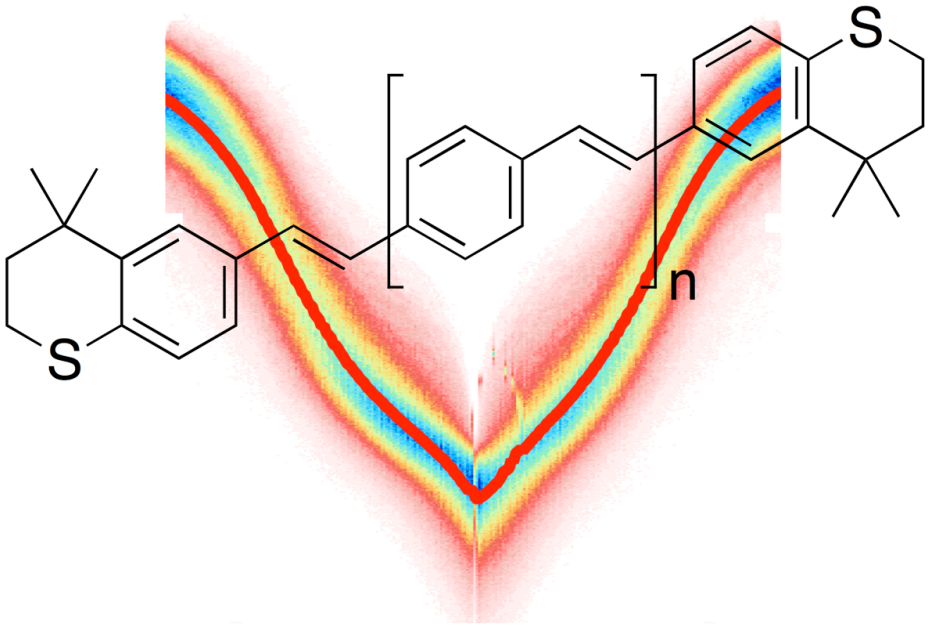
Chapter 6. Promising Molecular Wires for Current-Voltage Measurements of Molecular Junctions

In this chapter, molecules were synthesized by myself, while the physical investigations were preformed by Eek Huisman and Jonathan Widawsky. Pierre Darancet is responsible for modeling and calculations. Other DFT calculations were run by Michael Steigerwald and myself.



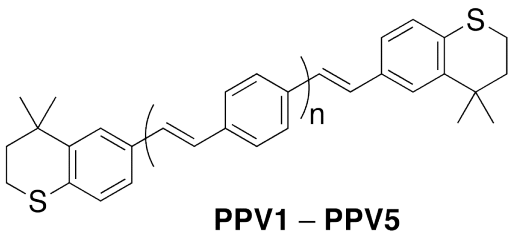
6.1. Background and Motivation

The electronic properties of molecular junctions have been studied using a variety of linear chemical structures and it is commonly found for organic molecules that the through-molecule current decays exponentially as the length of the molecules increase.[1] This decrease is a result of the longer tunneling barriers in the molecules of increased

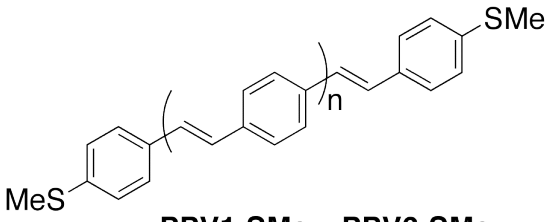
length. The other parameters that govern zero-bias conductance in the Landauer-Büttiker model,[2] are the energy of the conducting orbitals and their coupling to the metal electrodes.[3] In fact, it is often found that a single molecular orbital dominates the charge transport properties.[4] The molecular level broadens, due to its interaction with the electrodes, resulting in a finite conductance at the Fermi energy. However, the relationship between broadening and conductance decay as the molecular length is systemically changed is not well understood.

In this chapter, we outline the synthesis of two families of conjugated molecules that show promise for understanding the current-voltage (IV) characteristics of single-molecule junctions, which may aid in understanding the relationship between junction conductance and molecular level broadening. A series of symmetric molecules, oligo(p-phenylenevinylene)[5] (PPV) derivatives (Figure 6.1A), as well as a series of asymmetric oligoene derivatives (Figure 6.1C) are prepared and range in length from 1.2 to 4.0 nm. Their prototypical molecular wire structures are linear and fully conjugated. We believe these molecules to have promising current-voltage (IV) characteristics.

(A) Oligo(p-phenylenevinylene) (**PPVn**) Derivatives

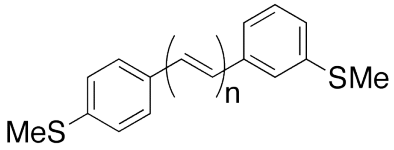


PPV1 – **PPV5**



PPV1-SMe – **PPV6-SMe**

(B) Asymmetric 3,4-Methylthio-diphenyl-0ligoenes



DPO1 – **DPO5**

Figure 6.1: Two different families of oligo(p-phenylenevinylene) derivatives, the **PPVn** series was synthesized while the **PPVn-SMe** derivatives comprise our theoretical control group. Asymmetric oligoene were synthesized from the stilbene to the diphenyl pentene and are end-functionalized with one *meta*- and one *para*-methylsulfide linker group.

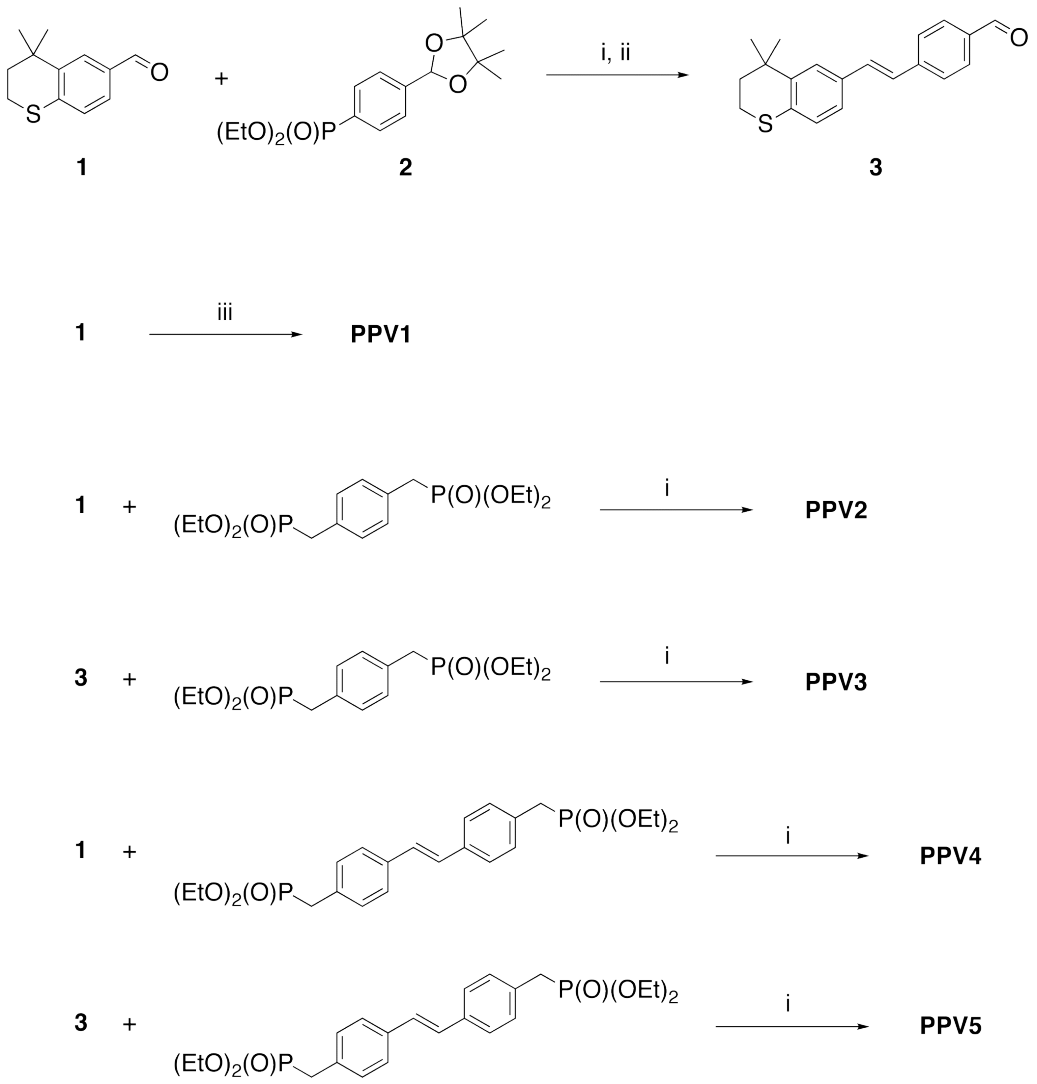
6.2. PPV Molecular Wire Design

A series of five PPV molecular wires (**PPV1**-**PPV5**, Figure 6.1A) and studied their charge transport characteristics using the scanning tunneling microscopy (STM) break-junction technique.[6,7] The molecular wires are terminated with alkylsulfide linker groups, which bind to the electrodes through the formation of a donor-acceptor bond between the sulfur lone pairs and under-coordinated Au surface atoms. Alkylsulfide linkers are embedded inside a six-membered ring locking the orientation of the sulfur lone pair with respect to the π-system.[8] The two protruding methyl groups added to this ring simplify the synthesis[9] as well as endows these otherwise unfunctionalized PPV's with superior solubility by disrupting intermolecular π-π stacking interactions; without these specially designed end-groups **PPVn** molecules, where n > 2 are too insoluble to measure using our STM-BJ method.

6.3. Synthesis of PPV Molecular Wires

Shown in Scheme 6.1A, each member of the **PPVn** series was synthesized in one step from the end-functionalized benzaldehyde (**1**; see also Ch. 1 and Appendix A) or extended (*E*)-4-styrylbenzaldehyde (**3**). Compound **3** is also prepared from compound **1** through Hörner-Wadsworth-Emmons (H.W.E.)[10] chemistry from the acetal-protected phosphonate (**2)**. The smallest homologue, **PPV1**, was synthesized by McMurray coupling[11] from two molar equivalents of **1**. Similarly, **PPV2** and **PPV4** were also prepared from two molar equivalents of **1,** however through H.W.E. conditions with the appropriate bisphosphonate. Using the same conditions, the longer odd-numbered oligomers, **PPV3** and **PPV5**, were obtained from compound **2**. Each compound was

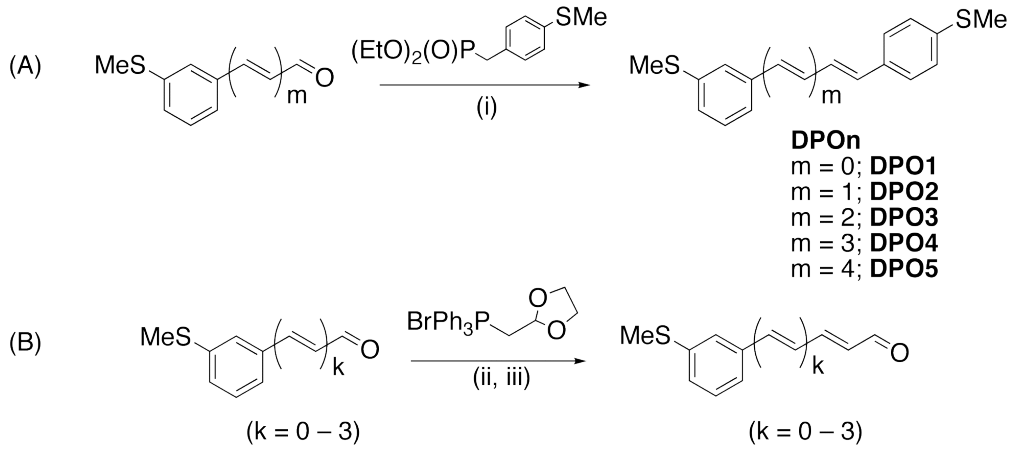
characterized by mass spectrometry, and UV-vis absorption spectroscopy, ^{1}H- and ^{13}C-, as well as ^{31}P-NMR (when applicable).



Scheme 6.1: Synthetic route to end-functionalized oligo(p-phenylenevinylene) molecular wires (**PPVn**). (i) H.W.E. reaction: tBuOK, THF, 0° C to 25° C, 16 h; (ii) conc. HCl, THF, 25° C, 3 h; (iii) McMurray coupling: Zn powder, $TiCl_4$, THF, reflux, 16 h. Cyclic thioethers are more soluble than the MeS-terminated analogues due to the disruption of intermolecular attractive forces by distal out-of-plane methyl groups. For a comparison, **PPV5** and the smaller methylthio derivative, 1,4-bis(4-(4-(methylthio)styryl)styryl)-benzene (**PPV2-SMe**), have comparable solubilities in chlorinated organic solvents.

6.4. Synthesis of Asymmetric Oligoene Wires

A family of oligoene rectifier candidates baring one *meta*- and one *para*-methylsulfide linker were prepared from the appropriate oligoenals and dimethyl 4-(methylthio)benzylphosphonate through a Hoerner-Wadsorth-Emmons olefination using potassium *tert*-butoxide as a base. Oligoenals were extended through iterative Wittig homologation cycles (see Chapter 2) starting from 3-(methylthio)benzaldehyde.



Scheme 7.1: Synthetic route to asymmetric oligoene rectifier candidates. (i) Hoerner-Wadsworth-Emmons reaction: tBuOK, THF, 0˚ to 25˚ C over 12 h; (ii) Wittig Homologation reaction: LiOMe, THF, reflux, 16 h; (iii) Acidolylsis: 10% aq. HCl, THF, 60 min.

6.5. STM-break Junctions

We plan to carry out STM-BJ experiments to measure the conductance as a function of voltage of these oligomers. This procedure is similar to that described in the

previous chapters. For each experiment on PPV molecules a point-contact between a gold tip and substrate will be broken repeatedly (typically 5000 times) in a dilute molecular solution in 1,2,4-trichlorobenzene. The conductance of our PPV molecules was found to be concentration dependent. Because of this we measured them at the lower limit of concentration (10 μM); below this concentration the formation of molecular junctions was not observed. Conductance (current/voltage) traces are recorded while the tip is retracted with a constant speed of 16 nm/s over a distance of 5-8 nm at a bias of 250-700 mV.

6.6. Theoretical Methods

To determine the molecular length and HOMO-LUMO energy gaps of the **PPVn** series, electronic structure calculations[12] using the B3LYP hybrid functional and the 6-31G** basis sets. Besides the **PPVn** series, we also ran calculations of their *para*-methylthio analogues (**MeS-PPVn**) as a reference. The geometries of both series were fully optimized. The final geometries, total energies, bond distances, bond angles and torsional angles may be found in the Appendix D. Below in Table 6.1 is a summary of the HOMO-LUMO energy differences (band gap) results of our calculations on our **PPVn** series (from n = 1 to 5) and our reference molecules (**MeS-PPVn**; n = 1 to 6). As expected, molecular band gaps converge as oligomer length (n) increases (Figure 6.2). Previous experimental studies on oligo(p-phenylenevinylene) compounds have predicted the saturation of the electronic properties at oligomeric lengths of $n \approx 10$.[13,14] Geometry optimizations of the longer **PPVn** molecules (**PPV3**, **PPV4** and **PPV5**) were found to

converge on a distribution of geometries, all of which were energetically similar. The geometries differed from each other by small degrees of twists and bends along the conjugated backbone. Incorporation of even the smallest distortions gave large variations in the molecular length (i.e. S-S distance). **MeS-PPVn** molecules, however, converged on reliable linear geometries, which are expected for fully elongated break junction. In such cases, sulfur-to-sulfur (S-S) distances were taken from the **MeS-PPVn** calculations and not from those of the **PPVn** molecules.

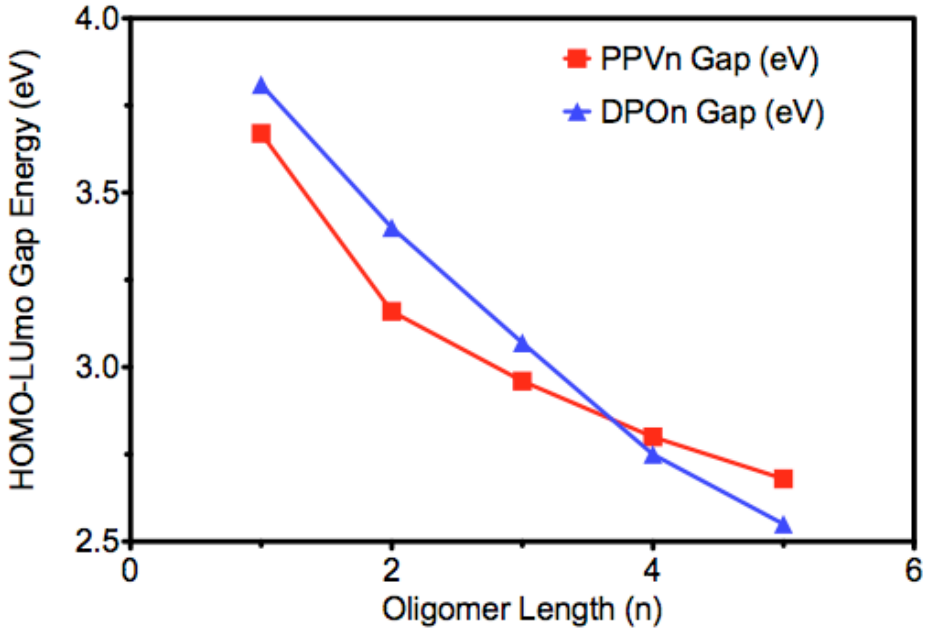


Figure 6.2: DFT estimations of the molecular band gap of **PPVn** and asymmetric **DPOn** series.

PPVn	S-S Length[b] (nm)	HOMO (eV)	LUMO (eV)	HOMO-LUMO gap
PPV1	1.30	-4.90	-1.23	3.67
PPV2	1.97	-4.84	-1.68	3.16
PPV3[a]	2.65[a]	-4.82	-1.86	2.96
PPV4[a]	3.31[a]	-4.86	-2.06	2.80
PPV5[a]	3.99[a]	-4.79	-2.11	2.68
DPOn				
DPO1	1.20	-5.22	-1.41	3.81
DPO2	1.42	-5.06	-1.66	3.40
DPO3	1.70	-4.93	-1.86	3.07
DPO4	1.95	-4.70	-1.95	2.75
DPO5	2.17	-4.62	-2.07	2.55

Table 6.1: DFT calculation results on **PPVn** and **DPOn** series. [a]Due to unreliable convergence in the geometry optimization, sulfur-to-sulfur (S-S) distances for the longer oligomers, **PPV3-PPV5**, were estimated from DFT calculations performed on the model series **MeS-PPV** (see Appendix E). [b]Through-space sulfur-to-sulfur distance.

6.7. Conclusions and Future Outlook

A set of oligo(p-phenylenevinylene) oligomers (**PPVn**) was end-functionalized with cyclic alkylsulfides making them soluble for STM-BJ studies. This is a work in progress and we are currently investigating the single-molecule conductance and IV curves for **PPVn** molecular junctions. Future studies include modeling the electronic properties (i.e. the IV and transmission characteristics) of **PPVn** junctions in greater detail.

The asymmetric end-functionalization of oligoene molecular wires (**DPOn**) is also a significant achievement since they may lead to large rectification ratios[15] as a result of asymmetric electronic coupling between the electrodes and molecule. As gap energies decrease (molecular length increases) more asymmetric transmission profiles may be accessed in the scanned bias window, resulting in asymmetric IV properties. We are currently investigating the IV characteristics of the single-molecule junctions of these molecules.

Molecular rectification[16] is definitely one of the basic steps toward controlling molecular electronics, since electronic components are essential in the construction of logic switches. Such rectifiers are rare due to the difficulties in building and orienting them between electrical leads. Additionally, contact asymmetry can be adapted to molecules outside of oligoenes. It is also compatible with other molecular rectification strategies such as those employed in donor-acceptor designs and may aid in the generation of high-performance single-molecule rectifiers in the future.

6.8. References and Footnotes

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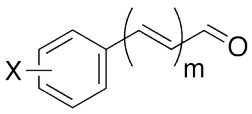
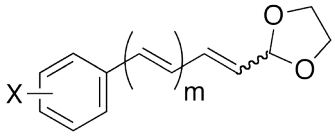
Appendix A (Part 1)

A1. List of Compounds

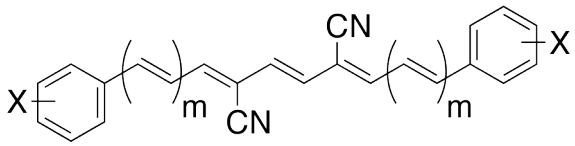


X	m	Molecule
H	2	**1a**
H	3	**1b**
H	4	**1c**
H	5	**1d**
4-SMe	1	**2a**
4-SMe	2	**2b**
4-SMe	3	**2c**4
4-SMe	4	**2d**
4-SC_4H_8	0	**3a**
4-SC_4H_8	1	**3b**
4-SC_4H_8	2	**3c**
4-SC_4H_8	3	**3d**
4-SC_4H_8	4	**3e**
4-SC_5H_{10}	0	**4a**
4-SC_5H_{10}	1	**4b**
4-SC_5H_{10}	2	**4c**
4-SC_5H_{10}	3	**4d**
4-SC_5H_{10}	4	**4e**
4-SC_5H_{10}	5	**4f**
4-Me_2N	2	**5a**
4-Ph_2N	1	**6a**
4-Br	1	**7a**
4-Br	2	**7b**
4-Br	3	**7c**
4-CO_2H	0	**8a**
4-CO_2H	1	**8b**



X	m	E/Z	Molecule
H	2	*E*	***E*-1e**
H	2	*Z*	***Z*-1e**
Br	1	*E*	***E*-7d**
Br	1	*Z*	***Z*-7d**
Br	2	*E*	***E*-7e**
Br	2	*Z*	***Z*-7e**

4-CO_2H	2	**8c**
4-CO_2Et	0	**9a**
4-CO_2Et	1	**9b**
4-CO_2Et	2	**9c**
3,5-OC_6H_{13}	0	**10a**
3,5-OC_6H_{13}	1	**10b**
3,5-OC_6H_{13}	2	**10c**
3,5-$OC_{10}H_{21}$	0	**11a**
3,5-$OC_{10}H_{21}$	1	**11b**
3,5-$OC_{10}H_{21}$	2	**11c**
3,5-$OC_{14}H_{29}$	0	**12a**
3,5-$OC_{14}H_{29}$	1	**12b**
4-C≡C-C_6H_{13}	0	**13a**
4-C≡C-C_6H_{13}	1	**13b**
4-C≡C-C_6H_{13}	2	**13c**
4-CN	1	**14a**



DPDCn-X

X	**m**	**Total n**	**Molecule**
H	0	3	**DPDC3**
H	1	5	**DPDC5**
H	2	7	**DPDC7**
H	3	9	**DPDC9**
H	4	11	**DPDC11**
H	5	13	**DPDC13**
4-SMe	0	3	**DPDC3-SMe**
4-SMe	1	5	**DPDC5-SMe**
4-SMe	2	7	**DPDC7-SMe**
4-SMe	3	9	**DPDC9-SMe**
4-SMe	4	11	**DPDC11-SMe**
4-SC_4H_8	0	3	**DPDC3-SC_4H_8**

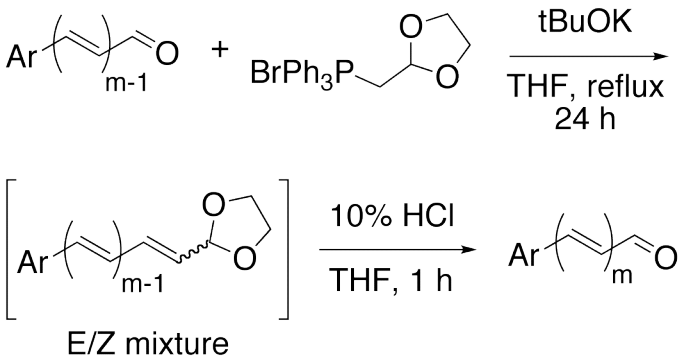
4-SC_4H_8	1	5	**DPDC5-SC_4H_8**
4-SC_4H_8	2	7	**DPDC7-SC_4H_8**
4-SC_4H_8	3	9	**DPDC9-SC_4H_8**
4-SC_4H_8	4	11	**DPDC11-SC_4H_8**
4-SC_5H_{10}	0	3	**DPDC3-SC_5H_{10}**
4-SC_5H_{10}	1	5	**DPDC5-SC_5H_{10}**
4-SC_5H_{10}	2	7	**DPDC7-SC_5H_{10}**
4-SC_5H_{10}	3	9	**DPDC9-SC_5H_{10}**
4-SC_5H_{10}	4	11	**DPDC11-SC_5H_{10}**
4-SC_5H_{10}	5	13	**DPDC13-SC_5H_{10}**
4-Me_2N	0	3	**DPDC3-NMe_2**
4-Me_2N	1	5	**DPDC5-NMe_2**
4-Me_2N	2	7	**DPDC7-NMe_2**
4-Ph_2N	0	3	**DPDC3-NPh_2**
4-Ph_2N	1	5	**DPDC5-NPh_2**
4-Br	0	3	**DPDC3-Br**
4-Br	1	5	**DPDC5-Br**
4-Br	2	7	**DPDC7-Br**
4-Br	3	9	**DPDC9-Br**
4-CO_2H	0	3	**DPDC3-CO_2H**
4-CO_2H	1	5	**DPDC5-CO_2H**
4-CO_2H	2	7	**DPDC7-CO_2H**
4-CO_2Et	0	3	**DPDC3-CO_2Et**
4-CO_2Et	1	5	**DPDC5-CO_2Et**
4-CO_2Et	2	7	**DPDC7-CO_2Et**
3,5-OC_6H_{13}	0	3	**DPDC3-OC_6H_{13}**
3,5-OC_6H_{13}	1	5	**DPDC5-OC_6H_{13}**
3,5-OC_6H_{13}	2	7	**DPDC7-OC_6H_{13}**
3,5-$OC_{10}H_{21}$	0	3	**DPDC3-$OC_{10}H_{21}$**
3,5-$OC_{10}H_{21}$	1	5	**DPDC5-$OC_{10}H_{21}$**
3,5-$OC_{10}H_{21}$	2	7	**DPDC7-$OC_{10}H_{21}$**
3,5-$OC_{14}H_{29}$	0	3	**DPDC3-$OC_{14}H_{29}$**
3,5-$OC_{14}H_{29}$	1	5	**DPDC5-$OC_{14}H_{29}$**
4-C≡C-C_6H_{13}	0	3	**DPDC3-C_8H_{13}**
4-C≡C-C_6H_{13}	1	5	**DPDC5-C_8H_{13}**

4-C≡C-C_6H_{13}	2	7	**DPDC7-C_8H_{13}**
4-CN	0	3	**DPDC3-CN**
4-CN	1	5	**DPDC5-CN**
2-Br	0	3	***ortho*-DPDC3-Br**
3-Br	0	3	***meta*-DPDC3-Br**
2-OMe	0	3	***ortho*-DPDC3-OMe**
3-OMe	0	3	***meta*-DPDC3-OMe**
4-OMe	0	3	**DPDC3-OMe**
3-NO_2	0	3	***meta*-DPDC3-NO_2**
4-NO_2	0	3	**DPDC3-NO_2**
4-NO2	0	5	**DPDC5-NO_2**
4-F	0	5	**DPDC5-NO_2**

A2. Synthetic Details

General Information:

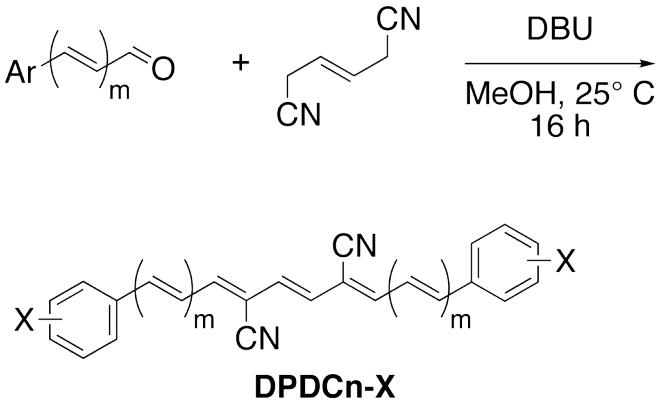
(1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide was purchased from TCI America and stored in a desiccator. Benzaldehyde, 4-bromobenzaldehyde, 3-bromobenzaldehyde, 2-bromobenzaldehyde, 4-methoxybenzaldehyde, 3-methoxybenzaldehyde, 2-methoxybenzaldehyde, 4-(methylthio)-benzaldehyde, 4-(dimethylamino)-benzaldehyde, 4-formal benzoic acid, 4-fluorobenzaldehyde, 4-nitrobenzaldehyde, 3-nitrobenzaldehyde, 4-cyanobenzaldehyde, *trans*-cinnamaldehyde, trans-(4-dimethylamino)cinnamaldehyde and trans-(4-nitro)cinnamaldehyde, 1,4-dicyano-2-butene, 1,2-epoxy-2-methylpropane, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), 3,3-dimethylallyl bromide and all other reagents were purchased from Sigma-Aldrich Chemical. Alkoxybenzaldehydes,[1] α,ω-diphenyl-oligoenes (**DPOn**) and α,ω-(4-dimethylamino)phenyl-deca-pentaene[2] (**DPO-NMe$_2$**) were synthesized according to the literature. All reactions were carried out under nitrogen unless otherwise noted. All chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica columns. ^{1}H and ^{13}C NMRs were recorded on a Bruker DRX300 (300MHz), DRX400 (400MHz) or Bruker DMX500 (500MHz). In general, mass spectrometry for the oligoenes was difficult to interpret. ^{1}H and ^{13}C NMR spectra for the compounds prepared here are contained at the end of the Supporting Information.



General Procedure for Wittig Homologation of Aldehydes: As an example, lithium methoxide (0.149 g, 3.93 mmol, 2.6 eq.) was added to a stirring solution of (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide (1.62 g, 3.78 mmol, 2.5 eq.) in 50 mL of anhydrous tetrahydrofuran (THF) in a 100-mL round-bottom flask. The suspension was heated to reflux stirred for 30 minutes, changing color from off-white to light orange/pink. *trans*-cinnamaldehyde (0.200 g, 1.51 mmol, 1.0 eq.) in 20 mL of dry THF solution was added dropwise over 30-60 min. The suspension was refluxed for 24 h. The reaction suspension was then cooled to room temperature, at which point 10% aqueous hydrochloric acid (HCl) was added. Stirring was continued for 1 hour in order to hydrolyze the intermediate acetals (mixture of *E*- and *Z*-stereoisomers) to the all-*trans* configuration. The organic layer was extracted with CH_2Cl_2 (25 mL x3) and the combined fractions were washed with water, sat. aqueous sodium bicarbonate solution and brine, and then dried over $MgSO_4$. Solvent was removed by rotary evaporation and the product was purified via column chromatography using an eluent gradient from 0% to 10% ethyl acetate in hexanes over 25 column volumes. The product, in this case (2*E*,4*E*)-5-phenylpenta-2,4-dienal, was obtained in 92% yield (0.199 g) as a yellow oil. This reaction was typically carried out on 0.200 g of starting aldehyde for quick work up and

separation, but can easily be scaled up to multi-gram quantities. We have attempted this reaction on a 5.00 g scale without significant loss in yield (~3.7%).

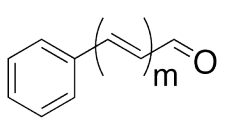
Alternatively, the (*E*)- and (*Z*)-acetals may be isolated by column chromatography. As in the reaction above, *trans*-cinnamaldehyde is reacted with the triphenylphosphonium salt. After refluxing for 24 h the reaction was cooled to room temperature, diluted with water, extracted with CH_2Cl_2 (3x) and dried over $MgSO_4$. The organic solvent was removed by rotary evaporation. The (*E*)- and (*Z*)--diene-acetals were isolated by column chromatography 5% ethyl acetate in hexanes (Rf_E/Rf_Z = 0.2/0.1) in 16.6% and 70.8%, respectively. (*Z*)-isomer is produced in 14:3 ratio compared with the (*E*)-isomer. When 10% aq. HCl solution is added to a solution of either stereoisomer or a mixture of isomers only the *E*-enal, the desired product, is obtained (see ^1H and ^{13}C NMR for compound **1a**). In the route to most DPDC's we did not isolate the intermediate acetals. In few circumstances it was synthetically necessary to isolate these acetals in order to synthesize the carboxylic acid polyenals for our **DPDCn-CO_2H** series (see **7e** and **7d**).



DPDCn-X

General Procedure for Double Knoevenagel Condensation: The appropriate oligoenal (150 mg) and 1,4-dicyano-2-butene (0.75 eq.) were dissolved in wet methanol (25-50 mL) in a 100-mL round-bottomed flask (anhydrous solvents do not effect isolated yield). In some cases, the aryl-oligoenals were insoluble in methanol and a methanol/tetrahydrofuran mixture was used instead. The flask was sealed with a rubber septum and purged by bubbling nitrogen through the reaction solution for 10 minutes. 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU; 1.0 eq.) were added via syringe and the solution was left stirring for 16 hours, over which the product usually precipitated out. The crude product was filtered off and washed with methanol and then purified either by recrystallization from dichloromethane/methanol or by flash column chromatography using dichloromethane/hexanes (1:1) as eluent. To test whether this procedure was scalable we prepared **DPDC5** on gram quantities without a significant loss in yield (~4%).

Synthetic Experimentals and Characterization:



1a; m = 2
1b; m = 3
1c; m = 4
1d; m = 5

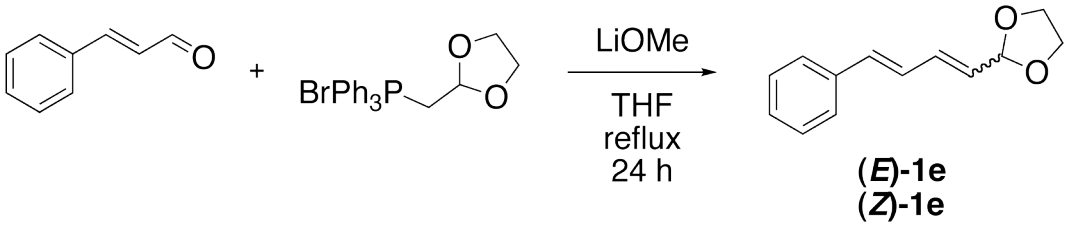
(2E,4E)-5-phenylpenta-2,4-dienal (**1a**; m = 2): General Wittig homologation procedure. The product was prepared from *trans*-cinnamaldehyde and isolated as a yellow oil in 92.0% yield. This compound is known and agrees with spectroscopic data in literature.[3] ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.63 (d, *J* = 8.1 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.34 (m, 4H), 7.07-7.10 (m, 2H), 6.30 (dd, *J* = 7.9 Hz, 15.2 Hz, 1H); ^{13}C NMR (400 MHz, CD_2Cl_2): δ 194.1, 152.6, 142.9, 136.0, 132.0, 130.1, 129.4, 128.0, 126.6.

(2E,4E,6E)-7-phenylhepta-2,4,6-trienal (**1b**; m = 3): General Wittig homologation procedure. The product was prepared from **1a** and isolated as a dark yellow solid in 88.0% yield. This compound is known and agrees with spectrocopic data in literature.[4,5] ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.40-7.28 (m, 3H), 7.23 (dd, *J* = 11.6 Hz, 15.2 Hz, 1H), 6.96-6.86 (m, 3H), 6.61 (dd, *J* = 11.2 Hz, 14.0 Hz, 1H), 6.22 (dd, *J* = 8.0 Hz, 15.2 Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 193.45, 151.67, 142.71, 138.34, 136.36, 131.23, 130.15, 128.85, 128.83, 127.72, 127.02.

(2E,4E,6E,8E)-9-phenylnona-2,4,6,8-tetraenal (**1c**; m = 4): General Wittig homologation procedure. The product was prepared from **1b** and isolated as an orange solid in 70.0% yield. This compound is known and agrees with spectroscopic data in literature.[4,5] ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.59 (d, *J* = 8.1 Hz, 1H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.37-7.24

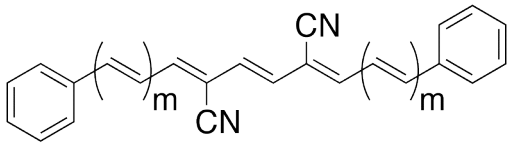
(m, 3H), 7.17 (dd, *J* = 11.4 Hz, 15.0 Hz, 1H), 6.90 (dd, *J* = 10.8 Hz, 15.3 Hz, 1H), 6.82-6.42 (m, 5H), 6.19 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.45, 151.72, 142.61, 138.93, 136.76, 136.06, 131.86, 131.02, 129.98, 128.78, 128.36, 128.35, 126.77.

(2E,4E,6E,8E,10E)-11-phenylundeca-2,4,6,8,10-pentaenal (**1d**; m = 5): General Wittig homologation procedure. The product was prepared from **1c** and isolated as a dark orange solid in 55.0% yield. This compound is known and agrees with spectroscopic data in literature.[4,6] ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.61 (d, *J* = 7.2 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 8.1 Hz, 2H), 7.27 (t, *J* = 6.5 Hz, 1H), 7.18 (dd, *J* = 11.2 Hz, 15.1 Hz, 1H), 6.90 (dd, *J* = 10.8 Hz, 15.4 Hz, 1H), 6.77 (dd, *J* = 11.4 Hz, 14.6 Hz, 1H), 6.68 (d, *J* = 15.6 Hz, 1H), 6.64-6.30 (m, 5H), 6.18 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.44, 151.72, 142.67, 138.83, 137.00, 136.76, 134.78, 132.63, 131.75, 130.92, 129.93, 128.73, 128.71, 128.05, 126.61.



2-((1E,3E)-4-phenylbuta-1,3-dienyl)-1,3-dioxolane (***E*-1e**) and *2-((1Z,3E)-4-phenylbuta-1,3-dienyl)-1,3-dioxolane* (***Z*-1e**): Using the modified general Wittig homologation procedure outlined above (pp. S6-S7) The (*E*)- and (*Z*)-products were prepared from *trans*-cinnamaldehyde and isolated by column chromatography 5% ethyl acetate in

hexanes (Rf_E/Rf_Z = 0.2/0.1) in 16.6% and 70.8% yield, respectively. The (*Z*)-isomer is selectively formed in a 14:3 ratio compared with the (*E*)-isomer. ***E*-1e** was isolated as a pale yellow oil in 16.6% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 6.79 (dd, *J* = 11.6 Hz, 15.2 Hz, 1H), 6.62 (d, *J* = 15.7 Hz, 1H), 6.52 (dd, *J* = 15.5 Hz, 10.6 Hz, 1H), 5.75 (dd, *J* = 15.5 Hz, 4.9 Hz, 1H), 4.90 (dd, *J* = 4.9 Hz, 0.7 Hz, 1H), 3.35 (s, 4H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 137.0, 134.7, 133.9, 129.4, 128.6, 127.8, 127.7, 126.5, 102.6, 52.6. ***Z*-1e** was isolated as a pale yellow oil in 70.8% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.42 (d, *J* = 7.4 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.14 (ddd, *J* = 15.5 Hz, 11.3 Hz, 0.9 Hz, 1H), 6.60 (d, *J* = 15.6 Hz, 1H), 6.34 (t, *J* = 11.2 Hz, 1H), 5.48 (dd, *J* = 11.1 Hz, 5.9 Hz, 1H), 5.32 (dd, *J* = 5.9 Hz, 1.2 Hz, 1H), 3.34 (s, 4H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 136.9, 135.5, 132.5, 128.7, 128.1, 127.4, 126.7, 123.9, 99.8, 52.2.



DPDCn; m = 0, 1, 2, 3, 4, 5

(1Z,3E,5Z)-2,5-dicyano-1,6-diphenyl-hexa-1,3,5-triene (**DPDC3**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from benzaldehyde and isolated as a yellow crystalline solid in 55.0% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 7.87-7.84 (m, 4H), 7.47 (m, 6H), 7.22 (s, 2H), 6.87 (s, 2H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): δ 145.60, 133.12, 131.07, 130.08, 129.29, 129.02, 116.02, 109.31.

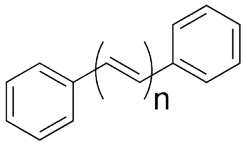
(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-diphenyl-deca-1,3,5,7,9-pentaene (**DPDC5**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from *trans*-cinnamaldehyde and isolated as an orange crystalline solid in 60.1% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 7.59 (d, J = 6.6 Hz, 4H), 7.44-7.28 (m, 8H), 7.08-7.01 (m, 4H), 6.76 (s, 2H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): δ 145.0, 142.0, 135.6, 129.7, 129.0, 128.8, 127.5, 124.7, 114.8, 111.9.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-diphenyl-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7**; m = 2): General double Knoevenagel condensation procedure was run at 55° C. The product was prepared from **1a** and isolated as a red solid in 53.8% yield. ^{1}H NMR (400 MHz, 350 K, DMSO-d_6): δ 7.59 (d, J = 7.6 Hz, 4H), 7.44-7.30 (m, 8H), 7.24 (dd, J = 10.8 Hz, 15.6 Hz, 2H), 7.04-6.95 (m, 4H), 6.84 (dd, J = 11.6 Hz, 14.0 Hz, 2H), 6.75 (s, 2H); ^{13}C NMR (300 MHz, 370 K, DMSO-d_6): δ 146.22, 143.44, 138.76, 137.06, 129.23, 129.18, 129.16, 129.13, 127.59, 115.49, 111.03.

(1E,3E,5E,7Z,9E,11Z,13E,15E,17E)-8,11-dicyano-1,18-diphenyl-octadeca-1,3,5,7,9,11,13,15,17-nonaene (**DPDC9**; m = 3): General double Knoevenagel condensation procedure was run at 55° C. The product was prepared from **1b** and isolated as a dark purple solid in 45.4% yield. ^{1}H NMR (400 MHz, 350 K, DMSO-d_6): δ 7.53 (d, J = 7.6 Hz, 4H), 7.39-7.27 (m, 8H), 7.10-6.68 (m, 14H); ^{13}C NMR (300 MHz, 380 K, DMSO-d_6): δ 146.25, 143.50, 140.26, 140.00, 137.79, 136.63, 133.42, 129.81, 129.53, 129.27, 128.98, 127.58, 115.86, 111.27.

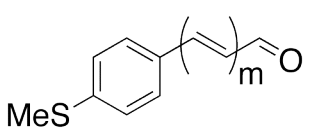
(1E,3E,5E,7E,9Z,11E,13Z,15E,17E,19E,21E)-10,13-dicyano-1,22-diphenyl-docosa-1,3,5,7,9,11,13,15,17,19,21-undecaene (**DPDC11**; m = 4): General double Knoevenagel condensation procedure was run at 55° C. The product was prepared from **1c** and isolated as a lustrous dark purple-black solid in 40.4% yield. ^{1}H NMR (400 MHz, 350 K, $C_2H_2Cl_4$): δ 7.47 (d, J = 7.6 Hz, 4H), 7.37 (t, J = 7.2 Hz, 4H), 7.28 (t, J = 7.2 Hz, 2H), 6.95-6.47 (m, 20H); ^{13}C NMR (400 MHz, 350 K, $C_2D_2Cl_4$): δ 144.0, 141.6, 136.6, 136.4, 134.4, 132.3, 131.7, 128.6, 128.4, 128.2, 127.5, 126.1; due to insolubility four carbon signals were not observed (see crystal structure in supporting information).

(1E,3E,5E,7E,9E,11Z,13E,15Z,17E,19E,21E,23E,25E)-12,15-dicyano-1,26-diphenyl-hexacosa-1,3,5,7,9,11,13,15,17,19,21,23,25-tridecaene (**DPDC13**; m = 5): General double Knoevenagel condensation procedure was run at 55° C. The product was prepared from **1d** and isolated as a lustrous dark black solid in 10.0% yield; ^{1}H and ^{13}H NMR data unavailable due to insolubility (see crystal structure in supporting information).



DPOn; n = 3, 5, 7

(1E,3E,5E)-1,6-diphenyl-hexa-1,3,5-triene (**DPO3**; n = 3), *(1E,3E,5E,7E,9E)-1,10-diphenyl-deca-1,3,5,7,9-pentaene* (**DPO5**; n = 5), and *(1E,3E,5E,7E,9E,11E,13E)-1,14-diphenyl-tetradeca-1,3,5,7,9,11,13-heptaene* (**DPO7**; n = 7) were prepared according to the procedure reported by Spangler and coworkers.[2] Longer **DPOn** molecules, where n > 7, were insoluble and difficult to characterize.



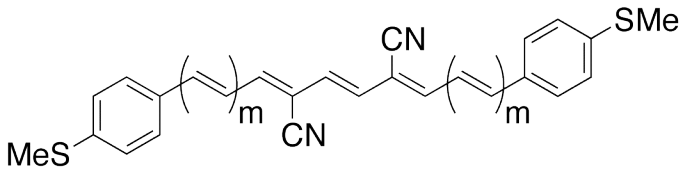
2a; m = 1
2b; m = 2
2c; m = 3
2d; m = 4

trans-4-(methylthio)cinnamaldehyde (**2a**; m = 1): General Wittig homologation procedure. The product was prepared from (4-methylthio)benzaldehyde and isolated as a pale yellow oil in 96.0% yield. The molecule is known, however specific characterizations have not been reported.**Error! Bookmark not defined.**,[7] ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.70 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 16.0 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 6.69 (dd, *J* = 7.6 Hz, 15.6 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.9, 152.2, 144.0, 130.8, 129.2, 128.0, 126.3, 15.4.

(2E,4E)-5-(4-(methylthio)phenyl)penta-2,4-dienal (**2b**; m = 2): General Wittig homologation procedure. The product was prepared from **2a** and isolated as a yellow solid in 99.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.62 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.26 (m, 3H), 6.95 (m, 2H), 6.27 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.8, 152.1, 143.2, 140.3, 138.1, 131.4, 130.2, 127.7, 127.4, 126.8, 15.8.

(2E,4E,6E)-7-(4-(methylthio)phenyl)hepta-2,4,6-trienal (**2c**; m = 3): General Wittig homologation procedure. The product was prepared from **2b** and isolated as an orange solid in 73.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.60 (d, *J* = 8.1 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.19 (m, 3H), 6.83 (m, 3H), 6.55 (dd, *J* = 11.1 Hz, 15.3 Hz, 1H), 6.19 (dd, *J* = 8.1 Hz, 15.3 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.48, 151.78, 142.83, 139.88, 137.78, 133.10, 131.05, 129.85, 127.37, 127.01, 126.35, 15.45.

(2E,4E,6E,8E)-9-(4-(methylthio)phenyl)nona-2,4,6,8-tetraenal (**2d**; m = 4): General Wittig homologation procedure. The product was prepared from **2c** and isolated as an orange-red solid in 70.0% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.16 (dd, *J* = 12.0 Hz, 15.9 Hz, 1H), 6.84 (dd, *J* = 10.8 Hz, 15.4 Hz, 1H), 6.76 (dd, *J* = 11.2 Hz, 14.5 Hz, 1H), 6.70-6.58 (m, 2H), 6.47 (m, 2H), 6.17 (dd, *J* = 7.9 Hz, 15.1 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (300 MHz, $CDCl_3$), 400 MHz: δ 193.9, 152.2, 143.1, 139.4, 135.9, 134.6, 134.0, 132.0, 131.3, 130.3, 128.1, 127.5, 126.9, 16.0.



DPDCn-SMe; m = 0, 1, 2, 3, 4

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(methylthio)phenyl)-hexa-1,3,5-triene (**DPDC3-SMe**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from (4-methylthio)benzaldehyde and isolated as a lemon yellow solid in 70.0% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_3$): δ 7.78 (d, *J* = 8.3 Hz, 4H), 7.34 (d, *J* = 8.3 Hz, 4H), 7.18 (s, 2H), 6.86 (s, 2H), 2.58 (s, 6H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): δ 144.3, 143.3, 129.9, 129.8, 129.5, 126.1, 116.0, 108.5, 15.0.

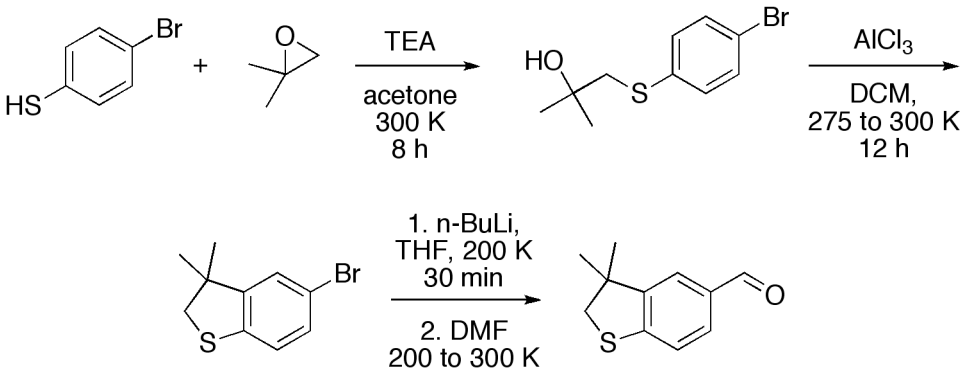
(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(methylthio)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-SMe**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **2a** and isolated as a red solid in 45.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.4 Hz, 4H), 7.26-7.18 (m, 6H), 7.00 (d, *J* = 11.4 Hz, 2H), 6.94 (d, *J* = 15.0 Hz, 2H), 6.68 (s, 2H), 2.52 (s, 6H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): δ 145.0, 141.4, 141.2, 132.5, 128.8, 127.9, 126.5, 124.1, 115.0, 111.4, 15.3.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-(methylthio)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-SMe**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **2b** and isolated as a purple crystalline solid in 20.3% yield. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$): δ 7.41 (d, *J* = 8.4 Hz, 4H), 7.23 (d, *J* = 8.4 Hz, 4H), 6.99-6.89 (m, 4H), 6.82-6.67 (m, 6H), 6.64 (s, 2H), 2.52 (s,

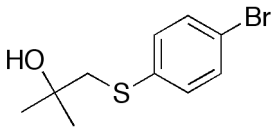
6H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): δ 144.21, 142.39, 139.47, 137.47, 132.76, 128.06, 128.5, 127.00, 126.96, 114.76, 110.63, 15.01.

(1E,3E,5E,7Z,9E,11Z,13E,15E,17E)-8,11-dicyano-1,18-di-(4-(methylthio)phenyl)-octadeca-1,3,5,7,9,11,13,15,17-nonaene (**DPDC9-SMe**; m = 3): General Double Knoevenagel Condensation Procedure was carried out at 55° C. The product was prepared from **2c** and isolated as a dark purple-black solid in 40.5% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.40 (d, J = 8.5 Hz, 4H), 7.29 (d, J = 8.5 Hz, 4H), 7.13-6.34 (m, 16H), 2.54 (s, 6H). ^{13}C NMR could not be obtained due to insolubility.

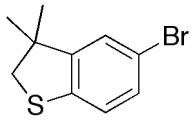
(1E,3E,5E,7E,9Z,11E,13Z,15E,17E,19E,21E)-10,13-dicyano-1,22-di-(4-(methylthio)-phenyl)-docosa-1,3,5,7,9,11,13,15,17,19,21-undecaene (**DPDC11-SMe**; m = 4): General double Knoevenagel condensation procedure. The product was prepared from **2d** and isolated as a lustrous dark black solid in 10.0% yield. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.37 (d, J = 8.0 Hz, 4H), 7.22 (d, J = 8.0 Hz, 4H), 6.92-6.45 (m, 16H), 6.49 (m, 4H), 2.51 (s, 6H); ^{13}C NMR could not be obtained due to compound insolubility.



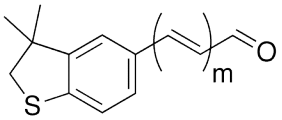
Scheme S1. Synthesis of 3,3-dimethyl-2,3-dihydrobenzo[*b*]thiophene-5-carbaldehyde from 4-bromothiophenol.



4-bromophenylthio 2-methyl-propan-2-ol: 4-bromothiophenol (1.0 g, 5.3 mmol) and 1,2-Epoxy-2-methylpropane (0.76 g, 10.5 mmol) were added to a 100-mL round-bottom flask with magnetic stir bar. The reaction flask was then charged with 50 mL of acetone (from drum) and nitrogen was bubbled through for 20 min. Triethylamine (3 mL) was added to reaction via syringe. The reaction was stirred overnight at room temperature. The organic solvent was removed by rotary evaporation. The product was isolated by column chromatography (20% ethyl acetate in hexanes) and 1.28 g (93%) of clear oil was isolated. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40 (d, J = 8.7 Hz, 2H), 7.28 (d, J = 8.7 Hz, 2H), 3.08 (s, 2H), 2.14 (bs, 1H), 1.30 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 136.8, 132.4, 131.3, 120.4, 71.2, 48.9, 29.1.



5-bromo-3,3-dimethyl-2,3-dihydrobenzo[b]thiophene: A solution of 4-bromophenylthio 2-methyl-propan-2-ol (0.36 g, 1.39 mmol) CH_2Cl_2 was added to a stirring suspension of aluminum chloride (0.20 g, 1.53 mmol) in CH_2Cl_2 cool in an ice bath. The suspension was left to stir overnight while warming to room temperature. Water was added to quench unreacted $AlCl_3$. The organic layer was washed with water and then sat. aqueous sodium chloride solution before drying over $MgSO_4$. The product was isolated by column chromatography (100% hexanes) and 1.90 g (57%) of clear oil was isolated. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.23 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 7.14 (d, *J* = 1.8 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 3.18 (s, 2H), 1.36 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 150.7, 140.1, 130.6, 126.4, 124.1, 118.2, 47.9, 47.8, 27.6.



3a; m = 1
3b; m = 2
3c; m = 3
3d; m = 4

3,3-dimethyl-2,3-dihydrobenzo[b]thiophene-5-carbaldehyde (**3a**; m = 0): A 100-mL round-bottom flask was flame dried and charged with 5-bromo-3,3-dimethyl-2,3-dihydrobenzo[*b*]thiophene (0.310 g, 1.20 mmol) and anhydrous THF (25 mL). The reaction flask was cooled to -78° C in an acetone/dry ice bath for 40 min. 0.9 mL of n-BuLi (1.6 M in hexanes) was dripped into the reaction slowly over 5 minutes. The reaction was allowed to stir at -78° C for 30 min before dry DMF (1 mL) was added dropwise. This reaction was allowed to warm to room temperature overnight. The reaction was then quenched with water, left to stir for 10 min and extracted with ether.

The organic layers were combined and washed with sat. sodium chloride solution and then dried over $MgSO_4$. Product was isolated by column chromatography to yield 0.203 g (94 %) of a colorless oil. NOTE: yields varied. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.88 (s, 1H), 7.62 (dd, *J* = 1.8 Hz, 8.1 Hz, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 3.24 (s, 2H), 1.41 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 191.6, 150.5, 149.6, 134.1, 131.1, 123.0, 122.9, 47.8, 47.3, 27.9.

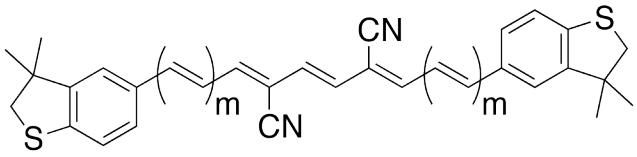
(E)-3-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophen-5-yl)acrylaldehyde (**3b**; m = 1): General Wittig homologation procedure. The product was prepared from **3a** and isolated as a pale yellow solid in 94.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.68 (d, J = 8.0 Hz, 1H), 7.44 (d, *J* = 15.8 Hz, 1H), 7.32 (dd, *J* = 1.4 Hz, 8.0 Hz, 1H), 7.22 (m, 2H), 6.68 (dd, *J* = 7.8 Hz, 15.8 Hz, 1H), 3.21 (s, 2H), 1.39 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.6, 152.8, 149.1, 145.9, 130.7, 128.3, 127.0, 122.8, 122.4, 47.5, 47.1, 27.5.

(2E,4E)-5-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophen-5-yl)penta-2,4-dienal (**3c**; m = 2): General Wittig homologation procedure. The product was prepared from **3b** and isolated as a yellow solid in 92.0% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (d, *J* = 8.0 Hz, 1H), 7.26-7.16 (m, 2H), 6.96 (m, 2H), 6.26 (dd, *J* = 8.0 Hz, 15.2 Hz, 1H), 3.22 (s, 2H), 1.40 (s, 6H); ^{13}C NMR (400 MHz, $CDC1_3$): δ 193.81, 152.80, 149.30, 143.94, 142.88, 132.73, 131.23, 127.77, 125.10, 123.07, 121.80, 47.82, 47.46, 27.80.

(2E,4E,6E)-7-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophen-5-yl)hepta-2,4,6-trienal (**3d**; m = 3): General Wittig homologation procedure. The product was prepared from **3c** and

isolated as an orange solid in 90.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.87 (d, *J* = 7.8 Hz, 1H), 7.16 (m, 4H), 6.80 (m, 3H), 6.50 (dt, *J* = 2.7 Hz, 11.1 Hz, 1H), 6.12 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H), 3.16 (s, 2H), 1.35 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.78, 152.27, 149.17, 143.44, 142.71, 138.77, 133.49, 131.21, 129.86, 127.10, 126.72, 123.04, 121.37, 47.84, 47.48, 27.81.

(2E,4E,6E,8E)-9-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophen-5-yl)nona-2,4,6,8-tetraenal (**3e**; m = 4): General Wittig homologation procedure. The product was prepared from **3d** and isolated as a red-orange solid in 63.0% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.55 (d, *J* = 8.1 Hz, 1H), 7.18-7.07 (m, 4H), 6.85-6.56 (m, 4H), 6.48 (d, *J* = 11.1 Hz, 1H), 6.41 (dd, *J* = 8.1 Hz, 11.7 Hz, 1H), 6.14 (dd, *J* = 8.1 Hz, 15.3 Hz, 1H), 3.16 (s, 2H), 1.36 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.9, 152.4, 149.1, 143.3, 142.0, 139.7, 136.5, 133.9, 131.6, 131.2, 130.0, 127.4, 126.9, 123.0, 121.1, 47.8, 47.5, 27.8.



DPDCn-SC$_4$H$_8$; m = 0, 1, 2, 3, 4

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophene)-hexa-1,3,5-triene (**DPDC3-SC$_4$H$_8$**; m = 0): General double Knoevenagel condensation procedure. This molecule was prepared from **3a** and isolated as a lemon yellow solid in 41.9% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.61 (d, *J* = 1.7 Hz, 2H), 7.57 (dd, *J* = 1.7 Hz, 8.2 Hz, 2H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.12 (s, 2H), 6.79 (s, 2H), 3.24 (s, 4H), 1.42 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 149.13, 145.70, 144.91, 130.13, 129.79, 129.39, 123.18, 122.75, 116.58, 107.63, 47.52, 47.22, 27.46.

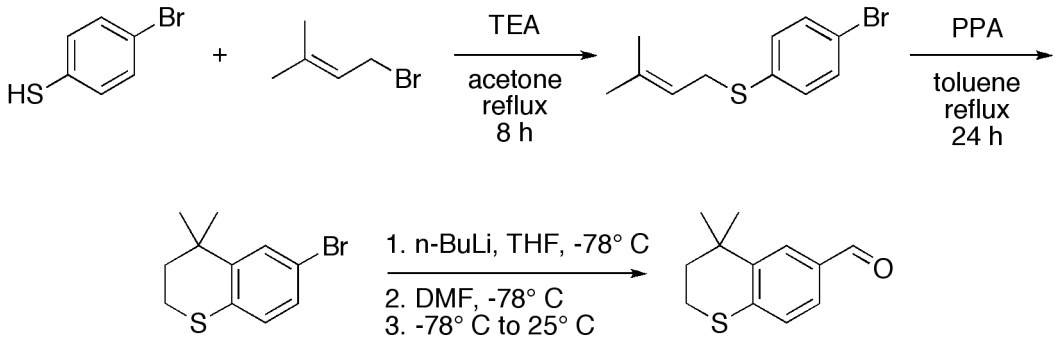
(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophene)-deca-1,3,5,7,9-pentaene (**DPDC5-SC$_4$H$_8$**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **3b** and isolated as a red solid in 30.0% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.33 (dd, *J* = 1.5 Hz, 8.1 Hz, 2H), 7.28-7.19 (m, 6H), 7.05 (d, *J* = 11.4 Hz, 2H), 6.98 (d, *J* = 15.3 Hz, 2H), 6.70 (s, 2H), 3.24 (s, 4H), 1.41 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 149.7, 146.0, 144.2, 142.2, 132.9, 129.3, 127.9, 123.8, 123.1, 122.0, 115.8, 111.3, 47.5, 47.0, 26.6.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophene)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-SC$_4$H$_8$**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **3c** and isolated as a purple solid in 17.0% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.12 (m,

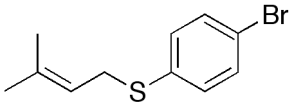
6H), 7.05-6.77 (m, 10H), 6.67 (s, 2H), 3.23 (s, 4H), 1.41 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 149.22, 145.17, 142.88, 142.87, 138.94, 133.57, 129.34, 128.73, 127.37, 127.14, 123.09, 121.29, 115.80, 111.35, 47.87, 47.50, 27.81.

(1E,3E,5E,7Z,9E,11Z,13E,15E,17E)-8,11-dicyano-1,18-di-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophene)-octadeca-1,3,5,7,9,11,13,15,17-nonaene (**DPDC9-SC$_4$H$_8$**; m = 3): General double Knoevenagel condensation procedure. The product was prepared from **3d** and isolated as a dark purple solid in 10.5% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.44 (d, *J* = 11.9 Hz, 2H), 7.35 (s, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 6.6 Hz, 2H), 7.09 (dd, *J* = 12.3 Hz, 17.2 Hz, 2H), 6.93 (dd, *J* = 13.5 Hz, 16.9 Hz, 2H), 6.85-6.62 (m, 12H), 3.22 (s, 4H), 2.08 (s, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 149.10, 145.00, 142.62, 142.07, 139.94, 136.72, 133.96, 132.09, 129.42, 128.86, 127.59, 126.95, 123.01, 121.14, 115.79, 111.33, 47.85, 47.49, 27.80.

(1E,3E,5E,7E,9Z,11E,13Z,15E,17E,19E,21E)-10,13-dicyano-1,22-di-(3,3-dimethyl-2,3-dihydrobenzo[b]thiophene)-phenyl)-docosa-1,3,5,7,9,11,13,15,17,19,21-undecaene (**DPDC11-SC$_4$H$_8$**; m = 4): General double Knoevenagel condensation procedure. The product was prepared from **3e** and isolated as a dark purple-black solid in 8.0% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.22-7.11 (m, 6H), 6.90-6.48 (m, 20H), 3.21 (s, 4H), 1.40 (s, 12H); ^{13}C NMR (500 MHz, CD_2Cl_2): δ 148.2, 144.0, 141.6, 140.7, 138.7, 136.7, 134.4, 133.4, 131.7, 128.6, 128.0, 127.1, 125.7, 122.0, 120.2, 114.8, 110.4, 47.0, 46.5, 26.9; one sp^2 carbon signal not observed.

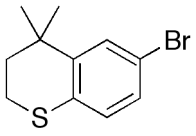


Scheme S2. Synthesis of 4,4-dimethylthiochroman-6-carbaldehyde.

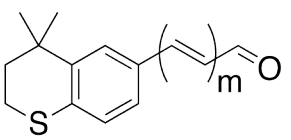


1-bromo-4-[(3-methyl-2-buten-1-yl)thio]benzene: This compound is known [8] in the literature and has been prepared in poor yields by Fe-catalyzed sulfenylation of 4-bromothiophenol with isobutyl 1,1-dimethylprop-2-enyl hydrogen carbonate. We chose a different method for our preparation. 4-bromothiophenol (5.00 g, 26.4 mmol) and 3,3-dimethylallyl bromide (7.88 g, 52.9 mmol) was added to a 250-mL round-bottom flask with magnetic stir bar. The reaction flask was then charged with 200 mL of acetone and nitrogen was bubbled through for 25 min. 5 mL of triethylamine was added to reaction via syringe and the a white precipitate crashed out immediately. The reaction was stirred overnight at room temperature before filtering off the white solid and washing with acetone. Solvent was removed from the organic layer by rotary evaporation and then loaded onto a silica gel loading column. Column chromatography (100% hexanes) was

used to isolate the product in quantitative yields. ^{1}H NMR (300 MHz, CD_2Cl_2): 7.39 (d, *J* = 8.7, 2H), 7.20 (d, *J* = 8.6 Hz, 2H), 5.27 (m, 1H), 3.50 (d, *J* = 7.7 Hz, 2H), 1.71 (s, 3H), 1.59 (s, 3H); ^{13}C NMR (300 MHz, $CDC1_3$): 150.7, 140.1, 130.6, 126.4, 124.1, 118.1, 53.8, 47.9, 47.8, 27.6.



6-bromo-4,4-dimethylthiochroman: This compound is known, however NMR characterization was provided.[9] (4-bromophenyl)(3-methylbut-2-enyl)sulfane (2.72 g, 10.58 mmol) was in a 100-mL round-bottom flask and dissolved in a minimal amount of toluene (not dry). Polyphosphonic acid (5-10 mL) was added and the mixture was refluxed for 24 hours. The reaction was cooled to room temperature and toluene was decanted off. The remaining mixture was dissolved in water and extracted with toluene. Organics were combined, washed with sat. aqueous sodium chloride solution and dried over $MgSO_4$. After column chromatography in 100% hexanes the product was isolated in 2.37 g (87%) as a white powder. ^{1}H NMR (300 MHz, $CDCl_3$): 7.45 (d, *J* = 1.5 Hz, 1H), 7.14 (dd, *J* = 1.5 Hz, 6.3 Hz, 1H), 6.95 (d, *J* = 6.3 Hz, 1H), 3.01 (m, 2H), 1.92 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): 144.5, 131.5, 129.8, 129.4, 128.4, 117.7, 37.5, 33.6, 30.4, 23.4.



4a; m = 0
4b; m = 1
4c; m = 2
4d; m = 3
4e; m = 4
4f; m = 5

4,4-dimethylthiochroman-6-carbaldehyde (**4a**; m = 0): This compound is known, however NMR characterization was provided.[9] A 100-mL round-bottom flask was flame dried and charged with 6-bromo-4,4-dimethylthiochroman (1.00 g, 3.89 mmol) and anhydrous THF (50 mL). The reaction flask was cooled to -78° C in an acetone/dry ice bath for 40 min. 2.67 mL of n-BuLi (1.6 M in hexanes) solution was dripped into the reaction very slowly over 10 minutes. The reaction was allowed to stir at -78° C for 30 min before dry DMF (1 mL) was added dropwise. This reaction was allowed to warm to room temperature overnight. Reaction was quenched with water, allowed to stir for 10 min and extracted with ether. The organic layers were combined and washed with sat. sodium chloride solution and then dried over $MgSO_4$. Product was isolated by column chromatography to yield 0.686 g (86 %) of a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): 9.87 (s, 1H), 7.85 (d, *J* = 1.8 Hz, 1H), 7.52 (dd, *J* = 1.8 Hz, 8.1 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 3.08 (m, 2H), 1.97 (m, 2H), 1.37 (s, 6H); ^{13}C NMR (500 MHz, $CDC1_3$): 191.5, 142.4, 141.7, 132.7, 127.6, 127.0, 126.9, 36.7, 33.1, 29.8, 23.3.

(E)-3-(4,4-dimethylthiochroman-6-carbaldehyde)acrylaldehyde (**4b**; m = 1): General Wittig homologation procedure. The product was prepared from **4a** and isolated as a pale yellow solid in 92.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.64 (d, *J* = 7.5 Hz, 1H), 7.54 (d, *J* = 1.8 Hz, 1H), 7.42 (d, *J* = 15.6 Hz, 1H), 7.24 (dd, *J* = 1.8 Hz, 8.1 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.63 (dd, *J* = 7.5 Hz, 15.9 Hz, 1H), 3.05 (m, 2H), 1.94 (m, 2H), 1.33 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.34, 153.81, 144.14, 138.88, 131.80, 128.94, 128.88, 128.85, 127.36, 41.45, 37.51, 34.28, 28.13.

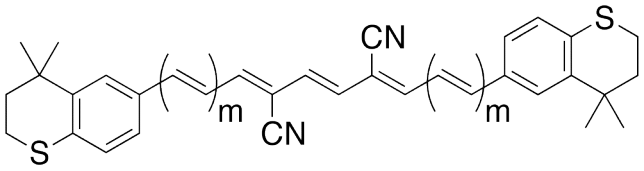
(2E,4E)-5-(4,4-dimethylthiochroman-6-carbaldehyde)penta-2,4-dienal (**4c**; m = 2): General Wittig homologation procedure. The product was prepared from **4b** and isolated as a yellow solid in 92.7% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.62 (d, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 1.8 Hz, 1H), 7.19-7.30 (m, 2H), 7.11 (d, *J* = 8.1 Hz, 1H), 6.97-6.99 (m, 2H), 6.29 (dd, *J* = 7.8 Hz, 15.0 Hz, 1H), 3.06 (m, 2H), 1.97 (m, 2H), 1.36 (s, 6H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.9, 152.9, 143.1, 142.8, 135.4, 131.9, 131.2, 127.5, 126.5, 125.1, 125.0, 37.6, 33.4, 30.4, 23.6.

(2E,4E,6E)-7-(4,4-dimethylthiochroman-6-carbaldehyde)hepta-2,4,6-trienal (**4d**; m = 3): General Wittig homologation procedure. The product was prepared from **4c** and isolated as a golden solid in 71.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.55 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 1.2 Hz, 1H), 7.17-7.01 (m, 3H), 6.82-6.67 (m, 3H), 6.52 (m, 1H), 6.16 (dd, *J* = 7.8 Hz, 15.0 Hz, 1H), 3.00 (m, 2H), 1.91 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.6, 152.3, 143.5, 142.7, 138.9, 134.0, 132.7, 131.1, 129.8, 127.3, 126.6, 126.0, 124.5, 37.7, 33.3, 30.3, 23.6.

(2E,4E,6E,8E)-9-(4,4-dimethylthiochroman-6-carbaldehyde)nona-2,4,6,8-tetraenal (**4e**; m = 4): General Wittig homologation procedure. The product was prepared from **4d** and isolated as an orange solid in 59.4% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.55 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 1.8 Hz, 1H), 7.20-7.08 (m, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.83-6.56 (m, 4H), 6.48-6.36 (m, 2H), 6.17 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H), 3.01 (m, 2H), 1.93 (m, 2H), 1.31 (s, 6H); ^{13}C NMR (500 MHz, $CDC1_3$): δ 193.42, 151.86, 142.87, 142.23,

139.29, 136.25, 132.90, 132.75, 131.10, 130.75, 129.52, 126.95, 126.88, 125.30, 123.97, 37.43, 33.00, 30.06, 23.20.

(2E,4E,6E,8E,10E)-9-(4,4-dimethylthiochroman-6-carbaldehyde)undeca-2,4,6,8,10-pentaenal (**4f**; m = 5): General Wittig homologation procedure. The product was prepared from **4e** and isolated as an orange solid in 41.3% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.60 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 1.8 Hz, 1H), 7.25-7.15 (m, 2H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.92-6.77 (m, 2H), 6.69-6.40 (m, 6H), 6.20 (dd, *J* = 8.1 Hz, 15.3 Hz, 1H), 3.07 (m, 2H), 1.98 (m, 2H), 1.37 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.7, 152.1, 143.0, 142.7, 139.3, 137.3, 135.1, 133.4, 132.9, 132.4, 131.9, 131.1, 130.1, 127.7, 127.1, 125.6, 124.1, 37.8, 33.3, 30.2, 23.6.



DPDCn-SC_8H_{10}; m = 0, 1, 2, 3, 4, 5

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4,4-dimethylthiochroman)-hexa-1,3,5-triene (**DPDC3-SC_5H_{10}**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from **4a** and isolated as a lemon yellow solid in 43.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.92 (d, *J* = 1.8 Hz, 2H), 7.50 (dd, *J* = 2.1 Hz, 8.4 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.09 (s, 2H), 6.79 (s, 2H), 3.07 (m, 4H), 1.98 (m, 4H), 1.38 (s, 12H); ^{13}C NMR (300 MHz, CD_2C1_2): δ 145.3, 143.0, 137.6, 130.0, 129.8, 127.9, 127.2, 127.1, 116.9, 108.0, 37.3, 33.5, 30.0, 23.7.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4,4-dimethylthiochroman)-deca-1,3,5,7,9-pentaene (**DPDC5-SC_5H_{10}**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **4b** and isolated as a bright red solid in 34.8% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.50 (d, *J* = 1.5 Hz, 2H), 7.32 (dd, *J* = 1.2 Hz, 8.4 Hz, 2H), 7.23 (dd, *J* = 11.4 Hz, 15.0 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 11.7 Hz, 2H), 6.97 (d, *J* = 15.3 Hz, 2H), 6.71 (s, 2H), 3.09 (m, 4H), 1.98 (m, 4H), 1.37 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 145.7, 143.0, 142.4, 135.7, 132.1, 129.2, 127.3, 126.8, 124.8, 123.6, 115.5, 111.2, 37.6, 33.3, 30.0, 23.6.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4,4-dimethylthiochroman)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-SC_5H_{10}**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **4c** and isolated as a red-purple

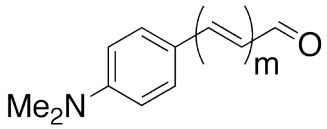
solid in 23.2%. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.43 (d, *J* = 1.8 Hz, 2H), 7.17 (dd, *J* = 1.8 Hz, 8.4 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.95-6.71 (m, 10H), 6.63 (s, 2H), 3.03 (m, 4H), 1.94 (m, 4H), 1.32 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 146.7, 144.4, 144.2, 140.6, 135.5, 134.1, 130.5, 129.9, 128.8, 128.4, 127.4, 126.1, 117.4, 112.4, 38.9, 34.7, 31.8, 25.1.

(1E,3E,5E,7Z,9E,11Z,13E,15E,17E)-8,11-dicyano-1,18-di-(4,4-dimethylthiochroman)-octadeca-1,3,5,7,9,11,13,15,17-nonaene (**DPDC9-SC_5H_{10}**; m = 3): General double Knoevenagel condensation procedure. The product was prepared from **4d** and isolated as a dark purple solid in 15.5% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.39 (s, 2H), 7.19 (d, *J* = 9.0 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.91-6.62 (m, 14H), 6.55-6.47 (m, 2H), 3.07 (m, 4H), 1.97 (m, 4H), 1.34 (s, 12H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 144.6, 142.3, 142.2, 139.5, 136.4, 132.8, 132.6, 131.5, 128.7, 128.2, 127.0, 126.8, 125.3, 123.9, 115.4, 110.5, 37.1, 32.8, 29.9, 23.1.

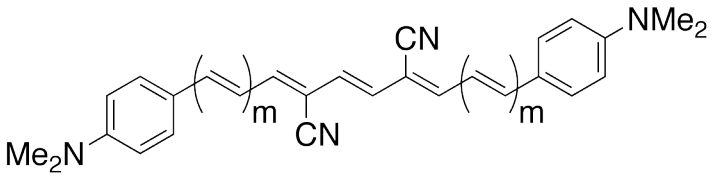
(1E,3E,5E,7E,9Z,11E,13Z,15E,17E,19E,21E)-10,13-dicyano-1,22-di-(4,4-dimethylthiochroman)-docosa-1,3,5,7,9,11,13,15,17,19,21-undecaene (**DPDC11-SC_5H_{10}**; m = 4): General double Knoevenagel condensation procedure. The product was prepared from **4e** and isolated as a lustrous blue-black solid in 6.0% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.41 (d, *J* = 1.2 Hz, 2H), 7.18 (bd, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 6.92-6.45 (m, 20H), 3.08 (m, 4H), 2.01 (m, 4H), 1.40 (s, 12H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 144.49, 142.19, 142.14, 139.32, 137.34, 135.09, 133.04, 133.02, 132.48,

132.21, 129.06, 128.61, 127.38, 126.93, 125.14, 123.92, 115.40, 110.93, 37.49, 33.00, 30.07, 23.20.

(1E,3E,5E,7E,9E,11Z,13E,15Z,17E,19E,21E,23E,25E)-12,15-dicyano-1,26-di-(4,4-dimethylthiochroman)-hexacosa-1,3,5,7,9,11,13,15,17,19,21,23,25-tridecaene (**DPDC13-SC$_5$H$_{10}$**; m = 5): General double Knoevenagel condensation procedure. The product was prepared from **4f** and isolated as a lustrous blue-black solid in 5.1% yield%. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$): δ 7.38 (bs, 2H), 7.27-7.14 (m, 6H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.88 (m, 2H), 6.82 (dd, *J* = 10.4 Hz, 15.3 Hz, 2H), 6.72-6.38 (m, 16H), 3.05 (m, 4H), 1.95 (m, 4H), 1.34 (s, 12H); ^{13}C NMR could not be obtained due to insolubility of product.



(2E,4E)-5-(4-(dimethylamino)phenyl)penta-2,4-dienal (**5a**; m = 2): Compound is known.[10] General Wittig homologation procedure. The product was prepared from *trans*-(4-dimethylamino)cinnamaldehyde and isolated as a golden-orange solid in 91.1% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.57 (d, *J* = 8.1 Hz, 1H), 7.41 (d, *J* = 8.9 Hz, 2H), 7.29 (dd, *J* = 7.5 Hz, 15.3 Hz, 1H), 6.97-6.73 (m, 2H), 6.71 (d, *J* = 8.9 Hz, 2H), 6.21 (dd, *J* = 8.1 Hz, 15.0 Hz, 1H), 3.02 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 194.0, 154.1, 151.8, 143.9, 129.6, 129.5, 124.0, 122.0, 112.4, 40.6.



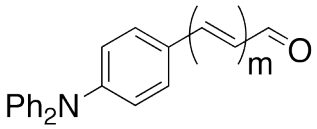
DPDCn-NMe$_2$; m = 0, 1, 2

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(dimethylamino)phenyl)-hexa-1,3,5-triene (**DPDC3-NMe$_2$**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from (4-dimethylamino)benzaldehyde and isolated as an orange-red solid in 8.1% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 7.78 (d, *J* = 8.7 Hz, 4H), 7.02 (s, 2H), 6.72 (d, *J* = 8.7 Hz, 4H), 6.66 (s, 2H), 3.06 (s, 12H); ^{13}C NMR (500 MHz, $C_2D_2Cl_4$): δ 151.2, 143.7, 130.7, 127.7, 121.1, 117.1, 111.2, 102.9, 39.4.

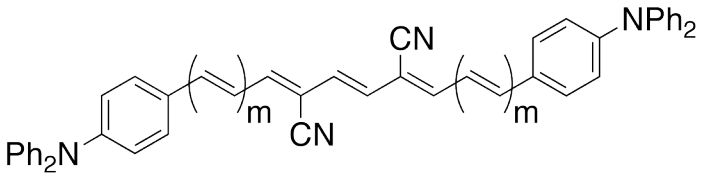
(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(dimethylamino)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-NMe$_2$**; m = 1): General double Knoevenagel condensation procedure.

The product was prepared from *trans*-(4-dimethylamino)cinnamaldehyde and isolated as a lustrous blue-black solid in 30.1% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.46 (d, J = 7.0 Hz, 4H), 7.17-6.83 (m, 6H), 6.73 (d, J = 7.0 Hz, 4H), 6.64 (s, 2H), 3.06 (s, 12H); ^{13}C NMR was not obtained due to insolubility.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-(dimethylamino)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-NMe$_2$**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **5a** and isolated as a black lustrous solid in 23.3% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 7.40 (d, J = 8.7 Hz, 4H), 6.97-6.66 (m, 14H), 6.61 (s, 2H), 3.05 (s, 12H); ^{13}C NMR was not obtained due to limited solubility.



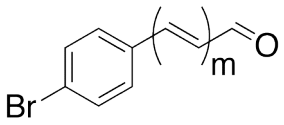
(E)-3-(4-(diphenylamino)phenyl)acrylaldehyde (**6a**; m = 1): Compound is known.[11] General Wittig homologation procedure. The product was prepared from 4-diphenylamino)benzaldehyde and isolated as a pale yellow solid in 55.3% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 9.65 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 2H), 7.35-7.25 (m, 5H), 7.15-7.09 (m, 6H), 7.02 (d, *J* = 8.7 Hz, 2H), 6.62 (dd, *J* = 7.8 Hz, 15.6 Hz, 1H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 194.0, 153.0, 151.2, 147.0, 130.2, 130.0, 127.1, 126.5, 126.1, 124.9, 121.4.



DPDCn-NPh$_2$; m = 0, 1

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(diphenylamino)phenyl)-hexa-1,3,5-triene (**DPDC3-NPh$_2$**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from 4-diphenylamino)benzaldehyde and isolated as a orange-red solid in 16.3% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 7.76 (d, *J* = 8.8 Hz, 4H), 7.40-7.38 (m, 8H), 7.21-7.11 (m, 14H), 7.03 (d, *J* = 8.8 Hz, 4H), 6.79 (s, 2H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 150.60, 146.87, 144.36, 131.06, 129.95, 129.61, 126.62, 126.27, 124.96, 120.84, 117.17, 106.53.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(diphenylamino)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-NPh$_2$**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **6a** and isolated as a dark purple solid in 51.6% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37 (d, *J* = 8.3 Hz, 4H), 7.29 (t, *J* = 7.5 Hz, 8H), 7.14-7.08 (m, 14H), 7.00 (d, *J* = 8.3 Hz, 4H), 6.95 (d, *J* = 11.5 Hz, 2H), 6.89 (d, *J* = 15.2 Hz, 2H), 6.63 (s, 2H); ^{13}C NMR (500 MHz, $CDC1_3$): δ 149.44, 146.87, 145.38, 141.52, 129.50, 128.95, 128.83, 128.57, 125.37, 124.04, 122.69, 121.88, 115.64, 110.21.



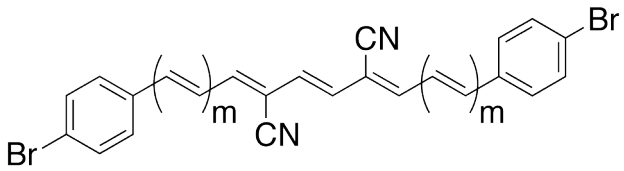
7a; m = 1
7b; m = 2
7c; m = 3

4-bromocinnamaldehyde (**7a**; m = 1): General Wittig homologation procedure. The product was prepared from 4-bromobenzaldehyde and isolated by column chromatograph (15% ethyl acetate in hexanes) as a white solid in 91.5% yield. This compound is known and matches the reported spectroscopic data.[12] ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.69 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.43-7.38 (m, 3H), 6.69 (dd, *J* = 7.6 Hz, 16.0 Hz, 1H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 193.4, 151.2, 133.1, 132.5, 129.9, 129.2, 125.8.

(2E,4E)-5-(4-bromophenyl)penta-2,4-dienal (**7b**; m = 2): General Wittig homologation procedure. The product was prepared from **7a** and isolated by column chromatography (15% ethyl acetate in hexanes) as a yellow solid in 96.0% yield. This compound is known and matches the reported spectroscopic data.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.36 (d, *J* = 8.8 Hz, 2H), 7.27-7.21 (dd, *J* = 9.6 Hz, 15 Hz, 1H), 7.02-6.91 (m, 2H), 6.31-6.25 (dd, *J* = 8.0 Hz, 15.0 Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 193.5, 151.5, 140.9, 134.5, 132.1, 132.0, 128.9, 126.8, 123.8.

(2E,4E,6E)-7-(4-bromophenyl)hepta-2,4,6-trienal (**7c**; m = 3): General Wittig homologation procedure. The product prepared from **7b** and was isolated by column chromatograph (15% ethyl acetate in hexanes) as a orange-yellow solid in 73.7% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.18 (dd, *J* = 11.0 Hz, 15.0 Hz, 1H), 6.92-6.72 (m, 3H), 6.58 (dd, *J* = 11.0 Hz, 14.0 Hz, 1H), 6.21, (dd, *J* = 7.6 Hz, 15.0 Hz, 1H); ^{13}C NMR (400 MHz,

$CDCl_3$): δ 193.4, 151.3, 142.1, 136.8 135.3, 132.0, 131.4, 130.6, 128.3(4), 128.3(2), 122.7.



DPDCn-Br; m = 0, 1, 2, 3

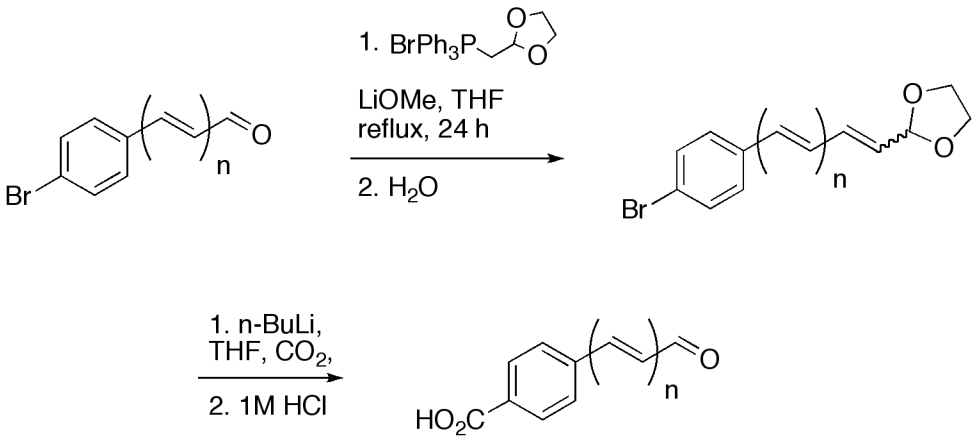
(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-bromophenyl)-hexa-1,3,5-triene (**DPDC3-Br**): General double Knoevenagel condensation procedure. The product was prepared from 4-bromobenzaldehyde and isolated as a yellow solid in 35.6% yield. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$): δ 7.72 (d, *J* = 8.4 Hz, 4H), 7.62 (d, *J* = 8.4 Hz, 4H), 7.19 (s, 2H), 6.86 (s, 2H); 13C NMR (400 MHz, DMSO-d_6): 7.81 (d, *J* = 8.4 Hz, 4H), 7.76 (s, 2H), 7.74 (d, *J* = 8.4 Hz, 4H), 6.97 (s, 2H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 145.7, 133.2, 132.6, 131.4, 130.6, 124.8, 116.1, 110.2.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-bromophenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-Br**): General double Knoevenagel condensation procedure. The product was prepared from **7a** and isolated as a peach-orange solid in 33.4% yield. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$): δ 7.58 (d, *J* = 8.4 Hz, 4H), 7.44 (d, *J* = 8.4 Hz, 4H), 7.28 (dd, *J* = 12.0 Hz, 15.0 Hz, 2H), 7.05 (d, *J* = 12.0 Hz, 2 H), 6.97 (d, *J* = 15.0 Hz, 2H), 6.75 (s, 2H); ^{13}C NMR (500 MHz, $C_2D_2Cl_4$): δ 146.2, 142.0, 136.2, 133.6, 130.8, 130.3, 126.8, 125.4, 116.2, 114.0

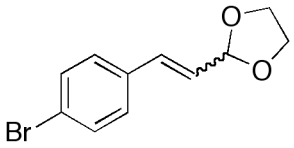
(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-bromophenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-Br**): General double Knoevenagel condensation procedure. The product was prepared from **7b** and isolated as a red solid in 15.5% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.54 (d, *J* = 8.5 Hz, 4H), 7.36 (d, *J* = 8.5 Hz, 4H), 6.98-

6.64 (m, 12H); ^{13}C NMR (500 MHz, $C_2D_2Cl_4$): δ 145.8, 143.5, 143.1, 138.6, 138.3, 133.5, 130.7, 130.2, 129.8, 124.2, 116.3, 113.4.

(1E,3E,5E,7Z,9E,11Z,13E,15E,17E)-8,11-dicyano-1,18-di-(4-bromophenyl)-octadeca-1,3,5,7,9,11,13,15,17-nonaene (**DPDC9-Br**): General double Knoevenagel condensation procedure. The product was prepared from **7c** and isolated as a red-purple solid in 7.6% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.52 (d, J = 8.4 Hz, 4H), 7.33 (d, J = 8.4 Hz, 4H), 6.99-6.55 (m, 16H); Limited solubility prevented acquisition of ^{13}C NMR.

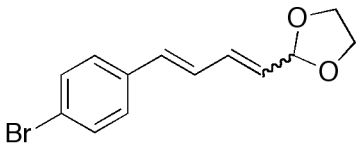


Scheme S3. General route to the synthesis of carboxylic acid aryl-enals through Wittig reaction and concomitant lithium-halogen exchange and carboxylation.



(E)-2-(4-bromostyryl)-1,3-dioxolane (***E*-7d**): Compound is known.[14] The product was synthesized from 4-bromobenzaldehyde using the general Wittig homologation procedure without acidic hydrolysis. Water was added to quench the reaction solution and the product was isolated by column chromatography (15% ethyl acetate in hexanes) as a white solid in 36.3% yield (both stereoisomers in overall 80.5% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, J = 8.8 Hz, 2H), 7.27 (d, J = 8.8 Hz, 2H), 6.73 (d, J = 16.0 Hz, 1H), 6.15 (dd, J = 6.0 Hz, 16.0 Hz, 1H), 5.41 (d, J = 6.0 Hz, 1H), 4.09-3.19 (m, 4H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 134.8, 133.5, 131.7, 128.4, 125.9, 122.3, 103.6, 65.1.

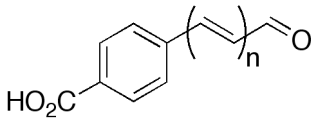
(Z)-2-(4-bromostyryl)-1,3-dioxolane (***Z*-7d**): Compound is known.[14] The product was synthesized from 4-bromobenzaldehyde using the general Wittig homologation procedure without acidic hydrolysis. The product was isolated by column chromatography (15% ethyl acetate in hexanes) as a colorless oil in 44.2% yield (both stereoisomers in overall 80.5% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 11.7 Hz, 1H), 5.73 (dd, *J* = 7.5 Hz, 11.7 Hz, 1H), 5.44 (d, *J* = 7.5 Hz, 1H), 4.09-3.84 (m, 4H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 135.0, 134.7, 131.8, 131.0, 129.0, 122.4, 99.9, 65.6.



2-((1E,3E)-4-(4-bromophenyl)buta-1,3-dienyl)-1,3-dioxolane (***E*-7e**): Acetals were synthesized from **7a** using the general Wittig homologation procedure without acidic hydrolysis. The product was isolated by column chromatography (15% ethyl acetate in hexanes) as a pale yellow solid in 36.4% yield (both stereoisomers in overall 93.5% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 6.77 (dd, *J* = 10.8 Hz, 15.6 Hz, 1H), 6.54 (m, 2H), 5.78 (dd, *J* = 6.0 Hz, 15.2 Hz, 1H), 5.35 (d, *J* = 6.0 Hz, 1H), 4.04-3.88 (m, 4H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 135.7, 135.5, 133.5, 131.8, 131.8, 129.4, 121.7, 103.4, 65.0; one sp^2-carbon signal not observed due to overlapping signals.

2-((1Z,3E)-4-(4-bromophenyl)buta-1,3-dienyl)-1,3-dioxolane (***Z*-7e**): Acetals were synthesized from **7a** using the general Wittig homologation procedure without acidic

hydrolysis. The product was isolated by column chromatography (15% ethyl acetate in hexanes) as a pale yellow solid in 93.5% yield (both stereoisomers in overall 80.5% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.14 (dd, *J* = 11.2 Hz, 15.2 Hz, 1H), 6.55 (d, *J* = 15.0 Hz, 1H), 6.40 (t, *J* = 11.0 Hz, 1H), 5.78 (d, *J* = 6.4 Hz, 1H), 5.54 (dd, *J* = 4.4 Hz, 11.0 Hz, 1H), 4.10-3.91 (m, 4H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 135.8, 134.6, 134.1, 131.8, 128.2, 127.2, 124.0, 121.9, 99.5, 65.1.

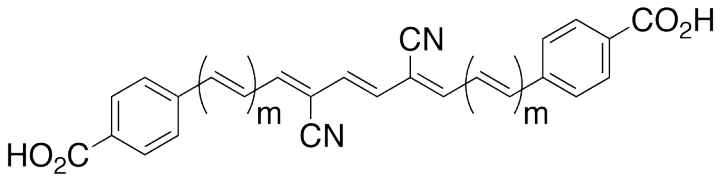


(E)-4-(3-oxoprop-1-enyl)benzoic acid (**8a**; m = 1): This compound has been previously prepared by the soponification of methyl 4-(3-Oxo-1-propenyl)benzoate using sodium hydroxide.[15] In our method, a three-neck round-bottomed flask was charged with acetal protected polyenal (either ***E*-7d** or ***Z*-7d**, 1.0 eq.) in dry THF and cooled to -78° C. n-butyl lithium (1.6 M in hexanes, 1.1 eq.) was added dropwise and the yellow solution was stirred for 15 minutes. Carbon dioxide gas (CO_2 tank, Matheson Tri-Gas; Product Grade) was bubbled into the solution until the yellow color disappeared, and then the reaction was left to warm to room temperature. The solution was diluted with diethyl ether, and then extracted (3x) with water. 1 M aq. hydrochloric acid was added to the aqueous layer and stirred for 1 h, during which time a precipitate formed. This was collected by vacuum filtration to yield pure product ($C_{10}O_2H_8$) as a white solid in 89.4% yield. [**Note**: When the Z-alkene is used, acetal hydrolysis may remain incomplete. In that event, the precipitate is dissolved in tetrahydrofuran before adding 1 M aq. hydrochloric acid. After stirring for 1 h, the solution was diluted with water and extracted (3x) with ethyl acetate.

The organic layer was washed with brine, dried over magnesium sulfate, and concentrated to yield the all-*trans* product. It is important to note that both the (*E*)- and (*Z*)-acetals yield the same all-*trans*-product. Therefore, the *E*/*Z* mixture can be used as the starting material for **8a**.] ^{1}H NMR (300 MHz, Acetone-d_6): δ 11.39 (bs, 1H), 9.76 (d, *J* = 7.5 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 16.2 Hz, 1H), 6.88 (dd, *J* = 7.5 Hz, 16.2 Hz, 1H); ^{13}C NMR (300 MHz, Acetone-d_6): δ 193.5, 166.4, 151.1, 139.0, 132.8, 130.9, 130.6, 128.9.

4-((1E,3E)-5-oxopenta-1,3-dienyl)benzoic acid (**8b**; m = 2): A three-neck round-bottomed flask was charged with acetal protected polyenal (either ***E*-7e** or ***Z*-7e**, 1.0 eq.) in dry THF and cooled to -78° C. n-butyl lithium (1.6 M in hexanes, 1.1 eq.) was added dropwise and the yellow solution was stirred for 15 minutes. Carbon dioxide gas (CO_2 tank, Matheson Tri-Gas; Product Grade) was bubbled into the solution until the yellow color disappeared, and then the reaction was left to warm to room temperature. The solution was diluted with diethyl ether, and then extracted (3x) with water. To the water layer was added 1 M aq. hydrochloric acid and this was stirred for one hour during which time a precipitate formed. This was collected by vacuum filtration to yield pure product ($C_{12}O_2H_{10}$) as a yellow solid in 90.7% yield. [**Note**: When the Z-alkene is used, acetal hydrolysis may remain incomplete. In that event, the precipitate is dissolved in tetrahydrofuran before adding 1 M aq. hydrochloric acid. After stirring for 1 h, the solution was diluted with water and extracted (3x) with ethyl acetate. The organic layer was washed with brine, dried over magnesium sulfate, and concentrated to yield the all-*trans* product. It is important to note that both the (*E*)- and (*Z*)-acetals yield the same all-

trans-product. Therefore, the *E*/*Z* mixture can be used as the starting material.] ^{1}H NMR (400 MHz, Acetone-d_6): δ 11.39 (bs, 1H), 9.68 (d, J = 8.0 Hz, 1H), 8.07 (d, J = 8.4 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.51 (dd, J = 10.8 Hz, 14.8 Hz, 1H), 7.43-7.36 (m, 1H), 7.26 (d, J = 15.6 Hz, 1H), 6.35 (dd, J = 8.0 Hz, 15.2 Hz, 1H); ^{13}C NMR (400 MHz, Acetone-d_6): δ 193.0, 166.3, 151.2, 137.3, 132.8, 130.8, 130.1, 129.0, 127.4, 125.2.



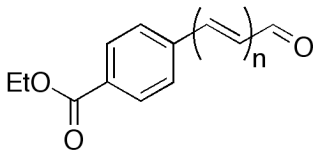
DPDCn-CO_2H; m = 0, 1, 2

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(carboxy)phenyl-hexa-1,3,5-triene (**DPDC3-CO_2H**; m = 0): A round-bottomed flask is charged with 4-formylbenzoic acid (1.0 eq.) and *trans*-1,4-dicyano-2-butene (1.0 eq.) in methanol under a nitrogen atmosphere. Sodium metal (>6.0 eq.) is dissolved in methanol and this is added directly to reaction solution. The reaction is stirred for 12 hours during which time a colored precipitate forms. The precipitate is collected by vacuum filtration, then suspended in methanol, and excess 1 M aq. hydrochloric acid is added. The reaction mixture is left to sit for one hour while the solid settles and is again collected by vacuum filtration. The yellow solid is pure product; 19.8% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.22 (bs, 2H), 8.05 (d, J = 8.4 Hz, 4H), 7.94 (m, 6H), 7.04 (s, 2H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 167.0, 146.2, 137.8, 132.9, 131.1, 130.4, 129.7, 116.1, 111.2.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(carboxy)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-CO_2H**; m = 1): A round-bottomed flask is charged with **8a** acid (1.0 eq.) and *trans*-1,4-dicyano-2-butene (1.0 eq.) in methanol under a nitrogen atmosphere. Sodium metal (>6.0 eq.) is dissolved in methanol and this is added directly to reaction solution. The reaction is stirred for 12 hours during which time a colored precipitate forms. The precipitate is collected by vacuum filtration, then suspended in methanol, and excess 1 M aq. hydrochloric acid is added. The reaction mixture is left to sit for one hour while the solid settles and is again collected by vacuum filtration. The dark orange solid is pure

product; 14.4% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.00 (bs, 2H) 7.95 (d, J = 8.0 Hz, 4H), 7.75 (d, J = 8.0 Hz, 4H), 7.61 (d, J = 10.4 Hz, 2H), 7.33-7.21 (m, 4H), 6.86 (s, 2H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 167.3, 146.7, 141.5, 139.9, 131.8, 130.4, 129.8, 128.2, 127.0, 115.2, 112.7.

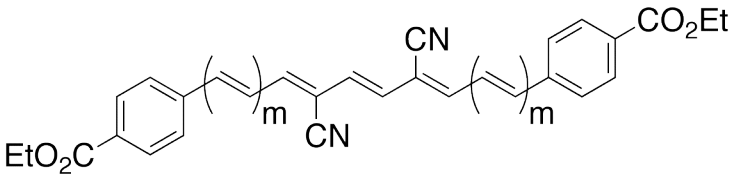
(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-(carboxy)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-CO_2H**; m = 2): A round-bottomed flask is charged with **8b** (1.0 eq.) and *trans*-1,4-dicyano-2-butene (1.0 eq.) in methanol under a nitrogen atmosphere. Sodium metal (>6.0 eq.) is dissolved in methanol and this is added directly to reaction solution. The reaction is stirred for 12 hours during which time a colored precipitate forms. The precipitate is collected by vacuum filtration, then suspended in methanol, and excess 1 M aq. hydrochloric acid is added. The reaction mixture is left to sit for one hour while the solid settles and is again collected by vacuum filtration. The dark red solid is pure product; 18.1% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.00 (bs, 2H), 7.91 (d, J = 8.4 Hz, 4H), 7.68 (d, J = 8.4 Hz, 4H), 7.51 (d, J = 11.6 Hz, 2H), 7.42 (dd, J = 11.0 Hz, 15.4 Hz, 2H), 7.04-7.00 (m, 4H), 6.87 (dd, J = 11.6 Hz, 14.8 Hz, 2H), 6.78 (s, 2H); Limited solubility prevented acquisition of ^{13}C NMR.



ethyl 4-formylbenzoate (**9a**; m = 0): Product prepared from reaction of 4-formylbenzoic acid with 1-bromoethane in the presence of base. Detailed preparation and characterization has been previously reported.[16]

(E)-ethyl 4-(3-oxoprop-1-enyl)benzoate (**9b**; m = 1): Product was prepared via Heck reaction involving ethyl 4-bromo-benzoate and acrolein diethyl acetal. Detailed preparation and characterization have been previously reported.[17] Yield: 85.1%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.73 (d, *J* = 7.6 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4, 2H), 7.50 (d, *J* = 16.0 Hz, 1H), 6.77 (dd, *J* = 7.6 Hz, 16.0 Hz, 1H), 4.39 (q, *J* = 6.8 Hz, 2H), 1.38 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 193.3, 165.8, 150.9, 138.0, 132.6, 130.3, 130.2, 128.3, 61.3, 14.3.

ethyl 4-((1E,3E)-5-oxopenta-1,3-dienyl)benzoate (**9c**; m = 2): General Wittig homologation procedure was modified by using 3.0 eq. of (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide and 3.3 eq. of LiOMe. The product was isolated by column chromatograph (15% ethyl acetate in hexanes) as a pale yellow solid in 64.6% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.64 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.28 (dd, *J* = 9.5 Hz, 15.5 Hz, 1H), 7.07 (m, 2H), 6.32 (dd, *J* = 7.5 Hz, 15.5 Hz, 1H), 4.39 (q, *J* = 7.5 Hz, 2H), 1.41 (t, J = 7.5 Hz, 3H); ^{13}C NMR (500 MHz, $CDCl_3$): 193.4 166.0, 151.0, 140.8, 139.7, 132.7, 131.1, 130.1, 128.3, 127.3, 61.2, 14.3.



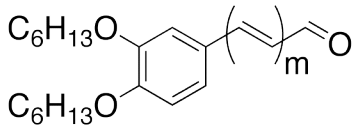
DPDCn-CO_2Et; m = 0, 1, 2

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(diethylbenzoate)-hexa-1,3,5-triene (**DPDC3-CO_2Et**; m = 0): General double Knoevenagel condensation procedure was modified by employing sodium methoxide as base; instead of DBU. The product was prepared from **9a** and was isolated as a bright yellow solid in 33.4% yield and was very insoluble. ^{1}H NMR (300 MHz, 355 K, $C_2D_2Cl_4$): δ 8.12 (bs, 4H), 7.92 (bs, 4H), 7.31 (bs, 2H), 6.94 (bs, 2H), 4.04 (bs, 4H), 1.42 (bs, 6H); ^{13}C NMR (400 MHz, $C_2D_2Cl_4$): δ 167.2, 145.9, 138.5, 134.0, 132.5, 131.5, 130.6, 116.7, 113.2, 62.7, 15.6.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(diethylbenzoate)-deca-1,3,5,7,9-pentaene (**DPDC5-CO_2Et**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **9b** and isolated as an orange solid in 32.4% yield. ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): δ 8.06 (d, *J* = 8.1 Hz, 4H), 7.62 (d, *J* = 8.1 Hz, 4H), 7.35 (dd, *J* = 11.5 Hz, 15.3 Hz, 2H), 7.08 (d, *J* = 11.5 Hz, 2H), 7.04 (d, *J* = 15.3 Hz, 2H), 6.75 (s, 2H), 4.39 (q, *J* = 7.2 Hz, 4H), 1.41 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (400 MHz, $C_2D_2Cl_4$): δ 165.49, 144.61, 140.36, 139.09, 130.58, 129.58, 129.08, 127.00, 126.15, 114.44, 112.45, 60.82, 13.86.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-(diethylbenzoate)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-CO_2Et**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **9c** and isolated as a red solid in

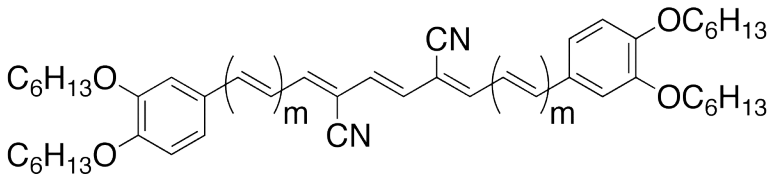
14.6% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.04 (d, J = 8.0 Hz, 4H), 7.54 (d, J = 8.0 Hz, 4H), 7.11-6.72 (m, 12H), 4.41 (q, J = 7.0 Hz, 4H), 1.43 (t, J = 7.0 Hz, 6H); ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 8.03 (d, J = 8.2 Hz, 4H), 7.53 (d, J = 8.2 Hz, 4H), 7.08 (dd, J = 10.5 Hz, 15.3 Hz, 2H), 6.97-6.80 (m, 8H), 6.68 (s, 2H), 4.38 (q, J = 7.1 Hz, 4H), 1.40 (t, J = 7.1 Hz, 6H); ^{13}C NMR (500 MHz, $C_2D_2Cl_4$): δ 165.64, 144.26, 141.34, 140.05, 136.69, 129.76, 129.62, 129.59, 129.53, 128.84, 126.39, 114.65, 111.51, 60.71, 13.89.



3,4-bis(hexyloxy)benzaldehyde (**10a**; m = 0): This product was prepared by reaction of 3,4-dihydroxybenzaldehyde with 1-bromodecane under basic conditions. Detailed preparation and characterization has been reported by Binnemanns and coworkers.[1]

(E)-3-(3,4-bis(hexyloxy)phenyl)acrylaldehyde (**10b**; m = 1): General Wittig Homologation procedure. The product was prepared from **10a** and isolated as a pale yellow solid in 91.1% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.68 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 15.9 Hz, 1H), 7.16 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 7.11 (d, *J* = 1.8 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.62 (dd, *J* = 7.8 Hz, 15.9 Hz, 1H), 4.04 (m, 4H), 1.84 (m, 4H), 1.51 (m, 4H), 1.39 (m, 8H), 0.95 (m, 6H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 194.1, 153.6, 152.7, 149.6, 127.2, 126.8, 123.9, 113.1, 112.7, 69.7, 69.4, 32.0, 31.9, 29.5, 29.4, 26.1, 26.0, 23.0, 22.9, 14.4 (2 -CH_3 carbon signals).

(2E,4E)-5-(3,4-bis(hexyloxy)phenyl)penta-2,4-dienal (**10c**; m = 2): General Wittig procedure. The product was prepared from **10b** and isolated as a lemon yellow solid in 42.0% yield. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 9.62 (d, *J* = 8.1 Hz, 1H), 7.32 (dd, *J* = 10.2 Hz, 15.3 Hz, 1H), 7.10-6.88 (m, 5H), 6.25 (dd, *J* = 7.8 Hz, 15.0 Hz, 1H), 4.06 (m, 4H), 1.86 (m, 4H), 1.50 (m, 4H), 1.37 (m, 8H), 0.93 (m, 6H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 195.73, 154.96, 152.97, 151.07, 144.77, 132.05, 130.25, 125.79, 124.04, 115.28, 114.24, 71.36, 70.96, 33.36, 33.33, 31.07, 30.94, 27.49, 27.46, 24.45, 24.43, 15.9 (2 -CH_3 signals).



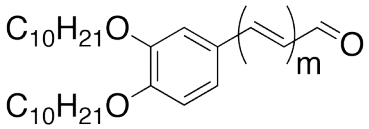
DPDCn-OC_6H_{13}; m = 0, 1, 2

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3,4-bis(hexyloxy)phenyl)-hexa-1,3,5-triene (**DPDC3-OC_6H_{13}**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from **10a** and isolated as a lemon yellow solid in 7.8% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.61 (d, *J* = 2.1 Hz, 2H), 7.32 (dd, *J* = 1.8 Hz, 8.4 Hz, 2H), 7.09 (s, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.77 (s, 2H), 4.06 (m, 8H), 1.86 (m, 8H), 1.52 (m, 8H), 1.37 (m, 16H), 0.94 (m, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 152.2, 149.4, 145.4, 139.3, 129.8, 126.8, 125.0, 113.1, 113.0, 107.0, 69.6, 69.4, 32.0, 31.9, 30.1, 29.6, 29.5, 26.1, 26.0, 23.0, 14.4 (2 -CH_3 carbon signals).

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(3,4-bis(hexyloxy)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-OC_6H_{13}**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **10b** and isolated as a dark red solid in 13.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.28 (s, 2H), 7.17-7.07 (m, 6H), 7.00-6.86 (m, 6H), 6.67 (s, 2H), 4.09 (m, 8H), 1.87 (m, 8H), 1.52 (m, 8H), 1.38 (m, 16H), 0.93 (m, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 151.6, 149.7, 145.9, 142.6, 129.1, 129.0, 123.0, 122.7, 116.0, 113.4, 112.1, 110.7, 69.8, 69.5, 32.0, 31.9, 29.6, 29.5, 26.1, 26.0, 23.0 (2 -CH_2- signals), 14.4 (2 -CH_3 carbon signals).

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(3,4-bis(hexyloxy)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-OC_6H_{13}**; m = 2): General double Knoevenagel

condensation procedure. The product was prepared from **10c** and isolated as a dark purple solid in 20.1% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.04 (d, J = 1.8 Hz, 2H), 7.01 (dd, J = 2.1 Hz, J = 8.7 Hz, 2H), 6.95-6.75 (m, 12H), 6.65 (s, 2H), 4.04 (m, 8H), 1.87 (m, 8H), 1.51 (m, 8H), 1.37 (m, 16H), 0.93 (m, 12H); ^{13}C NMR ($CDCl_3$); δ 300 MHz: 150.76, 149.67, 145.22, 142.99, 139.08, 129.21, 128.32, 126.53, 121.77, 115.88, 115.00, 113.65, 111.70, 111.06, 69.68, 69.54, 32.00, 31.98, 29.63, 29.54, 26.11, 26.08, 23.03, 23.02, 14.45, 14.43.

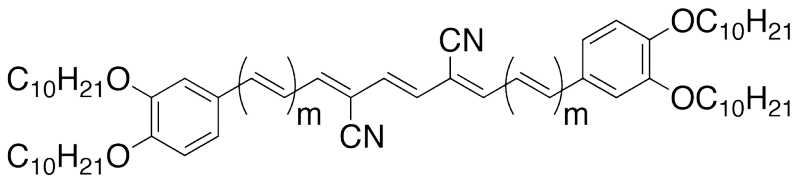


3,4-bis(decyloxy)benzaldehyde (**11a**; m = 0): This product was prepared by reaction of 3,4-dihydroxybenzaldehyde with 1-bromohexane under basic conditions. Detailed preparation and characterization has been reported by Binnemanns and coworkers.[1]

(E)-3,4-bis(decyloxy)cinnamaldehyde (**11b**; m = 1): General Wittig homologation procedure. The product was prepared from **11a** and isolated as a pale yellow solid in 98.8% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.68 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 15.6 Hz, 1H), 7.13 (dd, *J* = 2.0 Hz, 8.4 Hz, 1H), 7.09 (d, *J* = 1.6 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.60 (dd, *J* = 8.0 Hz, 16 Hz, 1H), 4.04 (m, 4H), 1.84 (m, 4H), 1.48 (m, 4H), 1.36-1.28 (m, 24H), 0.88 (t, *J* = 6.4 Hz, 6H); ^{13}C NMR (500 MHz, $CDC1_3$): δ 193.57, 153.06, 152.34, 149.34, 126.88, 126.52, 123.44, 112.93, 112.54, 69.43, 69.12, 31.91, 29.62, 29.60, 29.58, 29.40, 29.37, 29.35, 29.22, 29.20, 26.01, 25.98, 22.68 (2 -CH_2- carbon signals), 14.10 (2 -CH_3 carbon signals); three other aliphatic carbon signals not observed due to overlapping shifts.

(2E,4E)-5-(3,4-bis(decyloxy)phenyl)penta-2,4-dienal (**11c**; m = 2): General Wittig homologation procedure. The product was prepared from **11b** and isolated as a yellow solid in 96.4% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.58 (d, *J* = 8.1 Hz, 1H), 7.25 (dd, *J* = 10.4 Hz, 15.1 Hz, 1H), 7.05 (d, *J* = 1.9 Hz, 1H), 7.03 (dd, *J* = 1.9 Hz, 8.1 Hz, 1H), 6.97 (d, *J* = 15.4 Hz, 1H), 6.88-6.67 (m, 2H), 6.87-6.83 (m, 2H), 6.26 (d, *J* = 8.1 Hz, 15.3 Hz, 1H), 4.03 (m, 4H), 1.82 (m, 4H), 1.48 (m, 4H), 1.41-1.16 (m, 24H), 0.88 (t, *J* = 6.9 Hz,

6H); ^{13}C NMR (500 MHz, $CDC1_3$): δ 193.54, 152.62, 151.10, 149.35, 142.72, 130.53, 128.60, 124.06, 122.05, 113.23, 112.02, 69.46, 69.16, 31.92, 29.63, 29.62, 29.59, 29.57, 29.43, 29.35, 29.34, 29.30, 29.18, 26.05, 26.013, 22.69 (2 -CH_2- carbon signals), 14.10 (2 -CH_3 carbon signals); two other aliphatic carbon signals not observed due to overlapping shifts.



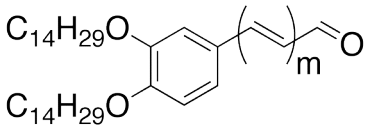
DPDCn-OC$_{10}$H$_{21}$; m = 0, 1, 2

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3,4-bis(decyloxy)phenyl)-hexa-1,3,5-triene (**DPDC3-OC$_{10}$H$_{21}$**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from **11a**. Reaction took longer than other double Knoevenagel condensations and was stirred for 48 h at 50° C. The product was isolated as a lemon yellow solid in 18.7% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 1.6 Hz, 2H), 7.30 (dd, J = 1.6 Hz, *J* = 8.4 Hz, 2H), 7.08 (s, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.76 (s, 2H), 4.07 (m, 8H), 1.85 (m, 8H), 1.49 (m, 8H), 1.40-1.20 (m, 48H), 0.88 (t, *J* = 6.4 Hz, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 152.17, 149.46, 145.32, 129.75, 126.77, 124.97, 117.24, 113.33, 113.11, 106.99, 69.64, 69.47, 32.32, 30.11, 30.03, 30.01, 29.99, 29.77, 29.54, 29.46, 28.77, 26.44, 26.37, 26.18, 23.10, 22.57, 14.52 (2 -CH_3 carbon signals); two aliphatic carbon signals were not observed due to overlapping chemical shifts.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(3,4-bis(decyloxy)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-OC$_{10}$H$_{21}$**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **11b**. Reaction took longer than other double Knoevenagel condensations and was run for 48 h at 50° C. The product was isolated as a purple solid in 9.6% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.16-7.04 (m, 6H), 6.97-6.84 (m, 6H), 6.52 (s, 2H), 4.04 (m, 8H), 1.86 (m, 8H), 1.50 (m, 8H), 1.38 (m, 48H), 0.88 (m, 12H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 151.27, 149.42, 145.49, 142.20, 128.71, 128.63, 122.68,

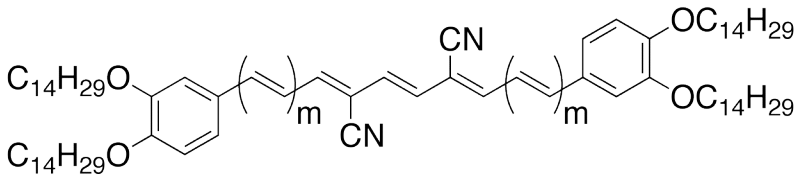
122.31, 115.59, 113.21, 111.99, 110.32, 69.48, 69.15, 31.92, 29.63, 29.61, 29.58, 29.44, 29.40, 29.36, 29.34, 29.32, 29.17, 26.05, 26.00, 22.69 (2 -CH_2- carbon signals), 14.10 (2 -CH_3 carbon signals); two aliphatic carbon signals were not observed due to overlapping chemical shifts.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(3,4-bis(decyloxy)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-OC$_{10}$H$_{21}$**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **11c**. Reaction took longer than other double Knoevenagel condensations and was run for 48 h at 50° C. The product was isolated as a purple solid in 25.6% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.03-6.65 (m, 18H), 4.05 (m, 8H), 1.86 (m, 8H), 1.51 (m, 8H), 1.30 (m, 48H), 0.91 (t, J = 6.4 Hz, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 150.1, 149.7, 145.2, 143.0, 139.1, 129.9, 129.2, 128.3, 126.5, 121.8, 115.9, 113.7, 111.8, 111.1, 69.7, 69.6, 32.3, 30.0 2 -CH_3 carbon signals, 29.8 (2 -CH_3 carbon signals), 29.7, 29.6, 26.4 (2 -CH_3 carbon signals), 23.1, 14.5 (2 -CH_3 carbon signals); five aliphatic carbon signals were not observed due to overlapping chemical shifts.



3,4-bis(tetradecyloxy)benzaldehyde (**12a**; m = 0): This product was prepared by reaction of 3,4-dihydroxybenzaldehyde with 1-bromotetradecane under basic conditions. Detailed preparation and characterization has been reported by Binnemanns and coworkers.[1]

3,4-bis(tetradecyloxy)cinnamaldehyde (**12b**; m = 1): General Wittig homologation procedure. The product was prepared from **12a** and isolated by column chromatography (5% ethylacetate in hexnes) as a light yellow solid in 53.4% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.66 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 15.9 Hz, 1H), 7.13 (dd, *J* = 2.1 Hz, 8.1 Hz, 1H), 7.08 (d, *J* = 1.8 Hz, 1H), 6.89 (d, *J* = 8.1 Hz, 1H), 6.63 (dd, *J* = 7.8 Hz, 15.9 Hz, 1H), 4.04 (m, 4H), 1.84 (m, 4H), 1.78-1.02 (m, 44H), 0.88 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.79, 153.31, 152.75, 149.78, 127.31, 126.93, 123.78, 113.32, 123.96, 69.81, 69.50, 35.06, 34.91, 32.33, 31.98, 30.11, 29.81, 29.77, 29.63, 29.51, 29.45, 26.42, 26.39, 25.66, 23.07, 23.03, 21.03 (2 -CH_2- carbon signals), 14.43 (2 -CH_3 carbon signals); seven aliphatic peaks not observed due to overlapping chemical shifts.

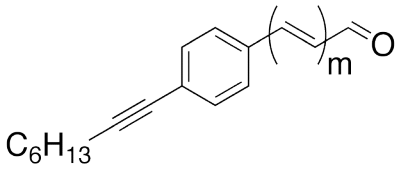


DPDCn-$OC_{14}H_{29}$; m = 0, 1

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3,4-bis(tetradecyloxy)phenyl)-hexa-1,3,5-triene (**DPDC3-$OC_{14}H_{29}$**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from **12a**. Reaction took longer than other double Knoevenagel condensations and was run for 36 h at 60° C. The product was isolated as a lemon yellow solid in 15.9% yield with a small amount of starting material as impurity. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.60 (d, *J* = 1.8 Hz, 2H), 7.33 (dd, *J* = 1.8 Hz, 8.4 Hz, 2H), 7.09 (s, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.78 (s, 2H), 4.08 (m, 8H), 1.86 (m, 8H), 1.49 (m, 8H), 1.28 (m, 80H), 0.90 (t, *J* = 6.9 Hz, 12H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 151.96, 149.26, 144.83, 129.40, 126.51, 124.52, 116.73, 113.43, 113.08, 106.73, 69.41, 69.20, 31.89, 29.67, 29.62, 29.59, 29.57, 29.38, 29.34, 29.31, 29.19, 29.12, 26.03, 25.96, 22.63 (2 -CH_2- signals), 14.01 (2 -CH_3 signals); ten carbon signals not observed due to overlapping chemical shifts.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(3,4-bis(tetradecyloxy)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-$OC_{14}H_{29}$**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **12b**. Reaction took longer than other double Knoevenagel condensations and was run for 36 h at 60° C. The product was isolated as a purple solid in 24.5% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.16 (dd, *J* = 11.4 Hz, 15.0 Hz, 2H), 7.07 (m, 4H), 6.98-6.84 (m, 6H), 6.65 (s, 2H), 4.04 (m, 8H), 1.84 (m, 8H), 1.50 (m, 8H), 1.42-1.18 (m, 80H), 0.88 (m, 12H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 151.27,

149.42, 145.49, 142.19, 128.71, 128.63, 122.67, 122.31, 115.59, 113.21, 111.99, 110.33, 69.48, 69.15, 31.93, 29.72, 29.67, 29.64, 29.62, 29.45, 29.40, 29.37, 29.32, 29.18, 26.05, 26.01, 22.69 (2 -CH_2- signals), 14.11 (2 -CH_3 signals); ten carbon signals not observed due to overlapping chemical shifts.

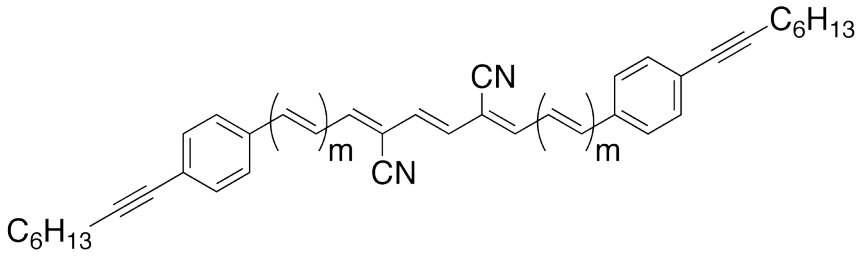


4-(oct-1-ynyl)benzaldehyde (**13a**; m = 0): This compound was prepared by modifying the reported procedure.[18] 4-bromobenzaldehyde (1.0 g, 5.4 mmol), PPh_3 (10 mol%), $PdCl_2(PPh_3)_2$ (5 mol%) and 25 mL of THF combined into a flame dried 100-mL round-bottomed flask to make a yellow suspension. The suspension was degassed with nitrogen gas for 10 min before copper(I) iodide (10 mol%) was added and the suspension was further degassed for another 10 min. During this time the suspended solid dissolved into an orange solution. 1-octyne was added via syringe and the reaction was heated at 40° C for 16 h. The resulting brown solution was cooled to room temperature and diluted with diethyl ether, washed with water and dried over $MgSO_4$. After removing the solvent under reduced pressure the product was isolated by flash column chromatography in hexanes/ethyl acetate (3:1), yielding a crude product as a light brown/yellow oil (99.0%). Spectroscopic data agrees with the literature. This product was not purified further but used in the next step as is. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.97 (s, 1H), 7.80 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 2.43 (t, J = 7.2 Hz, 2H), 1.60 (m, 2H), 1.45 (m, 2H), 1.30 (m, 4H), 0.91 (t, J = 6.9 Hz, 3H); ^{13}C NMR ($CDC1_3$): δ 191.7, 135.4, 132.4, 131.0, 129.8, 95.7, 80.5, 31.7, 29.0, 28.9, 22.9, 19.9, 14.5.

(E)-(4-(oct-1-ynyl)phenyl)acrylaldehyde (**13b**; m = 1): General Wittig homologation procedure. The product was prepared from **13a** and isolated by column chromatography (10% ethyl acetate in hexanes) as an orange oil in 31.6% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.73 (d, J = 7.8 Hz, 1H), 7.52-7.43 (m, 5H), 6.72 (dd, J = 7.8 Hz, 15.9 Hz,

1H), 2.44 (t, *J* = 7.2 Hz, 2H), 1.63 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.92 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR ($CDC1_3$): δ 193.9, 152.3, 133.3, 132.5, 129.0, 128.7, 127.6, 94.3, 80.7, 31.7, 29.0, 28.9, 23.0, 19.9, 14.5.

(2E,4E)-5-(4-(oct-1-ynyl)phenyl)penta-2,4-dienal (**13c**; m = 2): General Wittig homologation procedure. The product was prepared from **13b** and isolated by column chromatography (10% ethyl actete in hexanes) as a dark orange oil in 74.1% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.65 (d, *J* = 8.1 Hz, 1H), 7.45-7.38 (m, 4H), 7.31-7.22 (ddd, *J* = 4.8 Hz, 6.7 Hz, 10.3 Hz, 1H), 6.99 (m, 2H), 6.31 (dd, *J* = 7.8 Hz, 15.3 Hz, 1H), 2.44 (t, *J* = 6.9 Hz, 2H), 1.63 (m, 2H), 1.47 (m, 2H), 1.33 (m, 4H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.8, 152.1, 142.0, 135.0, 132.4, 132.1, 127.7, 126.9, 125.9, 93.5, 80.8, 31.7, 29.1, 29.0, 22.9, 19.9, 14.4.

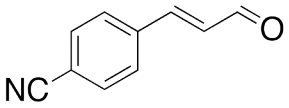


DPDCn-C_8H_{13}; m = 0, 1, 2

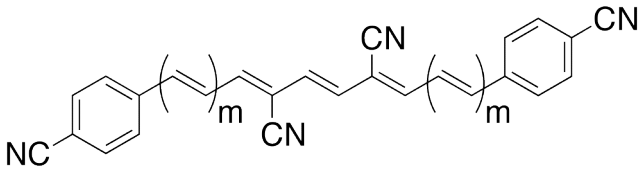
(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-(oct-1-ynyl)phenyl)-hexa-1,3,5-triene (**DPDC3-C_8H_{13}**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from **13a** and isolated as a lemon yellow solid in 45.6% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 4H), 7.46 (d, *J* = 8.1 Hz, 4H), 7.15 (s, 2H), 6.84 (s, 2H), 2.44 (d, *J* = 6.6 Hz, 4H), 1.62 (m, 4H), 1.49 (m, 4H), 1.34 (m, 8H), 0.91 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 145.1, 132.6, 132.5, 130.9, 129.7, 127.5, 116.4, 109.9, 94.8, 80.8, 31.7, 29.0, 28.9, 22.9, 20.0, 14.4.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-(oct-1-ynyl)phenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-C_8H_{13}**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **13b** and isolated as an orange-red solid in 7.6% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48 (d, *J* = 8.1 Hz, 4H), 7.42 (d, *J* = 8.4 Hz, 4H), 7.31 (dd, *J* = 11.7 Hz, 15.3 Hz, 2H), 7.02 (d, *J* = 15.6 Hz, 2H), 6.98 (d, *J* = 15.3 Hz, 2H), 6.71 (s, 2H), 2.45 (d, *J* = 6.9 Hz, 4H), 1.64 (m, 4H), 1.47 (m, 4H), 1.35 (m, 8H), 0.93 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 145.56, 141.77, 135.04, 132.48, 129.64, 127.90, 126.13, 125.39, 115.52, 112.41, 93.79, 80.92, 31.75, 29.03, 29.02, 22.94, 19.98, 14.44.

(1E,3E,5Z,7E,9Z,11E,13E)-6,9-dicyano-1,14-di-(4-(oct-1-ynyl)phenyl)-tetradeca-1,3,5,7,9,11,13-heptaene (**DPDC7-C_8H_{13}**; m = 2): General double Knoevenagel condensation procedure. The product was prepared from **13c** and isolated as a purple solid in 48.9% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.37 (s, 8H), 6.98-6.75 (m, 10H), 6.65 (s, 2H), 2.42 (d, *J* = 6.6 Hz, 4H), 1.63 (m, 4H), 1.47 (m, 4H), 1.33 (m, 8H), 0.91 (t, *J* = 6.6 Hz, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 145.1, 142.5, 138.3, 135.9, 132.4, 129.6, 129.5, 128.8, 127.3, 125.1, 115.6, 112.0, 93.1, 81.0, 31.7, 29.1, 29.0, 22.9, 20.0, 14.4.



trans-4-cyanocinnamaldehyde (**14a**): General Wittig homologation procedure. The product was prepared from 4-cyanobenzadehyde and isolated by column chromatography (15% ethyl actete in hexanes) as a dark orange oil in 98.0% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.78 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 16.2 Hz, 1H), 6.82 (dd, *J* = 7.8 Hz, 15.9 Hz, 1H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 193.3, 149.8, 138.6, 133.2, 131.6, 129.1, 118.5, 114.7.

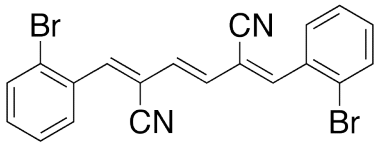


DPDCn-CN; m = 0, 1

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-cyanophenyl)-hexa-1,3,5-triene (**DPDC3-CN**; m = 0): General double Knoevenagel condensation procedure. The product was prepared from 4-cyanobenzaldehyde and isolated as a dull yellow solid in 21.8% yield. ^{1}H NMR (300 MHz, 355 K, DMSO-d_6): δ 8.01 (d, *J* = 7.8 Hz, 4H), 7.94 (d, *J* = 7.8 Hz, 4H), 7.85 (s, 2H), 7.06 (s, 2H); ^{13}C NMR (300 MHz, 355 K, DMSO-d_6): δ 145.7, 138.4, 133.5, 131.9, 130.6, 113.9, 113.1, 104.5, 106.0.

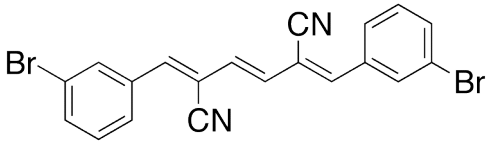
(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-cyanophenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-CN**; m = 1): General double Knoevenagel condensation procedure. The product was prepared from **14a** and isolated as an insoluble bright-orange solid in 25.8% yield.

^{1}H NMR (400 MHz, 355 K, DMF-d_7,): δ 8.05 (m, 8H), 7.81 (bd, 2H), 7.64 (bt, 2H), 7.53 (bd, 2H), 7.14 (bs, 2H); ^{13}C NMR was not obtained do to insolubility.



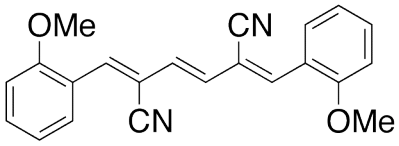
***ortho*-DPDC3-Br**

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(2-bromophenyl)-hexa-1,3,5-triene (***ortho*-DPDC3-Br**): General double Knoevenagel condensation procedure. The product was prepared from 2-bromobenzaldehyde and isolated as a pale yellow solid in 33.9% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.10 (dd, *J* = 1.5 Hz, 7.8 Hz, 2H), 7.70 (dd, *J* = 1.2 Hz, 8.1 Hz, 2H), 7.58 (s, 2H), 7.47 (td, *J* = 1.2 Hz, 7.8 Hz, 2H), 7.33 (td, *J* = 1.5 Hz, 7.8 Hz, 2H), 6.98 (s, 2H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2C1_4$): δ 144.5, 133.3, 133.2, 131.7, 130.7, 129.3, 127.7, 125.2, 115.0, 112.6.



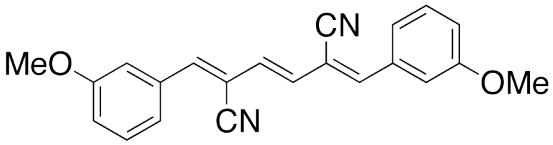
***meta*-DPDC3-Br**

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3-bromophenyl)-hexa-1,3,5-triene (***meta*-DPDC3-Br**): General double Knoevenagel condensation procedure. The product was prepared from 3-bromobenzaldehyde and isolated as a yellow solid in 24.9% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (dd, *J* = 1.7 Hz, 2H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.92 (t, *J* = 7.9 Hz, 2H), 7.15 (s, 2H), 6.88 (s, 2H); ^{13}C NMR (300 MHz, 350 K, $C_2D_2Cl_4$): d 143.3, 134.8, 133.3, 131.6, 130.2, 130.0, 127.1, 122.6, 114.7, 110.7.



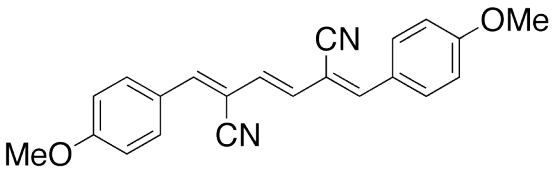
***ortho*-DPDC3-OMe**

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(2-methoxyphenyl)-hexa-1,3,5-triene (***ortho*-DPDC3-OMe**): General double Knoevenagel condensation procedure. The product was prepared from 2-methoxybenzaldehyde and isolated as a yellow solid in 8.5% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (dd, *J* = 1.4 Hz, 7.8 Hz, 2H), 7.66 (s, 2H), 7.43-7.39 (m, 2H), 7.04 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.3 Hz, 2H), 6.88 (s, 2H), 3.90 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 157.99, 140.11, 132.44, 130.28, 128.34, 122.69, 120.88, 116.47, 110.89, 109.46, 55.67.



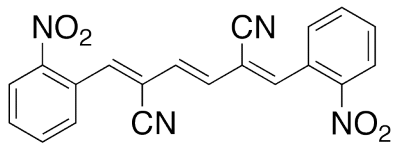
***meta*-DPDC3-OMe**

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3-methoxyphenyl)-hexa-1,3,5-triene (***meta*-DPDC3-OMe**): General double Knoevenagel condensation procedure. The product was prepared from 3-methoxybenzaldehyde and isolated as a neon yellow solid in 9.2% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (m, 2H), 7.40-7.33 (m, 4H), 7.19 (s, 2H), 7.00 (dt, *J* = 2.5 Hz, 6.6 Hz, 2H), 6.86 (s, 2H), 3.87 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 159.94, 145.60, 134.57, 130.42, 130.08, 122.52, 117.66, 116.06, 113.53, 109.76, 55.43.



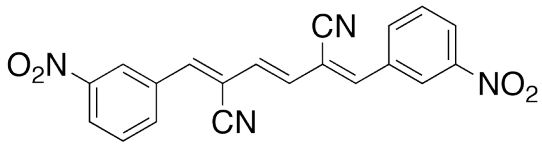
***para*-DPDC3-OMe**

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-methoxyphenyl)-hexa-1,3,5-triene (***para*-DPDC3-OMe**): General double Knoevenagel condensation procedure. The product was prepared from 4-methoxybenzaldehyde and isolated as a yellow solid in 11.4% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.83 (d, J = 8.4, 4H), 7.57 (s, 2H), 7.06 (d, J = 8.4, 4H), 6.82 (s, 2H), 3.85 (s, 6H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 161.1, 144.7, 130.6, 128.5, 125.9, 115.8, 114.3, 105.8, 55.1.



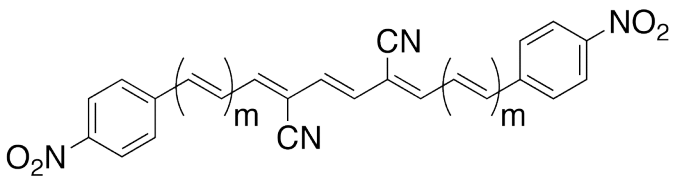
***ortho*-DPDC3-NO_2**

(1*Z*,3*E*,5*Z*)-2,5-dicyano-1,6-di-(2-nitrophenyl)-hexa-1,3,5-triene (***ortho*-DPDC3-NO_2**): This product could not be synthesized from 2-nitrobenzaldehyde using our method.



***meta*-DPDC3-NO_2**

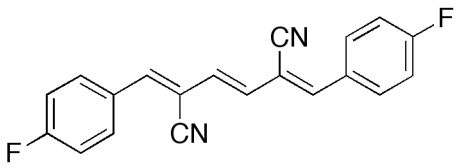
(1Z,3E,5Z)-2,5-dicyano-1,6-di-(3-nitrophenyl)-hexa-1,3,5-triene (***meta*-DPDC3-NO_2**): General double Knoevenagel condensation procedure was modified. The base, DBU, was substituted with catalytic amounts sodium methoxide. The product was prepared from 3-nitrobenzaldehyde and isolated as a yellow solid in 10.9% yield. ^{1}H NMR (500 MHz, $C_2D_2C1_4$): δ 8.67 (s, 2H), 8.33 (d, J = 8.2 Hz, 2H), 8.22 (d, J = 7.8 Hz, 2H), 7.71 (t, J = 8.0 Hz, 2H), 7.37 (s, 2H), 6.99 (s, 2H); ^{13}C NMR (500 MHz, $C_2D_2C1_4$): δ 149.9, 144.7, 136.0, 135.9, 132.6, 131.8, 126.8, 125.4, 116.5, 113.8.



DPDCn-NO_2; m = 0, 1

(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-nitrophenyl)-hexa-1,3,5-triene (**DPDC3-NO_2**; m = 0): General double Knoevenagel condensation procedure was modified. The base, DBU, was substituted with catalytic amounts sodium methoxide. The product was prepared from 4-nitrobenzaldehyde and isolated as a yellow solid in 24.0% yield. ^{1}H NMR (500 MHz, $C_2D_2C1_4$): δ 8.33 (d, *J* = 8.5 Hz, 4H), 8.02 (d, *J* = 8.5 Hz, 4H), 7.36 (s, 2H), 7.00 (s, 2H); ^{13}C NMR (500 MHz, $C_2D_2C1_4$): δ 147.89, 142.98, 138.37, 131.22, 129.65, 123.78, 114.51, 112.67.

(1E,3Z,5E,7Z,9E)-4,7-dicyano-1,10-di-(4-nitrophenyl)-deca-1,3,5,7,9-pentaene (**DPDC5-NO_2**; m = 1): General double Knoevenagel condensation procedure was modified. The base, DBU, was substituted with catalytic amounts sodium methoxide. The product was prepared from *trans*-4-nitrocinnamaldehyde and isolated as a dark orange solid in 11.4% yield. ^{1}H NMR (400 MHz, 350 K, $C_2D_2C1_4$): δ 8.26 (d, *J* = 8.0 Hz, 4H), 7.71 (d, *J* = 8.0 Hz, 4H), 7.48-7.33 (m, 2H), 7.18-6.80 (m, 6H); ^{1}H NMR (400 MHz, 373 K, DMSO-d_6): δ 8.26 (d, *J* = 8.3 Hz, 4H), 7.93 (d, *J* = 8.3 Hz, 4H), 7.64 (d, *J* = 10.8 Hz, 2H), 7.44-7.32 (m, 4H), 6.94 (s, 2H); ^{13}C NMR could not be obtained due to limited solubility.



(1Z,3E,5Z)-2,5-dicyano-1,6-di-(4-fluorophenyl)-hexa-1,3,5-triene (**DPDC3-F**): General double Knoevenagel condensation procedure. The product was prepared from 4-fluorobenzaldehyde and isolated as a pale yellow solid in 33.4% yield. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.92 (bs, 4H), 7.75 (s, 2H), 7.35 (bs, 2H), 6.93 (s, 2H); ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.92 (m, 4H), 7.18 (m, 6H), 6.84 (s, 2H); ^{13}C NMR (400 MHz, $C_2D_2Cl_4$): δ 165.0, 143.4, 131.0, 130.9, 129.7, 115.8, 115.6 109.1; ^{19}F NMR (400 MHz, $C_2D_2Cl_4$): δ 106.2.

A3. UV-Vis Absorption Spectroscopy

General Procedure and Instrumentation: Absorption spectra were taken on an Agilent Technologies 8453 UV-Vis spectrophotometer. Solutions of oligoenes were prepared in dichloromethane solution at a concentration between 10^{-5} and 10^{-6} M. A quartz quevette with path length equal to 1.0 cm was used in the collection of each spectrum.

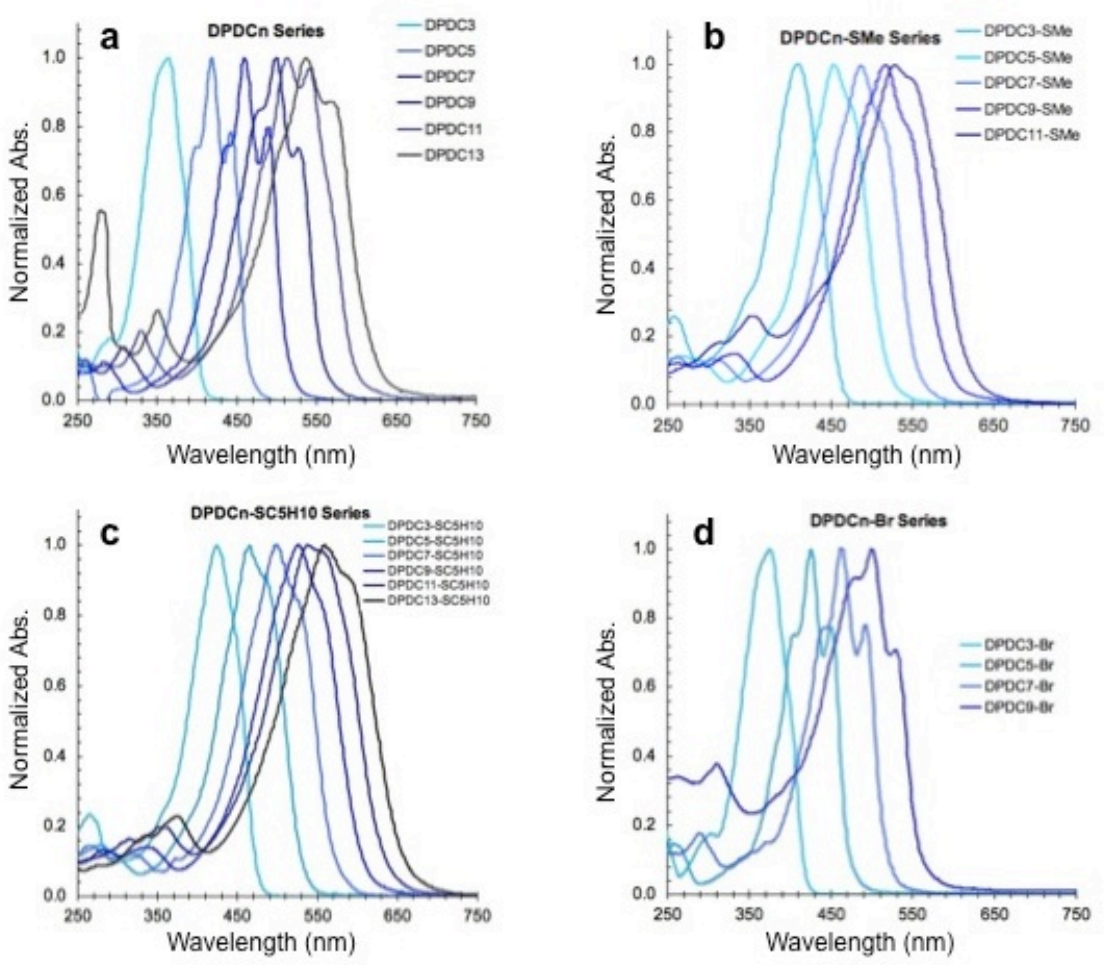


Figure A1: Optical abortion spectra of different families of α,ω-diphenyl-μ,ν-dicyano-oligoenes: (a) the unfunctionalized **DPDCn** series (n = 3 to 13), (b) **DPDCn-SMe** (n = 3 to 11), (c) **DPDCn-SC_5H_{10}** (n = 3 to 13) and (d) **DPDCn-Br** (n = 3 to 9). In all cases the spectra shift towards the red with increasing oligoene length (n). All spectra obtained in dichloromethane.

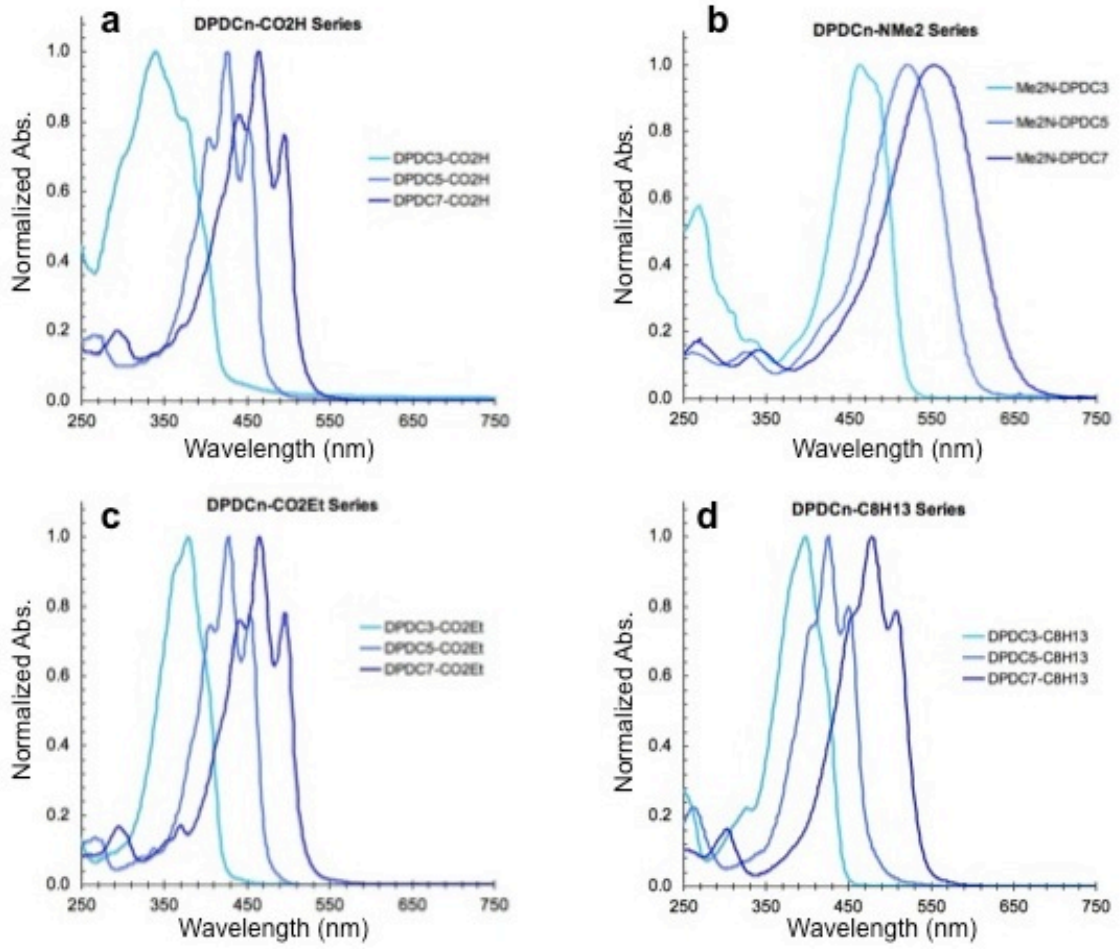


Figure A2: Optical abortion spectra of the (a) **DPDCn-CO_2H** series (n = 3, 5 and 7) in tetrahydrofuran solutions, as well as (b) **DPDCn-NMe_2** (n = 3, 5 and 7), (c) **DPDCn-CO_2Et** (n = 3, 5 and 7) and (d) **DPDCn-C_8H_{13}** (n = 3, 5 and 7) in dichloromethane solutions. In all cases the spectra shift towards the red with increasing oligoene length (n).

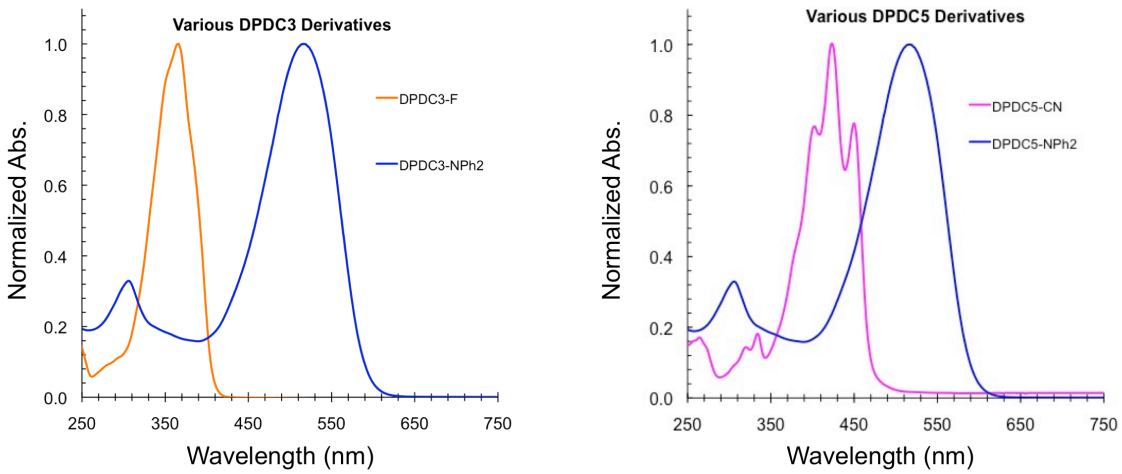


Figure A3: Optical abortion spectra of various (a) **DPDC3-X** derivatives, where X = **F** (orange line) and **NPh_2** (blue line); and (b) **DPDC5-X** derivatives, where X = **CN** (purple line) and **NPh_2** (dark blue line). All spectra obtained in dichloromethane solutions.

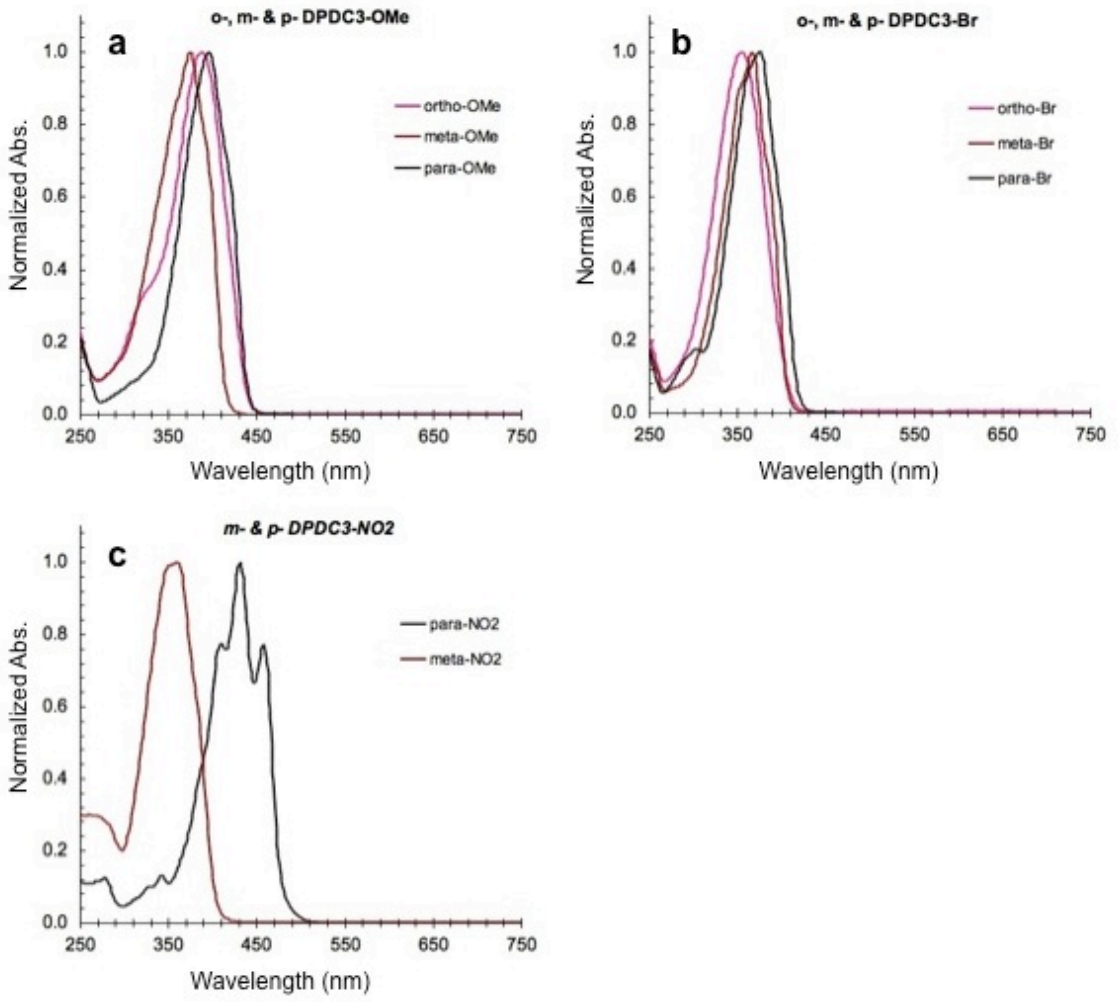


Figure A4: Effects on the substitution pattern of electron-donating and electron-withdrawing groups were investigated. UV-Vis absorption spectra (a) **DPDC3-OMe**, (b) **DPDC3-Br** and (c) **DPDC3-NO_2** derivatives were taken in dichloromethane solutions. Our observations agree well with Hammett coefficients suggesting that *para*-substitutions are most strongly coupled to the π-conjugated oligoene backbone.

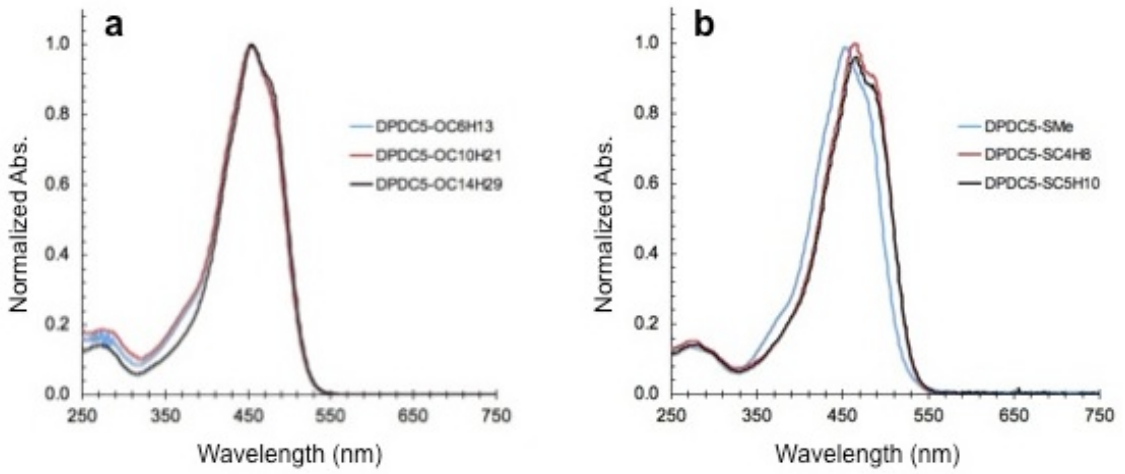


Figure A5: The physical properties can be tuned independently from the electronic structure as shown in the following collections of **DPDC5** derivatives: (a) **DPDC5-OC_6H_{13}**, **DPDC5-$OC_{10}H_{21}$**, **DPDC5-$OC_{14}H_{29}$**; and (b) **DPDC5-SMe**, **DPDC5-SC_4H_8**, **DPDC5-SC_5H_{10}**. Spectra obtained in dichloromethane solutions.

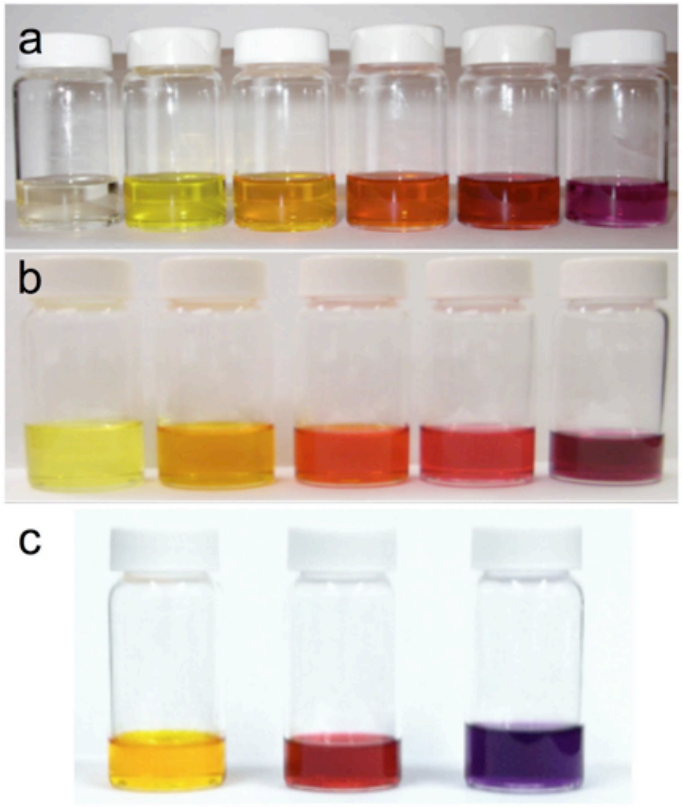


Figure A6: Photograph of dilute solutions (~10^{-4} M) of oligoene series (a) **DPDCn** (b) **DPDCn-SMe** and (c) **DPDCn-NMe_2** in dichloromethane.

Extinction Coefficient Values for DPDCn's and Their Derivatives:

Molecule	Wavelength (nm)	Extinction ($cm^{-1}*mol^{-1}$)
DPDC3	353[a]	5.00×10^4
	366	5.44×10^4
	383[a]	3.78×10^4
DPDC5	399[a]	7.51×10^4
	418	1.00×10^5
	442	7.85×10^4
DPDC7	284	1.34×10^4
	438	8.69×10^4
	460	1.16×10^5
	489	1.02×10^5
DPDC9	307	1.54×10^4
	480	9.69×10^4
	498	1.13×10^5
	526	8.40×10^4
DPDC11	330	2.73×10^4
	485[a]	9.36×10^4
	512	1.27×10^5
	540	1.22×10^5
DPDC13[c]	351	3.14×10^4
	510[a]	9.45×10^4
	536	1.24×10^5
	572	1.09×10^5
DPDC3-SMe	225	1.45×10^4
	412	7.33×10^4
DPDC5-SMe	267	1.18×10^4
	453	8.25×10^4
	476[a]	7.11×10^4
DPDC7-SMe	263	1.44×10^4
	309	1.46×10^4
	487	1.04×10^5
	513[a]	8.59×10^4
DPDC9-SMe[c]	308	2.34×10^4
	476[a]	1.22×10^5
	498	1.41×10^5
	526	1.03×10^5
DPDC11-SMe[c]	312[a]	1.93×10^4
	350	2.57×10^4
	497[a]	7.10×10^4
	527	9.00×10^4
	555[a]	8.12×10^4

DPDC3-SC_4H_8	263	3.87×10^4
	382	5.62×10^4
	485[a]	4.74×10^4
DPDC5-SC_4H_8	280	1.41×10^4
	463	9.61×10^4
	485[a]	8.57×10^4
DPDC7-SC_4H_8	274	5.38×10^4
	497	1.24×10^5
	525[a]	1.03×10^5
DPDC9-SC_4H_8	336	2.23×10^4
	523	1.07×10^5
	552[a]	8.82×10^4
DPDC11-SC_4H_8	353	2.52×10^4
	359	2.52×10^4
	537	1.22×10^5
	557	1.18×10^5
DPDC3-SC_5H_{10}	264	1.19×10^4
	424	6.72×10^4
	447[a]	5.29×10^4
DPDC5-SC_5H_{10}	280	1.18×10^4
	463	7.62×10^4
	484[a]	6.91×10^4
DPDC7-SC_5H_{10}	271	1.41×10^4
	317	1.32×10^4
	498	1.04×10^5
	526[a]	8.75×10^4
DPDC9-SC_5H_{10}	284	1.27×10^4
	339	1.38×10^4
	526	9.23×10^4
	555[a]	7.71×10^4
DPDC11-SC_5H_{10}	353	2.50×10^4
	360	2.54×10^4
	539	1.28×10^5
	558[a]	1.26×10^5
DPDC13-SC_5H_{10}	336	2.39×10^4
	375	3.12×10^4
	658	1.27×10^5
	589[a]	1.13×10^5
DPDC3-NMe_2	264	6.82×10^3
	383[a]	3.55×10^4
	464	3.19×10^4
	485[a]	7.38×10^3

DPDC5-NMe_2	264	1.33×10^4
	325	1.14×10^4
	521	8.82×10^4
DPDC7-NMe_2	328	1.25×10^4
	426[a]	2.26×10^4
	521	9.09×10^4
DPDC3-NPh_2	303	2.03×10^4
	476	4.84×10^4
DPDC5-NPh_2	306	2.80×10^4
	516	8.45×10^4
DPDC3-Br	242	1.08×10^4
	359[a]	5.59×10^4
	377	6.49×10^4
	396[a]	4.31×10^4
DPDC5-Br	258	1.37×10^4
	404[a]	7.67×10^4
	425	1.03×10^5
	450	8.00×10^4
DPDC7-Br	290	1.46×10^4
	371[a]	1.32×10^4
	441	7.58×10^4
	463	9.88×10^4
	492	7.76×10^4
DPDC9-Br[c]	311	1.24×10^4
	477[a]	6.01×10^4
	501	6.98×10^4
	529	5.08×10^4
DPDC3-CO_2H[b]	368[a]	5.13×10^4
	383	5.60×10^4
	404[a]	3.62×10^4
DPDC5-CO_2H[b]	343[a]	6.16×10^3
	384[a]	1.91×10^4
	411[a]	3.90×10^4
	434	5.17×10^4
	460	4.06×10^4
DPDC7-CO_2H[b]	296	1.27×10^4
	450	4.84×10^4
	474	6.19×10^4
	505	4.93×10^4
DPDC3-CO_2Et	362[a]	5.70×10^4
	378	6.18×10^4
	398[a]	3.94×10^4

DPDC5-CO_2Et	266	1.37×10^4
	337	1.38×10^4
	405	8.24×10^4
	427	1.10×10^5
	453	8.48×10^4
DPDC7-CO_2Et[c]	295	8.94×10^3
	370	9.18×10^3
	441	4.32×10^4
	465	5.68×10^4
	496	4.43×10^4
DPDC3-OC_6H_{13}	258	1.33×10^4
	411	6.40×10^4
	432[a]	5.03×10^4
DPDC5-OC_6H_{13}	276	9.53×10^3
	427[a]	5.27×10^4
	454	7.50×10^4
	476[a]	6.69×10^4
DPDC7-OC_6H_{13}	271	9.73×10^3
	305	9.20×10^3
	493	8.58×10^4
	521[a]	7.10×10^4
DPDC3-$OC_{10}H_{21}$	247	1.47×10^4
	411	3.47×10^4
	431[a]	2.73×10^4
DPDC5-$OC_{10}H_{21}$	278	1.38×10^4
	454	8.20×10^4
	474[a]	7.28×10^4
DPDC7-$OC_{10}H_{21}$	300	1.45×10^4
	492	4.96×10^4
	519[a]	4.14×10^4
DPDC3-C_8H_{13}	249	1.37×10^4
	379[a]	5.85×10^4
	399	7.16×10^4
	423[a]	4.64×10^4
DPDC5-C_8H_{13}	279	1.34×10^4
	420[a]	6.89×10^4
	443	9.08×10^4
	470	6.97×10^4
DPDC7-C_8H_{13}	303	2.36×10^4
	453[a]	1.10×10^5
	478	1.43×10^5
	508	1.13×10^5
DPDC3-CN	238	1.34×10^4

	361[a]	5.29 x 10^4
	376	5.68 x 10^4
	395[a]	3.74 x 10^4
DPDC5-CN	264	1.51 x 10^4
	402	7.61 x 10^4
	424	1.03 x 10^5
	450	8.12 x 10^4
***ortho*-DPDC3-Br**	230	9.26 x 10^3
	355	3.79 x 10^4
***meta*-DPDC3-Br**	240	9.92 x 10^3
	352[a]	4.96 x 10^4
	367	5.52 x 10^4
	385[a]	3.66 x 10^4
***ortho*-DPDC3-OMe**	242	8.57 x 10^3
	321[a]	1.10 x 10^4
	389	3.60 x 10^4
***meta*-DPDC3-OMe**	229	1.20 x 10^4
	374	4.76 x 10^4
***para*-DPDC3-OMe**	249	1.14 x 10^4
	396	5.72 x 10^4
***meta*-DPDC3-NO_2[c]**	281	1.81 x 10^3
	359	3.09 x 10^3
DPDC3-NO_2	236	7.29 x 10^3
	267	6.69 x 10^3
	390	4.59 x 10^4
	414[a]	2.89 x 10^4
DPDC5-NO_2	228	3.21 x 10^4
	415[a]	5.20 x 10^4
	437	6.77 x 10^4
	462	5.20 x 10^4
DPDC3-F	236	1.18 x 10^4
	367	5.60 x 10^4
	382[a]	4.27 x 10^4

Table A1: UV-vis spectra were obtained in dichloromethane solutions. [a]Peaks were not well-defined; absorption shoulder. [b]Spectra were obtained in DMSO due to limited solubility. [c]There is more error in these values due to their extreme insolubility.

#	Solvent	λmax (nm)
1	nitrobenzene	539
2	dimethyl sulfoxide	533
3	1,1',2,2'-Tetrachloroethane	529
4	dimethylformamide	523
5	chlorobenzene	523
6	methylene chloride	520
7	chloroform	518
8	tetrahydrofuran	514
9	acetonitrile	512
10	acetone	512
11	benzene	511
12	toluene	511
13	ethyl acetate	506
14	diethyl ether	500
15	n-heptane	484

Table A2: Solvatochromism survey in the UV-vis absorption maxima for **DPDC-NMe$_2$**.

A4. Cyclic Voltammetry

General Procedure and Data Analysis: Cyclic voltammetry (CV) was preformed using a CHI600c potentiometer. All electrodes were purchased from Bioanalytical Systems, Inc; working electrode was a glass carbon electrode (MF-2070), reference electrode was Ag/AgCl (MF-2062), and auxiliary electrode was a platinum electrode (MW-4130). All measurements were carried out under argon in dimethylformamide (DMF) solution with tetrabutylammonium hexafluorophosphate electrolyte (0.1 M) and oligoene (350 μM). Ferrocene was used as an internal standard. To assure that the addition of the internal standard did not affect the redox chemistry of the analyte, oligoene solutions were first measured without the presence of ferrocene and then again with the internal standard. Ionization potentials were then set relative to that of ferrocene at E^0 = -4.8 eV.

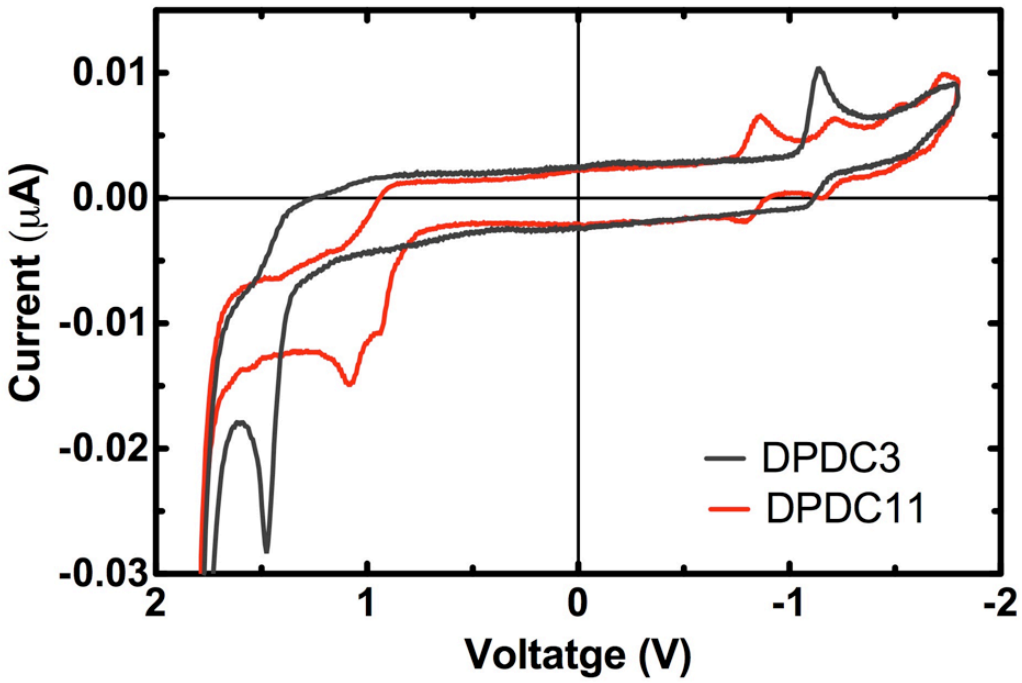


Figure A8: Comparison of ionization potentials obtained from cyclic voltammetry (CV). As a general trend, reductions become more reversible as the molecular length increases. Oxidations, on the other hand, are generally unstable, where apparent deposition of the oxidized material is observed on the electrode surface. The irreversibility of the oxidations does not change if the CV was stopped before reaching the solvent oxidation. Ferrocene was used as an internal standard.

Tabulated DPDCn Redox Potentials:

Molecule	Reductions								Oxidations			
	E_1	E^0_1	E_2	E^0_2	E_3	E^0_3	E_4	E^0_4	E_1	E^0_1	E_2	E^0_2
DPDC3	-3.09	-3.13	-	-	-	-	-	-	-5.74	-	-	-
DPDC5	-3.25	-3.28	-	-	-	-	-	-	-5.47	-	-	-
DPDC7	-3.29	-3.34	-2.85	-2.90	-2.51	-	-	-	-5.32	-	-5.57	-
DPDC9	-3.33	-3.38	-2.97	-3.02	-2.90	-2.76	-	-	-5.25	-	-5.42	-
DPDC11	-3.37	-3.43	-3.03	-3.07	-2.97	-2.84	-2.49	-	-5.19	-	-5.34	-
DPDC13	-3.38	-3.44	-3.06	-3.11	-3.06	-2.94	-2.59	-	-5.14	-	-5.27	-

Table A3. Ionization potentials obtained by CV. Oligoene solutions (350 μM) were prepared in DMF with tetrabutylammonium hexafluorophosphate electrolyte (0.1 M). All value are relative to ferrocene (E^0 = -4.8 eV) as internal standard.

DPDCn	**DPDC3**	**DPDC5**	**DPDC7**	**DPDC9**	**DPDC11**	**DPDC13**
LUMO	-3.125	-3.275	-3.335	-3.375	-3.425	-3.435
HOMO	-5.740	-5.470	-5.320	-5.250	-5.190	-5.140
DPOn	**DPO3**	**DPO5**	**DPO7**			
LUMO	-2.448	-2.650	-2.770			
HOMO	-5.298	-5.193	-4.969			
Difference in LUMO	0.677	0.625	0.565			
Difference in HOMO	0.442	0.277	0.351			

Table A4: Redox potentials estimate the HOMO and LUMO energy differences between series **DPDCn** and **DPOn**. The installation of nitriles lowers the energy of both the LUMO (up to 0.68 eV) and the HOMO (up to 0.44 eV) and shrinks the molecular band gap, E_{cv}, as much as 0.24 eV. Longer **DPOn** oligomers could not be synthesized/characterized due to their high insolubility.

A5. Particle in a Box: A Simple Model for Electron Confinement in DPDCn Series

As a simple model for small-scale confinement, the energies of a one-dimensional "particle in a box" were found to relate the optical absorptions and electrochemical redox potential gaps, E_{cv}, of the **DPDCn** series.

$$E_n = \frac{n^2\hbar^2\pi^2}{2m^*L^2} = \frac{n^2h^2}{8m^*L^2} \qquad \text{(eq. A1)}$$

where L is the molecular length, which was obtained directly from the crystal structures and measured between the *para*-positioned hydrogens at each end of the molecule (see Table S5). The strongest wavelength absorption (λ_{max}), solution optical band gap (E_{og}), and the electrochemical band gap (E_{CV}) can be described with this model. Linear regression analysis yielded fitted lines with R^2 values > 0.99. Simple extrapolative analysis to oligomers of infinite lengths predicts values that agree well with those obtained experimentally for the polymer, polyacetylene.

L (nm)	$1/L^2$ (nm^{-2})	λ_{max} (eV)	E_{OG} (eV)	E_{CV} (eV)
1.633	0.3752	3.39	2.86	2.62
2.104	0.2259	2.97	2.42	2.20
2.591	0.1490	2.70	2.13	1.99
3.077	0.1056	2.49	1.97	1.88
3.555	0.0791	2.42	1.86	1.77
4.043	0.0612	2.31	1.76	1.71
Extrapolation Results				
slope	n/a	3.40	3.47	2.86

y-intercept	n/a	2.15	1.59	1.55

Table A5: Values used for particle in a box modeling of **DPDCn** series. Molecular length (L) was obtained from crystal structures and measured between the *para*-positioned carbons at each end of the molecule. The values for the slope and y-intercept obtained from our simple extrapolative analysis are also tabulated.

In order to calculate the resulting effective mass, data was converted to standard units of energy (erg), time (s), mass (g) and length (cm). Given the equation above the slope obtained from our linear regression would have units [erg x s].

$$slope = \frac{h^2}{8m^*} \qquad \text{(eq. A2)}$$

Thus, the appropriate value for Planck's constant was chosen, 6.626 x 10^{-27} erg x s, providing mass in grams.

$$[erg] \times [cm^2] = \frac{[erg \times s]^2}{m^*}$$

$$[erg] = \frac{[g \times cm^2]}{s^2}$$

$$m^* = [g]$$

A sample calculation gives an effective mass; To a fi.st order approximation the exciton behaves as a spatially confined quantum mechanical particle relative to the length of the molecule.

$$m^* = \frac{h^2}{8 \times (slope)}$$

$$m^* = \frac{(6.626 \times 10^{-27} erg \cdot s)^2}{8 \cdot (2.551 \times 10^{-12} erg \times cm^2)} = 2.151 \times 10^{-42} g = 2.151 \times 10^{-45} kg$$

A6. Nanoparticle Synthetic Details and SAM Preparation

General information: Gallium Arsenide (100) single crystalline wafer was purchased from Sigma-Aldrich. Ammonium Hydroxide, 30% in water (NH_4OH) and Ethanol, 200 proof (EtOH) were purchased from Fischer Scientific. Dimethyl Sulfoxide (DMSO) 99% anhydrous was purchased from Sigma-Aldrich. EtOH and DMSO were degassed over several (three or greater) freeze pump thaw cycles before use. Iron (III) chloride 97%, and oleic acid 90% were purchased from Sigma-Aldrich. Sodium oleate 97% was purchased from TCI. 1-octadecene 90% was purchased from Acros Organics. Hexane was purchased from Fischer Scientific. Monolayer formation was observed using a Hitachi S-4700 FE-SEM.

Nanoparticle Synthesis. Fe_3O_4 nanoparticles were prepared using the method developed by Hyeon *et al.*[19] Iron oleate precursor was made by adding 10.8 g of iron (III) chloride and 36.5 g of sodium oleate into a mixed solvent of 30 mL of ethanol, 40 mL of DI water and 70 mL of hexane. The reaction was kept at 60 ºC for 4 hours and the product was purified with DI water and then dried under vacuum. The 10 nm Fe_3O_4 nanoparticles were synthesized by mixing 3.6 g of iron oleate, 1.28 mL of oleic acid and 20 mL of 1-octadecene into a three neck flask, and the solution was heated to 320 ºC at a heating rate of 200 ºC/hr and kept at 320 ºC for 30 minutes. After the reaction mixture was cooled to room temperature, ethanol was added as anti-solvent to precipitate the nanoparticles by centrifugation. The precipitated nanoparticles were re-dispersed in hexane.

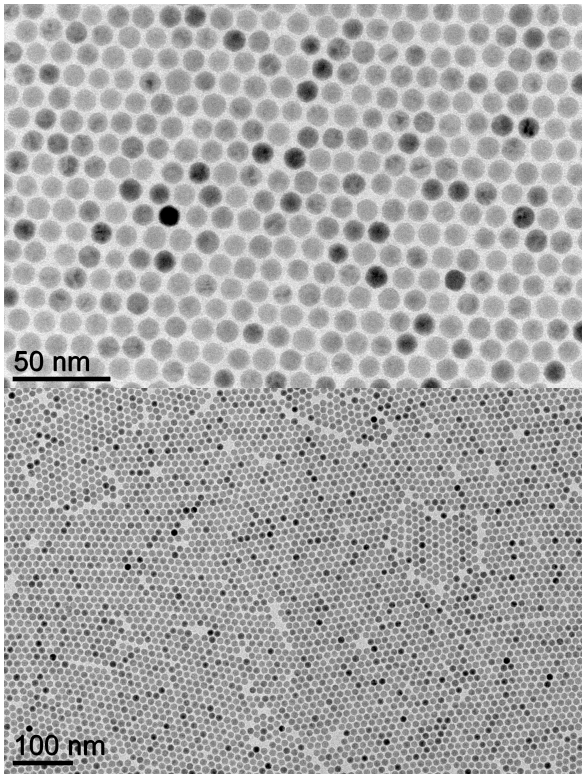


Figure A9: TEM images of as-synthesized 10-nm Fe_3O_4 nanoparticles.

Monolayer Formation Procedure. Gallium Arsenide crystal was cut into several 0.75-1.0 cm square wafers using a diamond scribe. The wafers were submerged in NH_4OH and allowed to stand covered for 10 minutes. Upon removal from the NH_4OH, a wafer is rinsed with ethanol, dried under an argon stream, rinsed and dried a second time, them immediately submerged in a 1.5 mM solution of **DPDC3-CO_2H** in dimethyl sulfoxide (DMSO). The solution is transferred to a nitrogen glove box and allowed to stand for 16 hours. After removal from the glove box, the wafer is removed from the solution, rinsed thoroughly with ethanol and dried under an argon stream. It is immediately submerged into a solution of 10-nm iron oxide (Fe_3O_4) nanoparticles in dimethylformamide, and allowed to stand 1-2 hours. Upon removal from the nanoparticle solution, the wafer is rinsed with ethanol and dried under an argon stream, at which point they are ready for microscopy (Figure S12a).

Controls. In order to probe the dependence of monolayer formation on oligoene concentration in DMSO, the above procedure was carried out using both 3.0 and 6.0 mM solutions. It was found that nanoparticle coverage increased with increasing concentration of **DPDC3-CO_2H** (Figure S12b and S12c).

We verified that monolayer formation is initiated by the oligoene connectors. Two controls were carried out: First, to eliminate the possibility that DMSO was acting as a inter-particle connector the above procedure was carried out using pure DMSO in place of the oligoene solution; secondly, in order to eliminate the possibility that submersion

into the nanoparticle solution was sufficient to generate monolayers, a wafer was placed into the nanoparticle solution directly after cleaning. No monolayer formation was observed in either case as seen in Figure S12c and S12d.

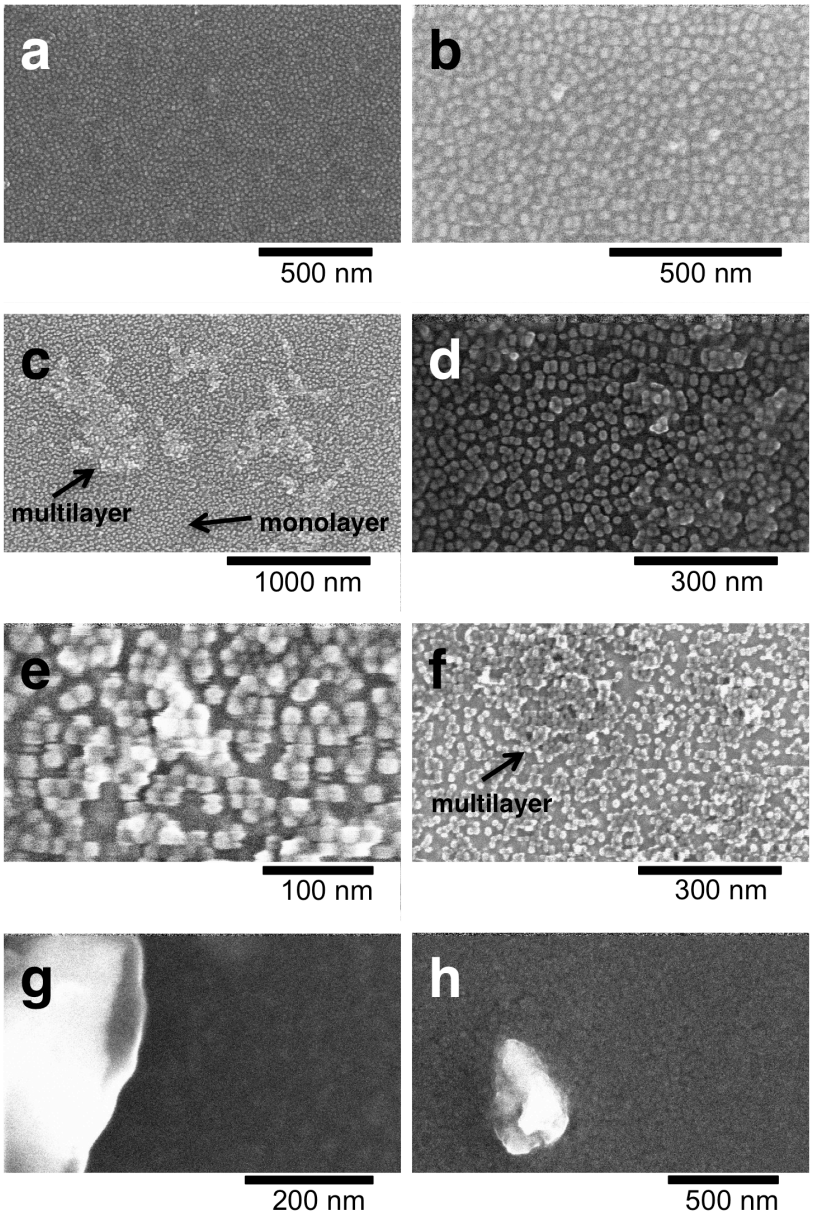


Figure A10: SEM images of monolayers of Fe_3O_4 nanoparticles formed after carrying out the above procedure using: (a) 1.5 mM **DPDC3-CO_2H,** where the scale bar represents a distance of 500 nm; (b) 1.5 mM **DPDC3-CO_2H,** where the scale bar represents a distance of 300 nm; (c) 3.0 mM **DPDC3-CO_2H,** where the scale bar represents a distance of 1 μm; (d) 3.0 mM **DPDC3-CO_2H,** where the scale bar represents a distance of 300 nm; (e) 6.0 mM **DPDC3-CO_2H,** where the scale bar represents a distance of 100 nm; (f) 6.0 mM **DPDC3-CO_2H,** where the scale bar represents a distance of at 300 nm; (g) DMSO only; (h) DMF only.

A7. Theoretical Methods and Details.

All electronic structure calculations used Jaguar (version 7.0, Schrodinger LLC, New York, NY, 2007) using the B3LYP hybrid functional and the 6-31G** basis sets. The geometries of **DPDCn** and **DPOn** were fully optimized. The final geometries, total energies, bond angles and bond distances can be found in a separate supporting information file. Below is a summary the results of our calculations on selected **DPDC5** and **DPO5** derivatives.

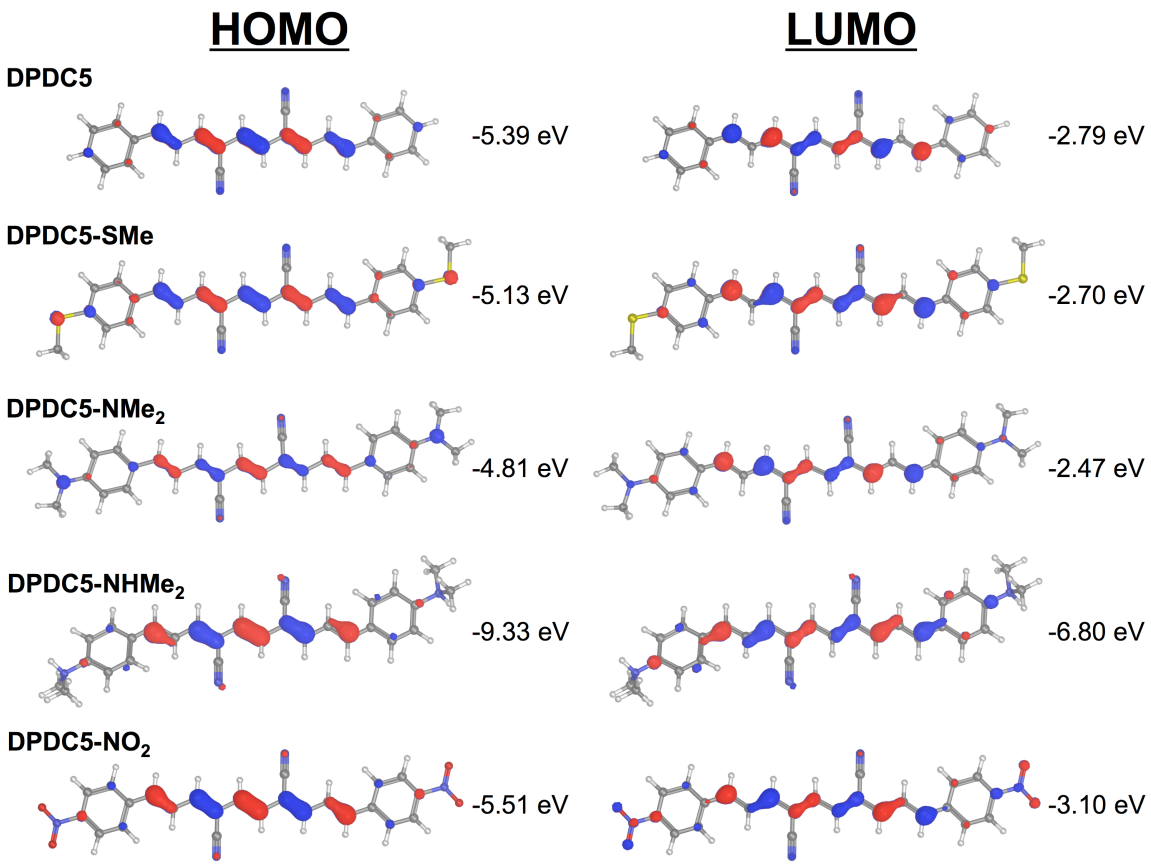


Figure A11: HOMO and LUMO topologies of selected **DPDC5** derivatives predicted by DFT B3LYP 6-31G** (gas phase).

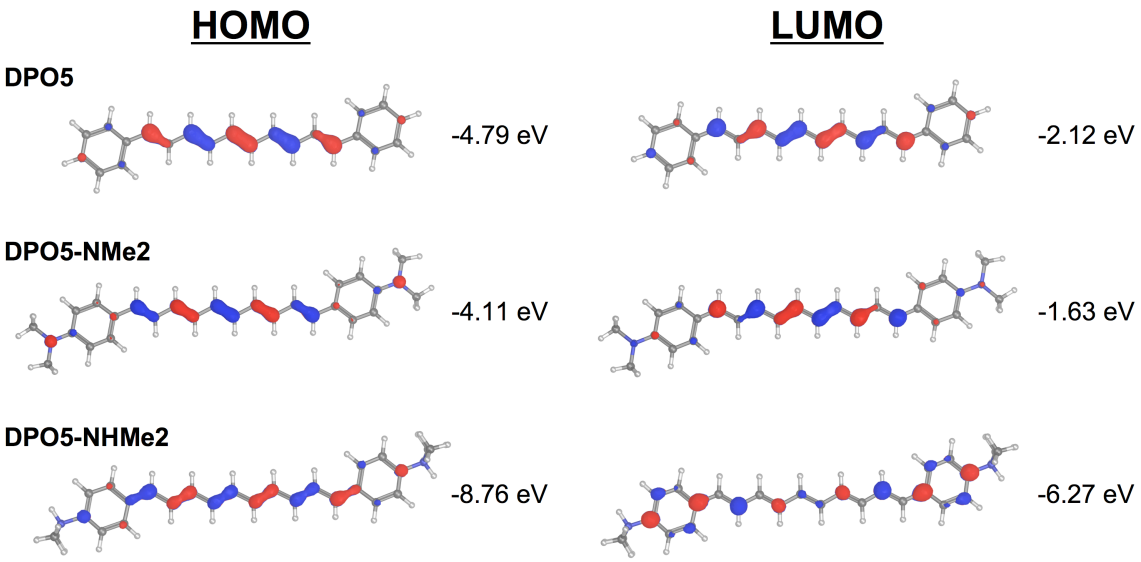


Figure A12: HOMO and LUMO topologies of selected **DPO5** derivatives predicted by DFT B3LYP 6-31G** (gas phase).

Molecule	lone pair sigma/pi	E(S1), nm	Oscillator strength
DPO5	-	413	4.3
DPDC5	-	431	3.8
DPO5- NH_2	sigma	418	4.5
DPO5- NH_2	pi	442	4.5
DPDC5- NH_2	sigma	437	3.9
DPDC5-NH_2	pi	471	4.1
DPO5-SMe	sigma	432	4.7
DPO5-SMe	pi	451	4.6
DPDC5-SMe	sigma	446	4.2
DPDC5-SMe	pi	482	4.0
DPO5-NO_2	sigma	-	-
DPO5-NO_2	pi	-	-
DPDC5-NO_2	sigma	436	4.0
DPDC5-NO_2	pi	474	3.7
DPO5-NMe_2	sigma	422	4.6
DPO5-NMe_2	pi	463	4.5
DPDC5-NMe_2	sigma	440	4.1
DPDC5-NMe_2	pi	498	4.2

Table A6. TD-DFT calculations results on the energy and character of the energy of the first excited state, E(S1), of selected DPOs and DPDCs.

A8. Comparison of DPDCn Band Gaps from Various Methods

# of Double Bonds	UV-Vis Eg (eV)†	CV Eg (eV)	DFT (eV)
3	3.01	2.62	3.14
5	2.44	2.20	2.60
7	2.15	1.99	2.24
9	2.02	1.88	2.03
11	1.81	1.77	1.86
13	1.77	1.71	1.75

Table A7: Bad Gap Estimations from various methods.

A9. References

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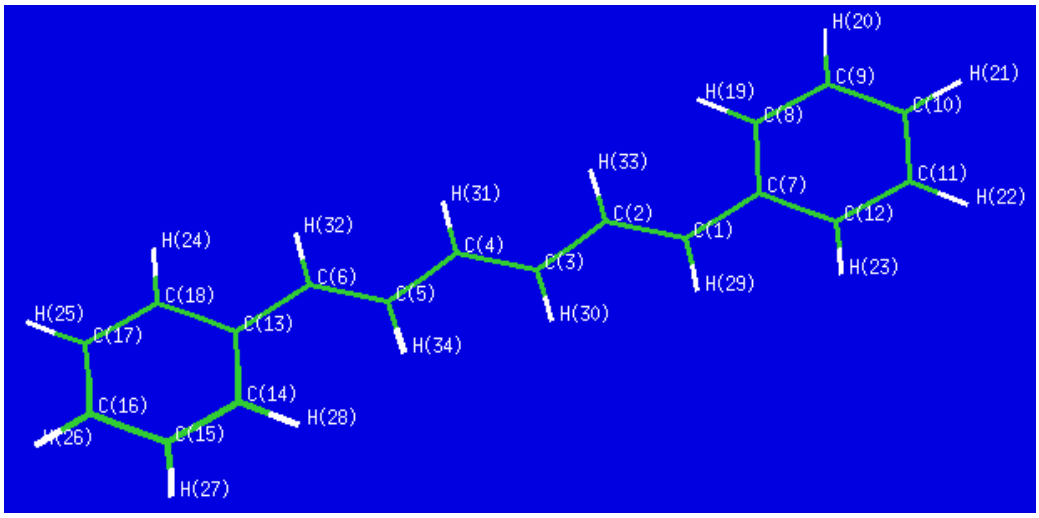
Appendix A (Part 2)

Density Functional Theory (DFT) Calculation Summary for DPDCn and DPOn

α,ω-diphenyl-oligoene Series (DPOn):

DPO3



final geometry:

	angstroms		
atom	x	y	z
C1	0.2639357739	-0.0045845578	-0.1806805468
C2	0.2807805026	-0.0019002222	1.1736092721
C3	1.4859075458	-0.0030603202	1.9566268003
C4	1.5181685464	-0.0001035078	3.3149372916
C5	2.7257553496	-0.0023191867	4.0940227597
C6	2.7510621393	0.0013705327	5.4479611439
C7	-0.9020386405	-0.0043846758	-1.0599649108
C8	-2.2319192227	-0.0016965938	-0.5920006510
C9	-3.2997549733	-0.0019110874	-1.4819850414
C10	-3.0750592389	-0.0047430685	-2.8618802365
C11	-1.7661961674	-0.0073228581	-3.3431798079
C12	-0.6962302123	-0.0071434489	-2.4529630024
C13	3.9253244806	-0.0013419265	6.3162972632
C14	5.2501270585	-0.0220463788	5.8346313761
C15	6.3274346958	-0.0234093366	6.7130483384
C16	6.1175451577	-0.0043629054	8.0951435668
C17	4.8138423461	0.0157874421	8.5900361479
C18	3.7343764119	0.0169534844	7.7112196326
H19	-2.4320654598	0.0005350516	0.4748481869
H20	-4.3164389799	0.0001402303	-1.0992188937
H21	-3.9129806966	-0.0049246081	-3.5527442902
H22	-1.5777007740	-0.0095027827	-4.4130677389
H23	0.3220220560	-0.0091726496	-2.8342280505
H24	2.7203423893	0.0326874053	8.1031689595

H25	4.6368098472	0.0304530146	9.6617738445
H26	6.9628209884	-0.0057327910	8.7770103887
H27	7.3398909800	-0.0399805421	6.3194891628
H28	5.4390349315	-0.0383040764	4.7658532635
H29	1.2252448105	-0.0073250412	-0.6936723388
H30	2.4300908700	-0.0068609272	1.4111814987
H31	0.5749260229	0.0039297217	3.8618834552
H32	1.7935082482	0.0080716467	5.9685092754
H33	-0.6556647085	0.0010842712	1.7290221234
H34	3.6594724525	-0.0067635386	3.5339054746

Final total energy: -695.549672

HOMO energy: -0.18543
LUMO energy: -0.06770

bond lengths (angstroms):

C1	-C2	:	1.354397	C1	-C7	:	1.460355
C1	-H29	:	1.089625	C2	-C3	:	1.437167
C2	-H33	:	1.088771	C3	-C4	:	1.358697
C3	-H30	:	1.090416	C4	-C5	:	1.437096
C4	-H31	:	1.090354	C5	-C6	:	1.354180
C5	-H34	:	1.088843	C6	-C13	:	1.460448
C6	-H32	:	1.089920	C7	-C8	:	1.409816
C7	-C12	:	1.408122	C8	-C9	:	1.390088
C8	-H19	:	1.085463	C9	-C10	:	1.398073
C9	-H20	:	1.086352	C10	-C11	:	1.394553
C10	-H21	:	1.086004	C11	-C12	:	1.391874
C11	-H22	:	1.086368	C12	-H23	:	1.087292
C13	-C14	:	1.409799	C13	-C18	:	1.408050
C14	-C15	:	1.390040	C14	-H28	:	1.085466
C15	-C16	:	1.398071	C15	-H27	:	1.086384
C16	-C17	:	1.394620	C16	-H26	:	1.086018
C17	-C18	:	1.391965	C17	-H25	:	1.086360
C18	-H24	:	1.087261				

bond angles:

C7	-C1	-C2	: 127.733172	H29	-C1	-C2	: 117.373669
H29	-C1	-C7	: 114.893158	C3	-C2	-C1	: 123.725750
H33	-C2	-C1	: 119.960065	H33	-C2	-C3	: 116.314184
C4	-C3	-C2	: 124.373676	H30	-C3	-C2	: 116.972059
H30	-C3	-C4	: 118.654263	C5	-C4	-C3	: 124.188644
H31	-C4	-C3	: 118.747289	H31	-C4	-C5	: 117.064064
C6	-C5	-C4	: 123.898774	H34	-C5	-C4	: 116.213026
H34	-C5	-C6	: 119.888193	C13	-C6	-C5	: 127.552151
H32	-C6	-C5	: 117.459115	H32	-C6	-C13	: 114.988708
C8	-C7	-C1	: 123.593104	C12	-C7	-C1	: 118.616229
C12	-C7	-C8	: 117.790667	C9	-C8	-C7	: 120.804331
H19	-C8	-C7	: 120.011776	H19	-C8	-C9	: 119.183894
C10	-C9	-C8	: 120.560756	H20	-C9	-C8	: 119.559915
H20	-C9	-C10	: 119.879329	C11	-C10	-C9	: 119.438386
H21	-C10	-C9	: 120.256840	H21	-C10	-C11	: 120.304774
C12	-C11	-C10	: 120.049653	H22	-C11	-C10	: 120.181742
H22	-C11	-C12	: 119.768605	C11	-C12	-C7	: 121.356206
H23	-C12	-C7	: 118.931935	H23	-C12	-C11	: 119.711859
C14	-C13	-C6	: 123.535731	C18	-C13	-C6	: 118.683018
C18	-C13	-C14	: 117.781244	C15	-C14	-C13	: 120.824052
H28	-C14	-C13	: 120.010880	H28	-C14	-C15	: 119.165033
C16	-C15	-C14	: 120.553983	H27	-C15	-C14	: 119.562054
H27	-C15	-C16	: 119.883955	C17	-C16	-C15	: 119.428754
H26	-C16	-C15	: 120.252998	H26	-C16	-C17	: 120.318242

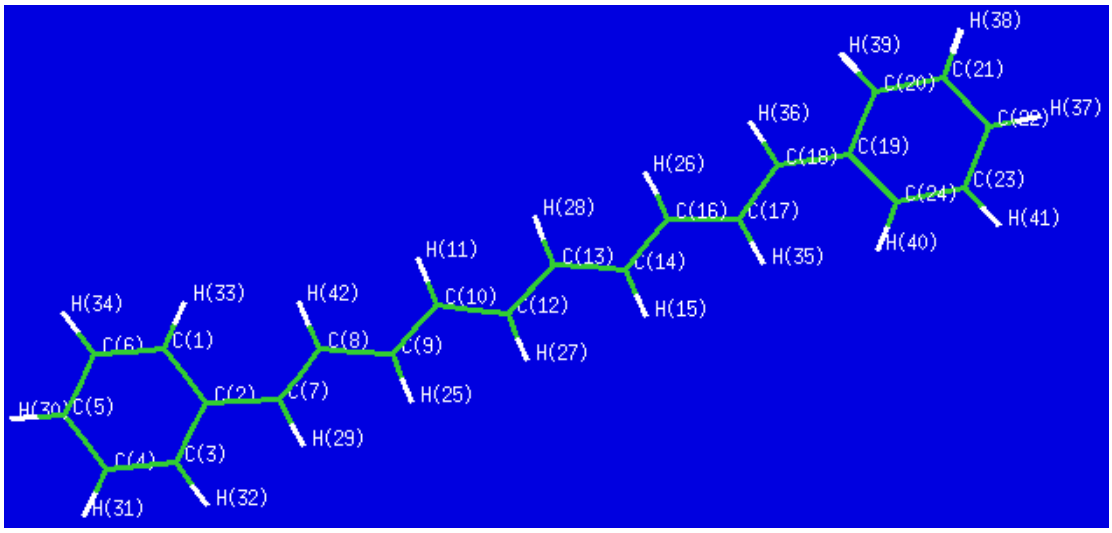
C18 -C17 -C16 : 120.060518 H25 -C17 -C16 : 120.173020
H25 -C17 -C18 : 119.766461 C17 -C18 -C13 : 121.351433
H24 -C18 -C13 : 118.933732 H24 -C18 -C17 : 119.714830

torsional angles:

C1 -C2 -C3 -C4 : 179.984705
C1 -C2 -C3 -H30 : -0.033129
C1 -C7 -C8 -C9 :-179.987721
C1 -C7 -C8 -H19 : 0.009784
C1 -C7 -C12 -C11 : 179.989576
C1 -C7 -C12 -H23 : -0.010047
C2 -C1 -C7 -C8 : -0.023714
C2 -C1 -C7 -C12 : 179.982498
C2 -C3 -C4 -C5 : 179.949833
C2 -C3 -C4 -H31 : -0.032006
C3 -C2 -C1 -C7 : 179.966372
C3 -C2 -C1 -H29 : -0.027938
C3 -C4 -C5 -C6 : 179.963304
C3 -C4 -C5 -H34 : -0.006437
C4 -C3 -C2 -H33 : -0.030365
C4 -C5 -C6 -C13 : 179.957084
C4 -C5 -C6 -H32 : -0.104545
C5 -C4 -C3 -H30 : -0.032055
C5 -C6 -C13 -C14 : -0.660280
C5 -C6 -C13 -C18 : 179.371863
C6 -C5 -C4 -H31 : -0.054576
C6 -C13 -C14 -C15 : 179.993369
C6 -C13 -C14 -H28 : -0.074970
C6 -C13 -C18 -C17 :-179.981163
C6 -C13 -C18 -H24 : -0.007252
C7 -C1 -C2 -H33 : -0.018036
C7 -C8 -C9 -C10 : -0.002898
C7 -C8 -C9 -H20 : 179.996933
C7 -C12 -C11 -C10 : -0.000229
C7 -C12 -C11 -H22 :-179.998727
C8 -C7 -C1 -H29 : 179.970717
C8 -C7 -C12 -C11 : -0.004574
C8 -C7 -C12 -H23 : 179.995802
C8 -C9 -C10 -C11 : -0.002057
C8 -C9 -C10 -H21 : 179.998351
C9 -C8 -C7 -C12 : 0.006114
C9 -C10 -C11 -C12 : 0.003601
C9 -C10 -C11 -H22 :-179.997907
C10 -C9 -C8 -H19 : 179.999576
C10 -C11 -C12 -H23 : 179.999391
C11 -C10 -C9 -H20 : 179.998114
C12 -C7 -C1 -H29 : -0.023071
C12 -C7 -C8 -H19 :-179.996380
C12 -C11 -C10 -H21 :-179.996807
C13 -C6 -C5 -H34 : -0.074228
C13 -C14 -C15 -C16 : 0.006762
C13 -C14 -C15 -H27 : 179.973441

C13 -C18 -C17 -C16 : -0.027729
C13 -C18 -C17 -H25 : 179.982494
C14 -C13 -C6 -H32 : 179.400053
C14 -C13 -C18 -C17 : 0.049120
C14 -C13 -C18 -H24 :-179.976968
C14 -C15 -C16 -C17 : 0.015867
C14 -C15 -C16 -H26 : 179.987082
C15 -C14 -C13 -C18 : -0.038503
C15 -C16 -C17 -C18 : -0.005519
C15 -C16 -C17 -H25 : 179.984216
C16 -C15 -C14 -H28 :-179.925469
C16 -C17 -C18 -H24 : 179.998560
C17 -C16 -C15 -H27 :-179.950705
C18 -C13 -C6 -H32 : -0.567804
C18 -C13 -C14 -H28 : 179.893157
C18 -C17 -C16 -H26 :-179.976714
H19 -C8 -C9 -H20 : -0.000594
H20 -C9 -C10 -H21 : -0.001478
H21 -C10 -C11 -H22 : 0.001685
H22 -C11 -C12 -H23 : 0.000894
H24 -C18 -C17 -H25 : 0.008784
H25 -C17 -C16 -H26 : 0.013020
H26 -C16 -C15 -H27 : 0.020509
H27 -C15 -C14 -H28 : 0.041210
H29 -C1 -C2 -H33 : 179.987653
H30 -C3 -C2 -H33 : 179.951802
H30 -C3 -C4 -H31 : 179.986106
H31 -C4 -C5 -H34 : 179.975683
H32 -C6 -C5 -H34 : 179.864144

DPO5



final geometry:

	angstroms		
atom	x	y	z
C1	0.0163039242	0.1219747686	-0.0673436152
C2	-0.0085225022	0.0327573420	1.3394044852
C3	1.2281652926	0.0277622743	2.0151536824
C4	2.4340563544	0.1067926781	1.3260253541
C5	2.4386373964	0.1949561000	-0.0664502972
C6	1.2221635666	0.2016768150	-0.7560710395
C7	-1.2273925745	-0.0458213317	2.1394122170
C8	-2.5220745548	-0.0755638252	1.7330084304
C9	-3.6172353688	-0.1302657674	2.6633129539
C10	-4.9394996950	-0.1484464518	2.3406592999
H11	-5.2259598542	-0.1329738331	1.2888015646
C12	-5.9969997976	-0.1691722514	3.3089618126
C13	-7.3236911053	-0.1670426561	3.0018602554
C14	-8.3990347696	-0.1501244239	3.9509391929
H15	-8.1404595019	-0.1449038033	5.0098093437
C16	-9.7086465941	-0.1271896249	3.5811443959
C17	-10.8526826619	-0.0752358489	4.4519640030
C18	-12.1171930038	-0.0409162234	3.9599415262
C19	-13.3925375702	0.0365112569	4.6655798476
C20	-14.5725403118	0.0353519105	3.8947235862
C21	-15.8284975173	0.1147893073	4.4872461346
C22	-15.9409912943	0.1990059155	5.8753939020
C23	-14.7823096266	0.2020903106	6.6579105658
C24	-13.5264523406	0.1217647553	6.0657110556
H25	-3.3502400723	-0.1490357981	3.7208598062
H26	-9.9307884880	-0.1366332309	2.5131983006
H27	-5.7048785956	-0.1761414153	4.3596010925
H28	-7.6070501723	-0.1637118598	1.9485975437
H29	-1.0553408716	-0.0805637198	3.2153609162
H30	3.3766516813	0.2581255376	-0.6098741162
H31	3.3705438937	0.1005141580	1.8766062495
H32	1.2329036894	-0.0391237539	3.1002994805

H33	-0.9152428914	0.1314672898	-0.6252853745
H34	1.2153398055	0.2707070232	-1.8402835395
H35	-10.6703758260	-0.0570809794	5.5257378770
H36	-12.2148203007	-0.0684199026	2.8744718254
H37	-16.9183749240	0.2626086644	6.3443190664
H38	-16.7191992849	0.1120465674	3.8652480157
H39	-14.4921871411	-0.0281680882	2.8123028671
H40	-12.6406998495	0.1294266602	6.6937112609
H41	-14.8602594194	0.2690742759	7.7394202869
H42	-2.7681299376	-0.0480118771	0.6721011399

Final total energy..... -850.37013

HOMO energy: -0.17577
LUMO energy: -0.07707

bond lengths (angstroms):

C1	-C2	: 1.409793	C1	-C6	: 1.390969
C1	-H33	: 1.085895	C2	-C3	: 1.409276
C2	-C7	: 1.460079	C3	-C4	: 1.391157
C3	-H32	: 1.087216	C4	-C5	: 1.395271
C4	-H31	: 1.086364	C5	-C6	: 1.398367
C5	-H30	: 1.085896	C6	-H34	: 1.086429
C7	-C8	: 1.357295	C7	-H29	: 1.090172
C8	-C9	: 1.437997	C8	-H42	: 1.089416
C9	-C10	: 1.361183	C9	-H25	: 1.090891
C10	-H11	: 1.090277	C10	-C12	: 1.433996
C12	-C13	: 1.361773	C12	-H27	: 1.090517
C13	-C14	: 1.434364	C13	-H28	: 1.090718
C14	-H15	: 1.089997	C14	-C16	: 1.361013
C16	-C17	: 1.438695	C16	-H26	: 1.090846
C17	-C18	: 1.357295	C17	-H35	: 1.089291
C18	-C19	: 1.459597	C18	-H36	: 1.090198
C19	-C20	: 1.409478	C19	-C24	: 1.409102
C20	-C21	: 1.390979	C20	-H39	: 1.087256
C21	-C22	: 1.395242	C21	-H38	: 1.086388
C22	-C23	: 1.398172	C22	-H37	: 1.085917
C23	-C24	: 1.390802	C23	-H41	: 1.086382
C24	-H40	: 1.085818			

bond angles:

C6	-C1	-C2	: 120.861549	H33	-C1	-C2	: 119.877325
H33	-C1	-C6	: 119.260952	C3	-C2	-C1	: 117.596138
C7	-C2	-C1	: 124.391456	C7	-C2	-C3	: 118.011177
C4	-C3	-C2	: 121.529732	H32	-C3	-C2	: 118.857363
H32	-C3	-C4	: 119.612898	C5	-C4	-C3	: 120.053380
H31	-C4	-C3	: 119.726044	H31	-C4	-C5	: 120.220549
C6	-C5	-C4	: 119.315660	H30	-C5	-C4	: 120.394253
H30	-C5	-C6	: 120.290083	C5	-C6	-C1	: 120.643514
H34	-C6	-C1	: 119.493678	H34	-C6	-C5	: 119.862781
C8	-C7	-C2	: 129.301951	H29	-C7	-C2	: 114.251271
H29	-C7	-C8	: 116.446206	C9	-C8	-C7	: 122.247604
H42	-C8	-C7	: 120.429185	H42	-C8	-C9	: 117.320335
C10	-C9	-C8	: 125.942238	H25	-C9	-C8	: 116.194906
H25	-C9	-C10	: 117.860197	H11	-C10	-C9	: 118.928998
C12	-C10	-C9	: 123.813927	C12	-C10	-H11	: 117.251696
C13	-C12	-C10	: 124.482180	H27	-C12	-C10	: 116.943021
H27	-C12	-C13	: 118.571345	C14	-C13	-C12	: 125.534122
H28	-C13	-C12	: 118.091119	H28	-C13	-C14	: 116.368879
H15	-C14	-C13	: 117.709251	C16	-C14	-C13	: 122.806618
C16	-C14	-H15	: 119.480800	C17	-C16	-C14	: 126.963589
H26	-C16	-C14	: 117.503747	H26	-C16	-C17	: 115.528263

C18 -C17 -C16 : 121.488463 H35 -C17 -C16 : 117.657055
H35 -C17 -C18 : 120.853091 C19 -C18 -C17 : 129.801114
H36 -C18 -C17 : 116.341500 H36 -C18 -C19 : 113.856231
C20 -C19 -C18 : 117.843819 C24 -C19 -C18 : 124.514697
C24 -C19 -C20 : 117.639972 C21 -C20 -C19 : 121.527589
H39 -C20 -C19 : 118.858795 H39 -C20 -C21 : 119.613578
C22 -C21 -C20 : 120.003746 H38 -C21 -C20 : 119.752780
H38 -C21 -C22 : 120.243440 C23 -C22 -C21 : 119.349930
H37 -C22 -C21 : 120.379968 H37 -C22 -C23 : 120.270072
C24 -C23 -C22 : 120.655236 H41 -C23 -C22 : 119.856907
H41 -C23 -C24 : 119.487810 C23 -C24 -C19 : 120.823507
H40 -C24 -C19 : 119.840416 H40 -C24 -C23 : 119.335561

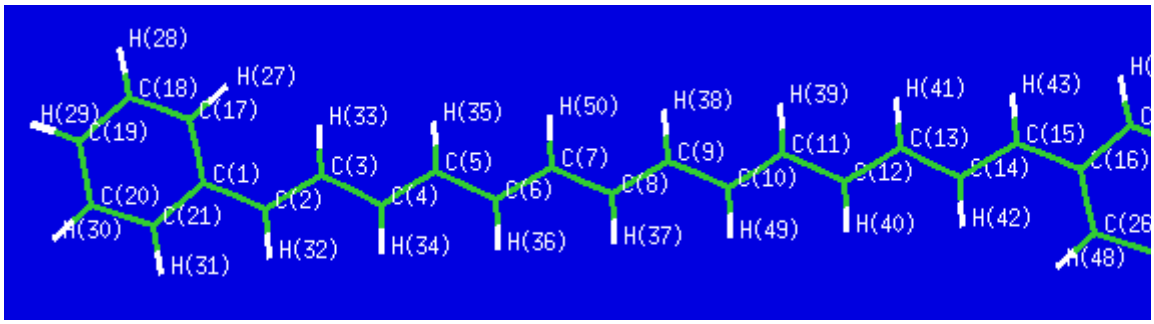
torsional angles:

C1 -C2 -C3 -C4 : -0.042043
C1 -C2 -C3 -H32 : 179.927330
C1 -C2 -C7 -C8 : 1.384365
C1 -C2 -C7 -H29 :-178.327221
C1 -C6 -C5 -C4 : 0.018483
C1 -C6 -C5 -H30 :-179.958080
C2 -C1 -C6 -C5 : 0.002891
C2 -C1 -C6 -H34 :-179.936435
C2 -C3 -C4 -C5 : 0.064369
C2 -C3 -C4 -H31 :-179.995337
C2 -C7 -C8 -C9 :-178.826512
C2 -C7 -C8 -H42 : 0.539868
C3 -C2 -C1 -C6 : 0.008349
C3 -C2 -C1 -H33 :-179.838947
C3 -C2 -C7 -C8 :-179.029471
C3 -C2 -C7 -H29 : 1.258943
C3 -C4 -C5 -C6 : -0.051498
C3 -C4 -C5 -H30 : 179.925040
C4 -C3 -C2 -C7 :-179.656709
C4 -C5 -C6 -H34 : 179.957586
C5 -C4 -C3 -H32 :-179.904777
C5 -C6 -C1 -H33 : 179.851117
C6 -C1 -C2 -C7 : 179.596091
C6 -C5 -C4 -H31 :-179.991494
C7 -C2 -C1 -H33 : -0.251206
C7 -C2 -C3 -H32 : 0.312664
C7 -C8 -C9 -C10 : 179.255058
C7 -C8 -C9 -H25 : -0.135986
C8 -C9 -C10 -H11 : 0.785725
C8 -C9 -C10 -C12 :-178.346206
C9 -C8 -C7 -H29 : 0.879791
C9 -C10 -C12 -C13 : 178.955998
C9 -C10 -C12 -H27 : -0.356292
C10 -C9 -C8 -H42 : -0.130006
C10 -C12 -C13 -C14 :-178.167295
C10 -C12 -C13 -H28 : 0.915711
H11 -C10 -C9 -H25 :-179.832328
H11 -C10 -C12 -C13 : -0.189394

H11 -C10 -C12 -H27 :-179.501683
C12 -C10 -C9 -H25 : 1.035741
C12 -C13 -C14 -H15 : -0.417548
C12 -C13 -C14 -C16 : 178.914270
C13 -C14 -C16 -C17 :-178.318199
C13 -C14 -C16 -H26 : 0.880440
C14 -C13 -C12 -H27 : 1.134629
C14 -C16 -C17 -C18 : 179.219199
C14 -C16 -C17 -H35 : -0.355131
H15 -C14 -C13 -H28 :-179.514631
H15 -C14 -C16 -C17 : 1.002260
H15 -C14 -C16 -H26 :-179.799101
C16 -C14 -C13 -H28 : -0.182814
C16 -C17 -C18 -C19 :-178.788659
C16 -C17 -C18 -H36 : 0.792026
C17 -C18 -C19 -C20 :-178.986299
C17 -C18 -C19 -C24 : 1.472817
C18 -C17 -C16 -H26 : 0.006890
C18 -C19 -C20 -C21 :-179.593741
C18 -C19 -C20 -H39 : 0.334465
C18 -C19 -C24 -C23 : 179.518797
C18 -C19 -C24 -H40 : -0.218031
C19 -C18 -C17 -H35 : 0.772156
C19 -C20 -C21 -C22 : 0.041580
C19 -C20 -C21 -H38 : 179.974324
C19 -C24 -C23 -C22 : 0.046119
C19 -C24 -C23 -H41 :-179.874742
C20 -C19 -C18 -H36 : 1.424581
C20 -C19 -C24 -C23 : -0.022945
C20 -C19 -C24 -H40 :-179.759773
C20 -C21 -C22 -C23 : -0.018287
C20 -C21 -C22 -H37 : 179.918673
C21 -C20 -C19 -C24 : -0.020777
C21 -C22 -C23 -C24 : -0.025087
C21 -C22 -C23 -H41 : 179.895483
C22 -C21 -C20 -H39 :-179.886095
C22 -C23 -C24 -H40 : 179.784260
C23 -C22 -C21 -H38 :-179.950698
C24 -C19 -C18 -H36 :-178.116302
C24 -C19 -C20 -H39 : 179.907429
C24 -C23 -C22 -H37 :-179.962118
H25 -C9 -C8 -H42 :-179.521051
H26 -C16 -C17 -H35 :-179.567440
H27 -C12 -C13 -H28 :-179.782365
H29 -C7 -C8 -H42 :-179.753829
H30 -C5 -C4 -H31 : -0.014956
H30 -C5 -C6 -H34 : -0.018977
H31 -C4 -C3 -H32 : 0.035517
H33 -C1 -C6 -H34 : -0.088209
H35 -C17 -C18 -H36 :-179.647159
H37 -C22 -C21 -H38 : -0.013738
H37 -C22 -C23 -H41 : -0.041548
H38 -C21 -C20 -H39 : 0.046650

H40 -C24 -C23 -H41 : -0.136601

DPO7



final geometry:

	angstroms		
atom	x	y	z
C1	-0.0704590910	0.1452901882	-0.0068445096
C2	-0.0892360394	0.0524084180	1.4492038362
C3	0.9726244166	-0.0225477331	2.2885196922
C4	0.8602944166	-0.0937659836	3.7166856229
C5	1.9252863220	-0.1463176660	4.5637558553
C6	1.8300036493	-0.1894787560	5.9900293113
C7	2.9067206997	-0.2089696859	6.8268423335
C8	2.8276132845	-0.2178701129	8.2531535101
C9	3.9121344308	-0.2003639910	9.0806793071
C10	3.8412435818	-0.1739951647	10.5070598868
C11	4.9263876852	-0.1204794662	11.3313665480
C12	4.8508813506	-0.0625892426	12.7583596638
C13	5.9278430399	0.0206982727	13.5878215699
C14	5.8353556035	0.1021121246	15.0172338255
C15	6.9060927478	0.2035869671	15.8417952335
C16	6.9012486201	0.3046939259	17.2973523779
C17	1.1131410930	0.1743027414	-0.7720322386
C18	1.0651330732	0.2682554979	-2.1582450492
C19	-0.1630392986	0.3362684977	-2.8232956090
C20	-1.3443851323	0.3089168549	-2.0818377362
C21	-1.2969321458	0.2146166759	-0.6946507366
C22	8.1337202332	0.3976194058	17.9717583160
C23	8.1957196138	0.4989194523	19.3575082667
C24	7.0222388935	0.5099841926	20.1107632407
C25	5.7872756478	0.4196819675	19.4613401753
C26	5.7252257297	0.3185742349	18.0759903726
H27	2.0786210173	0.1239717704	-0.2785946417
H28	1.9908676914	0.2892964054	-2.7265554132
H29	-0.1952943621	0.4100105104	-3.9064239371
H30	-2.3057517234	0.3615339151	-2.5848699724
H31	-2.2218953510	0.1940330402	-0.1237467205
H32	-1.0831837221	0.0489699528	1.8958001695
H33	1.9839685905	-0.0223917760	1.8852256990
H34	-0.1459519923	-0.0950986165	4.1366108218
H35	2.9290729432	-0.1426260725	4.1375530824
H36	0.8290978641	-0.1937703304	6.4226831890
H37	1.8317013482	-0.2250794616	8.6971129127
H38	4.9063745490	-0.1903081841	8.6328491185
H39	5.9201447670	-0.1074128043	10.8825625750

H40	3.8552962962	-0.0759690220	13.2031552485
H41	6.9256198423	0.0366533704	13.1484549316
H42	4.8305994290	0.0850378659	15.4364582022
H43	7.8941974253	0.2163005801	15.3819652360
H44	9.0526769862	0.3891352889	17.3915167921
H45	9.1614014057	0.5694874335	19.8500324212
H46	7.0653367351	0.5887023764	21.1930172657
H47	4.8684099006	0.4291422614	20.0412425083
H48	4.7546497406	0.2508291931	17.5940957588
H49	2.8479033937	-0.1842303044	10.9563047251
H50	3.9047514114	-0.2020405922	6.3878273811

Final total energy: -1005.193166 hartrees

HOMO energy: -0.17018
LUMO energy: -0.08455

bond lengths (angstroms):

C1	-C2	:	1.459129	C1	-C17	:	1.409703
C1	-C21	:	1.407878	C2	-C3	:	1.355587
C2	-H32	:	1.089675	C3	-C4	:	1.434346
C3	-H33	:	1.088790	C4	-C5	:	1.361799
C4	-H34	:	1.090354	C5	-C6	:	1.430104
C5	-H35	:	1.090527	C6	-C7	:	1.363802
C6	-H36	:	1.090422	C7	-C8	:	1.428531
C7	-H50	:	1.090343	C8	-C9	:	1.364292
C8	-H37	:	1.090409	C9	-C10	:	1.428385
C9	-H38	:	1.090489	C10	-C11	:	1.363775
C10	-H49	:	1.090252	C11	-C12	:	1.430161
C11	-H39	:	1.090481	C12	-C13	:	1.361907
C12	-H40	:	1.090510	C13	-C14	:	1.434713
C13	-H41	:	1.090347	C14	-C15	:	1.355240
C14	-H42	:	1.088841	C15	-C16	:	1.459073
C15	-H43	:	1.089934	C16	-C22	:	1.407993
C16	-C26	:	1.410496	C17	-C18	:	1.390222
C17	-H27	:	1.085433	C18	-C19	:	1.398329
C18	-H28	:	1.086464	C19	-C20	:	1.395022
C19	-H29	:	1.086115	C20	-C21	:	1.391198
C20	-H30	:	1.086294	C21	-H31	:	1.087158
C22	-C23	:	1.390830	C22	-H44	:	1.086846
C23	-C24	:	1.394479	C23	-H45	:	1.086325
C24	-C25	:	1.398227	C24	-H46	:	1.085969
C25	-C26	:	1.390420	C25	-H47	:	1.086596
C26	-H48	:	1.085739				

bond angles:

C17	-C1	-C2	: 123.625992	C21	-C1	-C2	: 118.648433
C21	-C1	-C17	: 117.725246	C3	-C2	-C1	: 127.682502
H32	-C2	-C1	: 114.892513	H32	-C2	-C3	: 117.424316
C4	-C3	-C2	: 123.909682	H33	-C3	-C2	: 119.884814
H33	-C3	-C4	: 116.203516	C5	-C4	-C3	: 124.056714
H34	-C4	-C3	: 117.116573	H34	-C4	-C5	: 118.823767
C6	-C5	-C4	: 124.709534	H35	-C5	-C4	: 118.464370
H35	-C5	-C6	: 116.821013	C7	-C6	-C5	: 124.040232
H36	-C6	-C5	: 117.193006	H36	-C6	-C7	: 118.761886
C8	-C7	-C6	: 124.680817	H50	-C7	-C6	: 118.392532
H50	-C7	-C8	: 116.919724	C9	-C8	-C7	: 124.160806
H37	-C8	-C7	: 117.202421	H37	-C8	-C9	: 118.630998
C10	-C9	-C8	: 124.506108	H38	-C9	-C8	: 118.411028
H38	-C9	-C10	: 117.076025	C11	-C10	-C9	: 124.389526
H49	-C10	-C9	: 117.162961	H49	-C10	-C11	: 118.442201

C12 -C11 -C10 : 124.240666 H39 -C11 -C10 : 118.478086
H39 -C11 -C12 : 117.276246 C13 -C12 -C11 : 124.640204
H40 -C12 -C11 : 117.044239 H40 -C12 -C13 : 118.312155
C14 -C13 -C12 : 124.006574 H41 -C13 -C12 : 118.627448
H41 -C13 -C14 : 117.363388 C15 -C14 -C13 : 124.020823
H42 -C14 -C13 : 116.243841 H42 -C14 -C15 : 119.734270
C16 -C15 -C14 : 127.555096 H43 -C15 -C14 : 117.415769
H43 -C15 -C16 : 115.028750 C22 -C16 -C15 : 118.652558
C26 -C16 -C15 : 123.652274 C26 -C16 -C22 : 117.694949
C18 -C17 -C1 : 120.906063 H27 -C17 -C1 : 119.941222
H27 -C17 -C18 : 119.152686 C19 -C18 -C17 : 120.520693
H28 -C18 -C17 : 119.568177 H28 -C18 -C19 : 119.911123
C20 -C19 -C18 : 119.343479 H29 -C19 -C18 : 120.243905
H29 -C19 -C20 : 120.412612 C21 -C20 -C19 : 120.159865
H30 -C20 -C19 : 120.156760 H30 -C20 -C21 : 119.683371
C20 -C21 -C1 : 121.344651 H31 -C21 -C1 : 118.927337
H31 -C21 -C20 : 119.728005 C23 -C22 -C16 : 121.403476
H44 -C22 -C16 : 118.939703 H44 -C22 -C23 : 119.656817
C24 -C23 -C22 : 120.083503 H45 -C23 -C22 : 119.741503
H45 -C23 -C24 : 120.174993 C25 -C24 -C23 : 119.462814
H46 -C24 -C23 : 120.364567 H46 -C24 -C25 : 120.172607
C26 -C25 -C24 : 120.456261 H47 -C25 -C24 : 119.897952
H47 -C25 -C26 : 119.645771 C25 -C26 -C16 : 120.898962
H48 -C26 -C16 : 119.980228 H48 -C26 -C25 : 119.120777

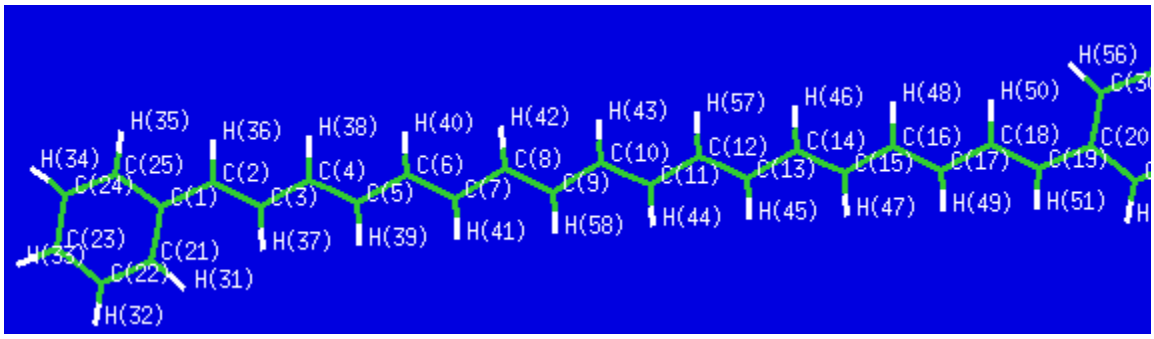
torsional angles:

C1 -C2 -C3 -C4 : 179.135057
C1 -C2 -C3 -H33 : -0.332030
C1 -C17 -C18 -C19 : 0.008663
C1 -C17 -C18 -H28 : 179.977364
C1 -C21 -C20 -C19 : 0.019513
C1 -C21 -C20 -H30 :-179.957195
C2 -C1 -C17 -C18 :-179.788420
C2 -C1 -C17 -H27 : 0.149586
C2 -C1 -C21 -C20 : 179.785178
C2 -C1 -C21 -H31 : -0.184464
C2 -C3 -C4 -C5 :-178.839000
C2 -C3 -C4 -H34 : 0.527756
C3 -C2 -C1 -C17 : -0.177000
C3 -C2 -C1 -C21 :-179.963552
C3 -C4 -C5 -C6 : 178.631355
C3 -C4 -C5 -H35 : -0.520531
C4 -C3 -C2 -H32 : -0.550441
C4 -C5 -C6 -C7 :-178.327235
C4 -C5 -C6 -H36 : 0.857520
C5 -C4 -C3 -H33 : 0.646026
C5 -C6 -C7 -C8 : 178.333526
C5 -C6 -C7 -H50 : -0.677341
C6 -C5 -C4 -H34 : -0.725300
C6 -C7 -C8 -C9 :-178.120372
C6 -C7 -C8 -H37 : 0.991238
C7 -C6 -C5 -H35 : 0.837298

C7 -C8 -C9 -C10 : 178.291347
C7 -C8 -C9 -H38 : -0.727429
C8 -C7 -C6 -H36 : -0.839283
C8 -C9 -C10 -C11 :-178.163739
C8 -C9 -C10 -H49 : 0.982483
C9 -C8 -C7 -H50 : 0.903732
C9 -C10 -C11 -C12 : 178.466427
C9 -C10 -C11 -H39 : -0.696244
C10 -C9 -C8 -H37 : -0.808447
C10 -C11 -C12 -C13 :-178.482504
C10 -C11 -C12 -H40 : 0.833080
C11 -C10 -C9 -H38 : 0.866992
C11 -C12 -C13 -C14 : 178.837662
C11 -C12 -C13 -H41 : -0.560410
C12 -C11 -C10 -H49 : -0.669682
C12 -C13 -C14 -C15 :-179.049518
C12 -C13 -C14 -H42 : 0.572779
C13 -C12 -C11 -H39 : 0.689408
C13 -C14 -C15 -C16 : 179.314902
C13 -C14 -C15 -H43 : -0.446966
C14 -C13 -C12 -H40 : -0.469930
C14 -C15 -C16 -C22 : 179.780095
C14 -C15 -C16 -C26 : -0.394369
C15 -C14 -C13 -H41 : 0.355573
C15 -C16 -C22 -C23 : 179.877009
C15 -C16 -C22 -H44 : -0.144260
C15 -C16 -C26 -C25 :-179.875822
C15 -C16 -C26 -H48 : 0.058368
C16 -C15 -C14 -H42 : -0.294961
C16 -C22 -C23 -C24 : 0.009294
C16 -C22 -C23 -H45 :-179.980411
C16 -C26 -C25 -C24 : 0.006431
C16 -C26 -C25 -H47 : 179.960809
C17 -C1 -C2 -H32 : 179.515252
C17 -C1 -C21 -C20 : -0.014038
C17 -C1 -C21 -H31 :-179.983680
C17 -C18 -C19 -C20 : -0.003393
C17 -C18 -C19 -H29 : 179.973725
C18 -C17 -C1 -C21 : -0.000033
C18 -C19 -C20 -C21 : -0.010522
C18 -C19 -C20 -H30 : 179.966075
C19 -C18 -C17 -H27 :-179.929825
C19 -C20 -C21 -H31 : 179.988916
C20 -C19 -C18 -H28 :-179.971987
C21 -C1 -C2 -H32 : -0.271300
C21 -C1 -C17 -H27 : 179.937973
C21 -C20 -C19 -H29 :-179.987601
C22 -C16 -C15 -H43 : -0.453200
C22 -C16 -C26 -C25 : -0.048731
C22 -C16 -C26 -H48 : 179.885459
C22 -C23 -C24 -C25 : -0.052735
C22 -C23 -C24 -H46 : 179.987692
C23 -C22 -C16 -C26 : 0.041026

C23 -C24 -C25 -C26 : 0.045048
C23 -C24 -C25 -H47 :-179.909214
C24 -C23 -C22 -H44 :-179.969287
C24 -C25 -C26 -H48 :-179.928316
C25 -C24 -C23 -H45 : 179.936925
C26 -C16 -C15 -H43 : 179.372337
C26 -C16 -C22 -H44 :-179.980243
C26 -C25 -C24 -H46 :-179.995300
H27 -C17 -C18 -H28 : 0.038876
H28 -C18 -C19 -H29 : 0.005131
H29 -C19 -C20 -H30 : -0.011003
H30 -C20 -C21 -H31 : 0.012207
H32 -C2 -C3 -H33 : 179.982472
H33 -C3 -C4 -H34 :-179.987218
H34 -C4 -C5 -H35 :-179.877186
H35 -C5 -C6 -H36 :-179.977947
H36 -C6 -C7 -H50 :-179.850150
H37 -C8 -C7 -H50 :-179.984658
H37 -C8 -C9 -H38 :-179.827224
H38 -C9 -C10 -H49 :-179.986786
H39 -C11 -C10 -H49 :-179.832354
H39 -C11 -C12 -H40 :-179.995009
H40 -C12 -C13 -H41 :-179.868002
H41 -C13 -C14 -H42 : 179.977870
H42 -C14 -C15 -H43 : 179.943171
H44 -C22 -C23 -H45 : 0.041008
H45 -C23 -C24 -H46 : -0.022648
H46 -C24 -C25 -H47 : 0.050437
H47 -C25 -C26 -H48 : 0.026061

DPO9



final geometry:

	angstroms		
atom	x	y	z
C1	-0.0011750393	-0.0296692541	-0.0023206387
C2	0.0195664490	-0.0076153987	1.4567000657
C3	1.1027336347	0.0159595469	2.2730233735
C4	1.0160377858	0.0447841354	3.7043307128
C5	2.0875533231	0.0637296577	4.5460251669
C6	1.9839581628	0.1000069001	5.9717434570
C7	3.0443129384	0.1140803612	6.8307609130
C8	2.9195726497	0.1559833125	8.2530619674
C9	3.9689814355	0.1637529965	9.1266730763
C10	3.8312883212	0.2092779491	10.5470242125
C11	4.8775018859	0.2106306659	11.4251161593
C12	4.7431798391	0.2581776619	12.8456397580
C13	5.7966360309	0.2542486184	13.7143570917
C14	5.6820929427	0.3030232019	15.1372055210
C15	6.7498657140	0.2955521292	15.9869917755
C16	6.6629583190	0.3459898471	17.4133389085
C17	7.7459833659	0.3375158701	18.2402660329
C18	7.6852303851	0.3911052724	19.6722526655
C19	8.7856016795	0.3820168689	20.4654789955
C20	8.8449450110	0.4370829410	21.9221958955
C21	1.1606889238	0.0153446751	-0.7997591468
C22	1.0748722891	-0.0054195780	-2.1868371762
C23	-0.1694653403	-0.0718408047	-2.8205675042
C24	-1.3302062220	-0.1170374911	-2.0484056260
C25	-1.2452854713	-0.0952974338	-0.6596295597
C26	10.1074355381	0.4003970213	22.5459952585
C27	10.2326100497	0.4517765437	23.9307906359
C28	9.0946141171	0.5419913327	24.7322425282
C29	7.8324737175	0.5796369416	24.1322804725
C30	7.7065117002	0.5281380950	22.7489197749
H31	2.1382126179	0.0715230848	-0.3306459522
H32	1.9838345440	0.0323427065	-2.7807166342
H33	-0.2308579302	-0.0872377588	-3.9047246236
H34	-2.3032879906	-0.1682560012	-2.5285775110
H35	-2.1537591931	-0.1299175866	-0.0634487534
H36	-0.9624751341	-0.0120717812	1.9297099499
H37	2.1046890279	0.0134694675	1.8474055483
H38	0.0154946650	0.0540807689	4.1377073211

H39	3.0904153233	0.0519233639	4.1182122398
H40	0.9780435557	0.1189308158	6.3923301678
H41	4.0530504970	0.0923674841	6.4174163589
H42	1.9079934674	0.1841794662	8.6593154381
H43	2.8175066888	0.2454256687	10.9469069829
H44	5.8910251442	0.1723372327	11.0245741367
H45	6.8052202881	0.2105544857	13.3019565759
H46	4.6775602453	0.3496340646	15.5584686875
H47	7.7506343368	0.2480879434	15.5563949927
H48	5.6666555644	0.3955301950	17.8534004164
H49	8.7386655165	0.2876202016	17.7917464623
H50	6.6927456697	0.4422972102	20.1166960844
H51	9.7550670049	0.3272684696	19.9709017445
H52	10.9980788616	0.3309534206	21.9263566110
H53	11.2190809096	0.4221132459	24.3847567754
H54	9.1872338780	0.5827731353	25.8135018469
H55	6.9414140229	0.6511476902	24.7496309660
H56	6.7160463692	0.5611198927	22.3054104158
H57	3.7320255105	0.3004031460	13.2513194011
H58	4.9822098553	0.1329330755	8.7249613190

Final total energy: -1160.015207 hartrees

HOMO energy: -0.16589
LUMO energy: -0.08866

bond lengths (angstroms):

C1	-C2	:	1.459335	C1	-C21	:	1.409916				
C1	-C25	:	1.408607	C2	-C3	:	1.356536				
C2	-H36	:	1.090029	C3	-C4	:	1.434220				
C3	-H37	:	1.088610	C4	-C5	:	1.362701				
C4	-H38	:	1.090407	C5	-C6	:	1.429937				
C5	-H39	:	1.090365	C6	-C7	:	1.364720				
C6	-H40	:	1.090466	C7	-C8	:	1.428375				
C7	-H41	:	1.090356	C8	-C9	:	1.365473				
C8	-H42	:	1.090472	C9	-C10	:	1.427736				
C9	-H58	:	1.090392	C10	-C11	:	1.365873				
C10	-H43	:	1.090397	C11	-C12	:	1.427652				
C11	-H44	:	1.090472	C12	-C13	:	1.365451				
C12	-H57	:	1.090317	C13	-C14	:	1.428285				
C13	-H45	:	1.090516	C14	-C15	:	1.364673				
C14	-H46	:	1.090285	C15	-C16	:	1.429882				
C15	-H47	:	1.090506	C16	-C17	:	1.362653				
C16	-H48	:	1.090288	C17	-C18	:	1.434276				
C17	-H49	:	1.090448	C18	-C19	:	1.356506				
C18	-H50	:	1.088658	C19	-C20	:	1.458965				
C19	-H51	:	1.089710	C20	-C26	:	1.408671				
C20	-C30	:	1.409891	C21	-C22	:	1.389885				
C21	-H31	:	1.085714	C22	-C23	:	1.397999				
C22	-H32	:	1.086430	C23	-C24	:	1.394846				
C23	-H33	:	1.086003	C24	-C25	:	1.391540				
C24	-H34	:	1.086313	C25	-H35	:	1.087177				
C26	-C27	:	1.391390	C26	-H52	:	1.087207				
C27	-C28	:	1.394811	C27	-H53	:	1.086319				
C28	-C29	:	1.397988	C28	-H54	:	1.085985				
C29	-C30	:	1.390038	C29	-H55	:	1.086381				
C30	-H56	:	1.085730								

bond angles:

C21	-C1	-C2	: 123.592079	C25	-C1	-C2	: 118.671982
C25	-C1	-C21	: 117.735644	C3	-C2	-C1	: 127.825035
H36	-C2	-C1	: 114.896618	H36	-C2	-C3	: 117.278311
C4	-C3	-C2	: 123.547688	H37	-C3	-C2	: 119.973812
H37	-C3	-C4	: 116.478500	C5	-C4	-C3	: 124.691659
H38	-C4	-C3	: 116.889749	H38	-C4	-C5	: 118.418458
C6	-C5	-C4	: 124.002562	H39	-C5	-C4	: 118.732312
H39	-C5	-C6	: 117.265089	C7	-C6	-C5	: 124.859112
H40	-C6	-C5	: 116.860955	H40	-C6	-C7	: 118.279879
C8	-C7	-C6	: 124.001742	H41	-C7	-C6	: 118.684918
H41	-C7	-C8	: 117.313340	C9	-C8	-C7	: 124.758368
H42	-C8	-C7	: 116.919266	H42	-C8	-C9	: 118.322355
C10	-C9	-C8	: 124.231674	H58	-C9	-C8	: 118.573143

H58 -C9 -C10 : 117.195175 C11 -C10 -C9 : 124.451947
H43 -C10 -C9 : 117.100763 H43 -C10 -C11 : 118.447289
C12 -C11 -C10 : 124.585522 H44 -C11 -C10 : 118.407881
H44 -C11 -C12 : 117.006587 C13 -C12 -C11 : 124.080167
H57 -C12 -C11 : 117.307225 H57 -C12 -C13 : 118.612604
C14 -C13 -C12 : 124.877320 H45 -C13 -C12 : 118.233263
H45 -C13 -C14 : 116.889415 C15 -C14 -C13 : 123.876025
H46 -C14 -C13 : 117.403696 H46 -C14 -C15 : 118.720258
C16 -C15 -C14 : 124.988684 H47 -C15 -C14 : 118.190839
H47 -C15 -C16 : 116.820472 C17 -C16 -C15 : 123.836452
H48 -C16 -C15 : 117.371918 H48 -C16 -C17 : 118.791553
C18 -C17 -C16 : 124.888689 H49 -C17 -C16 : 118.307907
H49 -C17 -C18 : 116.803367 C19 -C18 -C17 : 123.313062
H50 -C18 -C17 : 116.613519 H50 -C18 -C19 : 120.073377
C20 -C19 -C18 : 128.068130 H51 -C19 -C18 : 117.168487
H51 -C19 -C20 : 114.763383 C26 -C20 -C19 : 118.529889
C30 -C20 -C19 : 123.715180 C30 -C20 -C26 : 117.754806
C22 -C21 -C1 : 120.870061 H31 -C21 -C1 : 119.948432
H31 -C21 -C22 : 119.180936 C23 -C22 -C21 : 120.534936
H32 -C22 -C21 : 119.561167 H32 -C22 -C23 : 119.903789
C24 -C23 -C22 : 119.425424 H33 -C23 -C22 : 120.233989
H33 -C23 -C24 : 120.340568 C25 -C24 -C23 : 120.078915
H34 -C24 -C23 : 120.149451 H34 -C24 -C25 : 119.771603
C24 -C25 -C1 : 121.354964 H35 -C25 -C1 : 118.922974
H35 -C25 -C24 : 119.722054 C27 -C26 -C20 : 121.358795
H52 -C26 -C20 : 118.912425 H52 -C26 -C27 : 119.728773
C28 -C27 -C26 : 120.056966 H53 -C27 -C26 : 119.775272
H53 -C27 -C28 : 120.167747 C29 -C28 -C27 : 119.455277
H54 -C28 -C27 : 120.327399 H54 -C28 -C29 : 120.217324
C30 -C29 -C28 : 120.524982 H55 -C29 -C28 : 119.894383
H55 -C29 -C30 : 119.580575 C29 -C30 -C20 : 120.849171
H56 -C30 -C20 : 119.936976 H56 -C30 -C29 : 119.213707

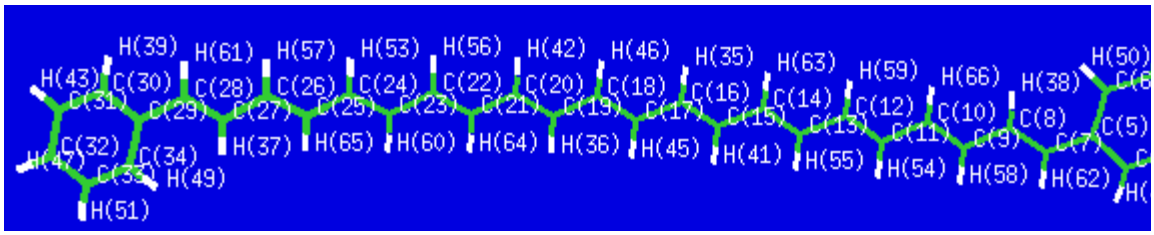
torsional angles:

C1 -C2 -C3 -C4 : 179.601638
C1 -C2 -C3 -H37 : -0.402522
C1 -C21 -C22 -C23 : -0.012759
C1 -C21 -C22 -H32 : 179.867686
C1 -C25 -C24 -C23 : -0.083447
C1 -C25 -C24 -H34 : 179.980376
C2 -C1 -C21 -C22 :-179.836086
C2 -C1 -C21 -H31 : -0.113291
C2 -C1 -C25 -C24 : 179.894440
C2 -C1 -C25 -H35 : -0.136760
C2 -C3 -C4 -C5 : 179.740458
C2 -C3 -C4 -H38 : -0.395053
C3 -C2 -C1 -C21 : -2.184076
C3 -C2 -C1 -C25 : 178.018246
C3 -C4 -C5 -C6 : 179.632943
C3 -C4 -C5 -H39 : -0.295193
C4 -C3 -C2 -H36 : -0.471597
C4 -C5 -C6 -C7 : 179.727153

C4 -C5 -C6 -H40 : -0.358811
C5 -C4 -C3 -H37 : -0.255517
C5 -C6 -C7 -C8 : 179.730856
C5 -C6 -C7 -H41 : -0.264071
C6 -C5 -C4 -H38 : -0.229639
C6 -C7 -C8 -C9 : 179.651357
C6 -C7 -C8 -H42 : -0.387165
C7 -C6 -C5 -H39 : -0.343740
C7 -C8 -C9 -C10 : 179.831656
C7 -C8 -C9 -H58 : -0.202070
C8 -C7 -C6 -H40 : -0.182062
C8 -C9 -C10 -C11 : 179.663958
C8 -C9 -C10 -H43 : -0.350249
C9 -C8 -C7 -H41 : -0.353653
C9 -C10 -C11 -C12 : 179.897863
C9 -C10 -C11 -H44 : -0.141655
C10 -C9 -C8 -H42 : -0.129325
C10 -C11 -C12 -C13 : 179.756500
C10 -C11 -C12 -H57 : -0.265510
C11 -C10 -C9 -H58 : -0.302742
C11 -C12 -C13 -C14 : 179.915431
C11 -C12 -C13 -H45 : -0.101846
C12 -C11 -C10 -H43 : -0.087753
C12 -C13 -C14 -C15 : 179.873231
C12 -C13 -C14 -H46 : -0.180125
C13 -C12 -C11 -H44 : -0.204487
C13 -C14 -C15 -C16 : 179.880657
C13 -C14 -C15 -H47 : -0.094158
C14 -C13 -C12 -H57 : -0.062292
C14 -C15 -C16 -C17 :-179.986352
C14 -C15 -C16 -H48 : -0.087928
C15 -C14 -C13 -H45 : -0.109702
C15 -C16 -C17 -C18 : 179.813487
C15 -C16 -C17 -H49 : -0.113998
C16 -C15 -C14 -H46 : -0.065329
C16 -C17 -C18 -C19 :-179.939026
C16 -C17 -C18 -H50 : -0.013704
C17 -C16 -C15 -H47 : -0.011225
C17 -C18 -C19 -C20 : 179.766174
C17 -C18 -C19 -H51 : -0.224907
C18 -C17 -C16 -H48 : -0.083585
C18 -C19 -C20 -C26 : 179.306112
C18 -C19 -C20 -C30 : -0.825647
C19 -C18 -C17 -H49 : -0.010553
C19 -C20 -C26 -C27 : 179.885359
C19 -C20 -C26 -H52 : -0.084199
C19 -C20 -C30 -C29 :-179.867897
C19 -C20 -C30 -H56 : -0.008096
C20 -C19 -C18 -H50 : -0.156674
C20 -C26 -C27 -C28 : -0.020516
C20 -C26 -C27 -H53 :-179.976165
C20 -C30 -C29 -C28 : -0.000480
C20 -C30 -C29 -H55 : 179.910281

C21 -C1 -C2 -H36 : 177.887684
C21 -C1 -C25 -C24 : 0.084851
C21 -C1 -C25 -H35 :-179.946349
C21 -C22 -C23 -C24 : 0.015945
C21 -C22 -C23 -H33 : 179.965590
C22 -C21 -C1 -C25 : -0.036642
C22 -C23 -C24 -C25 : 0.031537
C22 -C23 -C24 -H34 : 179.967471
C23 -C22 -C21 -H31 :-179.737652
C23 -C24 -C25 -H35 : 179.947998
C24 -C23 -C22 -H32 :-179.864091
C25 -C1 -C2 -H36 : -1.909995
C25 -C1 -C21 -H31 : 179.686153
C25 -C24 -C23 -H33 :-179.918053
C26 -C20 -C19 -H51 : -0.702626
C26 -C20 -C30 -C29 : 0.001294
C26 -C20 -C30 -H56 : 179.861095
C26 -C27 -C28 -C29 : 0.020974
C26 -C27 -C28 -H54 :-179.975079
C27 -C26 -C20 -C30 : 0.009206
C27 -C28 -C29 -C30 : -0.010654
C27 -C28 -C29 -H55 :-179.921135
C28 -C27 -C26 -H52 : 179.948797
C28 -C29 -C30 -H56 :-179.861281
C29 -C28 -C27 -H53 : 179.976447
C30 -C20 -C19 -H51 : 179.165615
C30 -C20 -C26 -H52 :-179.960352
C30 -C29 -C28 -H54 : 179.985403
H31 -C21 -C22 -H32 : 0.142793
H32 -C22 -C23 -H33 : 0.085554
H33 -C23 -C24 -H34 : 0.017881
H34 -C24 -C25 -H35 : 0.011821
H36 -C2 -C3 -H37 : 179.524243
H37 -C3 -C4 -H38 : 179.608973
H38 -C4 -C5 -H39 : 179.842225
H39 -C5 -C6 -H40 : 179.570297
H40 -C6 -C7 -H41 : 179.823012
H41 -C7 -C8 -H42 : 179.607825
H42 -C8 -C9 -H58 : 179.836949
H43 -C10 -C9 -H58 : 179.683050
H43 -C10 -C11 -H44 : 179.872730
H44 -C11 -C12 -H57 : 179.773503
H45 -C13 -C12 -H57 : 179.920431
H45 -C13 -C14 -H46 : 179.836942
H46 -C14 -C15 -H47 : 179.959856
H47 -C15 -C16 -H48 : 179.887199
H48 -C16 -C17 -H49 : 179.988930
H49 -C17 -C18 -H50 : 179.914768
H50 -C18 -C19 -H51 : 179.852245
H52 -C26 -C27 -H53 : -0.006852
H53 -C27 -C28 -H54 : -0.019606
H54 -C28 -C29 -H55 : 0.074923
H55 -C29 -C30 -H56 : 0.049479

DPO11



final geometry:

angstroms

atom	x	y	z
C1	0.1757747976	0.0217251870	0.2552688024
C2	0.2576219401	0.0121502934	1.6508916533
C3	1.5102908262	-0.0033722528	2.2641768354
C4	2.6658835273	-0.0090838996	1.4888016257
C5	2.6041565511	0.0004473396	0.0815873958
C6	1.3290191918	0.0159556639	-0.5203531192
C7	3.8524422865	-0.0058511114	-0.6739313406
C8	4.0032592174	0.0012925273	-2.0216296948
C9	5.2742169521	-0.0048643486	-2.6855481590
C10	5.4280303640	0.0024257364	-4.0393860504
C11	6.6869690376	-0.0027516707	-4.7157636854
C12	6.8269729299	0.0049894049	-6.0735017445
C13	8.0785414436	0.0007708704	-6.7589559862
C14	8.2134125663	0.0090070072	-8.1185104875
C15	9.4652293643	0.0055822710	-8.8014254579
C16	9.6119272284	0.0142475205	-10.1604335094
C17	10.8744575902	0.0113435593	-10.8229207066
C18	11.0513480433	0.0202395563	-12.1783490825
C19	12.3307956873	0.0176290296	-12.8082062718
C20	12.5446599038	0.0265576491	-14.1579157437
C21	13.8409290954	0.0241631669	-14.7540317383
C22	14.0865200293	0.0330024289	-16.0976780991
C23	15.3960125468	0.0307825206	-16.6665774958
C24	15.6666534011	0.0393918999	-18.0042554448
C25	16.9873504257	0.0373202362	-18.5520000821
C26	17.2768487941	0.0455222626	-19.8834523751
C27	18.6088145633	0.0434798834	-20.4159197978
C28	18.8947903575	0.0511641694	-21.7415963629
C29	20.2119619185	0.0498010325	-22.3702128890
C30	20.2894538006	0.0584113385	-23.7765967890
C31	21.5158114198	0.0575269520	-24.4343183757
C32	22.7023896506	0.0479462929	-23.7012470333
C33	22.6464805158	0.0393061599	-22.3044622108
C34	21.4221556621	0.0401434079	-21.6467302194
H35	8.7171205313	0.0244313829	-10.7831081449
H36	13.2007358762	0.0078560359	-12.1510099811
H37	19.4180581748	0.0352035379	-19.6876361109
H38	3.1247158495	0.0128355200	-2.6643784668
H39	19.3681424127	0.0659625265	-24.3538362132
H40	3.6396541083	-0.0211655754	1.9723434766
H41	10.3646666036	-0.0046376134	-8.1855134092
H42	11.6831973014	0.0363655562	-14.8260147563

H43	21.5451835828	0.0643348425	-25.5202159935
H44	1.5878433442	-0.0109937011	3.3477432183
H45	11.7617140304	0.0013257729	-10.1894132946
H46	10.1719054315	0.0302805376	-12.8225488566
H47	23.6616391962	0.0472064310	-24.2103213799
H48	-0.6468733913	0.0167675974	2.2518784775
H49	21.4048406347	0.0333386332	-20.5612094140
H50	1.2397074251	0.0234954267	-1.6021384198
H51	23.5657469261	0.0318476494	-21.7255337129
H52	-0.7962454480	0.0337791226	-0.2297090451
H53	14.8332029445	0.0485471329	-18.7070708018
H54	7.5851022393	-0.0135647090	-4.0982672758
H55	8.9808957963	-0.0096850950	-6.1475137909
H56	13.2403925507	0.0425586246	-16.7851083212
H57	16.4540387217	0.0542180615	-20.5987548625
H58	6.1644103279	-0.0161227070	-2.0566321761
H59	5.9260149676	0.0156211743	-6.6870237419
H60	16.2354013234	0.0215985837	-15.9704690442
H61	18.0546950673	0.0593231903	-22.4355185348
H62	4.7576330904	-0.0176521768	-0.0673937559
H63	7.3113475223	0.0193492644	-8.7302769469
H64	14.6943763802	0.0146587384	-14.0751911440
H65	17.8150295174	0.0285588165	-17.8419935837
H66	4.5335856429	0.0134613936	-4.6624300315

Final total energy: -1314.837227 hartrees

HOMO energy: -0.16343
LUMO energy: -0.09254

bond lengths (angstroms):

C1	-C2	:	1.398054	C1	-C6	:	1.389818				
C1	-H52	:	1.086357	C2	-C3	:	1.394826				
C2	-H48	:	1.085964	C3	-C4	:	1.391630				
C3	-H44	:	1.086365	C4	-C5	:	1.408600				
C4	-H40	:	1.087285	C5	-C6	:	1.410159				
C5	-C7	:	1.459132	C6	-H50	:	1.085492				
C7	-C8	:	1.356130	C7	-H62	:	1.089678				
C8	-C9	:	1.433931	C8	-H38	:	1.088622				
C9	-C10	:	1.362567	C9	-H58	:	1.090003				
C10	-C11	:	1.429140	C10	-H66	:	1.090109				
C11	-C12	:	1.364959	C11	-H54	:	1.089983				
C12	-C13	:	1.426986	C12	-H59	:	1.090068				
C13	-C14	:	1.366253	C13	-H55	:	1.090052				
C14	-C15	:	1.425984	C14	-H63	:	1.089994				
C15	-C16	:	1.366930	C15	-H41	:	1.090156				
C16	-C17	:	1.425791	C16	-H35	:	1.090186				
C17	-C18	:	1.366951	C17	-H45	:	1.090255				
C18	-C19	:	1.426083	C18	-H46	:	1.090190				
C19	-C20	:	1.366577	C19	-H36	:	1.090320				
C20	-C21	:	1.426770	C20	-H42	:	1.090216				
C21	-C22	:	1.365935	C21	-H64	:	1.090544				
C22	-C23	:	1.427733	C22	-H56	:	1.090222				
C23	-C24	:	1.364809	C23	-H60	:	1.090516				
C24	-C25	:	1.429779	C24	-H53	:	1.090263				
C25	-C26	:	1.362586	C25	-H65	:	1.090522				
C26	-C27	:	1.434454	C26	-H57	:	1.090298				
C27	-C28	:	1.356193	C27	-H37	:	1.088734				
C28	-C29	:	1.459487	C28	-H61	:	1.089658				
C29	-C30	:	1.408544	C29	-C34	:	1.409996				
C30	-C31	:	1.391600	C30	-H39	:	1.087234				
C31	-C32	:	1.394795	C31	-H43	:	1.086316				
C32	-C33	:	1.397930	C32	-H47	:	1.085964				
C33	-C34	:	1.389814	C33	-H51	:	1.086400				
C34	-H49	:	1.085680								

bond angles:

C6	-C1	-C2	: 120.563779	H52	-C1	-C2	: 119.874877
H52	-C1	-C6	: 119.561343	C3	-C2	-C1	: 119.444131
H48	-C2	-C1	: 120.242509	H48	-C2	-C3	: 120.313360
C4	-C3	-C2	: 120.054443	H44	-C3	-C2	: 120.181635
H44	-C3	-C4	: 119.763922	C5	-C4	-C3	: 121.346065
H40	-C4	-C3	: 119.732587	H40	-C4	-C5	: 118.921348
C6	-C5	-C4	: 117.784044	C7	-C5	-C4	: 118.669648

C7 -C5 -C6 : 123.546306 C5 -C6 -C1 : 120.807536
H50 -C6 -C1 : 119.200503 H50 -C6 -C5 : 119.991961
C8 -C7 -C5 : 127.566784 H62 -C7 -C5 : 114.992230
H62 -C7 -C8 : 117.440986 C9 -C8 -C7 : 123.964290
H38 -C8 -C7 : 119.805629 H38 -C8 -C9 : 116.230075
C10 -C9 -C8 : 124.060754 H58 -C9 -C8 : 117.178543
H58 -C9 -C10 : 118.760703 C11 -C10 -C9 : 124.726933
H66 -C10 -C9 : 118.379692 H66 -C10 -C11 : 116.893369
C12 -C11 -C10 : 124.132345 H54 -C11 -C10 : 117.243487
H54 -C11 -C12 : 118.624168 C13 -C12 -C11 : 124.593773
H59 -C12 -C11 : 118.367898 H59 -C12 -C13 : 117.038323
C14 -C13 -C12 : 124.371695 H55 -C13 -C12 : 117.170008
H55 -C13 -C14 : 118.458297 C15 -C14 -C13 : 124.277711
H63 -C14 -C13 : 118.480928 H63 -C14 -C15 : 117.241355
C16 -C15 -C14 : 124.773142 H41 -C15 -C14 : 116.983525
H41 -C15 -C16 : 118.243332 C17 -C16 -C15 : 123.846516
H35 -C16 -C15 : 118.674080 H35 -C16 -C17 : 117.479399
C18 -C17 -C16 : 125.120841 H45 -C17 -C16 : 116.785482
H45 -C17 -C18 : 118.093677 C19 -C18 -C17 : 123.644170
H46 -C18 -C17 : 118.789660 H46 -C18 -C19 : 117.566166
C20 -C19 -C18 : 125.212495 H36 -C19 -C18 : 116.720137
H36 -C19 -C20 : 118.067367 C21 -C20 -C19 : 123.698461
H42 -C20 -C19 : 118.793140 H42 -C20 -C21 : 117.508397
C22 -C21 -C20 : 125.052800 H64 -C21 -C20 : 116.804397
H64 -C21 -C22 : 118.142802 C23 -C22 -C21 : 123.838788
H56 -C22 -C21 : 118.735577 H56 -C22 -C23 : 117.425633
C24 -C23 -C22 : 124.918418 H60 -C23 -C22 : 116.848543
H60 -C23 -C24 : 118.233039 C25 -C24 -C23 : 123.962020
H53 -C24 -C23 : 118.703558 H53 -C24 -C25 : 117.334422
C26 -C25 -C24 : 124.791242 H65 -C25 -C24 : 116.850162
H65 -C25 -C26 : 118.358596 C27 -C26 -C25 : 124.055169
H57 -C26 -C25 : 118.736418 H57 -C26 -C27 : 117.208412
C28 -C27 -C26 : 123.961707 H37 -C27 -C26 : 116.224442
H37 -C27 -C28 : 119.813850 C29 -C28 -C27 : 127.684909
H61 -C28 -C27 : 117.384937 H61 -C28 -C29 : 114.930155
C30 -C29 -C28 : 118.665524 C34 -C29 -C28 : 123.614859
C34 -C29 -C30 : 117.719616 C31 -C30 -C29 : 121.358496
H39 -C30 -C29 : 118.916444 H39 -C30 -C31 : 119.725059
C32 -C31 -C30 : 120.086009 H43 -C31 -C30 : 119.754091
H43 -C31 -C32 : 120.159901 C33 -C32 -C31 : 119.417146
H47 -C32 -C31 : 120.336703 H47 -C32 -C33 : 120.246151
C34 -C33 -C32 : 120.536845 H51 -C33 -C32 : 119.910829
H51 -C33 -C34 : 119.552326 C33 -C34 -C29 : 120.881889
H49 -C34 -C29 : 119.959563 H49 -C34 -C33 : 119.158548

torsional angles:

C1 -C2 -C3 -C4 : 0.006580
C1 -C2 -C3 -H44 :-179.996509
C1 -C6 -C5 -C4 : 0.007405
C1 -C6 -C5 -C7 :-179.977759
C2 -C1 -C6 -C5 : -0.004375
C2 -C1 -C6 -H50 : 179.992663

C2 -C3 -C4 -C5 : -0.003419
C2 -C3 -C4 -H40 : 179.998269
C3 -C2 -C1 -C6 : -0.002732
C3 -C2 -C1 -H52 : 179.997059
C3 -C4 -C5 -C6 : -0.003536
C3 -C4 -C5 -C7 : 179.982372
C4 -C3 -C2 -H48 :-179.993350
C4 -C5 -C6 -H50 :-179.989610
C4 -C5 -C7 -C8 : 179.993909
C4 -C5 -C7 -H62 : -0.007775
C5 -C4 -C3 -H44 : 179.999658
C5 -C6 -C1 -H52 : 179.995833
C5 -C7 -C8 -C9 : 179.955748
C5 -C7 -C8 -H38 : -0.016921
C6 -C1 -C2 -H48 : 179.997198
C6 -C5 -C4 -H40 : 179.994790
C6 -C5 -C7 -C8 : -0.021051
C6 -C5 -C7 -H62 : 179.977266
C7 -C5 -C4 -H40 : -0.019303
C7 -C5 -C6 -H50 : 0.025226
C7 -C8 -C9 -C10 :-179.993271
C7 -C8 -C9 -H58 : 0.009314
C8 -C9 -C10 -C11 : 179.960831
C8 -C9 -C10 -H66 : -0.010544
C9 -C8 -C7 -H62 : -0.042533
C9 -C10 -C11 -C12 :-179.983588
C9 -C10 -C11 -H54 : 0.015586
C10 -C9 -C8 -H38 : -0.019709
C10 -C11 -C12 -C13 : 179.958835
C10 -C11 -C12 -H59 : -0.011405
C11 -C10 -C9 -H58 : -0.041792
C11 -C12 -C13 -C14 :-179.977234
C11 -C12 -C13 -H55 : 0.019269
C12 -C11 -C10 -H66 : -0.011827
C12 -C13 -C14 -C15 : 179.960483
C12 -C13 -C14 -H63 : -0.010348
C13 -C12 -C11 -H54 : -0.040328
C13 -C14 -C15 -C16 :-179.974063
C13 -C14 -C15 -H41 : 0.020903
C14 -C13 -C12 -H59 : -0.006635
C14 -C15 -C16 -C17 : 179.964374
C14 -C15 -C16 -H35 : -0.008310
C15 -C14 -C13 -H55 : -0.035978
C15 -C16 -C17 -C18 :-179.977628
C15 -C16 -C17 -H45 : 0.015250
C16 -C15 -C14 -H63 : -0.002901
C16 -C17 -C18 -C19 : 179.969203
C16 -C17 -C18 -H46 : -0.007698
C17 -C16 -C15 -H41 : -0.030534
C17 -C18 -C19 -C20 :-179.985496
C17 -C18 -C19 -H36 : 0.004465
C18 -C17 -C16 -H35 : -0.004642
C18 -C19 -C20 -C21 : 179.972652

C18 -C19 -C20 -H42 : -0.010139
C19 -C18 -C17 -H45 : -0.023591
C19 -C20 -C21 -C22 :-179.993691
C19 -C20 -C21 -H64 : -0.003194
C20 -C19 -C18 -H46 : -0.008333
C20 -C21 -C22 -C23 : 179.978239
C20 -C21 -C22 -H56 : -0.008127
C21 -C20 -C19 -H36 : -0.017186
C21 -C22 -C23 -C24 : 179.996860
C21 -C22 -C23 -H60 : -0.010386
C22 -C21 -C20 -H42 : -0.010695
C22 -C23 -C24 -C25 : 179.982576
C22 -C23 -C24 -H53 : -0.010327
C23 -C22 -C21 -H64 : -0.012142
C23 -C24 -C25 -C26 : 179.985960
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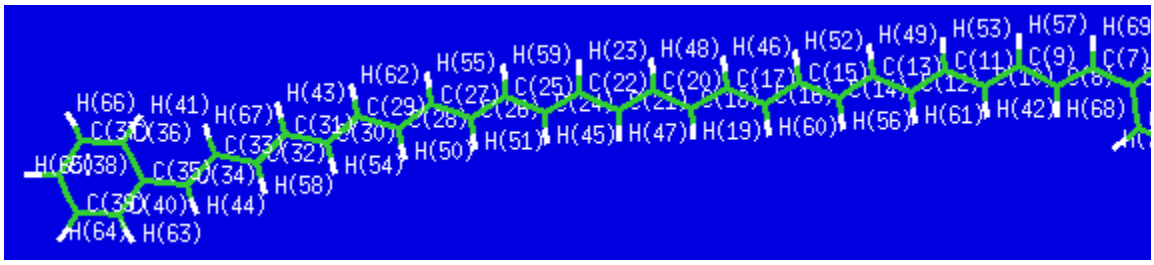
C24 -C23 -C22 -H56 : -0.016609
C24 -C25 -C26 -C27 : 179.990863
C24 -C25 -C26 -H57 : -0.008668
C25 -C24 -C23 -H60 : -0.010086
C25 -C26 -C27 -C28 : 179.974936
C25 -C26 -C27 -H37 : -0.026080
C26 -C25 -C24 -H53 : -0.021048
C26 -C27 -C28 -C29 :-179.998619
C26 -C27 -C28 -H61 : -0.002027
C27 -C26 -C25 -H65 : -0.005361
C27 -C28 -C29 -C30 : 179.976866
C27 -C28 -C29 -C34 : -0.015888
C28 -C27 -C26 -H57 : -0.025526
C28 -C29 -C30 -C31 :-179.996384
C28 -C29 -C30 -H39 : 0.008673
C28 -C29 -C34 -C33 : 179.997860
C28 -C29 -C34 -H49 : -0.008330
C29 -C28 -C27 -H37 : 0.002431
C29 -C30 -C31 -C32 : 0.001393
C29 -C30 -C31 -H43 :-179.997935
C29 -C34 -C33 -C32 : -0.005115
C29 -C34 -C33 -H51 : 179.995984
C30 -C29 -C28 -H61 : -0.019797
C30 -C29 -C34 -C33 : 0.005042
C30 -C29 -C34 -H49 : 179.998852
C30 -C31 -C32 -C33 : -0.001297
C30 -C31 -C32 -H47 : 179.999159
C31 -C30 -C29 -C34 : -0.003201
C31 -C32 -C33 -C34 : 0.003154
C31 -C32 -C33 -H51 :-179.997949
C32 -C31 -C30 -H39 : 179.996295
C32 -C33 -C34 -H49 :-179.998973
C33 -C32 -C31 -H43 : 179.998028
C34 -C29 -C28 -H61 : 179.987449
C34 -C29 -C30 -H39 :-179.998144
C34 -C33 -C32 -H47 :-179.997302
H35 -C16 -C15 -H41 : 179.996782

H35 -C16 -C17 -H45 : 179.988237
H36 -C19 -C18 -H46 : 179.981628
H36 -C19 -C20 -H42 :-179.999977
H37 -C27 -C26 -H57 : 179.973458
H37 -C27 -C28 -H61 : 179.999023
H38 -C8 -C7 -H62 : 179.984798
H38 -C8 -C9 -H58 : 179.982875
H39 -C30 -C31 -H43 : -0.003032
H40 -C4 -C3 -H44 : 0.001346
H41 -C15 -C14 -H63 : 179.992066
H42 -C20 -C21 -H64 : 179.979802
H43 -C31 -C32 -H47 : -0.001516
H44 -C3 -C2 -H48 : 0.003560
H45 -C17 -C18 -H46 : 179.999508
H47 -C32 -C33 -H51 : 0.001595
H48 -C2 -C1 -H52 : -0.003010
H49 -C34 -C33 -H51 : 0.002125
H50 -C6 -C1 -H52 : -0.007129
H53 -C24 -C23 -H60 : 179.997011
H53 -C24 -C25 -H65 : 179.975228
H54 -C11 -C10 -H66 : 179.987347
H54 -C11 -C12 -H59 : 179.989432
H55 -C13 -C12 -H59 : 179.989869
H55 -C13 -C14 -H63 : 179.993191
H56 -C22 -C21 -H64 :-179.998508
H56 -C22 -C23 -H60 : 179.976145
H57 -C26 -C25 -H65 : 179.995108
H58 -C9 -C10 -H66 : 179.986833

DPO13



final geometry:

angstroms

atom	x	y	z
C1	-0.1161583897	-0.0359749208	0.0993952798
C2	-0.0402995352	-0.2581481179	1.4901240851
C3	1.2388222534	-0.4116724682	2.0583393024
C4	2.3897718455	-0.3475352727	1.2776915117
C5	2.2942524481	-0.1273489406	-0.0964877558
C6	1.0328220662	0.0277590310	-0.6788480655
C7	-1.2153745734	-0.3319321445	2.3539814952
C8	-2.5093100390	-0.2084799292	1.9689249812
C9	-3.6438985927	-0.2788970108	2.8422467855
C10	-4.9234194712	-0.1363655647	2.3965202049
C11	-6.1011263881	-0.1858668685	3.2021928018
C12	-7.3582525476	-0.0253992236	2.6951678288
C13	-8.5606564874	-0.0610049960	3.4596671079
C14	-9.8087760332	0.1079731023	2.9300643579
C15	-11.0109560227	0.0739583806	3.6933645566
C16	-12.2673331405	0.2390315482	3.1816761547
C17	-13.4498067103	0.1931961624	3.9743918292
C18	-14.7225327513	0.3419299341	3.5006442040
H19	-14.8715928850	0.5150071503	2.4347595809
C20	-15.8813525132	0.2740035646	4.3263741874
C21	-17.1657857724	0.3969033915	3.8786835970
C22	-18.3171037943	0.3018304515	4.7128519401
H23	-18.1523373660	0.1320496166	5.7769697453
C24	-19.5994366052	0.3937829787	4.2528890385
C25	-20.7712682554	0.2710797760	5.0547900268
C26	-22.0333177138	0.3318843796	4.5372702324
C27	-23.2481501947	0.1838043517	5.2679803297
C28	-24.4720458161	0.2164751605	4.6638590422
C29	-25.7349197866	0.0464785161	5.3037340732
C30	-26.9117747462	0.0562292172	4.6129239551
C31	-28.2123020470	-0.1316153042	5.1706189694
C32	-29.3495859461	-0.1395157642	4.4199759610
C33	-30.6719936032	-0.3420507834	4.9309281295
C34	-31.7778040949	-0.3603223271	4.1456420770
C35	-33.1612811848	-0.5668286044	4.5561644993
C36	-33.5533393002	-0.7812770955	5.8937257467
C37	-34.8904518369	-0.9747572831	6.2193954458
C38	-35.8732879884	-0.9605850218	5.2251143791
C39	-35.5038362917	-0.7496172484	3.8968434067
C40	-34.1659876929	-0.5554575504	3.5688643305
H41	-32.8073258752	-0.7967393585	6.6821657232
H42	-5.0740326974	0.0354617016	1.3300765918

H43	-28.2862973634	-0.2842622935	6.2469867729
H44	-31.6341678447	-0.2068107654	3.0763547188
H45	-19.7520466737	0.5603329286	3.1859442180
H46	-13.3179614527	0.0192155342	5.0428065011
H47	-17.3340781922	0.5677318728	2.8150279888
H48	-15.7195334439	0.1008831855	5.3907017917
H49	-8.4690119871	-0.2331006775	4.5322817546
H50	-24.4978804448	0.3738680122	3.5848325374
H51	-22.1333594025	0.4936107415	3.4632734620
H52	-10.9111729317	-0.0991996604	4.7652780183
H53	-5.9802666521	-0.3574274907	4.2717757360
H54	-26.8658881210	0.2102829469	3.5344496450
H55	-23.1854489103	0.0239283376	6.3441858447
H56	-9.9004889675	0.2805023749	1.8573891154
H57	-3.4630808002	-0.4498007171	3.9034293401
H58	-29.2581665561	0.0121726014	3.3442853886
H59	-20.6417585275	0.1060886548	6.1243972955
H60	-12.3815391119	0.4123491022	2.1114433840
H61	-7.4612152858	0.1466301766	1.6232601369
H62	-25.7488347450	-0.1093020137	6.3822790143
H63	-33.8826604705	-0.3915445285	2.5320630653
H64	-36.2584834570	-0.7362912675	3.1156488936
H65	-36.9164033426	-1.1127914426	5.4858883223
H66	-35.1715722608	-1.1384848727	7.2558439553
H67	-30.7630600782	-0.4914556811	6.0053314998
H68	-2.7375218034	-0.0381172958	0.9179129043
H69	-1.0103042745	-0.5015259144	3.4109109331
H70	1.3224005749	-0.5833099405	3.1287799324
H71	3.3633903047	-0.4695228610	1.7439098586
H72	3.1900307245	-0.0762259868	-0.7079991208
H73	0.9464280609	0.2005162330	-1.7479517332
H74	-1.0826784888	0.0892434543	-0.3784042661

Final total energy: -1469.658033 hartrees

HOMO energy: -0.16068
LUMO energy: -0.09420

bond lengths (angstroms):

C1	-C2	:	1.410405	C1	-C6	:	1.389202				
C1	-H74	:	1.085418	C2	-C3	:	1.408045				
C2	-C7	:	1.460306	C3	-C4	:	1.392196				
C3	-H70	:	1.087331	C4	-C5	:	1.394982				
C4	-H71	:	1.086358	C5	-C6	:	1.398002				
C5	-H72	:	1.085808	C6	-H73	:	1.086412				
C7	-C8	:	1.355647	C7	-H69	:	1.089915				
C8	-C9	:	1.433506	C8	-H68	:	1.088912				
C9	-C10	:	1.362410	C9	-H57	:	1.089959				
C10	-C11	:	1.427779	C10	-H42	:	1.090647				
C11	-C12	:	1.364987	C11	-H53	:	1.089976				
C12	-C13	:	1.425308	C12	-H61	:	1.090496				
C13	-C14	:	1.366322	C13	-H49	:	1.090192				
C14	-C15	:	1.424437	C14	-H56	:	1.090326				
C15	-C16	:	1.366586	C15	-H52	:	1.090385				
C16	-C17	:	1.424339	C16	-H60	:	1.090174				
C17	-C18	:	1.366159	C17	-H46	:	1.090487				
C18	-H19	:	1.090085	C18	-C20	:	1.424538				
C20	-C21	:	1.365760	C20	-H48	:	1.090390				
C21	-C22	:	1.424924	C21	-H47	:	1.090352				
C22	-H23	:	1.090101	C22	-C24	:	1.365430				
C24	-C25	:	1.425234	C24	-H45	:	1.090596				
C25	-C26	:	1.365391	C25	-H59	:	1.089979				
C26	-C27	:	1.425371	C26	-H51	:	1.090703				
C27	-C28	:	1.365266	C27	-H55	:	1.089821				
C28	-C29	:	1.425900	C28	-H50	:	1.090751				
C29	-C30	:	1.364662	C29	-H62	:	1.089826				
C30	-C31	:	1.427473	C30	-H54	:	1.090388				
C31	-C32	:	1.362697	C31	-H43	:	1.089653				
C32	-C33	:	1.432081	C32	-H58	:	1.090173				
C33	-C34	:	1.356401	C33	-H67	:	1.088558				
C34	-C35	:	1.457801	C34	-H44	:	1.089758				
C35	-C36	:	1.410237	C35	-C40	:	1.408661				
C36	-C37	:	1.389736	C36	-H41	:	1.085547				
C37	-C38	:	1.398128	C37	-H66	:	1.086306				
C38	-C39	:	1.394742	C38	-H65	:	1.085937				
C39	-C40	:	1.391081	C39	-H64	:	1.086248				
C40	-H63	:	1.087244								

bond angles:

C6	-C1	-C2	: 121.006553	H74	-C1	-C2	: 120.008173
H74	-C1	-C6	: 118.985243	C3	-C2	-C1	: 117.642625
C7	-C2	-C1	: 123.228938	C7	-C2	-C3	: 119.128315

C4 -C3 -C2 : 121.313069 H70 -C3 -C2 : 118.967889
H70 -C3 -C4 : 119.719041 C5 -C4 -C3 : 120.200854
H71 -C4 -C3 : 119.676732 H71 -C4 -C5 : 120.122411
C6 -C5 -C4 : 119.317650 H72 -C5 -C4 : 120.379753
H72 -C5 -C6 : 120.302586 C5 -C6 -C1 : 120.519240
H73 -C6 -C1 : 119.525311 H73 -C6 -C5 : 119.955427
C8 -C7 -C2 : 126.542564 H69 -C7 -C2 : 115.474900
H69 -C7 -C8 : 117.982385 C9 -C8 -C7 : 125.305271
H68 -C8 -C7 : 119.237935 H68 -C8 -C9 : 115.456487
C10 -C9 -C8 : 122.606906 H57 -C9 -C8 : 118.004247
H57 -C9 -C10 : 119.388415 C11 -C10 -C9 : 125.904076
H42 -C10 -C9 : 117.779862 H42 -C10 -C11 : 116.315604
C12 -C11 -C10 : 123.092582 H53 -C11 -C10 : 117.886483
H53 -C11 -C12 : 119.020683 C13 -C12 -C11 : 125.083854
H61 -C12 -C11 : 118.074645 H61 -C12 -C13 : 116.841288
C14 -C13 -C12 : 124.030451 H49 -C13 -C12 : 117.435791
H49 -C13 -C14 : 118.533722 C15 -C14 -C13 : 124.076293
H56 -C14 -C13 : 118.538248 H56 -C14 -C15 : 117.385456
C16 -C15 -C14 : 124.916381 H52 -C15 -C14 : 116.958336
H52 -C15 -C16 : 118.125182 C17 -C16 -C15 : 123.433220
H60 -C16 -C15 : 118.887663 H60 -C16 -C17 : 117.678838
C18 -C17 -C16 : 125.233729 H46 -C17 -C16 : 116.746544
H46 -C17 -C18 : 118.018724 H19 -C18 -C17 : 118.930650
C20 -C18 -C17 : 123.479536 C20 -C18 -H19 : 117.588286
C21 -C20 -C18 : 124.801442 H48 -C20 -C18 : 116.913249
H48 -C20 -C21 : 118.282291 C22 -C21 -C20 : 124.192331
H47 -C21 -C20 : 118.621709 H47 -C21 -C22 : 117.182252
H23 -C22 -C21 : 117.369379 C24 -C22 -C21 : 123.856597
C24 -C22 -H23 : 118.768489 C25 -C24 -C22 : 125.228138
H45 -C24 -C22 : 118.116031 H45 -C24 -C25 : 116.649925
C26 -C25 -C24 : 122.880043 H59 -C25 -C24 : 117.870092
H59 -C25 -C26 : 119.242647 C27 -C26 -C25 : 126.075603
H51 -C26 -C25 : 117.684634 H51 -C26 -C27 : 116.233066
C28 -C27 -C26 : 122.324301 H55 -C27 -C26 : 118.193177
H55 -C27 -C28 : 119.475537 C29 -C28 -C27 : 126.337222
H50 -C28 -C27 : 117.543557 H50 -C28 -C29 : 116.113718
C30 -C29 -C28 : 122.395825 H62 -C29 -C28 : 118.193871
H62 -C29 -C30 : 119.405281 C31 -C30 -C29 : 125.942674
H54 -C30 -C29 : 117.736171 H54 -C30 -C31 : 116.317851
C32 -C31 -C30 : 123.087279 H43 -C31 -C30 : 117.789599
H43 -C31 -C32 : 119.120541 C33 -C32 -C31 : 125.096149
H58 -C32 -C31 : 118.212333 H58 -C32 -C33 : 116.690083
C34 -C33 -C32 : 123.240929 H67 -C33 -C32 : 116.667551
H67 -C33 -C34 : 120.090613 C35 -C34 -C33 : 127.775052
H44 -C34 -C33 : 117.304559 H44 -C34 -C35 : 114.920141
C36 -C35 -C34 : 123.536469 C40 -C35 -C34 : 118.578241
C40 -C35 -C36 : 117.885173 C37 -C36 -C35 : 120.724813
H41 -C36 -C35 : 119.999253 H41 -C36 -C37 : 119.275933
C38 -C37 -C36 : 120.549693 H66 -C37 -C36 : 119.574435
H66 -C37 -C38 : 119.875869 C39 -C38 -C37 : 119.510606
H65 -C38 -C37 : 120.202050 H65 -C38 -C39 : 120.287344
C40 -C39 -C38 : 120.026502 H64 -C39 -C38 : 120.180328
H64 -C39 -C40 : 119.793171 C39 -C40 -C35 : 121.303204

H63 -C40 -C35 : 118.928307 H63 -C40 -C39 : 119.768483

torsional angles:

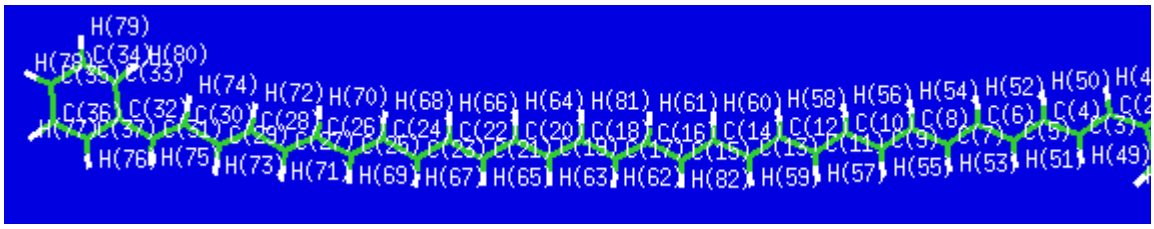
C1 -C2 -C3 -C4 : -0.027014
C1 -C2 -C3 -H70 : 179.962255
C1 -C2 -C7 -C8 : 0.256782
C1 -C2 -C7 -H69 :-179.597848
C1 -C6 -C5 -C4 : 0.003488
C1 -C6 -C5 -H72 :-179.958581
C2 -C1 -C6 -C5 : -0.021742
C2 -C1 -C6 -H73 :-179.967910
C2 -C3 -C4 -C5 : 0.009801
C2 -C3 -C4 -H71 : 179.991135
C2 -C7 -C8 -C9 :-179.669557
C2 -C7 -C8 -H68 : 0.119440
C3 -C2 -C1 -C6 : 0.032906
C3 -C2 -C1 -H74 :-179.903378
C3 -C2 -C7 -C8 :-179.873384
C3 -C2 -C7 -H69 : 0.271987
C3 -C4 -C5 -C6 : 0.002456
C3 -C4 -C5 -H72 : 179.964495
C4 -C3 -C2 -C7 :-179.904103
C4 -C5 -C6 -H73 : 179.949425
C5 -C4 -C3 -H70 :-179.979388
C5 -C6 -C1 -H74 : 179.915183
C6 -C1 -C2 -C7 : 179.904552
C6 -C5 -C4 -H71 :-179.978794
C7 -C2 -C1 -H74 : -0.031732
C7 -C2 -C3 -H70 : 0.085166
C7 -C8 -C9 -C10 : 179.463820
C7 -C8 -C9 -H57 : -0.295481
C8 -C9 -C10 -C11 :-179.611520
C8 -C9 -C10 -H42 : 0.132282
C9 -C8 -C7 -H69 : 0.181832
C9 -C10 -C11 -C12 : 179.497236
C9 -C10 -C11 -H53 : -0.317739
C10 -C9 -C8 -H68 : -0.332261
C10 -C11 -C12 -C13 :-179.715535
C10 -C11 -C12 -H61 : 0.111031
C11 -C10 -C9 -H57 : 0.144575
C11 -C12 -C13 -C14 : 179.715765
C11 -C12 -C13 -H49 : -0.214134
C12 -C11 -C10 -H42 : -0.249888
C12 -C13 -C14 -C15 :-179.932024
C12 -C13 -C14 -H56 : 0.046081
C13 -C12 -C11 -H53 : 0.097443
C13 -C14 -C15 -C16 :-179.913634
C13 -C14 -C15 -H52 : -0.032217
C14 -C13 -C12 -H61 : -0.112731
C14 -C15 -C16 -C17 : 179.716959
C14 -C15 -C16 -H60 : -0.086528
C15 -C14 -C13 -H49 : -0.002843

C15 -C16 -C17 -C18 :-179.420764
C15 -C16 -C17 -H46 : 0.206143
C16 -C15 -C14 -H56 : 0.108028
C16 -C17 -C18 -H19 : -0.287080
C16 -C17 -C18 -C20 : 179.251946
C17 -C16 -C15 -H52 : -0.163192
C17 -C18 -C20 -C21 :-178.877903
C17 -C18 -C20 -H48 : 0.477169
C18 -C17 -C16 -H60 : 0.384941
C18 -C20 -C21 -C22 : 178.770478
C18 -C20 -C21 -H47 : -0.508054
H19 -C18 -C17 -H46 :-179.909672
H19 -C18 -C20 -C21 : 0.666892
H19 -C18 -C20 -H48 :-179.978035
C20 -C18 -C17 -H46 : -0.370646
C20 -C21 -C22 -H23 : 0.771133
C20 -C21 -C22 -C24 :-178.360627
C21 -C22 -C24 -C25 : 178.409391
C21 -C22 -C24 -H45 : -0.674349
C22 -C21 -C20 -H48 : -0.576488
C22 -C24 -C25 -C26 :-177.996525
C22 -C24 -C25 -H59 : 1.017547
H23 -C22 -C21 -H47 :-179.940799
H23 -C22 -C24 -C25 : -0.710987
H23 -C22 -C24 -H45 :-179.794728
C24 -C22 -C21 -H47 : 0.927441
C24 -C25 -C26 -C27 : 178.279267
C24 -C25 -C26 -H51 : -0.739968
C25 -C26 -C27 -C28 :-177.870196
C25 -C26 -C27 -H55 : 1.162487
C26 -C25 -C24 -H45 : 1.099281
C26 -C27 -C28 -C29 : 178.404186
C26 -C27 -C28 -H50 : -0.705468
C27 -C26 -C25 -H59 : -0.721865
C27 -C28 -C29 -C30 :-178.068710
C27 -C28 -C29 -H62 : 1.110425
C28 -C27 -C26 -H51 : 1.161598
C28 -C29 -C30 -C31 : 178.724222
C28 -C29 -C30 -H54 : -0.587617
C29 -C28 -C27 -H55 : -0.616502
C29 -C30 -C31 -C32 :-178.525040
C29 -C30 -C31 -H43 : 0.884553
C30 -C29 -C28 -H50 : 1.052112
C30 -C31 -C32 -C33 : 179.100371
C30 -C31 -C32 -H58 : -0.448263
C31 -C30 -C29 -H62 : -0.445315
C31 -C32 -C33 -C34 :-179.087364
C31 -C32 -C33 -H67 : 0.565847
C32 -C31 -C30 -H54 : 0.795436
C32 -C33 -C34 -C35 : 179.505675
C32 -C33 -C34 -H44 : -0.303040
C33 -C32 -C31 -H43 : -0.301741
C33 -C34 -C35 -C36 : 0.243757

C33 -C34 -C35 -C40 :-179.629042
C34 -C33 -C32 -H58 : 0.467458
C34 -C35 -C36 -C37 :-179.859464
C34 -C35 -C36 -H41 : 0.127178
C34 -C35 -C40 -C39 : 179.851437
C34 -C35 -C40 -H63 : -0.121175
C35 -C34 -C33 -H67 : -0.136156
C35 -C36 -C37 -C38 : 0.012259
C35 -C36 -C37 -H66 : 179.991873
C35 -C40 -C39 -C38 : 0.016542
C35 -C40 -C39 -H64 :-179.984220
C36 -C35 -C34 -H44 :-179.943664
C36 -C35 -C40 -C39 : -0.028608
C36 -C35 -C40 -H63 : 179.998780
C36 -C37 -C38 -C39 : -0.024815
C36 -C37 -C38 -H65 : 179.974909
C37 -C36 -C35 -C40 : 0.014159
C37 -C38 -C39 -C40 : 0.010497
C37 -C38 -C39 -H64 :-179.988738
C38 -C37 -C36 -H41 :-179.974478
C38 -C39 -C40 -H63 : 179.988928
C39 -C38 -C37 -H66 : 179.995633
C40 -C35 -C34 -H44 : 0.183536
C40 -C35 -C36 -H41 :-179.999199
C40 -C39 -C38 -H65 :-179.989228
H41 -C36 -C37 -H66 : 0.005135
H42 -C10 -C9 -H57 : 179.888378
H42 -C10 -C11 -H53 : 179.935137
H43 -C31 -C30 -H54 :-179.794972
H43 -C31 -C32 -H58 :-179.850375
H44 -C34 -C33 -H67 :-179.944871
H45 -C24 -C25 -H59 :-179.886646
H46 -C17 -C16 -H60 :-179.988152
H47 -C21 -C20 -H48 :-179.855020
H49 -C13 -C12 -H61 : 179.957371
H49 -C13 -C14 -H56 : 179.975263
H50 -C28 -C27 -H55 :-179.726155
H50 -C28 -C29 -H62 :-179.768753
H51 -C26 -C25 -H59 :-179.741100
H51 -C26 -C27 -H55 :-179.805720
H52 -C15 -C14 -H56 : 179.989445
H52 -C15 -C16 -H60 :-179.966679
H53 -C11 -C12 -H61 : 179.924010
H54 -C30 -C29 -H62 :-179.757155
H57 -C9 -C8 -H68 : 179.908438
H58 -C32 -C33 -H67 :-179.879331
H63 -C40 -C39 -H64 : -0.011834
H64 -C39 -C38 -H65 : 0.011537
H65 -C38 -C37 -H66 : -0.004643
H68 -C8 -C7 -H69 : 179.970829
H70 -C3 -C4 -H71 : 0.001945
H71 -C4 -C5 -H72 : -0.016755
H72 -C5 -C6 -H73 : -0.012644

H73 -C6 -C1 -H74 : -0.030986

DPO15



final geometry:

	angstroms		
atom	x	y	z
C1	-0.0510348764	-0.0076449271	0.0400482352
C2	-0.0718001018	-0.0102797611	1.5000061528
C3	0.9897367409	-0.0178112697	2.3450309810
C4	0.8754699505	-0.0170924628	3.7752798248
C6	1.8359030298	-0.0184659793	6.0550066774
C5	1.9381407375	-0.0213884184	4.6289865952
C7	2.9057256452	-0.0188769752	6.9036139604
C8	2.8079617401	-0.0144261712	8.3278460600
C9	3.8781696884	-0.0107232689	9.1778793312
C10	3.7751918478	-0.0052031250	10.6003673066
C11	4.8392259620	0.0027114946	11.4591946784
C12	4.7172376759	0.0093148006	12.8793635345
C13	5.7645044182	0.0213674672	13.7590436820
C14	5.6078407131	0.0295597673	15.1761146088
C15	6.6312474522	0.0454861803	16.0839004942
C16	6.4384600882	0.0557739699	17.4964231596
C17	7.4407263632	0.0748817260	18.4276740321
C18	7.2192808532	0.0880565885	19.8359215402
C19	8.2042593200	0.1096415923	20.7852704590
C20	7.9589556015	0.1260051468	22.1894681362
C21	8.9289638955	0.1498404751	23.1532846254
C22	8.6642011165	0.1694430715	24.5538509181
C23	9.6221480550	0.1944789785	25.5290493829
C24	9.3393671963	0.2168089633	26.9266511705
C25	10.2824802302	0.2418345548	27.9152621781
C26	9.9756074108	0.2662835595	29.3091359370
C27	10.8992504973	0.2910548975	30.3138888506
C28	10.5647644506	0.3171897450	31.7034548254
C29	11.4669558177	0.3417893427	32.7242203123
C30	11.1026185188	0.3692327627	34.1111702942
C31	11.9926269462	0.3937907050	35.1342807372
C32	11.6988971888	0.4233987020	36.5640907960
C33	10.3905808884	0.4247999103	37.0906449735
C34	10.1739986458	0.4551937092	38.4630235769
C35	11.2524375471	0.4851997872	39.3519515992
C36	12.5537954065	0.4836081868	38.8500642983
C37	12.7720391355	0.4531212367	37.4759136055
C38	1.1341726391	-0.0105846534	-0.7239192545
C39	1.0887856019	-0.0069128446	-2.1129955372
C40	-0.1378795134	0.0003553839	-2.7833012438
C41	-1.3211730051	0.0033045006	-2.0447640019
C42	-1.2765836594	-0.0006569336	-0.6538795472

H43	-2.2030941155	0.0019639672	-0.0850441720
H44	-2.2811677508	0.0087758476	-2.5530837050
H45	-0.1681013785	0.0034720559	-3.8688509418
H46	2.0158257993	-0.0095108329	-2.6794947732
H47	2.0989717436	-0.0153707153	-0.2270350962
H48	-1.0665881870	-0.0050550836	1.9455717917
H49	2.0015493294	-0.0236360957	1.9432433844
H50	-0.1315699711	-0.0118500269	4.1932669255
H51	2.9431186004	-0.0258143247	4.2065302270
H52	0.8325340223	-0.0147794899	6.4816909257
H53	3.9083323064	-0.0213805910	6.4749770400
H54	1.8052483996	-0.0129788454	8.7561947305
H55	4.8810611616	-0.0108431564	8.7508126025
H56	2.7702281738	-0.0065605852	11.0234901253
H57	5.8461816762	0.0050438498	11.0419932102
H58	3.7057468494	0.0050513504	13.2860147623
H59	6.7804869045	0.0257547084	13.3635197034
H60	4.5860679904	0.0229968229	15.5567830161
H61	5.4076830115	0.0481957881	17.8519374079
H62	8.4746397801	0.0807207686	18.0821649305
H63	9.2439424307	0.1149778996	20.4575378615
H64	6.9162803689	0.1199561131	22.5077949772
H65	9.9732977818	0.1545081658	22.8412997560
H66	7.6173498027	0.1652276687	24.8589474131
H67	10.6704061455	0.1979284431	25.2305338588
H68	8.2884162090	0.2149240116	27.2173379337
H69	11.3356857959	0.2436226568	27.6335223014
H70	8.9195300571	0.2664987132	29.5807667409
H71	11.9575435497	0.2912779578	30.0529120213
H72	9.5031748944	0.3188482858	31.9530223220
H73	12.5306839844	0.3407517791	32.4862266499
H74	10.0350356643	0.3714429471	34.3246257884
H75	13.0525779974	0.3921092864	34.8798678942
H76	13.7891332898	0.4521818239	37.0915363904
H77	13.4008644133	0.5060914540	39.5298478788
H78	11.0775949952	0.5092212736	40.4234616487
H79	9.1570692042	0.4553306746	38.8452106106
H80	9.5367856000	0.4011108391	36.4212204792
H81	6.1820611585	0.0808689908	20.1709918222
H82	7.6573031265	0.0511375516	15.7161067494

Final total energy: -1624.481322 hartrees

HOMO energy: -0.15985
LUMO energy: -0.09683

bond lengths (angstroms):

C1	-C2	:	1.460108	C1	-C38	:	1.410096
C1	-C42	:	1.408387	C2	-C3	:	1.356829
C2	-H48	:	1.090027	C3	-C4	:	1.434806
C3	-H49	:	1.088684	C4	-C5	:	1.363122
C4	-H50	:	1.090353	C5	-C6	:	1.429683
C5	-H51	:	1.090169	C6	-C7	:	1.365524
C6	-H52	:	1.090331	C7	-C8	:	1.427591
C7	-H53	:	1.090393	C8	-C9	:	1.366717
C8	-H54	:	1.090375	C9	-C10	:	1.426221
C9	-H55	:	1.090035	C10	-C11	:	1.367412
C10	-H56	:	1.090407	C11	-C12	:	1.425414
C11	-H57	:	1.089964	C12	-C13	:	1.367754
C12	-H58	:	1.090182	C13	-C14	:	1.425728
C13	-H59	:	1.090266	C14	-C15	:	1.368097
C14	-H60	:	1.090399	C15	-C16	:	1.425655
C15	-H82	:	1.089997	C16	-C17	:	1.368258
C16	-H61	:	1.090389	C17	-C18	:	1.425613
C17	-H62	:	1.090132	C18	-C19	:	1.368178
C18	-H81	:	1.090022	C19	-C20	:	1.425557
C19	-H63	:	1.090128	C20	-C21	:	1.367635
C20	-H64	:	1.090202	C21	-C22	:	1.425507
C21	-H65	:	1.089949	C22	-C23	:	1.367224
C22	-H66	:	1.090412	C23	-C24	:	1.426098
C23	-H67	:	1.089940	C24	-C25	:	1.366543
C24	-H68	:	1.090413	C25	-C26	:	1.427464
C25	-H69	:	1.090240	C26	-C27	:	1.365012
C26	-H70	:	1.090451	C27	-C28	:	1.429496
C27	-H71	:	1.089997	C28	-C29	:	1.362540
C28	-H72	:	1.090532	C29	-C30	:	1.434268
C29	-H73	:	1.090027	C30	-C31	:	1.356272
C30	-H74	:	1.088715	C31	-C32	:	1.459969
C31	-H75	:	1.090057	C32	-C33	:	1.410302
C32	-C37	:	1.408523	C33	-C34	:	1.389696
C33	-H80	:	1.085199	C34	-C35	:	1.397900
C34	-H79	:	1.086376	C35	-C36	:	1.394785
C35	-H78	:	1.085947	C36	-C37	:	1.391708
C36	-H77	:	1.086341	C37	-H76	:	1.087303
C38	-C39	:	1.389822	C38	-H47	:	1.085244
C39	-C40	:	1.397880	C39	-H46	:	1.086431
C40	-C41	:	1.394858	C40	-H45	:	1.085975
C41	-C42	:	1.391605	C41	-H44	:	1.086282
C42	-H43	:	1.087199				

bond angles:

C38 -C1 -C2 : 123.619707 C42 -C1 -C2 : 118.704595
C42 -C1 -C38 : 117.675676 C3 -C2 -C1 : 127.706259
H48 -C2 -C1 : 114.941587 H48 -C2 -C3 : 117.352148
C4 -C3 -C2 : 123.952543 H49 -C3 -C2 : 119.821953
H49 -C3 -C4 : 116.225461 C5 -C4 -C3 : 124.208854
H50 -C4 -C3 : 117.109269 H50 -C4 -C5 : 118.681853
C6 -C5 -C4 : 124.675488 H51 -C5 -C4 : 118.423311
H51 -C5 -C6 : 116.901130 C7 -C6 -C5 : 124.321341
H52 -C6 -C5 : 117.138688 H52 -C6 -C7 : 118.539948
C8 -C7 -C6 : 124.495173 H53 -C7 -C6 : 118.429924
H53 -C7 -C8 : 117.074848 C9 -C8 -C7 : 124.532479
H54 -C8 -C7 : 117.058574 H54 -C8 -C9 : 118.408921
C10 -C9 -C8 : 124.318750 H55 -C9 -C8 : 118.474807
H55 -C9 -C10 : 117.206407 C11 -C10 -C9 : 124.768502
H56 -C10 -C9 : 116.972722 H56 -C10 -C11 : 118.258752
C12 -C11 -C10 : 123.999786 H57 -C11 -C10 : 118.586548
H57 -C11 -C12 : 117.413644 C13 -C12 -C11 : 125.120868
H58 -C12 -C11 : 116.809475 H58 -C12 -C13 : 118.069642
C14 -C13 -C12 : 123.722171 H59 -C13 -C12 : 118.700291
H59 -C13 -C14 : 117.577523 C15 -C14 -C13 : 125.266368
H60 -C14 -C13 : 116.738696 H60 -C14 -C15 : 117.994928
C16 -C15 -C14 : 123.804014 H82 -C15 -C14 : 118.707193
H82 -C15 -C16 : 117.488788 C17 -C16 -C15 : 125.126670
H61 -C16 -C15 : 116.796565 H61 -C16 -C17 : 118.076757
C18 -C17 -C16 : 123.963531 H62 -C17 -C16 : 118.626440
H62 -C17 -C18 : 117.410028 C19 -C18 -C17 : 125.011720
H81 -C18 -C17 : 116.833617 H81 -C18 -C19 : 118.154651
C20 -C19 -C18 : 124.040723 H63 -C19 -C18 : 118.559951
H63 -C19 -C20 : 117.399325 C21 -C20 -C19 : 124.912634
H64 -C20 -C19 : 116.880068 H64 -C20 -C21 : 118.207264
C22 -C21 -C20 : 124.118711 H65 -C21 -C20 : 118.550281
H65 -C21 -C22 : 117.331007 C23 -C22 -C21 : 124.813566
H66 -C22 -C21 : 116.946814 H66 -C22 -C23 : 118.239573
C24 -C23 -C22 : 124.081483 H67 -C23 -C22 : 118.591573
H67 -C23 -C24 : 117.326944 C25 -C24 -C23 : 124.919268
H68 -C24 -C23 : 116.894181 H68 -C24 -C25 : 118.186496
C26 -C25 -C24 : 123.942716 H69 -C25 -C24 : 118.671065
H69 -C25 -C26 : 117.386219 C27 -C26 -C25 : 125.001670
H70 -C26 -C25 : 116.836267 H70 -C26 -C27 : 118.161993
C28 -C27 -C26 : 123.884287 H71 -C27 -C26 : 118.733742
H71 -C27 -C28 : 117.381970 C29 -C28 -C27 : 125.004040
H72 -C28 -C27 : 116.760610 H72 -C28 -C29 : 118.235279
C30 -C29 -C28 : 123.820607 H73 -C29 -C28 : 118.853787
H73 -C29 -C30 : 117.325606 C31 -C30 -C29 : 124.271856
H74 -C30 -C29 : 116.022543 H74 -C30 -C31 : 119.705523
C32 -C31 -C30 : 127.381229 H75 -C31 -C30 : 117.516431
H75 -C31 -C32 : 115.102333 C33 -C32 -C31 : 123.525634
C37 -C32 -C31 : 118.759343 C37 -C32 -C33 : 117.715011
C34 -C33 -C32 : 120.884576 H80 -C33 -C32 : 119.969032
H80 -C33 -C34 : 119.146372 C35 -C34 -C33 : 120.545017
H79 -C34 -C33 : 119.558041 H79 -C34 -C35 : 119.896941
C36 -C35 -C34 : 119.403242 H78 -C35 -C34 : 120.245960
H78 -C35 -C36 : 120.350796 C37 -C36 -C35 : 120.107896

H77 -C36 -C35 : 120.153951 H77 -C36 -C37 : 119.738153
C36 -C37 -C32 : 121.344239 H76 -C37 -C32 : 118.935553
H76 -C37 -C36 : 119.720208 C39 -C38 -C1 : 120.933245
H47 -C38 -C1 : 119.945917 H47 -C38 -C39 : 119.120833
C40 -C39 -C38 : 120.525973 H46 -C39 -C38 : 119.556372
H46 -C39 -C40 : 119.917654 C41 -C40 -C39 : 119.376200
H45 -C40 -C39 : 120.249314 H45 -C40 -C41 : 120.374485
C42 -C41 -C40 : 120.133030 H44 -C41 -C40 : 120.129062
H44 -C41 -C42 : 119.737908 C41 -C42 -C1 : 121.355871
H43 -C42 -C1 : 118.932944 H43 -C42 -C41 : 119.711182

torsional angles:

C1 -C2 -C3 -C4 : 179.866435
C1 -C2 -C3 -H49 : -0.055862
C1 -C38 -C39 -C40 : 0.026616
C1 -C38 -C39 -H46 :-179.986622
C1 -C42 -C41 -C40 : 0.001221
C1 -C42 -C41 -H44 :-179.994338
C2 -C1 -C38 -C39 :-179.955528
C2 -C1 -C38 -H47 : 0.019218
C2 -C1 -C42 -C41 : 179.944439
C2 -C1 -C42 -H43 : -0.037118
C2 -C3 -C4 -C5 :-179.835121
C2 -C3 -C4 -H50 : 0.107954
C3 -C2 -C1 -C38 : -0.109877
C3 -C2 -C1 -C42 : 179.945436
C3 -C4 -C5 -C6 : 179.890131
C3 -C4 -C5 -H51 : -0.009300
C4 -C3 -C2 -H48 : -0.104065
C4 -C5 -C6 -C7 :-179.800244
C4 -C5 -C6 -H52 : 0.142939
C5 -C4 -C3 -H49 : 0.089730
C5 -C6 -C7 -C8 : 179.924993
C5 -C6 -C7 -H53 : 0.013323
C6 -C5 -C4 -H50 : -0.052110
C6 -C7 -C8 -C9 :-179.790811
C6 -C7 -C8 -H54 : 0.149520
C7 -C6 -C5 -H51 : 0.100579
C7 -C8 -C9 -C10 : 179.947481
C7 -C8 -C9 -H55 : 0.018652
C8 -C7 -C6 -H52 : -0.017451
C8 -C9 -C10 -C11 :-179.786811
C8 -C9 -C10 -H56 : 0.156324
C9 -C8 -C7 -H53 : 0.121952
C9 -C10 -C11 -C12 : 179.943265
C9 -C10 -C11 -H57 : -0.001343
C10 -C9 -C8 -H54 : 0.007894
C10 -C11 -C12 -C13 :-179.790397
C10 -C11 -C12 -H58 : 0.164206
C11 -C10 -C9 -H55 : 0.142845
C11 -C12 -C13 -C14 : 179.910560
C11 -C12 -C13 -H59 : -0.044186

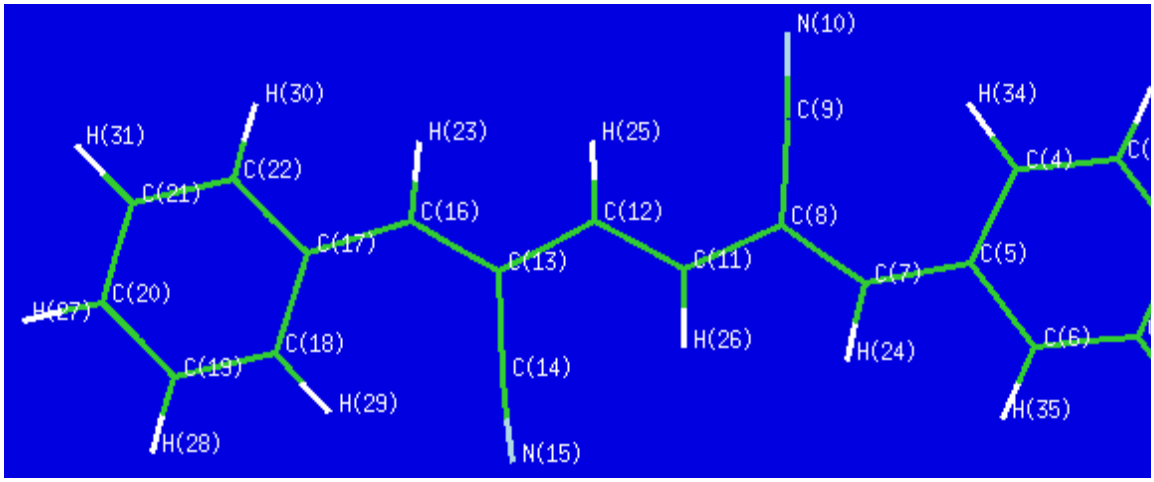
C12 -C11 -C10 -H56 : 0.000802
C12 -C13 -C14 -C15 :-179.803164
C12 -C13 -C14 -H60 : 0.164734
C13 -C12 -C11 -H57 : 0.154810
C13 -C14 -C15 -C16 : 179.880554
C13 -C14 -C15 -H82 : -0.095037
C14 -C13 -C12 -H58 : -0.043522
C14 -C15 -C16 -C17 :-179.838422
C14 -C15 -C16 -H61 : 0.129073
C15 -C14 -C13 -H59 : 0.152054
C15 -C16 -C17 -C18 : 179.843142
C15 -C16 -C17 -H62 : -0.144493
C16 -C15 -C14 -H60 : -0.086978
C16 -C17 -C18 -C19 :-179.875325
C16 -C17 -C18 -H81 : 0.083206
C17 -C16 -C15 -H82 : 0.137445
C17 -C18 -C19 -C20 : 179.830215
C17 -C18 -C19 -H63 : -0.159426
C18 -C17 -C16 -H61 : -0.123974
C18 -C19 -C20 -C21 :-179.887850
C18 -C19 -C20 -H64 : 0.043236
C19 -C18 -C17 -H62 : 0.112449
C19 -C20 -C21 -C22 : 179.829916
C19 -C20 -C21 -H65 : -0.158903
C20 -C19 -C18 -H81 : -0.127816
C20 -C21 -C22 -C23 :-179.942318
C20 -C21 -C22 -H66 : -0.023346
C21 -C20 -C19 -H63 : 0.101902
C21 -C22 -C23 -C24 : 179.856728
C21 -C22 -C23 -H67 : -0.135240
C22 -C21 -C20 -H64 : -0.100332
C22 -C23 -C24 -C25 : 179.993588
C22 -C23 -C24 -H68 : -0.093685
C23 -C22 -C21 -H65 : 0.046626
C23 -C24 -C25 -C26 : 179.884909
C23 -C24 -C25 -H69 : -0.105051
C24 -C23 -C22 -H66 : -0.061284
C24 -C25 -C26 -C27 : 179.977867
C24 -C25 -C26 -H70 : -0.120494
C25 -C24 -C23 -H67 : -0.014351
C25 -C26 -C27 -C28 : 179.906367
C25 -C26 -C27 -H71 : -0.086777
C26 -C25 -C24 -H68 : -0.026785
C26 -C27 -C28 -C29 : 179.980280
C26 -C27 -C28 -H72 : -0.118379
C27 -C26 -C25 -H69 : -0.032054
C27 -C28 -C29 -C30 : 179.927831
C27 -C28 -C29 -H73 : -0.077817
C28 -C27 -C26 -H70 : 0.005920
C28 -C29 -C30 -C31 : 179.997723
C28 -C29 -C30 -H74 : -0.104866
C29 -C28 -C27 -H71 : -0.026490
C29 -C30 -C31 -C32 : 179.950043

C29 -C30 -C31 -H75 : -0.020412
C30 -C29 -C28 -H72 : 0.027820
C30 -C31 -C32 -C33 : 0.283783
C30 -C31 -C32 -C37 :-179.676287
C31 -C30 -C29 -H73 : 0.003291
C31 -C32 -C33 -C34 :-179.929993
C31 -C32 -C33 -H80 : 0.120508
C31 -C32 -C37 -C36 : 179.928647
C31 -C32 -C37 -H76 : -0.063110
C32 -C31 -C30 -H74 : 0.056180
C32 -C33 -C34 -C35 : 0.005388
C32 -C33 -C34 -H79 :-179.980827
C32 -C37 -C36 -C35 : 0.001031
C32 -C37 -C36 -H77 : 179.997450
C33 -C32 -C31 -H75 :-179.745153
C33 -C32 -C37 -C36 : -0.033751
C33 -C32 -C37 -H76 : 179.974491
C33 -C34 -C35 -C36 : -0.038869
C33 -C34 -C35 -H78 : 179.979266
C34 -C33 -C32 -C37 : 0.030466
C34 -C35 -C36 -C37 : 0.035597
C34 -C35 -C36 -H77 :-179.960807
C35 -C34 -C33 -H80 : 179.955297
C35 -C36 -C37 -H76 : 179.992725
C36 -C35 -C34 -H79 : 179.947299
C37 -C32 -C31 -H75 : 0.294777
C37 -C32 -C33 -H80 :-179.919034
C37 -C36 -C35 -H78 :-179.982558
C38 -C1 -C2 -H48 : 179.861226
C38 -C1 -C42 -C41 : -0.003550
C38 -C1 -C42 -H43 :-179.985107
C38 -C39 -C40 -C41 : -0.028621
C38 -C39 -C40 -H45 : 179.983441
C39 -C38 -C1 -C42 : -0.010310
C39 -C40 -C41 -C42 : 0.014771
C39 -C40 -C41 -H44 :-179.989687
C40 -C39 -C38 -H47 :-179.948334
C40 -C41 -C42 -H43 : 179.982637
C41 -C40 -C39 -H46 : 179.984664
C42 -C1 -C2 -H48 : -0.083462
C42 -C1 -C38 -H47 : 179.964435
C42 -C41 -C40 -H45 :-179.997307
H43 -C42 -C41 -H44 : -0.012923
H44 -C41 -C40 -H45 : -0.001765
H45 -C40 -C39 -H46 : -0.003274
H46 -C39 -C38 -H47 : 0.038428
H48 -C2 -C3 -H49 : 179.973638
H49 -C3 -C4 -H50 :-179.967195
H50 -C4 -C5 -H51 :-179.951542
H51 -C5 -C6 -H52 :-179.956238
H52 -C6 -C7 -H53 :-179.929121
H53 -C7 -C8 -H54 :-179.937718
H54 -C8 -C9 -H55 :-179.920934

H55 -C9 -C10 -H56 :-179.914020
H56 -C10 -C11 -H57 :-179.943806
H57 -C11 -C12 -H58 :-179.890587
H58 -C12 -C13 -H59 :-179.998268
H59 -C13 -C14 -H60 :-179.880048
H60 -C14 -C15 -H82 : 179.937431
H61 -C16 -C15 -H82 :-179.895060
H61 -C16 -C17 -H62 : 179.888391
H62 -C17 -C18 -H81 :-179.929020
H63 -C19 -C18 -H81 : 179.882544
H63 -C19 -C20 -H64 :-179.967013
H64 -C20 -C21 -H65 : 179.910850
H65 -C21 -C22 -H66 : 179.965598
H66 -C22 -C23 -H67 : 179.946748
H67 -C23 -C24 -H68 : 179.898376
H68 -C24 -C25 -H69 : 179.983255
H69 -C25 -C26 -H70 : 179.869585
H70 -C26 -C27 -H71 :-179.987224
H71 -C27 -C28 -H72 : 179.874851
H72 -C28 -C29 -H73 :-179.977827
H73 -C29 -C30 -H74 : 179.900701
H74 -C30 -C31 -H75 :-179.914275
H76 -C37 -C36 -H77 : -0.010856
H77 -C36 -C35 -H78 : 0.021038
H78 -C35 -C34 -H79 : -0.034565
H79 -C34 -C33 -H80 : -0.030918

α,ω-diphenyl-μ,ν-dicyano-oligoene (DPDCn) Series:

DPDC3



final geometry:

	angstroms		
atom	x	y	z
C1	0.0381824916	-0.1227603836	-0.2673295124
C2	-0.2117708504	-0.6567283298	0.9975668046
C3	0.8459437885	-0.8475952316	1.8909054414
C4	2.1475446870	-0.5114388428	1.5347028258
C5	2.4182916768	0.0291818696	0.2593850383
C6	1.3362597060	0.2145640979	-0.6287728769
C7	3.7295080231	0.4183500785	-0.2316873774
C8	4.9798793012	0.3898709402	0.3206839049
C9	5.2494922254	-0.0870492097	1.6447285370
N10	5.5276665244	-0.4619501885	2.7110929237
C11	6.1152606212	0.8622925178	-0.4568587258
C12	7.4081776482	0.9023809817	-0.0653453624
C13	8.4928584952	1.3910825136	-0.9093782547
C14	8.1050839066	1.8418707965	-2.2153216392
N15	7.7128822233	2.1902684475	-3.2543543146
C16	9.7883969479	1.4163822232	-0.4757024823
C17	11.0205697875	1.8492569924	-1.1218434294
C18	11.1194781809	2.3458119328	-2.4398994431
C19	12.3500002450	2.7322988710	-2.9580994685
C20	13.5106560124	2.6370557537	-2.1868494556
C21	13.4332011212	2.1474417956	-0.8824679209
C22	12.2051938427	1.7589988316	-0.3596609423
H23	9.9297509456	1.0476423746	0.5385878616
H24	3.7084729765	0.8120977016	-1.2461391016
H25	7.6929352388	0.5591145947	0.9262003426
H26	5.8603420128	1.2122263831	-1.4541124432
H27	14.4676714308	2.9414896019	-2.6000853122
H28	12.4031549256	3.1112564405	-3.9742670771
H29	10.2401366793	2.4309301300	-3.0631843680
H30	12.1501325940	1.3778835930	0.6569136791
H31	14.3286351384	2.0680884280	-0.2732973270
H32	-1.2239867829	-0.9230947522	1.2872675723

H33	0.6538467648	-1.2629739733	2.8756649088
H34	2.9496325789	-0.6689066653	2.2451647884
H35	1.5294538228	0.6301711788	-1.6142993694
H36	-0.7763419456	0.0297764742	-0.9689999963

Final total energy: -880.026574 hartrees

HOMO energy: -0.21161
LUMO energy: -0.09611

bond lengths (angstroms):

C1	-C2	:	1.395550	C1	-C6	:	1.389041
C1	-H36	:	1.085845	C2	-C3	:	1.397585
C2	-H32	:	1.086029	C3	-C4	:	1.390700
C3	-H33	:	1.085906	C4	-C5	:	1.411386
C4	-H34	:	1.083004	C5	-C6	:	1.412085
C5	-C7	:	1.453235	C6	-H35	:	1.086883
C7	-C8	:	1.367243	C7	-H24	:	1.088390
C8	-C9	:	1.432912	C8	-C11	:	1.454938
C9	-N10	:	1.164072	C11	-C12	:	1.351490
C11	-H26	:	1.087176	C12	-C13	:	1.458682
C12	-H25	:	1.087236	C13	-C14	:	1.434945
C13	-C16	:	1.366431	C14	-N15	:	1.163955
C16	-C17	:	1.457096	C16	-H23	:	1.088455
C17	-C18	:	1.411957	C17	-C22	:	1.411525
C18	-C19	:	1.389996	C18	-H29	:	1.081189
C19	-C20	:	1.396789	C19	-H28	:	1.085832
C20	-C21	:	1.395397	C20	-H27	:	1.085966
C21	-C22	:	1.390042	C21	-H31	:	1.085904
C22	-H30	:	1.087062				

bond angles:

C6	-C1	-C2	: 119.745360	H36	-C1	-C2	: 120.337691
H36	-C1	-C6	: 119.916948	C3	-C2	-C1	: 119.739757
H32	-C2	-C1	: 120.169308	H32	-C2	-C3	: 120.090935
C4	-C3	-C2	: 120.770286	H33	-C3	-C2	: 119.869253
H33	-C3	-C4	: 119.360461	C5	-C4	-C3	: 120.236295
H34	-C4	-C3	: 119.340178	H34	-C4	-C5	: 120.423526
C6	-C5	-C4	: 118.139862	C7	-C5	-C4	: 125.520866
C7	-C5	-C6	: 116.339268	C5	-C6	-C1	: 121.368431
H35	-C6	-C1	: 119.664220	H35	-C6	-C5	: 118.967349
C8	-C7	-C5	: 133.082454	H24	-C7	-C5	: 113.228750
H24	-C7	-C8	: 113.688794	C9	-C8	-C7	: 123.525998
C11	-C8	-C7	: 119.405603	C11	-C8	-C9	: 117.068372
N10	-C9	-C8	: 176.989041	C12	-C11	-C8	: 126.967346
H26	-C11	-C8	: 114.314742	H26	-C11	-C12	: 118.717896
C13	-C12	-C11	: 123.620621	H25	-C12	-C11	: 120.357081
H25	-C12	-C13	: 116.022286	C14	-C13	-C12	: 115.525276
C16	-C13	-C12	: 121.842313	C16	-C13	-C14	: 122.632304
N15	-C14	-C13	: 175.957874	C17	-C16	-C13	: 131.799332
H23	-C16	-C13	: 114.368857	H23	-C16	-C17	: 113.831743
C18	-C17	-C16	: 125.286671	C22	-C17	-C16	: 116.824397
C22	-C17	-C18	: 117.888887	C19	-C18	-C17	: 120.518161
H29	-C18	-C17	: 120.587670	H29	-C18	-C19	: 118.894142

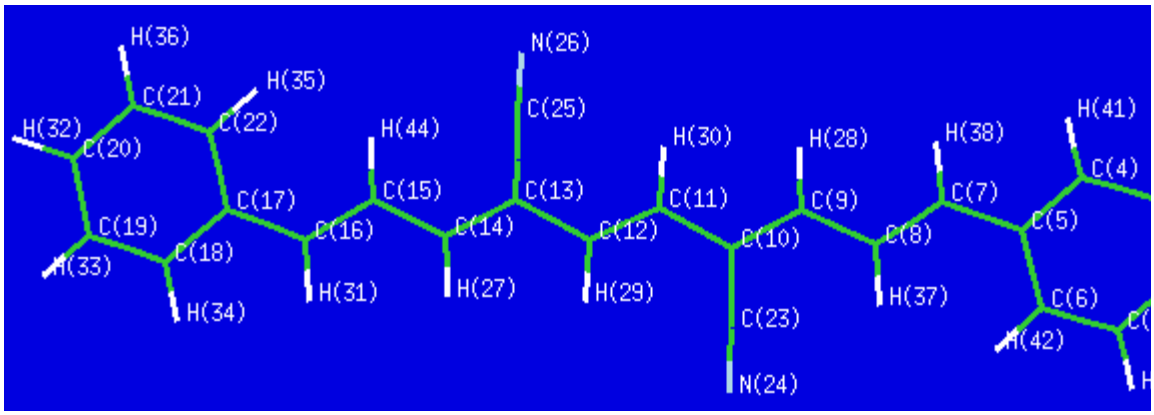
C20 -C19 -C18 : 120.717360 H28 -C19 -C18 : 119.292274
H28 -C19 -C20 : 119.990363 C21 -C20 -C19 : 119.600285
H27 -C20 -C19 : 120.202118 H27 -C20 -C21 : 120.197581
C22 -C21 -C20 : 119.911762 H31 -C21 -C20 : 120.282198
H31 -C21 -C22 : 119.806038 C21 -C22 -C17 : 121.363413
H30 -C22 -C17 : 119.003748 H30 -C22 -C21 : 119.632820

torsional angles:

C1 -C2 -C3 -C4 : -0.000219
C1 -C2 -C3 -H33 :-179.997425
C1 -C6 -C5 -C4 : -0.017565
C1 -C6 -C5 -C7 : 179.960127
C2 -C1 -C6 -C5 : -0.006699
C2 -C1 -C6 -H35 : 179.989223
C2 -C3 -C4 -C5 : -0.024626
C2 -C3 -C4 -H34 : 179.987319
C3 -C2 -C1 -C6 : 0.015819
C3 -C2 -C1 -H36 :-179.990527
C3 -C4 -C5 -C6 : 0.032998
C3 -C4 -C5 -C7 :-179.942439
C4 -C3 -C2 -H32 :-179.998206
C4 -C5 -C6 -H35 : 179.986485
C4 -C5 -C7 -C8 : -0.030917
C4 -C5 -C7 -H24 : 179.955720
C5 -C4 -C3 -H33 : 179.972594
C5 -C6 -C1 -H36 : 179.999621
C5 -C7 -C8 -C9 : -0.042298
C5 -C7 -C8 -C11 : 179.896028
C6 -C1 -C2 -H32 :-179.986195
C6 -C5 -C4 -H34 :-179.979078
C6 -C5 -C7 -C8 : 179.993251
C6 -C5 -C7 -H24 : -0.020111
C7 -C5 -C4 -H34 : 0.045485
C7 -C5 -C6 -H35 : -0.035823
C7 -C8 -C9 -N10 :-179.949241
C7 -C8 -C11 -C12 :-179.978082
C7 -C8 -C11 -H26 : -0.025894
C8 -C11 -C12 -C13 : 179.909171
C8 -C11 -C12 -H25 : -0.050135
C9 -C8 -C7 -H24 : 179.971111
C9 -C8 -C11 -C12 : -0.035821
C9 -C8 -C11 -H26 : 179.916368
N10 -C9 -C8 -C11 : 0.111096
C11 -C8 -C7 -H24 : -0.090563
C11 -C12 -C13 -C14 : 0.062118
C11 -C12 -C13 -C16 : 179.945939
C12 -C13 -C14 -N15 : 1.360596
C12 -C13 -C16 -C17 : 179.942251
C12 -C13 -C16 -H23 : -0.160563
C13 -C12 -C11 -H26 : -0.041148
C13 -C16 -C17 -C18 : -1.248127
C13 -C16 -C17 -C22 : 178.831136

C14 -C13 -C12 -H25 :-179.976958
C14 -C13 -C16 -C17 : -0.182238
C14 -C13 -C16 -H23 : 179.714947
N15 -C14 -C13 -C16 :-178.522211
C16 -C13 -C12 -H25 : -0.093137
C16 -C17 -C18 -C19 : 179.976028
C16 -C17 -C18 -H29 : -0.083873
C16 -C17 -C22 -C21 :-179.938052
C16 -C17 -C22 -H30 : 0.010966
C17 -C18 -C19 -C20 : 0.011914
C17 -C18 -C19 -H28 : 179.991092
C17 -C22 -C21 -C20 : -0.072942
C17 -C22 -C21 -H31 : 179.943250
C18 -C17 -C16 -H23 : 178.854257
C18 -C17 -C22 -C21 : 0.135150
C18 -C17 -C22 -H30 :-179.915832
C18 -C19 -C20 -C21 : 0.053432
C18 -C19 -C20 -H27 :-179.993012
C19 -C18 -C17 -C22 : -0.104001
C19 -C20 -C21 -C22 : -0.023155
C19 -C20 -C21 -H31 : 179.960575
C20 -C19 -C18 -H29 :-179.929188
C20 -C21 -C22 -H30 : 179.978356
C21 -C20 -C19 -H28 :-179.925601
C22 -C17 -C16 -H23 : -1.066480
C22 -C17 -C18 -H29 : 179.836099
C22 -C21 -C20 -H27 :-179.976714
H25 -C12 -C11 -H26 : 179.999546
H27 -C20 -C19 -H28 : 0.027955
H27 -C20 -C21 -H31 : 0.007017
H28 -C19 -C18 -H29 : 0.049990
H30 -C22 -C21 -H31 : -0.005453
H32 -C2 -C1 -H36 : 0.007458
H32 -C2 -C3 -H33 : 0.004588
H33 -C3 -C4 -H34 : -0.015461
H35 -C6 -C1 -H36 : -0.004457

DPDC5



final geometry:

	angstroms		
atom	x	y	z
C1	-0.1162094820	-0.0069872294	0.0075163409
C2	-0.0971985878	0.0551256162	1.4043488578
C3	1.1240553839	0.1004591200	2.0769409569
C4	2.3145713883	0.0838401412	1.3573900706
C5	2.3153503036	0.0218035298	-0.0498604949
C6	1.0716494531	-0.0236013473	-0.7129172555
C7	3.5961934258	0.0084899811	-0.7437397582
C8	3.8160788025	-0.0425768383	-2.0833050998
C9	5.1321719836	-0.0471446615	-2.6403519872
C10	5.4473262951	-0.0953593792	-3.9762893570
C11	6.8163323676	-0.0917403839	-4.4464336255
C12	7.1972279364	-0.1338986058	-5.7470852309
C13	8.5693978625	-0.1259842123	-6.2079260596
C14	8.9030445836	-0.1689513257	-7.5393040282
C15	10.2298178425	-0.1623663843	-8.0702239561
C16	10.4844024034	-0.2085424413	-9.4032722639
C17	11.7861634243	-0.2037394032	-10.0578137895
C18	11.8332372278	-0.2764519445	-11.4634862502
C19	13.0464418358	-0.2775817909	-12.1445604870
C20	14.2446453825	-0.2043562558	-11.4342009295
C21	14.2176642251	-0.1304677267	-10.0382588868
C22	13.0072780005	-0.1302707711	-9.3564651336
C23	4.3955218310	-0.1505472314	-4.9509694692
N24	3.5540482242	-0.1966854697	-5.7541516885
C25	9.6110730655	-0.0707111669	-5.2219269690
N26	10.4438745279	-0.0252934473	-4.4098672882
H27	8.0799789576	-0.2133159652	-8.2504122342
H28	5.9669642668	-0.0073327401	-1.9424402754
H29	6.4382401775	-0.1762378124	-6.5251467709
H30	7.5779565851	-0.0501786756	-3.6708158762
H31	9.6294346747	-0.2589597250	-10.0772067483
H32	15.1937345768	-0.2042497639	-11.9617497767
H33	13.0572219538	-0.3353392913	-13.2288788118
H34	10.9015384182	-0.3335477252	-12.0204068243
H35	13.0099184544	-0.0715733850	-8.2726988053
H36	15.1475334032	-0.0723760513	-9.4803697847

H37	2.9814102474	-0.0798848027	-2.7782705864
H38	4.4705502530	0.0456153114	-0.0946658394
H39	-1.0288392745	0.0678339467	1.9619880112
H40	1.1488472140	0.1487768212	3.1615009654
H41	3.2646135822	0.1195135516	1.8843673351
H42	1.0343280881	-0.0723702119	-1.7965716567
H43	-1.0644270195	-0.0426095752	-0.5205492836
H44	11.0480052084	-0.1138829669	-7.3569537537

Final total energy: -1034.854828 hartrees

HOMO energy: -0.19793
LUMO energy: -0.10237

bond lengths (angstroms):

C1	-C2	:	1.398342	C1	-C6	:	1.389356
C1	-H43	:	1.085928	C2	-C3	:	1.394954
C2	-H39	:	1.085853	C3	-C4	:	1.391171
C3	-H40	:	1.085919	C4	-C5	:	1.408618
C4	-H41	:	1.086995	C5	-C6	:	1.410141
C5	-C7	:	1.456779	C6	-H42	:	1.085393
C7	-C8	:	1.358452	C7	-H38	:	1.089576
C8	-C9	:	1.429134	C8	-H37	:	1.086757
C9	-C10	:	1.373454	C9	-H28	:	1.088827
C10	-C11	:	1.447490	C10	-C23	:	1.435040
C11	-C12	:	1.355933	C11	-H30	:	1.087833
C12	-C13	:	1.447511	C12	-H29	:	1.087766
C13	-C14	:	1.373220	C13	-C25	:	1.435387
C14	-C15	:	1.429072	C14	-H27	:	1.088614
C15	-C16	:	1.357926	C15	-H44	:	1.086525
C16	-C17	:	1.457062	C16	-H31	:	1.089816
C17	-C18	:	1.408339	C17	-C22	:	1.410109
C18	-C19	:	1.391305	C18	-H34	:	1.086960
C19	-C20	:	1.394871	C19	-H33	:	1.085909
C20	-C21	:	1.398157	C20	-H32	:	1.085854
C21	-C22	:	1.389200	C21	-H36	:	1.085943
C22	-H35	:	1.085358	C23	-N24	:	1.164177
C25	-N26	:	1.164071				

bond angles:

C6	-C1	-C2	: 120.456608	H43	-C1	-C2	: 119.939422
H43	-C1	-C6	: 119.603969	C3	-C2	-C1	: 119.668843
H39	-C2	-C1	: 120.122487	H39	-C2	-C3	: 120.208670
C4	-C3	-C2	: 119.962325	H40	-C3	-C2	: 120.198076
H40	-C3	-C4	: 119.839599	C5	-C4	-C3	: 121.179705
H41	-C4	-C3	: 119.788582	H41	-C4	-C5	: 119.031709
C6	-C5	-C4	: 118.078450	C7	-C5	-C4	: 118.472511
C7	-C5	-C6	: 123.449033	C5	-C6	-C1	: 120.654066
H42	-C6	-C1	: 119.264778	H42	-C6	-C5	: 120.081154
C8	-C7	-C5	: 127.759477	H38	-C7	-C5	: 114.929567
H38	-C7	-C8	: 117.310914	C9	-C8	-C7	: 122.245080
H37	-C8	-C7	: 120.501929	H37	-C8	-C9	: 117.252873
C10	-C9	-C8	: 126.196473	H28	-C9	-C8	: 117.135124
H28	-C9	-C10	: 116.668347	C11	-C10	-C9	: 122.198869
C23	-C10	-C9	: 119.591692	C23	-C10	-C11	: 118.209424
C12	-C11	-C10	: 125.250989	H30	-C11	-C10	: 115.510951
H30	-C11	-C12	: 119.238019	C13	-C12	-C11	: 124.855413
H29	-C12	-C11	: 119.427852	H29	-C12	-C13	: 115.716703

C14 -C13 -C12 : 122.603119 C25 -C13 -C12 : 117.998910
C25 -C13 -C14 : 119.397970 C15 -C14 -C13 : 125.847062
H27 -C14 -C13 : 116.801164 H27 -C14 -C15 : 117.351717
C16 -C15 -C14 : 122.589108 H44 -C15 -C14 : 117.093556
H44 -C15 -C16 : 120.316840 C17 -C16 -C15 : 127.472165
H31 -C16 -C15 : 117.487631 H31 -C16 -C17 : 115.039803
C18 -C17 -C16 : 118.558897 C22 -C17 -C16 : 123.395441
C22 -C17 -C18 : 118.045658 C19 -C18 -C17 : 121.183687
H34 -C18 -C17 : 119.042381 H34 -C18 -C19 : 119.773901
C20 -C19 -C18 : 119.980591 H33 -C19 -C18 : 119.835042
H33 -C19 -C20 : 120.184366 C21 -C20 -C19 : 119.647092
H32 -C20 -C19 : 120.225111 H32 -C20 -C21 : 120.127791
C22 -C21 -C20 : 120.452597 H36 -C21 -C20 : 119.948825
H36 -C21 -C22 : 119.598574 C21 -C22 -C17 : 120.690329
H35 -C22 -C17 : 120.103719 H35 -C22 -C21 : 119.205915
N24 -C23 -C10 : 179.152182 N26 -C25 -C13 : 179.149764

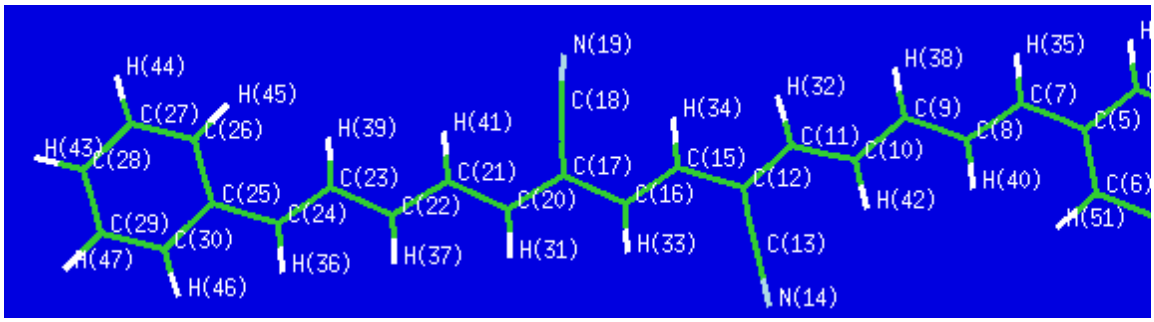
torsional angles:

C1 -C2 -C3 -C4 : 0.004838
C1 -C2 -C3 -H40 :-179.997744
C1 -C6 -C5 -C4 : 0.014070
C1 -C6 -C5 -C7 :-179.956406
C2 -C1 -C6 -C5 : -0.001078
C2 -C1 -C6 -H42 : 179.982384
C2 -C3 -C4 -C5 : 0.008622
C2 -C3 -C4 -H41 : 179.985348
C3 -C2 -C1 -C6 : -0.008586
C3 -C2 -C1 -H43 : 179.989954
C3 -C4 -C5 -C6 : -0.017896
C3 -C4 -C5 -C7 : 179.954080
C4 -C3 -C2 -H39 : 179.996583
C4 -C5 -C6 -H42 :-179.969257
C4 -C5 -C7 -C8 :-179.731967
C4 -C5 -C7 -H38 : 0.190537
C5 -C4 -C3 -H40 :-179.988805
C5 -C6 -C1 -H43 :-179.999623
C5 -C7 -C8 -C9 : 179.863616
C5 -C7 -C8 -H37 : -0.008116
C6 -C1 -C2 -H39 : 179.999663
C6 -C5 -C4 -H41 :-179.994795
C6 -C5 -C7 -C8 : 0.238400
C6 -C5 -C7 -H38 :-179.839097
C7 -C5 -C4 -H41 : -0.022818
C7 -C5 -C6 -H42 : 0.060267
C7 -C8 -C9 -C10 :-179.927227
C7 -C8 -C9 -H28 : -0.016851
C8 -C9 -C10 -C11 : 179.808953
C8 -C9 -C10 -C23 : -0.146896
C9 -C8 -C7 -H38 : -0.057292
C9 -C10 -C11 -C12 :-179.815392
C9 -C10 -C11 -H30 : 0.110056
C9 -C10 -C23 -N24 :-176.491045

C10 -C9 -C8 -H37 : -0.051544
C10 -C11 -C12 -C13 : 179.811853
C10 -C11 -C12 -H29 : -0.121229
C11 -C10 -C9 -H28 : -0.101792
C11 -C10 -C23 -N24 : 3.551351
C11 -C12 -C13 -C14 :-179.939335
C11 -C12 -C13 -C25 : 0.056896
C12 -C11 -C10 -C23 : 0.141041
C12 -C13 -C14 -C15 : 179.897512
C12 -C13 -C14 -H27 : -0.192045
C12 -C13 -C25 -N26 : -1.164141
C13 -C12 -C11 -H30 : -0.111040
C13 -C14 -C15 -C16 : 179.921159
C13 -C14 -C15 -H44 : -0.334685
C14 -C13 -C12 -H29 : -0.004027
C14 -C13 -C25 -N26 : 178.832214
C14 -C15 -C16 -C17 : 179.827182
C14 -C15 -C16 -H31 : -0.415836
C15 -C14 -C13 -C25 : -0.098667
C15 -C16 -C17 -C18 : 179.127671
C15 -C16 -C17 -C22 : -0.852543
C16 -C15 -C14 -H27 : 0.011157
C16 -C17 -C18 -C19 :-179.910704
C16 -C17 -C18 -H34 : 0.025305
C16 -C17 -C22 -C21 : 179.960496
C16 -C17 -C22 -H35 : -0.109410
C17 -C16 -C15 -H44 : 0.091033
C17 -C18 -C19 -C20 : -0.069786
C17 -C18 -C19 -H33 : 179.943137
C17 -C22 -C21 -C20 : -0.031528
C17 -C22 -C21 -H36 : 179.946527
C18 -C17 -C16 -H31 : -0.634382
C18 -C17 -C22 -C21 : -0.019813
C18 -C17 -C22 -H35 : 179.910281
C18 -C19 -C20 -C21 : 0.016888
C18 -C19 -C20 -H32 :-179.956852
C19 -C18 -C17 -C22 : 0.070579
C19 -C20 -C21 -C22 : 0.033350
C19 -C20 -C21 -H36 :-179.944629
C20 -C19 -C18 -H34 : 179.994666
C20 -C21 -C22 -H35 :-179.962243
C21 -C20 -C19 -H33 :-179.996081
C22 -C17 -C16 -H31 : 179.385404
C22 -C17 -C18 -H34 :-179.993411
C22 -C21 -C20 -H32 :-179.992885
C23 -C10 -C9 -H28 : 179.942359
C23 -C10 -C11 -H30 :-179.933511
C25 -C13 -C12 -H29 : 179.992204
C25 -C13 -C14 -H27 : 179.811775
H27 -C14 -C15 -H44 : 179.755313
H28 -C9 -C8 -H37 : 179.858832
H29 -C12 -C11 -H30 : 179.955878
H31 -C16 -C15 -H44 : 179.848016

H32 -C20 -C19 -H33 : 0.030179
H32 -C20 -C21 -H36 : 0.029137
H33 -C19 -C18 -H34 : 0.007590
H35 -C22 -C21 -H36 : 0.015812
H37 -C8 -C7 -H38 :-179.929024
H39 -C2 -C1 -H43 : -0.001797
H39 -C2 -C3 -H40 : -0.005999
H40 -C3 -C4 -H41 : -0.012079
H42 -C6 -C1 -H43 : -0.016161

DPDC7



final geometry:

	angstroms		
atom	x	y	z
C1	0.0758788280	-0.0963861364	-0.1259788144
C2	-0.0010154487	-0.1261026227	1.2691602386
C3	1.1715276728	-0.0953052956	2.0234684011
C4	2.4106114462	-0.0361143624	1.3908297581
C5	2.5070182105	-0.0052728190	-0.0118206090
C6	1.3090832837	-0.0368575468	-0.7567592075
C7	3.8177626736	0.0478662714	-0.6504145160
C8	4.0077008268	0.0844900955	-1.9910243664
C9	5.2477631261	0.1104392573	-2.6968638262
C10	5.2529066684	0.1223500341	-4.0617289000
C11	6.4117517755	0.1147927644	-4.8752304006
C12	6.4118759274	0.1022248826	-6.2529128979
C13	5.1633648911	0.1127970051	-6.9577744888
N14	4.1369937483	0.1218181781	-7.5076247676
C15	7.6541347974	0.0674140456	-6.9742741256
C16	7.8519345917	0.0403046056	-8.3161981898
C17	9.1785863179	-0.0011965258	-8.8892561238
C18	10.2758951120	-0.0232050524	-7.9629024707
N19	11.1329879155	-0.0419034352	-7.1756901390
C20	9.4464635203	-0.0182985792	-10.2370344449
C21	10.7538989871	-0.0457944348	-10.8025034664
C22	10.9984852476	-0.0485910648	-12.1431265934
C23	12.3064019178	-0.0563923320	-12.7273097480
C24	12.4993415940	-0.0447949656	-14.0700319766
C25	13.7536129439	-0.0349691506	-14.8106351404
C26	15.0277077250	-0.0382114769	-14.2066158174
C27	16.1788618750	-0.0230967302	-14.9859326027
C28	16.0924252165	-0.0042749374	-16.3815178882
C29	14.8398553387	-0.0012424228	-16.9951107542
C30	13.6873138685	-0.0166098988	-16.2174965040
H31	8.5964043583	-0.0032649747	-10.9167757062
H32	7.3822315259	0.1065337226	-4.3839162652
H33	7.0117396999	0.0483591698	-9.0058581491
H34	8.5318832618	0.0583134866	-6.3336937345
H35	4.6825023331	0.0509709734	0.0113840405
H36	11.6062899897	-0.0359339287	-14.6944155544
H37	10.1517321381	-0.0364290332	-12.8299320659
H38	6.1842634225	0.1073386954	-2.1406389854

H39	13.1539790211	-0.0652811078	-12.0451897306
H40	3.1333798866	0.0847426368	-2.6362908565
H41	11.5978783058	-0.0575651724	-10.1159027669
H42	4.2921052200	0.1245128870	-4.5724540265
H43	16.9961191052	0.0077294511	-16.9835750433
H44	17.1526150450	-0.0256876346	-14.5047968688
H45	15.1166993436	-0.0516310944	-13.1247310177
H46	12.7121147903	-0.0133386367	-16.6978271791
H47	14.7612730485	0.0132559366	-18.0782833274
H48	-0.9673785229	-0.1733307534	1.7621393935
H49	1.1213532040	-0.1181465813	3.1081767838
H50	3.3204316703	-0.0137153235	1.9849285082
H51	1.3373876195	-0.0176080699	-1.8402973007
H52	-0.8315412700	-0.1208032974	-0.7222925819

Final total energy: -1189.672379 hartrees

HOMO energy: -0.18875
LUMO energy: -0.10648

bond lengths (angstroms):

C1	-C2	:	1.397572	C1	-C6	:	1.386442
C1	-H52	:	1.086093	C2	-C3	:	1.394556
C2	-H48	:	1.085871	C3	-C4	:	1.392503
C3	-H49	:	1.086108	C4	-C5	:	1.406298
C4	-H50	:	1.086843	C5	-C6	:	1.411021
C5	-C7	:	1.458999	C6	-H51	:	1.084079
C7	-C8	:	1.354493	C7	-H35	:	1.088927
C8	-C9	:	1.427108	C8	-H40	:	1.086649
C9	-C10	:	1.364927	C9	-H38	:	1.089233
C10	-C11	:	1.415897	C10	-H42	:	1.088110
C11	-C12	:	1.377740	C11	-H32	:	1.087791
C12	-C13	:	1.433779	C12	-C15	:	1.436935
C13	-N14	:	1.164412	C15	-C16	:	1.356694
C15	-H34	:	1.086678	C16	-C17	:	1.445726
C16	-H33	:	1.087025	C17	-C18	:	1.436211
C17	-C20	:	1.374248	C18	-N19	:	1.163899
C20	-C21	:	1.424745	C20	-H31	:	1.088520
C21	-C22	:	1.362755	C21	-H41	:	1.088053
C22	-C23	:	1.432472	C22	-H37	:	1.090340
C23	-C24	:	1.356563	C23	-H39	:	1.088004
C24	-C25	:	1.456635	C24	-H36	:	1.089713
C25	-C26	:	1.410024	C25	-C30	:	1.408542
C26	-C27	:	1.390223	C26	-H45	:	1.085622
C27	-C28	:	1.398386	C27	-H44	:	1.086137
C28	-C29	:	1.394789	C28	-H43	:	1.085946
C29	-C30	:	1.390421	C29	-H47	:	1.086116
C30	-H46	:	1.087079				

bond angles:

C6	-C1	-C2	: 120.266522	H52	-C1	-C2	: 120.108718
H52	-C1	-C6	: 119.624735	C3	-C2	-C1	: 119.552623
H48	-C2	-C1	: 120.204839	H48	-C2	-C3	: 120.242532
C4	-C3	-C2	: 120.222927	H49	-C3	-C2	: 120.058971
H49	-C3	-C4	: 119.718088	C5	-C4	-C3	: 121.002287
H50	-C4	-C3	: 119.829811	H50	-C4	-C5	: 119.167894
C6	-C5	-C4	: 117.896896	C7	-C5	-C4	: 119.930189
C7	-C5	-C6	: 122.171439	C5	-C6	-C1	: 121.058729
H51	-C6	-C1	: 118.601995	H51	-C6	-C5	: 120.339063
C8	-C7	-C5	: 124.067610	H35	-C7	-C5	: 116.584802
H35	-C7	-C8	: 119.346384	C9	-C8	-C7	: 127.724500
H40	-C8	-C7	: 118.353155	H40	-C8	-C9	: 113.919066
C10	-C9	-C8	: 119.868104	H38	-C9	-C8	: 119.634909
H38	-C9	-C10	: 120.492074	C11	-C10	-C9	: 125.279128

H42 -C10 -C9 : 117.777389 H42 -C10 -C11 : 116.938217
C12 -C11 -C10 : 125.074923 H32 -C11 -C10 : 118.081492
H32 -C11 -C12 : 116.839572 C13 -C12 -C11 : 119.435598
C15 -C12 -C11 : 120.151752 C15 -C12 -C13 : 120.410575
N14 -C13 -C12 : 178.731407 C16 -C15 -C12 : 128.541084
H34 -C15 -C12 : 113.739375 H34 -C15 -C16 : 117.719019
C17 -C16 -C15 : 121.764311 H33 -C16 -C15 : 120.977551
H33 -C16 -C17 : 117.258124 C18 -C17 -C16 : 116.479505
C20 -C17 -C16 : 124.609144 C20 -C17 -C18 : 118.911267
N19 -C18 -C17 : 177.604665 C21 -C20 -C17 : 124.636197
H31 -C20 -C17 : 117.389695 H31 -C20 -C21 : 117.972898
C22 -C21 -C20 : 123.723577 H41 -C21 -C20 : 117.488274
H41 -C21 -C22 : 118.786502 C23 -C22 -C21 : 124.407571
H37 -C22 -C21 : 118.702706 H37 -C22 -C23 : 116.887985
C24 -C23 -C22 : 122.240021 H39 -C23 -C22 : 117.106744
H39 -C23 -C24 : 120.651952 C25 -C24 -C23 : 128.738894
H36 -C24 -C23 : 116.785027 H36 -C24 -C25 : 114.475129
C26 -C25 -C24 : 124.073020 C30 -C25 -C24 : 117.864697
C30 -C25 -C26 : 118.061933 C27 -C26 -C25 : 120.534182
H45 -C26 -C25 : 120.066165 H45 -C26 -C27 : 119.399627
C28 -C27 -C26 : 120.558045 H44 -C27 -C26 : 119.604591
H44 -C27 -C28 : 119.837362 C29 -C28 -C27 : 119.641747
H43 -C28 -C27 : 120.132949 H43 -C28 -C29 : 120.225303
C30 -C29 -C28 : 119.890253 H47 -C29 -C28 : 120.247026
H47 -C29 -C30 : 119.862721 C29 -C30 -C25 : 121.313827
H46 -C30 -C25 : 118.920212 H46 -C30 -C29 : 119.765922

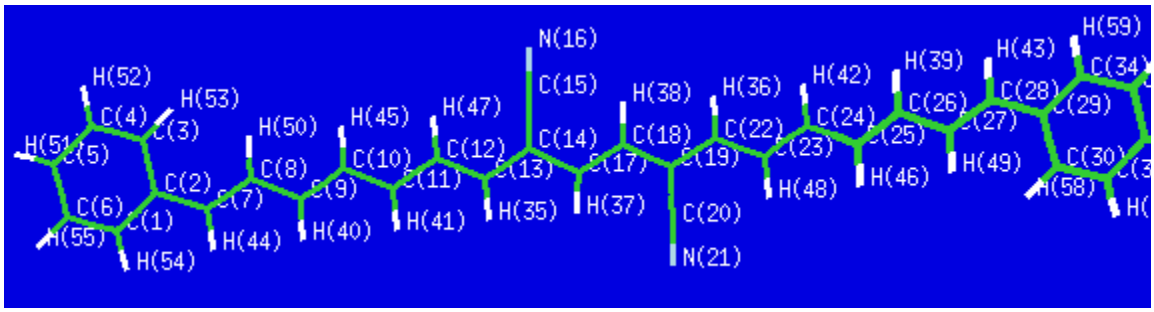
torsional angles:

C1 -C2 -C3 -C4 : -0.036450
C1 -C2 -C3 -H49 :-179.993428
C1 -C6 -C5 -C4 : 0.001399
C1 -C6 -C5 -C7 : 179.558875
C2 -C1 -C6 -C5 : 0.009508
C2 -C1 -C6 -H51 : 179.842328
C2 -C3 -C4 -C5 : 0.048095
C2 -C3 -C4 -H50 :-179.919025
C3 -C2 -C1 -C6 : 0.007933
C3 -C2 -C1 -H52 : 179.949783
C3 -C4 -C5 -C6 : -0.030138
C3 -C4 -C5 -C7 :-179.597915
C4 -C3 -C2 -H48 : 179.934535
C4 -C5 -C6 -H51 :-179.828531
C4 -C5 -C7 -C8 :-179.789335
C4 -C5 -C7 -H35 : 0.613572
C5 -C4 -C3 -H49 :-179.994780
C5 -C6 -C1 -H52 :-179.932623
C5 -C7 -C8 -C9 :-178.646533
C5 -C7 -C8 -H40 : 0.651019
C6 -C1 -C2 -H48 :-179.963063
C6 -C5 -C4 -H50 : 179.937197
C6 -C5 -C7 -C8 : 0.661951
C6 -C5 -C7 -H35 :-178.935143

C7 -C5 -C4 -H50 : 0.369419
C7 -C5 -C6 -H51 : -0.271055
C7 -C8 -C9 -C10 : 178.825274
C7 -C8 -C9 -H38 : -0.372525
C8 -C9 -C10 -C11 :-178.357280
C8 -C9 -C10 -H42 : 0.779686
C9 -C8 -C7 -H35 : 0.940114
C9 -C10 -C11 -C12 : 178.747225
C9 -C10 -C11 -H32 : -0.498956
C10 -C9 -C8 -H40 : -0.498470
C10 -C11 -C12 -C13 : 0.773403
C10 -C11 -C12 -C15 :-178.704898
C11 -C10 -C9 -H38 : 0.833541
C11 -C12 -C13 -N14 : 0.133552
C11 -C12 -C15 -C16 : 179.439957
C11 -C12 -C15 -H34 : -0.288193
C12 -C11 -C10 -H42 : -0.396258
C12 -C15 -C16 -C17 :-179.636845
C12 -C15 -C16 -H33 : 0.320003
C13 -C12 -C11 -H32 :-179.971972
C13 -C12 -C15 -C16 : -0.033209
C13 -C12 -C15 -H34 :-179.761359
N14 -C13 -C12 -C15 : 179.610475
C15 -C12 -C11 -H32 : 0.549727
C15 -C16 -C17 -C18 : 0.490015
C15 -C16 -C17 -C20 :-179.402853
C16 -C17 -C18 -N19 : 2.435192
C16 -C17 -C20 -C21 : 179.344865
C16 -C17 -C20 -H31 : -0.245736
C17 -C16 -C15 -H34 : 0.082047
C17 -C20 -C21 -C22 :-179.300356
C17 -C20 -C21 -H41 : 0.226215
C18 -C17 -C16 -H33 :-179.468365
C18 -C17 -C20 -C21 : -0.545590
C18 -C17 -C20 -H31 : 179.863809
N19 -C18 -C17 -C20 :-177.665536
C20 -C17 -C16 -H33 : 0.638766
C20 -C21 -C22 -C23 : 179.046608
C20 -C21 -C22 -H37 : -0.458030
C21 -C22 -C23 -C24 :-179.295248
C21 -C22 -C23 -H39 : 0.294942
C22 -C21 -C20 -H31 : 0.288053
C22 -C23 -C24 -C25 : 179.219577
C22 -C23 -C24 -H36 : -0.403248
C23 -C22 -C21 -H41 : -0.474191
C23 -C24 -C25 -C26 : 0.102562
C23 -C24 -C25 -C30 :-179.677470
C24 -C23 -C22 -H37 : 0.217593
C24 -C25 -C26 -C27 :-179.754754
C24 -C25 -C26 -H45 : 0.186395
C24 -C25 -C30 -C29 : 179.755420
C24 -C25 -C30 -H46 : -0.173281
C25 -C24 -C23 -H39 : -0.356379

C25 -C26 -C27 -C28 : 0.007381
C25 -C26 -C27 -H44 : 179.990738
C25 -C30 -C29 -C28 : 0.018776
C25 -C30 -C29 -H47 :-179.970558
C26 -C25 -C24 -H36 : 179.732614
C26 -C25 -C30 -C29 : -0.038102
C26 -C25 -C30 -H46 :-179.966802
C26 -C27 -C28 -C29 : -0.027425
C26 -C27 -C28 -H43 : 179.983385
C27 -C26 -C25 -C30 : 0.024876
C27 -C28 -C29 -C30 : 0.014396
C27 -C28 -C29 -H47 :-179.996312
C28 -C27 -C26 -H45 :-179.934157
C28 -C29 -C30 -H46 : 179.946882
C29 -C28 -C27 -H44 : 179.989258
C30 -C25 -C24 -H36 : -0.047418
C30 -C25 -C26 -H45 : 179.966025
C30 -C29 -C28 -H43 :-179.996424
H31 -C20 -C21 -H41 : 179.814623
H32 -C11 -C10 -H42 :-179.642438
H33 -C16 -C15 -H34 :-179.961105
H35 -C7 -C8 -H40 :-179.762334
H36 -C24 -C23 -H39 :-179.979204
H37 -C22 -C21 -H41 :-179.978828
H37 -C22 -C23 -H39 : 179.807782
H38 -C9 -C8 -H40 :-179.696269
H38 -C9 -C10 -H42 : 179.970508
H43 -C28 -C27 -H44 : 0.000067
H43 -C28 -C29 -H47 : -0.007131
H44 -C27 -C26 -H45 : 0.049199
H46 -C30 -C29 -H47 : -0.042452
H48 -C2 -C1 -H52 : -0.021213
H48 -C2 -C3 -H49 : -0.022443
H49 -C3 -C4 -H50 : 0.038100
H51 -C6 -C1 -H52 : -0.099803

DPDC9



final geometry:

angstroms

atom	x	y	z
C1	0.1960386397	0.2858460312	0.3519596121
C2	0.1948422846	0.2390581649	1.6992741428
C3	1.3814750432	0.0789003086	2.5024865347
C4	1.3966531730	0.0465999345	3.8622464284
C5	2.5888453871	-0.0943257407	4.6415591165
C6	2.6271119244	-0.1016665843	6.0067373826
C7	3.8367461520	-0.2154273783	6.7498529646
C8	3.9541249676	-0.1948233960	8.1215082920
C9	5.2297405595	-0.2827936665	8.7948134666
C10	5.4077420935	-0.2148811336	10.1394099157
C11	6.6833477181	-0.2694344571	10.8158013080
C12	6.7994744236	-0.1426954576	12.1818078799
C13	8.0102577153	-0.1542718794	12.9312956106
C14	8.0469062065	0.0081139443	14.2869742143
C15	9.2429339321	0.0245794738	15.0728105109
C16	9.2604002158	0.2070774818	16.4207645875
C17	10.4548191019	0.2389596172	17.2278642124
C18	10.4602096186	0.4296149020	18.5624408184
C19	2.7755291655	-0.0633001522	8.9283110972
N20	1.8311337202	0.0418608332	9.6009917298
C21	7.8622584985	-0.4465250334	10.0186992416
N22	8.8066247366	-0.5920683319	9.3535126823
H23	1.1496330358	0.1935718346	-0.1692860668
H24	-0.7522343985	0.3312623256	2.2311314888
H25	2.3272284393	-0.0152865567	1.9684943321
H26	0.4555401022	0.1421391391	4.4026651345
H27	3.5270212914	-0.1914045917	4.0948496798
H28	1.6965569216	-0.0026298301	6.5622034637
H29	4.7611600885	-0.3153213683	6.1840700533
H30	6.0967345684	-0.3963504788	8.1482865572
H31	4.5399879694	-0.0941670936	10.7836318637
H32	5.8727485697	-0.0091257388	12.7370074855
H33	8.9439631252	-0.2881115986	12.3885543471
H34	7.1051168010	0.1438079096	14.8191124658
H35	10.1872660610	-0.1116308041	14.5469451301
H36	8.3119231340	0.3443954500	16.9403955855
H37	11.4038303187	0.1010499365	16.7095339265
H38	9.5049772081	0.5674876821	19.0704713763
C39	-1.0171136675	0.4599419857	-0.5056506262
C40	11.6838331619	0.4711819400	19.4223889894

H41	11.6471442329	-0.3022209700	20.2007610103
H42	12.5957730128	0.3225537373	18.8369833781
H43	11.7665729300	1.4324295628	19.9463817690
H44	-0.9370012829	1.3624919050	-1.1257393132
H45	-1.1348073930	-0.3818050830	-1.2002412954
H46	-1.9285660189	0.5381220628	0.0936880158

Final total energy: -1344.499258 hartrees

HOMO energy: -0.18270
LUMO energy: -0.10794

bond lengths (angstroms):

C1	-C2	: 1.408511	C1	-C6	: 1.391560			
C1	-H54	: 1.087115	C2	-C3	: 1.409929			
C2	-C7	: 1.458727	C3	-C4	: 1.389495			
C3	-H53	: 1.085541	C4	-C5	: 1.398020			
C4	-H52	: 1.086203	C5	-C6	: 1.394816			
C5	-H51	: 1.085911	C6	-H55	: 1.086127			
C7	-C8	: 1.356858	C7	-H44	: 1.089934			
C8	-C9	: 1.432842	C8	-H50	: 1.088248			
C9	-C10	: 1.363835	C9	-H40	: 1.090260			
C10	-C11	: 1.427048	C10	-H45	: 1.089792			
C11	-C12	: 1.367455	C11	-H41	: 1.090297			
C12	-C13	: 1.421442	C12	-H47	: 1.088593			
C13	-C14	: 1.378091	C13	-H35	: 1.088721			
C14	-C15	: 1.433976	C14	-C17	: 1.442605			
C15	-N16	: 1.164277	C17	-C18	: 1.359086			
C17	-H37	: 1.087392	C18	-C19	: 1.442340			
C18	-H38	: 1.087331	C19	-C20	: 1.433747			
C19	-C22	: 1.378110	C20	-N21	: 1.164284			
C22	-C23	: 1.421302	C22	-H36	: 1.088367			
C23	-C24	: 1.367629	C23	-H48	: 1.088486			
C24	-C25	: 1.426817	C24	-H42	: 1.090333			
C25	-C26	: 1.363929	C25	-H46	: 1.089704			
C26	-C27	: 1.432685	C26	-H39	: 1.090287			
C27	-C28	: 1.356947	C27	-H49	: 1.088163			
C28	-C29	: 1.458657	C28	-H43	: 1.089968			
C29	-C30	: 1.410014	C29	-C34	: 1.408471			
C30	-C31	: 1.389410	C30	-H58	: 1.085497			
C31	-C32	: 1.398066	C31	-H57	: 1.086200			
C32	-C33	: 1.394959	C32	-H56	: 1.085934			
C33	-C34	: 1.391533	C33	-H60	: 1.086126			
C34	-H59	: 1.087107						

bond angles:

C6	-C1	-C2	: 121.264169	H54	-C1	-C2	: 118.981327	
H54	-C1	-C6	: 119.754442	C3	-C2	-C1	: 117.873161	
C7	-C2	-C1	: 118.653843	C7	-C2	-C3	: 123.472629	
C4	-C3	-C2	: 120.808088	H53	-C3	-C2	: 120.025099	
H53	-C3	-C4	: 119.166179	C5	-C4	-C3	: 120.482266	
H52	-C4	-C3	: 119.588901	H52	-C4	-C5	: 119.928728	
C6	-C5	-C4	: 119.532881	H51	-C5	-C4	: 120.185174	
H51	-C5	-C6	: 120.281878	C5	-C6	-C1	: 120.039203	
H55	-C6	-C1	: 119.797964	H55	-C6	-C5	: 120.162813	
C8	-C7	-C2	: 127.556195	H44	-C7	-C2	: 115.050316	
H44	-C7	-C8	: 117.393455	C9	-C8	-C7	: 123.655814	

H50 -C8 -C7 : 119.961475 H50 -C8 -C9 : 116.382552
C10 -C9 -C8 : 124.044894 H40 -C9 -C8 : 117.244831
H40 -C9 -C10 : 118.709764 C11 -C10 -C9 : 124.239425
H45 -C10 -C9 : 118.656146 H45 -C10 -C11 : 117.103436
C12 -C11 -C10 : 123.933483 H41 -C11 -C10 : 117.332399
H41 -C11 -C12 : 118.733597 C13 -C12 -C11 : 123.522667
H47 -C12 -C11 : 118.772448 H47 -C12 -C13 : 117.704115
C14 -C13 -C12 : 125.731810 H35 -C13 -C12 : 117.540532
H35 -C13 -C14 : 116.727262 C15 -C14 -C13 : 119.330151
C17 -C14 -C13 : 122.746641 C17 -C14 -C15 : 117.922926
N16 -C15 -C14 : 179.009352 C18 -C17 -C14 : 124.947265
H37 -C17 -C14 : 115.762094 H37 -C17 -C18 : 119.290437
C19 -C18 -C17 : 125.194249 H38 -C18 -C17 : 119.187140
H38 -C18 -C19 : 115.618508 C20 -C19 -C18 : 118.064843
C22 -C19 -C18 : 122.505155 C22 -C19 -C20 : 119.429876
N21 -C20 -C19 : 179.036825 C23 -C22 -C19 : 126.060107
H36 -C22 -C19 : 116.580401 H36 -C22 -C23 : 117.359492
C24 -C23 -C22 : 123.205697 H48 -C23 -C22 : 117.871314
H48 -C23 -C24 : 118.922987 C25 -C24 -C23 : 124.194042
H42 -C24 -C23 : 118.601397 H42 -C24 -C25 : 117.204528
C26 -C25 -C24 : 124.077612 H46 -C25 -C24 : 117.226171
H46 -C25 -C26 : 118.696199 C27 -C26 -C25 : 124.129346
H39 -C26 -C25 : 118.668221 H39 -C26 -C27 : 117.202378
C28 -C27 -C26 : 123.622760 H49 -C27 -C26 : 116.394620
H49 -C27 -C28 : 119.982519 C29 -C28 -C27 : 127.557420
H43 -C28 -C27 : 117.399569 H43 -C28 -C29 : 115.042794
C30 -C29 -C28 : 123.450201 C34 -C29 -C28 : 118.672163
C34 -C29 -C30 : 117.877631 C31 -C30 -C29 : 120.814875
H58 -C30 -C29 : 120.018476 H58 -C30 -C31 : 119.166617
C32 -C31 -C30 : 120.472210 H57 -C31 -C30 : 119.593762
H57 -C31 -C32 : 119.934023 C33 -C32 -C31 : 119.537109
H56 -C32 -C31 : 120.181675 H56 -C32 -C33 : 120.281202
C34 -C33 -C32 : 120.040148 H60 -C33 -C32 : 120.165280
H60 -C33 -C34 : 119.794571 C33 -C34 -C29 : 121.257967
H59 -C34 -C29 : 119.002630 H59 -C34 -C33 : 119.739342

torsional angles:

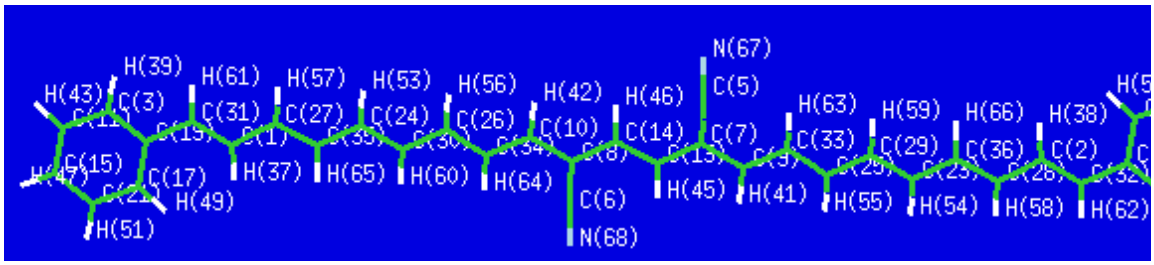
C1 -C2 -C3 -C4 : -0.141430
C1 -C2 -C3 -H53 : 179.566456
C1 -C2 -C7 -C8 : 177.585710
C1 -C2 -C7 -H44 : -2.345640
C1 -C6 -C5 -C4 : -0.007551
C1 -C6 -C5 -H51 :-179.913692
C2 -C1 -C6 -C5 : -0.112548
C2 -C1 -C6 -H55 : 179.937955
C2 -C3 -C4 -C5 : 0.026832
C2 -C3 -C4 -H52 : 179.908394
C2 -C7 -C8 -C9 : 179.413216
C2 -C7 -C8 -H50 : -0.436644
C3 -C2 -C1 -C6 : 0.184739
C3 -C2 -C1 -H54 :-179.905788
C3 -C2 -C7 -C8 : -2.639488

C3 -C2 -C7 -H44 : 177.429162
C3 -C4 -C5 -C6 : 0.049891
C3 -C4 -C5 -H51 : 179.956125
C4 -C3 -C2 -C7 :-179.917875
C4 -C5 -C6 -H55 : 179.941761
C5 -C4 -C3 -H53 :-179.683530
C5 -C6 -C1 -H54 : 179.978669
C6 -C1 -C2 -C7 : 179.972236
C6 -C5 -C4 -H52 :-179.831268
C7 -C2 -C1 -H54 : -0.118291
C7 -C2 -C3 -H53 : -0.209990
C7 -C8 -C9 -C10 :-179.997636
C7 -C8 -C9 -H40 : -0.262029
C8 -C9 -C10 -C11 : 179.267036
C8 -C9 -C10 -H45 : -0.359238
C9 -C8 -C7 -H44 : -0.656831
C9 -C10 -C11 -C12 :-179.805215
C9 -C10 -C11 -H41 : -0.071585
C10 -C9 -C8 -H50 : -0.142835
C10 -C11 -C12 -C13 : 179.278258
C10 -C11 -C12 -H47 : -0.394824
C11 -C10 -C9 -H40 : -0.464955
C11 -C12 -C13 -C14 :-179.902654
C11 -C12 -C13 -H35 : -0.139990
C12 -C11 -C10 -H45 : -0.173621
C12 -C13 -C14 -C15 : -0.443454
C12 -C13 -C14 -C17 : 179.359180
C13 -C12 -C11 -H41 : -0.451881
C13 -C14 -C15 -N16 :-177.614471
C13 -C14 -C17 -C18 :-179.897468
C13 -C14 -C17 -H37 : -0.063459
C14 -C13 -C12 -H47 : -0.226315
C14 -C17 -C18 -C19 : 179.650129
C14 -C17 -C18 -H38 : -0.227782
C15 -C14 -C13 -H35 : 179.792162
C15 -C14 -C17 -C18 : -0.092206
C15 -C14 -C17 -H37 : 179.741803
N16 -C15 -C14 -C17 : 2.573400
C17 -C14 -C13 -H35 : -0.405204
C17 -C18 -C19 -C20 : -0.253039
C17 -C18 -C19 -C22 : 179.877121
C18 -C19 -C20 -N21 : -2.826718
C18 -C19 -C22 -C23 : 179.897335
C18 -C19 -C22 -H36 : -0.111398
C19 -C18 -C17 -H37 : -0.178464
C19 -C22 -C23 -C24 : 179.893146
C19 -C22 -C23 -H48 : -0.088892
C20 -C19 -C18 -H38 : 179.628752
C20 -C19 -C22 -C23 : 0.029207
C20 -C19 -C22 -H36 :-179.979525
N21 -C20 -C19 -C22 : 177.047248
C22 -C19 -C18 -H38 : -0.241088
C22 -C23 -C24 -C25 :-179.984494

C22 -C23 -C24 -H42 : -0.053030
C23 -C24 -C25 -C26 : 179.781045
C23 -C24 -C25 -H46 : -0.169508
C24 -C23 -C22 -H36 : -0.098061
C24 -C25 -C26 -C27 :-179.929179
C24 -C25 -C26 -H39 : -0.016551
C25 -C24 -C23 -H48 : -0.002636
C25 -C26 -C27 -C28 : 179.759877
C25 -C26 -C27 -H49 : -0.124100
C26 -C25 -C24 -H42 : -0.151298
C26 -C27 -C28 -C29 :-179.946290
C26 -C27 -C28 -H43 : -0.125066
C27 -C26 -C25 -H46 : 0.020695
C27 -C28 -C29 -C30 : -1.150121
C27 -C28 -C29 -C34 : 178.822516
C28 -C27 -C26 -H39 : -0.153929
C28 -C29 -C30 -C31 : 179.908996
C28 -C29 -C30 -H58 : -0.156794
C28 -C29 -C34 -C33 :-179.880783
C28 -C29 -C34 -H59 : 0.029413
C29 -C28 -C27 -H49 : -0.066275
C29 -C30 -C31 -C32 : 0.002440
C29 -C30 -C31 -H57 : 179.977929
C29 -C34 -C33 -C32 : -0.061138
C29 -C34 -C33 -H60 : 179.953428
C30 -C29 -C28 -H43 : 179.025069
C30 -C29 -C34 -C33 : 0.093389
C30 -C29 -C34 -H59 :-179.996415
C30 -C31 -C32 -C33 : 0.031946
C30 -C31 -C32 -H56 : 179.989142
C31 -C30 -C29 -C34 : -0.063845
C31 -C32 -C33 -C34 : -0.002912
C31 -C32 -C33 -H60 : 179.982468
C32 -C31 -C30 -H58 :-179.932323
C32 -C33 -C34 -H59 :-179.970682
C33 -C32 -C31 -H57 :-179.943460
C34 -C29 -C28 -H43 : -1.002294
C34 -C29 -C30 -H58 : 179.870365
C34 -C33 -C32 -H56 :-179.960065
H35 -C13 -C12 -H47 : 179.536349
H36 -C22 -C23 -H48 : 179.919902
H37 -C17 -C18 -H38 : 179.943625
H39 -C26 -C25 -H46 : 179.933323
H39 -C26 -C27 -H49 : 179.962094
H40 -C9 -C8 -H50 : 179.592772
H40 -C9 -C10 -H45 : 179.908771
H41 -C11 -C10 -H45 : 179.560009
H41 -C11 -C12 -H47 : 179.875037
H42 -C24 -C23 -H48 : 179.928828
H42 -C24 -C25 -H46 : 179.898149
H43 -C28 -C27 -H49 : 179.754949
H44 -C7 -C8 -H50 : 179.493309
H51 -C5 -C4 -H52 : 0.074965

H51 -C5 -C6 -H55 : 0.035619
H52 -C4 -C3 -H53 : 0.198032
H54 -C1 -C6 -H55 : 0.029172
H56 -C32 -C31 -H57 : 0.013736
H56 -C32 -C33 -H60 : 0.025315
H57 -C31 -C30 -H58 : 0.043166
H59 -C34 -C33 -H60 : 0.043884

DPDC11



final geometry:

	angstroms		
atom	x	y	z
C1	-11.5596556375	2.1321136710	-0.2237190568
C2	11.5596556375	-2.1321136710	0.2237190568
C3	-15.2992366101	1.9754701035	0.0970934069
C4	15.2992366101	-1.9754701035	-0.0970934069
C5	1.5983947691	-1.8906199282	0.7889341316
C6	-1.5983947691	1.8906199282	-0.7889341316
C7	1.8045681034	-0.6150266305	0.1671700931
C8	-1.8045681034	0.6150266305	-0.1671700931
C9	3.0906744061	-0.2038817456	-0.1179974105
C10	-3.0906744061	0.2038817456	0.1179974105
C11	-16.4884936245	2.6555731434	-0.1475192009
C12	16.4884936245	-2.6555731434	0.1475192009
C13	0.6420620873	0.1825237890	-0.1313851967
C14	-0.6420620873	-0.1825237890	0.1313851967
C15	-16.4626435737	3.9144054140	-0.7478133337
C16	16.4626435737	-3.9144054140	0.7478133337
C17	-14.0475176641	3.8059882283	-0.8560762681
C18	14.0475176641	-3.8059882283	0.8560762681
C19	-14.0532133857	2.5326867686	-0.2503326080
C20	14.0532133857	-2.5326867686	0.2503326080
C21	-15.2355095994	4.4841352260	-1.0999210370
C22	15.2355095994	-4.4841352260	1.0999210370
C23	7.9844319544	-0.8897732044	-0.1265253567
C24	-7.9844319544	0.8897732044	0.1265253567
C25	5.5363462480	-0.5172763993	-0.1377170203
C26	-5.5363462480	0.5172763993	0.1377170203
C27	-10.4215986368	1.3175063719	0.0860354048
C28	10.4215986368	-1.3175063719	-0.0860354048
C29	6.7043116764	-1.2830689953	0.1446240491
C30	-6.7043116764	1.2830689953	-0.1446240491
C31	-12.8418065074	1.7698518783	0.0317354907
C32	12.8418065074	-1.7698518783	-0.0317354907
C33	4.2693566754	-0.9475364588	0.1529603761
C34	-4.2693566754	0.9475364588	-0.1529603761
C35	-9.1337616286	1.6834870334	-0.1712502808
C36	9.1337616286	-1.6834870334	0.1712502808
H37	-11.3509797636	3.0924395275	-0.6913630857
H38	11.3509797636	-3.0924395275	0.6913630857
H39	-15.3253122360	0.9945862552	0.5651668455
H40	15.3253122360	-0.9945862552	-0.5651668455

H41	3.2019836857	0.7712267454	-0.5890478363
H42	-3.2019836857	-0.7712267454	0.5890478363
H43	-17.4358750117	2.2028248269	0.1304456489
H44	17.4358750117	-2.2028248269	-0.1304456489
H45	0.8353397389	1.1437756659	-0.6021179099
H46	-0.8353397389	-1.1437756659	0.6021179099
H47	-17.3881945520	4.4486801451	-0.9406202819
H48	17.3881945520	-4.4486801451	0.9406202819
H49	-13.1070664958	4.2688933316	-1.1383974234
H50	13.1070664958	-4.2688933316	1.1383974234
H51	-15.2072376137	5.4640448473	-1.5678152572
H52	15.2072376137	-5.4640448473	1.5678152572
H53	-8.1495174303	-0.0804388403	0.5946226210
H54	8.1495174303	0.0804388403	-0.5946226210
H55	5.6693918655	0.4573369989	-0.6076996863
H56	-5.6693918655	-0.4573369989	0.6076996863
H57	-10.6106902461	0.3514641743	0.5537529104
H58	10.6106902461	-0.3514641743	-0.5537529104
H59	6.5520566702	-2.2548761648	0.6132331594
H60	-6.5520566702	2.2548761648	-0.6132331594
H61	-13.0058522699	0.8000849720	0.5013870966
H62	13.0058522699	-0.8000849720	-0.5013870966
H63	4.1501484730	-1.9219259191	0.6227514052
H64	-4.1501484730	1.9219259191	-0.6227514052
H65	-8.9544283439	2.6512209802	-0.6391930066
H66	8.9544283439	-2.6512209802	0.6391930066
N67	1.4102674640	-2.9226237176	1.2937235252
N68	-1.4102674640	2.9226237176	-1.2937235252

Final total energy: -1499.321022 hartrees

HOMO energy: -0.17812
LUMO energy: -0.10982

bond lengths (angstroms):

C1	-C27	:	1.433425	C1	-C31	:	1.356614
C1	-H37	:	1.088330	C2	-C28	:	1.433425
C2	-C32	:	1.356614	C2	-H38	:	1.088330
C3	-C11	:	1.391656	C3	-C19	:	1.408463
C3	-H39	:	1.087155	C4	-C12	:	1.391656
C4	-C20	:	1.408463	C4	-H40	:	1.087155
C5	-C7	:	1.433958	C5	-N67	:	1.164146
C6	-C8	:	1.433958	C6	-N68	:	1.164146
C7	-C9	:	1.380011	C7	-C13	:	1.441056
C8	-C10	:	1.380011	C8	-C14	:	1.441056
C9	-C33	:	1.419765	C9	-H41	:	1.088630
C10	-C34	:	1.419765	C10	-H42	:	1.088630
C11	-C15	:	1.394876	C11	-H43	:	1.086175
C12	-C16	:	1.394876	C12	-H44	:	1.086175
C13	-C14	:	1.360619	C13	-H45	:	1.087635
C14	-H46	:	1.087635	C15	-C21	:	1.398009
C15	-H47	:	1.085941	C16	-C22	:	1.398009
C16	-H48	:	1.085941	C17	-C19	:	1.410055
C17	-C21	:	1.389485	C17	-H49	:	1.085557
C18	-C20	:	1.410055	C18	-C22	:	1.389485
C18	-H50	:	1.085557	C19	-C31	:	1.459105
C20	-C32	:	1.459105	C21	-H51	:	1.086254
C22	-H52	:	1.086254	C23	-C29	:	1.366350
C23	-C36	:	1.428149	C23	-H54	:	1.089807
C24	-C30	:	1.366350	C24	-C35	:	1.428149
C24	-H53	:	1.089807	C25	-C29	:	1.424885
C25	-C33	:	1.369262	C25	-H55	:	1.090163
C26	-C30	:	1.424885	C26	-C34	:	1.369262
C26	-H56	:	1.090163	C27	-C35	:	1.363328
C27	-H57	:	1.089841	C28	-C36	:	1.363328
C28	-H58	:	1.089841	C29	-H59	:	1.089580
C30	-H60	:	1.089580	C31	-H61	:	1.089923
C32	-H62	:	1.089923	C33	-H63	:	1.088278
C34	-H64	:	1.088278	C35	-H65	:	1.089789
C36	-H66	:	1.089789				

bond angles:

C31	-C1	-C27	: 123.912001	H37	-C1	-C27	: 116.236508
H37	-C1	-C31	: 119.851486	C32	-C2	-C28	: 123.912001
H38	-C2	-C28	: 116.236508	H38	-C2	-C32	: 119.851486
C19	-C3	-C11	: 121.285783	H39	-C3	-C11	: 119.742989
H39	-C3	-C19	: 118.971228	C20	-C4	-C12	: 121.285783
H40	-C4	-C12	: 119.742989	H40	-C4	-C20	: 118.971228
N67	-C5	-C7	: 178.963814	N68	-C6	-C8	: 178.963814

C9 -C7 -C5 : 119.249986 C13 -C7 -C5 : 117.786061
C13 -C7 -C9 : 122.963950 C10 -C8 -C6 : 119.249986
C14 -C8 -C6 : 117.786061 C14 -C8 -C10 : 122.963950
C33 -C9 -C7 : 125.325131 H41 -C9 -C7 : 116.844100
H41 -C9 -C33 : 117.830769 C34 -C10 -C8 : 125.325131
H42 -C10 -C8 : 116.844100 H42 -C10 -C34 : 117.830769
C15 -C11 -C3 : 120.055859 H43 -C11 -C3 : 119.780492
H43 -C11 -C15 : 120.163649 C16 -C12 -C4 : 120.055859
H44 -C12 -C4 : 119.780492 H44 -C12 -C16 : 120.163649
C14 -C13 -C7 : 124.949348 H45 -C13 -C7 : 115.813950
H45 -C13 -C14 : 119.236701 C13 -C14 -C8 : 124.949348
H46 -C14 -C8 : 115.813950 H46 -C14 -C13 : 119.236701
C21 -C15 -C11 : 119.501128 H47 -C15 -C11 : 120.306240
H47 -C15 -C21 : 120.192632 C22 -C16 -C12 : 119.501128
H48 -C16 -C12 : 120.306240 H48 -C16 -C22 : 120.192632
C21 -C17 -C19 : 120.841088 H49 -C17 -C19 : 120.019058
H49 -C17 -C21 : 119.139855 C22 -C18 -C20 : 120.841088
H50 -C18 -C20 : 120.019058 H50 -C18 -C22 : 119.139855
C17 -C19 -C3 : 117.826229 C31 -C19 -C3 : 118.683280
C31 -C19 -C17 : 123.490489 C18 -C20 -C4 : 117.826229
C32 -C20 -C4 : 118.683280 C32 -C20 -C18 : 123.490489
C17 -C21 -C15 : 120.489914 H51 -C21 -C15 : 119.931627
H51 -C21 -C17 : 119.578460 C18 -C22 -C16 : 120.489914
H52 -C22 -C16 : 119.931627 H52 -C22 -C18 : 119.578460
C36 -C23 -C29 : 123.547589 H54 -C23 -C29 : 118.908725
H54 -C23 -C36 : 117.543671 C35 -C24 -C30 : 123.547589
H53 -C24 -C30 : 118.908725 H53 -C24 -C35 : 117.543671
C33 -C25 -C29 : 123.197231 H55 -C25 -C29 : 117.766196
H55 -C25 -C33 : 119.036567 C34 -C26 -C30 : 123.197231
H56 -C26 -C30 : 117.766196 H56 -C26 -C34 : 119.036567
C35 -C27 -C1 : 123.823919 H57 -C27 -C1 : 117.304997
H57 -C27 -C35 : 118.871075 C36 -C28 -C2 : 123.823919
H58 -C28 -C2 : 117.304997 H58 -C28 -C36 : 118.871075
C25 -C29 -C23 : 125.025350 H59 -C29 -C23 : 118.229114
H59 -C29 -C25 : 116.745528 C26 -C30 -C24 : 125.025350
H60 -C30 -C24 : 118.229114 H60 -C30 -C26 : 116.745528
C19 -C31 -C1 : 127.492599 H61 -C31 -C1 : 117.450735
H61 -C31 -C19 : 115.056663 C20 -C32 -C2 : 127.492599
H62 -C32 -C2 : 117.450735 H62 -C32 -C20 : 115.056663
C25 -C33 -C9 : 124.269322 H63 -C33 -C9 : 117.414205
H63 -C33 -C25 : 118.316469 C26 -C34 -C10 : 124.269322
H64 -C34 -C10 : 117.414205 H64 -C34 -C26 : 118.316469
C27 -C35 -C24 : 124.866413 H65 -C35 -C24 : 116.783310
H65 -C35 -C27 : 118.350271 C28 -C36 -C23 : 124.866413
H66 -C36 -C23 : 116.783310 H66 -C36 -C28 : 118.350271

torsional angles:

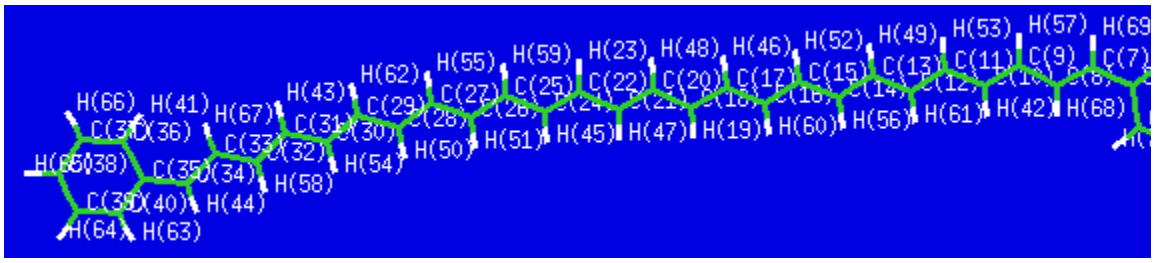
C1 -C27 -C35 -C24 :-179.939193
C1 -C27 -C35 -H65 : 0.031077
C1 -C31 -C19 -C3 :-179.916516
C1 -C31 -C19 -C17 : 0.100215
C2 -C28 -C36 -C23 : 179.939193

C2 -C28 -C36 -H66 : -0.031077
C2 -C32 -C20 -C4 : 179.916516
C2 -C32 -C20 -C18 : -0.100215
C3 -C11 -C15 -C21 : -0.003874
C3 -C11 -C15 -H47 : 179.996266
C3 -C19 -C17 -C21 : -0.004260
C3 -C19 -C17 -H49 : 179.998234
C3 -C19 -C31 -H61 : 0.104602
C4 -C12 -C16 -C22 : 0.003874
C4 -C12 -C16 -H48 :-179.996266
C4 -C20 -C18 -C22 : 0.004260
C4 -C20 -C18 -H50 :-179.998234
C4 -C20 -C32 -H62 : -0.104602
C5 -C7 -C9 -C33 : 0.055898
C5 -C7 -C9 -H41 :-179.945230
C5 -C7 -C13 -C14 : -0.033837
C5 -C7 -C13 -H45 : 179.975781
C6 -C8 -C10 -C34 : -0.055898
C6 -C8 -C10 -H42 : 179.945230
C6 -C8 -C14 -C13 : 0.033837
C6 -C8 -C14 -H46 :-179.975781
C7 -C9 -C33 -C25 :-179.897942
C7 -C9 -C33 -H63 : 0.077435
C7 -C13 -C14 -C8 : 180.000000
C7 -C13 -C14 -H46 : 0.009922
C8 -C10 -C34 -C26 : 179.897942
C8 -C10 -C34 -H64 : -0.077435
C8 -C14 -C13 -H45 : -0.009922
C9 -C7 -C5 -N67 : 179.322019
C9 -C7 -C13 -C14 : 179.984942
C9 -C7 -C13 -H45 : -0.005441
C9 -C33 -C25 -C29 : 179.992632
C9 -C33 -C25 -H55 : 0.021957
C10 -C8 -C6 -N68 :-179.322019
C10 -C8 -C14 -C13 :-179.984942
C10 -C8 -C14 -H46 : 0.005441
C10 -C34 -C26 -C30 :-179.992632
C10 -C34 -C26 -H56 : -0.021957
C11 -C3 -C19 -C17 : 0.000871
C11 -C3 -C19 -C31 :-179.983351
C11 -C15 -C21 -C17 : 0.000508
C11 -C15 -C21 -H51 : 179.996185
C12 -C4 -C20 -C18 : -0.000871
C12 -C4 -C20 -C32 : 179.983351
C12 -C16 -C22 -C18 : -0.000508
C12 -C16 -C22 -H52 :-179.996185
C13 -C7 -C5 -N67 : -0.659923
C13 -C7 -C9 -C33 :-179.963143
C13 -C7 -C9 -H41 : 0.035729
C14 -C8 -C6 -N68 : 0.659923
C14 -C8 -C10 -C34 : 179.963143
C14 -C8 -C10 -H42 : -0.035729
C15 -C11 -C3 -C19 : 0.003182

C15 -C11 -C3 -H39 :-179.996191
C15 -C21 -C17 -C19 : 0.003624
C15 -C21 -C17 -H49 :-179.998849
C16 -C12 -C4 -C20 : -0.003182
C16 -C12 -C4 -H40 : 179.996191
C16 -C22 -C18 -C20 : -0.003624
C16 -C22 -C18 -H50 : 179.998849
C17 -C19 -C3 -H39 :-179.999752
C17 -C19 -C31 -H61 :-179.878666
C17 -C21 -C15 -H47 :-179.999631
C18 -C20 -C4 -H40 : 179.999752
C18 -C20 -C32 -H62 : 179.878666
C18 -C22 -C16 -H48 : 179.999631
C19 -C3 -C11 -H43 : 179.998960
C19 -C17 -C21 -H51 :-179.992068
C19 -C31 -C1 -C27 :-179.929021
C19 -C31 -C1 -H37 : 0.047025
C20 -C4 -C12 -H44 :-179.998960
C20 -C18 -C22 -H52 : 179.992068
C20 -C32 -C2 -C28 : 179.929021
C20 -C32 -C2 -H38 : -0.047025
C21 -C15 -C11 -H43 :-179.999636
C21 -C17 -C19 -C31 : 179.979142
C22 -C16 -C12 -H44 : 179.999636
C22 -C18 -C20 -C32 :-179.979142
C23 -C29 -C25 -C33 :-179.864634
C23 -C29 -C25 -H55 : 0.106391
C23 -C36 -C28 -H58 : -0.025922
C24 -C30 -C26 -C34 : 179.864634
C24 -C30 -C26 -H56 : -0.106391
C24 -C35 -C27 -H57 : 0.025922
C25 -C29 -C23 -C36 : 179.955124
C25 -C29 -C23 -H54 : -0.001167
C25 -C33 -C9 -H41 : 0.103197
C26 -C30 -C24 -C35 :-179.955124
C26 -C30 -C24 -H53 : 0.001167
C26 -C34 -C10 -H42 : -0.103197
C27 -C1 -C31 -H61 : 0.049421
C27 -C35 -C24 -C30 : 179.931173
C27 -C35 -C24 -H53 : -0.025674
C28 -C2 -C32 -H62 : -0.049421
C28 -C36 -C23 -C29 :-179.931173
C28 -C36 -C23 -H54 : 0.025674
C29 -C23 -C36 -H66 : 0.039519
C29 -C25 -C33 -H63 : 0.017461
C30 -C24 -C35 -H65 : -0.039519
C30 -C26 -C34 -H64 : -0.017461
C31 -C1 -C27 -C35 :-179.986337
C31 -C1 -C27 -H57 : 0.048043
C31 -C19 -C3 -H39 : 0.016026
C31 -C19 -C17 -H49 : -0.018364
C32 -C2 -C28 -C36 : 179.986337
C32 -C2 -C28 -H58 : -0.048043

C32 -C20 -C4 -H40 : -0.016026
C32 -C20 -C18 -H50 : 0.018364
C33 -C25 -C29 -H59 : 0.101179
C34 -C26 -C30 -H60 : -0.101179
C35 -C24 -C30 -H60 : 0.010226
C35 -C27 -C1 -H37 : 0.036824
C36 -C23 -C29 -H59 : -0.010226
C36 -C28 -C2 -H38 : -0.036824
H37 -C1 -C27 -H57 :-179.928796
H37 -C1 -C31 -H61 :-179.974533
H38 -C2 -C28 -H58 : 179.928796
H38 -C2 -C32 -H62 : 179.974533
H39 -C3 -C11 -H43 : -0.000412
H40 -C4 -C12 -H44 : 0.000412
H41 -C9 -C33 -H63 :-179.921426
H42 -C10 -C34 -H64 : 179.921426
H43 -C11 -C15 -H47 : 0.000503
H44 -C12 -C16 -H48 : -0.000503
H45 -C13 -C14 -H46 : 180.000000
H47 -C15 -C21 -H51 : -0.003954
H48 -C16 -C22 -H52 : 0.003954
H49 -C17 -C21 -H51 : 0.005459
H50 -C18 -C22 -H52 : -0.005459
H53 -C24 -C30 -H60 : 179.966516
H53 -C24 -C35 -H65 :-179.996366
H54 -C23 -C29 -H59 :-179.966516
H54 -C23 -C36 -H66 : 179.996366
H55 -C25 -C29 -H59 :-179.927796
H55 -C25 -C33 -H63 :-179.953214
H56 -C26 -C30 -H60 : 179.927796
H56 -C26 -C34 -H64 : 179.953214
H57 -C27 -C35 -H65 : 179.996192
H58 -C28 -C36 -H66 :-179.996192

DPDC13



final geometry:

	angstroms		
atom	x	y	z
H1	0.1242624540	0.0150421899	0.5865098031
C2	0.3850863448	0.0250929874	1.6402352085
C3	1.7396168862	0.0329418828	2.0318719685
C4	2.8508643276	0.0287933485	1.0878793636
C5	2.7911169950	0.0186572859	-0.2667712591
C6	3.9537327364	0.0151470650	-1.1041124963
C7	3.9303071067	0.0065608895	-2.4672861728
C8	5.1040714492	0.0032495473	-3.2804754163
C9	5.1114488082	-0.0034655099	-4.6468614969
C10	6.3064057372	-0.0063338274	-5.4241778506
C11	6.3608905734	-0.0108904201	-6.7914597214
C12	7.5847002125	-0.0131631903	-7.5184897030
C13	7.6968144209	-0.0152948449	-8.8844424189
C14	8.9548457411	-0.0170783218	-9.5417705311
C15	9.1802653906	-0.0168742075	-10.9036605620
C16	10.5138611047	-0.0183447485	-11.4505621737
C17	10.8343736617	-0.0151752019	-12.7723080024
C18	12.1807252979	-0.0160263006	-13.2882620706
C19	12.4677303978	-0.0090254524	-14.6382762487
C20	13.7697663125	-0.0083757132	-15.2038836318
C21	14.0222212360	0.0017101588	-16.5503309271
C22	15.3344236483	0.0036015386	-17.1043138010
C23	15.6141236702	0.0162742451	-18.4431385758
C24	16.9355246616	0.0191405779	-18.9804864866
C25	17.2301103182	0.0340946143	-20.3142291251
C26	18.5588291531	0.0377992166	-20.8403193241
C27	18.8648646870	0.0546502776	-22.1686956473
C28	20.2028826653	0.0590496104	-22.6846008122
C29	20.5029597499	0.0774153291	-24.0069253245
C30	21.8277895077	0.0837172452	-24.6194129957
C31	8.0671223050	-0.0154098135	-11.8070504246
N32	7.1735759637	-0.0142832887	-12.5536775094
C33	13.2625644502	-0.0237301017	-12.3457395004
N34	14.1286076973	-0.0298127726	-11.5675885368
H35	19.3768872159	0.0267165538	-20.1199023690
H36	2.9670613203	0.0015086118	-2.9763732436
H37	3.8408936490	0.0352413781	1.5428514767
H38	9.8416208745	-0.0183276713	-8.9103138109
H39	11.6184749817	-0.0037419973	-15.3193538636
H40	11.3172828141	-0.0219917590	-10.7175987718
H41	10.0391382471	-0.0118716965	-13.5138877841

H42	14.7846839025	0.0245291335	-19.1501864536
H43	7.2487417876	-0.0040182194	-4.8757690434
H44	8.5033703935	-0.0125345349	-6.9312713214
H45	13.1803293693	0.0085084092	-17.2429850149
H46	16.4080893468	0.0436738402	-21.0300804767
H47	6.0625857369	0.0070709656	-2.7614048088
H48	5.4305110136	-0.0133401830	-7.3583358152
H49	16.1681183091	-0.0050787035	-16.4024831994
H50	18.0501469521	0.0653507604	-22.8933150787
H51	4.9214762027	0.0203594998	-0.6023075016
H52	6.7948816566	-0.0161534140	-9.4931768626
H53	14.6160695512	-0.0155783421	-14.5197710290
H54	17.7607879165	0.0091647666	-18.2684979497
H55	4.1603256306	-0.0072575384	-5.1787292911
C56	-0.6285729693	0.0298331104	2.5905957180
C57	-0.3233536112	0.0425436466	3.9546503764
C58	1.0109571620	0.0503940621	4.3602802150
C59	2.0267117889	0.0455543140	3.4103918563
H60	3.0655784264	0.0517195343	3.7308904329
H61	1.2601892458	0.0602918914	5.4174918503
H62	-1.1196207648	0.0462458914	4.6930310020
H63	-1.6657762329	0.0235620060	2.2680805844
H64	1.8262640341	0.0122715197	-0.7699861521
H65	21.0043358502	0.0472498064	-21.9484500438
H66	19.6705725904	0.0886034971	-24.7099626625
C67	21.9222574169	0.1049098322	-26.0249210560
C68	23.1570655385	0.1120322585	-26.6675832122
C69	24.3346599261	0.0979372552	-25.9193023435
C70	24.2603743322	0.0766042548	-24.5229240838
C71	23.0280980037	0.0695687295	-23.8798414949
H72	21.0082216227	0.1156729900	-26.6137562199
H73	23.1996291224	0.1285689307	-27.7529154758
H74	25.2999830298	0.1034798874	-26.4162335614
H75	25.1721064445	0.0654034509	-23.9326750767
H76	22.9970329887	0.0526643376	-22.7949100974

Final total energy: -1654.143389 hartrees

HOMO energy: -0.17442
LUMO energy: -0.10994

bond lengths (angstroms):

H1	-C2	:	1.085572	C2	-C3	:	1.410033
C2	-C56	:	1.389501	C3	-C4	:	1.458084
C3	-C59	:	1.408155	C4	-C5	:	1.356005
C4	-H37	:	1.089587	C5	-C6	:	1.432769
C5	-H64	:	1.088213	C6	-C7	:	1.363402
C6	-H51	:	1.090121	C7	-C8	:	1.427939
C7	-H36	:	1.089513	C8	-C9	:	1.366422
C8	-H47	:	1.090045	C9	-C10	:	1.425535
C9	-H55	:	1.089740	C10	-C11	:	1.368375
C10	-H43	:	1.090300	C11	-C12	:	1.423477
C11	-H48	:	1.089477	C12	-C13	:	1.370548
C12	-H44	:	1.090312	C13	-C14	:	1.419411
C13	-H52	:	1.088137	C14	-C15	:	1.380420
C14	-H38	:	1.088627	C15	-C16	:	1.441382
C15	-C31	:	1.433598	C16	-C17	:	1.360055
C16	-H40	:	1.087536	C17	-C18	:	1.441829
C17	-H41	:	1.087360	C18	-C19	:	1.380203
C18	-C33	:	1.434846	C19	-C20	:	1.419581
C19	-H39	:	1.088636	C20	-C21	:	1.369947
C20	-H53	:	1.088251	C21	-C22	:	1.424351
C21	-H45	:	1.090228	C22	-C23	:	1.367788
C22	-H49	:	1.089811	C23	-C24	:	1.426482
C23	-H42	:	1.089934	C24	-C25	:	1.365970
C24	-H54	:	1.089994	C25	-C26	:	1.429083
C25	-H46	:	1.090070	C26	-C27	:	1.363277
C26	-H35	:	1.090111	C27	-C28	:	1.434040
C27	-H50	:	1.090391	C28	-C29	:	1.356070
C28	-H65	:	1.088294	C29	-C30	:	1.459573
C29	-H66	:	1.089612	C30	-C67	:	1.408839
C30	-C71	:	1.409931	C31	-N32	:	1.164422
C33	-N34	:	1.164297	C56	-C57	:	1.397843
C56	-H63	:	1.086207	C57	-C58	:	1.394626
C57	-H62	:	1.085938	C58	-C59	:	1.390708
C58	-H61	:	1.086237	C59	-H60	:	1.087199
C67	-C68	:	1.392055	C67	-H72	:	1.087338
C68	-C69	:	1.395296	C68	-H73	:	1.086292
C69	-C70	:	1.398516	C69	-H74	:	1.085735
C70	-C71	:	1.390003	C70	-H75	:	1.086174
C71	-H76	:	1.085508				

bond angles:

C3	-C2	-H1	: 120.030425	C56	-C2	-H1	: 119.251827
C56	-C2	-C3	: 120.717747	C4	-C3	-C2	: 123.524411

C59 -C3 -C2 : 117.892202 C59 -C3 -C4 : 118.583388
C5 -C4 -C3 : 127.822245 H37 -C4 -C3 : 114.969478
H37 -C4 -C5 : 117.208269 C6 -C5 -C4 : 123.236936
H64 -C5 -C4 : 120.070918 H64 -C5 -C6 : 116.692140
C7 -C6 -C5 : 124.777915 H51 -C6 -C5 : 116.828433
H51 -C6 -C7 : 118.393642 C8 -C7 -C6 : 123.730027
H36 -C7 -C6 : 118.842449 H36 -C7 -C8 : 117.427519
C9 -C8 -C7 : 125.023944 H47 -C8 -C7 : 116.847661
H47 -C8 -C9 : 118.128383 C10 -C9 -C8 : 123.353390
H55 -C9 -C8 : 118.905106 H55 -C9 -C10 : 117.741499
C11 -C10 -C9 : 125.326033 H43 -C10 -C9 : 116.757698
H43 -C10 -C11 : 117.916256 C12 -C11 -C10 : 122.995407
H48 -C11 -C10 : 119.072025 H48 -C11 -C12 : 117.932563
C13 -C12 -C11 : 125.405584 H44 -C12 -C11 : 116.699666
H44 -C12 -C13 : 117.894739 C14 -C13 -C12 : 122.279555
H52 -C13 -C12 : 119.324133 H52 -C13 -C14 : 118.396305
C15 -C14 -C13 : 126.985632 H38 -C14 -C13 : 116.958753
H38 -C14 -C15 : 116.055610 C16 -C15 -C14 : 121.696656
C31 -C15 -C14 : 119.663256 C31 -C15 -C16 : 118.640088
C17 -C16 -C15 : 125.928663 H40 -C16 -C15 : 115.327470
H40 -C16 -C17 : 118.743864 C18 -C17 -C16 : 124.598466
H41 -C17 -C16 : 119.369992 H41 -C17 -C18 : 116.031541
C19 -C18 -C17 : 122.969395 C33 -C18 -C17 : 117.968626
C33 -C18 -C19 : 119.061968 C20 -C19 -C18 : 125.481930
H39 -C19 -C18 : 116.727386 H39 -C19 -C20 : 117.790683
C21 -C20 -C19 : 124.098908 H53 -C20 -C19 : 117.568429
H53 -C20 -C21 : 118.332645 C22 -C21 -C20 : 123.507500
H45 -C21 -C20 : 118.827376 H45 -C21 -C22 : 117.665122
C23 -C22 -C21 : 124.687720 H49 -C22 -C21 : 117.018234
H49 -C22 -C23 : 118.294033 C24 -C23 -C22 : 123.928881
H42 -C23 -C22 : 118.647748 H42 -C23 -C24 : 117.423370
C25 -C24 -C23 : 124.583243 H54 -C24 -C23 : 117.082715
H54 -C24 -C25 : 118.334033 C26 -C25 -C24 : 124.055038
H46 -C25 -C24 : 118.598921 H46 -C25 -C26 : 117.346040
C27 -C26 -C25 : 124.573185 H35 -C26 -C25 : 117.027677
H35 -C26 -C27 : 118.399132 C28 -C27 -C26 : 124.058445
H50 -C27 -C26 : 118.680672 H50 -C27 -C28 : 117.260882
C29 -C28 -C27 : 123.870183 H65 -C28 -C27 : 116.342626
H65 -C28 -C29 : 119.787181 C30 -C29 -C28 : 127.597218
H66 -C29 -C28 : 117.403574 H66 -C29 -C30 : 114.999204
C67 -C30 -C29 : 118.657397 C71 -C30 -C29 : 123.543633
C71 -C30 -C67 : 117.798970 N32 -C31 -C15 : 179.180262
N34 -C33 -C18 : 179.122984 C57 -C56 -C2 : 120.541829
H63 -C56 -C2 : 119.571011 H63 -C56 -C57 : 119.887160
C58 -C57 -C56 : 119.523443 H62 -C57 -C56 : 120.227642
H62 -C57 -C58 : 120.248915 C59 -C58 -C57 : 120.007925
H61 -C58 -C57 : 120.175717 H61 -C58 -C59 : 119.816358
C58 -C59 -C3 : 121.316853 H60 -C59 -C3 : 118.911390
H60 -C59 -C58 : 119.771756 C68 -C67 -C30 : 121.340928
H72 -C67 -C30 : 118.949618 H72 -C67 -C68 : 119.709453
C69 -C68 -C67 : 120.066326 H73 -C68 -C67 : 119.741694
H73 -C68 -C69 : 120.191980 C70 -C69 -C68 : 119.392711
H74 -C69 -C68 : 120.322650 H74 -C69 -C70 : 120.284638

C71 -C70 -C69 : 120.604462 H75 -C70 -C69 : 119.878359
H75 -C70 -C71 : 119.517179 C70 -C71 -C30 : 120.796601
H76 -C71 -C30 : 120.003899 H76 -C71 -C70 : 119.199497

torsional angles:

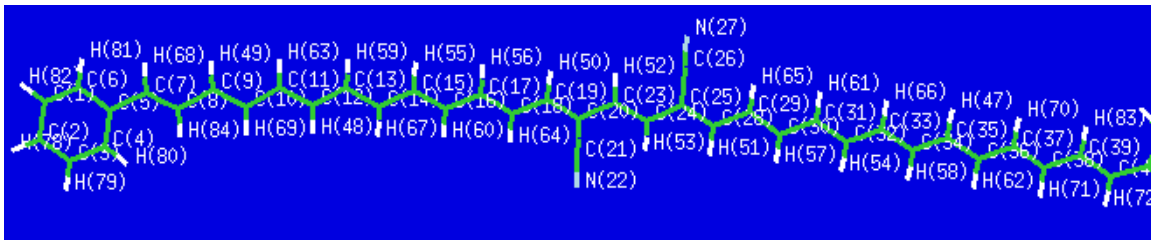
H1 -C2 -C3 -C4 : 0.021524
H1 -C2 -C3 -C59 :-179.983458
H1 -C2 -C56 -C57 : 179.991052
H1 -C2 -C56 -H63 : -0.007301
C2 -C3 -C4 -C5 : 0.074942
C2 -C3 -C4 -H37 :-179.959362
C2 -C3 -C59 -C58 : -0.010401
C2 -C3 -C59 -H60 : 179.998515
C2 -C56 -C57 -C58 : -0.004849
C2 -C56 -C57 -H62 : 179.997030
C3 -C2 -C56 -C57 : 0.002467
C3 -C2 -C56 -H63 :-179.995886
C3 -C4 -C5 -C6 :-179.986724
C3 -C4 -C5 -H64 : -0.014430
C3 -C59 -C58 -C57 : 0.008214
C3 -C59 -C58 -H61 :-179.991919
C4 -C3 -C2 -C56 :-179.989979
C4 -C3 -C59 -C58 : 179.984869
C4 -C3 -C59 -H60 : -0.006215
C4 -C5 -C6 -C7 :-179.921754
C4 -C5 -C6 -H51 : 0.042062
C5 -C4 -C3 -C59 :-179.920044
C5 -C6 -C7 -C8 : 179.998520
C5 -C6 -C7 -H36 : -0.024930
C6 -C5 -C4 -H37 : 0.048242
C6 -C7 -C8 -C9 :-179.905567
C6 -C7 -C8 -H47 : 0.052765
C7 -C6 -C5 -H64 : 0.105083
C7 -C8 -C9 -C10 : 179.987769
C7 -C8 -C9 -H55 : -0.037195
C8 -C7 -C6 -H51 : 0.035225
C8 -C9 -C10 -C11 :-179.890933
C8 -C9 -C10 -H43 : 0.066803
C9 -C8 -C7 -H36 : 0.117576
C9 -C10 -C11 -C12 : 179.979108
C9 -C10 -C11 -H48 : -0.047419
C10 -C9 -C8 -H47 : 0.029925
C10 -C11 -C12 -C13 :-179.876224
C10 -C11 -C12 -H44 : 0.085095
C11 -C10 -C9 -H55 : 0.133759
C11 -C12 -C13 -C14 : 179.979968
C11 -C12 -C13 -H52 : -0.050687
C12 -C11 -C10 -H43 : 0.021816
C12 -C13 -C14 -C15 :-179.875244
C12 -C13 -C14 -H38 : 0.097084
C13 -C12 -C11 -H48 : 0.150018
C13 -C14 -C15 -C16 : 179.977427

C13 -C14 -C15 -C31 : -0.033979
C14 -C13 -C12 -H44 : 0.019067
C14 -C15 -C16 -C17 :-179.838798
C14 -C15 -C16 -H40 : 0.138852
C14 -C15 -C31 -N32 :-179.807630
C15 -C14 -C13 -H52 : 0.155139
C15 -C16 -C17 -C18 : 179.964248
C15 -C16 -C17 -H41 : -0.044350
C16 -C15 -C14 -H38 : 0.004883
C16 -C15 -C31 -N32 : 0.181312
C16 -C17 -C18 -C19 :-179.817194
C16 -C17 -C18 -C33 : 0.144806
C17 -C16 -C15 -C31 : 0.172495
C17 -C18 -C19 -C20 : 179.946130
C17 -C18 -C19 -H39 : -0.063832
C17 -C18 -C33 -N34 : -0.664552
C18 -C17 -C16 -H40 : -0.012711
C18 -C19 -C20 -C21 :-179.846551
C18 -C19 -C20 -H53 : 0.103272
C19 -C18 -C17 -H41 : 0.191145
C19 -C18 -C33 -N34 : 179.298975
C19 -C20 -C21 -C22 : 179.934114
C19 -C20 -C21 -H45 : -0.078269
C20 -C19 -C18 -C33 : -0.015473
C20 -C21 -C22 -C23 :-179.862582
C20 -C21 -C22 -H49 : 0.095537
C21 -C20 -C19 -H39 : 0.163508
C21 -C22 -C23 -C24 : 179.943466
C21 -C22 -C23 -H42 : -0.070415
C22 -C21 -C20 -H53 : -0.015352
C22 -C23 -C24 -C25 :-179.879836
C22 -C23 -C24 -H54 : 0.085495
C23 -C22 -C21 -H45 : 0.149667
C23 -C24 -C25 -C26 : 179.952084
C23 -C24 -C25 -H46 : -0.061112
C24 -C23 -C22 -H49 : -0.014161
C24 -C25 -C26 -C27 :-179.898941
C24 -C25 -C26 -H35 : 0.072992
C25 -C24 -C23 -H42 : 0.133888
C25 -C26 -C27 -C28 : 179.958887
C25 -C26 -C27 -H50 : -0.054223
C26 -C25 -C24 -H54 : -0.012847
C26 -C27 -C28 -C29 :-179.919433
C26 -C27 -C28 -H65 : 0.044221
C27 -C26 -C25 -H46 : 0.114102
C27 -C28 -C29 -C30 : 179.976141
C27 -C28 -C29 -H66 : -0.048772
C28 -C27 -C26 -H35 : -0.012690
C28 -C29 -C30 -C67 :-179.941882
C28 -C29 -C30 -C71 : 0.064975
C29 -C28 -C27 -H50 : 0.093506
C29 -C30 -C67 -C68 : 179.992522
C29 -C30 -C67 -H72 : -0.017736

C29 -C30 -C71 -C70 :-179.997691
C29 -C30 -C71 -H76 : 0.020329
C30 -C29 -C28 -H65 : 0.013671
C30 -C67 -C68 -C69 : 0.007889
C30 -C67 -C68 -H73 :-179.993544
C30 -C71 -C70 -C69 : 0.001708
C30 -C71 -C70 -H75 :-179.999035
C31 -C15 -C14 -H38 : 179.993477
C31 -C15 -C16 -H40 :-179.849855
C33 -C18 -C17 -H41 :-179.846856
C33 -C18 -C19 -H39 : 179.974564
H35 -C26 -C25 -H46 :-179.913965
H35 -C26 -C27 -H50 : 179.974199
H36 -C7 -C6 -H51 :-179.988225
H36 -C7 -C8 -H47 :-179.924093
H37 -C4 -C3 -C59 : 0.045652
H37 -C4 -C5 -H64 :-179.979464
H38 -C14 -C13 -H52 :-179.872534
H39 -C19 -C20 -H53 :-179.886670
H40 -C16 -C17 -H41 : 179.978691
H42 -C23 -C22 -H49 : 179.971958
H42 -C23 -C24 -H54 :-179.900781
H43 -C10 -C9 -H55 :-179.908505
H43 -C10 -C11 -H48 : 179.995289
H44 -C12 -C11 -H48 :-179.888663
H44 -C12 -C13 -H52 : 179.988412
H45 -C21 -C20 -H53 : 179.972264
H45 -C21 -C22 -H49 :-179.892214
H46 -C25 -C24 -H54 : 179.973957
H47 -C8 -C9 -H55 :-179.995039
H50 -C27 -C28 -H65 :-179.942840
H51 -C6 -C5 -H64 :-179.931101
C56 -C2 -C3 -C59 : 0.005038
C56 -C57 -C58 -C59 : -0.000441
C56 -C57 -C58 -H61 : 179.999693
C57 -C58 -C59 -H60 : 179.999223
C58 -C57 -C56 -H63 : 179.993499
C59 -C58 -C57 -H62 : 179.997680
H60 -C59 -C58 -H61 : -0.000910
H61 -C58 -C57 -H62 : -0.002187
H62 -C57 -C56 -H63 : -0.004622
H65 -C28 -C29 -H66 : 179.988758
H66 -C29 -C30 -C67 : 0.082521
H66 -C29 -C30 -C71 :-179.910622
C67 -C30 -C71 -C70 : 0.009111
C67 -C30 -C71 -H76 :-179.972869
C67 -C68 -C69 -C70 : 0.003293
C67 -C68 -C69 -H74 :-179.996416
C68 -C67 -C30 -C71 : -0.013938
C68 -C69 -C70 -C71 : -0.008052
C68 -C69 -C70 -H75 : 179.992694
C69 -C68 -C67 -H72 :-179.981776
C69 -C70 -C71 -H76 : 179.983831

C70	-C69	-C68	-H73	:-179.995268
C71	-C30	-C67	-H72	: 179.975804
C71	-C70	-C69	-H74	: 179.991656
H72	-C67	-C68	-H73	: 0.016791
H73	-C68	-C69	-H74	: 0.005024
H74	-C69	-C70	-H75	: -0.007598
H75	-C70	-C71	-H76	: -0.016912

DPDC15



final geometry:

	angstroms		
atom	x	y	z
C1	0.0073500156	0.0047503020	-0.0006584579
C2	0.0086184680	0.0038894649	1.3945911631
C3	1.2276598240	0.0041060930	2.0794162974
C4	2.4297248283	0.0050837280	1.3820581493
C5	2.4489977482	0.0060203897	-0.0276970055
C6	1.2110167620	0.0059421132	-0.6999343693
C7	3.6763532591	0.0071987370	-0.8181254438
C8	4.9542547086	0.0013413434	-0.3627867723
C9	6.1079483170	0.0049499252	-1.2152200082
C10	7.3920582237	-0.0014454812	-0.7582132057
C11	8.5559246359	0.0035782093	-1.5879591414
C12	9.8324100370	-0.0044059632	-1.1026147599
C13	11.0142176653	0.0013568950	-1.9019562962
C14	12.2785448708	-0.0098907329	-1.3811202626
C15	13.4811758974	-0.0041049335	-2.1454994314
C16	14.7305306142	-0.0203793515	-1.5860435925
C17	15.9531473417	-0.0152059436	-2.3143465320
C18	17.1861732252	-0.0382654854	-1.7153087855
C19	18.4171147435	-0.0340755637	-2.4212245848
C20	19.6710488826	-0.0646928264	-1.8425396110
C21	19.7789292821	-0.1055443696	-0.4121018522
N22	19.8854384364	-0.1386923223	0.7468736445
C23	20.8909743748	-0.0603482652	-2.6096248690
C24	22.1424390981	-0.1008239056	-2.0764620686
C25	23.3717649400	-0.1017219497	-2.8267822626
C26	23.2921006393	-0.0442286500	-4.2569609854
N27	23.2103586155	0.0044148728	-5.4174303238
C28	24.6098999218	-0.1559179760	-2.2180632633
C29	25.8651377903	-0.1662182933	-2.8782703102
C30	27.0649077365	-0.2209714727	-2.2174191954
C31	28.3321115495	-0.2348836984	-2.8636308226
C32	29.5318572012	-0.2875561316	-2.2066050705
C33	30.7998528521	-0.3031920355	-2.8558248921
C34	32.0007589522	-0.3534724785	-2.2038456254
C35	33.2691234676	-0.3703627342	-2.8566534694
C36	34.4688985696	-0.4188715899	-2.2060208195
C37	35.7415172814	-0.4369713452	-2.8562043628
C38	36.9346648385	-0.4847438000	-2.1988298436
C39	38.2182334628	-0.5044120441	-2.8380425528
C40	39.3893495615	-0.5520724739	-2.1545722381
C41	40.7439688765	-0.5771483762	-2.6957936498

C42	41.0344019199	-0.5605714273	-4.0751820655
C43	42.3482422248	-0.5871265493	-4.5273490511
C44	43.4102261182	-0.6311240392	-3.6194408323
C45	43.1428048958	-0.6482032477	-2.2507162961
C46	41.8276727942	-0.6216005111	-1.7970137604
H47	33.2683087943	-0.3426974507	-3.9464315965
H48	9.9709068872	-0.0164435681	-0.0212571011
H49	5.9331435442	0.0136377185	-2.2913320768
H50	18.3783531861	-0.0056786598	-3.5089776549
H51	24.6149304734	-0.1954097295	-1.1300850184
H52	20.7724309035	-0.0234723420	-3.6903168184
H53	22.2527575614	-0.1391417329	-0.9949429498
H54	29.5267339031	-0.3196781072	-1.1167182035
H55	13.3908950595	0.0135520839	-3.2318290018
H56	15.8952026296	0.0073460416	-3.4028880618
H57	27.0577604953	-0.2563358296	-1.1276425539
H58	31.9997915854	-0.3827489835	-1.1138659837
H59	10.8914921776	0.0150680283	-2.9850841081
H60	14.8060676851	-0.0398261415	-0.4988001225
H61	28.3366257014	-0.2012100425	-3.9528686414
H62	34.4679079385	-0.4460308512	-1.1159712601
H63	8.4040174038	0.0143439221	-2.6674124115
H64	17.2311563344	-0.0628017844	-0.6276246343
H65	25.8673839220	-0.1291645967	-3.9662177646
H66	30.8013599175	-0.2728770389	-3.9454191131
H67	12.3861729477	-0.0251753517	-0.2963359487
H68	3.5280855166	0.0135712896	-1.8980389550
H69	7.5569860272	-0.0110362488	0.3195432887
H70	35.7444375883	-0.4110990509	-3.9460830988
H71	36.9263173992	-0.5104882763	-1.1087691597
H72	39.3305609791	-0.5749516344	-1.0662897432
H73	44.4350393301	-0.6520066881	-3.9779631268
H74	42.5481500360	-0.5737874586	-5.5950534299
H75	40.2259424666	-0.5275012104	-4.7984563085
H76	41.6253656432	-0.6354438898	-0.7289211182
H77	43.9594886034	-0.6824568962	-1.5354434123
H78	-0.9278704925	0.0031173125	1.9441549479
H79	1.2387093356	0.0036270407	3.1656305779
H80	3.3626231030	0.0058086777	1.9371898024
H81	1.2023455993	0.0067306820	-1.7871878016
H82	-0.9323219276	0.0046615801	-0.5457818862
H83	38.2218526904	-0.4793193766	-3.9266254332
H84	5.1468286064	-0.0064916566	0.7088391469

Final total energy: -1808.965556 hartrees

HOMO energy: -0.17184
LUMO energy: -0.11123

bond lengths (angstroms):

C1	-C2	:	1.395250	C1	-C6	:	1.392050
C1	-H82	:	1.086344	C2	-C3	:	1.398230
C2	-H78	:	1.085833	C3	-C4	:	1.389701
C3	-H79	:	1.086271	C4	-C5	:	1.409887
C4	-H80	:	1.085574	C5	-C6	:	1.408723
C5	-C7	:	1.459856	C6	-H81	:	1.087288
C7	-C8	:	1.356613	C7	-H68	:	1.090063
C8	-C9	:	1.434456	C8	-H84	:	1.088820
C9	-C10	:	1.363024	C9	-H49	:	1.090252
C10	-C11	:	1.429366	C10	-H69	:	1.090345
C11	-C12	:	1.365664	C11	-H63	:	1.090143
C12	-C13	:	1.426762	C12	-H48	:	1.090257
C13	-C14	:	1.367450	C13	-H59	:	1.090145
C14	-C15	:	1.425002	C14	-H67	:	1.090218
C15	-C16	:	1.368993	C15	-H55	:	1.090218
C16	-C17	:	1.423111	C16	-H60	:	1.090038
C17	-C18	:	1.371033	C17	-H56	:	1.090316
C18	-C19	:	1.418997	C18	-H64	:	1.088890
C19	-C20	:	1.381363	C19	-H50	:	1.088814
C20	-C21	:	1.435082	C20	-C23	:	1.441061
C21	-N22	:	1.164331	C23	-C24	:	1.360906
C23	-H52	:	1.087799	C24	-C25	:	1.440216
C24	-H53	:	1.087806	C25	-C26	:	1.433549
C25	-C28	:	1.380744	C26	-N27	:	1.164361
C28	-C29	:	1.418309	C28	-H51	:	1.088706
C29	-C30	:	1.370828	C29	-H65	:	1.088581
C30	-C31	:	1.422529	C30	-H57	:	1.090374
C31	-C32	:	1.368885	C31	-H61	:	1.089768
C32	-C33	:	1.424621	C32	-H54	:	1.090372
C33	-C34	:	1.367399	C33	-H66	:	1.090017
C34	-C35	:	1.426602	C34	-H58	:	1.090373
C35	-C36	:	1.365700	C35	-H47	:	1.090130
C36	-C37	:	1.429204	C36	-H62	:	1.090388
C37	-C38	:	1.363094	C37	-H70	:	1.090190
C38	-C39	:	1.434060	C38	-H71	:	1.090397
C39	-C40	:	1.356804	C39	-H83	:	1.088878
C40	-C41	:	1.458953	C40	-H72	:	1.090109
C41	-C42	:	1.409730	C41	-C46	:	1.408615
C42	-C43	:	1.389725	C42	-H75	:	1.085277
C43	-C44	:	1.397871	C43	-H74	:	1.086340
C44	-C45	:	1.394709	C44	-H73	:	1.085917
C45	-C46	:	1.391447	C45	-H77	:	1.086168
C46	-H76	:	1.087171				

bond angles:

C6 -C1 -C2 : 120.102577 H82 -C1 -C2 : 120.171000
H82 -C1 -C6 : 119.726423 C3 -C2 -C1 : 119.378199
H78 -C2 -C1 : 120.353795 H78 -C2 -C3 : 120.268005
C4 -C3 -C2 : 120.554420 H79 -C3 -C2 : 119.908936
H79 -C3 -C4 : 119.536644 C5 -C4 -C3 : 120.902719
H80 -C4 -C3 : 119.125321 H80 -C4 -C5 : 119.971947
C6 -C5 -C4 : 117.719192 C7 -C5 -C4 : 123.565179
C7 -C5 -C6 : 118.715629 C5 -C6 -C1 : 121.342891
H81 -C6 -C1 : 119.697729 H81 -C6 -C5 : 118.959379
C8 -C7 -C5 : 127.605534 H68 -C7 -C5 : 114.964147
H68 -C7 -C8 : 117.430320 C9 -C8 -C7 : 123.927195
H84 -C8 -C7 : 119.800234 H84 -C8 -C9 : 116.272571
C10 -C9 -C8 : 123.948607 H49 -C9 -C8 : 117.233367
H49 -C9 -C10 : 118.818024 C11 -C10 -C9 : 124.921924
H69 -C10 -C9 : 118.291893 H69 -C10 -C11 : 116.786182
C12 -C11 -C10 : 123.694021 H63 -C11 -C10 : 117.476102
H63 -C11 -C12 : 118.829877 C13 -C12 -C11 : 125.106242
H48 -C12 -C11 : 118.118100 H48 -C12 -C13 : 116.775655
C14 -C13 -C12 : 123.533730 H59 -C13 -C12 : 117.609571
H59 -C13 -C14 : 118.856694 C15 -C14 -C13 : 125.167292
H67 -C14 -C13 : 118.058648 H67 -C14 -C15 : 116.774048
C16 -C15 -C14 : 123.431470 H55 -C15 -C14 : 117.688935
H55 -C15 -C16 : 118.879581 C17 -C16 -C15 : 125.089310
H60 -C16 -C15 : 118.103664 H60 -C16 -C17 : 116.806999
C18 -C17 -C16 : 123.296568 H56 -C17 -C16 : 117.733075
H56 -C17 -C18 : 118.970331 C19 -C18 -C17 : 124.245868
H64 -C18 -C17 : 118.292443 H64 -C18 -C19 : 117.461635
C20 -C19 -C18 : 125.378862 H50 -C19 -C18 : 117.786989
H50 -C19 -C20 : 116.834106 C21 -C20 -C19 : 119.106692
C23 -C20 -C19 : 123.051437 C23 -C20 -C21 : 117.841753
N22 -C21 -C20 : 179.062635 C24 -C23 -C20 : 124.738918
H52 -C23 -C20 : 115.892070 H52 -C23 -C24 : 119.368909
C25 -C24 -C23 : 125.509849 H53 -C24 -C23 : 118.934679
H53 -C24 -C25 : 115.555217 C26 -C25 -C24 : 118.183273
C28 -C25 -C24 : 122.395107 C28 -C25 -C26 : 119.421618
N27 -C26 -C25 : 179.154282 C29 -C28 -C25 : 126.063624
H51 -C28 -C25 : 116.496004 H51 -C28 -C29 : 117.440329
C30 -C29 -C28 : 123.399477 H65 -C29 -C28 : 117.826578
H65 -C29 -C30 : 118.773932 C31 -C30 -C29 : 124.128216
H57 -C30 -C29 : 118.514176 H57 -C30 -C31 : 117.357608
C32 -C31 -C30 : 124.269197 H61 -C31 -C30 : 117.221818
H61 -C31 -C32 : 118.508985 C33 -C32 -C31 : 124.178662
H54 -C32 -C31 : 118.474867 H54 -C32 -C33 : 117.346470
C34 -C33 -C32 : 124.388671 H66 -C33 -C32 : 117.159095
H66 -C33 -C34 : 118.452233 C35 -C34 -C33 : 124.269054
H58 -C34 -C33 : 118.479121 H58 -C34 -C35 : 117.251824
C36 -C35 -C34 : 124.296803 H47 -C35 -C34 : 117.160464
H47 -C35 -C36 : 118.542730 C37 -C36 -C35 : 124.469930
H62 -C36 -C35 : 118.447171 H62 -C36 -C37 : 117.082899
C38 -C37 -C36 : 124.088267 H70 -C37 -C36 : 117.186085
H70 -C37 -C38 : 118.725641 C39 -C38 -C37 : 124.679338

H71 -C38 -C37 : 118.440409 H71 -C38 -C39 : 116.880251
C40 -C39 -C38 : 123.265053 H83 -C39 -C38 : 116.633031
H83 -C39 -C40 : 120.101913 C41 -C40 -C39 : 127.963036
H72 -C40 -C39 : 117.198856 H72 -C40 -C41 : 114.838109
C42 -C41 -C40 : 123.646451 C46 -C41 -C40 : 118.565753
C46 -C41 -C42 : 117.787773 C43 -C42 -C41 : 120.857693
H75 -C42 -C41 : 119.932879 H75 -C42 -C43 : 119.209408
C44 -C43 -C42 : 120.498178 H74 -C43 -C42 : 119.572183
H74 -C43 -C44 : 119.929637 C45 -C44 -C43 : 119.479421
H73 -C44 -C43 : 120.207787 H73 -C44 -C45 : 120.312791
C46 -C45 -C44 : 120.064850 H77 -C45 -C44 : 120.164083
H77 -C45 -C46 : 119.771066 C45 -C46 -C41 : 121.312084
H76 -C46 -C41 : 118.953567 H76 -C46 -C45 : 119.734347

torsional angles:

C1 -C2 -C3 -C4 : -0.003999
C1 -C2 -C3 -H79 : 179.988692
C1 -C6 -C5 -C4 : -0.010825
C1 -C6 -C5 -C7 : 179.995492
C2 -C1 -C6 -C5 : 0.013726
C2 -C1 -C6 -H81 :-179.992562
C2 -C3 -C4 -C5 : 0.006751
C2 -C3 -C4 -H80 : 179.965171
C3 -C2 -C1 -C6 : -0.006120
C3 -C2 -C1 -H82 :-179.995875
C3 -C4 -C5 -C6 : 0.000595
C3 -C4 -C5 -C7 : 179.993947
C4 -C3 -C2 -H78 : 179.999571
C4 -C5 -C6 -H81 : 179.995418
C4 -C5 -C7 -C8 : 0.332891
C4 -C5 -C7 -H68 :-179.667051
C5 -C4 -C3 -H79 :-179.985967
C5 -C6 -C1 -H82 :-179.996473
C5 -C7 -C8 -C9 :-179.908807
C5 -C7 -C8 -H84 : 0.084397
C6 -C1 -C2 -H78 : 179.990307
C6 -C5 -C4 -H80 :-179.957476
C6 -C5 -C7 -C8 :-179.673819
C6 -C5 -C7 -H68 : 0.326239
C7 -C5 -C4 -H80 : 0.035876
C7 -C5 -C6 -H81 : 0.001734
C7 -C8 -C9 -C10 :-179.973986
C7 -C8 -C9 -H49 : 0.044209
C8 -C9 -C10 -C11 :-179.921440
C8 -C9 -C10 -H69 : 0.072912
C9 -C8 -C7 -H68 : 0.091134
C9 -C10 -C11 -C12 :-179.931593
C9 -C10 -C11 -H63 : 0.064574
C10 -C9 -C8 -H84 : 0.032591
C10 -C11 -C12 -C13 :-179.947015
C10 -C11 -C12 -H48 : 0.072889
C11 -C10 -C9 -H49 : 0.060095

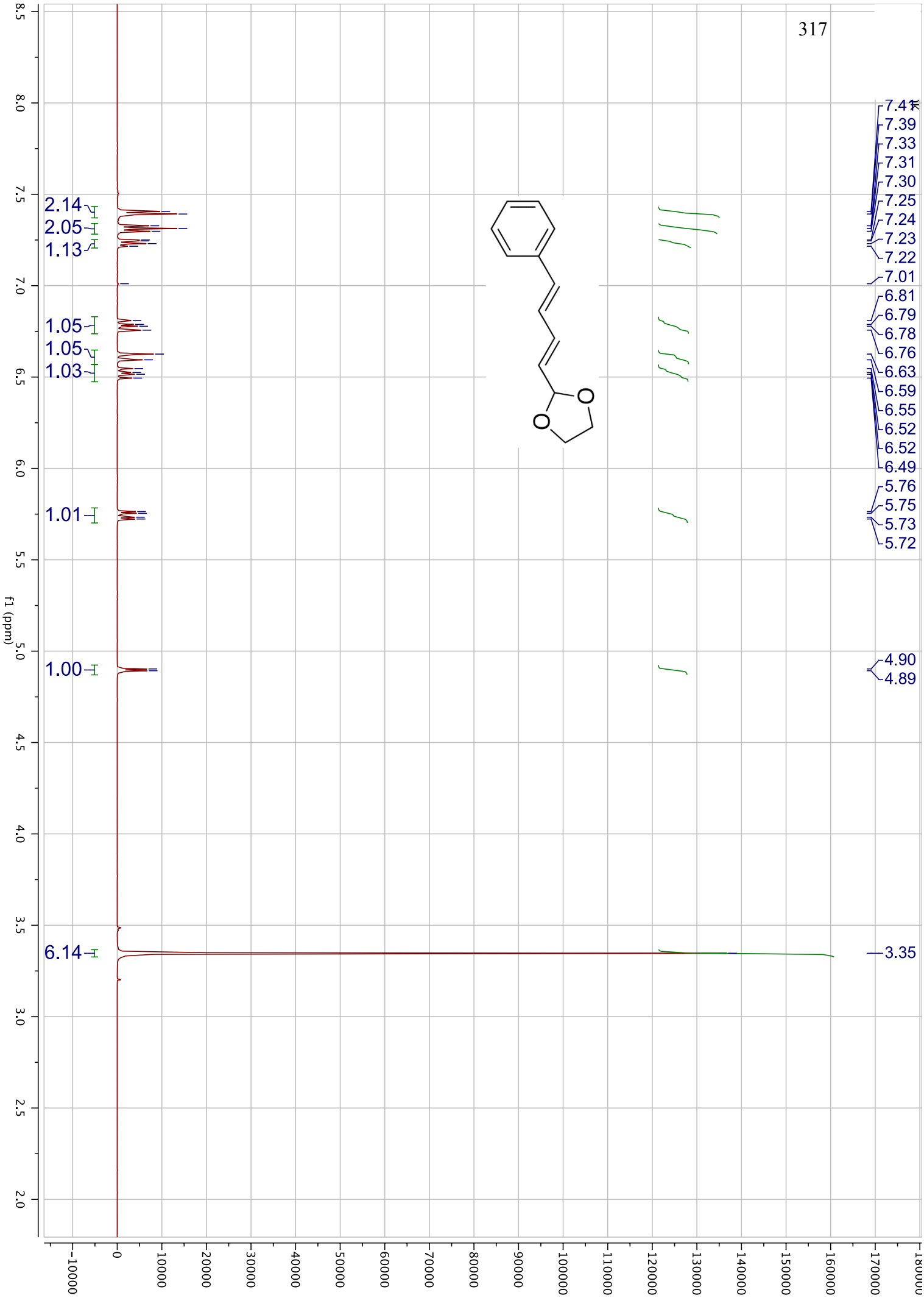
C11 -C12 -C13 -C14 :-179.853388
C11 -C12 -C13 -H59 : 0.120066
C12 -C11 -C10 -H69 : 0.073978
C12 -C13 -C14 -C15 :-179.973340
C12 -C13 -C14 -H67 : 0.069107
C13 -C12 -C11 -H63 : 0.056867
C13 -C14 -C15 -C16 :-179.770637
C13 -C14 -C15 -H55 : 0.185504
C14 -C13 -C12 -H48 : 0.126949
C14 -C15 -C16 -C17 :-179.995348
C14 -C15 -C16 -H60 : 0.066670
C15 -C14 -C13 -H59 : 0.053519
C15 -C16 -C17 -C18 :-179.688945
C15 -C16 -C17 -H56 : 0.250712
C16 -C15 -C14 -H67 : 0.187406
C16 -C17 -C18 -C19 : 179.978569
C16 -C17 -C18 -H64 : 0.065400
C17 -C16 -C15 -H55 : 0.049005
C17 -C18 -C19 -C20 :-179.603127
C17 -C18 -C19 -H50 : 0.319089
C18 -C17 -C16 -H60 : 0.249763
C18 -C19 -C20 -C21 : 0.050450
C18 -C19 -C20 -C23 : 179.923095
C19 -C18 -C17 -H56 : 0.039620
C19 -C20 -C21 -N22 :-179.478778
C19 -C20 -C23 -C24 :-179.433707
C19 -C20 -C23 -H52 : 0.447915
C20 -C19 -C18 -H64 : 0.310706
C20 -C23 -C24 -C25 : 179.780029
C20 -C23 -C24 -H53 : -0.027837
C21 -C20 -C19 -H50 :-179.872431
C21 -C20 -C23 -C24 : 0.440454
C21 -C20 -C23 -H52 :-179.677924
N22 -C21 -C20 -C23 : 0.641943
C23 -C20 -C19 -H50 : 0.000214
C23 -C24 -C25 -C26 : 0.558648
C23 -C24 -C25 -C28 :-179.426669
C24 -C25 -C26 -N27 : 5.251597
C24 -C25 -C28 -C29 : 179.738115
C24 -C25 -C28 -H51 : -0.183641
C25 -C24 -C23 -H52 : -0.097770
C25 -C28 -C29 -C30 : 179.987754
C25 -C28 -C29 -H65 : -0.054203
C26 -C25 -C24 -H53 :-179.627736
C26 -C25 -C28 -C29 : -0.247027
C26 -C25 -C28 -H51 : 179.831217
N27 -C26 -C25 -C28 :-174.762636
C28 -C25 -C24 -H53 : 0.386947
C28 -C29 -C30 -C31 : 179.863480
C28 -C29 -C30 -H57 : -0.139129
C29 -C30 -C31 -C32 : 179.901069
C29 -C30 -C31 -H61 : -0.105709
C30 -C29 -C28 -H51 : -0.091149

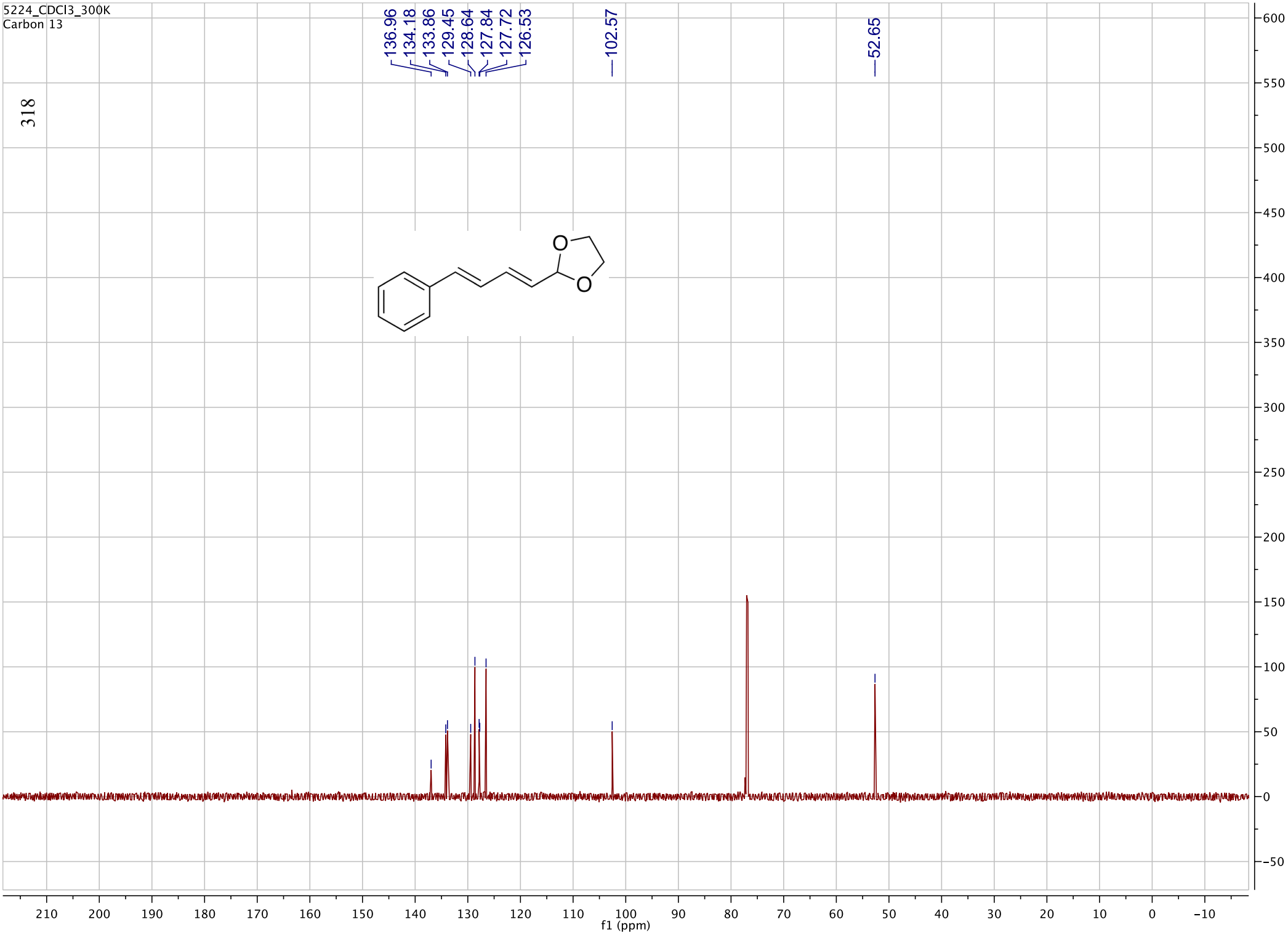
C30 -C31 -C32 -C33 : 179.912759
C30 -C31 -C32 -H54 : -0.099762
C31 -C30 -C29 -H65 : -0.094187
C31 -C32 -C33 -C34 : 179.884649
C31 -C32 -C33 -H66 : -0.124413
C32 -C31 -C30 -H57 : -0.096350
C32 -C33 -C34 -C35 : 179.934684
C32 -C33 -C34 -H58 : -0.072710
C33 -C32 -C31 -H61 : -0.080382
C33 -C34 -C35 -C36 : 179.913506
C33 -C34 -C35 -H47 : -0.104957
C34 -C33 -C32 -H54 : -0.102960
C34 -C35 -C36 -C37 : 179.949979
C34 -C35 -C36 -H62 : -0.046455
C35 -C34 -C33 -H66 : -0.056145
C35 -C36 -C37 -C38 : 179.963195
C35 -C36 -C37 -H70 : -0.069142
C36 -C35 -C34 -H58 : -0.079183
C36 -C37 -C38 -C39 : 179.950961
C36 -C37 -C38 -H71 : -0.031968
C37 -C36 -C35 -H47 : -0.031321
C37 -C38 -C39 -C40 : 179.993398
C37 -C38 -C39 -H83 : -0.027005
C38 -C37 -C36 -H62 : -0.040326
C38 -C39 -C40 -C41 : 179.940757
C38 -C39 -C40 -H72 : -0.062801
C39 -C38 -C37 -H70 : -0.016238
C39 -C40 -C41 -C42 : -0.319824
C39 -C40 -C41 -C46 : 179.738003
C40 -C39 -C38 -H71 : -0.023431
C40 -C41 -C42 -C43 :-179.953450
C40 -C41 -C42 -H75 : -0.004678
C40 -C41 -C46 -C45 : 179.954533
C40 -C41 -C46 -H76 : -0.029703
C41 -C40 -C39 -H83 : -0.038160
C41 -C42 -C43 -C44 : 0.009111
C41 -C42 -C43 -H74 : 179.991165
C41 -C46 -C45 -C44 : -0.005211
C41 -C46 -C45 -H77 :-179.994989
C42 -C41 -C40 -H72 : 179.683664
C42 -C41 -C46 -C45 : 0.008947
C42 -C41 -C46 -H76 :-179.975288
C42 -C43 -C44 -C45 : -0.005039
C42 -C43 -C44 -H73 : 179.983378
C43 -C42 -C41 -C46 : -0.010858
C43 -C44 -C45 -C46 : 0.003078
C43 -C44 -C45 -H77 : 179.992816
C44 -C43 -C42 -H75 :-179.940027
C44 -C45 -C46 -H76 : 179.978904
C45 -C44 -C43 -H74 :-179.987028
C46 -C41 -C40 -H72 : -0.258509
C46 -C41 -C42 -H75 : 179.937914
C46 -C45 -C44 -H73 :-179.985327

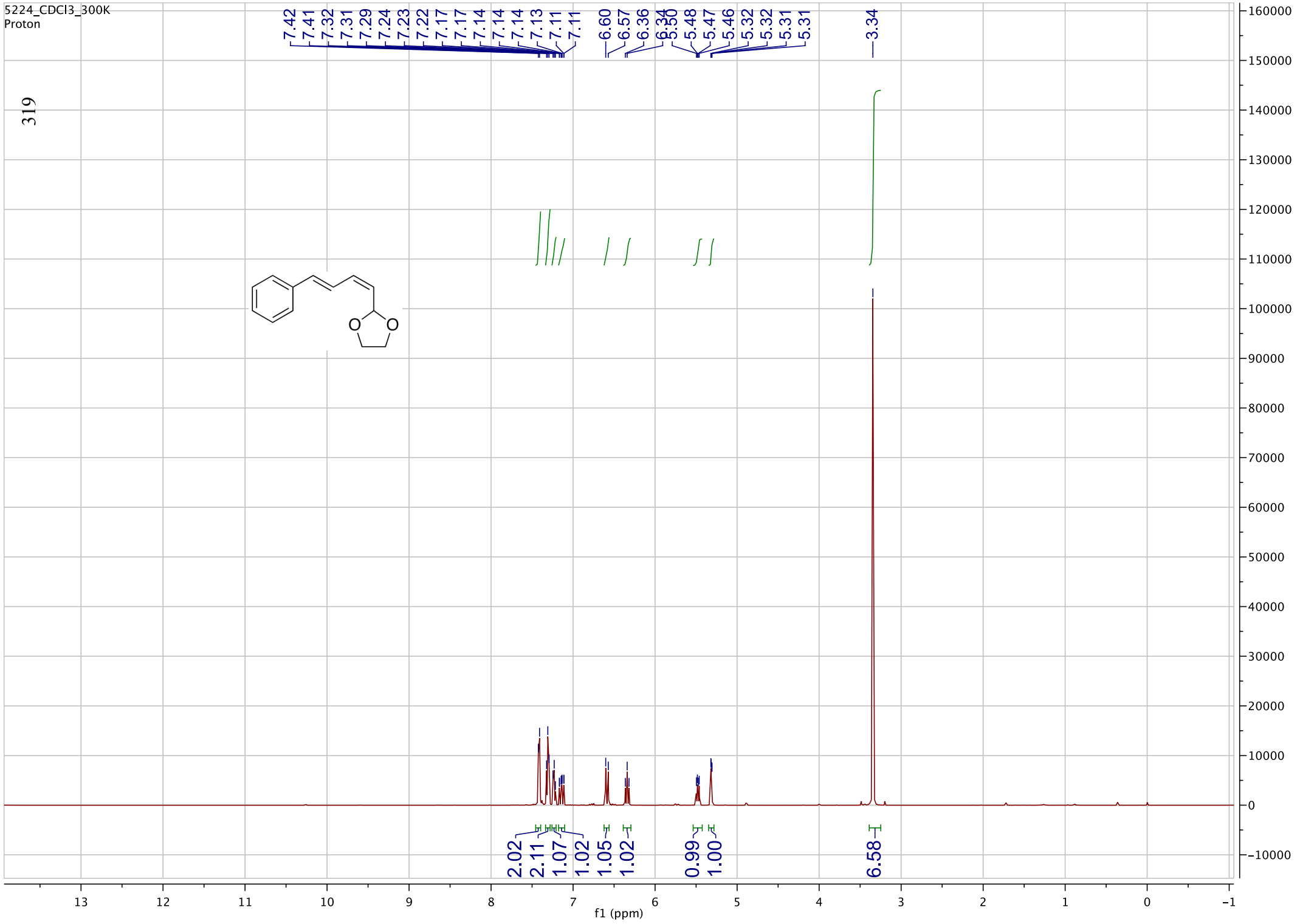
H47 -C35 -C34 -H58 : 179.902354
H47 -C35 -C36 -H62 : 179.972244
H48 -C12 -C11 -H63 :-179.923229
H48 -C12 -C13 -H59 :-179.899598
H49 -C9 -C8 -H84 :-179.949214
H49 -C9 -C10 -H69 :-179.945553
H50 -C19 -C18 -H64 :-179.767078
H51 -C28 -C29 -H65 : 179.866893
H52 -C23 -C24 -H53 :-179.905637
H54 -C32 -C31 -H61 : 179.907097
H54 -C32 -C33 -H66 : 179.887978
H55 -C15 -C14 -H67 :-179.856453
H55 -C15 -C16 -H60 :-179.888978
H56 -C17 -C16 -H60 :-179.810580
H56 -C17 -C18 -H64 :-179.873550
H57 -C30 -C29 -H65 : 179.903204
H57 -C30 -C31 -H61 : 179.896872
H58 -C34 -C33 -H66 : 179.936461
H59 -C13 -C14 -H67 :-179.904034
H62 -C36 -C37 -H70 : 179.927337
H63 -C11 -C10 -H69 :-179.929855
H68 -C7 -C8 -H84 :-179.915662
H70 -C37 -C38 -H71 :-179.999167
H71 -C38 -C39 -H83 : 179.956165
H72 -C40 -C39 -H83 : 179.958281
H73 -C44 -C43 -H74 : 0.001389
H73 -C44 -C45 -H77 : 0.004411
H74 -C43 -C42 -H75 : 0.042026
H76 -C46 -C45 -H77 : -0.010875
H78 -C2 -C1 -H82 : 0.000552
H78 -C2 -C3 -H79 : -0.007738
H79 -C3 -C4 -H80 : -0.027546
H81 -C6 -C1 -H82 : -0.002761

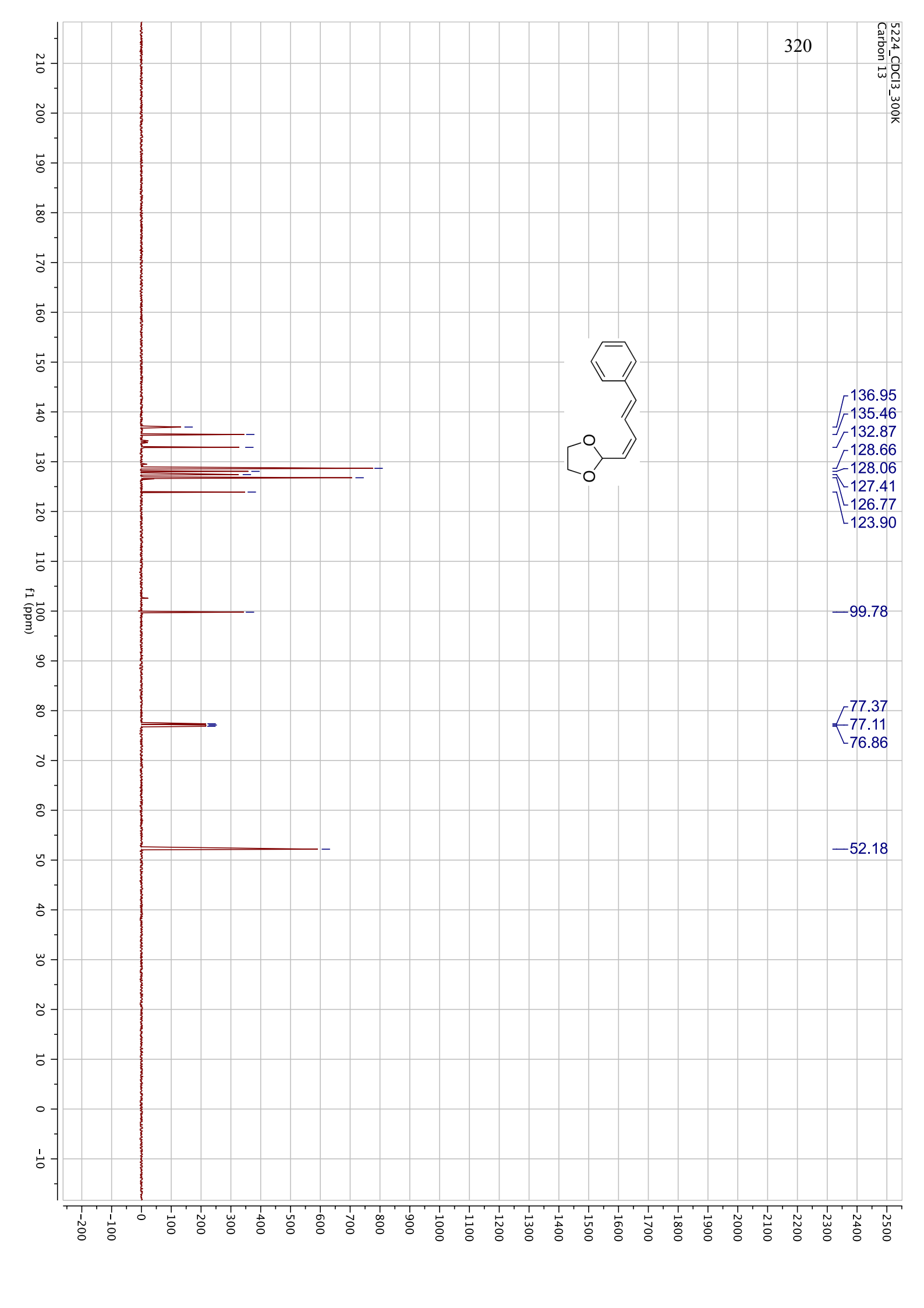
Appendix A (Part 3)

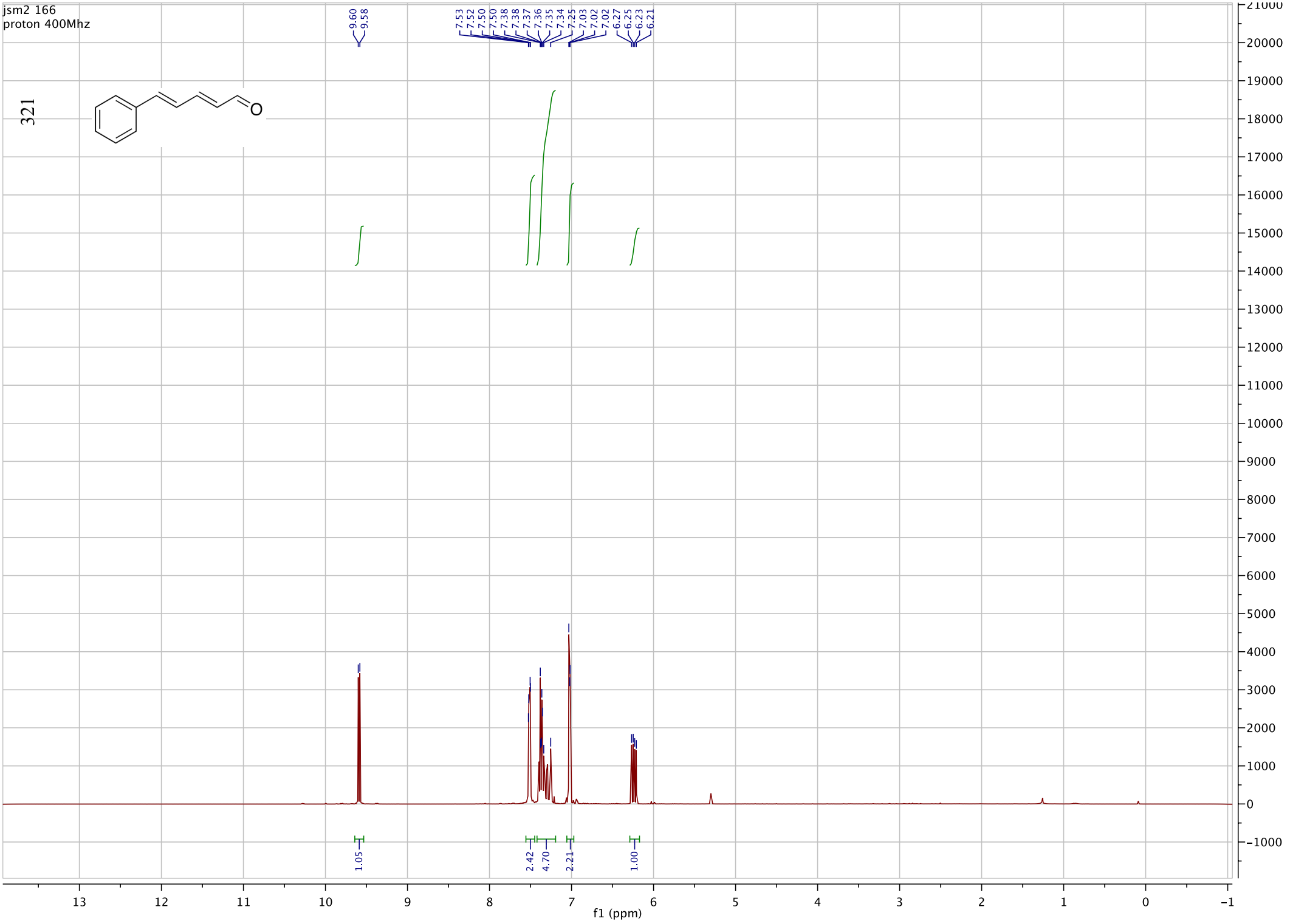
^{1}H-NNMR and ^{13}C-NMR Spectra:

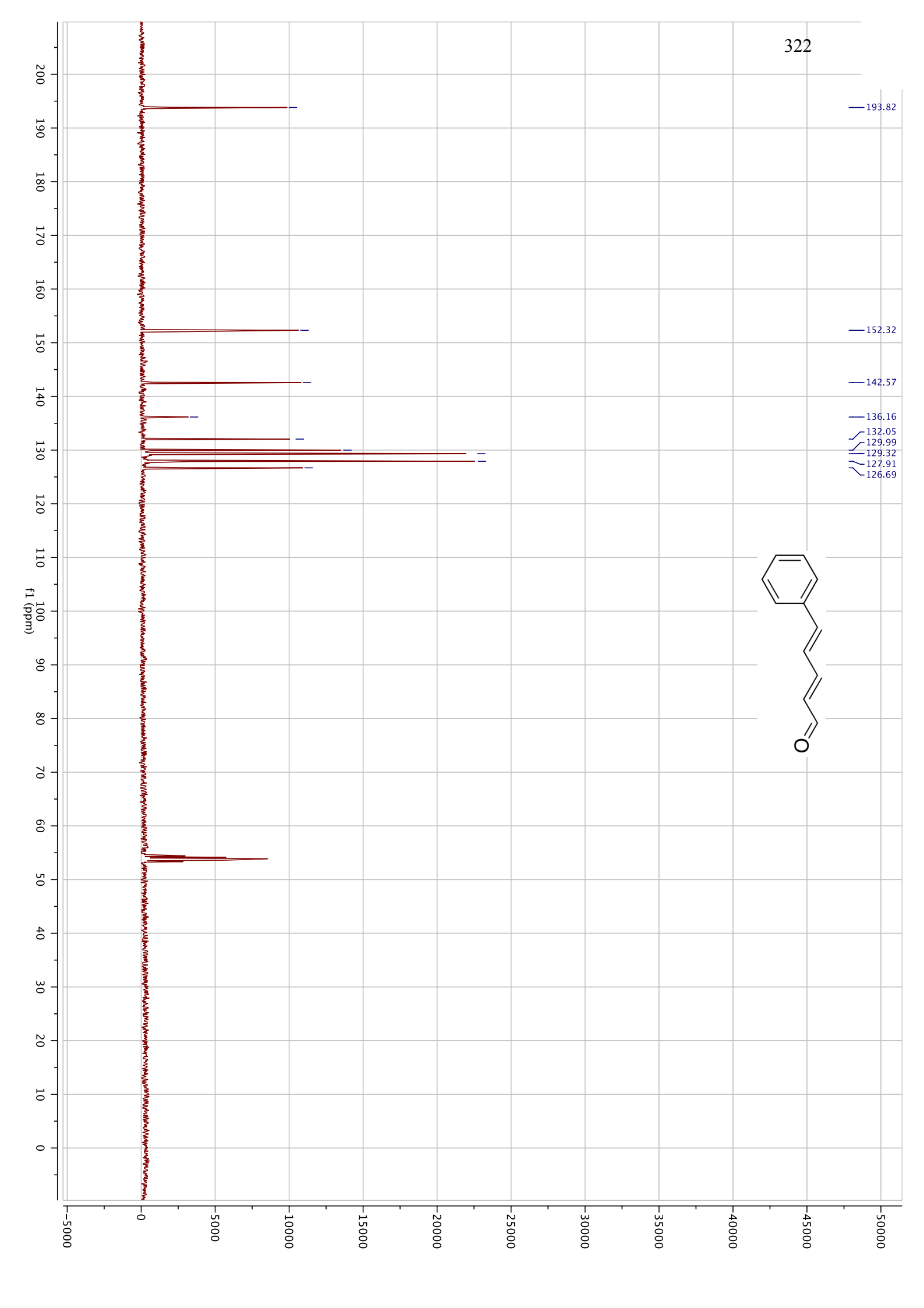

7.41
7.39
7.33
7.31
7.30
7.25
7.24
7.23
7.22
7.01
6.81
6.79
6.78
6.76
6.63
6.59
6.55
6.52
6.52
6.49
5.76
5.75
5.73
5.72
4.90
4.89
3.35
2.14
2.05
1.13
1.05
1.05
1.03
1.01
1.00
6.14
f1 (ppm)

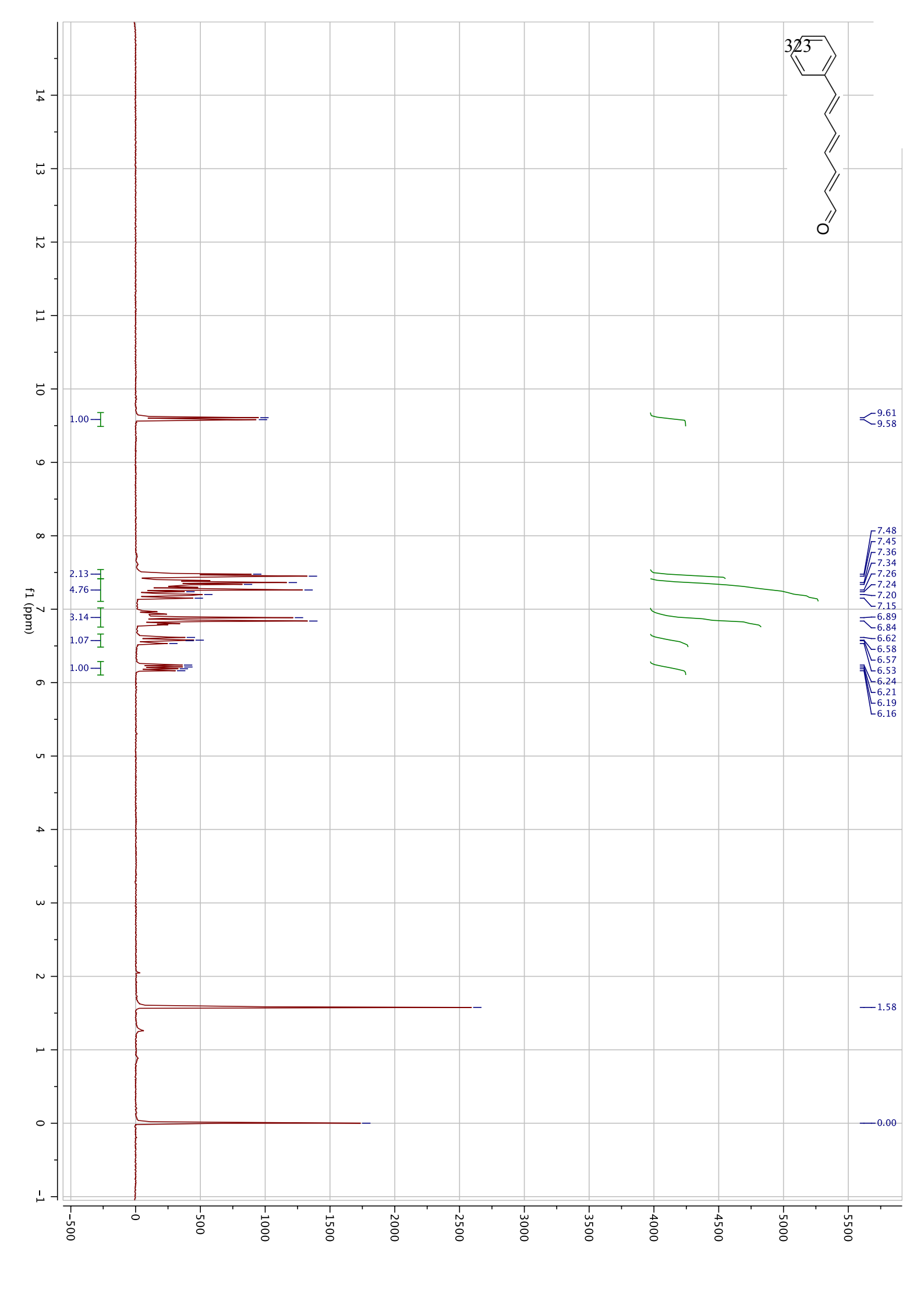

5224_CDCl3_300K
Carbon 13
318
136.96
134.18
133.86
129.45
128.64
127.84
127.72
126.53
102.57
52.65
O
O
f1 (ppm)

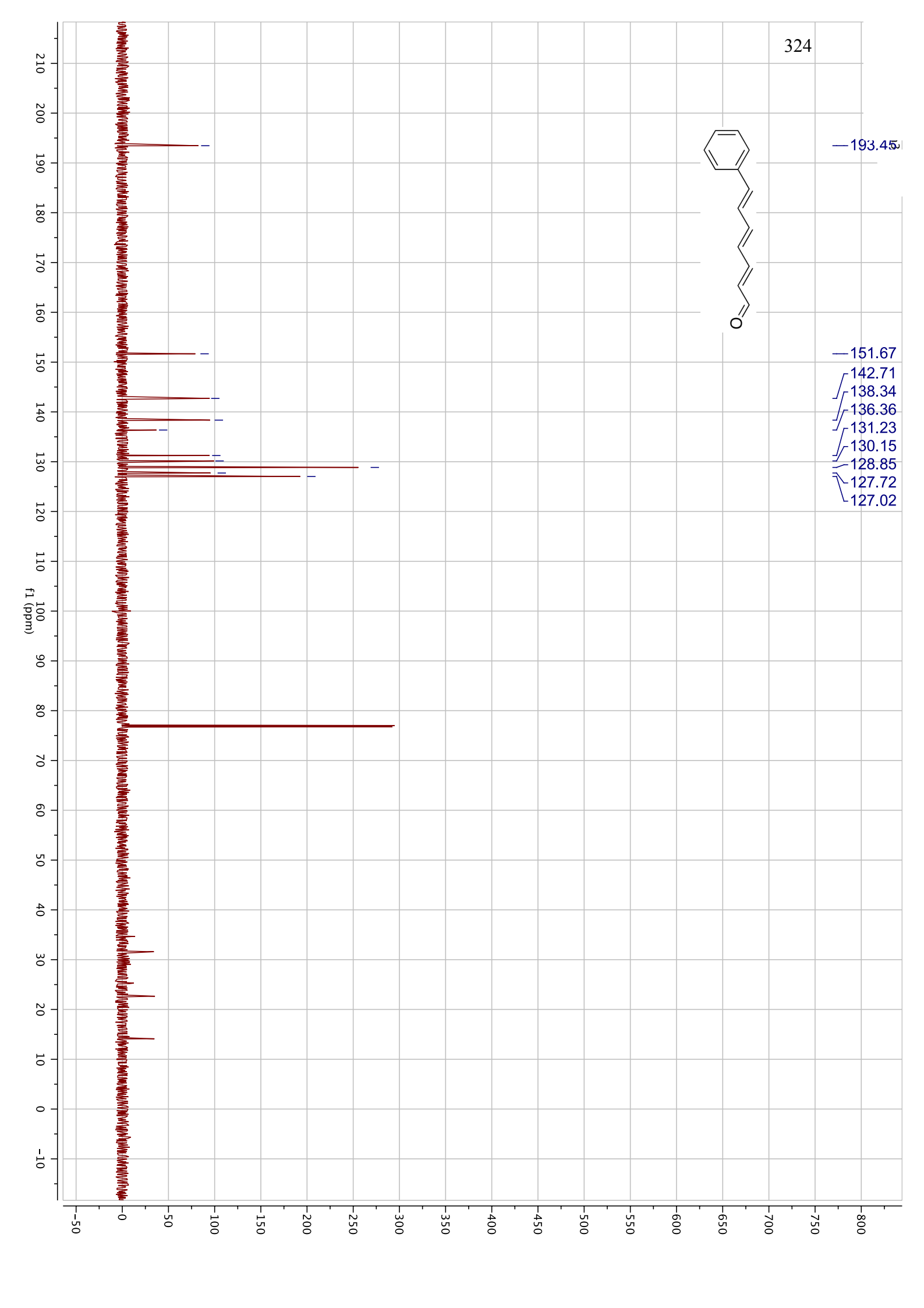

5224_CDCl3_300K
Proton
319
7.42
7.41
7.32
7.31
7.29
7.24
7.23
7.22
7.17
7.17
7.14
7.14
7.14
7.13
7.11
7.11
6.60
6.57
6.36
6.34
5.50
5.48
5.47
5.46
5.32
5.32
5.31
5.31
3.34
O
O
2.02
2.11
1.07
1.02
1.05
1.02
0.99
1.00
6.58
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

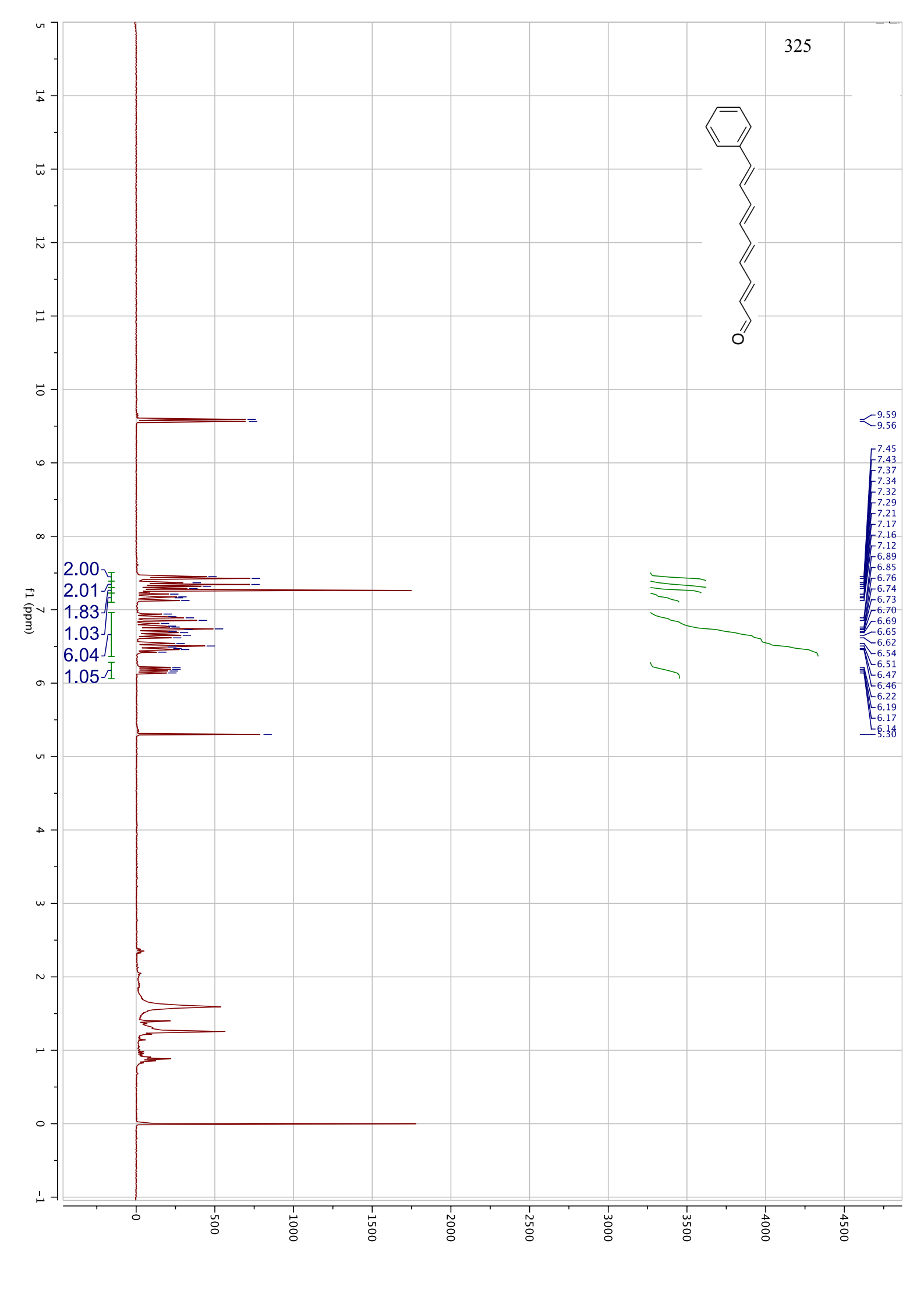

320
5224_CDCl3_300K
Carbon 13
136.95
135.46
132.87
128.66
128.06
127.41
126.77
123.90
99.78
77.37
77.11
76.86
52.18
f1 (ppm)

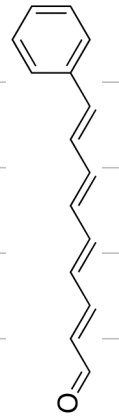

jsm2 166
proton 400Mhz
321
O
9.60
9.58
7.53
7.52
7.50
7.50
7.38
7.38
7.37
7.36
7.35
7.34
7.25
7.03
7.02
7.02
6.27
6.25
6.23
6.21
1.05
2.42
4.70
2.21
1.00
f1 (ppm)


193.82
152.32
142.57
136.16
132.05
129.99
129.32
127.91
126.69
O
f1 (ppm)


323
O
9.61
9.58
7.48
7.45
7.36
7.34
7.26
7.24
7.20
7.15
6.89
6.84
6.62
6.58
6.57
6.53
6.24
6.21
6.19
6.16
1.58
0.00
1.00
2.13
4.76
3.14
1.07
1.00
f1 (ppm)


193.45
151.67
142.71
138.34
136.36
131.23
130.15
128.85
127.72
127.02
O
f1 (ppm)

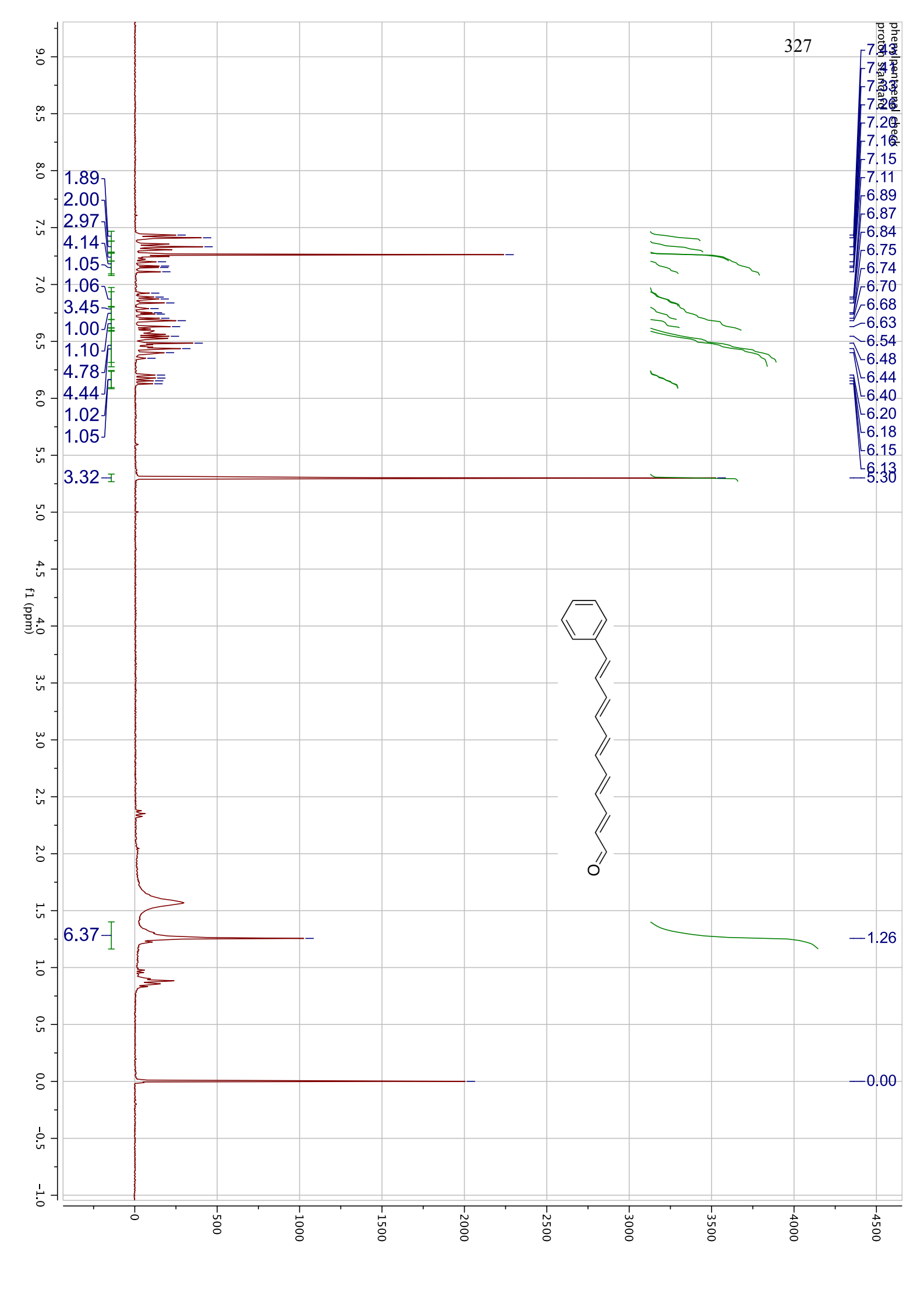

O
9.59
9.56
7.45
7.43
7.37
7.34
7.32
7.29
7.21
7.17
7.16
7.12
6.89
6.85
6.76
6.74
6.73
6.70
6.69
6.65
6.62
6.54
6.51
6.47
6.46
6.22
6.19
6.17
6.14
5.30
2.00
2.01
1.83
1.03
6.04
1.05
f1 (ppm)

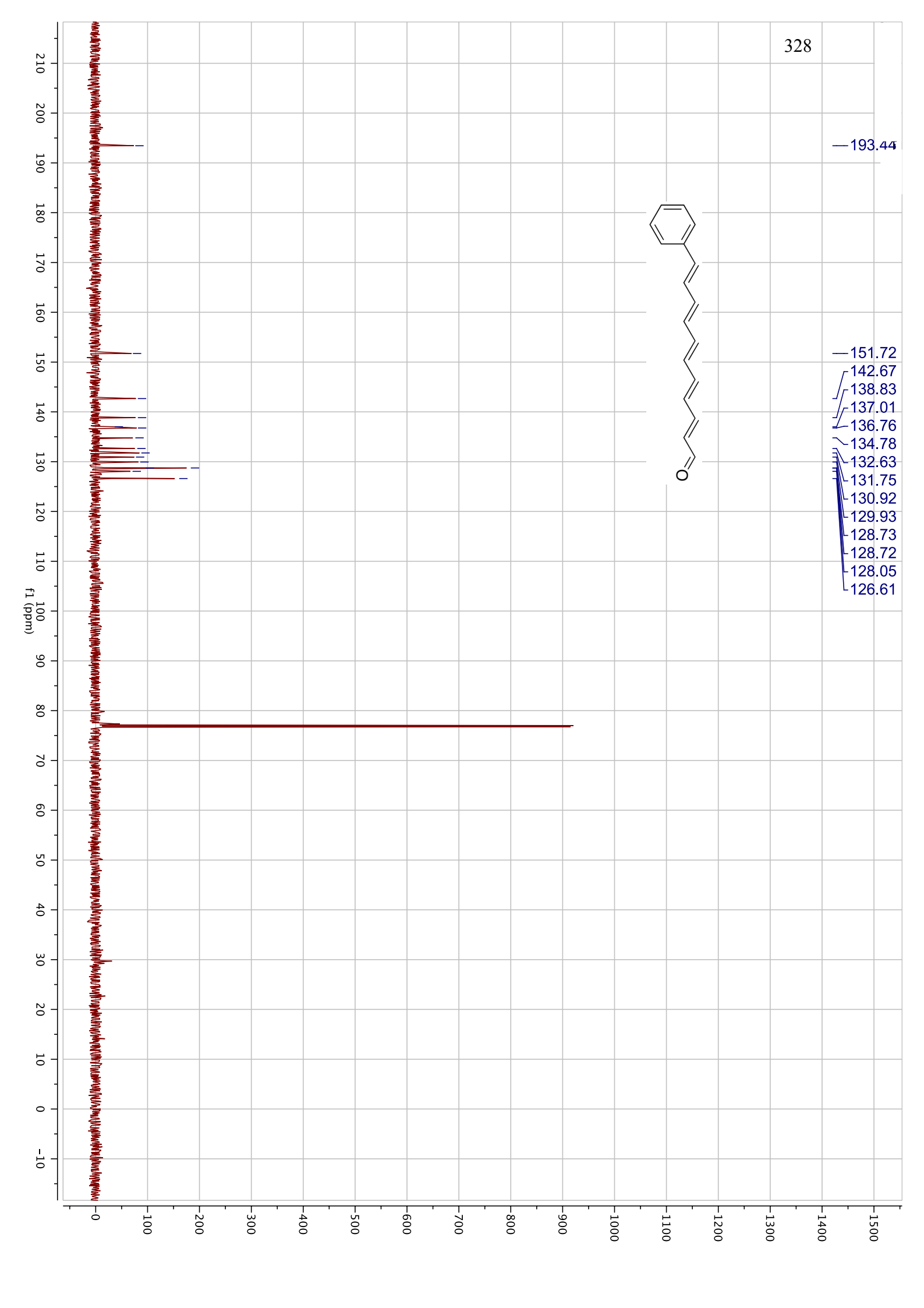


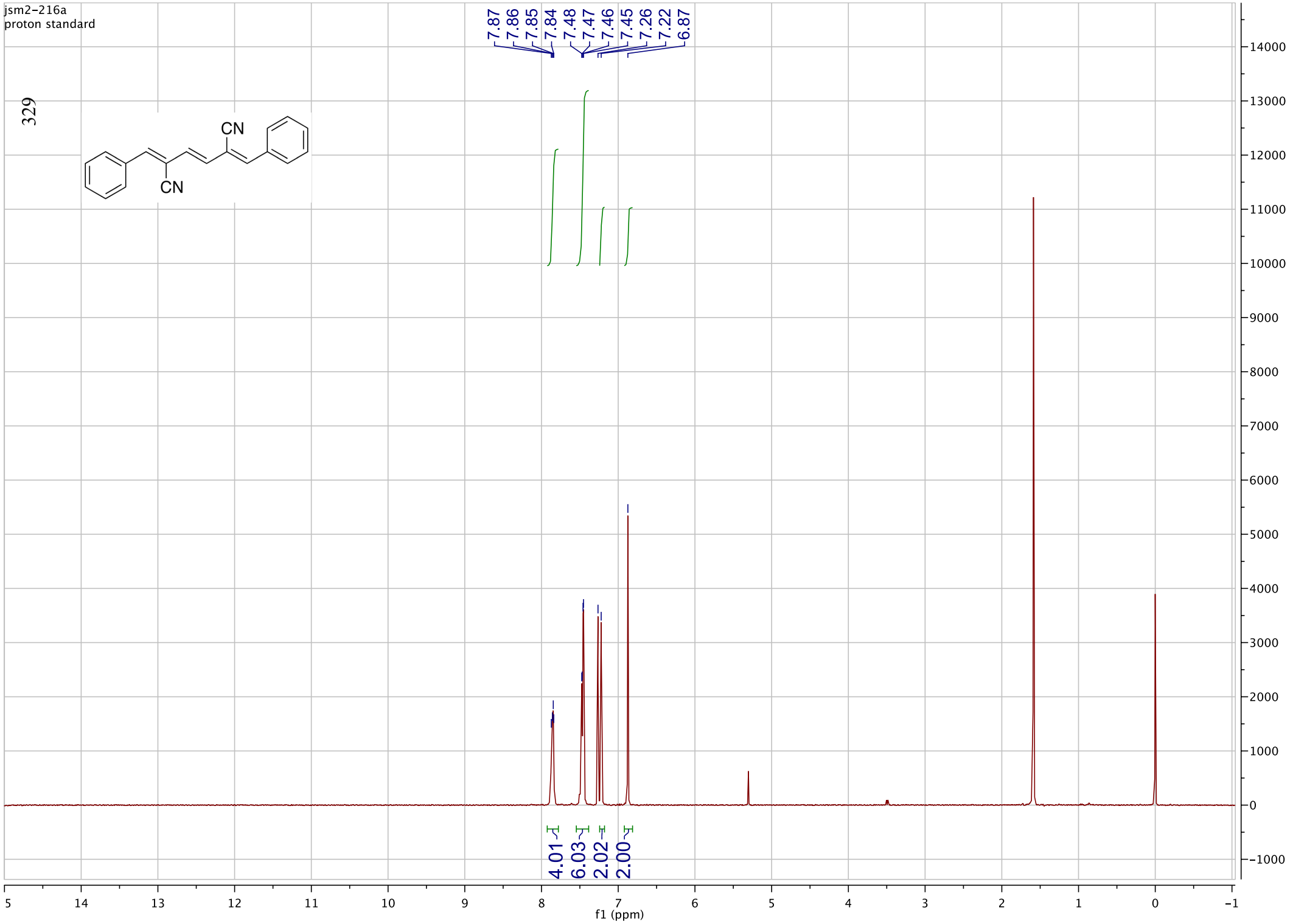
193.45

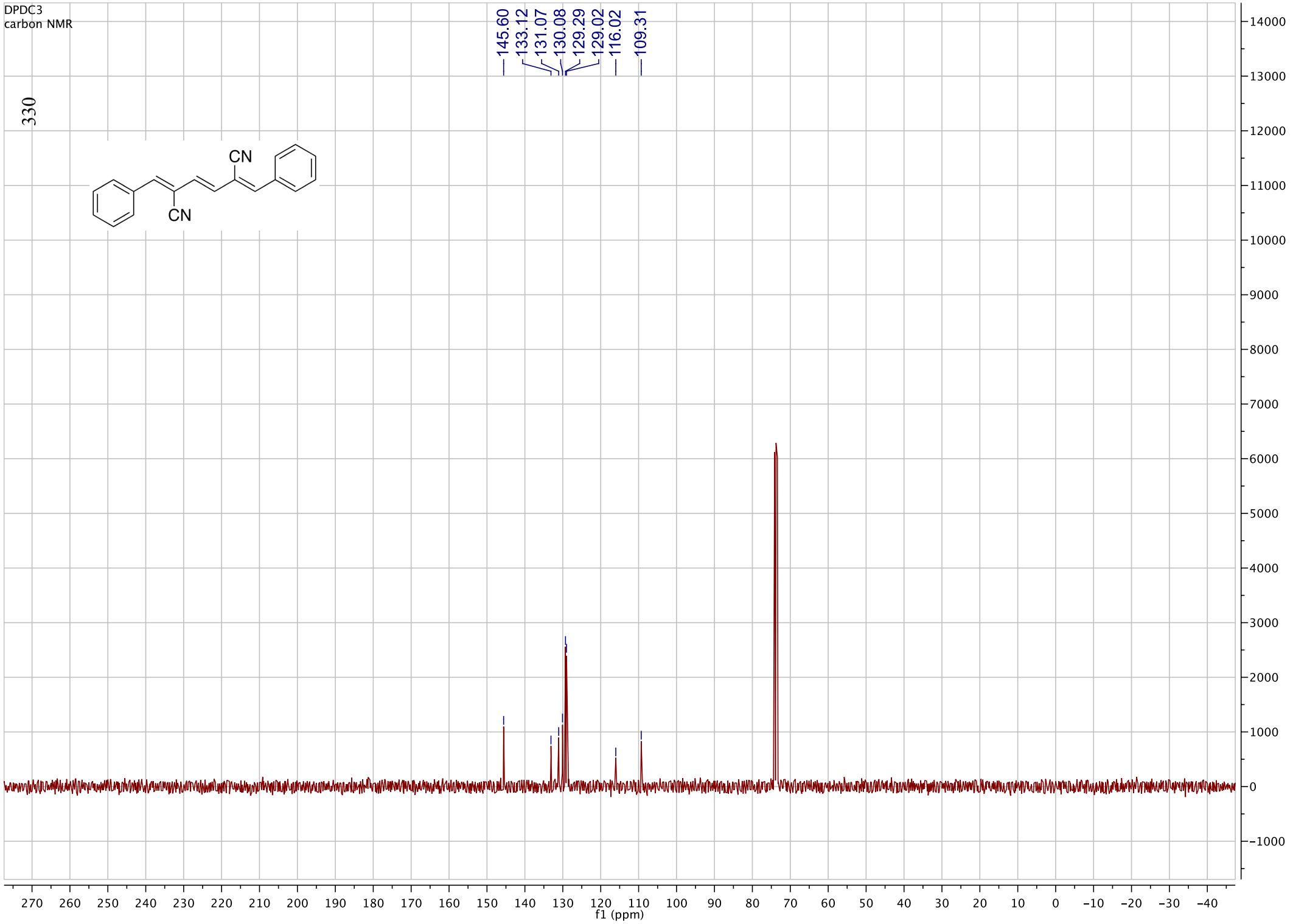
151.72
142.61
138.93
136.76
136.06
131.86
131.02
129.98
128.78
128.37
128.35
126.77

f1 (ppm)

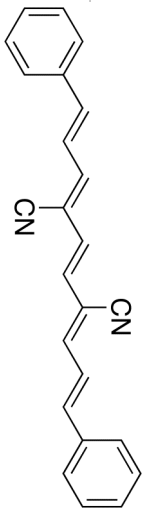

phenylpentenal deck
proton standard
7.26
7.16
7.15
7.11
6.89
6.87
6.84
6.75
6.74
6.70
6.68
6.63
6.54
6.48
6.44
6.40
6.20
6.18
6.15
6.13
5.30
1.89
2.00
2.97
4.14
1.05
1.06
3.45
1.00
1.10
4.78
4.44
1.02
1.05
3.32
6.37
1.26
0.00
O
f1 (ppm)


193.44
151.72
142.67
138.83
137.01
136.76
134.78
132.63
131.75
130.92
129.93
128.73
128.72
128.05
126.61
O
f1 (ppm)


jsm2-216a
proton standard
329
CN
CN
7.87
7.86
7.85
7.84
7.48
7.47
7.46
7.45
7.26
7.22
6.87
4.01
6.03
2.02
2.00
f1 (ppm)


DPDC3
carbon NMR
330
145.60
133.12
131.07
130.08
129.29
129.02
116.02
109.31
CN
CN
f1 (ppm)

jsm2-205
proton standard



4.00
7.64
4.01
1.69

7.53
7.38
7.36
7.06
7.02
6.71

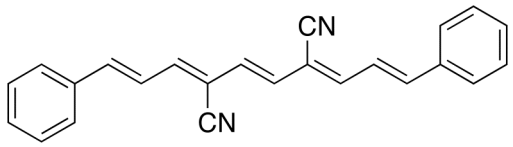
5.30
5.30
5.30

1.53

f1 (ppm)

DPDC5
carbon NMR

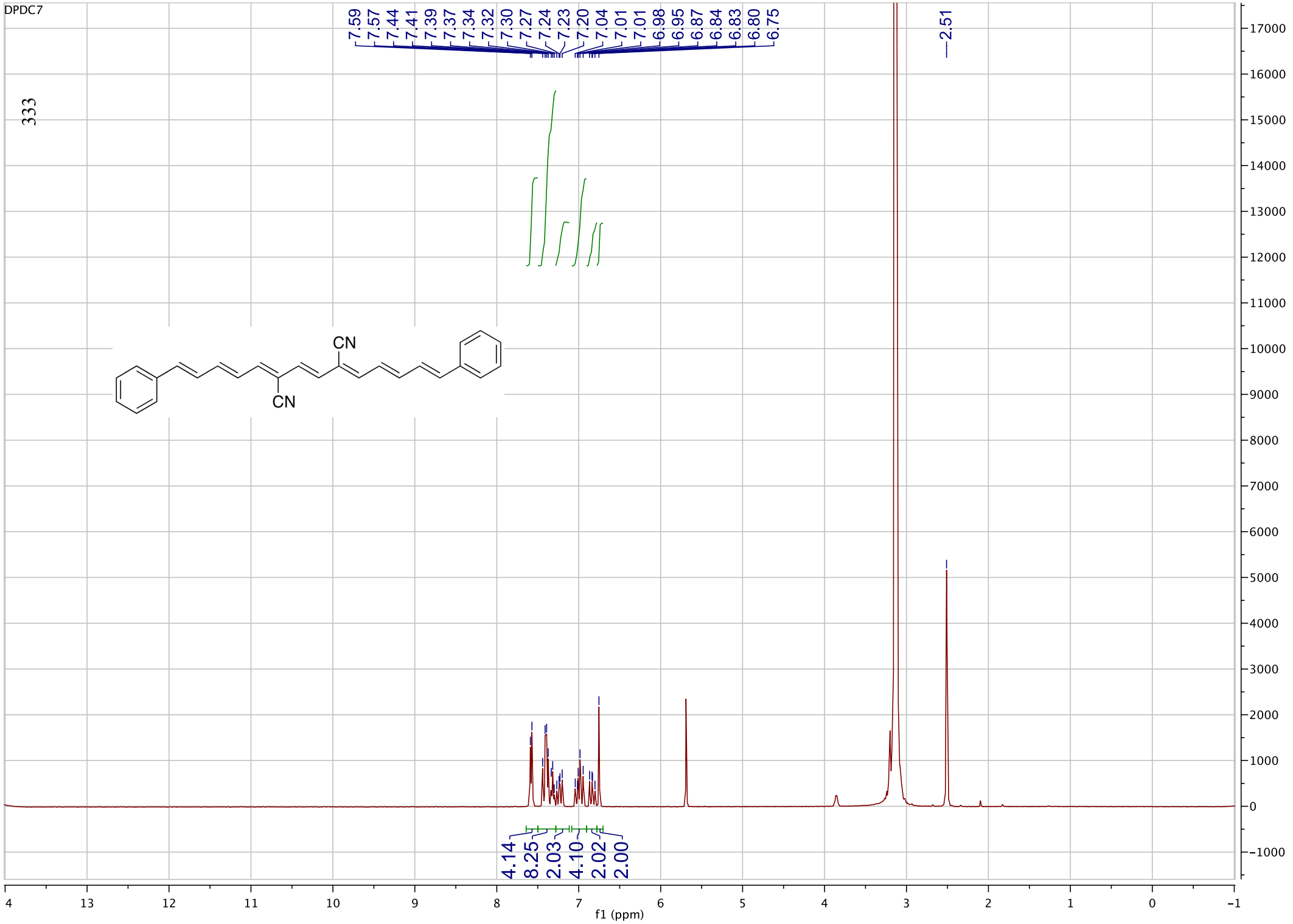
332



145.04
141.98
135.63
129.69
128.99
128.82
127.54
124.71
114.84
111.85

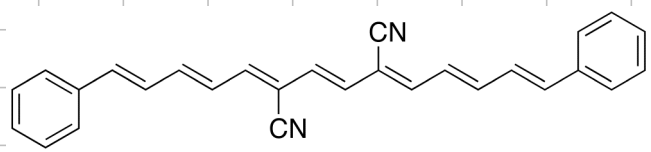
30000
25000
20000
15000
10000
5000
0

270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30 −40
f1 (ppm)


DPDC7
333
7.59
7.57
7.44
7.41
7.39
7.37
7.34
7.32
7.30
7.27
7.24
7.23
7.20
7.04
7.01
7.01
6.98
6.95
6.87
6.84
6.83
6.80
6.75
2.51
CN
CN
4.14
8.25
2.03
4.10
2.02
2.00
f1 (ppm)

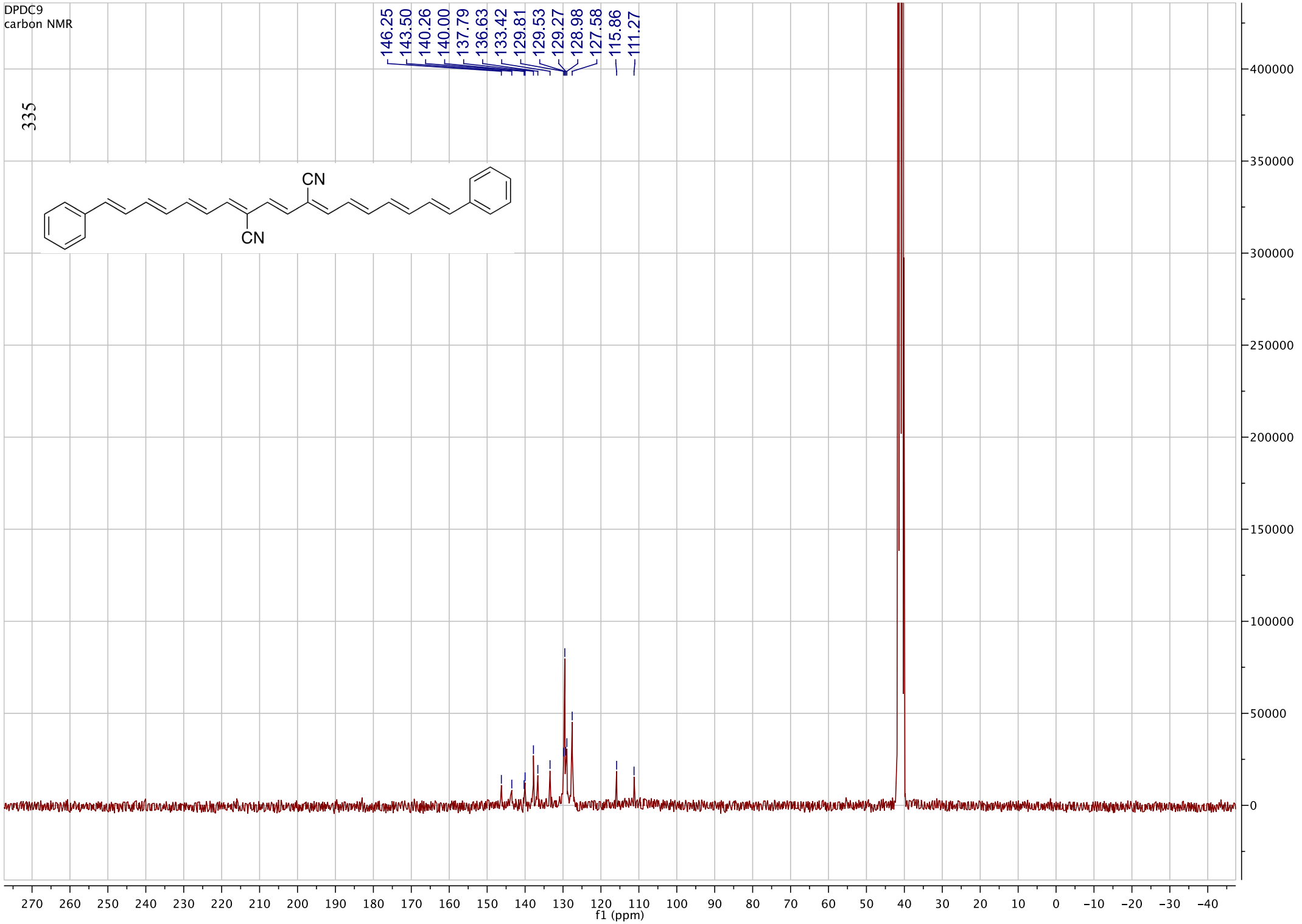
DPDC7
carbon 13

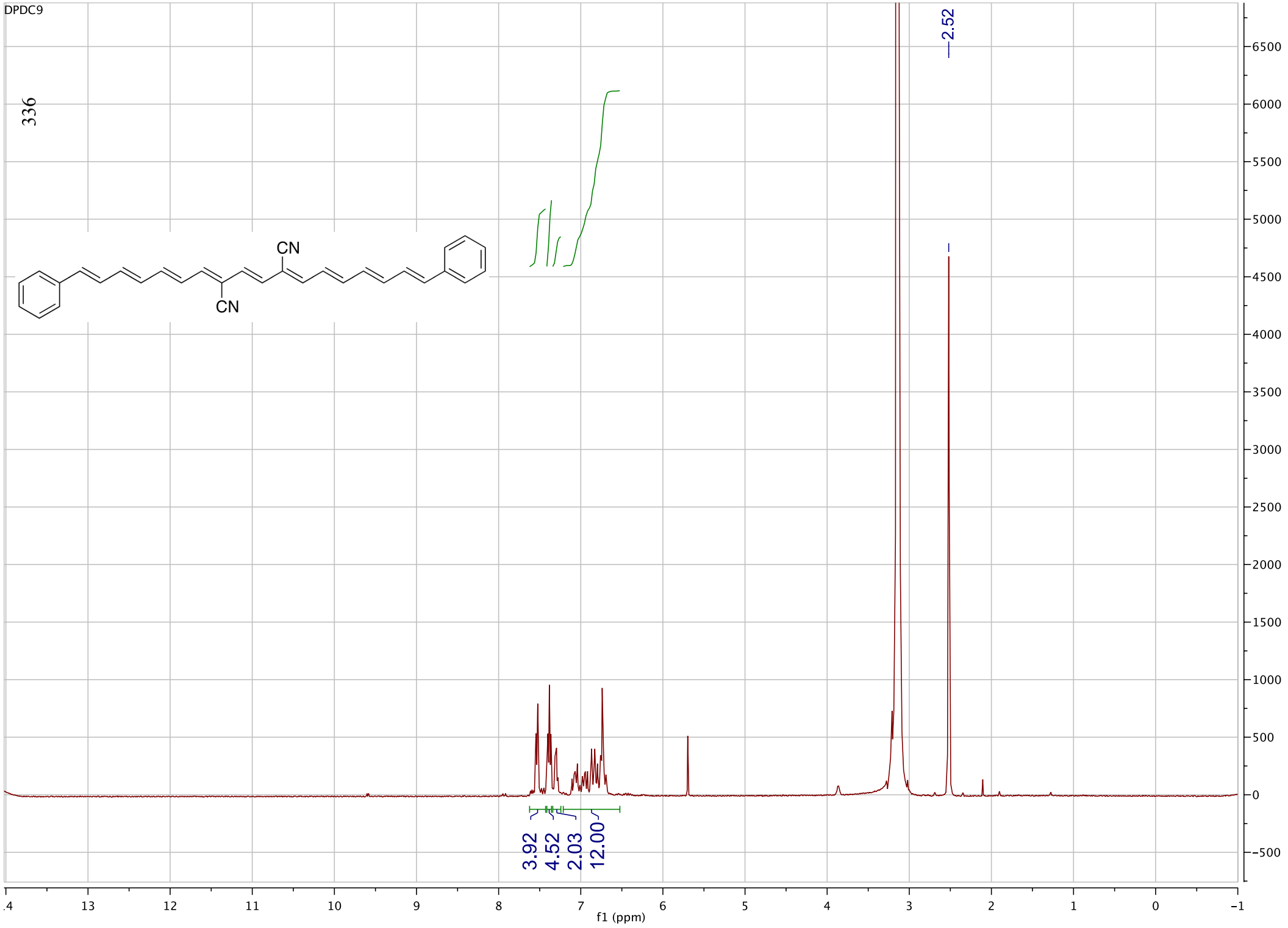
334

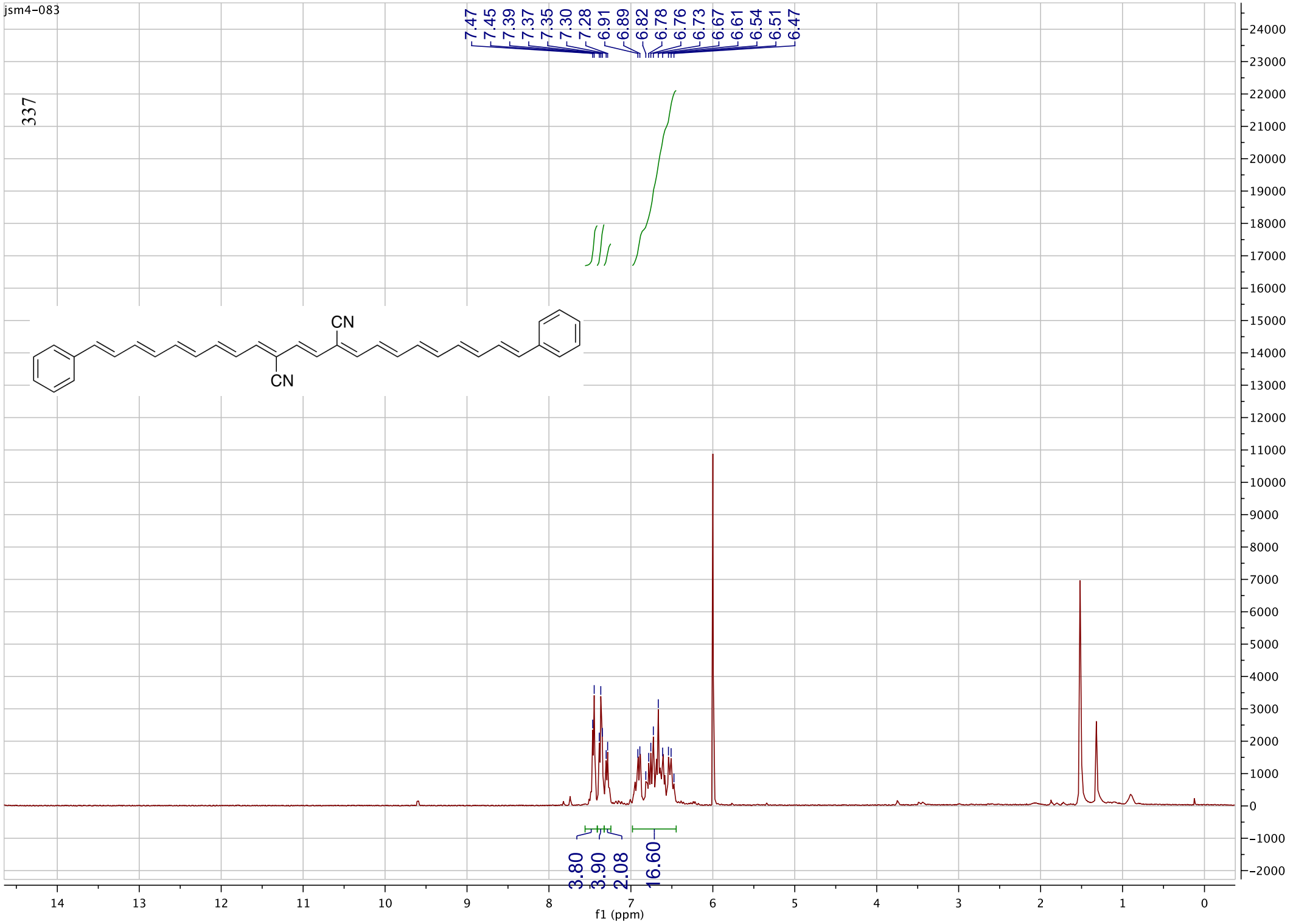


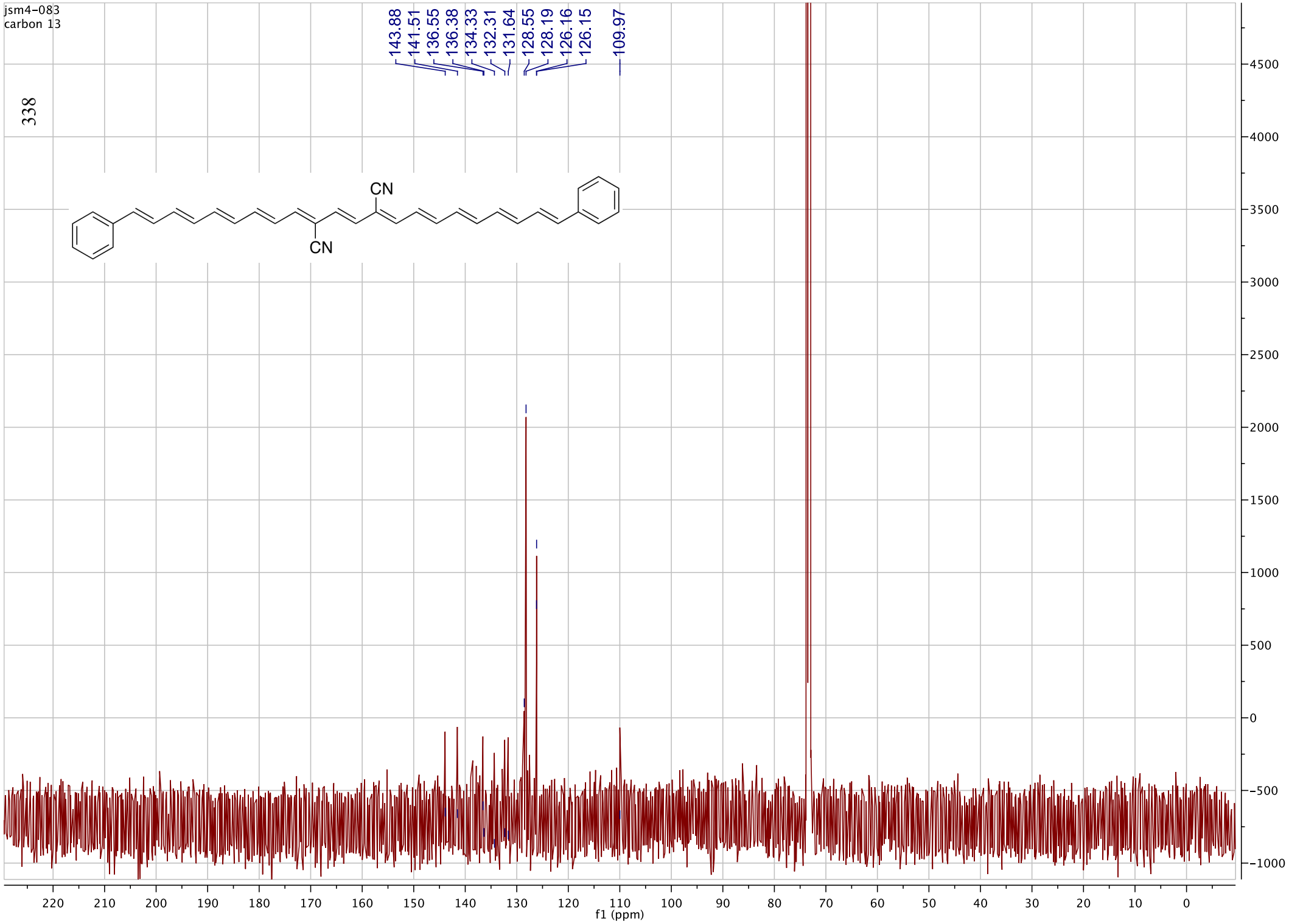
146.20
143.43
138.75
137.05
129.21
129.19
129.14
129.11
127.57
115.48
111.02

f1 (ppm)


DPDC9
carbon NMR
335
146.25
143.50
140.26
140.00
137.79
136.63
133.42
129.81
129.53
129.27
128.98
127.58
115.86
111.27
CN
CN
400000
350000
300000
250000
200000
150000
100000
50000
0
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20 −30 −40
f1 (ppm)

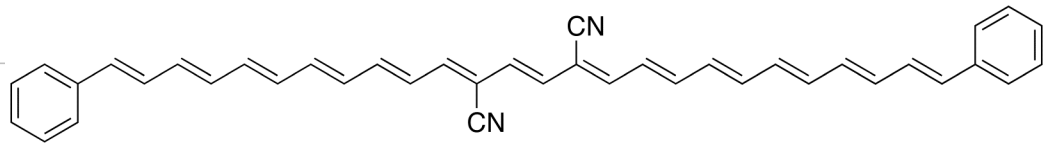

DPDC9
336
CN
CN
2.52
3.92
4.52
2.03
12.00
f1 (ppm)


jsm4-083
337
7.47
7.45
7.39
7.37
7.35
7.30
7.28
6.91
6.89
6.82
6.78
6.76
6.73
6.67
6.61
6.54
6.51
6.47
CN
CN
3.80
3.90
2.08
16.60
f1 (ppm)

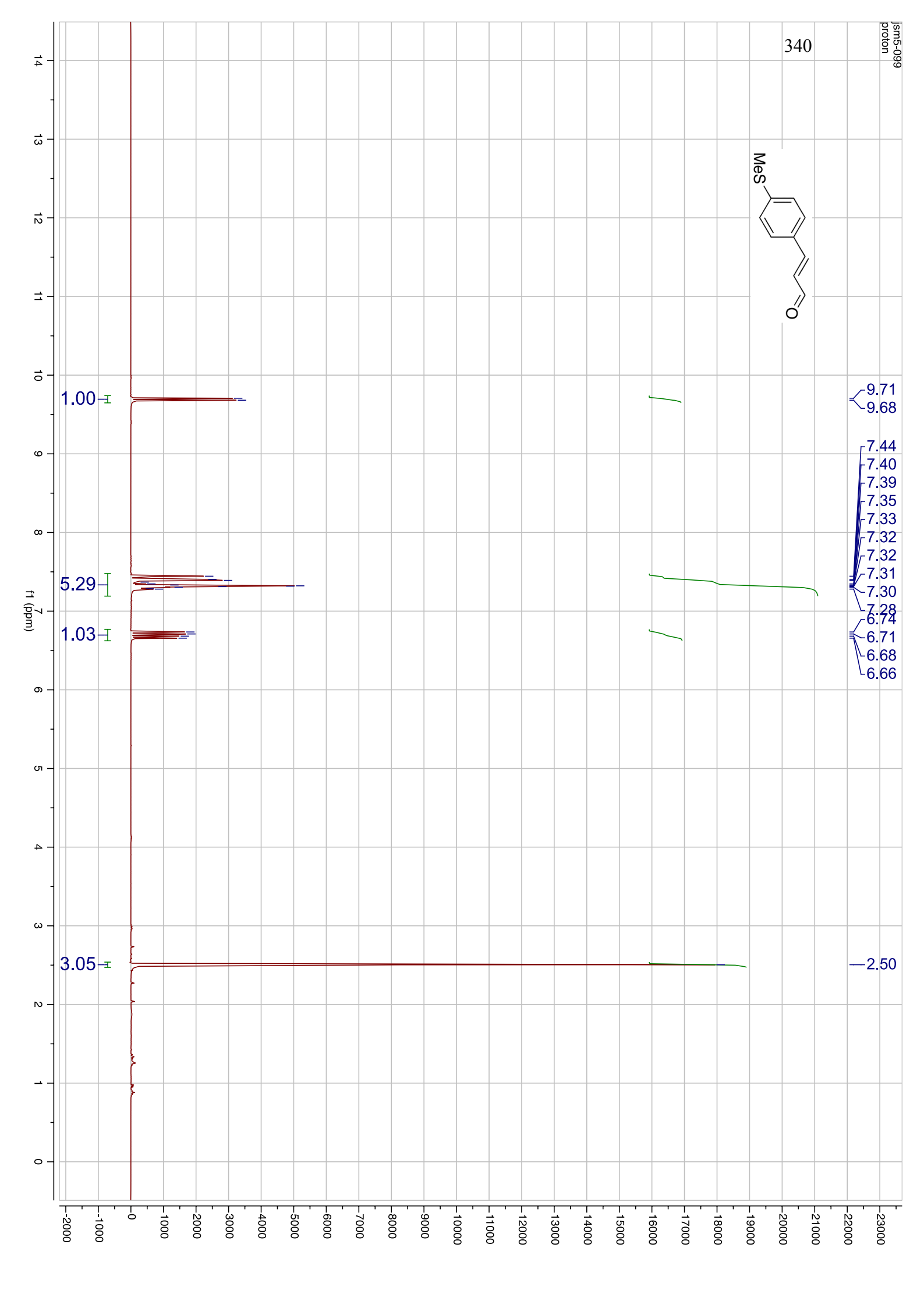

jsm4-083
carbon 13
338
143.88
141.51
136.55
136.38
134.33
132.31
131.64
128.55
128.19
126.16
126.15
109.97
CN
CN
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

jsm2-243
proton standard

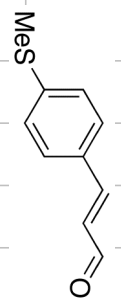
339



f1 (ppm)

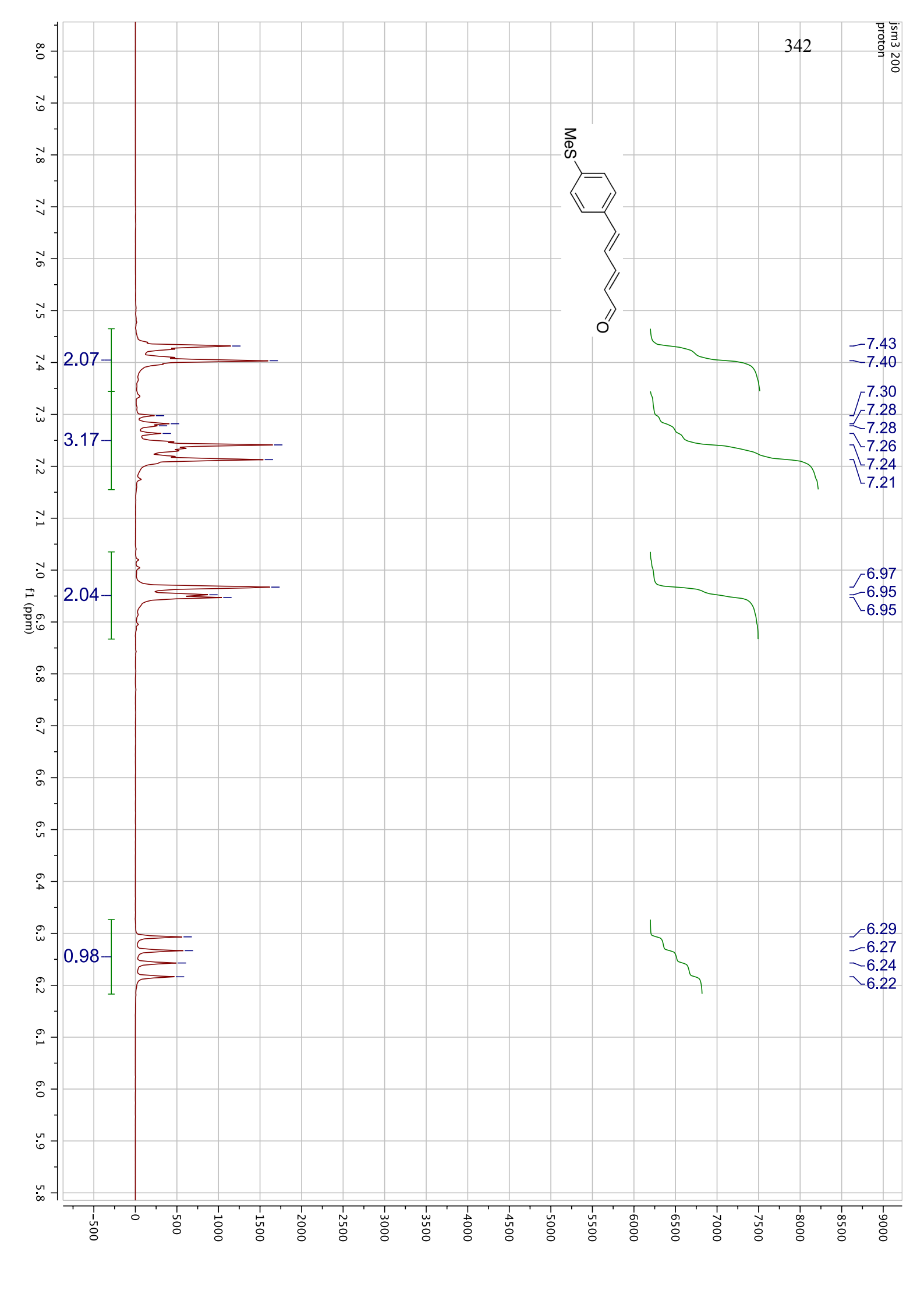

340
jsm5-099
proton
MeS
O
1.00
5.29
1.03
3.05
9.71
9.68
7.44
7.40
7.39
7.35
7.33
7.32
7.32
7.31
7.30
7.28
6.74
6.71
6.68
6.66
2.50
f1 (ppm)

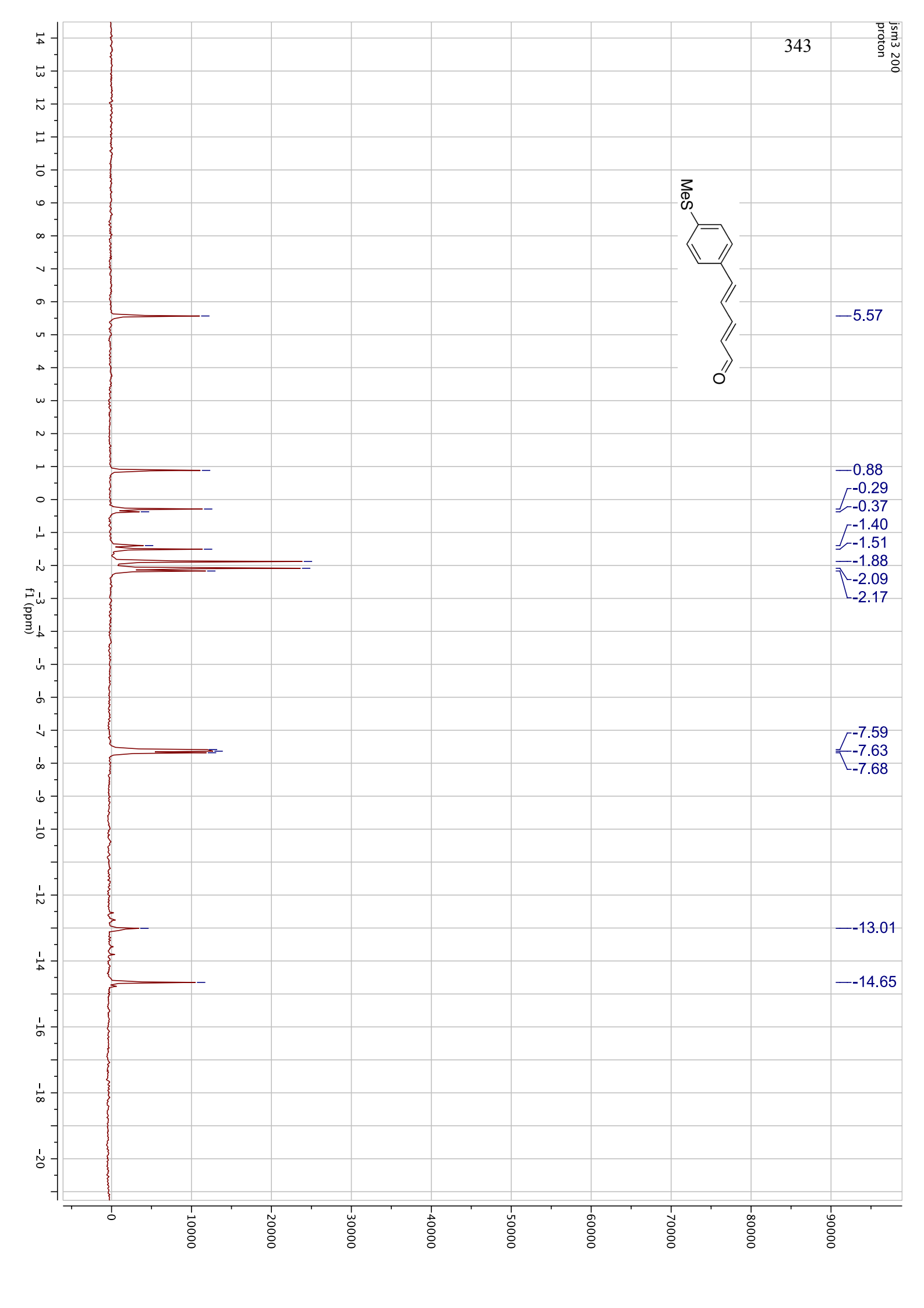
jsm5-099
carbon NMR

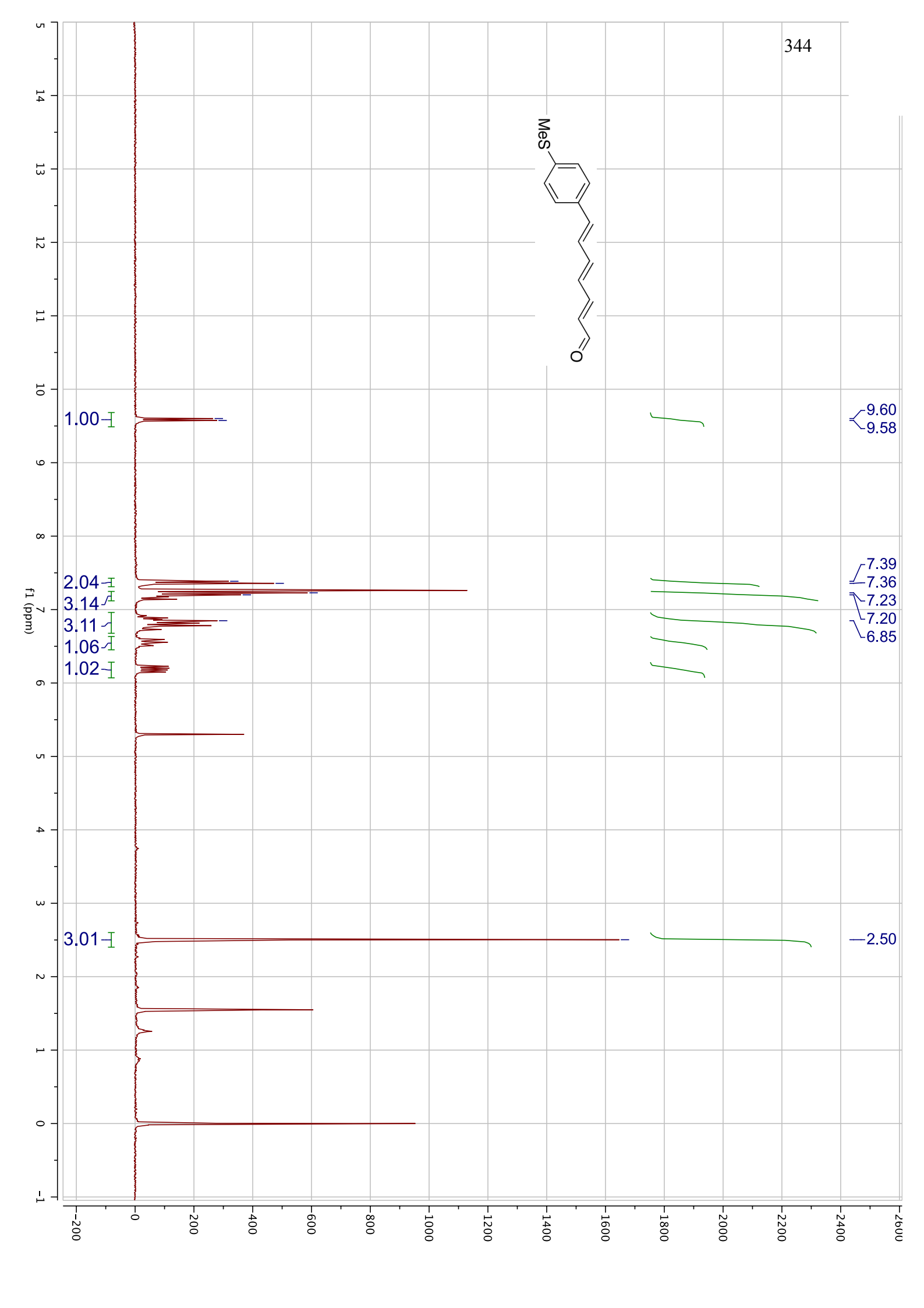


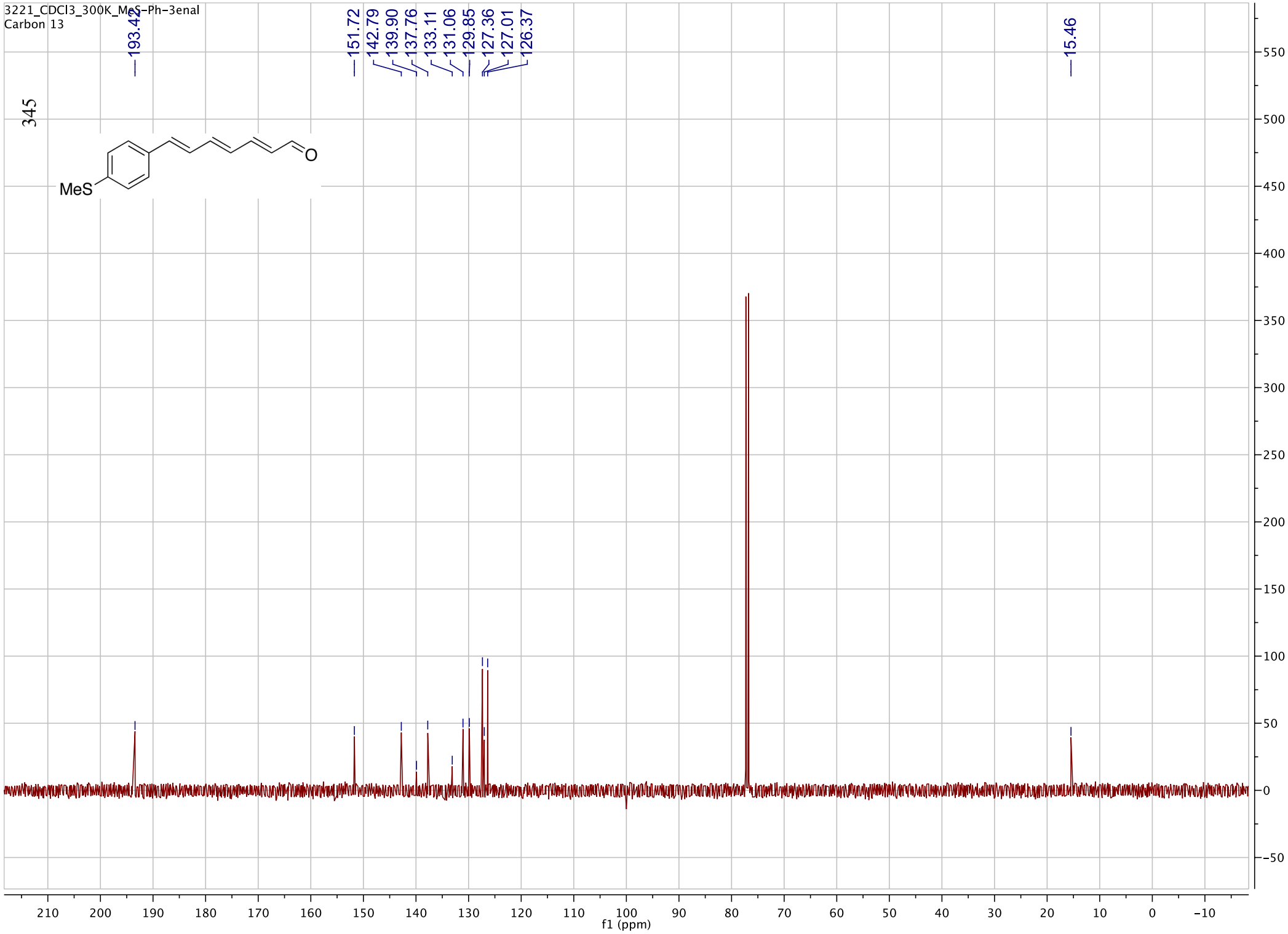
193.86
152.42
140.39
135.04
129.82
129.43
129.37
126.44
125.38
16.00

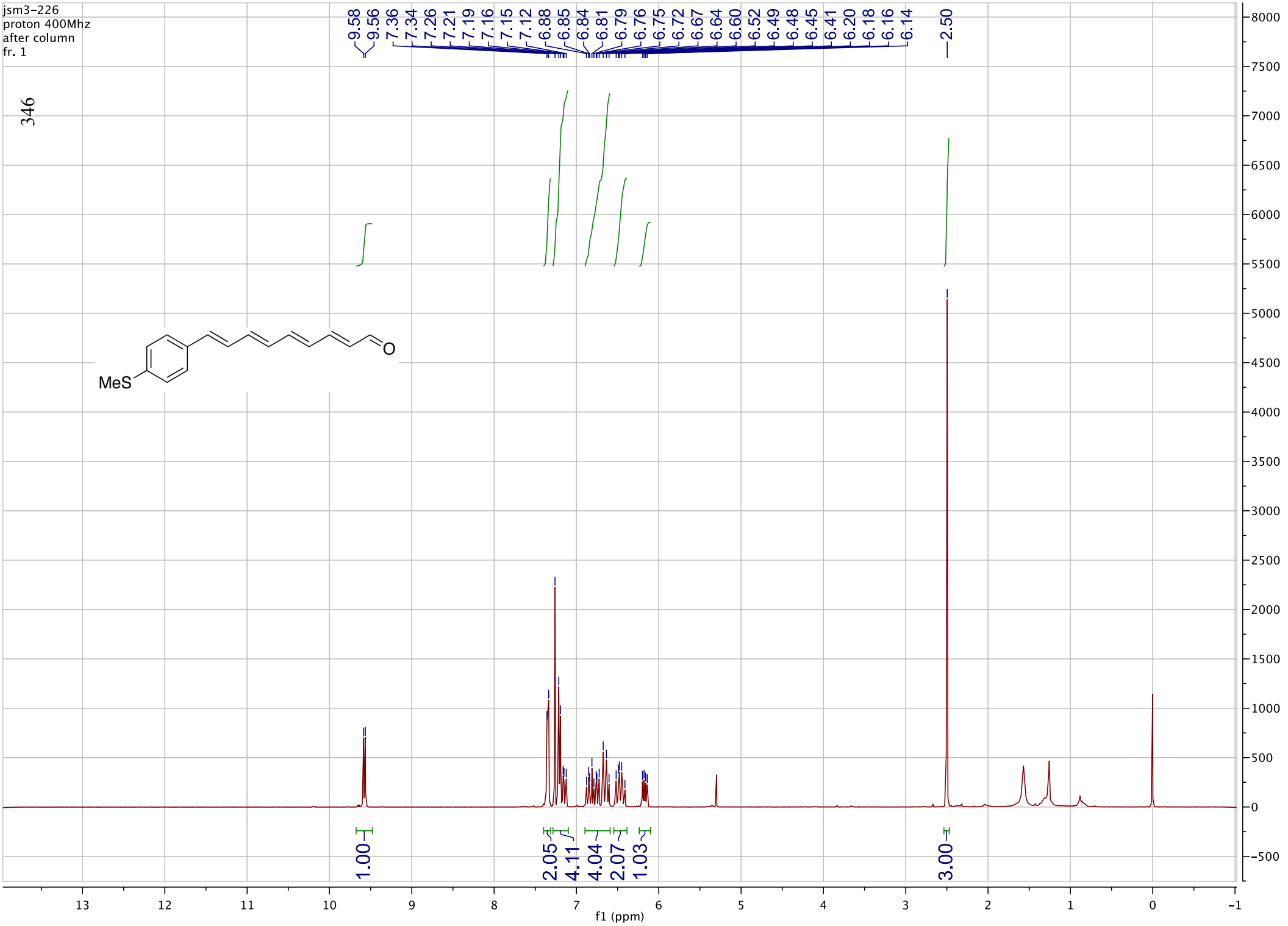
f1 (ppm)

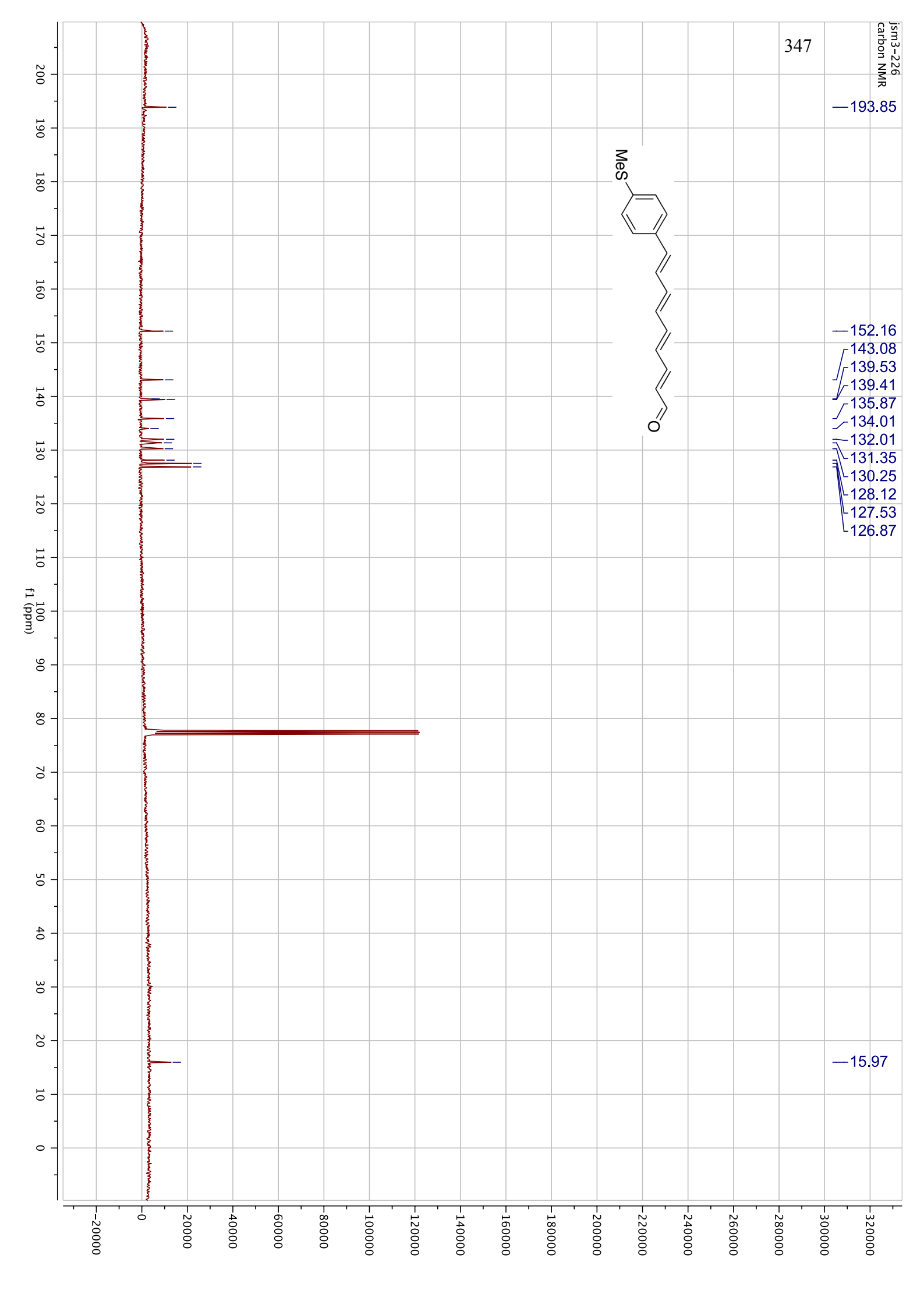

jsm3 200
proton
MeS
O
7.43
7.40
7.30
7.28
7.28
7.26
7.24
7.21
6.97
6.95
6.95
6.29
6.27
6.24
6.22
2.07
3.17
2.04
0.98
f1 (ppm)

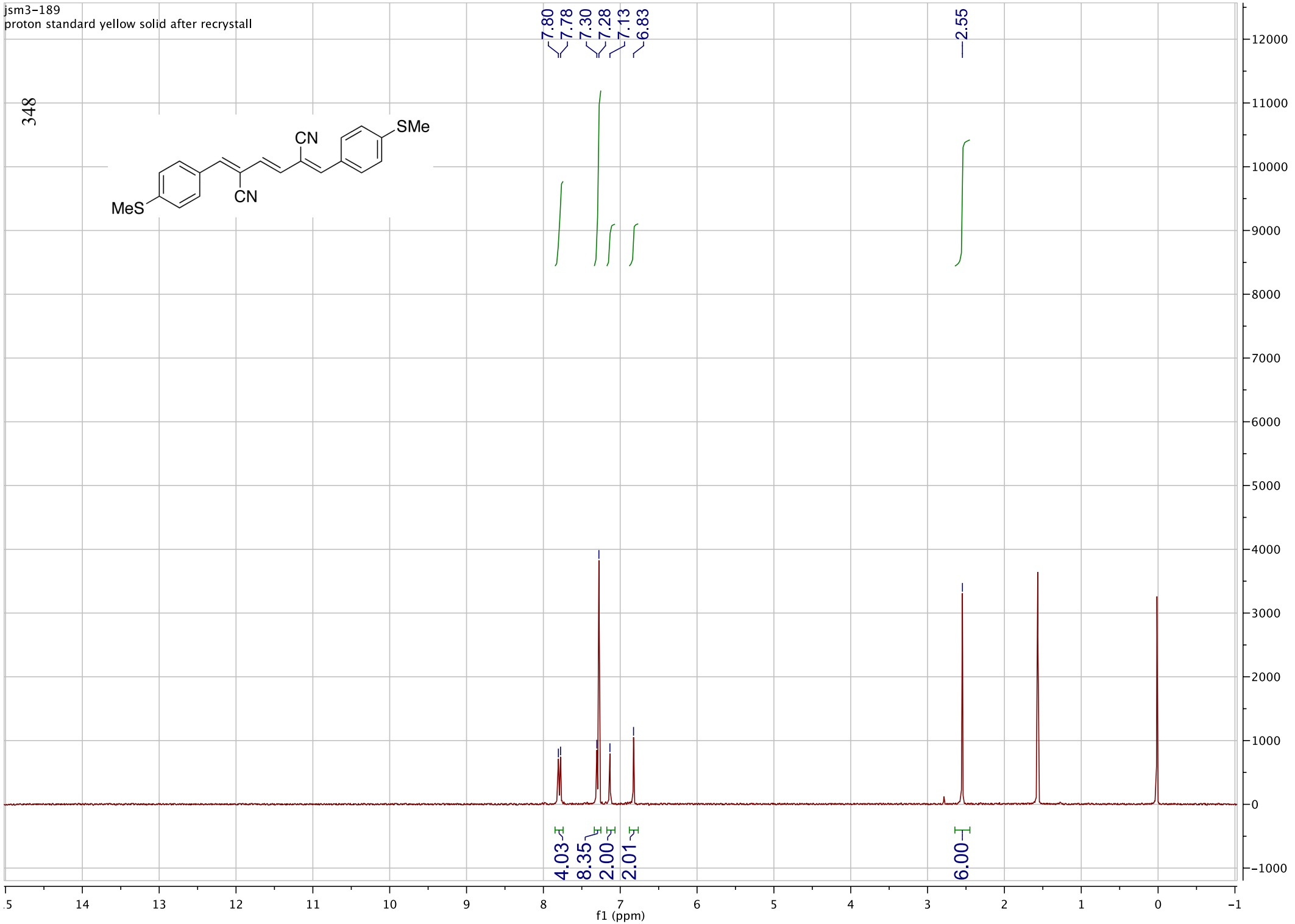

jsm3 200
proton
MeS
O
5.57
0.88
0.29
0.37
1.40
1.51
1.88
2.09
2.17
7.59
7.63
7.68
13.01
14.65
f1 (ppm)

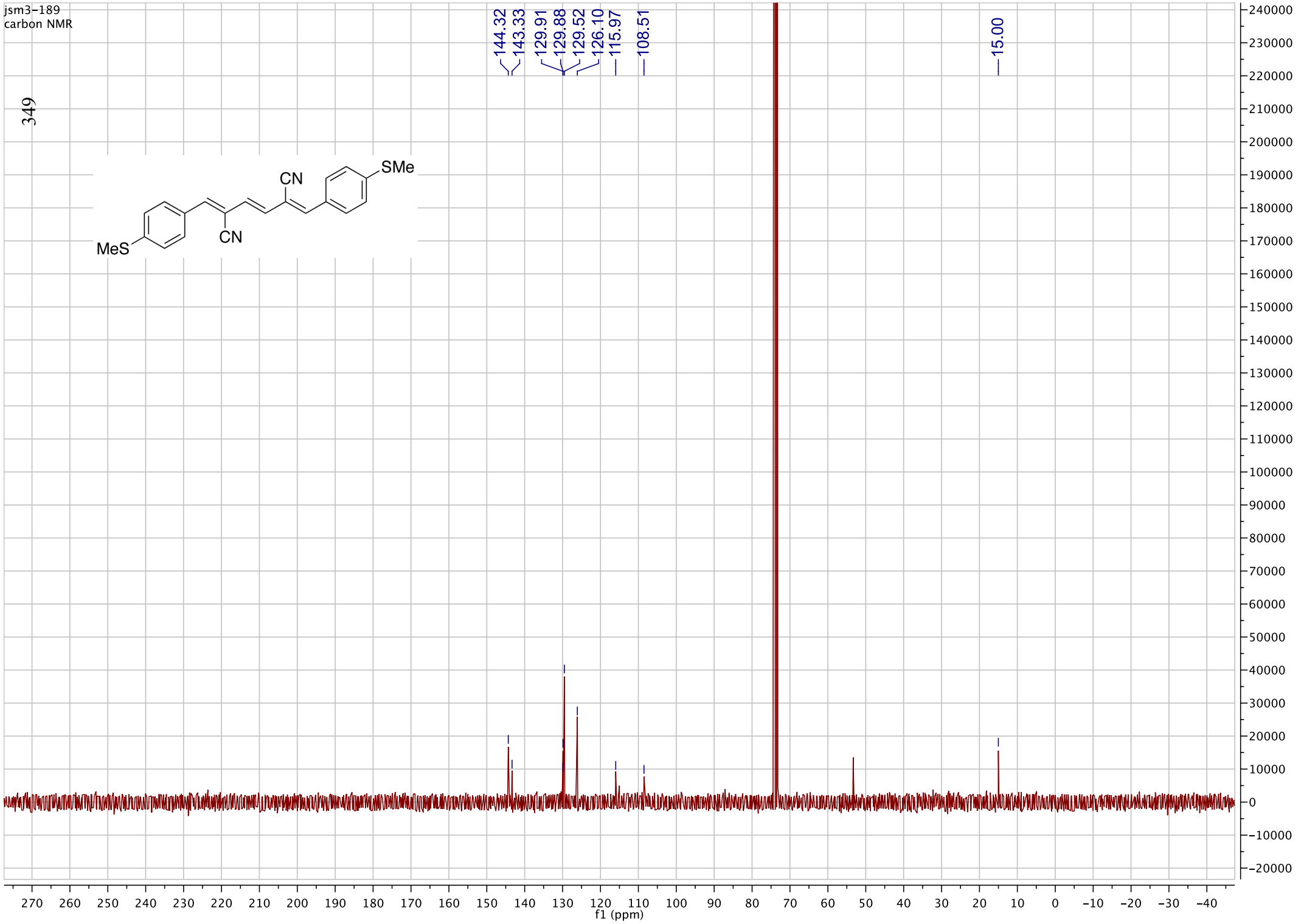

MeS
O
1.00
2.04
3.14
3.11
1.06
1.02
3.01
9.60
9.58
7.39
7.36
7.23
7.20
6.85
2.50
f1 (ppm)

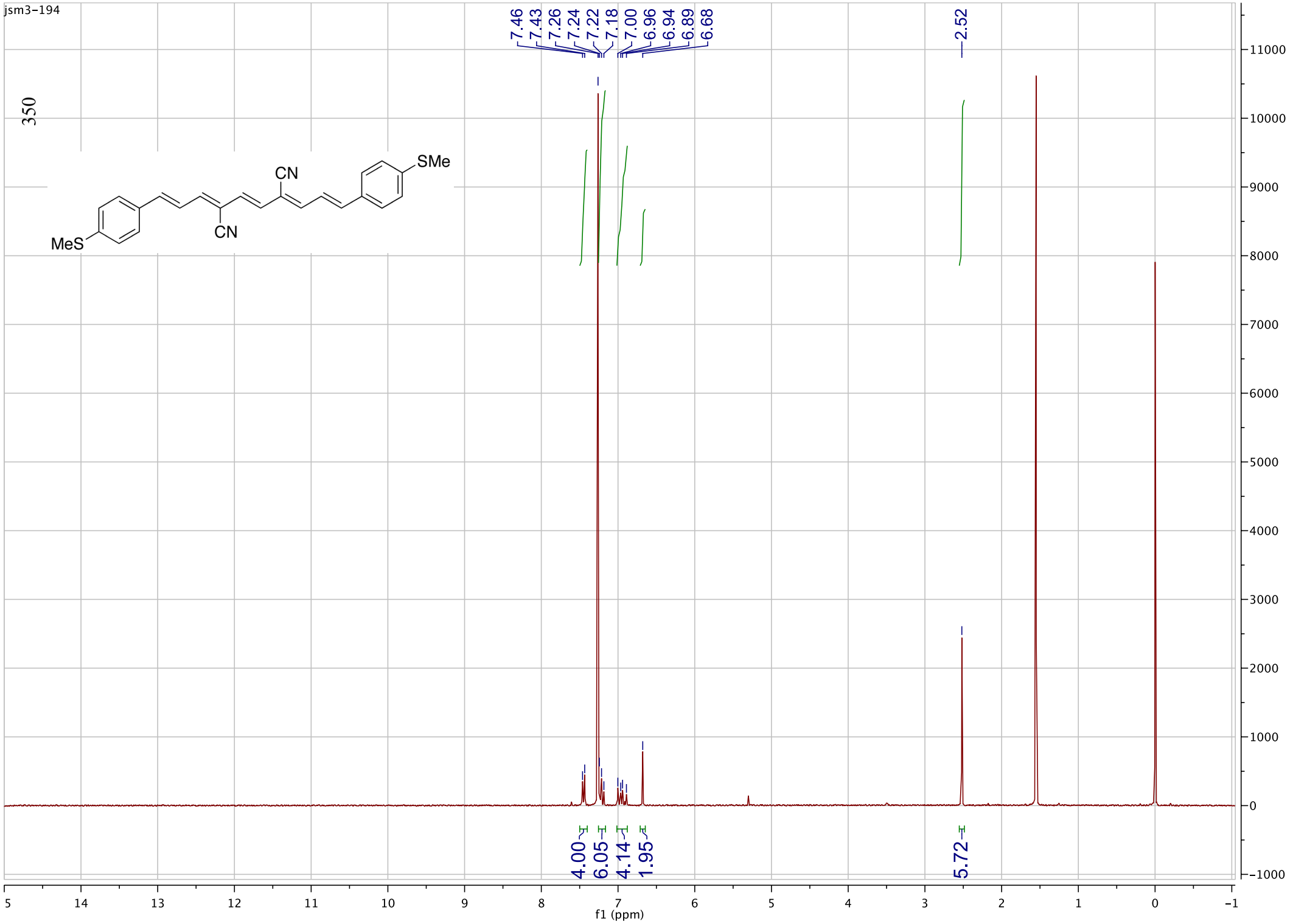

3221_CDCl3_300K_MeS-Ph-3enal
Carbon 13
193.42
151.72
142.79
139.90
137.76
133.11
131.06
129.85
127.36
127.01
126.37
15.46
345
MeS
O
f1 (ppm)

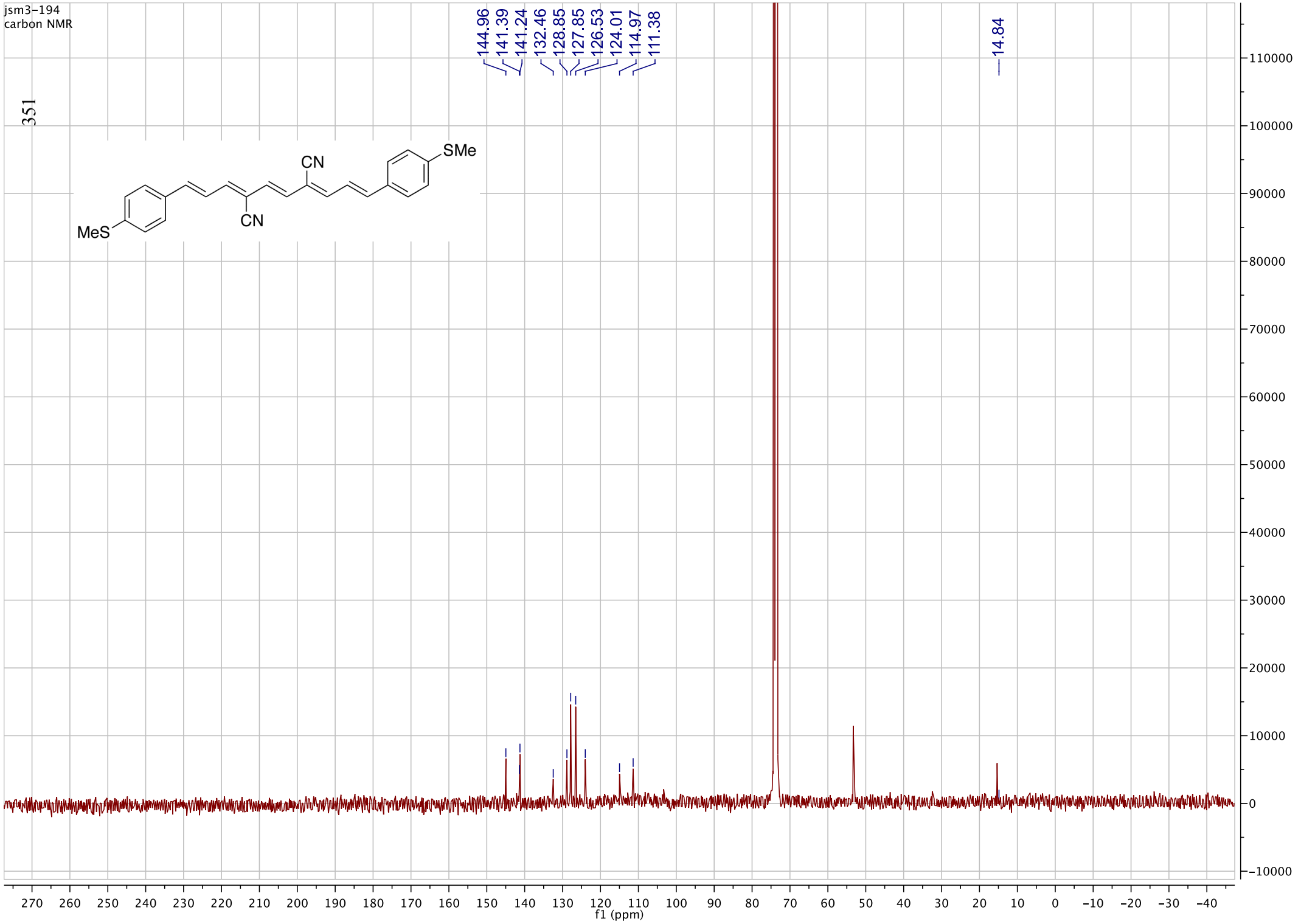

jsm3-226
proton 400Mhz
after column
fr. 1
346
9.58
9.56
7.36
7.34
7.26
7.21
7.19
7.16
7.15
7.12
6.88
6.85
6.84
6.81
6.79
6.76
6.75
6.72
6.67
6.64
6.60
6.52
6.49
6.48
6.45
6.41
6.20
6.18
6.16
6.14
2.50
MeS
O
1.00
2.05
4.11
4.04
2.07
1.03
3.00
f1 (ppm)

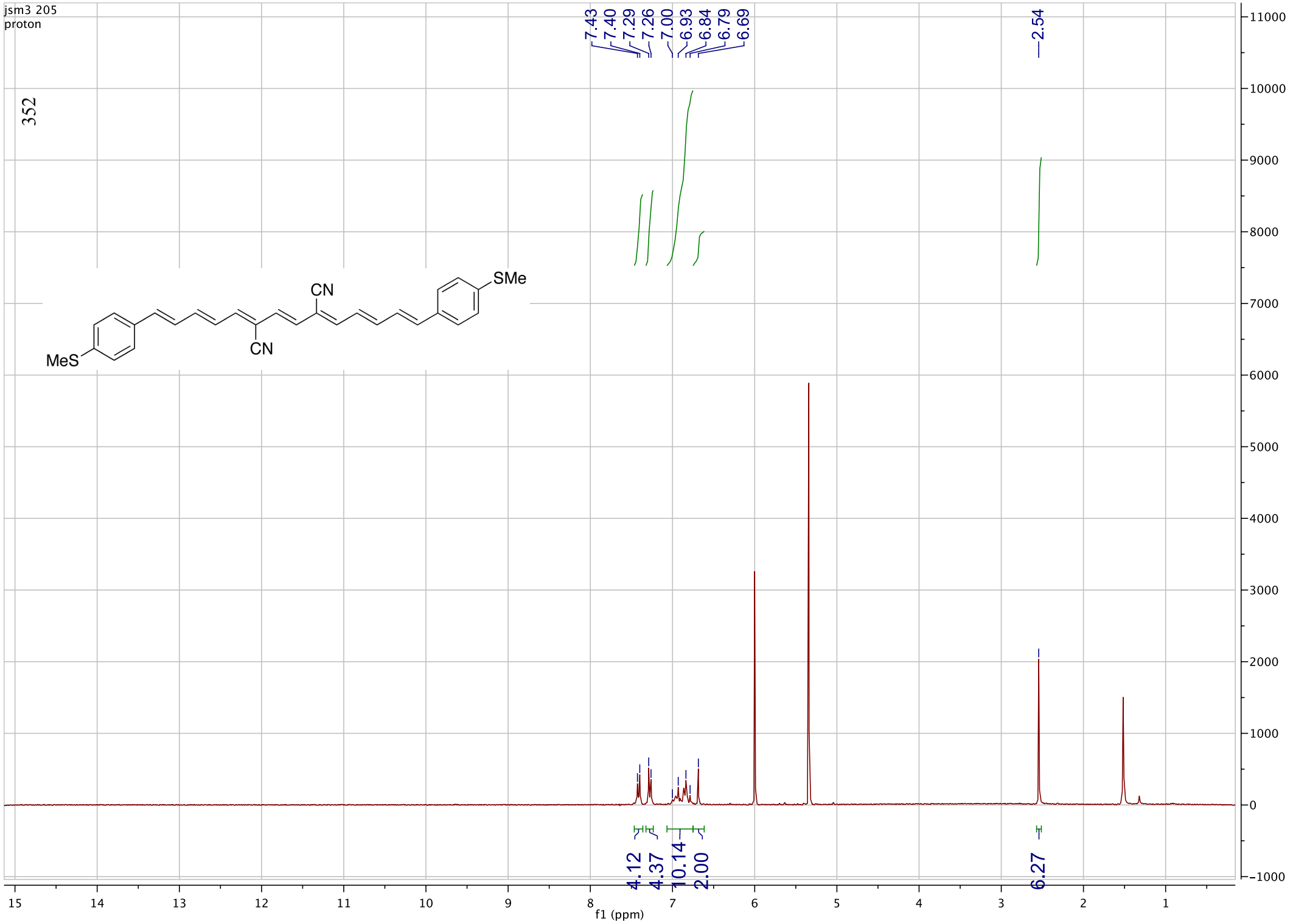

347
jsm3-226
carbon NMR
193.85
152.16
143.08
139.53
139.41
135.87
134.01
132.01
131.35
130.25
128.12
127.53
126.87
15.97
MeS
O
f1 (ppm)

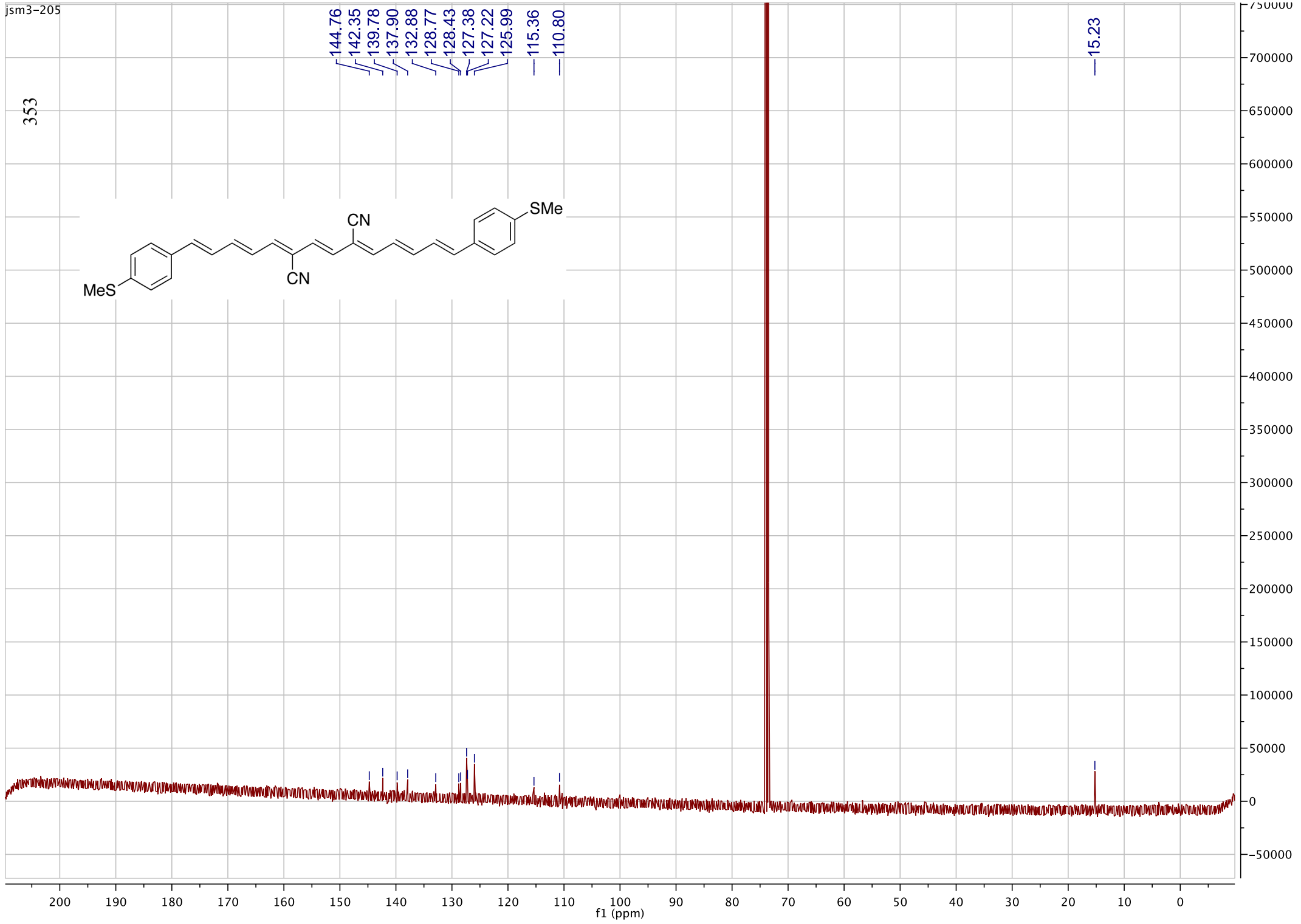

jsm3-189
proton standard yellow solid after recrystall
348
CN
SMe
CN
MeS
7.80
7.78
7.30
7.28
7.13
6.83
2.55
4.03
8.35
2.00
2.01
6.00
f1 (ppm)

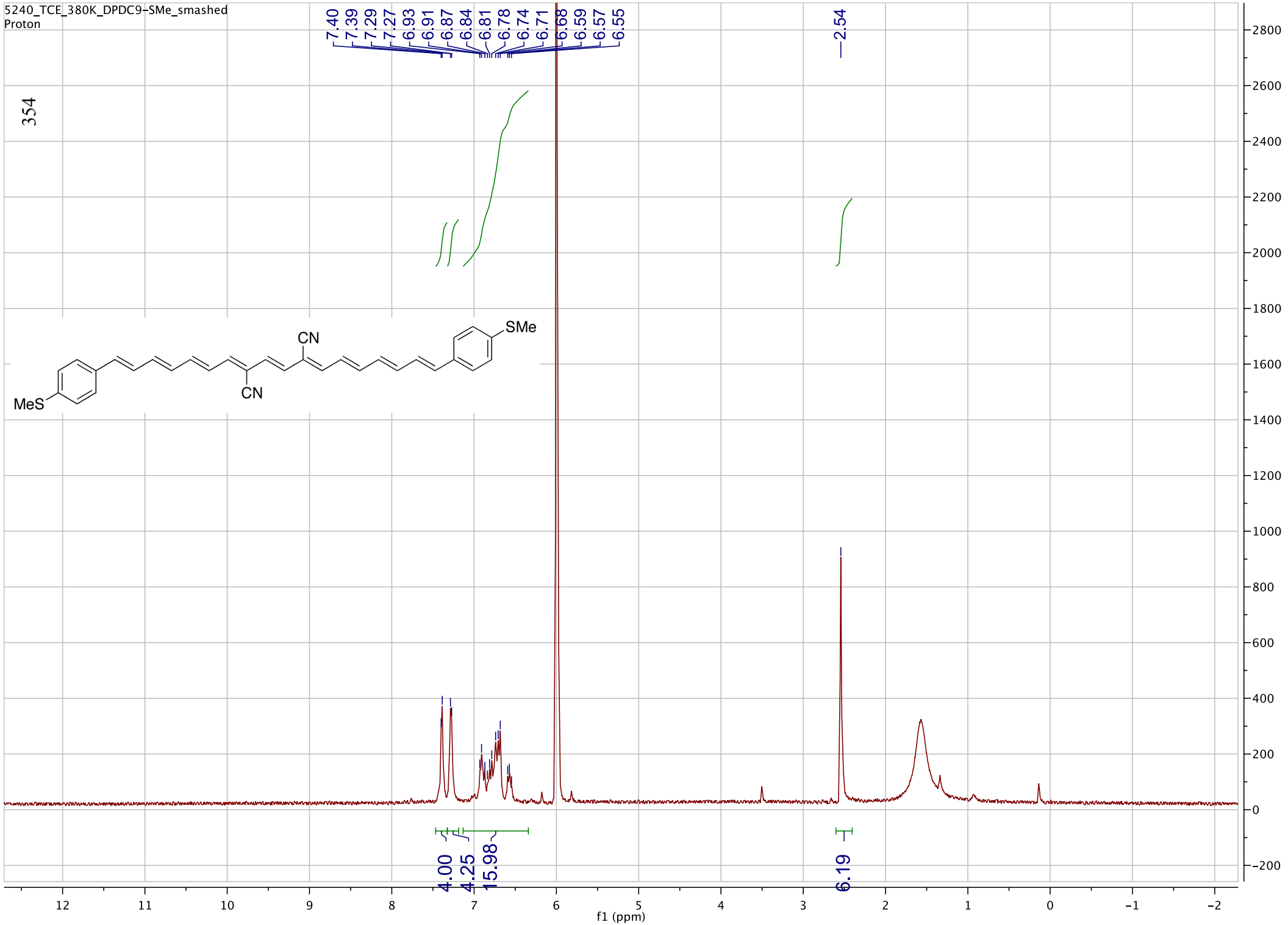

jsm3-189
carbon NMR
349
144.32
143.33
129.91
129.88
129.52
126.10
115.97
108.51
15.00
CN
SMe
MeS
CN
f1 (ppm)

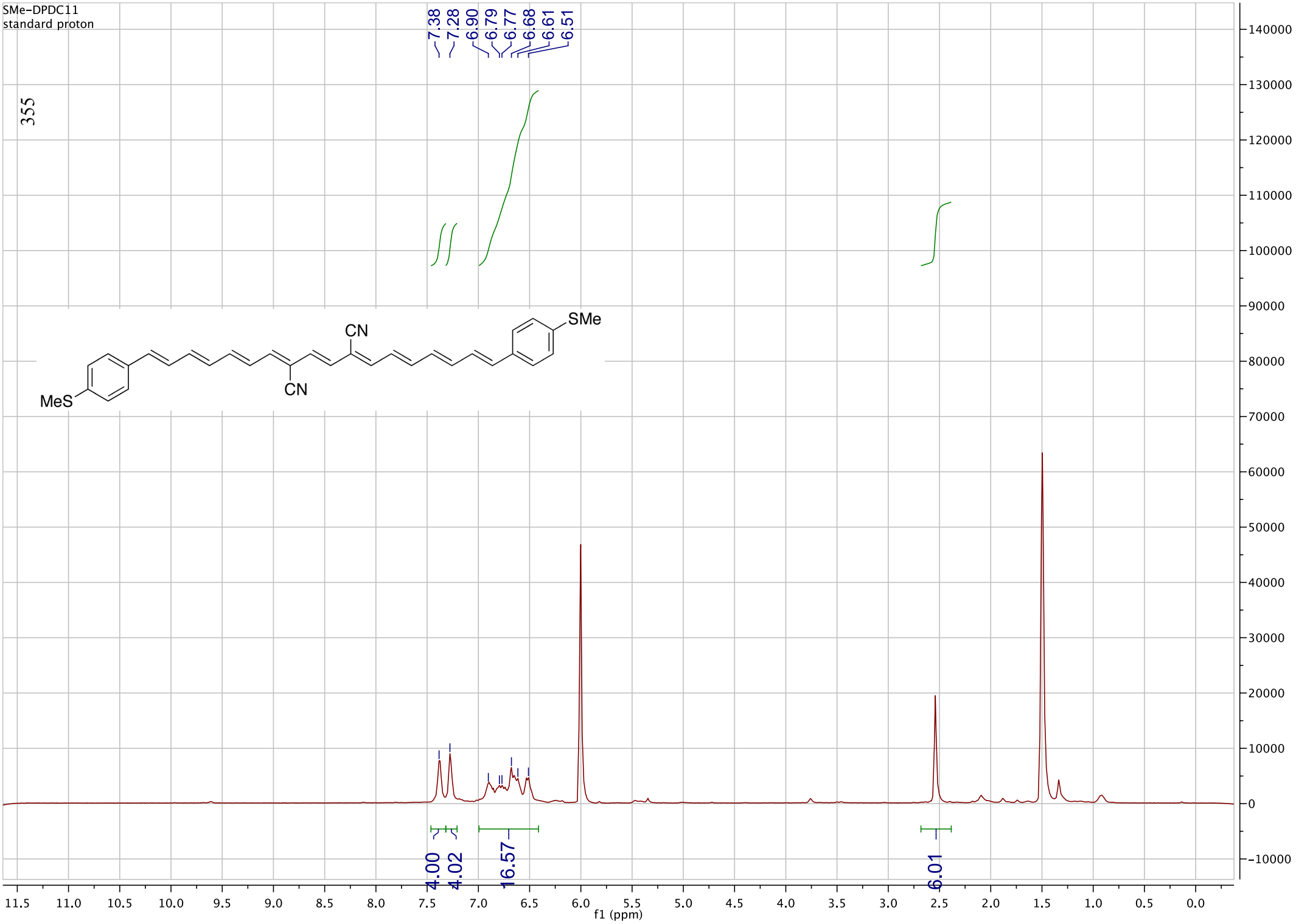

jsm3-194
350
CN
SMe
CN
MeS
7.46
7.43
7.26
7.24
7.22
7.18
7.00
6.96
6.94
6.89
6.68
2.52
4.00
6.05
4.14
1.95
5.72
f1 (ppm)


jsm3-194
carbon NMR
351
144.96
141.39
141.24
132.46
128.85
127.85
126.53
124.01
114.97
111.38
14.84
CN
SMe
CN
MeS
f1 (ppm)

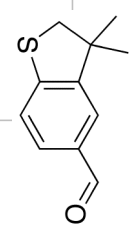

jsm3 205
proton
352
7.43
7.40
7.29
7.26
7.00
6.93
6.84
6.79
6.69
2.54
CN
SMe
CN
MeS
4.12
4.37
10.14
2.00
6.27
f1 (ppm)


jsm3-205
353
144.76
142.35
139.78
137.90
132.88
128.77
128.43
127.38
127.22
125.99
115.36
110.80
15.23
CN
CN
SMe
MeS
f1 (ppm)


5240_TCE_380K_DPDC9-SMe_smashed
Proton
7.40
7.39
7.29
7.27
6.93
6.91
6.87
6.84
6.81
6.78
6.74
6.71
6.68
6.59
6.57
6.55
2.54
354
CN
SMe
CN
MeS
4.00
4.25
15.98
6.19
f1 (ppm)


SMe-DPDC11
standard proton
355
7.38
7.28
6.90
6.79
6.77
6.68
6.61
6.51
CN
CN
SMe
MeS
4.00
4.02
16.57
6.01
f1 (ppm)

jsm4-082
proton standard

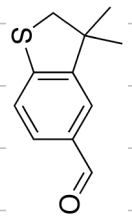


1.00
2.00
1.03
2.02
6.08

9.89
7.62
7.62
7.60
7.59
7.55
7.55
7.32
7.30
7.26
3.25
1.41

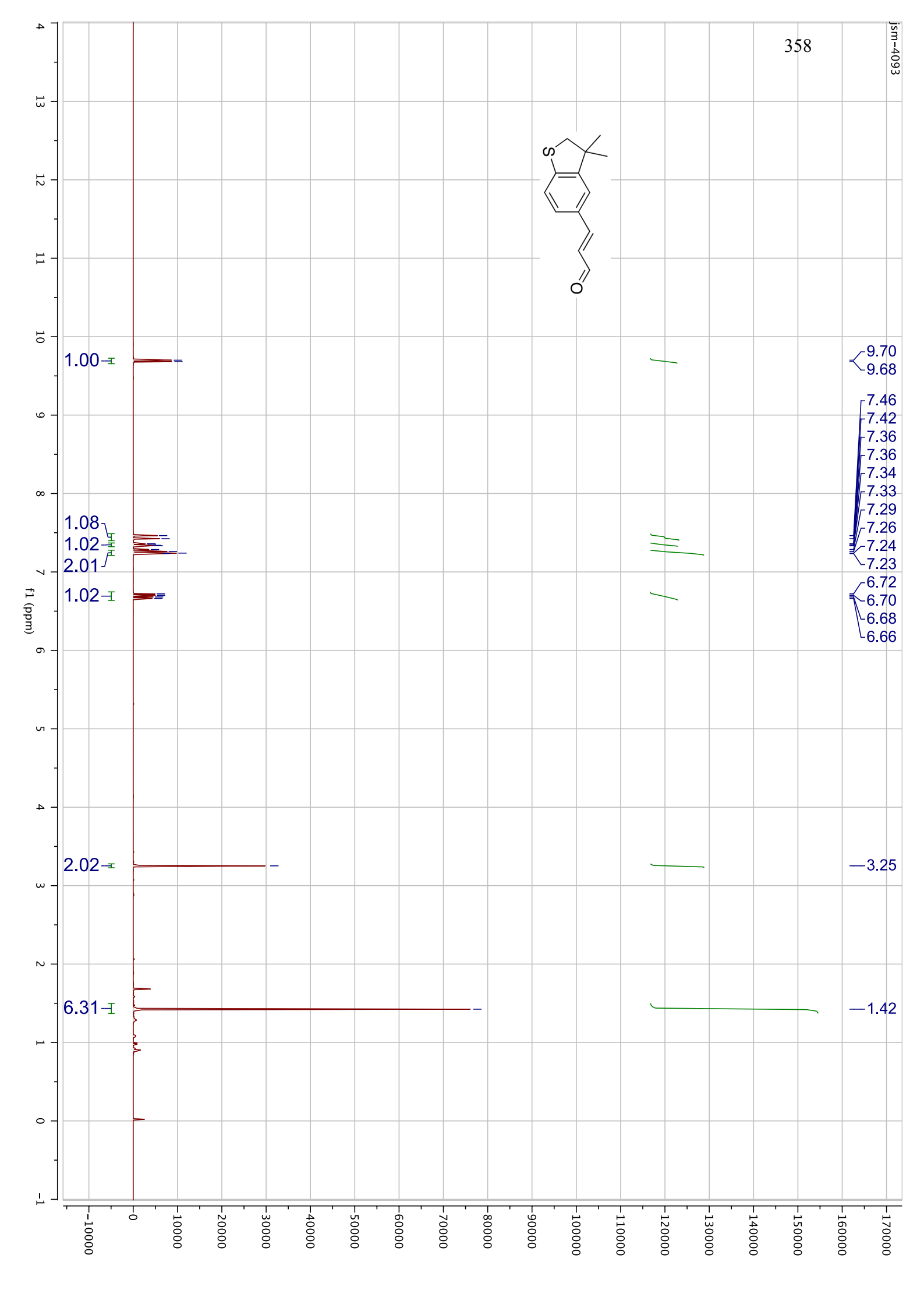
f1 (ppm)

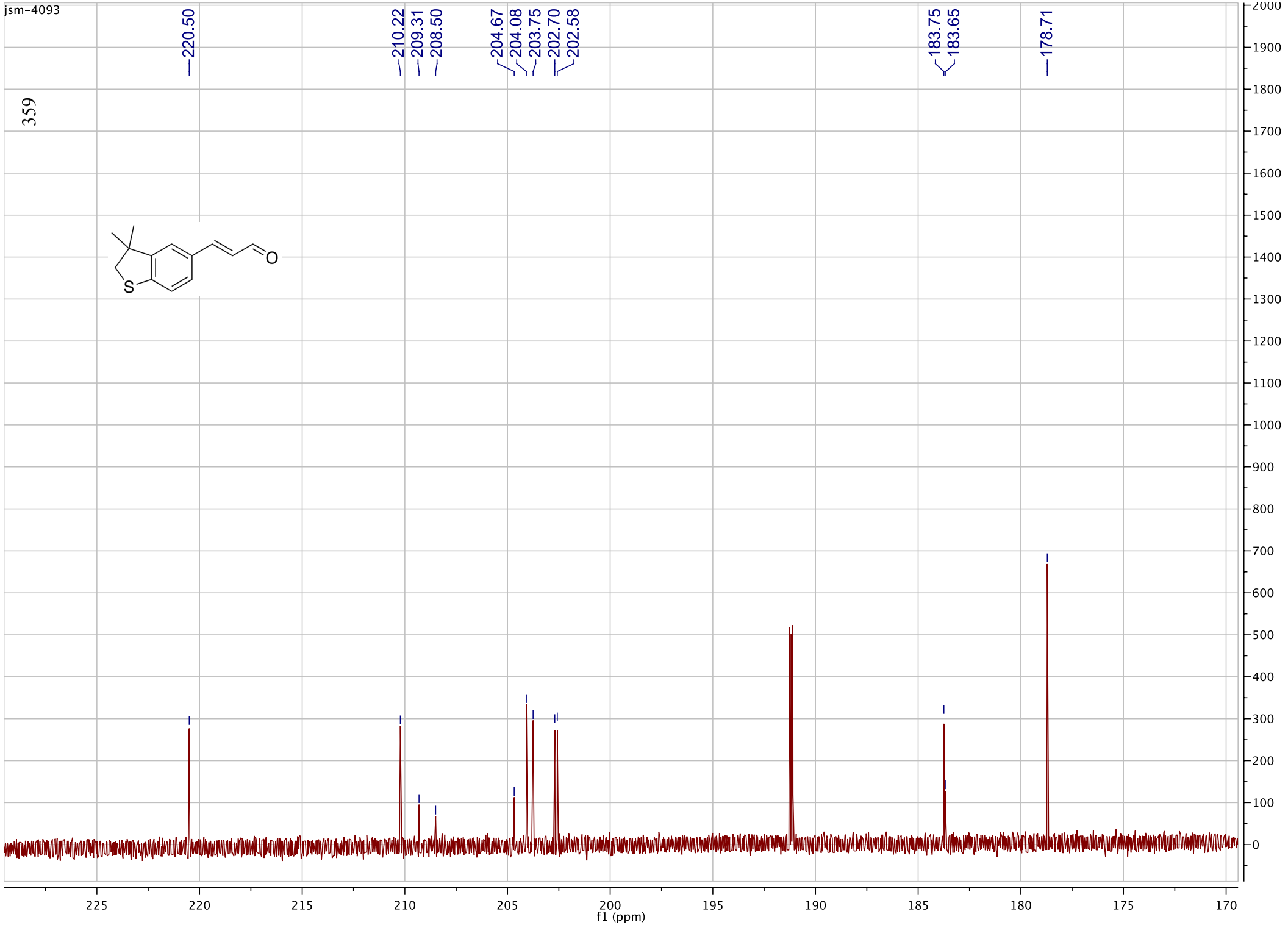
jsm4-082
carbon NMR



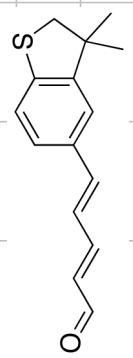
191.61
150.55
149.58
134.11
131.08
123.01
122.88
47.84
47.31
27.87

f1 (ppm)


jsm-4093
S
O
1.00
1.08
1.02
2.01
1.02
2.02
6.31
9.70
9.68
7.46
7.42
7.36
7.36
7.34
7.33
7.29
7.26
7.24
7.23
6.72
6.70
6.68
6.66
3.25
1.42
f1 (ppm)


jsm-4093
359
220.50
210.22
209.31
208.50
204.67
204.08
203.75
202.70
202.58
183.75
183.65
178.71
S
O
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
225
220
215
210
205
200
195
190
185
180
175
170
f1 (ppm)

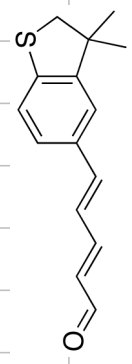
jsm3-287
proton 400Mhz
after column
fr 16



1.05
5.00
2.08
1.04
2.12
6.77

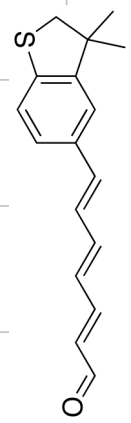
9.61
9.59
7.26
7.25
7.25
7.19
7.17
7.17
7.16
6.96
6.96
6.95
6.28
6.26
6.24
6.22
3.22
1.40

f1 (ppm)



193.81
152.80
149.30
143.94
142.88
132.73
131.23
127.77
125.10
123.07
121.80
47.82
47.46
27.80

jsm4-022
proton standard

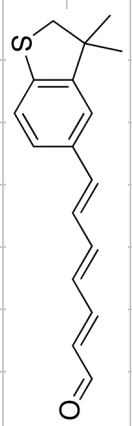


0.94
4.11
3.02
1.00
1.00
2.35
7.05

9.60
9.57
7.28
7.24
7.24
7.22
7.21
7.20
7.18
7.15
7.15
7.14
6.89
6.86
6.85
6.84
6.82
6.79
6.74
6.59
6.55
6.54
6.22
6.20
6.17
6.15
3.21
1.41
1.39

f1 (ppm)

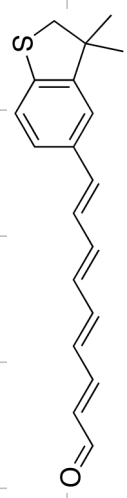
jsm4-mk124
carbon NMR



193.78
152.27
149.17
143.44
142.71
138.77
133.49
131.21
129.86
127.10
126.72
123.04
121.37
47.84
47.48
27.81

f1 (ppm)

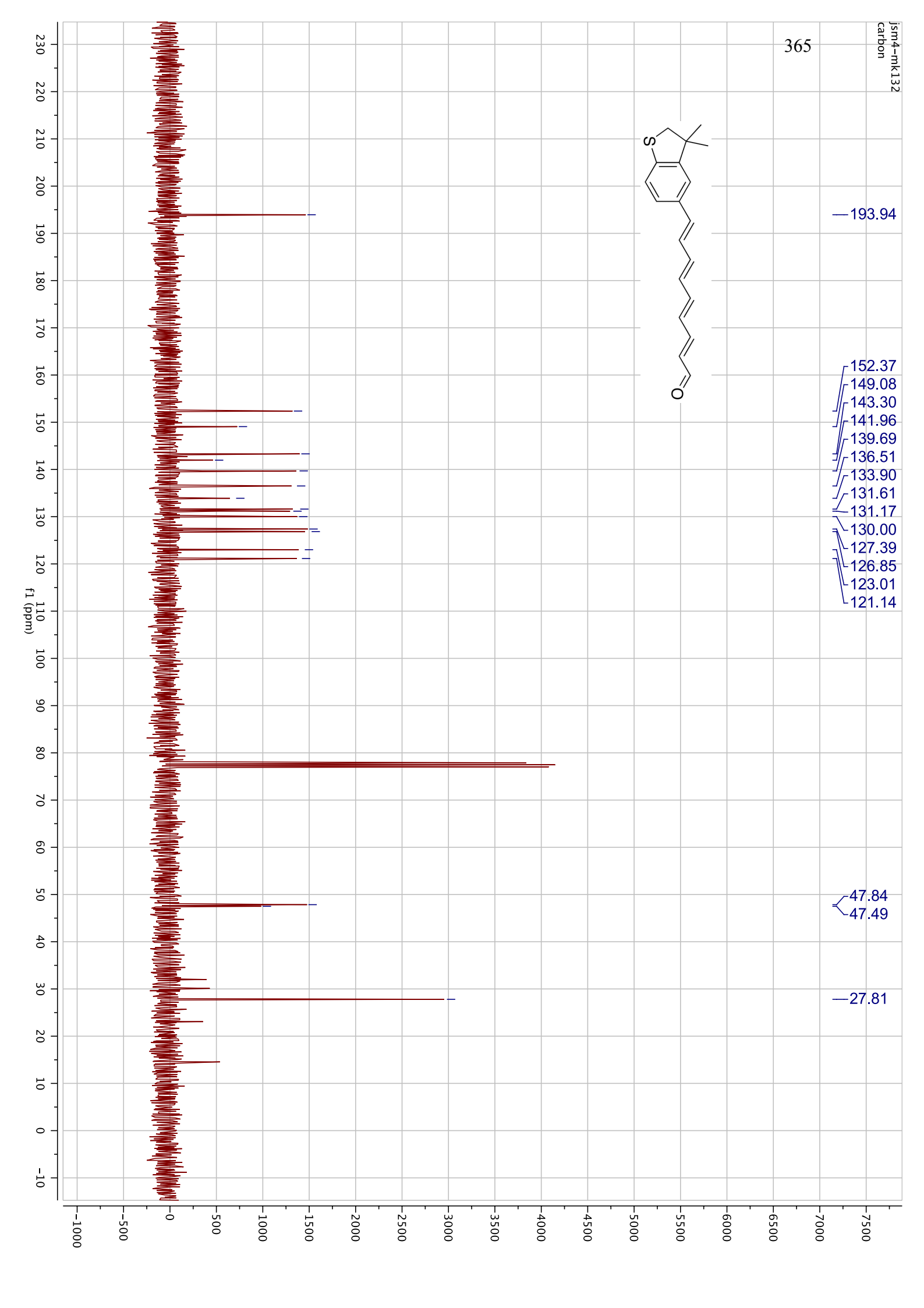
jsm4-mk132
proton standard

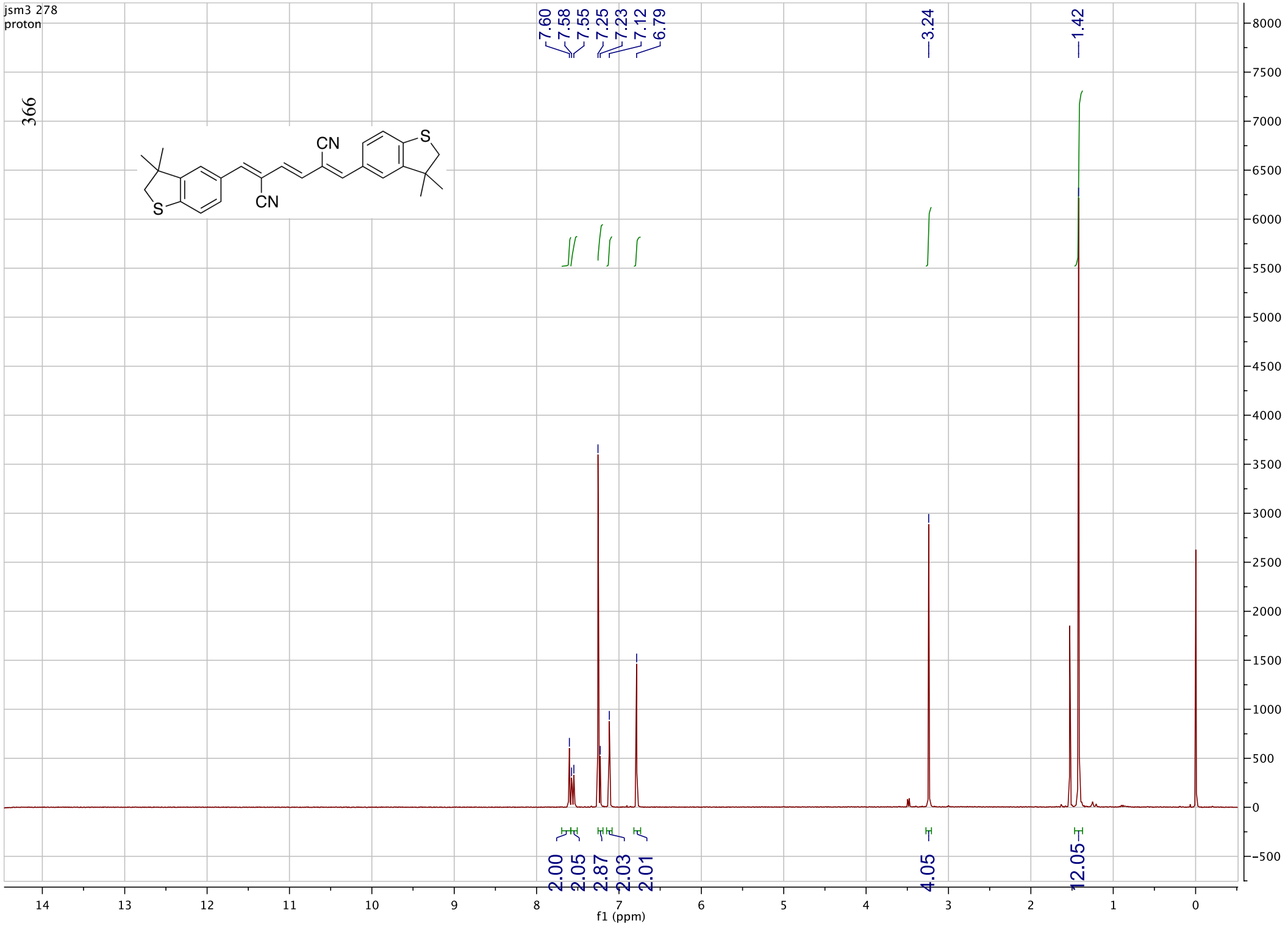


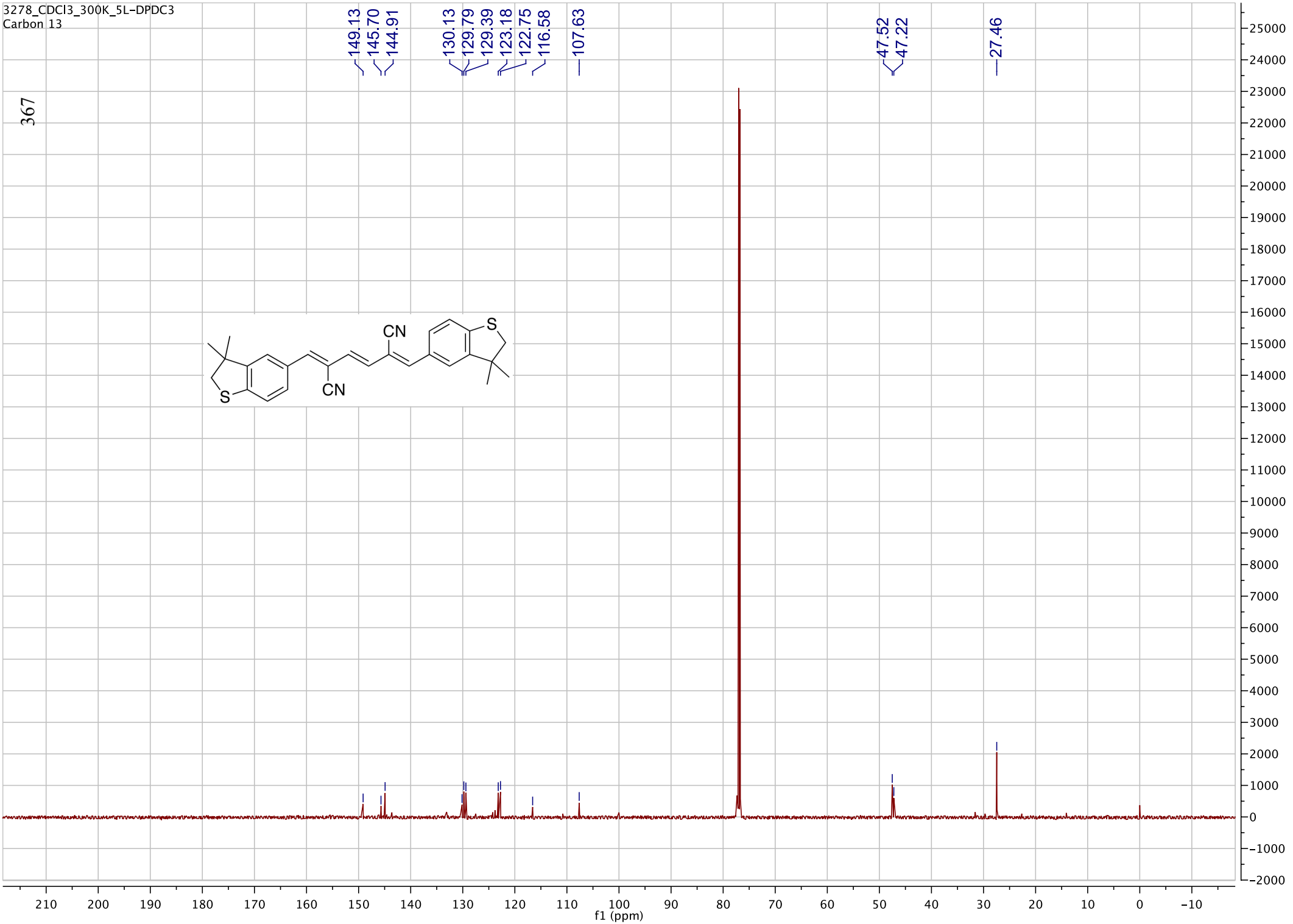
1.00
4.11
4.29
2.01
1.01
2.00
6.05

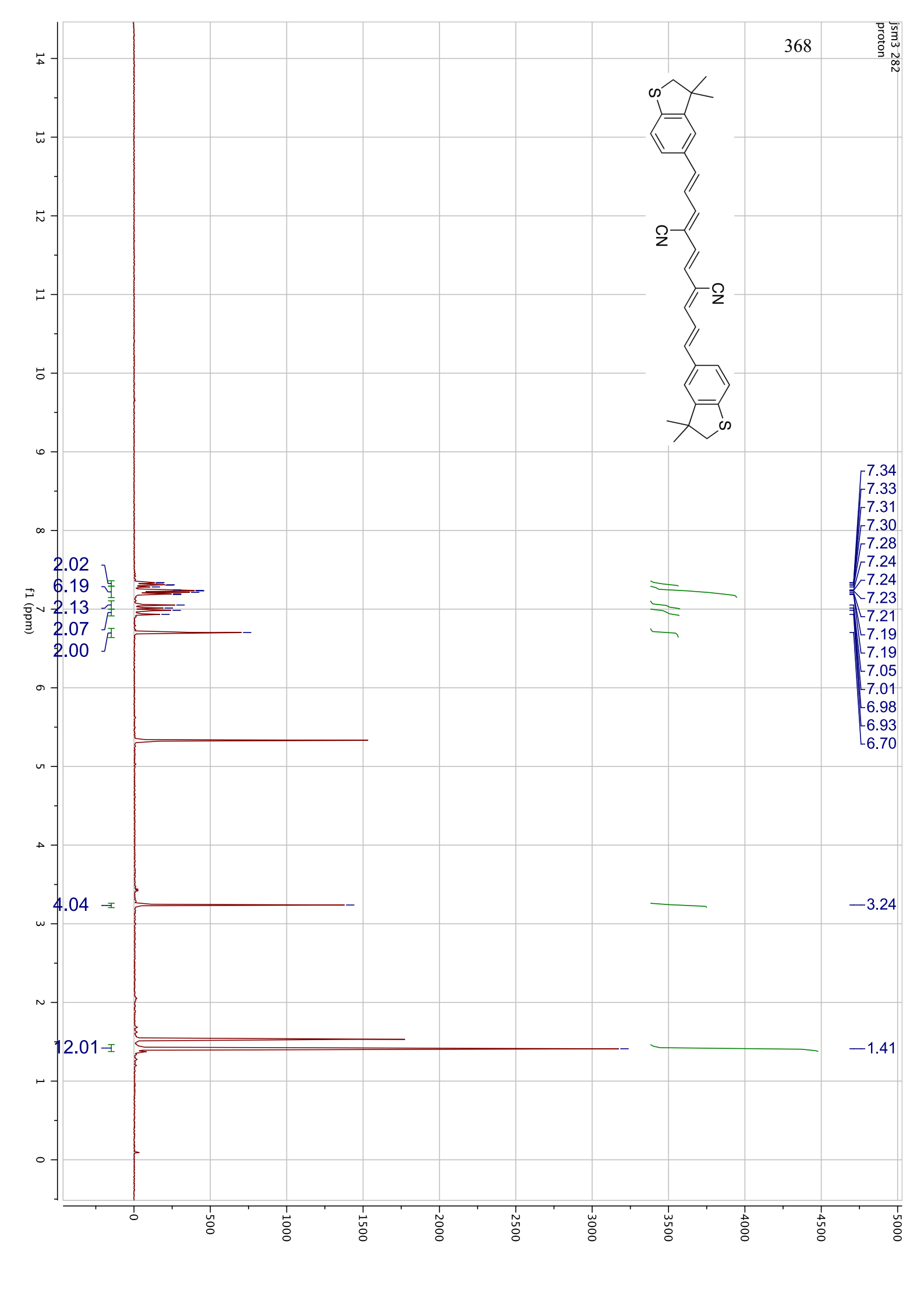
9.58
9.55
7.20
7.18
7.15
7.13
7.10
6.88
6.85
6.83
6.79
6.76
6.75
6.71
6.68
6.63
6.59
6.51
6.48
6.44
6.43
6.39
6.20
6.17
6.15
6.12
3.20
1.39
1.05

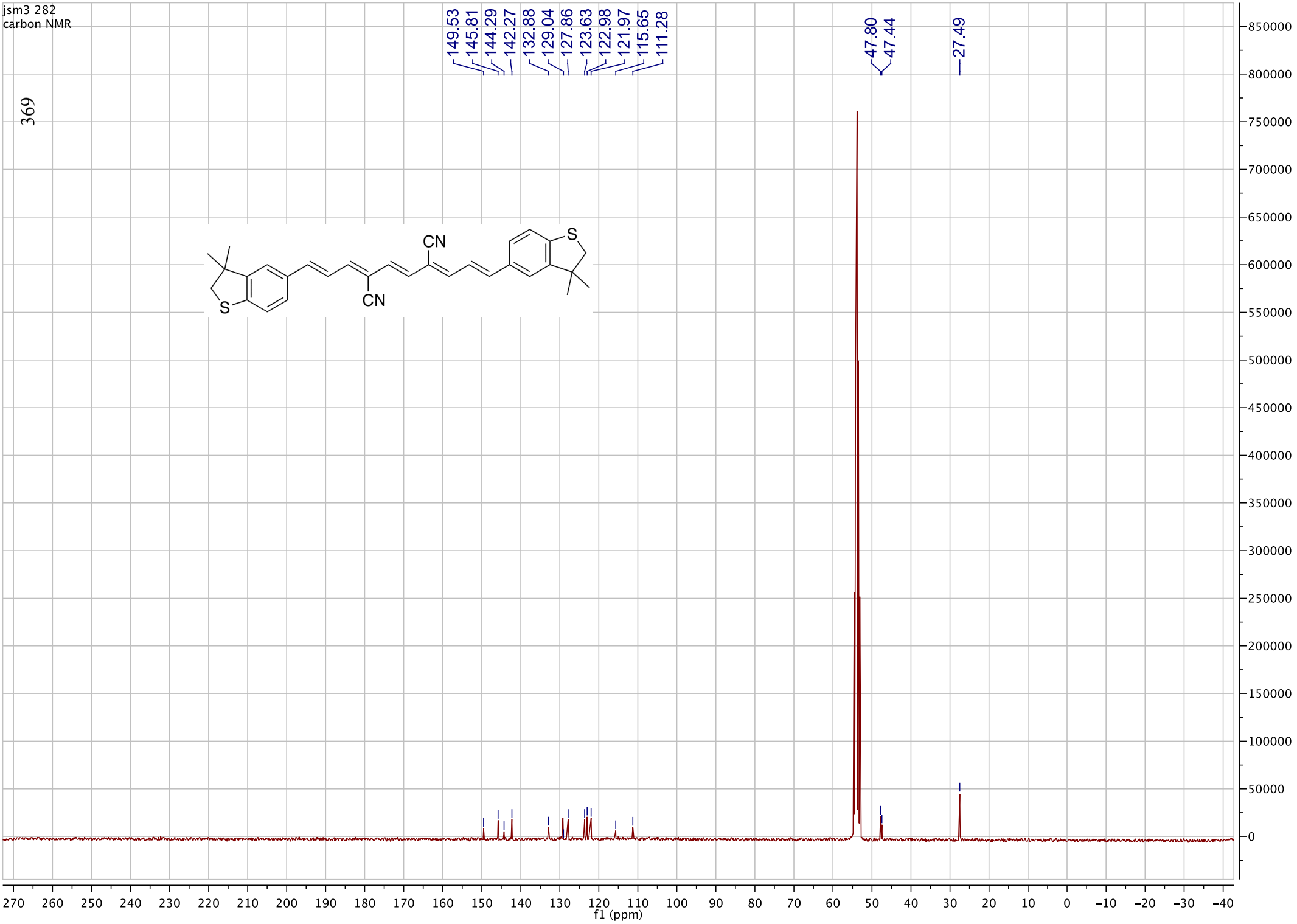
f1 (ppm)

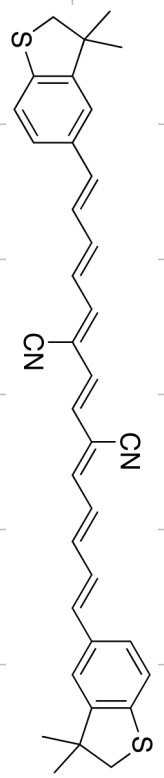

jsm4-mk132
carbon
193.94
152.37
149.08
143.30
141.96
139.69
136.51
133.90
131.61
131.17
130.00
127.39
126.85
123.01
121.14
47.84
47.49
27.81
f1 (ppm)


jsm3 278
proton
366
CN
CN
S
S
7.60
7.58
7.55
7.25
7.23
7.12
6.79
3.24
1.42
2.00
2.05
2.87
2.03
2.01
4.05
12.05
f1 (ppm)


3278_CDCl3_300K_5L-DPDC3
Carbon 13
367
149.13
145.70
144.91
130.13
129.79
129.39
123.18
122.75
116.58
107.63
47.52
47.22
27.46
CN
CN
S
S
f1 (ppm)


jsm3 282
proton
f1 (ppm)
2.02
6.19
2.13
2.07
2.00
4.04
12.01
7.34
7.33
7.31
7.30
7.28
7.24
7.24
7.23
7.21
7.19
7.19
7.05
7.01
6.98
6.93
6.70
3.24
1.41
CN
CN
S
S


jsm3 282
carbon NMR
369
149.53
145.81
144.29
142.27
132.88
129.04
127.86
123.63
122.98
121.97
115.65
111.28
47.80
47.44
27.49
CN
CN
S
S
f1 (ppm)



13.34

7.23
7.18
6.85
6.83
6.67

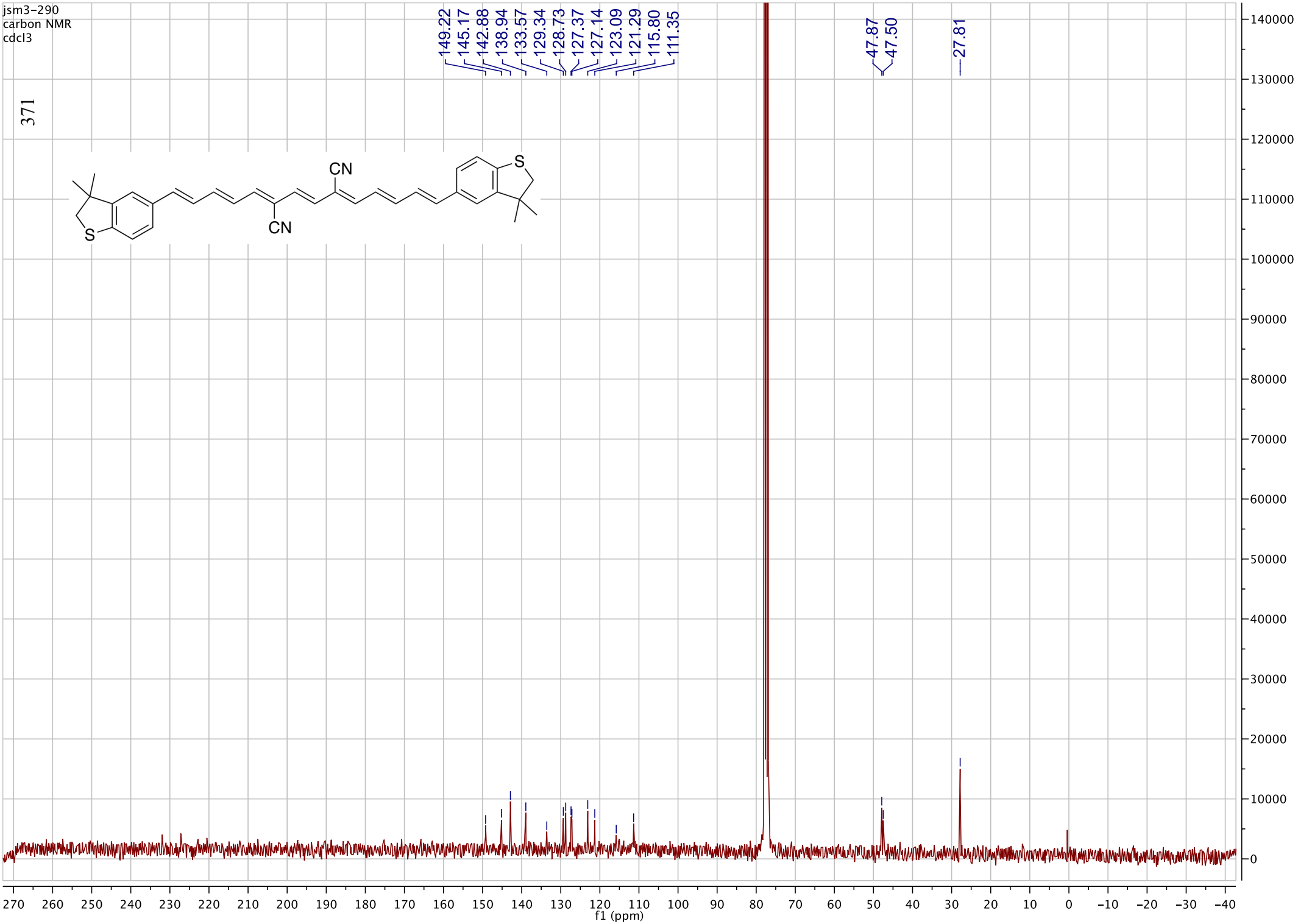
5.34
5.34
5.33

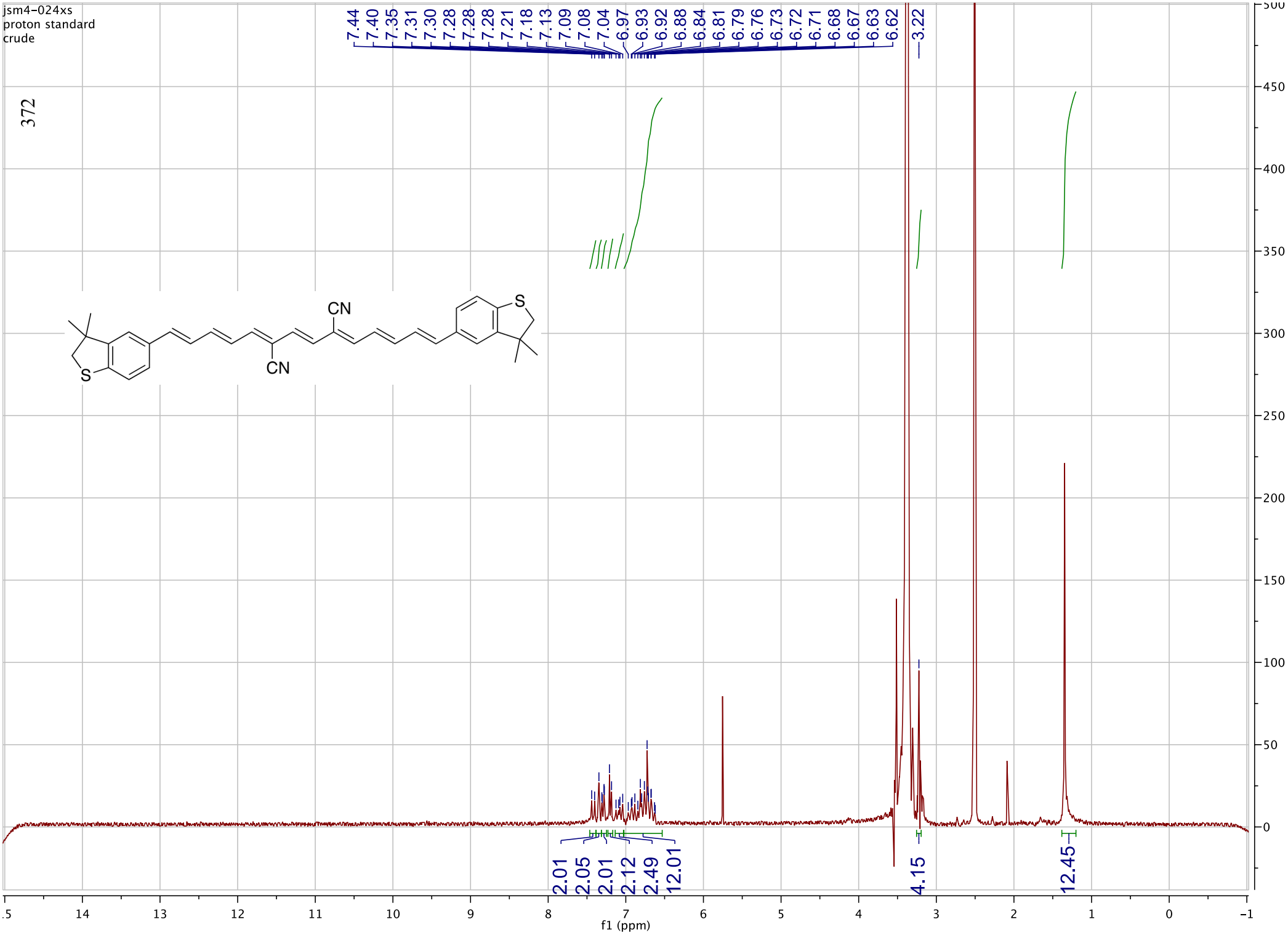
3.23

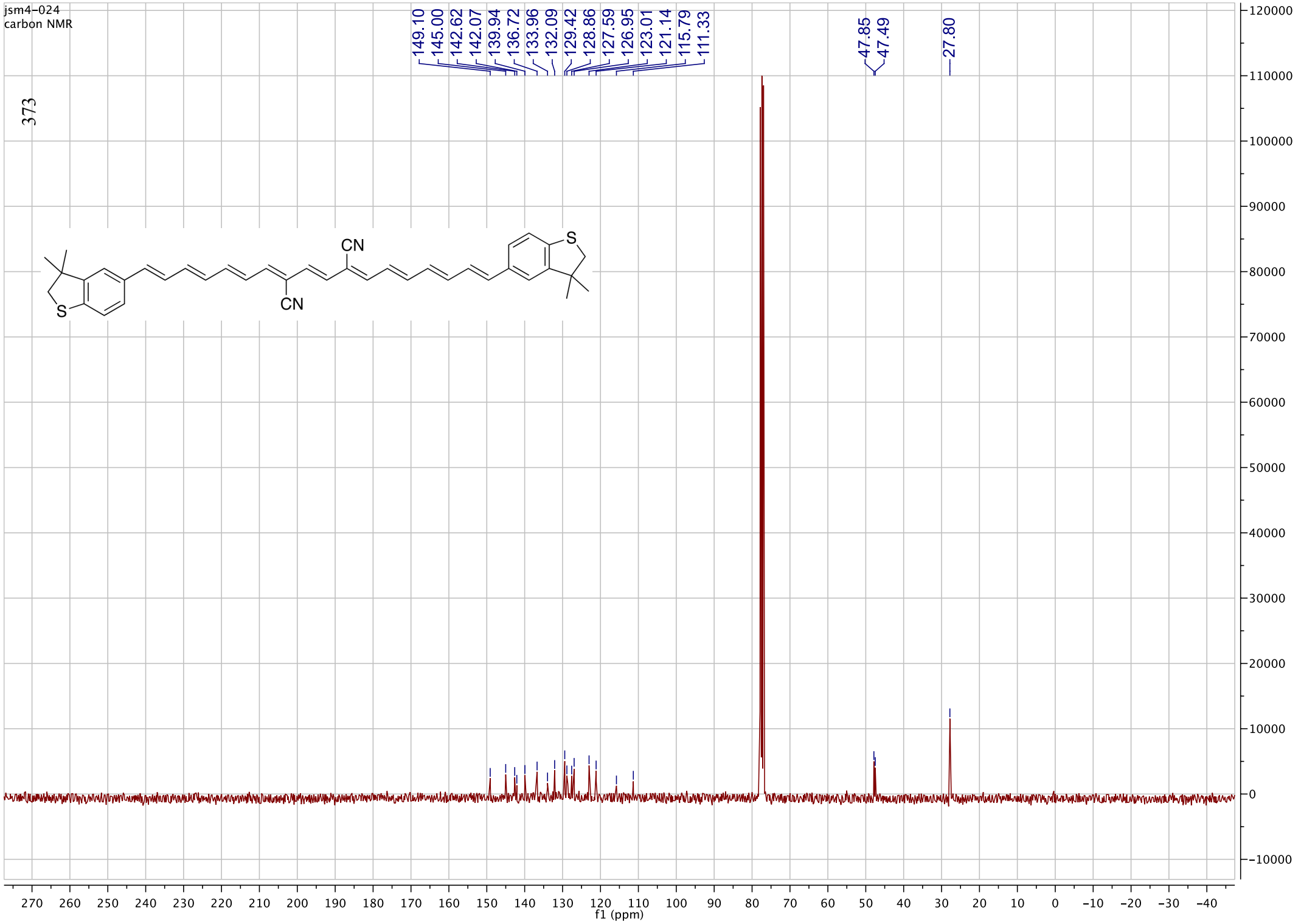
1.41

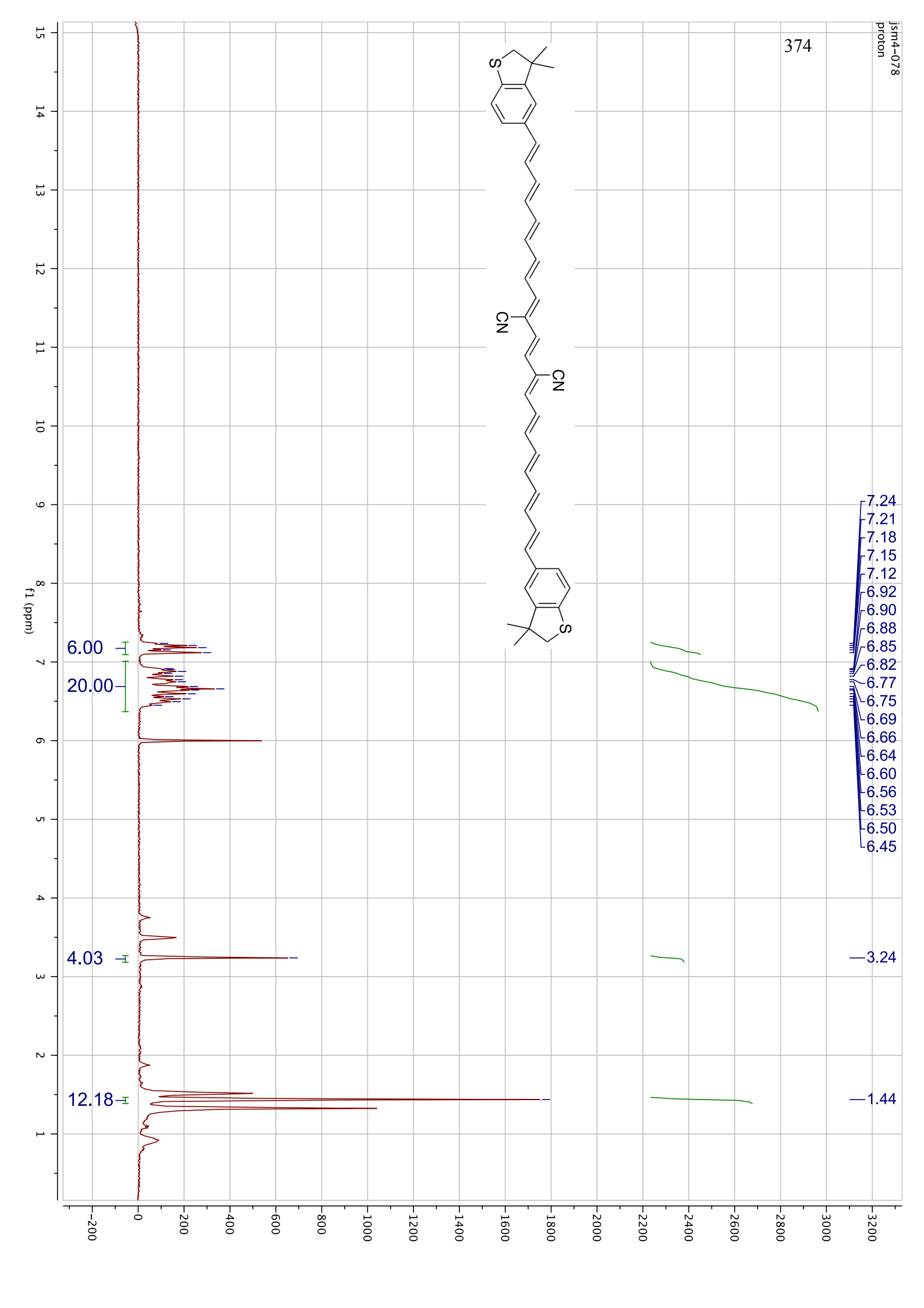
6.07
10.48
2.00
4.09
12.07

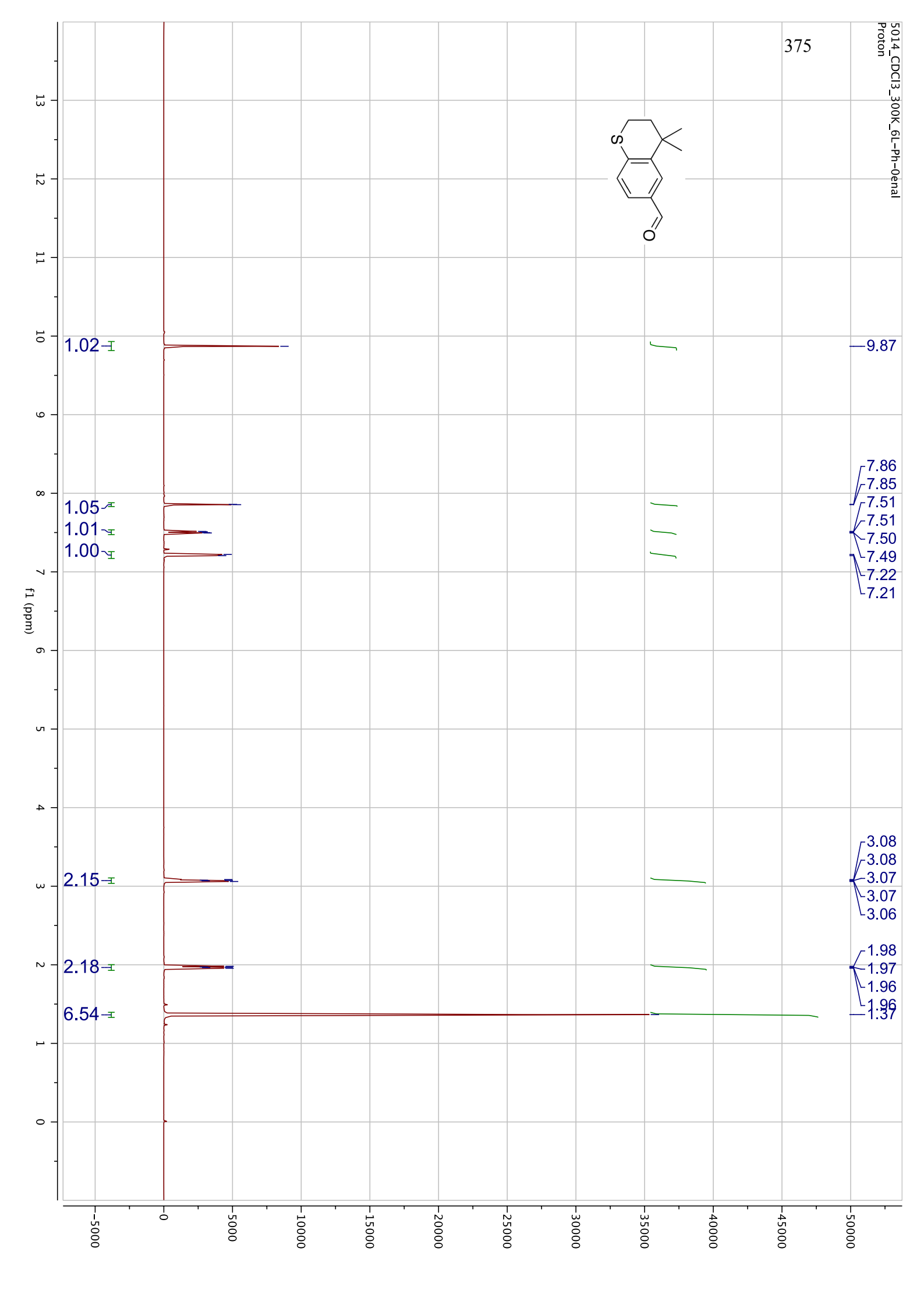
f1 (ppm)

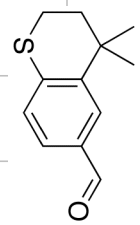

jsm3-290
carbon NMR
cdcl3
371
149.22
145.17
142.88
138.94
133.57
129.34
128.73
127.37
127.14
123.09
121.29
115.80
111.35
47.87
47.50
27.81
CN
CN
S
S
f1 (ppm)


jsm4-024xs
proton standard
crude
372
7.44
7.40
7.35
7.31
7.30
7.28
7.28
7.28
7.21
7.18
7.13
7.09
7.08
7.04
6.97
6.93
6.92
6.88
6.84
6.81
6.79
6.76
6.73
6.72
6.71
6.68
6.67
6.63
6.62
3.22
CN
CN
S
S
2.01
2.05
2.01
2.12
2.49
12.01
4.15
12.45
f1 (ppm)


jsm4-024
carbon NMR
373
149.10
145.00
142.62
142.07
139.94
136.72
133.96
132.09
129.42
128.86
127.59
126.95
123.01
121.14
115.79
111.33
47.85
47.49
27.80
CN
CN
S
S
f1 (ppm)


374
jsm4-078
proton
S
CN
CN
S
7.24
7.21
7.18
7.15
7.12
6.92
6.90
6.88
6.85
6.82
6.77
6.75
6.69
6.66
6.64
6.60
6.56
6.53
6.50
6.45
3.24
1.44
6.00
20.00
4.03
12.18
f1 (ppm)

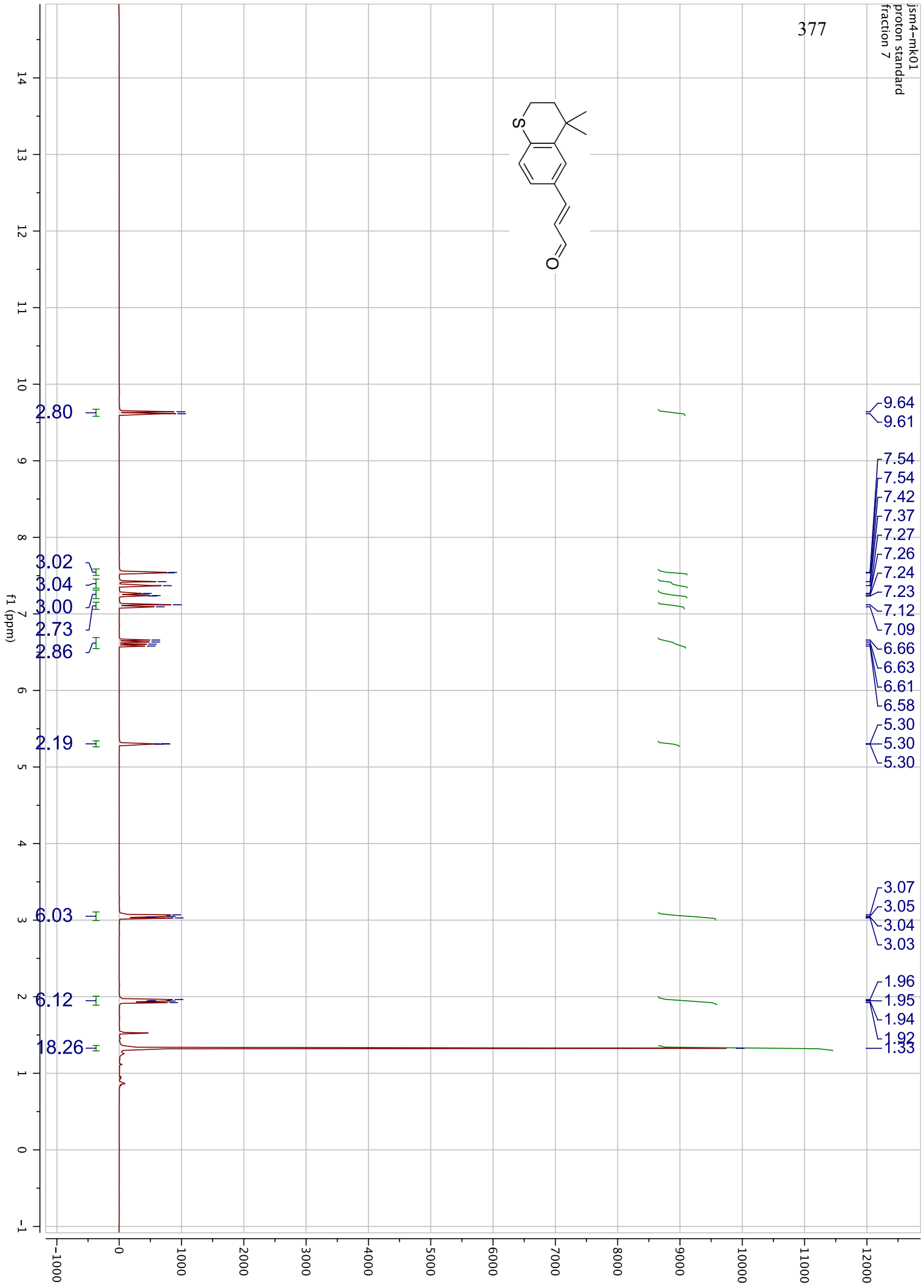

375
5014_CDCl3_300K_6L-Ph-0enal
Proton
S
O
1.02
1.05
1.01
1.00
2.15
2.18
6.54
9.87
7.86
7.85
7.51
7.51
7.50
7.49
7.22
7.21
3.08
3.08
3.07
3.07
3.06
1.98
1.97
1.96
1.96
1.37
f1 (ppm)



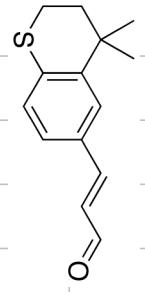
5014_CDCl3_300K_6L-Rh-0enal
Carbon 13

191.45
142.43
141.68
132.75
127.62
127.04
126.96
36.71
33.05
29.77
23.36

f1 (ppm)


jsm4-mk01
proton standard
fraction 7
f1 (ppm)
2.80
3.02
3.04
3.00
2.73
2.86
2.19
6.03
6.12
18.26
9.64
9.61
7.54
7.54
7.42
7.37
7.27
7.26
7.24
7.23
7.12
7.09
6.66
6.63
6.61
6.58
5.30
5.30
5.30
3.07
3.05
3.04
3.03
1.96
1.95
1.94
1.92
1.33
S
O

jsm4-mk1
carbon NMR

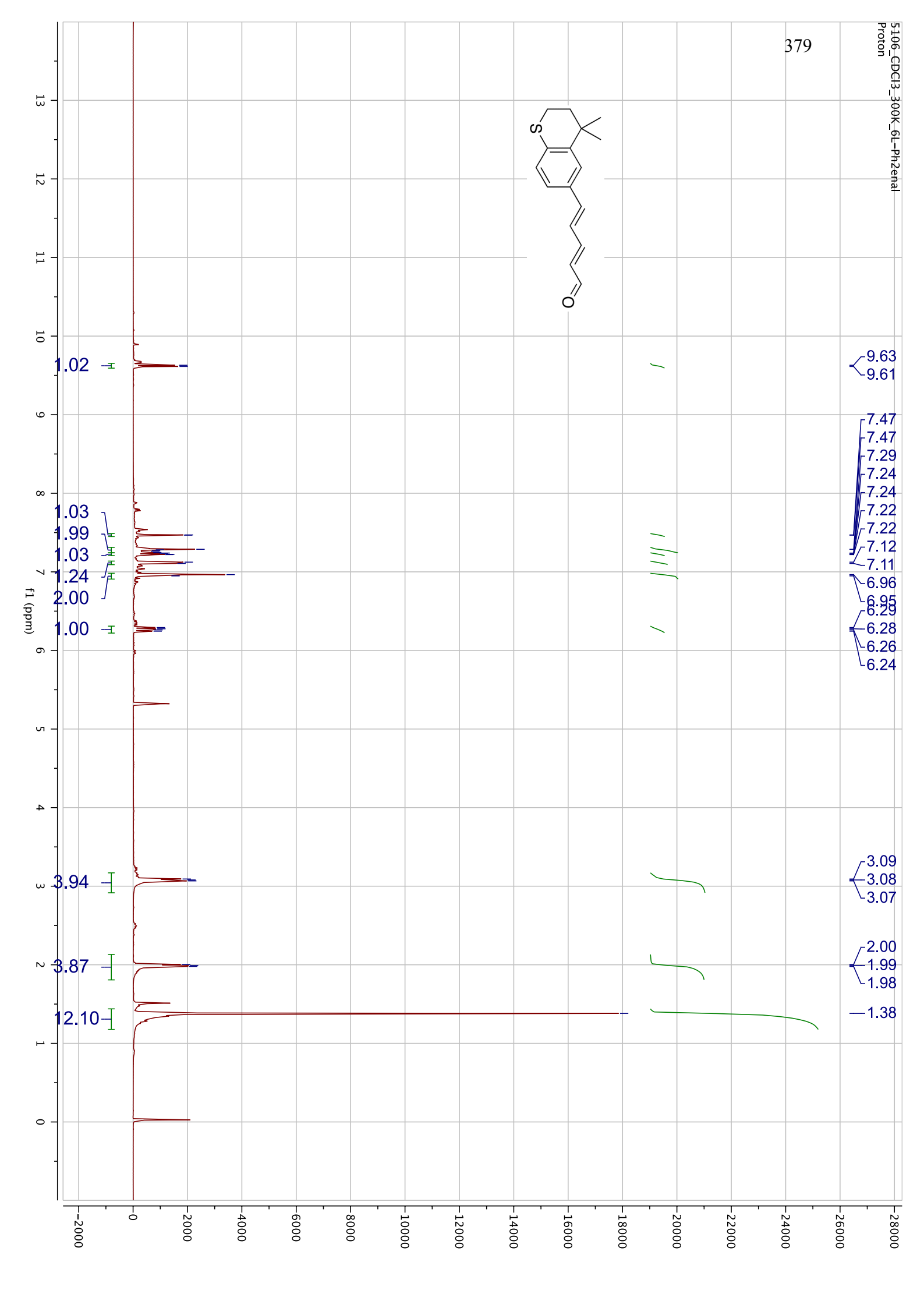


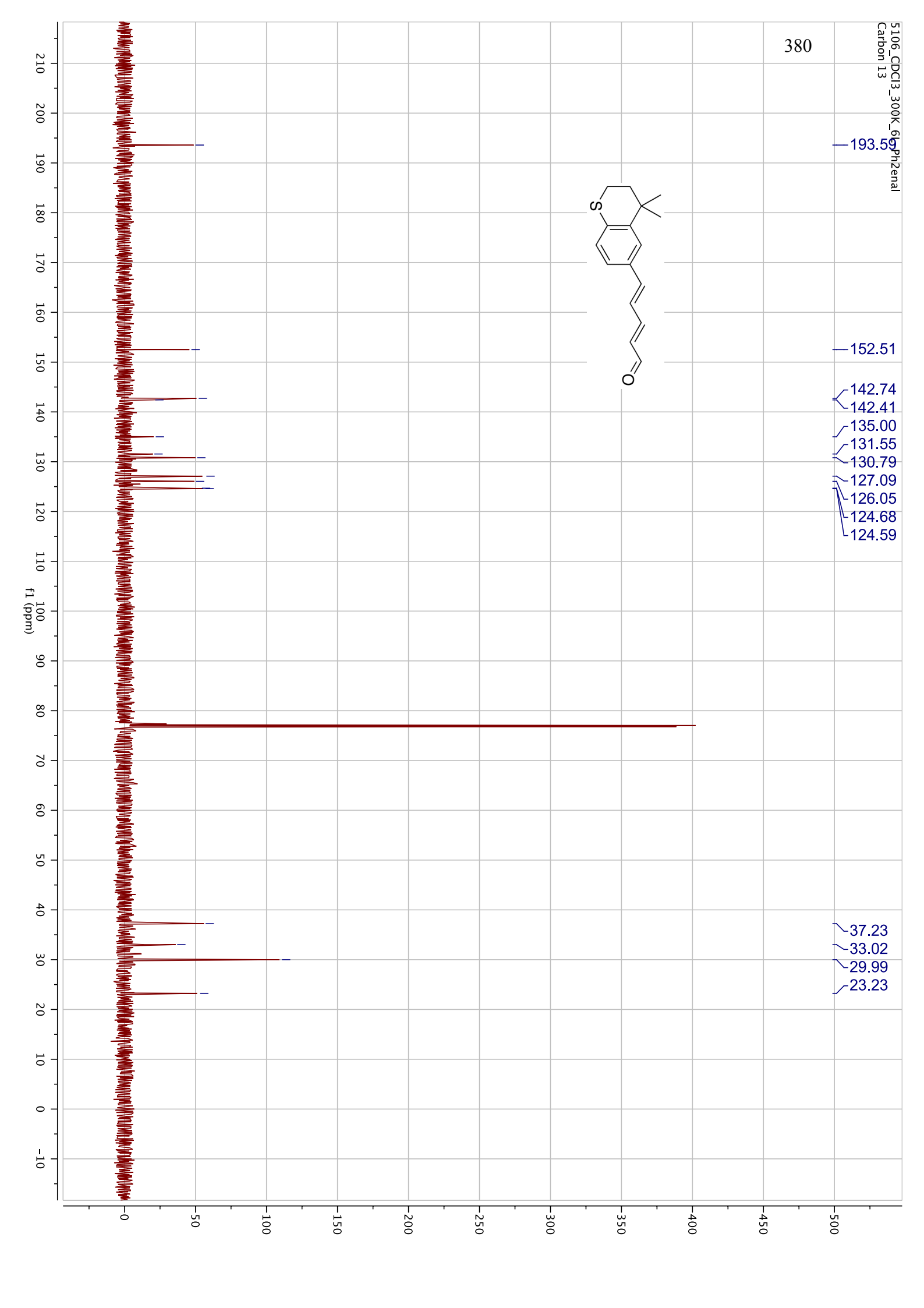
193.34

153.81
144.14
138.88
131.80
128.94
128.88
127.36

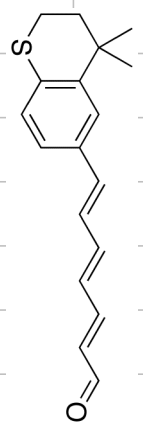
41.45
37.51
34.28
28.13

f1 (ppm)


5106_CDCl3_300K_6L-Ph2enal
Proton
f1 (ppm)
1.02
1.03
1.99
1.03
1.24
2.00
1.00
3.94
3.87
12.10
9.63
9.61
7.47
7.47
7.29
7.24
7.24
7.22
7.22
7.12
7.11
6.96
6.95
6.29
6.28
6.26
6.24
3.09
3.08
3.07
2.00
1.99
1.98
1.38
S
O


380
5106_CDCl3_300K_6b_Ph2enal
Carbon 13
193.55
152.51
142.74
142.41
135.00
131.55
130.79
127.09
126.05
124.68
124.59
37.23
33.02
29.99
23.23
S
O
f1 (ppm)

jsm4-mk127
carbon NMR

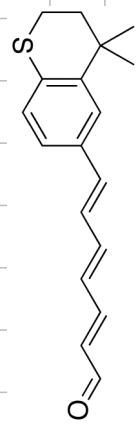


f1 (ppm)

1.00
1.13
2.21
1.07
3.19
1.08
1.04
2.14
2.14
6.34

168.64
168.08
122.91
118.61
117.81
117.34
116.76
115.77
115.20
111.19
110.43
109.02
107.95
104.93
104.15
103.19
97.34
96.78
96.28
95.72
31.12
30.70
30.27
8.25
7.83
7.40
-4.85

jsm4-mk127
carbon NMR

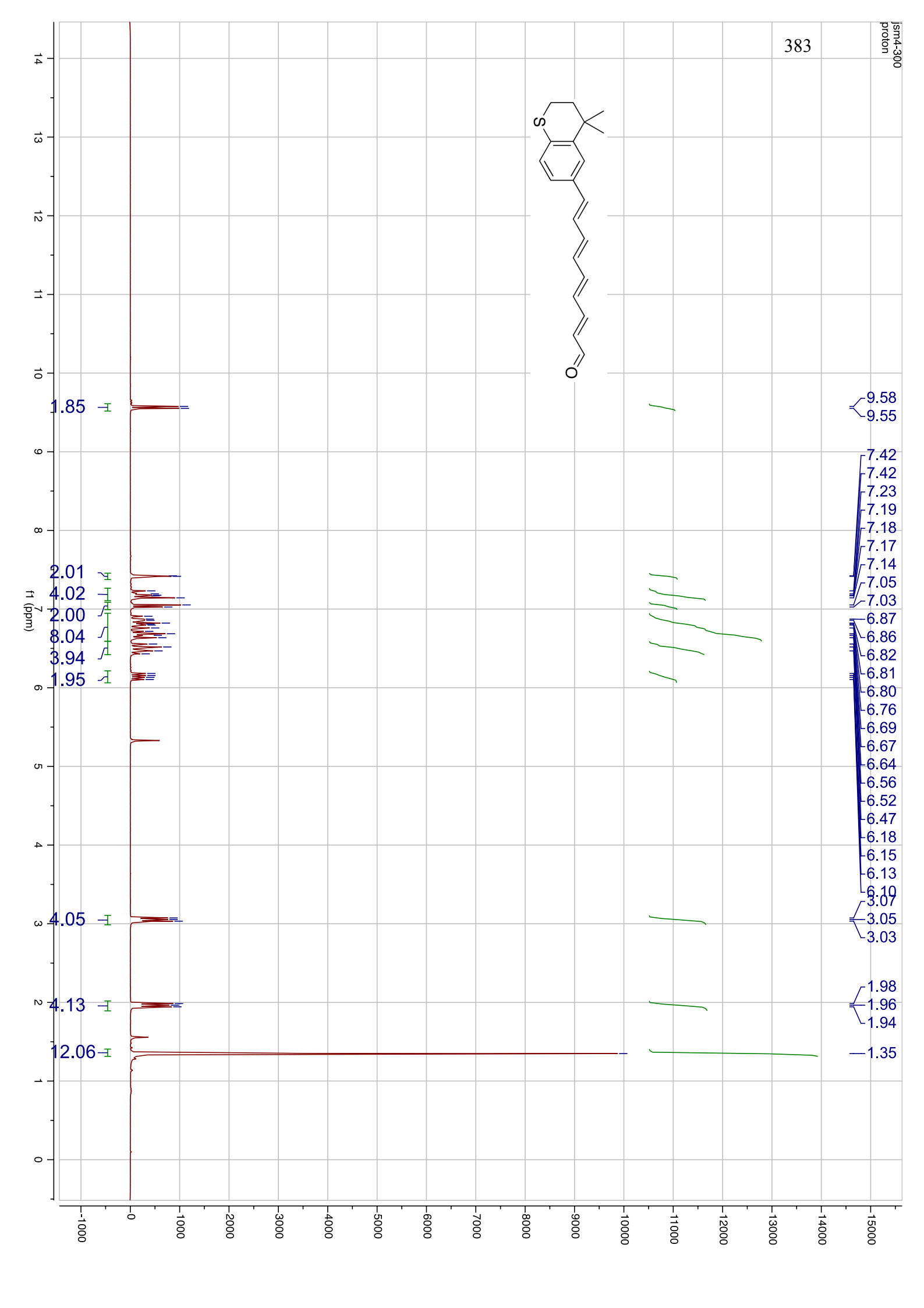


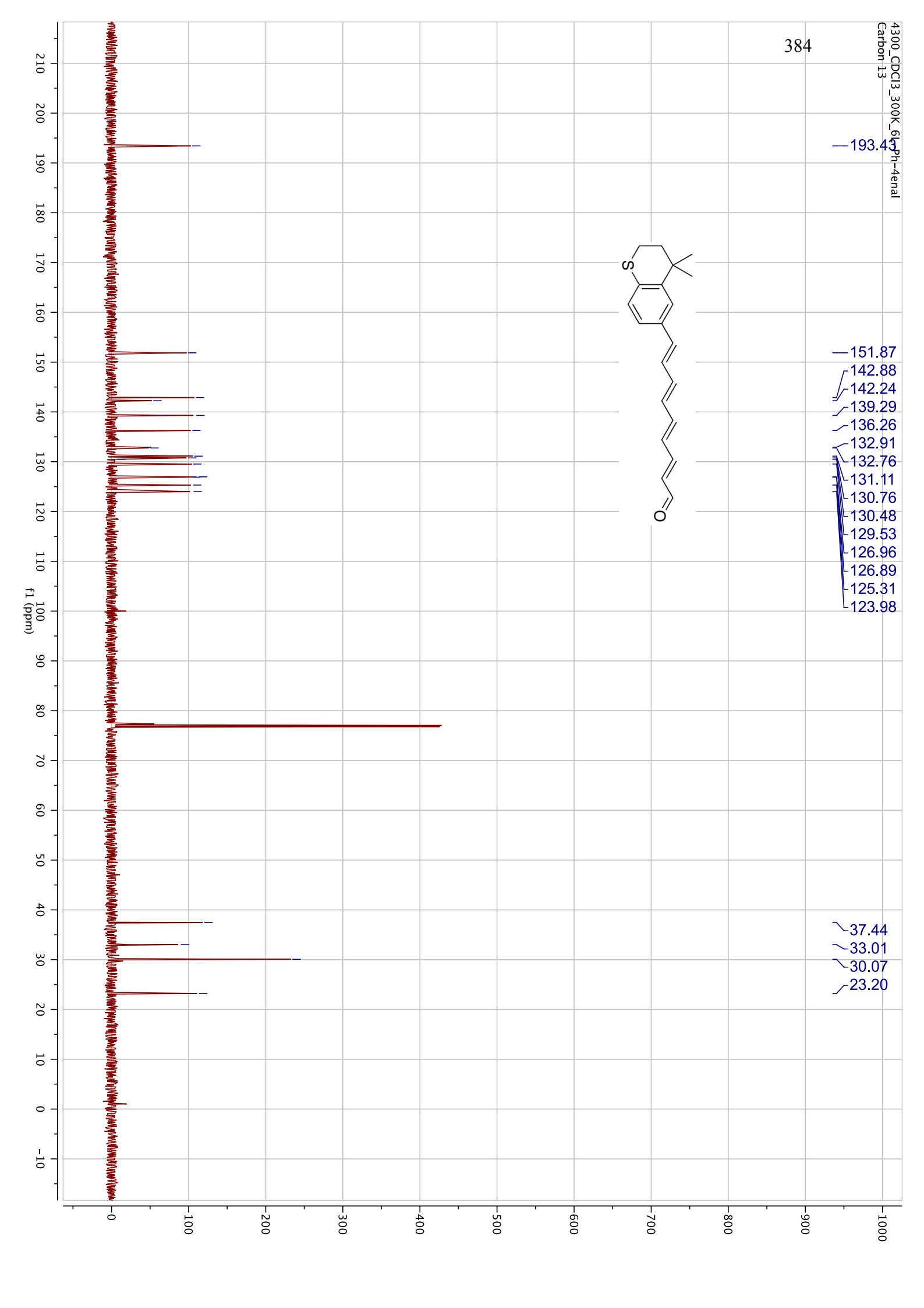
193.64

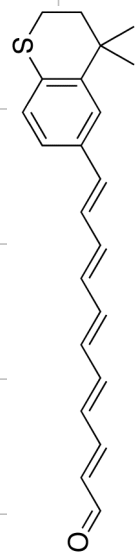
152.29
143.47
142.70
138.87
134.05
132.70
131.09
129.77
127.33
126.62
125.97
124.55

37.69
33.34
30.34
23.56

f1 (ppm)


jsm4-300
proton
S
O
1.85
2.01
4.02
2.00
8.04
3.94
1.95
4.05
4.13
12.06
9.58
9.55
7.42
7.42
7.23
7.19
7.18
7.17
7.14
7.05
7.03
6.87
6.86
6.82
6.81
6.80
6.76
6.69
6.67
6.64
6.56
6.52
6.47
6.18
6.15
6.13
6.10
3.07
3.05
3.03
1.98
1.96
1.94
1.35
f1 (ppm)


4300_CDCl3_300K_6c-Ph-4enal
Carbon 13
193.47
151.87
142.88
142.24
139.29
136.26
132.91
132.76
131.11
130.76
130.48
129.53
126.96
126.89
125.31
123.98
37.44
33.01
30.07
23.20
S
O
f1 (ppm)



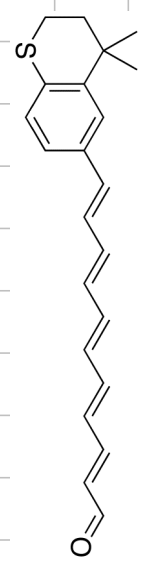
jsm4-077
proton

1.00
1.01
2.03
1.00
2.04
6.01
1.04
2.00
2.18
6.48

9.59
9.56
7.42
7.16
7.06
7.03
6.83
6.65
6.60
6.57
6.52
6.48
5.35
3.07
2.00
1.98
1.96
1.37

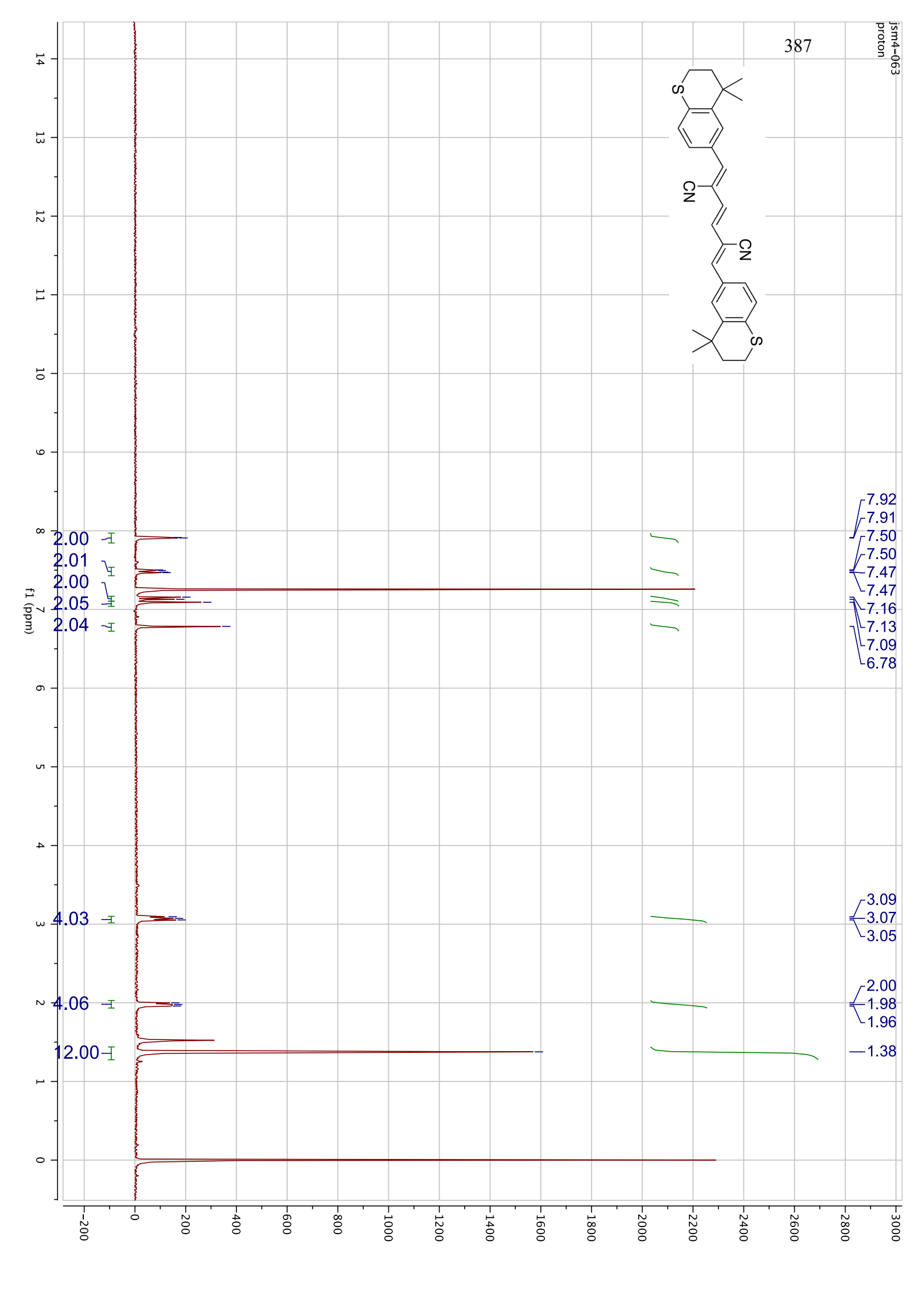
f1 (ppm)

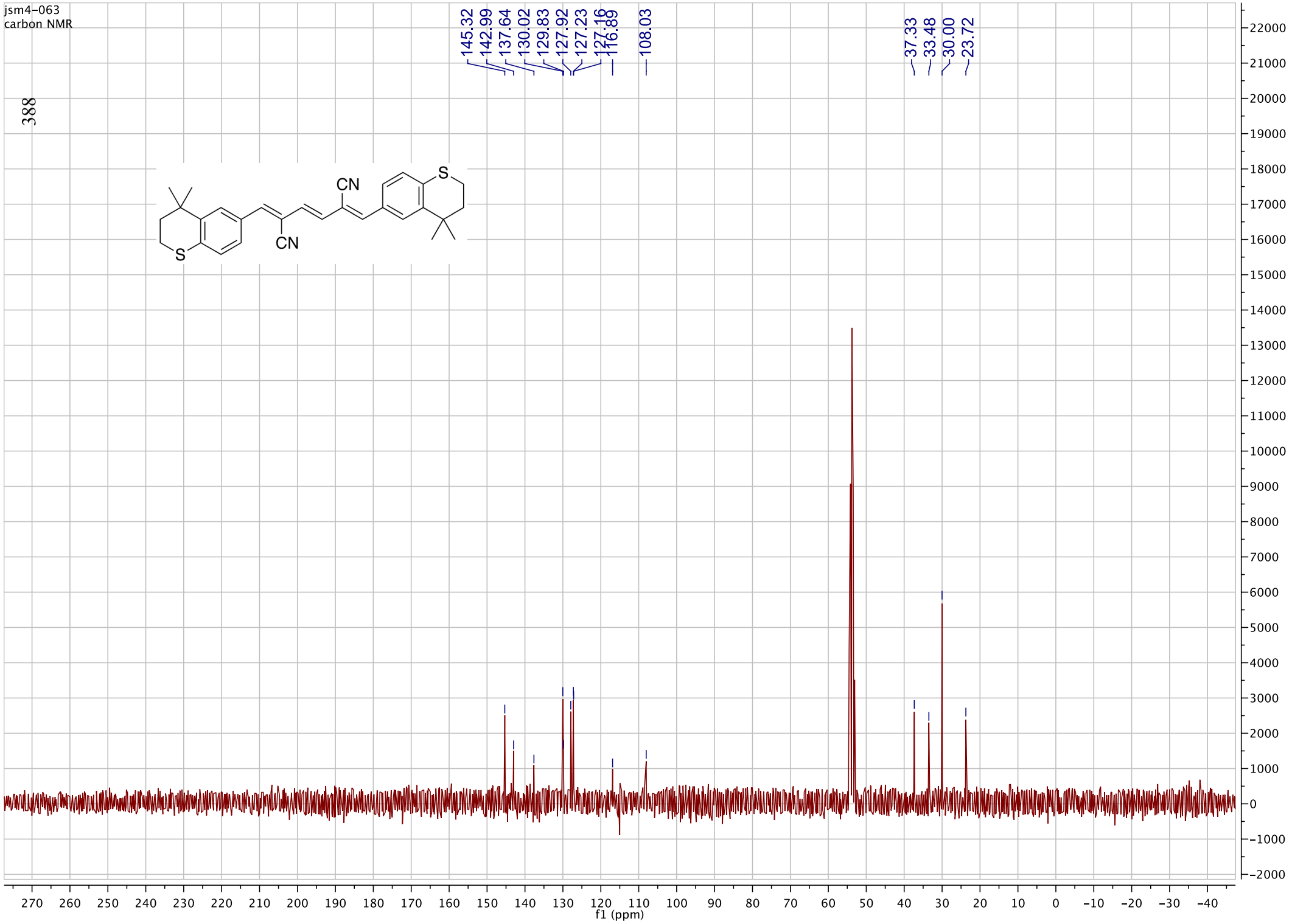
jsm4-077
carbon NMR

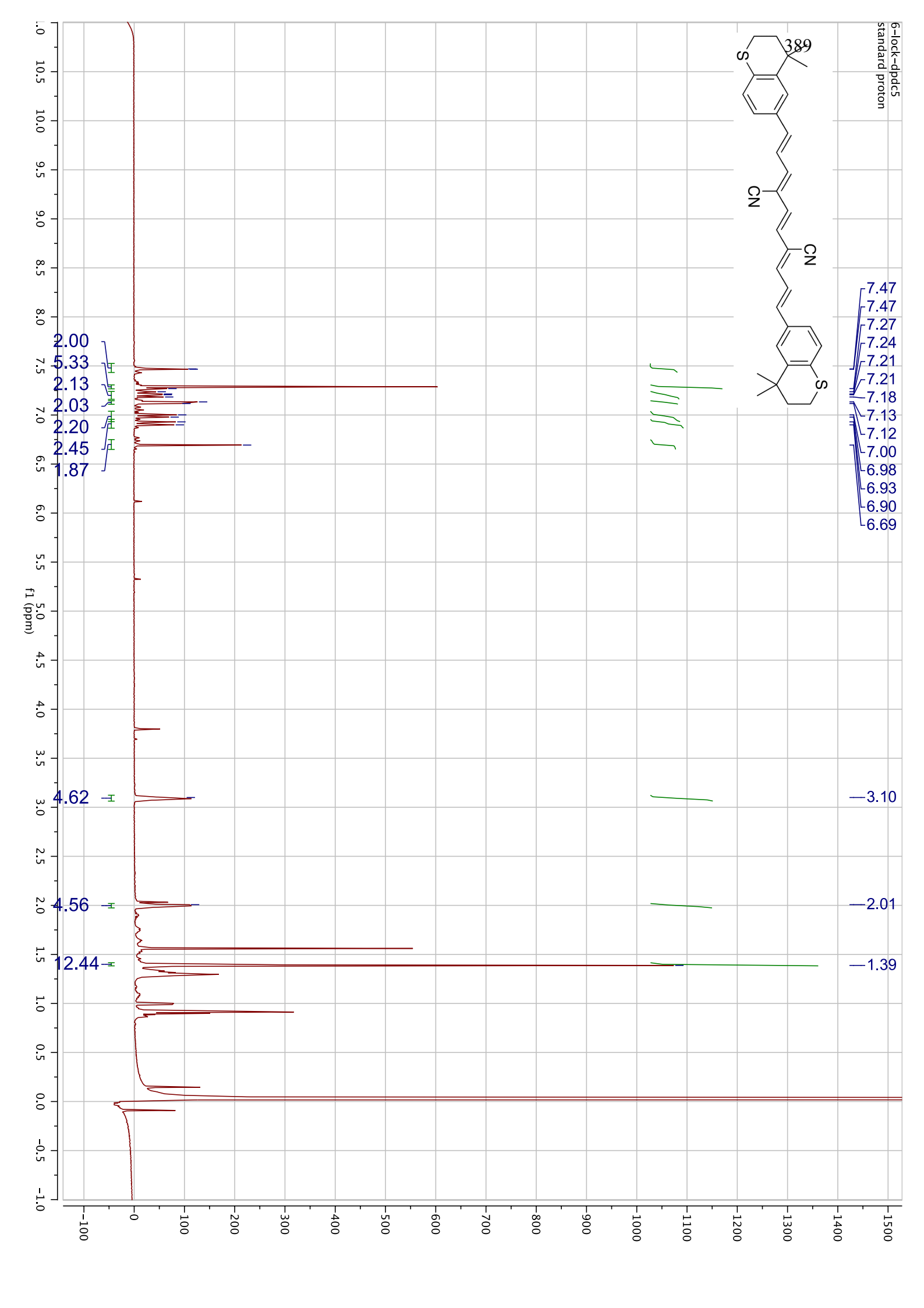


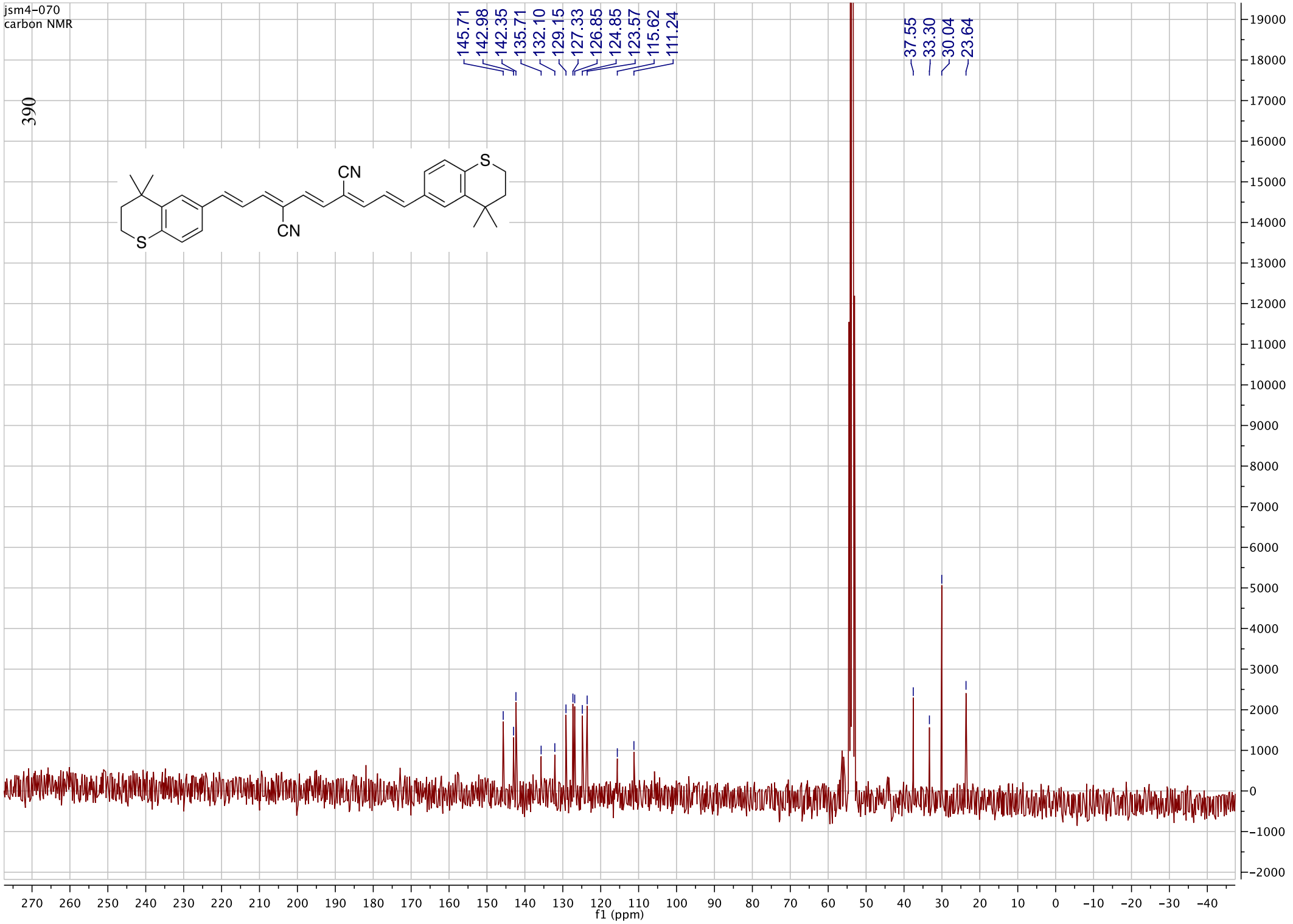
193.56
152.05
143.05
142.74
139.29
137.32
135.06
133.37
132.88
132.38
131.87
131.14
130.14
127.66
127.09
125.59
124.12
53.83
37.81
33.29
30.17
23.56

f1 (ppm)

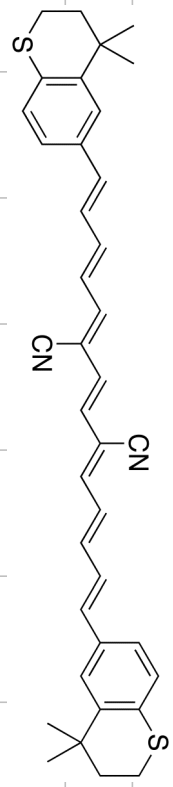

jsm4-063
proton
f1 (ppm)
2.00
2.01
2.00
2.05
2.04
4.03
4.06
12.00
7.92
7.91
7.50
7.50
7.47
7.47
7.16
7.13
7.09
6.78
3.09
3.07
3.05
2.00
1.98
1.96
1.38
CN
CN
S
S


jsm4-063
carbon NMR
388
145.32
142.99
137.64
130.02
129.83
127.92
127.23
127.16
116.89
108.03
37.33
33.48
30.00
23.72
CN
CN
S
S
f1 (ppm)


6-lock-dpdc5
standard proton
389
S
CN
CN
S
7.47
7.47
7.27
7.24
7.21
7.21
7.18
7.13
7.12
7.00
6.98
6.93
6.90
6.69
2.00
5.33
2.13
2.03
2.20
2.45
1.87
4.62
4.56
12.44
3.10
2.01
1.39
f1 (ppm)


jsm4-070
carbon NMR
390
145.71
142.98
142.35
135.71
132.10
129.15
127.33
126.85
124.85
123.57
115.62
111.24
37.55
33.30
30.04
23.64
CN
CN
S
S
f1 (ppm)

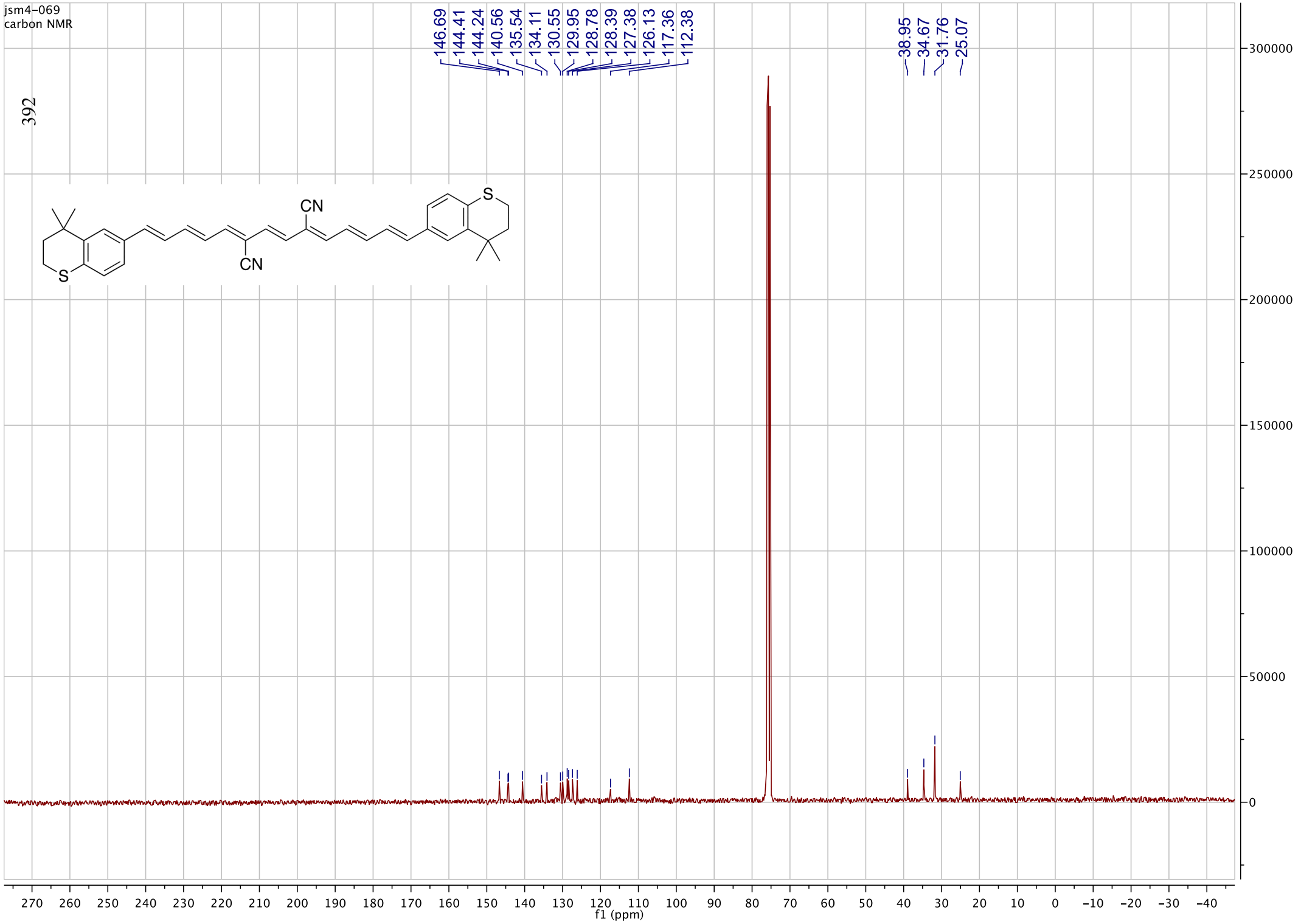
jsm4-069
proton standard

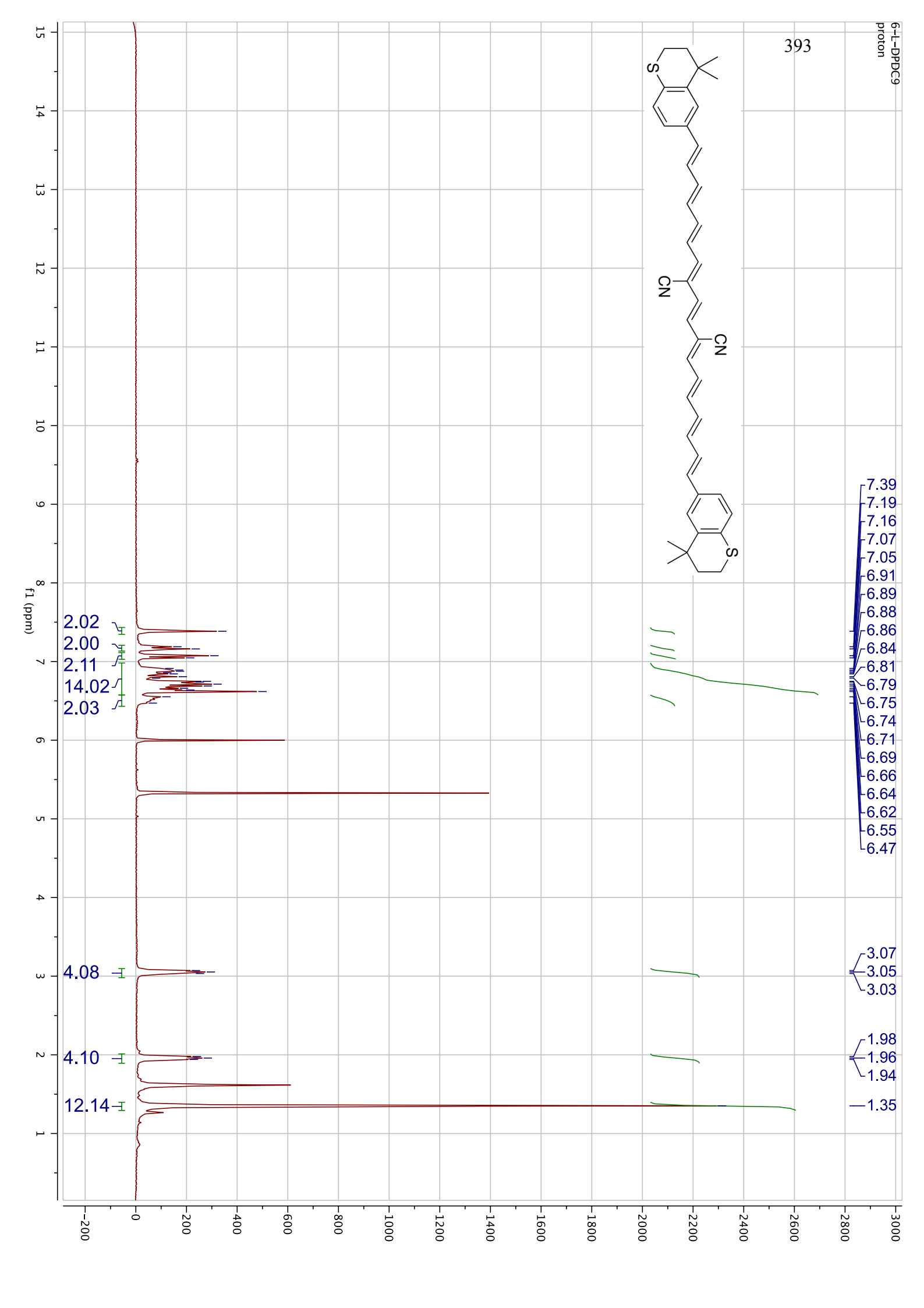


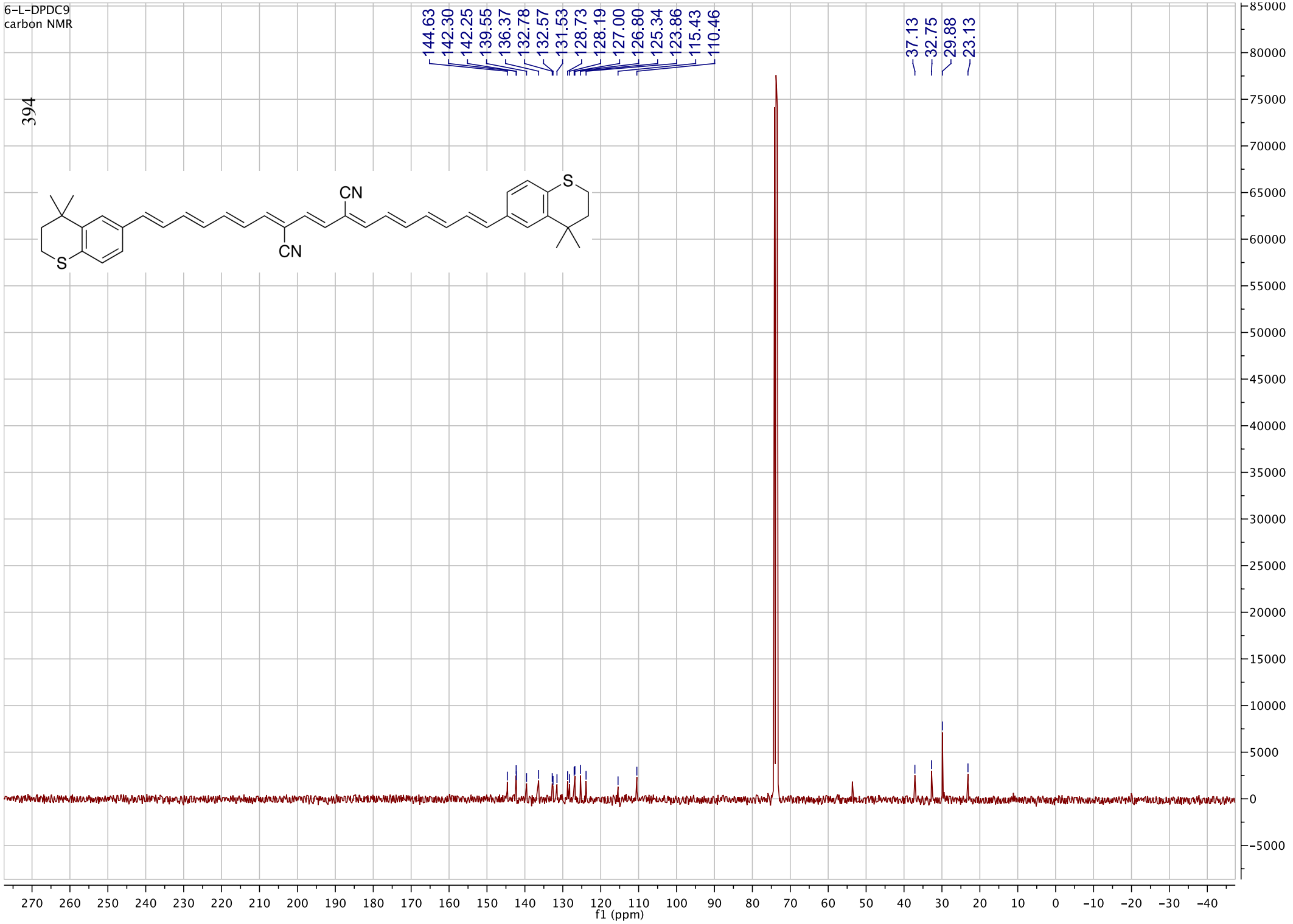
7.43
7.42
7.16
7.16
7.14
7.13
7.04
7.01
6.95
6.91
6.90
6.81
6.76
6.71
6.63

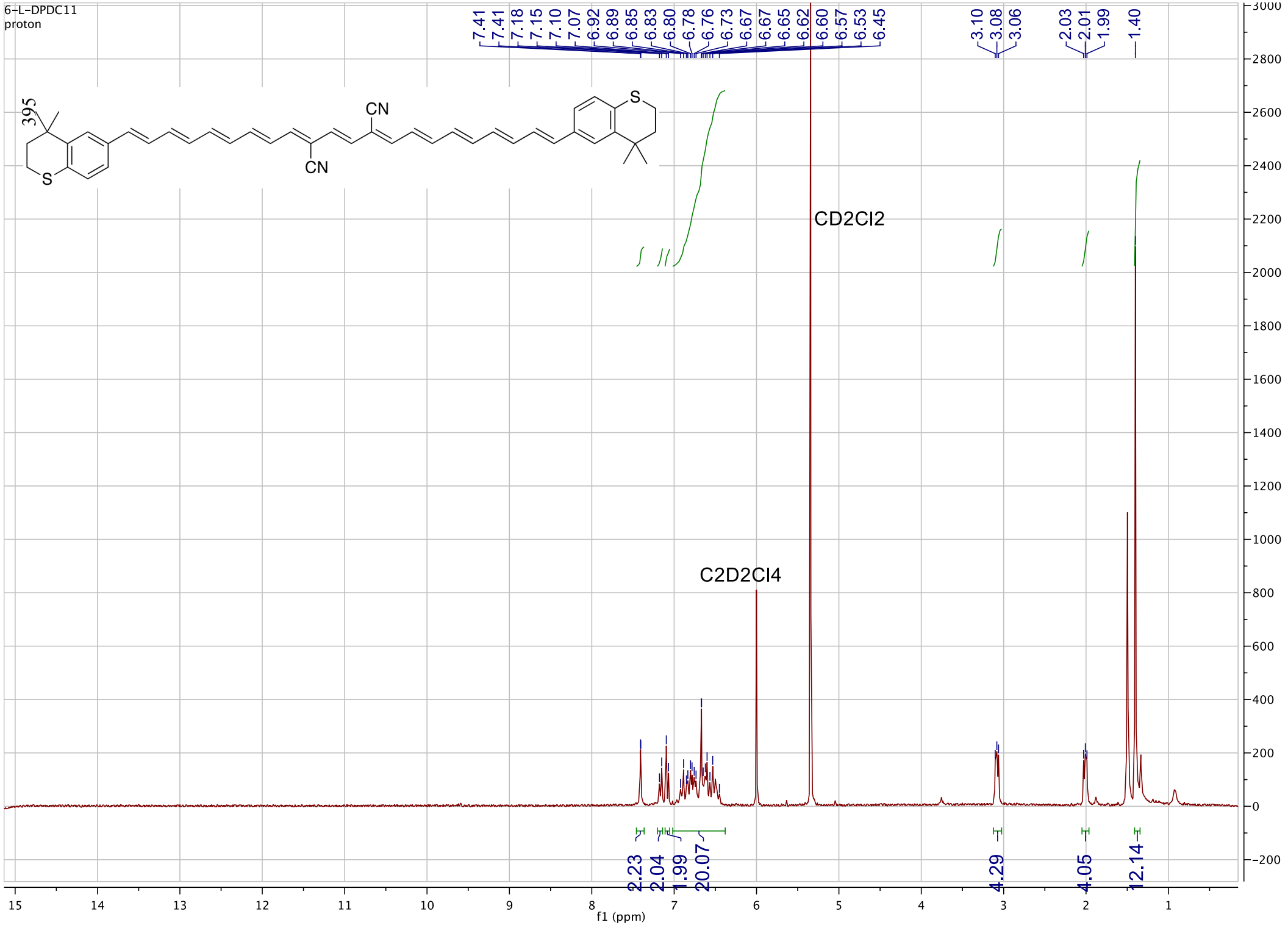
2.00
2.06
2.07
10.12
2.00
10.83
4.02
4.06
12.03
1.32

f1 (ppm)

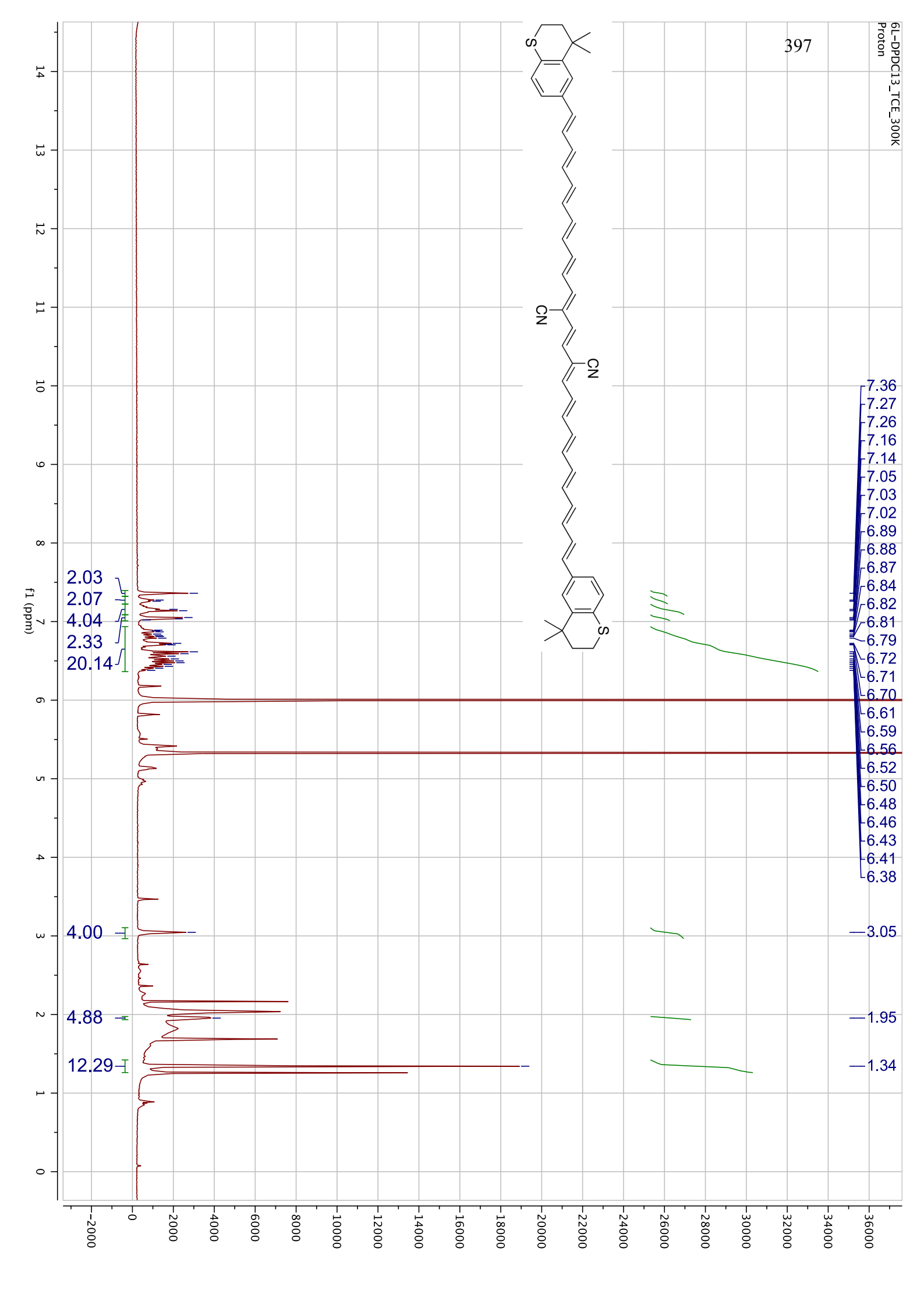

jsm4-069
carbon NMR
392
146.69
144.41
144.24
140.56
135.54
134.11
130.55
129.95
128.78
128.39
127.38
126.13
117.36
112.38
38.95
34.67
31.76
25.07
CN
CN
S
S
300000
250000
200000
150000
100000
50000
0
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)

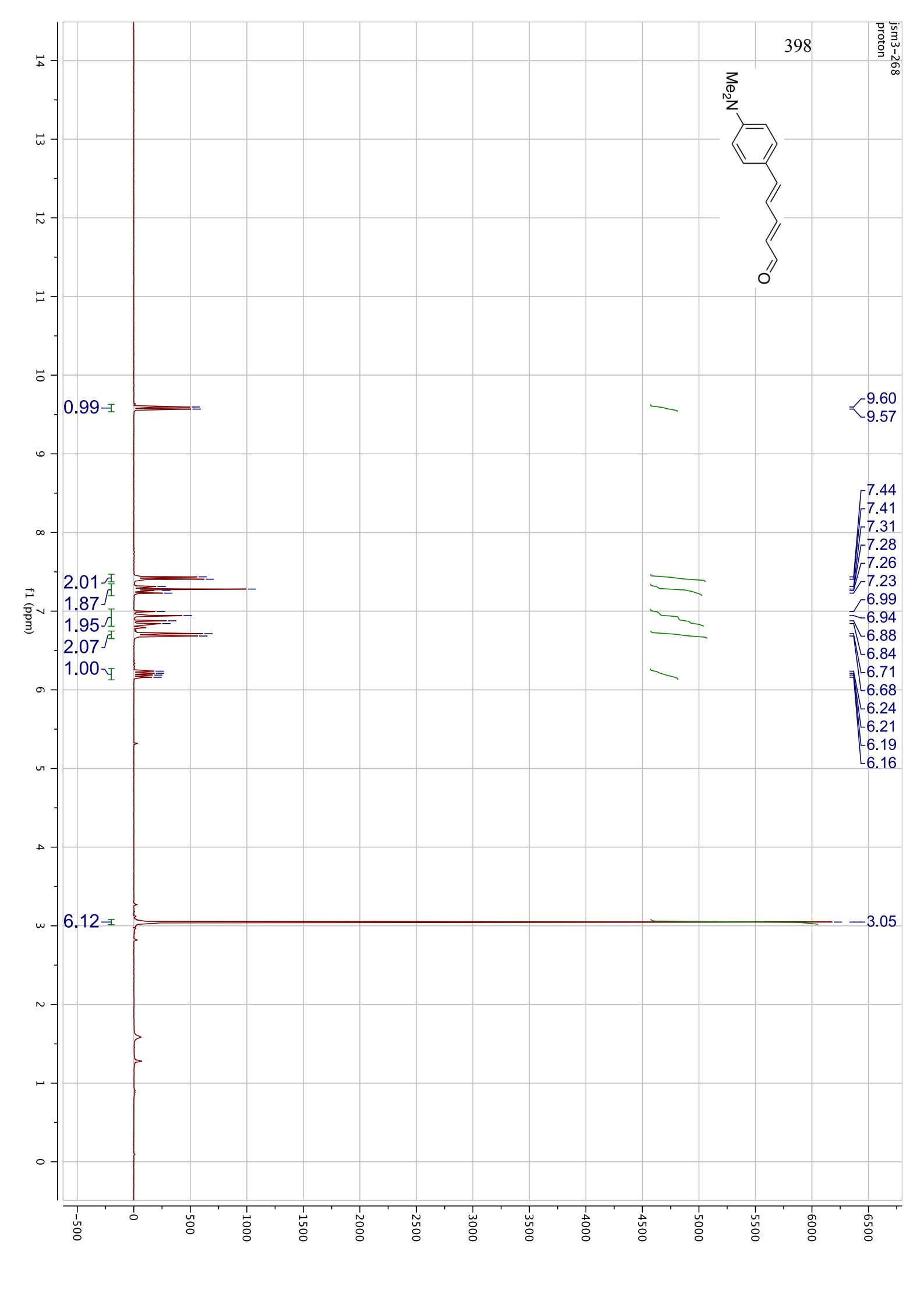

393
6-L-DPDC9
proton
S
CN
CN
S
f1 (ppm)
2.02
2.00
2.11
14.02
2.03
4.08
4.10
12.14
7.39
7.19
7.16
7.07
7.05
6.91
6.89
6.88
6.86
6.84
6.81
6.79
6.75
6.74
6.71
6.69
6.66
6.64
6.62
6.55
6.47
3.07
3.05
3.03
1.98
1.96
1.94
1.35

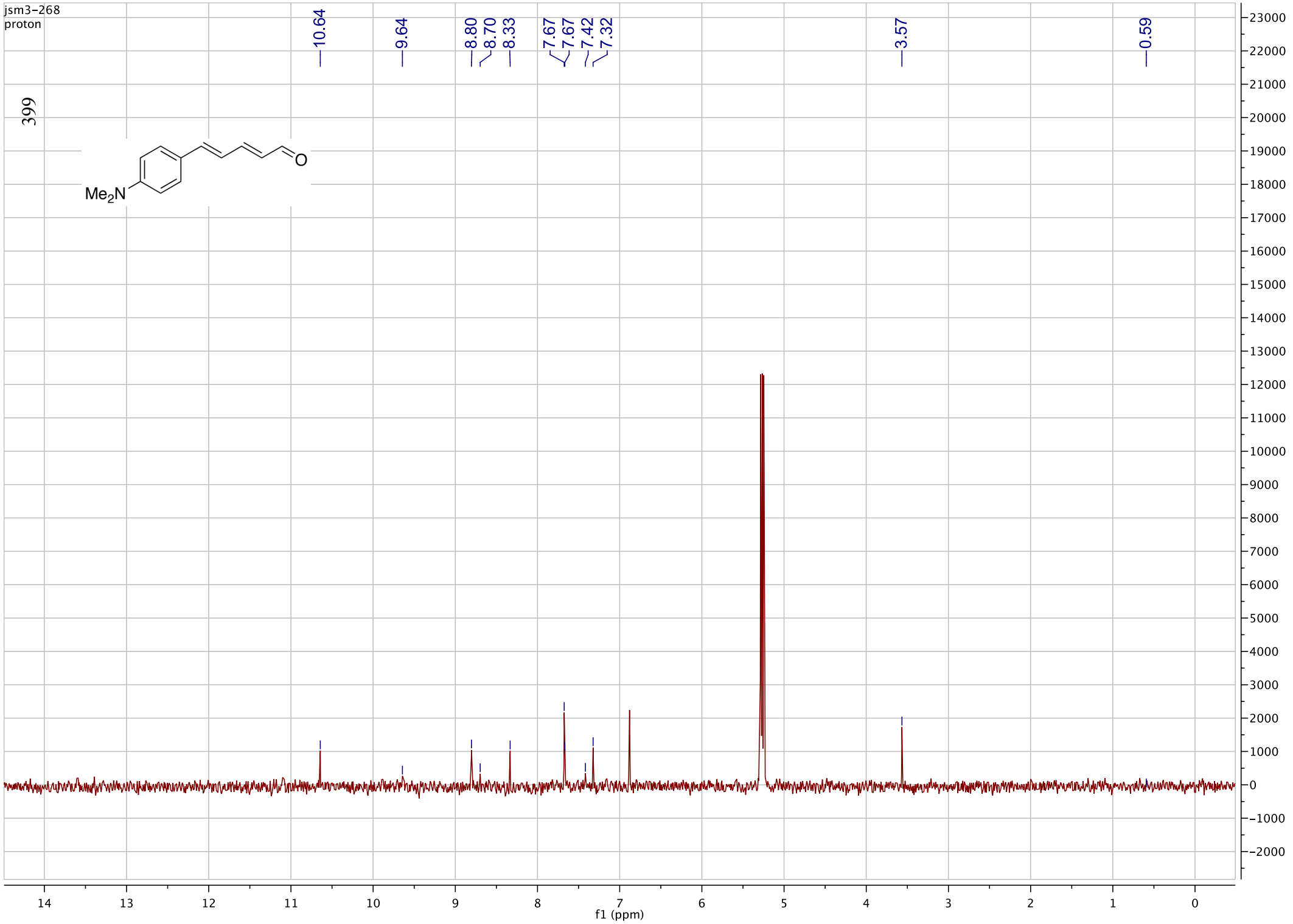

6-L-DPDC9
carbon NMR
394
144.63
142.30
142.25
139.55
136.37
132.78
132.57
131.53
128.73
128.19
127.00
126.80
125.34
123.86
115.43
110.46
37.13
32.75
29.88
23.13
CN
CN
S
S
f1 (ppm)

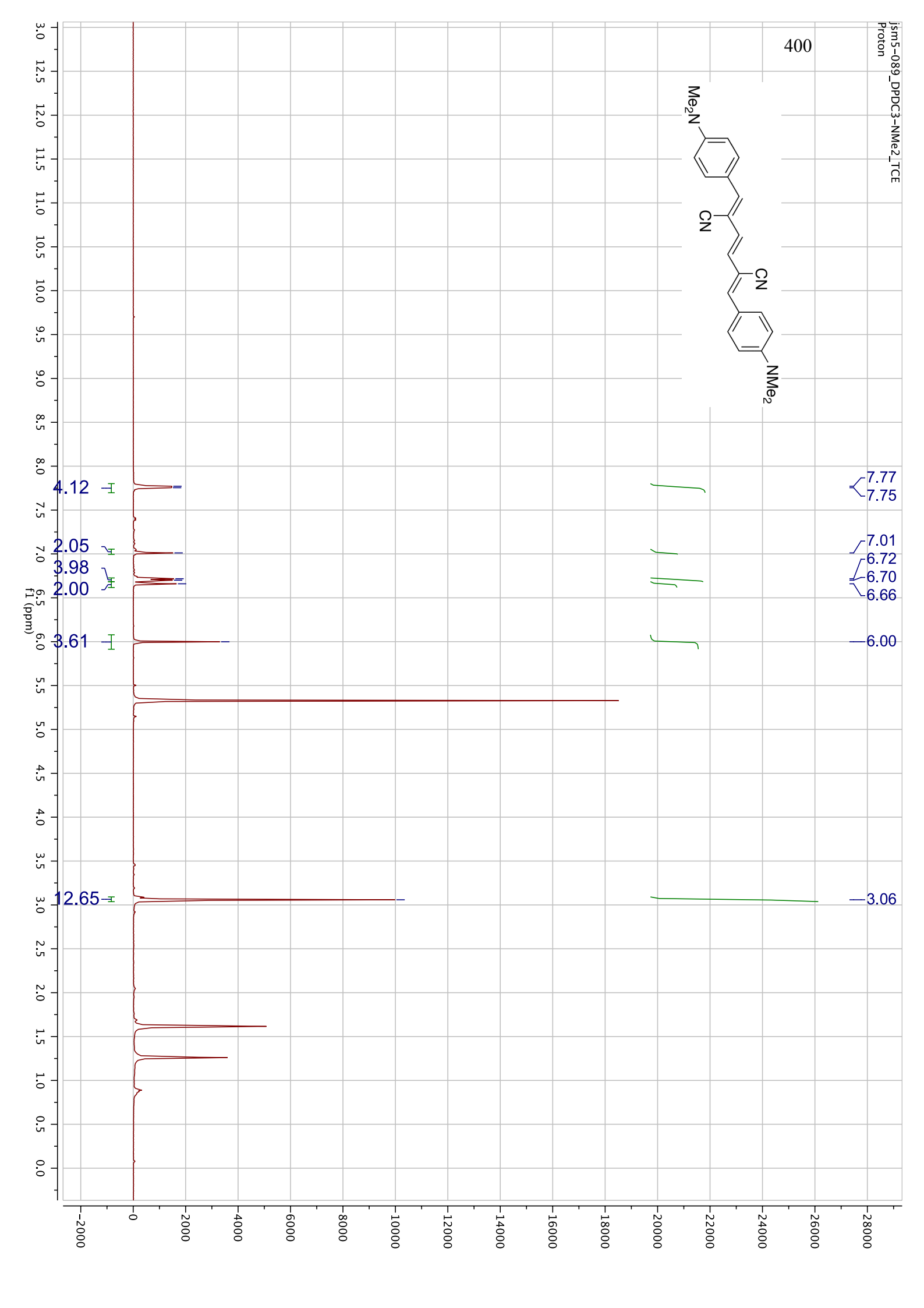

6-L-DPDC11
proton
7.41
7.41
7.18
7.15
7.10
7.07
6.92
6.89
6.85
6.83
6.80
6.78
6.76
6.73
6.67
6.67
6.65
6.62
6.60
6.57
6.53
6.45
3.10
3.08
3.06
2.03
2.01
1.99
1.40
395
CN
CN
S
S
CD2Cl2
C2D2Cl4
2.23
2.04
1.99
20.07
4.29
4.05
12.14
f1 (ppm)

396
jsm4-081-DPDC11-6Lock_CDCl3
144.49
142.19
142.14
139.32
137.34
135.09
133.04
133.02
132.48
132.21
129.06
128.61
127.38
126.93
125.14
123.92
115.40
110.93
37.49
33.00
30.07
23.20
CN
CN
S
S
f1 (ppm)

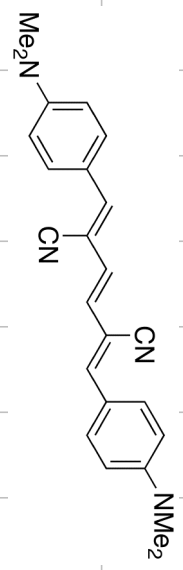

6L-DPDC13_TCE_300K
Proton
f1 (ppm)
CN
CN
S
S
7.36
7.27
7.26
7.16
7.14
7.05
7.03
7.02
6.89
6.88
6.87
6.84
6.82
6.81
6.79
6.72
6.71
6.70
6.61
6.59
6.56
6.52
6.50
6.48
6.46
6.43
6.41
6.38
2.03
2.07
4.04
2.33
20.14
4.00
4.88
12.29
3.05
1.95
1.34


jsm3-268
proton
Me2N
O
0.99
2.01
1.87
1.95
2.07
1.00
6.12
9.60
9.57
7.44
7.41
7.31
7.28
7.26
7.23
6.99
6.94
6.88
6.84
6.71
6.68
6.24
6.21
6.19
6.16
3.05
f1 (ppm)


jsm3-268
proton
399
10.64
9.64
8.80
8.70
8.33
7.67
7.67
7.42
7.32
3.57
0.59
Me2N
O
f1 (ppm)

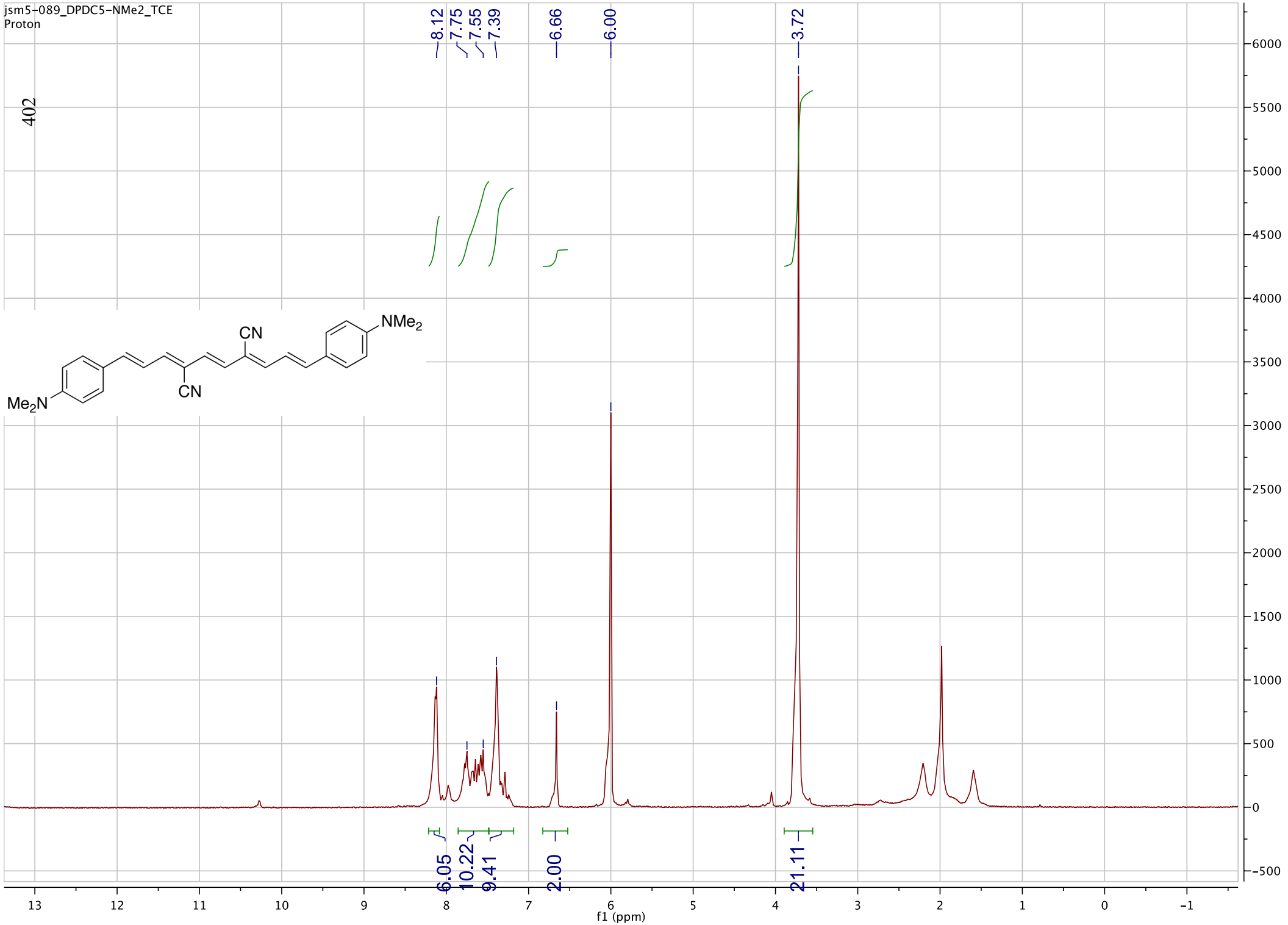

400
jsm5-089_DPDC3-NMe2_TCE
Proton
Me2N
CN
CN
NMe2
4.12
2.05
3.98
2.00
3.61
12.65
7.77
7.75
7.01
6.72
6.70
6.66
6.00
3.06
f1 (ppm)

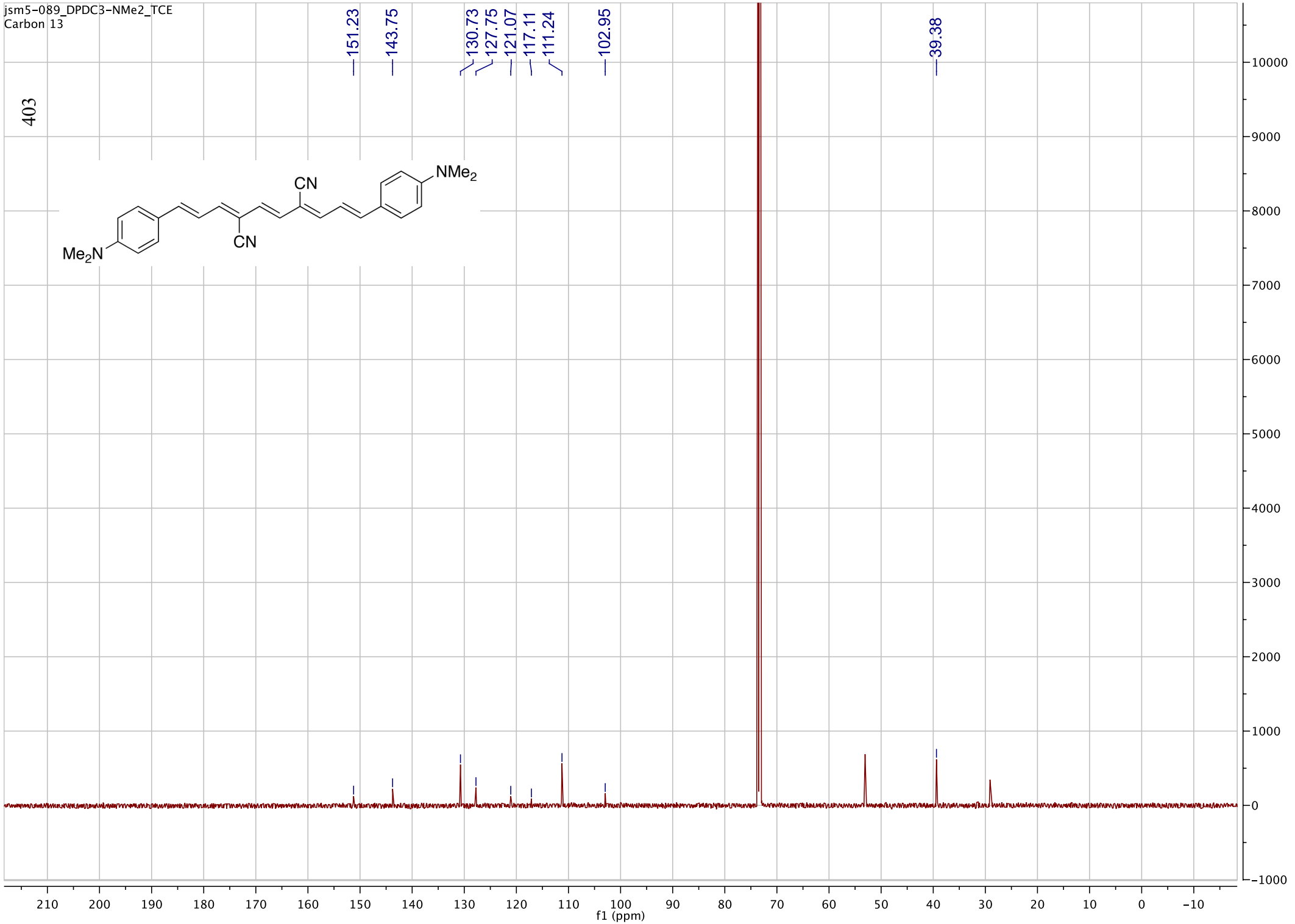
jsm5-089_DPDC3-NMe2_TCE
Carbon 13

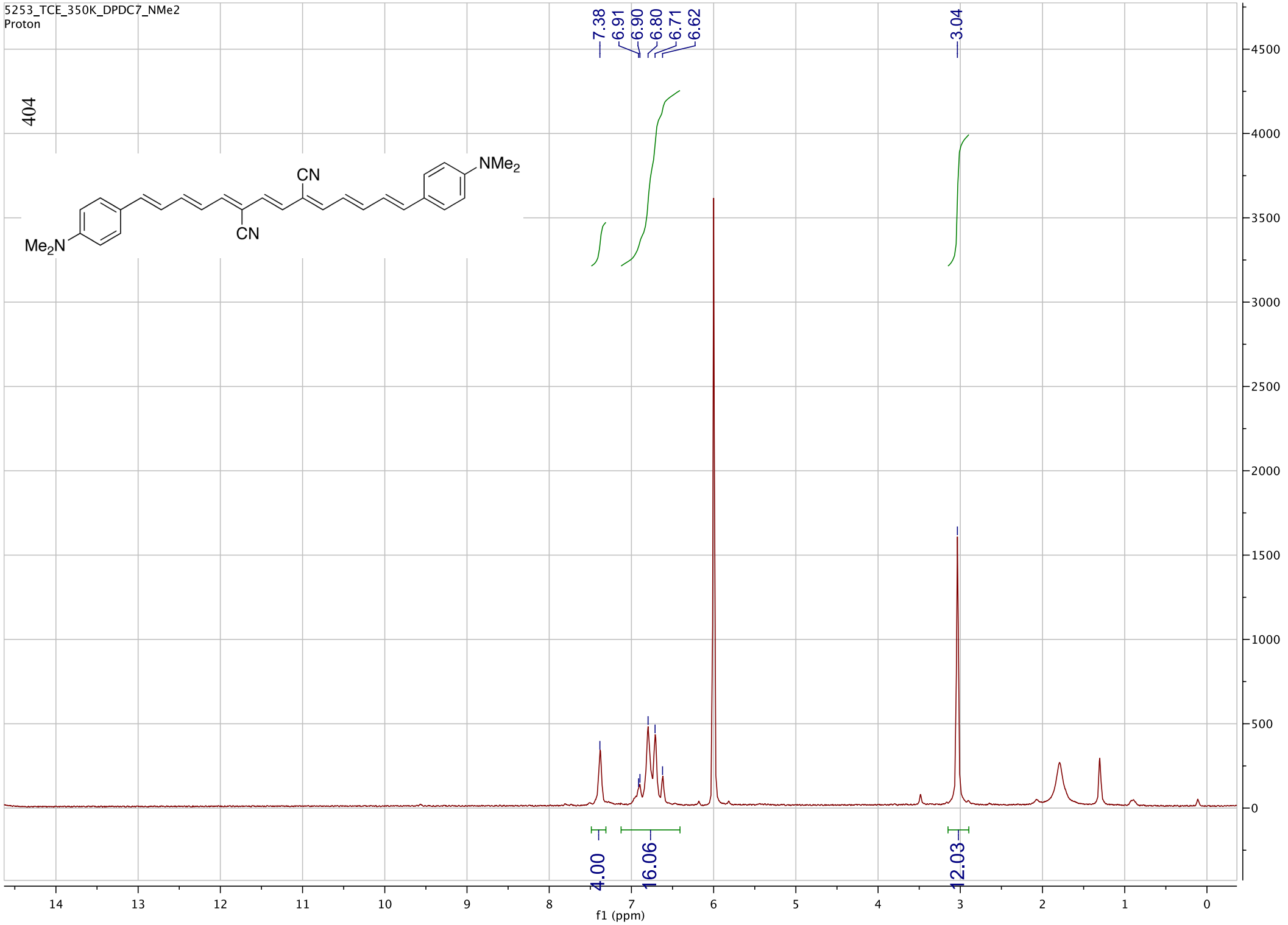


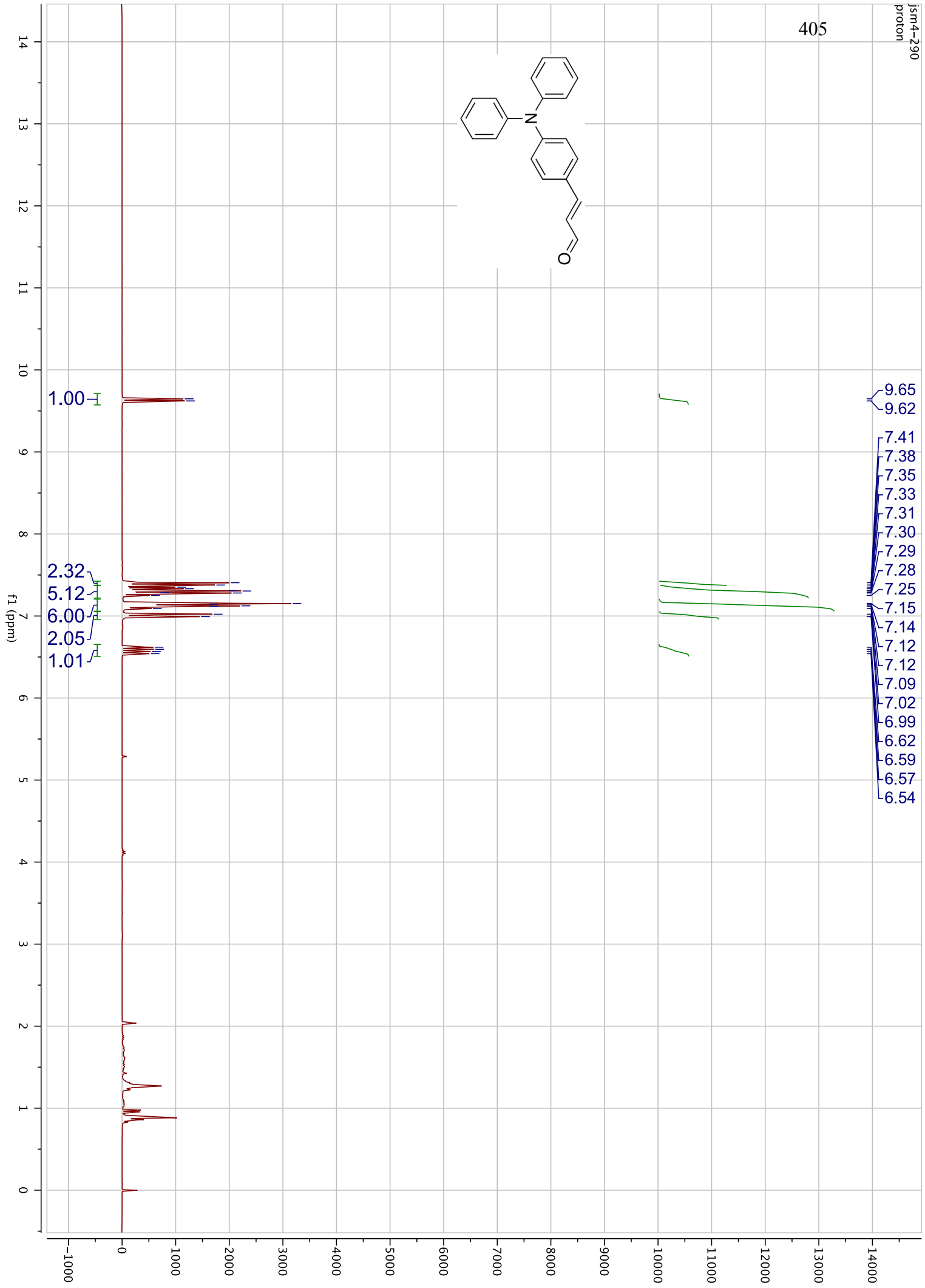
151.23
143.75
130.73
127.75
121.07
117.11
111.24
102.95
39.38

f1 (ppm)

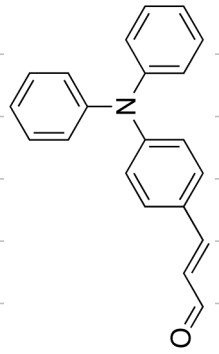

jsm5-089_DPDC5-NMe2_TCE
Proton
402
8.12
7.75
7.55
7.39
6.66
6.00
3.72
NMe2
CN
CN
Me2N
6.05
10.22
9.41
2.00
21.11
f1 (ppm)


jsm5-089_DPDC3-NMe2_TCE
Carbon 13
403
151.23
143.75
130.73
127.75
121.07
117.11
111.24
102.95
39.38
CN
CN
NMe2
Me2N
f1 (ppm)


5253_TCE_350K_DPDC7_NMe2
Proton
404
7.38
6.91
6.90
6.80
6.71
6.62
3.04
CN
CN
NMe2
Me2N
4.00
16.06
12.03
f1 (ppm)


jsm4-290
proton
f1 (ppm)
1.00
2.32
5.12
6.00
2.05
1.01
9.65
9.62
7.41
7.38
7.35
7.33
7.31
7.30
7.29
7.28
7.25
7.15
7.14
7.12
7.12
7.09
7.02
6.99
6.62
6.59
6.57
6.54
N
O

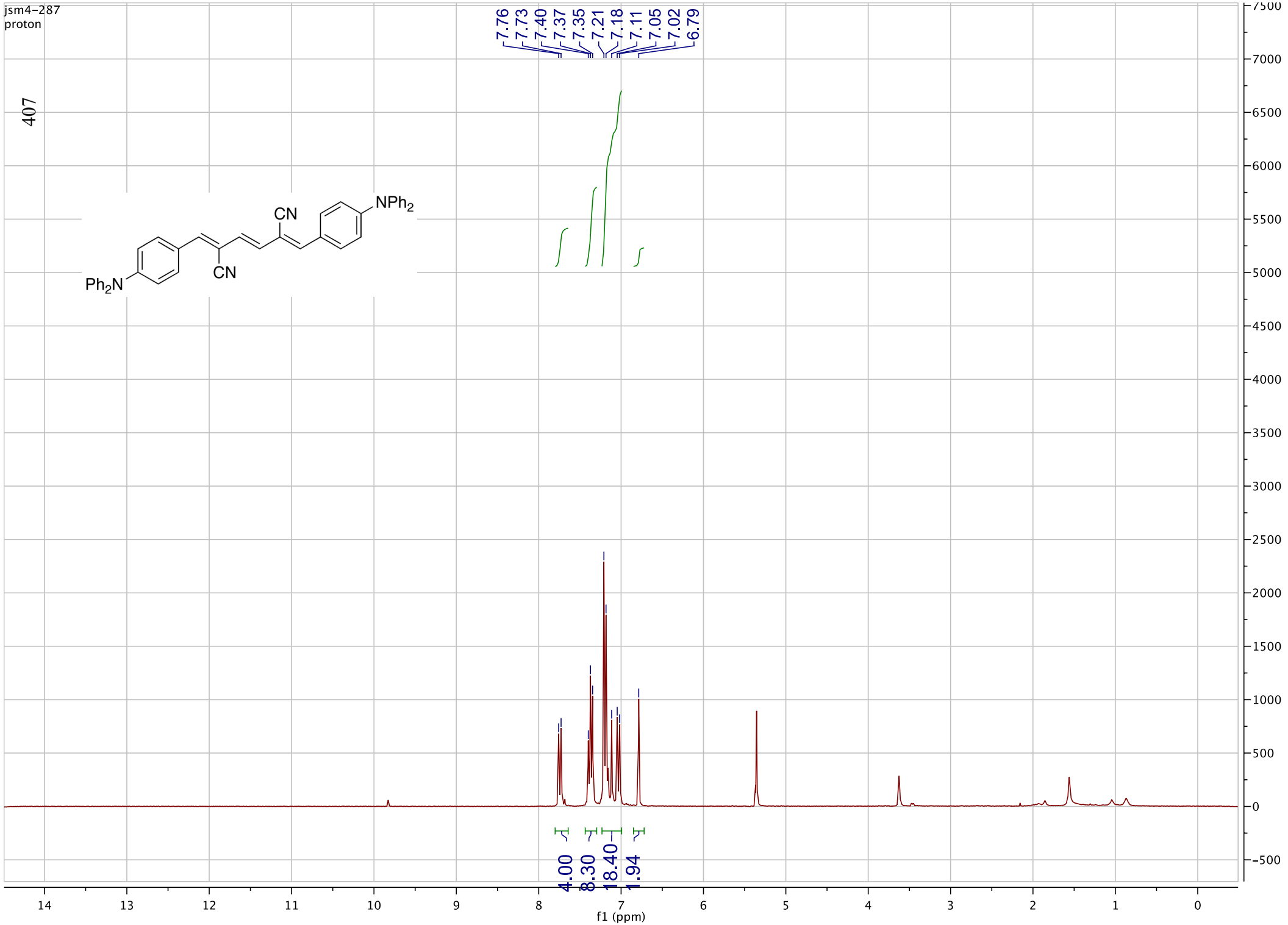
jsm4-290
carbon NMR

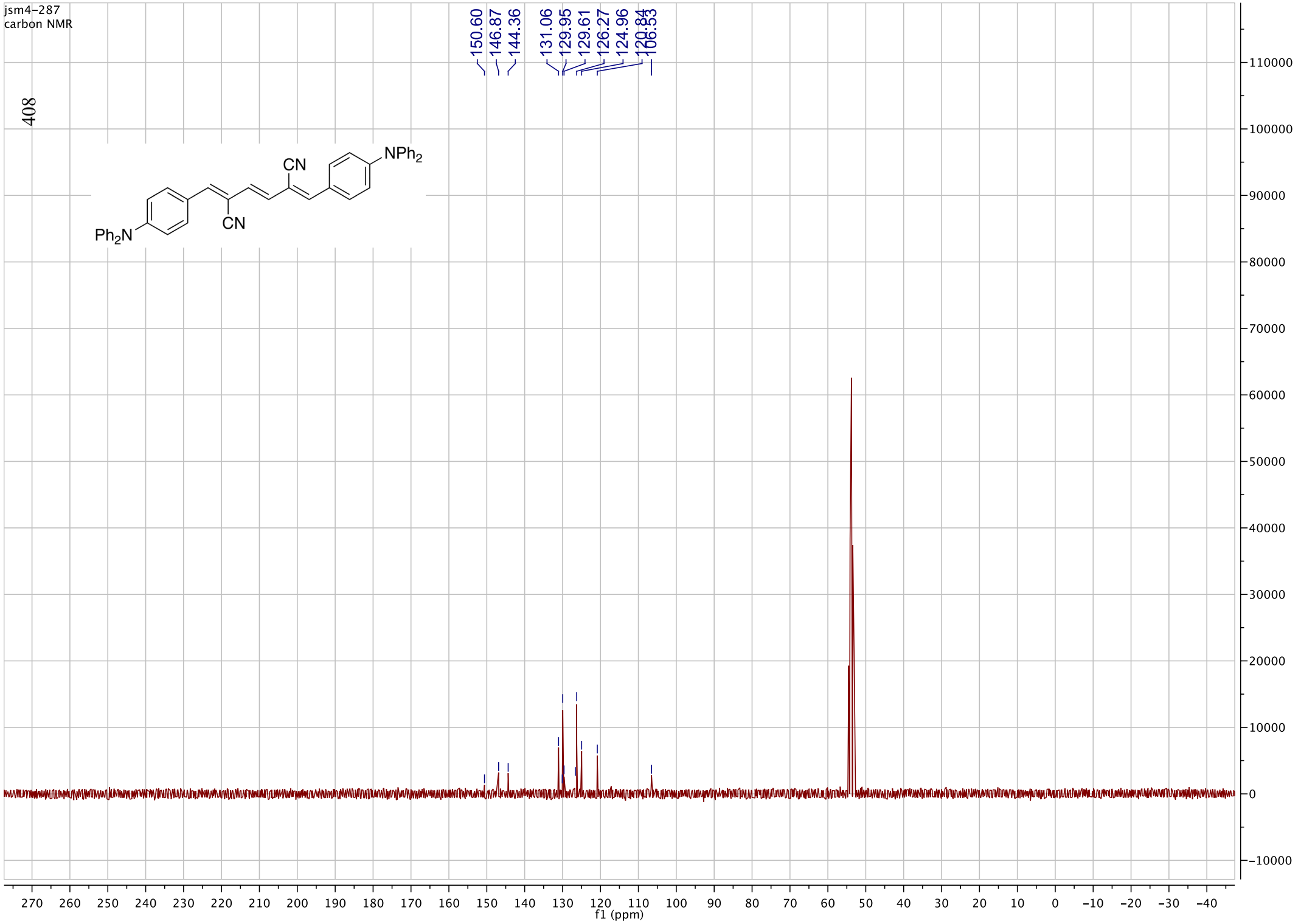


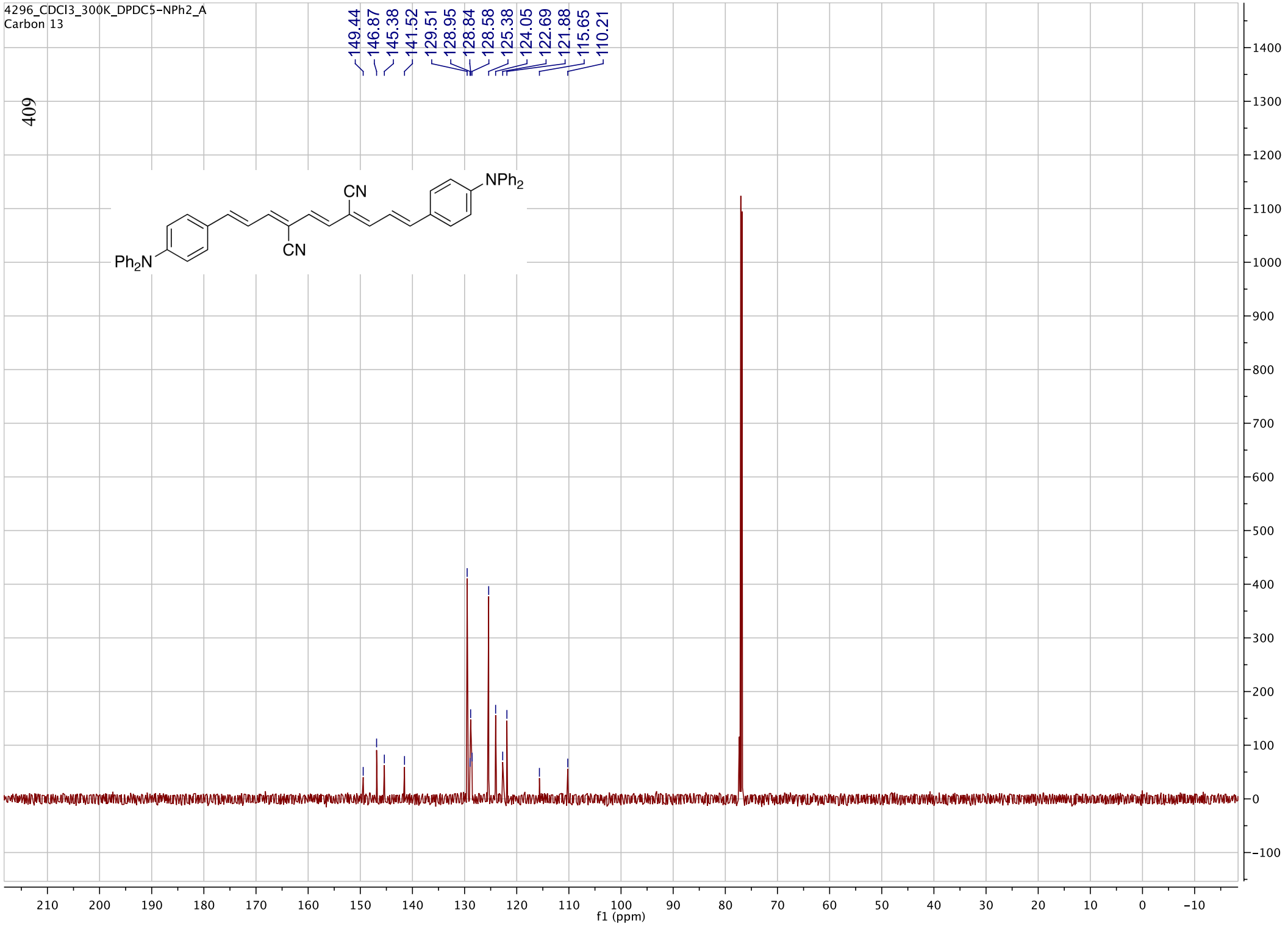
193.99

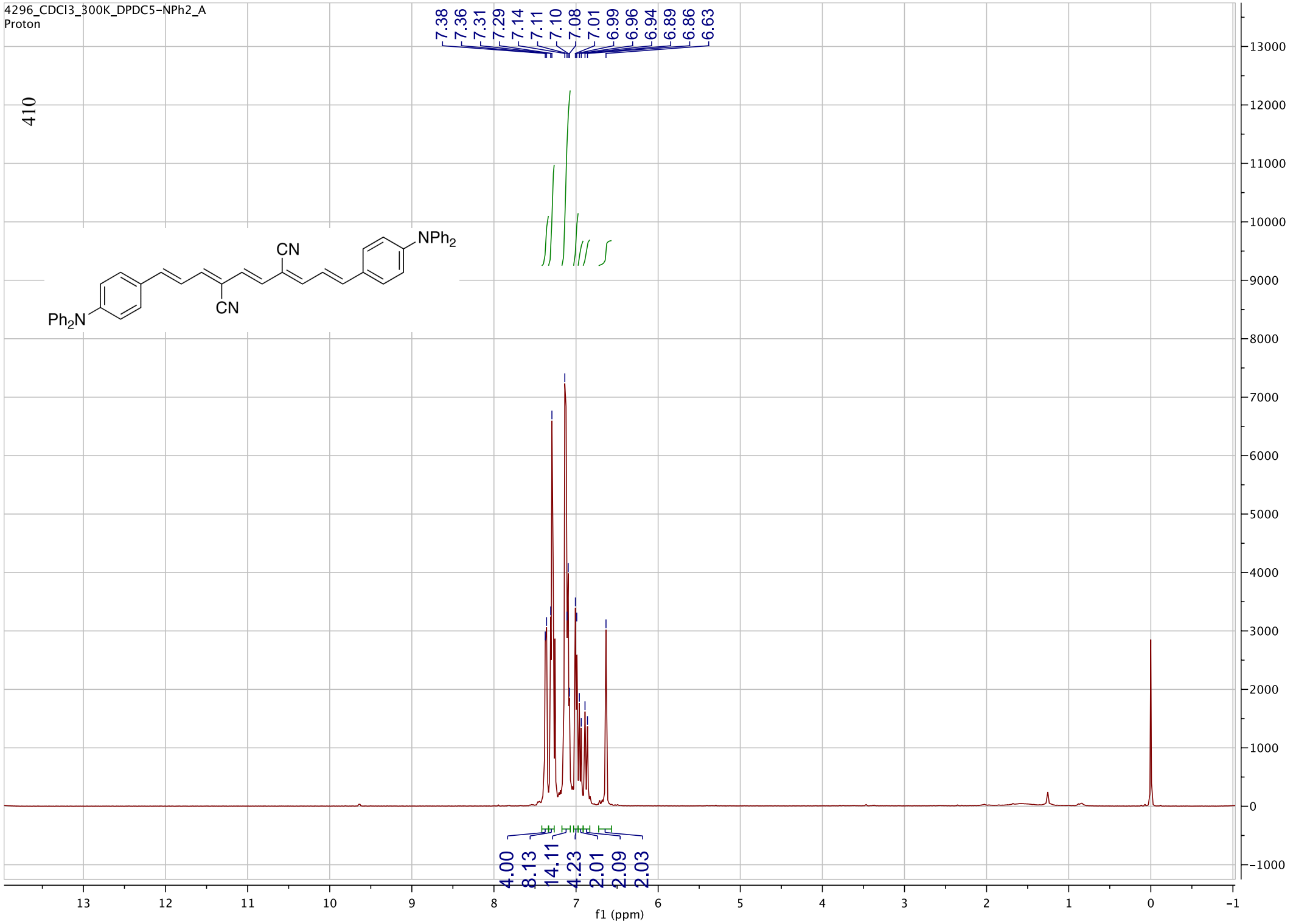
152.96
151.22
147.00
130.21
129.99
127.11
126.46
126.13
124.87
121.45

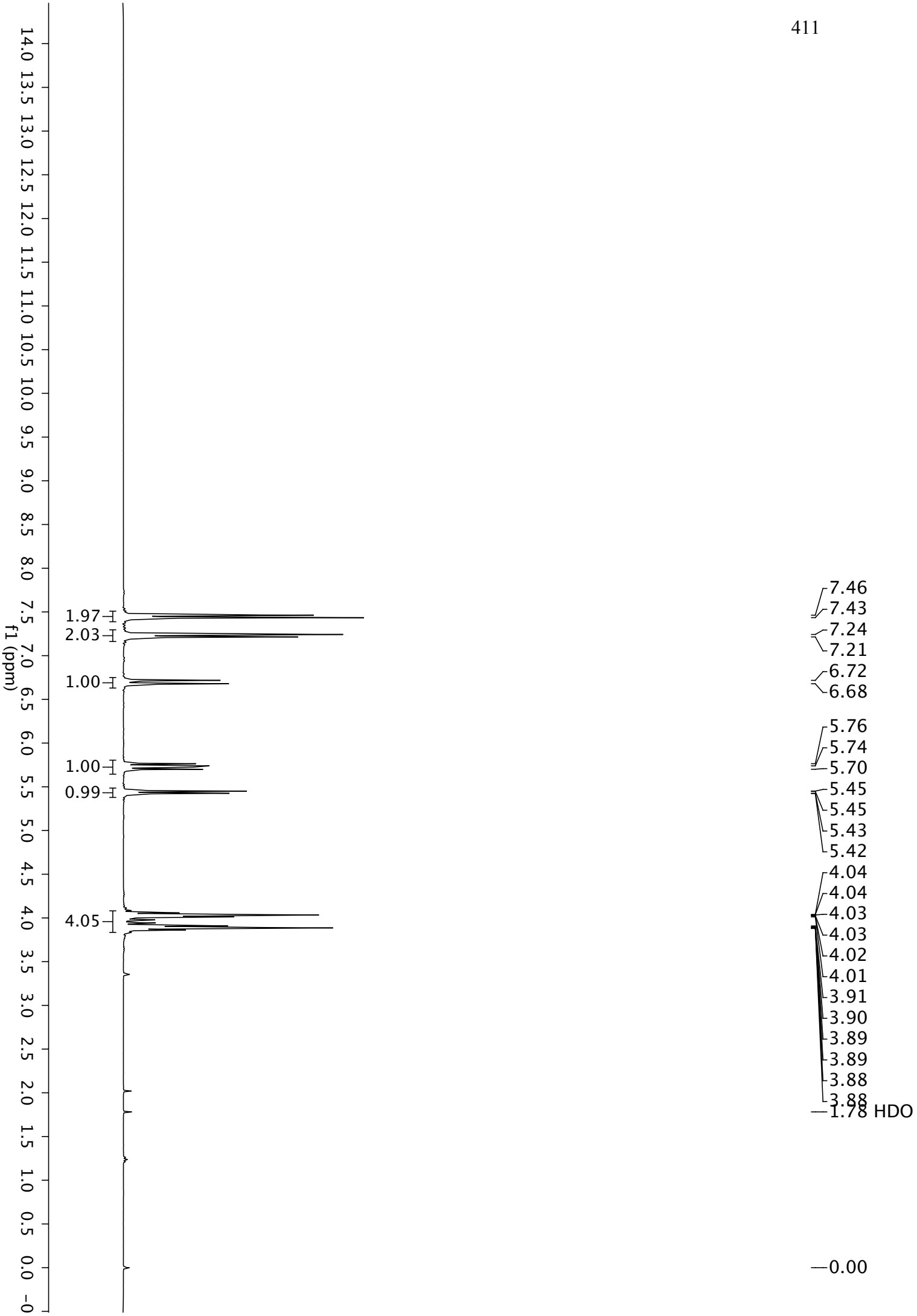
f1 (ppm)


jsm4-287
proton
407
7.76
7.73
7.40
7.37
7.35
7.21
7.18
7.11
7.05
7.02
6.79
CN
NPh2
CN
Ph2N
4.00
8.30
18.40
1.94
f1 (ppm)


jsm4-287
carbon NMR
408
150.60
146.87
144.36
131.06
129.95
129.61
126.27
124.96
120.84
116.53
CN
NPh2
CN
Ph2N
f1 (ppm)


4296_CDCl3_300K_DPDC5-NPh2_A
Carbon 13
149.44
146.87
145.38
141.52
129.51
128.95
128.84
128.58
125.38
124.05
122.69
121.88
115.65
110.21
409
CN
CN
NPh2
Ph2N
f1 (ppm)

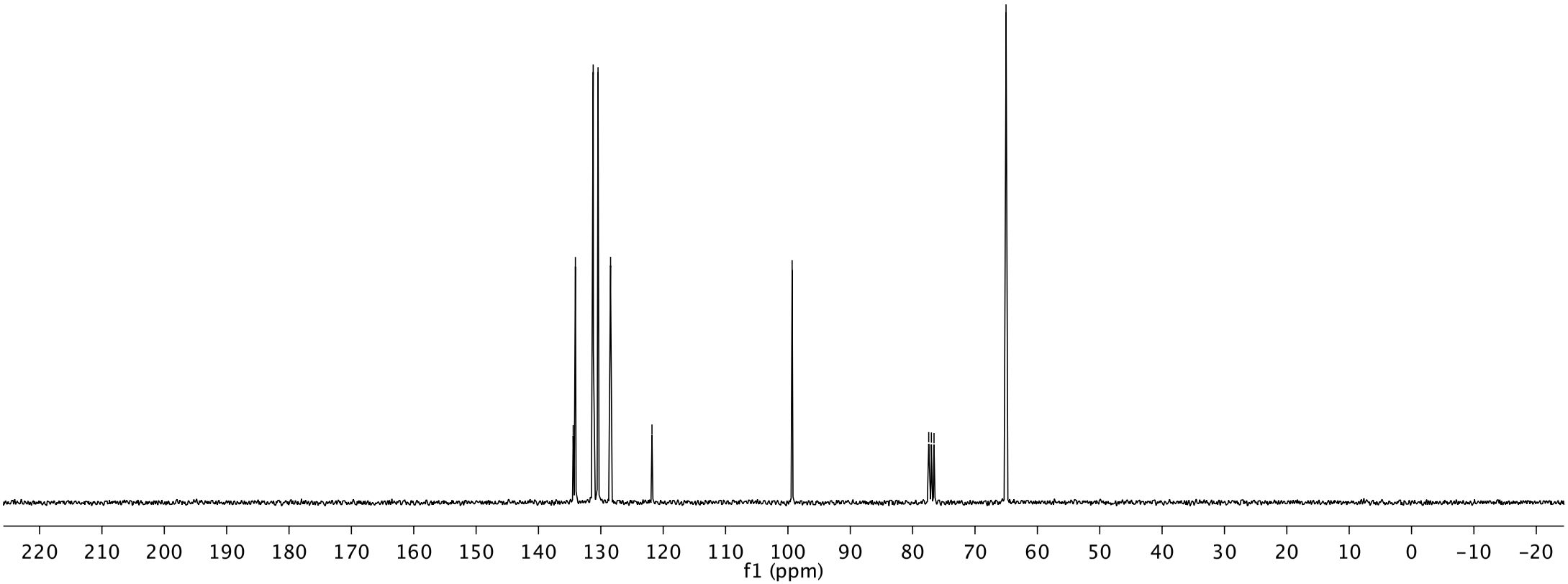

4296_CDCl3_300K_DPDC5-NPh2_A
Proton
410
7.38
7.36
7.31
7.29
7.14
7.11
7.10
7.08
7.01
6.99
6.96
6.94
6.89
6.86
6.63
CN
NPh2
CN
Ph2N
4.00
8.13
14.11
4.23
2.01
2.09
2.03
f1 (ppm)

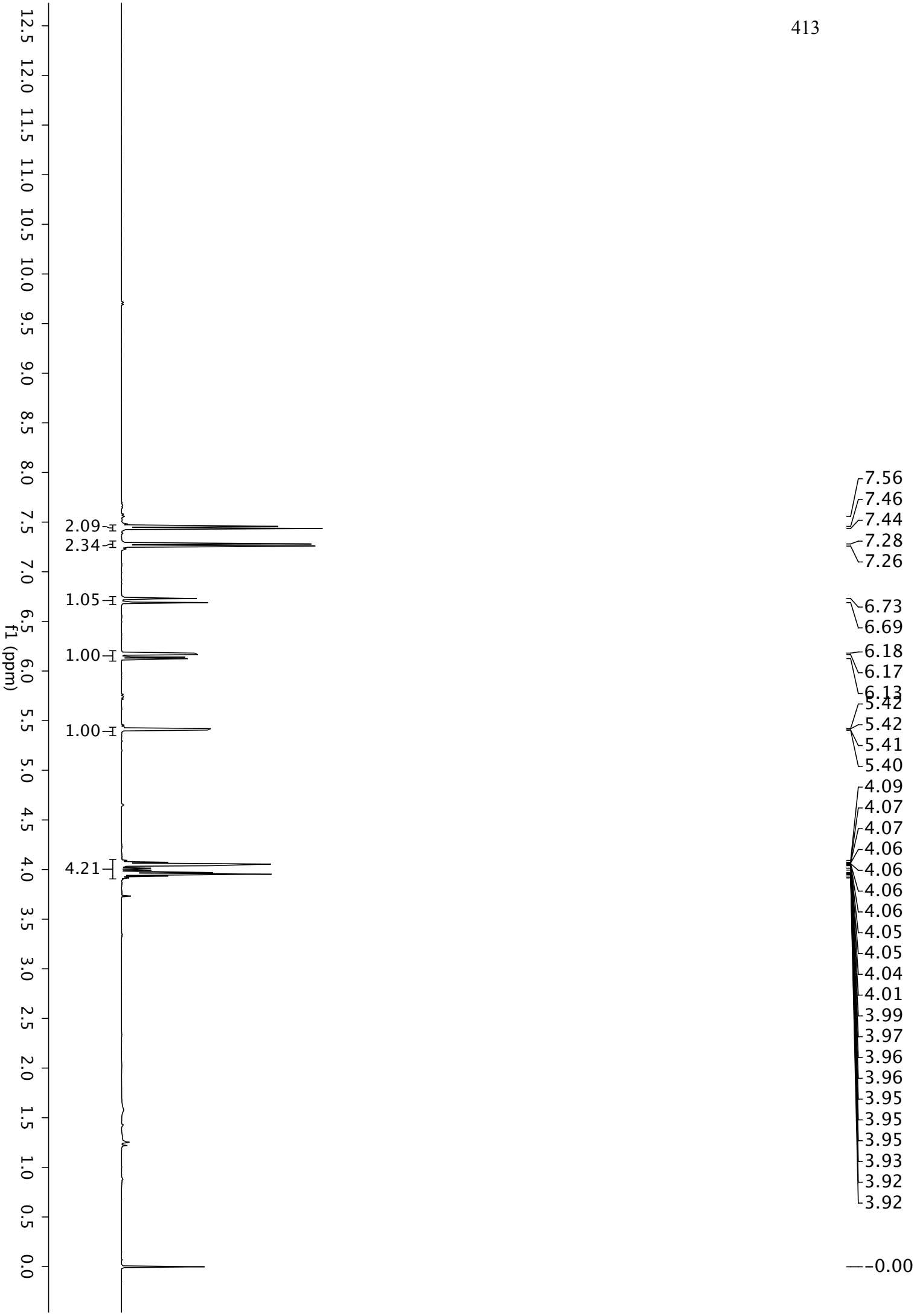

f1 (ppm)
1.97
2.03
1.00
1.00
0.99
4.05
7.46
7.43
7.24
7.21
6.72
6.68
5.76
5.74
5.70
5.45
5.45
5.43
5.42
4.04
4.04
4.03
4.03
4.02
4.01
3.91
3.90
3.89
3.89
3.88
3.88
1.78 HDO
0.00

dfs-2-161
carbon NMR

412

134.43
134.08
131.23
130.45
128.44
121.80
99.33
77.42
77.00
76.57 CDCl3
65.03




f1 (ppm)
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
2.09
2.34
1.05
1.00
1.00
4.21
7.56
7.46
7.44
7.28
7.26
6.73
6.69
6.18
6.17
6.13
5.42
5.42
5.41
5.40
4.09
4.07
4.07
4.06
4.06
4.06
4.06
4.05
4.05
4.04
4.01
3.99
3.97
3.96
3.96
3.95
3.95
3.95
3.93
3.92
3.92
0.00

dfs-1-247

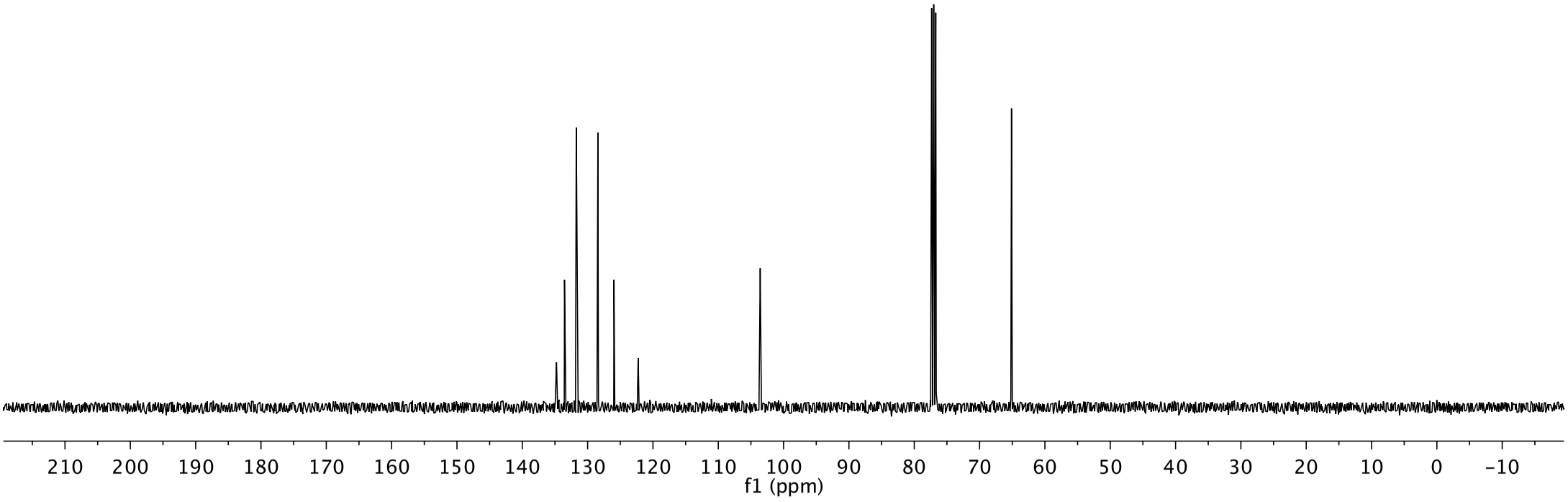
414

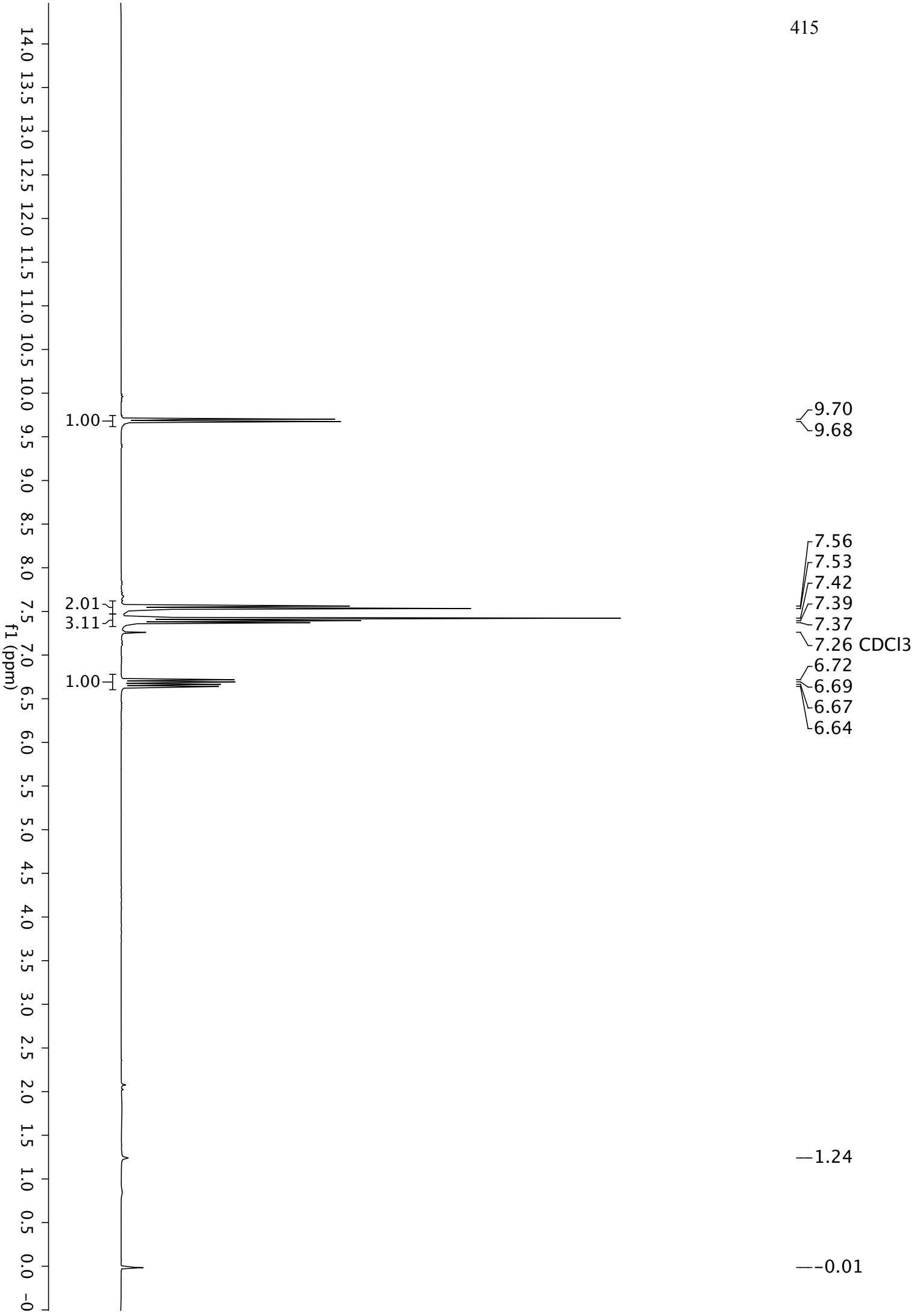
134.8
134.4
133.5
131.7
128.4
126.0
122.3

103.6

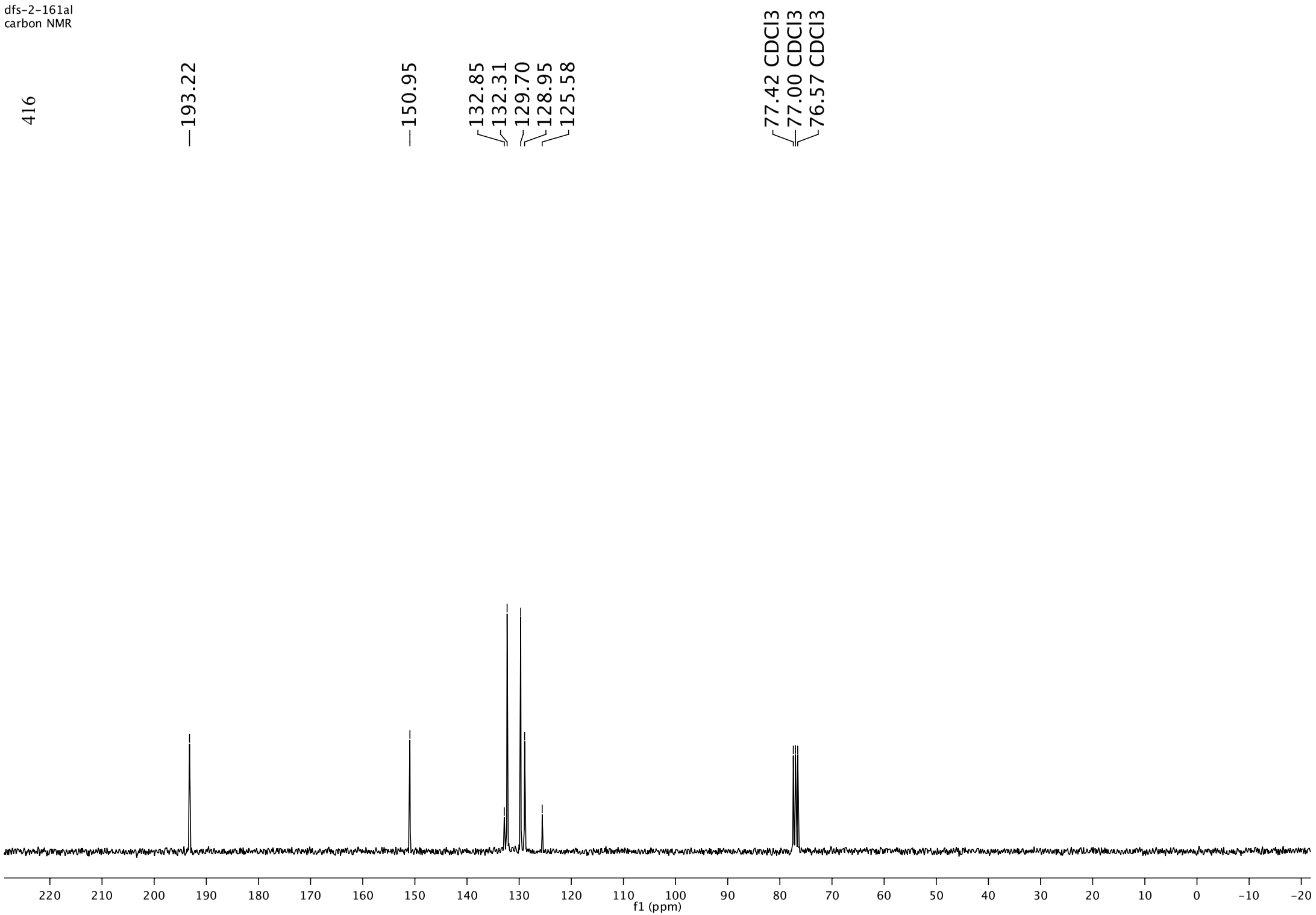
77.3 CDCl3
77.0 CDCl3
76.7 CDCl3

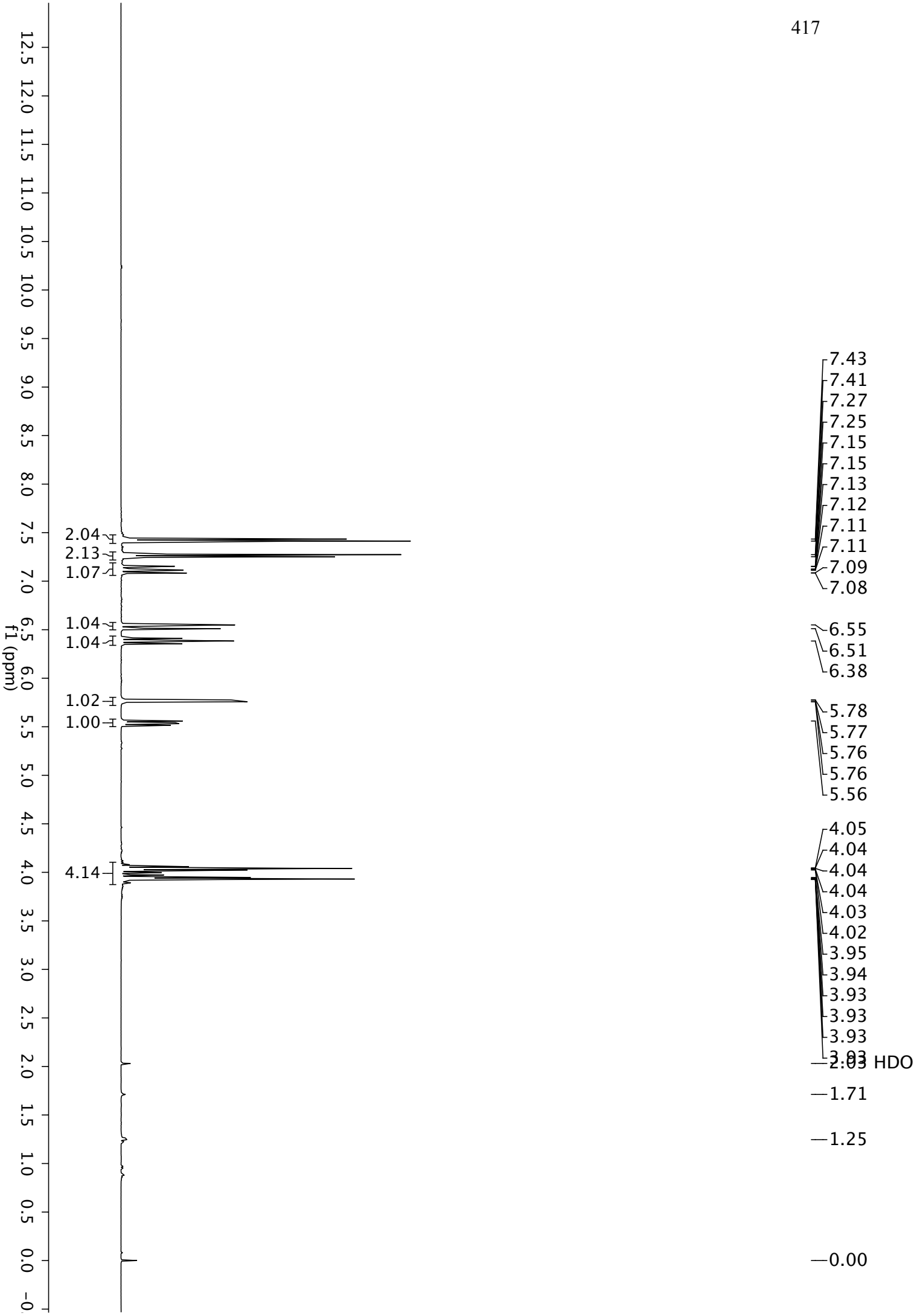
65.2
65.1

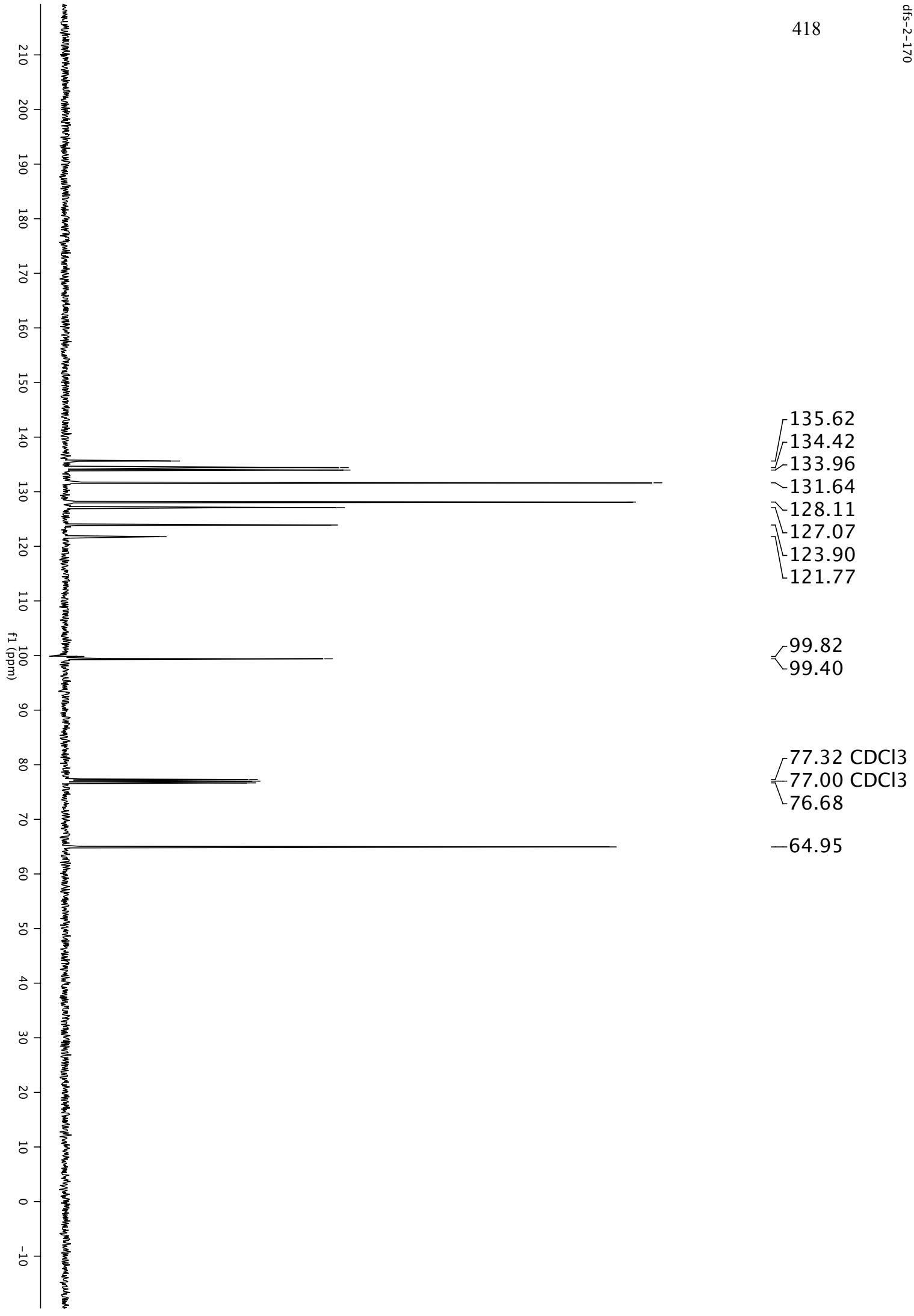


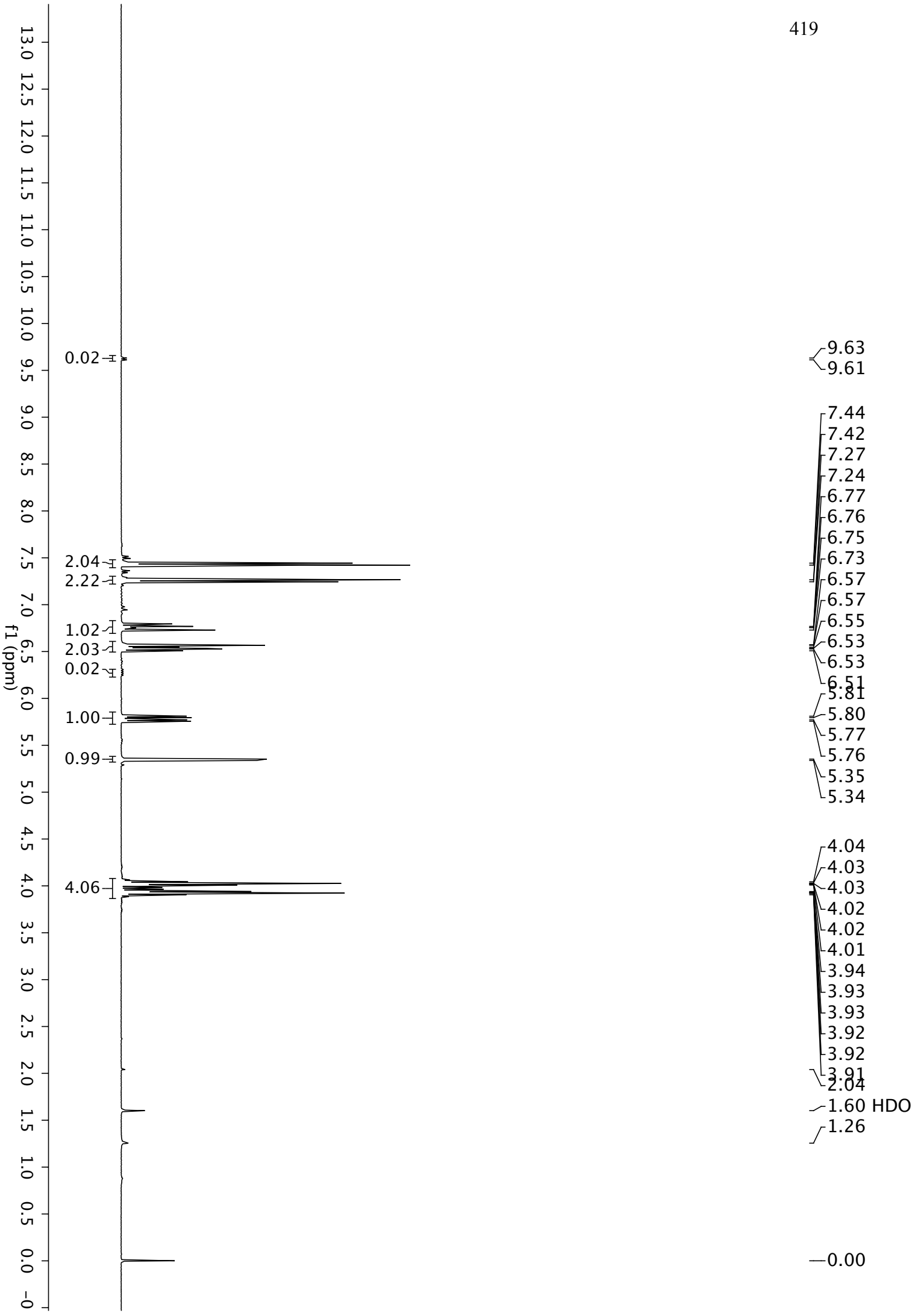

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)
1.00
2.01
3.11
1.00
9.70
9.68
7.56
7.53
7.42
7.39
7.37
7.26 CDCl3
6.72
6.69
6.67
6.64
1.24
-0.01

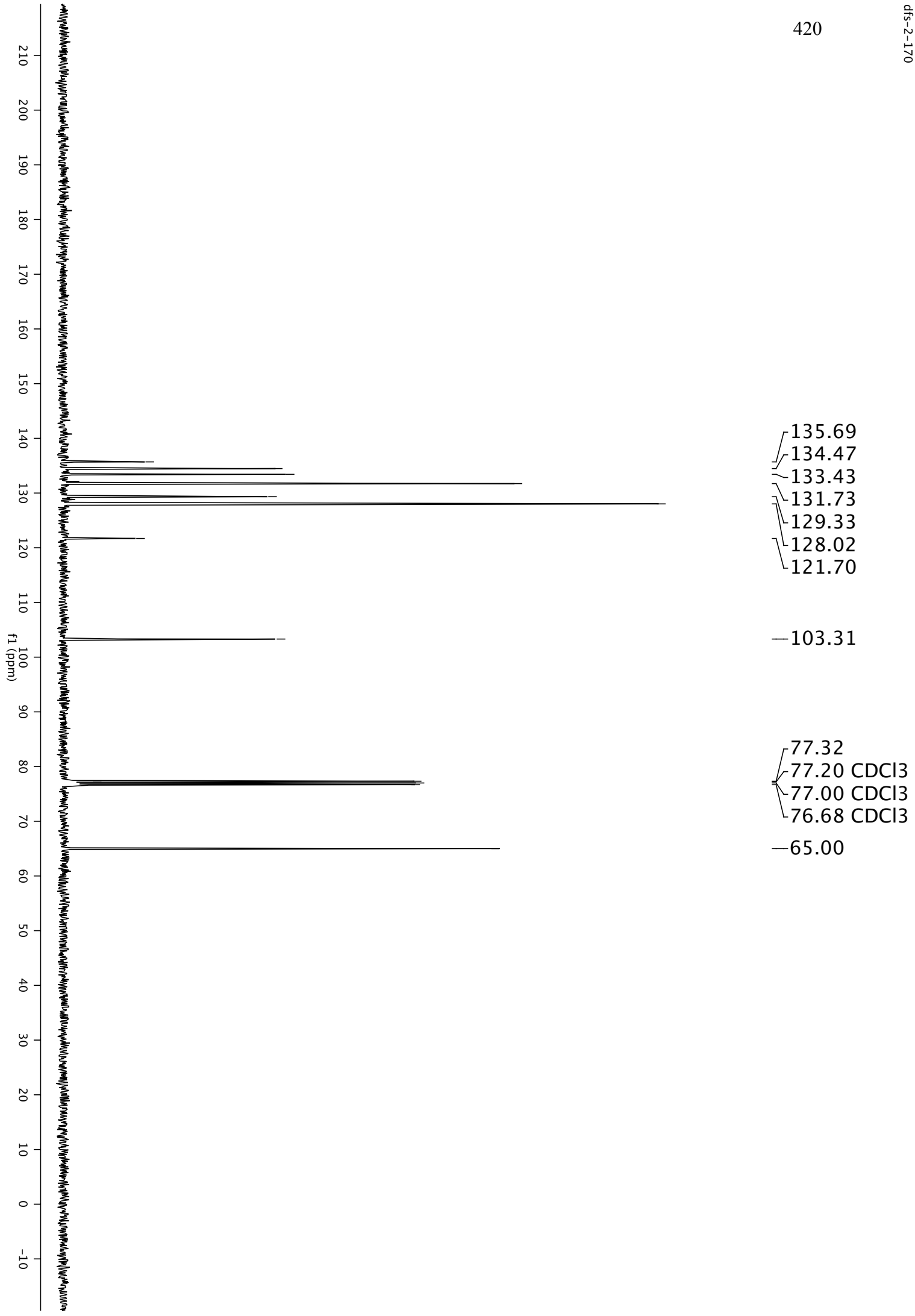
dfs-2-161al
carbon NMR

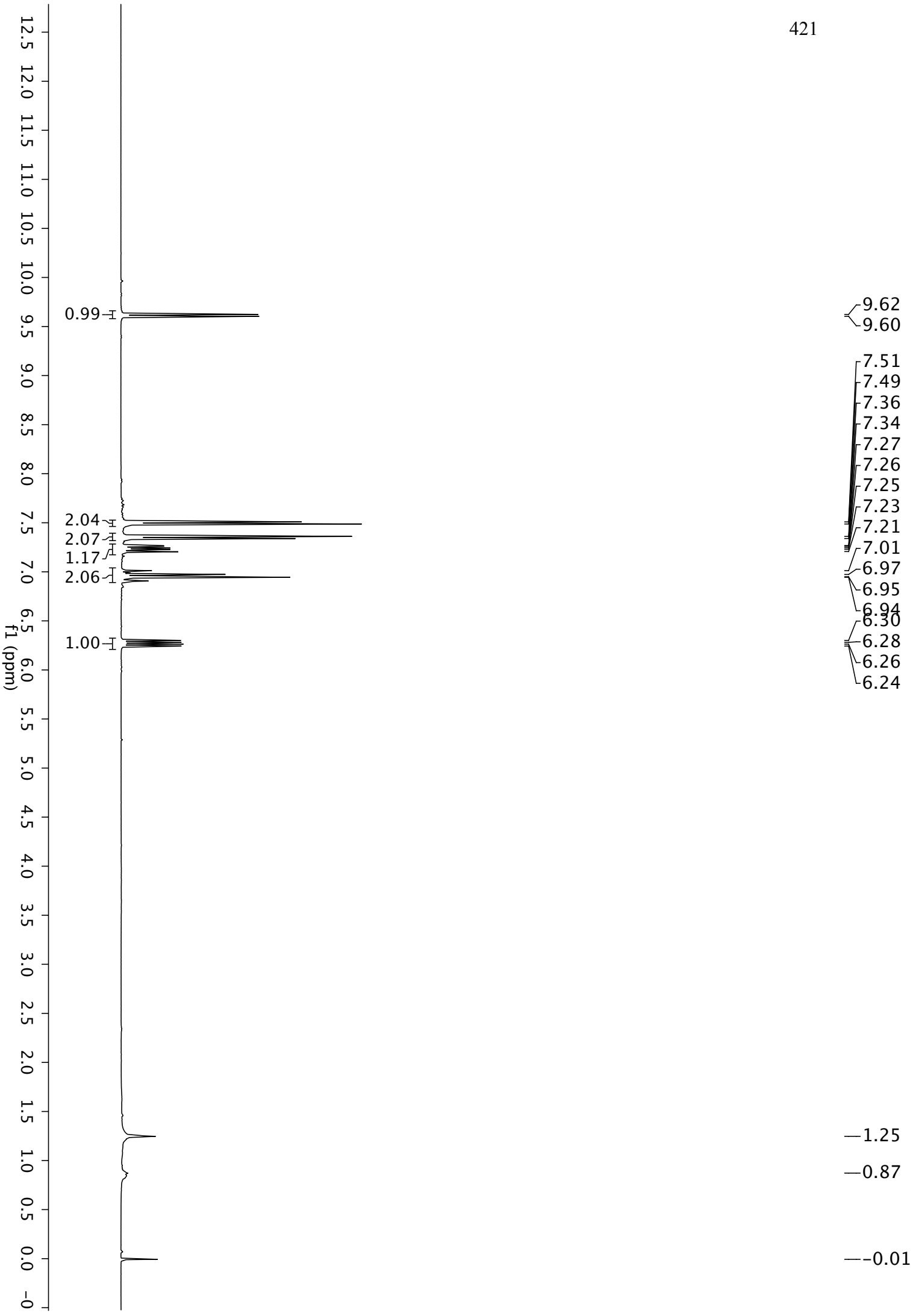


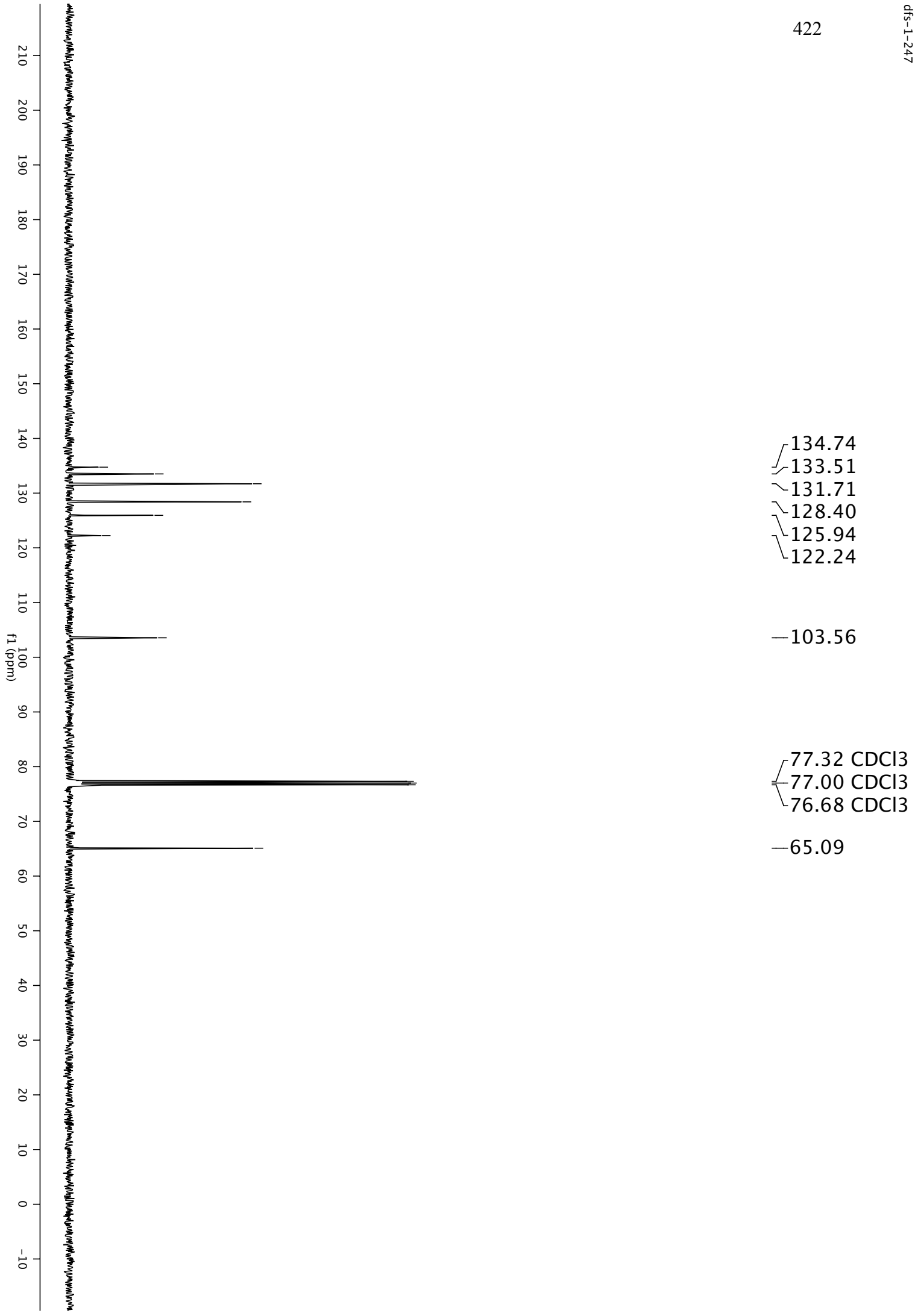

f1 (ppm)
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
2.04
2.13
1.07
1.04
1.04
1.02
1.00
4.14
7.43
7.41
7.27
7.25
7.15
7.15
7.13
7.12
7.11
7.11
7.09
7.08
6.55
6.51
6.38
5.78
5.77
5.76
5.76
5.56
4.05
4.04
4.04
4.04
4.03
4.02
3.95
3.94
3.93
3.93
3.93
3.93
2.03 HDO
1.71
1.25
0.00

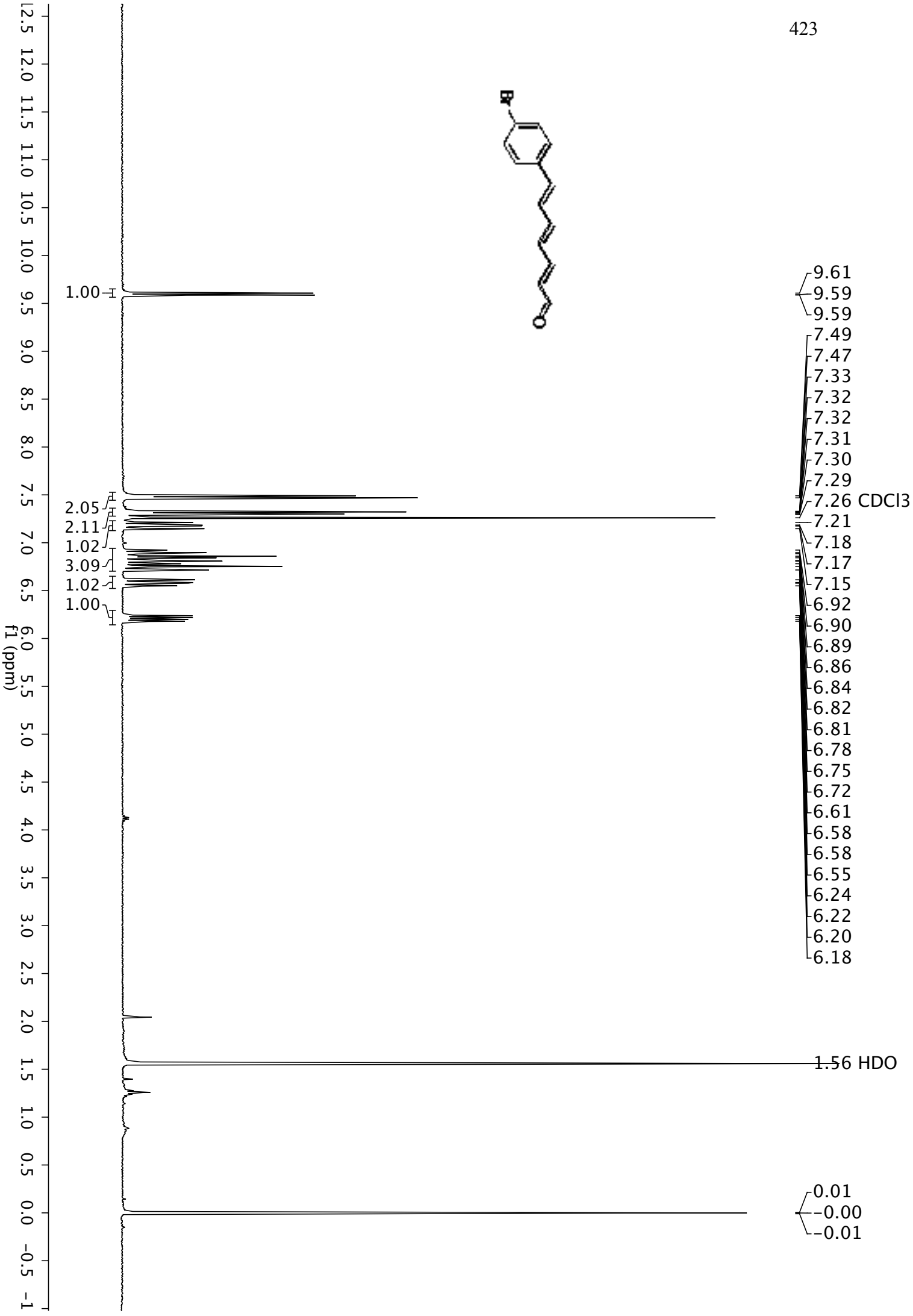

135.62
134.42
133.96
131.64
128.11
127.07
123.90
121.77
99.82
99.40
77.32 CDCl3
77.00 CDCl3
76.68
64.95
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

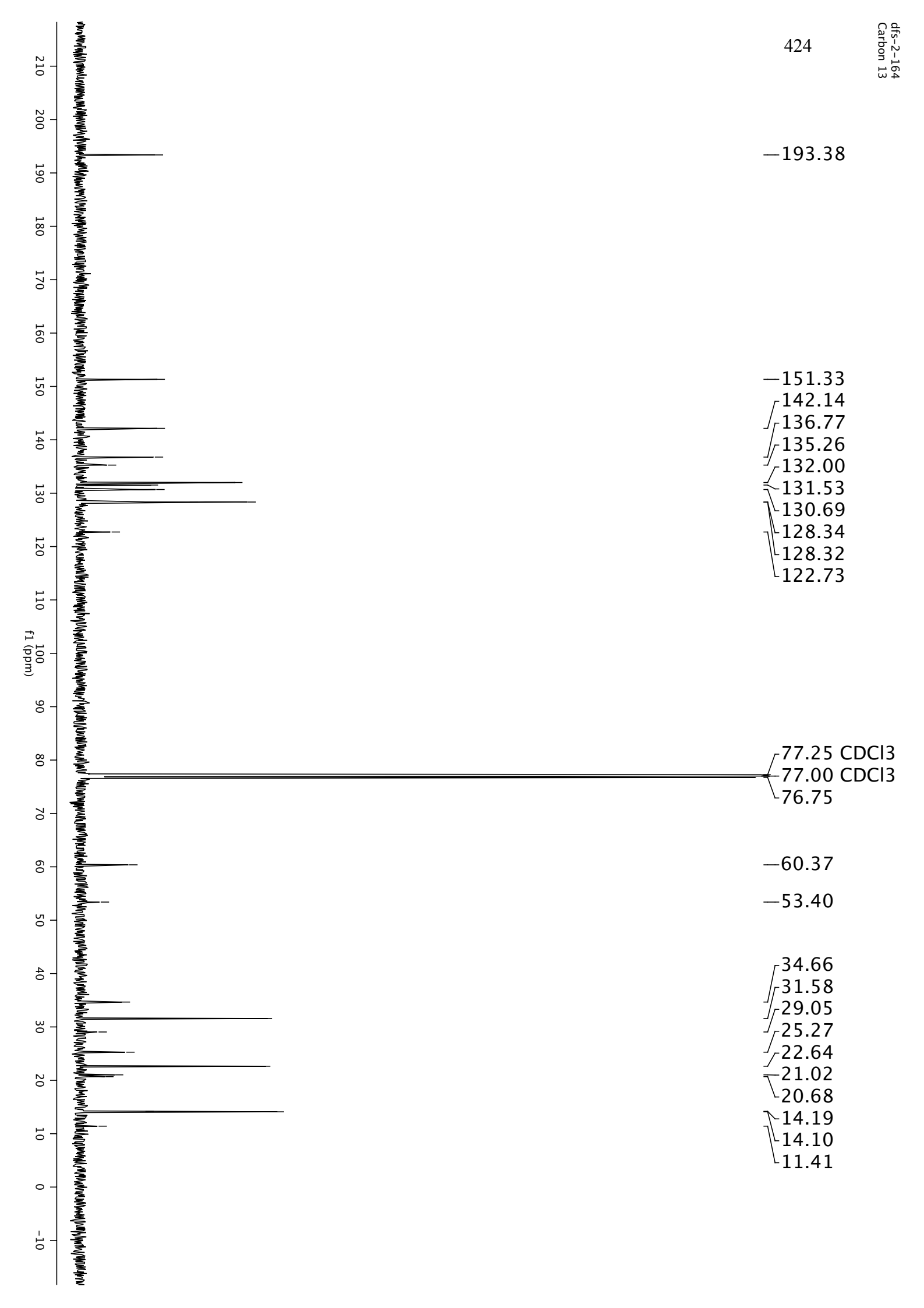

f1 (ppm)
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
0.02
2.04
2.22
1.02
2.03
0.02
1.00
0.99
4.06
9.63
9.61
7.44
7.42
7.27
7.24
6.77
6.76
6.75
6.73
6.57
6.57
6.55
6.53
6.53
6.51
5.81
5.80
5.77
5.76
5.35
5.34
4.04
4.03
4.03
4.02
4.02
4.01
3.94
3.93
3.93
3.92
3.92
3.91
2.04
1.60 HDO
1.26
0.00

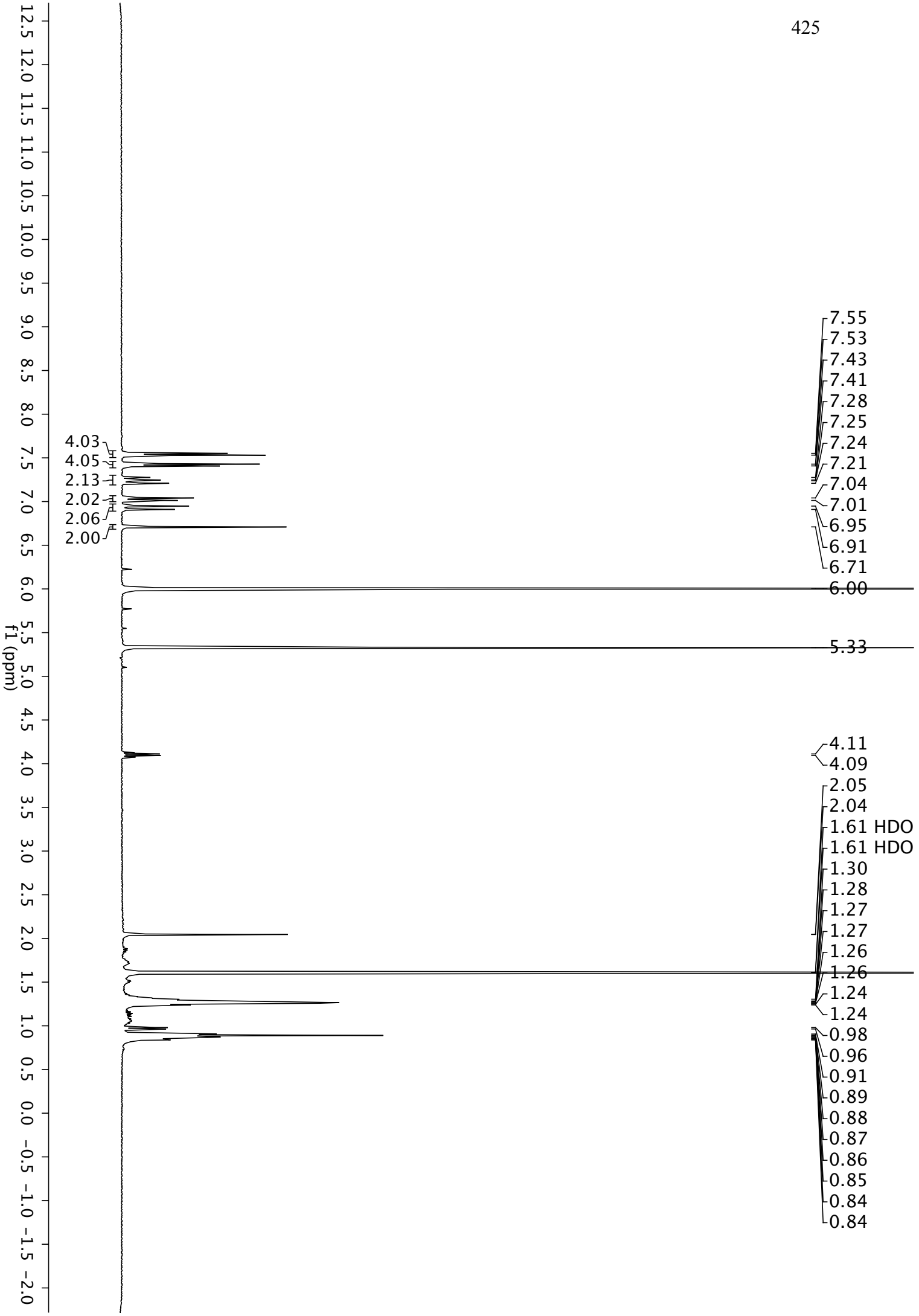

135.69
134.47
133.43
131.73
129.33
128.02
121.70
103.31
77.32
77.20 CDCl3
77.00 CDCl3
76.68 CDCl3
65.00
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10


0.99
2.04
2.07
1.17
2.06
1.00
9.62
9.60
7.51
7.49
7.36
7.34
7.27
7.26
7.25
7.23
7.21
7.01
6.97
6.95
6.94
6.30
6.28
6.26
6.24
1.25
0.87
-0.01
f1 (ppm)

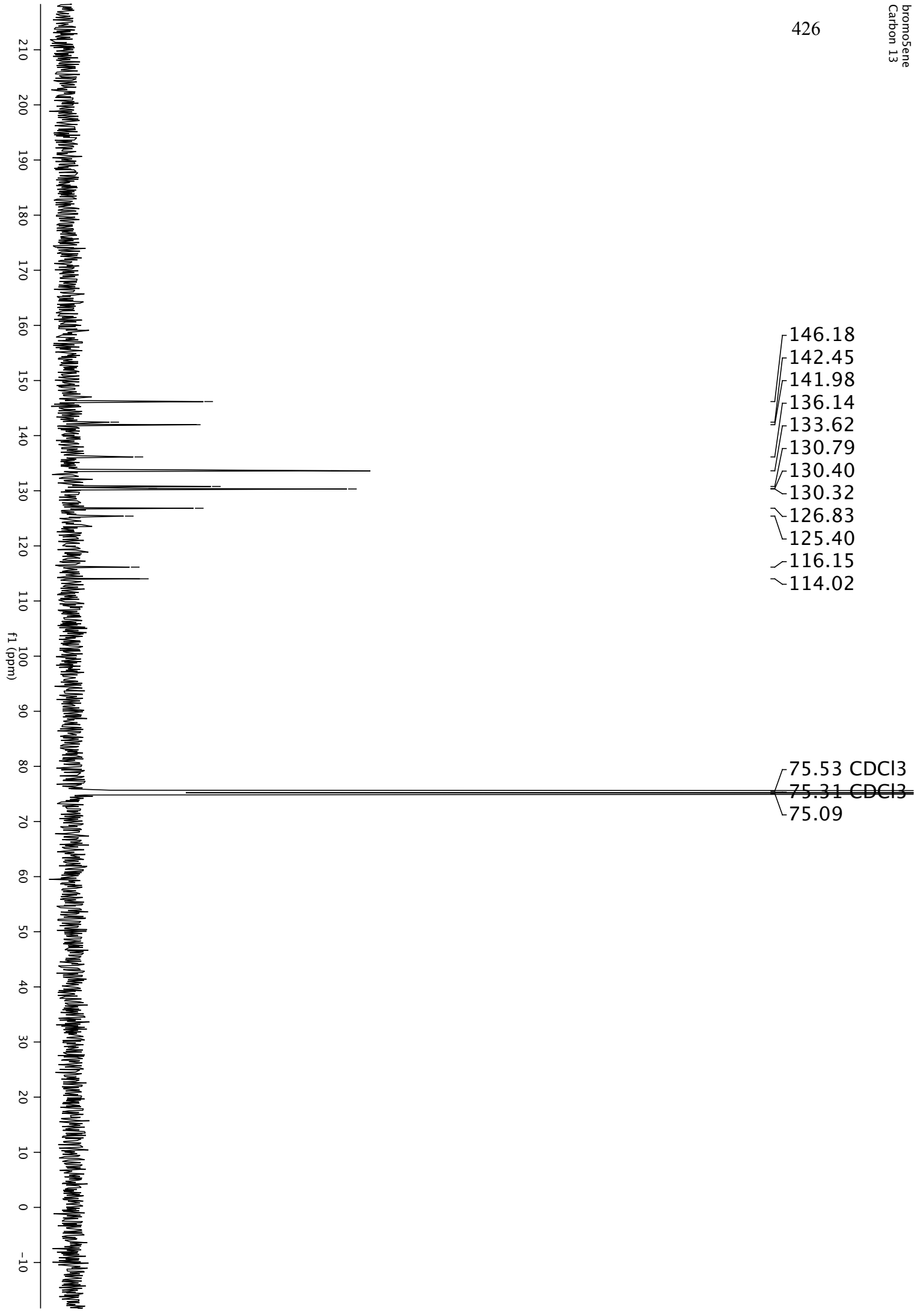

134.74
133.51
131.71
128.40
125.94
122.24
103.56
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
65.09
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

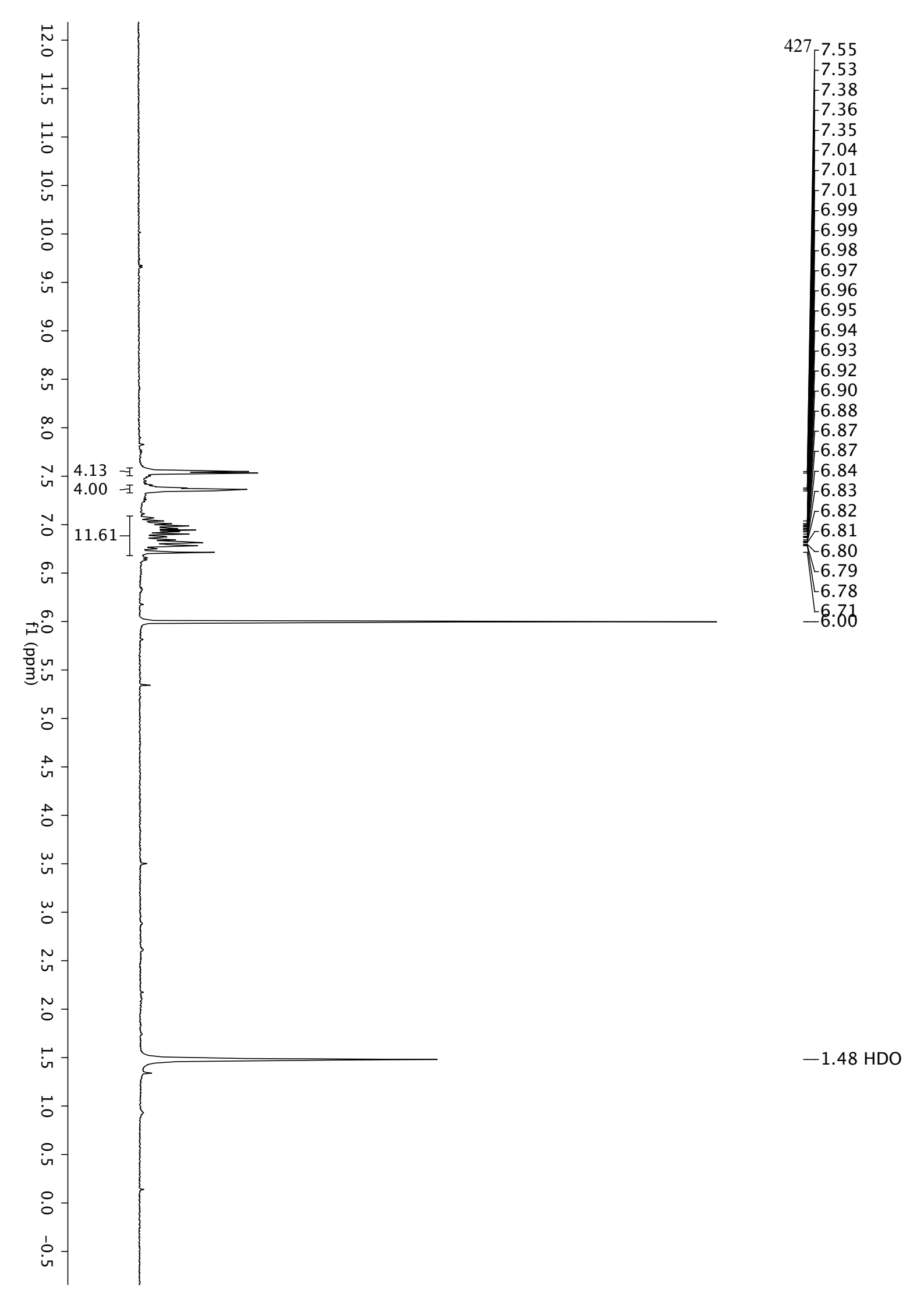

Br
1.00
2.05
2.11
1.02
3.09
1.02
1.00
9.61
9.59
9.59
7.49
7.47
7.33
7.32
7.32
7.31
7.30
7.29
7.26 CDCl3
7.21
7.18
7.17
7.15
6.92
6.90
6.89
6.86
6.84
6.82
6.81
6.78
6.75
6.72
6.61
6.58
6.58
6.55
6.24
6.22
6.20
6.18
1.56 HDO
0.01
-0.00
-0.01
f1 (ppm)

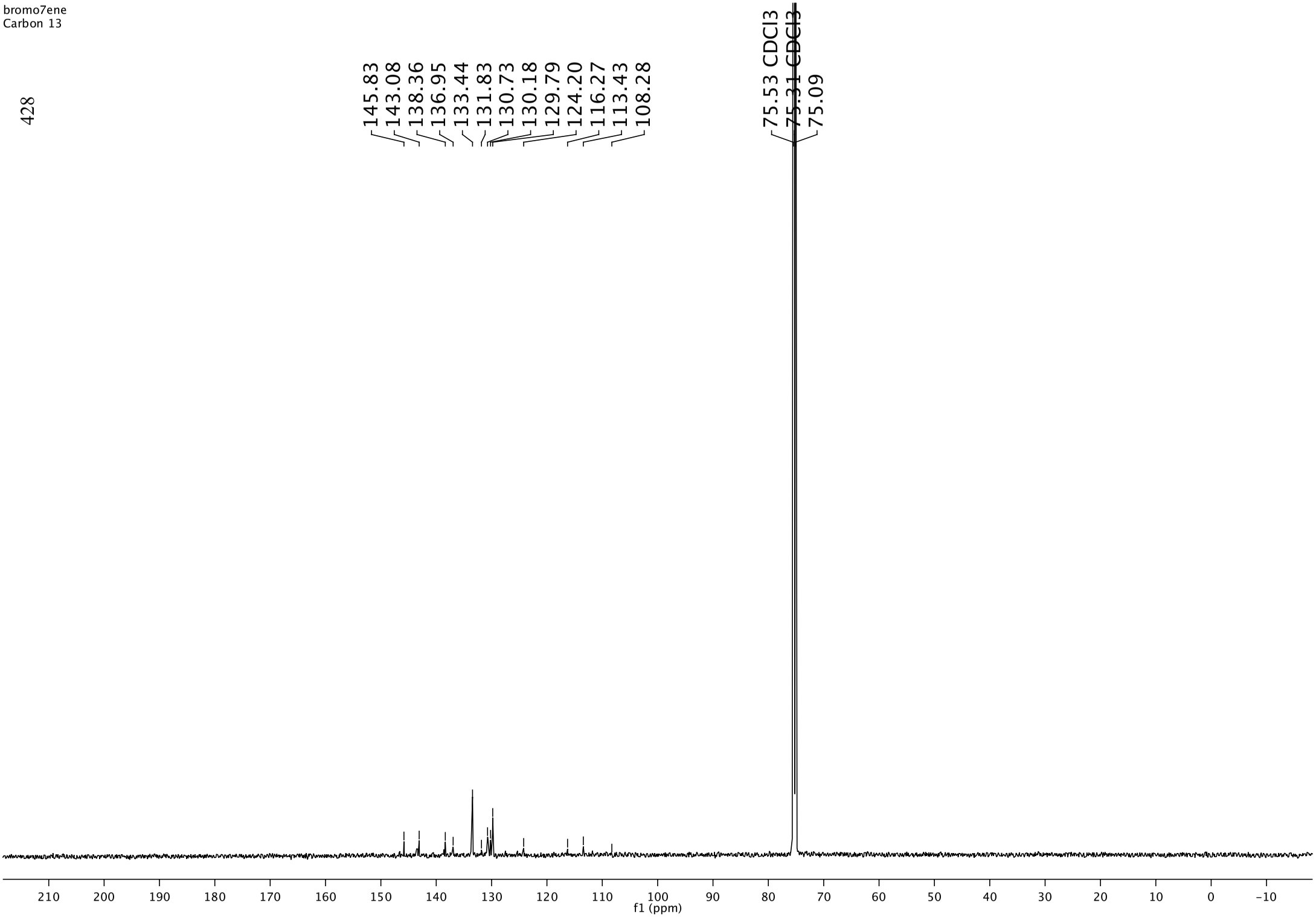

424
dfs-2-164
Carbon 13
193.38
151.33
142.14
136.77
135.26
132.00
131.53
130.69
128.34
128.32
122.73
77.25 CDCl3
77.00 CDCl3
76.75
60.37
53.40
34.66
31.58
29.05
25.27
22.64
21.02
20.68
14.19
14.10
11.41
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

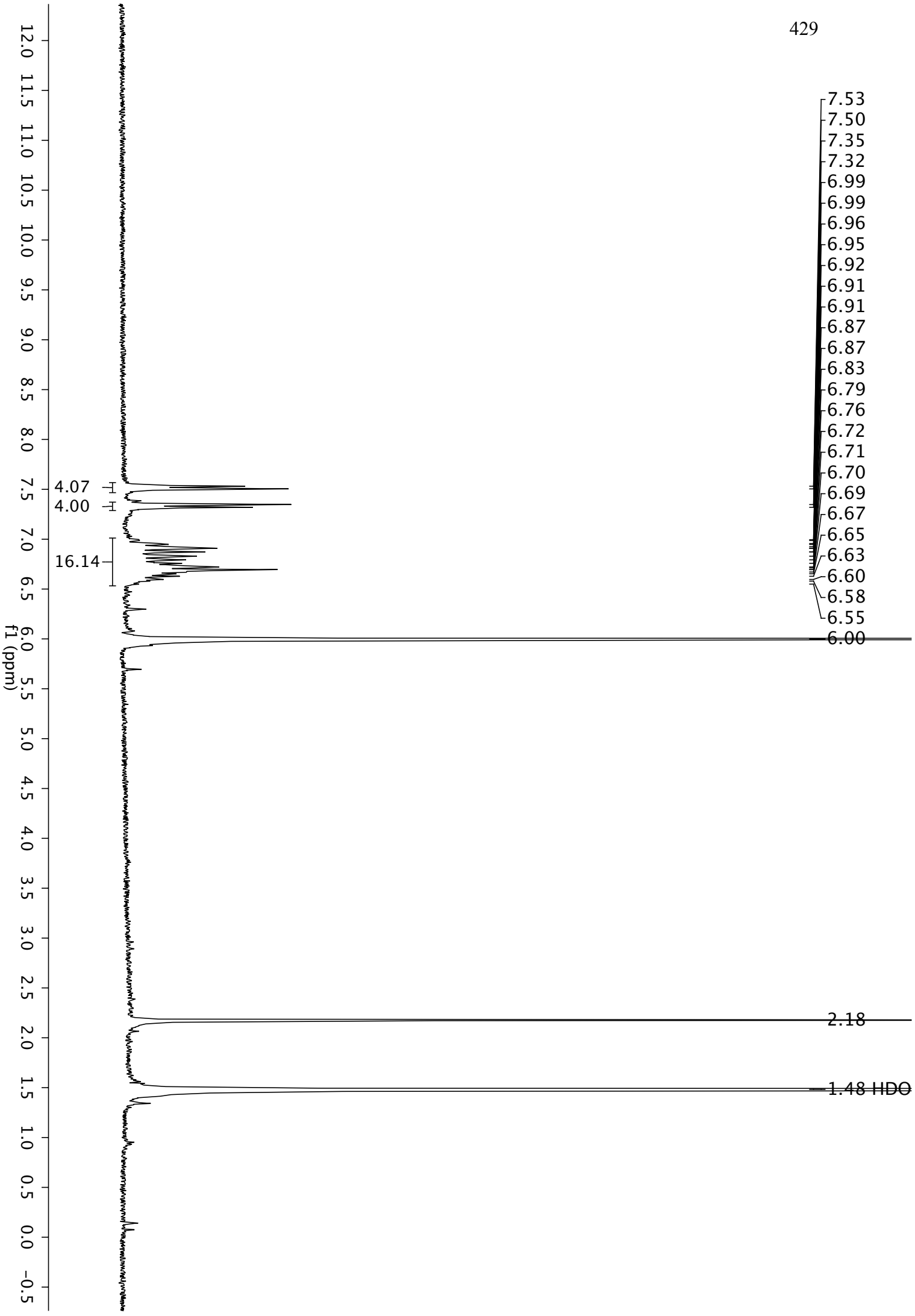

4.03
4.05
2.13
2.02
2.06
2.00
7.55
7.53
7.43
7.41
7.28
7.25
7.24
7.21
7.04
7.01
6.95
6.91
6.71
6.00
5.33
4.11
4.09
2.05
2.04
1.61 HDO
1.61 HDO
1.30
1.28
1.27
1.27
1.26
1.26
1.24
1.24
0.98
0.96
0.91
0.89
0.88
0.87
0.86
0.85
0.84
0.84
f1 (ppm)

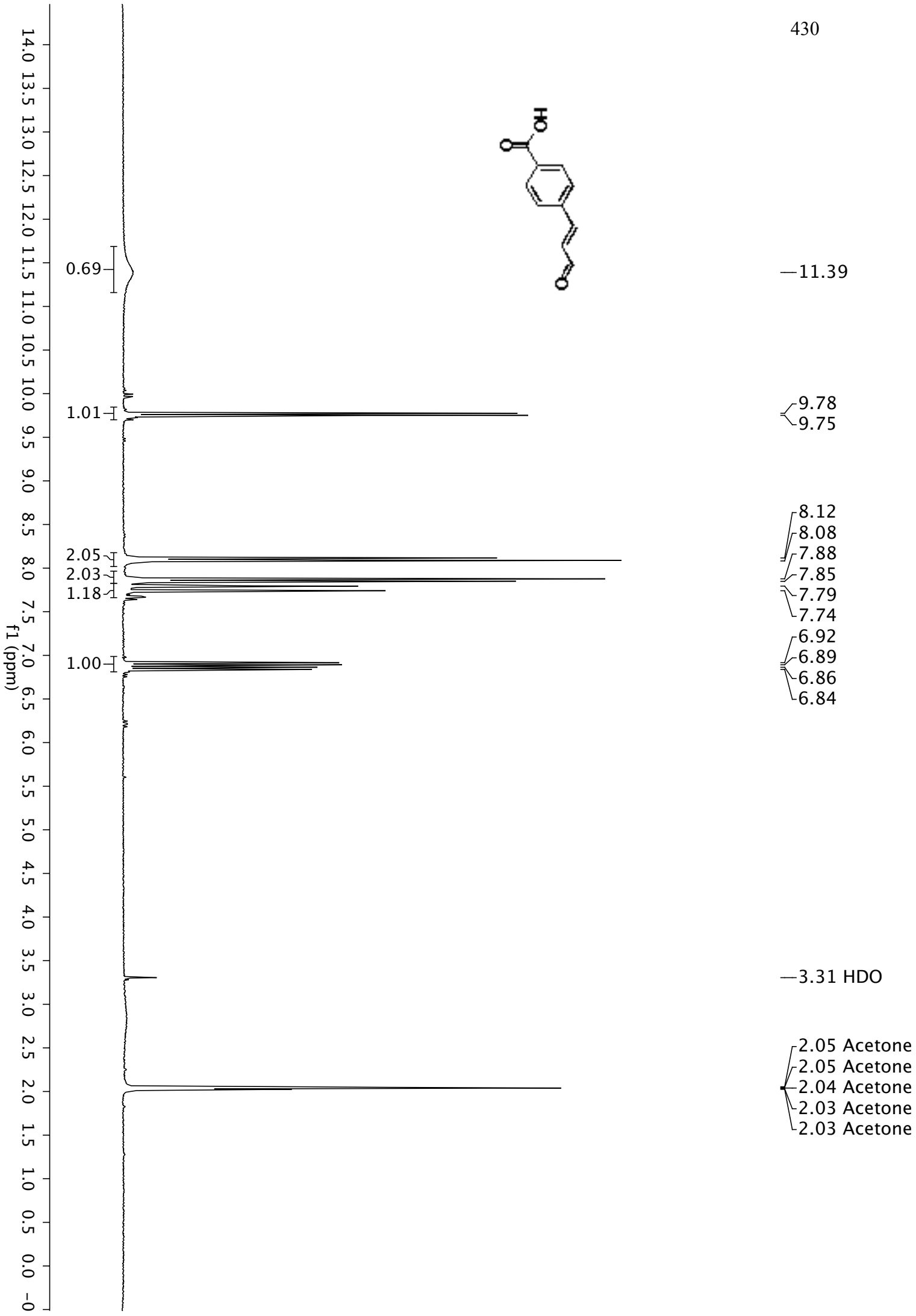
bromo5ene
Carbon 13

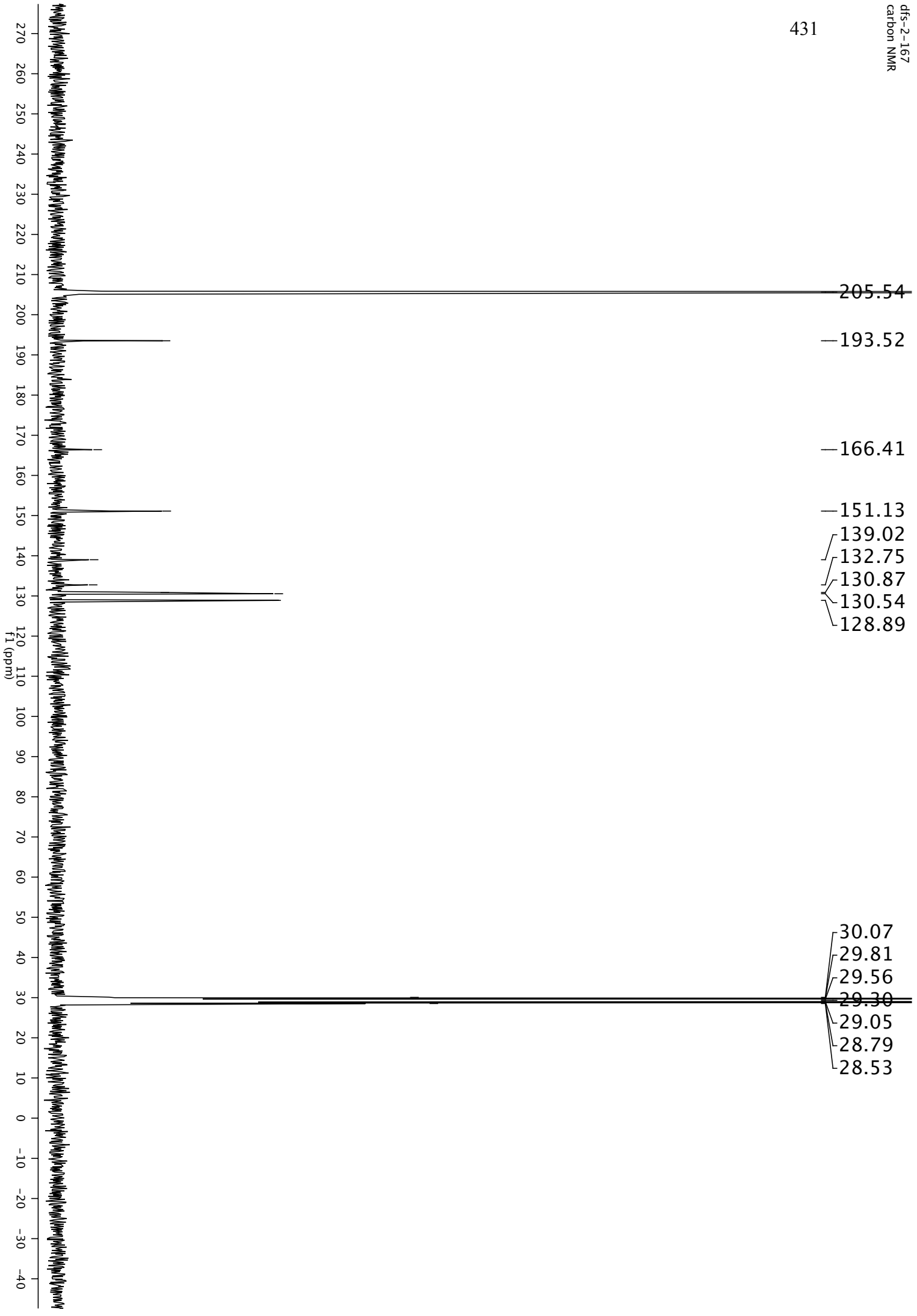


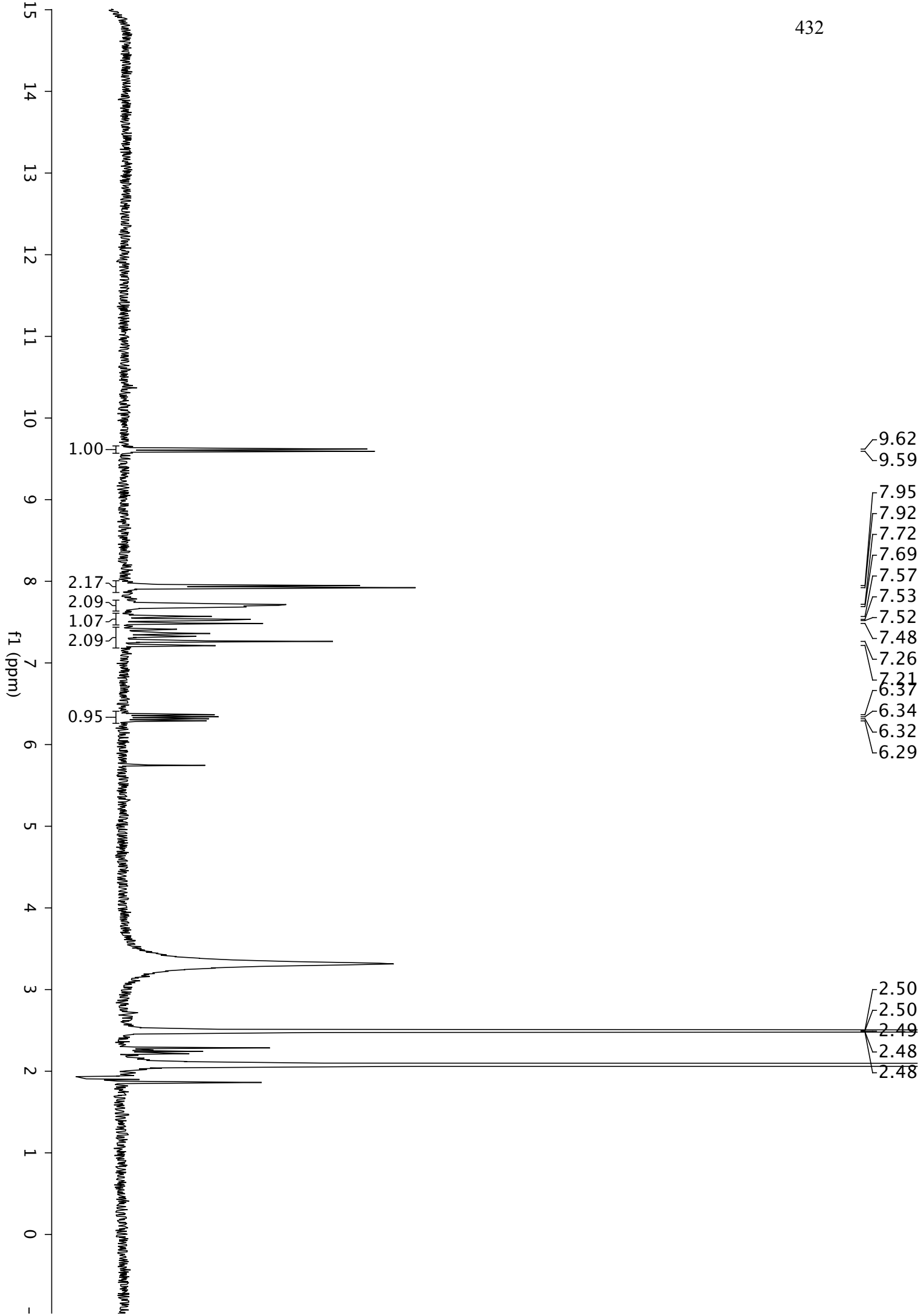

427
7.55
7.53
7.38
7.36
7.35
7.04
7.01
7.01
6.99
6.99
6.98
6.97
6.96
6.95
6.94
6.93
6.92
6.90
6.88
6.87
6.87
6.84
6.83
6.82
6.81
6.80
6.79
6.78
6.71
6.00
4.13
4.00
11.61
1.48 HDO
f1 (ppm)

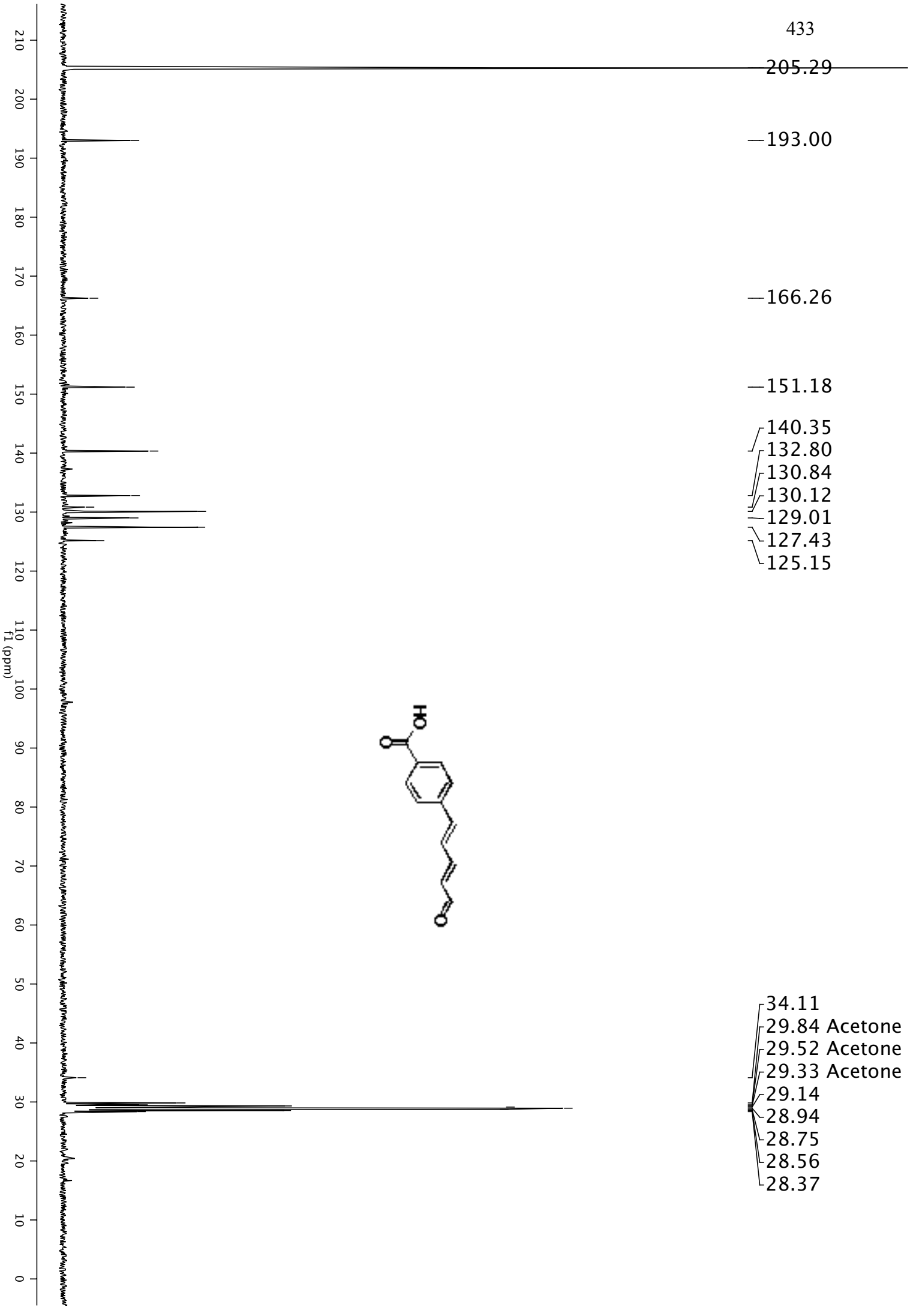

bromo7ene
Carbon 13
428
145.83
143.08
138.36
136.95
133.44
131.83
130.73
130.18
129.79
124.20
116.27
113.43
108.28
75.53 CDCl3
75.31 CDCl3
75.09
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

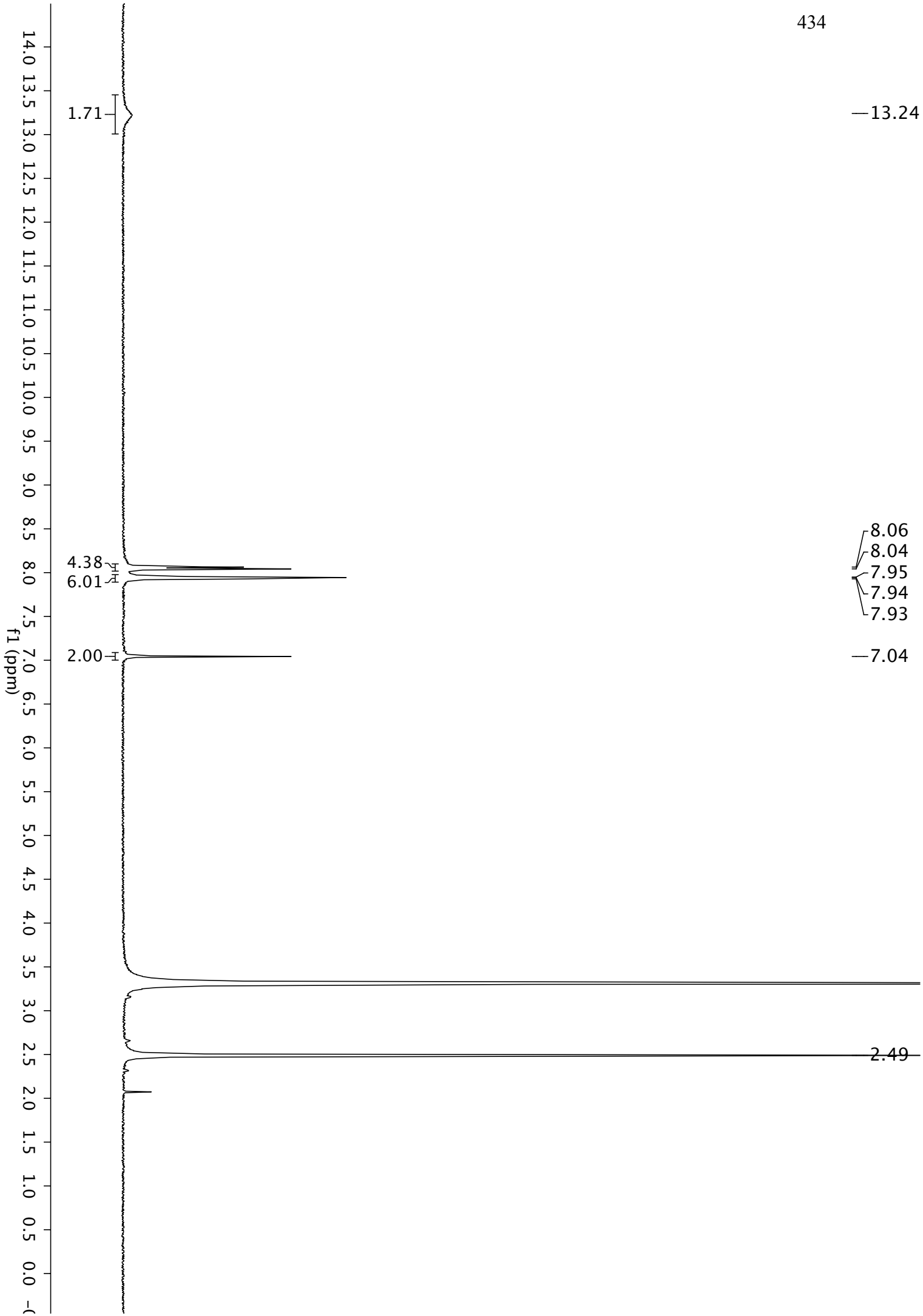

7.53
7.50
7.35
7.32
6.99
6.99
6.96
6.95
6.92
6.91
6.91
6.87
6.87
6.83
6.79
6.76
6.72
6.71
6.70
6.69
6.67
6.65
6.63
6.60
6.58
6.55
6.00
4.07
4.00
16.14
2.18
1.48 HDO
f1 (ppm)

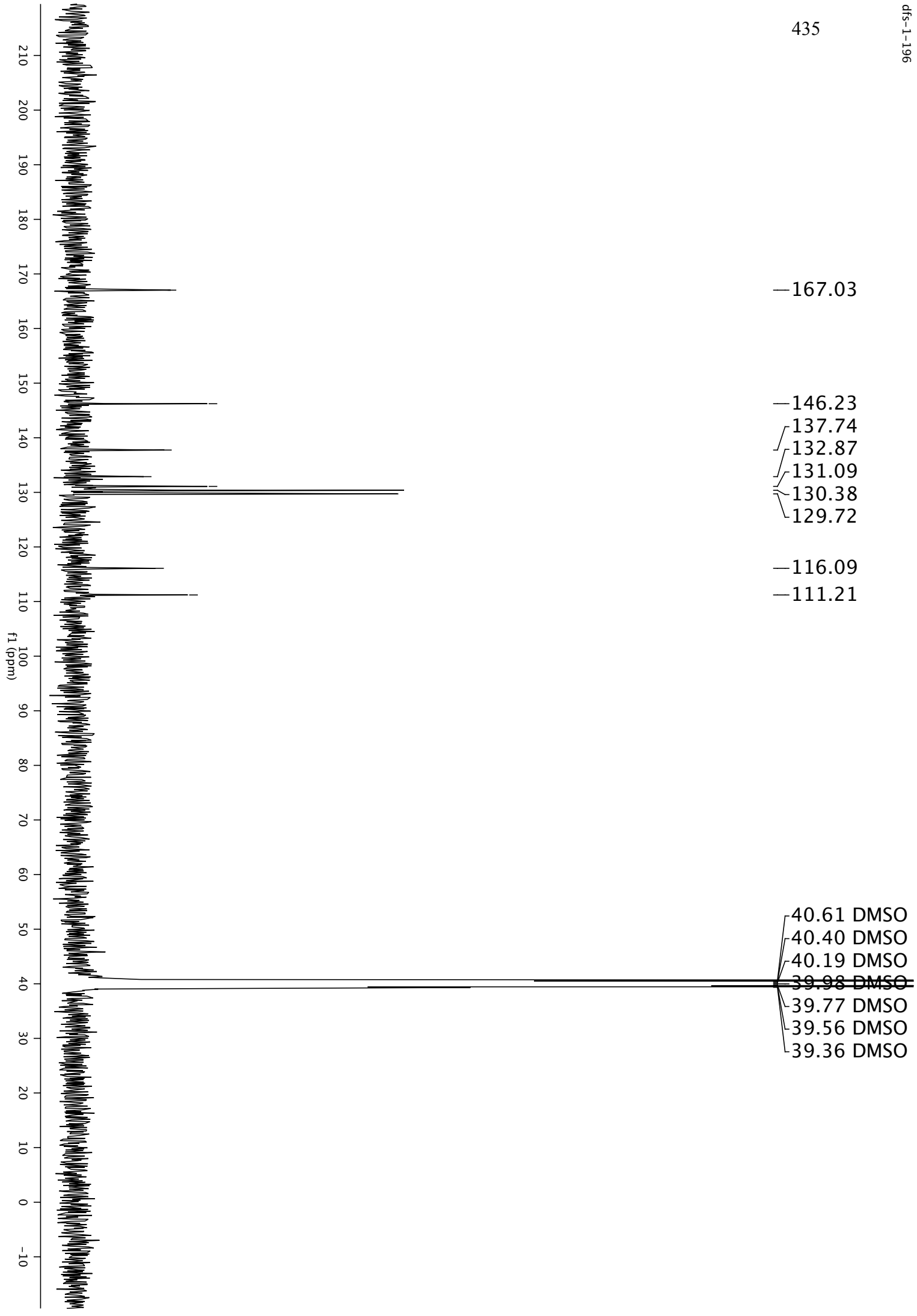

0.69
1.01
2.05
2.03
1.18
1.00
11.39
9.78
9.75
8.12
8.08
7.88
7.85
7.79
7.74
6.92
6.89
6.86
6.84
3.31 HDO
2.05 Acetone
2.05 Acetone
2.04 Acetone
2.03 Acetone
2.03 Acetone
f1 (ppm)

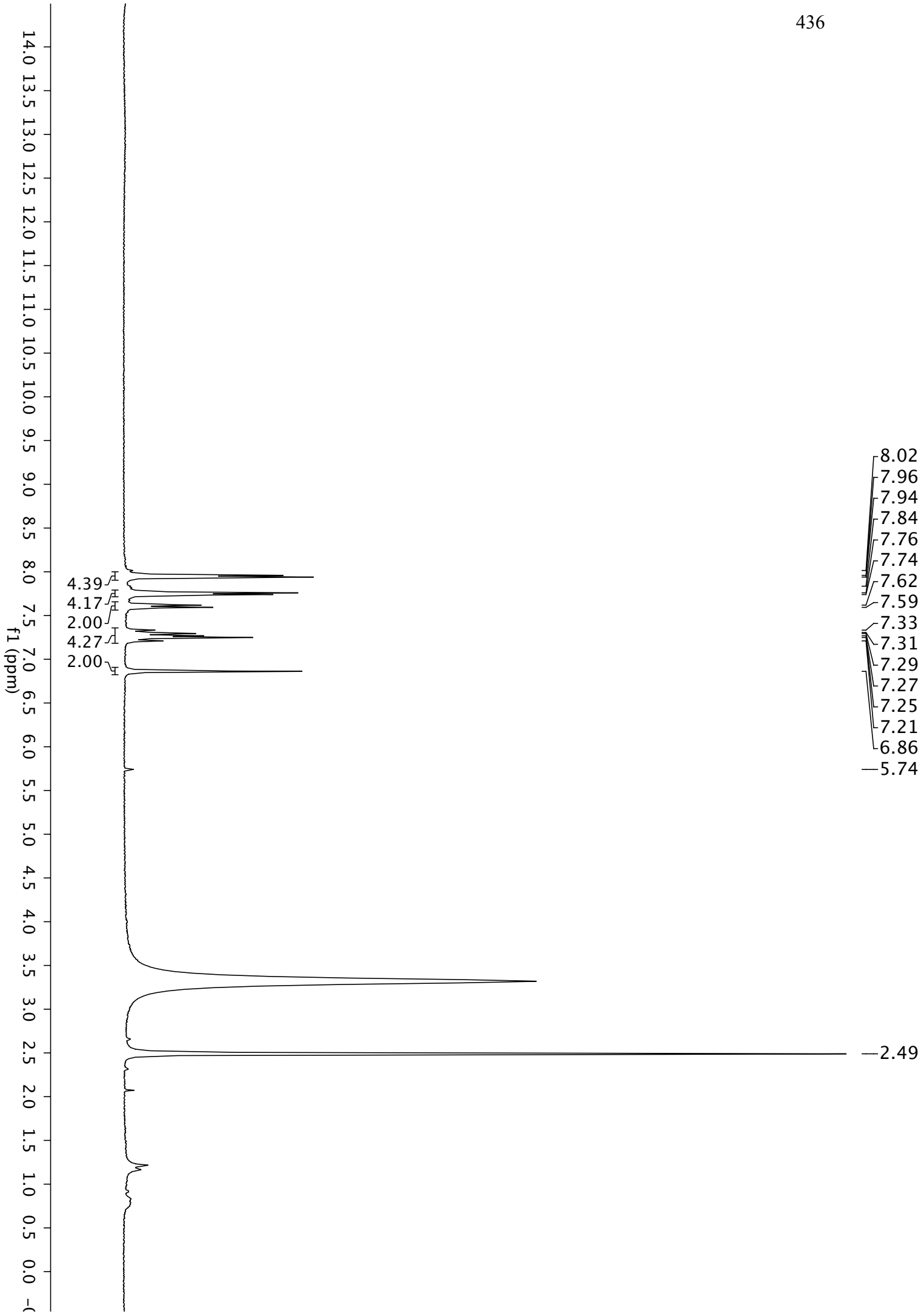

dfs-2-167
carbon NMR
205.54
193.52
166.41
151.13
139.02
132.75
130.87
130.54
128.89
30.07
29.81
29.56
29.30
29.05
28.79
28.53
f1 (ppm)

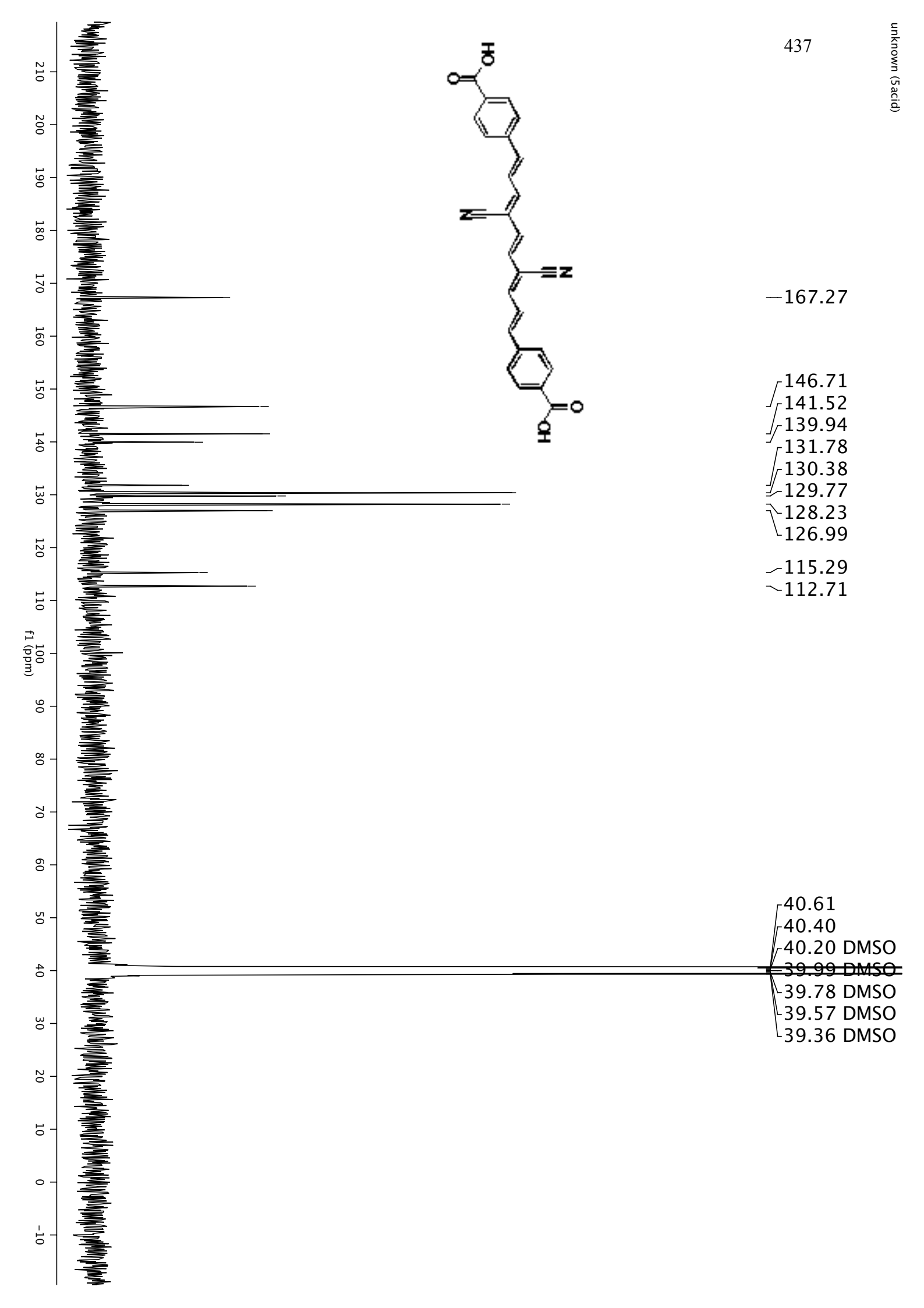

f1 (ppm)
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
1.00
2.17
2.09
1.07
2.09
0.95
9.62
9.59
7.95
7.92
7.72
7.69
7.57
7.53
7.52
7.48
7.26
7.21
6.37
6.34
6.32
6.29
2.50
2.50
2.49
2.48
2.48

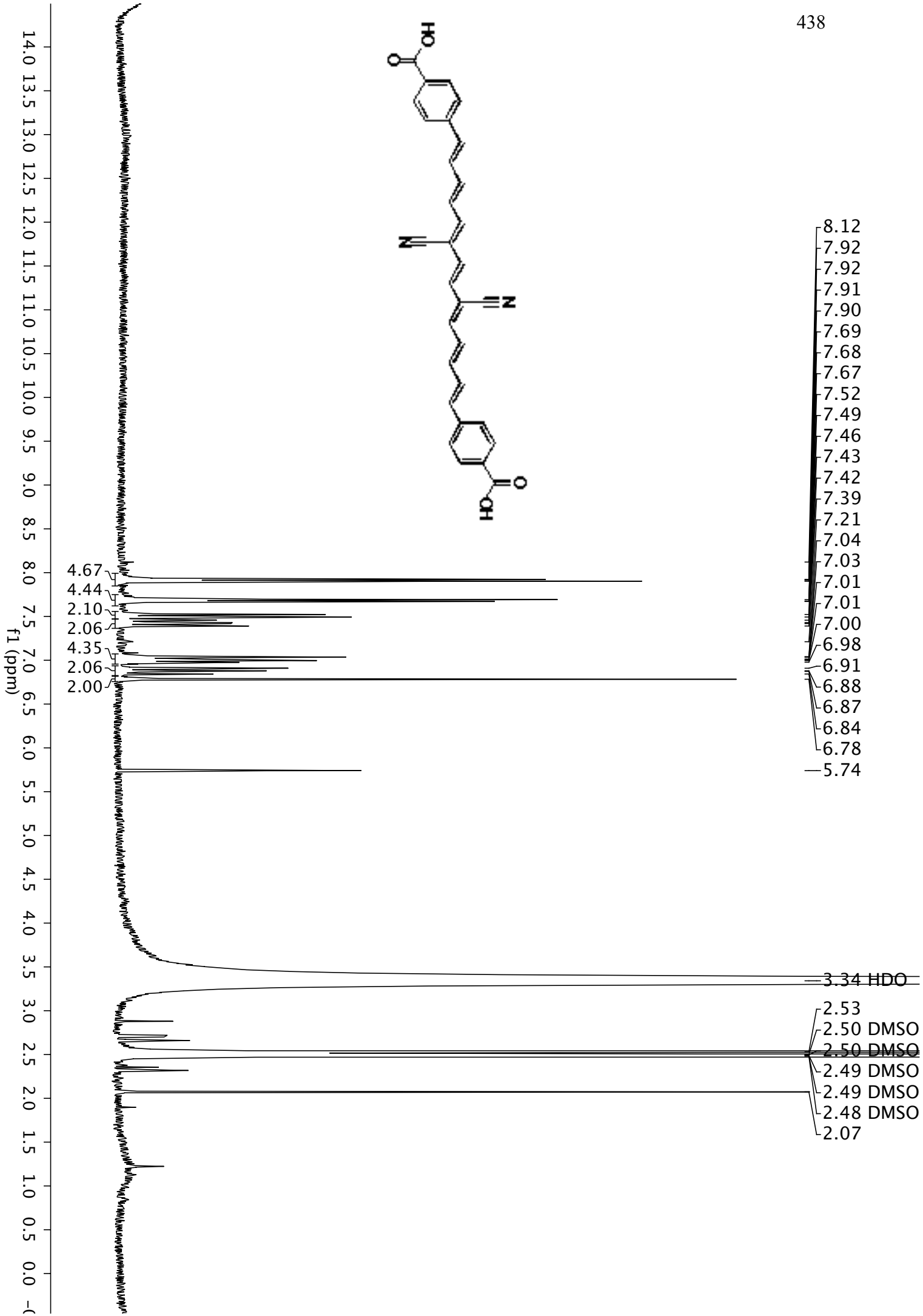

205.29
193.00
166.26
151.18
140.35
132.80
130.84
130.12
129.01
127.43
125.15
34.11
29.84 Acetone
29.52 Acetone
29.33 Acetone
29.14
28.94
28.75
28.56
28.37
f1 (ppm)

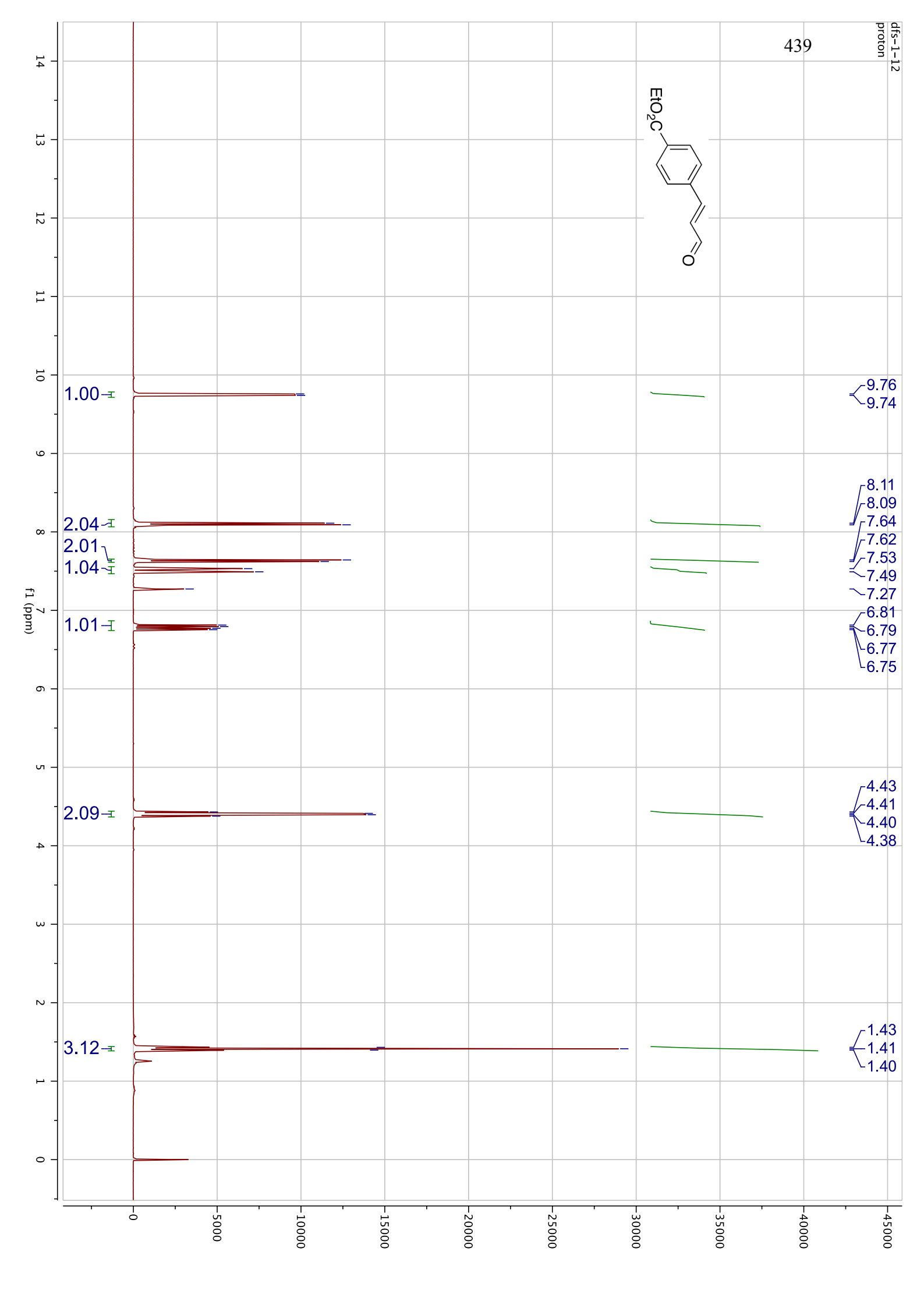

1.71
4.38
6.01
2.00
13.24
8.06
8.04
7.95
7.94
7.93
7.04
2.49
f1 (ppm)

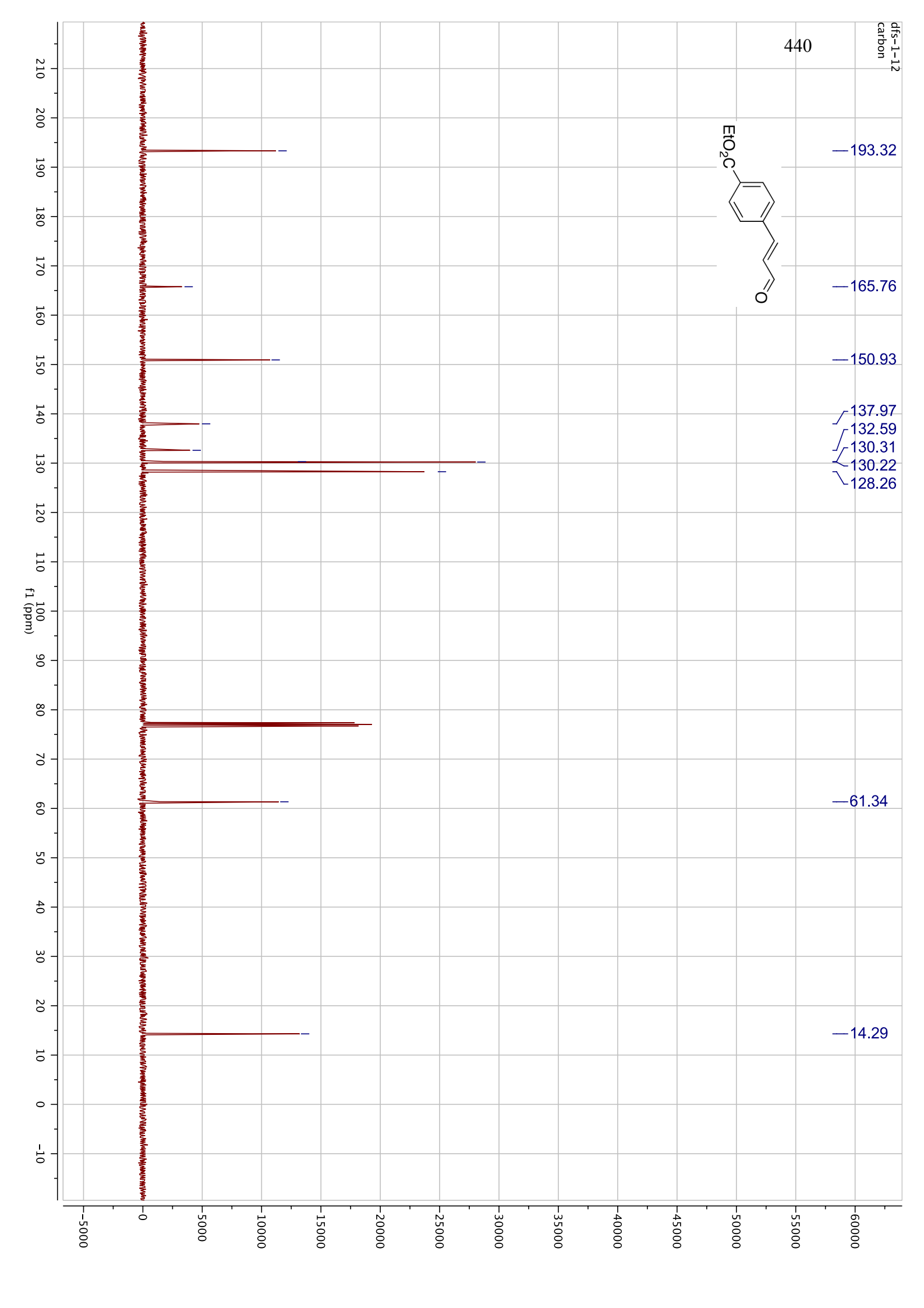

167.03
146.23
137.74
132.87
131.09
130.38
129.72
116.09
111.21
40.61 DMSO
40.40 DMSO
40.19 DMSO
39.98 DMSO
39.77 DMSO
39.56 DMSO
39.36 DMSO
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

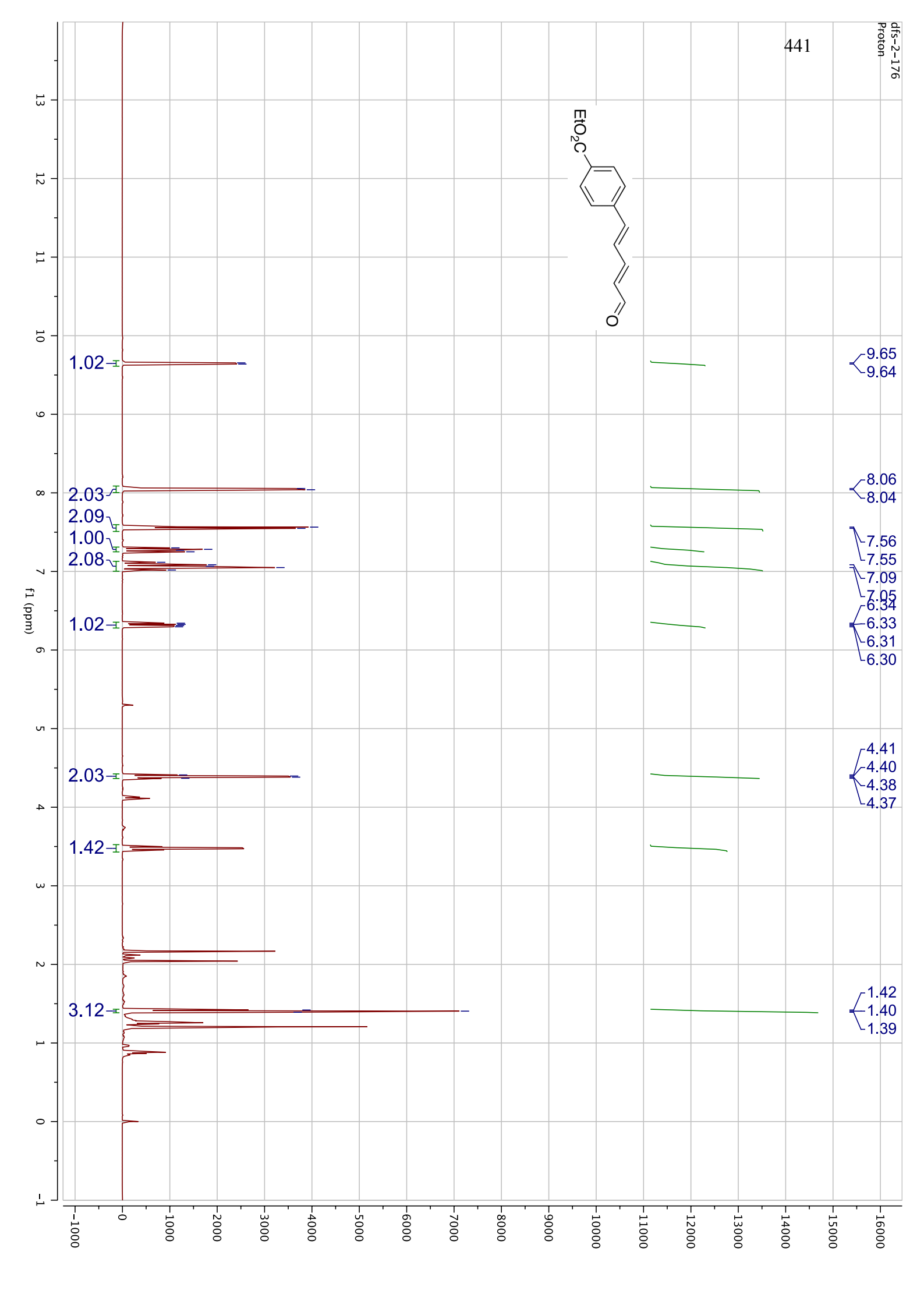

14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
4.39
4.17
2.00
4.27
2.00
8.02
7.96
7.94
7.84
7.76
7.74
7.62
7.59
7.33
7.31
7.29
7.27
7.25
7.21
6.86
5.74
2.49


unknown (5acid)
167.27
146.71
141.52
139.94
131.78
130.38
129.77
128.23
126.99
115.29
112.71
40.61
40.40
40.20 DMSO
39.99 DMSO
39.78 DMSO
39.57 DMSO
39.36 DMSO
f1 (ppm)


8.12
7.92
7.92
7.91
7.90
7.69
7.68
7.67
7.52
7.49
7.46
7.43
7.42
7.39
7.21
7.04
7.03
7.01
7.01
7.00
6.98
6.91
6.88
6.87
6.84
6.78
5.74
4.67
4.44
2.10
2.06
4.35
2.06
2.00
3.34 HDO
2.53
2.50 DMSO
2.50 DMSO
2.49 DMSO
2.49 DMSO
2.48 DMSO
2.07
f1 (ppm)


dfs-1-12
proton
EtO2C
O
1.00
2.04
2.01
1.04
1.01
2.09
3.12
9.76
9.74
8.11
8.09
7.64
7.62
7.53
7.49
7.27
6.81
6.79
6.77
6.75
4.43
4.41
4.40
4.38
1.43
1.41
1.40
f1 (ppm)

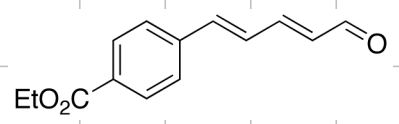

440
dfs-1-12
carbon
193.32
165.76
150.93
137.97
132.59
130.31
130.22
128.26
61.34
14.29
f1 (ppm)


dfs-2-176
Proton
EtO2C
O
1.02
2.03
2.09
1.00
2.08
1.02
2.03
1.42
3.12
9.65
9.64
8.06
8.04
7.56
7.55
7.09
7.05
6.34
6.33
6.31
6.30
4.41
4.40
4.38
4.37
1.42
1.40
1.39
f1 (ppm)

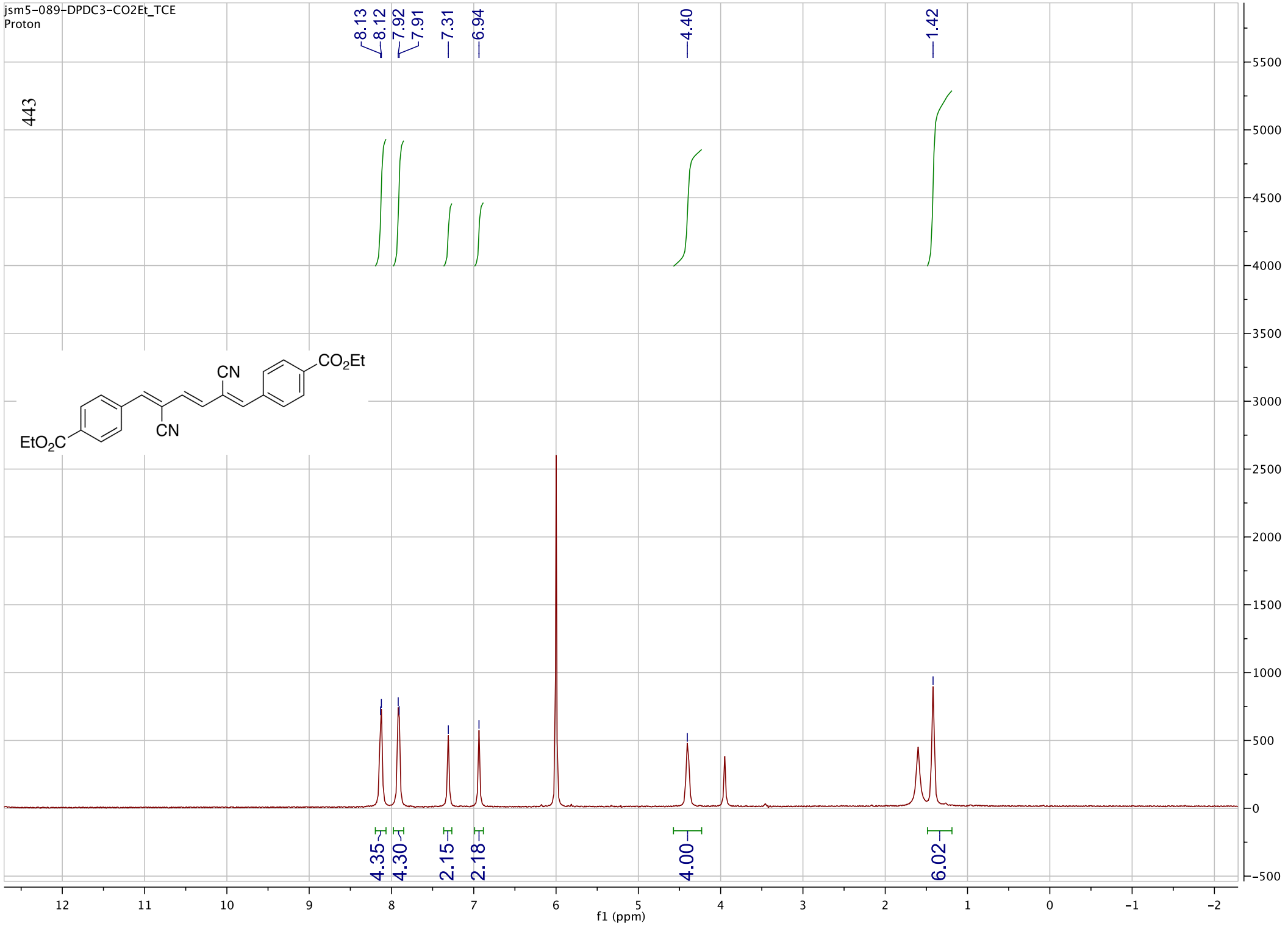
dfs-2-176
Carbon 13

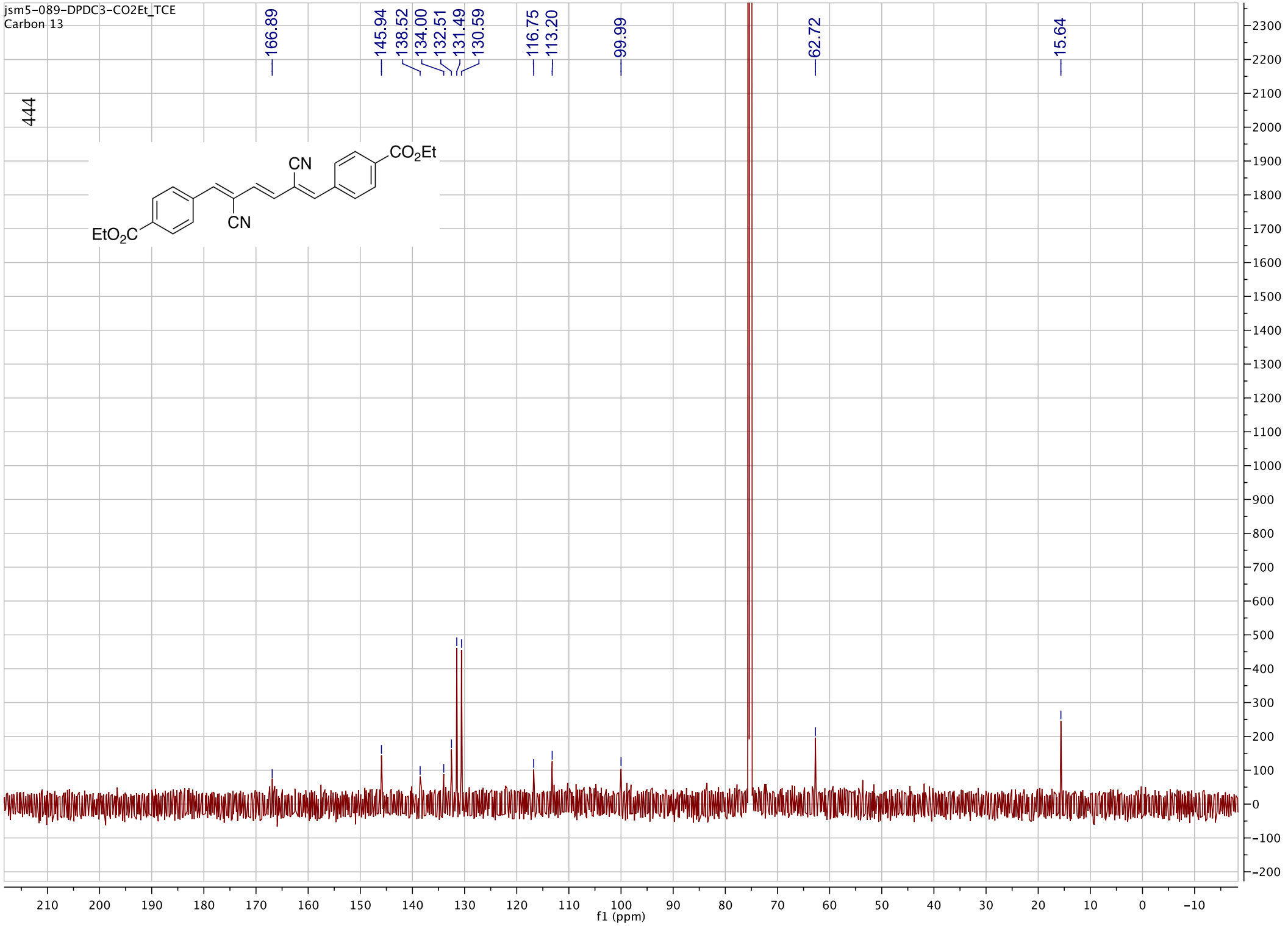
442

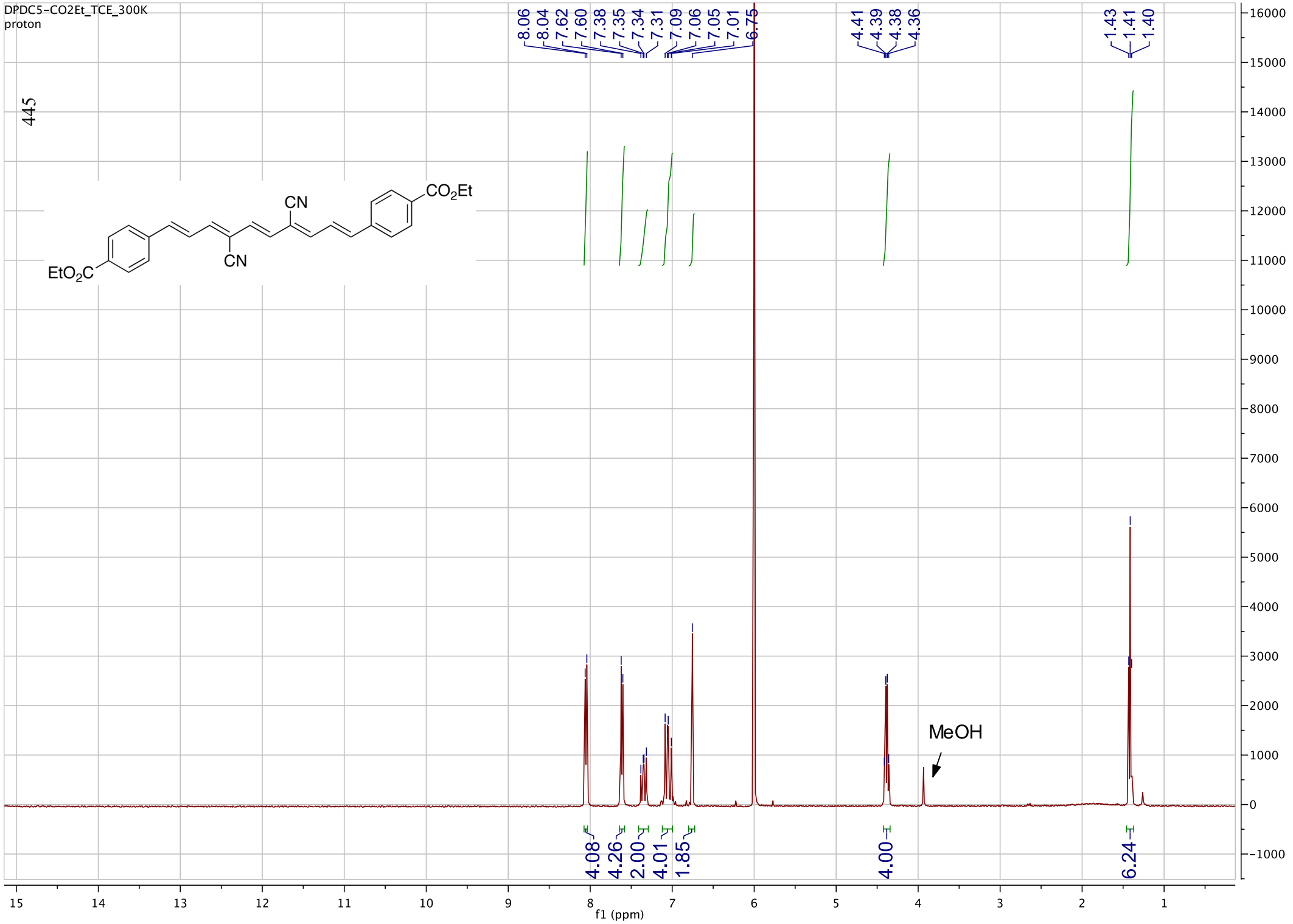
193.37
165.99
151.05
140.83
139.70
132.66
131.08
130.10
128.35
127.28
61.16
14.30

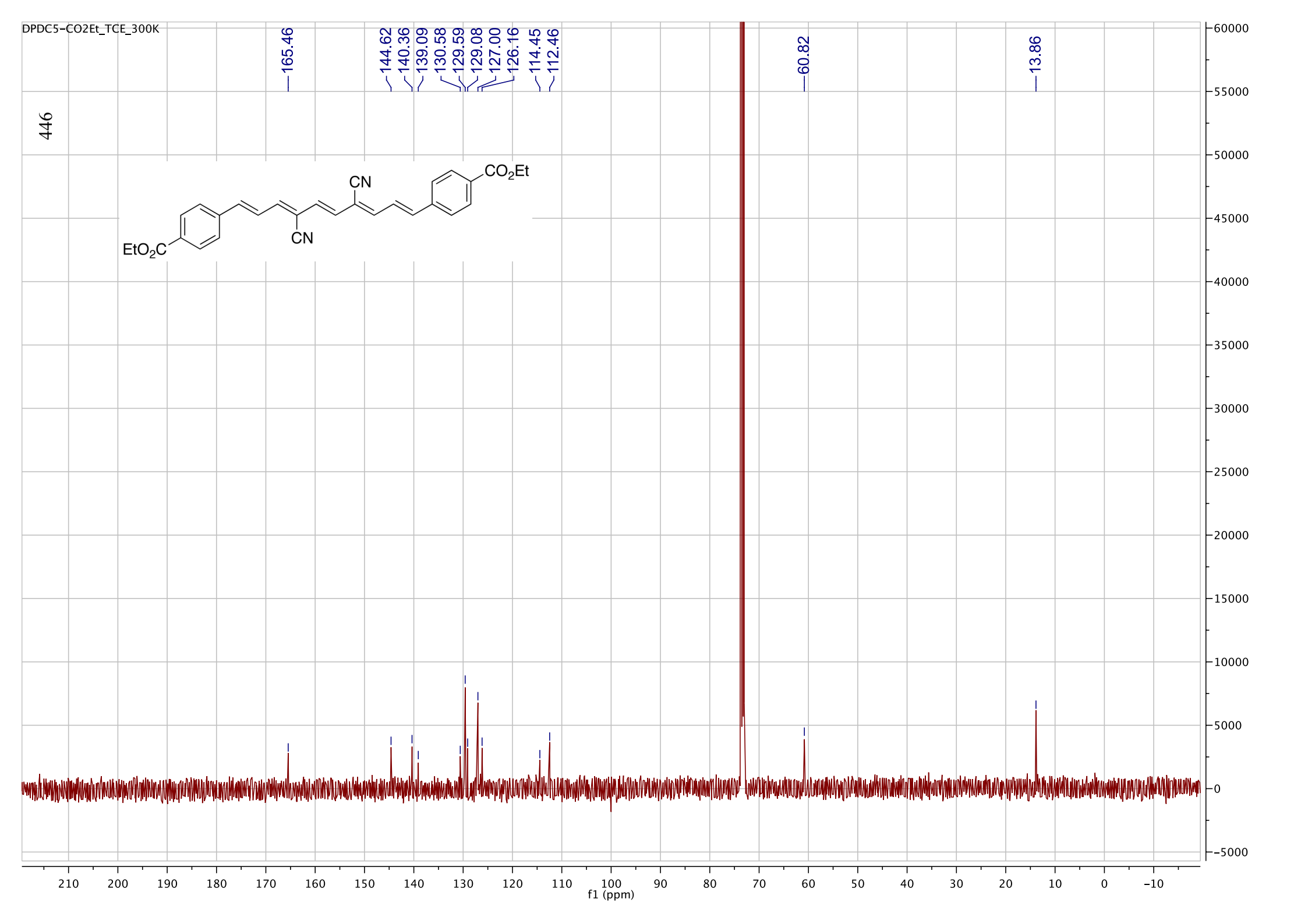


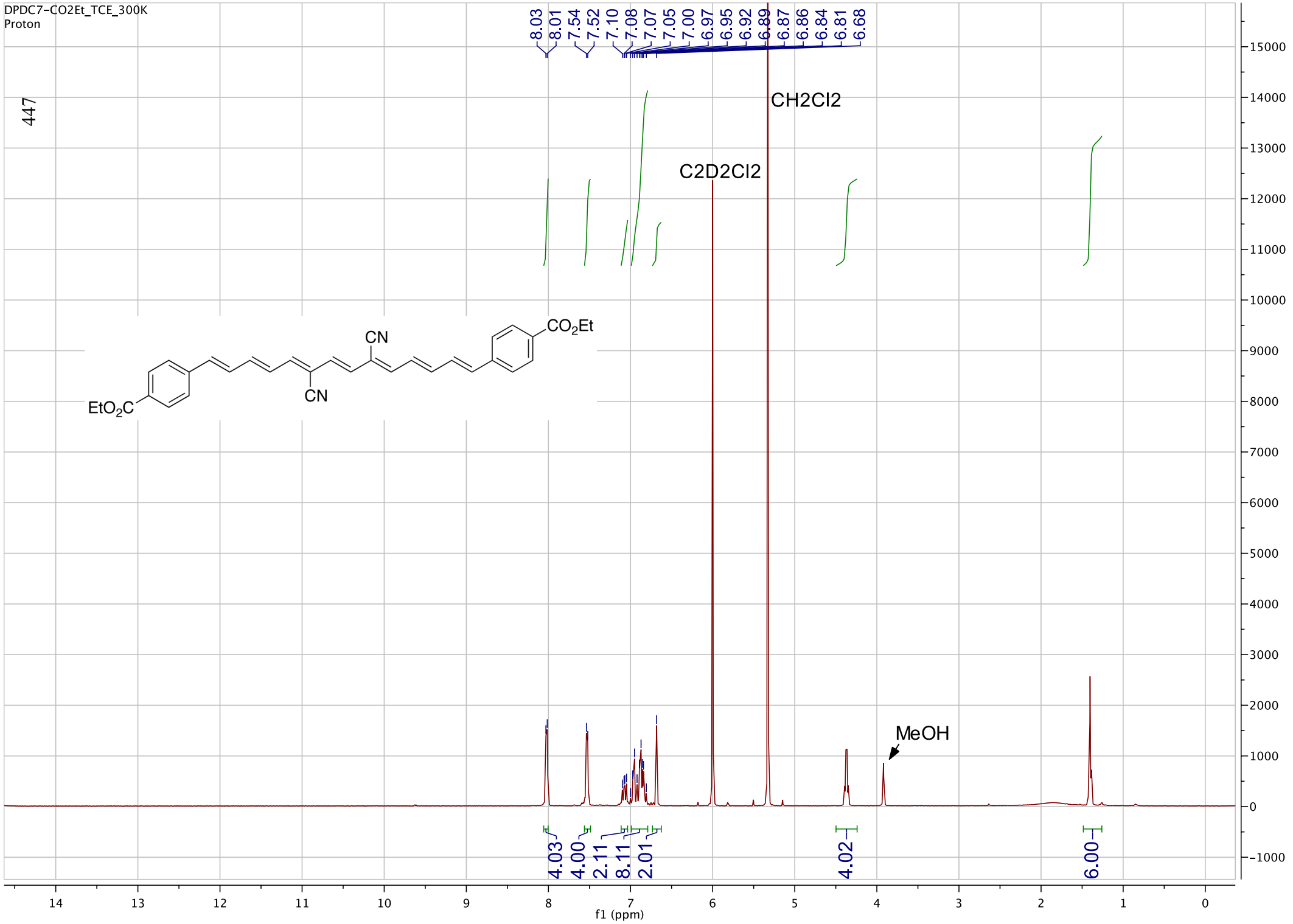
f1 (ppm)

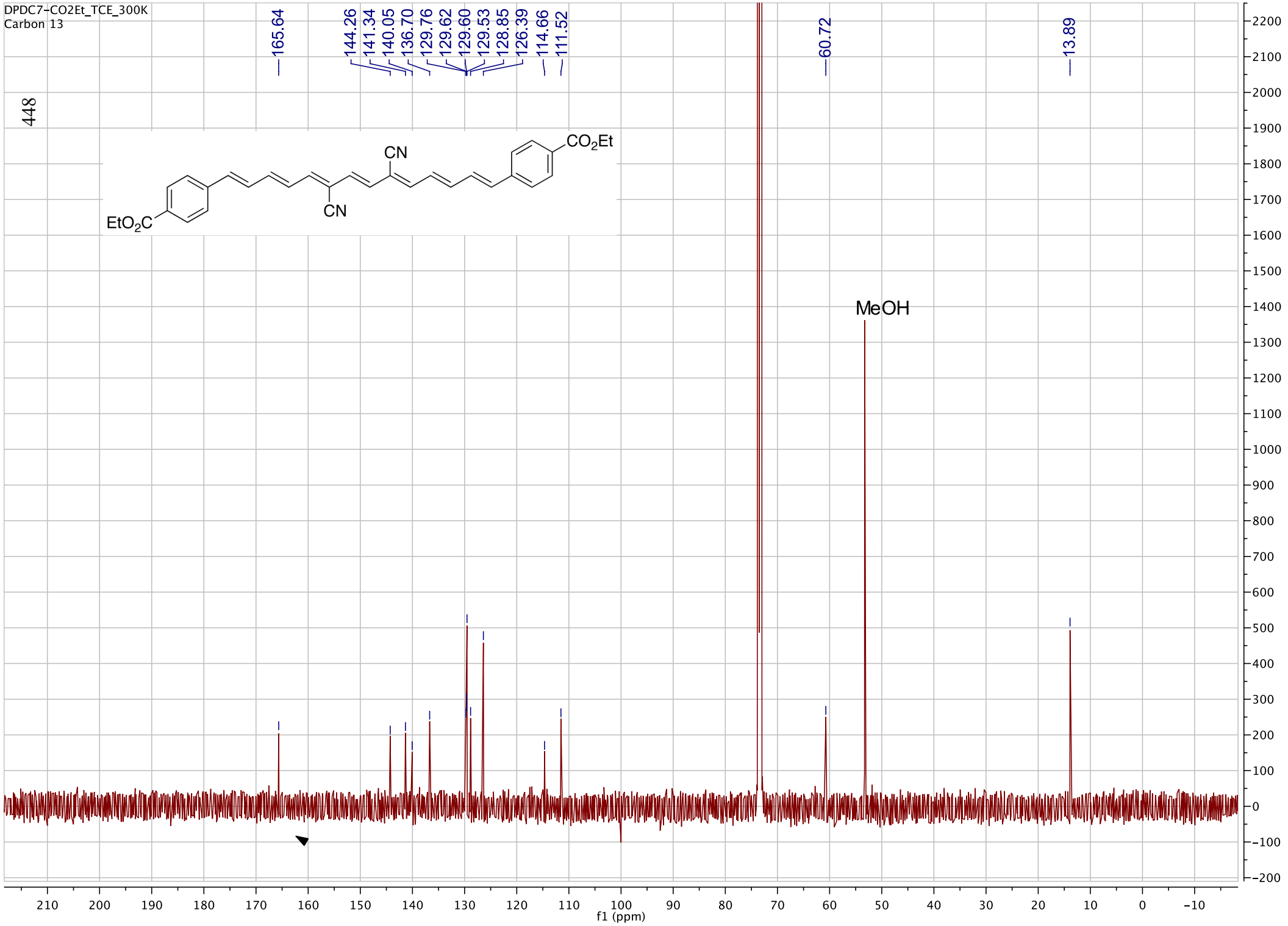

jsm5-089-DPDC3-CO2Et_TCE
Proton
443
8.13
8.12
7.92
7.91
7.31
6.94
4.40
1.42
CN
CO2Et
CN
EtO2C
4.35
4.30
2.15
2.18
4.00
6.02
f1 (ppm)

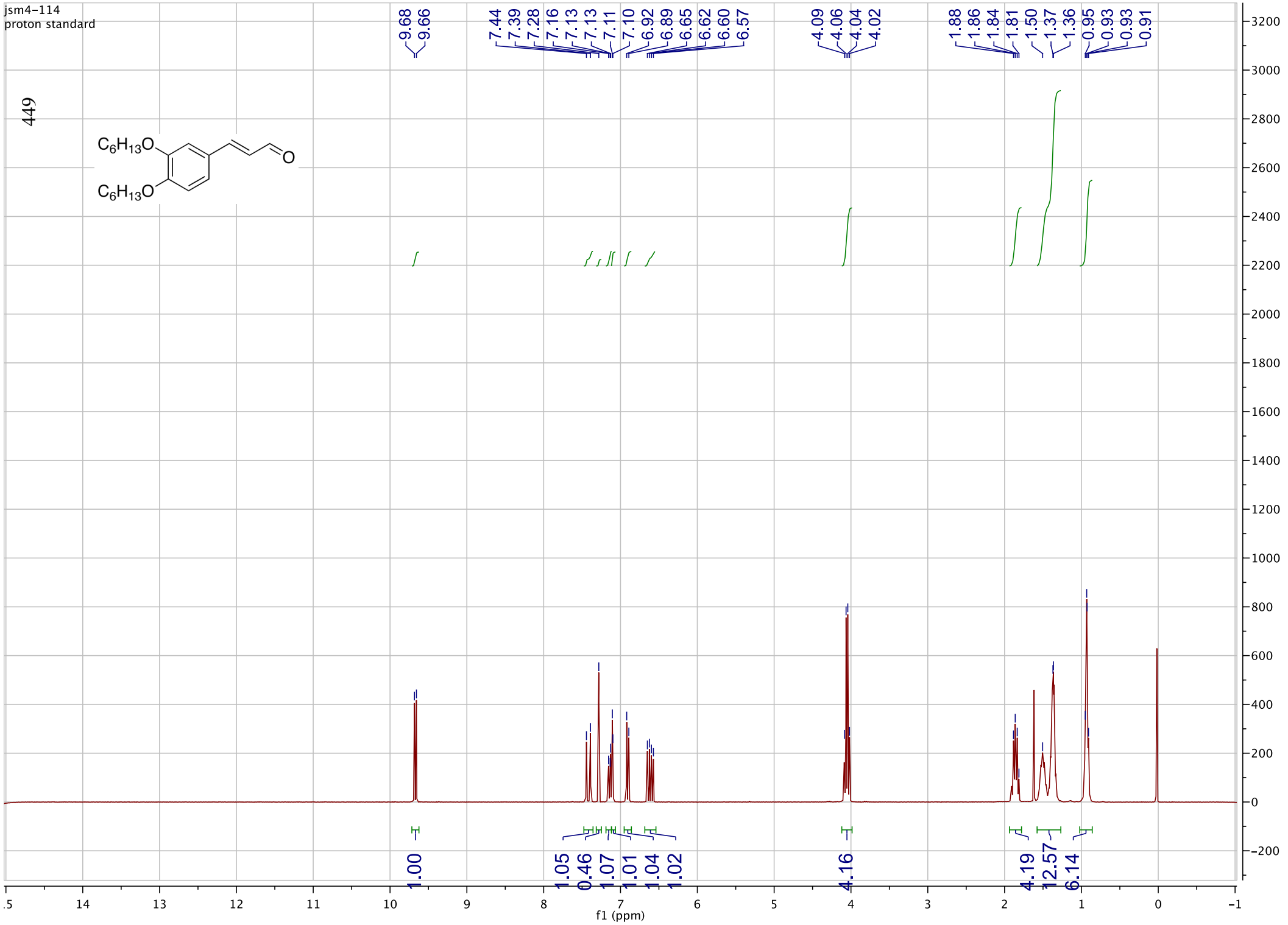

jsm5-089-DPDC3-CO2Et_TCE
Carbon 13
166.89
145.94
138.52
134.00
132.51
131.49
130.59
116.75
113.20
99.99
62.72
15.64
444
CN
CO2Et
CN
EtO2C
f1 (ppm)


DPDC5-CO2Et_TCE_300K
proton
445
8.06
8.04
7.62
7.60
7.38
7.35
7.34
7.31
7.09
7.06
7.05
7.01
6.75
4.41
4.39
4.38
4.36
1.43
1.41
1.40
CN
CN
CO2Et
EtO2C
MeOH
4.08
4.26
2.00
4.01
1.85
4.00
6.24
f1 (ppm)

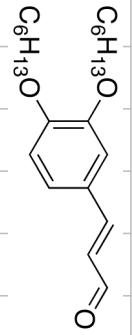

DPDC5-CO2Et_TCE_300K
446
165.46
144.62
140.36
139.09
130.58
129.59
129.08
127.00
126.16
114.45
112.46
60.82
13.86
CN
CN
CO2Et
EtO2C
f1 (ppm)


DPDC7-CO2Et_TCE_300K
Proton
447
8.03
8.01
7.54
7.52
7.10
7.08
7.07
7.05
7.00
6.97
6.95
6.92
6.89
6.87
6.86
6.84
6.81
6.68
CH2Cl2
C2D2Cl2
CN
CO2Et
EtO2C
CN
MeOH
4.03
4.00
2.11
8.11
2.01
4.02
6.00
f1 (ppm)


DPDC7-CO2Et_TCE_300K
Carbon 13
448
165.64
144.26
141.34
140.05
136.70
129.76
129.62
129.60
129.53
128.85
126.39
114.66
111.52
60.72
13.89
CN
CN
CO2Et
EtO2C
MeOH
f1 (ppm)


jsm4-114
proton standard
449
C6H13O
C6H13O
O
9.68
9.66
7.44
7.39
7.28
7.16
7.13
7.13
7.11
7.10
6.92
6.89
6.65
6.62
6.60
6.57
4.09
4.06
4.04
4.02
1.88
1.86
1.84
1.81
1.50
1.37
1.36
0.95
0.93
0.93
0.91
1.00
1.05
0.46
1.07
1.01
1.04
1.02
4.16
4.19
12.57
6.14
f1 (ppm)

jsm4-114
carbon NMR



194.06

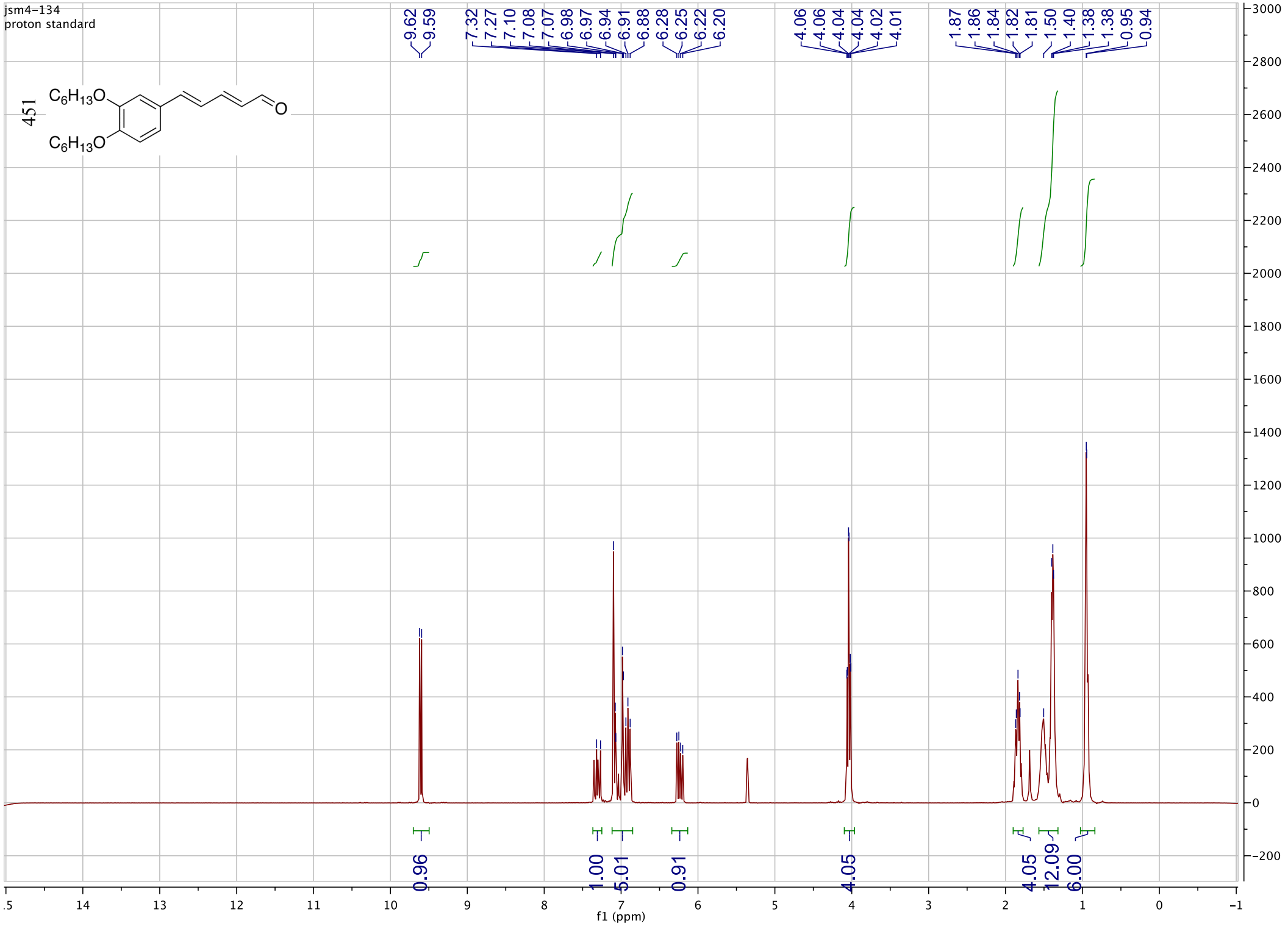
153.59
152.66
149.65

127.20
126.83
123.88
113.14
112.69

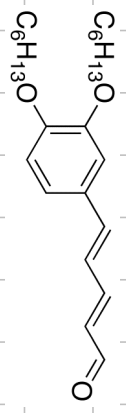
69.72
69.44

31.97
31.94
29.54
29.43
26.08
26.05
23.01
23.00
14.43

f1 (ppm)

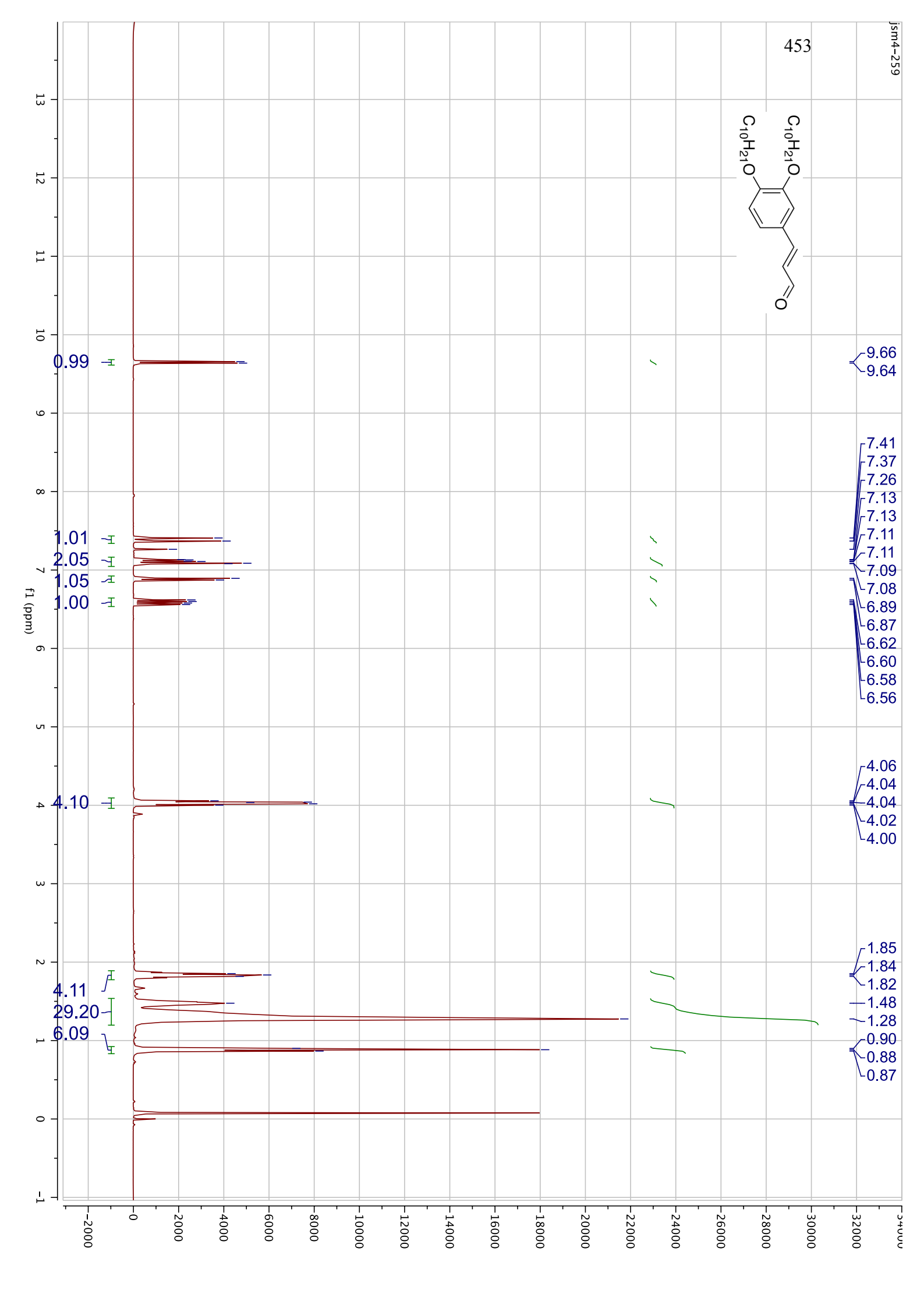

jsm4-134
proton standard
451
$C_6H_{13}O$
$C_6H_{13}O$
O
9.62
9.59
7.32
7.27
7.10
7.08
7.07
6.98
6.97
6.94
6.91
6.88
6.28
6.25
6.22
6.20
4.06
4.06
4.04
4.04
4.02
4.01
1.87
1.86
1.84
1.82
1.81
1.50
1.40
1.38
1.38
0.95
0.94
0.96
1.00
5.01
0.91
4.05
4.05
12.09
6.00
f1 (ppm)

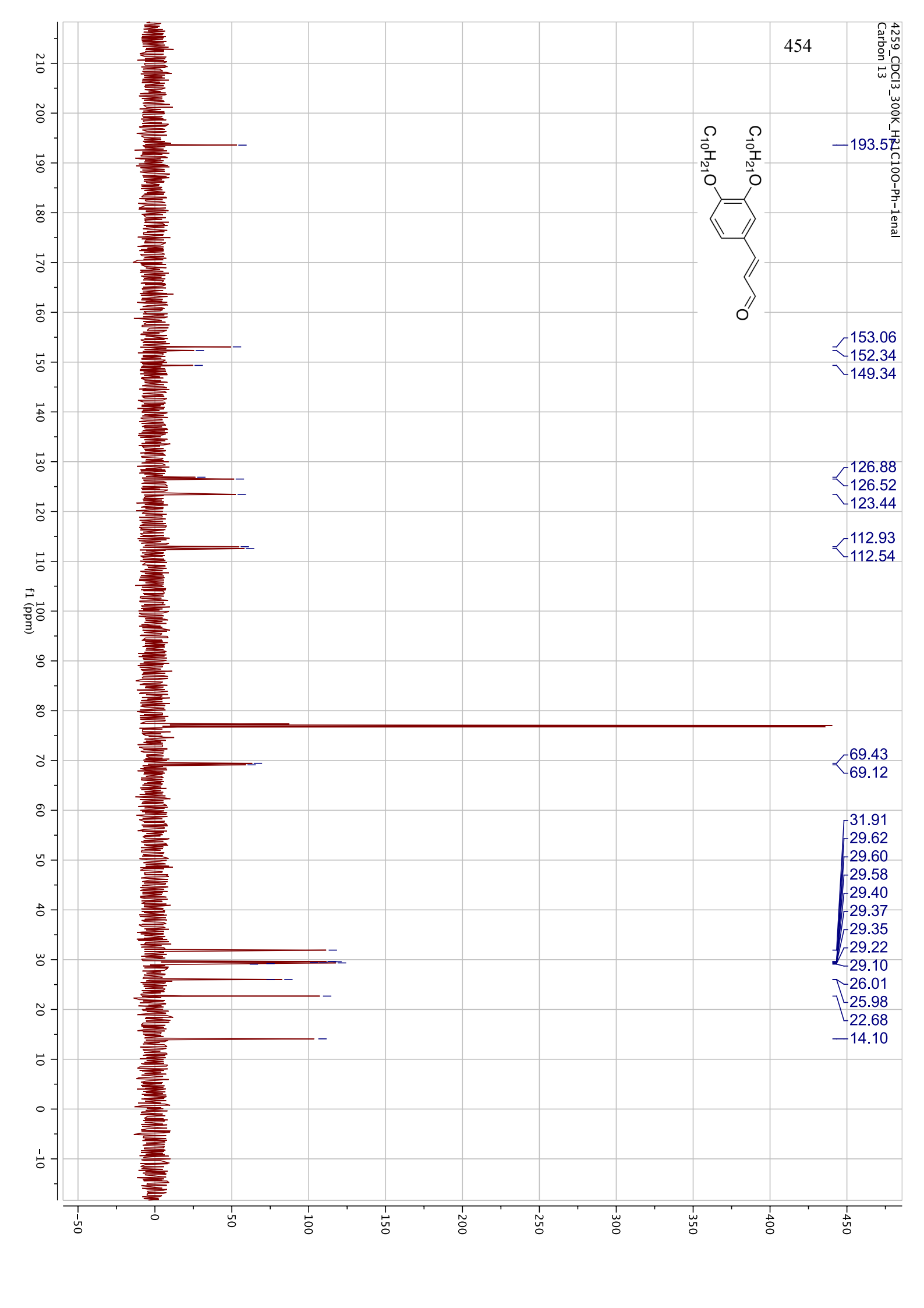
jsm4-134
carbon NMR

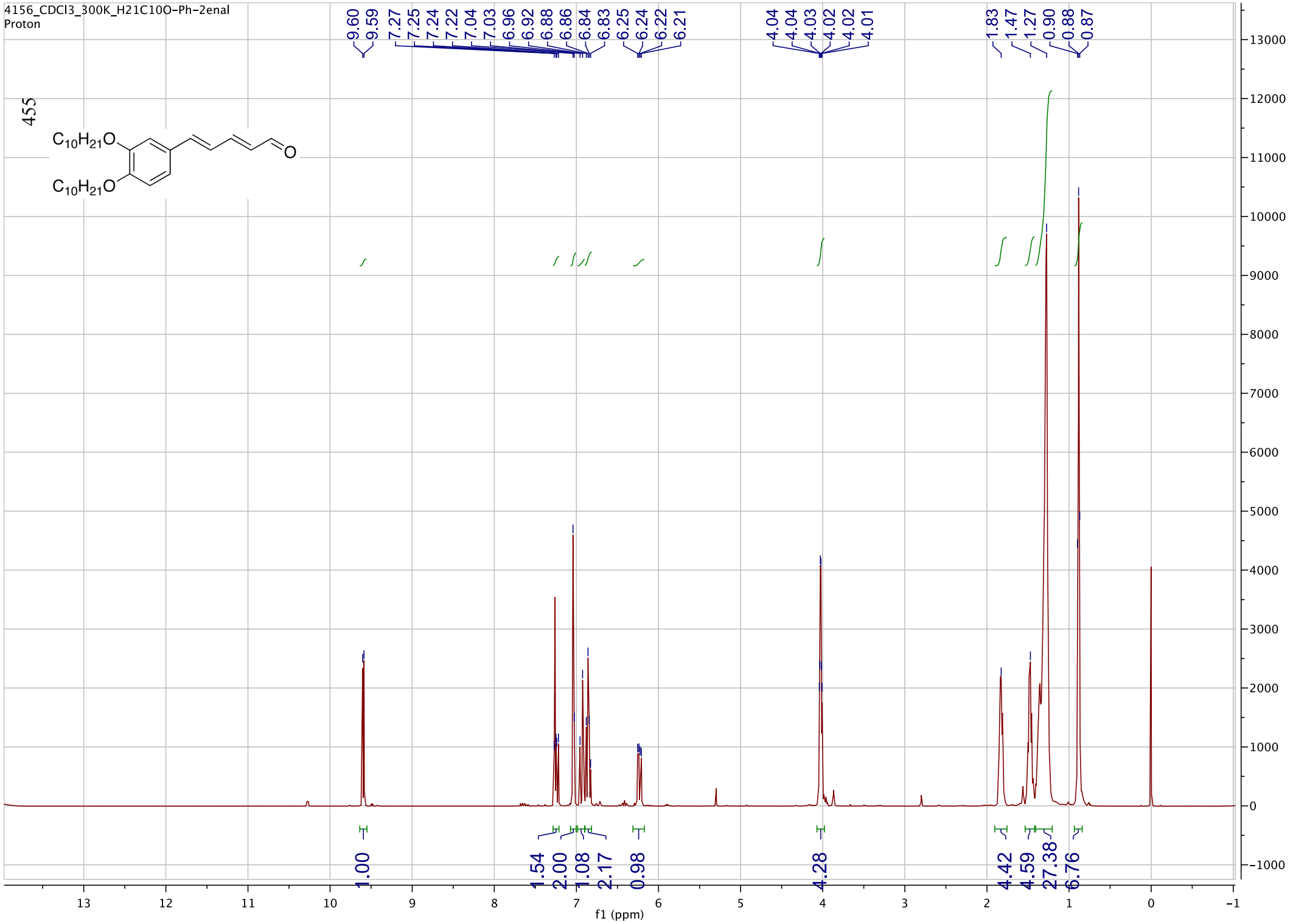


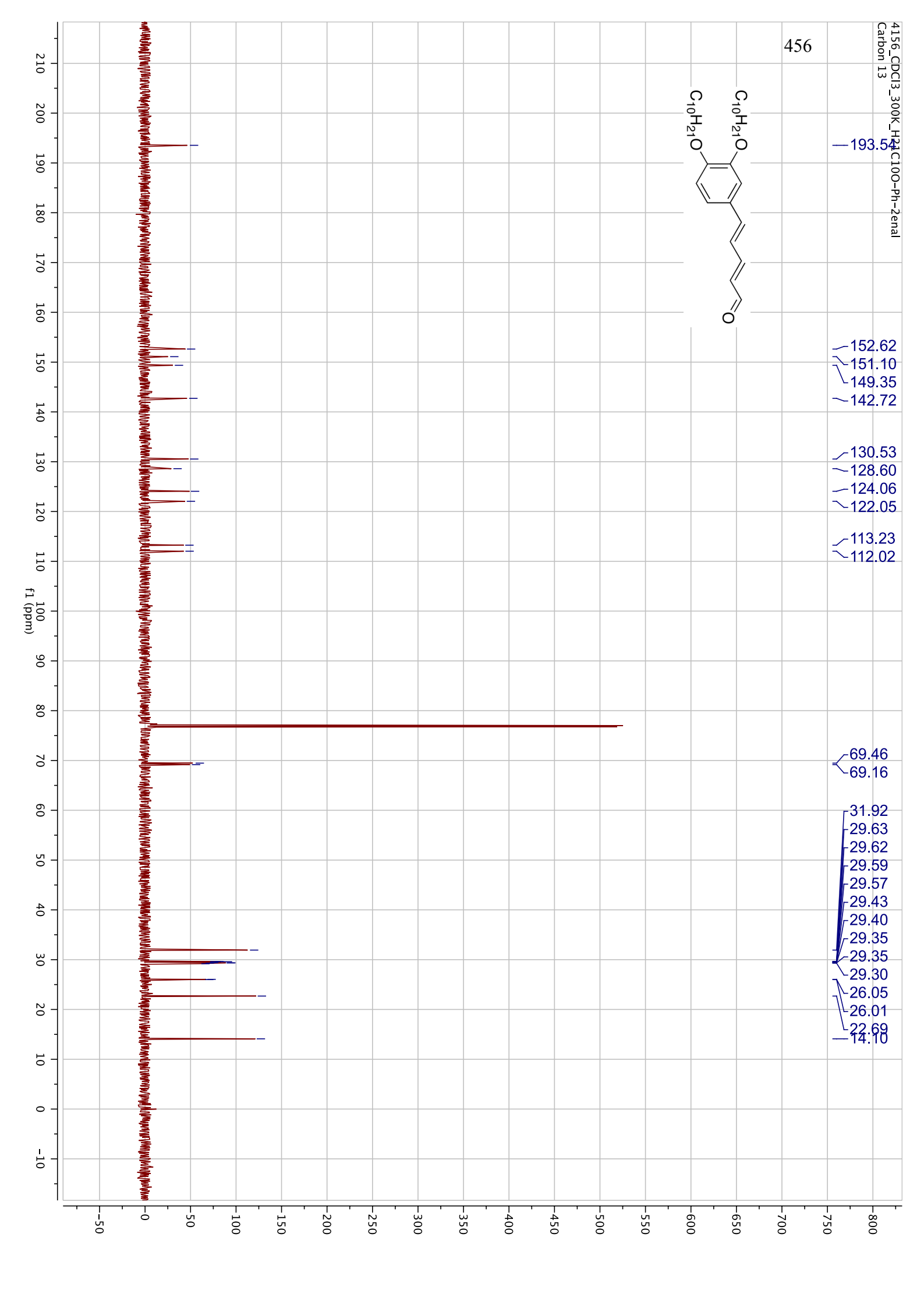
195.73
154.96
152.97
151.07
144.77
132.05
130.25
125.79
124.04
115.28
114.24
71.36
70.96
33.36
33.33
31.07
30.94
27.49
27.46
24.44
15.93

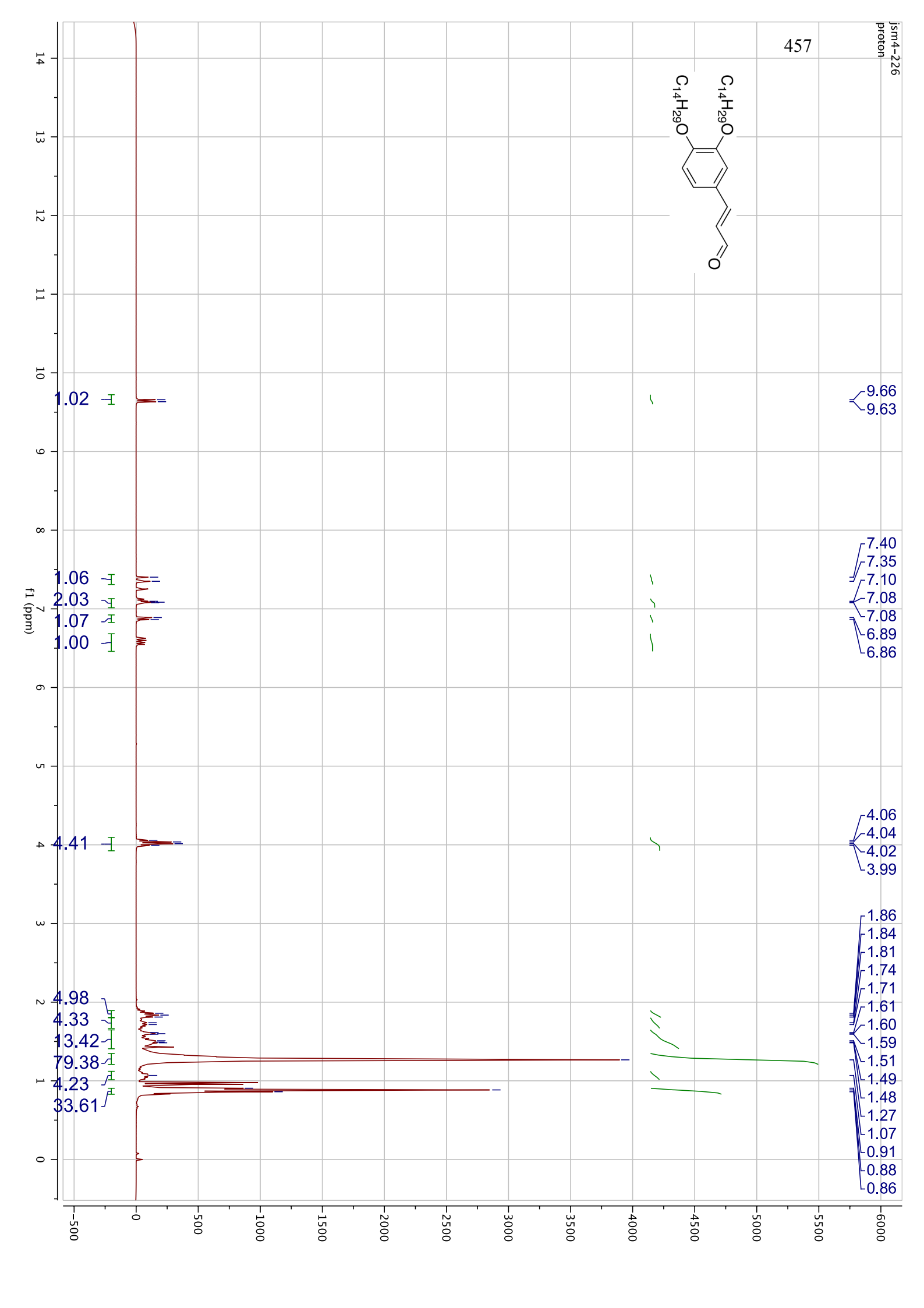
f1 (ppm)

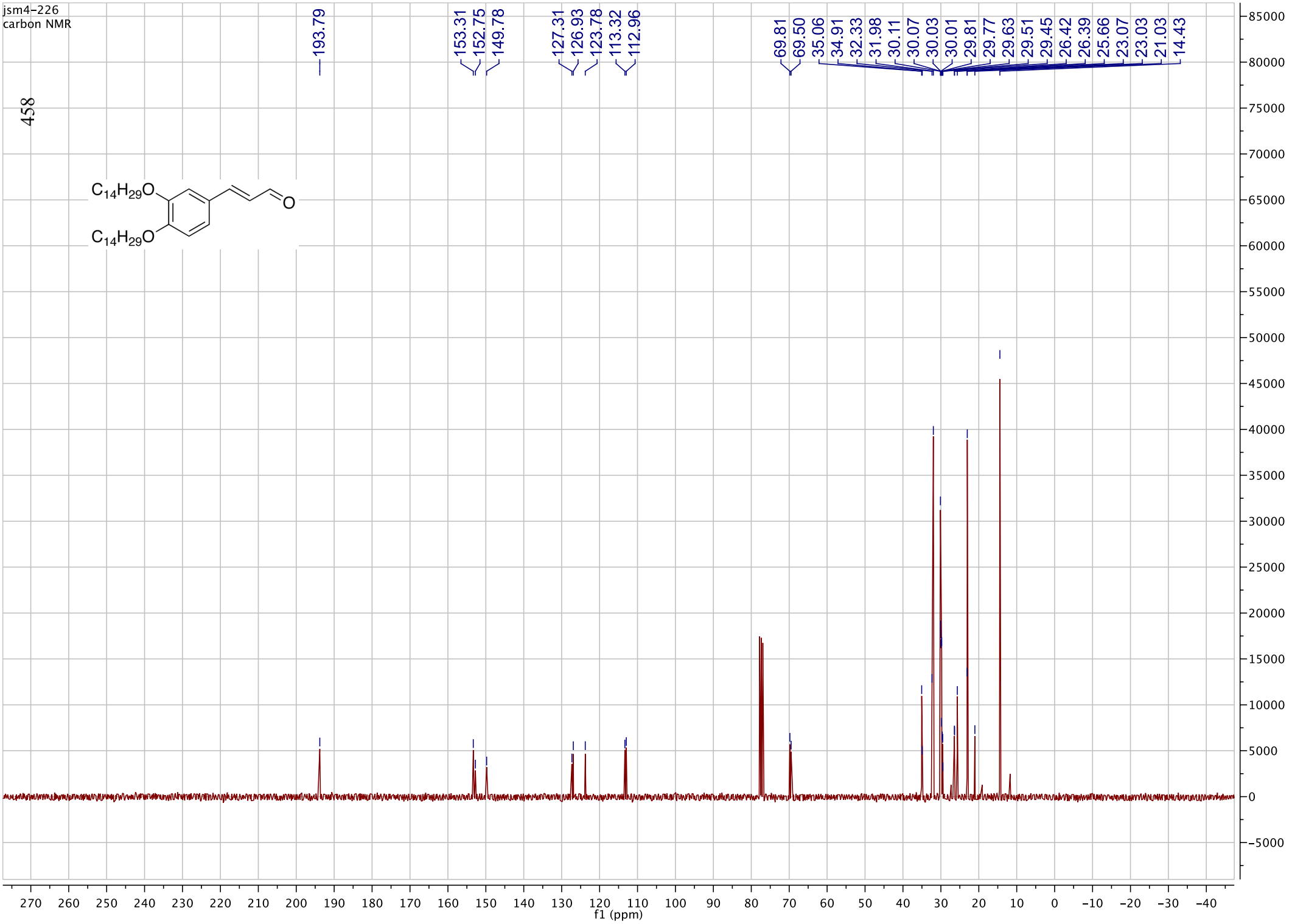

453
jsm4-259
$C_{10}H_{21}O$
$C_{10}H_{21}O$
O
f1 (ppm)
0.99
1.01
2.05
1.05
1.00
4.10
4.11
29.20
6.09
9.66
9.64
7.41
7.37
7.26
7.13
7.13
7.11
7.11
7.09
7.08
6.89
6.87
6.62
6.60
6.58
6.56
4.06
4.04
4.04
4.02
4.00
1.85
1.84
1.82
1.48
1.28
0.90
0.88
0.87

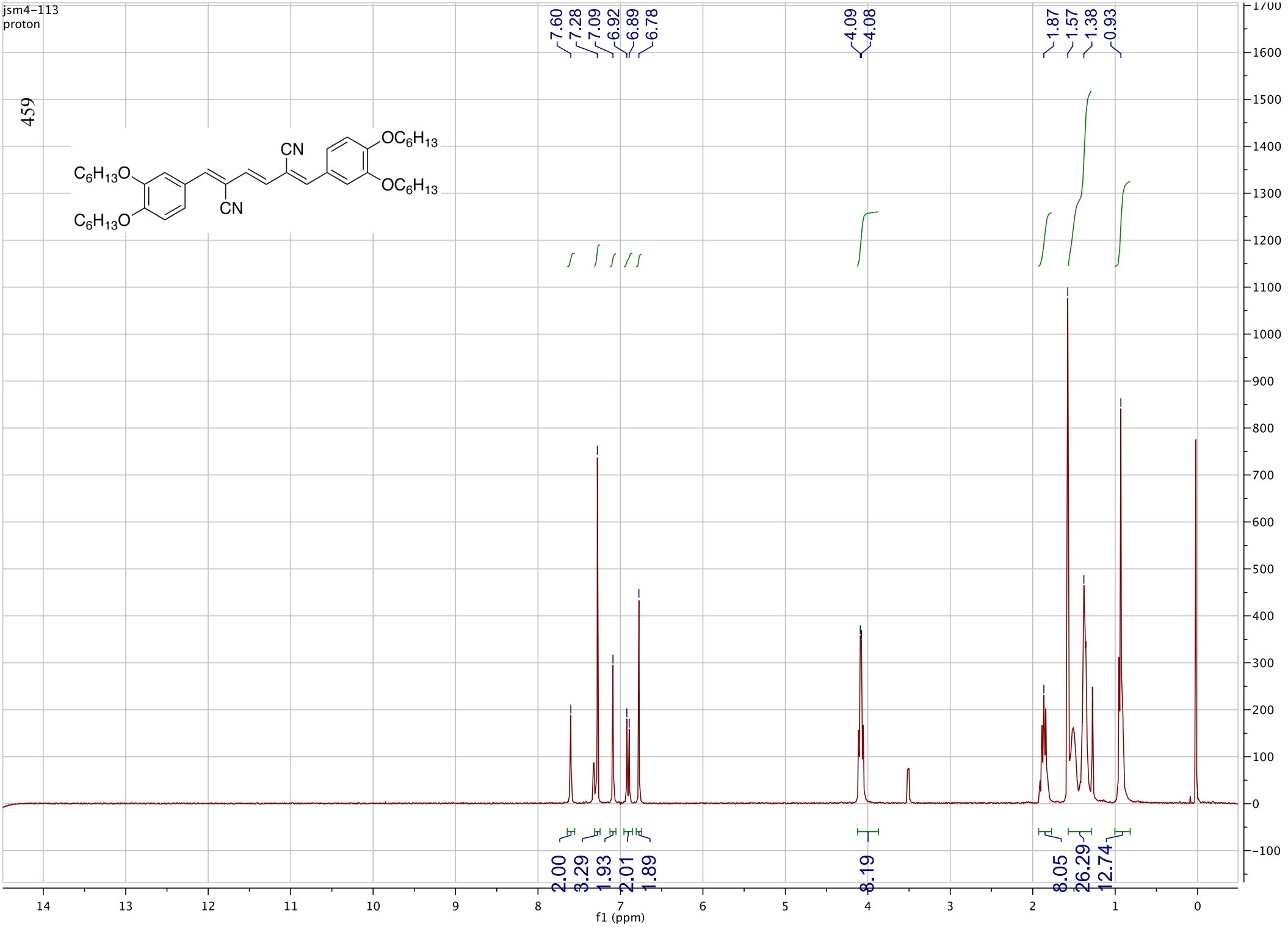

4259_CDCl3_300K_HR1C10O-Ph-1enal
Carbon 13
193.51
153.06
152.34
149.34
126.88
126.52
123.44
112.93
112.54
69.43
69.12
31.91
29.62
29.60
29.58
29.40
29.37
29.35
29.22
29.10
26.01
25.98
22.68
14.10
f1 (ppm)

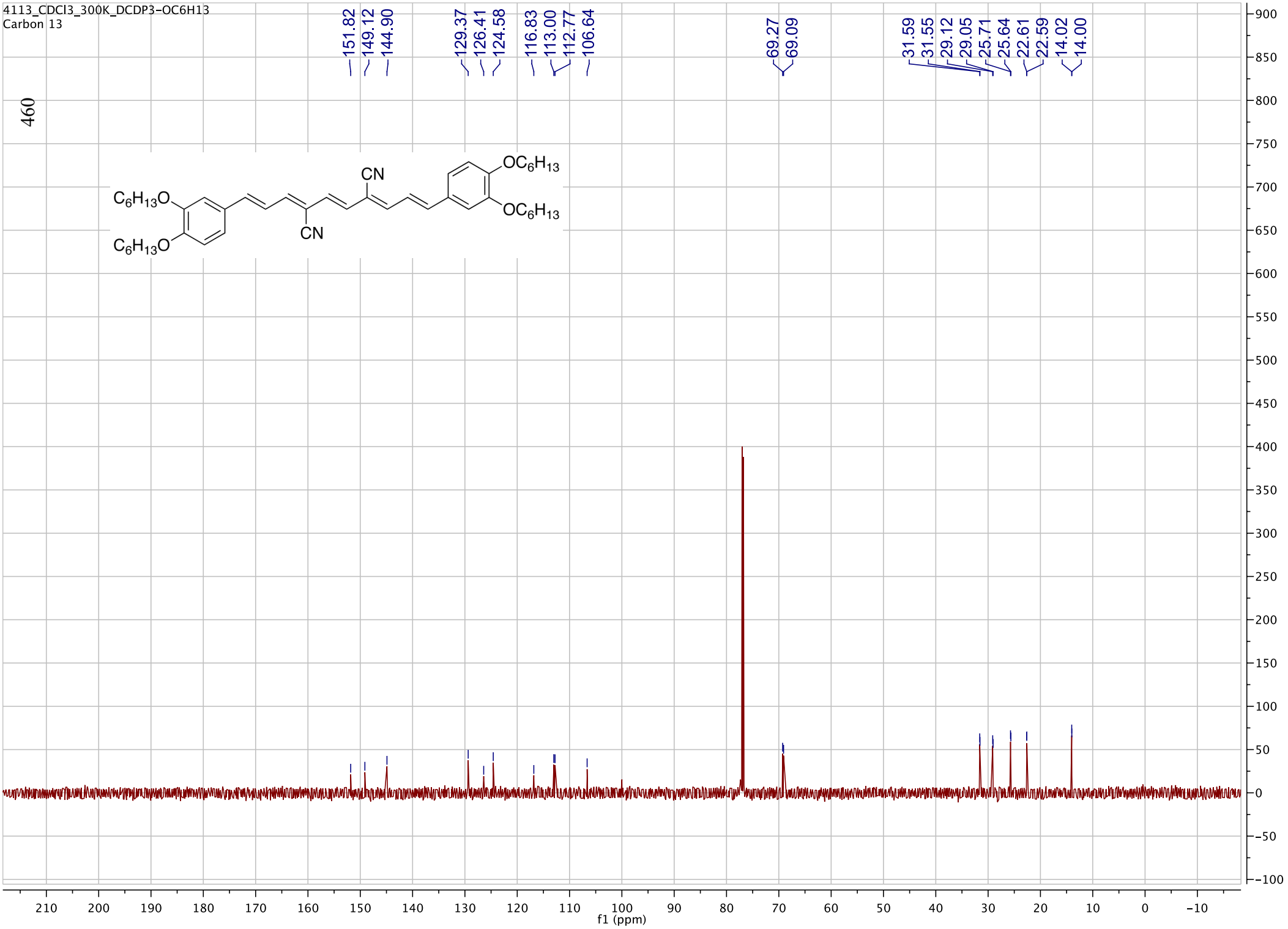

4156_CDCl3_300K_H21C10O-Ph-2enal
Proton
9.60
9.59
7.27
7.25
7.24
7.22
7.04
7.03
6.96
6.92
6.88
6.86
6.84
6.83
6.25
6.24
6.22
6.21
4.04
4.04
4.03
4.02
4.02
4.01
1.83
1.47
1.27
0.90
0.88
0.87
455
C10H21O
C10H21O
O
1.00
1.54
2.00
1.08
2.17
0.98
4.28
4.42
4.59
27.38
6.76
f1 (ppm)

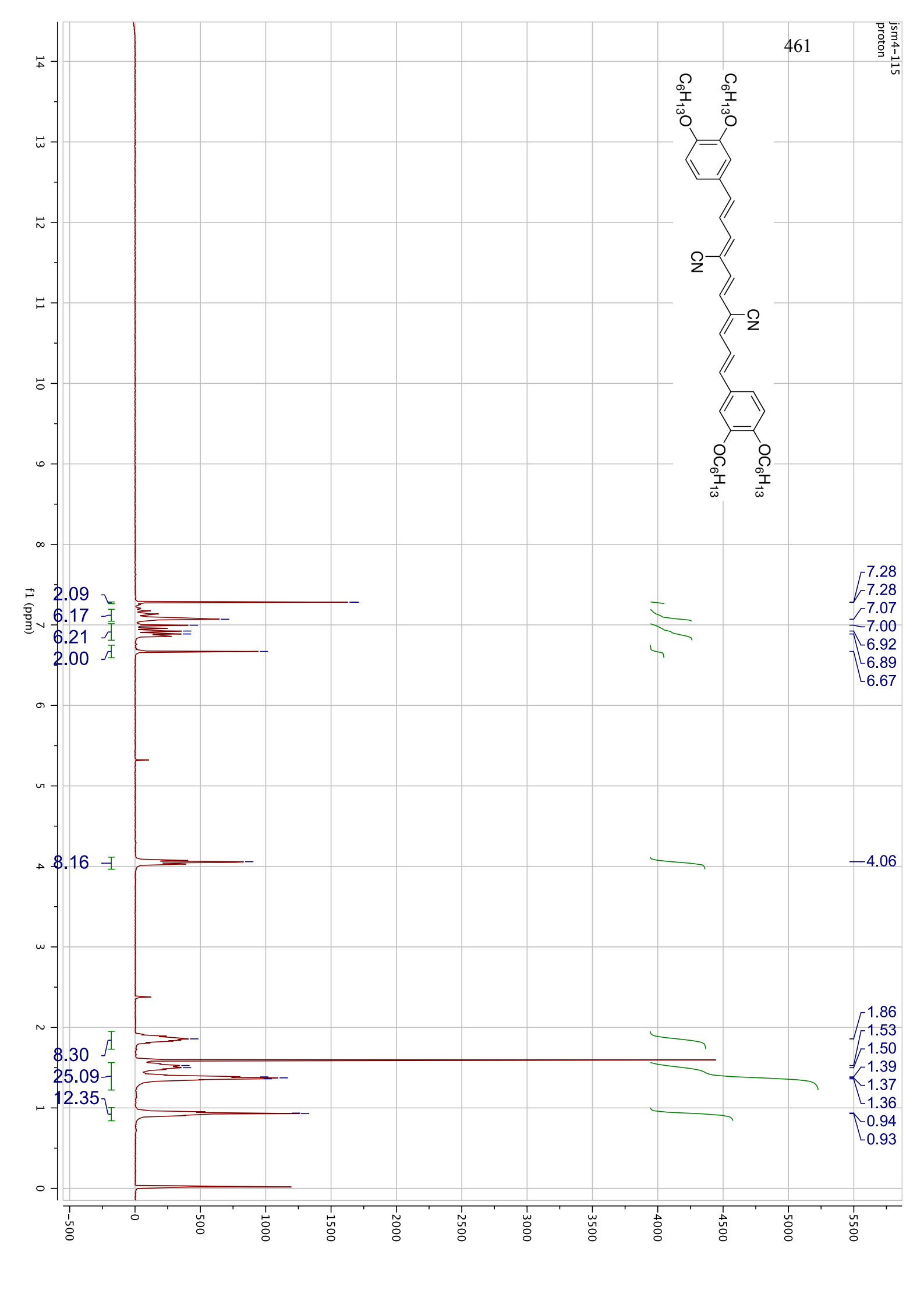

456
4156_CDCl3_300K_H24C10O-Ph-2enal
Carbon 13
193.54
152.62
151.10
149.35
142.72
130.53
128.60
124.06
122.05
113.23
112.02
69.46
69.16
31.92
29.63
29.62
29.59
29.57
29.43
29.40
29.35
29.35
29.30
26.05
26.01
22.69
14.10
f1 (ppm)


457
jsm4-226
proton
$C_{14}H_{29}O$
$C_{14}H_{29}O$
O
f1 (ppm)
1.02
1.06
2.03
1.07
1.00
4.41
4.98
4.33
13.42
79.38
4.23
33.61
9.66
9.63
7.40
7.35
7.10
7.08
7.08
6.89
6.86
4.06
4.04
4.02
3.99
1.86
1.84
1.81
1.74
1.71
1.61
1.60
1.59
1.51
1.49
1.48
1.27
1.07
0.91
0.88
0.86


jsm4-226
carbon NMR
458
193.79
153.31
152.75
149.78
127.31
126.93
123.78
113.32
112.96
69.81
69.50
35.06
34.91
32.33
31.98
30.11
30.07
30.03
30.01
29.81
29.77
29.63
29.51
29.45
26.42
26.39
25.66
23.07
23.03
21.03
14.43
C14H29O
C14H29O
O
f1 (ppm)

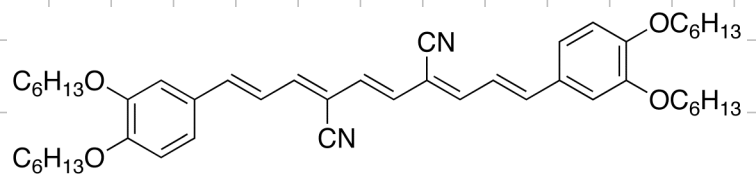

jsm4-113
proton
459
7.60
7.28
7.09
6.92
6.89
6.78
4.09
4.08
1.87
1.57
1.38
0.93
CN
CN
OC6H13
OC6H13
C6H13O
C6H13O
2.00
3.29
1.93
2.01
1.89
8.19
8.05
26.29
12.74
f1 (ppm)


4113_CDCl3_300K_DCDP3-OC6H13
Carbon 13
151.82
149.12
144.90
129.37
126.41
124.58
116.83
113.00
112.77
106.64
69.27
69.09
31.59
31.55
29.12
29.05
25.71
25.64
22.61
22.59
14.02
14.00
460
CN
CN
C6H13O
C6H13O
OC6H13
OC6H13
f1 (ppm)


jsm4-115
proton
f1 (ppm)
2.09
6.17
6.21
2.00
8.16
8.30
25.09
12.35
7.28
7.28
7.07
7.00
6.92
6.89
6.67
4.06
1.86
1.53
1.50
1.39
1.37
1.36
0.94
0.93
CN
CN
OC6H13
OC6H13
OC6H13
OC6H13

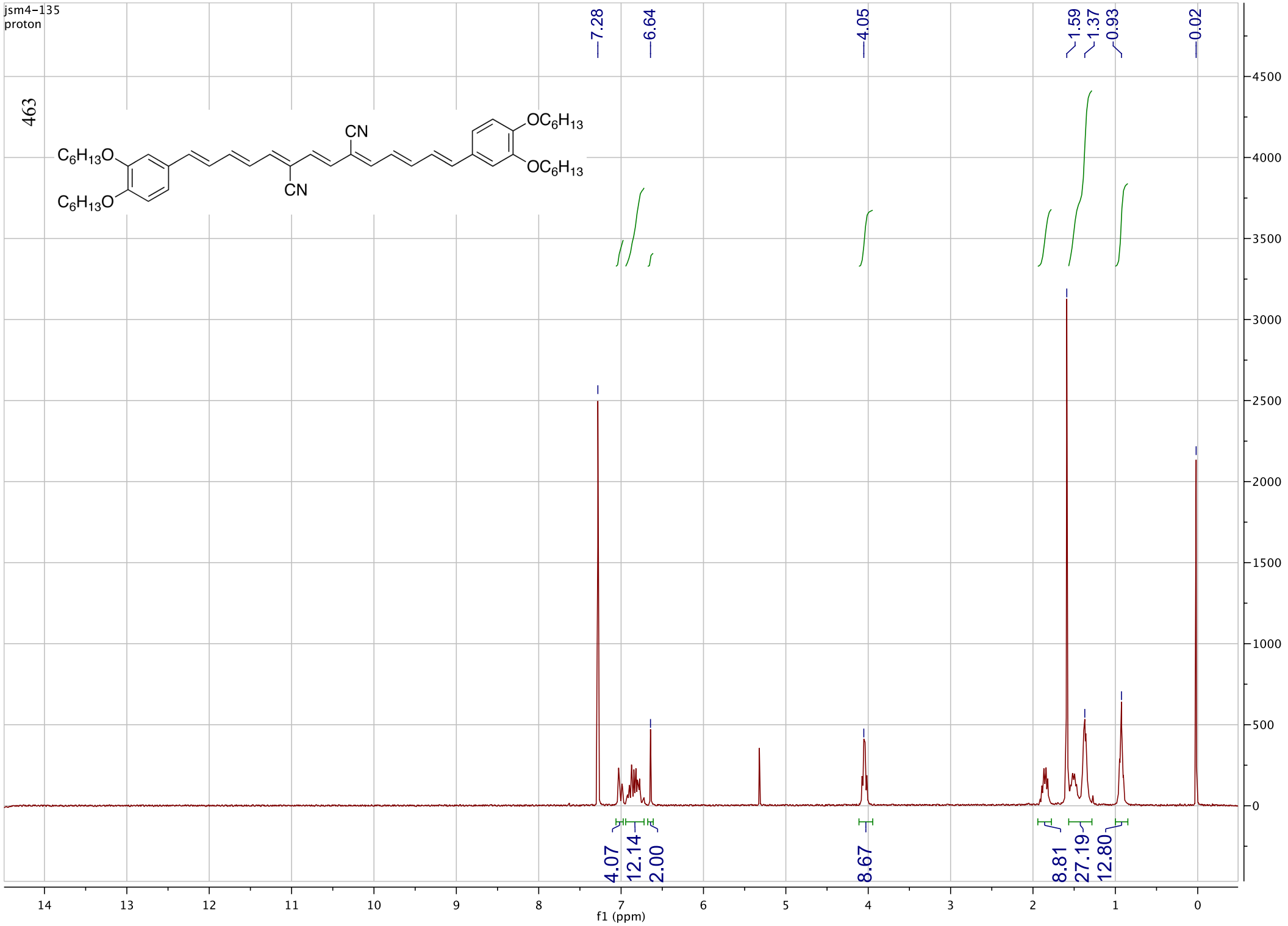
jsm4-115
carbon NMR

462

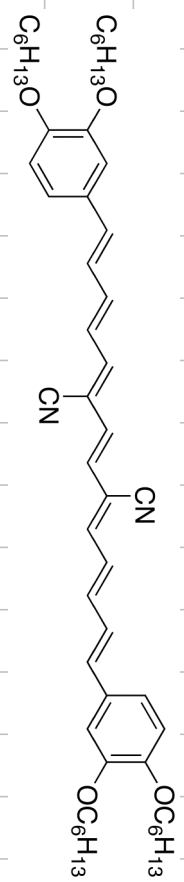


151.59
149.74
145.94
142.62
129.05
123.04
122.74
116.03
115.00
113.44
112.14
110.67
69.80
69.49
32.01
31.97
29.64
29.50
26.11
26.07
23.01
14.43

f1 (ppm)


jsm4-135
proton
463
7.28
6.64
4.05
1.59
1.37
0.93
0.02
CN
CN
OC6H13
OC6H13
C6H13O
C6H13O
4.07
12.14
2.00
8.67
8.81
27.19
12.80
f1 (ppm)

jsm4-135
carbon NMR

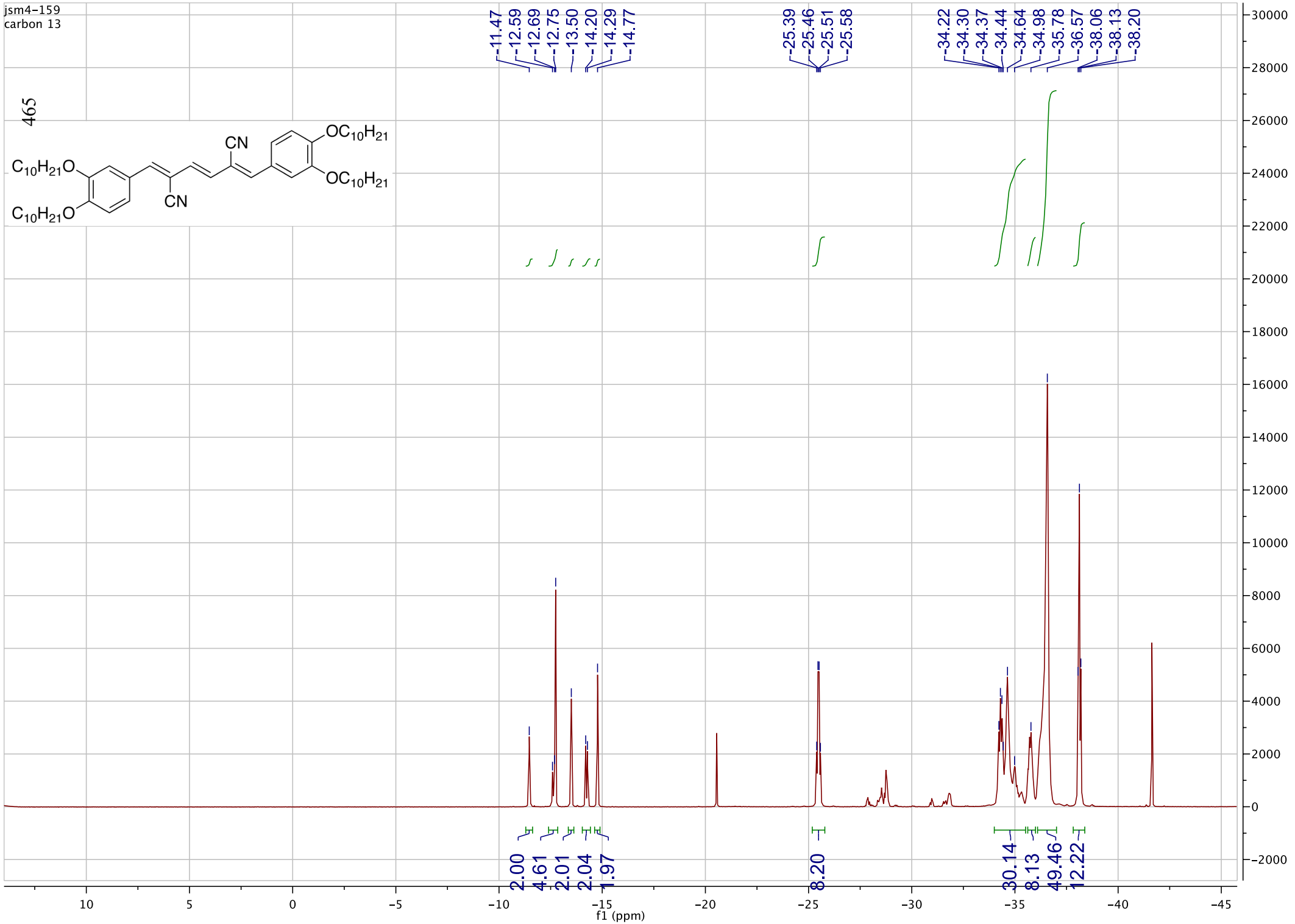


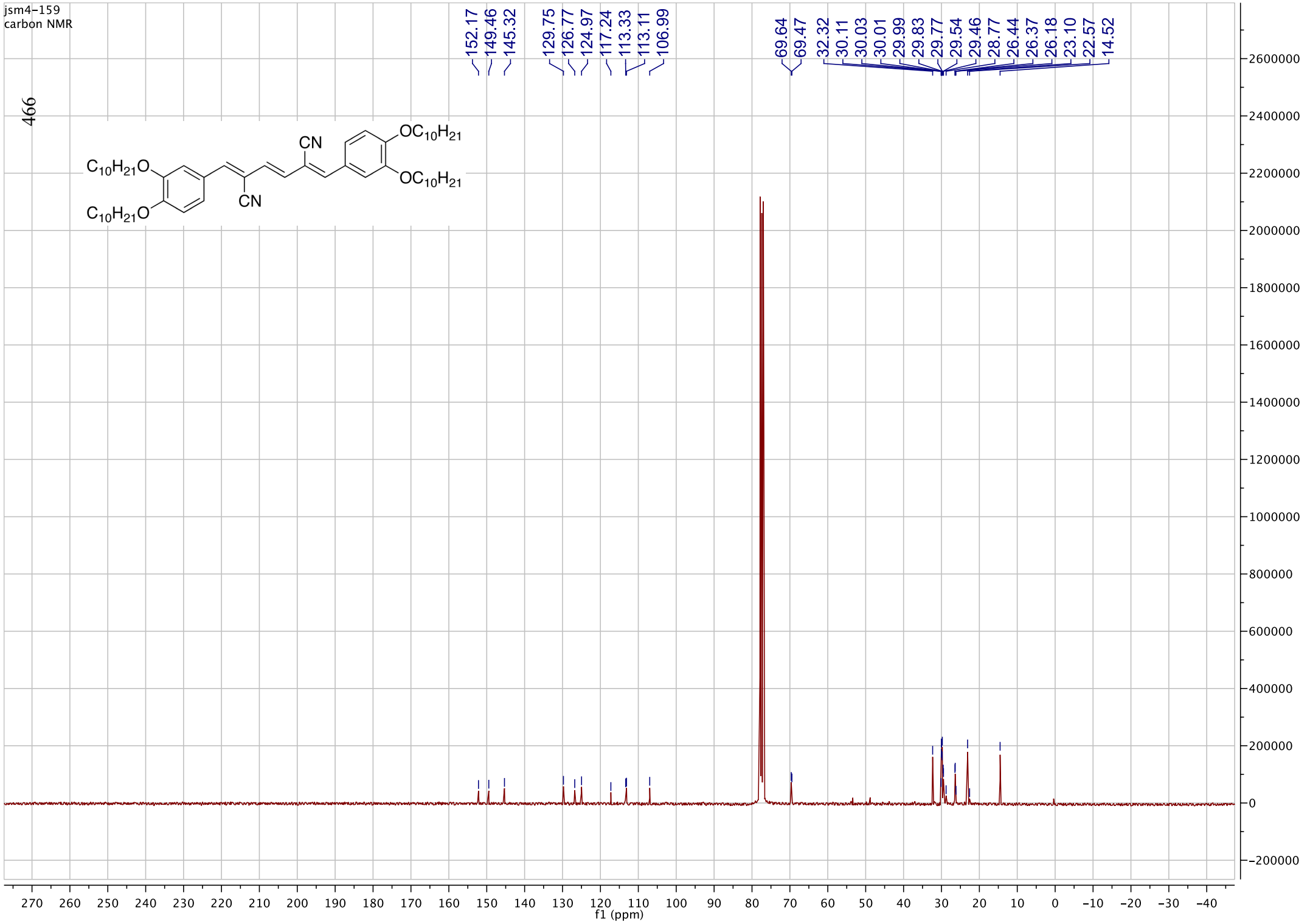
150.76
149.67
145.22
142.99
139.08
129.87
129.21
128.32
126.53
121.77
115.88
115.00
113.65
111.70
111.06

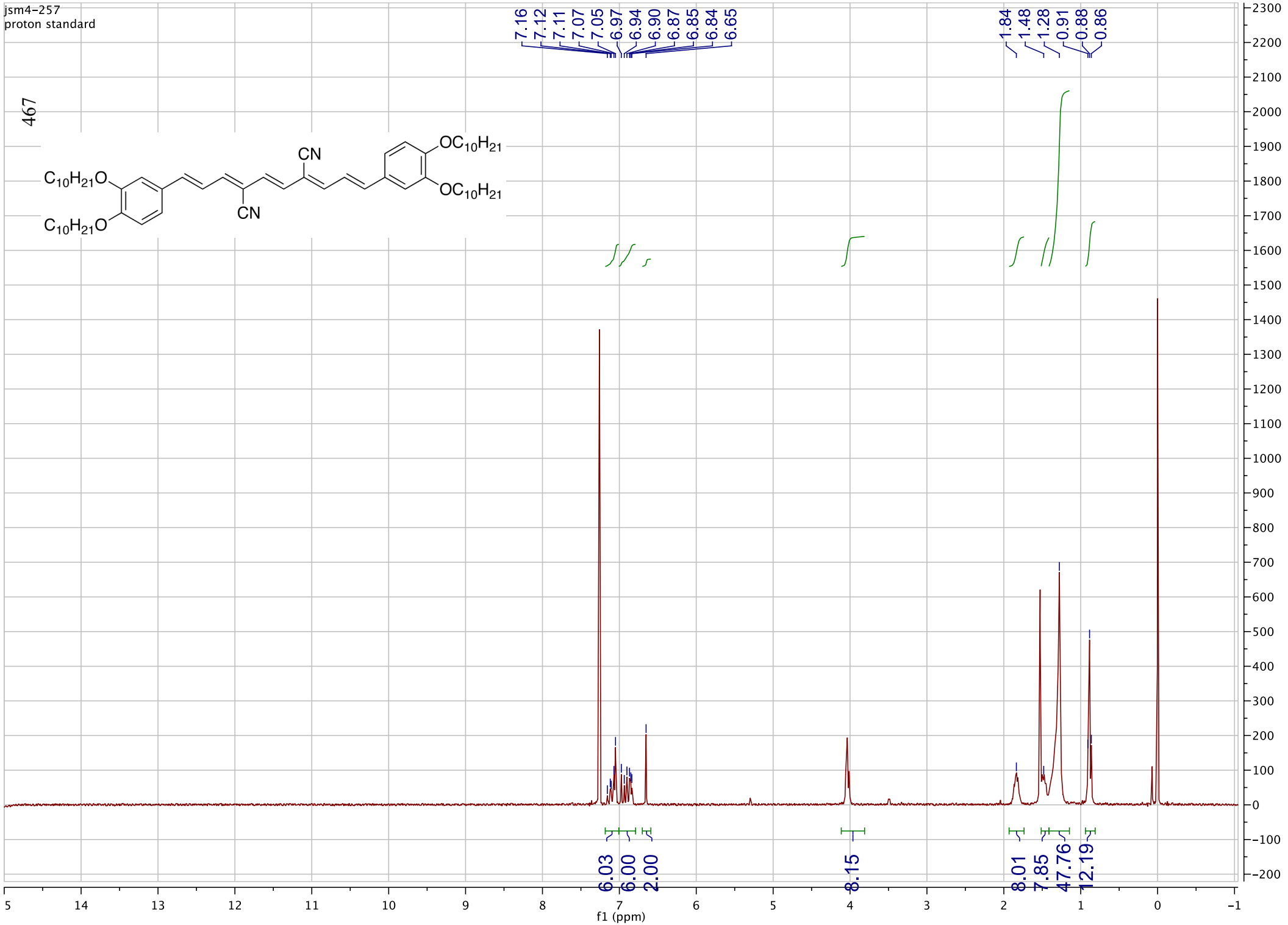
69.68
69.54

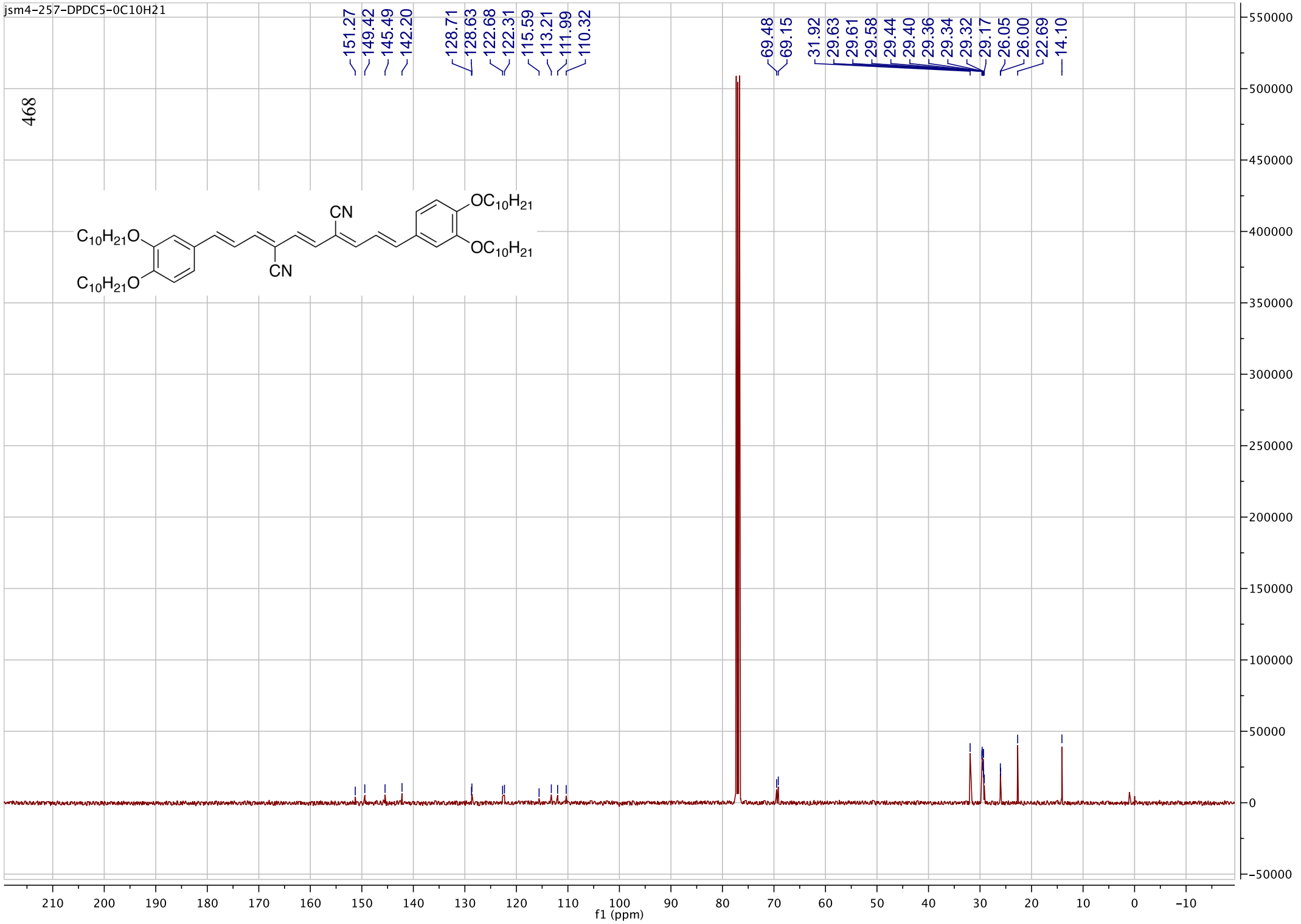
32.00
31.98
29.63
29.54
26.11
26.08
23.03
23.01
14.45
14.43

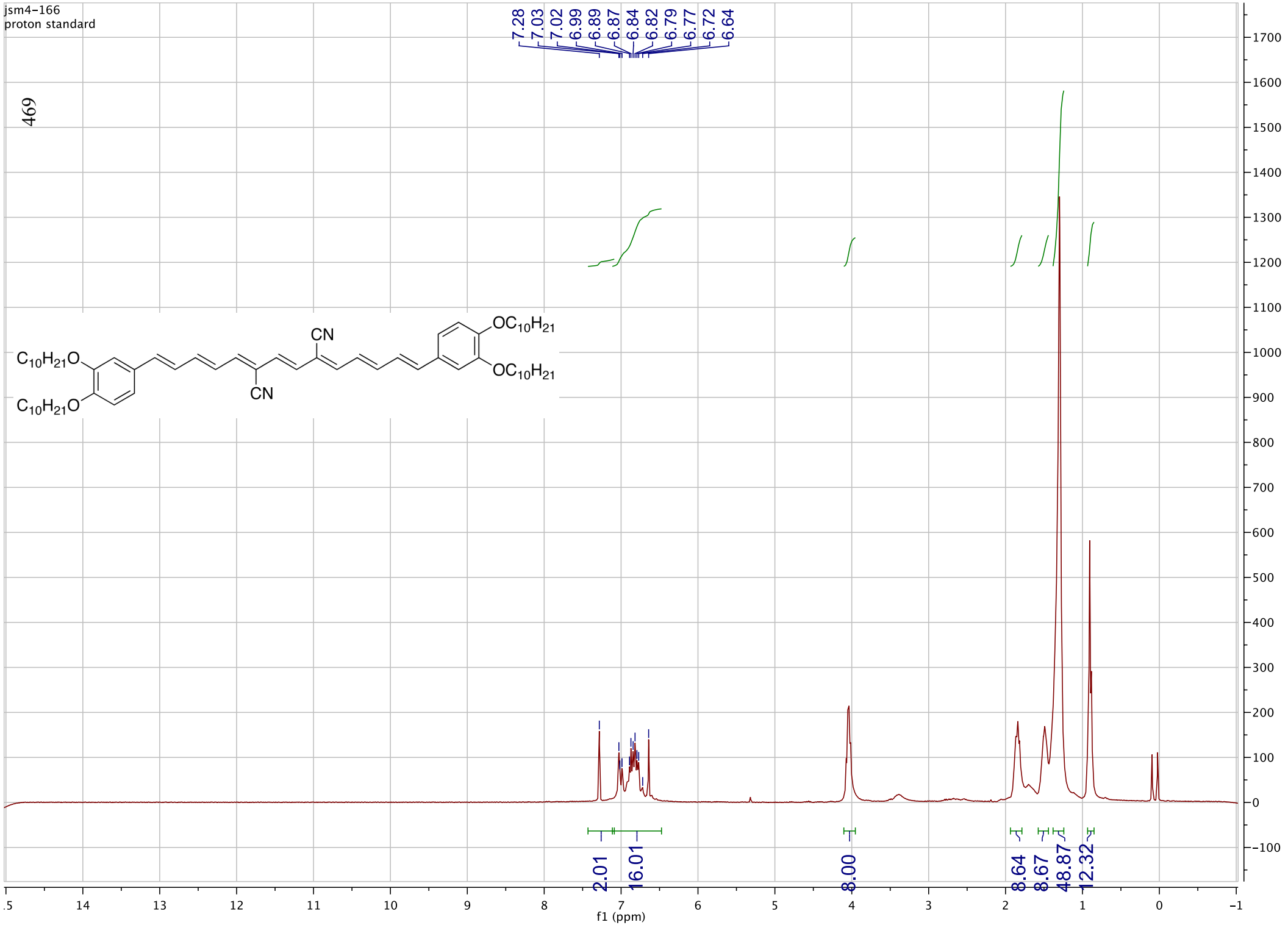
f1 (ppm)

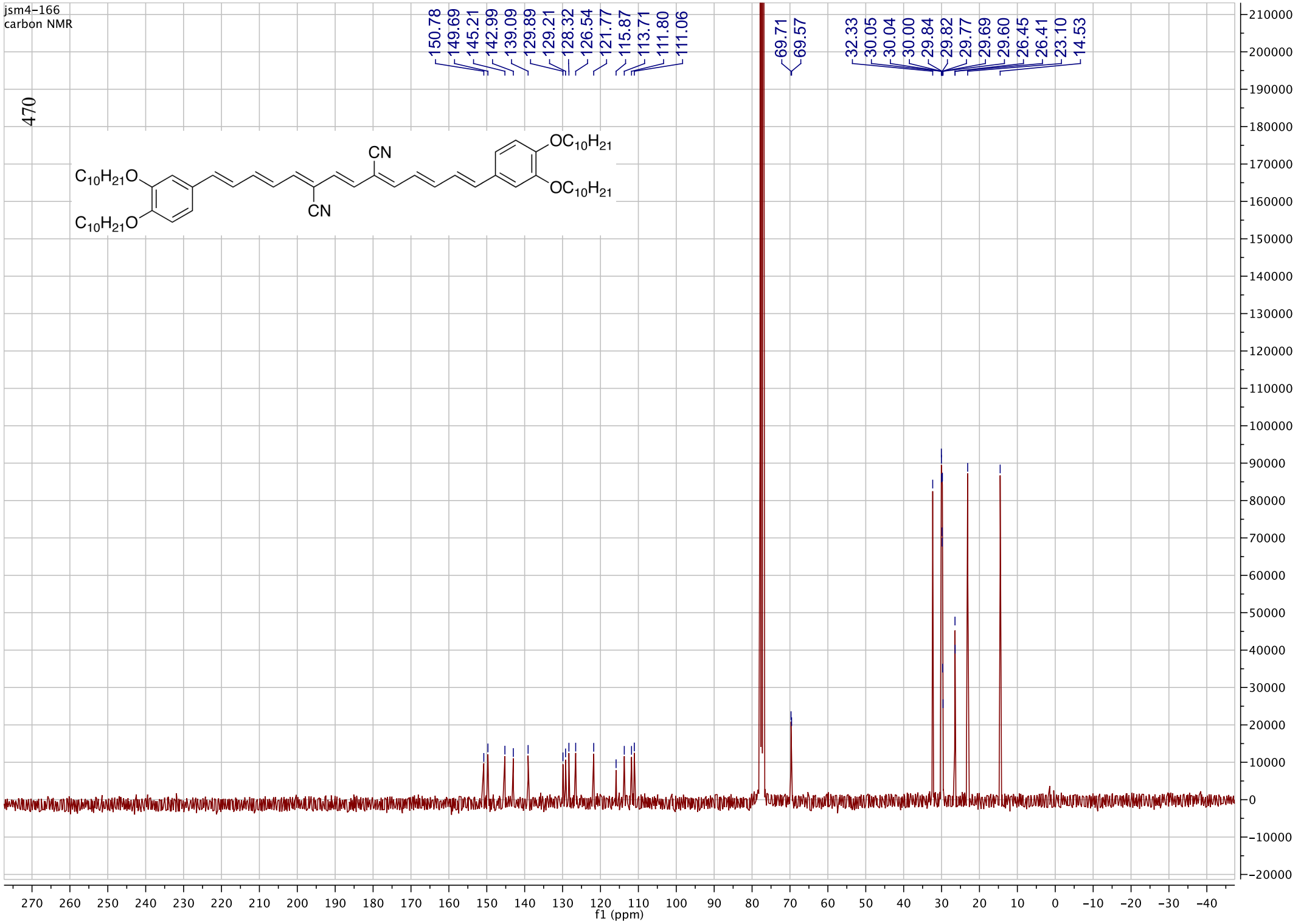

jsm4-159
carbon 13
465
CN
CN
$OC_{10}H_{21}$
$OC_{10}H_{21}$
$C_{10}H_{21}O$
$C_{10}H_{21}O$
11.47
12.59
12.69
12.75
13.50
14.20
14.29
14.77
25.39
25.46
25.51
25.58
34.22
34.30
34.37
34.44
34.64
34.98
35.78
36.57
38.06
38.13
38.20
2.00
4.61
2.01
2.04
1.97
8.20
30.14
8.13
49.46
12.22
f1 (ppm)

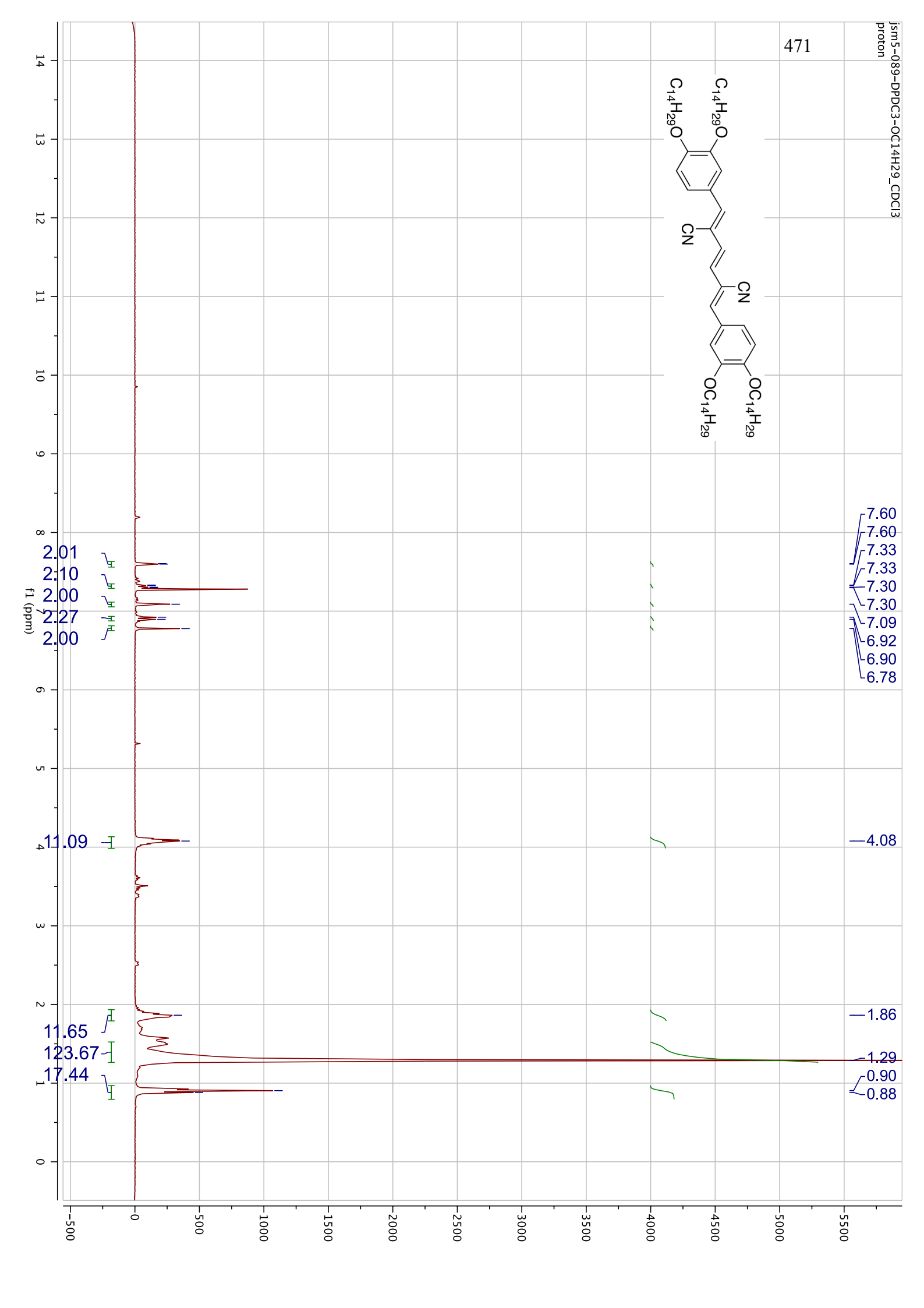

jsm4-159
carbon NMR
466
152.17
149.46
145.32
129.75
126.77
124.97
117.24
113.33
113.11
106.99
69.64
69.47
32.32
30.11
30.03
30.01
29.99
29.83
29.77
29.54
29.46
28.77
26.44
26.37
26.18
23.10
22.57
14.52
CN
CN
OC10H21
OC10H21
C10H21O
C10H21O
f1 (ppm)


jsm4-257
proton standard
467
CN
CN
$C_{10}H_{21}O$
$C_{10}H_{21}O$
$OC_{10}H_{21}$
$OC_{10}H_{21}$
7.16
7.12
7.11
7.07
7.05
6.97
6.94
6.90
6.87
6.85
6.84
6.65
1.84
1.48
1.28
0.91
0.88
0.86
6.03
6.00
2.00
8.15
8.01
7.85
47.76
12.19
f1 (ppm)

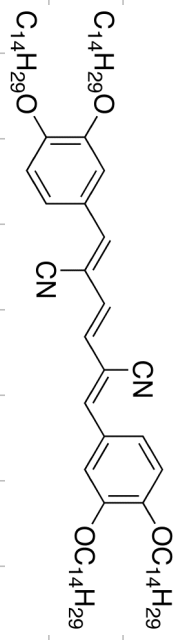

jsm4-257-DPDC5-0C10H21
468
151.27
149.42
145.49
142.20
128.71
128.63
122.68
122.31
115.59
113.21
111.99
110.32
69.48
69.15
31.92
29.63
29.61
29.58
29.44
29.40
29.36
29.34
29.32
29.17
26.05
26.00
22.69
14.10
CN
CN
OC10H21
OC10H21
C10H21O
C10H21O
f1 (ppm)


jsm4-166
proton standard
469
7.28
7.03
7.02
6.99
6.89
6.87
6.84
6.82
6.79
6.77
6.72
6.64
CN
CN
$OC_{10}H_{21}$
$OC_{10}H_{21}$
$C_{10}H_{21}O$
$C_{10}H_{21}O$
2.01
16.01
8.00
8.64
8.67
48.87
12.32
f1 (ppm)


jsm4-166
carbon NMR
470
150.78
149.69
145.21
142.99
139.09
129.89
129.21
128.32
126.54
121.77
115.87
113.71
111.80
111.06
69.71
69.57
32.33
30.05
30.04
30.00
29.84
29.82
29.77
29.69
29.60
26.45
26.41
23.10
14.53
CN
CN
OC10H21
OC10H21
C10H21O
C10H21O
f1 (ppm)

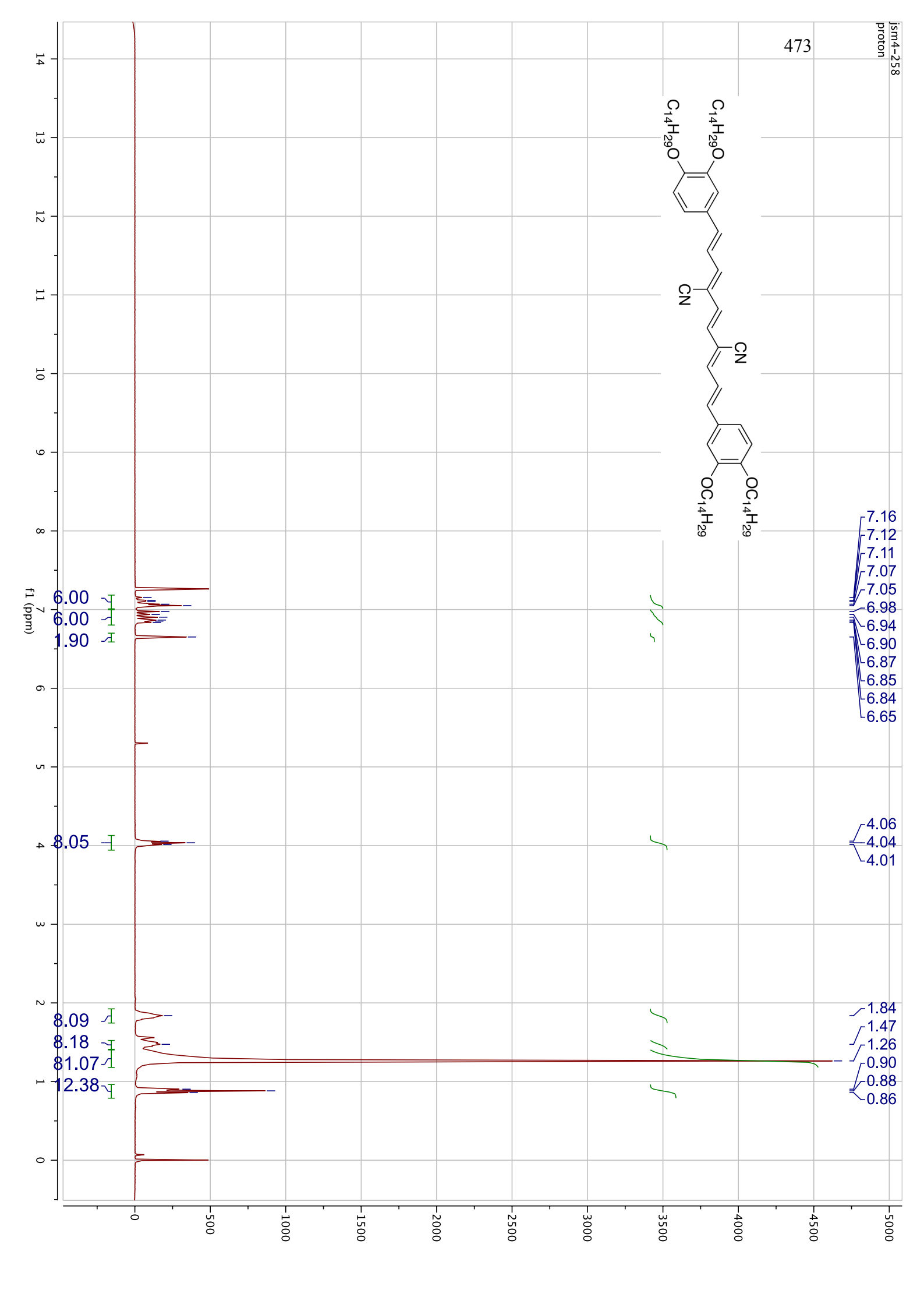

jsm5-089-DPDC3-OC14H29_CDCl3
proton
f1 (ppm)
2.01
2.10
2.00
2.27
2.00
11.09
11.65
123.67
17.44
7.60
7.60
7.33
7.33
7.30
7.30
7.09
6.92
6.90
6.78
4.08
1.86
1.29
0.90
0.88
CN
CN
OC14H29
OC14H29
C14H29O
C14H29O

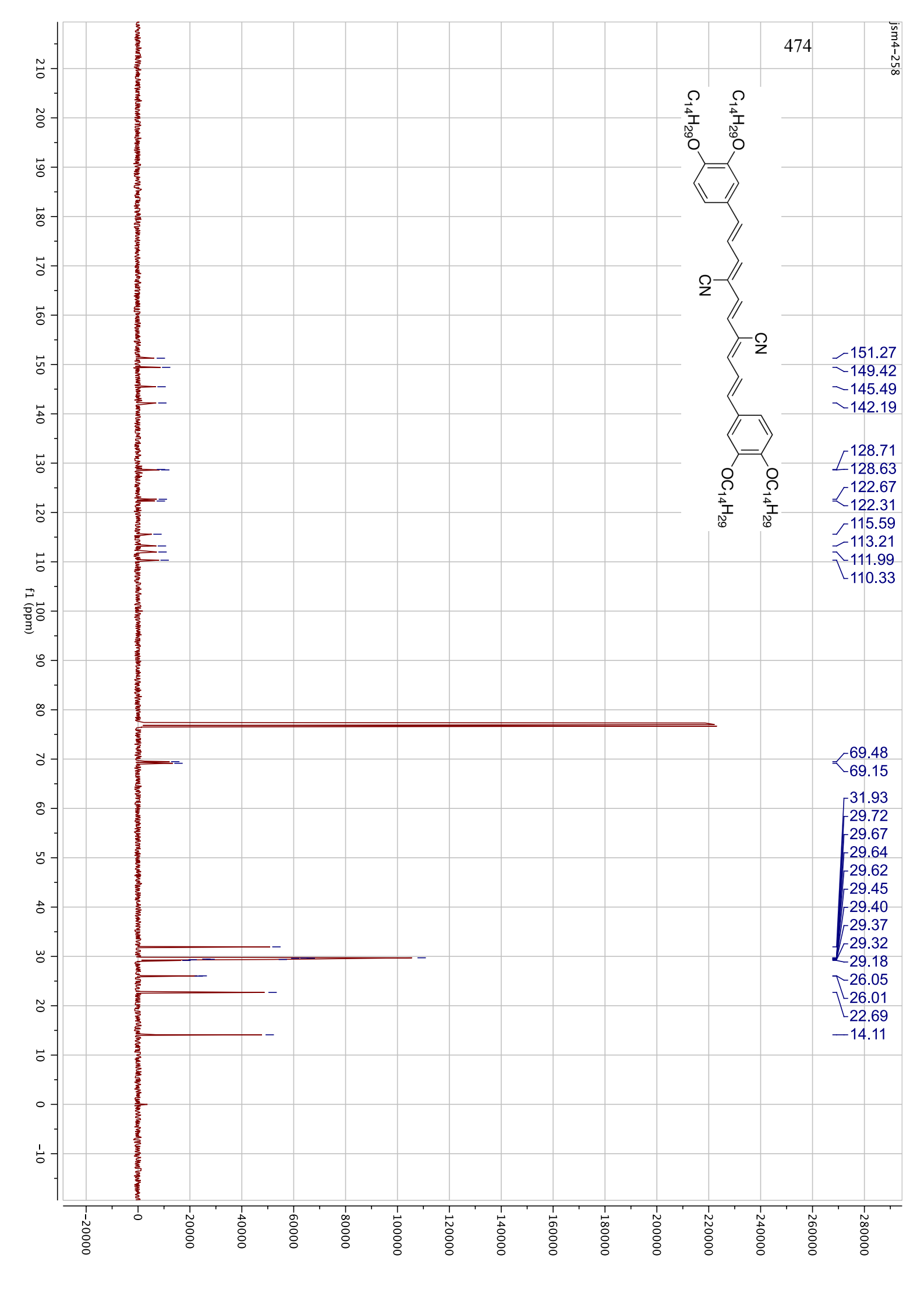
jsm5-089-DPDC3-OC14H29_CDCl3
Carbon 13

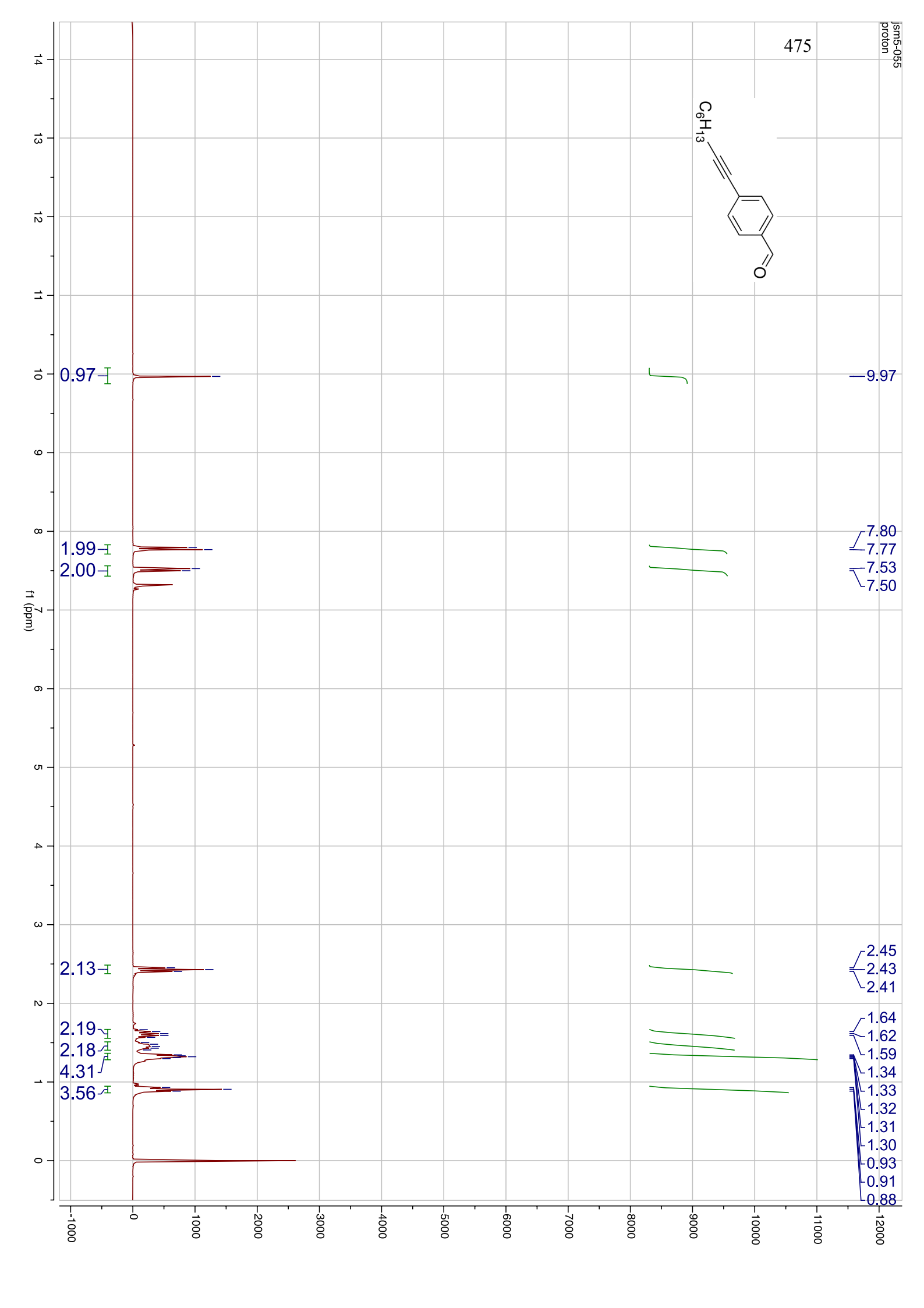


151.96
149.26
144.83
129.40
126.51
124.52
116.73
113.43
113.08
106.77
69.41
69.20
31.90
29.67
29.63
29.60
29.58
29.39
29.35
29.32
29.20
29.13
26.03
25.96
22.64
14.01

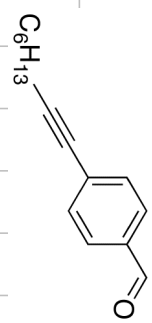
f1 (ppm)


jsm4-258
proton
f1 (ppm)
6.00
6.00
1.90
8.05
8.09
8.18
81.07
12.38
7.16
7.12
7.11
7.07
7.05
6.98
6.94
6.90
6.87
6.85
6.84
6.65
4.06
4.04
4.01
1.84
1.47
1.26
0.90
0.88
0.86
CN
CN
OC14H29
OC14H29
C14H29O
C14H29O


jsm4-258
151.27
149.42
145.49
142.19
128.71
128.63
122.67
122.31
115.59
113.21
111.99
110.33
69.48
69.15
31.93
29.72
29.67
29.64
29.62
29.45
29.40
29.37
29.32
29.18
26.05
26.01
22.69
14.11
f1 (ppm)

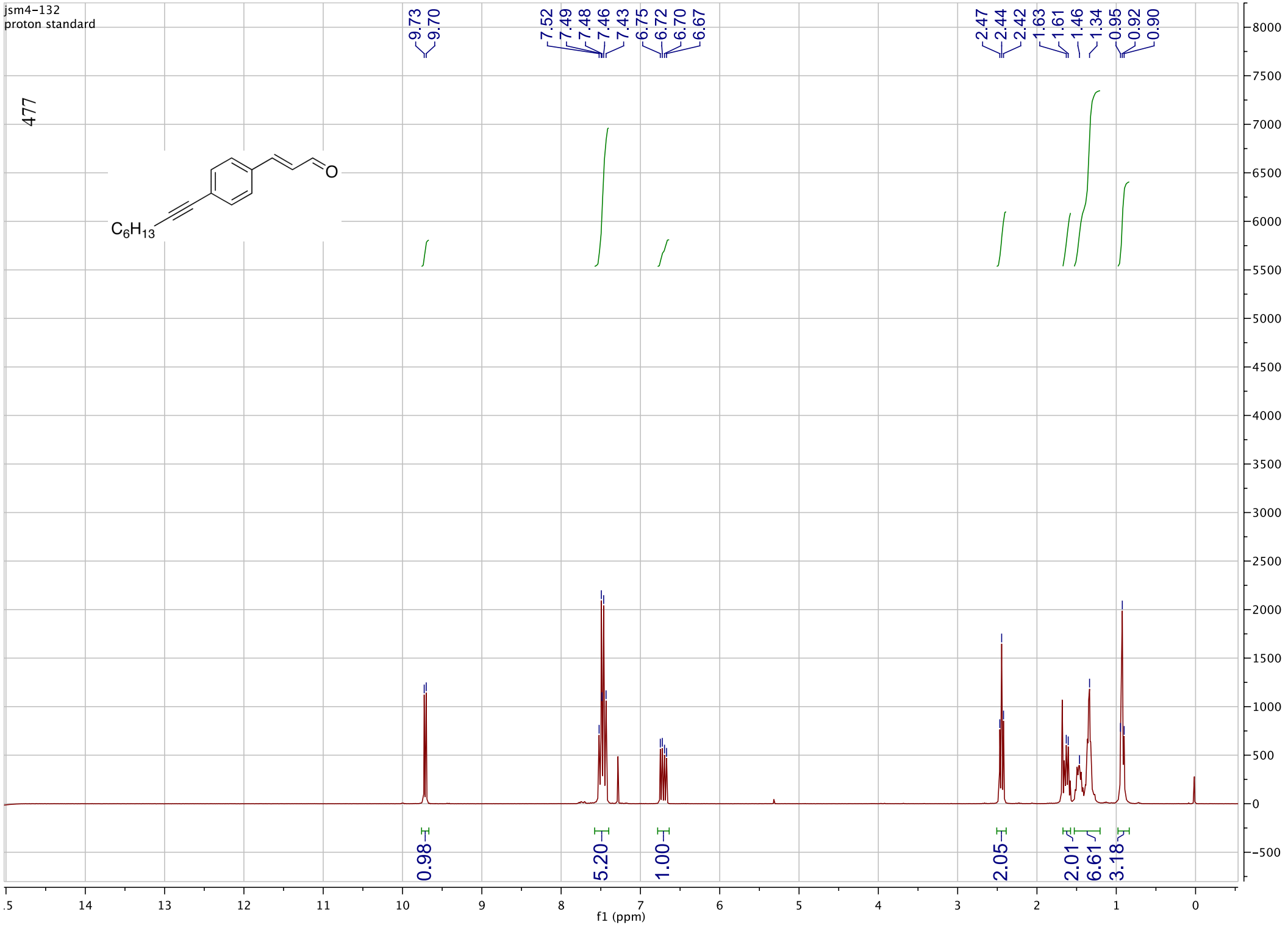

475
jsm5-055
proton
C_6H_{13}
O
0.97
1.99
2.00
2.13
2.19
2.18
4.31
3.56
9.97
7.80
7.77
7.53
7.50
2.45
2.43
2.41
1.64
1.62
1.59
1.34
1.33
1.32
1.31
1.30
0.93
0.91
0.88
f1 (ppm)

jsm5-055
carbon NMR

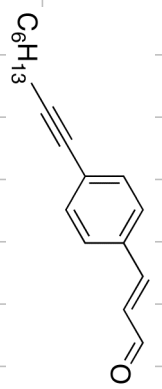


191.73
135.36
132.44
131.00
129.83
95.70
80.53
31.72
28.99
28.89
22.93
19.95
14.41

f1 (ppm)

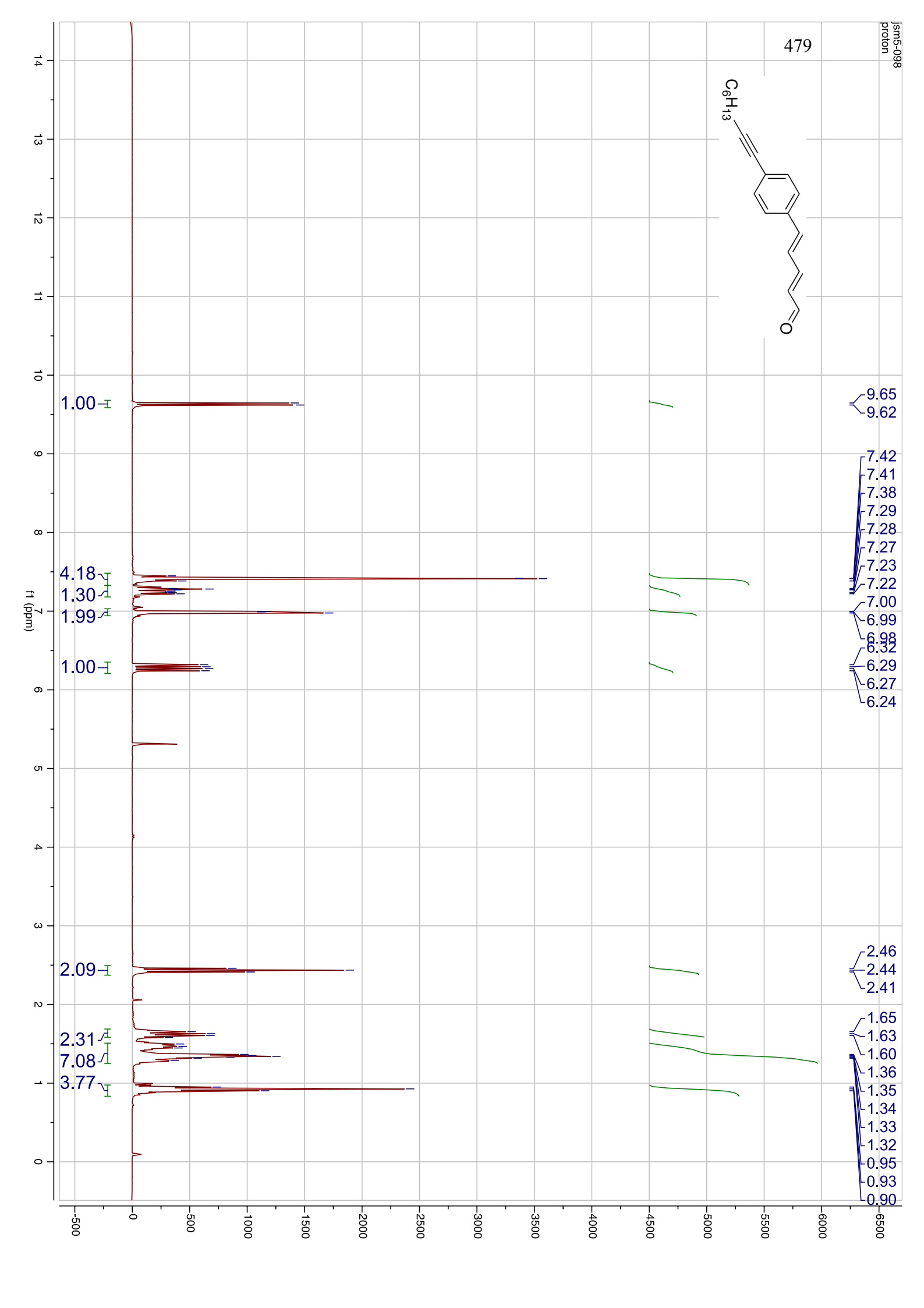

jsm4-132
proton standard
477
9.73
9.70
7.52
7.49
7.48
7.46
7.43
6.75
6.72
6.70
6.67
2.47
2.44
2.42
1.63
1.61
1.46
1.34
0.95
0.92
0.90
O
C6H13
0.98
5.20
1.00
2.05
2.01
6.61
3.18
f1 (ppm)

jsm4-132
carbon NMR

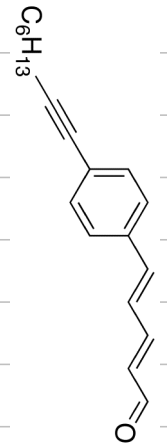


193.88
152.25
133.33
132.53
128.98
128.70
127.63
94.31
80.68
31.74
29.02
28.97
22.96
19.94
14.48

f1 (ppm)

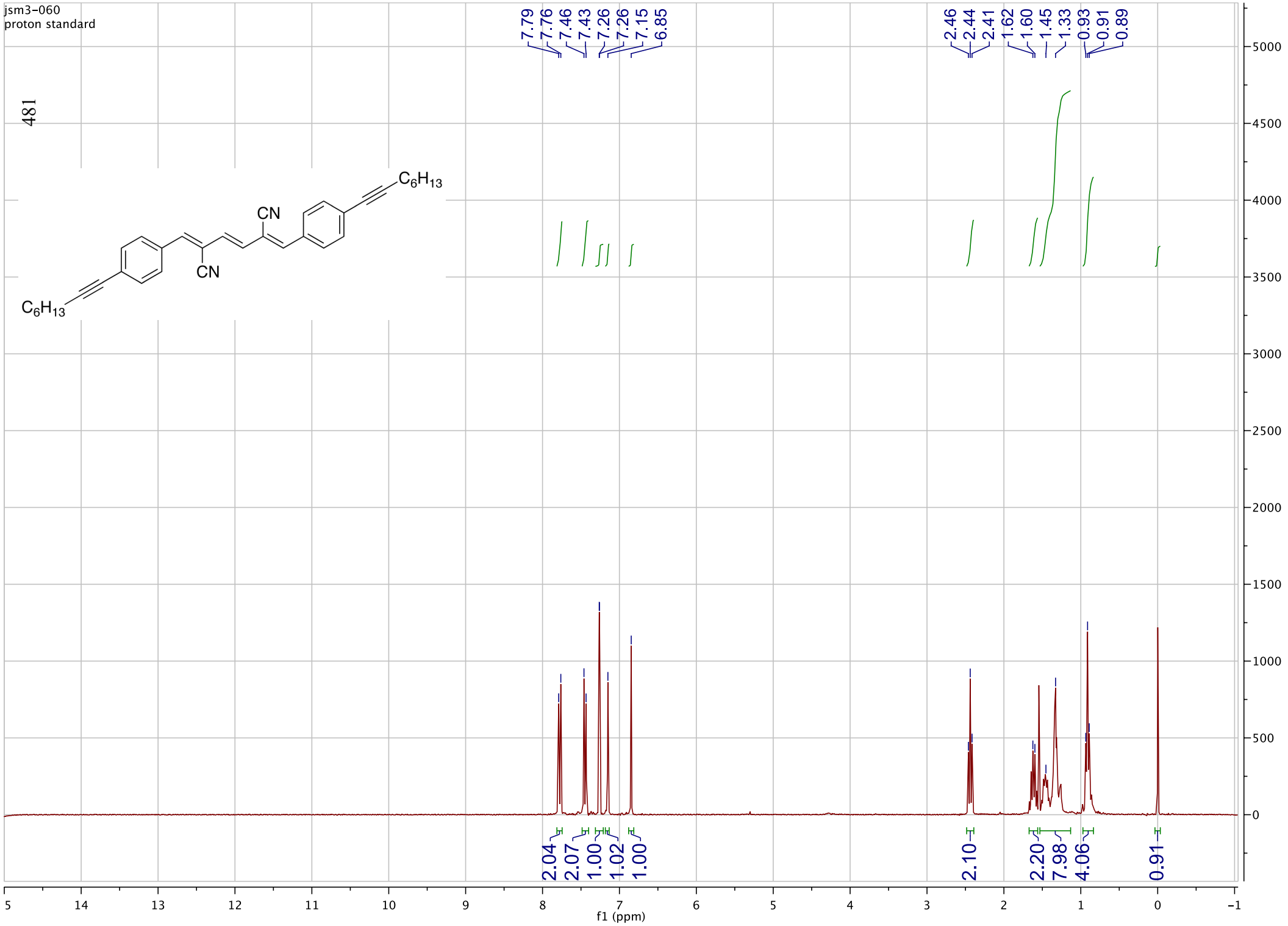

jsm5-098
proton
C6H13
O
1.00
4.18
1.30
1.99
1.00
2.09
2.31
7.08
3.77
9.65
9.62
7.42
7.41
7.38
7.29
7.28
7.27
7.23
7.22
7.00
6.99
6.98
6.32
6.29
6.27
6.24
2.46
2.44
2.41
1.65
1.63
1.60
1.36
1.35
1.34
1.33
1.32
0.95
0.93
0.90
f1 (ppm)

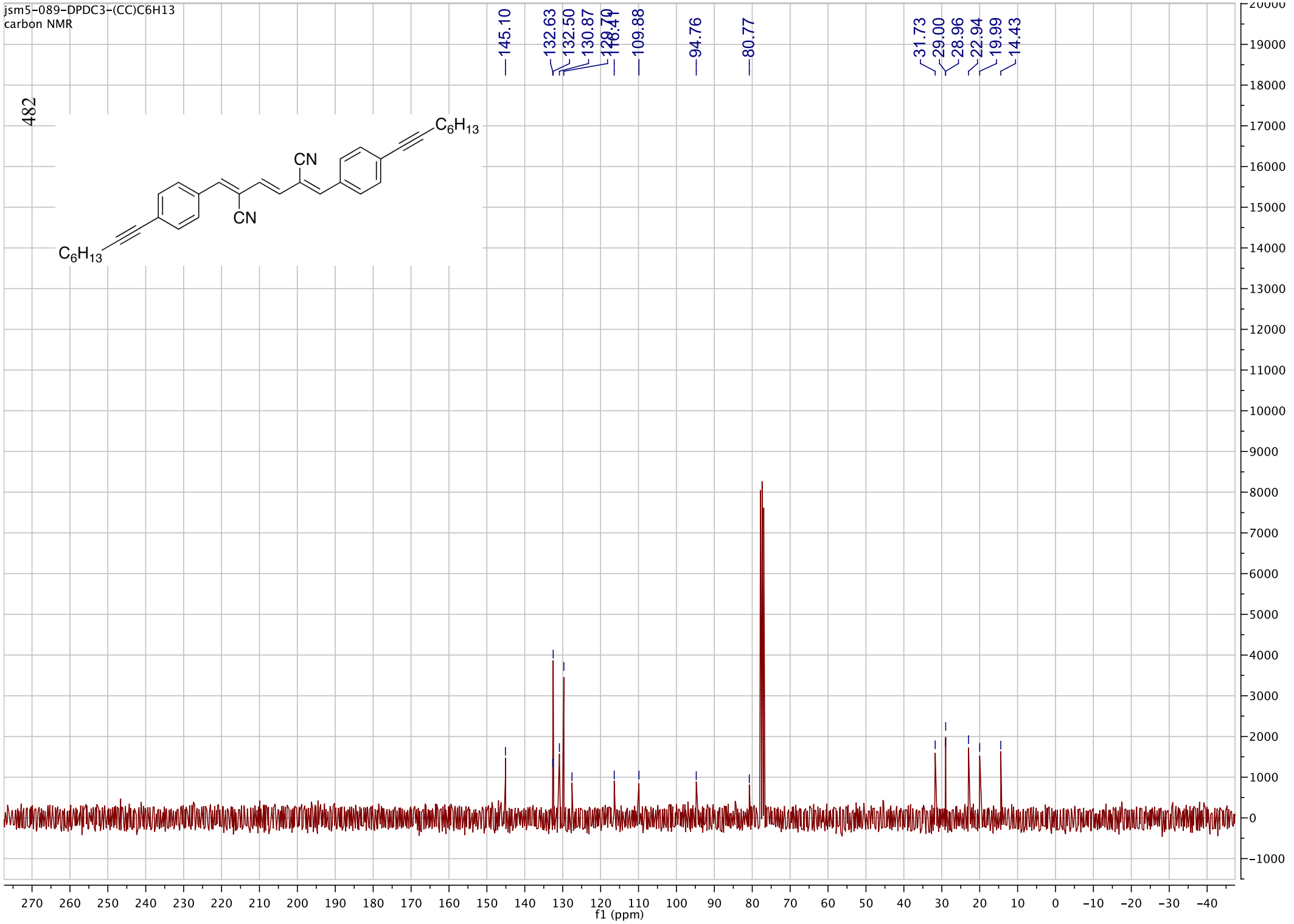
jsm5-098-H13C8-Ph-2enal
carbon NMR

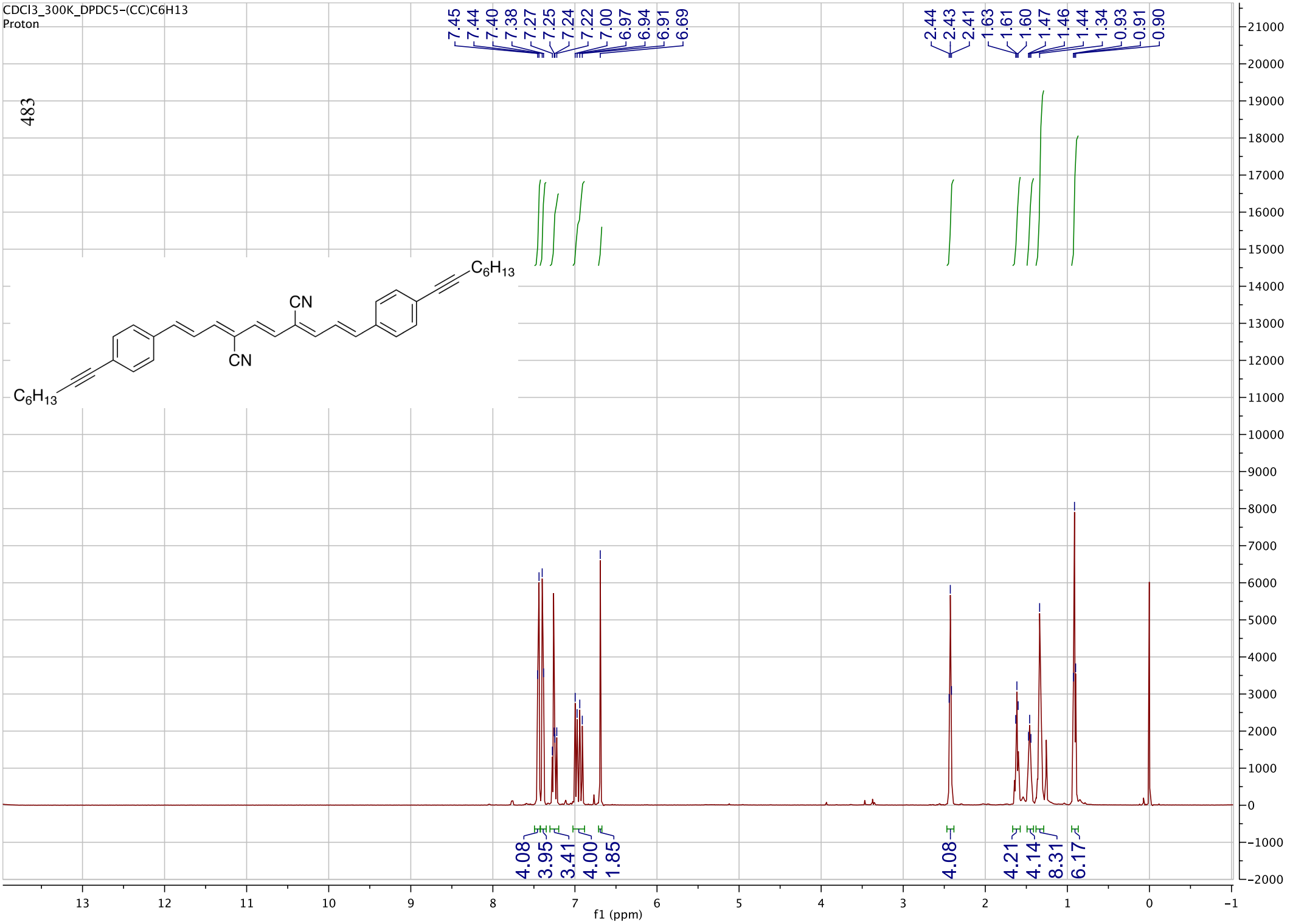


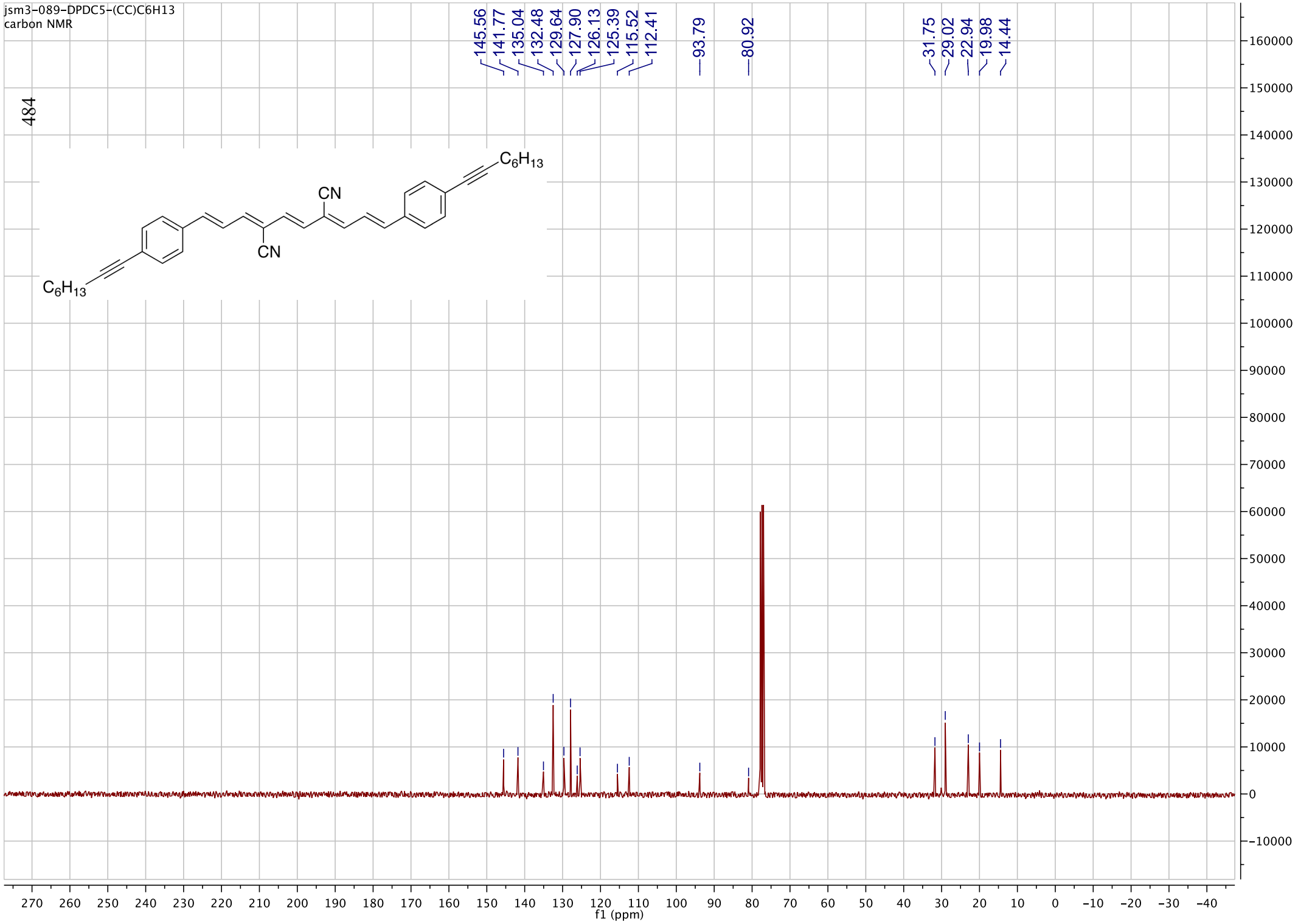
193.81
152.09
142.04
135.01
132.43
132.14
127.71
126.87
125.93
93.47
80.83
31.74
29.04
29.01
22.94
19.95
14.43

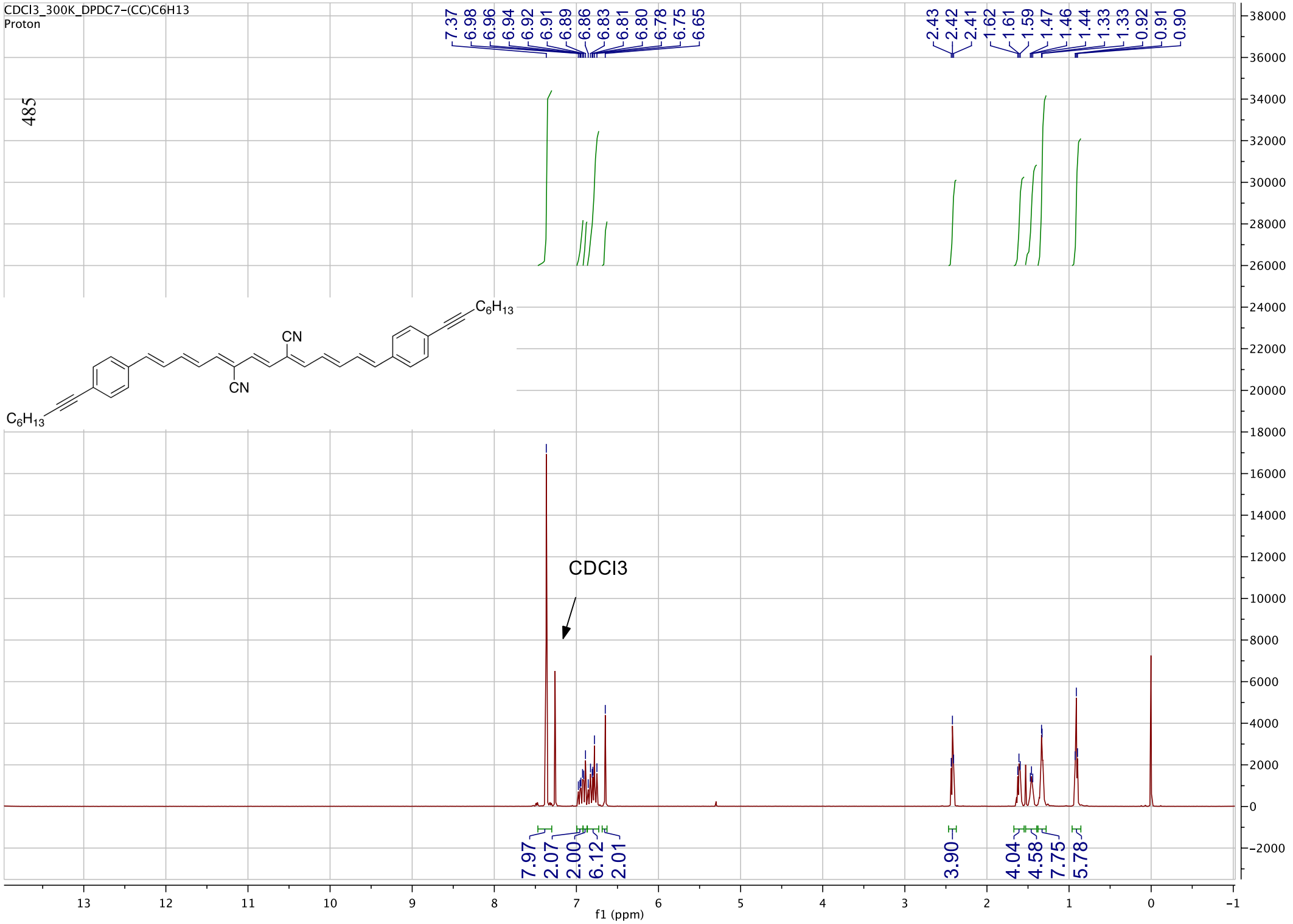
f1 (ppm)

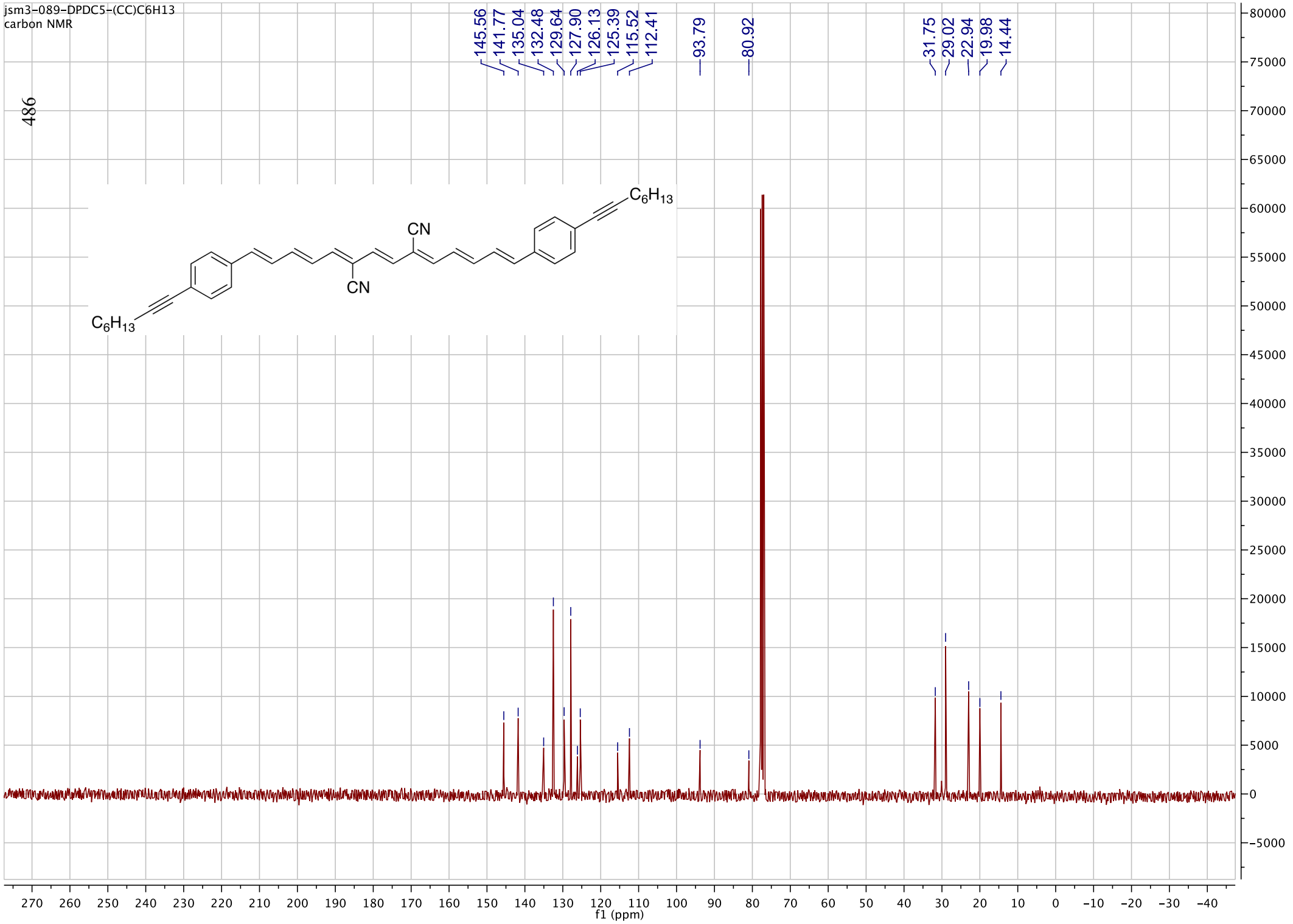

jsm3-060
proton standard
481
CN
CN
C6H13
C6H13
7.79
7.76
7.46
7.43
7.26
7.26
7.15
6.85
2.46
2.44
2.41
1.62
1.60
1.45
1.33
0.93
0.91
0.89
2.04
2.07
1.00
1.02
1.00
2.10
2.20
7.98
4.06
0.91
f1 (ppm)

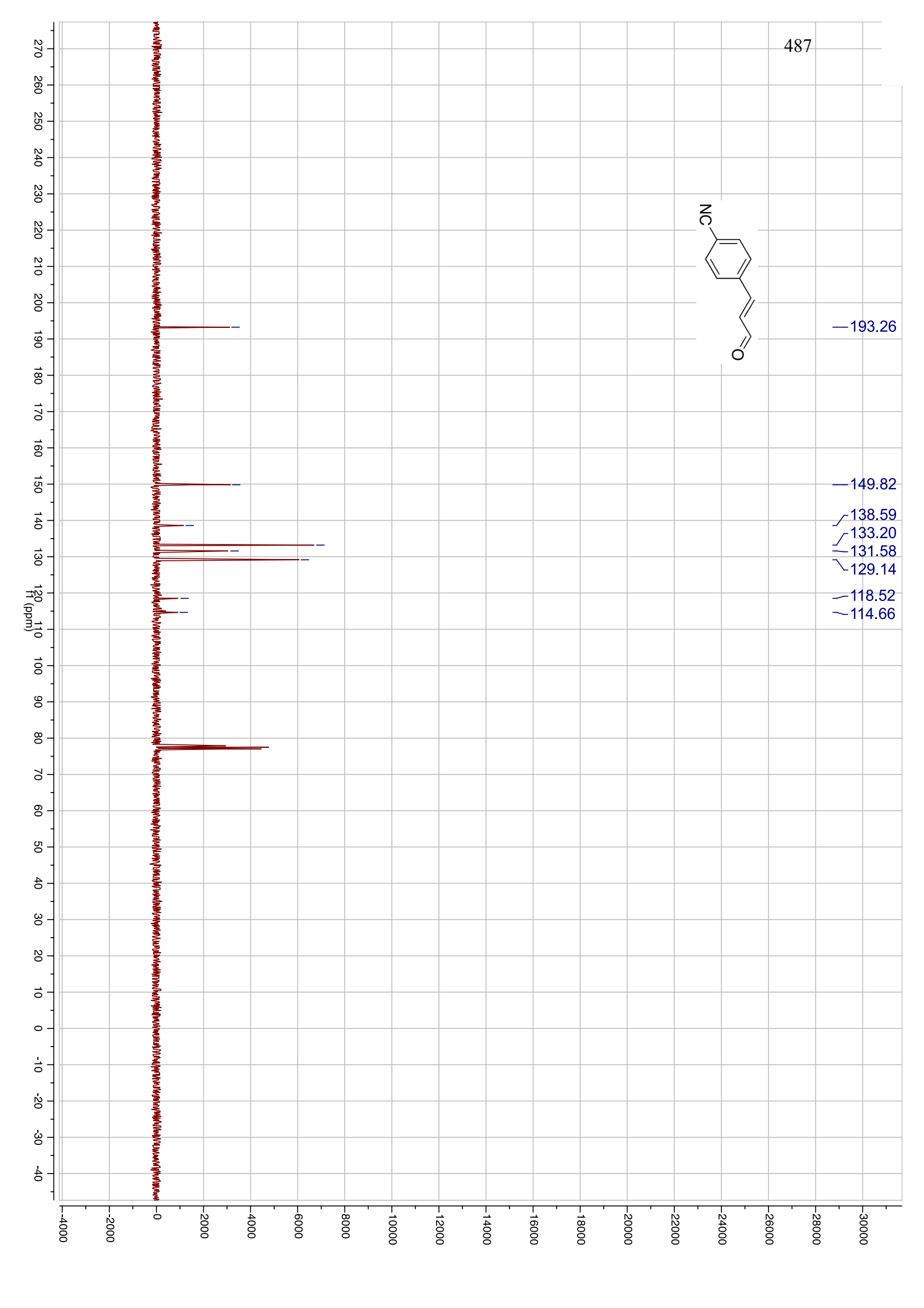

jsm5-089-DPDC3-(CC)C6H13
carbon NMR
482
145.10
132.63
132.50
130.87
128.70
128.41
109.88
94.76
80.77
31.73
29.00
28.96
22.94
19.99
14.43
CN
CN
C6H13
C6H13
f1 (ppm)

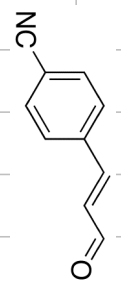

CDCl3_300K_DPDC5-(CC)C6H13
Proton
483
7.45
7.44
7.40
7.38
7.27
7.25
7.24
7.22
7.00
6.97
6.94
6.91
6.69
2.44
2.43
2.41
1.63
1.61
1.60
1.47
1.46
1.44
1.34
0.93
0.91
0.90
CN
CN
C6H13
C6H13
4.08
3.95
3.41
4.00
1.85
4.08
4.21
4.14
8.31
6.17
f1 (ppm)


jsm3-089-DPDC5-(CC)C6H13
carbon NMR
484
145.56
141.77
135.04
132.48
129.64
127.90
126.13
125.39
115.52
112.41
93.79
80.92
31.75
29.02
22.94
19.98
14.44
CN
CN
C6H13
C6H13
f1 (ppm)


CDCl3_300K_DPDC7-(CC)C6H13
Proton
485
7.37
6.98
6.96
6.94
6.92
6.91
6.89
6.86
6.83
6.81
6.80
6.78
6.75
6.65
2.43
2.42
2.41
1.62
1.61
1.59
1.47
1.46
1.44
1.33
1.33
0.92
0.91
0.90
C6H13
CN
CN
C6H13
CDCl3
7.97
2.07
2.00
6.12
2.01
3.90
4.04
4.58
7.75
5.78
f1 (ppm)

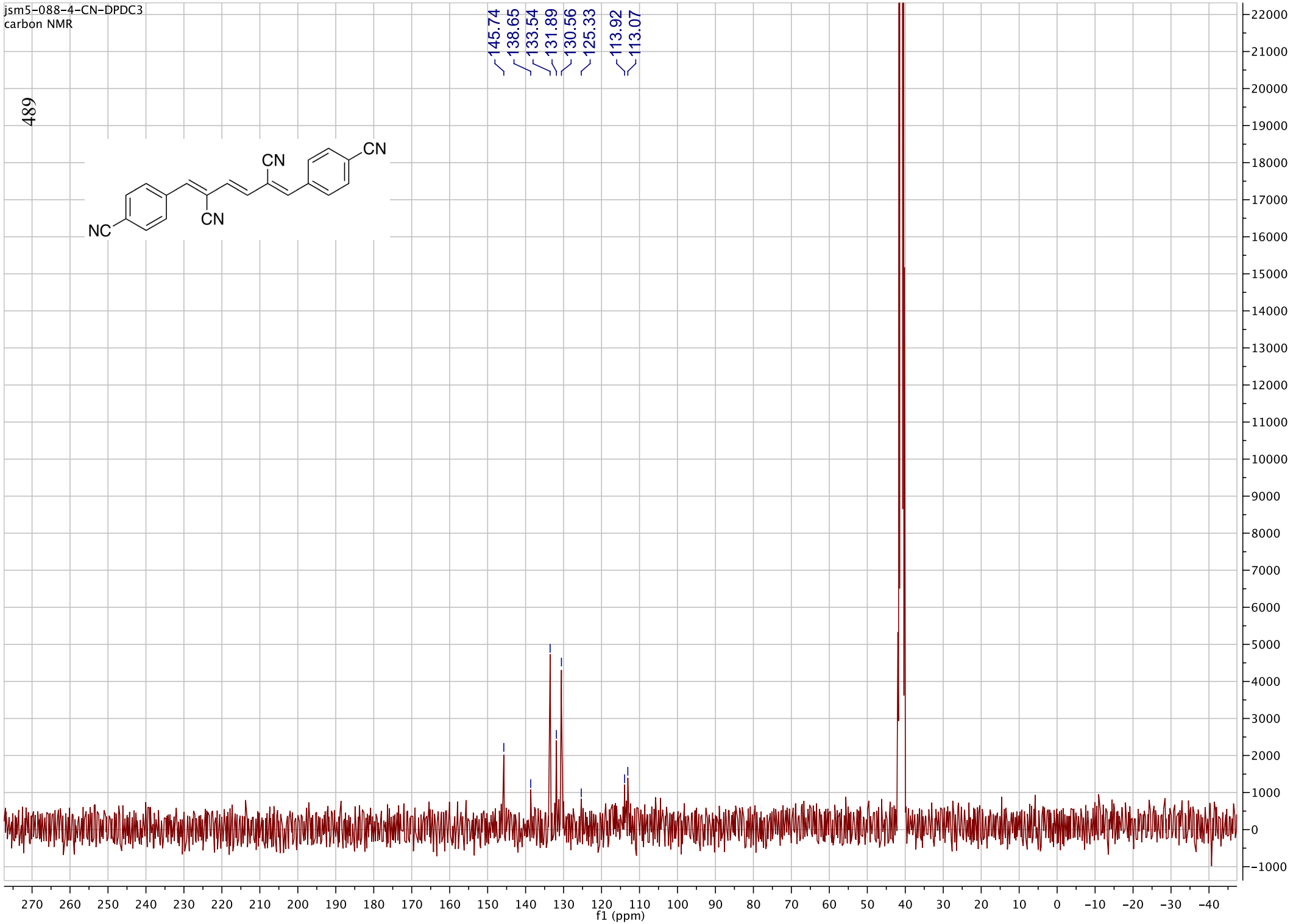

jsm3-089-DPDC5-(CC)C6H13
carbon NMR
486
145.56
141.77
135.04
132.48
129.64
127.90
126.13
125.39
115.52
112.41
93.79
80.92
31.75
29.02
22.94
19.98
14.44
CN
CN
C6H13
C6H13
f1 (ppm)


NC
O
193.26
149.82
138.59
133.20
131.58
129.14
118.52
114.66
f1 (ppm)



193.26
149.82
138.59
133.20
131.58
129.14
118.52
114.66

f1 (ppm)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carbon NMR
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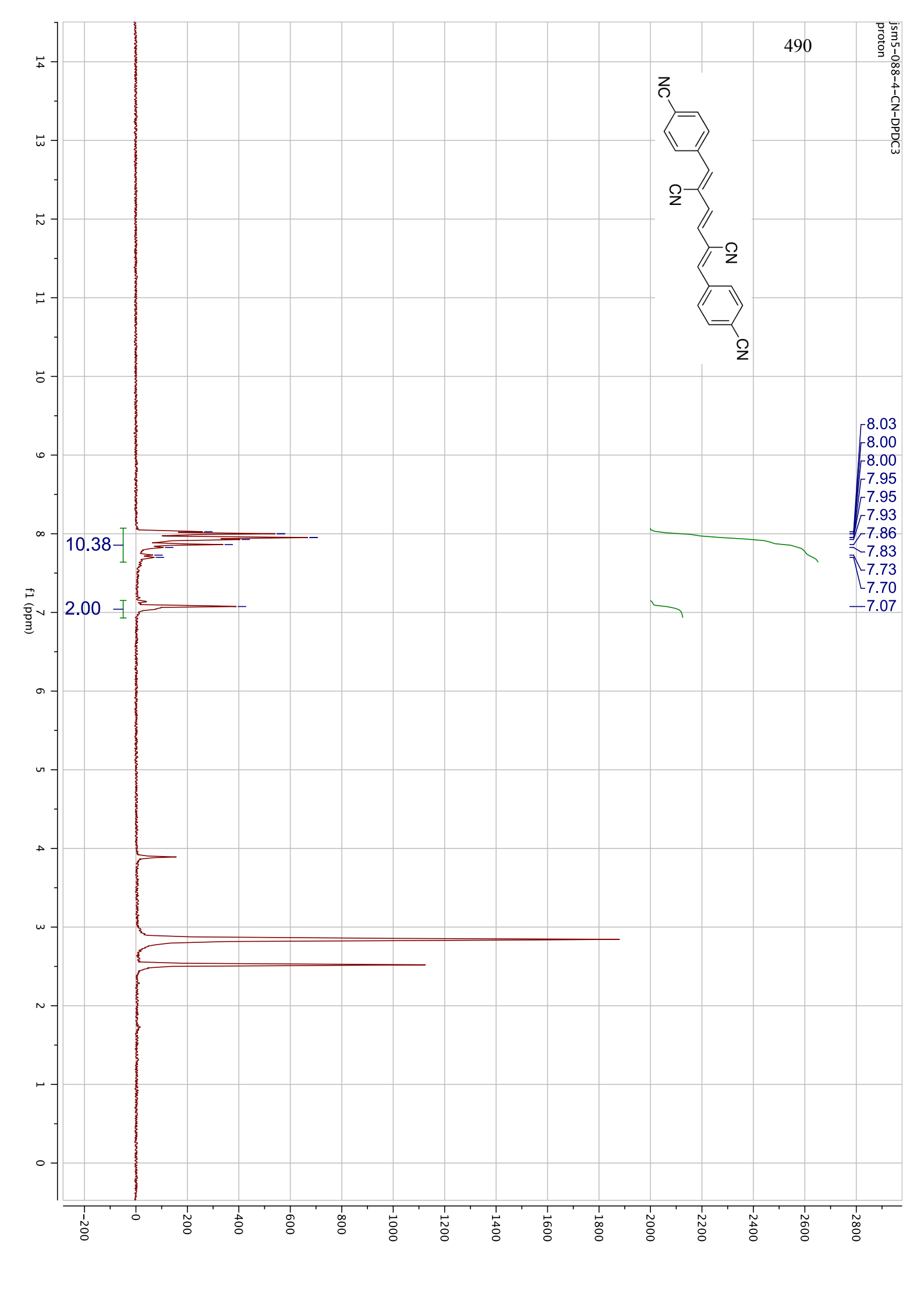
145.74
138.65
133.54
131.89
130.56
125.33
113.92
113.07
CN
CN
CN
NC
f1 (ppm)


jsm5-088-4-CN-DPDC3
proton
NC
CN
CN
CN
8.03
8.00
8.00
7.95
7.95
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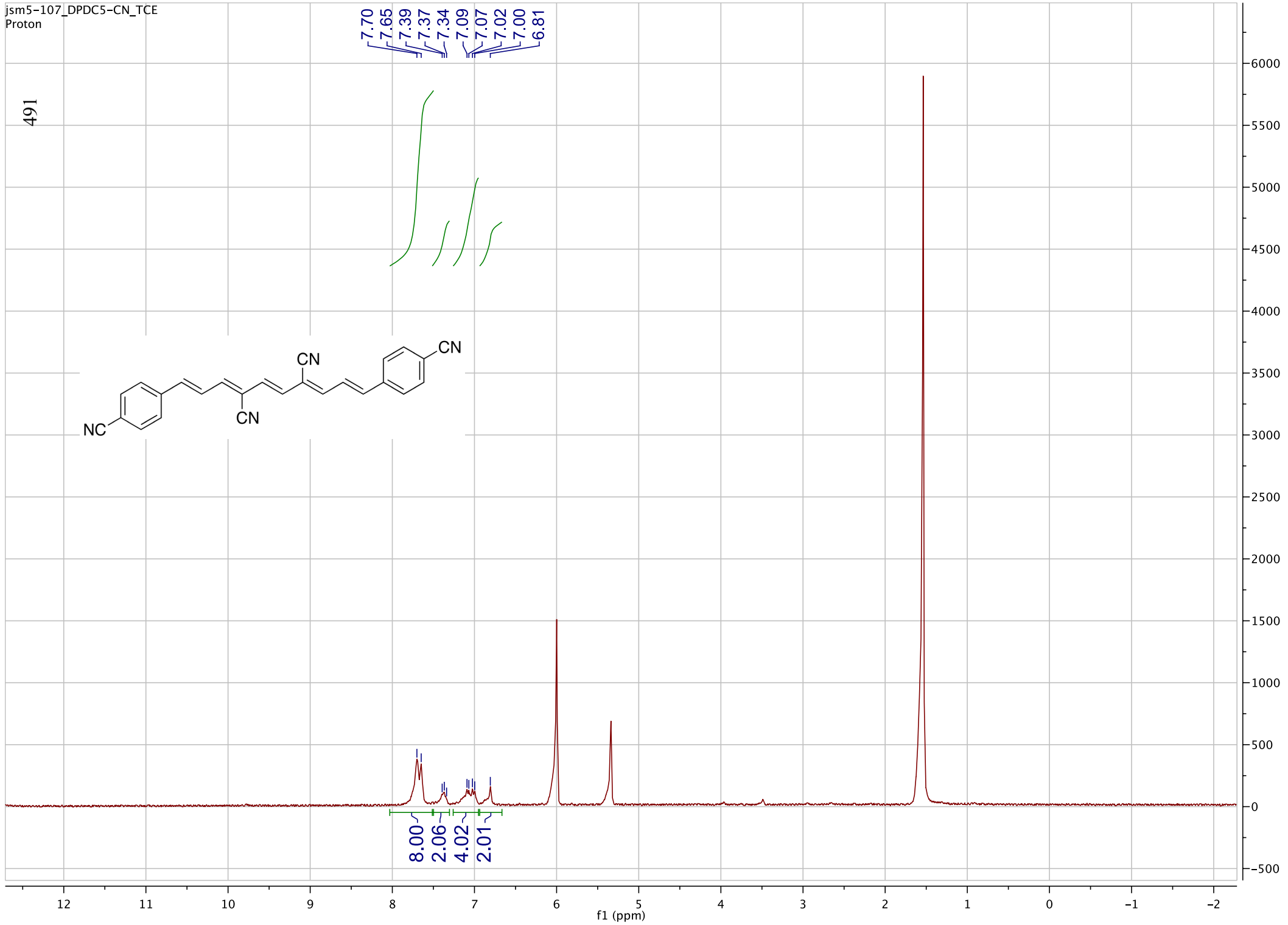
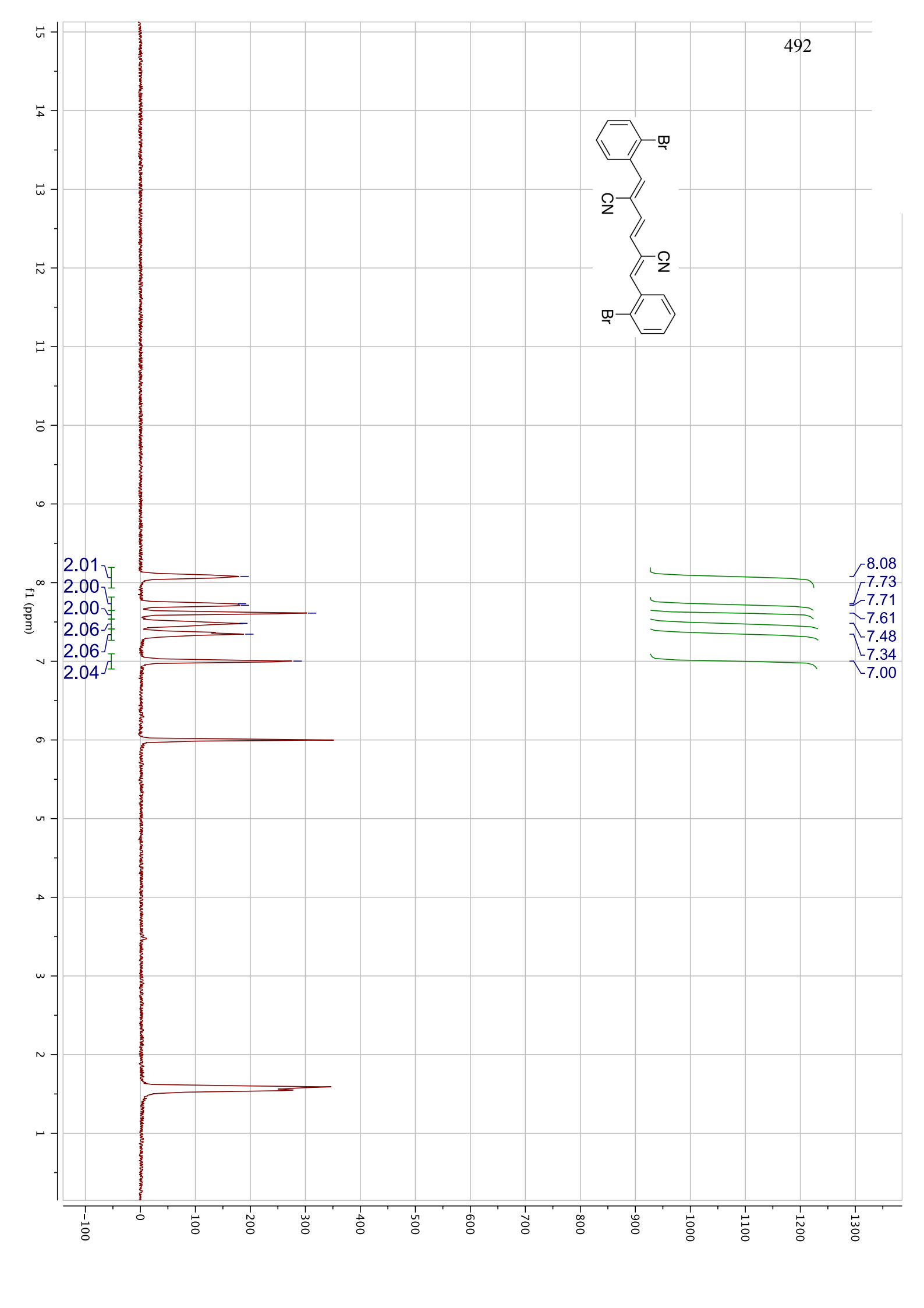
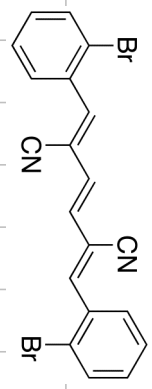
7.73
7.70
7.07
10.38
2.00
f1 (ppm)

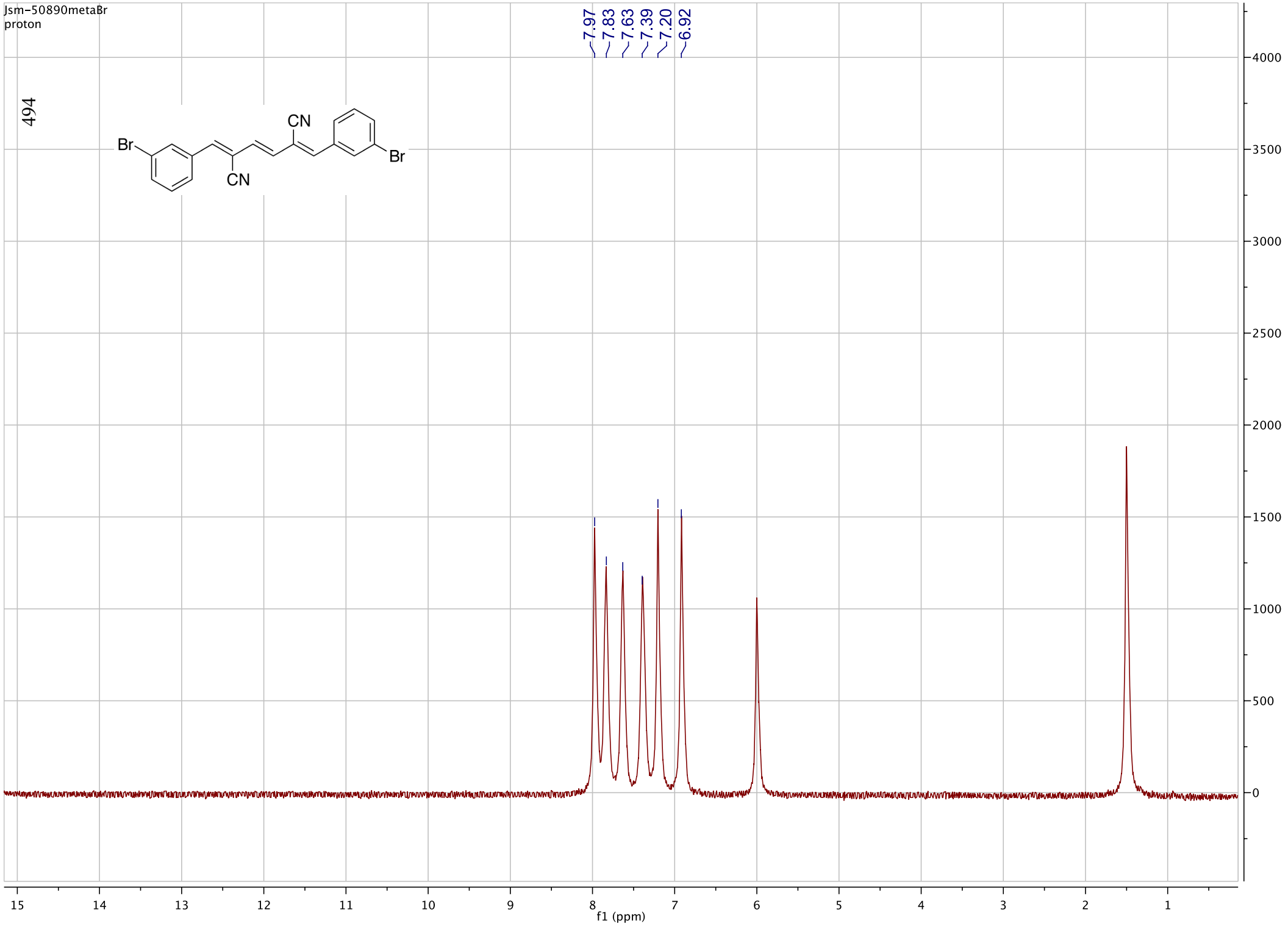

jsm5-107_DPDC5-CN_TCE
Proton
491
7.70
7.65
7.39
7.37
7.34
7.09
7.07
7.02
7.00
6.81
CN
CN
CN
NC
8.00
2.06
4.02
2.01
f1 (ppm)

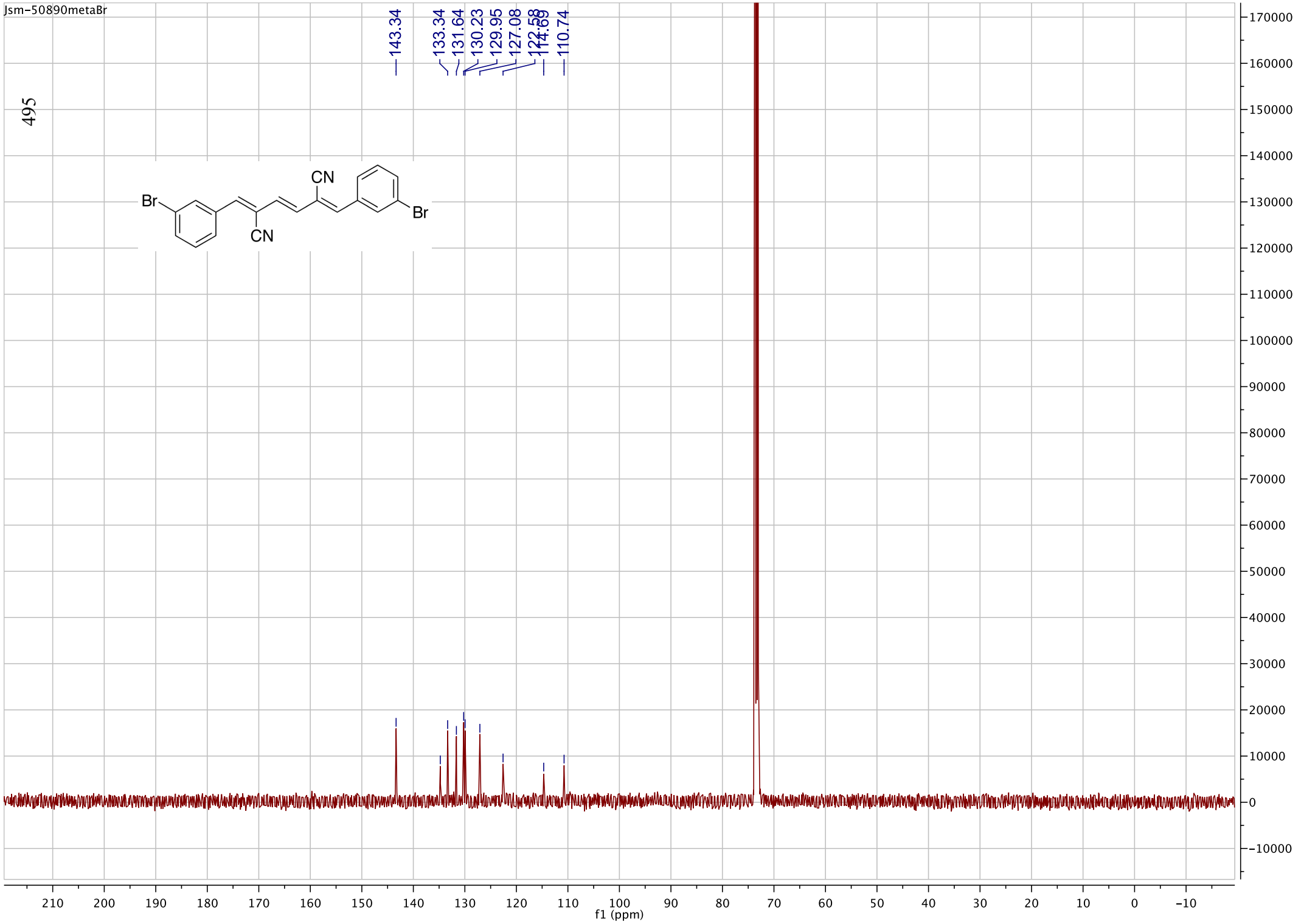

Br
CN
CN
Br
2.01
2.00
2.00
2.06
2.06
2.04
8.08
7.73
7.71
7.61
7.48
7.34
7.00
f1 (ppm)

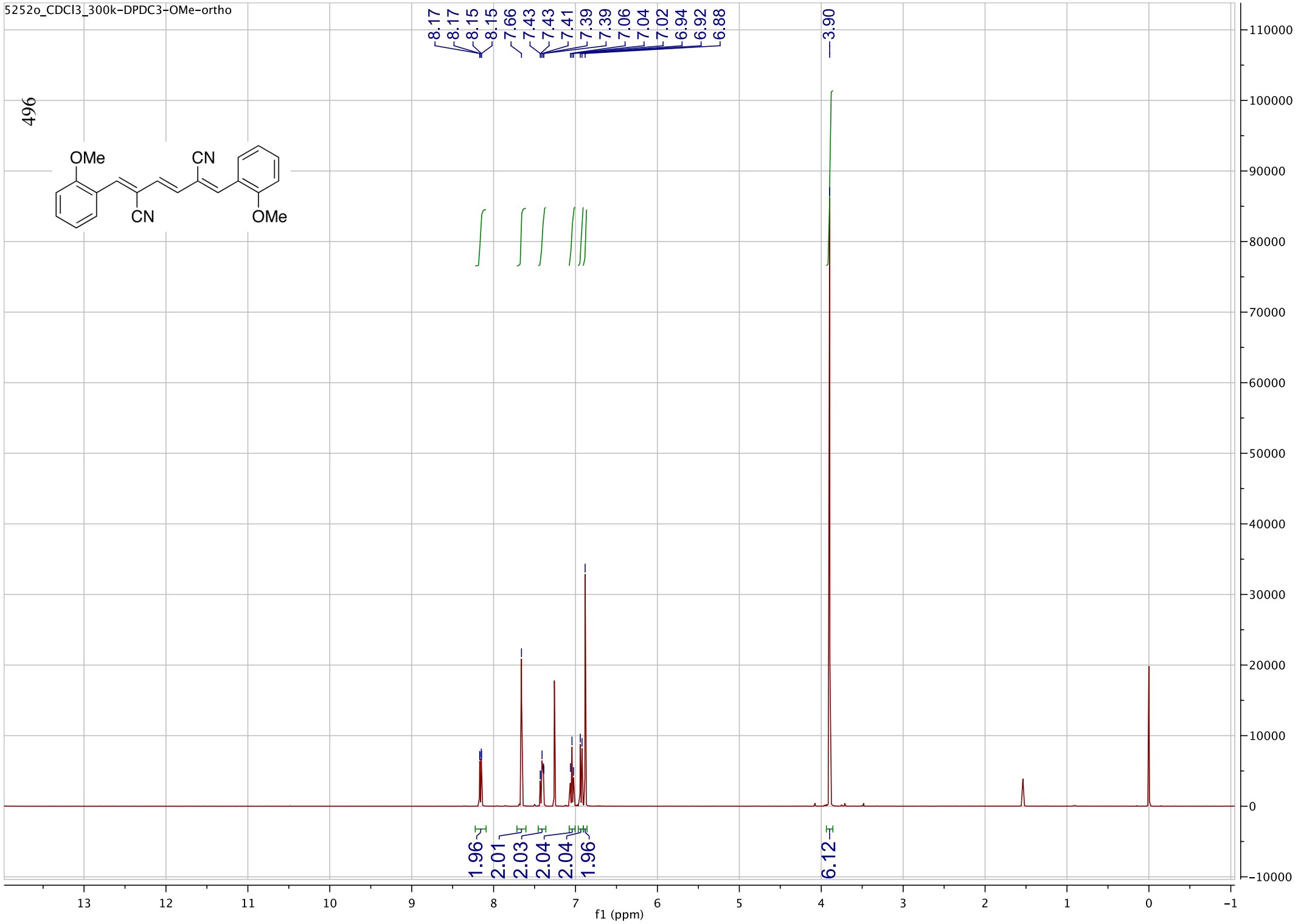


144.52
133.26
130.68
129.31
127.69
114.98
112.60

f1 (ppm)


Jsm-50890metaBr
proton
494
Br
CN
CN
Br
7.97
7.83
7.63
7.39
7.20
6.92
4000
3500
3000
2500
2000
1500
1000
500
0
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
f1 (ppm)


Jsm-50890metaBr
495
143.34
133.34
131.64
130.23
129.95
127.08
122.58
114.69
110.74
CN
Br
CN
Br
f1 (ppm)


5252o_CDCl3_300k-DPDC3-OMe-ortho
496
OMe
CN
CN
OMe
8.17
8.17
8.15
8.15
7.66
7.43
7.43
7.41
7.39
7.39
7.06
7.04
7.02
6.94
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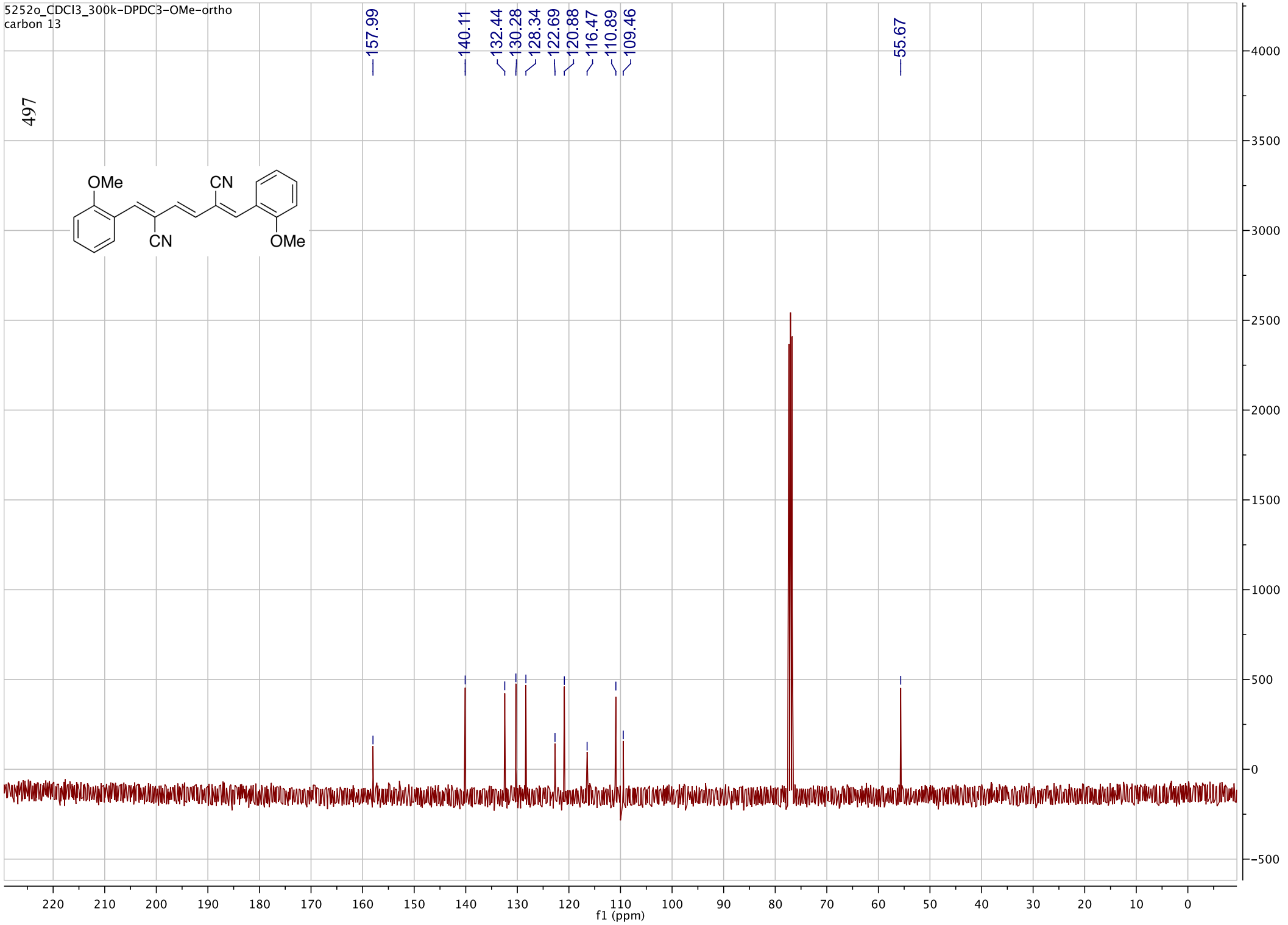
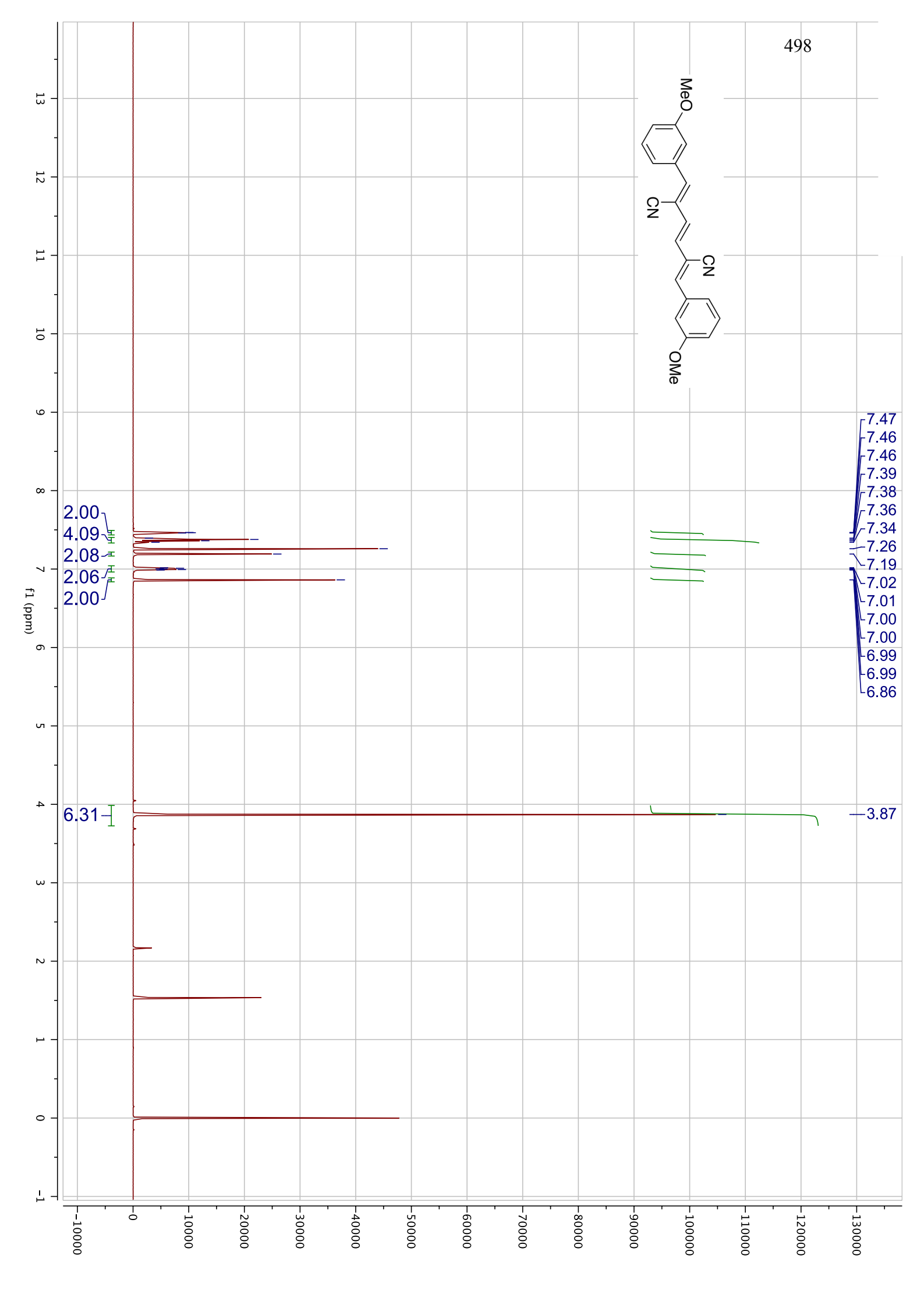
2.03
2.04
2.04
1.96
6.12
f1 (ppm)


5252o_CDCl3_300k-DPDC3-OMe-ortho
carbon 13
497
157.99
140.11
132.44
130.28
128.34
122.69
120.88
116.47
110.89
109.46
55.67
OMe
CN
CN
OMe
f1 (ppm)


MeO
CN
CN
OMe
7.47
7.46
7.46
7.39
7.38
7.36
7.34
7.26
7.19
7.02
7.01
7.00
7.00
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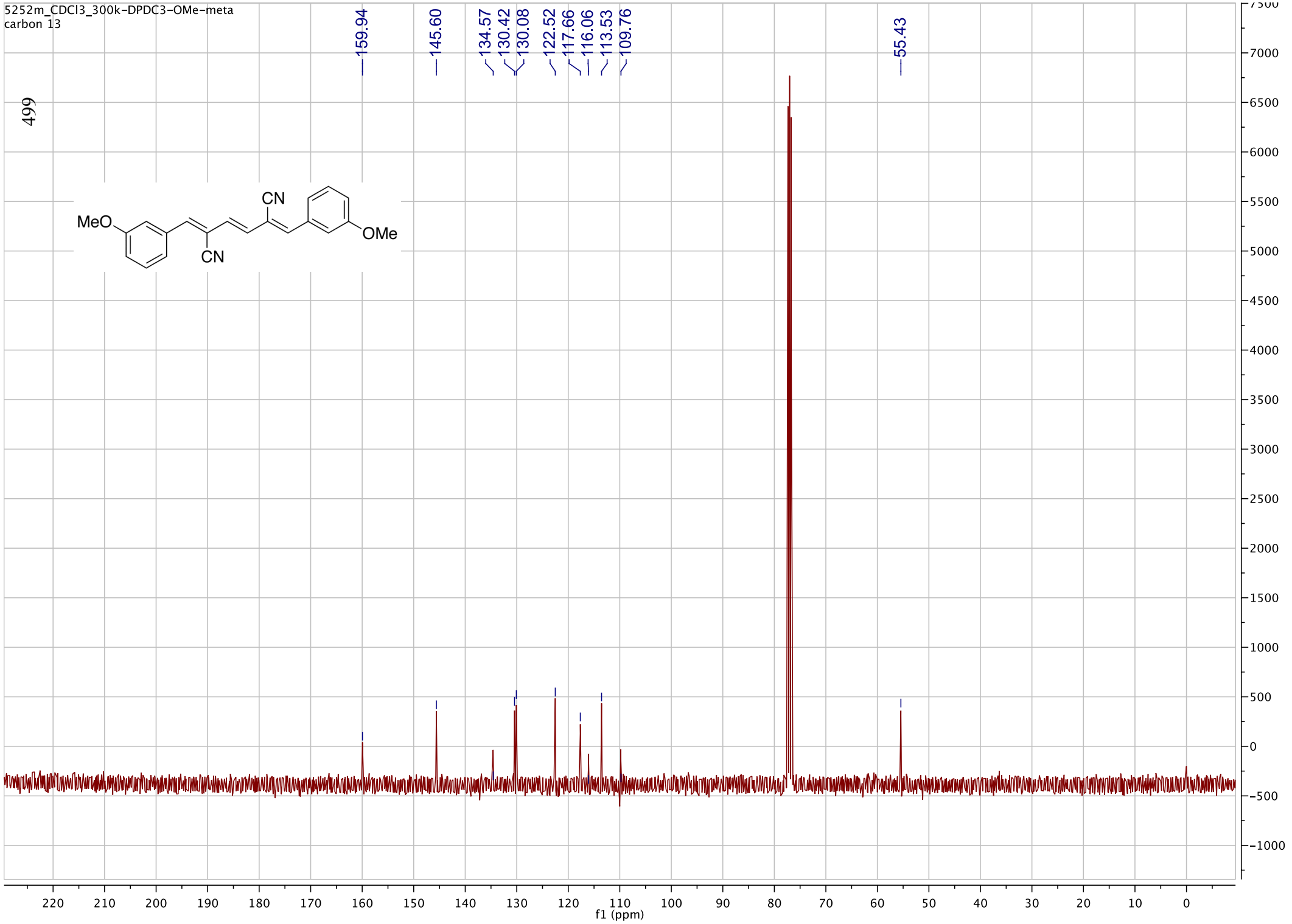
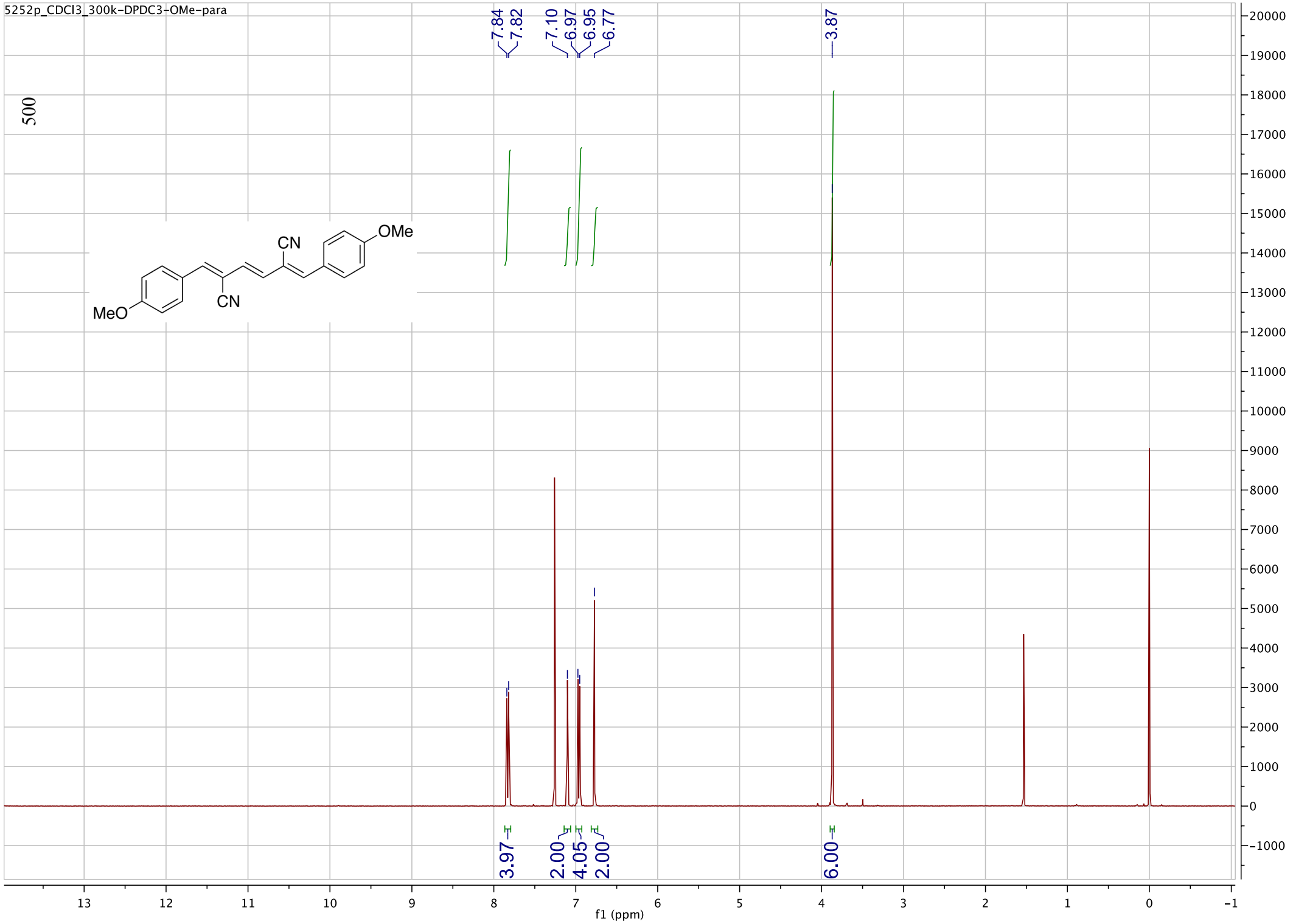
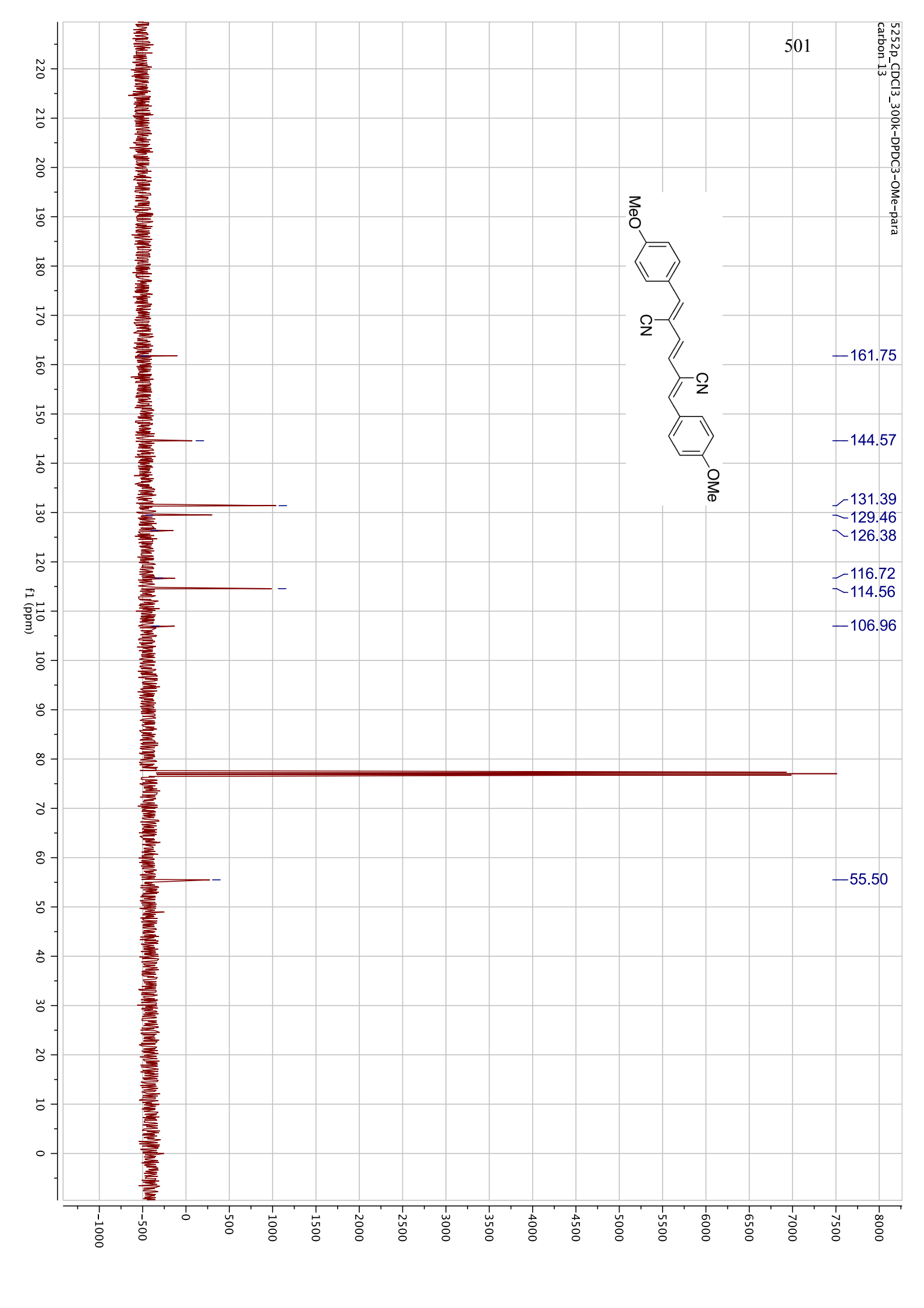
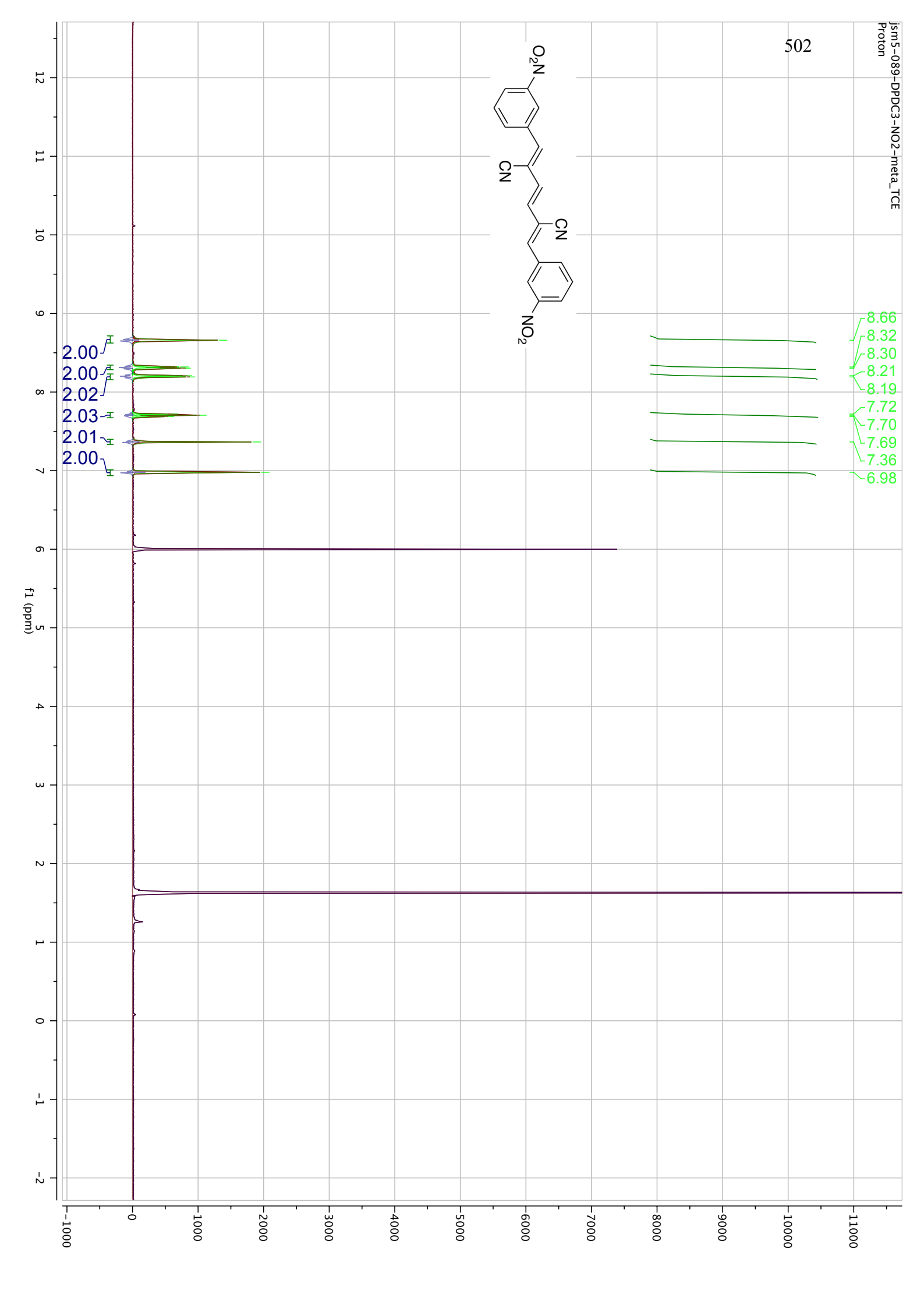
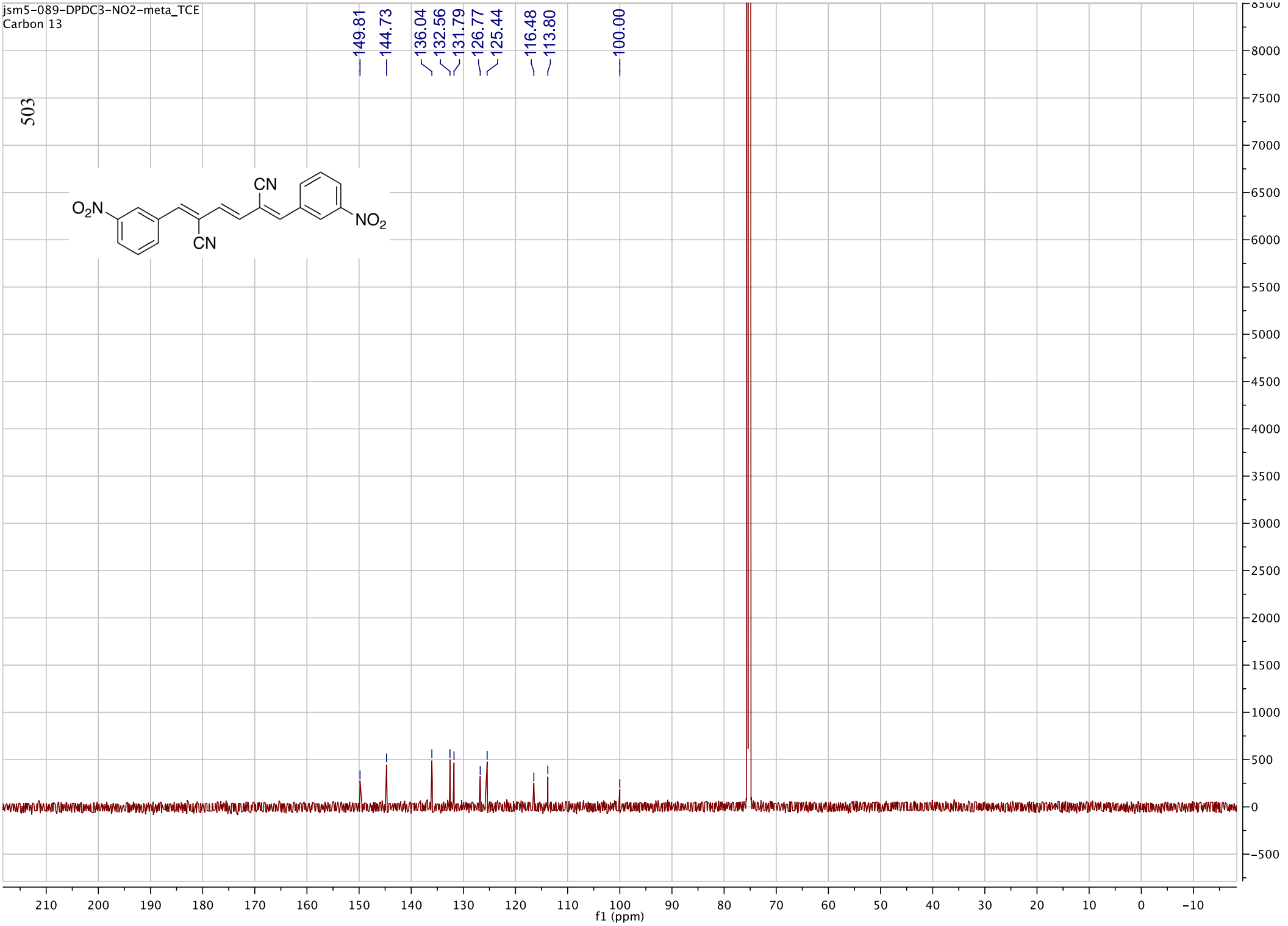
4.09
2.08
2.06
2.00
6.31
f1 (ppm)


5252m_CDCl3_300k-DPDC3-OMe-meta
carbon 13
499
159.94
145.60
134.57
130.42
130.08
122.52
117.66
116.06
113.53
109.76
55.43
MeO
CN
CN
OMe
f1 (ppm)


5252p_CDCl3_300k-DPDC3-OMe-para
500
7.84
7.82
7.10
6.97
6.95
6.77
3.87
CN
OMe
CN
MeO
3.97
2.00
4.05
2.00
6.00
f1 (ppm)


5252p_CDCl3_300k-DPDC3-OMe-para
carbon 13
MeO
CN
CN
OMe
161.75
144.57
131.39
129.46
126.38
116.72
114.56
106.96
55.50
f1 (ppm)


jsm5-089-DPDC3-NO2-meta_TCE
Proton
O2N
CN
CN
NO2
8.66
8.32
8.30
8.21
8.19
7.72
7.70
7.69
7.36
6.98
2.00
2.00
2.02
2.03
2.01
2.00
f1 (ppm)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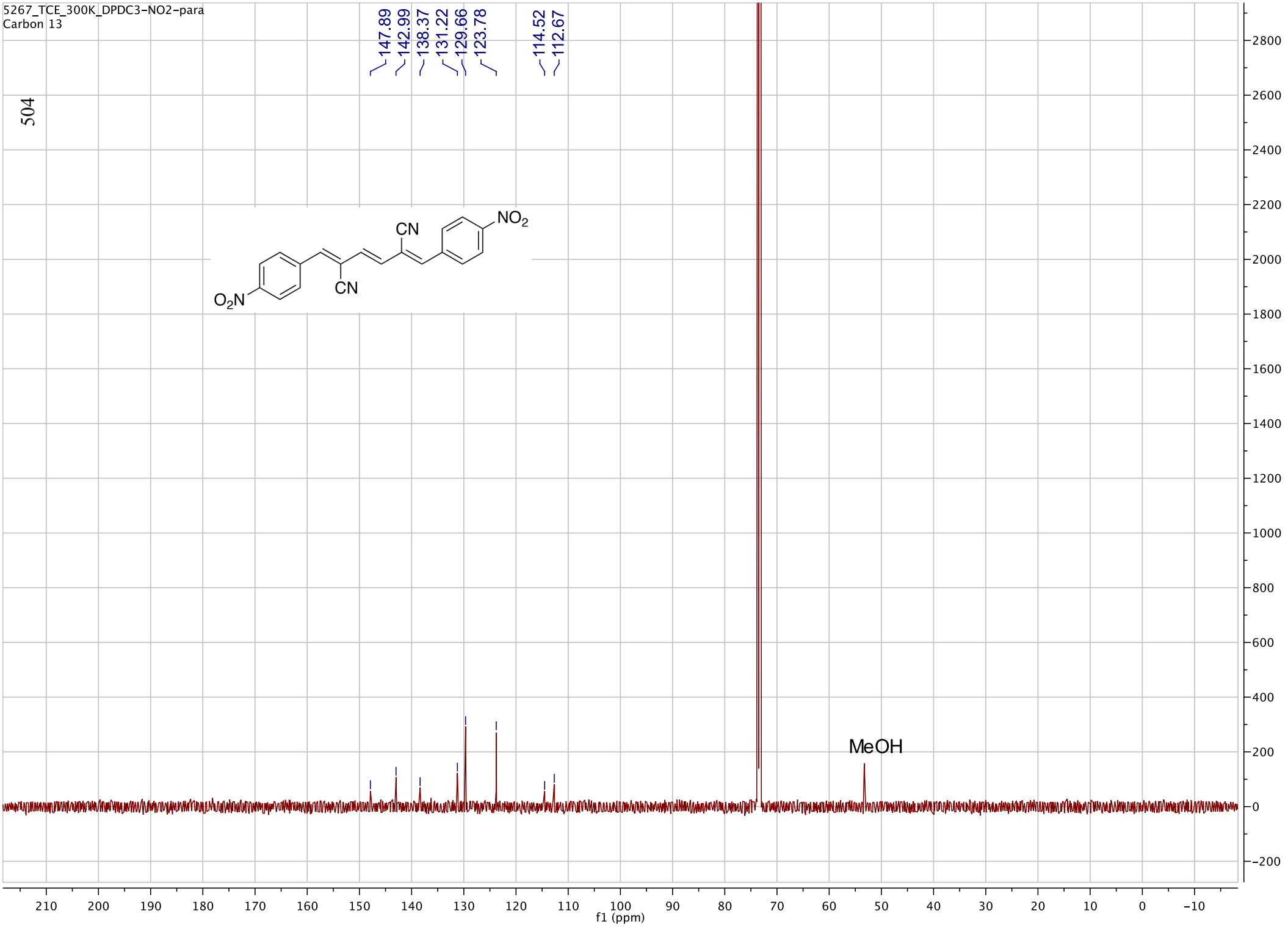
Carbon 13
503
149.81
144.73
136.04
132.56
131.79
126.77
125.44
116.48
113.80
100.00
CN
CN
O2N
NO2
f1 (ppm)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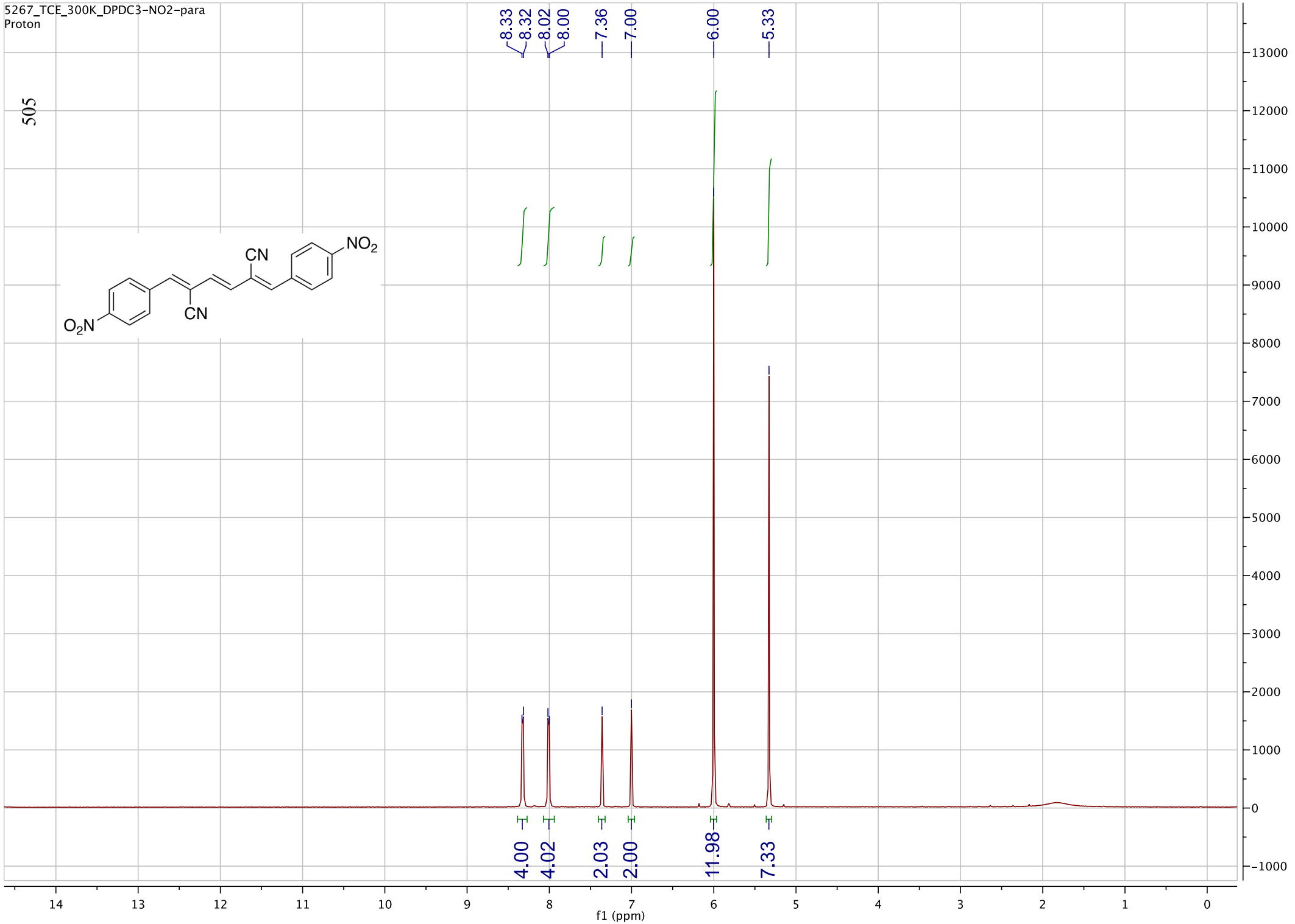
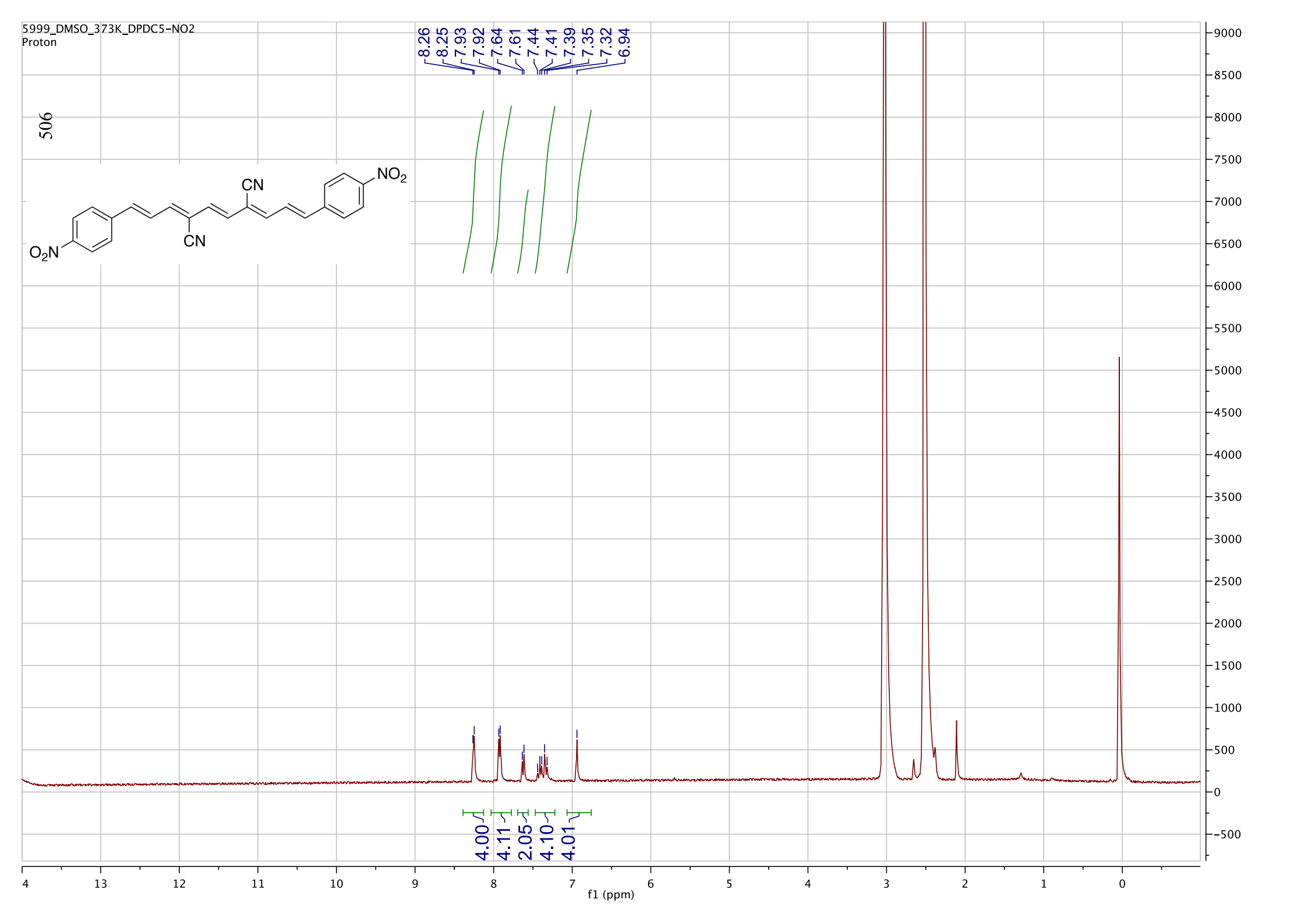
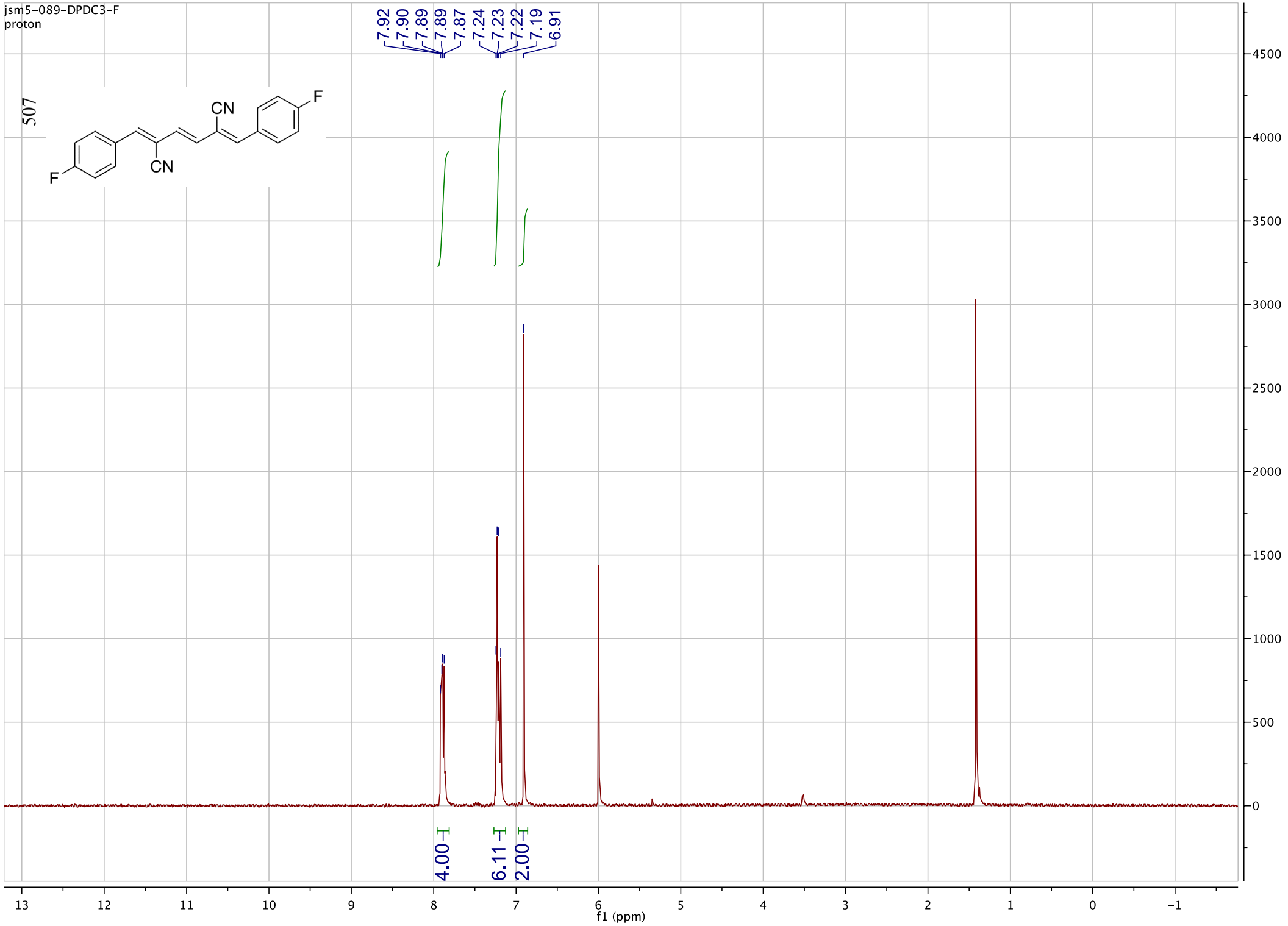
Carbon 13
504
147.89
142.99
138.37
131.22
129.66
123.78
114.52
112.67
CN
NO2
CN
O2N
MeOH
f1 (ppm)


5267_TCE_300K_DPDC3-NO2-para
Proton
505
8.33
8.32
8.02
8.00
7.36
7.00
6.00
5.33
CN
NO2
CN
O2N
4.00
4.02
2.03
2.00
11.98
7.33
f1 (ppm)


5999_DMSO_373K_DPDC5-NO2
Proton
506
8.26
8.25
7.93
7.92
7.64
7.61
7.44
7.41
7.39
7.35
7.32
6.94
CN
CN
NO2
O2N
4.00
4.11
2.05
4.10
4.01
f1 (ppm)


jsm5-089-DPDC3-F
proton
7.92
7.90
7.89
7.89
7.87
7.24
7.23
7.22
7.19
6.91
507
CN
F
CN
F
4.00
6.11
2.00
f1 (ppm)

Appendix B

B1. General Information

The synthesis and characterization of molecules **An** and **Bn** can be found in Appendix A, as well as all absorption spectra and electrochemical. However, they conform to the naming scheme in Chapter 1. The key below describes the relationship.

Chapter 1 Name	Chapter 2 Name
A0	**DPDC3-SMe**
A1	**DPDC5-SMe**
A2	**DPDC7-SMe**
A3	**DPDC9-SMe**
A4	**DPDC11-SMe**
B0	**DPDC3-SC_4H_8**
B1	**DPDC5- SC_4H_8**
B2	**DPDC7- SC_4H_8**
B3	**DPDC9- SC_4H_8**
B4	**DPDC11- SC_4H_8**

B2. Modified STM Break Junction Studies

Experimental Procedure and Data Analysis: The details of our experimental setup have been described previously.[1] We prepare gold samples by evaporating 100 nm of gold onto freshly cleaved mica. During measurement, the sample is mounted on top of a single-axis piezoelectric positioner below a hand-cut gold tip in a home-built STM setup. The sample-tip junction is stretched and compressed with sub-nanometer precision by moving the substrate relative to the tip at a rate of 15 nm/s with the piezoelectric (Mad City Labs) while applying constant bias to the sample through a series resistor. The current in the tip is captured by a Keithly 428 current-voltage amplifier. The sample position is manipulated and data acquired at 40 kHz using a data acquisition board (National Instruments, PXI-4461) and custom-built software written in Igor (Wavemetrics, Inc). All position determinations were based on measurements with a built-in position sensor within our custom piezoelectric positioner. This position sensor was calibrated both by the manufacturer and by us using laser interference measurements. We found the absolute values of the measured displacements to be accurate to within 5%.

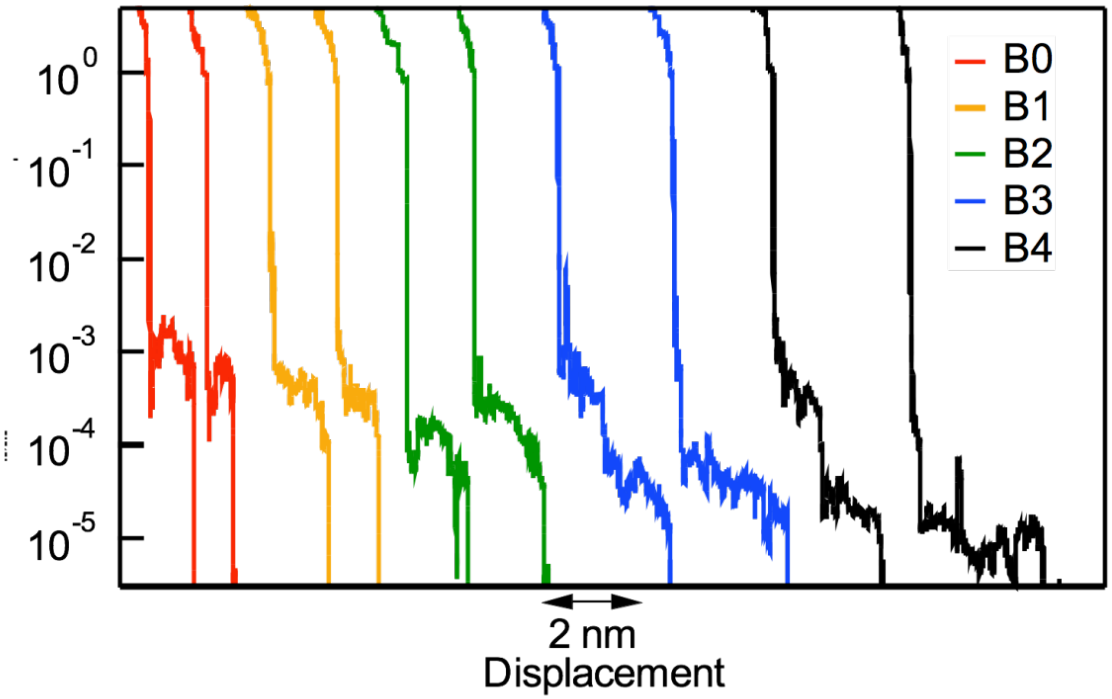


Figure B1: Sample conductance traces gained from STM-based break junction measurements on **Bn** series. Step lengths become longer as molecular length increases, showing that conductive junctions are sustained at larger electrode separations with longer molecules.

We form metal-molecule-metal junctions by smashing the tip and substrate together until conductance exceeds 5 G_0 and then pulling them apart. All conductance traces acquired that reach a conductance below $5x10^{-6}$ G_0 are then added to a linear binned histogram by an automated algorithm without any further data selection. Typically, 5000 traces are used to construct conductance histograms.

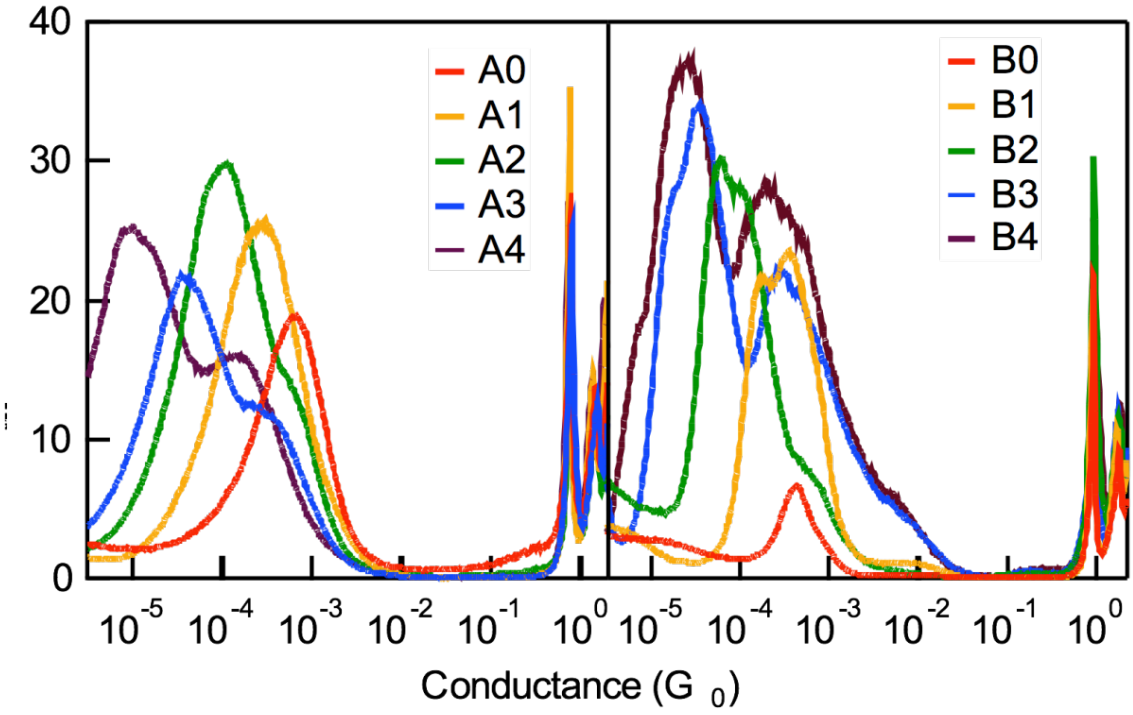


Figure B2: Logarithm binned conductance histograms for **An** and **Bn** series. Bin size is 100 per decade.

Two-dimensional (2D) conductance-displacement histograms are automatically generated[2,3] with the added requirement that a G_0 break is clearly identifiable in the trace (more than 90% of traces that start with a conductance greater than 1 G_0 and break satisfy this requirement). In 2D histograms conductance is binned logarithmically with 100 bins per decade, while displacement is binned linearly for image clarity.

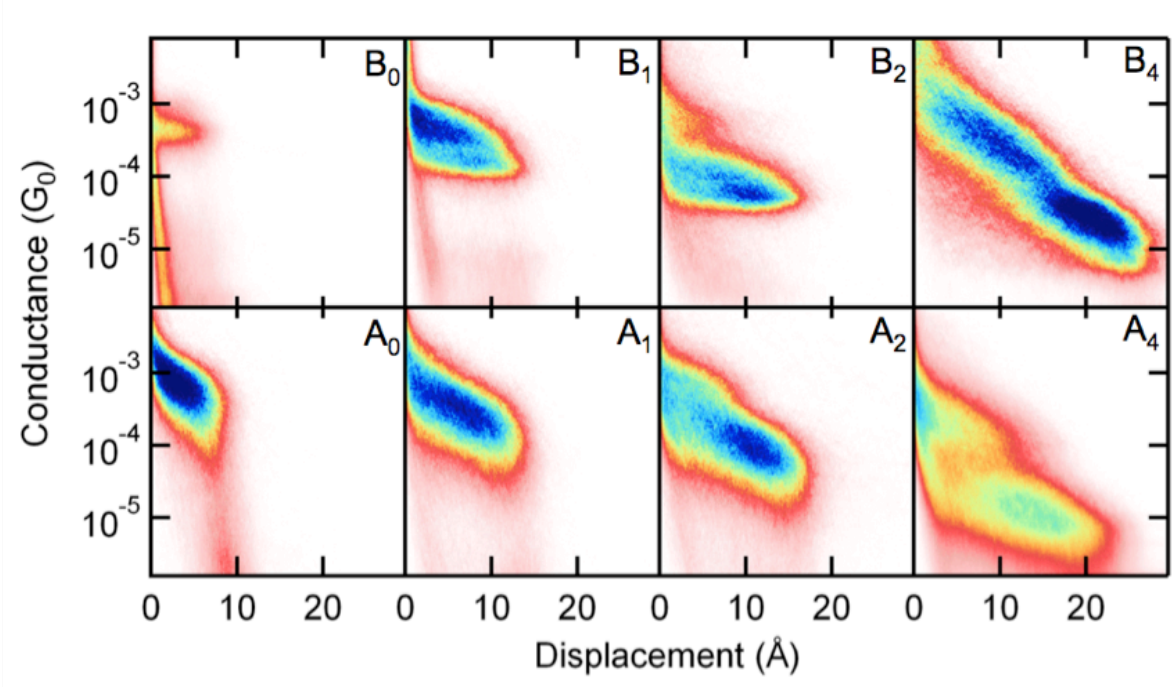


Figure B3: 2D conductance-displacement histograms for the **An** and **Bn** series. The displacement axis has linear bins while the conductance axis has logarithm bins (100 per decade). The higher conductance regime lengthens as the oligomer length increases.

We have not observed that cyano groups bind to gold. 1,4-dicyanobenzene, 1,4-dicyano-2-butene and oligoenes **DPDCn** do not show conductance peaks and likely do not form molecular junctions. Like the cyano-functionalized oligoenes, oligoenes without

cyano groups (**Cont-1**) contain 2 conductance peaks demonstrating that cyano groups do not play a direct role in junction formation.

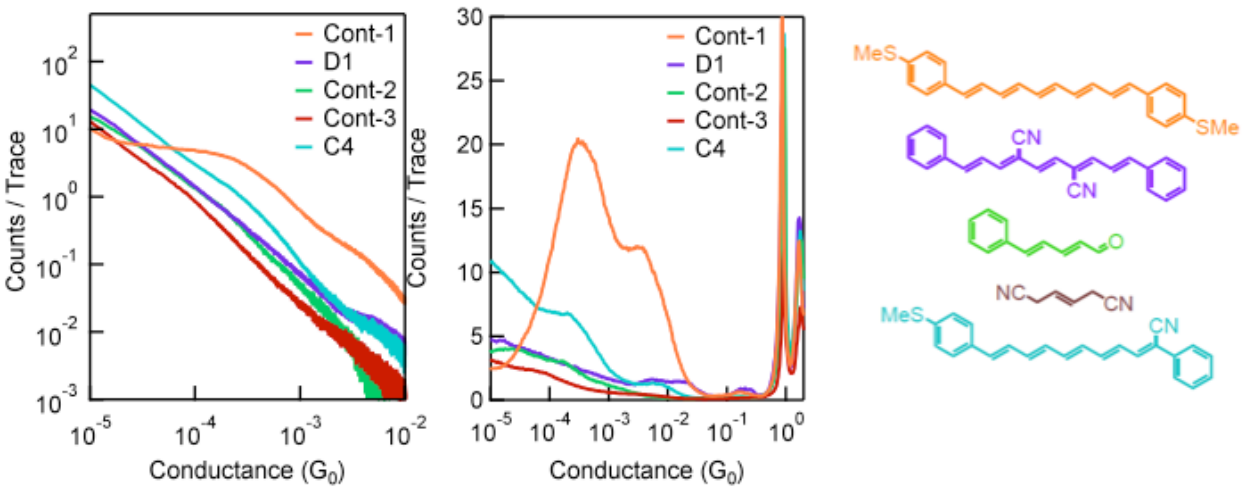


Figure B4: Linear and log binned conductance histograms of control compounds investigated. Structures are shown on the right.

B3. Variable Resistance Measurements and Controls

Traces were selected from all measured traces using an automated algorithm. The number of data points in the initial "hold" region of each trace (starting at time t = 0 s) that had a conductance within the required range was determined. Typically, 50% of all measured traces had a molecule during the initial “hold” region. All selected traces were used to construct a two-dimensional conductance vs. time histograms. Control measurements were carried out with 1,6-bis(methylsulfide)hexane, a saturated molecule. The zig-zag ramp used was chosen so that the proportional change in the in electrode-electrode separation relative to the length of the molecule was the same as in the ramp used in Figure 2.8 of Chapter 2. (Figure B5). The probability of having a junction start at the selected conductance with hexane is 15%, which is significantly lower than the 50% success rate with **B4**. In addition, no reproducible modulation in conductance during the ramp is observed. Traces collected without the presence of any molecules showed conductance oscillating between a closed and an open junction during the zig-zag ramp.

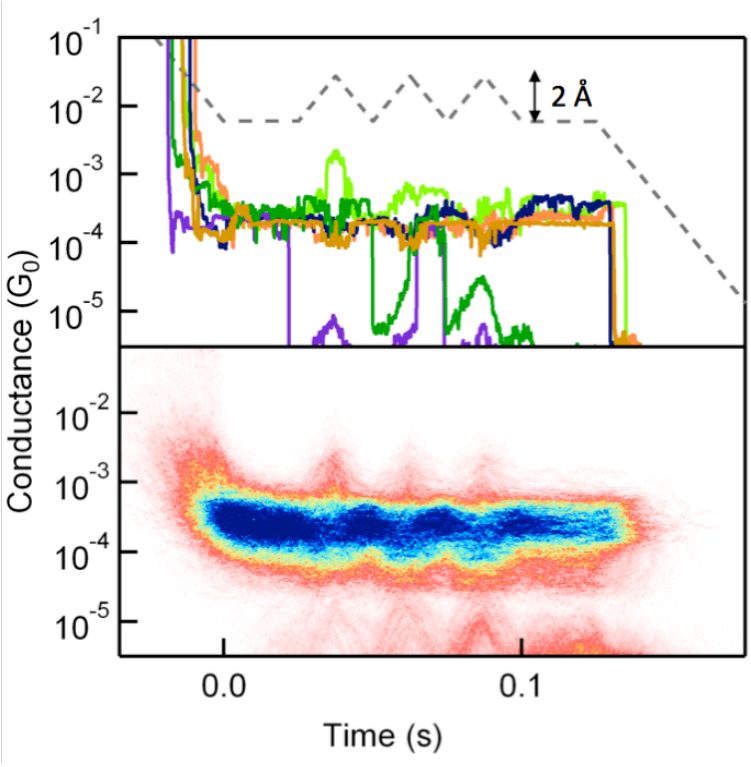


Figure B5: Upper panel: sample traces measured using the modified piezo ramp with a 2Å amplitude with 1,6-bis(methylsulfide)hexane. Lower panel: two-dimensional histograms of all selected traces (1477 out of 10000) measured with the zig-zag ramp.

B4. Theoretical Methods and Details

All electronic structure calculations used Jaguar (version 7.0, Schrodinger LLC, New York, NY, 2007) using the B3LYP hybrid functional and the 6-31G** basis sets. The Au atoms were described using the LACVP local potentials. The geometries of **A1**, **C4**, **Au_2-A1**, and **Au_2-C4** were fully optimized. The final geometries and total energies are given below.

Molecule: **A1**

DFT: B3LYP, 6-31G**

Final total energy: -1909.86419 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.0054586777	0.0160760258	-0.0169920773
C2	0.0027896249	0.0085385018	1.3914265084
C3	1.2617271719	0.0012497986	2.0283492339
C4	2.4438887757	0.0015085903	1.3053981250
C5	2.4188241032	0.0089772276	-0.0998196412
C6	1.1742433465	0.0163070722	-0.7499110173
C7	-1.2021440991	0.0072778950	2.2052531568
C8	-2.4927133813	0.0169740384	1.7749831566
C9	-3.6075929604	0.0127547254	2.6676183755
C10	-4.9334990519	0.0224029486	2.3021511411
C11	-5.2751397474	0.0392694232	0.9081509595
N12	-5.5621980629	0.0531364751	-0.2201717100
C13	-6.0101421145	0.0154862932	3.2699705747
C14	-7.3322358085	0.0233110312	2.9653261724
C15	-8.4151733561	0.0145807935	3.9266602800
C16	-8.0813278759	-0.0032513273	5.3218234957
N17	-7.7896758628	-0.0176148026	6.4488742453
C18	-9.7352003865	0.0222806138	3.5418266357
C19	-10.8782093540	0.0136783650	4.3994222849
C20	-12.1461860159	0.0220303112	3.9044895871
C21	-13.4021959869	0.0146818583	4.6351965919

C22	-14.6079289886	0.0263155388	3.9099862826
C23	-15.8483278911	0.0202660156	4.5387136047
C24	-15.9277001203	0.0017264220	5.9370020083
C25	-14.7299066618	-0.0103240334	6.6793230835
C26	-13.4999714035	-0.0041483078	6.0445455925
H27	-3.3938194979	0.0003963107	3.7351203893
H28	-9.9256264741	0.0358768554	2.4698511737
H29	-5.7046635080	0.0023889406	4.3139517264
H30	-7.6345826850	0.0364930545	1.9204393953
H31	-1.0316634905	-0.0025146717	3.2818925770
S32	3.9910988563	0.0084039910	-0.9274374134
H33	3.3957627930	-0.0044316048	1.8287255893
H34	1.3047841869	-0.0047694344	3.1145542437
H35	-0.9481970700	0.0214885691	-0.5550998814
H36	1.1158745968	0.0221111506	-1.8319398186
H37	-10.7015210857	-0.0001287768	5.4719983301
H38	-12.2526442300	0.0358262463	2.8196296730
S39	-17.4430232213	-0.0078399861	6.8645500296
H40	-16.7451674257	0.0300240106	3.9305929385
H41	-14.5699844983	0.0404738872	2.8235381871
H42	-12.6003534518	-0.0141466040	6.6514829712
H43	-14.7718464591	-0.0246611109	7.7647246498
H44	-2.7134702204	0.0283108250	0.7108404068
C45	-18.7342463992	0.0135341018	5.5795904309
H46	-19.6832765180	0.0068539840	6.1193210506
H47	-18.6792182189	0.9193772498	4.9717731839
H48	-18.6821711952	-0.8737282692	4.9446992281
C49	3.5500383513	0.0142213788	-2.6948981937
H50	4.5004270922	0.0121132100	-3.2322812278
H51	2.9861342170	-0.8798300083	-2.9698160773
H52	2.9926291711	0.9135017312	-2.9658734422

Molecule: **C4**

B3LYP, 6-31G**

Final total energy: -1380.11453 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.0221616271	0.0305191350	0.0657841755
C2	0.0505512825	0.0074467812	1.4712469394
C3	1.3277432101	-0.0214717221	2.0644324619
C4	2.4824111277	-0.0279251694	1.2886342811
C5	2.3940480177	-0.0052338919	-0.1022654048
C6	1.1349232644	0.0236065508	-0.7067546243
C7	-1.1500491919	0.0210224430	2.3322139375
C8	-2.4642172798	0.0200794862	1.9282325595
C9	-3.5626572514	0.0607782631	2.8408985884
C10	-4.8923875129	0.0687414444	2.5311564879
C11	-5.8881283931	0.1410966200	3.5564740442
C12	-7.2395506329	0.1665423464	3.3755156381
C13	-8.1765498464	0.2718719279	4.4542673537
C14	-9.5285250050	0.3102243306	4.2922088751
C15	-10.4967098987	0.4474326670	5.3441060724
C16	-11.8299166562	0.4874863103	5.0879124803
C17	-12.9519267843	0.6487222766	6.0013380875
C18	-12.8435524243	0.8223418732	7.3944075692
C19	-13.9702420162	0.9877303016	8.1954721673
C20	-15.2552778560	0.9855665195	7.6300934672
C21	-15.3785559738	0.8073841152	6.2428590091
C22	-14.2523666593	0.6442161835	5.4547805575

H23	-7.7653337333	0.3339907054	5.4618309675
H24	-5.2159161072	0.0299975693	1.4910745619
H25	-9.9250838102	0.2437572817	3.2783197951
H26	-3.3058197567	0.0970533638	3.8970299195
H27	-7.6416884426	0.1163793456	2.3633494258
H28	-5.5136371922	0.1890132931	4.5791158155
H29	-12.1223322999	0.3951920445	4.0415861458
S30	-16.7774130997	1.1948086860	8.5286893528
H31	-16.3632711996	0.8015210691	5.7840625660
H32	-14.3719619379	0.5107655764	4.3826476703
H33	-11.8645342439	0.8327906750	7.8648242297
H34	-13.8376736657	1.1201628395	9.2633471263
H35	-2.6853256881	-0.0050533406	0.8644066396
C36	-0.9120067742	0.0384788820	3.7478490561
H37	3.2935780054	-0.0090819695	-0.7105257126
H38	3.4529261387	-0.0501423745	1.7755083334
H39	1.4134213558	-0.0385732287	3.1459155885
H40	-0.9857224925	0.0579577247	-0.4330746723
H41	1.0535213299	0.0430039393	-1.7896751657
H42	-10.1230897813	0.5277065949	6.3638829573
N43	-0.7363902581	0.0501750068	4.8991437366
C44	-16.2411684638	1.4463029825	10.2504037037
H45	-17.1591222690	1.5911879998	10.8236836060
H46	-15.7157666983	0.5714214952	10.6400607049
H47	-15.6177881406	2.3377946450	10.3492541465

Molecule: **Au_2-A1**

B3LYP, 6-31G**/LACVP

Final total energy: -2180.81428 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.1516373949	0.1679875211	-0.0920807598
C2	-0.1554448482	0.1426712864	1.3189390134
C3	1.0950682395	0.0959268006	1.9662913092
C4	2.2834179216	0.0722650893	1.2466190464
C5	2.2685631129	0.0939093271	-0.1578716415
C6	1.0283367266	0.1450026652	-0.8179739000
C7	-1.4298578120	0.1556168426	2.0175984357
C8	-1.6479765191	0.1579270279	3.3611422960
C9	-2.9622376371	0.1481850783	3.9206759664
C10	-3.2784332203	0.1451744227	5.2595695653
C11	-2.2256593264	0.1715243113	6.2341693894
N12	-1.3825923233	0.1950646990	7.0369549542
S13	3.7168477442	0.0609847888	-1.1863319944
C14	5.0901887530	-0.1068559426	-0.0023258630
C15	-4.6464451705	0.1045807583	5.7315867670
C16	-5.0255135231	0.0790647660	7.0345937175
C17	-6.3937433972	0.0239428273	7.5051142778
C18	-7.4441699552	-0.0080536046	6.5279112199
N19	-8.2840057906	-0.0353541022	5.7221000288
C20	-6.7115130661	-0.0132685978	8.8430009027
C21	-8.0256896009	-0.0812680369	9.4003620940
C22	-8.2437773535	-0.1239383696	10.7434470448

C23	-9.5174855466	-0.1938231748	11.4406077574
C24	-10.7729390874	-0.2106831967	10.7900000803
C25	-11.9527239137	-0.2787178759	11.5105828581
C26	-11.9345078346	-0.3325500112	12.9174044466
C27	-10.7015192229	-0.3151262038	13.5799404261
C28	-9.5202313733	-0.2476393486	12.8466948642
S29	-13.5277210425	-0.3528084540	13.7409995325
C30	-13.0603518622	-0.3164940106	15.5108257009
Au31	-14.5024901338	-2.6095863740	13.4571867019
H32	3.2218390586	0.0336526329	1.7879740759
H33	1.1452791694	0.0736161875	3.0507683321
H34	-1.0999330274	0.2039259268	-0.6228532913
H35	0.9941922861	0.1605641450	-1.9039558313
H36	-2.3072802772	0.1596859296	1.3702118362
H37	-0.8108994067	0.1618803954	4.0550936332
H38	-3.7981752710	0.1291394194	3.2228255261
H39	-5.4087535267	0.0872652434	4.9556374629
H40	-4.2630557325	0.0899286556	7.8105133488
H41	-5.8768160363	0.0099773858	9.5422295413
H42	-8.8616179730	-0.1007964511	8.7051387280
H43	-7.3670894811	-0.1046560205	11.3914968636
H44	-8.5712925854	-0.2372100081	13.3777291444
H45	-10.6450344931	-0.3569231448	14.6612106335
H46	-12.9045312944	-0.2987525020	10.9871035551
H47	-10.8253190860	-0.1688656503	9.7062787616
H48	5.1557753051	0.7553652430	0.6654996964
H49	5.0082487114	-1.0296409468	0.5767940192
H50	5.9958057167	-0.1510484786	-0.6111780022
H51	-12.4899264306	-1.2026905582	15.7924293051
H52	-14.0044300352	-0.3082362637	16.0571946543
H53	-12.5005591224	0.5952144728	15.7349863339

Au54	-15.6041498559	-4.9343391061	13.2321392566

Molecule: **Au_2-C4**

B3LYP, 6-31G**/LACVP

Final total energy: -1651.074011 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.0157017963	0.0713846205	0.0100088942
C2	-0.0118780466	0.0574814708	1.4167733522
C3	1.2404537151	0.0046851532	2.0705008407
C4	2.4275782274	0.0119996515	1.3502056867
C5	2.3943929024	0.0397774758	-0.0495957415
C6	1.1662093791	0.0546989829	-0.7199962650
C7	-1.2925818092	0.1475882933	2.1042742997
C8	-1.5445809720	0.0547421499	3.4348586239
C9	-2.8580297143	0.2437167487	3.9826887694
C10	-3.1844232823	0.1319396223	5.3000704689
C11	-4.4990801142	0.3756221425	5.8111019268
C12	-4.8574738253	0.2164532870	7.1164697956
C13	-6.1630000042	0.4864148915	7.6337069042
C14	-6.5143059703	0.2593894971	8.9324159169
C15	-7.8043499020	0.5445691560	9.4770163200
C16	-8.2013856165	0.2527364866	10.7570880070
C17	-7.2855822889	-0.4687689976	11.5941527484
N18	-6.5455373448	-1.0662493374	12.2662795552
S19	3.8714400398	0.2111589482	-1.0640110846
C20	4.9903736624	-1.0844467160	-0.4077782114
C21	-9.5126099593	0.6012157947	11.3377247039
C22	-10.3310782986	1.5966127061	10.7696238294

C23	-11.5618579051	1.9129444833	11.3374705296
C24	-12.0029360574	1.2502985388	12.4839933743
C25	-11.1987587534	0.2660184912	13.0606093806
C26	-9.9667531961	-0.0537118197	12.4969875873
H27	-2.4147493587	-0.1571741925	6.0159303128
H28	-6.9079680580	0.8887811008	6.9464122007
H29	-3.6437981061	0.5070433353	3.2738701458
H30	-5.7686471574	-0.1722184270	9.5981027247
H31	-5.2542664826	0.7082690098	5.0980360509
H32	-4.1091763819	-0.1462937171	7.8217503301
H33	-2.1424095822	0.3253711826	1.4455936853
H34	1.1353606077	0.0733025681	-1.8036737409
H35	-0.9674620536	0.1073238813	-0.5168104552
H36	1.2889975403	0.0083579577	3.1536287791
H37	3.3765622903	0.0336033088	1.8790898024
H38	-8.5304716919	1.0212860850	8.8235923062
H39	-12.9611702550	1.5060690611	12.9275935091
H40	-11.5281163260	-0.2545725451	13.9542156847
H41	-9.3493007561	-0.8221582988	12.9532240181
H42	-9.9947464398	2.1452441082	9.8961649563
H43	-12.1750177976	2.6907268560	10.8898848717
H44	-0.7430734747	-0.1635173370	4.1387137927
H45	5.9164448599	-0.9988878072	-0.9785381181
H46	5.2009031202	-0.9300127831	0.6503336885
H47	4.5364919704	-2.0624752090	-0.5760763271
Au48	4.7641825117	2.3655582803	-0.2666378145
Au49	5.5058118799	4.6126128264	0.7780153528

B5. References

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2. Kamenetska, M.; Koentopp, M.; Whalley, A.; Park, Y. S.; Steigerwald, M.; Nuckolls, C.; Hybertsen, M.; Venkataraman, L. *Phys. Rev. Lett.,* **2009**, *102*, 126803.

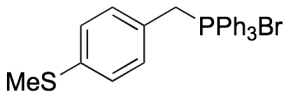
3. Quek, S. Y.; Kamenetska, M.; Steigerwald, M. L.; Choi, H. J.; Louie, S. G.; Hybertsen, M. S.; Neaton, J. B.; Venkataraman, L. *Nature Nanotech.,* **2009**, *4*, 230–234.

Appendix C

C1. Synthetic Details

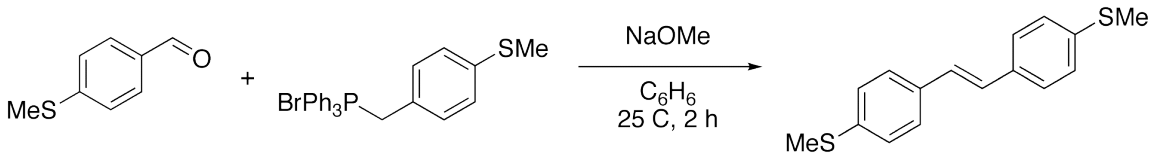
General Information: 4-(methylthio)benzaldehyde, 3-(methylthio)benzoic acid, 4-(methylthio)benzyl bromide, and all other starting materials and reagents were all purchased from Sigma-Aldrich. All reactions were carried out under nitrogen unless otherwise noted. (3-(methylthio)benzaldehyde,[1] (3-(methylthio)phenyl)methanol,[1] and (3-methylthio)benzyl chloride[2] were prepared according to the reported procedures. Sodium methoxide solution was made fresh by dissolving sodium metal into 5 mL of methanol. Flash column chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica columns. All ^{1}H and ^{13}C NMR spectra were taken on a Bruker DRX300 (300MHz), DRX400 (400MHz) and DMX500 (500MHz).

Synthetic Experimentals:

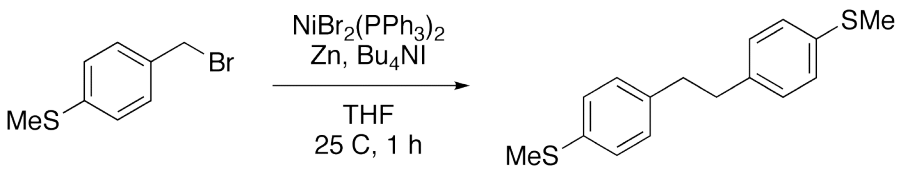


4-(methylthio)benzyltriphenylphosphonium bromide: Adapted from known procedure.[3] To a flame dried 25-mL round-bottom flask was added triphenylphosphine (3.91 g, 14.9 mmol) and anhydrous benzene (10 mL). The reaction flask was purged with nitrogen gas and then heated to reflux, at which point a solution of (4-methylthio)benzyl bromide (3.23 g, 14.9 mmol) in 5 mL of anhydrous benzene was added to the reaction solution via syringe. The reaction was stirred at reflux for 12 hours as product precipitated out. The

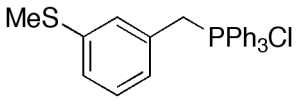
crude product was isolated by filtration, washed with benzene and recrystallized from CH_2Cl_2/benzene mixture. The product was isolated as white powder in quantitative yields. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.81-7.74 (m, 9H), 7.69-7.62 (m, 6H), 7.08-6.98 (m, 4H), 5.45 (d, *J* = 14.4 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (300 MHz, DMSO-*d*$_6$): δ 139.73, 139.68, 135.0, 134.9, 132.2, 132.1, 131.1, 130.9, 126.7, 124.8, 124.7, 119.3, 118.2, 28.9, 28.3, 15.2.



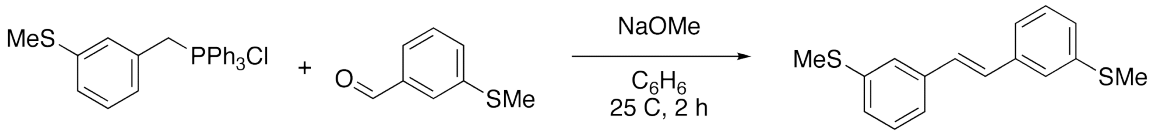
(E)-4,4'-di-(methylthio)stilbene (**1**): In a 100-mL round-bottom flask, (4-methylthio)-benzaldehyde (0.100 g, 6.62 mmol) and (4-methylthio)benzyltriphenylphosphonium bromide (3.20 g, 6.62 mmol) were dissolved in 50 mL of anhydrous methanol under a nitrogen atmosphere. Sodium methoxide (13.2 mmol) in methanol solution was added to the reaction slowly over 10 min by syringe. An off-white precipitate forms while the reaction was stirred for an additional 2 hours at room temperature. The pure product was collected by vacuum filtration as pale yellow needles in 31.0% yield. No further purification was necessary. UV-vis: 223 nm (ε = 1.38 x 10^4 mol^{-1}*cm^{-1}), 347 nm (ε = 4.42 x 10^4 mol^{-1}*cm^{-1}), 362 nm (shoulder, ε = 3.21 x 10^4 mol^{-1}*cm^{-1}); ^{1}H NMR (300 MHz, $CDC1_3$): δ 7.44 (d, *J* = 8.4 Hz, 4H), 7.23 (d, *J* = 7.8 Hz, 4H), 7.02 (s, 2H), 2.50 (s, 6H); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ 7.54 (d, *J* = 8.4 Hz, 4H), 7.26 (d, *J* = 8.3 Hz, 4H), 7.18 (s, 2H), 2.50 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 138.2, 134.7, 127.8, 127.2, 127.1, 16.2; HR-MS: m/z calcd for ($C_{16}H_{16}S_2$): 272.0693, found: 272.0686.



1,2-bis(4-(methylthio)phenyl)ethane (**2**): This procedure was modified from the reported preparation of *1,2-bis(4-(methoxy)phenyl)ethane*.[4] In a 100-mL round-bottom flask, dibromobis(triphenylphosphine)nickel(II) (0.086 g, 0.12 mmol), zinc powder (0.112 g, 1.73 mmol) and tetrabutylammonium iodide (0.296 g, 1.15 mmol) were combined in a with 25 mL of tetrahydrofuran. The green slurry was stirred for 30 min at room temperature as the color changes to grey-brown. Then, a solution of 4-(methylthio)benzyl bromide (0.250 g, 1.15 mmol) in 5 mL of tetrahydrofuran was added dropwise to the reaction slurry. The reaction turns red and later dark purple. The reaction was monitored by TLC and finished in less than 1 hour. The zinc solid was filtered off and washed with dichloromethane. The organic solvents were removed by rotary evaporation and the product was isolated by flash column chromatography (hexanes) as a colorless crystalline solid in 46.2% yield. UV-vis: 261 nm (ε = 2.66 x 10^4 $mol^{-1}*cm^{-1}$); ^{1}H NMR (300 MHz, $CDC1_3$): δ 7.19 (d, J = 8.4 Hz, 4H), 7.08 (d, J = 8.4 Hz, 4H), 2.85 (s, 4H), 2.45 (s, 6H); ^{13}C NMR (300 MHz, $CDC1_3$): δ 139.10, 135.91, 129.43, 127.53, 37.66, 16.71; HR-MS: m/z calcd for ($C_{16}H_{18}S_2$): 274.0850, found: 274.0841.



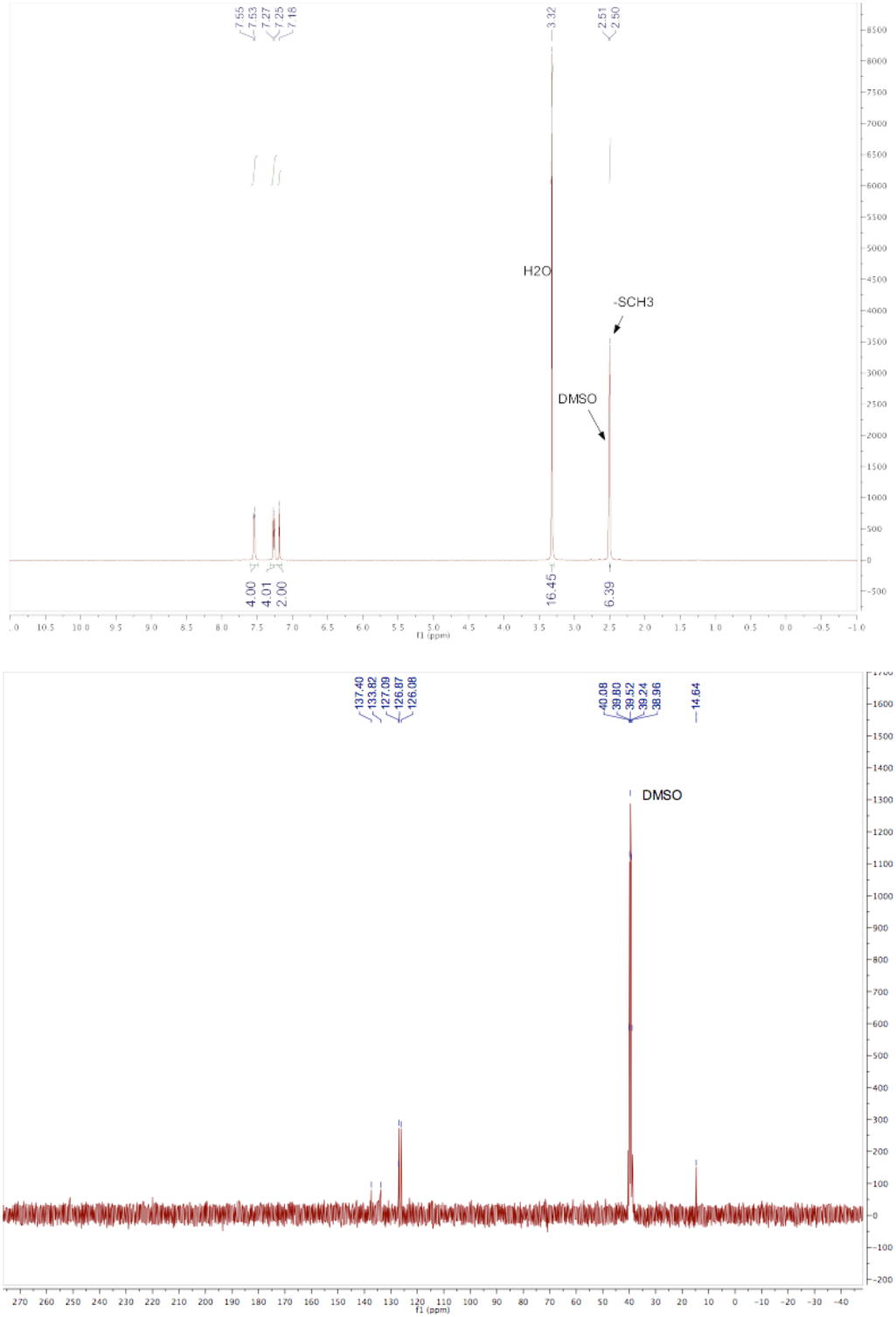
3-(methylthio)benzyltriphenylphosphonium chloride: Similar to the synthesis of *4-(methylthio)benzyltriphenylphosphonium bromide* above. 3-(methylthio)benzyl chloride (0.230 g, 1.33 mmol) and triphenylphosphine (0.348 g, 1.33 mmol) were combined in anhydrous benzene (12 mL). The solution was refluxed for 24 hours. The reaction was cooled to room temperature, during which a white precipitate formed. The solid was isolated by vacuum filtration and washed with cold benzene. The white crystalline product (0.258 g, 45%) was dried in air. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.94 (t, J = 7.5 Hz, 3H), 7.78-7.73 (m, 6H), 7.70-7.65 (m, 6H), 7.19 (m, 2H), 6.82 (bs, 1H), 6.74 (bs, 1H), 5.16 (d, J = 15.7 Hz, 2H), 2.19 (s, 3H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 139.43, 135.61, 135.58, 134.57, 134.47, 130.63, 130.51, 129.70, 129.28, 128.33, 127.58, 126.26, 118.59, 117.74, 28.81, 28.32, 14.75.



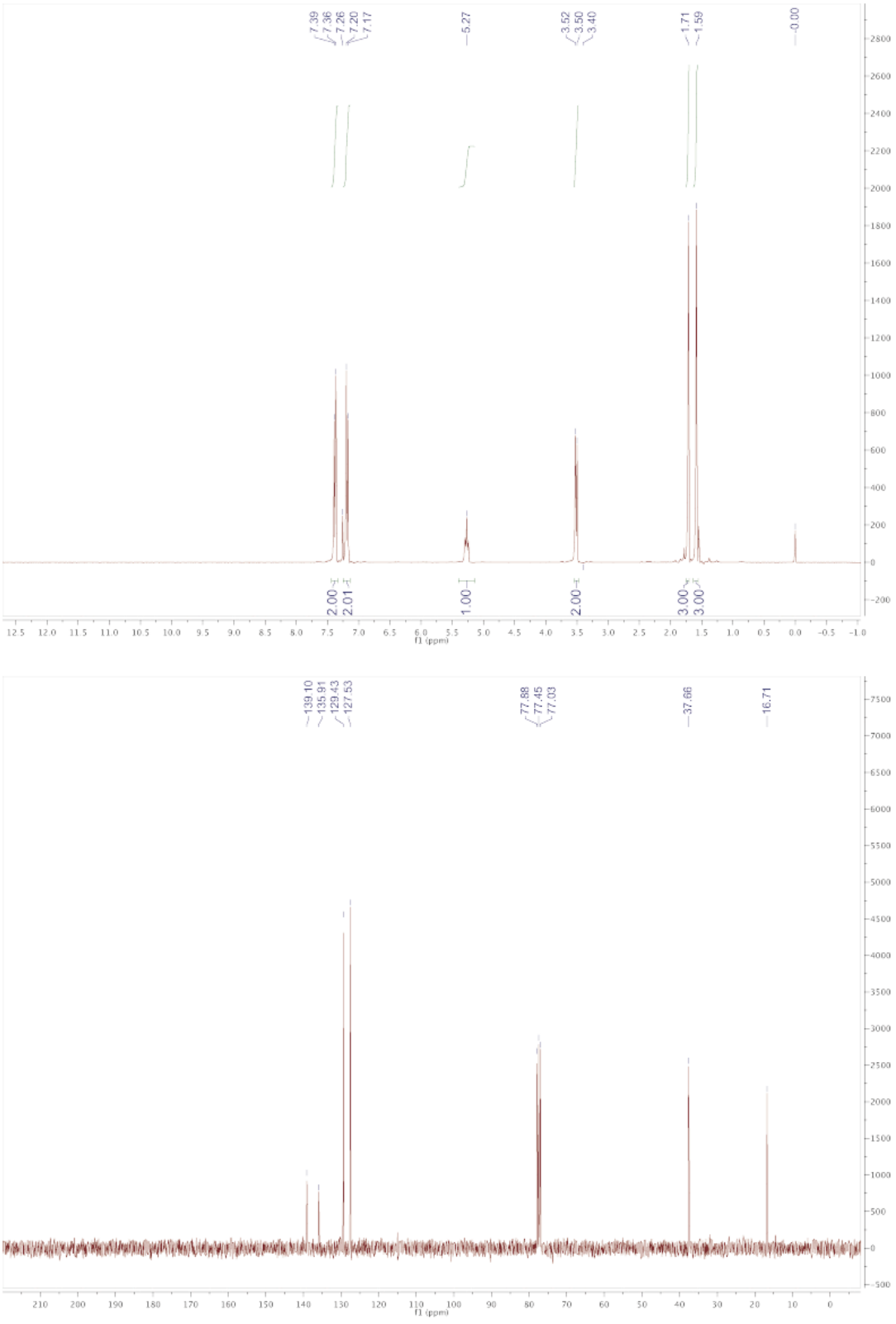
(E)-3,3'-di-(methylthio)stilbene (**3**): In a 50-mL round-bottom flask, (3-methylthio)benzaldehyde (0.10 g, 0.66 mmol) and (3-methylthio)triphenyl-phosphonium chloride (0.29 g, 0.66 mmol) were dissolved in 25 mL of anhydrous methanol under nitrogen. Sodium methoxide (1.32 mmol) was added to the solution slowly over 15 min via syringe. A colorful (usually yellow) precipitate forms while the reaction was stirred for an additional 2 hours at room temperature. The resultant *E*/*Z*-mixture of stereoisomers was collected by filtration and separated by flash column chromatography (25% CH_2Cl_2

in hexanes). The (*E*)-stilbene was isolated as a white solid in overall 30% yield. UV-vis: 267 nm (ε = 3.48 x 10^4 $mol^{-1}*cm^{-1}$), 302 nm (ε = 2.68 x 10^4 $mol^{-1}*cm^{-1}$); ^{1}H NMR (300MHz, $CDCl_3$): δ 7.39 (bs, 2H), 7.28-7.24 (m, 4H), 7.17-7.14 (m, 2H), 7.05 (s, 2H), 2.51 (s, 6H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 139.46, 138.18, 129.49, 129.19, 126.34, 125.14, 123.81, 16.31; HR-MS: m/z calcd for ($C_{16}H_{16}S_2$): 272.0693, found: 272.0692.

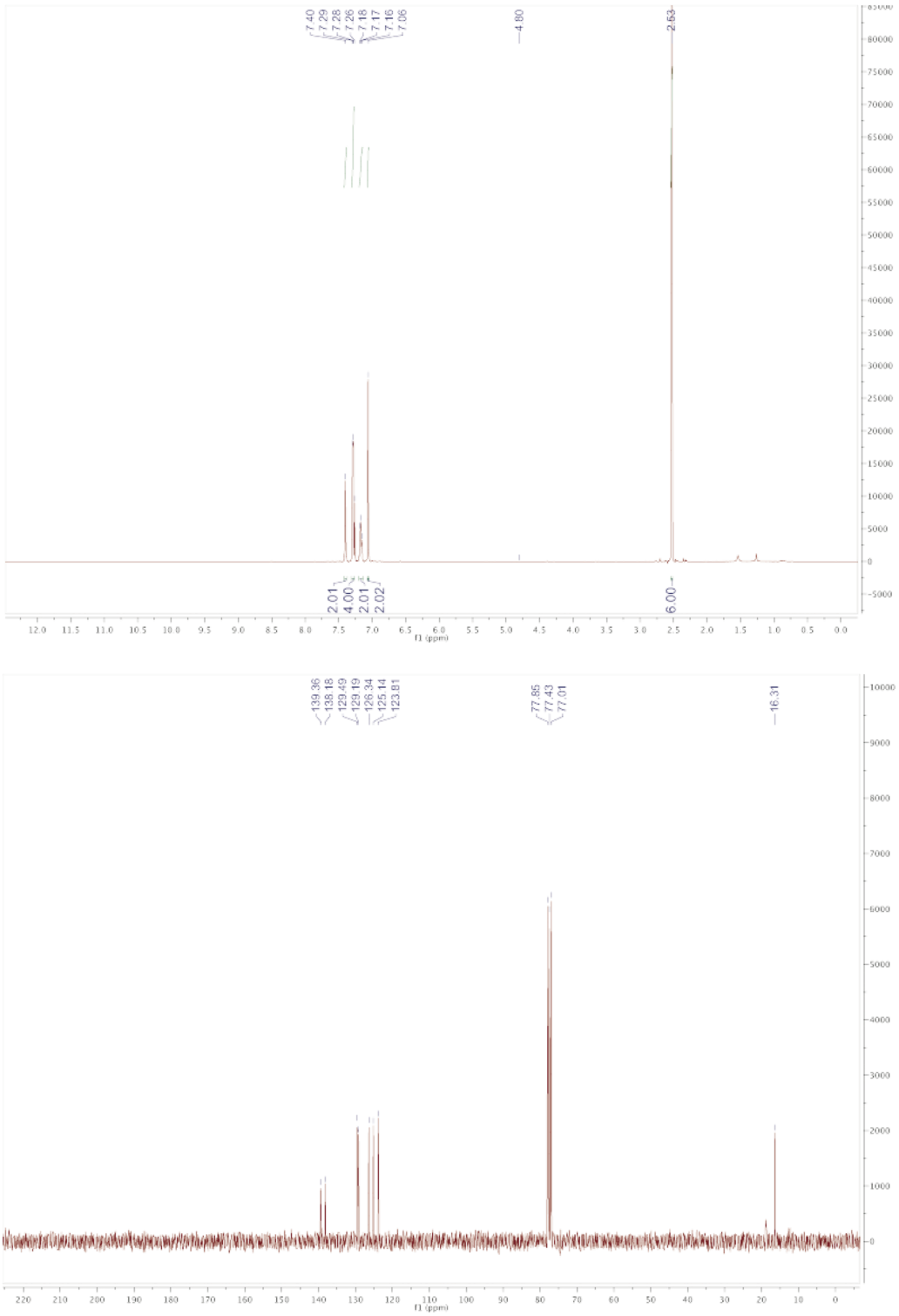
C2. NMR Spectra



1H and 13C NMR of (E)-4,4’-di-(methylthio)stilbene (1) in DMSO



^{1}H and ^{13}C NMR of *1,2-bis(4-(methylthio)phenyl)ethane* (**2**) in $CDCl_3$



^{1}H and ^{13}C NMR of *(E)-3,3'-di-(methylthio)stilbene* (**3**) in $CDCl_3$

C3. Optical Absorption Spectroscopy

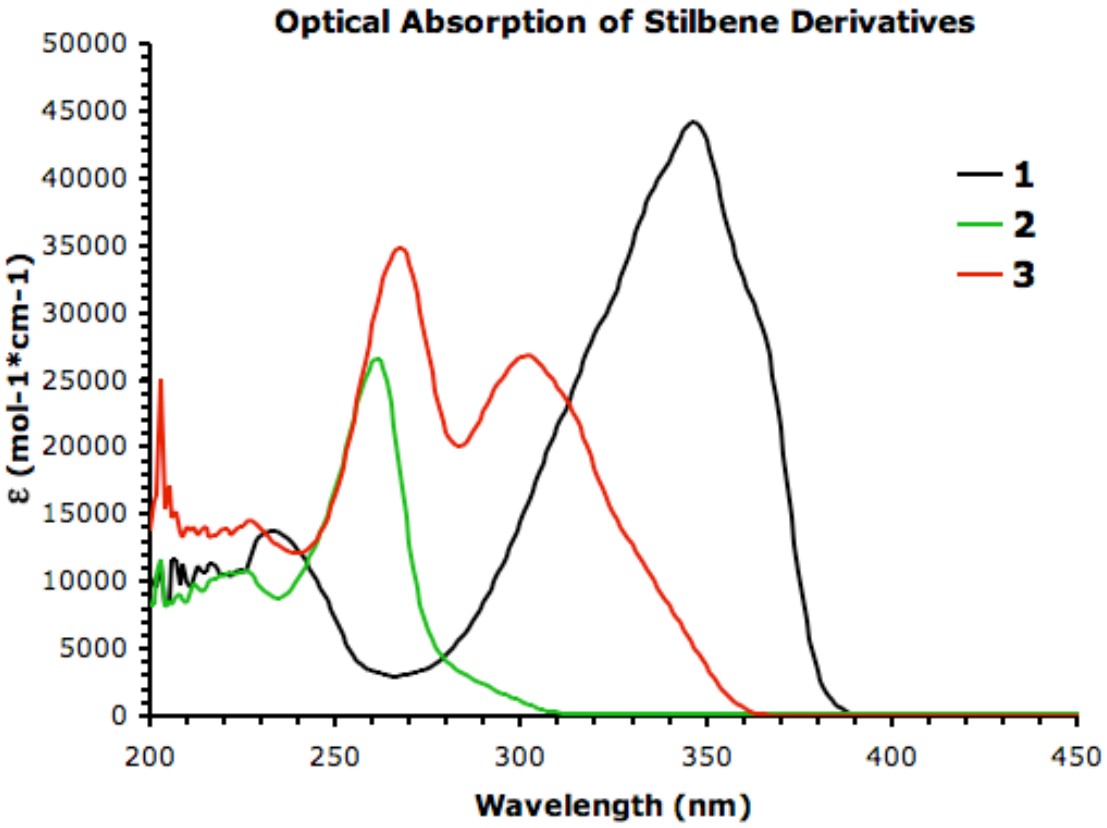


Figure C1. UV-vis spectra of each stilbene derivative (**1**-**3**) show conjugated molecules to have longest-wavelength absorption edges residing in the near UV spectrum (>350 nm), while molecule **2** (not fully conjugated) has an absorption edge at 310 nm. Absorption spectra were taken on an Agilent Technologies 8453 UV-Vis spectrophotometer using a quatz cuvette with path length equal to 1.0 cm. Solutions of oligoenes were prepared in CH_2Cl_2 solution at a concentration of 5.00 x 10^{-5} M. Solution optical band gaps, E_{OP}, are found to be 4.00, 3.42, 3.18 eV.

C4. AFM-based Single-molecule Break Junction Studies

Experimental Procedure

We use a custom-built conducting AFM to perform the simultaneous conductance and force measurements. All the experiments are performed in ambient and at room temperature. We use commercial tapping mode silicon AFM cantilevers (NanoAndMore) on which we sequentially thermally evaporate a ~10 nm of chromium adhesion layer and an gold layer of ~100 nm. Using the thermal spectrum method, we obtain nominal spring constants of ~50 N/m (resonant frequency ~200 kHz) after Au evaporation.[5] The substrates are cleaved mica surfaces coated with ~100 nm of evaporated Au. The substrate is mounted on top of a single-axis piezoelectric stage (Mad City Labs). The substrate-tip junction is stretched and compressed with sub-angstrom precision by moving the substrate relative to the tip at a rate of 18 nm/s using the piezoelectric stage. A constant bias of 75 mV is applied to the substrate through a 10 kΩ series resistor. The current through the tip/substrate junction is measured by a current-voltage amplifier (Keithley 428). Both the conductance and force data are acquired at 100 kHz through data acquisition cards (National Instruments, PXI-4461 and PXI 6251) and custom-built software written in Igor Pro (Wavemetrics). All position determinations were based on measurements with a built-in position sensor within the piezoelectric positioner. This position sensor was calibrated both by the manufacturer and by us using laser interference measurements. We found the absolute values of the measured displacements to be accurate to within 5%. The details of our AFM based experimental setup have been described previously.[6]

Analysis Technique

The measured conductance and force traces are analyzed using an automated algorithm (using Igor Pro software). The algorithm performs three sequential operations on every individual simultaneously measured conductance and force traces: (1) identifying the location of the end of the $1G_0$ conductance plateau, (2) analyzing the force data beyond this point to find the last force event within 1 nm of this point and (3) setting the origin of conductance and force traces at this location and creating 2D histograms of force and conductance. Figure C2 demonstrates application of this technique on a sample individual elongation measurement of molecule **3**. The conductance drop from 1 G_0 is easily identified since the conductance decreases by more than two orders of magnitude upon the rupture of Au point-contacts. Analyzing the force data to identify significant events is carried out by the following procedure. First, the force trace F (Figure C2, blue trace) is transformed to a trace F* (Figure S2, green trace) where every data point F*[p] with index p is defined as:

$$F^*[p] = \sqrt{F[p]_{avg,10} \times F[p]_{avg,50}} \qquad \text{(eq. C1)}$$

where,

$$F_{avg,n}[p] = \frac{1}{n}\left(\sum_{i=p-n}^{p} F[i] - \sum_{j=p}^{p+n} F[j] \right) \qquad \text{(eq. C2)}$$

F* shows clearly defined spikes at the positions where there are large changes in the force, and is much less sensitive to random noise compared to the original data, due to the averaging. We note that due to high frequency noise in the raw force trace, a simple numerical derivative cannot reliably indentify the location of these sharp drops in force. We classify every spike of F* that corresponds to a change in force greater than 0.3 nN (which is 2× the experimental noise level of the force data) as a significant force event, and use this threshold to consistently analyze all data collected here for all three molecule types. F* is used to identify all the significant force events within a 1 nm elongation beyond the 1 G_0 point-contact rupture. Figure C2 demonstrates the high sensitivity of F* to significant force events which are heuristically identified in the force data. It also demonstrates the insensitivity of F* towards high frequency noise in the force data. The algorithm then identifies the last force event as the rupture of the molecular junction, irrespective of the conductance. This molecular rupture location is used as the origin to construct the displacement-preserving 2D histograms in (Figures 3.3 and 3.4 in Chapter 3).

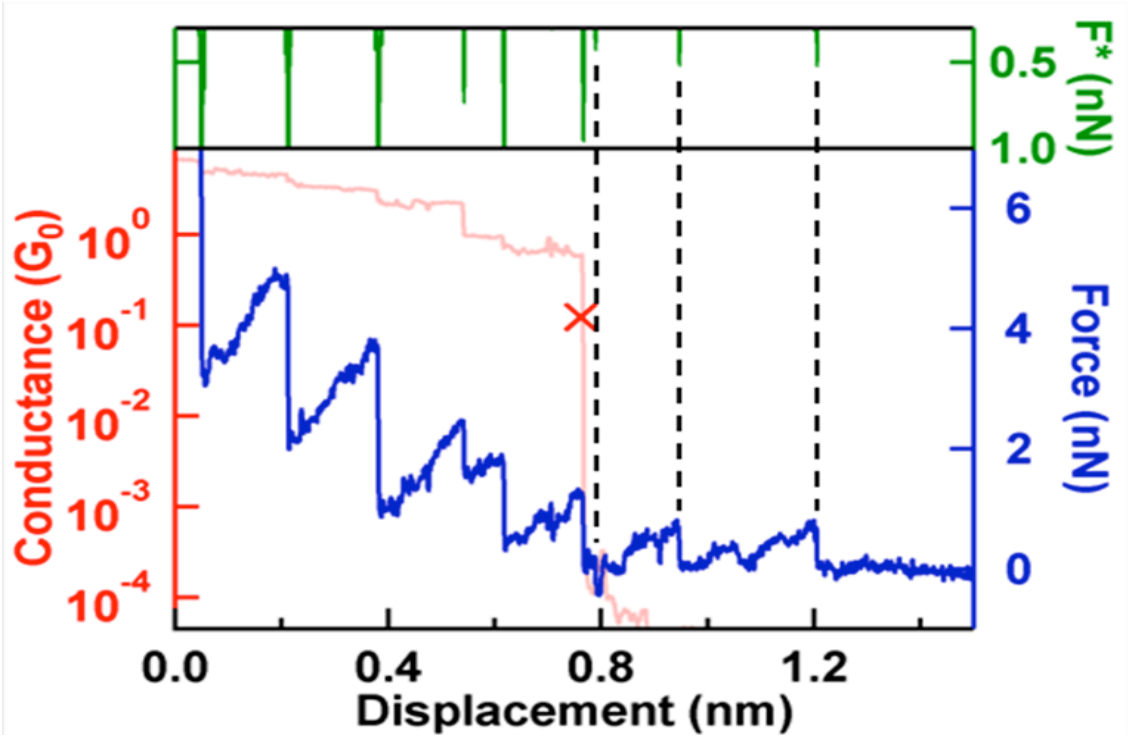


Figure C2. Analysis technique applied to a sample pullout experiment. The rupture from 1 G_0 is shown by the red ×. Dashed lines are provided as visual guides to the force events identified through F*, the auxiliary force trace (green) within a 1 nm displacement from the 1 G_0 rupture location.

Force, Conductance and Elongation Length Histograms:

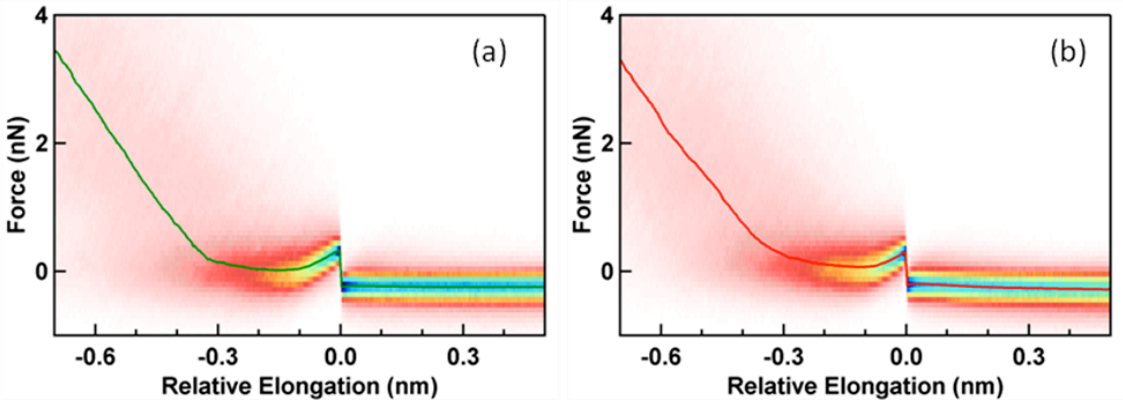


Figure C3. 2D force histograms for molecule **2** (a) and **3** (b), with the statistically averaged force profiles overlaid.

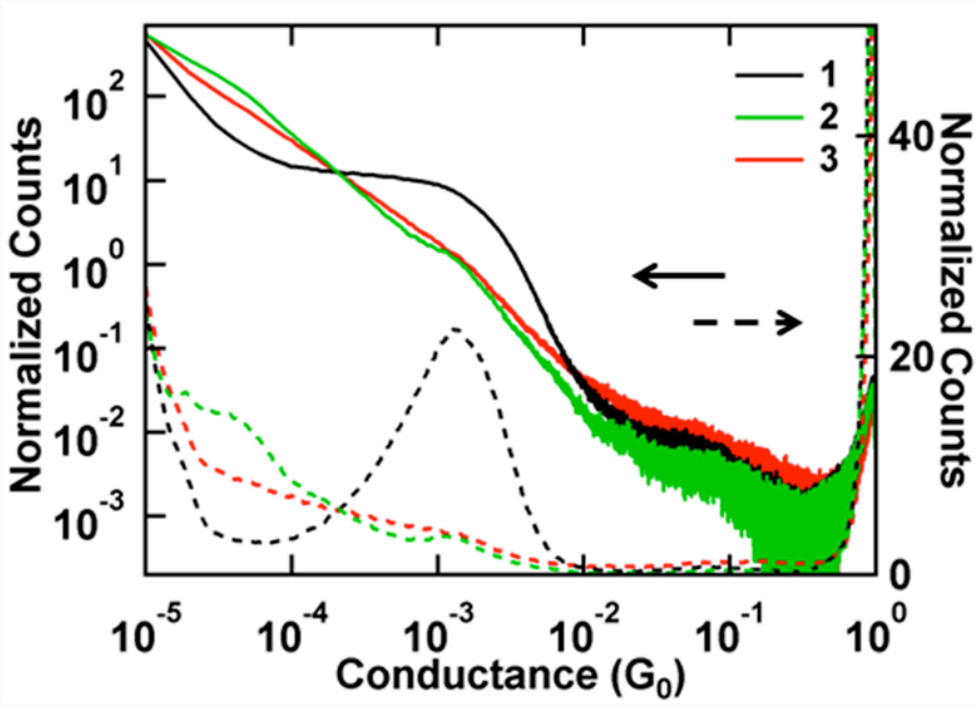


Figure C4. Histograms of conductance for all the measured traces for molecules **1-3**. Solid lines present a log-log plot of linearly binned conductance histograms with bin size = 10^{-5} G_0 and dashed lines present the logarithmically binned conductance histograms with 100 bins/decade. Conductance feature for **1** is prominent in both histograms, while **3** has no discernable feature in either representation.

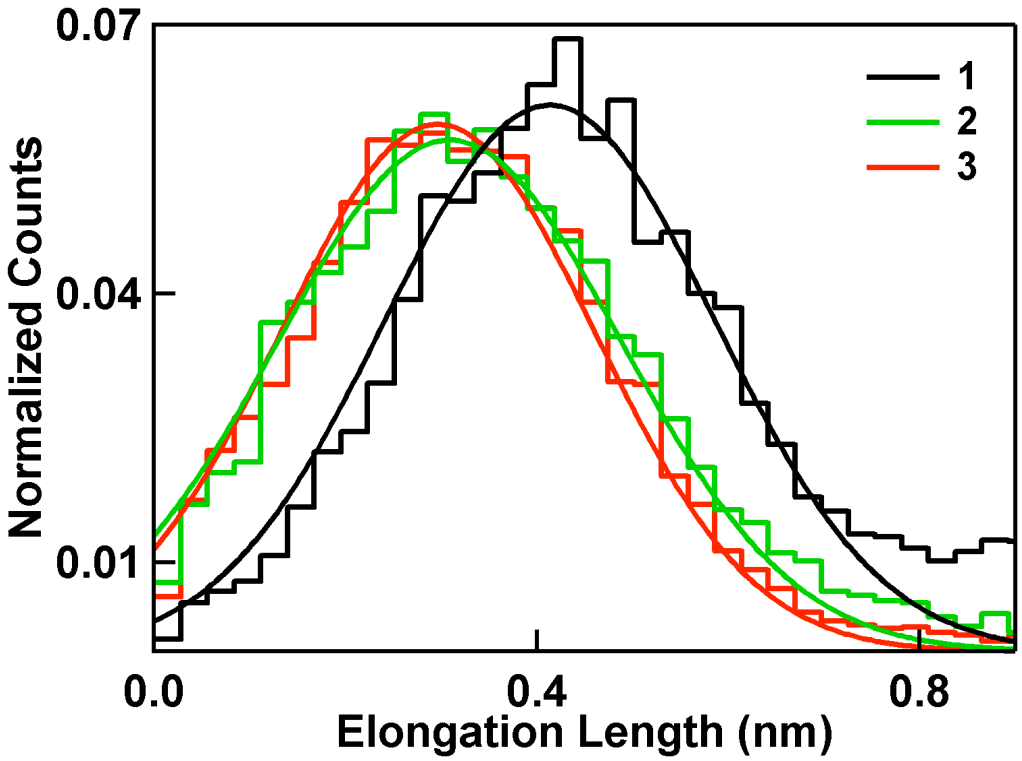


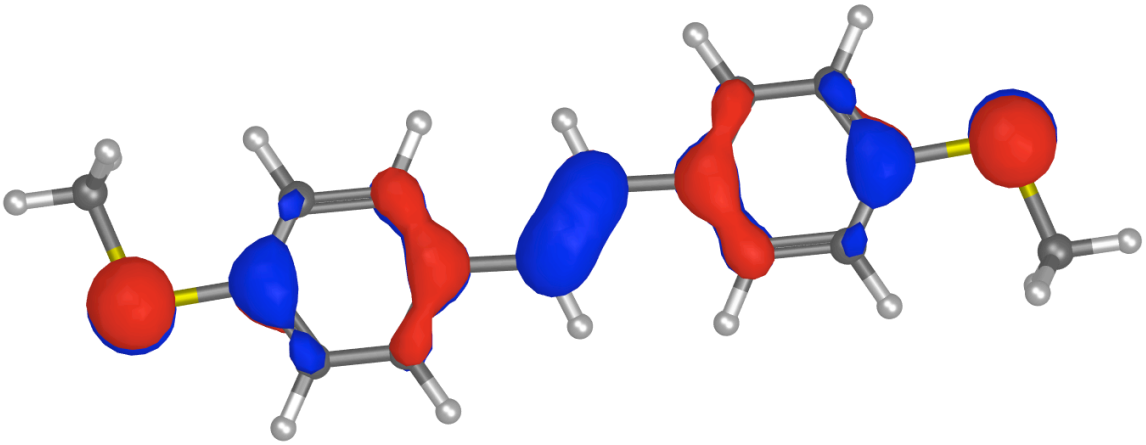
Figure C5. Elongation length distributions for molecules **1**-**3**, normalized by total number of traces (**1**-6788, **2**-6332 and **3**-5965) for each case (0.03 nm/bin). Gaussian fits to the histograms are overlaid.

C5. Theoretical Methods and Details

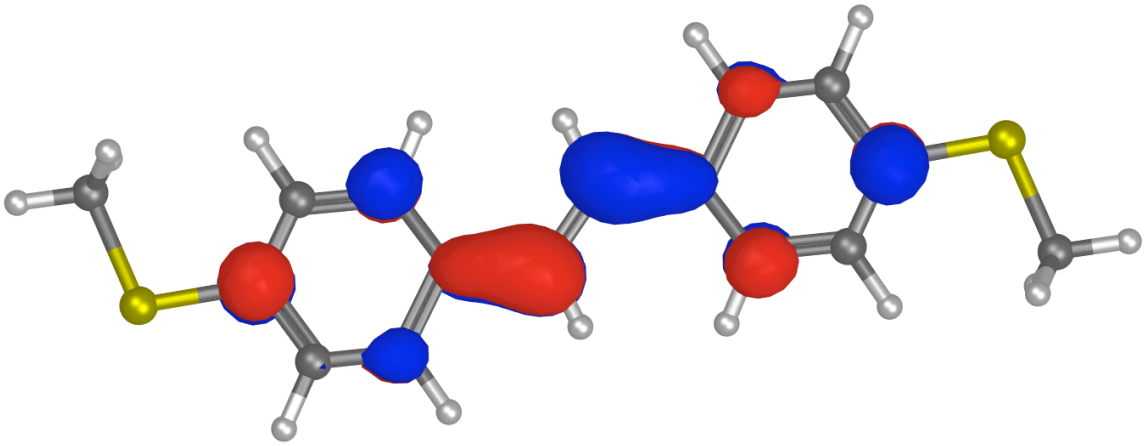
All electronic structure calculations used Jaguar (version 7.0, Schrodinger LLC, New York, NY, 2007) using the B3LYP hybrid functional and the 6-31G** basis sets. The geometries of **1**, **2**, and **3** were fully optimized. The final geometries and total energies are given below.

(E)-4,4'-di-(methylthio)stilbene (**1**):

HOMO:



LUMO:



Final Geometry:

		angstroms	
atom	x	y	z
C1	-3.8434657906	-1.8489488923	-0.0120387531

C2	-4.5597978043	-0.6660921203	-0.2805624712
C3	-5.9467255545	-0.6325681374	-0.2796433503
C4	-6.6855502592	-1.7937947552	-0.0064348986
C5	-5.9902287827	-2.9808488469	0.2650085261
C6	-4.5991963175	-3.0026449136	0.2621135588
H8	-4.0097134678	0.2469096457	-0.4949240973
H9	-6.4629515231	0.2996396986	-0.4916892543
H11	-6.5258516266	-3.8979328936	0.4823056343
H12	-4.0982714329	-3.9407699265	0.4812263322
C12	-1.5316801901	-2.8421871117	0.1511900371
C13	-2.3802636501	-1.8091183580	-0.0312521643
H15	-1.9652880229	-0.8205089096	-0.2198575523
H16	-1.9486865576	-3.8323927158	0.3259489543
C16	2.7734875957	-2.8774915889	0.1311408256
C17	2.0277379167	-4.0554884837	0.2888181918
C18	0.6411749301	-4.0140393968	0.2921141524
C19	-0.0682757996	-2.8065055585	0.1381972998
C20	0.6946137979	-1.6350753330	-0.0162369530
C21	2.0856456257	-1.6651369891	-0.0209750767
H23	2.5383213377	-5.0068558627	0.4096633569
H24	0.0856855673	-4.9404056715	0.4159550123
H25	0.1994174010	-0.6754224880	-0.1305297622
H26	2.6273682700	-0.7339753005	-0.1424063707
S26	-8.4609420801	-1.6384944700	-0.0311872223
C27	-9.0457398363	-3.3122035795	0.3862641249
H28	-10.1358266120	-3.2488756365	0.3880750438
H29	-8.7357642632	-4.0449031320	-0.3622958347
H30	-8.7077887729	-3.6191342554	1.3787457348
S30	4.5474530372	-3.0472519226	0.1422375258
C31	5.1465915681	-1.3400388869	-0.0658394496
H32	6.2362572697	-1.4100408636	-0.0593391970
H33	4.8255885854	-0.9149795515	-1.0193301512
H34	4.8286735152	-0.6998453415	0.7601083900

Total Energy (hartrees): -1415.73607449062
HOMO energy (hartrees): -0.18483
LUMO energy (hartrees): -0.04928

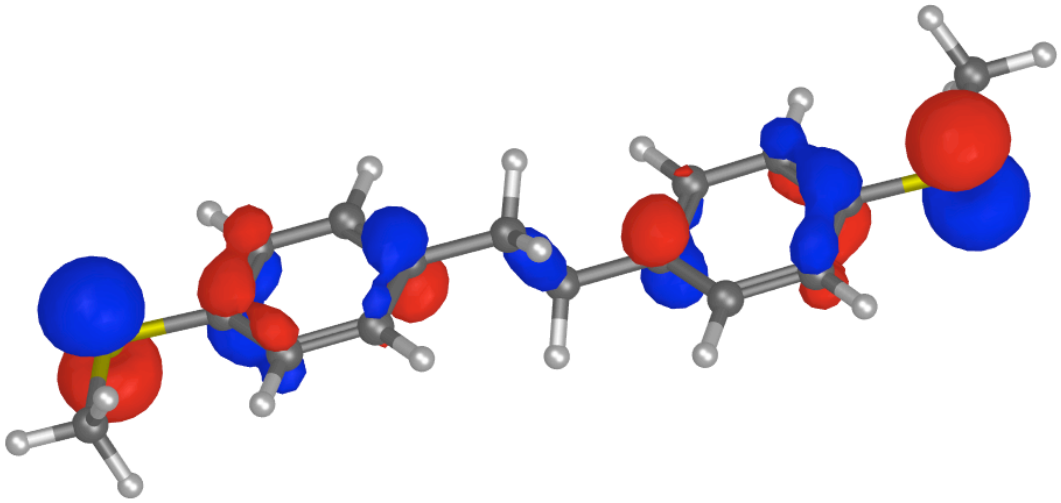
Orbital energies (hartrees):

-88.88533	-88.88533	-10.22391	-10.22390	-10.22024	-10.22022
-10.19744	-10.19727	-10.19490	-10.19484	-10.19299	-10.19283
-10.19270	-10.19270	-10.19168	-10.19162	-10.19059	-10.18982
-7.94627	-7.94626	-5.91154	-5.91154	-5.90741	-5.90741
-5.90116	-5.90115	-0.86678	-0.86337	-0.81690	-0.80337
-0.77646	-0.74930	-0.74811	-0.74693	-0.71289	-0.66634
-0.64406	-0.62146	-0.61013	-0.59317	-0.57536	-0.55401

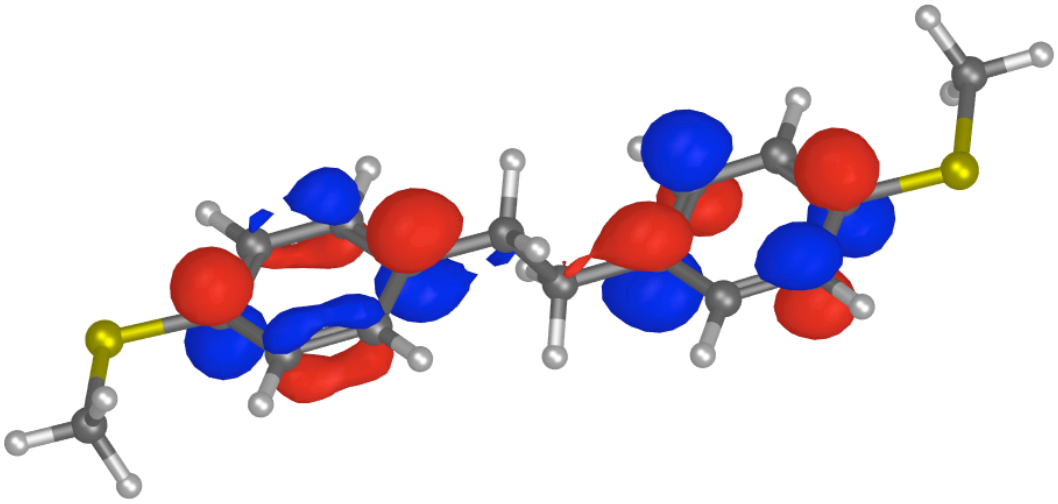
-0.50733	-0.50164	-0.46834	-0.46315	-0.45534	-0.44748
-0.44163	-0.43725	-0.43718	-0.43554	-0.42303	-0.41971
-0.40553	-0.40003	-0.38175	-0.37464	-0.36866	-0.36828
-0.35153	-0.34528	-0.33545	-0.32320	-0.32060	-0.31940
-0.29357	-0.25459	-0.25419	-0.25029	-0.21622	-0.18483
-0.04928	-0.00270	-0.00263	0.01549	0.03558	0.03569
0.07273	0.07408	0.07412	0.09542		

1,2-bis(4-(methylthio)phenyl)ethane (**2**):

HOMO:



LUMO:



Final geometry:

		angstroms	
atom	x	y	z
C1	-2.0391223094	1.2619882597	0.2193244174
C2	-2.8429749263	2.0991273975	1.0072999068
C3	-4.2260745163	2.1113982422	0.8766424497
C4	-4.8599744865	1.2766399086	-0.0573181820
C5	-4.0717195107	0.4348307044	-0.8483758009
C6	-2.6821766960	0.4352886669	-0.7053876456
H8	-2.3772837900	2.7505411937	1.7431049756
H9	-4.8212531005	2.7681295433	1.5054024702
H11	-4.5246266736	-0.2287710339	-1.5762136209
H12	-2.0902480058	-0.2315183662	-1.3284610878

C12	-0.5318415897	1.2887850243	0.3460289145
H14	-0.2462663513	1.3803959869	1.4008232137
H15	-0.1086833348	0.3412859558	-0.0070304016
C15	0.1223094402	2.4539771393	-0.4433388058
H17	-0.1460269167	2.3543676346	-1.5018567924
H18	-0.3143949014	3.3992059037	-0.1011071460
C18	4.4402506542	2.5006518576	0.0495365811
C19	3.6205429879	3.2573621143	0.8934719110
C20	2.2352549305	3.2479458921	0.7187248637
C21	1.6265435738	2.4957170014	-0.2900060273
C22	2.4609976782	1.7451693037	-1.1306174682
C23	3.8415616660	1.7432791542	-0.9693360679
H25	4.0461817048	3.8612139509	1.6869369067
H26	1.6185232166	3.8478362191	1.3844878603
H27	2.0217598623	1.1530356593	-1.9303269106
H28	4.4615207037	1.1532452065	-1.6389004654
S28	6.2213643407	2.4242741773	0.1599858314
C29	6.6084822162	3.4853959305	1.5886467743
H30	7.6949071026	3.4507610684	1.6935820496
H31	6.3037293338	4.5200117629	1.4154965819
H32	6.1526080023	3.1062241112	2.5062533120
S32	-6.6416943423	1.3745702949	-0.1354578962
C33	-7.0820854404	0.1519479999	-1.4113037884
H34	-8.1712724770	0.1825905912	-1.4836298930
H35	-6.6561344384	0.4133711927	-2.3827759112
H36	-6.7752854926	-0.8563889808	-1.1236142931

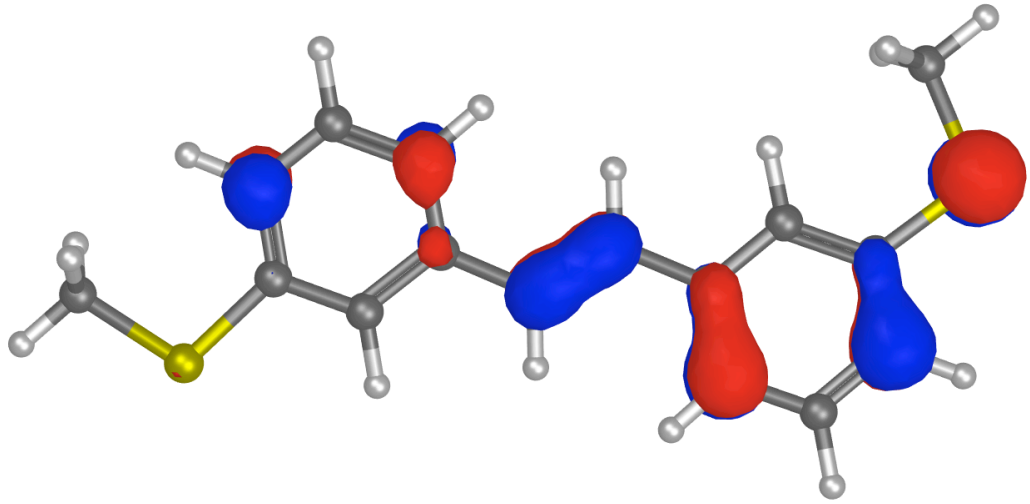
Total Energy (hartrees): -1416.95778765468
HOMO energy: -0.20125
LUMO energy: -0.00500

Orbital energies (hartrees):

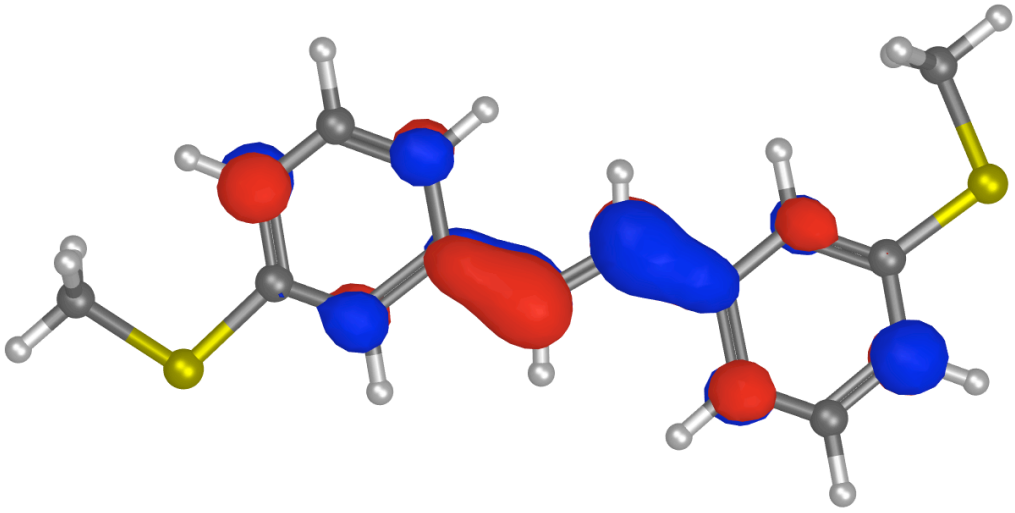
-88.88189	-88.88188	-10.22092	-10.22081	-10.21803	-10.21799
-10.19190	-10.19182	-10.19161	-10.19157	-10.19084	-10.19078
-10.18945	-10.18943	-10.18894	-10.18874	-10.18870	-10.18864
-7.94285	-7.94284	-5.90816	-5.90814	-5.90404	-5.90402
-5.89767	-5.89765	-0.86375	-0.86036	-0.81338	-0.79993
-0.77341	-0.74710	-0.74495	-0.74232	-0.70947	-0.66622
-0.64111	-0.61385	-0.60667	-0.60545	-0.57055	-0.56655
-0.50044	-0.49205	-0.47815	-0.46031	-0.45356	-0.45022
-0.44136	-0.43488	-0.43480	-0.43288	-0.42087	-0.41615
-0.41266	-0.39824	-0.39736	-0.38188	-0.36915	-0.35851
-0.35777	-0.35461	-0.34133	-0.33632	-0.32900	-0.31765
-0.31515	-0.28134	-0.27265	-0.25091	-0.25046	-0.20663
-0.20125	-0.00500	-0.00233	-0.00165	0.00757	0.03770

0.03789 0.07171 0.07587 0.10732 0.10821

(E)-3,3'-di-(methylthio)stilbene (**3**):
HOMO:



LUMO:



Final Geometry:

		angstroms	
atom	x	y	z
C1	5.1445385010	-3.9313429181	2.2477499737
H2	6.0325375266	-4.4076372247	2.6682275355
H3	4.2585198521	-4.4739417722	2.5854357091
H4	5.1051384506	-2.8944674834	2.5891610324
S5	5.3426962042	-4.0349223237	0.4398560535
C6	1.5933339214	-2.1002631841	-1.3634677608
C7	1.7311136406	-2.1387232848	0.0161653010
C8	2.8529826542	-2.7171924821	0.6176900994
C9	3.8563150607	-3.2670897512	-0.1858178537
C10	3.7153360307	-3.2265107604	-1.5797833468
C11	2.5914510743	-2.6519535977	-2.1916495372

H12	0.7143541038	-1.6372538703	-1.7983644784
H13	0.9564255323	-1.7093655157	0.6454880562
H14	2.9299791236	-2.7292326065	1.6983686761
H15	4.4936068666	-3.6556800048	-2.2062883232
C16	1.4828296366	-2.2340023005	-4.4124944882
C17	2.5151314098	-2.6576279424	-3.6571012808
H19	3.3961469356	-3.0616085484	-4.1515398712
H20	0.5952018574	-1.8513909917	-3.9127592499
C20	1.0784016235	-2.1959102633	-8.6739565317
C21	2.2842817319	-2.5936219787	-8.1021572564
C22	2.4504008160	-2.6160642719	-6.7208510805
C23	1.3937985010	-2.2357263830	-5.8767761677
C24	0.1790943734	-1.8302158310	-6.4638104111
C25	0.0112666086	-1.8082598090	-7.8500840287
H26	0.9643853184	-2.1840800203	-9.7540838175
H27	3.1068042182	-2.8890971336	-8.7473788256
H28	3.4028447885	-2.9233262834	-6.3028848964
H29	-0.6324595076	-1.5343680030	-5.8077887956
S30	-1.4908402163	-1.3104803060	-8.6786025325
C31	-2.6280561353	-0.9139195680	-7.3125201402
H32	-3.5632991529	-0.6133465599	-7.7893867509
H33	-2.8172227925	-1.7856303585	-6.6817892623
H34	-2.2570580741	-0.0829439805	-6.7081032292

Total Energy (hartrees): -1415.73474599105
HOMO energy (hartrees): -0.20060
LUMO energy (hartrees): -0.05312

Orbital Energies (hartrees):

-88.88445	-88.88366	-10.22502	-10.22401	-10.21998	-10.21943
-10.20369	-10.20330	-10.19514	-10.19484	-10.19435	-10.19402
-10.19327	-10.19325	-10.19307	-10.19222	-10.18855	-10.18759
-7.94541	-7.94459	-5.91071	-5.90990	-5.90660	-5.90577
-5.90023	-5.89940	-0.86825	-0.86405	-0.81523	-0.80135
-0.78538	-0.76030	-0.74202	-0.73738	-0.71284	-0.65842
-0.65499	-0.63239	-0.60247	-0.59561	-0.57759	-0.53237
-0.51613	-0.51053	-0.47476	-0.46933	-0.45154	-0.44594
-0.44546	-0.43722	-0.43689	-0.43637	-0.42249	-0.41736
-0.39871	-0.39539	-0.38344	-0.37850	-0.37529	-0.36254
-0.35407	-0.34962	-0.33838	-0.32093	-0.31961	-0.31781
-0.29000	-0.27703	-0.26241	-0.21845	-0.21000	-0.20060
-0.05312	-0.00297	0.00009	0.01334	0.03529	0.03672
0.07177	0.07260	0.07546	0.09345		

C6. References

1. Cody, J.; Fahrni, C. J. *Tetrahedron*, **2004**, *60*, 11099–11107.

2. Laufer, S. A.; Wergner, G. K. *J. Med. Chem.*, **2002**, *45*, 2733–2740.

3. Ngwendson, J. N.; Schultze, C. M.; Bollinger, J. C., Banerjee, A. *Can. J. Chem.,* **2008**, *86*, 7, 668–675.

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Appendix D

D1. General Information

(*E*)-4-nitrostilbene, diethyl benzylphosphonate and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide were purchased from TCI America and the latter was stored in a desiccator. 3-nitrobenzaldehyde, 4-nitrobenzaldehyde, 3-nitrobenzyl bromide, 4-nitrobenzyltriphenylphosphonium bromide, (*E*)-4,4'-diaminostilbene (**PP1A**), 4-nitrostilbene, 4-(methylthio)benzaldehyde, 4-(methylthio)benzyl bromide, 3-(methylthio)benzyl bromide, n-butyl lithium (1.6 M) in hexanes and all other reagents were purchased from Sigma-Aldrich. All reactions were carried out under nitrogen unless otherwise noted.

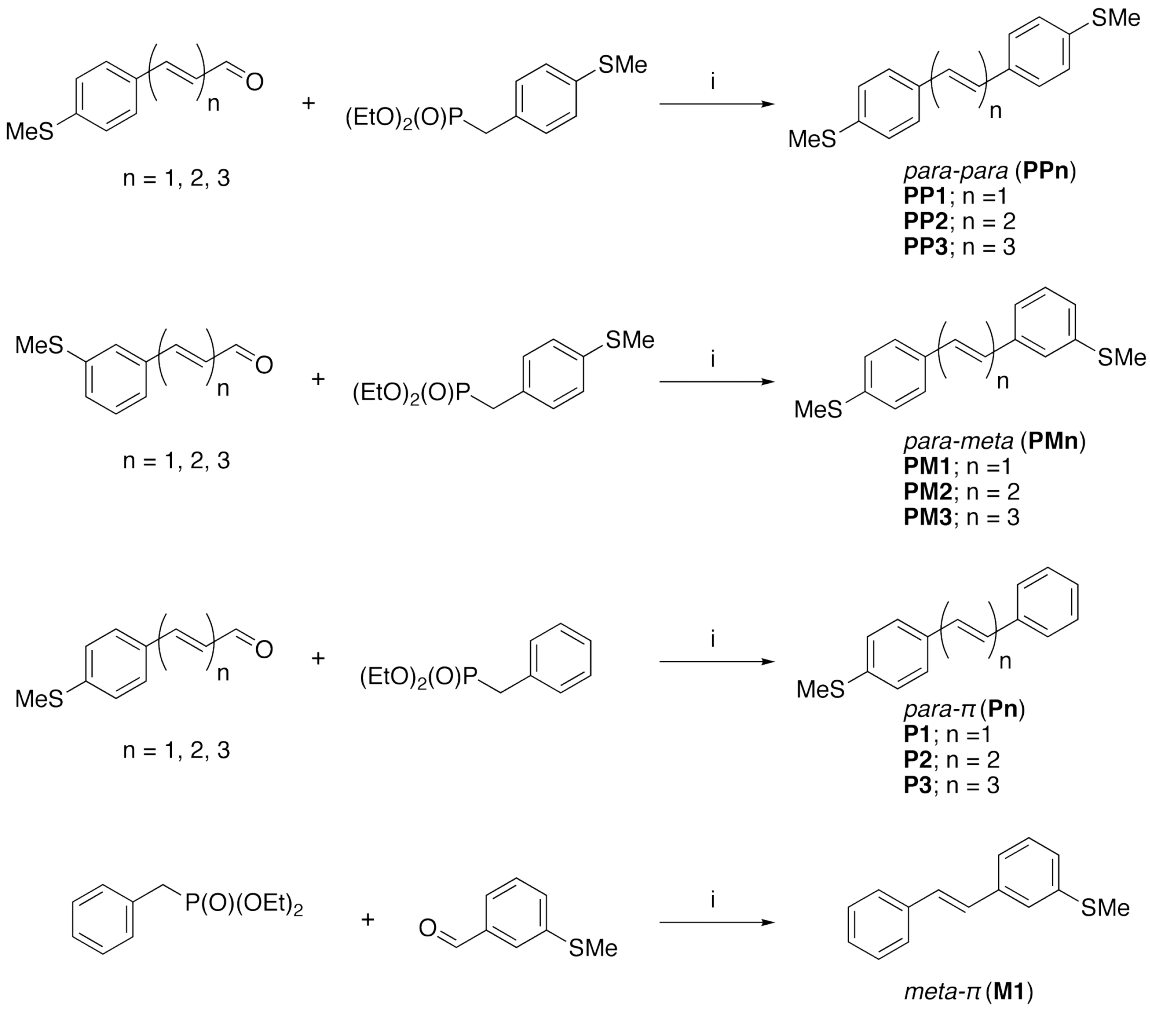
Compounds were prepared by the reported procedures: 3-(methylthio)benzaldehyde;[1] (*E*)-4-(methylthio)cinnamaldehyde and (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal;[2] (*E*)-4,4'-di-(methylthio)stilbene (**PP1**);[1] 3-(dimethylamino)benzaldehyde;[3] (*E*)-methyl(4-styrylphenyl)sulfane (**P1**);[4] dimethyl 4-(methylthio)benzylphosphonate;[5] and (*E*)-4-aminostilbene (**P1A**).[6]

Chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica columns. ^{1}H, ^{13}C and ^{31}P NMR spectra were taken on a Bruker DRX300 (300MHz), DRX400 (400MHz) and DMX500 (500MHz).

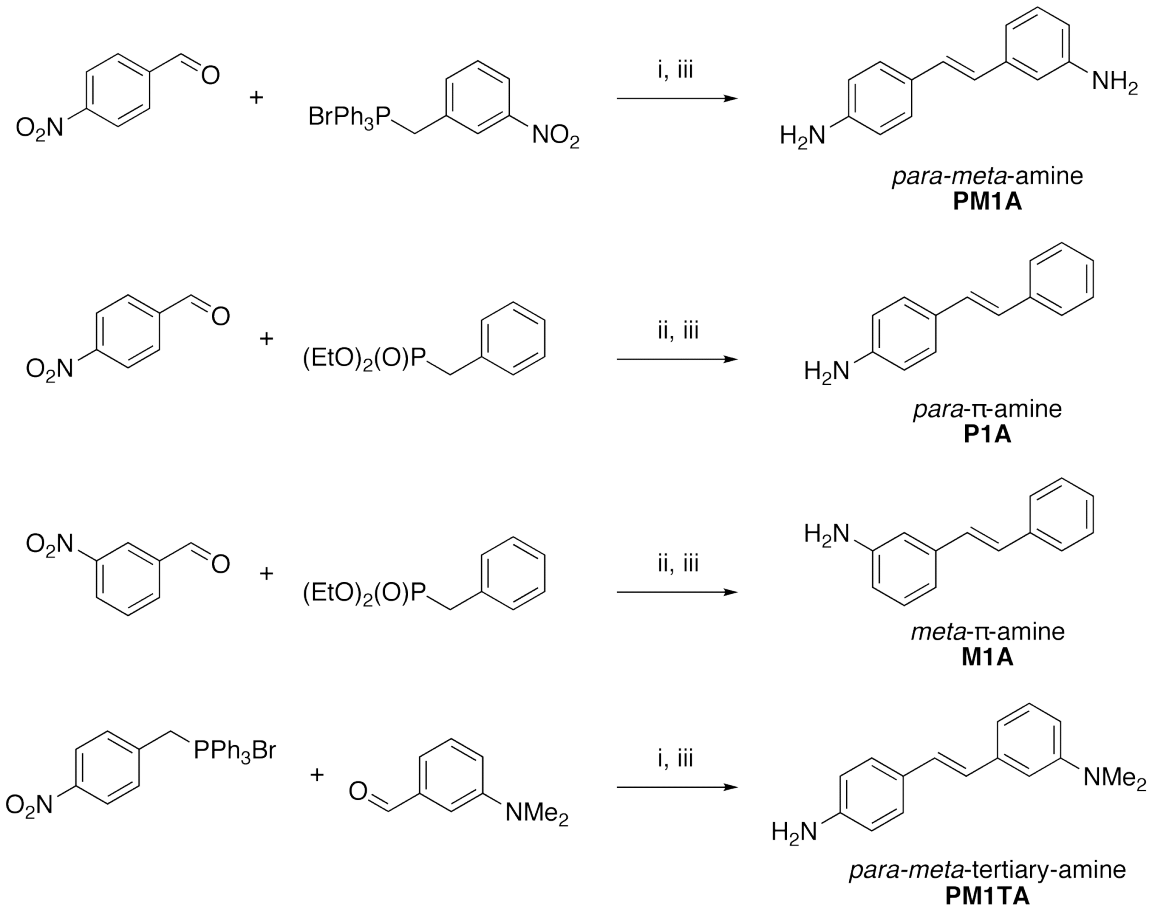
High resolution mass spectrometry (HR-MS) were obtained for all target molecules on a double focusing mass spectrometer (JMS-HX110A; JEOL, ltd.; Tokyo, Japan); Ionization method: FAB, High energy Xe* beam (3 kV); Matix: *meta*-nitrobenzyl

alcohol (m-NBA); MS Acceleration-Voltage: 10 kJ; Resolution: 3,000/10,000 (Low-Res/High-Res).

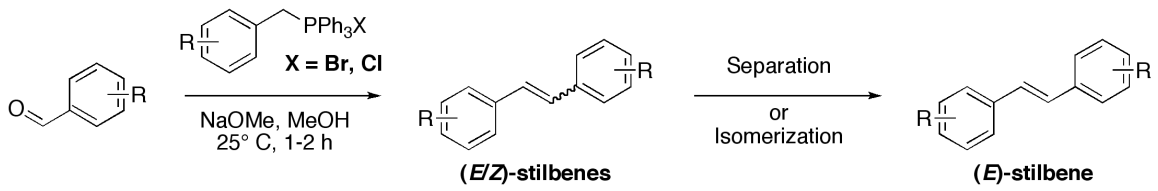
D2. Synthetic Experimentals



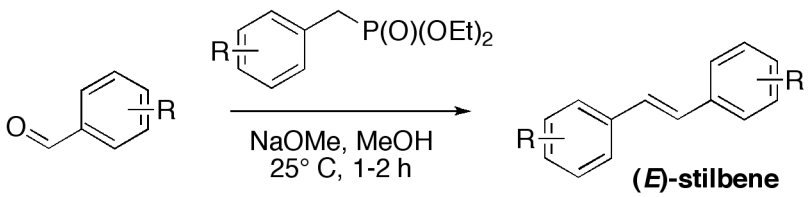
Scheme D1: Synthesis of *trans*-α,ω-diphenyl-μ,ν-oligoenes, where n = 1-3; (i) General H.W.E. reaction: General H.W.E. reaction: ^{t}BuOK (1.1 eq.), THF, 0° C, 1 h, let warm to room temperature overnight.



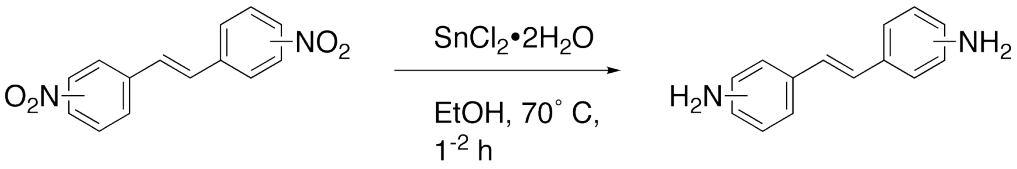
Scheme D2: Amine-functionalized stilbene derivative through Wittig Reaction or H.W.E. and $SnCl_2$ reduction. Compound **M1A** was prepared as a control molecule to verify conductance trends found in the methylsulfide molecular wires; (i) NaOMe (1.2 eq.), MeOH, 1 h, produces a mixture of (E/Z)-stereoisomers that may be separated by flash column chromatography or by isomerization using I_2, acetone, reflux, 12 h; (ii) General H.W.E. reaction: ^{t}BuOK (1.1 eq.), THF, 0˚ C, 1 h, let warm to room temperature overnight; (iii) $SnCl_2 \bullet 2H_2O$, EtOH (anhydrous), 70˚ C, 2 h (50-90%).



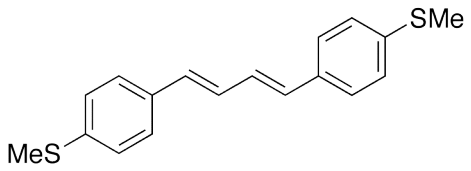
General Wittig Procedure: Adapted from the reported procedure.[7] In a 100-mL round-bottom flask, 3-nitrobenzaldehyde (0.100 g, 6.62 mmol) and 3-nitrobenzyltriphenyl-phosphonium bromide (3.20 g, 6.62 mmol) were dissolved in 50 mL of anhydrous methanol under nitrogen. Sodium methoxide (13.2 mmol) was added to the solution slowly over 15 min. A colorful (usually yellow) precipitate forms while the reaction was stirred for an additional 1-2 hours at room temperature. The resultant E/Z mixture of isomers was collected by filtration as a light yellow solid that was air-dried. The stereoisomers were separated (by chromatography or recrystallization) or where isomerized completely to the E isomer.



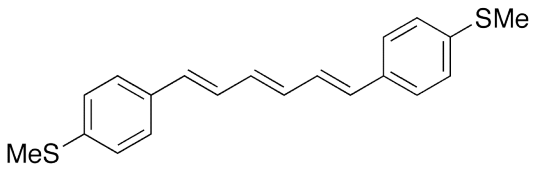
General Hoerner-Wadsworth-Emmons (H.W.E.) Procedure: Inside a flame-dried flask, aldehyde (0.150 g, 1.0 eq.) and phosphonate (1.1 eq.) were dissolved in 25 mL of dry THF. After being cooled to 0° C, a solution of tBuOK (1.1 eq.) in 5 mL of THF was slowly added to the stirred reaction solution. The reaction was left overnight and warmed to room temperature. The reaction was stopped by adding a large portion of water. Dichloromethane was added and the organic layer was extracted and then washed with brine and dried over magnesium sulfate. The product was isolated by column chromatography (usually 10% ethyl acetate in hexanes).



General Reduction of Aryl-NO_2 Group to Aryl-NH_2 Group: The dinitrostilbene (0.100 g, 0.370 mmol, 1.0 eq.), tin(II) chloride dihydrate (0.835 g, 3.70 mmol, 10.0 eq.), and 10 mL of anhydrous ethanol were added to a flame-dried, 25-mL RBF with stir bar and sealed with a septum. The suspension was purged with nitrogen for 10 minutes before heating to 80° C under an inert atmosphere. After 2-3 hours all solids dissolved and the reaction, which was monitored by TLC, was complete. The reaction solution was cooled to room temperature and water was added followed by extraction with ethyl acetate. The organic layers were combined, washed with aq. brine solution and dried with magnesium sulfate. Product was isolated by column chromatography on silica gel (usually in 50% ethyl acetate in hexanes).

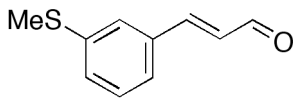


(1E,3E)-1,4-bis(4-(methylthio)phenyl)buta-1,3-diene (**PP2**): General H.W.E. Procedure. The product was prepared from (*E*)-3-(4-(methylthio)phenyl)acrylaldehyde[2] and dimethyl 4-(methylthio)benzylphosphonate and was isolated by column chromatography (10% ethyl acetate in hexanes) as a pale yellow solid in 67.7% yield. ^{1}H NMR (400MHz, $C_2D_2C1_4$): δ 7.38 (d, *J* = 8.4 Hz, 4H), 7.22 (d, *J* = 8.4 Hz, 4H), 6.97-6.87 (m, 2H), 6.68-6.52 (m, 2H), 2.51 (s, 6H); ^{13}C NMR (400MHz, $C_2D_2C1_4$): δ 137.18, 133.64, 131.43, 128.15, 126.28, 125.93, 15.17; HR-MS: m/z calcd for ($C_{18}H_{18}S_2$): 298.0850, found: 298.0841.

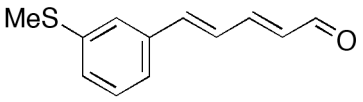


(1E,3E,5E)-1,6-bis(4-(methylthio)phenyl)hexa-1,3,5-triene (**PP3**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal[2] and *dimethyl 4-(methylthio)benzylphosphonate* and was isolated by column chromatography (10% ethyl acetate in hexanes) as a yellowish-green solid in 54.0% yield. This compound was previously prepared by Spangler and coworkers.[8] Our NMR characterization data agrees with their report. ^{1}H NMR (400MHz, 350K, $C_2D_2C1_4$): δ 7.36 (bs, 4H), 7.26 (bs, 4H), 7.35 (t, *J* = 7.5 Hz, 2H), 6.85 (bm, 2H), 6.72-6.33 (m, 4H), 2.53 (bs, 6H), note: spectral shifts appeared broad; ^{13}C NMR (400MHz, 350K, $C_2D_2C1_4$):

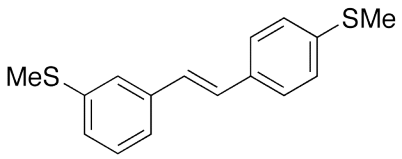
δ 137.30, 137.04, 132.83, 131.43, 128.24, 126.56, 126.25, 15.46; HR-MS: m/z calcd for ($C_{20}H_{20}S_2$): 324.1006, found: 324.1011.



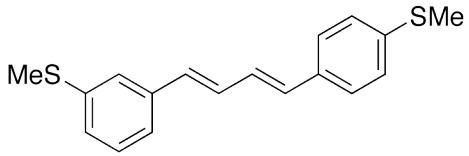
(E)-3-(methylthio)cinnamaldehyde: General Wittig homologation procedure. Product was prepared from 3-(methylthio)benzaldehyde and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide and isolated as a pale yellow solid (yield: 0.456 g, 38.9%). ^{1}H NMR (300MHz, $CDCl_3$): δ 9.70 (d, *J* = 7.8 Hz, 1H), 7.44-7.30 (m, 5H), 6.70 (dd, *J* = 7.8 Hz, *J* = 16.2 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (300MHz, $CDCl_3$): δ 194.0, 152.5, 140.4, 135.0, 129.8, 129.4, 129.3, 126.3, 125.4, 15.9; HR-MS: m/z calcd for ($C_{10}H_{10}OS$): 178.0452, found: 178.0460.



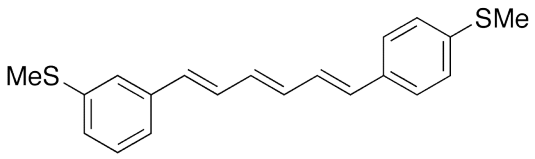
(2E,4E)-5-(3-(methylthio)phenyl)penta-2,4-dienal: General Wittig homologation procedure. Product was prepared from (*E*)-3-(methylthio)cinnamaldehyde and (1,3-dioxolan-2-yl)methyl-triphenylphosphonium bromide and isolated as a yellow solid (yield: 0.501 g, 96.2%). ^{1}H NMR (300MHz, $CDCl_3$): δ 9.59 (d, *J* = 8.1 Hz, 1H), 7.32 (s, 1H), 7.28-7.14 (m, 4H), 6.98-6.86 (m, 2H), 6.23 (dd, *J* = 7.8 Hz, J = 15.3 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (300MHz, $CDCl_3$): δ 194.0, 152.2, 142.2, 139.9, 136.6, 132.2, 129.7, 127.8, 127.1, 125.7, 124.6, 16.1; HR-MS: m/z calcd for ($C_{12}H_{12}OS$): 204.0609, found: 204.0636.



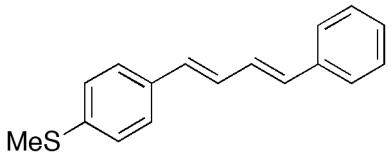
(E)-3,4'-di-(methylthio)stilbene (**PM1**): General Wittig Procedure. The product was prepared from 3-(methylthio)benzaldehyde and dimethyl 4-(methylthio)benzyl-phosphonate. Pure product as collected by filtration from the reaction suspension as a white solid (43.0%). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.36 (bs, 1H), 7.30-7.20 (m, 5H), 7.20-7.09 (m, 1H), 7.04 (d, *J* = 16.4 Hz, 1H), 7.03 (d, *J* = 16.4 Hz, 1H), 2.52 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (400MHz, $CDCl_3$): δ 138.9, 138.1, 138.0, 134.1, 129.1, 128.7, 127.5, 127.0, 126.7, 125.7, 124.6, 123.3, 15.9, 15.7; HR-MS: m/z calcd for ($C_{16}H_{16}S_2$): 272.0693, found: 272.0686.



(1E,3E)-1-(3-(methylthio)phenyl)-4-(4-methylthio)phenyl)-buta-1,3-diene (**PM2**): General H.W.E. Procedure. The product was prepared from (*E*)-3-(methylthio)cinnamaldehyde and dimethyl 4-(methylthio)benzylphosphonate and isolated by column chromatography (10% ethyl acetate in hexanes) as an off-white solid in 86.5% yield. ^{1}H NMR (500MHz, $CDC1_3$): δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 1.6 Hz, 1H), 7.29-7.15 (m, 4H), 7.13 (dt, *J* = 1.6 Hz, 7.5 Hz, 1H), 7.00-6.84 (m, 2H), 6.68-6.53 (m, 2H), 2.51 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (500MHz, $CDCl_3$): δ 138.97, 138.16, 138.12, 134.34, 132.78, 32.09, 130.02, 129.19, 128.60, 126.94, 126.78, 125.78, 124.58, 123.34, 16.02, 15.91; HR-MS: m/z calcd for ($C_{18}H_{18}S_2$): 298.0850, found: 298.0848.

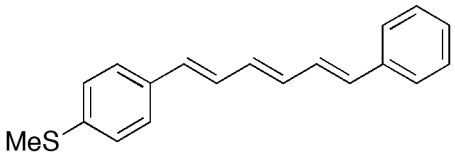


(1E,3E,5E)-1-(3-(methylthio)phenyl)-6-(4-methylthio)phenyl)-hexa-1,3,5-triene (**PM3**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(3-(methylthio)phenyl)penta-2,4-dienal and dimethyl 4-(methylthio)benzylphosphonate and isolated by column chromatography (10% ethyl acetate in hexanes) as a yellow solid in 40.5% yield. ^{1}H NMR (300MHz, CDC1$_3$): δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.30 (t, J = 1.5 Hz, 1H), 7.24-7.18 (m, 4H), 7.12 (dt, *J* = 1.5 Hz, 7.5 Hz, 1H), 6.91-6.81 (m, 2H), 6.75-6.40 (m, 4H), 2.51 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (500MHz, $CDCl_3$): δ 138.96, 138.20, 138.07, 134.47, 134.17, 133.30, 132.49, 132.08, 129.93, 129.18, 128.63, 126.92, 126.82, 125.84, 124.66, 123.37, 16.05, 15.94; HR-MS: m/z calcd for ($C_{20}H_{20}S_2$): 324.1006, found: 324.0997.

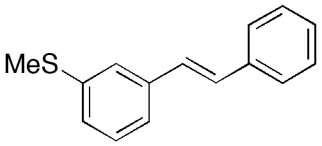


(1E,3E)-1-(4-(methylthio)phenyl)-4-phenyl-buta-1,3-diene (**3b**): General H.W.E. Procedure. The product was previously prepared from cyclopropyl carbinols through indium triflate catalyzed rearrangements by Ranu and Banerjee.[9] Our ^{1}H and ^{13}C NMR data agrees with their findings. We prepared the product from (*E*)-4-(methylthio)cinnamaldehyde[2] and diethyl benzylphosphonate and isolated it as a white solid in 45.0% yield. ^{1}H NMR (300MHz, CDC1$_3$): δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.44-7.35

(m, 4H), 7.30-7.24 (m, 3H), 7.07-6.94 (m, 2H), 6.74-6.66 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (300MHz, CD_2Cl_2): δ 138.5, 137.8, 134.6, 132.9, 132.5, 130.8, 129.6, 129.0, 127.9, 127.1, 126.9, 126.7, 15.8; HR-MS: m/z calcd for ($C_{17}H_{16}S$): 252.0973, found: 252.0979.

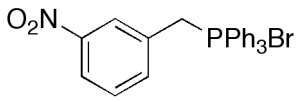


(1E,3E,5E)-1-(4-(methylthio)phenyl)-6-phenyl-hexaa-1,3,5-triene (**3c**): General H.W.E. Procedure. The product was prepared from (2*E*,4*E*)-5-(4-(methylthio)phenyl)penta-2,4-dienal[2] and diethyl benzylphosphonate and isolated as a yellow solid in 31.3% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.48 (d, *J* = 7.5 Hz, 2H), 7.41-7.33 (m, 4H), 7.28-7.23 (m, 3H), 7.00-6.88 (m, 2H), 6.7-6.56 (m, 4H), 2.53 (s, 3H); ^{13}C NMR (500MHz, $C_2D_2Cl_4$): δ 137.36, 136.85, 133.81, 133.24, 133.02, 132.18, 131.66, 128.78, 128.35, 128.18, 127.27 , 126.42, 126.10, 126.01, 15.32; HR-MS: m/z calcd for ($C_{19}H_{18}S$): 278.1129, found: 278.1134.

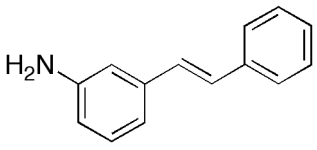


(E)-3-(methtylthio)stilbene (**4**): The compound is known in the literature and was initially synthesized by cationic cycloaromatization of the respective styryl *ß,ß*-bis(methylthio)vinyl ketones.[10] General H.W.E. Procedure. The product was prepared from 3-(methylthio)benzaldehyde and diethyl benzylphosphonate and isolated by column

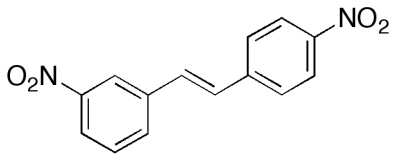
chromatography (5% ethyl acetate in hexanes) as a white solid in 98% yield. ^{1}H NMR (400MHz, $CDC1_3$): δ 7.52 (d, *J* = 7.6 Hz, 2H), 7.40 (bs, 1H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.30-7.24 (m, 3H), 7.15 (m, 1H), 7.09 (d, *J* = 16.0 Hz, 1H), 7.07 (d, *J* = 16.4 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (400MHz, $CDC1_3$): δ 138.9, 138.0, 137.1, 129.3, 129.1, 128.7, 128.1, 127.8, 126.6, 125.7, 124.6, 123.4, 15.9; HR-MS: m/z calcd for ($C_{15}H_{14}S$): 226.0816, found: 226.0808.



3-nitrobenzyltriphenylphosphonium bromide: This compound is known in the literature,[11] however detailed characterization was not given. General Synthesis of triphenylphosphonium Halide Salts (above). Product was prepared from 3-nitrobenzyl bromide and triphenylphosphine and isolated as a white powder in quantitative yields. ^{1}H NMR (300MHz, DMSO-d_6): δ 8.16 (d, *J* = 7.2 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 3H), 7.79-7.65 (m, 14H), 7.55 (t, *J* = 8.1 Hz, 1H), 7.47 (bd, *J* = 7.8 Hz, 2H), 5.36 (d, *J* = 15.9 Hz, 2H); ^{13}C NMR (300MHz, DMSO-d_6): δ 138.2, 136.2, 135.0, 134.9, 131.2, 131.0, 126.4, 126.4, 124.1, 118.7, 117.5, 28.8, 28.2; HR-MS: m/z calcd for triphenylphosphonium cation ($C_{25}H_{21}NO_2P$): 398.1310, found: 398.1301.

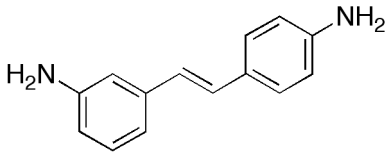


(E)-3-aminostilbene (**7**): This compound is known[12] and was synthesized as a control molecule to verify the trends in conductance found within the methylsulfide molecular wires. It was prepared by the General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. (*E*)-3-dinitrostilbene[13] (0.100 g, 0.370 mmol), tin(II) chloride dihydrate (0.835 g), and 12 mL of anhydrous ethanol were added to a flame dried, 25-mL round-bottomed flask with stir bar and sealed with a septum. The suspension was purged with nitrogen for 10 minutes before heating to 70° C under an inert atmosphere. After 16 h the reaction was cooled to room temperature and the ethanol was removed under reduced pressure. Water was added followed by sat. aqueous $NaHCO_3$. The aqueous layer was extracted three times with dichloromethane. The solvent was remove and leaving a off-white solid (0.059 g, 68%). ^{1}H NMR (400MHz, $CDC1_3$): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 8.4 Hz, 2H), 7.29 (td, *J* = 1.6 Hz, 7.2 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 16.4 Hz, 1H), 7,07 (d, *J* = 16.4 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.87 (s, 1H), 6.64 (dd, *J* = 2.0 Hz, 8.0 Hz, 1H), 3.70 (bs, 2H); ^{13}C NMR (400MHz, $CDC1_3$): δ 146.7, 138.4, 137.4, 129.6, 128.9, 128.7, 128.5, 127.6, 126.5, 117.3, 114.7, 112.9; HR-MS: m/z calcd for ($C_{14}H_{13}N$): 195.1048, found: 195.0461.

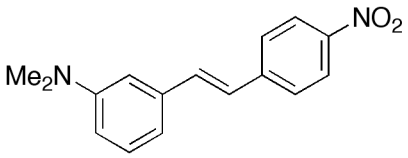


(E)-3,4'-dinitrostilbene: This compound is known in the literature,[14] however HR-MS, ^{1}H and ^{13}C NMR data was not provided. General Wittig Procedure. The product was prepared from 4-nitrobenzyltriphosphonium bromide and 3-nitrobenzaldehyde. A mixture

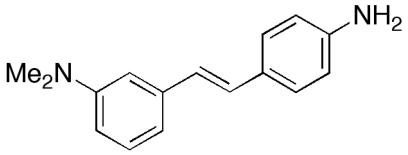
of E/Z isomers was collected by vacuum filtration from the reaction suspension as a pale yellow precipitate. The E/Z mixture was placed in a 50-mL round-bottom flask with 20 mL of acetone and a crystal of iodine. The mixture was heated at reflux under a nitrogen atmosphere for 12 hours. The solution was cooled, and the product was collected by filtration to give yellow needles in overall 29% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 8.43 (t, *J* = 1.9 Hz, 1H), 8.27 (d, *J* = 8.9 Hz, 2H), 8.18 (d, *J* = 6.9 Hz, 1H), 7.88-7.81 (m, 1H), 7.69 (d, *J* = 8.9 Hz, 2H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.29 (s, 2H); ^{13}C NMR (300MHz, $CDC1_3$): δ 148.5, 147.4, 142.6, 138.0, 132.7, 130.5, 129.9, 129.3, 127.3, 124.3, 123.1, 121.3; HR-MS: m/z calcd for ($C_{14}H_{10}N_2O_4$): 270.0641, found: 270.0636.



(E)-3,4'-diaminostilbene (**5**): This compound is known in the literature.[15] General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. The product was prepared from (*E)*-3,4'-dinitrostilbene and stannous chloride dihydrate and isolated by column chromatography (50% ethyl acetate in hexanes) as an off-white solid in 23.6% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 16.2 Hz, 1H), 6.89 (d, *J* = 7.8 Hz, 1H), 6.84 (d, *J* = 15.9 Hz, 1H), 6.79 (s, 1H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 7.5 Hz, 1H), 3.71 (bs, 4H); ^{13}C NMR (CDC13): δ 147.0, 146.5, 139.4, 129.8, 128.9, 128.5, 128.1, 125.7, 117.3, 115.6, 114.4, 112.9; HR-MS: m/z calcd for ($C_{14}H_{14}N_2$): 210.1157, found: 210.1152.



(E)-3-dimethylamino-4'-nitrostilbene: The product was prepared from 3-dimethylaminobenzaldehyde and 4-nitrobenzyltriphenylphosphonium bromide using the General Wittig Procedure. Pure product was isolated by column chromatography (10% ethyl acetate in hexanes) as an orange solid in 20.0% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 8.22 (d, *J* = 8.7 Hz, 2H), 7.63 (d, *J* = 8.7 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 16.2 Hz, 1H), 7.13 (d, *J* = 16.2 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.85 (bs, 1H), 6.74 (dd, *J* = 2.4 Hz, 8.1 Hz, 1H), 3.00 (s, 6H); ^{13}C NMR (300MHz, $CDCl_3$): δ 151.4, 147.1, 144.6, 137.3, 134.8, 129.9, 127.2, 126.2, 124.5, 115.7, 113.7, 111.5, 40.9; HR-MS: m/z calcd for ($C_{16}H_{16}N_2O_2$): 268.1212, found: 268.1225.



(E)-3-dimethylamino-4'-aminostilbene (**8**): General Reduction of Aryl-NO_2 to Aryl-NH_2 Group. The product was prepared from (*E*)-3-dimethylamino-4'-nitrostilbene and tin(II) chloride dihydrate isolated by column chromatography (25% ethyl acetate in hexanes) as a off-white solid in 5.3% yield. ^{1}H NMR (300MHz, $CDC1_3$): δ 7.35 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.03 (d, *J* = 16.2 Hz, 1H), 6.92 (d, *J* = 16.2 Hz, 1H), 6.89 (d, *J* = 7.2 Hz, 1H), 6.82 (bs, 1H), 6.67 (d, *J* = 8.4 Hz, 2H), 6.62 (dd, *J* = 2.4 Hz, 8.4 Hz, 1H), 3.62 (bs, 2H), 2.97 (s, 6H); ^{13}C NMR (300MHz, $CDCl_3$): δ 151.3, 146.4, 139.1, 129.6,

128.7, 128.6, 128.1, 126.5, 115.6, 115.2, 112.1, 111.0, 41.1; HR-MS: m/z calcd for ($C_{16}H_{18}N_2$): 238.1470, found: 238.1480.

D3. Optical Absorption Spectroscopy

The HOMO-LUMO gap of all our molecular wires was estimated using solution-phase UV-vis absorption spectroscopy. Absorption spectra were taken on an Agilent Technologies 8453 UV-Vis spectrophotometer using a quartz cuvette with path length equal to 1.0 cm. Solutions of molecular wires were prepared in CH_2Cl_2 at concentrations of ~1 mM. All spectra were normalized to 1.0 Abs for clarity.

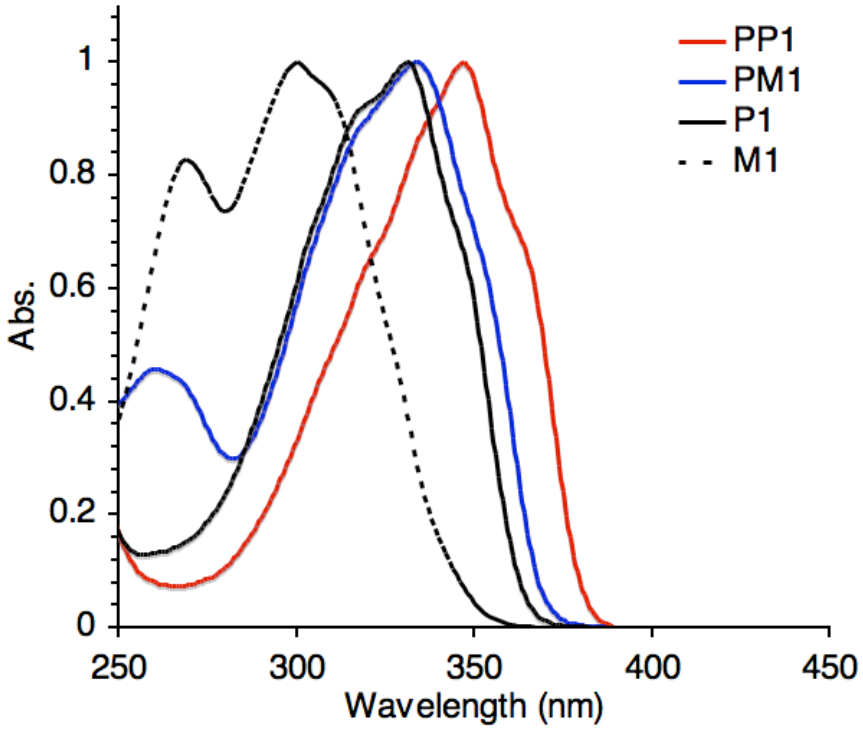


Figure D1: Optical absorption spectra of the methylsulfide-functionalized stilbenes.

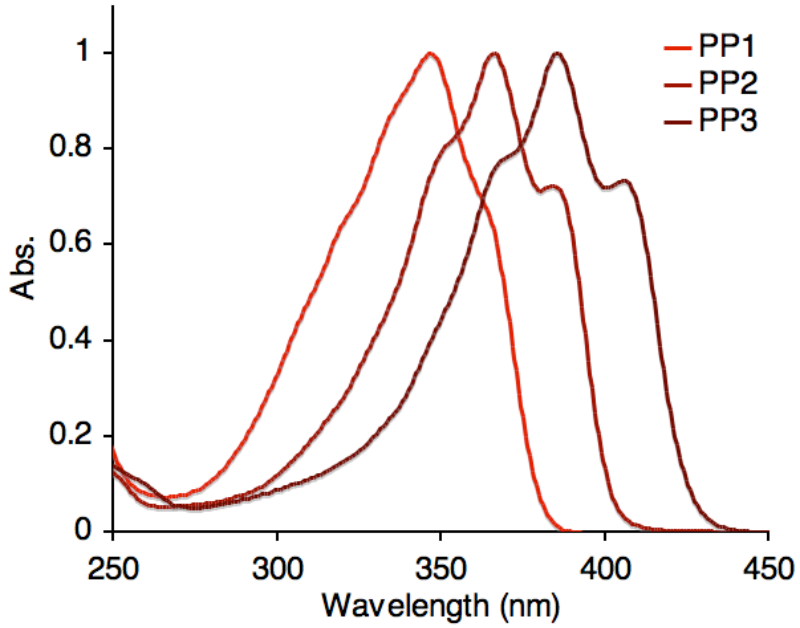


Figure D2: Optical absorption spectra of the *para-para* series (**PPn**).

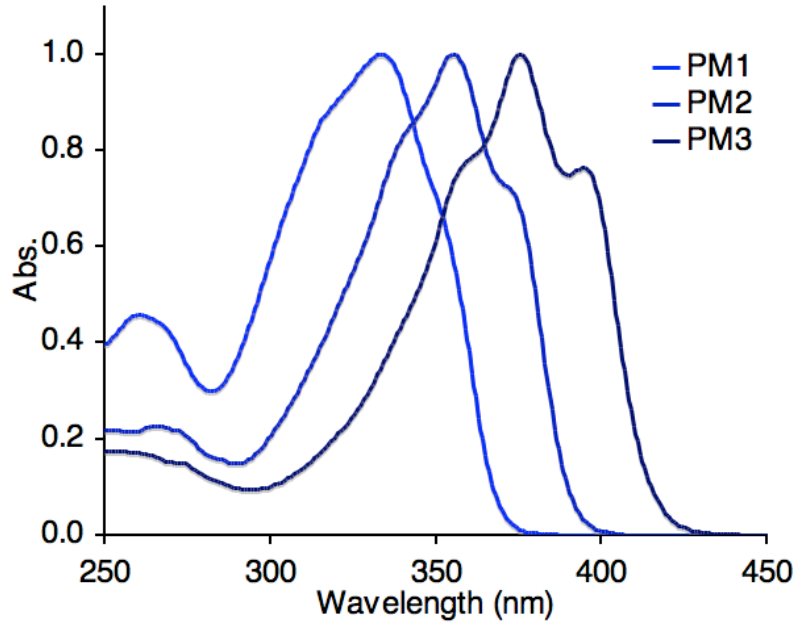


Figure D3: Optical absorption spectra of the *para-meta* series (**PMn**).

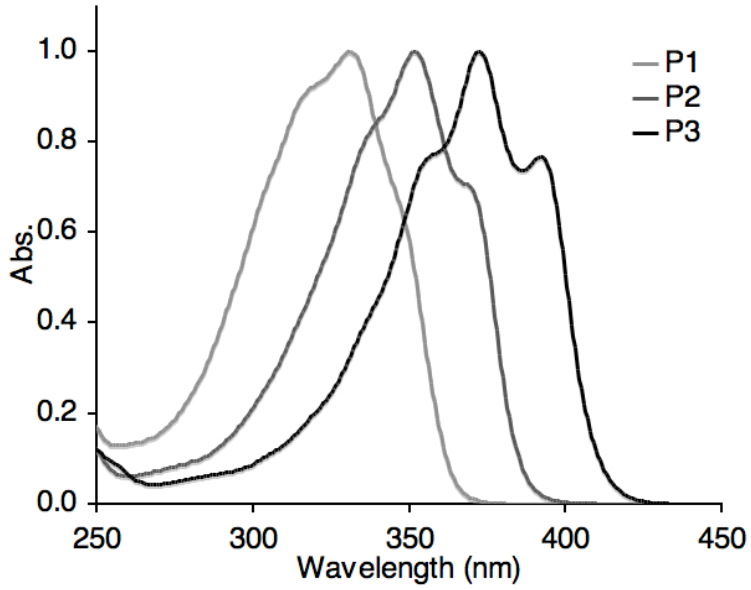


Figure D4: Optical absorption spectra of the *para*-π series (**Pn**).

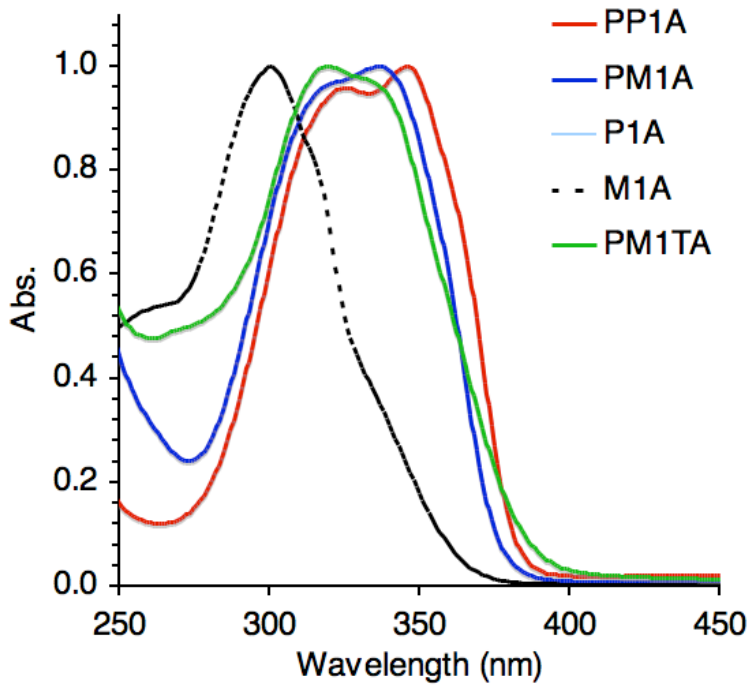


Figure D5: Optical absorption spectra of the amine-functionalized stilbene derivatives.

Molecule	E_{OP} (nm)	E_{OP} (eV)
PP1	389	3.19
PP2	416	2.98
PP3	435	2.85
PM1	380	3.26
PM2	403	3.08
PM3	430	2.88
P1	373	3.32
P2	395	3.14
P3	428	2.90
M1	358	3.46
PM1A	395	3.14
P1A	389	3.19
PM1TA	411	3.02

Table D1: Solution optical band gaps (E_{OP}) for target molecules range from 2.88-3.46 eV.

D4. Single-molecule Conductance and Force Measurement and Analysis

STM Break Junction Conductance Measurement. Gold substrates were prepared by evaporating 100 nm of gold on freshly cleaved mica. A freshly cut gold wire was used as the STM tip. The junctions were repeatedly formed and broken in dilute solution of stilbene derivatives (1 ± 0.1 mM in 1,2,4-trichlorobenzene). The junction conductance (current/voltage) was measured at a constant bias of 500 mV. Over 5000 traces were used to construct 2D conductance-displacement (Figures D6 and D7) and 1D (Figure D8) conductance histograms.

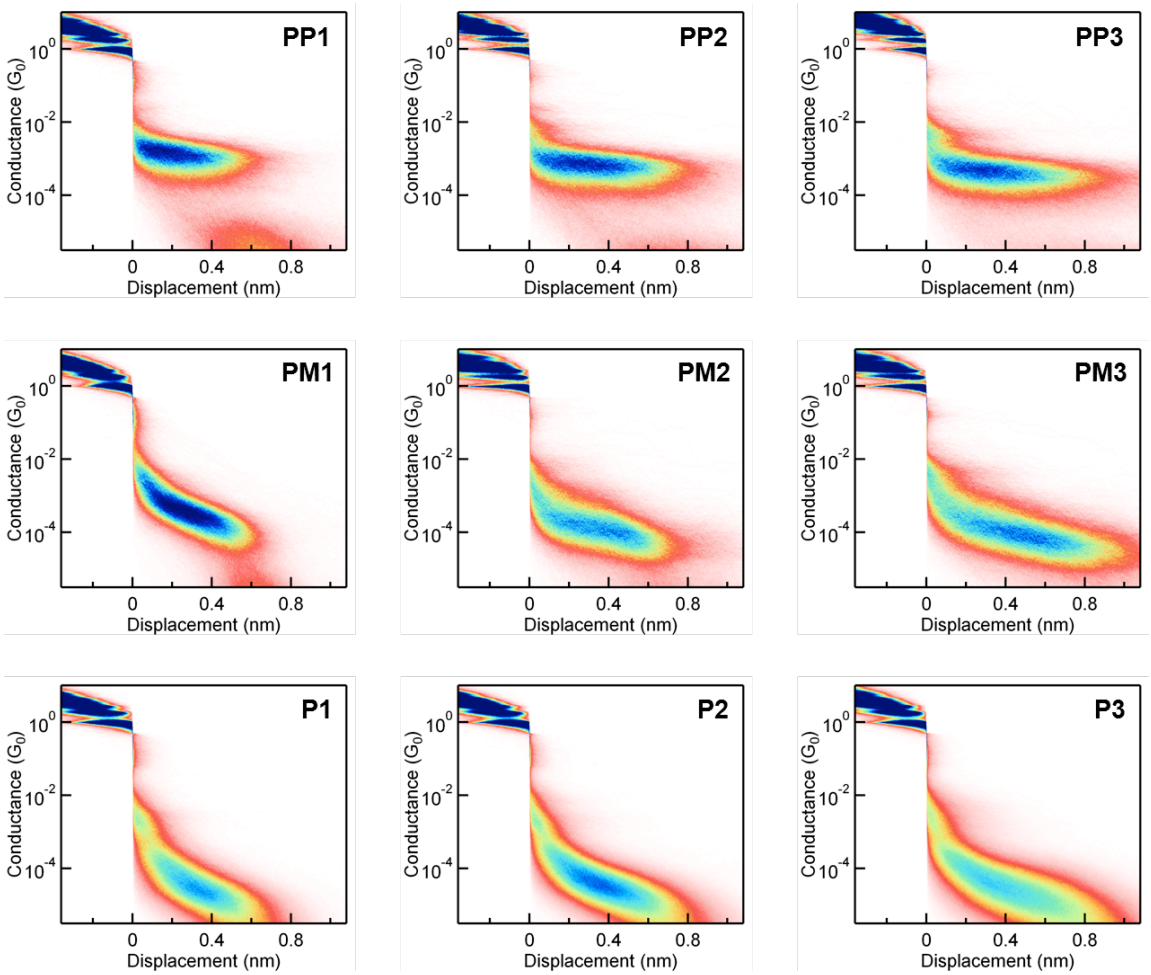


Figure D6: 2D conductance-displacement histograms for **PPn**, **PMn** and **Pn** molecular junctions.

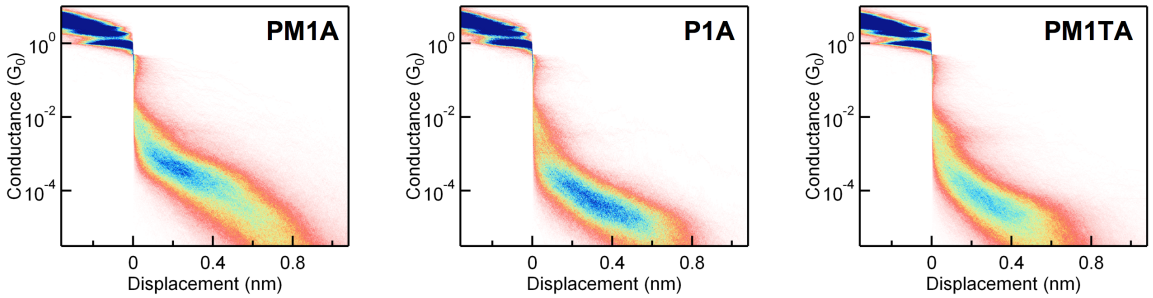


Figure D7: 2D conductance-displacement histograms for molecular junctions of amine-terminated molecular wires.

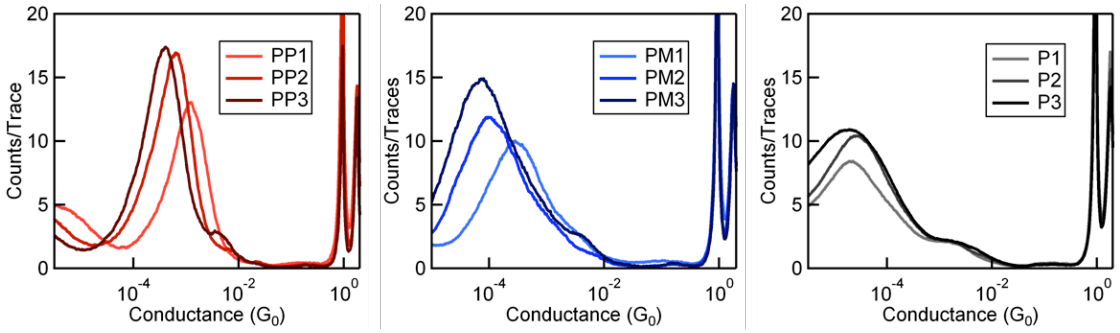


Figure D8: 1D conductance histograms of molecular junctions of **PPn**, **PMn** and **Pn** series of molecular wires.

Junction Variation Analysis. The variability of the mono-substituted series, **Pn**, is quantified in two steps. First, we construct separate (logarithmically binned) 1D histograms, 1000 traces at a time, for each molecule. The peak position of each of these histograms is well defined, and is extracted using a Gaussian fit in the neighborhood of

the molecular conductance feature. Then, peak values from these individual histograms are compiled from at least three separate experiments with different tip-sample combinations, totaling more than 30,000 individual measurements. The arithmetic mean as well as the 10^{th}, 25^{th}, 75^{th} and 90^{th} percentiles are computed from these peak positions, and are used to construct Figure 2 in the manuscript. Table D2 provides a summary of these statistics, along with the variation– defined as (75^{th} – 25^{th} percentile)/(mean value) for **Pn** series. The largest variation among the difunctionalized compounds was observed in **PM3**, and is given in the table for comparison.

Table D2: Comparison of Conductance Variation in STM-BJ's.

Molecule	Mean	25th %ile	75th %ile	% variation
P1	1.95×10^{-5}	1.71×10^{-5}	2.56×10^{-5}	44
P2	2.74×10^{-5}	1.56×10^{-5}	3.39×10^{-5}	67
P3	1.31×10^{-5}	8.25×10^{-6}	3.65×10^{-5}	216
PM3	8.74×10^{-5}	7.28×10^{-5}	9.47×10^{-5}	25

Sloping of 2D conductance histograms. The slopes of the molecular

conductance features from 2D conductance histograms can be obtained from the "average conductance profile," which corresponds to the maximum value of counts of conductance at each value of displacement in the 2D histogram. Figure S9 demonstrates this procedure for the 2D histogram of **PM1**, where the dashed white line is the average conductance profile, as obtained by fitting a Gaussian line shape at each displacement value. A line is then fitted to the linear section of this profile, which in turn yields the decay constant, $ß_s$, such that where 'G' is the conductance and 'L' is the displacement.

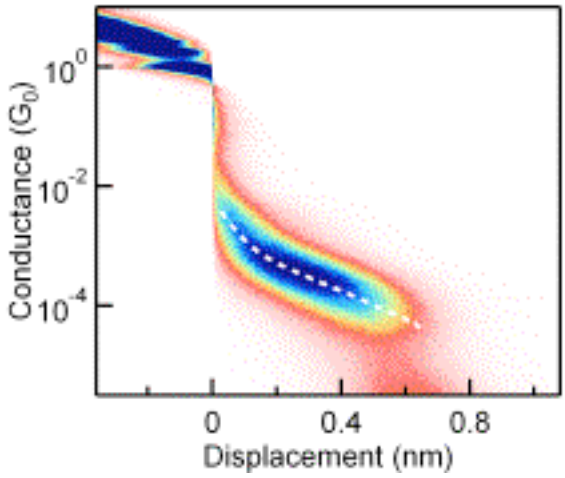


Figure D9: Maximum likelihood conductance profile overlaid on the 2D conductance histogram for **PM1**.

AFM Simultaneous Force and Conductance Measurement: A home-built conducting atomic force microscope (AFM) is used to simultaneously measure conductance and force across single molecule junctions. Au coated (100 nm) mica substrates and Au coated (100 nm) commercial AFM cantilevers (~50 N/m, NanoAndMore Inc.) are used as the two electrodes. Dilute solutions of the molecules (1 mM in 1,2,4-trichlorobenzene) are deposited on the substrates to perform single-molecule measurements. A constant voltage bias of 75 mV is used to obtain conductance measurements, while minimizing electrostatic tip-substrate interactions. The details of the experimental setup[16] and analysis technique[1] have been described in detail previously.

For junctions of **PP1** and **PM1**, the algorithm finds significant force fluctuations due to molecular junctions in more than 90% of the measured traces, in contrast to **P1** where only 12% of the measurements have such events. The rupture force for **PP1** and **PM1** are found to be 0.5 nN, whereas for **P1**, we obtain 0.3 nN, which is same as the threshold used to detect the force events (inset of Figure D10B). Together, the low probability of molecular force events, and the null value of the rupture force imply that the rupture force for **P1** is smaller than 0.3 nN.

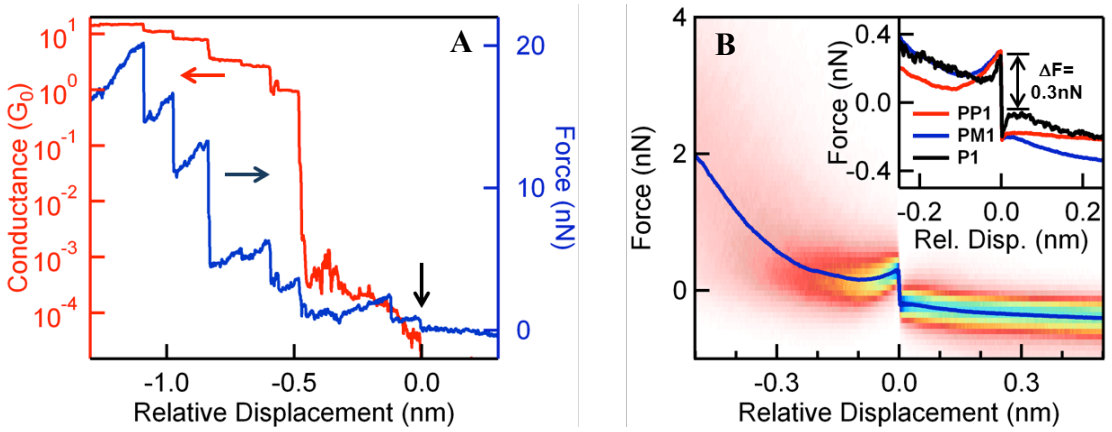


Figure D10: (A) A sample simultaneous measurement of conductance (red, left axis) and force (blue, right axis) with **PM1** molecule. The downward arrow indicates the rupture of the **PM1** molecular junction in force; a highly correlated drop in conductance is also observed in the conductance at the same location (zero of the displacement axis). (B) 2D force histogram for **PM1** constructed from 8242 traces. The averaged force profile is overlaid. Inset: Comparison of averaged force profiles for **PP1**, **PM1** and **P1**.

D5. Theoretical Methods and Details

All electronic structure calculations used Jaguar (version 7.8, Schrodinger LLC, New York, NY, 2011) using the B3LYP hybrid functional and the 6-31G** basis sets. Final geometries and energies, as well as orbital energies are given below.

Molecule	HOMO (eV)	LUMO (eV)	E_{DFT} (eV)
PP1	-5.03	-1.34	3.69
PP2	-4.89	-1.58	3.31
PP3	-4.79	-1.79	3.00
PM1	-5.22	-1.41	3.81
PM2	-5.06	-1.66	3.40
PM3	-4.93	-1.86	3.07
P1	-5.21	-1.35	3.85
P2	-5.04	-1.62	3.42
P3	-4.90	-1.82	3.08
M1	-5.47	-1.44	4.04
PP1A	-4.54	-0.75	3.79
PM1A	-4.82	-0.93	3.89
P1A	-4.93	-1.05	3.88
M1A	-5.11	-1.17	3.94
PM1TA	-4.98	-1.19	3.79

Table D2: Summary of DFT calculations. Energy of the HOMO (E_{HOMO}) and LUMO (E_{LUMO}) and the HOMO-LUMO energy gap (E_{DFT}) energies of all derivatives.

PP1

Final total energy: -1415.73607449062 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-3.8434657906	-1.8489488923	-0.0120387531
C2	-4.5597978043	-0.6660921203	-0.2805624712
C3	-5.9467255545	-0.6325681374	-0.2796433503
C4	-6.6855502592	-1.7937947552	-0.0064348986
C5	-5.9902287827	-2.9808488469	0.2650085261
C6	-4.5991963175	-3.0026449136	0.2621135588
H8	-4.0097134678	0.2469096457	-0.4949240973
H9	-6.4629515231	0.2996396986	-0.4916892543
H11	-6.5258516266	-3.8979328936	0.4823056343
H12	-4.0982714329	-3.9407699265	0.4812263322
C12	-1.5316801901	-2.8421871117	0.1511900371
C13	-2.3802636501	-1.8091183580	-0.0312521643
H15	-1.9652880229	-0.8205089096	-0.2198575523
H16	-1.9486865576	-3.8323927158	0.3259489543
C16	2.7734875957	-2.8774915889	0.1311408256
C17	2.0277379167	-4.0554884837	0.2888181918
C18	0.6411749301	-4.0140393968	0.2921141524
C19	-0.0682757996	-2.8065055585	0.1381972998
C20	0.6946137979	-1.6350753330	-0.0162369530
C21	2.0856456257	-1.6651369891	-0.0209750767
H23	2.5383213377	-5.0068558627	0.4096633569
H24	0.0856855673	-4.9404056715	0.4159550123
H25	0.1994174010	-0.6754224880	-0.1305297622
H26	2.6273682700	-0.7339753005	-0.1424063707
S26	-8.4609420801	-1.6384944700	-0.0311872223
C27	-9.0457398363	-3.3122035795	0.3862641249
H28	-10.1358266120	-3.2488756365	0.3880750438
H29	-8.7357642632	-4.0449031320	-0.3622958347
H30	-8.7077887729	-3.6191342554	1.3787457348
S30	4.5474530372	-3.0472519226	0.1422375258
C31	5.1465915681	-1.3400388869	-0.0658394496
H32	6.2362572697	-1.4100408636	-0.0593391970
H33	4.8255885854	-0.9149795515	-1.0193301512
H34	4.8286735152	-0.6998453415	0.7601083900

HOMO energy: -0.18483 hartrees
LUMO energy: -0.04928 hartrees

Orbital energies (hartrees):

-88.88533	-88.88533	-10.22391	-10.22390	-10.22024	-10.22022
-10.19744	-10.19727	-10.19490	-10.19484	-10.19299	-10.19283
-10.19270	-10.19270	-10.19168	-10.19162	-10.19059	-10.18982
-7.94627	-7.94626	-5.91154	-5.91154	-5.90741	-5.90741
-5.90116	-5.90115	-0.86678	-0.86337	-0.81690	-0.80337
-0.77646	-0.74930	-0.74811	-0.74693	-0.71289	-0.66634
-0.64406	-0.62146	-0.61013	-0.59317	-0.57536	-0.55401
-0.50733	-0.50164	-0.46834	-0.46315	-0.45534	-0.44748
-0.44163	-0.43725	-0.43718	-0.43554	-0.42303	-0.41971
-0.40553	-0.40003	-0.38175	-0.37464	-0.36866	-0.36828
-0.35153	-0.34528	-0.33545	-0.32320	-0.32060	-0.31940
-0.29357	-0.25459	-0.25419	-0.25029	-0.21622	-0.18483
-0.04928	-0.00270	-0.00263	0.01549	0.03558	0.03569
0.07273	0.07408	0.07412	0.09542		

PP2

Final total energy: -1493.14718671261 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-2.3426775229	0.3995095608	0.2271635527
C2	-3.0478500144	1.6139813026	0.1671225268
C3	-4.4559283131	1.5375564676	0.2236024395
C4	-5.1094032871	0.3209868684	0.3336649073
C5	-4.3867386852	-0.8851527425	0.3925295337
C6	-2.9896899681	-0.8288809901	0.3374113222
H7	-1.2562442673	0.4182435637	0.1862575986
H9	-5.0508083675	2.4449004000	0.1812964131
H10	-6.1949642165	0.2986233620	0.3751764357
H12	-2.3939219123	-1.7334528963	0.3790083062
C12	-2.7918756553	4.1254521647	-0.0162133438
C13	-2.3021963745	2.8637794382	0.0524918686
H15	-1.2187522020	2.7464803418	0.0200902986
H16	-3.8676876486	4.2937979399	0.0125048882
C16	-2.4443747228	6.5643786043	-0.1968484366
C17	-1.9629571924	5.2996381087	-0.1280939073
H19	-0.8877721980	5.1271682639	-0.1565392351
H20	-3.5265966465	6.6919774791	-0.1654450995
C20	-0.3049851916	10.2844717219	-0.5322354923
C21	-1.7029789238	10.2492150939	-0.4815755756
C22	-2.3696077966	9.0306797560	-0.3725988926
C23	-1.6836926068	7.8052647531	-0.3103159240
C24	-0.2741033785	7.8611504965	-0.3626713669
C25	0.3985830592	9.0672098383	-0.4705632110
H27	-2.2844765369	11.1629551894	-0.5259612429
H28	-3.4563184210	9.0293368098	-0.3350256829
H29	0.3075175889	6.9454721734	-0.3173875929
H30	1.4845883058	9.0726916977	-0.5071149586
S30	0.6745435159	11.7661241977	-0.6714303558
S31	-5.3407273913	-2.3829791615	0.5323163287
C32	-0.5657889538	13.0994612142	-0.7048297948
H33	0.0037994124	14.0278260094	-0.7824793883
H34	-1.2232856043	13.0144143901	-1.5730491862
H35	-1.1548726080	13.1215346676	0.2148660257
C35	-4.0751165783	-3.6914743480	0.5912039609
H36	-4.6268065871	-4.6293897572	0.6814976262
H37	-3.4816895207	-3.7170720836	-0.3256451807
H38	-3.4230535777	-3.5792297134	1.4604472093

HOMO energy: -0.17989 hartrees
LUMO energy: -0.05819 hartrees

Orbital energies (hartrees):

-88.88601	-88.88588	-10.22447	-10.22425	-10.22057	-10.22050
-10.19725	-10.19723	-10.19413	-10.19405	-10.19398	-10.19375
-10.19270	-10.19268	-10.19246	-10.19226	-10.19081	-10.19078
-10.18983	-10.18946	-7.94694	-7.94681	-5.91220	-5.91207
-5.90808	-5.90794	-5.90186	-5.90172	-0.86558	-0.86476
-0.82047	-0.80901	-0.79180	-0.76513	-0.74978	-0.74851
-0.73865	-0.70716	-0.66780	-0.64956	-0.61125	-0.61004
-0.60663	-0.58150	-0.56194	-0.54973	-0.51334	-0.49343
-0.47655	-0.46312	-0.45779	-0.45268	-0.44704	-0.44006
-0.43752	-0.43742	-0.42570	-0.42117	-0.41798	-0.40503
-0.38873	-0.38726	-0.37988	-0.37744	-0.36963	-0.35834
-0.34567	-0.34181	-0.33736	-0.33359	-0.32096	-0.32057
-0.30755	-0.27847	-0.25434	-0.25395	-0.23881	-0.21178
-0.17989	-0.05819	-0.00481	-0.00258	0.00028	0.03521
0.03540	0.04919	0.07278	0.07419	0.09198	

PP3

Final total energy: -1570.55777722054 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-3.1551496645	-0.6879559967	0.0298618562
C2	-3.8331293924	0.5370730239	-0.0962281767
C3	-5.2228585531	0.6212940323	-0.0665630512
C4	-5.9934697400	-0.5356753780	0.0926084957
C5	-5.3320694910	-1.7712854312	0.2194653054
C6	-3.9494693277	-1.8440539426	0.1886412849
H8	-3.2545191227	1.4492428745	-0.2207461730
H9	-5.6921724636	1.5930939161	-0.1683384951
H11	-5.9135644082	-2.6807345772	0.3438048701
H12	-3.4783510527	-2.8169266177	0.2899312979
C12	-0.8723064740	-1.7732230234	0.1020687380
C13	-1.6969243605	-0.7019811848	-0.0077536449
H15	-1.2325168067	0.2754924195	-0.1391683053
H16	-1.2928066323	-2.7688387784	0.2351041179
C16	1.3962637767	-2.7598903379	0.1684609068
C17	0.5624780039	-1.6911897147	0.0564464166
H19	0.9972679888	-0.7000366234	-0.0767287034
H20	0.9581320534	-3.7497195073	0.3016018597
C20	3.6408452228	-3.7704801249	0.2427604174
C21	2.8316557782	-2.6880505007	0.1264906468
H23	3.2646124641	-1.6973844820	-0.0064163587
H24	3.1597096911	-4.7398825885	0.3743251359
C24	7.9335142822	-4.0201546780	0.1792768013
C25	7.1327097530	-5.1617697156	0.3418825608
C26	5.7503478782	-5.0538382762	0.3586689862
C27	5.0987091406	-3.8116301104	0.2154009235
C28	5.9166104051	-2.6782479235	0.0530805644
C29	7.3037137505	-2.7754150869	0.0348220496
H31	7.5981676516	-6.1369399235	0.4553998180
H32	5.1512769576	-5.9520865853	0.4860159106
H33	5.4664591196	-1.6972202701	-0.0620145632
H34	7.8884172616	-1.8716544615	-0.0931652146
S34	-7.7736393134	-0.5751673799	0.1480717571
S35	9.6970797157	-4.2727603815	0.1731346389
C36	10.3718983264	-2.5972341185	-0.0609335293
H37	11.4570840218	-2.7178796934	-0.0713936708
H38	10.0548913316	-2.1663199301	-1.0133891647
H39	10.0978857909	-1.9351469426	0.7636288567

C39	-8.2481010201	1.1731158198	-0.0402055755
H40	-9.3394650905	1.1862091481	-0.0087950934
H41	-7.8633221428	1.7833973846	0.7799505496
H42	-7.9170999999	1.5772378425	-0.9994620603

HOMO energy: -0.17597 hartrees
LUMO energy: -0.06587 hartrees

Orbital energies (hartrees):

-88.88634	-88.88628	-10.22501	-10.22480	-10.22090	-10.22087
-10.19776	-10.19755	-10.19555	-10.19457	-10.19420	-10.19363
-10.19339	-10.19328	-10.19277	-10.19231	-10.19152	-10.19150
-10.19055	-10.19003	-10.18975	-10.18953	-7.94727	-7.94721
-5.91253	-5.91248	-5.90840	-5.90834	-5.90219	-5.90212
-0.86588	-0.86569	-0.82335	-0.81312	-0.80103	-0.78040
-0.75762	-0.74938	-0.74891	-0.73375	-0.70373	-0.66695
-0.65086	-0.61964	-0.61114	-0.60818	-0.58537	-0.56898
-0.55545	-0.54884	-0.50969	-0.49922	-0.47893	-0.46574
-0.46033	-0.45538	-0.45073	-0.44285	-0.43786	-0.43786
-0.43428	-0.42655	-0.42086	-0.41497	-0.40402	-0.39260
-0.38555	-0.37971	-0.37888	-0.37037	-0.35954	-0.35813
-0.34697	-0.34081	-0.33968	-0.33928	-0.32118	-0.32075
-0.31813	-0.29534	-0.26489	-0.25488	-0.25449	-0.23099
-0.20760	-0.17597	-0.06587	-0.01572	-0.00322	-0.00218
0.03069	0.03496	0.03504	0.07243	0.07311	0.07326

PM1

Final total energy: -1415.73537949533 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-4.1841626791	1.5569152376	0.1876405253
H2	-4.8681849692	2.1476792536	0.8002559953
H4	-3.5310557600	2.2345545285	-0.3669654053
H5	-3.5926357479	0.9112819201	0.8407662029
S5	-5.2447620944	0.5862788618	-0.9305507327
C6	-2.3823785809	-1.9177229951	-3.5570237809
C7	-3.7844491201	-1.9666890719	-3.6834427426
C8	-4.6197022234	-1.2029753234	-2.8809826322
C9	-4.0829755879	-0.3486244001	-1.9053112009
C10	-2.6889818901	-0.2887247417	-1.7631528553
C11	-1.8610176290	-1.0591520904	-2.5731102603
H13	-4.2245698321	-2.6208744022	-4.4320987891
H14	-5.6965058426	-1.2683829515	-3.0096548134
H15	-2.2361014097	0.3563953038	-1.0191008976
H16	-0.7872595727	-0.9878255599	-2.4280142244
C16	-0.2166891382	-2.8021124764	-4.4961546441
C17	-1.5629807732	-2.7490076915	-4.4409475680
H19	-2.1367771807	-3.3756844631	-5.1215955134
H20	0.3582907936	-2.1623091605	-3.8287710090
C20	2.2951312176	-5.1603142055	-7.0404801091
C21	0.9139641993	-5.3366790344	-7.0833230429
C22	0.0675872953	-4.5900090945	-6.2688007359
C23	0.6001639505	-3.6354947902	-5.3846752709
C24	1.9986199116	-3.4671145401	-5.3448578342
C25	2.8479013190	-4.2165362547	-6.1615582525
H26	2.9419420299	-5.7526805353	-7.6810011348
H27	0.4938780097	-6.0732378099	-7.7625410961
H28	-1.0032460330	-4.7569812191	-6.3168710225
H29	2.4050003077	-2.7312507175	-4.6593427007
S30	4.6277835112	-4.0636045686	-6.1743032869
C31	4.9616803185	-2.7851081655	-4.9205730380
H32	6.0476767973	-2.6723956119	-4.9002796841
H33	4.5125037958	-1.8272913686	-5.1931900786
H34	4.6202373396	-3.0942580685	-3.9298415359

HOMO energy: -0.19201 hartrees
LUMO energy: -0.05198 hartrees

Orbital energies (hartrees):

-88.88746	-88.88300	-10.22661	-10.22306	-10.22202	-10.21902
-10.20222	-10.19962	-10.19723	-10.19551	-10.19498	-10.19406
-10.19377	-10.19234	-10.19214	-10.19182	-10.19105	-10.18648
-7.94839	-7.94393	-5.91366	-5.90953	-5.90924	-5.90511
-5.90329	-5.89874	-0.86837	-0.86348	-0.81707	-0.80198
-0.78236	-0.75441	-0.75061	-0.73640	-0.71449	-0.66063
-0.65402	-0.62388	-0.60948	-0.59341	-0.57814	-0.54317
-0.51293	-0.50491	-0.47107	-0.46640	-0.45517	-0.44585
-0.44386	-0.43904	-0.43713	-0.43586	-0.42558	-0.41866
-0.40479	-0.39467	-0.38316	-0.37503	-0.37209	-0.36662
-0.35597	-0.34634	-0.33625	-0.32313	-0.32257	-0.31755
-0.29178	-0.27053	-0.25646	-0.23700	-0.21015	-0.19201
-0.05198	-0.00496	0.00104	0.01355	0.03367	0.03727
0.07153	0.07222	0.07460	0.09410		

PM2

Final total energy: -1493.14628820380 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	3.4309097782	-2.6742507232	-0.0445427170
C2	2.5858524868	-1.6221888849	0.0730163638
H3	3.0285750210	-0.6350856798	0.2075180118
H4	3.0323966266	-3.6783857411	-0.1798668317
C5	5.7072258229	-3.6165548353	-0.1211760795
C6	4.8672005688	-2.5614230687	-0.0029803294
H7	5.2693188189	-1.5585090740	0.1306008651
H8	5.2582754989	-4.6005685628	-0.2570214150
C9	9.9835303964	-3.7265535331	-0.0571460621
C10	9.2403428278	-4.9023263880	-0.2421129830
C11	7.8461417671	-4.8313837265	-0.2569875890
C12	7.1698681221	-3.6052080974	-0.0929508361
C13	7.9348211422	-2.4397050911	0.0908049013
C14	9.3242046084	-2.5106970002	0.1073491009
H15	11.0689058255	-3.7655739556	-0.0415250075
H16	7.2516000592	-5.7276615182	-0.3972100526
H17	7.4474516624	-1.4797181811	0.2249292723
H18	9.9072374063	-1.6052765001	0.2507602410
S19	10.1789174143	-6.4096989895	-0.4391533848
C20	8.9033085215	-7.6904505167	-0.6618136303
H21	9.4494681120	-8.6275149673	-0.7884150734
H22	8.2588917337	-7.7732585189	0.2163770056
H23	8.3024934736	-7.5084615313	-1.5558648984
C24	-1.7142516165	-1.5642160130	-0.0101675885
C25	-1.0213289917	-2.7807127837	-0.1512348766
C26	0.3624864690	-2.8167710817	-0.1258793556
C27	1.1265067181	-1.6421870324	0.0410959452
C28	0.4182519244	-0.4366410456	0.1809809238
C29	-0.9737426442	-0.3889636394	0.1573772335
H30	-1.5787877651	-3.7039888423	-0.2830047986
H31	0.8584053613	-3.7754774787	-0.2393656009
H32	0.9731481005	0.4892386087	0.3121587236
H33	-1.4680648502	0.5689931485	0.2707910000
S34	-3.4925301763	-1.6522694111	-0.0581361428
C35	-4.0137918152	0.0811330683	0.1413373017
H36	-5.1050381604	0.0648937336	0.1096878573
H37	-3.6938141556	0.4876739165	1.1032856899

H38 -3.6453074801 0.7064700900 -0.6748589477

HOMO energy: -0.18603 hartrees
LUMO energy: -0.06110 hartrees

Orbital energies (hartrees):

-88.88766	-88.88260	-10.22648	-10.22270	-10.22195	-10.21846
-10.20187	-10.19941	-10.19614	-10.19587	-10.19501	-10.19453
-10.19401	-10.19344	-10.19261	-10.19208	-10.19202	-10.19176
-10.19093	-10.18662	-7.94861	-7.94353	-5.91386	-5.90973
-5.90884	-5.90471	-5.90353	-5.89834	-0.86763	-0.86430
-0.82173	-0.80760	-0.79356	-0.77168	-0.75197	-0.74474
-0.73585	-0.70852	-0.66304	-0.65368	-0.62425	-0.61289
-0.59445	-0.58687	-0.55923	-0.54472	-0.51379	-0.50050
-0.48069	-0.46451	-0.45931	-0.45168	-0.44456	-0.44324
-0.43901	-0.43533	-0.42895	-0.42279	-0.41729	-0.39707
-0.39346	-0.38668	-0.38155	-0.37759	-0.36674	-0.36074
-0.35206	-0.34196	-0.33836	-0.33488	-0.32264	-0.31764
-0.30621	-0.28098	-0.26283	-0.25616	-0.22770	-0.20869
-0.18603	-0.06110	-0.00628	-0.00268	0.00190	0.03379
0.03776	0.04783	0.07179	0.07510	0.08987	

PM3

Final total energy: -1570.55698523588 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.1214174131	-0.5496530163	-0.1421607584
C2	-1.9001919380	-1.7258257742	-0.1936817260
C3	-3.2834508741	-1.6741721547	-0.2293588137
C4	-3.9607073966	-0.4406197988	-0.2151470989
C5	-3.2054229588	0.7361770033	-0.1636312596
C6	-1.8147633186	0.6731104147	-0.1281622186
H8	-1.4163744755	-2.6976184912	-0.2061226513
H9	-3.8530224789	-2.5986170235	-0.2688857519
H11	-3.6874124894	1.7069506489	-0.1506857277
H12	-1.2478555418	1.6001010588	-0.0885594658
S12	-5.7395675213	-0.5083250317	-0.2654271733
C13	-6.2362483257	1.2435577975	-0.2344455922
H14	-7.3276436229	1.2395804495	-0.2646318884
H15	-5.9094981105	1.7365168155	0.6838635087
H16	-5.8602332270	1.7821032315	-1.1071461148
C16	1.1738665274	-1.6085319089	-0.1099699765
C17	0.3365626975	-0.5417718681	-0.1041437221
H19	0.7891279905	0.4492863493	-0.0673123014
H20	0.7664547045	-2.6175886665	-0.1457429997
C20	3.4565476790	-2.5642195597	-0.0772933417
C21	2.6070923235	-1.5026593544	-0.0715352384
H23	3.0277071992	-0.4971960234	-0.0356951856
H24	3.0359175572	-3.5696464281	-0.1127364341
C24	5.7237014967	-3.5284870603	-0.0454439044
C25	4.8902679352	-2.4599237635	-0.0396985916
H27	5.3007783018	-1.4521846187	-0.0052862828
H28	5.2673327592	-4.5177756381	-0.0808368635
C28	9.9985608557	-3.6650738906	0.0544182194
C29	9.2449052948	-4.8481614661	0.0049838393
C30	7.8516394427	-4.7671879714	-0.0266147217
C31	7.1852568012	-3.5244732234	-0.0100516582
C32	7.9600816236	-2.3514923509	0.0397254081
C33	9.3488468432	-2.4327556513	0.0712834146
H34	11.0833252990	-3.7111547758	0.0798298231
H36	7.2494542945	-5.6684899257	-0.0650609156
H37	7.4808841818	-1.3783068197	0.0544626917
H38	9.9396869824	-1.5219005612	0.1101052170
S38	10.1671572344	-6.3780466925	-0.0131781070

C39	8.8764800127	-7.6616286812	-0.0775953370
H40	9.4116810129	-8.6134289617	-0.0887541255
H41	8.2323539104	-7.6291314697	0.8042028085
H42	8.2763354500	-7.5834368827	-0.9871154871

HOMO energy: -0.18110 hartrees
LUMO energy: -0.06838 hartrees

Orbital energies (hartrees):

-88.88788	-88.88275	-10.22678	-10.22303	-10.22203	-10.21863
-10.20205	-10.19954	-10.19631	-10.19605	-10.19512	-10.19475
-10.19413	-10.19347	-10.19336	-10.19278	-10.19218	-10.19215
-10.19195	-10.19177	-10.19129	-10.18675	-7.94882	-7.94368
-5.91407	-5.90994	-5.90899	-5.90486	-5.90375	-5.89849
-0.86769	-0.86447	-0.82497	-0.81250	-0.80028	-0.78455
-0.76331	-0.75141	-0.73904	-0.73475	-0.70442	-0.66362
-0.65390	-0.62980	-0.61297	-0.59650	-0.59224	-0.56831
-0.55723	-0.53965	-0.51326	-0.50457	-0.47979	-0.47022
-0.46122	-0.45589	-0.44789	-0.44419	-0.43914	-0.43544
-0.43506	-0.43149	-0.42133	-0.41000	-0.39854	-0.39277
-0.38735	-0.38126	-0.37826	-0.37313	-0.36001	-0.35965
-0.35008	-0.34249	-0.34164	-0.33865	-0.32276	-0.31784
-0.31782	-0.29387	-0.27437	-0.25688	-0.25258	-0.22107
-0.20764	-0.18110	-0.06838	-0.01702	-0.00480	0.00133
0.02933	0.03363	0.03757	0.07122	0.07177	0.07498

P1

Final total energy: -978.23224126891 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	2.0459081377	0.4276365722	-0.0033426950
C2	1.3357180151	1.6440195419	-0.0032010887
C3	-0.0509626423	1.6827516209	-0.0043976047
C4	-0.7949471235	0.4930725167	-0.0057504205
C5	-0.1054134668	-0.7279813582	-0.0058315340
C6	1.2853240827	-0.7547205650	-0.0047644557
H8	1.8906094781	2.5790452759	-0.0021160369
H9	-0.5626683380	2.6411109630	-0.0042185370
H11	-0.6448710554	-1.6681824002	-0.0067592443
H12	1.7820003632	-1.7199402003	-0.0049731160
C12	4.3565611442	-0.5836143713	-0.0031851937
C13	3.5091188302	0.4651646844	-0.0019358149
H15	3.9261363203	1.4704971079	0.0003770118
H16	3.9426085933	-1.5902623916	-0.0059349083
C16	8.6461496155	-0.5837977461	0.0026889973
C17	7.9253881781	-1.7773089379	-0.0017504087
C18	6.5331388321	-1.7519178731	-0.0036753571
C19	5.8216071913	-0.5376343723	-0.0012014785
C20	6.5674223129	0.6575897095	0.0031382380
C21	7.9575194646	0.6324310976	0.0050957687
H22	9.7321370603	-0.5981631253	0.0043013150
H23	8.4472423474	-2.7301744527	-0.0036965366
H24	5.9784854030	-2.6871478172	-0.0071477200
H25	6.0575640714	1.6160273577	0.0050404350
H26	8.5102615451	1.5677966082	0.0085199717
S26	-2.5692484006	0.6578768678	-0.0073705386
C27	-3.1620558017	-1.0642160476	0.0066487642
H28	-4.2519946798	-0.9987417114	0.0092229984
H29	-2.8427859704	-1.6057339193	-0.8866139095
H30	-2.8375598464	-1.5928114655	0.9057416875

HOMO energy: -0.19140 hartrees
LUMO energy: -0.04978 hartrees

Orbital energies (hartrees):
-88.88605 -10.22510 -10.22073 -10.19829 -10.19791 -10.19560
-10.19370 -10.19348 -10.19245 -10.19143 -10.18997 -10.18924
-10.18880 -10.18807 -10.18794 -10.18777 -7.94699 -5.91226

-5.90812	-5.90188	-0.86639	-0.85434	-0.81273	-0.78538
-0.75183	-0.74903	-0.74254	-0.71061	-0.65808	-0.62398
-0.60859	-0.60066	-0.57900	-0.55231	-0.51218	-0.50381
-0.46992	-0.46098	-0.45569	-0.44382	-0.43779	-0.43495
-0.42517	-0.41757	-0.41477	-0.40152	-0.38078	-0.36983
-0.36882	-0.36377	-0.34479	-0.34107	-0.33284	-0.32059
-0.31770	-0.27920	-0.25495	-0.24926	-0.23260	-0.19140
-0.04978	-0.00337	0.00157	0.01631	0.03503	0.07321
0.07500	0.09514	0.09722	0.10780		

P2

Final total energy: -1055.64297608260 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	2.8973854205	-0.4443906152	-0.1831191150
H2	2.1970329203	0.1579681372	0.3989276309
H4	3.5114362165	0.2204662576	-0.7948510606
H5	3.5267705594	-1.0165161671	0.5023183332
S5	1.8644758597	-1.5374438418	-1.2111918286
C6	4.7999241016	-4.1456015661	-3.6511417726
C7	3.3992281022	-4.2782860333	-3.7351491977
C8	2.5419533889	-3.4816912974	-2.9900771823
C9	3.0523015305	-2.5062489895	-2.1187563074
C10	4.4437506303	-2.3589915839	-2.0223349818
C11	5.2939417983	-3.1632213857	-2.7732566971
H13	2.9790440950	-5.0269831043	-4.4022237057
H14	1.4677589366	-3.6160828947	-3.0814617644
H15	4.8772719135	-1.6172547051	-1.3615056586
H16	6.3647112429	-3.0185615614	-2.6692786264
C16	7.0013969925	-5.0313840855	-4.5188869564
C17	5.6483797033	-5.0154281452	-4.4602167591
H19	5.1105003154	-5.7294557356	-5.0841794250
H20	7.5793866300	-4.3344543659	-3.9140130575
C20	9.1127623910	-5.9437484210	-5.4039763198
C21	7.7600831444	-5.9320135220	-5.3493989552
H23	7.1848576830	-6.6309883102	-5.9544538115
H24	9.6455241721	-5.2264740881	-4.7794887427
C24	11.7293982254	-8.4357731511	-7.7080428338
C25	10.3458184511	-8.5964101881	-7.8237255724
C26	9.4784234639	-7.7989931974	-7.0861572139
C27	9.9706063371	-6.8133435733	-6.2072903554
C28	11.3672679908	-6.6665382750	-6.1053234127
C29	12.2357494690	-7.4652975610	-6.8438792508
H30	12.4032313170	-9.0609799261	-8.2863648288
H31	9.9419125411	-9.3492254975	-8.4948693297
H32	8.4080152396	-7.9420409230	-7.1944555221
H33	11.7694786509	-5.9120831771	-5.4336771646
H34	13.3090166275	-7.3296322298	-6.7446284783

HOMO energy: -0.18521 hartrees
LUMO energy: -0.05953 hartrees

Orbital energies (hartrees):

-88.88657	-10.22529	-10.22116	-10.19829	-10.19815	-10.19577
-10.19402	-10.19384	-10.19293	-10.19241	-10.19156	-10.19081
-10.19061	-10.18952	-10.18907	-10.18848	-10.18834	-10.18812
-7.94749	-5.91276	-5.90863	-5.90240	-0.86626	-0.85526
-0.81868	-0.80021	-0.77172	-0.74949	-0.74407	-0.74169
-0.70563	-0.65924	-0.62474	-0.61445	-0.60273	-0.58502
-0.56214	-0.54984	-0.51716	-0.49874	-0.47693	-0.46217
-0.45748	-0.45183	-0.43976	-0.43811	-0.43153	-0.42378
-0.41703	-0.41020	-0.39958	-0.38000	-0.37984	-0.37141
-0.36220	-0.35855	-0.34280	-0.33986	-0.33478	-0.33130
-0.32103	-0.29967	-0.26358	-0.25511	-0.24961	-0.22364
-0.18521	-0.05953	-0.00602	-0.00055	0.00305	0.03462
0.05007	0.07292	0.09114	0.09391	0.09629	

P3

Final total energy: -1133.05366167212 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.0698586648	2.1599637374	0.6695269374
H2	-1.8175361083	2.6015366693	1.3314113209
H4	-0.3339965142	2.9236838039	0.4079257627
H5	-0.5852566007	1.3292716903	1.1876646061
S5	-1.9908574827	1.5888324925	-0.7943259717
C6	1.1356252020	-0.3088822037	-3.6157988250
C7	-0.2390748395	-0.2447349763	-3.9213569268
C8	-1.1547952013	0.3320731935	-3.0548180697
C9	-0.7309406481	0.8751932235	-1.8316170211
C10	0.6332691168	0.8204321149	-1.5098262489
C11	1.5437782995	0.2400786071	-2.3860730676
H13	-0.5896129526	-0.6591269932	-4.8633469430
H14	-2.2066172740	0.3631751435	-3.3250485412
H15	0.9969667255	1.2286948988	-0.5738795252
H16	2.5911447770	0.2146165946	-2.1022017493
C16	3.3863725785	-1.0819427407	-4.4730796369
C17	2.0426602878	-0.9310210281	-4.5726489431
H19	1.5635581306	-1.3167731946	-5.4726854704
H20	3.9129159188	-0.7122485867	-3.5946824855
C20	5.5355100701	-1.8861293380	-5.4100089716
C21	4.1885764005	-1.7184344025	-5.4808218196
H23	3.6647102056	-2.0906768177	-6.3615791014
H24	6.0666624958	-1.5167344543	-4.5323777263
C24	7.6621111493	-2.6973203201	-6.3615524555
C25	6.3197093365	-2.5284338518	-6.4290881232
H27	5.7723220073	-2.8915284435	-7.2973913803
H28	8.1732332106	-2.3179259120	-5.4767153983
C28	10.3031827474	-4.5495930945	-9.1802564836
C29	8.9333816406	-4.4925851242	-9.4534648870
C30	8.0573712795	-3.8966378024	-8.5535216593
C31	8.5289099888	-3.3373048524	-7.3481763529
C32	9.9118569438	-3.4051393650	-7.0909529020
C33	10.7881291877	-4.0020630737	-7.9927142924
H34	10.9830803070	-5.0164784144	-9.8867791907
H35	8.5473810589	-4.9173414135	-10.3758883145
H36	6.9979789213	-3.8656061704	-8.7881527355
H37	10.2963869402	-2.9799883481	-6.1670738855
H38	11.8503309505	-4.0396795834	-7.7679459868

HOMO energy: -0.18009 hartrees
LUMO energy: -0.06687 hartrees

Orbital energies (hartrees):

-88.88700	-10.22598	-10.22145	-10.19843	-10.19825	-10.19648
-10.19474	-10.19425	-10.19327	-10.19284	-10.19172	-10.19129
-10.19089	-10.19072	-10.19042	-10.18957	-10.18909	-10.18853
-10.18841	-10.18811	-7.94794	-5.91320	-5.90907	-5.90285
-0.86688	-0.85527	-0.82293	-0.80842	-0.78740	-0.76206
-0.75016	-0.74318	-0.73537	-0.70171	-0.66041	-0.62883
-0.61596	-0.60444	-0.59077	-0.57028	-0.55649	-0.54740
-0.51387	-0.50383	-0.47753	-0.46843	-0.45777	-0.45518
-0.44779	-0.43850	-0.43451	-0.42968	-0.42184	-0.41693
-0.40891	-0.39453	-0.38622	-0.38040	-0.37184	-0.36646
-0.36026	-0.35364	-0.34278	-0.34010	-0.34009	-0.33480
-0.32164	-0.31361	-0.28521	-0.25606	-0.25084	-0.24947
-0.21680	-0.18009	-0.06687	-0.01596	-0.00333	0.00180
0.03138	0.03425	0.07264	0.07337	0.08889	0.09623

M1

Final total energy: -978.23150103717 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	0.3642957432	0.8695936629	-0.2724815267
C2	-0.3381187969	2.0868137688	-0.2048729813
C3	-1.7284326436	2.1262271657	-0.2694616638
C4	-2.4550064930	0.9438346947	-0.4037590078
C5	-1.7749181289	-0.2752980164	-0.4717365436
C6	-0.3867561617	-0.3140860954	-0.4066117776
H8	0.2219301637	3.0129532474	-0.1005743682
H9	-2.2438677293	3.0808832409	-0.2149218739
H10	-3.5395052064	0.9690055540	-0.4545330883
H11	-2.3325348759	-1.2018725777	-0.5753061860
H12	0.1173585509	-1.2737648617	-0.4593138594
C12	2.6734725212	-0.1446155163	-0.2608163758
C13	1.8277462033	0.9025539758	-0.2001425573
H15	2.2421603871	1.9029215422	-0.0911925563
H16	2.2611696912	-1.1439588559	-0.3850426175
C16	6.9503433696	-0.1435051994	-0.0774355543
C17	6.2571340082	1.0659714963	0.1084786340
C18	4.8644337747	1.0772638636	0.0536671860
C19	4.1377404230	-0.1065255413	-0.1881644399
C20	4.8494776065	-1.3031338228	-0.3661164480
C21	6.2421032368	-1.3153577877	-0.3119856006
H22	8.0355382503	-0.1590426267	-0.0347459601
H24	4.3255761644	2.0040488248	0.2055571759
H25	4.3049859927	-2.2251287029	-0.5507944634
H26	6.7808340536	-2.2478945375	-0.4537809942
S26	7.2665089081	2.5086421731	0.4101439572
C27	6.0517307707	3.8484449315	0.6206949933
H28	6.6394484610	4.7491308494	0.8093946318
H29	5.4572603416	3.9974770632	-0.2837673200
H30	5.3983390158	3.6667585827	1.4773240499

HOMO energy: -0.20120 hartrees
LUMO energy: -0.05288 hartrees

Orbital energies (hartrees):
-88.88355 -10.22441 -10.21947 -10.20292 -10.20105 -10.19440
-10.19361 -10.19288 -10.19243 -10.19231 -10.19192 -10.19159
-10.19098 -10.19079 -10.19074 -10.18770 -7.94449 -5.90980

-5.90567	-5.89931	-0.86636	-0.85701	-0.80977	-0.79098
-0.75924	-0.74554	-0.73735	-0.71167	-0.65791	-0.63563
-0.60720	-0.59741	-0.57493	-0.55060	-0.51429	-0.51140
-0.47081	-0.46602	-0.45339	-0.44550	-0.43647	-0.43445
-0.43016	-0.41809	-0.41387	-0.39575	-0.38139	-0.37292
-0.37076	-0.36304	-0.34804	-0.34259	-0.33602	-0.31824
-0.31598	-0.28292	-0.26149	-0.25203	-0.21545	-0.20120
-0.05288	-0.00121	0.00022	0.01416	0.03646	0.07307
0.07421	0.09338	0.09535	0.10465		

PP1A

Final total energy: -651.44626208994 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	1.1442166194	0.6818031711	0.0618402600
C2	0.4349865101	1.8927137851	0.1689828716
C3	-0.9528991953	1.9405994128	0.1511604126
C4	-1.7057625323	0.7628362013	0.0253036694
C5	-1.0120326688	-0.4561260144	-0.0799565693
C6	0.3743543041	-0.4917973466	-0.0604132470
H8	0.9920927291	2.8212882178	0.2697079892
H9	-1.4633079257	2.8975295717	0.2318308755
H11	-1.5739540019	-1.3820826899	-0.1790102014
H12	0.8672520333	-1.4560874434	-0.1350551349
C12	3.4507572035	-0.3347242966	-0.0676129751
C13	2.6071100538	0.7072413817	0.0880184901
H15	3.0299227942	1.6982830684	0.2464297822
H16	3.0279676494	-1.3229871983	-0.2425299026
C16	7.7635194306	-0.3900583980	-0.0031124859
C17	7.0675693135	0.8123219703	0.2168336693
C18	5.6811935930	0.8472179354	0.2002329020
C19	4.9134226630	-0.3097383282	-0.0380141590
C20	5.6246016162	-1.5042911189	-0.2559899793
C21	7.0125420231	-1.5517678536	-0.2403880042
H23	7.6279385954	1.7265065387	0.3992224210
H24	5.1864160518	1.7966641990	0.3794197770
H25	5.0689973284	-2.4206627025	-0.4409032259
H26	7.5246838985	-2.4947702672	-0.4170373943
N26	9.1589954654	-0.4144683407	-0.0422163230
H27	9.6148922453	0.3218547733	0.4793262979
H28	9.5749818376	-1.3169542279	0.1438104207
N28	-3.0990859751	0.8045346980	-0.0513485923
H29	-3.5690509264	-0.0478846485	0.2214319464
H30	-3.5258491168	1.6184497277	0.3699096669

HOMO energy: -0.16682 hartrees
LUMO energy: -0.02741 hartrees

Orbital energies (hartrees):
-14.33989 -14.33988 -10.22270 -10.22266 -10.18030 -10.18030
-10.17989 -10.17988 -10.17948 -10.17947 -10.17801 -10.17799

-10.17661	-10.17659	-10.17467	-10.17391	-0.91473	-0.91467
-0.83818	-0.83074	-0.77372	-0.73657	-0.73578	-0.73112
-0.68527	-0.62017	-0.60580	-0.60412	-0.57896	-0.54415
-0.51525	-0.51354	-0.50521	-0.50081	-0.46685	-0.45835
-0.43572	-0.42778	-0.41410	-0.41278	-0.40881	-0.40461
-0.37820	-0.37768	-0.36580	-0.36324	-0.33713	-0.33155
-0.32841	-0.32026	-0.30882	-0.25769	-0.24196	-0.24180
-0.20944	-0.16682	-0.02741	0.00909	0.00941	0.03907
0.07807	0.08359	0.09919	0.10478	0.11036	0.11191

PM1A

Final total energy: -651.44579983956 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	0.9022076285	-0.2088632304	0.0340343948
C2	0.2103317063	1.0127703760	0.0649771006
C3	-1.1901454641	1.0739459415	0.0677182325
C4	-1.9159794967	-0.1261423215	0.0375693172
C5	-1.2384644954	-1.3442607682	0.0064085838
C6	0.1503435750	-1.3998306379	0.0043269629
H8	0.7786545271	1.9408538365	0.0841512159
H10	-3.0028199342	-0.1012362234	0.0319223919
H11	-1.8111900401	-2.2675586331	-0.0173094659
H12	0.6467918854	-2.3635176622	-0.0213235811
C12	3.2089220325	-1.2294237409	0.0398884893
C13	2.3685416501	-0.1740592938	0.0367716031
H15	2.7915570935	0.8289790533	0.0392032070
H16	2.7827908732	-2.2312182216	0.0441252324
C16	7.5205416186	-1.2877533810	0.0458864424
C17	6.8292113899	-0.0622884967	0.0265702129
C18	5.4433046847	-0.0262257033	0.0242362819
C19	4.6716835614	-1.2048576484	0.0424279065
C20	5.3777833133	-2.4219712895	0.0615939482
C21	6.7653999535	-2.4710789936	0.0631663589
H23	7.3933157273	0.8673772614	0.0168130205
H24	4.9513554702	0.9411180787	0.0045770635
H25	4.8188390341	-3.3544002289	0.0729194637
H26	7.2740368978	-3.4320170201	0.0817409004
N26	8.9128575323	-1.3229776680	0.1055042654
H27	9.3821593327	-0.5083392571	-0.2655236629
H28	9.3355592761	-2.1826225310	-0.2170010959
N28	-1.8478638654	2.3087964095	0.0419166426
H29	-2.7868380898	2.2926346861	0.4167277742
H30	-1.3130472212	3.0780154316	0.4223007057

HOMO energy: -0.17707 hartrees
LUMO energy: -0.03402 hartrees

Orbital energies (hartrees):
-14.34379 -14.33452 -10.22729 -10.21882 -10.18742 -10.18437
-10.18402 -10.18347 -10.18166 -10.18047 -10.18030 -10.17858
-10.17696 -10.17264 -10.17217 -10.16792 -0.91893 -0.91017

-0.84042	-0.82975	-0.77832	-0.74110	-0.73925	-0.71731
-0.69156	-0.62481	-0.60965	-0.59486	-0.58379	-0.54488
-0.51744	-0.51327	-0.50094	-0.49536	-0.46837	-0.46434
-0.43791	-0.43371	-0.41513	-0.41425	-0.40815	-0.40146
-0.38172	-0.37485	-0.36849	-0.35375	-0.34407	-0.33194
-0.32892	-0.32334	-0.30678	-0.27095	-0.24580	-0.23147
-0.19817	-0.17707	-0.03402	0.00547	0.02108	0.03496
0.07692	0.08462	0.09737	0.10404	0.10784	0.11434

P1A

Final total energy: -596.08770091935 hartrees

Final geometry:

		angstroms	
atom	x	y	z
N1	1.6499256042	1.3024215562	0.0759396850
H2	2.5875266164	1.5499405815	-0.2085590009
H4	1.6409178744	0.7740372203	0.9374759812
C4	-0.9048579788	-0.1141201096	-3.0001118396
C5	-1.1300291782	-0.4309674901	-1.6475705049
C6	-0.2891079537	0.0125644342	-0.6357000029
C7	0.8308969524	0.8046424790	-0.9358688524
C8	1.0688507934	1.1302016844	-2.2842420818
C9	0.2224771102	0.6810707322	-3.2859608153
H11	-1.9894574321	-1.0440322485	-1.3866891314
H12	-0.4994882283	-0.2499493487	0.3984011830
H13	1.9280729193	1.7457455486	-2.5399878084
H14	0.4467559460	0.9538154821	-4.3126489929
C14	-1.7812695632	-0.4192687079	-5.3456986335
C15	-1.8313741330	-0.6192989618	-4.0124312702
H17	-2.6442358542	-1.2212163793	-3.6085737273
H18	-0.9718210368	0.1841606089	-5.7532560950
C18	-4.4401662431	-1.8527756973	-8.3966146760
C19	-4.6765175330	-2.1908790287	-7.0609769118
C20	-3.8293614819	-1.7386172488	-6.0550703804
C21	-2.7143561888	-0.9303684403	-6.3541008097
C22	-2.4934503819	-0.6011326144	-7.7048612068
C23	-3.3415606373	-1.0538386431	-8.7123229103
H24	-5.1045023940	-2.2085224623	-9.1785313246
H25	-5.5290522117	-2.8130583826	-6.8025782472
H26	-4.0369753093	-2.0177284883	-5.0265634792
H27	-1.6396182572	0.0215715110	-7.9610089553
H28	-3.1432629305	-0.7816128383	-9.7453092903

HOMO energy: -0.18127 hartrees
LUMO energy: -0.03876 hartrees

Orbital energies (hartrees):

-14.34584 -10.22964 -10.19214 -10.18691 -10.18649 -10.18597
-10.18439 -10.18387 -10.18368 -10.18316 -10.18240 -10.18209
-10.18178 -10.18145 -10.18056 -0.92097 -0.84952 -0.83981
-0.78511 -0.74447 -0.74192 -0.73643 -0.69567 -0.62672
-0.61119 -0.59808 -0.58244 -0.54702 -0.51911 -0.51521

-0.49903 -0.47489 -0.45330 -0.44502 -0.43067 -0.42272
-0.41483 -0.41136 -0.40529 -0.38410 -0.37200 -0.36437
-0.35708 -0.33620 -0.33531 -0.32728 -0.32529 -0.28412
-0.24805 -0.24345 -0.23330 -0.18127 -0.03876 0.00323
0.00747 0.02862 0.07488 0.08964 0.10011 0.10196
0.10559 0.12581

M1A

Final total energy: -596.08503296076 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-0.2895692466	0.3590289273	-0.0932129658
C2	-0.9758155339	1.5196733895	-0.4804834983
C3	-2.3782522905	1.5942184994	-0.4606696530
C4	-3.1014732961	0.4661396360	-0.0359225663
C5	-2.4242053173	-0.6878562516	0.3522146310
C6	-1.0357932746	-0.7577054339	0.3290445405
H7	-0.4055143116	2.3872086762	-0.8067539301
H8	-4.1878056885	0.4992673269	-0.0115590031
H9	-2.9981123789	-1.5513089248	0.6776757863
H10	-0.5384096527	-1.6698535949	0.6400528411
C11	2.0153322259	-0.6341230807	0.1444437440
C12	1.1761636393	0.3779546906	-0.1502197804
H13	1.5985727958	1.3279701325	-0.4723044226
H14	1.5941438711	-1.5859748902	0.4625481972
C15	6.3034869834	-0.7001430455	0.0104189899
C16	5.6211943033	0.4671931991	-0.3427329346
C17	4.2320262224	0.5120021452	-0.3062046422
C18	3.4806837301	-0.6129945291	0.0854860142
C19	4.1857629553	-1.7788129174	0.4372752591
C20	5.5771321542	-1.8242450929	0.4012118348
H21	6.1773984575	1.3490813217	-0.6483351226
H22	3.7272259296	1.4313861870	-0.5853417944
H23	3.6269732208	-2.6601883963	0.7423518947
H24	6.0938000611	-2.7389034138	0.6781771323
N25	-3.0270859254	2.7469965583	-0.8480711070
H26	-4.0294972101	2.8060298144	-0.8344345723
H27	-2.5127276021	3.5515003032	-1.1592360387
H28	7.3887440385	-0.7305032580	-0.0196203385

HOMO energy: -0.18789 hartrees
LUMO energy: -0.04314 hartrees

Orbital energies (hartrees):

-14.34056 -10.22659 -10.19499 -10.19093 -10.18659 -10.18602
-10.18577 -10.18535 -10.18505 -10.18497 -10.18471 -10.18150
-10.17578 -10.17577 -10.16986 -0.91561 -0.85234 -0.83488
-0.78791 -0.75019 -0.73974 -0.72299 -0.70038 -0.63027
-0.60381 -0.59932 -0.58675 -0.54965 -0.51883 -0.50742

-0.50432 -0.47329 -0.45985 -0.44902 -0.43519 -0.42021
-0.41488 -0.40955 -0.40154 -0.38031 -0.36766 -0.36702
-0.35168 -0.34230 -0.33377 -0.32713 -0.32175 -0.28806
-0.25357 -0.24643 -0.20403 -0.18789 -0.04314 0.00441
0.01934 0.02852 0.07923 0.08719 0.09828 0.10294
0.11059 0.12577

PM1TA

Final total energy: -1112.20499561224 hartrees

Final geometry:

		angstroms	
atom	x	y	z
C1	-1.2106703531	-0.5803126647	-0.0882786851
C2	-2.5315992428	-0.7769215720	0.0968129706
H3	-0.5826405231	-1.4358836992	-0.3302271185
H5	-3.1594587183	0.0884337127	0.3008329027
C6	1.0065903020	3.1119110051	0.0652895781
C7	1.6142701591	1.9032859301	-0.3082254053
C8	0.8780954871	0.7271329729	-0.3468227401
C9	-0.4916347679	0.6941654280	-0.0200035872
C10	-1.0831444844	1.9132458634	0.3570645407
C11	-0.3554237643	3.0984380091	0.3986410873
H13	2.6687498220	1.8864039324	-0.5698243125
H14	1.3728756392	-0.1952622666	-0.6411124325
H15	-2.1329392874	1.9447093059	0.6324677552
H16	-0.8607527293	4.0098336107	0.6974845644
C16	-4.7948221688	-4.4026172427	-0.0665453956
C17	-5.4162645425	-3.1636194629	0.0382833813
C18	-4.6747386462	-1.9881042634	0.0899227764
C19	-3.2713838379	-2.0427450682	0.0357666965
C20	-2.6446638477	-3.2957385709	-0.0622981972
C21	-3.3844839253	-4.4925966102	-0.1289696412
H22	-5.4061790136	-5.2956476214	-0.0931271049
H23	-6.5010183965	-3.1202451988	0.0858130036
H24	-5.1732972093	-1.0266602541	0.1731428798
H25	-1.5633908251	-3.3348378746	-0.0687436771
S26	2.0436697153	4.5620176615	0.0819697073
C27	0.9166304275	5.8915888591	0.6110378542
H28	1.5240096460	6.7988066879	0.6320303258
H29	0.0980484972	6.0307342358	-0.0988439203
H30	0.5210598526	5.7079511923	1.6126572514
N30	-2.7513271705	-5.7274952909	-0.2558076542
C32	-1.3105489286	-5.8035709535	-0.0957018341
H33	-0.8012074257	-5.1787148549	-0.8376362887
H34	-0.9684572779	-5.4896549681	0.9035131249
H35	-0.9867032585	-6.8329371841	-0.2592487188
C35	-3.5195254187	-6.9412737351	-0.0390624690
H36	-2.8690389293	-7.8054591714	-0.1844162616
H37	-3.9535168609	-7.0039917746	0.9717578671
H38	-4.3378348475	-7.0244896689	-0.7627696868

HOMO energy: -0.18301 hartrees
LUMO energy: -0.04357 hartrees

Orbital energies (hartrees):

-88.88330	-14.34937	-10.22178	-10.22152	-10.21848	-10.21639
-10.21602	-10.19420	-10.19224	-10.19032	-10.18976	-10.18963
-10.18891	-10.18571	-10.18416	-10.18029	-10.17593	-10.17380
-10.17100	-7.94422	-5.90949	-5.90537	-5.89910	-0.94253
-0.86235	-0.84047	-0.80813	-0.77960	-0.74803	-0.74518
-0.73967	-0.72400	-0.70260	-0.65666	-0.65304	-0.61832
-0.60381	-0.58084	-0.56618	-0.54628	-0.51733	-0.50076
-0.47559	-0.46971	-0.46293	-0.46078	-0.45053	-0.44481
-0.43532	-0.43190	-0.42110	-0.41878	-0.41245	-0.40522
-0.39469	-0.39209	-0.38150	-0.37624	-0.36514	-0.36185
-0.35829	-0.34668	-0.33404	-0.32831	-0.31762	-0.31509
-0.28555	-0.26348	-0.25127	-0.22856	-0.19273	-0.18301
-0.04357	0.00011	0.01637	0.02745	0.03748	0.07575
0.08155	0.08591	0.09984	0.10937		

D6. References

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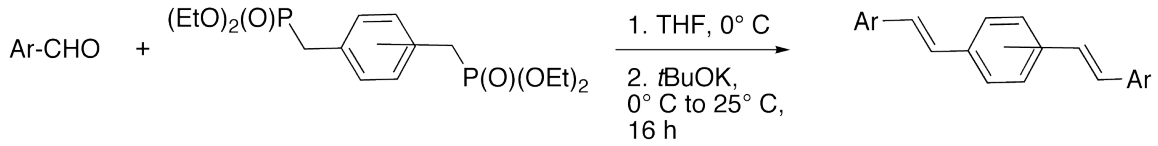
Appendix E

E1. Synthetic Experimentals

General Information: 4-(diethoxymethyl)-benzaldehyde, triethyl phosphite, potassium *tert*-butoxide and all other starting materials and reagents were all purchased from Sigma-Aldrich. THF was freshly distilled under reduced pressure over an SG Water USA, LLC (formerly known as Contour Glass) purification column. Potassium *tert*-butoxide was stored in a glove box under an anhydrous argon atmosphere. Compounds **DPO1**-**DPO3** and dimethyl 4-(methylthio)benzyl phosphonate were prepared for in chapter 5 (see Appendix D). All reactions were carried out under nitrogen unless otherwise noted. 4,4-dimethylthiochroman-6-carbaldehyde (1),[1] (4,4'-dibromomethylstilbene, (*E)*-4,4'-bis(diethyl-phosphonatemethyl)stilbene,[2] and diethyl 4-(4,4,5,5-tetramethyl-1,3-dioxolan-2-yl)benzyl-phosphonate[3] were prepared according to the reported procedures.

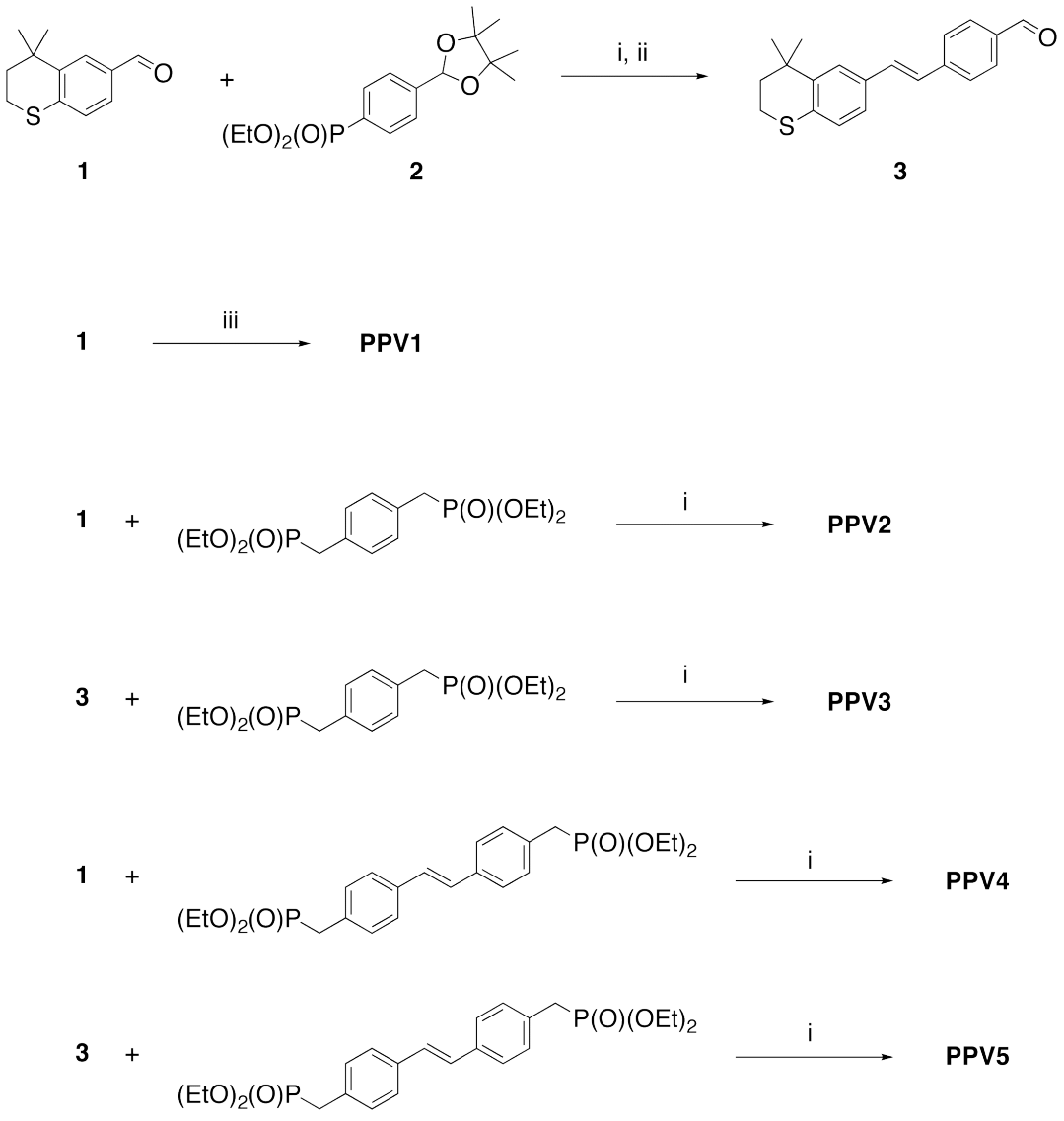
Flash column chromatography was performed on a Teledyne ISCO Combiflash RF using Redisep RF silica columns. Spectra for ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy (NMR) were taken on a Bruker DRX300 (300MHz), DRX400 (400MHz) and DMX500 (500MHz).

Low-resoltuion mass spectroscopy (LR-MS) and High-resolution mass spectrometry (HR-MS) was obtained on a double focusing mass spectrometer (JMS-HX110A; JEOL, ltd.; Tokyo, Japan); Ionization method: FAB, High energy Xe* beam (3 kV); Matix: *meta*-nitrobenzyl alcohol (m-NBA); MS Acceleration-Voltage: 10 kJ; Resolution: 3,000/10,000 (Low-Res/High-Res).

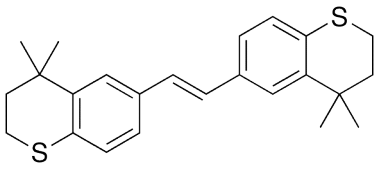


General Horner-Wadsworth-Emmons (H.W.E.) Reaction Procedure: In a 100-mL round-bottom flask 1.0 mmol of aryl-aldehyde was combined with a tetraethyl bisbenzylphosphonate (0.5 mmol) and dissolved in 50 mL of anhydrous tetrahydrofuran (THF). The solution was stirred while cooled in an ice bath for 25 min, at which time a solution of potassium *tert*-butoxide (1.1 mmol) in THF (5 mL) was added dropwise to the reaction solution. An immediate color is observed (usually yellow to orange in color) and followed by the precipitation of a colored solid. The reaction was left stirring overnight (16 h) as it warmed to room temperature. Water (50 mL) was added and the reaction was stirred vigorously for 30 min. The THF was removed under reduced pressure and the crude product was isolated by vacuum filtration. Lastly, the product was isolated by either flash column chromatography or recrystallized from THF/methanol. See specific experimentals for exact isolation procedure and characterization.

Preparation of PPVn Oligomers

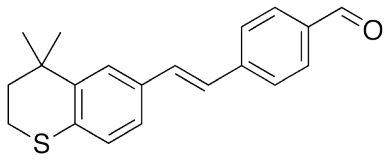


Scheme E1: Synthetic Route to end-functionalized oligo-*para*-phenylenevinylene (**PPVn**) molecular wires. Cyclic thioethers are more soluble than the methylthio derivatives due to the disruption of intermolecular attractive forces by distal out-of-plane methyl groups. For a comparison, **PPV4** and its 4-methylthio derivative, 1,4-bis(4-(4-(methylthio)styryl)styryl)benzene, have comparable solubilities in chlorinated organic solvents. An additional advantage to the cyclic thioether derivatives is that rotational freedom about the aryl-S bond is restricted in a cyclic system, as opposed to the linear alkylthio ether (i.e. MeS-Ar).[4]



(E)-1,2-bis(4,4-dimethylthiochroman-6-yl)ethane (**PPV1**): This experimental was modified from the reported McMurray coupling procedure.[5] Zinc powder (0.415 g, 6.35 mmol) was aded to a flame dried 200-mL round-bottom flask under nitrogen atmosphere. Anhydrous THF (60 mL) was also added and the suspension was cooled in an ice bath while stirring vigorously for 30 min. Titanium(IV) chloride (0.600 g, 3.16 mmol) was added dropwise to the suspension during which a violently evolution of yellow gas occurs. This suspenion was refluxed for 2 hours as the solution become dark. Next the reaction was cooled in an ice bath for 30 min. While stirring a solution of **1** (0.327 g, 1.59 mmol) in 10 mL of anhydrous THF was added slowly and the reaction was refluxed. After 16 h the reaction was cooled to room temperature and poured into saturated aq. sodium bicarbonate solution and left stirring for 30 min. The resulting suspension was filtered through a pad of celite and washed through with CH_2Cl_2. The organic layer was separate and aqueuos layer was extracted with CH_2Cl_2, three times. The organic layers were combined, dried over magnesium sulfate and the solvent removed under reduced pressure. The product was isolate by flash column chromatography in 33% CH_2Cl_2 in hexanes (R_f = 0.50) as a white solid. Yield: 0.246 g (81%). ^{1}H NMR (300 MHz, $C_2D_2Cl_4$): d 7.45 (d, J = 1.7 Hz, 2H, Ph_C), 7.25 (dd, J = 8.2 Hz, 1.7 Hz, 2H, Ph_B), 7.08 (d, J = 8.2 Hz, 2H, Ph_A), 6.97 (s, 2H, -CH=CH-), 3.12-3.10 (m, 4H, -SCH_2-), 2.03-1.92 (m, 4H, -CH_2-), 1.38 (s, 12H, -CH_3); ^{13}C NMR (300 MHz, $C_2D_2Cl_4$): d 141.53, 132.58,

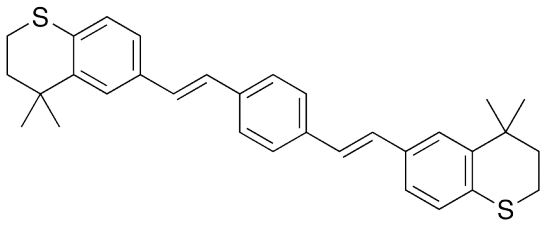
130.34, 126.35, 126.09, 124.40, 122.71, 36.75, 32.19, 29.42, 22.48; HR-MS: m/z calcd for ($C_{24}H_{28}S_2$): 380.1632. Found: 380.1648; 380.1632 (100.0%), 381.1664 (28.7%), 382.1623 (12.8%), 383.1636 (2.8%), 384.1619 (0.6%), 385.1621 (0.1%).



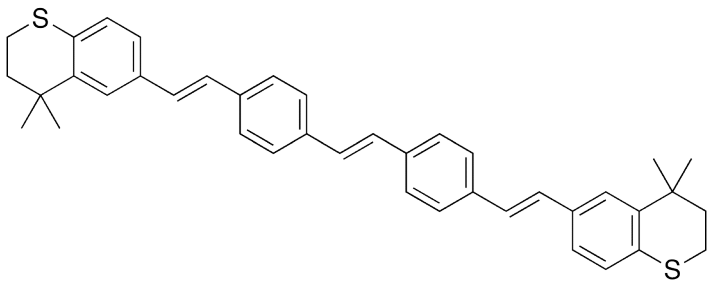
(E)-4-(2-(4,4-dimethylthiochroman-6-yl)vinyl)benzaldehyde (**3**): Using the general H.W.E. procedure from compound **1** and 4-(diethoxymethyl)benzaldehyde gives the acetal protected product, (*E*)-2-(4-(2-(4,4-dimethylthiochroman-6-yl)vinyl)phenyl)-4,4,5,5-tetramethyl-1,3-dioxolane, which may be isolated by column chromatography in 10% ethyl acetate in hexanes (R_f = 0.55). ^{1}H NMR (400 MHz, CD_2Cl_2): d 7.56-7.41 (m, 5H), 7.25 (d, *J* = 8.1 Hz, 1H, Ph), 7.15-7.01 (m, 3H), 5.95 (s, 1H, -CH^{acetal}), 3.08-3.03 (m, 2H, -CH_2-), 2.01-1.94 (m, 2H, -CH_2-), 1.37 (s, 6H, -CH_3), 1.32 (s, 6H, -CH_3^{acetal}), 1.36 (s, 6H, -CH_3^{acetal}); ^{13}C NMR (400 MHz, CD_2Cl_2): d 142.32, 139.24, 137.84, 133.17, 131.80, 128.82, 126.68, 126.55, 126.05, 125.21, 123.65, 99.60, 82.57, 37.57, 32.96, 29.89, 24.14, 23.16, 21.99.

The acetal was dissolved in 10 mL of THF and conc. hydrochloric acid (4 mL) was added to the reaction solution and stirred for 3 h; the solution will immediately turn a darker color of yellow. Cleavage of the acetal protecting group may be easily monitored by TLC, where the product, a yellow spot, will emerge with a lower R_f than the acetal (blue spot). After completion the reaction solution was diluted with water (50 mL), extracted with CH_2CL_2 (3x 20 mL)and dried over magnesium sulfate. The solvent was removed under reduced pressure and the product was isolated by flash column chromatography in 5% ethyl acetate in hexanes (R_f = 0.30) as a bright yellow solid in 59% overall yield. ^{1}H NMR (400 MHz, CD_2Cl_2): d. 9.97 (s, 1H, CHO), 7.85 (d, *J* = 8.1 Hz, 2H, Ph), 7.66 (d, *J* = 8.1 Hz, 2H, Ph), 7.53 (d, *J* = 1.0 Hz, 1H, Ph_C), 7.27 (dd, *J* = 8.2

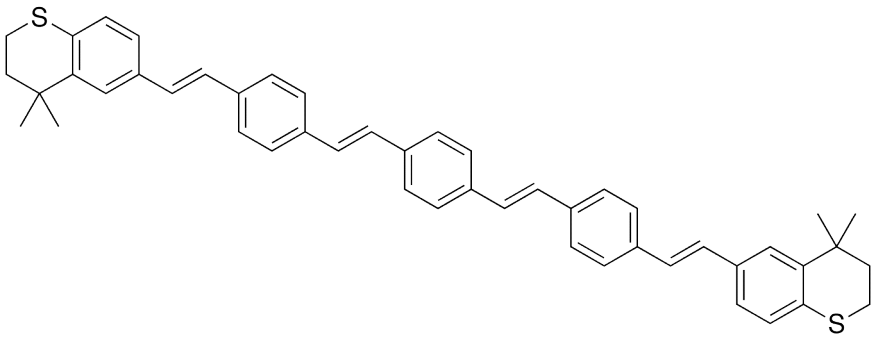
Hz, 1.0 Hz, 1H, Ph_B), 7.23 (d, *J* = 16.4 Hz, 1H, -C(H_a)=CH_b-), 7.10 (d, *J* = 16.3 Hz, 1H, -CH_a=C(H_b)-), 7.09 (d, *J* = 8.2 Hz, 1H, Ph_A), 3.10-3.01 (m, 2H, -SCH_2-), 2.02-1.93 (m, 2H, -CH_2-), 1.32 (s, 6H, -CH_3); ^{13}C NMR (400 MHz, CD_2Cl_2): d 191.93, 144.25, 143.05, 135.82, 133.65, 133.12, 132.66, 130.65, 127.40, 127.21, 126.21, 126.17, 124.51, 38.03, 33.55, 30.41, 23.78; HR-MS: m/z calcd for ($C_{20}H_{20}OS$): 308.1235. Found: 308.1230; 308.1235 (100.0%), 309.1267 (23.4%), 310.1234 (7.2%), 311.1246 (1.2%), 312.1258 (0.2%).



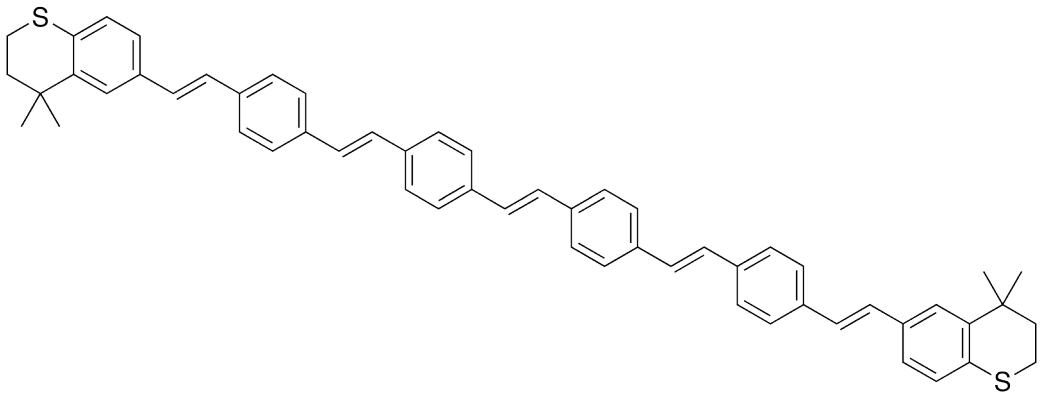
1,4-bis((E)-2-(4,4-dimethylthiochroman-6-yl)vinyl)benzene (**PPV2**): This compound was prepared by the general H.W.E. procedure from **1** and tetraethyl 1,4-phenylenebis(methylene)diphosphonate. The product was isolated by flash column chromatography in ethyl acetate/hexanes (1:9; R_f = 0.50) as a yellow solid in 91% yield. ^{1}H NMR (300 MHz, $CDCl_3$): d 7.47 (s, 4H, Ph), 7.46 (d, *J* = 1.8 Hz, 2H, Ph_C), 7.24 (dd, *J* = 8.2 Hz, 1.8 Hz, 2H, Ph_B), 7.24 (d, *J* = 8.2 Hz, 2H, Ph_A), 7.04 (d, *J* = 16.3 Hz, 2H, -$C(H_a)$=CH_b-), 7.00 (d, *J* = 16.3 Hz, 2H, -CH_a=$C(H_b)$-), 3.11-2.98 (m, 4H, -SCH_2-), 2.03-1.89 (m, 4H -CH_2-) 1.37 (s, 12H, -CH_3); ^{13}C NMR (300 MHz, $CDCl_3$): d 136.84, 133.56, 128.60, 127.05, 126.95, 126.80 (2 peaks), 125.30, 123.84, 118.21, 37.82, 33.21, 30.33, 23.34; HR-MS: m/z calcd for ($C_{32}H_{34}S_2$): 482.2102. Found: 482.2116; 482.2102 (100.0%), 483.2134 (37.7%), 484.2107 (15.8%), 485.2114 (4.1%), 486.2107 (0.9%), 487.2107 (0.2%).



(E)-1,2-bis(4-((E)-2-(4,4-dimethylthiochroman-6-yl)vinyl)phenyl)ethane (**PPV3**): This compound was prepared by the general H.W.E. procedure from compound **1** and (*E*)-4,4'-bis(diethylphosphonatemethyl)stilbene. The product may be monitored by TLC (10% ethyl acetate in hexanes; R_f = 0.70). Recrystallization from THF/methanol gave a bright yellow solid in 57% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): d 7.53 (s, 8H, Ph), 7.48 (dd, *J* = 1.5 Hz, 2H, Ph_C), 7.28 (dd, *J* = 8.3 Hz, 1.6 Hz, 2H, Ph_B), 7.14 (s, 2H, -CH=), 7.13-7.07 (d, *J* = 16.5 Hz, 2H, -C(H_a)=CH_b-), 7.10 (d, *J* = 8.2 Hz, 2H, Ph_C), 7.06-7.00 (d, *J* = 16.4 Hz, 2H, -CH_a=C(H_b)-), 3.14-2.97 (m, 4H, -SCH_2-), 2.04-1.91 (m, 4H -CH_2-) 1.39 (s, 12H, -CH_3); ^{13}C NMR (500 MHz, 320K, $C_2D_2Cl_4$): d 141.83, 136.37, 135.90, 132.68, 131.11, 128.18, 127.58, 126.37 (2 peaks), 126.22, 126.18, 124.77, 123.09, 37.01, 32.44; 29.59, 22.73; HR-MS: m/z calcd for ($C_{40}H_{40}S_2$): 584.2571. Found: 584.2593; 584.2571 (100.0%), 585.2604 (46.7%), 586.2588 (19.5%), 587.2592 (5.6%), 588.2591 (1.3%), 589.2592 (0.3%).

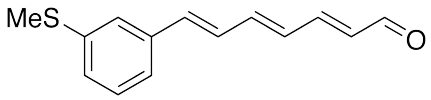


1,4-bis(4-((E)-2-(4,4-dimethylthiochroman-6-yl)vinyl)styryl)benzene (**PPV4**): This compound was prepared by the general H.W.E. procedure from compound **2** and (*E*)-4,4'-bis(diethylphosphonatemethyl)stilbene. The product was isolated by recrystallization from THF/methanol giving a sparingly soluble lemon-yellow solid in 74% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): d 7.58-7.47 (m, 14H), 7.28 (d, *J* = 8.0 Hz, 2H, Ph), 7.18-7.02 (m, 10H), 3.11-3.05 (m, 4H, -CH_2-), 2.05-1.99 (m, 4H, -CH_2-), 1.42 (s, 12H, -CH_3); ^{13}C NMR (500 MHz, 373 K, $C_2D_2Cl_4$): d 141.92, 136.60, 136.37, 136.04, 132.91, 131.24, 128.41, 127.94, 127.60, 126.42, 126.37 (3 overlapping C's signals), 126.22, 124.62, 123.19, 37.28, 32.51, 29.54, 22.74; HR-MS could not be obtained; LR-MS: m/z calcd for ($C_{48}H_{46}S_2$): 686.3041. Found: 686.30.

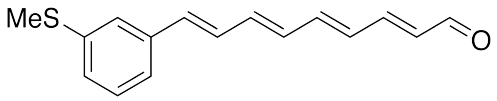


(E)-1,2-bis(4-(4-((E)-2-(4,4-dimethylthiochroman-6-yl)vinyl)styryl)phenyl)ethane (**PPV5**): This compound was prepared by the general H.W.E. procedure from compound **2** and 1,4-phenylenebis(methylene)diphosphonate. The product may be monitored by TLC (10% ethyl acetate in hexanes; R_f = 0.55). Recrystallization from THF/methanol gave a sparingly soluble lemon-yellow solid in 52% yield. ^{1}H NMR (500 MHz, 300 K, 1000 scans, $C_2D_2Cl_4$): d 7.58-7.46 (m, 14H), 7.31-7.00 (m, 20H), 3.09-3.04 (m, 4H, -CH_2-), 2.03-1.96 (m, 4H, -CH_2-), 1.38 (s, 12H, -CH_3); due to limited solubility the ^{13}C NMR could not be obtained; due to limited solubility in methanol, LR and HR-MS could not be obtained.

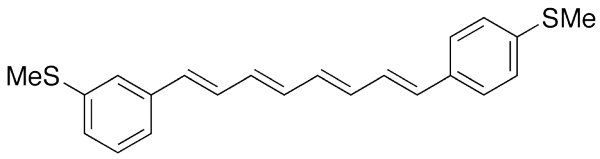
Preparation of Oligoenes (DPOn)



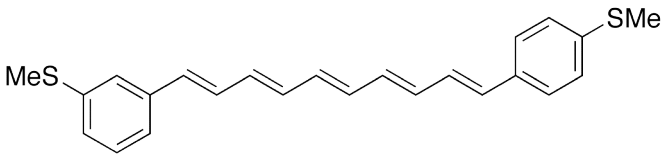
7-(3-(methylthio)phenyl)hepta-2,4,6-trienal: General Wittig Homologation Procedure. HR-MS: m/z calcd for ($C_{14}H_{14}OS$): 230.0765, found: 230.0754. See Appendix D for preparation and further characterization information.



9-(3-(methylthio)phenyl)nona-2,4,6,8-tetraenal: General Wittig Homologation Procedure. HR-MS: m/z calcd for ($C_{16}H_{16}OS$): 256.0922, found: 256.0922. See Appendix D for preparation and further characterization information.

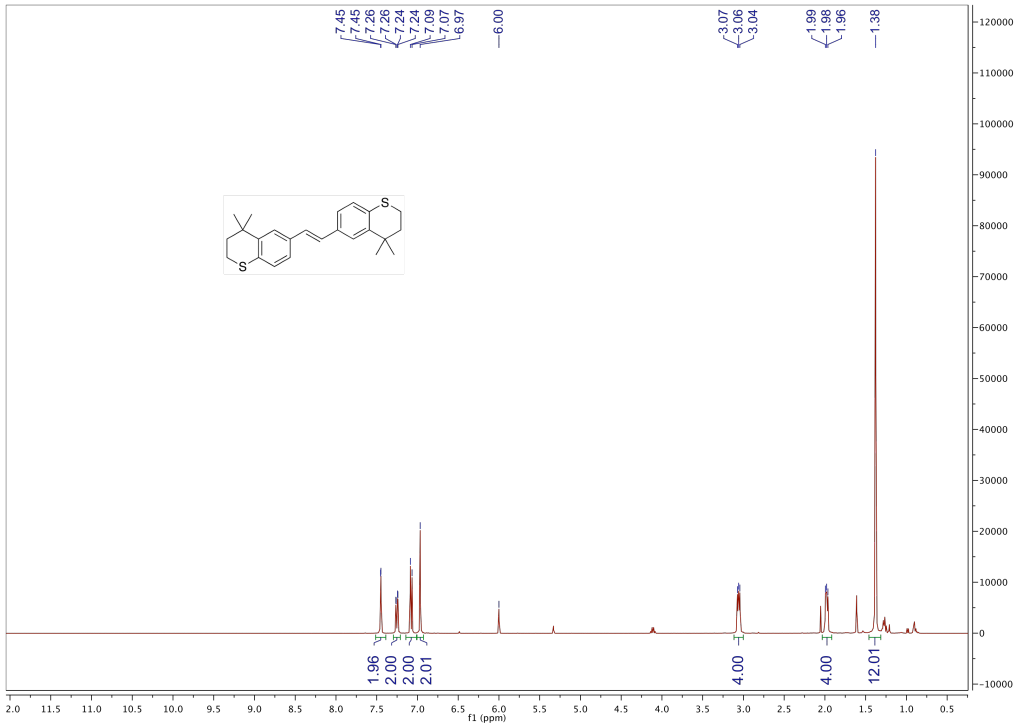


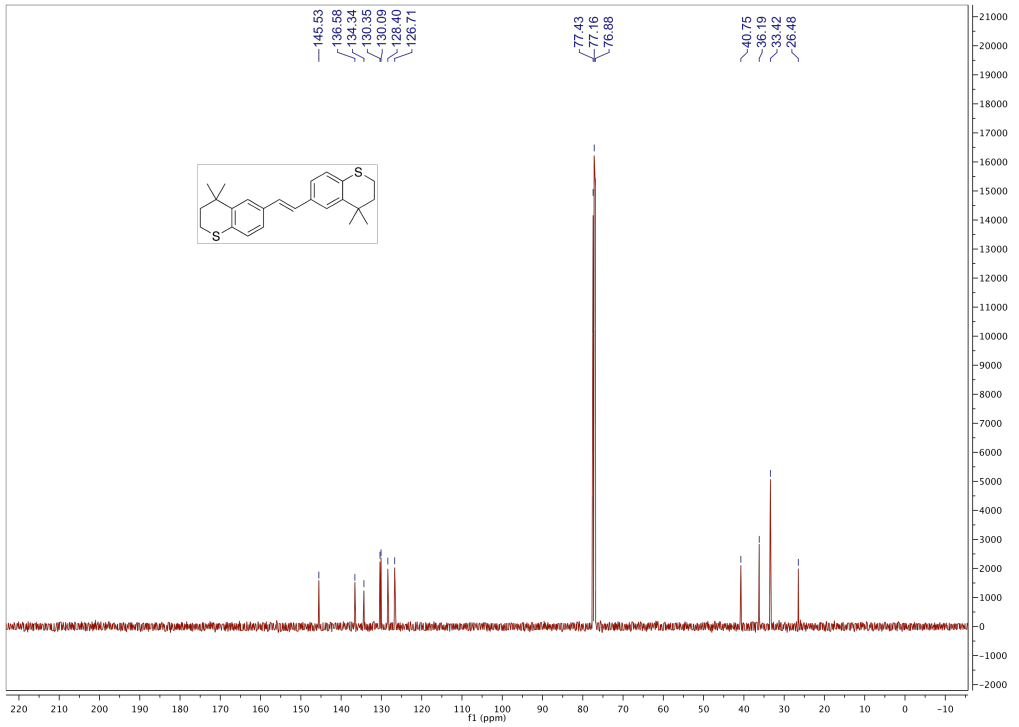
1-(3-(methylthio)phenyl)-8-(4-(methylthio)phenyl)-octa-1,3,5,7-tetraene (**4**): The General HWE Procedure was followed (see Appendix D). The product was prepared from the corresponding trienal and dimethyl 4-(methylthio)benzyl phosphonate and was isolated by recrystallization from CH_2Cl_2/MeOH as a yellow solid in 49% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 7.35 (d, *J* = 8.4 Hz, 2H), 7.28 (bs, 1H), 7.26 (d, *J* = 7.7 Hz, 1H), 7.21 (m, 3H), 7.12 (d, *J* = 7.7 Hz, 1H), 6.94-6.78 (m, 2H), 6.56 (d, *J* = 15.5 Hz, 1H), 6.55 (d, *J* = 15.5 Hz, 1H), 6.47 (m, 4H), 2.52 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (500 MHz, $C_2D_2Cl_4$): δ 138.21, 137.43, 137.29, 133.66, 133.54, 133.33, 132.74, 132.69, 131.67, 131.35, 129.38, 128.64, 128.08, 126.30, 125.95, 124.93, 123.66, 122.68, 15.24, 15.17; HR-MS: m/z calcd for ($C_{22}H_{22}S_2$): 350.1163, found: 350.1169.

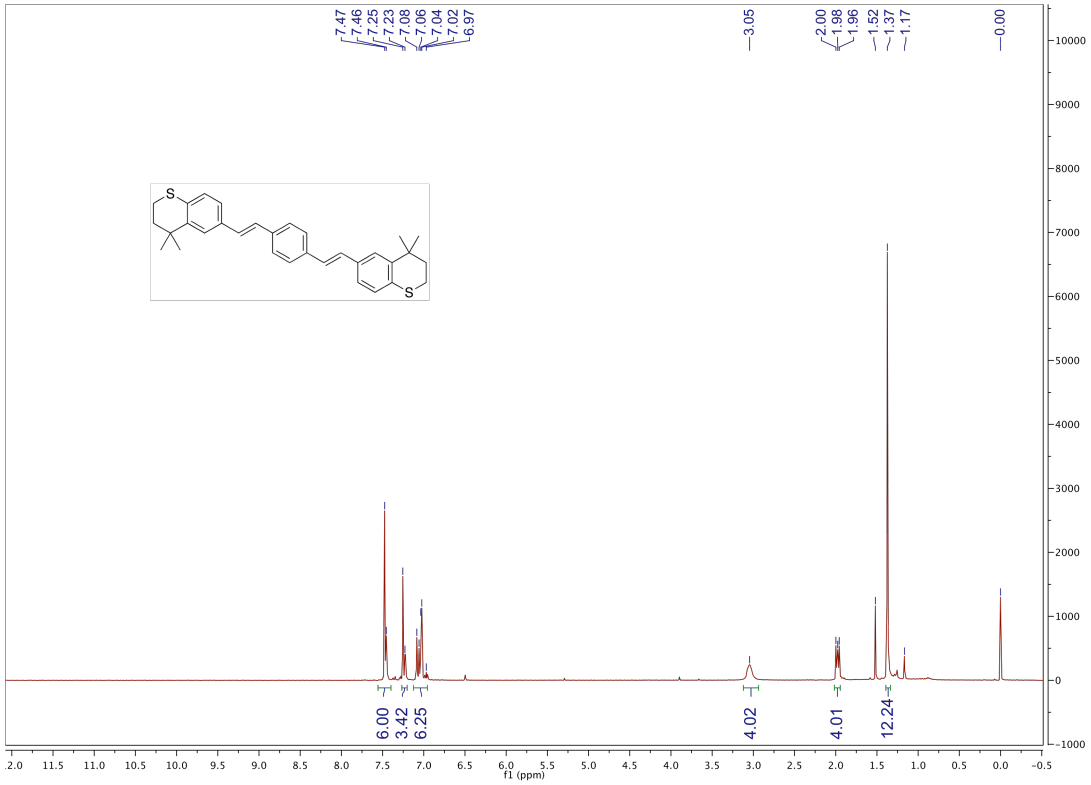


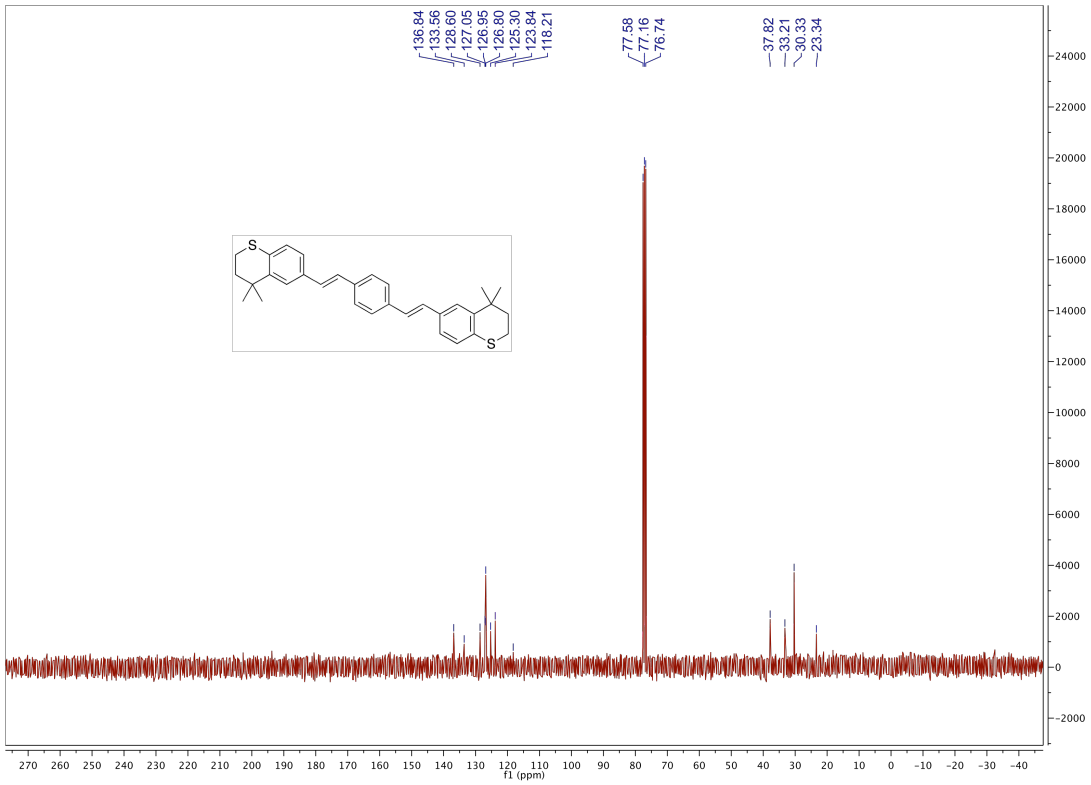
1-(3-(methylthio)phenyl)-10-(4-(methylthio)phenyl)-deca-1,3,5,7,9-pentaene (**5**): The General HWE Procedure was followed (see Appendix D). The product was prepared from the corresponding trienal and dimethyl 4-(methylthio)benzyl phosphonate and was isolated by recrystallization from CH_2Cl_2/MeOH as a light orange solid in 40% yield. ^{1}H NMR (500 MHz, $C_2D_2C1_4$): δ 7.34 (d, *J* = 8.3 Hz, 2H), 7.28 (bs, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.20 (m, 3H), 7.12 (d, *J* = 7.7 Hz, 1H), 6.91-6.79 (m, 2H), 6.54 (d, *J* = 15.5 Hz, 1H), 6.53 (d, *J* = 15.5 Hz, 1H), 6.49-6.37 (m, 6H), 2.51 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (500 MHz, $C_2D_2C1_4$): δ 138.21, 137.44, 137.26, 133.69, 133.63, 133.31, 133.23, 132.90, 132.79, 132.73, 131.59, 131.35, 129.41, 128.64, 128.14, 126.29, 125.95, 124.94, 123.66, 122.68, 15.24, 15.18; HRMS could not be obtained due to insolubility in methanol.

E2. NMR Spectra






7.47
7.46
7.25
7.23
7.08
7.06
7.04
7.02
6.97
3.05
2.00
1.98
1.96
1.52
1.37
1.17
0.00
6.00
3.42
6.25
4.02
4.01
12.24
f1 (ppm)


136.84
133.56
128.60
127.05
126.95
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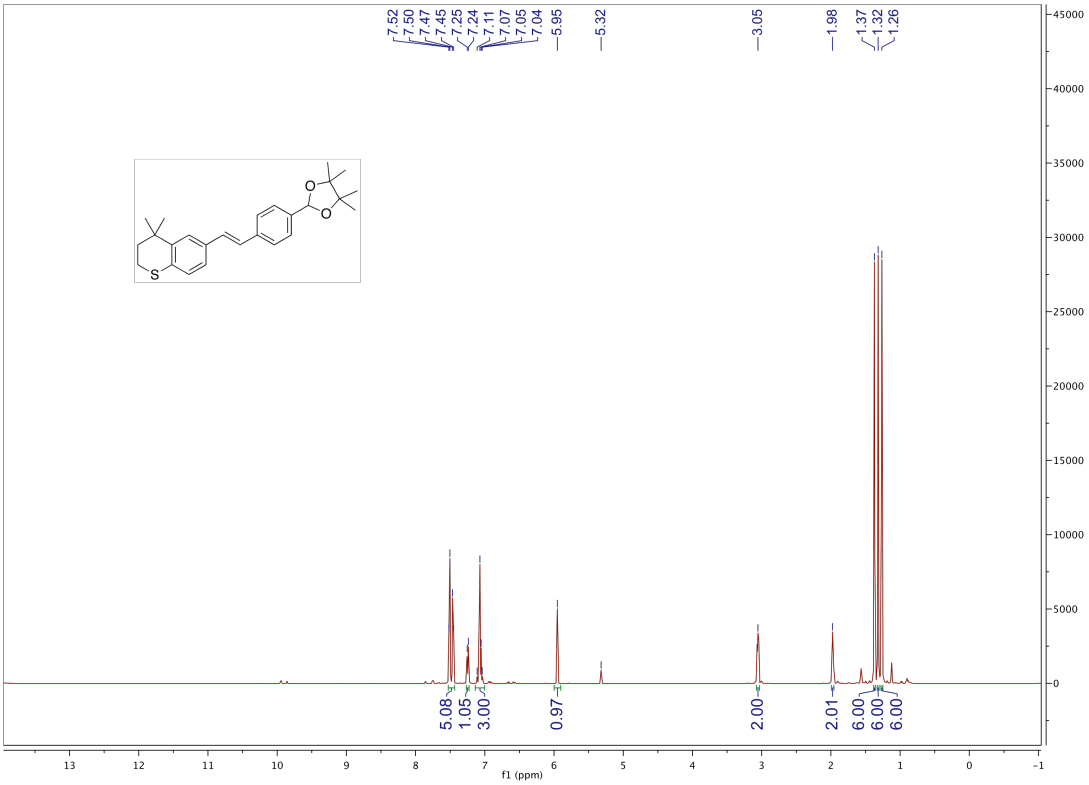
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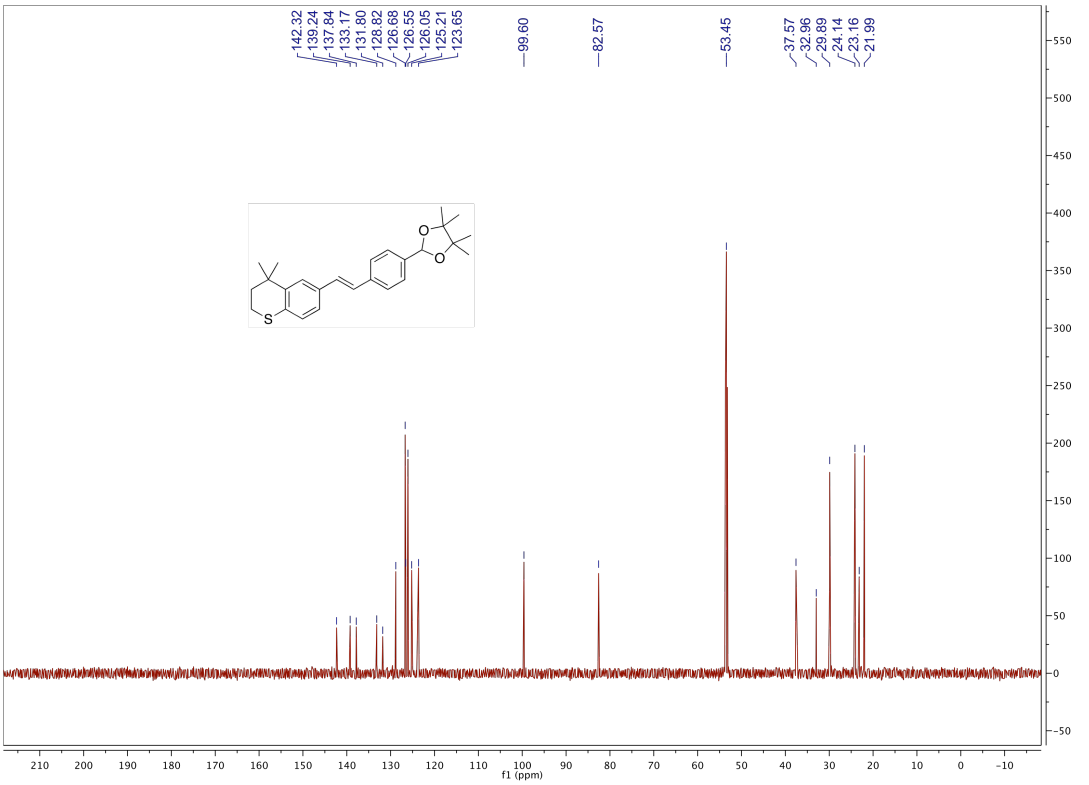
f1 (ppm)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24.14
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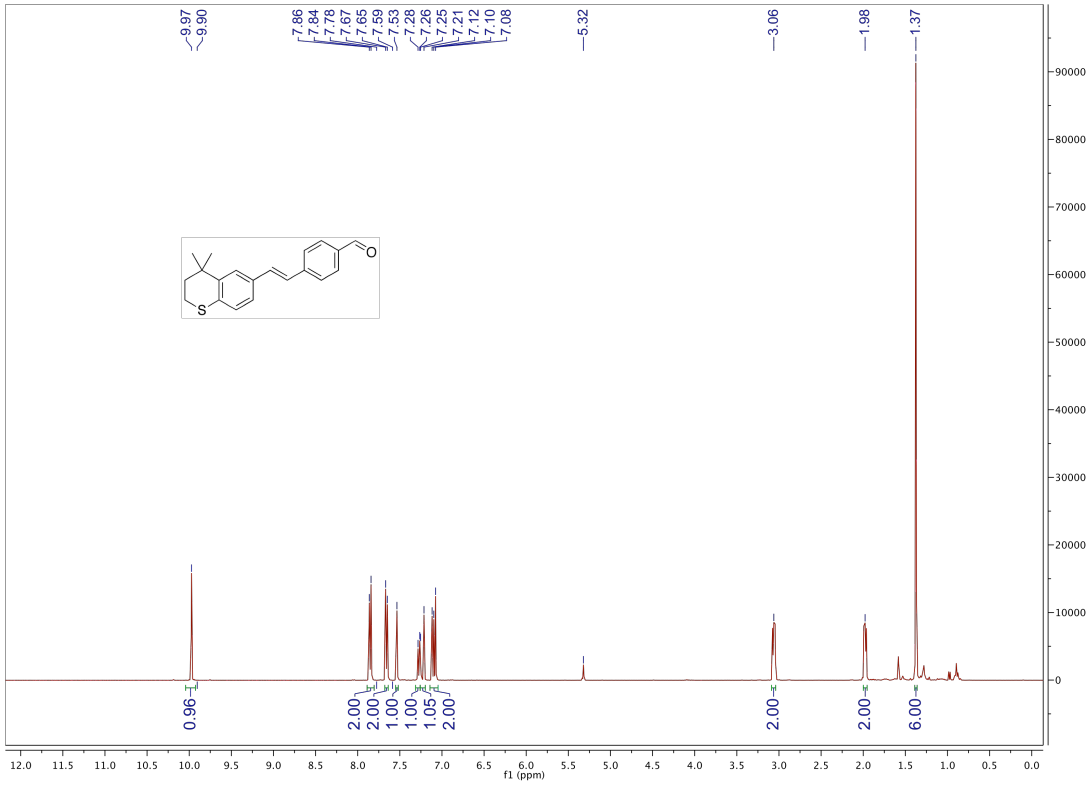
21.99
f1 (ppm)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7.21
7.12
7.10
7.08
5.32
3.06
1.98
1.37
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0.96
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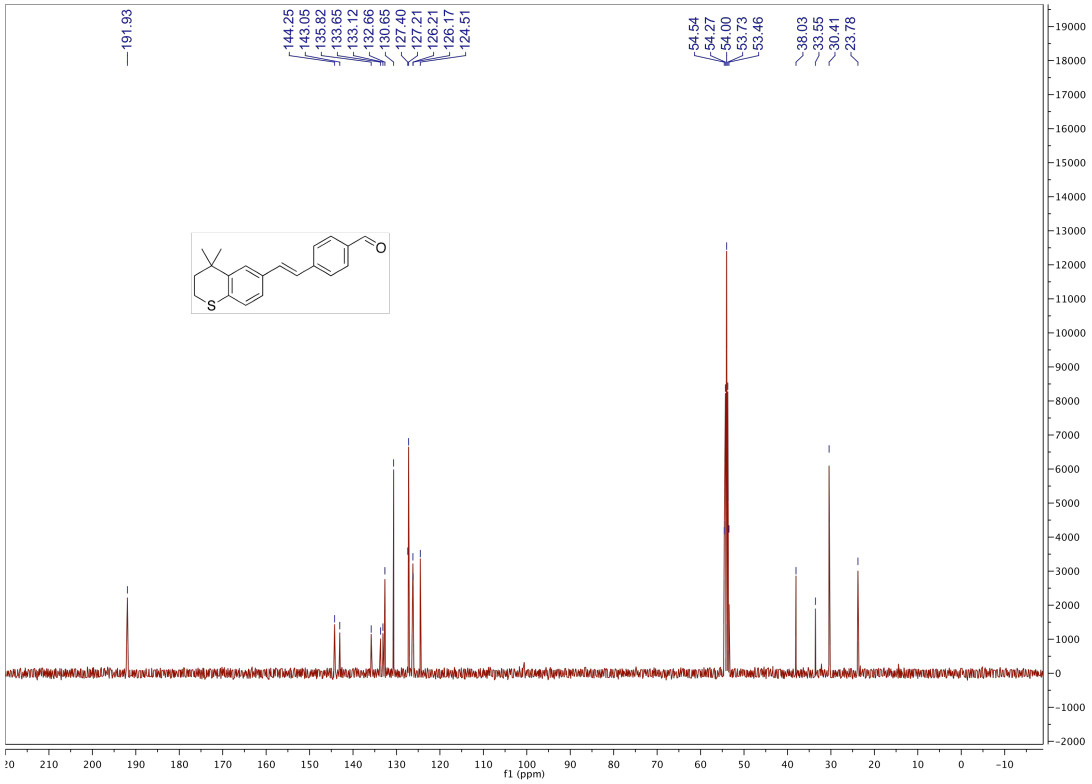
2.00
1.00
1.00
1.05
2.00
2.00
2.00
6.00
f1 (ppm)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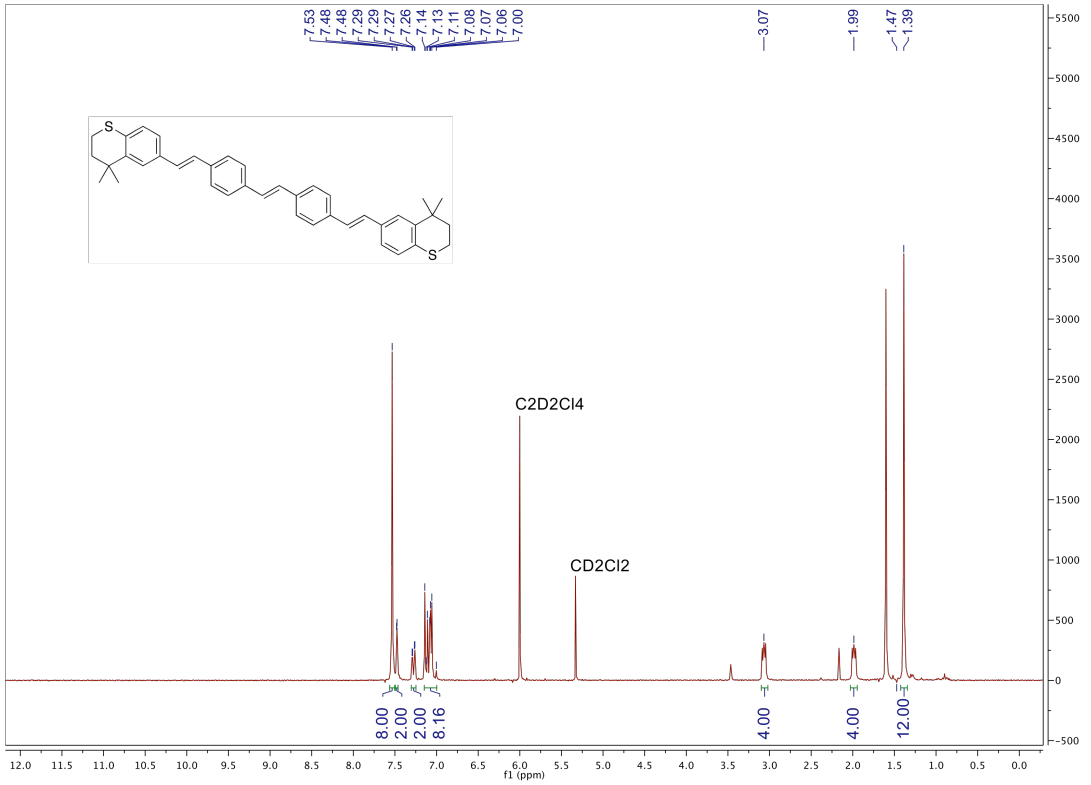
O
S
f1 (ppm)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7.00
3.07
1.99
1.47
1.39
S
S
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CD2Cl2
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2.00
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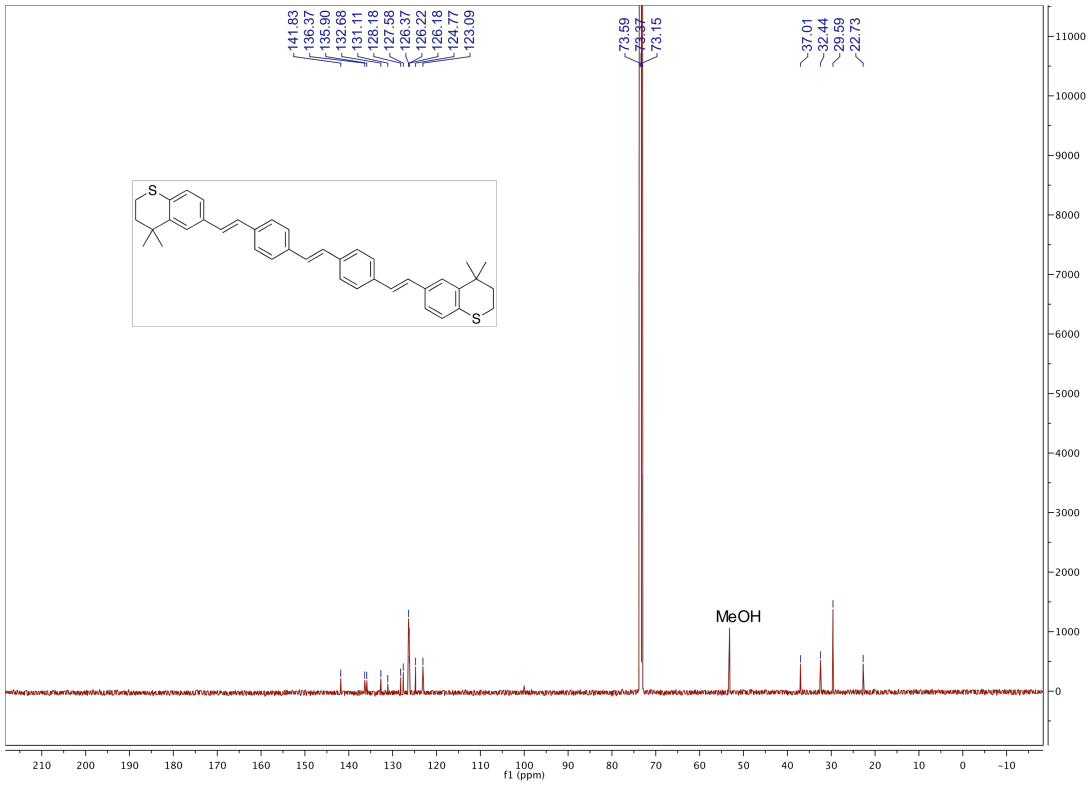
4.00
12.00
f1 (ppm)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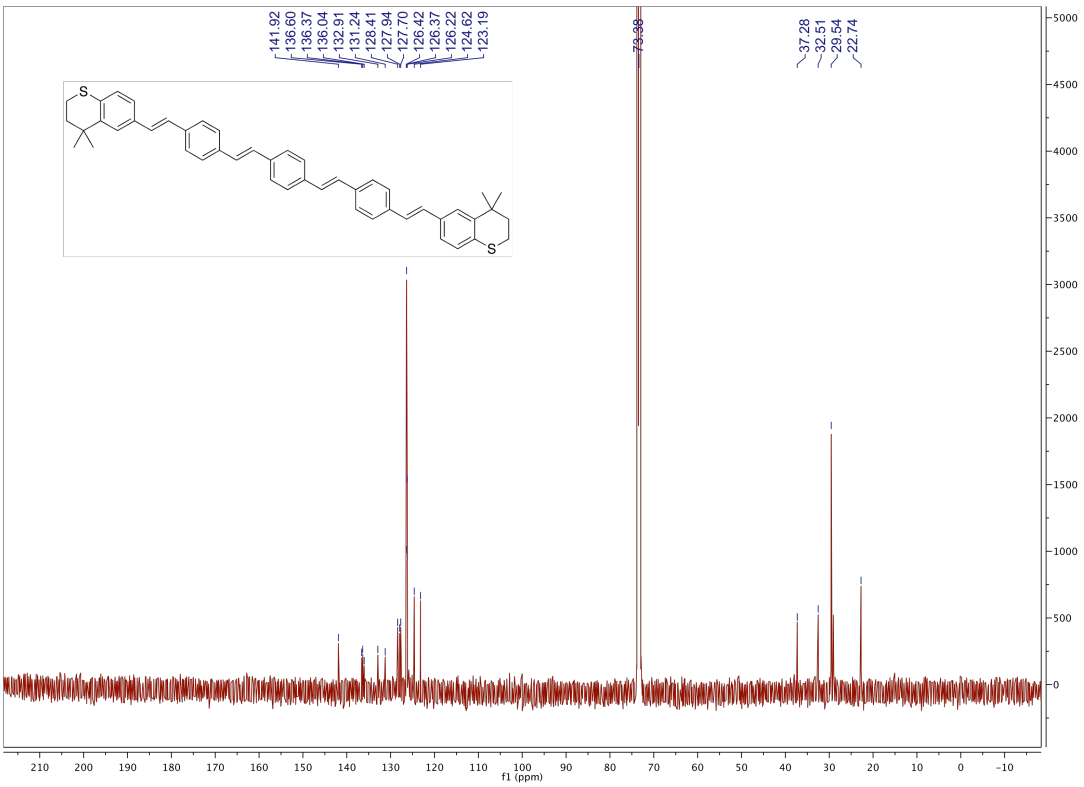
29.59
22.73
S
S
MeOH
f1 (ppm)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29.54
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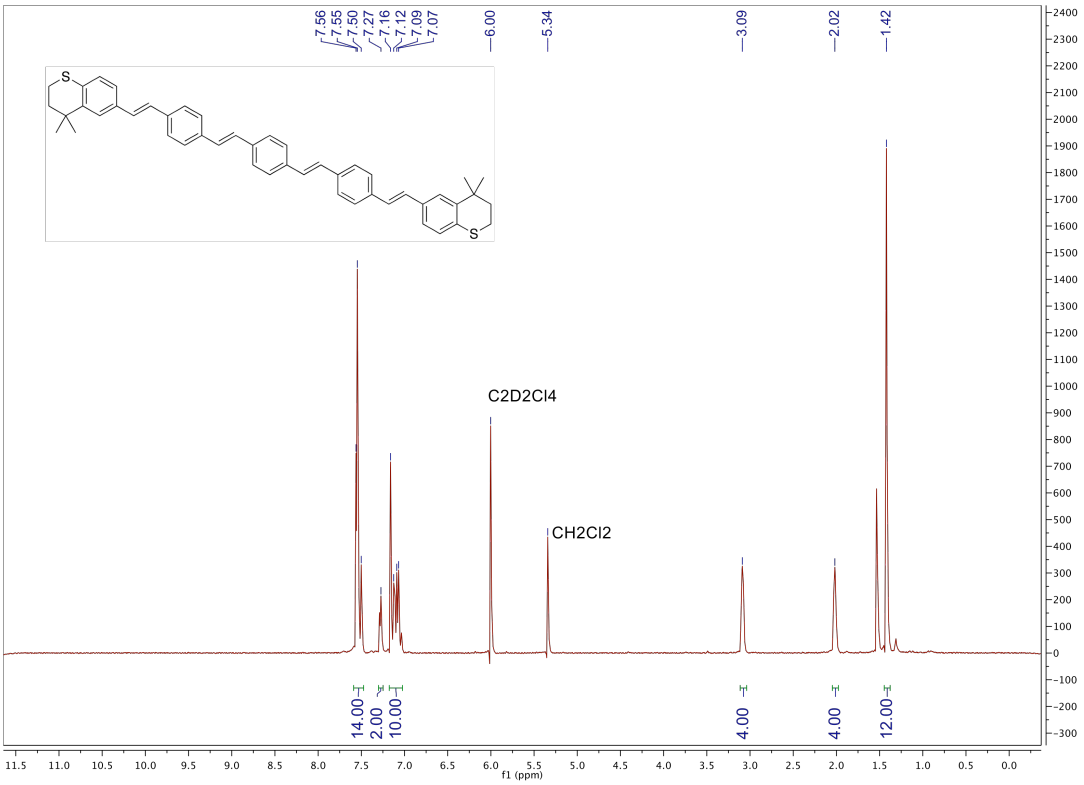
S
S
f1 (ppm)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CH2Cl2
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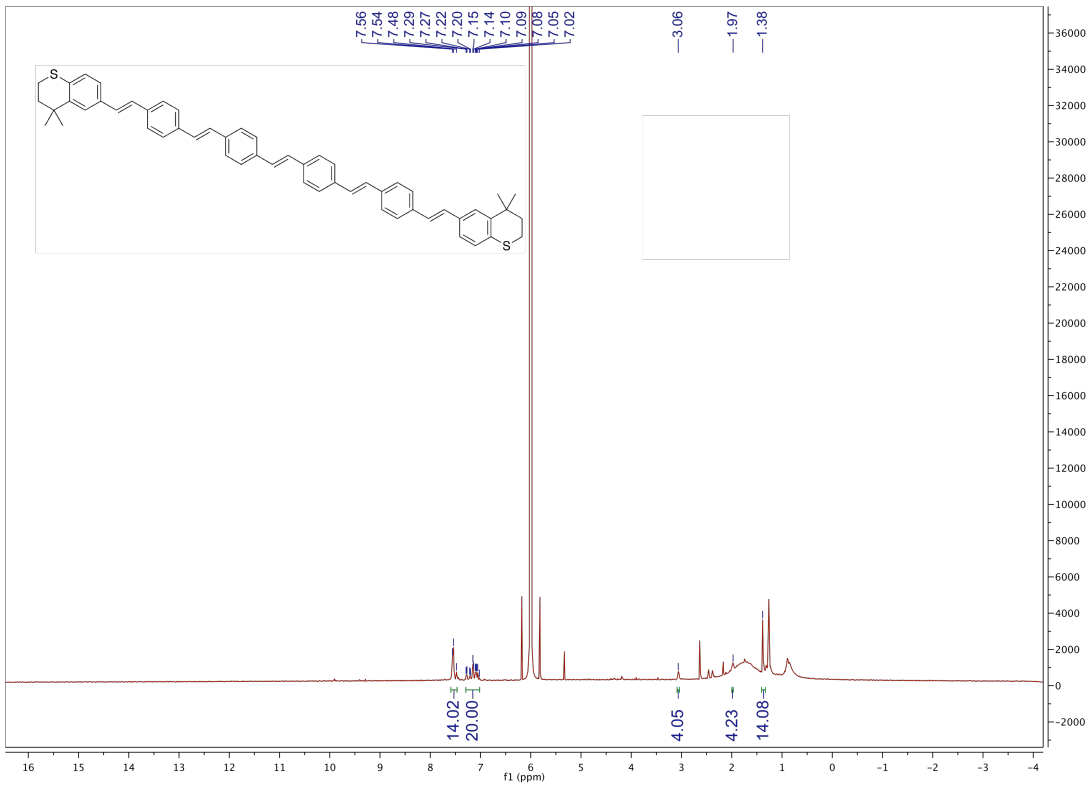
2.00
10.00
4.00
4.00
12.00
f1 (ppm)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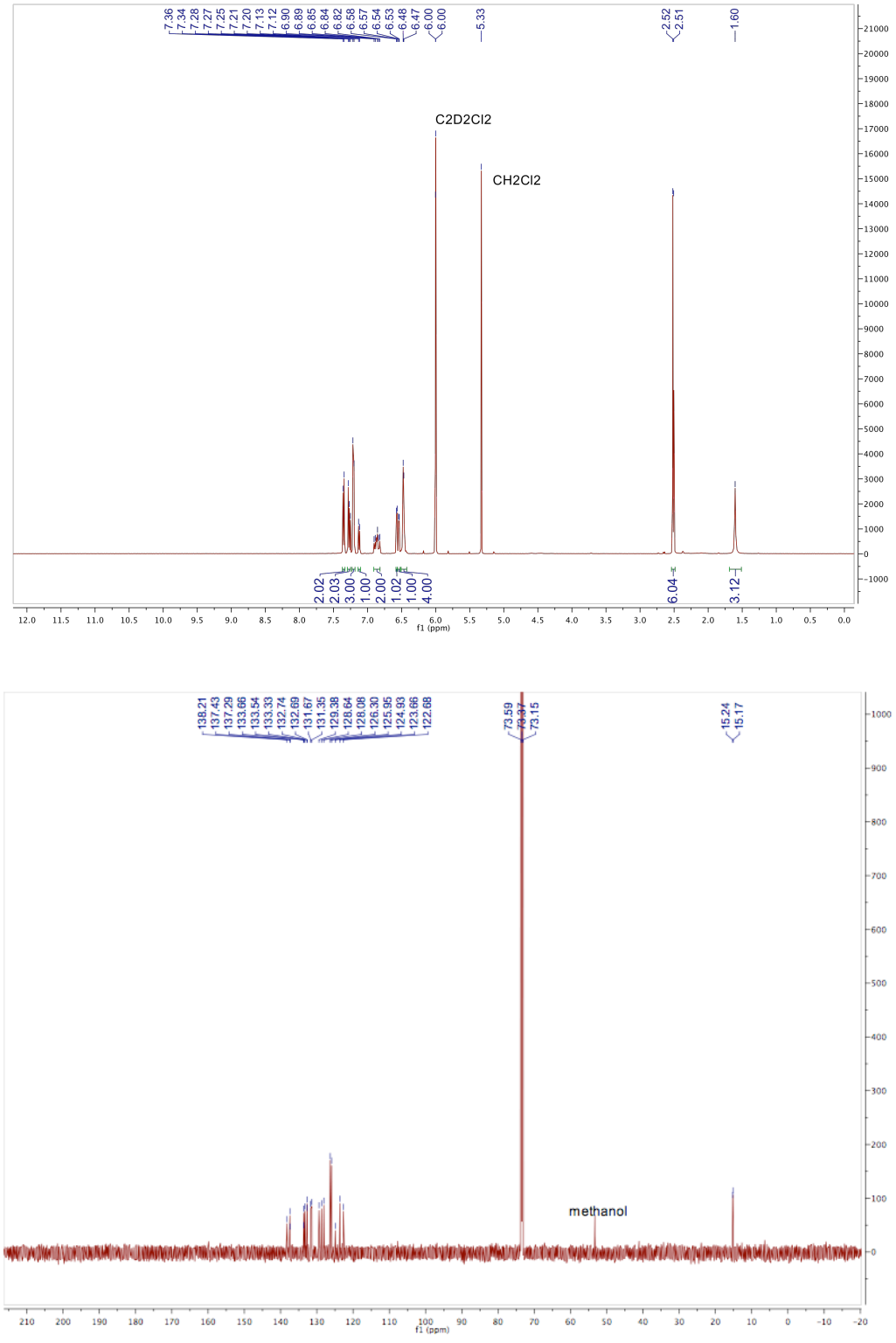
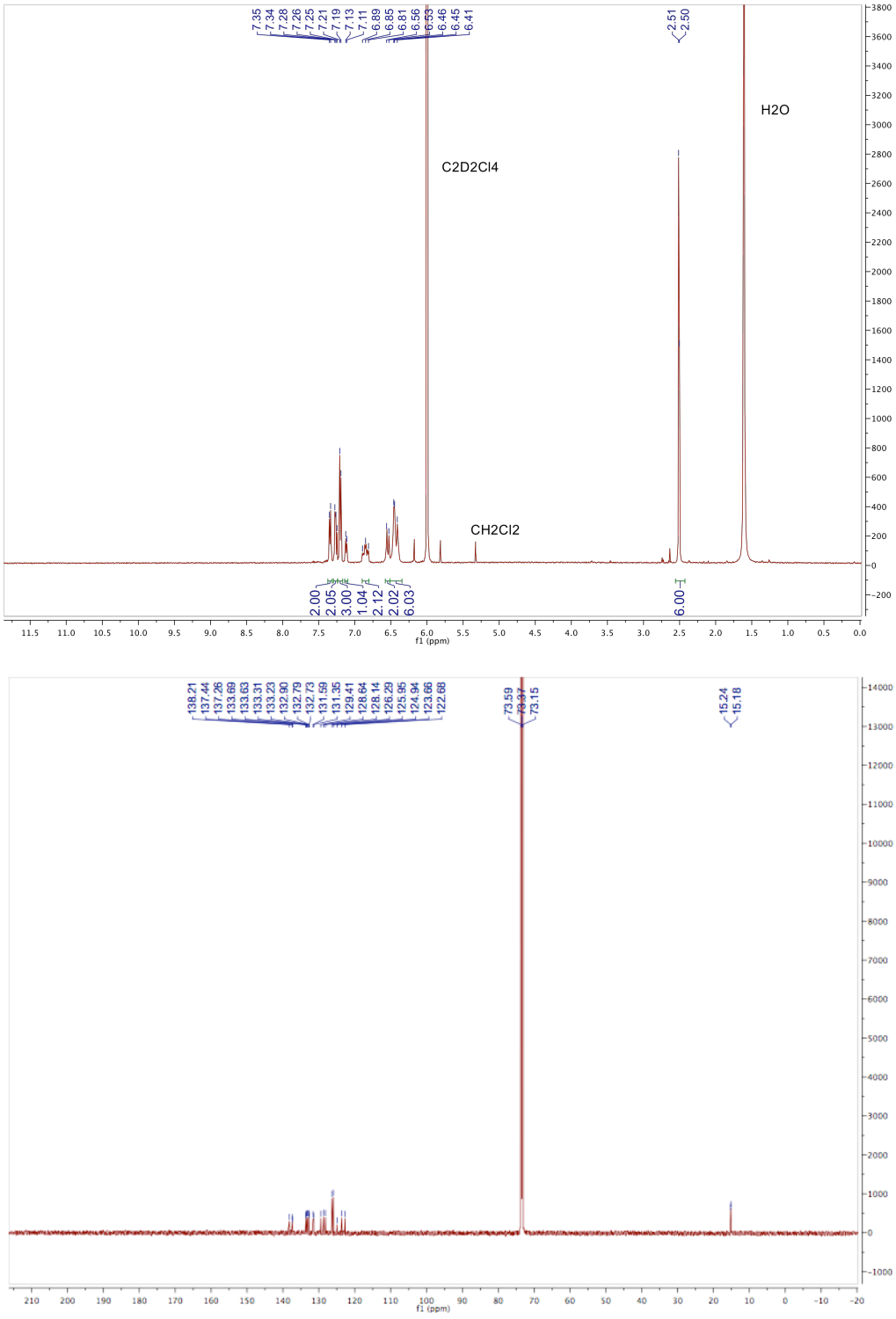
f1 (ppm)



^{1}H and ^{13}C NMR of *1-(3-(methylthio)phenyl)-8-(4-(methylthio)phenyl)-octa-1,3,5,7-tetraene* (**DPO4**) in $C_2D_2Cl_4$.



^{1}H and ^{13}C NMR of *1-(3-(methylthio)phenyl)-10-(4-(methylthio)phenyl)-deca-1,3,5,7,9-pentaene* (**DPO5**) in $C_2D_2Cl_4$.

E3. Optical Absorption Spectroscopy

Absorption spectra were taken on an Agilent Technologies 8453 UV-Vis spectrophotometer using a quartz cuvette with path length equal to 1.0 cm. Solutions of oligomers were prepared in CH_2Cl_2 at concentrations between 10^{-4} and 10^{-5} M.

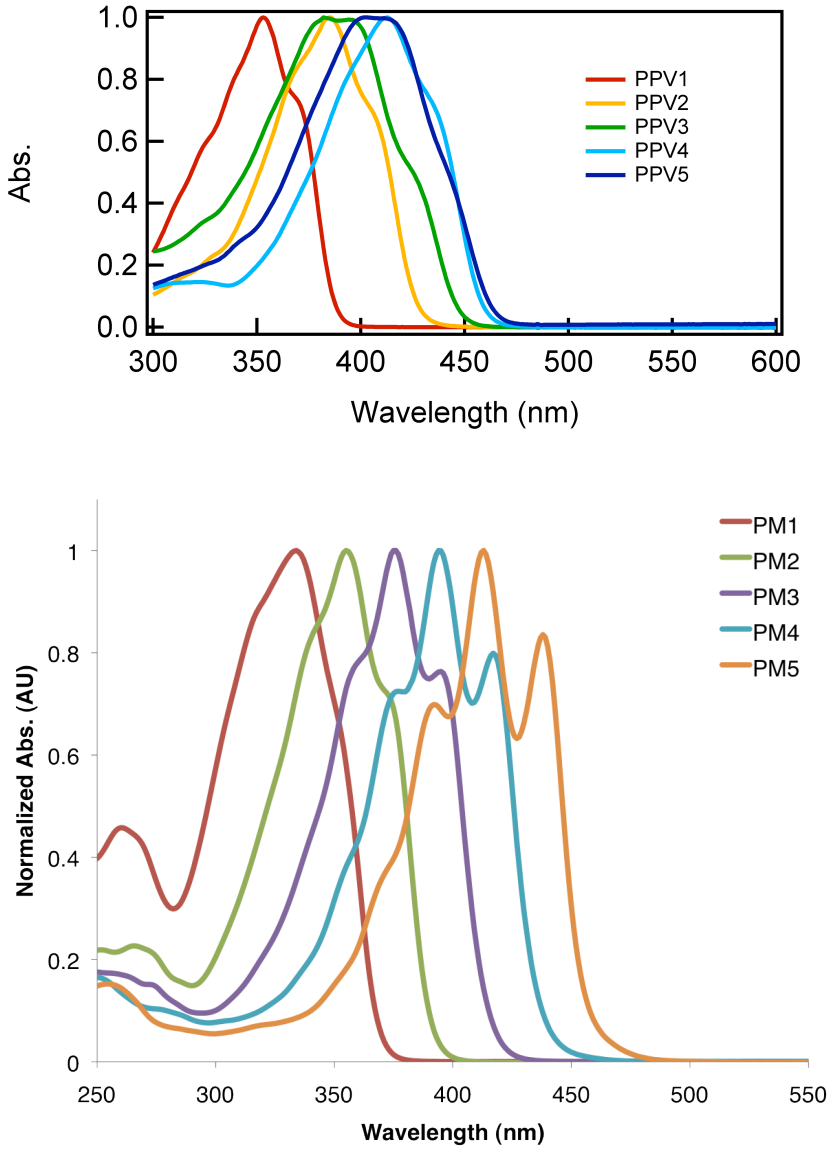


Figure E1: UV-vis optical absorption spectra of (top panel) **PPVn** series, from n = 1 to 5. Due to increased conjugation the longest-wavelength absorptions shift to lower energies. (bottom panel) Spectra of Asymmetric Oligoenes (**DPOn**), from the stilbene to pentaene. For easy comparison, each spectrum was normalized to 1.0 abs.

E4. STM and AFM-BJ Measurement and Analysis

Modified STM-BJ Technique

Details on the experimental technique have been published before.[6] The setups consist of a gold substrate on top of a single axis piezoelectric nanopositioner equipped with a position sensor (Mad City Labs) below a hand-cut gold tip (Alfa-Aesar) with an accuracy of within 5%. During measurement, the conductance of the junction (current/voltage) is measured as a function of piezo displacement. This is done by applying a bias through the junction in series with a fixed resistor (either 100KΩ or 1MΩ) while measuring the current through the junction and the voltage across the junction. The current through the junction is measured using a current amplifier (Keithley 428). A national instruments data acquisition board (PXI-4461) controlled by a Igor (Wavemetrics Inc.) software code controls the bias voltage and piezo position while recording the junction current, piezo position and voltage drop across the junction (sample rate = 40 kHz). The substrates are prepared by evaporating 100nm gold (Alfa-Aesar) on freshly-cleaved mica in a home-build thermal evaporator at a base pressure of 1×10^{-6} mbar. Sample and tip-holder are cleaned in a UV-ozone cleaner prior to measurement. For each tip-sample pair, the quality of the gold and the tunneling background is tested by recording the conductance histogram of typically 1000 traces in air and verifying the presence of (1) peaks at integer values of the conductance quantum and a (2) a featureless background out of contact. Subsequently, one or two droplets of freshly prepared 10^{-5} M solutions of PPV1-PPV5 in 1,2,4-trichlorobenzene (SureSeal, Sigma-Aldrich) are added.

Two-Dimensional Conductance-Displacement Histograms for PPVn

Two-dimensional conductance-displacement were generated by using an automated algorithm by setting the rupture of the G_0 contact as the origin of the displacement axis on each trace; conductance and displacement relative to this origin are then binned to generate 2D maps. In all cases, the same traces used to create linear-binned conductance histograms in Figure 5.3D of Chapter 5 were used to create these histograms.

The most probable length shown in Figure 5.3C (Ch. 5) were determined from a displacement profile of each 2D histogram[7]. Displacement profiles (Figure E3) were created by adding all counts for each displacement along the conductance axis within 1 decade centered around the peak value of the 1D conductance histogram (see Figure E5). Each profile is normalized with respect to its maximum value. The most probable length was taken to be the length at which the profile has an amplitude of 20% of the maximum number of counts.

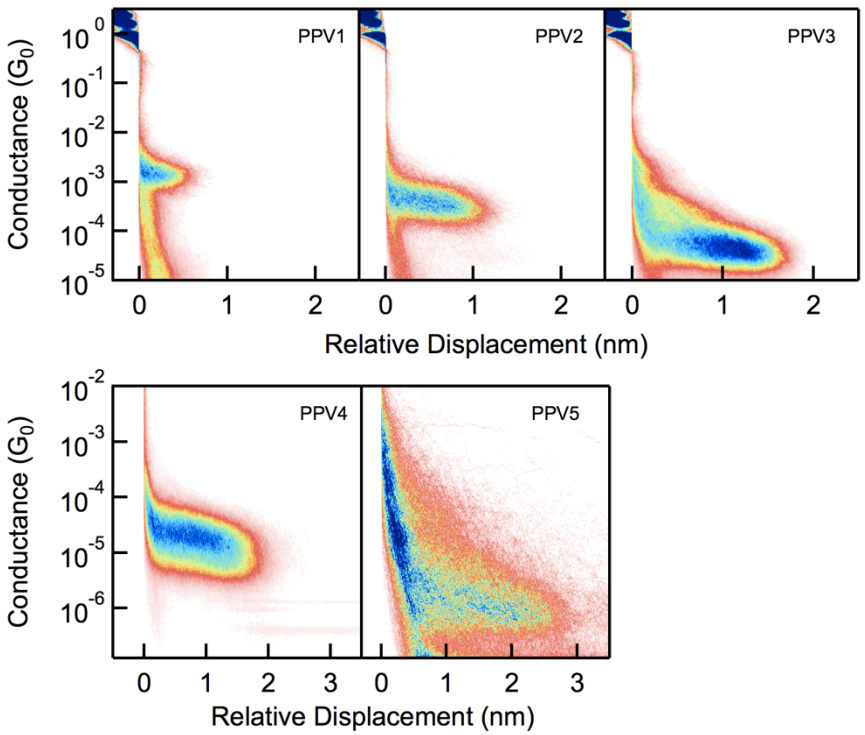


Figure E2: Two-dimensional conductance-displacement histograms for **PPV1-PPV5**.

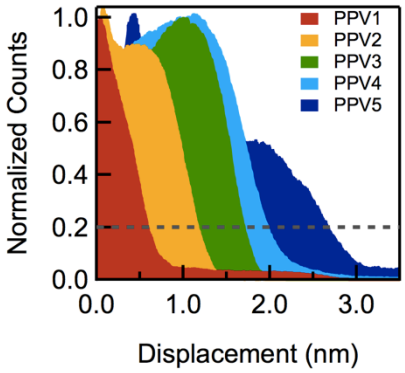


Figure E3: Length profiles of the 2D conductance histograms displayed in Figure E2.

Most-probable conductance from conductance histograms

In the main text, we determined the most probable conductance value for each of the PPV molecules by determining the peak of the linear-binned conductance histograms after subtracting a background from the data and fitting the peak with a log-normal distribution. We show here the details of this method and two other methods that give comparable conductance and beta values for this series.

Method A: Linearly Binned Histograms

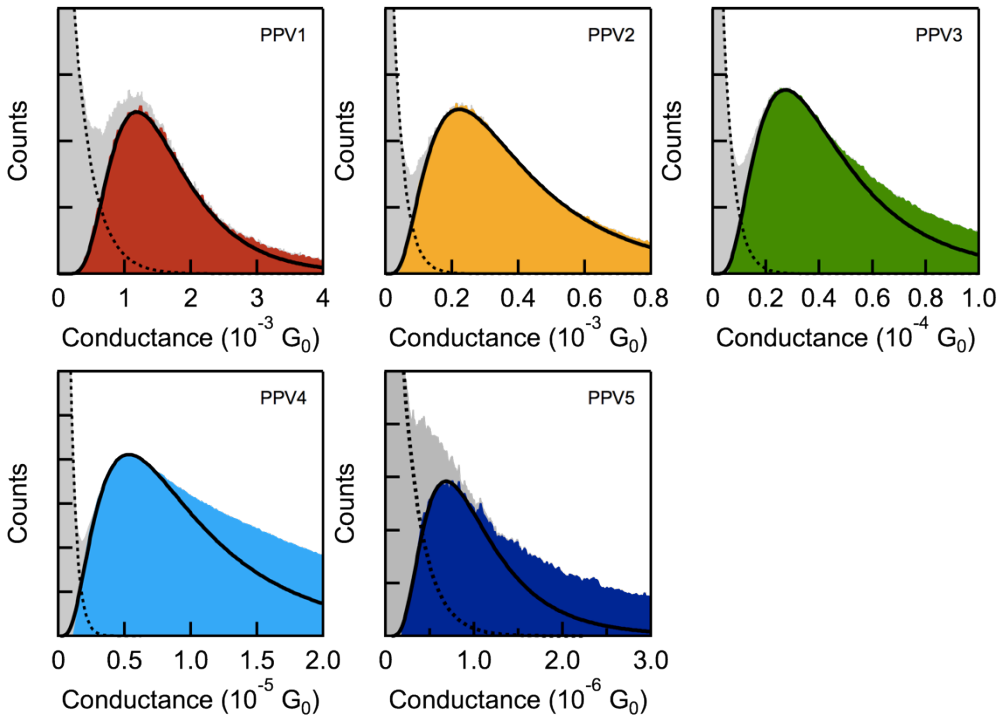


Figure E4: Linearly binned conductance histograms from Figure 5.3D showing the fits and conductance background. Conductance bin size varies from 10^{-4} G_0 for **PPV1** to 10^{-7} G_0 for **PPV5**.

Figure E4 shows *linearly* binned 1D conductance histograms for all five compounds. The most probable conductance value, G_c, for each **PPVn** in the main text was determined by fitting the 1D *linearly* binned histogram (colored areas) with a lognormal distribution (black line) after subtracting an exponential tunneling background (dashed line) from the raw data (grey area).

Method B: Log Binned Histograms

Alternatively, the most-probable conductance can be obtained from a Gaussian [$Ng(g) = C \cdot \exp(-(g - g_c)^2/2w^2)$] fit to the molecular peaks in *logarithmically* binned histograms (Figure E5). From g_c and w, the center of the conductance peak of a lognormal distribution in a linear histogram can is determined[8] as $\log(G_c) = g_c - \ln(10)w^2$.

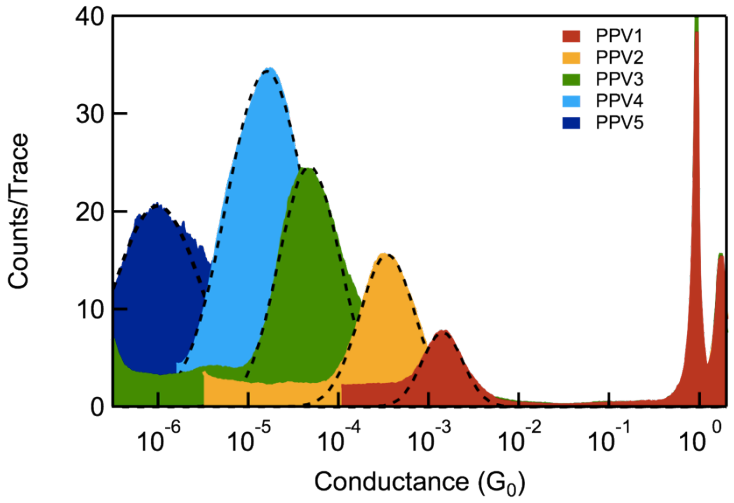


Figure E5: Logarithmically binned conductance histograms with a bin size of 100/decade.

Method C: 2D Histograms

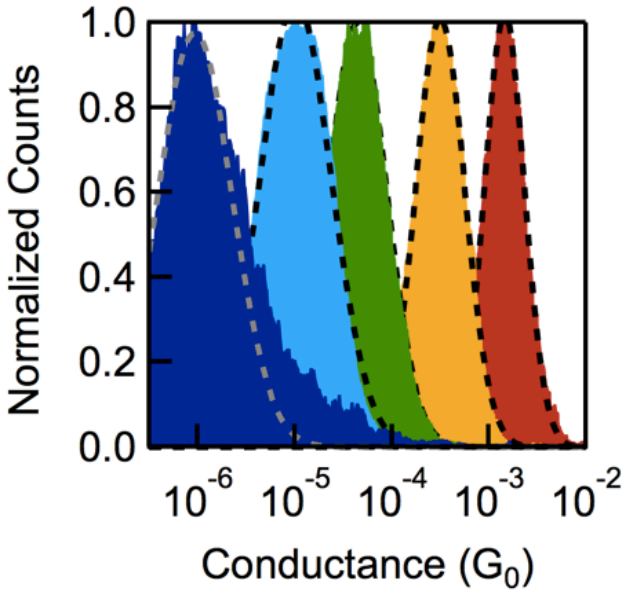


Figure E6: Conductance profiles of the 2D conductance histograms displayed in Figure E2 at two/thirds of the molecular plateau, averaged over 0.2 nm.

Finally, the most probable conductance can be determined from the conductance profile at a specific displacement in a 2D histogram. A displacement profile was created by adding all counts at roughly two thirds of the molecular plateau along the displacement axis for each of the 2D histograms shown in Figure E3. Figure E6 shows conductance profiles for all compounds, scaled to have the same maximum value. The most probable conductance was determined by fitting a Gaussian to these profiles and correcting their peak values as in method B.

Results from the three methods are summarized in Table E1.

	# of	Method A	Method B (Fig S5)			Method C (Fig S6)		
		g_c [G_0]	log(G_c)	w	g_c [G_0]	log(G_c)	w	g_c [G_0]
PPV1	5000	1.2e-3	-2.8	0.23	1.1e-3	-2.8	0.21	1.2e-3
PPV2	5000	2.2e-4	-3.5	0.31	2.2e-4	-3.5	0.25	2.2e-4
PPV3	5000	2.7e-5	-4.3	0.34	2.5e-5	-4.3	0.30	2.7e-5
PPV4	5000	5.3e-6	-4.8	0.45	5.5e-6	-5.0	0.37	5.0e-6
PPV5	2000	6.8e-7	-6.0	0.48	2.9e-7	-6.0	0.38	4.3e-7

Table E1: Comparison between the most-probable conductance value on a linear scale (g_c) determined from a linearly binned histogram (Figure E3) and a logarithmically binned histogram using the conversion method proposed by Huber[8] (Figure E4 and Figure E6).

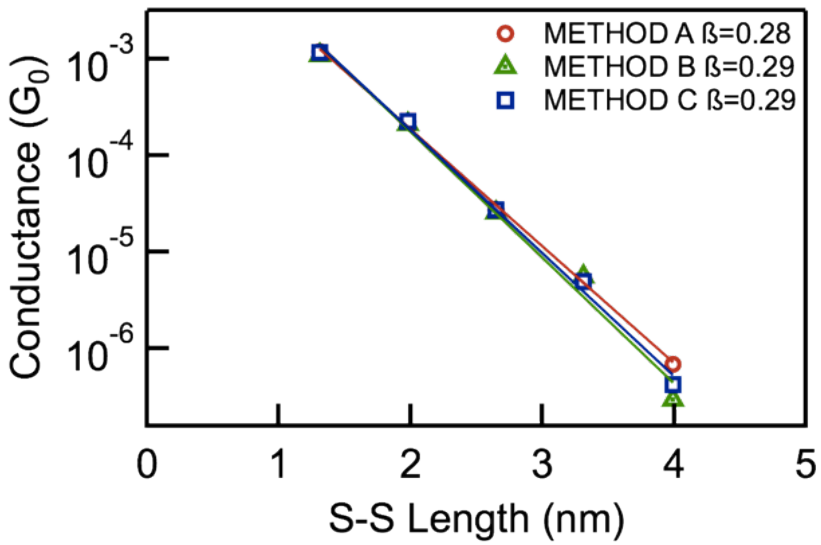


Figure E7: Conductance and corresponding β-values from 3 methods detailed above.

Current-voltage Traces and Histograms

Figure E6 shows 2 sample current-voltage curves for each **PPVn** (n = 1-5). Each trace was recorded after smashing the Au tip into the Au substrate until a conductance value of 5 G_0 was reached. Subsequently, the tip was retracted for 3 nm after which the bias was swept. Just before and after the bias sweep, the conductance was determined. Traces were added into a 2D histogram (see below) when the conductance before and after the bias sweep was found to be in between 10^{-6} and 1 G_0 and differed by no more than 20%.

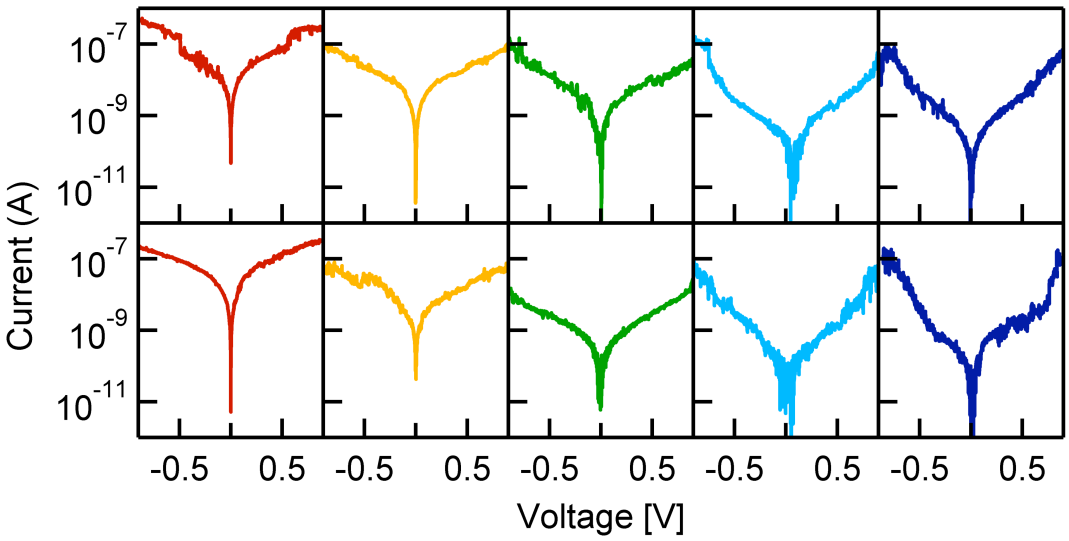


Figure E8: Sample current-voltage Curves for **PPV1-PPV5** (left to right). Only the down sweep is displayed for clarity.

Table E2 list the number of tip-sample pairs, the total number of traces that and the percentage those attempts that resulted in successful current-voltage traces for making

the 2D current-voltage histograms of the main text for each **PPVn**. Histograms were constructed by binning both the measured voltage (bin size = 0.01) and the logarithm of the current (bin size = 0.01) of all measurement points of a trace. The statistical IV curve was determined by fitting the 2D current/voltage map with a at each voltage was determined by fitting the logarithmically binned current distribution with a Gaussian and taking the center of this distribution as the most probable current value.

	# Tip-Sample	Total Traces	% Selected
PPV1	3	68000	4
PPV2	3	90638	18
PPV3	4	120000	23
PPV4	4	120975	14
PPV5	4	80736	10

Table E2: Current-voltage analysis details. Number of tip-sample pairs, total number of traces analyzed and percentage of traces maintaining a molecular plateau during a voltage sweep.

Although the most probable current-voltage curve resulting from each histogram is close to perfectly symmetric with respect to the bias polarity, individual current-voltage characteristics can show some asymmetry with respect to the bias polarity. To give an impression of the spread in individually obtained IVs, we determined the rectification ratio for each individual current-voltage characteristic of **PPV2**. The rectification ratio is defined as $^{10}\log(I(V=+0.7))/^{10}\log(I(V=-0.7))$. Figure S7 displays the rectification ratio for each current-voltage trace and also shows the resulting histogram. The histogram is centered around 1 and no time dependence on the rectification ratio is observed.

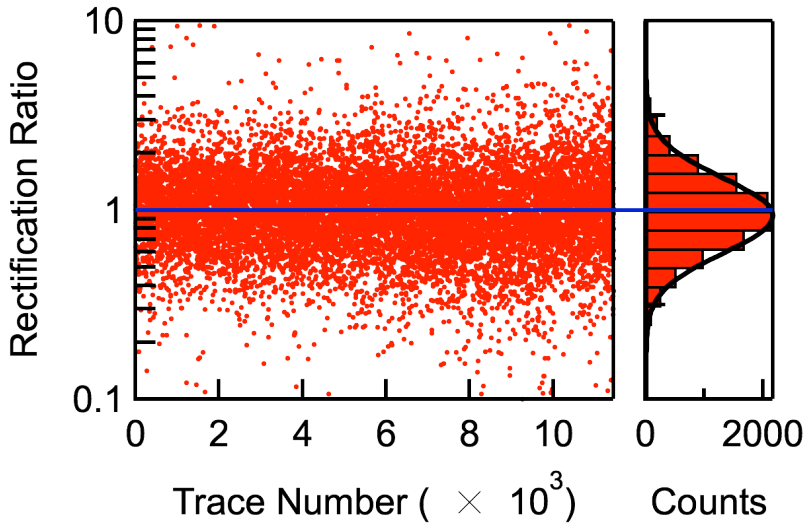


Figure E9: Rectification ratio as a number of the measured trace number for **PPV2**.

To check for any dependency of the most-probable IV on the sweep direction we constructed a 2D IV histogram for both positive and negative sweep direction: from 0 to 0.8 V and 0.8 to 0 V, respectively. Figure E10 shows the resulting histograms and most-probable IV curve for 11445 IV traces of **PPV2**. The traces are close to identical.

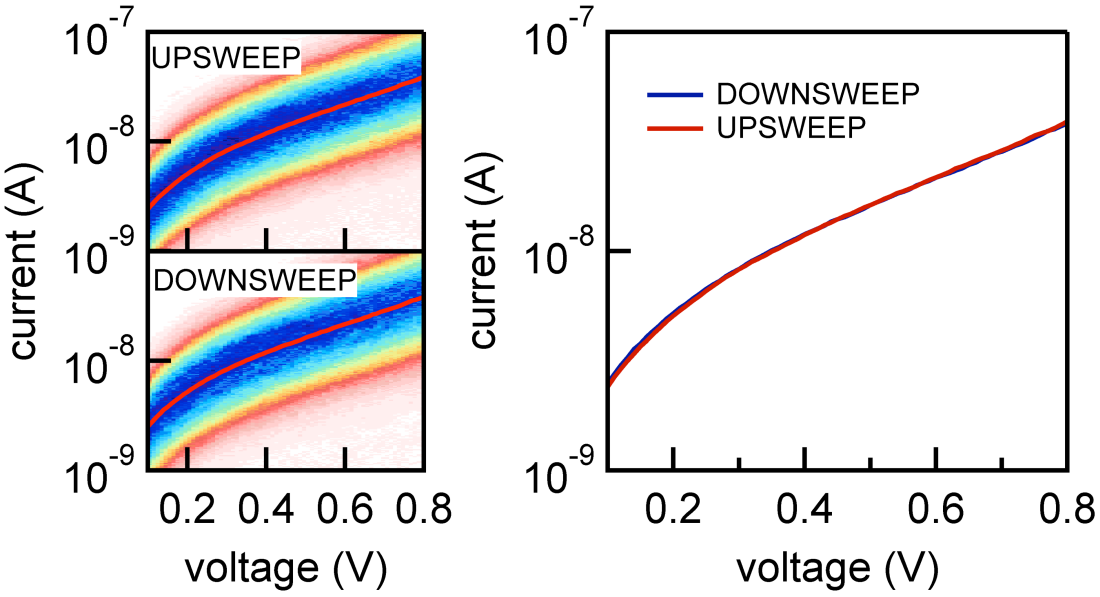


Figure E10: Dependence of sweep direction for 11455 IV traces of **PPV2**.

We find the number of selected IVs to decrease with the maximum amplitude of the bias voltage ramp. Figure E11 summarizes the bridging probability as a function of maximum applied bias voltage for **PPV4**.

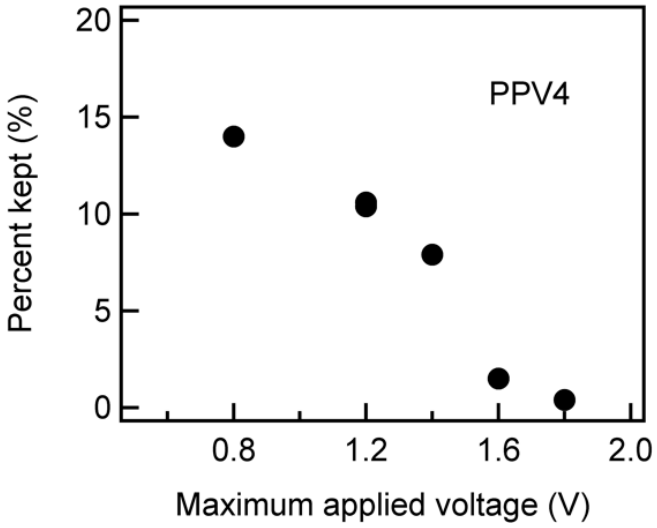


Figure E11: Bridging probability for **PPV4** as a function of applied maximum bias voltage in the ramp. For V = 1.2, 1.4, 1.6, and 1.8 V, a total of 1000 curves were recorded and traces were selected as described above. The data point at 1.2 was reproduced before and after ramping the maximum bias to 1.8 V. The data point at V = 0.8 V was determined from the analysis described above using 120975 traces (solid data point).

Current-voltage Fitting Procedure

The most-probable current-voltage characteristics were fit to equation 5.1 and 5.2 of the main text.

T [K]	ϵ [meV]					Γ [meV]					Fit error [-]				
	PPV1	**PPV2**	**PPV3**	**PPV4**	**PPV5**	**PPV1**	**PPV2**	**PPV3**	**PPV4**	**PPV5**	**PPV1**	**PPV2**	**PPV3**	**PPV4**	**PPV5**
300	790	620	550	500	500	34.5	11.6	5.1	2.4	1.0	0.013	0.183	0.508	5.990	4.168
350	770	640	570	520	520	33.3	12.0	5.3	2.5	1.0	0.014	0.194	0.435	4.799	2.126
400	780	660	590	530	540	33.7	12.4	5.4	2.4	1.0	0.013	0.207	0.366	3.826	1.082
450	790	680	610	550	570	34.1	12.8	5.6	2.4	1.0	0.013	0.213	0.291	3.219	0.762
500	**800**	**690**	**630**	**560**	**590**	**34.5**	**12.8**	**5.7**	**2.3**	**0.9**	**0.014**	**0.217**	**0.218**	**3.098**	**0.688**
550	820	710	650	580	610	35.4	13.2	5.8	2.3	0.9	0.012	0.201	0.172	3.185	1.039
600	840	740	670	590	630	36.2	13.8	5.9	2.0	0.9	0.014	0.214	0.125	3.508	1.780
650	850	750	690	610	630	36.6	13.8	6.0	2.0	0.6	0.014	0.193	0.096	3.858	2.566
700	870	770	710	610	630	37.4	14.0	6.0	1.6	0.5	0.014	0.198	0.067	4.353	3.627
750	870	790	730	630	650	37.0	14.4	6.0	1.5	0.5	0.016	0.194	0.056	4.978	5.291
800	900	810	750	650	670	38.2	14.6	6.0	1.5	0.5	0.015	0.181	0.051	6.110	7.642

Table E3: Results from fits at different temperatures.

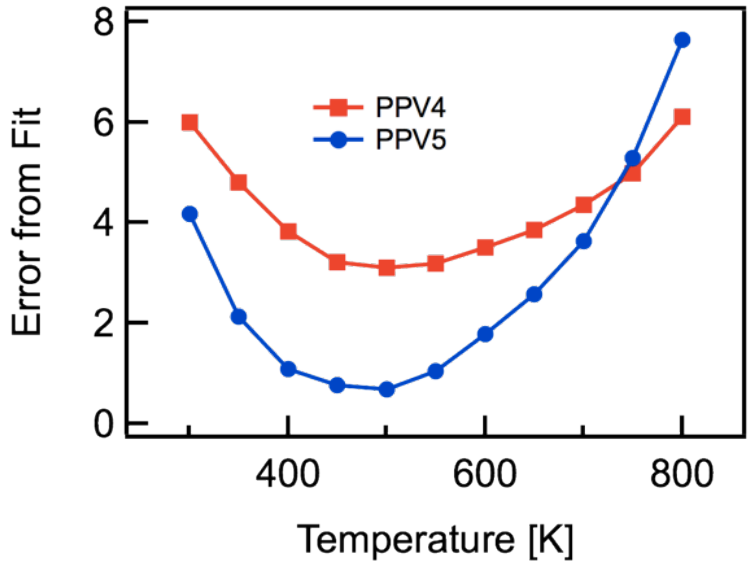


Figure E12: For **PPV4** and **PPV5**, the fit error parameter shows a clear minimum around T = 500. In this case, $\Gamma \ll k_B T$. Therefore, the width of the voltage range, over which the current increases, is determined by the electronic temperature of the leads (Fermi functions).

C5. Theoretical Methods and Details

All electronic structure calculations used Jaguar (version 7.8, Schrodinger LLC, New York, NY, 2011) using the B3LYP hybrid functional and the 6-31G** basis sets. The geometries of MeS-**PPVn**, **PPVn** and **DPO1**-**DPO5** were fully optimized. The final geometries, total energies, bond distances, bond angles and torsional angles may be found in the following sections. Below is a summary of the HOMO-LUMO energy differences (band gap) results of our calculations on methylthio-derivatives (**MeS-PPVn**; n = 1 to 6) and our **PPVn** series (from n = 1 to 5). **MeS-PPVn** molecules are model compounds for our PPV series. Geometry optimizations of the longer **PPVn** molecules (**PPV3**, **PPV4** and **PPV5**) were found to converge on a distribution of geometries, all of which were energetically similar. The geometries differed from each other by small degrees of twists and bends along the backbone. Incorporation of even the smallest twist and bend gave larger variations in the molecular length (i.e. S-S distance). **MeS-PPVn**'s however converged on reliable linear geometries, which are expected during break junction experiments. In such cases, sulfur-to-sulfur (S-S) distances were taken from the **MeS-PPVn** series calculations and not from the **PPVn** calculations and are shown in Table E4.

PPVn	S-S Length [nm]	HOMO [eV]	LUMO [eV]	HOMO-LUMO gap [eV]
n = 1	1.30	-4.90	-1.23	3.67
n = 2	1.97	-4.84	-1.68	3.16
n = 3	2.65[a]	-4.82	-1.86	2.96
n = 4	3.31[a]	-4.86	-2.06	2.80
n = 5	3.99[a]	-4.79	-2.11	2.68
MeS-PPVn	S-S Length [nm][a]	HOMO [eV]	LUMO [eV]	HOMO-LUMO gap [eV]
n = 1	1.31	-5.03	-1.34	3.69
n = 2	1.98	-4.93	-1.75	3.18
n = 3	2.65	-4.88	-1.95	2.93
n = 4	3.31	-4.85	-2.06	2.79
n = 5	3.99	-4.84	-2.13	2.71
N = 6	4.65	-4.82	-2.18	2.64
DPOn	S-S Length [nm]	HOMO [eV]	LUMO [eV]	HOMO-LUMO gap [eV]
n = 1	1.20	-5.22	-1.41	3.81
n = 2	1.45	-5.06	-1.66	3.40
n = 3	1.70	-4.93	-1.86	3.07
n = 4	1.95	-4.70	-1.95	2.75
n = 5	2.17	-4.62	-2.07	2.55

Table E4: DFT calculation results on **PPVn**, **MeS-PPVn** and **DPOn** series. [a]Due to unreliable geometry optimization convergence, sulfur-to-sulfur (S-S) distances for the longer oligomers, **PPV3-PPV5**, were estimated from DFT calculations performed on the model series **MeS-PPV**.

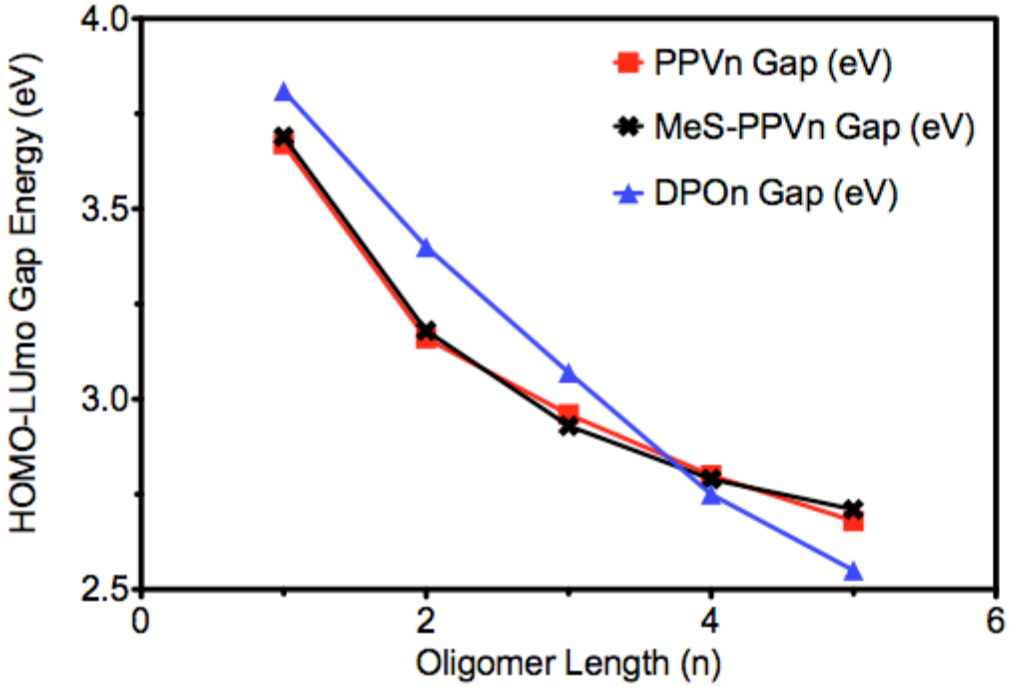
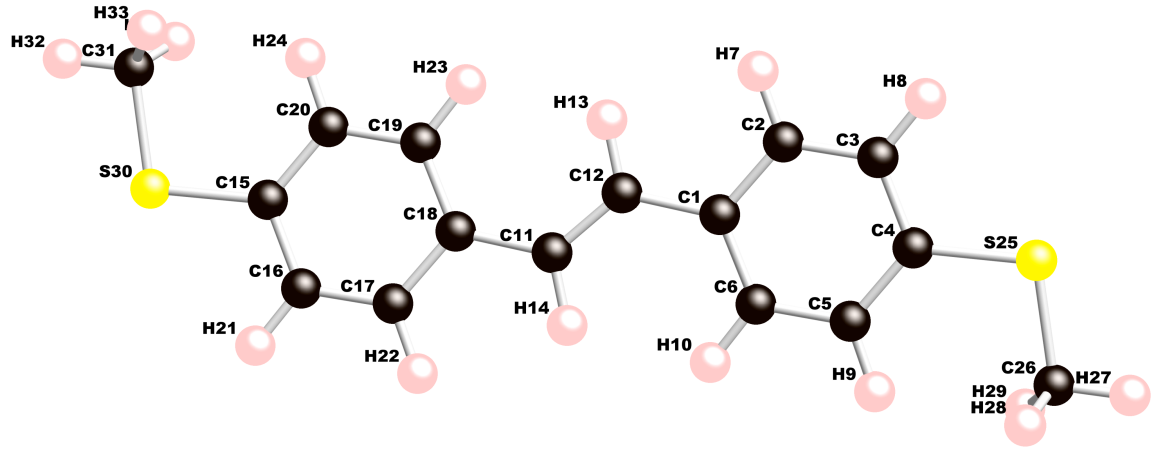


Figure E13: DFT estimations of the molecular band gap of **PPVn** series. Molecular band gap converges as oligomer length (n) increases. Simpler methylthio-derivatives (**MeS-PPVn**) are an adequate model series for exploring our **PPVn** series, since they predict very similar electronic properties. Length-dependent electronic properties of oligo-phenylenevinylene compounds have been previously studied. Experimental results have predicted the saturation of the electronic properties at oligomeric lengths of $n \approx 10$.[2,6]

DFT Summary PPVn and MeS-PPVn Molecules:

MeS-PPV1



Final geometry:

		angstroms	
atom	x	y	z
C1	-3.8434660000	-1.8489490000	-0.0120390000
C2	-4.5597980000	-0.6660920000	-0.2805620000
C3	-5.9467260000	-0.6325680000	-0.2796430000
C4	-6.6855500000	-1.7937950000	-0.0064350000
C5	-5.9902290000	-2.9808490000	0.2650090000
C6	-4.5991960000	-3.0026450000	0.2621140000
H8	-4.0097130000	0.2469100000	-0.4949240000
H9	-6.4629520000	0.2996400000	-0.4916890000
H11	-6.5258520000	-3.8979330000	0.4823060000
H12	-4.0982710000	-3.9407700000	0.4812260000
C12	-1.5316800000	-2.8421870000	0.1511900000
C13	-2.3802640000	-1.8091180000	-0.0312520000
H15	-1.9652880000	-0.8205090000	-0.2198580000
H16	-1.9486870000	-3.8323930000	0.3259490000
C16	2.7734880000	-2.8774920000	0.1311410000
C17	2.0277380000	-4.0554880000	0.2888180000

C18	0.6411750000	-4.0140390000	0.2921140000
C19	-0.0682760000	-2.8065060000	0.1381970000
C20	0.6946140000	-1.6350750000	-0.0162370000
C21	2.0856460000	-1.6651370000	-0.0209750000
H23	2.5383210000	-5.0068560000	0.4096630000
H24	0.0856860000	-4.9404060000	0.4159550000
H25	0.1994170000	-0.6754220000	-0.1305300000
H26	2.6273680000	-0.7339750000	-0.1424060000
S26	-8.4609420000	-1.6384940000	-0.0311870000
C27	-9.0457400000	-3.3122040000	0.3862640000
H28	-10.1358270000	-3.2488760000	0.3880750000
H29	-8.7357640000	-4.0449030000	-0.3622960000
H30	-8.7077890000	-3.6191340000	1.3787460000
S30	4.5474530000	-3.0472520000	0.1422380000
C31	5.1465920000	-1.3400390000	-0.0658390000
H32	6.2362570000	-1.4100410000	-0.0593390000
H33	4.8255890000	-0.9149800000	-1.0193300000
H34	4.8286740000	-0.6998450000	0.7601080000

Total energy (hartrees): -1415.73607450152

HOMO energy (hartrees): -0.18483

LUMO energy (hartrees): -0.04926

Bond lengths (angstroms):

C1	-C2	:	1.408683	C1	-C6	:	1.406166
C1	-C13	:	1.463870	C2	-C3	:	1.387333

C2 -H8 : 1.087252 C3 -C4 : 1.403193

C3 -H9 : 1.086492 C4 -C5 : 1.402230

C4 -S26 : 1.782343 C5 -C6 : 1.391207

C5 -H11 : 1.084045 C6 -H12 : 1.085824

C12 -C13 : 1.349300 C12 -H16 : 1.088551

C12 -C19 : 1.463897 C13 -H15 : 1.088634

C16 -C17 : 1.403096 C16 -C21 : 1.402166

C16 -S30 : 1.782104 C17 -C18 : 1.387186

C17 -H23 : 1.086462 C18 -C19 : 1.408952

C18 -H24 : 1.087226 C19 -C20 : 1.406450

C20 -C21 : 1.391365 C20 -H25 : 1.085918

C21 -H26 : 1.084099 S26 -C27 : 1.821417

C27 -H28 : 1.091926 C27 -H29 : 1.092371

C27 -H30 : 1.092446 S30 -C31 : 1.821219

C31 -H32 : 1.091931 C31 -H33 : 1.092183

C31 -H34 : 1.092295

Bond angles:

C6 -C1 -C2 : 116.923317 C13 -C1 -C2 : 118.876979

C13 -C1 -C6 : 124.199617 C3 -C2 -C1 : 121.906029

H8 -C2 -C1 : 119.040098 H8 -C2 -C3 : 119.053871

C4 -C3 -C2 : 120.431514 H9 -C3 -C2 : 119.709051

H9 -C3 -C4 : 119.859433 C5 -C4 -C3 : 118.500734

S26 -C4 -C3 : 116.722201 S26 -C4 -C5 : 124.777037

C6 -C5 -C4 : 120.575007 H11 -C5 -C4 : 120.661252

H11 -C5 -C6 : 118.763685 C5 -C6 -C1 : 121.663176

H12 -C6 -C1 : 120.017019 H12 -C6 -C5 : 118.319632

H16 -C12 -C13 : 118.505622 C19 -C12 -C13 : 127.505200

C19 -C12 -H16 : 113.988445 C12 -C13 -C1 : 127.301743

H15 -C13 -C1 : 114.079178 H15 -C13 -C12 : 118.618703

C21 -C16 -C17 : 118.514128 S30 -C16 -C17 : 116.641084

S30 -C16 -C21 : 124.844764 C18 -C17 -C16 : 120.427320

H23 -C17 -C16 : 119.860759 H23 -C17 -C18 : 119.711915

C19 -C18 -C17 : 121.914514 H24 -C18 -C17 : 119.045577

H24 -C18 -C19 : 119.039873 C18 -C19 -C12 : 118.783561

C20 -C19 -C12 : 124.299272 C20 -C19 -C18 : 116.917000

C21 -C20 -C19 : 121.646087 H25 -C20 -C19 : 120.017018

H25 -C20 -C21 : 118.336142 C20 -C21 -C16 : 120.580679

H26 -C21 -C16 : 120.642222 H26 -C21 -C20 : 118.776986

C27 -S26 -C4 : 103.683925 H28 -C27 -S26 : 105.522306

H29 -C27 -S26 : 111.603754 H29 -C27 -H28 : 108.864039

H30 -C27 -S26 : 111.534903 H30 -C27 -H28 : 108.881948

H30 -C27 -H29 : 110.262660 C31 -S30 -C16 : 103.737140

H32 -C31 -S30 : 105.516675 H33 -C31 -S30 : 111.584580

H33 -C31 -H32 : 108.871487 H34 -C31 -S30 : 111.547237

H34 -C31 -H32 : 108.876169 H34 -C31 -H33 : 110.272905

Torsional angles:

C1 -C2 -C3 -C4 : 0.027461

C1 -C2 -C3 -H9 :-179.992791

C1 -C6 -C5 -C4 : -0.100423

C1 -C6 -C5 -H11 : 179.984987

C1 -C13 -C12 -H16 : 0.596812

C1 -C13 -C12 -C19 :-179.734991

C2 -C1 -C6 -C5 : 0.177313

C2 -C1 -C6 -H12 :-179.668757

C2 -C1 -C13 -C12 :-177.369845

C2 -C1 -C13 -H15 : 2.401878

C2 -C3 -C4 -C5 : 0.055742

C2 -C3 -C4 -S26 : 179.997672

C3 -C2 -C1 -C6 : -0.141275

C3 -C2 -C1 -C13 : 179.961316

C3 -C4 -C5 -C6 : -0.020014

C3 -C4 -C5 -H11 : 179.892947

C3 -C4 -S26 -C27 :-179.158176

C4 -C3 -C2 -H8 :-179.985191

C4 -C5 -C6 -H12 : 179.748171

C4 -S26 -C27 -H28 : 179.518535

C4 -S26 -C27 -H29 : -62.388479

C4 -S26 -C27 -H30 : 61.440312

C5 -C4 -C3 -H9 :-179.923975

C5 -C4 -S26 -C27 : 0.779693

C5 -C6 -C1 -C13 :-179.931303

C6 -C1 -C2 -H8 : 179.871376

C6 -C1 -C13 -C12 : 2.740750

C6 -C1 -C13 -H15 :-177.487527

C6 -C5 -C4 -S26 :-179.956866

H8 -C2 -C1 -C13 : -0.026033

H8 -C2 -C3 -H9 : -0.005444

H9 -C3 -C4 -S26 : 0.017955

H11 -C5 -C4 -S26 : -0.043906

H11 -C5 -C6 -H12 : -0.166419

H12 -C6 -C1 -C13 : 0.222627

C12 -C19 -C18 -C17 : 179.959990

C12 -C19 -C18 -H24 : 0.029538

C12 -C19 -C20 -C21 :-179.972064

C12 -C19 -C20 -H25 : 0.349004

C13 -C12 -C19 -C18 :-177.231741

C13 -C12 -C19 -C20 : 2.921653

H15 -C13 -C12 -H16 :-179.165768

H15 -C13 -C12 -C19 : 0.502429

H16 -C12 -C19 -C18 : 2.449115

H16 -C12 -C19 -C20 :-177.397491

C16 -C17 -C18 -C19 : 0.071874

C16 -C17 -C18 -H24 :-179.997678

C16 -C21 -C20 -C19 : -0.065908

C16 -C21 -C20 -H25 : 179.618242

C16 -S30 -C31 -H32 : 179.794649

C16 -S30 -C31 -H33 : -62.116894

C16 -S30 -C31 -H34 : 61.720215

C17 -C16 -C21 -C20 : -0.051328

C17 -C16 -C21 -H26 : 179.824959

C17 -C16 -S30 -C31 :-179.439229

C17 -C18 -C19 -C20 : -0.182126

C18 -C17 -C16 -C21 : 0.048406

C18 -C17 -C16 -S30 : 179.994581

C18 -C19 -C20 -C21 : 0.178712

C18 -C19 -C20 -H25 :-179.500220

C19 -C18 -C17 -H23 :-179.956366

C19 -C20 -C21 -H26 :-179.944472

C20 -C19 -C18 -H24 : 179.887422

C20 -C21 -C16 -S30 :-179.992706

C21 -C16 -C17 -H23 :-179.923311

C21 -C16 -S30 -C31 : 0.503142

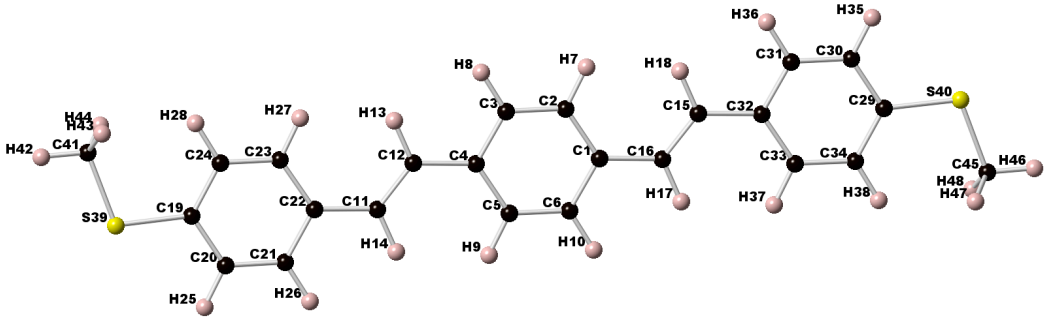
H23 -C17 -C16 -S30 : 0.022863

H23 -C17 -C18 -H24 : -0.025918

H25 -C20 -C21 -H26 : -0.260322

H26 -C21 -C16 -S30 : -0.116420

MeS-PPV2



Final geometry:

angstroms

atom	x	y	z
C1	-2.8120865413	-0.2582606753	-0.3594449378
C2	-3.5789177950	0.9212626521	-0.2955934493
C3	-4.9617572948	0.8717848038	-0.2085965705
C4	-5.6656061523	-0.3501221241	-0.1788807713
C5	-4.8985048154	-1.5293881361	-0.2433538414
C6	-3.5162848113	-1.4796007215	-0.3306522037
H8	-3.0897152017	1.8897740262	-0.3150011667
H9	-5.5240094867	1.8012903938	-0.1614588915
H11	-5.3871056571	-2.4982075993	-0.2269536452
H12	-2.9547910301	-2.4090092701	-0.3794959964
C12	-7.9558096639	-1.3874909787	-0.0294016933
C13	-7.1247483046	-0.3246595101	-0.0859297329
H15	-7.5532792313	0.6756449293	-0.0601970325
H16	-7.5224192755	-2.3856209604	-0.0501838113
C16	-0.5139426978	0.7685180414	-0.4896095661
C17	-1.3533603872	-0.2885265498	-0.4539127556

H19	-0.9311097261	-1.2907886870	-0.4985582321
H20	-0.9379250567	1.7699235391	-0.4434744408
C20	-12.2502351860	-1.4978266518	0.2417106259
C21	-11.4824237091	-2.6723485360	0.2180381438
C22	-10.0998682827	-2.6062311244	0.1298982367
C23	-9.4157900535	-1.3762331780	0.0618191011
C24	-10.2003160884	-0.2093471765	0.0855677265
C25	-11.5876104606	-0.2637040073	0.1738384504
H27	-11.9731556314	-3.6403455158	0.2684473907
H28	-9.5271153592	-3.5301656680	0.1129167848
H29	-9.7254821113	0.7653593536	0.0330081940
H30	-12.1462449578	0.6652098869	0.1884459035
C30	3.7812981531	0.8377265105	-0.7726096544
C31	3.0285912502	2.0196087274	-0.6949183833
C32	1.6454787333	1.9672860188	-0.6041542497
C33	0.9459194360	0.7441402746	-0.5861118780
C34	1.7157461269	-0.4302757333	-0.6649436869
C35	3.1032567932	-0.3896100655	-0.7560680276
H37	3.5314225605	2.9826124709	-0.7062359104
H38	1.0846218680	2.8968158617	-0.5453872208
H39	1.2288903266	-1.4003950929	-0.6558917170
H40	3.6497981713	-1.3239891158	-0.8143002712
S40	-14.0168789273	-1.6998941581	0.3580277440
S41	5.5500783688	1.0219696634	-0.8858729748
C42	-14.6499483821	0.0077036231	0.3423750859
H43	-15.7361225956	-0.0824628134	0.4081729857
H44	-14.2900886943	0.5773342327	1.2019704126
H45	-14.3935808136	0.5219938068	-0.5864411626
C45	6.1593968022	-0.6921035646	-0.9751382788
H46	7.2458586524	-0.6127533886	-1.0497923991

H47	5.9073784973	-1.2553995148	-0.0739639793
H48	5.7811336624	-1.2068103395	-1.8610583530

Total energy (hartrees): -1724.20777757151

HOMO energy (hartrees): -0.18125

LUMO energy (hartrees): -0.06433

Bond lengths (angstroms):

C1	-C2	: 1.408326	C1	-C6	:	1.410105	
C1	-C17	: 1.462095	C2	-C3	:	1.386456	
C2	-H8	: 1.085224	C3	-C4	:	1.410441	
C3	-H9	: 1.087350	C4	-C5	:	1.408286	
C4	-C13	: 1.462321	C5	-C6	:	1.385869	
C5	-H11	: 1.085178	C6	-H12	:	1.086950	
C12	-C13	: 1.350359	C12	-H16	:	1.088358	
C12	-C23	: 1.462871	C13	-H15	:	1.088536	
C16	-C17	: 1.350274	C16	-H20	:	1.088440	
C16	-C33	: 1.463251	C17	-H19	:	1.088494	
C20	-C21	: 1.403423	C20	-C25	:	1.402404	
C20	-S40	: 1.781963	C21	-C22	:	1.386939	
C21	-H27	: 1.086452	C22	-C23	:	1.409075	
C22	-H28	: 1.087193	C23	-C24	:	1.406296	
C24	-C25	: 1.391162	C24	-H29	:	1.085487	
C25	-H30	: 1.084051	C30	-C31	:	1.403371	
C30	-C35	: 1.402273	C30	-S41	:	1.781953	
C31	-C32	: 1.387075	C31	-H37	:	1.086436	
C32	-C33	: 1.409182	C32	-H38	:	1.087216	

C33 -C34 : 1.406450 C34 -C35 : 1.391094

C34 -H39 : 1.085469 C35 -H40 : 1.084049

S40 -C42 : 1.821239 S41 -C45 : 1.821341

C42 -H43 : 1.091895 C42 -H44 : 1.092191

C42 -H45 : 1.092208 C45 -H46 : 1.091911

C45 -H47 : 1.092214 C45 -H48 : 1.092182

Bond angles:

C6 -C1 -C2 : 116.908895 C17 -C1 -C2 : 124.298913

C17 -C1 -C6 : 118.792147 C3 -C2 -C1 : 121.066594

H8 -C2 -C1 : 120.079352 H8 -C2 -C3 : 118.854030

C4 -C3 -C2 : 122.003029 H9 -C3 -C2 : 119.205922

H9 -C3 -C4 : 118.791048 C5 -C4 -C3 : 116.914273

C13 -C4 -C3 : 118.959871 C13 -C4 -C5 : 124.125826

C6 -C5 -C4 : 121.069175 H11 -C5 -C4 : 120.108796

H11 -C5 -C6 : 118.821937 C5 -C6 -C1 : 122.038002

H12 -C6 -C1 : 118.796755 H12 -C6 -C5 : 119.165220

H16 -C12 -C13 : 118.421402 C23 -C12 -C13 : 127.645542

C23 -C12 -H16 : 113.932960 C12 -C13 -C4 : 127.089035

H15 -C13 -C4 : 114.225210 H15 -C13 -C12 : 118.685682

H20 -C16 -C17 : 118.487064 C33 -C16 -C17 : 127.511908

C33 -C16 -H20 : 114.001026 C16 -C17 -C1 : 127.281780

H19 -C17 -C1 : 114.125629 H19 -C17 -C16 : 118.592591

C25 -C20 -C21 : 118.499959 S40 -C20 -C21 : 116.653637

S40 -C20 -C25 : 124.846401 C22 -C21 -C20 : 120.434013

H27 -C21 -C20 : 119.851502 H27 -C21 -C22 : 119.714475

C23 -C22 -C21 : 121.912888 H28 -C22 -C21 : 119.053929

H28 -C22 -C23 : 119.033183 C22 -C23 -C12 : 118.738725

C24 -C23 -C12 : 124.346991 C24 -C23 -C22 : 116.914248

C25 -C24 -C23 : 121.665980 H29 -C24 -C23 : 120.014973

H29 -C24 -C25 : 118.318990 C24 -C25 -C20 : 120.572862

H30 -C25 -C20 : 120.659256 H30 -C25 -C24 : 118.767868

C35 -C30 -C31 : 118.497051 S41 -C30 -C31 : 116.668934

S41 -C30 -C35 : 124.834014 C32 -C31 -C30 : 120.442855

H37 -C31 -C30 : 119.846370 H37 -C31 -C32 : 119.710771

C33 -C32 -C31 : 121.910290 H38 -C32 -C31 : 119.056888

H38 -C32 -C33 : 119.032821 C32 -C33 -C16 : 118.794090

C34 -C33 -C16 : 124.311708 C34 -C33 -C32 : 116.894169

C35 -C34 -C33 : 121.682119 H39 -C34 -C33 : 120.021110

H39 -C34 -C35 : 118.296767 C34 -C35 -C30 : 120.573511

H40 -C35 -C30 : 120.663349 H40 -C35 -C34 : 118.763137

C42 -S40 -C20 : 103.752842 C45 -S41 -C30 : 103.761529

H43 -C42 -S40 : 105.535740 H44 -C42 -S40 : 111.574502

H44 -C42 -H43 : 108.868621 H45 -C42 -S40 : 111.543557

H45 -C42 -H43 : 108.882206 H45 -C42 -H44 : 110.265933

H46 -C45 -S41 : 105.535432 H47 -C45 -S41 : 111.575827

H47 -C45 -H46 : 108.873516 H48 -C45 -S41 : 111.555335

H48 -C45 -H46 : 108.868542 H48 -C45 -H47 : 110.261541

Torsional angles:

C1 -C2 -C3 -C4 : 0.043587

C1 -C2 -C3 -H9 :-179.968951

C1 -C6 -C5 -C4 : -0.009391

C1 -C6 -C5 -H11 : 179.880607

C1 -C17 -C16 -H20 : 0.085776

C1 -C17 -C16 -C33 :-179.898358

C2 -C1 -C6 -C5 : -0.018650

C2 -C1 -C6 -H12 : 179.925637

C2 -C1 -C17 -C16 : 0.295902

C2 -C1 -C17 -H19 :-179.701660

C2 -C3 -C4 -C5 : -0.069537

C2 -C3 -C4 -C13 : 179.990681

C3 -C2 -C1 -C6 : 0.001852

C3 -C2 -C1 -C17 : 179.922822

C3 -C4 -C5 -C6 : 0.052242

C3 -C4 -C5 -H11 :-179.836351

C3 -C4 -C13 -C12 :-179.108931

C3 -C4 -C13 -H15 : 0.790835

C4 -C3 -C2 -H8 : 179.987654

C4 -C5 -C6 -H12 :-179.953479

C4 -C13 -C12 -H16 : 0.210726

C4 -C13 -C12 -C23 :-179.909614

C5 -C4 -C3 -H9 : 179.942950

C5 -C4 -C13 -C12 : 0.955933

C5 -C4 -C13 -H15 :-179.144300

C5 -C6 -C1 -C17 :-179.944153

C6 -C1 -C2 -H8 :-179.941534

C6 -C1 -C17 -C16 :-179.784513

C6 -C1 -C17 -H19 : 0.217925

C6 -C5 -C4 -C13 : 179.988594

H8 -C2 -C1 -C17 : -0.020565

H8 -C2 -C3 -H9 : -0.024884

H9 -C3 -C4 -C13 : 0.003168

H11 -C5 -C4 -C13 : 0.100001

H11 -C5 -C6 -H12 : -0.063481

H12 -C6 -C1 -C17 : 0.000134

C12 -C23 -C22 -C21 : 179.991169

C12 -C23 -C22 -H28 : -0.003375

C12 -C23 -C24 -C25 :-179.991536

C12 -C23 -C24 -H29 : 0.096972

C13 -C12 -C23 -C22 :-179.073363

C13 -C12 -C23 -C24 : 0.998462

H15 -C13 -C12 -H16 :-179.685079

H15 -C13 -C12 -C23 : 0.194582

H16 -C12 -C23 -C22 : 0.810847

H16 -C12 -C23 -C24 :-179.117329

C16 -C33 -C32 -C31 :-179.948657

C16 -C33 -C32 -H38 : 0.040738

C16 -C33 -C34 -C35 : 179.954595

C16 -C33 -C34 -H39 : -0.024478

C17 -C16 -C33 -C32 :-179.750829

C17 -C16 -C33 -C34 : 0.318819

H19 -C17 -C16 -H20 :-179.916758

H19 -C17 -C16 -C33 : 0.099107

H20 -C16 -C33 -C32 : 0.264435

H20 -C16 -C33 -C34 :-179.665917

C20 -C21 -C22 -C23 : 0.024720

C20 -C21 -C22 -H28 :-179.980737

C20 -C25 -C24 -C23 : -0.032606

C20 -C25 -C24 -H29 : 179.880337

C20 -S40 -C42 -H43 : 179.749034

C20 -S40 -C42 -H44 : -62.159868

C20 -S40 -C42 -H45 : 61.657952

C21 -C20 -C25 -C24 : -0.021011

C21 -C20 -C25 -H30 : 179.935864

C21 -C20 -S40 -C42 :-179.372075

C21 -C22 -C23 -C24 : -0.075335

C22 -C21 -C20 -C25 : 0.024867

C22 -C21 -C20 -S40 :-179.955584

C22 -C23 -C24 -C25 : 0.079091

C22 -C23 -C24 -H29 :-179.832401

C23 -C22 -C21 -H27 : 179.989192

C23 -C24 -C25 -H30 :-179.990287

C24 -C23 -C22 -H28 : 179.930121

C24 -C25 -C20 -S40 : 179.957699

C25 -C20 -C21 -H27 :-179.939556

C25 -C20 -S40 -C42 : 0.648859

H27 -C21 -C20 -S40 : 0.079993

H27 -C21 -C22 -H28 : -0.016266

H29 -C24 -C25 -H30 : -0.077344

H30 -C25 -C20 -S40 : -0.085425

C30 -C31 -C32 -C33 : 0.005338

C30 -C31 -C32 -H38 :-179.984054

C30 -C35 -C34 -C33 : -0.025224

C30 -C35 -C34 -H39 : 179.954198

C30 -S41 -C45 -H46 : 179.775833

C30 -S41 -C45 -H47 : -62.126695

C30 -S41 -C45 -H48 : 61.695094

C31 -C30 -C35 -C34 : 0.016246

C31 -C30 -C35 -H40 : 179.997338

C31 -C30 -S41 -C45 :-179.720486

C31 -C32 -C33 -C34 : -0.013162

C32 -C31 -C30 -C35 : -0.006495

C32 -C31 -C30 -S41 :-179.997613

C32 -C33 -C34 -C35 : 0.023034

C32 -C33 -C34 -H39 :-179.956039

C33 -C32 -C31 -H37 : 179.981774

C33 -C34 -C35 -H40 : 179.993330

C34 -C33 -C32 -H38 : 179.976232

C34 -C35 -C30 -S41 :-179.993425

C35 -C30 -C31 -H37 :-179.982900

C35 -C30 -S41 -C45 : 0.289025

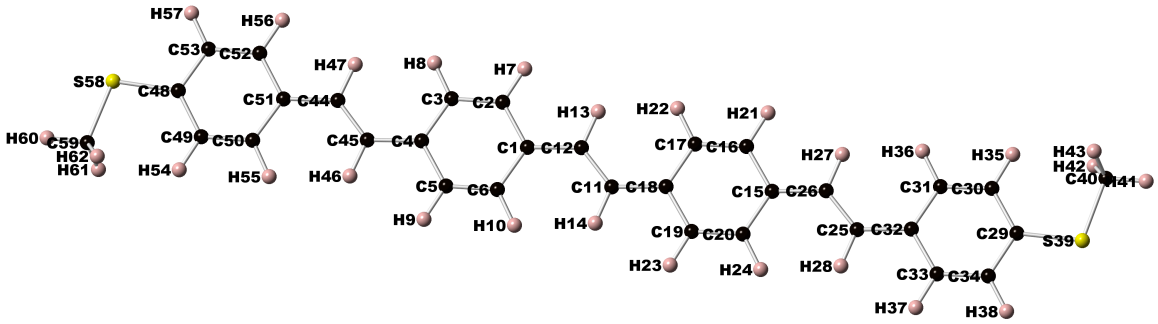
H37 -C31 -C30 -S41 : 0.025983

H37 -C31 -C32 -H38 : -0.007618

H39 -C34 -C35 -H40 : -0.027248

H40 -C35 -C30 -S41 : -0.012333

MeS-PPV3



Final geometry:

angstroms

atom	x	y	z
C1	-2.7675470000	-0.4598810000	-0.3083940000
C2	-3.4299300000	0.7854490000	-0.2887840000
C3	-4.8119210000	0.8827600000	-0.3002390000
C4	-5.6206460000	-0.2699890000	-0.3323540000
C5	-4.9584140000	-1.5156030000	-0.3513080000
C6	-3.5752520000	-1.6135290000	-0.3396710000
H8	-2.8340650000	1.6945860000	-0.2644080000
H9	-5.2673370000	1.8675260000	-0.2845130000
H11	-5.5545020000	-2.4246280000	-0.3758760000
H12	-3.1176970000	-2.5980190000	-0.3551430000
C12	-0.4917440000	-1.5512220000	-0.3124910000
C13	-1.3069830000	-0.4738430000	-0.2961390000
H15	-0.8558160000	0.5161660000	-0.2719540000
H16	-0.9377880000	-2.5437100000	-0.3371680000
C16	3.8264650000	-1.6822310000	-0.2863260000
C17	3.1398730000	-0.4505140000	-0.2637720000
C18	1.7562020000	-0.3798810000	-0.2711970000
C19	0.9697080000	-1.5479350000	-0.3017970000

C20	1.6558880000	-2.7802180000	-0.3237380000
C21	3.0404710000	-2.8504780000	-0.3164480000
H23	3.7171930000	0.4700770000	-0.2400640000
H24	1.2820150000	0.5959230000	-0.2529910000
H25	1.0779090000	-3.7008930000	-0.3472950000
H26	3.5159940000	-3.8257450000	-0.3342550000
C26	6.1164640000	-2.7372140000	-0.2953690000
C27	5.2882330000	-1.6708520000	-0.2775230000
H29	5.7243060000	-0.6738740000	-0.2543660000
H30	5.6799670000	-3.7340060000	-0.3183310000
C30	10.4200850000	-2.8458330000	-0.2764770000
C31	9.7531850000	-1.6122850000	-0.2565900000
C32	8.3632420000	-1.5592500000	-0.2623210000
C33	7.5795580000	-2.7267780000	-0.2876290000
C34	8.2677370000	-3.9562040000	-0.3072770000
C35	9.6533040000	-4.0210870000	-0.3019160000
H37	10.3106590000	-0.6827590000	-0.2367040000
H38	7.8856240000	-0.5847200000	-0.2468310000
H39	7.6959560000	-4.8806810000	-0.3275830000
H40	10.1471530000	-4.9886670000	-0.3180970000
S40	12.1909730000	-3.0451890000	-0.2715710000
C41	12.8192900000	-1.3357620000	-0.2456140000
H42	13.9076190000	-1.4240630000	-0.2450630000
H43	12.5103260000	-0.7810590000	-1.1342880000
H44	12.5073700000	-0.8069920000	0.6577060000
C44	-7.8768560000	0.8477580000	-0.3320930000
C45	-7.0827620000	-0.2445480000	-0.3477610000
H47	-7.5473750000	-1.2285110000	-0.3752410000
H48	-7.4065600000	1.8288250000	-0.3039450000
C48	-12.1719730000	1.1253600000	-0.3826410000

C49	-11.5548720000	-0.1336470000	-0.4069580000
C50	-10.1680510000	-0.2426020000	-0.3907570000
C51	-9.3389140000	0.8925630000	-0.3495720000
C52	-9.9777850000	2.1484690000	-0.3252700000
C53	-11.3593230000	2.2687840000	-0.3412840000
H55	-12.1490250000	-1.0398000000	-0.4388260000
H56	-9.7290170000	-1.2351410000	-0.4109940000
H57	-9.3697530000	3.0491980000	-0.2936600000
H58	-11.8141540000	3.2552740000	-0.3220520000
S58	-13.9328430000	1.3971210000	-0.3999710000
C59	-14.6306490000	-0.2840350000	-0.4625930000
H60	-15.7142770000	-0.1503580000	-0.4780600000
H61	-14.3265990000	-0.8110110000	-1.3696680000
H62	-14.3591770000	-0.8649550000	0.4215760000

Total energy (hartrees): -2032.67948856201

HOMO energy (hartrees): -0.17933

LUMO energy (hartrees): -0.07150

Bond lengths (angstroms):

C1	-C2	:	1.410667	C1	-C6	:	1.408641
C1	-C13	:	1.460682	C2	-C3	:	1.385460
C2	-H8	:	1.087281	C3	-C4	:	1.408509
C3	-H9	:	1.085088	C4	-C5	:	1.410838
C4	-C45	:	1.462418	C5	-C6	:	1.386673
C5	-H11	:	1.087314	C6	-H12	:	1.085733

C12	-C13	:	1.351158	C12	-H16	:	1.088392
C12	-C19	:	1.461495	C13	-H15	:	1.088235
C16	-C17	:	1.410335	C16	-C21	:	1.408366
C16	-C27	:	1.461839	C17	-C18	:	1.385493
C17	-H23	:	1.086898	C18	-C19	:	1.408495
C18	-H24	:	1.085071	C19	-C20	:	1.410619
C20	-C21	:	1.386384	C20	-H25	:	1.087316
C21	-H26	:	1.085166	C26	-C27	:	1.350338
C26	-H30	:	1.088417	C26	-C33	:	1.463152
C27	-H29	:	1.088421	C30	-C31	:	1.402424
C30	-C35	:	1.403504	C30	-S40	:	1.782081
C31	-C32	:	1.390966	C31	-H37	:	1.084062
C32	-C33	:	1.406386	C32	-H38	:	1.085388
C33	-C34	:	1.409065	C34	-C35	:	1.387096
C34	-H39	:	1.087200	C35	-H40	:	1.086444
S40	-C41	:	1.821427	C41	-H42	:	1.091905
C41	-H43	:	1.092198	C41	-H44	:	1.092190
C44	-C45	:	1.350542	C44	-H48	:	1.088330
C44	-C51	:	1.462849	C45	-H47	:	1.088487
C48	-C49	:	1.402321	C48	-C53	:	1.403399
C48	-S58	:	1.781802	C49	-C50	:	1.391189
C49	-H55	:	1.084042	C50	-C51	:	1.406330
C50	-H56	:	1.085493	C51	-C52	:	1.409272
C52	-C53	:	1.386860	C52	-H57	:	1.087205
C53	-H58	:	1.086464	S58	-C59	:	1.821302
C59	-H60	:	1.091952	C59	-H61	:	1.092216
C59	-H62	:	1.092209				

Bond angles:

C6 -C1 -C2 : 117.004542 C13 -C1 -C2 : 118.544198

C13 -C1 -C6 : 124.451245 C3 -C2 -C1 : 122.023522

H8 -C2 -C1 : 118.759641 H8 -C2 -C3 : 119.216831

C4 -C3 -C2 : 121.026756 H9 -C3 -C2 : 118.834232

H9 -C3 -C4 : 120.139004 C5 -C4 -C3 : 116.960051

C45 -C4 -C3 : 124.059587 C45 -C4 -C5 : 118.980347

C6 -C5 -C4 : 122.034979 H11 -C5 -C4 : 118.756953

H11 -C5 -C6 : 119.208068 C5 -C6 -C1 : 120.950129

H12 -C6 -C1 : 120.085051 H12 -C6 -C5 : 118.964820

H16 -C12 -C13 : 118.693131 C19 -C12 -C13 : 126.974798

C19 -C12 -H16 : 114.332051 C12 -C13 -C1 : 127.649879

H15 -C13 -C1 : 113.956524 H15 -C13 -C12 : 118.393565

C21 -C16 -C17 : 116.942559 C27 -C16 -C17 : 118.679592

C27 -C16 -C21 : 124.377847 C18 -C17 -C16 : 122.047839

H23 -C17 -C16 : 118.782228 H23 -C17 -C18 : 119.169931

C19 -C18 -C17 : 121.030724 H24 -C18 -C17 : 118.828696

H24 -C18 -C19 : 120.140580 C18 -C19 -C12 : 124.083517

C20 -C19 -C12 : 118.969643 C20 -C19 -C18 : 116.946832

C21 -C20 -C19 : 122.005251 H25 -C20 -C19 : 118.780512

H25 -C20 -C21 : 119.214235 C20 -C21 -C16 : 121.026783

H26 -C21 -C16 : 120.085556 H26 -C21 -C20 : 118.887660

H30 -C26 -C27 : 118.523764 C33 -C26 -C27 : 127.417912

C33 -C26 -H30 : 114.058323 C26 -C27 -C16 : 127.379711

H29 -C27 -C16 : 114.072106 H29 -C27 -C26 : 118.548174

C35 -C30 -C31 : 118.489309 S40 -C30 -C31 : 124.813329

S40 -C30 -C35 : 116.697360 C32 -C31 -C30 : 120.574787

H37 -C31 -C30 : 120.658158 H37 -C31 -C32 : 118.767054

C33 -C32 -C31 : 121.684672 H38 -C32 -C31 : 118.287417

H38 -C32 -C33 : 120.027910 C32 -C33 -C26 : 124.279243

C34 -C33 -C26 : 118.821192 C34 -C33 -C32 : 116.899555

C35 -C34 -C33 : 121.911898 H39 -C34 -C33 : 119.033801

H39 -C34 -C35 : 119.054298 C34 -C35 -C30 : 120.439776

H40 -C35 -C30 : 119.847223 H40 -C35 -C34 : 119.712991

C41 -S40 -C30 : 103.759270 H42 -C41 -S40 : 105.541714

H43 -C41 -S40 : 111.559674 H43 -C41 -H42 : 108.870990

H44 -C41 -S40 : 111.569958 H44 -C41 -H42 : 108.868072

H44 -C41 -H43 : 110.260036 H48 -C44 -C45 : 118.378630

C51 -C44 -C45 : 127.755810 C51 -C44 -H48 : 113.865540

C44 -C45 -C4 : 126.999504 H47 -C45 -C4 : 114.286192

H47 -C45 -C44 : 118.714298 C53 -C48 -C49 : 118.501374

S58 -C48 -C49 : 124.865494 S58 -C48 -C53 : 116.633132

C50 -C49 -C48 : 120.583094 H55 -C49 -C48 : 120.650098

H55 -C49 -C50 : 118.766808 C51 -C50 -C49 : 121.658023

H56 -C50 -C49 : 118.332036 H56 -C50 -C51 : 120.009939

C50 -C51 -C44 : 124.394191 C52 -C51 -C44 : 118.697058

C52 -C51 -C50 : 116.908722 C53 -C52 -C51 : 121.918205

H57 -C52 -C51 : 119.031460 H57 -C52 -C53 : 119.050325

C52 -C53 -C48 : 120.430579 H58 -C53 -C48 : 119.860474

H58 -C53 -C52 : 119.708943 C59 -S58 -C48 : 103.779453

H60 -C59 -S58 : 105.527573 H61 -C59 -S58 : 111.546430

H61 -C59 -H60 : 108.878313 H62 -C59 -S58 : 111.585292

H62 -C59 -H60 : 108.858831 H62 -C59 -H61 : 110.272684

Torsional angles:

C1 -C2 -C3 -C4 : -0.003839

C1 -C2 -C3 -H9 :-179.972973

C1 -C6 -C5 -C4 : -0.013831

C1 -C6 -C5 -H11 : 179.980668

C1 -C13 -C12 -H16 : -0.040714

C1 -C13 -C12 -C19 : 179.904696

C2 -C1 -C6 -C5 : 0.043388

C2 -C1 -C6 -H12 :-179.960964

C2 -C1 -C13 -C12 :-179.921512

C2 -C1 -C13 -H15 : 0.011622

C2 -C3 -C4 -C5 : 0.033871

C2 -C3 -C4 -C45 :-179.921537

C3 -C2 -C1 -C6 : -0.034959

C3 -C2 -C1 -C13 : 179.923555

C3 -C4 -C5 -C6 : -0.025306

C3 -C4 -C5 -H11 : 179.980171

C3 -C4 -C45 -C44 : -0.118360

C3 -C4 -C45 -H47 : 179.854224

C4 -C3 -C2 -H8 : 179.967265

C4 -C5 -C6 -H12 : 179.990473

C4 -C45 -C44 -H48 : -0.068512

C4 -C45 -C44 -C51 : 179.875982

C5 -C4 -C3 -H9 :-179.997394

C5 -C4 -C45 -C44 : 179.927075

C5 -C4 -C45 -H47 : -0.100341

C5 -C6 -C1 -C13 :-179.912417

C6 -C1 -C2 -H8 : 179.993810

C6 -C1 -C13 -C12 : 0.033663

C6 -C1 -C13 -H15 : 179.966797

C6 -C5 -C4 -C45 : 179.932463

H8 -C2 -C1 -C13 : -0.047676

H8 -C2 -C3 -H9 : -0.001870

H9 -C3 -C4 -C45 : 0.047198

H11 -C5 -C4 -C45 : -0.062060

H11 -C5 -C6 -H12 : -0.015027

H12 -C6 -C1 -C13 : 0.083230

C12 -C19 -C18 -C17 :-179.945533

C12 -C19 -C18 -H24 : 0.052858

C12 -C19 -C20 -C21 : 179.939676

C12 -C19 -C20 -H25 : -0.045850

C13 -C12 -C19 -C18 : 0.035694

C13 -C12 -C19 -C20 :-179.932822

H15 -C13 -C12 -H16 :-179.971252

H15 -C13 -C12 -C19 : -0.025842

H16 -C12 -C19 -C18 : 179.983140

H16 -C12 -C19 -C20 : 0.014623

C16 -C17 -C18 -C19 : 0.005302

C16 -C17 -C18 -H24 :-179.993110

C16 -C21 -C20 -C19 : 0.009595

C16 -C21 -C20 -H25 : 179.995060

C16 -C27 -C26 -H30 : -0.048525

C16 -C27 -C26 -C33 : 179.948208

C17 -C16 -C21 -C20 : 0.019474

C17 -C16 -C21 -H26 :-179.971639

C17 -C16 -C27 -C26 : 179.983377

C17 -C16 -C27 -H29 : -0.052164

C17 -C18 -C19 -C20 : 0.023568

C18 -C17 -C16 -C21 : -0.026950

C18 -C17 -C16 -C27 : 179.958610

C18 -C19 -C20 -C21 : -0.031073

C18 -C19 -C20 -H25 : 179.983401

C19 -C18 -C17 -H23 : 179.991951

C19 -C20 -C21 -H26 :-179.999189

C20 -C19 -C18 -H24 :-179.978041

C20 -C21 -C16 -C27 :-179.965177

C21 -C16 -C17 -H23 : 179.986351

C21 -C16 -C27 -C26 : -0.032220

C21 -C16 -C27 -H29 : 179.932239

H23 -C17 -C16 -C27 : -0.028088

H23 -C17 -C18 -H24 : -0.006462

H25 -C20 -C21 -H26 : -0.013724

H26 -C21 -C16 -C27 : 0.043710

C26 -C33 -C32 -C31 :-179.976985

C26 -C33 -C32 -H38 : 0.012538

C26 -C33 -C34 -C35 : 179.972841

C26 -C33 -C34 -H39 : -0.005078

C27 -C26 -C33 -C32 : -0.144134

C27 -C26 -C33 -C34 : 179.893352

H29 -C27 -C26 -H30 : 179.988416

H29 -C27 -C26 -C33 : -0.014850

H30 -C26 -C33 -C32 : 179.852723

H30 -C26 -C33 -C34 : -0.109791

C30 -C31 -C32 -C33 : 0.017236

C30 -C31 -C32 -H38 :-179.972463

C30 -C35 -C34 -C33 : -0.004671

C30 -C35 -C34 -H39 : 179.973244

C30 -S40 -C41 -H42 :-179.840460

C30 -S40 -C41 -H43 : -61.750765

C30 -S40 -C41 -H44 : 62.067927

C31 -C30 -C35 -C34 : 0.007400

C31 -C30 -C35 -H40 : 179.972862

C31 -C30 -S40 -C41 : -0.297310

C31 -C32 -C33 -C34 : -0.013813

C32 -C31 -C30 -C35 : -0.013564

C32 -C31 -C30 -S40 :-179.997118

C32 -C33 -C34 -C35 : 0.007574

C32 -C33 -C34 -H39 :-179.970345

C33 -C32 -C31 -H37 :-179.996514

C33 -C34 -C35 -H40 :-179.970179

C34 -C33 -C32 -H38 : 179.975711

C34 -C35 -C30 -S40 : 179.992286

C35 -C30 -C31 -H37 :-179.999552

C35 -C30 -S40 -C41 : 179.718869

H37 -C31 -C30 -S40 : 0.016894

H37 -C31 -C32 -H38 : 0.013786

H39 -C34 -C35 -H40 : 0.007735

H40 -C35 -C30 -S40 : -0.042251

C44 -C51 -C50 -C49 :-179.931703

C44 -C51 -C50 -H56 : 0.054625

C44 -C51 -C52 -C53 : 179.926432

C44 -C51 -C52 -H57 : -0.035534

C45 -C44 -C51 -C50 : -0.193940

C45 -C44 -C51 -C52 : 179.869721

H47 -C45 -C44 -H48 : 179.959981

H47 -C45 -C44 -C51 : -0.095525

H48 -C44 -C51 -C50 : 179.752659

H48 -C44 -C51 -C52 : -0.183680

C48 -C49 -C50 -C51 : 0.011435

C48 -C49 -C50 -H56 :-179.975115

C48 -C53 -C52 -C51 : 0.006537

C48 -C53 -C52 -H57 : 179.968496

C48 -S58 -C59 -H60 :-179.795566

C48 -S58 -C59 -H61 : -61.712499

C48 -S58 -C59 -H62 : 62.124252

C49 -C48 -C53 -C52 : 0.010792

C49 -C48 -C53 -H58 : 179.986369

C49 -C48 -S58 -C59 : -0.292713

C49 -C50 -C51 -C52 : 0.005675

C50 -C49 -C48 -C53 : -0.019608

C50 -C49 -C48 -S58 : 179.990834

C50 -C51 -C52 -C53 : -0.014659

C50 -C51 -C52 -H57 :-179.976625

C51 -C50 -C49 -H55 :-179.995324

C51 -C52 -C53 -H58 :-179.969076

C52 -C51 -C50 -H56 : 179.992004

C52 -C53 -C48 -S58 :-179.998792

C53 -C48 -C49 -H55 : 179.987279

C53 -C48 -S58 -C59 : 179.717553

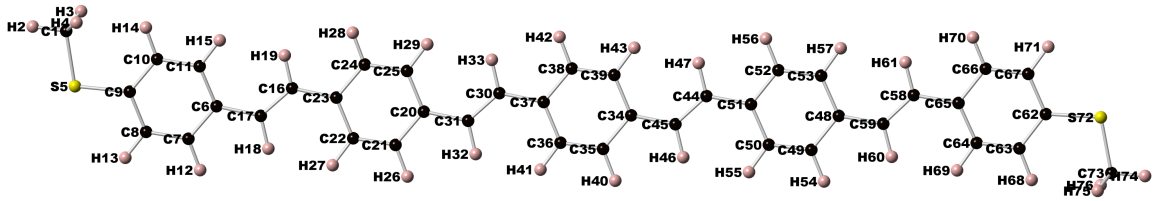
H55 -C49 -C48 -S58 : -0.002279

H55 -C49 -C50 -H56 : 0.018126

H57 -C52 -C53 -H58 : -0.007117

H58 -C53 -C48 -S58 : -0.023216

MeS-PPV4



Final geometry:

		angstroms	
atom	x	y	z
C1	-7.8000230000	2.6608420000	0.1427530000
H2	-8.4725620000	3.2839440000	0.7358560000
H4	-6.9699760000	3.2758070000	-0.2125690000
H5	-7.4270090000	1.8476990000	0.7696240000
S5	-8.8081710000	2.0326510000	-1.2385040000
C6	-5.9947040000	-0.6160170000	-3.7762290000
C7	-7.3523910000	-0.4113990000	-4.0927460000
C8	-8.1739020000	0.3899950000	-3.3129560000
C9	-7.6687400000	1.0267410000	-2.1686920000
C10	-6.3206940000	0.8319690000	-1.8353550000
C11	-5.5065890000	0.0266730000	-2.6241790000
H13	-7.7676390000	-0.8936680000	-4.9743030000
H14	-9.2156860000	0.5239330000	-3.5906720000
H15	-5.8943360000	1.3028450000	-0.9569560000
H16	-4.4710870000	-0.1049270000	-2.3268980000
C16	-3.8603290000	-1.7183240000	-4.5339430000
C17	-5.1832880000	-1.4703710000	-4.6423340000
H19	-5.7361020000	-1.9359060000	-5.4566230000
H20	-3.3043700000	-1.2376020000	-3.7306990000
C20	-1.3443290000	-4.2164840000	-7.0028960000

C21	-2.7314960000	-4.1268780000	-7.2428660000
C22	-3.5616610000	-3.3336310000	-6.4660990000
C23	-3.0490730000	-2.5754950000	-5.3949460000
C24	-1.6623160000	-2.6670580000	-5.1533900000
C25	-0.8323420000	-3.4600770000	-5.9299120000
H27	-3.1594570000	-4.7007100000	-8.0613440000
H28	-4.6232370000	-3.3069520000	-6.6920710000
H29	-1.2351450000	-2.0963110000	-4.3323340000
H30	0.2275580000	-3.4931810000	-5.6974660000
C30	0.8040330000	-5.2685160000	-7.7854890000
C31	-0.5312050000	-5.0748750000	-7.8603030000
H33	-1.0919990000	-5.5995170000	-8.6320240000
H34	1.3638440000	-4.7388060000	-7.0166130000
C34	3.3437170000	-7.7673520000	-10.2288110000
C35	1.9514660000	-7.7166210000	-10.4507750000
C36	1.1132140000	-6.9238220000	-9.6822260000
C37	1.6220680000	-6.1274940000	-8.6369840000
C38	3.0142050000	-6.1794100000	-8.4140370000
C39	3.8520200000	-6.9716430000	-9.1825630000
H41	1.5263780000	-8.3196910000	-11.2494640000
H42	0.0487680000	-6.9252600000	-9.8959620000
H43	3.4390240000	-5.5776820000	-7.6141700000
H44	4.9156580000	-6.9719780000	-8.9655650000
C44	5.5063230000	-8.7877890000	-11.0082110000
C45	4.1667720000	-8.6249790000	-11.0779000000
H47	3.6116010000	-9.1751880000	-11.8357970000
H48	6.0566270000	-8.2350030000	-10.2494230000
C48	8.1112970000	-11.2473430000	-13.4216590000
C49	6.7202480000	-11.2240100000	-13.6556240000
C50	5.8598600000	-10.4459860000	-12.8959350000

C51	6.3445970000	-9.6372500000	-11.8489760000
C52	7.7355140000	-9.6612230000	-11.6146040000
C53	8.5947820000	-10.4390020000	-12.3739780000
H55	6.3138310000	-11.8364610000	-14.4569070000
H56	4.7975930000	-10.4665420000	-13.1196950000
H57	8.1422450000	-9.0477350000	-10.8142520000
H58	9.6564510000	-10.4146320000	-12.1510650000
C58	10.2964380000	-12.2514670000	-14.1671700000
C59	8.9590390000	-12.0892650000	-14.2634660000
H61	8.4219660000	-12.6307090000	-15.0405080000
H62	10.8300980000	-11.7154350000	-13.3840940000
C62	12.9188110000	-14.6704120000	-16.5796930000
C63	11.5469760000	-14.6240830000	-16.8676030000
C64	10.6875730000	-13.8480170000	-16.0971960000
C65	11.1521530000	-13.0864770000	-15.0095580000
C66	12.5333000000	-13.1456700000	-14.7357250000
C67	13.3998560000	-13.9163980000	-15.4976510000
H69	11.1360780000	-15.1910000000	-17.6951170000
H70	9.6334650000	-13.8377930000	-16.3557510000
H71	12.9316090000	-12.5706020000	-13.9033410000
H72	14.4585300000	-13.9348040000	-15.2541330000
S72	14.1164890000	-15.6230380000	-17.4918630000
C73	13.1265400000	-16.4264100000	-18.7930180000
H74	13.8351270000	-17.0184380000	-19.3758990000
H75	12.3725150000	-17.0938990000	-18.3696760000
H76	12.6554910000	-15.6915790000	-19.4499210000

Total energy (hartrees): -2341.15120336664

HOMO energy (hartrees): -0.17817

LUMO energy (hartrees): -0.07571

Bond lengths (angstroms):

C1	-H2	:	1.091941	C1	-H4	:	1.092435
C1	-H5	:	1.092386	C1	-S5	:	1.821773
S5	-C9	:	1.781967	C6	-C7	:	1.409030
C6	-C11	:	1.406601	C6	-C17	:	1.462346
C7	-C8	:	1.387510	C7	-H13	:	1.087270
C8	-C9	:	1.403558	C8	-H14	:	1.086453
C9	-C10	:	1.402240	C10	-C11	:	1.390508
C10	-H15	:	1.084016	C11	-H16	:	1.085338
C16	-C17	:	1.350352	C16	-H20	:	1.088754
C16	-C23	:	1.460892	C17	-H19	:	1.088757
C20	-C21	:	1.410619	C20	-C25	:	1.409105
C20	-C31	:	1.460532	C21	-C22	:	1.386283
C21	-H27	:	1.087355	C22	-C23	:	1.408860
C22	-H28	:	1.085688	C23	-C24	:	1.410613
C24	-C25	:	1.385901	C24	-H29	:	1.087364
C25	-H30	:	1.085594	C30	-C31	:	1.351279
C30	-H34	:	1.088647	C30	-C37	:	1.460160
C31	-H33	:	1.088711	C34	-C35	:	1.410746
C34	-C39	:	1.409312	C34	-C45	:	1.460786
C35	-C36	:	1.386313	C35	-H41	:	1.087335
C36	-C37	:	1.409114	C36	-H42	:	1.085694
C37	-C38	:	1.410832	C38	-C39	:	1.385713
C38	-H43	:	1.087352	C39	-H44	:	1.085548
C44	-C45	:	1.351207	C44	-H48	:	1.088194

C44 -C51 : 1.459854 C45 -H47 : 1.088739

C48 -C49 : 1.410780 C48 -C53 : 1.408832

C48 -C59 : 1.461553 C49 -C50 : 1.386620

C49 -H55 : 1.087348 C50 -C51 : 1.408952

C50 -H56 : 1.085773 C51 -C52 : 1.410729

C52 -C53 : 1.385616 C52 -H57 : 1.087364

C53 -H58 : 1.085092 C58 -C59 : 1.350636

C58 -H62 : 1.088729 C58 -C65 : 1.462569

C59 -H61 : 1.088762 C62 -C63 : 1.402487

C62 -C67 : 1.403836 C62 -S72 : 1.781568

C63 -C64 : 1.390820 C63 -H69 : 1.083979

C64 -C65 : 1.406675 C64 -H70 : 1.085403

C65 -C66 : 1.409275 C66 -C67 : 1.387614

C66 -H71 : 1.087298 C67 -H72 : 1.086476

S72 -C73 : 1.821650 C73 -H74 : 1.091945

C73 -H75 : 1.092389 C73 -H76 : 1.092422

Bond angles:

H4 -C1 -H2 : 108.869679 H5 -C1 -H2 : 108.867641

H5 -C1 -H4 : 110.256848 S5 -C1 -H2 : 105.530692

S5 -C1 -H4 : 111.590863 S5 -C1 -H5 : 111.554078

C9 -S5 -C1 : 103.684741 C11 -C6 -C7 : 116.872293

C17 -C6 -C7 : 119.107626 C17 -C6 -C11 : 124.019907

C8 -C7 -C6 : 121.879207 H13 -C7 -C6 : 119.059752

H13 -C7 -C8 : 119.060928 C9 -C8 -C7 : 120.471590

H14 -C8 -C7 : 119.688084 H14 -C8 -C9 : 119.840298

C8 -C9 -S5 : 116.841212 C10 -C9 -S5 : 124.682635

C10 -C9 -C8 : 118.476109 C11 -C10 -C9 : 120.559509

H15 -C10 -C9 : 120.690733 H15 -C10 -C11 : 118.749422

C10 -C11 -C6 : 121.740605 H16 -C11 -C6 : 120.001293

H16 -C11 -C10 : 118.256962 H20 -C16 -C17 : 118.582505

C23 -C16 -C17 : 127.191549 C23 -C16 -H20 : 114.224792

C16 -C17 -C6 : 127.110495 H19 -C17 -C6 : 114.270036

H19 -C17 -C16 : 118.618008 C25 -C20 -C21 : 116.919636

C31 -C20 -C21 : 119.008673 C31 -C20 -C25 : 124.071402

C22 -C21 -C20 : 121.999640 H27 -C21 -C20 : 118.787639

H27 -C21 -C22 : 119.212553 C23 -C22 -C21 : 121.067888

H28 -C22 -C21 : 118.880181 H28 -C22 -C23 : 120.051239

C22 -C23 -C16 : 124.179906 C24 -C23 -C16 : 118.887118

C24 -C23 -C22 : 116.932745 C25 -C24 -C23 : 122.001164

H29 -C24 -C23 : 118.779395 H29 -C24 -C25 : 119.219436

C24 -C25 -C20 : 121.078658 H30 -C25 -C20 : 120.093791

H30 -C25 -C24 : 118.827421 H34 -C30 -C31 : 118.522093

C37 -C30 -C31 : 127.272085 C37 -C30 -H34 : 114.205740

C30 -C31 -C20 : 127.001976 H33 -C31 -C20 : 114.366596

H33 -C31 -C30 : 118.631411 C39 -C34 -C35 : 116.900825

C45 -C34 -C35 : 119.058681 C45 -C34 -C39 : 124.040489

C36 -C35 -C34 : 122.010514 H41 -C35 -C34 : 118.779853

H41 -C35 -C36 : 119.209617 C37 -C36 -C35 : 121.068012

H42 -C36 -C35 : 118.877113 H42 -C36 -C37 : 120.054752

C36 -C37 -C30 : 124.243163 C38 -C37 -C30 : 118.836226

C38 -C37 -C36 : 116.920542 C39 -C38 -C37 : 122.005056

H43 -C38 -C37 : 118.776583 H43 -C38 -C39 : 119.218355

C38 -C39 -C34 : 121.094976 H44 -C39 -C34 : 120.107302

H44 -C39 -C38 : 118.797706 H48 -C44 -C45 : 118.430758

C51 -C44 -C45 : 127.565862 C51 -C44 -H48 : 114.003297

C44 -C45 -C34 : 126.822293 H47 -C45 -C34 : 114.457471

H47 -C45 -C44 : 118.720203 C53 -C48 -C49 : 116.886199

C59 -C48 -C49 : 119.073034 C59 -C48 -C53 : 124.040617

C50 -C49 -C48 : 122.021340 H55 -C49 -C48 : 118.779257

H55 -C49 -C50 : 119.199399 C51 -C50 -C49 : 121.044372

H56 -C50 -C49 : 118.916203 H56 -C50 -C51 : 120.039407

C50 -C51 -C44 : 124.360616 C52 -C51 -C44 : 118.708947

C52 -C51 -C50 : 116.930303 C53 -C52 -C51 : 121.999738

H57 -C52 -C51 : 118.783104 H57 -C52 -C53 : 119.217023

C52 -C53 -C48 : 121.117980 H58 -C53 -C48 : 120.094630

H58 -C53 -C52 : 118.787075 H62 -C58 -C59 : 118.523363

C65 -C58 -C59 : 127.361482 C65 -C58 -H62 : 114.115120

C58 -C59 -C48 : 127.046132 H61 -C59 -C48 : 114.293576

H61 -C59 -C58 : 118.660228 C67 -C62 -C63 : 118.402444

S72 -C62 -C63 : 124.758919 S72 -C62 -C67 : 116.838626

C64 -C63 -C62 : 120.605672 H69 -C63 -C62 : 120.678416

H69 -C63 -C64 : 118.715866 C65 -C64 -C63 : 121.755739

H70 -C64 -C63 : 118.255279 H70 -C64 -C65 : 119.988797

C64 -C65 -C58 : 124.137781 C66 -C65 -C58 : 119.042932

C66 -C65 -C64 : 116.819134 C67 -C66 -C65 : 121.915389

H71 -C66 -C65 : 119.048881 H71 -C66 -C67 : 119.035729

C66 -C67 -C62 : 120.501614 H72 -C67 -C62 : 119.838373

H72 -C67 -C66 : 119.659997 C73 -S72 -C62 : 103.662108

H74 -C73 -S72 : 105.529816 H75 -C73 -S72 : 111.578478

H75 -C73 -H74 : 108.874632 H76 -C73 -S72 : 111.542190

H76 -C73 -H74 : 108.876344 H76 -C73 -H75 : 110.268675

Torsional angles:

C1 -S5 -C9 -C8 : 179.615450

C1 -S5 -C9 -C10 : -0.306620

H2 -C1 -S5 -C9 :-179.957530

H4 -C1 -S5 -C9 : 61.944508

H5 -C1 -S5 -C9 : -61.881357

S5 -C9 -C8 -C7 :-179.990905

S5 -C9 -C8 -H14 : -0.051795

S5 -C9 -C10 -C11 : 179.986255

S5 -C9 -C10 -H15 : 0.199757

C6 -C7 -C8 -C9 : -0.120496

C6 -C7 -C8 -H14 : 179.940301

C6 -C11 -C10 -C9 : 0.117422

C6 -C11 -C10 -H15 : 179.908010

C6 -C17 -C16 -H20 : -0.673589

C6 -C17 -C16 -C23 : 179.741608

C7 -C6 -C11 -C10 : -0.289389

C7 -C6 -C11 -H16 : 179.315409

C7 -C6 -C17 -C16 : 176.177937

C7 -C6 -C17 -H19 : -3.372414

C7 -C8 -C9 -C10 : -0.063808

C8 -C7 -C6 -C11 : 0.291340

C8 -C7 -C6 -C17 :-179.854305

C8 -C9 -C10 -C11 : 0.065359

C8 -C9 -C10 -H15 :-179.721139

C9 -C8 -C7 -H13 :-179.996490

C9 -C10 -C11 -H16 :-179.494024

C10 -C9 -C8 -H14 : 179.875302

C10 -C11 -C6 -C17 : 179.864140

C11 -C6 -C7 -H13 :-179.832664

C11 -C6 -C17 -C16 : -3.978809

C11 -C6 -C17 -H19 : 176.470840

H13 -C7 -C6 -C17 : 0.021690

H13 -C7 -C8 -H14 : 0.064307

H15 -C10 -C11 -H16 : 0.296564

H16 -C11 -C6 -C17 : -0.531062

C16 -C23 -C22 -C21 :-179.998850

C16 -C23 -C22 -H28 : -0.305063

C16 -C23 -C24 -C25 :-179.989890

C16 -C23 -C24 -H29 : -0.015079

C17 -C16 -C23 -C22 : -2.755979

C17 -C16 -C23 -C24 : 177.424573

H19 -C17 -C16 -H20 : 178.859455

H19 -C17 -C16 -C23 : -0.725348

H20 -C16 -C23 -C22 : 177.643823

H20 -C16 -C23 -C24 : -2.175625

C20 -C21 -C22 -C23 : 0.062969

C20 -C21 -C22 -H28 :-179.634333

C20 -C25 -C24 -C23 : -0.063450

C20 -C25 -C24 -H29 : 179.961847

C20 -C31 -C30 -H34 : -0.279898

C20 -C31 -C30 -C37 : 179.830364

C21 -C20 -C25 -C24 : -0.055910

C21 -C20 -C25 -H30 : 179.811618

C21 -C20 -C31 -C30 : 179.236750

C21 -C20 -C31 -H33 : -0.714423

C21 -C22 -C23 -C24 : -0.176168

C22 -C21 -C20 -C25 : 0.056174

C22 -C21 -C20 -C31 : 179.868389

C22 -C23 -C24 -C25 : 0.177648

C22 -C23 -C24 -H29 :-179.847541

C23 -C22 -C21 -H27 : 179.912463

C23 -C24 -C25 -H30 :-179.932621

C24 -C23 -C22 -H28 : 179.517618

C24 -C25 -C20 -C31 :-179.857650

C25 -C20 -C21 -H27 :-179.793938

C25 -C20 -C31 -C30 : -0.965386

C25 -C20 -C31 -H33 : 179.083441

H27 -C21 -C20 -C31 : 0.018277

H27 -C21 -C22 -H28 : 0.215161

H29 -C24 -C25 -H30 : 0.092675

H30 -C25 -C20 -C31 : 0.009878

C30 -C37 -C36 -C35 :-179.983413

C30 -C37 -C36 -H42 : -0.112234

C30 -C37 -C38 -C39 :-179.992903

C30 -C37 -C38 -H43 : -0.021357

C31 -C30 -C37 -C36 : -1.173722

C31 -C30 -C37 -C38 : 178.924843

H33 -C31 -C30 -H34 : 179.669429

H33 -C31 -C30 -C37 : -0.220310

H34 -C30 -C37 -C36 : 178.932497

H34 -C30 -C37 -C38 : -0.968938

C34 -C35 -C36 -C37 : 0.010563

C34 -C35 -C36 -H42 :-179.862103

C34 -C39 -C38 -C37 : -0.046312

C34 -C39 -C38 -H43 : 179.982264

C34 -C45 -C44 -H48 : 0.024060

C34 -C45 -C44 -C51 :-179.864548

C35 -C34 -C39 -C38 : -0.026155

C35 -C34 -C39 -H44 : 179.926751

C35 -C34 -C45 -C44 : 179.700303

C35 -C34 -C45 -H47 : -0.232156

C35 -C36 -C37 -C38 : -0.080250

C36 -C35 -C34 -C39 : 0.043834

C36 -C35 -C34 -C45 :-179.978964

C36 -C37 -C38 -C39 : 0.098479

C36 -C37 -C38 -H43 :-179.929975

C37 -C36 -C35 -H41 : 179.964319

C37 -C38 -C39 -H44 :-179.999822

C38 -C37 -C36 -H42 : 179.790929

C38 -C39 -C34 -C45 : 179.997894

C39 -C34 -C35 -H41 :-179.910114

C39 -C34 -C45 -C44 : -0.324233

C39 -C34 -C45 -H47 : 179.743308

H41 -C35 -C34 -C45 : 0.067088

H41 -C35 -C36 -H42 : 0.091653

H43 -C38 -C39 -H44 : 0.028754

H44 -C39 -C34 -C45 : -0.049200

C44 -C51 -C50 -C49 : 179.770172

C44 -C51 -C50 -H56 : -0.180136

C44 -C51 -C52 -C53 :-179.784500

C44 -C51 -C52 -H57 : 0.080455

C45 -C44 -C51 -C50 : -0.147711

C45 -C44 -C51 -C52 : 179.714761

H47 -C45 -C44 -H48 : 179.953955

H47 -C45 -C44 -C51 : 0.065347

H48 -C44 -C51 -C50 : 179.959520

H48 -C44 -C51 -C52 : -0.178009

C48 -C49 -C50 -C51 : 0.062909

C48 -C49 -C50 -H56 :-179.986236

C48 -C53 -C52 -C51 : -0.048434

C48 -C53 -C52 -H57 :-179.912821

C48 -C59 -C58 -H62 : 0.406067

C48 -C59 -C58 -C65 :-179.666674

C49 -C48 -C53 -C52 : 0.011355

C49 -C48 -C53 -H58 :-179.782015

C49 -C48 -C59 -C58 :-178.723701

C49 -C48 -C59 -H61 : 1.182467

C49 -C50 -C51 -C52 : -0.094535

C50 -C49 -C48 -C53 : -0.018814

C50 -C49 -C48 -C59 :-179.883409

C50 -C51 -C52 -C53 : 0.088161

C50 -C51 -C52 -H57 : 179.953117

C51 -C50 -C49 -H55 :-179.957823

C51 -C52 -C53 -H58 : 179.747580

C52 -C51 -C50 -H56 : 179.955158

C52 -C53 -C48 -C59 : 179.868537

C53 -C48 -C49 -H55 :-179.998167

C53 -C48 -C59 -C58 : 1.422043

C53 -C48 -C59 -H61 :-178.671789

H55 -C49 -C48 -C59 : 0.137238

H55 -C49 -C50 -H56 : -0.006967

H57 -C52 -C53 -H58 : -0.116807

H58 -C53 -C48 -C59 : 0.075167

C58 -C65 -C64 -C63 : 179.883903

C58 -C65 -C64 -H70 : 0.043029

C58 -C65 -C66 -C67 :-179.887894

C58 -C65 -C66 -H71 : 0.101880

C59 -C58 -C65 -C64 : 1.319734

C59 -C58 -C65 -C66 :-178.827417

H61 -C59 -C58 -H62 :-179.496469

H61 -C59 -C58 -C65 : 0.430790

H62 -C58 -C65 -C64 :-178.750289

H62 -C58 -C65 -C66 : 1.102560

C62 -C63 -C64 -C65 : -0.027616

C62 -C63 -C64 -H70 : 179.815918

C62 -C67 -C66 -C65 : 0.020108

C62 -C67 -C66 -H71 :-179.969667

C62 -S72 -C73 -H74 : 179.786408

C62 -S72 -C73 -H75 : -62.116740

C62 -S72 -C73 -H76 : 61.706590

C63 -C62 -C67 -C66 : -0.017943

C63 -C62 -C67 -H72 :-179.971688

C63 -C62 -S72 -C73 : 0.513166

C63 -C64 -C65 -C66 : 0.028057

C64 -C63 -C62 -C67 : 0.021628

C64 -C63 -C62 -S72 :-179.938191

C64 -C65 -C66 -C67 : -0.024369

C64 -C65 -C66 -H71 : 179.965404

C65 -C64 -C63 -H69 :-179.950594

C65 -C66 -C67 -H72 : 179.973935

C66 -C65 -C64 -H70 :-179.812817

C66 -C67 -C62 -S72 : 179.945061

C67 -C62 -C63 -H69 : 179.943087

C67 -C62 -S72 -C73 :-179.447223

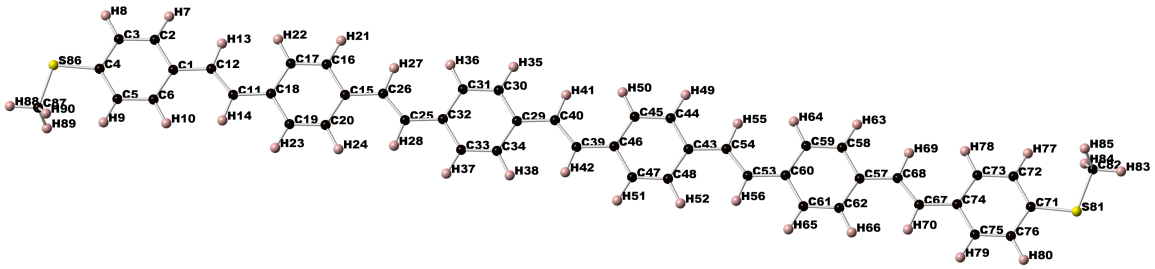
H69 -C63 -C62 -S72 : -0.016733

H69 -C63 -C64 -H70 : -0.107060

H71 -C66 -C67 -H72 : -0.015840

H72 -C67 -C62 -S72 : -0.008684

MeS-PPV5



Final geometry:

angstroms

atom	x	y	z
C1	-1.2260462267	0.3579924365	-1.1912687316
C2	-1.9451433869	1.5143222637	-1.5543536908
C3	-3.3321508011	1.5410139852	-1.5701760686
C4	-4.0705439251	0.4000316963	-1.2183763534
C5	-3.3721415961	-0.7601042313	-0.8529060455
C6	-1.9811820900	-0.7754703468	-0.8407813309
H8	-1.3969118741	2.4116030011	-1.8309148448
H9	-3.8491786577	2.4527437179	-1.8563300523
H11	-3.9053294589	-1.6612156475	-0.5724085057
H12	-1.4797458221	-1.6922188305	-0.5472549862
C12	1.0918339132	-0.6041957352	-0.9198185506
C13	0.2368338773	0.4039955776	-1.1969272103
H15	0.6485756540	1.3761171091	-1.4618195927
H16	0.6806413772	-1.5794524541	-0.6641081912
C16	5.4147608938	-0.6024479784	-0.8876820356
C17	4.6945115194	0.5740241529	-1.1831882778
C18	3.3084940056	0.6026909642	-1.2009440220
C19	2.5536688516	-0.5535371990	-0.9222683998
C20	3.2740981866	-1.7296689250	-0.6263111559

C21	4.6597629397	-1.7584708977	-0.6087400194
H23	5.2466793137	1.4847742903	-1.4021966151
H24	2.8073417747	1.5370630217	-1.4321623078
H25	2.7217603493	-2.6398725301	-0.4056319262
H26	5.1606415211	-2.6919616033	-0.3739334541
C26	7.7273579553	-1.5733739918	-0.6332940222
C27	6.8760813399	-0.5544614498	-0.8859579157
H29	7.2903618256	0.4250637935	-1.1173247246
H30	7.3103555804	-2.5517566025	-0.4027266921
C30	12.0483092562	-1.6091203386	-0.5823905903
C31	11.3401213969	-0.4247293994	-0.8763946008
C32	9.9545642494	-0.3831413110	-0.8998252667
C33	9.1883728472	-1.5336974394	-0.6282465483
C34	9.8967456999	-2.7179317532	-0.3341162049
C35	11.2817554598	-2.7594374319	-0.3107023479
H37	11.9017745401	0.4811894066	-1.0911462125
H38	9.4624516558	0.5556206204	-1.1326924229
H39	9.3351303207	-3.6238936863	-0.1196959966
H40	11.7732093934	-3.6985422157	-0.0784892773
C40	14.3498606676	-2.6031632798	-0.3209317082
C41	13.5099421846	-1.5757599180	-0.5775211892
H43	13.9348931399	-0.6012550486	-0.8105032772
H44	13.9218363060	-3.5759942567	-0.0870903932
C44	18.6696625864	-2.6920840947	-0.2749081179
C45	17.9760221626	-1.5007583110	-0.5759388410
C46	16.5911274781	-1.4414686036	-0.5971138743
C47	15.8112028399	-2.5804297775	-0.3163186010
C48	16.5053392926	-3.7710522034	-0.0149223257
C49	17.8895204012	-3.8304733906	0.0065107307
H51	18.5489258936	-0.6038380058	-0.7984274229

H52	16.1104119800	-0.4984508817	-0.8363063024
H53	15.9333805736	-4.6683356002	0.2062712880
H54	18.3694690216	-4.7743136979	0.2436745257
C54	20.9615160980	-3.7095949664	-0.0072326084
C55	20.1312303931	-2.6771027434	-0.2747767119
H57	20.5663642354	-1.7108060607	-0.5222479947
H58	20.5260926786	-4.6750287705	0.2433465503
C58	25.2815426443	-3.8174408025	0.0099915749
C59	24.5893847811	-2.6301538937	-0.3082450180
C60	23.2049436103	-2.5666037726	-0.3198601524
C61	22.4232061833	-3.6970160140	-0.0117781507
C62	23.1151581254	-4.8845527265	0.3066618195
C63	24.5000564114	-4.9479121473	0.3185374567
H65	25.1633298329	-1.7394486312	-0.5519656294
H66	22.7259778238	-1.6265495444	-0.5735709569
H67	22.5412729936	-5.7758907869	0.5485455237
H68	24.9792664616	-5.8889739753	0.5684347970
C68	27.5790772656	-4.8231292481	0.2879227543
C69	26.7437724510	-3.8024106347	-0.0026686605
H71	27.1744191668	-2.8424490759	-0.2812172855
H72	27.1495525946	-5.7814216884	0.5741504797
C72	31.8859560224	-4.9072791869	0.2699393884
C73	31.2079833664	-3.7363717980	-0.0997563201
C74	29.8175832205	-3.6922896216	-0.0989498611
C75	29.0426988532	-4.8067246313	0.2692217275
C76	29.7414098694	-5.9739374486	0.6372478416
C77	31.1277083091	-6.0292793946	0.6399566537
H79	31.7570144202	-2.8489471369	-0.3931520683
H80	29.3325697853	-2.7676958613	-0.3953734722
H81	29.1775722988	-6.8571197957	0.9274591397

H82	31.6286179231	-6.9488666468	0.9296047283
S82	33.6579830330	-5.0872275326	0.3077330446
C83	34.2675575354	-3.4661305320	-0.2565826101
H84	35.3565051829	-3.5466357272	-0.2552257079
H85	33.9306148517	-3.2424404176	-1.2713734128
H86	33.9716979743	-2.6657485909	0.4254238860
S86	-5.8453208476	0.5448123940	-1.2711008498
C87	-6.4278390181	-1.0922097916	-0.7247303911
H88	-7.5181066773	-1.0338043504	-0.7375546737
H89	-6.1081631481	-1.8813738382	-1.4090783883
H90	-6.0976724341	-1.3164478165	0.2921755196

Total energy (hartrees): -2649.62277737387

HOMO energy (hartrees): -0.17781

LUMO energy (hartrees): -0.07821

Bond lengths (angstroms):

C1	-C2	: 1.409266	C1	-C6	:	1.406346	
C1	-C13	: 1.463614	C2	-C3	:	1.387354	
C2	-H8	: 1.087270	C3	-C4	:	1.403862	
C3	-H9	: 1.086487	C4	-C5	:	1.402587	
C4	-S86	: 1.781453	C5	-C6	:	1.391097	
C5	-H11	: 1.083960	C6	-H12	:	1.085368	
C12	-C13	: 1.350653	C12	-H16	:	1.088849	
C12	-C19	: 1.462714	C13	-H15	:	1.088448	
C16	-C17	: 1.410734	C16	-C21	:	1.408623	
C16	-C27	: 1.462109	C17	-C18	:	1.386428	

C17	-H23	:	1.087345	C18	-C19	:	1.408646
C18	-H24	:	1.085203	C19	-C20	:	1.410636
C20	-C21	:	1.386075	C20	-H25	:	1.087312
C21	-H26	:	1.085089	C26	-C27	:	1.351552
C26	-H30	:	1.088249	C26	-C33	:	1.461562
C27	-H29	:	1.088406	C30	-C31	:	1.410940
C30	-C35	:	1.408776	C30	-C41	:	1.462022
C31	-C32	:	1.386379	C31	-H37	:	1.087318
C32	-C33	:	1.408753	C32	-H38	:	1.085208
C33	-C34	:	1.410927	C34	-C35	:	1.385829
C34	-H39	:	1.087269	C35	-H40	:	1.085066
C40	-C41	:	1.351613	C40	-H44	:	1.088249
C40	-C47	:	1.461526	C41	-H43	:	1.088358
C44	-C45	:	1.411033	C44	-C49	:	1.408456
C44	-C55	:	1.461645	C45	-C46	:	1.386325
C45	-H51	:	1.087284	C46	-C47	:	1.408673
C46	-H52	:	1.085165	C47	-C48	:	1.410761
C48	-C49	:	1.385622	C48	-H53	:	1.086821
C49	-H54	:	1.085095	C54	-C55	:	1.351664
C54	-H58	:	1.088323	C54	-C61	:	1.461751
C55	-H57	:	1.088261	C58	-C59	:	1.410676
C58	-C63	:	1.408505	C58	-C69	:	1.462362
C59	-C60	:	1.385948	C59	-H65	:	1.087276
C60	-C61	:	1.408496	C60	-H66	:	1.085117
C61	-C62	:	1.410831	C62	-C63	:	1.386398
C62	-H67	:	1.087352	C63	-H68	:	1.085213
C68	-C69	:	1.350572	C68	-H72	:	1.088459
C68	-C75	:	1.463833	C69	-H71	:	1.088381
C72	-C73	:	1.402621	C72	-C77	:	1.403829
C72	-S82	:	1.781541	C73	-C74	:	1.391099

C73 -H79 : 1.083992 C74 -C75 : 1.406400

C74 -H80 : 1.085347 C75 -C76 : 1.409264

C76 -C77 : 1.387405 C76 -H81 : 1.087266

C77 -H82 : 1.086484 S82 -C83 : 1.821535

C83 -H84 : 1.091920 C83 -H85 : 1.092414

C83 -H86 : 1.092372 S86 -C87 : 1.821453

C87 -H88 : 1.091906 C87 -H89 : 1.092385

C87 -H90 : 1.092424

Bond angles:

C6 -C1 -C2 : 116.841992 C13 -C1 -C2 : 118.896035

C13 -C1 -C6 : 124.261814 C3 -C2 -C1 : 121.928502

H8 -C2 -C1 : 119.037847 H8 -C2 -C3 : 119.033635

C4 -C3 -C2 : 120.487250 H9 -C3 -C2 : 119.663210

H9 -C3 -C4 : 119.849517 C5 -C4 -C3 : 118.401629

S86 -C4 -C3 : 116.777841 S86 -C4 -C5 : 124.820494

C6 -C5 -C4 : 120.617027 H11 -C5 -C4 : 120.671187

H11 -C5 -C6 : 118.711653 C5 -C6 -C1 : 121.723513

H12 -C6 -C1 : 120.005352 H12 -C6 -C5 : 118.270699

H16 -C12 -C13 : 118.535385 C19 -C12 -C13 : 127.333322

C19 -C12 -H16 : 114.131105 C12 -C13 -C1 : 127.477848

H15 -C13 -C1 : 114.023196 H15 -C13 -C12 : 118.498690

C21 -C16 -C17 : 116.886946 C27 -C16 -C17 : 118.891401

C27 -C16 -C21 : 124.221582 C18 -C17 -C16 : 122.027370

H23 -C17 -C16 : 118.778846 H23 -C17 -C18 : 119.193747

C19 -C18 -C17 : 121.076872 H24 -C18 -C17 : 118.829175

H24 -C18 -C19 : 120.093782 C18 -C19 -C12 : 124.352847

C20 -C19 -C12 : 118.762368 C20 -C19 -C18 : 116.884708

C21 -C20 -C19 : 122.042337 H25 -C20 -C19 : 118.757211

H25 -C20 -C21 : 119.200452 C20 -C21 -C16 : 121.081745

H26 -C21 -C16 : 120.096609 H26 -C21 -C20 : 118.821611

H30 -C26 -C27 : 118.426490 C33 -C26 -C27 : 127.574705

C33 -C26 -H30 : 113.998803 C26 -C27 -C16 : 127.228066

H29 -C27 -C16 : 114.186692 H29 -C27 -C26 : 118.585240

C35 -C30 -C31 : 116.904374 C41 -C30 -C31 : 118.903298

C41 -C30 -C35 : 124.192314 C32 -C31 -C30 : 122.027859

H37 -C31 -C30 : 118.768726 H37 -C31 -C32 : 119.203409

C33 -C32 -C31 : 121.050884 H38 -C32 -C31 : 118.867153

H38 -C32 -C33 : 120.081956 C32 -C33 -C26 : 124.414870

C34 -C33 -C26 : 118.672916 C34 -C33 -C32 : 116.912211

C35 -C34 -C33 : 122.034181 H39 -C34 -C33 : 118.760263

H39 -C34 -C35 : 119.205556 C34 -C35 -C30 : 121.070490

H40 -C35 -C30 : 120.100675 H40 -C35 -C34 : 118.828832

H44 -C40 -C41 : 118.417422 C47 -C40 -C41 : 127.597929

C47 -C40 -H44 : 113.984641 C40 -C41 -C30 : 127.195857

H43 -C41 -C30 : 114.208954 H43 -C41 -C40 : 118.595185

C49 -C44 -C45 : 116.919766 C55 -C44 -C45 : 118.876490

C55 -C44 -C49 : 124.203651 C46 -C45 -C44 : 122.035410

H51 -C45 -C44 : 118.757727 H51 -C45 -C46 : 119.206845

C47 -C46 -C45 : 121.028475 H52 -C46 -C45 : 118.885677

H52 -C46 -C47 : 120.085788 C46 -C47 -C40 : 124.439553

C48 -C47 -C40 : 118.653709 C48 -C47 -C46 : 116.906626

C49 -C48 -C47 : 122.074075 H53 -C48 -C47 : 118.771375

H53 -C48 -C49 : 119.154535 C48 -C49 -C44 : 121.035633

H54 -C49 -C44 : 120.113367 H54 -C49 -C48 : 118.850942

H58 -C54 -C55 : 118.517534 C61 -C54 -C55 : 127.376855

C61 -C54 -H58 : 114.105601 C54 -C55 -C44 : 127.331500

H57 -C55 -C44 : 114.135919 H57 -C55 -C54 : 118.532577

C63 -C58 -C59 : 116.916487 C69 -C58 -C59 : 118.685993

C69 -C58 -C63 : 124.397384 C60 -C59 -C58 : 122.046418

H65 -C59 -C58 : 118.753633 H65 -C59 -C60 : 119.199940

C61 -C60 -C59 : 121.049555 H66 -C60 -C59 : 118.855251

H66 -C60 -C61 : 120.095090 C60 -C61 -C54 : 124.234358

C62 -C61 -C54 : 118.848225 C62 -C61 -C60 : 116.917184

C63 -C62 -C61 : 122.027583 H67 -C62 -C61 : 118.773446

H67 -C62 -C63 : 119.198931 C62 -C63 -C58 : 121.042763

H68 -C63 -C58 : 120.094739 H68 -C63 -C62 : 118.862315

H72 -C68 -C69 : 118.548578 C75 -C68 -C69 : 127.385494

C75 -C68 -H72 : 114.065850 C68 -C69 -C58 : 127.502497

H71 -C69 -C58 : 114.011617 H71 -C69 -C68 : 118.485825

C77 -C72 -C73 : 118.398594 S82 -C72 -C73 : 124.798496

S82 -C72 -C77 : 116.802909 C74 -C73 -C72 : 120.625160

H79 -C73 -C72 : 120.659968 H79 -C73 -C74 : 118.714795

C75 -C74 -C73 : 121.717721 H80 -C74 -C73 : 118.260845

H80 -C74 -C75 : 120.021188 C74 -C75 -C68 : 124.271496

C76 -C75 -C68 : 118.888636 C76 -C75 -C74 : 116.839672

C77 -C76 -C75 : 121.934561 H81 -C76 -C75 : 119.036801

H81 -C76 -C77 : 119.028637 C76 -C77 -C72 : 120.484268

H82 -C77 -C72 : 119.849136 H82 -C77 -C76 : 119.666549

C83 -S82 -C72 : 103.673985 H84 -C83 -S82 : 105.529686

H85 -C83 -S82 : 111.518704 H85 -C83 -H84 : 108.895943

H86 -C83 -S82 : 111.593478 H86 -C83 -H84 : 108.865567

H86 -C83 -H85 : 110.267371 C87 -S86 -C4 : 103.691339

H88 -C87 -S86 : 105.529431 H89 -C87 -S86 : 111.577921

H89 -C87 -H88 : 108.873836 H90 -C87 -S86 : 111.533994

H90 -C87 -H88 : 108.886347 H90 -C87 -H89 : 110.269075

Torsional angles:

C1 -C2 -C3 -C4 : 0.063144

C1 -C2 -C3 -H9 :-179.991645

C1 -C6 -C5 -C4 : -0.045624

C1 -C6 -C5 -H11 :-179.913486

C1 -C13 -C12 -H16 : 0.380777

C1 -C13 -C12 -C19 :-179.787230

C2 -C1 -C6 -C5 : 0.100505

C2 -C1 -C6 -H12 :-179.655226

C2 -C1 -C13 -C12 :-177.916404

C2 -C1 -C13 -H15 : 1.891823

C2 -C3 -C4 -C5 : -0.003120

C2 -C3 -C4 -S86 : 179.930595

C3 -C2 -C1 -C6 : -0.109467

C3 -C2 -C1 -C13 :-179.970634

C3 -C4 -C5 -C6 : -0.005453

C3 -C4 -C5 -H11 : 179.859806

C3 -C4 -S86 -C87 :-178.776849

C4 -C3 -C2 -H8 :-179.984271

C4 -C5 -C6 -H12 : 179.714196

C4 -S86 -C87 -H88 : 179.517230

C4 -S86 -C87 -H89 : -62.387394

C4 -S86 -C87 -H90 : 61.429977

C5 -C4 -C3 -H9 :-179.948229

C5 -C4 -S86 -C87 : 1.152127

C5 -C6 -C1 -C13 : 179.953438

C6 -C1 -C2 -H8 : 179.937951

C6 -C1 -C13 -C12 : 2.233479

C6 -C1 -C13 -H15 :-177.958295

C6 -C5 -C4 -S86 :-179.933369

H8 -C2 -C1 -C13 : 0.076783

H8 -C2 -C3 -H9 : -0.039060

H9 -C3 -C4 -S86 : -0.014514

H11 -C5 -C4 -S86 : -0.068110

H11 -C5 -C6 -H12 : -0.153666

H12 -C6 -C1 -C13 : 0.197706

C12 -C19 -C18 -C17 : 179.941395

C12 -C19 -C18 -H24 : 0.093370

C12 -C19 -C20 -C21 :-179.958011

C12 -C19 -C20 -H25 : 0.041138

C13 -C12 -C19 -C18 : 1.232000

C13 -C12 -C19 -C20 :-178.872310

H15 -C13 -C12 -H16 :-179.419910

H15 -C13 -C12 -C19 : 0.412083

H16 -C12 -C19 -C18 :-178.929731

H16 -C12 -C19 -C20 : 0.965960

C16 -C17 -C18 -C19 : -0.021387

C16 -C17 -C18 -H24 : 179.828521

C16 -C21 -C20 -C19 : 0.042144

C16 -C21 -C20 -H25 :-179.957003

C16 -C27 -C26 -H30 : 0.049204

C16 -C27 -C26 -C33 :-179.936114

C17 -C16 -C21 -C20 : -0.016463

C17 -C16 -C21 -H26 :-179.947612

C17 -C16 -C27 -C26 :-179.722401

C17 -C16 -C27 -H29 : 0.296968

C17 -C18 -C19 -C20 : 0.043916

C18 -C17 -C16 -C21 : 0.006444

C18 -C17 -C16 -C27 :-179.900947

C18 -C19 -C20 -C21 : -0.054562

C18 -C19 -C20 -H25 : 179.944588

C19 -C18 -C17 -H23 :-179.951398

C19 -C20 -C21 -H26 : 179.974152

C20 -C19 -C18 -H24 :-179.804110

C20 -C21 -C16 -C27 : 179.885477

C21 -C16 -C17 -H23 : 179.936734

C21 -C16 -C27 -C26 : 0.377492

C21 -C16 -C27 -H29 :-179.603139

H23 -C17 -C16 -C27 : 0.029343

H23 -C17 -C18 -H24 : -0.101489

H25 -C20 -C21 -H26 : -0.024994

H26 -C21 -C16 -C27 : -0.045672

C26 -C33 -C32 -C31 :-179.972614

C26 -C33 -C32 -H38 : -0.003315

C26 -C33 -C34 -C35 : 179.974086

C26 -C33 -C34 -H39 : -0.028083

C27 -C26 -C33 -C32 : -0.166887

C27 -C26 -C33 -C34 : 179.852790

H29 -C27 -C26 -H30 :-179.970918

H29 -C27 -C26 -C33 : 0.043765

H30 -C26 -C33 -C32 : 179.847247

H30 -C26 -C33 -C34 : -0.133076

C30 -C31 -C32 -C33 : -0.000876

C30 -C31 -C32 -H38 :-179.970541

C30 -C35 -C34 -C33 : 0.000136

C30 -C35 -C34 -H39 :-179.997685

C30 -C41 -C40 -H44 : -0.100490

C30 -C41 -C40 -C47 : 179.863889

C31 -C30 -C35 -C34 : 0.007064

C31 -C30 -C35 -H40 : 179.986039

C31 -C30 -C41 -C40 :-179.976856

C31 -C30 -C41 -H43 : -0.001257

C31 -C32 -C33 -C34 : 0.008025

C32 -C31 -C30 -C35 : -0.006736

C32 -C31 -C30 -C41 : 179.951227

C32 -C33 -C34 -C35 : -0.007710

C32 -C33 -C34 -H39 : 179.990120

C33 -C32 -C31 -H37 : 179.969705

C33 -C34 -C35 -H40 :-179.979102

C34 -C33 -C32 -H38 : 179.977325

C34 -C35 -C30 -C41 :-179.948446

C35 -C30 -C31 -H37 :-179.977441

C35 -C30 -C41 -C40 : -0.022175

C35 -C30 -C41 -H43 : 179.953424

H37 -C31 -C30 -C41 : -0.019477

H37 -C31 -C32 -H38 : 0.000040

H39 -C34 -C35 -H40 : 0.023077

H40 -C35 -C30 -C41 : 0.030529

C40 -C47 -C46 -C45 :-179.835521

C40 -C47 -C46 -H52 : 0.074371

C40 -C47 -C48 -C49 : 179.853327

C40 -C47 -C48 -H53 : -0.102317

C41 -C40 -C47 -C46 : -0.394904

C41 -C40 -C47 -C48 : 179.730906

H43 -C41 -C40 -H44 : 179.924856

H43 -C41 -C40 -C47 : -0.110764

H44 -C40 -C47 -C46 : 179.570807

H44 -C40 -C47 -C48 : -0.303382

C44 -C45 -C46 -C47 : -0.017734

C44 -C45 -C46 -H52 :-179.928687

C44 -C49 -C48 -C47 : -0.003802

C44 -C49 -C48 -H53 : 179.951677

C44 -C55 -C54 -H58 : -0.215402

C44 -C55 -C54 -C61 : 179.747062

C45 -C44 -C49 -C48 : 0.027439

C45 -C44 -C49 -H54 : 179.938996

C45 -C44 -C55 -C54 : 179.687812

C45 -C44 -C55 -H57 : -0.333506

C45 -C46 -C47 -C48 : 0.040673

C46 -C45 -C44 -C49 : -0.016927

C46 -C45 -C44 -C55 : 179.877254

C46 -C47 -C48 -C49 : -0.030318

C46 -C47 -C48 -H53 :-179.985961

C47 -C46 -C45 -H51 : 179.931161

C47 -C48 -C49 -H54 :-179.916454

C48 -C47 -C46 -H52 : 179.950565

C48 -C49 -C44 -C55 :-179.860521

C49 -C44 -C45 -H51 :-179.966043

C49 -C44 -C55 -C54 : -0.426273

C49 -C44 -C55 -H57 : 179.552410

H51 -C45 -C44 -C55 : -0.071862

H51 -C45 -C46 -H52 : 0.020208

H53 -C48 -C49 -H54 : 0.039024

H54 -C49 -C44 -C55 : 0.051036

C54 -C61 -C60 -C59 :-179.785513

C54 -C61 -C60 -H66 : 0.095572

C54 -C61 -C62 -C63 : 179.809879

C54 -C61 -C62 -H67 : -0.115960

C55 -C54 -C61 -C60 : -0.651823

C55 -C54 -C61 -C62 : 179.529244

H57 -C55 -C54 -H58 : 179.806741

H57 -C55 -C54 -C61 : -0.230795

H58 -C54 -C61 -C60 : 179.312044

H58 -C54 -C61 -C62 : -0.506889

C58 -C59 -C60 -C61 : -0.032274

C58 -C59 -C60 -H66 :-179.914804

C58 -C63 -C62 -C61 : 0.002569

C58 -C63 -C62 -H67 : 179.928103

C58 -C69 -C68 -H72 : -0.374722

C58 -C69 -C68 -C75 : 179.733348

C59 -C58 -C63 -C62 : 0.003497

C59 -C58 -C63 -H68 : 179.846325

C59 -C58 -C69 -C68 : 179.049823

C59 -C58 -C69 -H71 : -0.858350

C59 -C60 -C61 -C62 : 0.036620

C60 -C59 -C58 -C63 : 0.011239

C60 -C59 -C58 -C69 : 179.882908

C60 -C61 -C62 -C63 : -0.022236

C60 -C61 -C62 -H67 :-179.948076

C61 -C60 -C59 -H65 : 179.933786

C61 -C62 -C63 -H68 :-179.842160

C62 -C61 -C60 -H66 : 179.917705

C62 -C63 -C58 -C69 :-179.860066

C63 -C58 -C59 -H65 :-179.954966

C63 -C58 -C69 -C68 : -1.088855

C63 -C58 -C69 -H71 : 179.002972

H65 -C59 -C58 -C69 : -0.083297

H65 -C59 -C60 -H66 : 0.051255

H67 -C62 -C63 -H68 : 0.083374

H68 -C63 -C58 -C69 : -0.017237

C68 -C75 -C74 -C73 :-179.890689

C68 -C75 -C74 -H80 : -0.074502

C68 -C75 -C76 -C77 : 179.892672

C68 -C75 -C76 -H81 : -0.098125

C69 -C68 -C75 -C74 : -1.650358

C69 -C68 -C75 -C76 : 178.516120

H71 -C69 -C68 -H72 : 179.529844

H71 -C69 -C68 -C75 : -0.362086

H72 -C68 -C75 -C74 : 178.453609

H72 -C68 -C75 -C76 : -1.379913

C72 -C73 -C74 -C75 : 0.044902

C72 -C73 -C74 -H80 :-179.774407

C72 -C77 -C76 -C75 : -0.030221

C72 -C77 -C76 -H81 : 179.960577

C72 -S82 -C83 -H84 :-179.405003

C72 -S82 -C83 -H85 : -61.314152

C72 -S82 -C83 -H86 : 62.501182

C73 -C72 -C77 -C76 : 0.018154

C73 -C72 -C77 -H82 : 179.939215

C73 -C72 -S82 -C83 : -1.072894

C73 -C74 -C75 -C76 : -0.054049

C74 -C73 -C72 -C77 : -0.025364

C74 -C73 -C72 -S82 : 179.961637

C74 -C75 -C76 -C77 : 0.046855

C74 -C75 -C76 -H81 :-179.943942

C75 -C74 -C73 -H79 : 179.945158

C75 -C76 -C77 -H82 :-179.951425

C76 -C75 -C74 -H80 : 179.762138

C76 -C77 -C72 -S82 :-179.969887

C77 -C72 -C73 -H79 :-179.923670

C77 -C72 -S82 -C83 : 178.914295

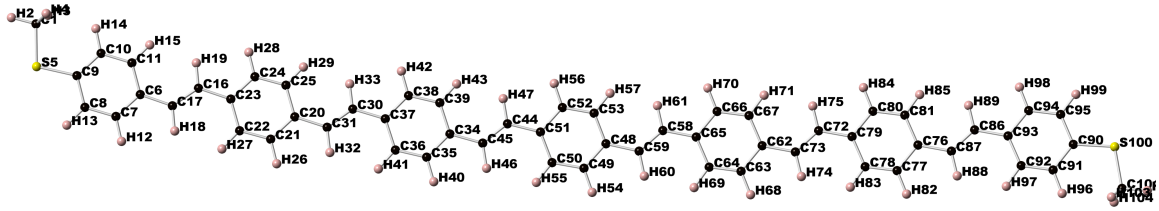
H79 -C73 -C72 -S82 : 0.063331

H79 -C73 -C74 -H80 : 0.125849

H81 -C76 -C77 -H82 : 0.039373

H82 -C77 -C72 -S82 : -0.048826

MeS-PPV6



Final geometry:

		angstroms	
atom	x	y	z
C1	-5.0888493610	-0.5592865372	0.9740341311
H2	-5.6962096409	0.0665081993	1.6310116332
H4	-4.4338883222	0.0826632153	0.3806170836
H5	-4.4954173951	-1.2427496108	1.5857124329
S5	-6.2739682755	-1.4596185847	-0.0763442714
C6	-3.7296418350	-4.1362479476	-2.8590503940
C7	-5.1380682033	-4.1111001234	-2.8913718687
C8	-5.8766021681	-3.2971388435	-2.0442254446
C9	-5.2326992161	-2.4636911649	-1.1160752228
C10	-3.8310436829	-2.4765478519	-1.0683647756
C11	-3.1011376883	-3.2960263789	-1.9222904745
H13	-5.6613468548	-4.7466379316	-3.6016434991
H14	-6.9615435525	-3.3065022925	-2.1006809015
H15	-3.2953224731	-1.8494059207	-0.3650649260
H16	-2.0183770143	-3.2774179959	-1.8503103874
C16	-1.6738260256	-5.1447720259	-3.9079411331
C17	-3.0118912883	-5.0160260509	-3.7809200835
H19	-3.6569779252	-5.6146004004	-4.4214008757
H20	-1.0312957026	-4.5398715915	-3.2703194140
C20	0.6147028985	-7.6700408501	-6.5650935163

C21	-0.7957861219	-7.6983142780	-6.5819365092
C22	-1.5575763944	-6.9006239966	-5.7406140255
C23	-0.9476051528	-6.0194690848	-4.8253985362
C24	0.4625353126	-5.9924420499	-4.8086991312
C25	1.2227073824	-6.7892392673	-5.6488785843
H27	-1.2979431556	-8.3671429724	-7.2768960926
H28	-2.6394054899	-6.9642322531	-5.7964572435
H29	0.9651850265	-5.3236416429	-4.1142342553
H30	2.3041891561	-6.7243218640	-5.5919647671
C30	2.7025592895	-8.6295149892	-7.5855258832
C31	1.3586722811	-8.5349327166	-7.4784903841
H33	0.7364594770	-9.1515369440	-8.1245011595
H34	3.3164263730	-8.0096756997	-6.9344667324
C34	5.1263209065	-11.0802138269	-10.1919741447
C35	3.7178421500	-11.1408978818	-10.2520747893
C36	2.9117351178	-10.3679382231	-9.4285675970
C37	3.4726140724	-9.4805584186	-8.4880815779
C38	4.8810224318	-9.4203294271	-8.4290163065
C39	5.6848554994	-10.1920448118	-9.2512175957
H41	3.2529345819	-11.8153486505	-10.9672227179
H42	1.8337436201	-10.4545663699	-9.5187483601
H43	5.3465695560	-8.7451652999	-7.7151592956
H44	6.7620772271	-10.1008170623	-9.1611611776
C44	7.2695625369	-11.9828442681	-11.1425179714
C45	5.9205874277	-11.9201356134	-11.0871682746
H47	5.3369089996	-12.5445335489	-11.7611010912
H48	7.8411746625	-11.3551304407	-10.4612920234
C48	9.8737851915	-14.3492186184	-13.6518370175
C49	8.4711944684	-14.4473300314	-13.7771263240
C50	7.6063857604	-13.7012582027	-12.9881179629

C51	8.0995810159	-12.8053952657	-12.0178649026
C52	9.5017709499	-12.7078783122	-11.8939935672
C53	10.3634815031	-13.4523022279	-12.6816424121
H55	8.0583890241	-15.1300524938	-14.5160155346
H56	6.5357071211	-13.8166957493	-13.1273048701
H57	9.9155603692	-12.0263808349	-11.1547274102
H58	11.4324752057	-13.3355820670	-12.5382546686
C58	12.0853244874	-15.1767798142	-14.5140185129
C59	10.7332308015	-15.1641343261	-14.5097741514
H61	10.1997354772	-15.8155406489	-15.2002311173
H62	12.6085739794	-14.5206021016	-13.8207588761
C62	14.8447572743	-17.4962627794	-16.8980780286
C63	13.4503677744	-17.6380599990	-17.0660186632
C64	12.5390566040	-16.9067228494	-16.3183054924
C65	12.9741671304	-15.9808085120	-15.3488245347
C66	14.3687075714	-15.8373852904	-15.1831316200
C67	15.2788463210	-16.5682374027	-15.9301185628
H69	13.0825939365	-18.3459802025	-17.8049126700
H70	11.4774669064	-17.0584188412	-16.4880115801
H71	14.7372668632	-15.1311531109	-14.4430513190
H72	16.3392277087	-16.4175697803	-15.7567908699
C72	17.0961719172	-18.3061544886	-17.6883301656
C73	15.7444988108	-18.3070736863	-17.7160945208
H75	15.2386738178	-18.9764243077	-18.4100076649
H76	17.6015595980	-17.6357392009	-16.9951213785
C76	19.8797514592	-20.6660299625	-20.0057434247
C77	18.4871881906	-20.8113191975	-20.1797863644
C78	17.5720557355	-20.0661297665	-19.4522400250
C79	17.9993098215	-19.1216406875	-18.4975598141
C80	19.3922746895	-18.9753485131	-18.3242176469

C81	20.3074859786	-19.7208283640	-19.0518687067
H83	18.1238837646	-21.5330874525	-20.9073680377
H84	16.5127094322	-20.2228981722	-19.6266331320
H85	19.7561714970	-18.2557967599	-17.5946569213
H86	21.3668823799	-19.5681196020	-18.8735485822
C86	22.1308163918	-21.4877425073	-20.7860190758
C87	20.7804284125	-21.4926885071	-20.8072361959
H89	20.2730822193	-22.1770492679	-21.4853029958
H90	22.6376398040	-20.7999482226	-20.1117491460
C90	24.9018826383	-23.8661794432	-23.0696395741
C91	23.5210780672	-24.0500865077	-23.2350173614
C92	22.6120130266	-23.2898860113	-22.5058137752
C93	23.0355960273	-22.3161975994	-21.5826650511
C94	24.4264283360	-22.1469749248	-21.4296006617
C95	25.3414502451	-22.8989127138	-22.1521011770
H97	23.1419831346	-24.7888474443	-23.9319824292
H98	21.5525990865	-23.4661047496	-22.6619012877
H99	24.7936148973	-21.4044841437	-20.7252929591
H100	26.4058129406	-22.7369242951	-22.0056545201
S100	26.1626877725	-24.7767222561	-23.9387710010
C101	25.2189824348	-25.9036640257	-25.0144532173
H102	25.9677240215	-26.4768507713	-25.5651093236
H103	24.6037054881	-26.5936925196	-24.4326187125
H104	24.6003356684	-25.3533869219	-25.7269841404

Total energy (hartrees): -2958.09426200184

HOMO energy (hartrees): -0.17724

LUMO energy (hartrees): -0.08011

Bond lengths (angstroms):

C1	-H2	:	1.091845	C1	-H4	:	1.092345
C1	-H5	:	1.092444	C1	-S5	:	1.821647
S5	-C9	:	1.781416	C6	-C7	:	1.409022
C6	-C11	:	1.406595	C6	-C17	:	1.462539
C7	-C8	:	1.387668	C7	-H13	:	1.087297
C8	-C9	:	1.403819	C8	-H14	:	1.086450
C9	-C10	:	1.402526	C10	-C11	:	1.390502
C10	-H15	:	1.083944	C11	-H16	:	1.085310
C16	-C17	:	1.350233	C16	-H20	:	1.088720
C16	-C23	:	1.460897	C17	-H19	:	1.088413
C20	-C21	:	1.410873	C20	-C25	:	1.408876
C20	-C31	:	1.461445	C21	-C22	:	1.387248
C21	-H27	:	1.087411	C22	-C23	:	1.409297
C22	-H28	:	1.085135	C23	-C24	:	1.410498
C24	-C25	:	1.385153	C24	-H29	:	1.087305
C25	-H30	:	1.084922	C30	-C31	:	1.351457
C30	-H34	:	1.088536	C30	-C37	:	1.460091
C31	-H33	:	1.088430	C34	-C35	:	1.411066
C34	-C39	:	1.409194	C34	-C45	:	1.462088
C35	-C36	:	1.387602	C35	-H41	:	1.087410
C36	-C37	:	1.409447	C36	-H42	:	1.085220
C37	-C38	:	1.410932	C38	-C39	:	1.384813
C38	-H43	:	1.087278	C39	-H44	:	1.084822
C44	-C45	:	1.351566	C44	-H48	:	1.088501
C44	-C51	:	1.460052	C45	-H47	:	1.088457
C48	-C49	:	1.411589	C48	-C53	:	1.409092

C48 -C59 : 1.462460 C49 -C50 : 1.388183

C49 -H55 : 1.087417 C50 -C51 : 1.409682

C50 -H56 : 1.085841 C51 -C52 : 1.411025

C52 -C53 : 1.384595 C52 -H57 : 1.087279

C53 -H58 : 1.084865 C58 -C59 : 1.352159

C58 -H62 : 1.088562 C58 -C65 : 1.460618

C59 -H61 : 1.088889 C62 -C63 : 1.411606

C62 -C67 : 1.409472 C62 -C73 : 1.461540

C63 -C64 : 1.387234 C63 -H69 : 1.087370

C64 -C65 : 1.409444 C64 -H70 : 1.085718

C65 -C66 : 1.411654 C66 -C67 : 1.385816

C66 -H71 : 1.087345 C67 -H72 : 1.084966

C72 -C73 : 1.351959 C72 -H76 : 1.088766

C72 -C79 : 1.461345 C73 -H75 : 1.088763

C76 -C77 : 1.410898 C76 -C81 : 1.409340

C76 -C87 : 1.461839 C77 -C78 : 1.386398

C77 -H83 : 1.087343 C78 -C79 : 1.409262

C78 -H84 : 1.084990 C79 -C80 : 1.411311

C80 -C81 : 1.386661 C80 -H85 : 1.087398

C81 -H86 : 1.085099 C86 -C87 : 1.350564

C86 -H90 : 1.088380 C86 -C93 : 1.462740

C87 -H89 : 1.088818 C90 -C91 : 1.402780

C90 -C95 : 1.403817 C90 -S100 : 1.781602

C91 -C92 : 1.391417 C91 -H97 : 1.084085

C92 -C93 : 1.407016 C92 -H98 : 1.085253

C93 -C94 : 1.409425 C94 -C95 : 1.387329

C94 -H99 : 1.087275 C95 -H100 : 1.086533

S100 -C101 : 1.821447 C101 -H102 : 1.091961

C101 -H103 : 1.092354 C101 -H104 : 1.092350

Bond angles:

H4 -C1 -H2 : 108.879857 H5 -C1 -H2 : 108.895622

H5 -C1 -H4 : 110.251238 S5 -C1 -H2 : 105.565133

S5 -C1 -H4 : 111.548702 S5 -C1 -H5 : 111.533502

C9 -S5 -C1 : 103.582189 C11 -C6 -C7 : 116.824138

C17 -C6 -C7 : 119.132214 C17 -C6 -C11 : 124.043643

C8 -C7 -C6 : 121.900959 H13 -C7 -C6 : 119.052765

H13 -C7 -C8 : 119.046205 C9 -C8 -C7 : 120.514559

H14 -C8 -C7 : 119.649678 H14 -C8 -C9 : 119.835756

C8 -C9 -S5 : 116.898706 C10 -C9 -S5 : 124.713067

C10 -C9 -C8 : 118.388217 C11 -C10 -C9 : 120.604459

H15 -C10 -C9 : 120.710098 H15 -C10 -C11 : 118.685407

C10 -C11 -C6 : 121.767575 H16 -C11 -C6 : 120.012439

H16 -C11 -C10 : 118.219813 H20 -C16 -C17 : 118.475261

C23 -C16 -C17 : 127.502496 C23 -C16 -H20 : 114.022034

C16 -C17 -C6 : 127.084224 H19 -C17 -C6 : 114.259465

H19 -C17 -C16 : 118.655896 C25 -C20 -C21 : 116.854568

C31 -C20 -C21 : 119.314613 C31 -C20 -C25 : 123.830798

C22 -C21 -C20 : 122.020665 H27 -C21 -C20 : 118.791328

H27 -C21 -C22 : 119.188007 C23 -C22 -C21 : 121.044025

H28 -C22 -C21 : 118.851966 H28 -C22 -C23 : 120.104009

C22 -C23 -C16 : 124.543992 C24 -C23 -C16 : 118.559568

C24 -C23 -C22 : 116.896410 C25 -C24 -C23 : 122.036348

H29 -C24 -C23 : 118.784736 H29 -C24 -C25 : 119.178892

C24 -C25 -C20 : 121.147949 H30 -C25 -C20 : 120.113039

H30 -C25 -C24 : 118.738977 H34 -C30 -C31 : 118.265503

C37 -C30 -C31 : 127.893660 C37 -C30 -H34 : 113.840837

C30 -C31 -C20 : 126.664652 H33 -C31 -C20 : 114.532005

H33 -C31 -C30 : 118.803322 C39 -C34 -C35 : 116.818316

C45 -C34 -C35 : 119.436708 C45 -C34 -C39 : 123.744959

C36 -C35 -C34 : 122.048465 H41 -C35 -C34 : 118.779366

H41 -C35 -C36 : 119.172168 C37 -C36 -C35 : 121.033861

H42 -C36 -C35 : 118.899976 H42 -C36 -C37 : 120.066123

C36 -C37 -C30 : 124.720307 C38 -C37 -C30 : 118.404925

C38 -C37 -C36 : 116.874645 C39 -C38 -C37 : 122.058270

H43 -C38 -C37 : 118.777102 H43 -C38 -C39 : 119.164602

C38 -C39 -C34 : 121.166436 H44 -C39 -C34 : 120.132079

H44 -C39 -C38 : 118.701385 H48 -C44 -C45 : 118.147622

C51 -C44 -C45 : 128.176548 C51 -C44 -H48 : 113.675759

C44 -C45 -C34 : 126.436222 H47 -C45 -C34 : 114.666242

H47 -C45 -C44 : 118.897490 C53 -C48 -C49 : 116.786269

C59 -C48 -C49 : 119.546302 C59 -C48 -C53 : 123.667236

C50 -C49 -C48 : 122.086933 H55 -C49 -C48 : 118.760383

H55 -C49 -C50 : 119.152683 C51 -C50 -C49 : 120.983617

H56 -C50 -C49 : 118.965753 H56 -C50 -C51 : 120.050621

C50 -C51 -C44 : 124.874337 C52 -C51 -C44 : 118.252577

C52 -C51 -C50 : 116.873060 C53 -C52 -C51 : 122.097537

H57 -C52 -C51 : 118.763672 H57 -C52 -C53 : 119.138752

C52 -C53 -C48 : 121.172561 H58 -C53 -C48 : 120.127657

H58 -C53 -C52 : 118.699652 H62 -C58 -C59 : 118.230481

C65 -C58 -C59 : 127.984719 C65 -C58 -H62 : 113.784647

C58 -C59 -C48 : 126.490895 H61 -C59 -C48 : 114.670879

H61 -C59 -C58 : 118.838076 C67 -C62 -C63 : 116.876355

C73 -C62 -C63 : 119.064190 C73 -C62 -C67 : 124.058895

C64 -C63 -C62 : 122.129372 H69 -C63 -C62 : 118.707579

H69 -C63 -C64 : 119.162921 C65 -C64 -C63 : 120.949122

H70 -C64 -C63 : 118.974451 H70 -C64 -C65 : 120.076277

C64 -C65 -C58 : 124.534058 C66 -C65 -C58 : 118.564576

C66 -C65 -C64 : 116.900889 C67 -C66 -C65 : 122.136731

H71 -C66 -C65 : 118.732587 H71 -C66 -C67 : 119.130558

C66 -C67 -C62 : 121.007304 H72 -C67 -C62 : 120.142133

H72 -C67 -C66 : 118.850343 H76 -C72 -C73 : 118.527458

C79 -C72 -C73 : 127.310655 C79 -C72 -H76 : 114.161768

C72 -C73 -C62 : 127.128926 H75 -C73 -C62 : 114.316065

H75 -C73 -C72 : 118.554567 C81 -C76 -C77 : 116.879103

C87 -C76 -C77 : 118.832696 C87 -C76 -C81 : 124.287862

C78 -C77 -C76 : 122.101288 H83 -C77 -C76 : 118.729592

H83 -C77 -C78 : 119.169022 C79 -C78 -C77 : 121.038429

H84 -C78 -C77 : 118.846677 H84 -C78 -C79 : 120.114635

C78 -C79 -C72 : 124.177782 C80 -C79 -C72 : 118.955193

C80 -C79 -C78 : 116.866302 C81 -C80 -C79 : 122.090125

H85 -C80 -C79 : 118.770058 H85 -C80 -C81 : 119.139697

C80 -C81 -C76 : 121.024709 H86 -C81 -C76 : 120.127253

H86 -C81 -C80 : 118.847734 H90 -C86 -C87 : 118.532288

C93 -C86 -C87 : 127.433524 C93 -C86 -H90 : 114.034118

C86 -C87 -C76 : 127.254854 H89 -C87 -C76 : 114.191252

H89 -C87 -C86 : 118.553889 C95 -C90 -C91 : 118.398785

S100 -C90 -C91 : 124.895247 S100 -C90 -C95 : 116.705741

C92 -C91 -C90 : 120.643216 H97 -C91 -C90 : 120.620378

H97 -C91 -C92 : 118.736277 C93 -C92 -C91 : 121.684755

H98 -C92 -C91 : 118.274274 H98 -C92 -C93 : 120.040710

C92 -C93 -C86 : 124.267584 C94 -C93 -C86 : 118.897435

C94 -C93 -C92 : 116.834835 C95 -C94 -C93 : 121.952928

H99 -C94 -C93 : 119.051617 H99 -C94 -C95 : 118.995422

C94 -C95 -C90 : 120.485421 H100 -C95 -C90 : 119.838297

H100 -C95 -C94 : 119.676281 C101 -S100 -C90 : 103.748113

H102 -C101 -S100 : 105.504902 H103 -C101 -S100 : 111.598412

H103 -C101 -H102 : 108.858767 H104 -C101 -S100 : 111.528931

H104 -C101 -H102 : 108.894344 H104 -C101 -H103 : 110.282998

Torsional angles:

C1 -S5 -C9 -C8 : 179.415273

C1 -S5 -C9 -C10 : -0.547750

H2 -C1 -S5 -C9 :-179.756075

H4 -C1 -S5 -C9 : 62.135424

H5 -C1 -S5 -C9 : -61.636705

S5 -C9 -C8 -C7 :-179.990916

S5 -C9 -C8 -H14 : -0.020309

S5 -C9 -C10 -C11 :-179.997632

S5 -C9 -C10 -H15 : 0.073064

C6 -C7 -C8 -C9 : -0.052013

C6 -C7 -C8 -H14 : 179.977326

C6 -C11 -C10 -C9 : 0.022667

C6 -C11 -C10 -H15 : 179.953382

C6 -C17 -C16 -H20 : -0.143611

C6 -C17 -C16 -C23 :-179.966213

C7 -C6 -C11 -C10 : -0.095827

C7 -C6 -C11 -H16 : 179.750664

C7 -C6 -C17 -C16 : 178.403494

C7 -C6 -C17 -H19 : -1.357113

C7 -C8 -C9 -C10 : -0.025466

C8 -C7 -C6 -C11 : 0.110597

C8 -C7 -C6 -C17 :-179.913926

C8 -C9 -C10 -C11 : 0.039852

C8 -C9 -C10 -H15 :-179.889453

C9 -C8 -C7 -H13 :-179.954178

C9 -C10 -C11 -H16 :-179.826476

C10 -C9 -C8 -H14 : 179.945141

C10 -C11 -C6 -C17 : 179.930024

C11 -C6 -C7 -H13 :-179.987244

C11 -C6 -C17 -C16 : -1.622917

C11 -C6 -C17 -H19 : 178.616476

H13 -C7 -C6 -C17 : -0.011767

H13 -C7 -C8 -H14 : 0.075161

H15 -C10 -C11 -H16 : 0.104239

H16 -C11 -C6 -C17 : -0.223484

C16 -C23 -C22 -C21 : 179.867650

C16 -C23 -C22 -H28 : -0.137238

C16 -C23 -C24 -C25 :-179.877429

C16 -C23 -C24 -H29 : 0.065437

C17 -C16 -C23 -C22 : -0.603026

C17 -C16 -C23 -C24 : 179.332275

H19 -C17 -C16 -H20 : 179.607672

H19 -C17 -C16 -C23 : -0.214930

H20 -C16 -C23 -C22 : 179.567697

H20 -C16 -C23 -C24 : -0.497001

C20 -C21 -C22 -C23 : 0.033899

C20 -C21 -C22 -H28 :-179.961273

C20 -C25 -C24 -C23 : -0.021061

C20 -C25 -C24 -H29 :-179.963709

C20 -C31 -C30 -H34 : 0.121628

C20 -C31 -C30 -C37 :-179.877689

C21 -C20 -C25 -C24 : -0.016394

C21 -C20 -C25 -H30 :-179.947383

C21 -C20 -C31 -C30 :-179.842973

C21 -C20 -C31 -H33 : 0.210967

C21 -C22 -C23 -C24 : -0.068631

C22 -C21 -C20 -C25 : 0.009999

C22 -C21 -C20 -C31 :-179.939812

C22 -C23 -C24 -C25 : 0.062816

C22 -C23 -C24 -H29 :-179.994318

C23 -C22 -C21 -H27 :-179.972502

C23 -C24 -C25 -H30 : 179.910855

C24 -C23 -C22 -H28 : 179.926480

C24 -C25 -C20 -C31 : 179.930924

C25 -C20 -C21 -H27 :-179.983625

C25 -C20 -C31 -C30 : 0.210929

C25 -C20 -C31 -H33 :-179.735131

H27 -C21 -C20 -C31 : 0.066564

H27 -C21 -C22 -H28 : 0.032327

H29 -C24 -C25 -H30 : -0.031793

H30 -C25 -C20 -C31 : -0.000064

C30 -C37 -C36 -C35 : 179.877187

C30 -C37 -C36 -H42 : -0.049290

C30 -C37 -C38 -C39 :-179.885013

C30 -C37 -C38 -H43 : 0.056390

C31 -C30 -C37 -C36 : 0.227438

C31 -C30 -C37 -C38 :-179.904340

H33 -C31 -C30 -H34 :-179.934371

H33 -C31 -C30 -C37 : 0.066312

H34 -C30 -C37 -C36 :-179.771904

H34 -C30 -C37 -C38 : 0.096318

C34 -C35 -C36 -C37 : 0.010633

C34 -C35 -C36 -H42 : 179.937951

C34 -C39 -C38 -C37 : -0.012035

C34 -C39 -C38 -H43 :-179.953219

C34 -C45 -C44 -H48 : 0.074328

C34 -C45 -C44 -C51 : 179.970456

C35 -C34 -C39 -C38 : 0.028667

C35 -C34 -C39 -H44 :-179.854897

C35 -C34 -C45 -C44 :-179.439886

C35 -C34 -C45 -H47 : 0.480737

C35 -C36 -C37 -C38 : 0.007134

C36 -C35 -C34 -C39 : -0.028168

C36 -C35 -C34 -C45 :-179.981542

C36 -C37 -C38 -C39 : -0.006441

C36 -C37 -C38 -H43 : 179.934962

C37 -C36 -C35 -H41 :-179.980894

C37 -C38 -C39 -H44 : 179.873157

C38 -C37 -C36 -H42 :-179.919343

C38 -C39 -C34 -C45 : 179.979832

C39 -C34 -C35 -H41 : 179.963392

C39 -C34 -C45 -C44 : 0.610157

C39 -C34 -C45 -H47 :-179.469220

H41 -C35 -C34 -C45 : 0.010018

H41 -C35 -C36 -H42 : -0.053576

H43 -C38 -C39 -H44 : -0.068027

H44 -C39 -C34 -C45 : 0.096268

C44 -C51 -C50 -C49 :-179.882132

C44 -C51 -C50 -H56 : 0.082567

C44 -C51 -C52 -C53 : 179.897795

C44 -C51 -C52 -H57 : -0.029604

C45 -C44 -C51 -C50 : 0.152574

C45 -C44 -C51 -C52 :-179.786036

H47 -C45 -C44 -H48 :-179.843279

H47 -C45 -C44 -C51 : 0.052850

H48 -C44 -C51 -C50 :-179.947431

H48 -C44 -C51 -C52 : 0.113960

C48 -C49 -C50 -C51 : -0.035019

C48 -C49 -C50 -H56 : 179.999906

C48 -C53 -C52 -C51 : 0.010726

C48 -C53 -C52 -H57 : 179.937862

C48 -C59 -C58 -H62 : -0.237434

C48 -C59 -C58 -C65 : 179.610905

C49 -C48 -C53 -C52 : 0.013801

C49 -C48 -C53 -H58 : 179.881318

C49 -C48 -C59 -C58 : 179.622308

C49 -C48 -C59 -H61 : -0.520993

C49 -C50 -C51 -C52 : 0.057244

C50 -C49 -C48 -C53 : -0.001744

C50 -C49 -C48 -C59 : 179.843916

C50 -C51 -C52 -C53 : -0.045742

C50 -C51 -C52 -H57 :-179.973141

C51 -C50 -C49 -H55 : 179.955800

C51 -C52 -C53 -H58 :-179.858640

C52 -C51 -C50 -H56 :-179.978057

C52 -C53 -C48 -C59 :-179.824870

C53 -C48 -C49 -H55 :-179.992598

C53 -C48 -C59 -C58 : -0.543238

C53 -C48 -C59 -H61 : 179.313461

H55 -C49 -C48 -C59 : -0.146938

H55 -C49 -C50 -H56 : -0.009275

H57 -C52 -C53 -H58 : 0.068496

H58 -C53 -C48 -C59 : 0.042647

C58 -C65 -C64 -C63 :-179.632105

C58 -C65 -C64 -H70 : 0.225939

C58 -C65 -C66 -C67 : 179.638494

C58 -C65 -C66 -H71 : -0.232156

C59 -C58 -C65 -C64 : -0.053281

C59 -C58 -C65 -C66 :-179.793443

H61 -C59 -C58 -H62 : 179.911222

H61 -C59 -C58 -C65 : -0.240440

H62 -C58 -C65 -C64 : 179.800695

H62 -C58 -C65 -C66 : 0.060533

C62 -C63 -C64 -C65 : 0.012969

C62 -C63 -C64 -H70 :-179.846613

C62 -C67 -C66 -C65 : 0.004644

C62 -C67 -C66 -H71 : 179.874796

C62 -C73 -C72 -H76 : -0.331551

C62 -C73 -C72 -C79 : 179.535336

C63 -C62 -C67 -C66 : 0.119900

C63 -C62 -C67 -H72 : 179.947496

C63 -C62 -C73 -C72 :-179.809170

C63 -C62 -C73 -H75 : -0.056728

C63 -C64 -C65 -C66 : 0.111993

C64 -C63 -C62 -C67 : -0.129405

C64 -C63 -C62 -C73 : 179.609481

C64 -C65 -C66 -C67 : -0.121481

C64 -C65 -C66 -H71 :-179.992131

C65 -C64 -C63 -H69 : 179.881242

C65 -C66 -C67 -H72 :-179.825137

C66 -C65 -C64 -H70 : 179.970038

C66 -C67 -C62 -C73 :-179.604610

C67 -C62 -C63 -H69 :-179.998255

C67 -C62 -C73 -C72 : -0.090304

C67 -C62 -C73 -H75 : 179.662137

H69 -C63 -C62 -C73 : -0.259369

H69 -C63 -C64 -H70 : 0.021659

H71 -C66 -C67 -H72 : 0.045016

H72 -C67 -C62 -C73 : 0.222986

C72 -C79 -C78 -C77 :-179.630542

C72 -C79 -C78 -H84 : 0.182275

C72 -C79 -C80 -C81 : 179.640641

C72 -C79 -C80 -H85 : -0.232361

C73 -C72 -C79 -C78 : -0.407372

C73 -C72 -C79 -C80 : 179.912206

H75 -C73 -C72 -H76 : 179.925287

H75 -C73 -C72 -C79 : -0.207826

H76 -C72 -C79 -C78 : 179.464447

H76 -C72 -C79 -C80 : -0.215975

C76 -C77 -C78 -C79 : -0.000949

C76 -C77 -C78 -H84 :-179.816093

C76 -C81 -C80 -C79 : 0.014329

C76 -C81 -C80 -H85 : 179.886876

C76 -C87 -C86 -H90 : -0.333408

C76 -C87 -C86 -C93 : 179.769114

C77 -C76 -C81 -C80 : 0.041485

C77 -C76 -C81 -H86 : 179.838366

C77 -C76 -C87 -C86 : 179.524173

C77 -C76 -C87 -H89 : -0.502025

C77 -C78 -C79 -C80 : 0.055993

C78 -C77 -C76 -C81 : -0.048322

C78 -C77 -C76 -C87 : 179.749009

C78 -C79 -C80 -C81 : -0.062983

C78 -C79 -C80 -H85 :-179.935984

C79 -C78 -C77 -H83 : 179.883636

C79 -C80 -C81 -H86 :-179.785101

C80 -C79 -C78 -H84 : 179.868810

C80 -C81 -C76 -C87 :-179.743628

C81 -C76 -C77 -H83 :-179.933395

C81 -C76 -C87 -C86 : -0.694623

C81 -C76 -C87 -H89 : 179.279179

H83 -C77 -C76 -C87 : -0.136063

H83 -C77 -C78 -H84 : 0.068491

H85 -C80 -C81 -H86 : 0.087446

H86 -C81 -C76 -C87 : 0.053253

C86 -C93 -C92 -C91 :-179.912175

C86 -C93 -C92 -H98 : -0.101189

C86 -C93 -C94 -C95 : 179.959825

C86 -C93 -C94 -H99 : -0.106871

C87 -C86 -C93 -C92 : -1.101143

C87 -C86 -C93 -C94 : 179.042723

H89 -C87 -C86 -H90 : 179.693798

H89 -C87 -C86 -C93 : -0.203679

H90 -C86 -C93 -C92 : 178.997478

H90 -C86 -C93 -C94 : -0.858656

C90 -C91 -C92 -C93 : -0.003626

C90 -C91 -C92 -H98 :-179.817836

C90 -C95 -C94 -C93 : -0.075721

C90 -C95 -C94 -H99 : 179.990938

C90 -S100 -C101 -H102 : 179.860644

C90 -S100 -C101 -H103 : -62.065879

C90 -S100 -C101 -H104 : 61.781086

C91 -C90 -C95 -C94 : 0.014914

C91 -C90 -C95 -H100 :-179.987527

C91 -C90 -S100 -C101 : 0.366027

C91 -C92 -C93 -C94 : -0.053328

C92 -C91 -C90 -C95 : 0.023915

C92 -C91 -C90 -S100 : 179.844604

C92 -C93 -C94 -C95 : 0.093066

C92 -C93 -C94 -H99 :-179.973629

C93 -C92 -C91 -H97 : 179.866514

C93 -C94 -C95 -H100 : 179.926716

C94 -C93 -C92 -H98 : 179.757659

C94 -C95 -C90 -S100 :-179.820453

C95 -C90 -C91 -H97 :-179.843768

C95 -C90 -S100 -C101 :-179.810541

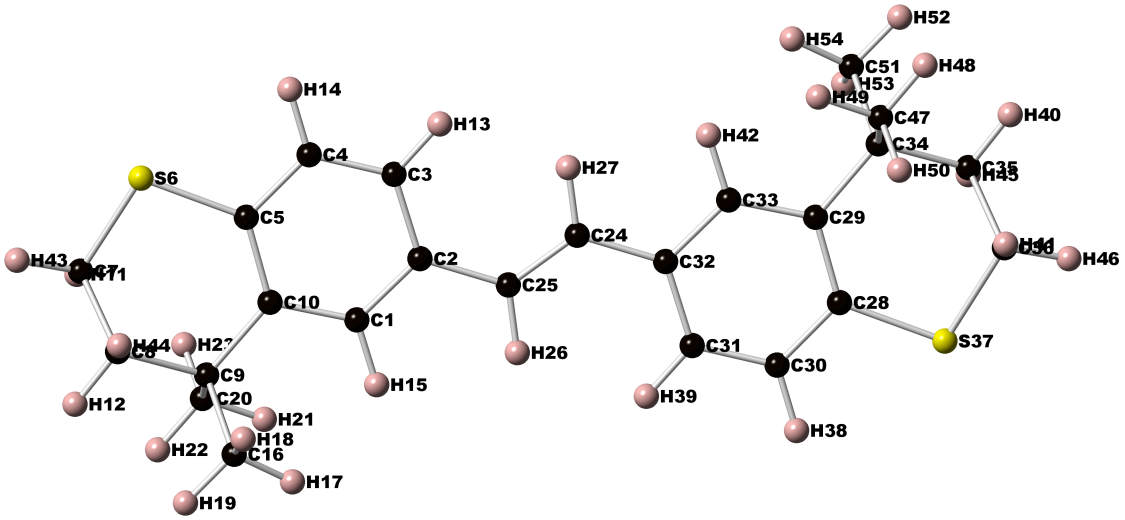
H97 -C91 -C90 -S100 : -0.023080

H97 -C91 -C92 -H98 : 0.052304

H99 -C94 -C95 -H100 : -0.006625

H100 -C95 -C90 -S100 : 0.177106

PPV1



Final geometry:

angstroms

atom	x	y	z
C1	1.1804350000	-1.8512460000	0.0196610000
C2	2.4748730000	-1.3095190000	0.0337080000
C3	2.5819370000	0.0944610000	0.0305200000
C4	1.4449970000	0.8798280000	-0.0009440000
C5	0.1554660000	0.3154630000	-0.0191090000
S6	-1.1712080000	1.5074060000	-0.0471810000
C7	-2.6210960000	0.4380600000	-0.3550130000
C8	-2.5176350000	-0.8769010000	0.4075670000
C9	-1.3595510000	-1.8041640000	-0.0361400000
C10	0.0050010000	-1.0858070000	0.0061380000
H11	-2.7348350000	0.2770070000	-1.4305930000
H12	-3.4586720000	-1.4279710000	0.2812820000
H13	3.5544880000	0.5759530000	0.0435830000
H14	1.5438160000	1.9619600000	-0.0189260000

H15	1.0945400000	-2.9336650000	0.0192170000
C16	-1.3823630000	-3.0151080000	0.9247300000
H17	-0.6928870000	-3.8059010000	0.6188140000
H18	-1.1230970000	-2.7156230000	1.9450280000
H19	-2.3858650000	-3.4543360000	0.9437840000
C20	-1.6107060000	-2.3108440000	-1.4773470000
H21	-0.8343990000	-3.0209610000	-1.7776490000
H22	-2.5800680000	-2.8192580000	-1.5453940000
H23	-1.6005990000	-1.4948520000	-2.2057600000
C24	4.9300340000	-1.8797280000	0.0493290000
C25	3.6232500000	-2.2174060000	0.0502510000
H26	3.3579900000	-3.2730080000	0.0647050000
H27	5.1940270000	-0.8238650000	0.0338610000
C28	8.4056110000	-4.4015780000	0.1323610000
C29	8.5509440000	-3.0003290000	0.0912470000
C30	7.1181050000	-4.9704180000	0.1221700000
C31	5.9792070000	-4.1886920000	0.0847680000
C32	6.0806640000	-2.7845390000	0.0690180000
C33	7.3731250000	-2.2387270000	0.0746720000
C34	9.9109180000	-2.2723870000	0.1157100000
C35	11.0792750000	-3.2042190000	-0.2894150000
C36	11.1730250000	-4.5035150000	0.5009240000
S37	9.7378920000	-5.5864950000	0.1748100000
H38	7.0222750000	-6.0525170000	0.1522850000
H39	5.0078490000	-4.6732560000	0.0778730000
H40	12.0159120000	-2.6466210000	-0.1594530000
H41	11.2569500000	-4.3220600000	1.5760900000
H42	7.4557020000	-1.1560300000	0.0652730000
H43	-3.4827510000	1.0187610000	-0.0145910000
H44	-2.4197420000	-0.6583580000	1.4775390000

H45	10.9999800000	-3.4459030000	-1.3559210000
H46	12.0467150000	-5.0847890000	0.1939730000
C47	10.1508130000	-1.7137580000	1.5393550000
H48	11.1125800000	-1.1895240000	1.5922290000
H49	9.3638170000	-1.0052570000	1.8145990000
H50	10.1506350000	-2.5052430000	2.2945060000
C51	9.9268570000	-1.0959880000	-0.8877770000
H52	10.9261490000	-0.6479330000	-0.9191410000
H53	9.6743160000	-1.4348870000	-1.8973890000
H54	9.2278850000	-0.3019460000	-0.6134220000

bond lengths (angstroms):

C1	-C2	:	1.403294	C1	-C10	:	1.402756
C1	-H15	:	1.085822	C2	-C3	:	1.408060
C2	-C25	:	1.464002	C3	-C4	:	1.382181
C3	-H13	:	1.085293	C4	-C5	:	1.407739
C4	-H14	:	1.086783	C5	-S6	:	1.783698
C5	-C10	:	1.409551	S6	-C7	:	1.827686
C7	-C8	:	1.523599	C7	-H11	:	1.093502
C7	-H43	:	1.093412	C8	-C9	:	1.548500
C8	-H12	:	1.097805	C8	-H44	:	1.096442
C9	-C10	:	1.542669	C9	-C16	:	1.546020
C9	-C20	:	1.548186	C16	-H17	:	1.092847
C16	-H18	:	1.094494	C16	-H19	:	1.095582
C20	-H21	:	1.094121	C20	-H22	:	1.096712
C20	-H23	:	1.093860	C24	-C25	:	1.349708
C24	-H27	:	1.088475	C24	-C32	:	1.463906
C25	-H26	:	1.088516	C28	-C29	:	1.409365

C28 -C30 : 1.407606 C28 -S37 : 1.783481

C29 -C33 : 1.402701 C29 -C34 : 1.542734

C30 -C31 : 1.381877 C30 -H38 : 1.086751

C31 -C32 : 1.407902 C31 -H39 : 1.085535

C32 -C33 : 1.402996 C33 -H42 : 1.085882

C34 -C35 : 1.548385 C34 -C47 : 1.548025

C34 -C51 : 1.546336 C35 -C36 : 1.523678

C35 -H40 : 1.097768 C35 -H45 : 1.096419

C36 -S37 : 1.827239 C36 -H41 : 1.093596

C36 -H46 : 1.093358 C47 -H48 : 1.096637

C47 -H49 : 1.094119 C47 -H50 : 1.093939

C51 -H52 : 1.095592 C51 -H53 : 1.094507

C51 -H54 : 1.092856

Total energy (hartrees): -1727.85570961920

HOMO energy (hartrees): -0.18021

LUMO energy (hartrees): -0.04525

bond angles:

C10 -C1 -C2 : 124.221386 H15 -C1 -C2 : 117.245450

H15 -C1 -C10 : 118.533164 C3 -C2 -C1 : 117.067279

C25 -C2 -C1 : 118.965020 C25 -C2 -C3 : 123.967698

C4 -C3 -C2 : 120.269527 H13 -C3 -C2 : 120.695586

H13 -C3 -C4 : 119.032599 C5 -C4 -C3 : 121.735349

H14 -C4 -C3 : 119.429925 H14 -C4 -C5 : 118.833452

S6 -C5 -C4 : 114.432798 C10 -C5 -C4 : 119.742220

C10 -C5 -S6 : 125.817302 C7 -S6 -C5 : 101.636755

C8 -C7 -S6 : 111.517982 H11 -C7 -S6 : 109.533118

H11 -C7 -C8 : 111.854982 H43 -C7 -S6 : 105.187450

H43 -C7 -C8 : 110.857675 H43 -C7 -H11 : 107.607181

C9 -C8 -C7 : 115.098885 H12 -C8 -C7 : 108.508807

H12 -C8 -C9 : 107.910210 H44 -C8 -C7 : 108.812132

H44 -C8 -C9 : 109.402731 H44 -C8 -H12 : 106.788723

C10 -C9 -C8 : 112.013777 C16 -C9 -C8 : 106.254659

C16 -C9 -C10 : 111.146451 C20 -C9 -C8 : 109.961681

C20 -C9 -C10 : 108.747879 C20 -C9 -C16 : 108.652657

C5 -C10 -C1 : 116.948324 C9 -C10 -C1 : 119.167602

C9 -C10 -C5 : 123.838492 H17 -C16 -C9 : 112.550084

H18 -C16 -C9 : 111.196050 H18 -C16 -H17 : 108.029138

H19 -C16 -C9 : 109.775889 H19 -C16 -H17 : 107.016172

H19 -C16 -H18 : 108.086959 H21 -C20 -C9 : 110.659292

H22 -C20 -C9 : 110.662592 H22 -C20 -H21 : 108.012750

H23 -C20 -C9 : 111.978563 H23 -C20 -H21 : 107.147481

H23 -C20 -H22 : 108.220119 H27 -C24 -C25 : 118.523637

C32 -C24 -C25 : 127.326712 C32 -C24 -H27 : 114.149593

C24 -C25 -C2 : 127.178853 H26 -C25 -C2 : 114.229123

H26 -C25 -C24 : 118.592024 C30 -C28 -C29 : 119.729206

S37 -C28 -C29 : 125.748001 S37 -C28 -C30 : 114.516620

C33 -C29 -C28 : 116.973899 C34 -C29 -C28 : 124.026447

C34 -C29 -C33 : 118.960093 C31 -C30 -C28 : 121.697486

H38 -C30 -C28 : 118.871355 H38 -C30 -C31 : 119.429470

C32 -C31 -C30 : 120.338239 H39 -C31 -C30 : 119.021326

H39 -C31 -C32 : 120.637593 C31 -C32 -C24 : 124.051902

C33 -C32 -C24 : 118.925735 C33 -C32 -C31 : 117.022304

C32 -C33 -C29 : 124.218174 H42 -C33 -C29 : 118.529380

H42 -C33 -C32 : 117.252445 C35 -C34 -C29 : 112.151811

C47 -C34 -C29 : 108.751736 C47 -C34 -C35 : 109.929259

C51 -C34 -C29 : 110.962998 C51 -C34 -C35 : 106.276051

C51 -C34 -C47 : 108.703597 C36 -C35 -C34 : 115.080821

H40 -C35 -C34 : 107.887716 H40 -C35 -C36 : 108.616460

H45 -C35 -C34 : 109.426110 H45 -C35 -C36 : 108.725477

H45 -C35 -H40 : 106.787862 S37 -C36 -C35 : 111.377124

H41 -C36 -C35 : 111.912783 H41 -C36 -S37 : 109.516708

H46 -C36 -C35 : 110.909605 H46 -C36 -S37 : 105.213182

H46 -C36 -H41 : 107.631809 C36 -S37 -C28 : 101.372515

H48 -C47 -C34 : 110.656089 H49 -C47 -C34 : 110.705573

H49 -C47 -H48 : 108.007977 H50 -C47 -C34 : 111.945363

H50 -C47 -H48 : 108.223782 H50 -C47 -H49 : 107.142106

H52 -C51 -C34 : 109.822239 H53 -C51 -C34 : 111.141407

H53 -C51 -H52 : 108.099987 H54 -C51 -C34 : 112.534941

H54 -C51 -H52 : 107.062243 H54 -C51 -H53 : 107.997266

torsional angles:

C1 -C2 -C3 -C4 : -0.724231

C1 -C2 -C3 -H13 : 179.831336

C1 -C2 -C25 -C24 : 179.162595

C1 -C2 -C25 -H26 : -0.840167

C1 -C10 -C5 -C4 : -1.340328

C1 -C10 -C5 -S6 : 179.726451

C1 -C10 -C9 -C8 : 161.564451

C1 -C10 -C9 -C16 : 42.872326

C1 -C10 -C9 -C20 : -76.693365

C2 -C1 -C10 -C5 : 1.188476

C2 -C1 -C10 -C9 : 178.827749

C2 -C3 -C4 -C5 : 0.548539

C2 -C3 -C4 -H14 :-179.036050

C2 -C25 -C24 -H27 : -0.063155

C2 -C25 -C24 -C32 : 179.843325

C3 -C2 -C1 -C10 : -0.160854

C3 -C2 -C1 -H15 : 179.830209

C3 -C2 -C25 -C24 : -0.819990

C3 -C2 -C25 -H26 : 179.177248

C3 -C4 -C5 -S6 : 179.578129

C3 -C4 -C5 -C10 : 0.528241

C4 -C3 -C2 -C25 : 179.258659

C4 -C5 -S6 -C7 : 170.687783

C4 -C5 -C10 -C9 :-178.858488

C5 -C4 -C3 -H13 :-179.997845

C5 -S6 -C7 -C8 : 38.901741

C5 -S6 -C7 -H11 : -85.463017

C5 -S6 -C7 -H43 : 159.140352

C5 -C10 -C1 -H15 :-178.802481

C5 -C10 -C9 -C8 : -20.969202

C5 -C10 -C9 -C16 :-139.661327

C5 -C10 -C9 -C20 : 100.772982

S6 -C5 -C4 -H14 : -0.834879

S6 -C5 -C10 -C9 : 2.208291

S6 -C7 -C8 -C9 : -65.433396

S6 -C7 -C8 -H12 : 173.574297

S6 -C7 -C8 -H44 : 57.736099

C7 -S6 -C5 -C10 : -10.329567

C7 -C8 -C9 -C10 : 54.535693

C7 -C8 -C9 -C16 : 176.083151

C7 -C8 -C9 -C20 : -66.507769

C8 -C9 -C16 -H17 : 172.003957

C8 -C9 -C16 -H18 : -66.632507

C8 -C9 -C16 -H19 : 52.924343

C8 -C9 -C20 -H21 :-176.140195

C8 -C9 -C20 -H22 : -56.444294

C8 -C9 -C20 -H23 : 64.389940

C9 -C8 -C7 -H11 : 57.616472

C9 -C8 -C7 -H43 : 177.721636

C9 -C10 -C1 -H15 : -1.163207

C10 -C1 -C2 -C25 : 179.855365

C10 -C5 -C4 -H14 :-179.884767

C10 -C9 -C8 -H12 : 175.853728

C10 -C9 -C8 -H44 : -68.318890

C10 -C9 -C16 -H17 : -65.895809

C10 -C9 -C16 -H18 : 55.467727

C10 -C9 -C16 -H19 : 175.024577

C10 -C9 -C20 -H21 : 60.875319

C10 -C9 -C20 -H22 :-179.428780

C10 -C9 -C20 -H23 : -58.594547

H11 -C7 -C8 -H12 : -63.375835

H11 -C7 -C8 -H44 :-179.214033

H12 -C8 -C7 -H43 : 56.729329

H12 -C8 -C9 -C16 : -62.598814

H12 -C8 -C9 -C20 : 54.810267

H13 -C3 -C2 -C25 : -0.185774

H13 -C3 -C4 -H14 : 0.417567

H15 -C1 -C2 -C25 : -0.153572

C16 -C9 -C8 -H44 : 53.228567

C16 -C9 -C20 -H21 : -60.233052

C16 -C9 -C20 -H22 : 59.462849

C16 -C9 -C20 -H23 :-179.702918

H17 -C16 -C9 -C20 : 53.726634

H18 -C16 -C9 -C20 : 175.090170

H19 -C16 -C9 -C20 : -65.352980

C20 -C9 -C8 -H44 : 170.637648

C24 -C32 -C31 -C30 :-179.075000

C24 -C32 -C31 -H39 : 0.305728

C24 -C32 -C33 -C29 :-179.908880

C24 -C32 -C33 -H42 : 0.076066

C25 -C24 -C32 -C31 : 0.384068

C25 -C24 -C32 -C33 :-179.525151

H26 -C25 -C24 -H27 : 179.939713

H26 -C25 -C24 -C32 : -0.153806

H27 -C24 -C32 -C31 :-179.705981

H27 -C24 -C32 -C33 : 0.384801

C28 -C29 -C33 -C32 : -1.349962

C28 -C29 -C33 -H42 : 178.665271

C28 -C29 -C34 -C35 : 19.428740

C28 -C29 -C34 -C47 :-102.365032

C28 -C29 -C34 -C51 : 138.115664

C28 -C30 -C31 -C32 : -0.635304

C28 -C30 -C31 -H39 : 179.974030

C28 -S37 -C36 -C35 : -40.253839

C28 -S37 -C36 -H41 : 84.074877

C28 -S37 -C36 -H46 :-160.494195

C29 -C28 -C30 -C31 : -0.595518

C29 -C28 -C30 -H38 : 179.880056

C29 -C28 -S37 -C36 : 11.291322

C29 -C33 -C32 -C31 : 0.175553

C29 -C34 -C35 -C36 : -53.435085

C29 -C34 -C35 -H40 :-174.863058

C29 -C34 -C35 -H45 : 69.310528

C29 -C34 -C47 -H48 : 179.935847

C29 -C34 -C47 -H49 : -60.348388

C29 -C34 -C47 -H50 : 59.124026

C29 -C34 -C51 -H52 :-175.080629

C29 -C34 -C51 -H53 : -55.512071

C29 -C34 -C51 -H54 : 65.760158

C30 -C28 -C29 -C33 : 1.523989

C30 -C28 -C29 -C34 : 179.206693

C30 -C28 -S37 -C36 :-169.620753

C30 -C31 -C32 -C33 : 0.835806

C31 -C30 -C28 -S37 :-179.743089

C31 -C32 -C33 -H42 :-179.839501

C32 -C31 -C30 -H38 : 178.886532

C32 -C33 -C29 -C34 :-179.155028

C33 -C29 -C28 -S37 :-179.431638

C33 -C29 -C34 -C35 :-162.931635

C33 -C29 -C34 -C47 : 75.274593

C33 -C29 -C34 -C51 : -44.244711

C33 -C32 -C31 -H39 :-179.783466

C34 -C29 -C28 -S37 : -1.748935

C34 -C29 -C33 -H42 : 0.860205

C34 -C35 -C36 -S37 : 65.945423

C34 -C35 -C36 -H41 : -57.021835

C34 -C35 -C36 -H46 :-177.232944

C35 -C34 -C47 -H48 : 56.798173

C35 -C34 -C47 -H49 : 176.513938

C35 -C34 -C47 -H50 : -64.013648

C35 -C34 -C51 -H52 : -52.905717

C35 -C34 -C51 -H53 : 66.662841

C35 -C34 -C51 -H54 :-172.064930

C36 -C35 -C34 -C47 : 67.683066

C36 -C35 -C34 -C51 :-174.852379

S37 -C28 -C30 -H38 : 0.732485

S37 -C36 -C35 -H40 :-173.022980

S37 -C36 -C35 -H45 : -57.174241

H38 -C30 -C31 -H39 : -0.504134

H40 -C35 -C34 -C47 : -53.744907

H40 -C35 -C34 -C51 : 63.719648

H40 -C35 -C36 -H41 : 64.009762

H40 -C35 -C36 -H46 : -56.201347

H41 -C36 -C35 -H45 : 179.858501

H43 -C7 -C8 -H44 : -59.108869

H45 -C35 -C34 -C47 :-169.571320

H45 -C35 -C34 -C51 : -52.106765

H45 -C35 -C36 -H46 : 59.647392

C47 -C34 -C51 -H52 : 65.371261

C47 -C34 -C51 -H53 :-175.060182

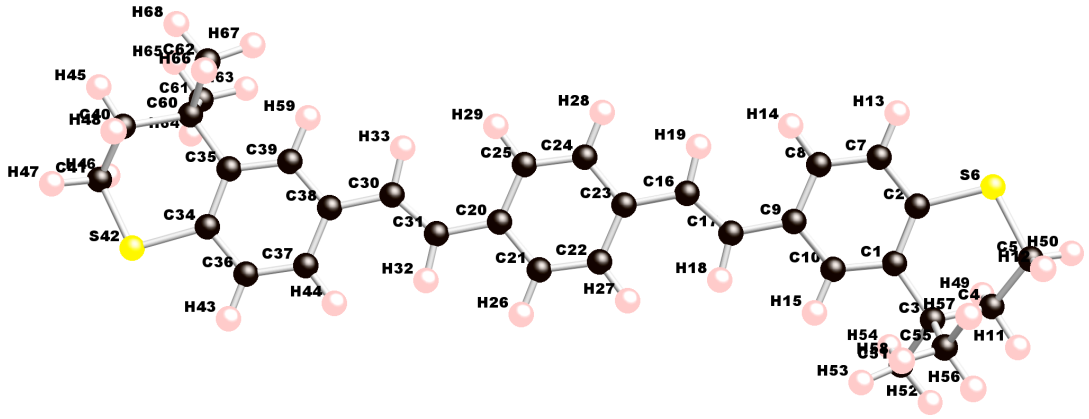
C47 -C34 -C51 -H54 : -53.787952

H48 -C47 -C34 -C51 : -59.145631

H49 -C47 -C34 -C51 : 60.570134

H50 -C47 -C34 -C51 :-179.957452

PPV2



Final geometry:

angstroms

atom	x	y	z
C1	-0.7269977200	-1.5243657451	-0.1496497698
C2	0.4835853395	-0.8027626381	-0.1162801904
C3	-0.8082881727	-3.0642958000	-0.1553707709
C4	0.5082005310	-3.7098469442	-0.6528757114
C5	1.7609304718	-3.2869395643	0.1041302030
S6	2.1204585923	-1.5097019823	-0.1291171863
C7	0.4576818391	0.6048875893	-0.0914759975
C8	-0.7309113706	1.3101648368	-0.0885060441
C9	-1.9614099095	0.6253722108	-0.0993718438
C10	-1.9129511542	-0.7768395614	-0.1271968181
H11	0.4032449139	-4.7994070638	-0.5699120157
H12	1.6841892248	-3.5066382262	1.1725118185
H13	1.3997370927	1.1461792383	-0.0682832674
H14	-0.7004229487	2.3948688282	-0.0695802166
H15	-2.8605450179	-1.3067486302	-0.1328725647
C16	-3.5094207236	2.6140801378	-0.0654957701

C17	-3.2661323636	1.2859180360	-0.0865924300
H18	-4.1131877298	0.6019036009	-0.1000686853
H19	-2.6629645195	3.2987033764	-0.0531758253
C20	-7.2971139943	4.6902965505	-0.0703046137
C21	-7.2457117365	3.2803474169	-0.0752802385
C22	-6.0453526225	2.5875120856	-0.0719077875
C23	-4.8145818170	3.2728362964	-0.0624455644
C24	-4.8658888640	4.6828233983	-0.0529505950
C25	-6.0668285645	5.3760495025	-0.0563197756
H26	-8.1796526538	2.7235018512	-0.0843807827
H27	-6.0652319626	1.5021336238	-0.0779643686
H28	-3.9318318206	5.2393858546	-0.0430026595
H29	-6.0482377495	6.4615520266	-0.0466860755
C30	-8.8680690857	6.6659609057	-0.1162872968
C31	-8.6051168832	5.3417997685	-0.0809655757
H32	-9.4434920992	4.6481486478	-0.0635818821
H33	-8.0335626841	7.3648968865	-0.1468914333
C34	-12.6735406129	8.6538582842	-0.1869241137
C35	-11.4836662108	9.4076230417	-0.2399058221
C36	-12.6076500742	7.2512332814	-0.0873778450
C37	-11.3993602156	6.5821148019	-0.0516019940
C38	-10.1883254619	7.2969364036	-0.1271434194
C39	-10.2763589331	8.6942468619	-0.2190119162
C40	-12.7746434512	11.5938289587	0.0908346289
C41	-14.0264985093	11.0713078745	-0.6025891414
S42	-14.3301213478	9.3130257200	-0.2061199477
H43	-13.5336181670	6.6840620915	-0.0428712442
H44	-11.3996233960	5.5003640164	0.0293279006
H45	-12.7024571412	12.6742400127	-0.0895518662
H46	-13.9729753807	11.1966620606	-1.6874913590

H47	-14.9160080437	11.6015478429	-0.2517929659
H48	-12.8872837509	11.4600387706	1.1732571181
H49	0.6443247813	-3.4847294737	-1.7173097174
H50	2.6418310425	-3.8094821582	-0.2785153595
C51	-1.9211779678	-3.5613836086	-1.1063626893
H52	-1.8994695815	-4.6552434707	-1.1622743889
H53	-2.9204698721	-3.2786734427	-0.7659501366
H54	-1.7834104044	-3.1665108386	-2.1178288404
C55	-1.1286391417	-3.5509015197	1.2789130120
H56	-1.1821240002	-4.6457370925	1.3134026976
H57	-0.3754711357	-3.2221905309	2.0008431945
H58	-2.0915990028	-3.1543524887	1.6145864707
H59	-9.3446936401	9.2485424623	-0.2787414951
C60	-11.4478859808	10.9433605629	-0.3717742181
C61	-11.1644760360	11.3087854339	-1.8491263030
C62	-10.3353742119	11.5529232003	0.5115278136
H63	-10.1959483757	10.9102170506	-2.1658178825
H64	-11.9191770935	10.8961782423	-2.5249317031
H65	-11.1432691884	12.3972000748	-1.9818718610
H66	-10.4454380421	11.2445131784	1.5558775627
H67	-9.3343296228	11.2685051501	0.1784956304
H68	-10.3876252895	12.6464324366	0.4721161069

Total energy (hartrees): -2036.32737837009

HOMO energy (hartrees): -0.17772

LUMO energy (hartrees): -0.06158

Bond lengths (angstroms):

C1 -C2 : 1.409729 C1 -C3 : 1.542085

C1 -C10 : 1.402065 C2 -S6 : 1.783054

C2 -C7 : 1.408107 C3 -C4 : 1.548351

C3 -C51 : 1.545964 C3 -C55 : 1.548089

C4 -C5 : 1.523562 C4 -H11 : 1.097743

C4 -H49 : 1.096461 C5 -S6 : 1.828179

C5 -H12 : 1.093433 C5 -H50 : 1.093368

C7 -C8 : 1.382092 C7 -H13 : 1.086739

C8 -C9 : 1.408256 C8 -H14 : 1.085297

C9 -C10 : 1.403325 C9 -C17 : 1.462458

C10 -H15 : 1.085712 C16 -C17 : 1.350425

C16 -H19 : 1.088737 C16 -C23 : 1.461990

C17 -H18 : 1.088834 C20 -C21 : 1.410895

C20 -C25 : 1.408565 C20 -C31 : 1.461315

C21 -C22 : 1.385963 C21 -H26 : 1.087385

C22 -C23 : 1.408743 C22 -H27 : 1.085577

C23 -C24 : 1.410952 C24 -C25 : 1.386661

C24 -H28 : 1.087347 C25 -H29 : 1.085704

C30 -C31 : 1.350479 C30 -H33 : 1.088967

C30 -C38 : 1.463327 C31 -H32 : 1.088268

C34 -C35 : 1.409528 C34 -C36 : 1.407696

C34 -S42 : 1.783011 C35 -C39 : 1.402474

C35 -C60 : 1.541804 C36 -C37 : 1.381653

C36 -H43 : 1.086775 C37 -C38 : 1.408290

C37 -H44 : 1.084774 C38 -C39 : 1.403092

C39 -H59 : 1.085731 C40 -C41 : 1.523485

C40 -H45 : 1.097742 C40 -H48 : 1.096461

C40 -C60 : 1.548354 C41 -S42 : 1.827821

C41 -H46 : 1.093431 C41 -H47 : 1.093362

C51 -H52 : 1.095503 C51 -H53 : 1.092882

C51 -H54 : 1.094517 C55 -H56 : 1.096684

C55 -H57 : 1.093845 C55 -H58 : 1.094175

C60 -C61 : 1.548039 C60 -C62 : 1.545792

C61 -H63 : 1.094165 C61 -H64 : 1.093861

C61 -H65 : 1.096685 C62 -H66 : 1.094485

C62 -H67 : 1.092655 C62 -H68 : 1.095466

Bond angles:

C3 -C1 -C2 : 123.815066 C10 -C1 -C2 : 116.941529

C10 -C1 -C3 : 119.201738 S6 -C2 -C1 : 125.818266

C7 -C2 -C1 : 119.757311 C7 -C2 -S6 : 114.416248

C4 -C3 -C1 : 111.883278 C51 -C3 -C1 : 111.181248

C51 -C3 -C4 : 106.281486 C55 -C3 -C1 : 108.745114

C55 -C3 -C4 : 110.034490 C55 -C3 -C51 : 108.656311

C5 -C4 -C3 : 115.070296 H11 -C4 -C3 : 107.953416

H11 -C4 -C5 : 108.455735 H49 -C4 -C3 : 109.383191

H49 -C4 -C5 : 108.861554 H49 -C4 -H11 : 106.799365

S6 -C5 -C4 : 111.601669 H12 -C5 -C4 : 111.839138

H12 -C5 -S6 : 109.499013 H50 -C5 -C4 : 110.849171

H50 -C5 -S6 : 105.159604 H50 -C5 -H12 : 107.606043

C5 -S6 -C2 : 101.769452 C8 -C7 -C2 : 121.734887

H13 -C7 -C2 : 118.839346 H13 -C7 -C8 : 119.424795

C9 -C8 -C7 : 120.217492 H14 -C8 -C7 : 119.071199

H14 -C8 -C9 : 120.709457 C10 -C9 -C8 : 117.120576

C17 -C9 -C8 : 124.044186 C17 -C9 -C10 : 118.835078

C9 -C10 -C1 : 124.212548 H15 -C10 -C1 : 118.551608

H15 -C10 -C9 : 117.235785 H19 -C16 -C17 : 118.591870

C23 -C16 -C17 : 127.158649 C23 -C16 -H19 : 114.248964

C16 -C17 -C9 : 127.234888 H18 -C17 -C9 : 114.216801

H18 -C17 -C16 : 118.547826 C25 -C20 -C21 : 117.047738

C31 -C20 -C21 : 118.562633 C31 -C20 -C25 : 124.389608

C22 -C21 -C20 : 122.080102 H26 -C21 -C20 : 118.717491

H26 -C21 -C22 : 119.202252 C23 -C22 -C21 : 120.896939

H27 -C22 -C21 : 118.942350 H27 -C22 -C23 : 120.160665

C22 -C23 -C16 : 124.106383 C24 -C23 -C16 : 118.865637

C24 -C23 -C22 : 117.027772 C25 -C24 -C23 : 122.077059

H28 -C24 -C23 : 118.706828 H28 -C24 -C25 : 119.216111

C24 -C25 -C20 : 120.869709 H29 -C25 -C20 : 120.119073

H29 -C25 -C24 : 119.011171 H33 -C30 -C31 : 118.740862

C38 -C30 -C31 : 126.773761 C38 -C30 -H33 : 114.484158

C30 -C31 -C20 : 127.706617 H32 -C31 -C20 : 113.907817

H32 -C31 -C30 : 118.384504 C36 -C34 -C35 : 119.734556

S42 -C34 -C35 : 125.888039 S42 -C34 -C36 : 114.368973

C39 -C35 -C34 : 117.008420 C60 -C35 -C34 : 123.742750

C60 -C35 -C39 : 119.206004 C37 -C36 -C34 : 121.689065

H43 -C36 -C34 : 118.882767 H43 -C36 -C37 : 119.427432

C38 -C37 -C36 : 120.319934 H44 -C37 -C36 : 118.990100

H44 -C37 -C38 : 120.688949 C37 -C38 -C30 : 123.820533

C39 -C38 -C30 : 119.111434 C39 -C38 -C37 : 117.067995

C38 -C39 -C35 : 124.162818 H59 -C39 -C35 : 118.566944

H59 -C39 -C38 : 117.270168 H45 -C40 -C41 : 108.469720

H48 -C40 -C41 : 108.848344 H48 -C40 -H45 : 106.802295

C60 -C40 -C41 : 115.089244 C60 -C40 -H45 : 107.940348

C60 -C40 -H48 : 109.372991 S42 -C41 -C40 : 111.573649

H46 -C41 -C40 : 111.842963 H46 -C41 -S42 : 109.489173

H47 -C41 -C40 : 110.863167 H47 -C41 -S42 : 105.175612

H47 -C41 -H46 : 107.611726 C41 -S42 -C34 : 101.749341

H52 -C51 -C3 : 109.766475 H53 -C51 -C3 : 112.546821

H53 -C51 -H52 : 106.996391 H54 -C51 -C3 : 111.214171

H54 -C51 -H52 : 108.093783 H54 -C51 -H53 : 108.035862

H56 -C55 -C3 : 110.672523 H57 -C55 -C3 : 111.995432

H57 -C55 -H56 : 108.229714 H58 -C55 -C3 : 110.635970

H58 -C55 -H56 : 108.013336 H58 -C55 -H57 : 107.133224

C40 -C60 -C35 : 111.901426 C61 -C60 -C35 : 108.723388

C61 -C60 -C40 : 110.049927 C62 -C60 -C35 : 111.137921

C62 -C60 -C40 : 106.278844 C62 -C60 -C61 : 108.692221

H63 -C61 -C60 : 110.627312 H64 -C61 -C60 : 111.978094

H64 -C61 -H63 : 107.127479 H65 -C61 -C60 : 110.691260

H65 -C61 -H63 : 108.021227 H65 -C61 -H64 : 108.235148

H66 -C62 -C60 : 111.208021 H67 -C62 -C60 : 112.491800

H67 -C62 -H66 : 108.035867 H68 -C62 -C60 : 109.800504

H68 -C62 -H66 : 108.108336 H68 -C62 -H67 : 107.011764

Torsional angles:

C1 -C2 -S6 -C5 : -9.545939

C1 -C2 -C7 -C8 : 0.505920

C1 -C2 -C7 -H13 :-179.854882

C1 -C3 -C4 -C5 : 55.149222

C1 -C3 -C4 -H11 : 176.412105

C1 -C3 -C4 -H49 : -67.734586

C1 -C3 -C51 -H52 : 174.920991

C1 -C3 -C51 -H53 : -66.032742

C1 -C3 -C51 -H54 : 55.350282

C1 -C3 -C55 -H56 :-179.332405

C1 -C3 -C55 -H57 : -58.467547

C1 -C3 -C55 -H58 : 60.979656

C1 -C10 -C9 -C8 : -0.252001

C1 -C10 -C9 -C17 : 179.608876

C2 -C1 -C3 -C4 : -21.658242

C2 -C1 -C3 -C51 :-140.321304

C2 -C1 -C3 -C55 : 100.089034

C2 -C1 -C10 -C9 : 1.238310

C2 -C1 -C10 -H15 :-178.852042

C2 -S6 -C5 -C4 : 38.099196

C2 -S6 -C5 -H12 : -86.279194

C2 -S6 -C5 -H50 : 158.355973

C2 -C7 -C8 -C9 : 0.527313

C2 -C7 -C8 -H14 :-179.964152

C3 -C1 -C2 -S6 : 2.140900

C3 -C1 -C2 -C7 :-178.959892

C3 -C1 -C10 -C9 : 178.980603

C3 -C1 -C10 -H15 : -1.109749

C3 -C4 -C5 -S6 : -65.211041

C3 -C4 -C5 -H12 : 57.844342

C3 -C4 -C5 -H50 : 177.931585

C4 -C3 -C1 -C10 : 160.764318

C4 -C3 -C51 -H52 : 52.942698

C4 -C3 -C51 -H53 : 171.988965

C4 -C3 -C51 -H54 : -66.628010

C4 -C3 -C55 -H56 : -56.465181

C4 -C3 -C55 -H57 : 64.399678

C4 -C3 -C55 -H58 :-176.153120

C5 -C4 -C3 -C51 : 176.679974

C5 -C4 -C3 -C55 : -65.853860

C5 -S6 -C2 -C7 : 171.503552

S6 -C2 -C1 -C10 : 179.768811

S6 -C2 -C7 -C8 : 179.525656

S6 -C2 -C7 -H13 : -0.835146

S6 -C5 -C4 -H11 : 173.799647

S6 -C5 -C4 -H49 : 57.951026

C7 -C2 -C1 -C10 : -1.331980

C7 -C8 -C9 -C10 : -0.650085

C7 -C8 -C9 -C17 : 179.496998

C8 -C9 -C10 -H15 : 179.837259

C8 -C9 -C17 -C16 : 0.128064

C8 -C9 -C17 -H18 : 179.869021

C9 -C8 -C7 -H13 :-179.109825

C9 -C17 -C16 -H19 : -0.199151

C9 -C17 -C16 -C23 : 179.522951

C10 -C1 -C3 -C51 : 42.101256

C10 -C1 -C3 -C55 : -77.488406

C10 -C9 -C8 -H14 : 179.849526

C10 -C9 -C17 -C16 :-179.722497

C10 -C9 -C17 -H18 : 0.018460

H11 -C4 -C3 -C51 : -62.057143

H11 -C4 -C3 -C55 : 55.409023

H11 -C4 -C5 -H12 : -63.144970

H11 -C4 -C5 -H50 : 56.942273

H12 -C5 -C4 -H49 :-178.993591

H13 -C7 -C8 -H14 : 0.398709

H14 -C8 -C9 -C17 : -0.003391

H15 -C10 -C9 -C17 : -0.301864

C16 -C23 -C22 -C21 :-179.662820

C16 -C23 -C22 -H27 : 0.258919

C16 -C23 -C24 -C25 : 179.670089

C16 -C23 -C24 -H28 : -0.310455

C17 -C16 -C23 -C22 : 0.486828

C17 -C16 -C23 -C24 :-179.341802

H18 -C17 -C16 -H19 :-179.930205

H18 -C17 -C16 -C23 : -0.208103

H19 -C16 -C23 -C22 :-179.780793

H19 -C16 -C23 -C24 : 0.390577

C20 -C21 -C22 -C23 : 0.039199

C20 -C21 -C22 -H27 :-179.883478

C20 -C25 -C24 -C23 : -0.037240

C20 -C25 -C24 -H28 : 179.943209

C20 -C31 -C30 -H33 : 0.384658

C20 -C31 -C30 -C38 : 179.959161

C21 -C20 -C25 -C24 : 0.241443

C21 -C20 -C25 -H29 :-179.678664

C21 -C20 -C31 -C30 :-177.971126

C21 -C20 -C31 -H32 : 1.644162

C21 -C22 -C23 -C24 : 0.168702

C22 -C21 -C20 -C25 : -0.244362

C22 -C21 -C20 -C31 : 179.705268

C22 -C23 -C24 -C25 : -0.170620

C22 -C23 -C24 -H28 : 179.848835

C23 -C22 -C21 -H26 : 179.893640

C23 -C24 -C25 -H29 : 179.883738

C24 -C23 -C22 -H27 :-179.909559

C24 -C25 -C20 -C31 :-179.704948

C25 -C20 -C21 -H26 : 179.900517

C25 -C20 -C31 -C30 : 1.974512

C25 -C20 -C31 -H32 :-178.410200

H26 -C21 -C20 -C31 : -0.149853

H26 -C21 -C22 -H27 : -0.029037

H28 -C24 -C25 -H29 : -0.135813

H29 -C25 -C20 -C31 : 0.374945

C30 -C38 -C37 -C36 :-179.051929

C30 -C38 -C37 -H44 : 0.577549

C30 -C38 -C39 -C35 : 179.911630

C30 -C38 -C39 -H59 : 0.009870

C31 -C30 -C38 -C37 : 2.434062

C31 -C30 -C38 -C39 :-177.492682

H32 -C31 -C30 -H33 :-179.215578

H32 -C31 -C30 -C38 : 0.358925

H33 -C30 -C38 -C37 :-177.975879

H33 -C30 -C38 -C39 : 2.097377

C34 -C35 -C39 -C38 : -1.104260

C34 -C35 -C39 -H59 : 178.796314

C34 -C35 -C60 -C40 : 21.645723

C34 -C35 -C60 -C61 :-100.117887

C34 -C35 -C60 -C62 : 140.288431

C34 -C36 -C37 -C38 : -0.583993

C34 -C36 -C37 -H44 : 179.780280

C34 -S42 -C41 -C40 : -38.105792

C34 -S42 -C41 -H46 : 86.250808

C34 -S42 -C41 -H47 :-158.374044

C35 -C34 -C36 -C37 : -0.593383

C35 -C34 -C36 -H43 : 179.720524

C35 -C34 -S42 -C41 : 9.562991

C35 -C39 -C38 -C37 : -0.020025

C35 -C60 -C40 -C41 : -55.168956

C35 -C60 -C40 -H45 :-176.452692

C35 -C60 -C40 -H48 : 67.703093

C35 -C60 -C61 -H63 : -60.933203

C35 -C60 -C61 -H64 : 58.489436

C35 -C60 -C61 -H65 : 179.362458

C35 -C60 -C62 -H66 : -55.295102

C35 -C60 -C62 -H67 : 66.044577

C35 -C60 -C62 -H68 :-174.902182

C36 -C34 -C35 -C39 : 1.382733

C36 -C34 -C35 -C60 : 178.978210

C36 -C34 -S42 -C41 :-171.503212

C36 -C37 -C38 -C39 : 0.876197

C37 -C36 -C34 -S42 :-179.598611

C37 -C38 -C39 -H59 :-179.921785

C38 -C37 -C36 -H43 : 179.100431

C38 -C39 -C35 -C60 :-178.813655

C39 -C35 -C34 -S42 :-179.735753

C39 -C35 -C60 -C40 :-160.808606

C39 -C35 -C60 -C61 : 77.427785

C39 -C35 -C60 -C62 : -42.165897

C39 -C38 -C37 -H44 :-179.494325

C40 -C60 -C61 -H63 : 176.181360

C40 -C60 -C61 -H64 : -64.396000

C40 -C60 -C61 -H65 : 56.477022

C40 -C60 -C62 -H66 : 66.678294

C40 -C60 -C62 -H67 :-171.982027

C40 -C60 -C62 -H68 : -52.928787

C41 -C40 -C60 -C61 : 65.829315

C41 -C40 -C60 -C62 :-176.655466

S42 -C34 -C35 -C60 : -2.140277

S42 -C34 -C36 -H43 : 0.715296

S42 -C41 -C40 -H45 :-173.776361

S42 -C41 -C40 -H48 : -57.923785

S42 -C41 -C40 -C60 : 65.228063

H43 -C36 -C37 -H44 : -0.535296

H45 -C40 -C41 -H46 : 63.198880

H45 -C40 -C41 -H47 : -56.907729

H45 -C40 -C60 -C61 : -55.454420

H45 -C40 -C60 -C62 : 62.060798

H46 -C41 -C40 -H48 : 179.051457

H46 -C41 -C40 -C60 : -57.796696

H47 -C41 -C40 -H48 : 58.944848

H47 -C41 -C40 -C60 :-177.903305

H48 -C40 -C60 -C61 :-171.298635

H48 -C40 -C60 -C62 : -53.783417

H49 -C4 -C3 -C51 : 53.796166

H49 -C4 -C3 -C55 : 171.262332

H49 -C4 -C5 -H50 : -58.906348

C51 -C3 -C55 -H56 : 59.516434

C51 -C3 -C55 -H57 :-179.618707

C51 -C3 -C55 -H58 : -60.171505

H52 -C51 -C3 -C55 : -65.436467

H53 -C51 -C3 -C55 : 53.609800

H54 -C51 -C3 -C55 : 174.992824

H59 -C39 -C35 -C60 : 1.086920

C61 -C60 -C62 -H66 :-174.907361

C61 -C60 -C62 -H67 : -53.567682

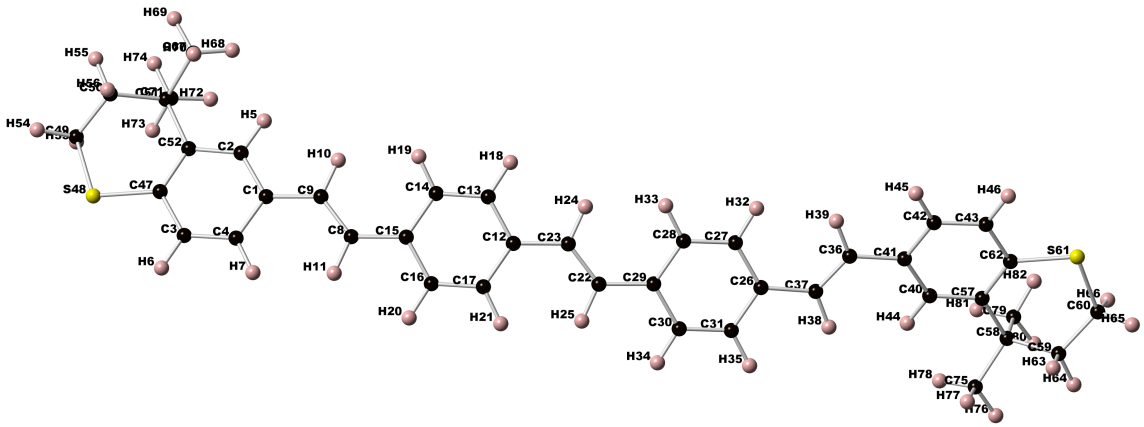
C61 -C60 -C62 -H68 : 65.485559

C62 -C60 -C61 -H63 : 60.173873

C62 -C60 -C61 -H64 : 179.596512

C62 -C60 -C61 -H65 : -59.530466

PPV3



Final geometry:

angstroms

atom	x	y	z
C1	-1.7503402346	0.1387931046	0.3811012728
C2	-2.4134342473	1.2997925062	-0.0448516430
C3	-3.9271411774	-0.8936947218	0.6118315532
C4	-2.5516750933	-0.9666523341	0.7230921189
H5	-1.7993179132	2.1553933212	-0.3066403970
H6	-4.5304468549	-1.7593866220	0.8718134368
H7	-2.0998621518	-1.8860806443	1.0805223035
C8	0.5164512012	-0.9262464533	0.6584752786
C9	-0.2878208970	0.1363266177	0.4384355124
H10	0.1710655141	1.1059713774	0.2535228970
H11	0.0590375119	-1.9038344289	0.7987758960
C12	4.8328726426	-1.1068520189	0.7156104152
C13	4.1624036209	0.1340757648	0.6948137618
C14	2.7788555925	0.2212654021	0.6834949584
C15	1.9785691723	-0.9373989478	0.6952793661
C16	2.6489786935	-2.1777580195	0.7428375886
C17	4.0325685162	-2.2651699690	0.7505466850

H18	4.7521311410	1.0475240779	0.6840736477
H19	2.3136974143	1.2017138485	0.6746663524
H20	2.0592725007	-3.0908756128	0.7687721967
H21	4.4974223091	-3.2449391164	0.7913840404
C22	7.1057963304	-2.1896579037	0.5620215821
C23	6.2943432380	-1.1172645935	0.6952459118
H24	6.7470581842	-0.1304663749	0.7704018333
H25	6.6548184592	-3.1735772257	0.4473231340
C26	11.4232968023	-2.2832485256	0.3334491473
C27	10.7420630536	-1.0904848652	0.6608963965
C28	9.3614414105	-1.0447427509	0.7507469954
C29	8.5665223273	-2.1873768522	0.5135890505
C30	9.2459520101	-3.3784279340	0.1972213202
C31	10.6309362345	-3.4231681282	0.1039142922
H32	11.3051032003	-0.1794189559	0.8363557629
H33	8.8883791120	-0.1031111048	1.0102326652
H34	8.6698021836	-4.2815696835	0.0112623395
H35	11.1173381935	-4.3614199090	-0.1497055569
C36	13.7853091607	-1.4449270308	0.5608415409
C37	12.8778586670	-2.3842036578	0.2169855271
H38	13.2337948186	-3.3354046834	-0.1749402520
H39	13.4271003389	-0.5194590438	1.0081864592
C40	15.9137932678	-2.5012447163	-0.3124786623
C41	15.2416480965	-1.5196414154	0.4349251698
C42	16.0303658400	-0.5563765317	1.0873461911
C43	17.4117725431	-0.5969951538	1.0067376570
H44	15.3176709709	-3.2318938489	-0.8449621558
H45	15.5505670018	0.2235210973	1.6731876377
H46	18.0031292727	0.1493757167	1.5302197341
C47	-4.5712713728	0.2756988567	0.1663226180

S48	-6.3491825706	0.1566092668	0.1038227552
C49	-6.8079790578	1.7284658503	-0.7103189459
C50	-5.9023713220	2.8734158114	-0.2744107457
C51	-4.4162760320	2.7287042965	-0.6845843390
C52	-3.8060600840	1.4137565958	-0.1604608786
H53	-6.7985204721	1.5937477474	-1.7952165145
H54	-7.8422070418	1.9150828279	-0.4086865766
H55	-6.2861120699	3.8042055386	-0.7116997304
H56	-5.9684622788	2.9835044599	0.8142501828
C57	17.3065393285	-2.5672935235	-0.4236926787
C58	17.9736984959	-3.6356141475	-1.3064951080
C59	19.3467427727	-4.0411218324	-0.7114502805
C60	20.3890220701	-2.9306512074	-0.6863559734
S61	19.8439097063	-1.4631795276	0.2707298950
C62	18.0650054747	-1.5880851372	0.2578248194
H63	19.1968455175	-4.4272802269	0.3038012305
H64	19.7541307565	-4.8664467823	-1.3092078363
H65	21.3049103097	-3.2735285422	-0.1976076633
H66	20.6519847500	-2.6127124056	-1.6983164473
C67	-3.6848318205	3.9588558318	-0.1015743320
H68	-2.6508892728	4.0349801038	-0.4472610681
H69	-4.1951255747	4.8762694387	-0.4144439021
H70	-3.6756097548	3.9311283946	0.9923215448
C71	-4.2835920777	2.7583203573	-2.2265768241
H72	-3.2304032424	2.7313807132	-2.5221162551
H73	-4.7722082775	1.8999214517	-2.6964242430
H74	-4.7281670662	3.6733277929	-2.6363952127
C75	17.1290483601	-4.9235960812	-1.3919896205
H76	17.6750848979	-5.6870014584	-1.9559921102
H77	16.9129695982	-5.3258178386	-0.3972478465

H78	16.1791497971	-4.7650092407	-1.9092746339
C79	18.1474295549	-3.0633782577	-2.7341891647
H80	18.6847377078	-3.7722845687	-3.3758761876
H81	17.1697254962	-2.8703976588	-3.1861047656
H82	18.6958743041	-2.1171751599	-2.7332042923

Total energy (hartrees): -2344.79833221306

HOMO energy (hartrees): -0.17726

LUMO energy (hartrees): -0.06852

Bond lengths (angstroms):

C1	-C2	: 1.403228	C1	-C4	: 1.407517		
C1	-C9	: 1.463645	C2	-H5	: 1.085230		
C2	-C52	: 1.402056	C3	-C4	: 1.381886		
C3	-H6	: 1.086734	C3	-C47	: 1.407431		
C4	-H7	: 1.085007	C8	-C9	: 1.350679		
C8	-H11	: 1.088389	C8	-C15	: 1.462624		
C9	-H10	: 1.088568	C12	-C13	: 1.410625		
C12	-C17	: 1.408335	C12	-C23	: 1.461650		
C13	-C14	: 1.386339	C13	-H18	: 1.087328		
C14	-C15	: 1.408226	C14	-H19	: 1.085232		
C15	-C16	: 1.410745	C16	-C17	: 1.386370		
C16	-H20	: 1.087295	C17	-H21	: 1.085221		
C22	-C23	: 1.351382	C22	-H25	: 1.088409		
C22	-C29	: 1.461530	C23	-H24	: 1.088288		
C26	-C27	: 1.412086	C26	-C31	: 1.407103		
C26	-C37	: 1.462705	C27	-C28	: 1.384298		

C27	-H32	:	1.085284	C28	-C29	:	1.412003
C28	-H33	:	1.085261	C29	-C30	:	1.407237
C30	-C31	:	1.388845	C30	-H34	:	1.087288
C31	-H35	:	1.086842	C36	-C37	:	1.350535
C36	-H39	:	1.088541	C36	-C41	:	1.463680
C37	-H38	:	1.088614	C40	-C41	:	1.404969
C40	-H44	:	1.082935	C40	-C57	:	1.398740
C41	-C42	:	1.405563	C42	-C43	:	1.384353
C42	-H45	:	1.087041	C43	-H46	:	1.086649
C43	-C62	:	1.403511	C47	-S48	:	1.782991
C47	-C52	:	1.409791	S48	-C49	:	1.828675
C49	-C50	:	1.523500	C49	-H53	:	1.093271
C49	-H54	:	1.093360	C50	-C51	:	1.548439
C50	-H55	:	1.097656	C50	-H56	:	1.096207
C51	-C52	:	1.541479	C51	-C67	:	1.545375
C51	-C71	:	1.547974	C57	-C58	:	1.538100
C57	-C62	:	1.413714	C58	-C59	:	1.550408
C58	-C75	:	1.542608	C58	-C79	:	1.547885
C59	-C60	:	1.523194	C59	-H63	:	1.096505
C59	-H64	:	1.097470	C60	-S61	:	1.834839
C60	-H65	:	1.093294	C60	-H66	:	1.092840
S61	-C62	:	1.783331	C67	-H68	:	1.092855
C67	-H69	:	1.095415	C67	-H70	:	1.094286
C71	-H72	:	1.094201	C71	-H73	:	1.093778
C71	-H74	:	1.096739	C75	-H76	:	1.095008
C75	-H77	:	1.094524	C75	-H78	:	1.093179
C79	-H80	:	1.096818	C79	-H81	:	1.094246
C79	-H82	:	1.093660				

Bond angles:

C4 -C1 -C2 : 117.034879 C9 -C1 -C2 : 119.043316

C9 -C1 -C4 : 123.920767 H5 -C2 -C1 : 117.266195

C52 -C2 -C1 : 124.170187 C52 -C2 -H5 : 118.561668

H6 -C3 -C4 : 119.423255 C47 -C3 -C4 : 121.660815

C47 -C3 -H6 : 118.915801 C3 -C4 -C1 : 120.374667

H7 -C4 -C1 : 120.563898 H7 -C4 -C3 : 119.061123

H11 -C8 -C9 : 118.512941 C15 -C8 -C9 : 127.254019

C15 -C8 -H11 : 114.206666 C8 -C9 -C1 : 127.064034

H10 -C9 -C1 : 114.397909 H10 -C9 -C8 : 118.516312

C17 -C12 -C13 : 116.987829 C23 -C12 -C13 : 118.770505

C23 -C12 -C17 : 124.241302 C14 -C13 -C12 : 121.991197

H18 -C13 -C12 : 118.775843 H18 -C13 -C14 : 119.232645

C15 -C14 -C13 : 121.019865 H19 -C14 -C13 : 118.989447

H19 -C14 -C15 : 119.988259 C14 -C15 -C8 : 124.167441

C16 -C15 -C8 : 118.855660 C16 -C15 -C14 : 116.976745

C17 -C16 -C15 : 121.997825 H20 -C16 -C15 : 118.779655

H20 -C16 -C17 : 119.221695 C16 -C17 -C12 : 121.005973

H21 -C17 -C12 : 120.004726 H21 -C17 -C16 : 118.987845

H25 -C22 -C23 : 118.617528 C29 -C22 -C23 : 127.024732

C29 -C22 -H25 : 114.332838 C22 -C23 -C12 : 127.402825

H24 -C23 -C12 : 114.111628 H24 -C23 -C22 : 118.461792

C31 -C26 -C27 : 116.772912 C37 -C26 -C27 : 123.814651

C37 -C26 -C31 : 119.411434 C28 -C27 -C26 : 121.608487

H32 -C27 -C26 : 119.755136 H32 -C27 -C28 : 118.632161

C29 -C28 -C27 : 121.589910 H33 -C28 -C27 : 118.615495

H33 -C28 -C29 : 119.794594 C28 -C29 -C22 : 123.942446

C30 -C29 -C22 : 119.253490 C30 -C29 -C28 : 116.798999

C31 -C30 -C29 : 121.590054 H34 -C30 -C29 : 119.054508

H34 -C30 -C31 : 119.352090 C30 -C31 -C26 : 121.634138

H35 -C31 -C26 : 119.039487 H35 -C31 -C30 : 119.326132

H39 -C36 -C37 : 118.347498 C41 -C36 -C37 : 127.672316

C41 -C36 -H39 : 113.964709 C36 -C37 -C26 : 126.863048

H38 -C37 -C26 : 114.463635 H38 -C37 -C36 : 118.663700

H44 -C40 -C41 : 118.008993 C57 -C40 -C41 : 123.479886

C57 -C40 -H44 : 118.499798 C40 -C41 -C36 : 123.878536

C42 -C41 -C36 : 118.908447 C42 -C41 -C40 : 117.212033

C43 -C42 -C41 : 120.851170 H45 -C42 -C41 : 119.614727

H45 -C42 -C43 : 119.529625 H46 -C43 -C42 : 119.659205

C62 -C43 -C42 : 121.079521 C62 -C43 -H46 : 119.261267

S48 -C47 -C3 : 114.328020 C52 -C47 -C3 : 119.714804

C52 -C47 -S48 : 125.946520 C49 -S48 -C47 : 102.026821

C50 -C49 -S48 : 111.682445 H53 -C49 -S48 : 109.494042

H53 -C49 -C50 : 111.801703 H54 -C49 -S48 : 105.141886

H54 -C49 -C50 : 110.797800 H54 -C49 -H53 : 107.636659

C51 -C50 -C49 : 115.116839 H55 -C50 -C49 : 108.389824

H55 -C50 -C51 : 108.013658 H56 -C50 -C49 : 108.892186

H56 -C50 -C51 : 109.288203 H56 -C50 -H55 : 106.822305

C52 -C51 -C50 : 111.689727 C67 -C51 -C50 : 106.255868

C67 -C51 -C52 : 111.309120 C71 -C51 -C50 : 110.141932

C71 -C51 -C52 : 108.728787 C71 -C51 -C67 : 108.663174

C47 -C52 -C2 : 117.026547 C51 -C52 -C2 : 119.378476

C51 -C52 -C47 : 123.543268 C58 -C57 -C40 : 120.685819

C62 -C57 -C40 : 117.591870 C62 -C57 -C58 : 121.673173

C59 -C58 -C57 : 110.213257 C75 -C58 -C57 : 111.976894

C75 -C58 -C59 : 106.726420 C79 -C58 -C57 : 108.741444

C79 -C58 -C59 : 110.566321 C79 -C58 -C75 : 108.602706

C60 -C59 -C58 : 114.937901 H63 -C59 -C58 : 109.050591

H63 -C59 -C60 : 109.574782 H64 -C59 -C58 : 108.444707

H64 -C59 -C60 : 107.651345 H64 -C59 -H63 : 106.870587

S61 -C60 -C59 : 112.853548 H65 -C60 -C59 : 110.607333

H65 -C60 -S61 : 105.457493 H66 -C60 -C59 : 111.192062

H66 -C60 -S61 : 108.773103 H66 -C60 -H65 : 107.675159

C62 -S61 -C60 : 103.683637 C57 -C62 -C43 : 119.778328

S61 -C62 -C43 : 114.264644 S61 -C62 -C57 : 125.956916

H68 -C67 -C51 : 112.576184 H69 -C67 -C51 : 109.781128

H69 -C67 -H68 : 106.980744 H70 -C67 -C51 : 111.158278

H70 -C67 -H68 : 108.058891 H70 -C67 -H69 : 108.099149

H72 -C71 -C51 : 110.553588 H73 -C71 -C51 : 111.999480

H73 -C71 -H72 : 107.135581 H74 -C71 -C51 : 110.698027

H74 -C71 -H72 : 108.046045 H74 -C71 -H73 : 108.249735

H76 -C75 -C58 : 109.730660 H77 -C75 -C58 : 111.380108

H77 -C75 -H76 : 108.080677 H78 -C75 -C58 : 112.388349

H78 -C75 -H76 : 106.900659 H78 -C75 -H77 : 108.169099

H80 -C79 -C58 : 110.833795 H81 -C79 -C58 : 110.233003

H81 -C79 -H80 : 108.063575 H82 -C79 -C58 : 112.042740

H82 -C79 -H80 : 108.303465 H82 -C79 -H81 : 107.208980

Torsional angles:

C1 -C2 -C52 -C47 : -0.521918

C1 -C2 -C52 -C51 :-177.999720

C1 -C4 -C3 -H6 : 179.467950

C1 -C4 -C3 -C47 : -0.400360

C1 -C9 -C8 -H11 : 0.917163

C1 -C9 -C8 -C15 : 178.931891

C2 -C1 -C4 -C3 : 1.149801

C2 -C1 -C4 -H7 :-178.645386

C2 -C1 -C9 -C8 :-171.052848

C2 -C1 -C9 -H10 : 7.211397

C2 -C52 -C47 -C3 : 1.292473

C2 -C52 -C47 -S48 :-179.965516

C2 -C52 -C51 -C50 :-159.359843

C2 -C52 -C51 -C67 : -40.771743

C2 -C52 -C51 -C71 : 78.894114

C3 -C4 -C1 -C9 :-178.475008

C3 -C47 -S48 -C49 :-172.758745

C3 -C47 -C52 -C51 : 178.655416

C4 -C1 -C2 -H5 : 179.821481

C4 -C1 -C2 -C52 : -0.695112

C4 -C1 -C9 -C8 : 8.564890

C4 -C1 -C9 -H10 :-173.170866

C4 -C3 -C47 -S48 :-179.755041

C4 -C3 -C47 -C52 : -0.872694

H5 -C2 -C1 -C9 : -0.534636

H5 -C2 -C52 -C47 : 178.955263

H5 -C2 -C52 -C51 : 1.477461

H6 -C3 -C4 -H7 : -0.733808

H6 -C3 -C47 -S48 : 0.376000

H6 -C3 -C47 -C52 : 179.258348

H7 -C4 -C1 -C9 : 1.729805

H7 -C4 -C3 -C47 : 179.397882

C8 -C15 -C14 -C13 :-178.765774

C8 -C15 -C14 -H19 : 1.806981

C8 -C15 -C16 -C17 : 178.586174

C8 -C15 -C16 -H20 : -1.080719

C9 -C1 -C2 -C52 : 178.948771

C9 -C8 -C15 -C14 : 9.136954

C9 -C8 -C15 -C16 :-170.715773

H10 -C9 -C8 -H11 :-177.283814

H10 -C9 -C8 -C15 : 0.730914

H11 -C8 -C15 -C14 :-172.775670

H11 -C8 -C15 -C16 : 7.371603

C12 -C13 -C14 -C15 : 0.137043

C12 -C13 -C14 -H19 : 179.569907

C12 -C17 -C16 -C15 : 0.228878

C12 -C17 -C16 -H20 : 179.894344

C12 -C23 -C22 -H25 : 0.485535

C12 -C23 -C22 -C29 : 178.559404

C13 -C12 -C17 -C16 : 1.002225

C13 -C12 -C17 -H21 :-178.554458

C13 -C12 -C23 -C22 :-172.083016

C13 -C12 -C23 -H24 : 6.100266

C13 -C14 -C15 -C16 : 1.089490

C14 -C13 -C12 -C17 : -1.188964

C14 -C13 -C12 -C23 : 178.601295

C14 -C15 -C16 -C17 : -1.277095

C14 -C15 -C16 -H20 : 179.056013

C15 -C14 -C13 -H18 : 179.930440

C15 -C16 -C17 -H21 : 179.789990

C16 -C15 -C14 -H19 :-178.337756

C16 -C17 -C12 -C23 :-178.775379

C17 -C12 -C13 -H18 : 179.016728

C17 -C12 -C23 -C22 : 7.690896

C17 -C12 -C23 -H24 :-174.125822

H18 -C13 -C12 -C23 : -1.193014

H18 -C13 -C14 -H19 : -0.636695

H20 -C16 -C17 -H21 : -0.544545

H21 -C17 -C12 -C23 : 1.667938

C22 -C29 -C28 -C27 :-178.437526

C22 -C29 -C28 -H33 : 1.554462

C22 -C29 -C30 -C31 : 178.316042

C22 -C29 -C30 -H34 : -1.013783

C23 -C22 -C29 -C28 : 7.340950

C23 -C22 -C29 -C30 :-171.812993

H24 -C23 -C22 -H25 :-177.628255

H24 -C23 -C22 -C29 : 0.445614

H25 -C22 -C29 -C28 :-174.514697

H25 -C22 -C29 -C30 : 6.331360

C26 -C27 -C28 -C29 : -0.280808

C26 -C27 -C28 -H33 : 179.727112

C26 -C31 -C30 -C29 : 0.611793

C26 -C31 -C30 -H34 : 179.939669

C26 -C37 -C36 -H39 : 2.449838

C26 -C37 -C36 -C41 :-179.075434

C27 -C26 -C31 -C30 : -0.116252

C27 -C26 -C31 -H35 :-179.935735

C27 -C26 -C37 -C36 : 9.189756

C27 -C26 -C37 -H38 :-171.962492

C27 -C28 -C29 -C30 : 0.735496

C28 -C27 -C26 -C31 : -0.045951

C28 -C27 -C26 -C37 : 179.586581

C28 -C29 -C30 -C31 : -0.897615

C28 -C29 -C30 -H34 : 179.772560

C29 -C28 -C27 -H32 : 178.970165

C29 -C30 -C31 -H35 :-179.569229

C30 -C29 -C28 -H33 :-179.272516

C30 -C31 -C26 -C37 :-179.765773

C31 -C26 -C27 -H32 :-179.288676

C31 -C26 -C37 -C36 :-171.186859

C31 -C26 -C37 -H38 : 7.660893

H32 -C27 -C26 -C37 : 0.343856

H32 -C27 -C28 -H33 : -1.021915

H34 -C30 -C31 -H35 : -0.241353

H35 -C31 -C26 -C37 : 0.414744

C36 -C41 -C40 -H44 : 1.453580

C36 -C41 -C40 -C57 :-179.790829

C36 -C41 -C42 -C43 : 179.330449

C36 -C41 -C42 -H45 : 0.103927

C37 -C36 -C41 -C40 : 12.889168

C37 -C36 -C41 -C42 :-167.482273

H38 -C37 -C36 -H39 :-176.354870

H38 -C37 -C36 -C41 : 2.119858

H39 -C36 -C41 -C40 :-168.579821

H39 -C36 -C41 -C42 : 11.048738

C40 -C41 -C42 -C43 : -1.016308

C40 -C41 -C42 -H45 : 179.757170

C40 -C57 -C58 -C59 :-148.394320

C40 -C57 -C58 -C75 : -29.754077

C40 -C57 -C58 -C79 : 90.258082

C40 -C57 -C62 -C43 : -0.192745

C40 -C57 -C62 -S61 : 179.936509

C41 -C40 -C57 -C58 :-177.472586

C41 -C40 -C57 -C62 : 0.020055

C41 -C42 -C43 -H46 :-179.147536

C41 -C42 -C43 -C62 : 0.881488

C42 -C41 -C40 -H44 :-178.180796

C42 -C41 -C40 -C57 : 0.574795

C42 -C43 -C62 -C57 : -0.251949

C42 -C43 -C62 -S61 : 179.633287

C43 -C62 -C57 -C58 : 177.273596

C43 -C62 -S61 -C60 : 176.533930

H44 -C40 -C57 -C58 : 1.277262

H44 -C40 -C57 -C62 : 178.769904

H45 -C42 -C43 -H46 : 0.079637

H45 -C42 -C43 -C62 :-179.891339

H46 -C43 -C62 -C57 : 179.776962

H46 -C43 -C62 -S61 : -0.337802

C47 -S48 -C49 -C50 : -36.567986

C47 -S48 -C49 -H53 : 87.815334

C47 -S48 -C49 -H54 :-156.795884

C47 -C52 -C51 -C50 : 23.335960

C47 -C52 -C51 -C67 : 141.924060

C47 -C52 -C51 -C71 : -98.410084

S48 -C47 -C52 -C51 : -2.602573

S48 -C49 -C50 -C51 : 64.666846

S48 -C49 -C50 -H55 :-174.284049

S48 -C49 -C50 -H56 : -58.427513

C49 -S48 -C47 -C52 : 8.440287

C49 -C50 -C51 -C52 : -56.418668

C49 -C50 -C51 -C67 :-177.975934

C49 -C50 -C51 -C71 : 64.508428

C50 -C51 -C67 -H68 :-171.993934

C50 -C51 -C67 -H69 : -52.938623

C50 -C51 -C67 -H70 : 66.612898

C50 -C51 -C71 -H72 : 175.800007

C50 -C51 -C71 -H73 : -64.802809

C50 -C51 -C71 -H74 : 56.108118

C51 -C50 -C49 -H53 : -58.414035

C51 -C50 -C49 -H54 :-178.479921

C52 -C51 -C50 -H55 :-177.672402

C52 -C51 -C50 -H56 : 66.464550

C52 -C51 -C67 -H68 : 66.205856

C52 -C51 -C67 -H69 :-174.738833

C52 -C51 -C67 -H70 : -55.187313

C52 -C51 -C71 -H72 : -61.515132

C52 -C51 -C71 -H73 : 57.882052

C52 -C51 -C71 -H74 : 178.792979

H53 -C49 -C50 -H55 : 62.635071

H53 -C49 -C50 -H56 : 178.491606

H54 -C49 -C50 -H55 : -57.430815

H54 -C49 -C50 -H56 : 58.425720

H55 -C50 -C51 -C67 : 60.770332

H55 -C50 -C51 -C71 : -56.745306

H56 -C50 -C51 -C67 : -55.092716

H56 -C50 -C51 -C71 :-172.608354

C57 -C58 -C59 -C60 : -64.621458

C57 -C58 -C59 -H63 : 58.845961

C57 -C58 -C59 -H64 : 174.874792

C57 -C58 -C75 -H76 :-175.189097

C57 -C58 -C75 -H77 : -55.552823

C57 -C58 -C75 -H78 : 66.010170

C57 -C58 -C79 -H80 : 176.021081

C57 -C58 -C79 -H81 : -64.385469

C57 -C58 -C79 -H82 : 54.916817

C57 -C62 -S61 -C60 : -3.589128

C58 -C57 -C62 -S61 : -2.597151

C58 -C59 -C60 -S61 : 58.560220

C58 -C59 -C60 -H65 : 176.430904

C58 -C59 -C60 -H66 : -63.985574

C59 -C58 -C57 -C62 : 34.216850

C59 -C58 -C75 -H76 : -54.503535

C59 -C58 -C75 -H77 : 65.132739

C59 -C58 -C75 -H78 :-173.304268

C59 -C58 -C79 -H80 : 54.889836

C59 -C58 -C79 -H81 : 174.483286

C59 -C58 -C79 -H82 : -66.214428

C59 -C60 -S61 -C62 : -22.759653

C60 -C59 -C58 -C75 : 173.571570

C60 -C59 -C58 -C79 : 55.632811

S61 -C60 -C59 -H63 : -64.627836

S61 -C60 -C59 -H64 : 179.498995

C62 -C57 -C58 -C75 : 152.857093

C62 -C57 -C58 -C79 : -87.130748

C62 -S61 -C60 -H65 :-143.611688

C62 -S61 -C60 -H66 : 101.129549

H63 -C59 -C58 -C75 : -62.961011

H63 -C59 -C58 -C79 : 179.100230

H63 -C59 -C60 -H65 : 53.242848

H63 -C59 -C60 -H66 : 172.826369

H64 -C59 -C58 -C75 : 53.067820

H64 -C59 -C58 -C79 : -64.870939

H64 -C59 -C60 -H65 : -62.630321

H64 -C59 -C60 -H66 : 56.953200

C67 -C51 -C71 -H72 : 59.785688

C67 -C51 -C71 -H73 : 179.182872

C67 -C51 -C71 -H74 : -59.906200

H68 -C67 -C51 -C71 : -53.498951

H69 -C67 -C51 -C71 : 65.556360

H70 -C67 -C51 -C71 :-174.892120

C75 -C58 -C79 -H80 : -61.894222

C75 -C58 -C79 -H81 : 57.699229

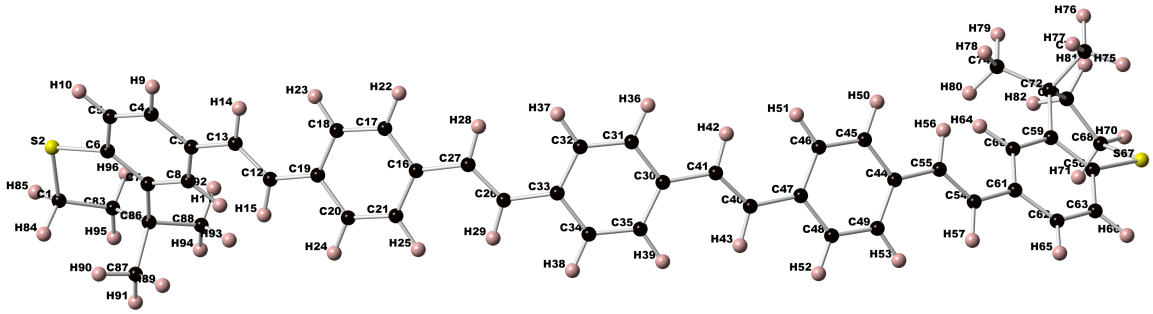
C75 -C58 -C79 -H82 : 177.001515

H76 -C75 -C58 -C79 : 64.717709

H77 -C75 -C58 -C79 :-175.646017

H78 -C75 -C58 -C79 : -54.083024

PPV4



Final geometry:

		angstroms	
atom	x	y	z
C1	0.1311759001	-4.8233740321	1.4399943570
S2	-0.9890420911	-4.3641105345	0.0698979678
C3	1.6580420060	-4.0156632387	-3.6837177687
C4	0.2925651842	-3.6829789008	-3.6670074669
C5	-0.4444921163	-3.7924394563	-2.5001795780
C6	0.1355228307	-4.2634152201	-1.3098970055
C7	1.4962042125	-4.6455218474	-1.2972765329
C8	2.2177456374	-4.4905926153	-2.4868594269
H9	-0.1870697937	-3.3260759650	-4.5748137483
H10	-1.4947215977	-3.5134239266	-2.5009360953
H11	3.2565520563	-4.7972966951	-2.5013596546
C12	3.7701423245	-3.8967026348	-5.0263730297
C13	2.4238894138	-3.9249560804	-4.9282922064
H14	1.8251189494	-3.8989081426	-5.8377398164
H15	4.3469499557	-3.8470089357	-4.1038683134
C16	6.3214375181	-4.4362718062	-8.4603722525
C17	4.9175032206	-4.4686350670	-8.5972176616
C18	4.0700547648	-4.2494966753	-7.5209240575

C19	4.5837393494	-3.9831692690	-6.2361536865
C20	5.9853146105	-3.8855063064	-6.1151584374
C21	6.8309888425	-4.1011771326	-7.1903733964
H22	4.4912725235	-4.7126309537	-9.5673759684
H23	2.9983975874	-4.3326020761	-7.6700862346
H24	6.4122928717	-3.6648601823	-5.1398197563
H25	7.9028339584	-4.0477694320	-7.0314022839
C26	8.5036465354	-4.9671990367	-9.5903093500
C27	7.1568284422	-4.8518903029	-9.5847543647
H28	6.6009723305	-5.1714012355	-10.4641285912
H29	9.0544660957	-4.6444994437	-8.7086852474
C30	11.0076317524	-7.1610955887	-12.3242428398
C31	9.6550623189	-6.9064778181	-12.6372080706
C32	8.8393060693	-6.1491522716	-11.8105338918
C33	9.3338831274	-5.6009952338	-10.6100572752
C34	10.7067649175	-5.7844468154	-10.3413864126
C35	11.5213406605	-6.5404877645	-11.1684606827
H36	9.2331091596	-7.3508079277	-13.5349678465
H37	7.7967819242	-6.0163068121	-12.0804164888
H38	11.1244511709	-5.3550195272	-9.4339784502
H39	12.5596776579	-6.6862764057	-10.8891329569
C40	13.0197504572	-8.5514201002	-12.9244824431
C41	11.7542235268	-8.1234582926	-13.1309231382
H42	11.1726836148	-8.5821463434	-13.9282208061
H43	13.6115705098	-8.0743142010	-12.1451424981
C44	14.9875759823	-12.0507673095	-14.4968600814
C45	13.6726760266	-11.7249540376	-14.8905082989
C46	13.0364862768	-10.5762959660	-14.4465993670
C47	13.6842483765	-9.6808586208	-13.5720992456
C48	15.0192058561	-9.9777671188	-13.2257444298

C49	15.6564611713	-11.1257146527	-13.6722110739
H50	13.1331314573	-12.4157148055	-15.5339516028
H51	12.0090021282	-10.3986841535	-14.7459604852
H52	15.5486866754	-9.3046751325	-12.5565273697
H53	16.6682937239	-11.3307695883	-13.3374978510
C54	16.7841375028	-13.8187358957	-14.6631758770
C55	15.5360861940	-13.3506145645	-14.8763336595
H56	14.8185967060	-14.0117687876	-15.3590480454
H57	17.5425232882	-13.1508418805	-14.2583695928
C58	18.1196925823	-17.8328441977	-15.3300325468
C59	16.7329974114	-17.5890246393	-15.1935798692
C60	16.3300062022	-16.2696597034	-14.9739737376
C61	17.2333267675	-15.1909289168	-14.9187326338
C62	18.6013873763	-15.4713268663	-15.0684126080
C63	19.0352628803	-16.7767471159	-15.2650190003
H64	15.2795312438	-16.0608339288	-14.8151330875
H65	19.3267552358	-14.6636808275	-15.0147559102
H66	20.0963751346	-16.9920632477	-15.3474995786
S67	18.7368927211	-19.4965405212	-15.5245009274
C68	17.5983695271	-20.2476885976	-14.2942171550
C69	16.1125393370	-20.0390398110	-14.6145201573
H70	17.8468433317	-21.3114587414	-14.2527495718
H71	17.8551648959	-19.8092023059	-13.3263549210
C72	15.7110543368	-18.7244406595	-15.3729780168
C73	15.6113978289	-19.0195106031	-16.8951064867
C74	14.3027610960	-18.3357360639	-14.8816723561
H75	16.5638310376	-19.3640900916	-17.3025773186
H76	14.8605214861	-19.7965969833	-17.0791221320
H77	15.3101488177	-18.1185816215	-17.4389564079
H78	13.8608270376	-17.5357335699	-15.4833121635

H79	13.6378591363	-19.2020318827	-14.9608623683
H80	14.3123317839	-18.0158609950	-13.8344174606
H81	15.7436773510	-20.8839589516	-15.2063898629
H82	15.5742478065	-20.0745222520	-13.6592874282
C83	1.2199254274	-5.7833844435	0.9783704079
H84	0.5511509823	-3.9186465296	1.8877071942
H85	-0.5116818836	-5.2951510987	2.1880497128
C86	2.2173742473	-5.1974034315	-0.0507206029
C87	3.0406978736	-4.0567189724	0.5950943297
C88	3.1787109640	-6.3495953829	-0.4247362875
H89	3.7971752139	-3.6861974547	-0.1034038374
H90	2.4135505118	-3.2045638581	0.8726221168
H91	3.5553251350	-4.4119394414	1.4960293734
H92	2.6562006803	-7.1410385739	-0.9711255417
H93	4.0185909080	-6.0136562998	-1.0380938162
H94	3.6030306827	-6.7875596844	0.4852654702
H95	1.7918007363	-6.1081536374	1.8571890388
H96	0.7490240011	-6.6799402055	0.5577915813

Total energy (hartrees): -2653.25687824603

HOMO energy (hartrees): -0.17849

LUMO energy (hartrees): -0.07562

Bond lengths (angstroms):

C1	-S2	:	1.828381	C1	-C83	:	1.523185
C1	-H84	:	1.093324	C1	-H85	:	1.093356

S2 -C6 : 1.782868 C3 -C4 : 1.405519

C3 -C8 : 1.404028 C3 -C13 : 1.464143

C4 -C5 : 1.384457 C4 -H9 : 1.086987

C5 -C6 : 1.405350 C5 -H10 : 1.086661

C6 -C7 : 1.413371 C7 -C8 : 1.399904

C7 -C86 : 1.542258 C8 -H11 : 1.083234

C12 -C13 : 1.350117 C12 -H15 : 1.089124

C12 -C19 : 1.460475 C13 -H14 : 1.089174

C16 -C17 : 1.410959 C16 -C21 : 1.408839

C16 -C27 : 1.461113 C17 -C18 : 1.387299

C17 -H22 : 1.087388 C18 -C19 : 1.409055

C18 -H23 : 1.085175 C19 -C20 : 1.410174

C20 -C21 : 1.384834 C20 -H24 : 1.087327

C21 -H25 : 1.084885 C26 -C27 : 1.351757

C26 -H29 : 1.088484 C26 -C33 : 1.459752

C27 -H28 : 1.088284 C30 -C31 : 1.411461

C30 -C35 : 1.408859 C30 -C41 : 1.460916

C31 -C32 : 1.386503 C31 -H36 : 1.086944

C32 -C33 : 1.409336 C32 -H37 : 1.085054

C33 -C34 : 1.410901 C34 -C35 : 1.385346

C34 -H38 : 1.087317 C35 -H39 : 1.085091

C40 -C41 : 1.351787 C40 -H43 : 1.088693

C40 -C47 : 1.461710 C41 -H42 : 1.088240

C44 -C45 : 1.410700 C44 -C49 : 1.408253

C44 -C55 : 1.460981 C45 -C46 : 1.386076

C45 -H50 : 1.087326 C46 -C47 : 1.409310

C46 -H51 : 1.084844 C47 -C48 : 1.410754

C48 -C49 : 1.386799 C48 -H52 : 1.086855

C49 -H53 : 1.085304 C54 -C55 : 1.349891

C54 -H57 : 1.088623 C54 -C61 : 1.466286

C55 -H56 : 1.088545 C58 -C59 : 1.414564

C58 -C63 : 1.399227 C58 -S67 : 1.785116

C59 -C60 : 1.396908 C59 -C72 : 1.538090

C60 -C61 : 1.408084 C60 -H64 : 1.082745

C61 -C62 : 1.404499 C62 -C63 : 1.389613

C62 -H65 : 1.086890 C63 -H66 : 1.085874

S67 -C68 : 1.836861 C68 -C69 : 1.534216

C68 -H70 : 1.093191 C68 -H71 : 1.093147

C69 -C72 : 1.569911 C69 -H81 : 1.095563

C69 -H82 : 1.097035 C72 -C73 : 1.553664

C72 -C74 : 1.541351 C73 -H75 : 1.091740

C73 -H76 : 1.096148 C73 -H77 : 1.094622

C74 -H78 : 1.094203 C74 -H79 : 1.094913

C74 -H80 : 1.095059 C83 -C86 : 1.548324

C83 -H95 : 1.097651 C83 -H96 : 1.096561

C86 -C87 : 1.547934 C86 -C88 : 1.546481

C87 -H89 : 1.094278 C87 -H90 : 1.093848

C87 -H91 : 1.096680 C88 -H92 : 1.094505

C88 -H93 : 1.092914 C88 -H94 : 1.095428

Bond angles:

C83 -C1 -S2 : 111.663131 H84 -C1 -S2 : 109.532871

H84 -C1 -C83 : 111.782338 H85 -C1 -S2 : 105.119899

H85 -C1 -C83 : 110.834284 H85 -C1 -H84 : 107.622597

C6 -S2 -C1 : 101.985576 C8 -C3 -C4 : 117.207568

C13 -C3 -C4 : 120.239038 C13 -C3 -C8 : 122.482983

C5 -C4 -C3 : 120.565196 H9 -C4 -C3 : 119.766679

H9 -C4 -C5 : 119.664604 C6 -C5 -C4 : 121.372510

H10 -C5 -C4 : 119.580357 H10 -C5 -C6 : 119.046648

C5 -C6 -S2 : 114.461563 C7 -C6 -S2 : 125.807735

C7 -C6 -C5 : 119.702664 C8 -C7 -C6 : 117.303204

C86 -C7 -C6 : 123.651087 C86 -C7 -C8 : 119.040033

C7 -C8 -C3 : 123.803195 H11 -C8 -C3 : 117.817386

H11 -C8 -C7 : 118.315222 H15 -C12 -C13 : 117.873022

C19 -C12 -C13 : 127.909809 C19 -C12 -H15 : 114.160398

C12 -C13 -C3 : 125.776151 H14 -C13 -C3 : 115.068169

H14 -C13 -C12 : 119.144571 C21 -C16 -C17 : 116.921286

C27 -C16 -C17 : 119.192338 C27 -C16 -C21 : 123.680876

C18 -C17 -C16 : 121.934733 H22 -C17 -C16 : 118.796692

H22 -C17 -C18 : 119.221023 C19 -C18 -C17 : 120.967343

H23 -C18 -C17 : 118.980757 H23 -C18 -C19 : 119.988330

C18 -C19 -C12 : 124.290301 C20 -C19 -C12 : 118.587899

C20 -C19 -C18 : 116.978766 C21 -C20 -C19 : 121.974413

H24 -C20 -C19 : 118.770987 H24 -C20 -C21 : 119.226054

C20 -C21 -C16 : 121.069698 H25 -C21 -C16 : 120.075145

H25 -C21 -C20 : 118.808923 H29 -C26 -C27 : 118.396856

C33 -C26 -C27 : 127.342733 C33 -C26 -H29 : 113.999157

C26 -C27 -C16 : 126.661614 H28 -C27 -C16 : 114.412274

H28 -C27 -C26 : 118.720217 C35 -C30 -C31 : 116.862535

C41 -C30 -C31 : 119.085794 C41 -C30 -C35 : 123.836346

C32 -C31 -C30 : 122.014713 H36 -C31 -C30 : 118.776913

H36 -C31 -C32 : 119.165917 C33 -C32 -C31 : 120.920430

H37 -C32 -C31 : 118.938437 H37 -C32 -C33 : 120.094094

C32 -C33 -C26 : 124.355855 C34 -C33 -C26 : 118.480088

C34 -C33 -C32 : 116.943055 C35 -C34 -C33 : 121.966451

H38 -C34 -C33 : 118.774078 H38 -C34 -C35 : 119.202316

C34 -C35 -C30 : 121.049284 H39 -C35 -C30 : 120.060498

H39 -C35 -C34 : 118.835534 H43 -C40 -C41 : 118.652656

C47 -C40 -C41 : 127.053157 C47 -C40 -H43 : 114.120287

C40 -C41 -C30 : 127.060424 H42 -C41 -C30 : 114.148996

H42 -C41 -C40 : 118.602637 C49 -C44 -C45 : 117.027082

C55 -C44 -C45 : 118.878289 C55 -C44 -C49 : 123.931787

C46 -C45 -C44 : 121.995111 H50 -C45 -C44 : 118.745483

H50 -C45 -C46 : 119.224557 C47 -C46 -C45 : 120.951046

H51 -C46 -C45 : 118.817360 H51 -C46 -C47 : 120.167853

C46 -C47 -C40 : 123.842703 C48 -C47 -C40 : 118.948502

C48 -C47 -C46 : 116.972184 C49 -C48 -C47 : 122.005428

H52 -C48 -C47 : 118.804614 H52 -C48 -C49 : 119.144135

C48 -C49 -C44 : 120.931205 H53 -C49 -C44 : 119.954243

H53 -C49 -C48 : 119.046296 H57 -C54 -C55 : 119.343743

C61 -C54 -C55 : 125.467638 C61 -C54 -H57 : 115.185290

C54 -C55 -C44 : 127.925599 H56 -C55 -C44 : 114.085829

H56 -C55 -C54 : 117.956216 C63 -C58 -C59 : 120.455655

S67 -C58 -C59 : 120.669474 S67 -C58 -C63 : 118.833031

C60 -C59 -C58 : 117.436477 C72 -C59 -C58 : 120.853431

C72 -C59 -C60 : 121.592806 C61 -C60 -C59 : 123.001924

H64 -C60 -C59 : 119.019917 H64 -C60 -C61 : 117.962559

C60 -C61 -C54 : 121.819635 C62 -C61 -C54 : 120.251918

C62 -C61 -C60 : 117.888612 C63 -C62 -C61 : 120.447737

H65 -C62 -C61 : 119.765625 H65 -C62 -C63 : 119.779878

C62 -C63 -C58 : 120.751333 H66 -C63 -C58 : 119.092882

H66 -C63 -C62 : 120.140943 C68 -S67 -C58 : 95.385122

C69 -C68 -S67 : 113.880346 H70 -C68 -S67 : 106.406545

H70 -C68 -C69 : 111.123549 H71 -C68 -S67 : 106.461860

H71 -C68 -C69 : 110.965098 H71 -C68 -H70 : 107.658819

C72 -C69 -C68 : 117.543045 H81 -C69 -C68 : 109.510126

H81 -C69 -C72 : 107.378999 H82 -C69 -C68 : 106.799153

H82 -C69 -C72 : 108.800413 H82 -C69 -H81 : 106.275820

C69 -C72 -C59 : 113.071470 C73 -C72 -C59 : 107.282623

C73 -C72 -C69 : 109.310450 C74 -C72 -C59 : 112.564714

C74 -C72 -C69 : 106.908128 C74 -C72 -C73 : 107.551863

H75 -C73 -C72 : 111.693392 H76 -C73 -C72 : 110.062451

H76 -C73 -H75 : 108.131300 H77 -C73 -C72 : 110.370749

H77 -C73 -H75 : 108.326459 H77 -C73 -H76 : 108.152832

H78 -C74 -C72 : 112.218374 H79 -C74 -C72 : 109.406020

H79 -C74 -H78 : 107.063732 H80 -C74 -C72 : 111.747367

H80 -C74 -H78 : 108.409221 H80 -C74 -H79 : 107.793737

C86 -C83 -C1 : 115.047759 H95 -C83 -C1 : 108.435585

H95 -C83 -C86 : 107.967963 H96 -C83 -C1 : 108.940986

H96 -C83 -C86 : 109.339083 H96 -C83 -H95 : 106.792286

C83 -C86 -C7 : 111.802235 C87 -C86 -C7 : 108.798187

C87 -C86 -C83 : 110.135391 C88 -C86 -C7 : 111.211037

C88 -C86 -C83 : 106.214622 C88 -C86 -C87 : 108.620214

H89 -C87 -C86 : 110.542169 H90 -C87 -C86 : 112.023387

H90 -C87 -H89 : 107.128802 H91 -C87 -C86 : 110.710569

H91 -C87 -H89 : 108.038743 H91 -C87 -H90 : 108.237118

H92 -C88 -C86 : 111.267097 H93 -C88 -C86 : 112.608150

H93 -C88 -H92 : 107.997215 H94 -C88 -C86 : 109.740204

H94 -C88 -H92 : 108.090789 H94 -C88 -H93 : 106.943866

Torsional angles:

C1 -S2 -C6 -C5 :-174.131013

C1 -S2 -C6 -C7 : 7.813344

C1 -C83 -C86 -C7 : -55.860997

C1 -C83 -C86 -C87 : 65.224637

C1 -C83 -C86 -C88 :-177.337314

S2 -C1 -C83 -C86 : 65.084267

S2 -C1 -C83 -H95 :-173.937759

S2 -C1 -C83 -H96 : -58.065829

S2 -C6 -C5 -C4 :-178.695051

S2 -C6 -C5 -H10 : 1.050263

S2 -C6 -C7 -C8 : 179.964275

S2 -C6 -C7 -C86 : -0.912508

C3 -C4 -C5 -C6 : -1.385404

C3 -C4 -C5 -H10 : 178.870618

C3 -C8 -C7 -C6 : -1.747213

C3 -C8 -C7 -C86 : 179.087593

C3 -C13 -C12 -H15 : -5.838516

C3 -C13 -C12 -C19 : 171.244222

C4 -C3 -C8 -C7 : -0.063728

C4 -C3 -C8 -H11 : 176.967863

C4 -C3 -C13 -C12 : 162.981345

C4 -C3 -C13 -H14 : -18.248636

C4 -C5 -C6 -C7 : -0.510374

C5 -C4 -C3 -C8 : 1.648410

C5 -C4 -C3 -C13 : 178.672384

C5 -C6 -C7 -C8 : 2.001861

C5 -C6 -C7 -C86 :-178.874922

C6 -S2 -C1 -C83 : -36.955848

C6 -S2 -C1 -H84 : 87.417167

C6 -S2 -C1 -H85 :-157.203648

C6 -C5 -C4 -H9 : 179.298800

C6 -C7 -C8 -H11 :-178.765007

C6 -C7 -C86 -C83 : 21.772342

C6 -C7 -C86 -C87 :-100.085475

C6 -C7 -C86 -C88 : 140.317304

C7 -C6 -C5 -H10 : 179.234939

C7 -C8 -C3 -C13 :-177.015731

C7 -C86 -C83 -H95 :-177.093813

C7 -C86 -C83 -H96 : 67.076699

C7 -C86 -C87 -H89 : -61.210923

C7 -C86 -C87 -H90 : 58.185716

C7 -C86 -C87 -H91 : 179.105608

C7 -C86 -C88 -H92 : -54.927505

C7 -C86 -C88 -H93 : 66.487320

C7 -C86 -C88 -H94 :-174.510917

C8 -C3 -C4 -H9 :-179.036490

C8 -C3 -C13 -C12 : -20.156438

C8 -C3 -C13 -H14 : 158.613581

C8 -C7 -C86 -C83 :-159.118794

C8 -C7 -C86 -C87 : 79.023389

C8 -C7 -C86 -C88 : -40.573832

H9 -C4 -C3 -C13 : -2.012516

H9 -C4 -C5 -H10 : -0.445178

H11 -C8 -C3 -C13 : 0.015860

H11 -C8 -C7 -C86 : 2.069799

C12 -C19 -C18 -C17 :-172.524606

C12 -C19 -C18 -H23 : 4.546292

C12 -C19 -C20 -C21 : 172.908980

C12 -C19 -C20 -H24 : -5.131646

C13 -C12 -C19 -C18 : -6.706481

C13 -C12 -C19 -C20 : 177.780366

H14 -C13 -C12 -H15 : 175.437115

H14 -C13 -C12 -C19 : -7.480146

H15 -C12 -C19 -C18 : 170.467192

H15 -C12 -C19 -C20 : -5.045961

C16 -C17 -C18 -C19 : 0.009326

C16 -C17 -C18 -H23 :-177.090578

C16 -C21 -C20 -C19 : -0.294607

C16 -C21 -C20 -H24 : 177.737371

C16 -C27 -C26 -H29 : -5.626922

C16 -C27 -C26 -C33 : 168.119645

C17 -C16 -C21 -C20 : 3.343803

C17 -C16 -C21 -H25 :-179.158716

C17 -C16 -C27 -C26 :-175.172876

C17 -C16 -C27 -H28 : -0.494423

C17 -C18 -C19 -C20 : 3.054588

C18 -C17 -C16 -C21 : -3.219227

C18 -C17 -C16 -C27 : 171.764727

C18 -C19 -C20 -C21 : -2.931935

C18 -C19 -C20 -H24 : 179.027439

C19 -C18 -C17 -H22 : 177.470292

C19 -C20 -C21 -H25 :-177.823132

C20 -C19 -C18 -H23 :-179.874515

C20 -C21 -C16 -C27 :-171.393245

C21 -C16 -C17 -H22 : 179.309395

C21 -C16 -C27 -C26 : -0.548542

C21 -C16 -C27 -H28 : 174.129910

H22 -C17 -C16 -C27 : -5.706651

H22 -C17 -C18 -H23 : 0.370388

H24 -C20 -C21 -H25 : 0.208846

H25 -C21 -C16 -C27 : 6.104236

C26 -C33 -C32 -C31 :-170.404769

C26 -C33 -C32 -H37 : 7.074343

C26 -C33 -C34 -C35 : 170.741479

C26 -C33 -C34 -H38 : -6.485864

C27 -C26 -C33 -C32 : 3.237468

C27 -C26 -C33 -C34 :-171.185263

H28 -C27 -C26 -H29 : 179.899248

H28 -C27 -C26 -C33 : -6.354185

H29 -C26 -C33 -C32 : 177.216802

H29 -C26 -C33 -C34 : 2.794071

C30 -C31 -C32 -C33 : -0.175937

C30 -C31 -C32 -H37 :-177.683691

C30 -C35 -C34 -C33 : 0.118426

C30 -C35 -C34 -H38 : 177.334255

C30 -C41 -C40 -H43 : -6.956239

C30 -C41 -C40 -C47 : 167.947794

C31 -C30 -C35 -C34 : 3.813173

C31 -C30 -C35 -H39 :-178.907586

C31 -C30 -C41 -C40 :-175.416936

C31 -C30 -C41 -H42 : -0.512127

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C32 -C31 -C30 -C35 : -3.805225

C32 -C31 -C30 -C41 : 171.068948

C32 -C33 -C34 -C35 : -4.094765

C32 -C33 -C34 -H38 : 178.677891

C33 -C32 -C31 -H36 : 177.424221

C33 -C34 -C35 -H39 :-177.193484

C34 -C33 -C32 -H37 :-178.424639

C34 -C35 -C30 -C41 :-170.793262

C35 -C30 -C31 -H36 : 178.585608

C35 -C30 -C41 -C40 : -0.923175

C35 -C30 -C41 -H42 : 173.981634

H36 -C31 -C30 -C41 : -6.540220

H36 -C31 -C32 -H37 : -0.083533

H38 -C34 -C35 -H39 : 0.022345

H39 -C35 -C30 -C41 : 6.485979

C40 -C47 -C46 -C45 :-171.488710

C40 -C47 -C46 -H51 : 5.573523

C40 -C47 -C48 -C49 : 171.879389

C40 -C47 -C48 -H52 : -5.636367

C41 -C40 -C47 -C46 : -5.783805

C41 -C40 -C47 -C48 : 179.981686

H42 -C41 -C40 -H43 : 178.339870

H42 -C41 -C40 -C47 : -6.756097

H43 -C40 -C47 -C46 : 169.316959

H43 -C40 -C47 -C48 : -4.917551

C44 -C45 -C46 -C47 : -0.173183

C44 -C45 -C46 -H51 :-177.274357

C44 -C49 -C48 -C47 : -0.069162

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C44 -C55 -C54 -H57 : -7.257325

C44 -C55 -C54 -C61 : 172.045468

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C45 -C44 -C49 -H53 : 179.720624

C45 -C44 -C55 -C54 : 176.060407

C45 -C44 -C55 -H56 : -6.072128

C45 -C46 -C47 -C48 : 2.850761

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C46 -C45 -C44 -C55 : 172.894957

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C46 -C47 -C48 -H52 : 179.735526

C47 -C46 -C45 -H50 : 177.651905

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C48 -C47 -C46 -H51 : 179.912994

C48 -C49 -C44 -C55 :-172.544879

C49 -C44 -C45 -H50 : 179.514020

C49 -C44 -C55 -C54 : -8.722490

C49 -C44 -C55 -H56 : 169.144975

H50 -C45 -C44 -C55 : -4.940186

H50 -C45 -C46 -H51 : 0.550731

H52 -C48 -C49 -H53 : 0.444423

H53 -C49 -C44 -C55 : 4.422024

C54 -C61 -C60 -C59 :-178.905969

C54 -C61 -C60 -H64 : -0.358626

C54 -C61 -C62 -C63 : 177.785836

C54 -C61 -C62 -H65 : -1.266290

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C55 -C54 -C61 -C62 : 159.891602

H56 -C55 -C54 -H57 : 174.946777

H56 -C55 -C54 -C61 : -5.750429

H57 -C54 -C61 -C60 : 156.875555

H57 -C54 -C61 -C62 : -20.779993

C58 -C59 -C60 -C61 : 1.640443

C58 -C59 -C60 -H64 :-176.892273

C58 -C59 -C72 -C69 : 45.924558

C58 -C59 -C72 -C73 : -74.669828

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C58 -C63 -C62 -C61 : 0.598954

C58 -C63 -C62 -H65 : 179.650945

C58 -S67 -C68 -C69 : 58.412878

C58 -S67 -C68 -H70 :-178.821360

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C59 -C58 -C63 -C62 : -0.129584

C59 -C58 -C63 -H66 : 178.470911

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C59 -C60 -C61 -C62 : -1.197235

C59 -C72 -C69 -C68 : -23.402957

C59 -C72 -C69 -H81 :-147.314032

C59 -C72 -C69 -H82 : 98.055276

C59 -C72 -C73 -H75 : 62.262631

C59 -C72 -C73 -H76 :-177.615839

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C59 -C72 -C74 -H78 : 65.660286

C59 -C72 -C74 -H79 :-175.657248

C59 -C72 -C74 -H80 : -56.359408

C60 -C59 -C58 -C63 : -0.952677

C60 -C59 -C58 -S67 : 176.667323

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C60 -C59 -C72 -C74 : -16.826972

C60 -C61 -C62 -C63 : 0.039665

C60 -C61 -C62 -H65 :-179.012460

C61 -C60 -C59 -C72 :-174.453326

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C62 -C61 -C60 -H64 : 177.350107

C62 -C63 -C58 -S67 :-177.792817

C63 -C58 -C59 -C72 : 175.171576

C63 -C58 -S67 -C68 : 136.998341

H64 -C60 -C59 -C72 : 7.013959

H65 -C62 -C63 -H66 : 1.065082

H66 -C63 -C58 -S67 : 0.807677

S67 -C58 -C59 -C72 : -7.208425

S67 -C68 -C69 -C72 : -31.035529

S67 -C68 -C69 -H81 : 91.796340

S67 -C68 -C69 -H82 :-153.523177

C68 -C69 -C72 -C73 : 96.030655

C68 -C69 -C72 -C74 :-147.833706

C69 -C72 -C73 -H75 : -60.686565

C69 -C72 -C73 -H76 : 59.434965

C69 -C72 -C73 -H77 : 178.736959

C69 -C72 -C74 -H78 :-169.599732

C69 -C72 -C74 -H79 : -50.917266

C69 -C72 -C74 -H80 : 68.380575

H70 -C68 -C69 -C72 :-151.180501

H70 -C68 -C69 -H81 : -28.348632

H70 -C68 -C69 -H82 : 86.331851

H71 -C68 -C69 -C72 : 89.064845

H71 -C68 -C69 -H81 :-148.103286

H71 -C68 -C69 -H82 : -33.422803

C73 -C72 -C69 -H81 : -27.880419

C73 -C72 -C69 -H82 :-142.511112

C73 -C72 -C74 -H78 : -52.299681

C73 -C72 -C74 -H79 : 66.382785

C73 -C72 -C74 -H80 :-174.319375

C74 -C72 -C69 -H81 : 88.255220

C74 -C72 -C69 -H82 : -26.375473

C74 -C72 -C73 -H75 :-176.411616

C74 -C72 -C73 -H76 : -56.290085

C74 -C72 -C73 -H77 : 63.011908

C83 -C86 -C87 -H89 : 175.923144

C83 -C86 -C87 -H90 : -64.680218

C83 -C86 -C87 -H91 : 56.239674

C83 -C86 -C88 -H92 : 66.926518

C83 -C86 -C88 -H93 :-171.658656

C83 -C86 -C88 -H94 : -52.656893

H84 -C1 -C83 -C86 : -58.018789

H84 -C1 -C83 -H95 : 62.959185

H84 -C1 -C83 -H96 : 178.831115

H85 -C1 -C83 -C86 :-178.078730

H85 -C1 -C83 -H95 : -57.100756

H85 -C1 -C83 -H96 : 58.771174

C87 -C86 -C83 -H95 : -56.008179

C87 -C86 -C83 -H96 :-171.837667

C87 -C86 -C88 -H92 :-174.630608

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C87 -C86 -C88 -H94 : 65.785980

C88 -C86 -C83 -H95 : 61.429870

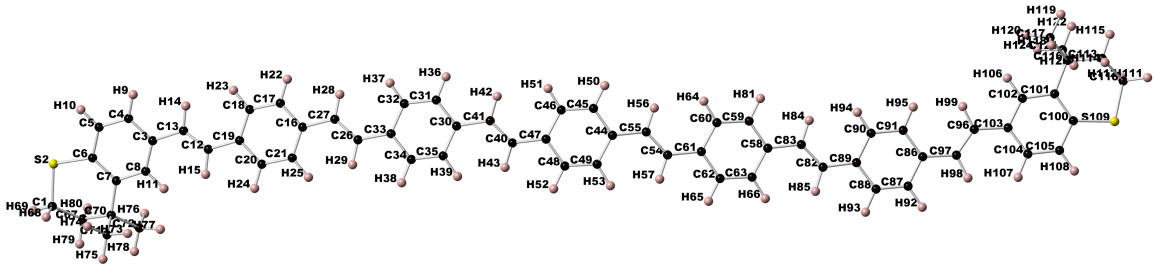
C88 -C86 -C83 -H96 : -54.399618

C88 -C86 -C87 -H89 : 59.986551

C88 -C86 -C87 -H90 : 179.383189

C88 -C86 -C87 -H91 : -59.696919

PPV5



Final geometry:

		angstroms	
atom	x	y	z
C1	-0.8228682975	-2.1534157401	1.3720545370
S2	-1.8090592213	-1.9925479834	-0.1584315924
C3	0.9859230210	-3.2186652657	-3.6107066183
C4	-0.2940248788	-2.6707657077	-3.8054971413
C5	-1.0824531648	-2.3122876158	-2.7260180642
C6	-0.6396747609	-2.4963894231	-1.4063935059
C7	0.6312393404	-3.0681630824	-1.1672011581
C8	1.4084979114	-3.3985972057	-2.2834340028
H9	-0.6656410410	-2.5174552357	-4.8154573410
H10	-2.0625485147	-1.8759729689	-2.8985677822
H11	2.3860638694	-3.8320499632	-2.1117777595
C12	3.0677406988	-4.0254391290	-4.7679625093
C13	1.7928851553	-3.5830149818	-4.7768066173
H14	1.2802295216	-3.4752668858	-5.7317420426
H15	3.5769514209	-4.1035888405	-3.8087861224
C16	5.6169915369	-5.3765978543	-7.9803662542
C17	4.3013159013	-4.9421944961	-8.2471312468
C18	3.4588214031	-4.4856153982	-7.2421504898
C19	3.8894495078	-4.4428078427	-5.9010369544

C20	5.2099177854	-4.8615522932	-5.6384401784
C21	6.0486998761	-5.3157957829	-6.6403791807
H22	3.9362371515	-4.9760243589	-9.2709850331
H23	2.4516912339	-4.1724191121	-7.5003924034
H24	5.5718803393	-4.8377698672	-4.6134530123
H25	7.0472692772	-5.6465385898	-6.3735680202
C26	7.7250463999	-6.3228989220	-8.9440784258
C27	6.4473279621	-5.9008401623	-9.0635860596
H28	5.9528136678	-5.9671064964	-10.0315607526
H29	8.2040066542	-6.2362845994	-7.9707988231
C30	10.3406313668	-8.2806674458	-11.7651499110
C31	9.0685289794	-7.8209854680	-12.1698770247
C32	8.2092017424	-7.1673209817	-11.2970135939
C33	8.5785358652	-6.9374821244	-9.9561777147
C34	9.8597562832	-7.3741795007	-9.5600261877
C35	10.7142930205	-8.0284696885	-10.4305201662
H36	8.7511553609	-7.9955494293	-13.1952165938
H37	7.2374867533	-6.8440754346	-11.6577528971
H38	10.1755395807	-7.2051733411	-8.5334695191
H39	11.6787206218	-8.3647554827	-10.0627703468
C40	12.4133153887	-9.5113376068	-12.4666779607
C41	11.1809567060	-9.0138339915	-12.7098373799
H42	10.7287543251	-9.1731040041	-13.6870904892
H43	12.8553494888	-9.3397164992	-11.4873401243
C44	15.0098013228	-11.9118002323	-14.9497930828
C45	13.7895959512	-11.4132115412	-15.4562516998
C46	12.9381656336	-10.6317014056	-14.6889795095
C47	13.2613753521	-10.2971766067	-13.3587213379
C48	14.4893647433	-10.7788115257	-12.8597153375
C49	15.3378584868	-11.5615410664	-13.6254357466

H50	13.5076700733	-11.6586026193	-16.4772860931
H51	12.0085385240	-10.2820864559	-15.1277875194
H52	14.7742453828	-10.5297635841	-11.8402977768
H53	16.2669907342	-11.9094780560	-13.1857956828
C54	17.0049038518	-13.3644380382	-15.4587885040
C55	15.8456264949	-12.7581828106	-15.7983142589
H56	15.4514679588	-12.9086886376	-16.8021022875
H57	17.3953732081	-13.2214071993	-14.4525024887
C58	19.5111216333	-15.9698112103	-17.8254484967
C59	18.3441784586	-15.3950868922	-18.3717236074
C60	17.5261072437	-14.5522648144	-17.6376435562
C61	17.8291669371	-14.2299909803	-16.3007032542
C62	19.0002582789	-14.7976179862	-15.7549068119
C63	19.8194433721	-15.6419577201	-16.4896048251
H64	16.6379348405	-14.1447215475	-18.1089805241
H65	19.2652297514	-14.5642952986	-14.7264007629
H66	20.7056715373	-16.0557763598	-16.0180492049
C67	0.0992546031	-3.3645898140	1.3202894020
H68	-0.2685527238	-1.2277842882	1.5493530838
H69	-1.5574344106	-2.2578627845	2.1751954221
C70	1.2103336869	-3.2971596418	0.2439734198
C71	2.1952429316	-2.1475602091	0.5687697496
C72	1.9733143004	-4.6391961233	0.3257970439
H73	3.0229431045	-2.1365425499	-0.1468210581
H74	1.7126848228	-1.1672295980	0.5176017667
H75	2.6168211616	-2.2701481604	1.5737884481
H76	1.3397904220	-5.4753846331	0.0136605926
H77	2.8744654473	-4.6482645758	-0.2924987060
H78	2.2926968029	-4.8210417885	1.3577994543
H79	0.5825832783	-3.4747678956	2.2996767718

H80	-0.5057834528	-4.2653996794	1.1626905319
H81	18.0793777934	-15.6273858621	-19.4003899327
C82	21.4447924204	-17.5110188558	-18.3260013500
C83	20.3088975090	-16.8618634258	-18.6603215959
H84	19.9083602873	-17.0009358004	-19.6629909013
H85	21.8573803310	-17.3751248984	-17.3276083489
C86	23.8118961556	-20.1680562267	-20.7751414055
C87	24.1847454901	-19.8214955254	-19.4629600150
C88	23.4107632141	-18.9672497414	-18.6892450973
C89	22.2182822402	-18.4060157612	-19.1823114455
C90	21.8456155338	-18.7536410790	-20.4998580987
C91	22.6166860085	-19.6039951085	-21.2727956918
H92	25.0993084011	-20.2368619638	-19.0469147597
H93	23.7306590039	-18.7244431236	-17.6786495615
H94	20.9335188299	-18.3483574353	-20.9272319390
H95	22.2877437525	-19.8349403934	-22.2811517604
C96	24.4406254028	-21.5579663946	-22.7791381214
C97	24.6663195791	-21.0758544914	-21.5376650278
H99	25.5723231538	-21.3797459853	-21.0171219119
H100	23.5264007155	-21.2629732966	-23.2917842522
C100	26.8293259834	-24.2288502195	-25.1425621316
C101	25.5991608935	-23.7534476121	-25.6405958817
C102	24.8677359319	-22.8909772209	-24.8118894296
C103	25.2957813393	-22.4635400935	-23.5461417304
C104	26.5403621197	-22.9424417878	-23.0944546152
C105	27.2801881591	-23.8079961930	-23.8770700342
H108	23.9072193645	-22.5251443839	-25.1614283398
H109	26.9306490826	-22.6424110219	-22.1270522215
H110	28.2324757038	-24.1798644416	-23.5084931512
S110	27.9424738943	-25.3324685941	-25.9914687496

C111	26.9229257126	-25.8642277886	-27.4118290490
H112	27.6371318462	-26.2207947376	-28.1589254724
H113	26.3005710176	-26.7135603124	-27.1170170523
C114	26.0894996511	-24.7142050368	-27.9630689214
H116	26.7611989173	-23.8976067710	-28.2534305599
H117	25.5892296102	-25.0543309452	-28.8789717157
C117	25.0051703821	-24.1700033337	-27.0010667840
C120	24.3545935056	-22.9647771267	-27.7180548154
H121	25.0660754501	-22.1408494723	-27.8322809705
H122	24.0182222748	-23.2645406885	-28.7165771606
H123	23.4787436786	-22.5838800713	-27.1868201352
C123	23.9211256285	-25.2483725043	-26.7583695284
H124	23.4837014118	-25.5794175601	-27.7079869777
H125	24.3246057576	-26.1250635191	-26.2433673560
H126	23.1149266848	-24.8511118780	-26.1342525335

Total energy (hartrees): -3270.21268240747

HOMO energy (hartrees): -0.17622

LUMO energy (hartrees): -0.07934

Bond lengths (angstroms):

C1	-S2	: 1.827796	C1	-C67	: 1.523133
C1	-H68	: 1.093387	C1	-H69	: 1.093404
S2	-C6	: 1.782898	C3	-C4	: 1.405846
C3	-C8	: 1.404492	C3	-C13	: 1.464147
C4	-C5	: 1.383980	C4	-H9	: 1.087025

C5 -C6 : 1.404050 C5 -H10 : 1.086614

C6 -C7 : 1.413988 C7 -C8 : 1.399748

C7 -C70 : 1.542467 C8 -H11 : 1.083043

C12 -C13 : 1.349472 C12 -H15 : 1.088771

C12 -C19 : 1.460568 C13 -H14 : 1.089186

C16 -C17 : 1.410983 C16 -C21 : 1.409125

C16 -C27 : 1.462072 C17 -C18 : 1.388614

C17 -H22 : 1.087522 C18 -C19 : 1.409205

C18 -H23 : 1.085860 C19 -C20 : 1.409943

C20 -C21 : 1.383392 C20 -H24 : 1.087282

C21 -H25 : 1.085228 C26 -C27 : 1.350918

C26 -H29 : 1.088199 C26 -C33 : 1.459624

C27 -H28 : 1.088995 C30 -C31 : 1.411863

C30 -C35 : 1.408710 C30 -C41 : 1.461545

C31 -C32 : 1.388384 C31 -H36 : 1.087437

C32 -C33 : 1.409636 C32 -H37 : 1.085749

C33 -C34 : 1.410378 C34 -C35 : 1.384228

C34 -H38 : 1.087245 C35 -H39 : 1.085564

C40 -C41 : 1.351053 C40 -H43 : 1.088095

C40 -C47 : 1.460305 C41 -H42 : 1.088521

C44 -C45 : 1.412088 C44 -C49 : 1.408625

C44 -C55 : 1.461149 C45 -C46 : 1.387227

C45 -H50 : 1.087295 C46 -C47 : 1.409240

C46 -H51 : 1.085813 C47 -C48 : 1.410297

C48 -C49 : 1.385256 C48 -H52 : 1.087379

C49 -H53 : 1.085187 C54 -C55 : 1.351572

C54 -H57 : 1.088823 C54 -C61 : 1.461989

C55 -H56 : 1.088854 C58 -C59 : 1.410844

C58 -C63 : 1.409620 C58 -C83 : 1.459184

C59 -C60 : 1.385086 C59 -H81 : 1.087307

C60 -C61 : 1.408231 C60 -H64 : 1.084943

C61 -C62 : 1.411223 C62 -C63 : 1.386995

C62 -H65 : 1.087416 C63 -H66 : 1.085823

C67 -C70 : 1.548386 C67 -H79 : 1.097700

C67 -H80 : 1.096525 C70 -C71 : 1.548263

C70 -C72 : 1.545929 C71 -H73 : 1.094203

C71 -H74 : 1.093859 C71 -H75 : 1.096731

C72 -H76 : 1.094529 C72 -H77 : 1.092907

C72 -H78 : 1.095492 C82 -C83 : 1.350344

C82 -H85 : 1.088800 C82 -C89 : 1.460333

C83 -H84 : 1.088631 C86 -C87 : 1.407459

C86 -C91 : 1.412215 C86 -C97 : 1.461362

C87 -C88 : 1.388315 C87 -H92 : 1.087220

C88 -C89 : 1.407163 C88 -H93 : 1.087470

C89 -C90 : 1.412676 C90 -C91 : 1.383866

C90 -H94 : 1.085736 C91 -H95 : 1.085505

C96 -C97 : 1.350787 C96 -H100 : 1.088868

C96 -C103 : 1.462754 C97 -H99 : 1.088190

C100 -C101 : 1.409735 C100 -C105 : 1.407787

C100 -S110 : 1.782614 C101 -C102 : 1.401996

C101 -C117 : 1.541825 C102 -C103 : 1.402869

C102 -H108 : 1.085635 C103 -C104 : 1.407959

C104 -C105 : 1.381671 C104 -H109 : 1.085454

C105 -H110 : 1.086732 S110 -C111 : 1.827476

C111 -H112 : 1.093336 C111 -H113 : 1.093437

C111 -C114 : 1.523488 C114 -H116 : 1.096505

C114 -H117 : 1.097649 C114 -C117 : 1.548345

C117 -C120 : 1.545928 C117 -C123 : 1.548204

C120 -H121 : 1.094583 C120 -H122 : 1.095468

C120 -H123 : 1.092889 C123 -H124 : 1.096679

C123 -H125 : 1.093897 C123 -H126 : 1.094210

Bond angles:

C67 -C1 -S2 : 111.603373 H68 -C1 -S2 : 109.560864

H68 -C1 -C67 : 111.824672 H69 -C1 -S2 : 105.128284

H69 -C1 -C67 : 110.838155 H69 -C1 -H68 : 107.598897

C6 -S2 -C1 : 101.966982 C8 -C3 -C4 : 117.051939

C13 -C3 -C4 : 119.236914 C13 -C3 -C8 : 123.706687

C5 -C4 -C3 : 120.766471 H9 -C4 -C3 : 119.666513

H9 -C4 -C5 : 119.564248 C6 -C5 -C4 : 121.296351

H10 -C5 -C4 : 119.602829 H10 -C5 -C6 : 119.100412

C5 -C6 -S2 : 114.455054 C7 -C6 -S2 : 125.830602

C7 -C6 -C5 : 119.700121 C8 -C7 -C6 : 117.365078

C70 -C7 -C6 : 123.520958 C70 -C7 -C8 : 119.081654

C7 -C8 -C3 : 123.799968 H11 -C8 -C3 : 118.204809

H11 -C8 -C7 : 117.988357 H15 -C12 -C13 : 118.108262

C19 -C12 -C13 : 128.322644 C19 -C12 -H15 : 113.565926

C12 -C13 -C3 : 126.658095 H14 -C13 -C3 : 114.471376

H14 -C13 -C12 : 118.870466 C21 -C16 -C17 : 116.883300

C27 -C16 -C17 : 119.991724 C27 -C16 -C21 : 123.093693

C18 -C17 -C16 : 122.014459 H22 -C17 -C16 : 118.779511

H22 -C17 -C18 : 119.203585 C19 -C18 -C17 : 120.886961

H23 -C18 -C17 : 119.041586 H23 -C18 -C19 : 120.065890

C18 -C19 -C12 : 125.103344 C20 -C19 -C12 : 117.857601

C20 -C19 -C18 : 117.027320 C21 -C20 -C19 : 122.037452

H24 -C20 -C19 : 118.741526 H24 -C20 -C21 : 119.215806

C20 -C21 -C16 : 121.140471 H25 -C21 -C16 : 120.168578

H25 -C21 -C20 : 118.679715 H29 -C26 -C27 : 118.069722

C33 -C26 -C27 : 128.554276 C33 -C26 -H29 : 113.348331

C26 -C27 -C16 : 125.706036 H28 -C27 -C16 : 114.990770

H28 -C27 -C26 : 119.282597 C35 -C30 -C31 : 116.890841

C41 -C30 -C31 : 119.741028 C41 -C30 -C35 : 123.344439

C32 -C31 -C30 : 122.055389 H36 -C31 -C30 : 118.750115

H36 -C31 -C32 : 119.191248 C33 -C32 -C31 : 120.837411

H37 -C32 -C31 : 119.026918 H37 -C32 -C33 : 120.131057

C32 -C33 -C26 : 125.099857 C34 -C33 -C26 : 117.826331

C34 -C33 -C32 : 117.045774 C35 -C34 -C33 : 122.040689

H38 -C34 -C33 : 118.745517 H38 -C34 -C35 : 119.205048

C34 -C35 -C30 : 121.109003 H39 -C35 -C30 : 120.075600

H39 -C35 -C34 : 118.805542 H43 -C40 -C41 : 118.324479

C47 -C40 -C41 : 128.165815 C47 -C40 -H43 : 113.500572

C40 -C41 -C30 : 126.358403 H42 -C41 -C30 : 114.509038

H42 -C41 -C40 : 119.119514 C49 -C44 -C45 : 116.785552

C55 -C44 -C45 : 119.376644 C55 -C44 -C49 : 123.834388

C46 -C45 -C44 : 122.066549 H50 -C45 -C44 : 118.761959

H50 -C45 -C46 : 119.169365 C47 -C46 -C45 : 121.001629

H51 -C46 -C45 : 118.904431 H51 -C46 -C47 : 120.093087

C46 -C47 -C40 : 124.832093 C48 -C47 -C40 : 118.249265

C48 -C47 -C46 : 116.912804 C49 -C48 -C47 : 122.054308

H52 -C48 -C47 : 118.791178 H52 -C48 -C49 : 119.153994

C48 -C49 -C44 : 121.167786 H53 -C49 -C44 : 120.037667

H53 -C49 -C48 : 118.793921 H57 -C54 -C55 : 118.740010

C61 -C54 -C55 : 127.191477 C61 -C54 -H57 : 114.066825

C54 -C55 -C44 : 127.199675 H56 -C55 -C44 : 114.101128

H56 -C55 -C54 : 118.690145 C63 -C58 -C59 : 116.942826

C83 -C58 -C59 : 118.666566 C83 -C58 -C63 : 124.388973

C60 -C59 -C58 : 122.086016 H81 -C59 -C58 : 118.732431

H81 -C59 -C60 : 119.180868 C61 -C60 -C59 : 121.017946

H64 -C60 -C59 : 118.805474 H64 -C60 -C61 : 120.175668

C60 -C61 -C54 : 124.116132 C62 -C61 -C54 : 118.899372

C62 -C61 -C60 : 116.982162 C63 -C62 -C61 : 122.012877

H65 -C62 -C61 : 118.796928 H65 -C62 -C63 : 119.190184

C62 -C63 -C58 : 120.956231 H66 -C63 -C58 : 120.095028

H66 -C63 -C62 : 118.947786 C70 -C67 -C1 : 115.050824

H79 -C67 -C1 : 108.424850 H79 -C67 -C70 : 107.975839

H80 -C67 -C1 : 108.910322 H80 -C67 -C70 : 109.378640

H80 -C67 -H79 : 106.782020 C67 -C70 -C7 : 111.901862

C71 -C70 -C7 : 108.694313 C71 -C70 -C67 : 110.058977

C72 -C70 -C7 : 111.259733 C72 -C70 -C67 : 106.233662

C72 -C70 -C71 : 108.633626 H73 -C71 -C70 : 110.578129

H74 -C71 -C70 : 112.024282 H74 -C71 -H73 : 107.102963

H75 -C71 -C70 : 110.718239 H75 -C71 -H73 : 108.038051

H75 -C71 -H74 : 108.217035 H76 -C72 -C70 : 111.250753

H77 -C72 -C70 : 112.594537 H77 -C72 -H76 : 108.033926

H78 -C72 -C70 : 109.745999 H78 -C72 -H76 : 108.094426

H78 -C72 -H77 : 106.928643 H85 -C82 -C83 : 119.063722

C89 -C82 -C83 : 126.512689 C89 -C82 -H85 : 114.423185

C82 -C83 -C58 : 127.744189 H84 -C83 -C58 : 113.823101

H84 -C83 -C82 : 118.431955 C91 -C86 -C87 : 117.025791

C97 -C86 -C87 : 118.982334 C97 -C86 -C91 : 123.991872

C88 -C87 -C86 : 121.560650 H92 -C87 -C86 : 119.047394

H92 -C87 -C88 : 119.391620 C89 -C88 -C87 : 121.505229

H93 -C88 -C87 : 119.425833 H93 -C88 -C89 : 119.068938

C88 -C89 -C82 : 119.198106 C90 -C89 -C82 : 123.916151

C90 -C89 -C88 : 116.885692 C91 -C90 -C89 : 121.677989

H94 -C90 -C89 : 119.793573 H94 -C90 -C91 : 118.528412

C90 -C91 -C86 : 121.344016 H95 -C91 -C86 : 119.923094

H95 -C91 -C90 : 118.732862 H100 -C96 -C97 : 118.443856

C103 -C96 -C97 : 127.243324 C103 -C96 -H100 : 114.311968

C96 -C97 -C86 : 127.127251 H99 -C97 -C86 : 114.246639

H99 -C97 -C96 : 118.625529 C105 -C100 -C101 : 119.750770

S110 -C100 -C101 : 125.834536 S110 -C100 -C105 : 114.404204

C102 -C101 -C100 : 116.992991 C117 -C101 -C100 : 123.834616

C117 -C101 -C102 : 119.129135 C103 -C102 -C101 : 124.164326

H108 -C102 -C101 : 118.591642 H108 -C102 -C103 : 117.244009

C102 -C103 -C96 : 118.904534 C104 -C103 -C96 : 123.996271

C104 -C103 -C102 : 117.099155 C105 -C104 -C103 : 120.310768

H109 -C104 -C103 : 120.646464 H109 -C104 -C105 : 119.042132

C104 -C105 -C100 : 121.665801 H110 -C105 -C100 : 118.896220

H110 -C105 -C104 : 119.437261 C111 -S110 -C100 : 101.647689

H112 -C111 -S110 : 105.161979 H113 -C111 -S110 : 109.512124

H113 -C111 -H112 : 107.620975 C114 -C111 -S110 : 111.516629

C114 -C111 -H112 : 110.872601 C114 -C111 -H113 : 111.871816

H116 -C114 -C111 : 108.836419 H117 -C114 -C111 : 108.501921

H117 -C114 -H116 : 106.798113 C117 -C114 -C111 : 115.063005

C117 -C114 -H116 : 109.376566 C117 -C114 -H117 : 107.948727

C114 -C117 -C101 : 111.924822 C120 -C117 -C101 : 111.145447

C120 -C117 -C114 : 106.294250 C123 -C117 -C101 : 108.639405

C123 -C117 -C114 : 110.056257 C123 -C117 -C120 : 108.727213

H121 -C120 -C117 : 111.204464 H122 -C120 -C117 : 109.793649

H122 -C120 -H121 : 108.086033 H123 -C120 -C117 : 112.552570

H123 -C120 -H121 : 108.016967 H123 -C120 -H122 : 106.999169

H124 -C123 -C117 : 110.719772 H125 -C123 -C117 : 111.947872

H125 -C123 -H124 : 108.231633 H126 -C123 -C117 : 110.635879

H126 -C123 -H124 : 108.035816 H126 -C123 -H125 : 107.109322

Torsional angles:

C1 -S2 -C6 -C5 :-172.480496

C1 -S2 -C6 -C7 : 8.904530

C1 -C67 -C70 -C7 : -55.821384

C1 -C67 -C70 -C71 : 65.146552

C1 -C67 -C70 -C72 :-177.428358

S2 -C1 -C67 -C70 : 65.101758

S2 -C1 -C67 -H79 :-173.916049

S2 -C1 -C67 -H80 : -58.078563

S2 -C6 -C5 -C4 :-179.202866

S2 -C6 -C5 -H10 : 1.030589

S2 -C6 -C7 -C8 :-179.995419

S2 -C6 -C7 -C70 : -2.085893

C3 -C4 -C5 -C6 : -0.722216

C3 -C4 -C5 -H10 : 179.043175

C3 -C8 -C7 -C6 : -1.308835

C3 -C8 -C7 -C70 :-179.314667

C3 -C13 -C12 -H15 : -1.676205

C3 -C13 -C12 -C19 : 177.630466

C4 -C3 -C8 -C7 : 0.145710

C4 -C3 -C8 -H11 : 179.171689

C4 -C3 -C13 -C12 : 174.839515

C4 -C3 -C13 -H14 : -5.253751

C4 -C5 -C6 -C7 : -0.495588

C5 -C4 -C3 -C8 : 0.889013

C5 -C4 -C3 -C13 :-179.850653

C5 -C6 -C7 -C8 : 1.456040

C5 -C6 -C7 -C70 : 179.365567

C6 -S2 -C1 -C67 : -37.465073

C6 -S2 -C1 -H68 : 86.940638

C6 -S2 -C1 -H69 :-157.690201

C6 -C5 -C4 -H9 : 179.884994

C6 -C7 -C8 -H11 : 179.663223

C6 -C7 -C70 -C67 : 22.279883

C6 -C7 -C70 -C71 : -99.475544

C6 -C7 -C70 -C72 : 140.947362

C7 -C6 -C5 -H10 : 179.737868

C7 -C8 -C3 -C13 :-179.078418

C7 -C70 -C67 -H79 :-177.048264

C7 -C70 -C67 -H80 : 67.109119

C7 -C70 -C71 -H73 : -61.107342

C7 -C70 -C71 -H74 : 58.281525

C7 -C70 -C71 -H75 : 179.181739

C7 -C70 -C72 -H76 : -55.159486

C7 -C70 -C72 -H77 : 66.281364

C7 -C70 -C72 -H78 :-174.740848

C8 -C3 -C4 -H9 :-179.718814

C8 -C3 -C13 -C12 : -5.952351

C8 -C3 -C13 -H14 : 173.954383

C8 -C7 -C70 -C67 :-159.844496

C8 -C7 -C70 -C71 : 78.400077

C8 -C7 -C70 -C72 : -41.177017

H9 -C4 -C3 -C13 : -0.458480

H9 -C4 -C5 -H10 : -0.349615

H11 -C8 -C3 -C13 : -0.052439

H11 -C8 -C7 -C70 : 1.657392

C12 -C19 -C18 -C17 :-177.736766

C12 -C19 -C18 -H23 : 1.397041

C12 -C19 -C20 -C21 : 177.844464

C12 -C19 -C20 -H24 : -1.317765

C13 -C12 -C19 -C18 : -1.722206

C13 -C12 -C19 -C20 : 179.564712

H14 -C13 -C12 -H15 : 178.420732

H14 -C13 -C12 -C19 : -2.272598

H15 -C12 -C19 -C18 : 177.610593

H15 -C12 -C19 -C20 : -1.102489

C16 -C17 -C18 -C19 : -0.231729

C16 -C17 -C18 -H23 :-179.374273

C16 -C21 -C20 -C19 : 0.190654

C16 -C21 -C20 -H24 : 179.349033

C16 -C27 -C26 -H29 : -2.478728

C16 -C27 -C26 -C33 : 175.467260

C17 -C16 -C21 -C20 : 0.583745

C17 -C16 -C21 -H25 : 179.348208

C17 -C16 -C27 -C26 : 178.666559

C17 -C16 -C27 -H28 : -3.005850

C17 -C18 -C19 -C20 : 0.985966

C18 -C17 -C16 -C21 : -0.564699

C18 -C17 -C16 -C27 : 177.463642

C18 -C19 -C20 -C21 : -0.973625

C18 -C19 -C20 -H24 : 179.864146

C19 -C18 -C17 -H22 : 179.192244

C19 -C20 -C21 -H25 :-178.591789

C20 -C19 -C18 -H23 :-179.880227

C20 -C21 -C16 -C27 :-177.377922

C21 -C16 -C17 -H22 :-179.991029

C21 -C16 -C27 -C26 : -3.432596

C21 -C16 -C27 -H28 : 174.894996

H22 -C17 -C16 -C27 : -1.962689

H22 -C17 -C18 -H23 : 0.049700

H24 -C20 -C21 -H25 : 0.566590

H25 -C21 -C16 -C27 : 1.386541

C26 -C33 -C32 -C31 :-176.720561

C26 -C33 -C32 -H37 : 2.490482

C26 -C33 -C34 -C35 : 176.701310

C26 -C33 -C34 -H38 : -2.213749

C27 -C26 -C33 -C32 : 2.073725

C27 -C26 -C33 -C34 :-175.937570

H28 -C27 -C26 -H29 : 179.259196

H28 -C27 -C26 -C33 : -2.794816

H29 -C26 -C33 -C32 :-179.900304

H29 -C26 -C33 -C34 : 2.088400

C30 -C31 -C32 -C33 : -0.120975

C30 -C31 -C32 -H37 :-179.340603

C30 -C35 -C34 -C33 : 0.436620

C30 -C35 -C34 -H38 : 179.346850

C30 -C41 -C40 -H43 : -1.730384

C30 -C41 -C40 -C47 : 177.091986

C31 -C30 -C35 -C34 : 0.773625

C31 -C30 -C35 -H39 : 179.617947

C31 -C30 -C41 -C40 : 179.973246

C31 -C30 -C41 -H42 : -1.361737

C31 -C32 -C33 -C34 : 1.304756

C32 -C31 -C30 -C35 : -0.931897

C32 -C31 -C30 -C41 : 177.356794

C32 -C33 -C34 -C35 : -1.471910

C32 -C33 -C34 -H38 : 179.613030

C33 -C32 -C31 -H36 : 179.215038

C33 -C34 -C35 -H39 :-178.422073

C34 -C33 -C32 -H37 :-179.484200

C34 -C35 -C30 -C41 :-177.447658

C35 -C30 -C31 -H36 : 179.729266

C35 -C30 -C41 -C40 : -1.853820

C35 -C30 -C41 -H42 : 176.811197

H36 -C31 -C30 -C41 : -1.982043

H36 -C31 -C32 -H37 : -0.004590

H38 -C34 -C35 -H39 : 0.488156

H39 -C35 -C30 -C41 : 1.396665

C40 -C47 -C46 -C45 :-178.332760

C40 -C47 -C46 -H51 : 1.327448

C40 -C47 -C48 -C49 : 178.245151

C40 -C47 -C48 -H52 : -1.490234

C41 -C40 -C47 -C46 : 2.717911

C41 -C40 -C47 -C48 :-176.373761

H42 -C41 -C40 -H43 : 179.660065

H42 -C41 -C40 -C47 : -1.517566

H43 -C40 -C47 -C46 :-178.412480

H43 -C40 -C47 -C48 : 2.495848

C44 -C45 -C46 -C47 : 0.148315

C44 -C45 -C46 -H51 :-179.515859

C44 -C49 -C48 -C47 : 0.142489

C44 -C49 -C48 -H52 : 179.876944

C44 -C55 -C54 -H57 : -0.645095

C44 -C55 -C54 -C61 : 178.852073

C45 -C44 -C49 -C48 : 0.774690

C45 -C44 -C49 -H53 :-179.516550

C45 -C44 -C55 -C54 :-176.857531

C45 -C44 -C55 -H56 : 2.023763

C45 -C46 -C47 -C48 : 0.769914

C46 -C45 -C44 -C49 : -0.922330

C46 -C45 -C44 -C55 : 178.431152

C46 -C47 -C48 -C49 : -0.918715

C46 -C47 -C48 -H52 : 179.345900

C47 -C46 -C45 -H50 : 179.611036

C47 -C48 -C49 -H53 :-179.569814

C48 -C47 -C46 -H51 :-179.569878

C48 -C49 -C44 -C55 :-178.547063

C49 -C44 -C45 -H50 : 179.612839

C49 -C44 -C55 -C54 : 2.447654

C49 -C44 -C55 -H56 :-178.671052

H50 -C45 -C44 -C55 : -1.033680

H50 -C45 -C46 -H51 : -0.053138

H52 -C48 -C49 -H53 : 0.164641

H53 -C49 -C44 -C55 : 1.161697

C54 -C61 -C60 -C59 :-179.106022

C54 -C61 -C60 -H64 : 0.542470

C54 -C61 -C62 -C63 : 179.113074

C54 -C61 -C62 -H65 : -0.848635

C55 -C54 -C61 -C60 : 0.778546

C55 -C54 -C61 -C62 :-178.648044

H56 -C55 -C54 -H57 :-179.480986

H56 -C55 -C54 -C61 : 0.016181

H57 -C54 -C61 -C60 :-179.704318

H57 -C54 -C61 -C62 : 0.869093

C58 -C59 -C60 -C61 : 0.032995

C58 -C59 -C60 -H64 :-179.620220

C58 -C63 -C62 -C61 : 0.011054

C58 -C63 -C62 -H65 : 179.972616

C58 -C83 -C82 -H85 : -0.663430

C58 -C83 -C82 -C89 : 179.581323

C59 -C58 -C63 -C62 : 0.351047

C59 -C58 -C63 -H66 : 179.991814

C59 -C58 -C83 -C82 :-179.657743

C59 -C58 -C83 -H84 : 0.017758

C59 -C60 -C61 -C62 : 0.330656

C60 -C59 -C58 -C63 : -0.375350

C60 -C59 -C58 -C83 : 179.180009

C60 -C61 -C62 -C63 : -0.354212

C60 -C61 -C62 -H65 : 179.684079

C61 -C60 -C59 -H81 : 179.728024

C61 -C62 -C63 -H66 :-179.633764

C62 -C61 -C60 -H64 : 179.979148

C62 -C63 -C58 -C83 :-179.176184

C63 -C58 -C59 -H81 : 179.928303

C63 -C58 -C83 -C82 : -0.138073

C63 -C58 -C83 -H84 : 179.537427

H64 -C60 -C59 -H81 : 0.074810

H65 -C62 -C63 -H66 : 0.327799

H66 -C63 -C58 -C83 : 0.464584

C67 -C70 -C71 -H73 : 176.019898

C67 -C70 -C71 -H74 : -64.591235

C67 -C70 -C71 -H75 : 56.308979

C67 -C70 -C72 -H76 : 66.856945

C67 -C70 -C72 -H77 :-171.702205

C67 -C70 -C72 -H78 : -52.724417

H68 -C1 -C67 -C70 : -58.024882

H68 -C1 -C67 -H79 : 62.957311

H68 -C1 -C67 -H80 : 178.794797

H69 -C1 -C67 -C70 :-178.085803

H69 -C1 -C67 -H79 : -57.103610

H69 -C1 -C67 -H80 : 58.733876

C71 -C70 -C67 -H79 : -56.080329

C71 -C70 -C67 -H80 :-171.922946

C71 -C70 -C72 -H76 :-174.772672

C71 -C70 -C72 -H77 : -53.331822

C71 -C70 -C72 -H78 : 65.645966

C72 -C70 -C67 -H79 : 61.344762

C72 -C70 -C67 -H80 : -54.497855

C72 -C70 -C71 -H73 : 60.095042

C72 -C70 -C71 -H74 : 179.483909

C72 -C70 -C71 -H75 : -59.615877

H81 -C59 -C58 -C83 : -0.516338

C82 -C89 -C88 -C87 :-179.856652

C82 -C89 -C88 -H93 : 0.148535

C82 -C89 -C90 -C91 : 179.790151

C82 -C89 -C90 -H94 : -0.149749

C83 -C82 -C89 -C88 : 177.793217

C83 -C82 -C89 -C90 : -2.122043

H84 -C83 -C82 -H85 : 179.674138

H84 -C83 -C82 -C89 : -0.081109

H85 -C82 -C89 -C88 : -1.971825

H85 -C82 -C89 -C90 : 178.112916

C86 -C87 -C88 -C89 : -0.122340

C86 -C87 -C88 -H93 : 179.872455

C86 -C91 -C90 -C89 : 0.247584

C86 -C91 -C90 -H94 :-179.811780

C86 -C97 -C96 -H100 : -0.546134

C86 -C97 -C96 -C103 : 179.810479

C87 -C86 -C91 -C90 : -0.288995

C87 -C86 -C91 -H95 : 179.649313

C87 -C86 -C97 -C96 : 177.072060

C87 -C86 -C97 -H99 : -2.644631

C87 -C88 -C89 -C90 : 0.064504

C88 -C87 -C86 -C91 : 0.227497

C88 -C87 -C86 -C97 :-179.789916

C88 -C89 -C90 -C91 : -0.126911

C88 -C89 -C90 -H94 : 179.933189

C89 -C88 -C87 -H92 :-179.909633

C89 -C90 -C91 -H95 :-179.691439

C90 -C89 -C88 -H93 :-179.930309

C90 -C91 -C86 -C97 : 179.729378

C91 -C86 -C87 -H92 :-179.984496

C91 -C86 -C97 -C96 : -2.946650

C91 -C86 -C97 -H99 : 177.336659

H92 -C87 -C86 -C97 : -0.001910

H92 -C87 -C88 -H93 : 0.085162

H94 -C90 -C91 -H95 : 0.249197

H95 -C91 -C86 -C97 : -0.332314

C96 -C103 -C102 -C101 : 179.834506

C96 -C103 -C102 -H108 : -0.222202

C96 -C103 -C104 -C105 : 179.305830

C96 -C103 -C104 -H109 : -0.401246

C97 -C96 -C103 -C102 : 177.917773

C97 -C96 -C103 -C104 : -2.157510

H99 -C97 -C96 -H100 : 179.159578

H99 -C97 -C96 -C103 : -0.483810

H100 -C96 -C103 -C102 : -1.738149

H100 -C96 -C103 -C104 : 178.186567

C100 -C101 -C102 -C103 : 1.153281

C100 -C101 -C102 -H108 :-178.789299

C100 -C101 -C117 -C114 : -21.278043

C100 -C101 -C117 -C120 :-139.960723

C100 -C101 -C117 -C123 : 100.451351

C100 -C105 -C104 -C103 : 0.543131

C100 -C105 -C104 -H109 :-179.745125

C100 -S110 -C111 -H112 : 158.981524

C100 -S110 -C111 -H113 : -85.628959

C100 -S110 -C111 -C114 : 38.741320

C101 -C100 -C105 -C104 : 0.564806

C101 -C100 -C105 -H110 :-179.745501

C101 -C100 -S110 -C111 : -10.192601

C101 -C102 -C103 -C104 : -0.095381

C101 -C117 -C114 -C111 : 54.811614

C101 -C117 -C114 -H116 : -68.028602

C101 -C117 -C114 -H117 : 176.125656

C101 -C117 -C120 -H121 : 55.526037

C101 -C117 -C120 -H122 : 175.098609

C101 -C117 -C120 -H123 : -65.829597

C101 -C117 -C123 -H124 :-179.272836

C101 -C117 -C123 -H125 : -58.405054

C101 -C117 -C123 -H126 : 60.980491

C102 -C101 -C100 -C105 : -1.357881

C102 -C101 -C100 -S110 : 179.889215

C102 -C101 -C117 -C114 : 161.189180

C102 -C101 -C117 -C120 : 42.506500

C102 -C101 -C117 -C123 : -77.081426

C102 -C103 -C104 -C105 : -0.768203

C102 -C103 -C104 -H109 : 179.524722

C103 -C102 -C101 -C117 : 178.853428

C103 -C104 -C105 -H110 :-179.144922

C104 -C103 -C102 -H108 : 179.847910

C104 -C105 -C100 -S110 : 179.454594

C105 -C100 -C101 -C117 :-178.939245

C105 -C100 -S110 -C111 : 170.996338

H108 -C102 -C101 -C117 : -1.089152

H109 -C104 -C105 -H110 : 0.566822

H110 -C105 -C100 -S110 : -0.855713

S110 -C100 -C101 -C117 : 2.307851

S110 -C111 -C114 -H116 : 57.655798

S110 -C111 -C114 -H117 : 173.514444

S110 -C111 -C114 -C117 : -65.472717

C111 -C114 -C117 -C120 : 176.331180

C111 -C114 -C117 -C123 : -66.100167

H112 -C111 -C114 -H116 : -59.166103

H112 -C111 -C114 -H117 : 56.692543

H112 -C111 -C114 -C117 : 177.705382

H113 -C111 -C114 -H116 :-179.310358

H113 -C111 -C114 -H117 : -63.451712

H113 -C111 -C114 -C117 : 57.561127

C114 -C117 -C120 -H121 : -66.490192

C114 -C117 -C120 -H122 : 53.082380

C114 -C117 -C120 -H123 : 172.154173

C114 -C117 -C123 -H124 : -56.409169

C114 -C117 -C123 -H125 : 64.458613

C114 -C117 -C123 -H126 :-176.155843

H116 -C114 -C117 -C120 : 53.490964

H116 -C114 -C117 -C123 : 171.059618

H117 -C114 -C117 -C120 : -62.354778

H117 -C114 -C117 -C123 : 55.213876

C120 -C117 -C123 -H124 : 59.640330

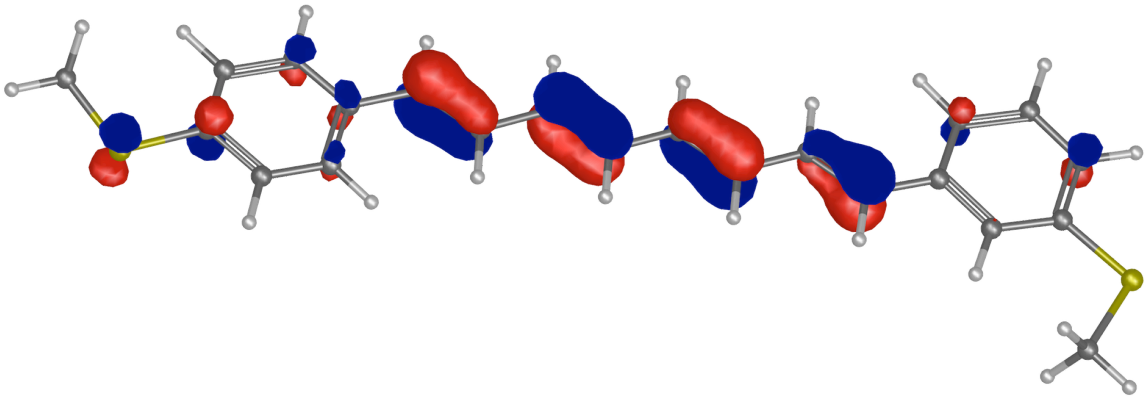
C120 -C117 -C123 -H125 :-179.491887

C120 -C117 -C123 -H126 : -60.106343

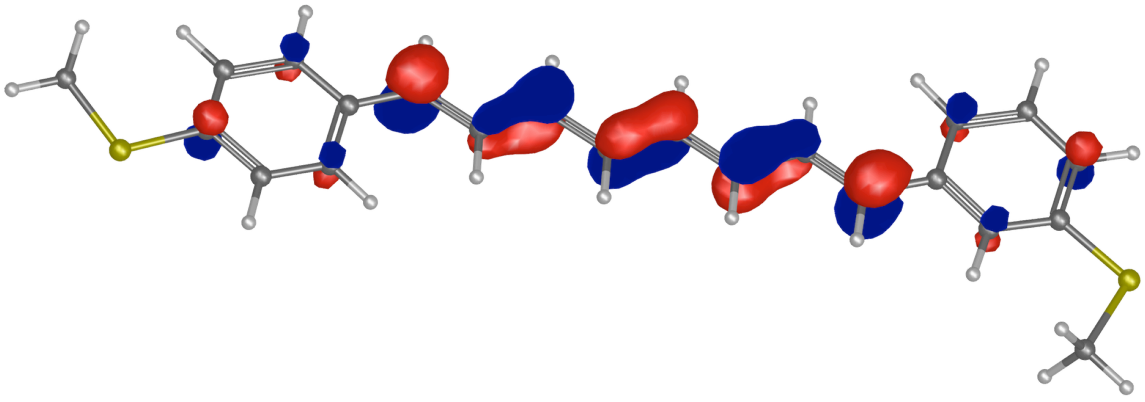
H121	-C120	-C117	-C123	: 175.061613
H122	-C120	-C117	-C123	: -65.365815
H123	-C120	-C117	-C123	: 53.705978

1-(3-(methylthio)phenyl)-8-(4-(methylthio)phenyl)-octa-1,3,5,7-tetraene (**4**):

HOMO:



LUMO:



Final Geometry:

angstroms

atom	x	y	z

C1	-1.2605521880	-0.4962683601	-0.1191088892
C2	-1.9538433705	-1.7182240942	-0.2579329767
C3	-3.3365392714	-1.7607597597	-0.3195444052
C4	-4.0996515448	-0.5807181456	-0.2449482062
C5	-3.4301443195	0.6402080296	-0.1067259292
C6	-2.0393160783	0.6720275557	-0.0461478384
H8	-1.4024684241	-2.6513865681	-0.3192516582
H9	-3.8386263780	-2.7183155838	-0.4274013595
H11	-3.9797141188	1.5724932972	-0.0451705165
H12	-1.5403396498	1.6321307884	0.0611036738
S12	-5.8686673613	-0.7685443637	-0.3353438500
C13	-6.4884814759	0.9396624444	-0.2129311912
H14	-7.5761777657	0.8620698582	-0.2678254642
H15	-6.2143169538	1.3985048215	0.7396240983
H16	-6.1352214210	1.5541502391	-1.0439655102
C16	1.1029942636	-1.3942191944	-0.1025609568
C17	0.1921182013	-0.3895794093	-0.0500588096
H19	0.5732255851	0.6261970978	0.0558515889
H20	0.7664305408	-2.4244307406	-0.2074964697
C20	3.4434997660	-2.1983118598	-0.0793651802
C21	2.5236277311	-1.1953648736	-0.0282084495
H23	2.8756200757	-0.1685724459	0.0758176978
H24	3.0877212716	-3.2239916122	-0.1829814042
C24	5.7734087193	-3.0221304909	-0.0572229441
C25	4.8633706520	-2.0102726502	-0.0068286890
H27	5.2244682489	-0.9864486731	0.0952269604
H28	5.4068985561	-4.0438636448	-0.1586742033
C28	8.0781508215	-3.8833566022	-0.0363976940
C29	7.1976518354	-2.8517538885	0.0137019870
H31	7.5611085395	-1.8301808272	0.1137404017

H32	7.6625386545	-4.8864355673	-0.1338539002
C32	12.3739261651	-3.8635756886	0.1395336134
C33	11.6469478444	-5.0597750945	0.0301587784
C34	10.2619694336	-5.0374521767	-0.0253615249
C35	9.5338067431	-3.8308544196	0.0260545726
C36	10.2778659591	-2.6413128560	0.1353921365
C37	11.6676295188	-2.6527142071	0.1911782669
H39	12.1725632384	-6.0097400616	-0.0118652338
H40	9.7208392961	-5.9764527444	-0.1106858901
H41	9.7666307144	-1.6842097787	0.1765828384
H42	12.1944873684	-1.7090119925	0.2748030860
S42	14.1481946616	-4.0114674541	0.2030153987
C43	14.7225183988	-2.2885504765	0.3393138682
H44	15.8122750001	-2.3455258762	0.3768638010
H45	14.4292893835	-1.6975352611	-0.5311705939
H46	14.3614996069	-1.8170025635	1.2559703467

bond lengths (angstroms):

C1	-C2	:	1.411772	C1	-C6	:	1.405956
C1	-C17	:	1.458219	C2	-C3	:	1.384721
C2	-H8	:	1.085618	C3	-C4	:	1.407268
C3	-H9	:	1.086572	C4	-C5	:	1.399288
C4	-S12	:	1.781254	C5	-C6	:	1.392510
C5	-H11	:	1.083961	C6	-H12	:	1.087326
S12	-C13	:	1.821298	C13	-H14	:	1.091841
C13	-H15	:	1.092275	C13	-H16	:	1.092248
C16	-C17	:	1.357112	C16	-H20	:	1.088863
C16	-C21	:	1.436409	C17	-H19	:	1.090074

C20 -C21 : 1.361868 C20 -H24 : 1.090566

C20 -C25 : 1.434104 C21 -H23 : 1.090423

C24 -C25 : 1.361824 C24 -H28 : 1.090211

C24 -C29 : 1.436150 C25 -H27 : 1.090423

C28 -C29 : 1.357200 C28 -H32 : 1.090137

C28 -C35 : 1.457941 C29 -H31 : 1.088908

C32 -C33 : 1.404049 C32 -C37 : 1.402750

C32 -S42 : 1.781553 C33 -C34 : 1.386271

C33 -H39 : 1.086495 C34 -C35 : 1.410228

C34 -H40 : 1.087117 C35 -C36 : 1.407334

C36 -C37 : 1.390929 C36 -H41 : 1.085866

C37 -H42 : 1.084042 S42 -C43 : 1.821227

C43 -H44 : 1.091891 C43 -H45 : 1.092257

C43 -H46 : 1.092223

bond angles:

C6 -C1 -C2 : 116.893257 C17 -C1 -C2 : 123.861918

C17 -C1 -C6 : 119.244814 C3 -C2 -C1 : 121.421060

H8 -C2 -C1 : 120.009053 H8 -C2 -C3 : 118.569882

C4 -C3 -C2 : 120.887593 H9 -C3 -C2 : 119.531042

H9 -C3 -C4 : 119.581359 C5 -C4 -C3 : 118.517792

S12 -C4 -C3 : 116.578863 S12 -C4 -C5 : 124.903341

C6 -C5 -C4 : 120.140352 H11 -C5 -C4 : 120.895293

H11 -C5 -C6 : 118.964355 C5 -C6 -C1 : 122.139939

H12 -C6 -C1 : 118.990601 H12 -C6 -C5 : 118.869460

C13 -S12 -C4 : 103.630941 H14 -C13 -S12 : 105.604197

H15 -C13 -S12 : 111.542401 H15 -C13 -H14 : 108.889818

H16 -C13 -S12 : 111.497010 H16 -C13 -H14 : 108.900451

H16 -C13 -H15 : 110.243445 H20 -C16 -C17 : 119.779904

C21 -C16 -C17 : 124.009494 C21 -C16 -H20 : 116.210600

C16 -C17 -C1 : 127.780628 H19 -C17 -C1 : 114.901757

H19 -C17 -C16 : 117.317608 H24 -C20 -C21 : 118.414572

C25 -C20 -C21 : 124.769911 C25 -C20 -H24 : 116.815517

C20 -C21 -C16 : 124.342122 H23 -C21 -C16 : 117.036396

H23 -C21 -C20 : 118.621481 H28 -C24 -C25 : 118.368204

C29 -C24 -C25 : 124.941111 C29 -C24 -H28 : 116.690682

C24 -C25 -C20 : 124.216492 H27 -C25 -C20 : 117.110778

H27 -C25 -C24 : 118.672729 H32 -C28 -C29 : 117.087870

C35 -C28 -C29 : 128.227929 C35 -C28 -H32 : 114.684105

C28 -C29 -C24 : 123.462152 H31 -C29 -C24 : 116.541699

H31 -C29 -C28 : 119.996117 C37 -C32 -C33 : 118.527801

S42 -C32 -C33 : 116.596697 S42 -C32 -C37 : 124.875497

C34 -C33 -C32 : 120.443670 H39 -C33 -C32 : 119.830439

H39 -C33 -C34 : 119.725883 C35 -C34 -C33 : 121.882580

H40 -C34 -C33 : 119.113197 H40 -C34 -C35 : 119.004220

C34 -C35 -C28 : 118.892103 C36 -C35 -C28 : 124.169229

C36 -C35 -C34 : 116.938664 C37 -C36 -C35 : 121.630939

H41 -C36 -C35 : 119.936837 H41 -C36 -C37 : 118.432152

C36 -C37 -C32 : 120.576313 H42 -C37 -C32 : 120.636124

H42 -C37 -C36 : 118.787557 C43 -S42 -C32 : 103.780057

H44 -C43 -S42 : 105.541924 H45 -C43 -S42 : 111.566703

H45 -C43 -H44 : 108.879489 H46 -C43 -S42 : 111.530837

H46 -C43 -H44 : 108.878101 H46 -C43 -H45 : 110.273983

torsional angles:

C1 -C2 -C3 -C4 : -0.019270

C1 -C2 -C3 -H9 : 179.952208

C1 -C6 -C5 -C4 : -0.019994

C1 -C6 -C5 -H11 : 179.978892

C1 -C17 -C16 -H20 : -0.057732

C1 -C17 -C16 -C21 : 179.922182

C2 -C1 -C6 -C5 : -0.002422

C2 -C1 -C6 -H12 : 179.995642

C2 -C1 -C17 -C16 : -0.057154

C2 -C1 -C17 -H19 : 179.913073

C2 -C3 -C4 -C5 : -0.003602

C2 -C3 -C4 -S12 :-179.983260

C3 -C2 -C1 -C6 : 0.021964

C3 -C2 -C1 -C17 :-179.941003

C3 -C4 -C5 -C6 : 0.022787

C3 -C4 -C5 -H11 :-179.976078

C3 -C4 -S12 -C13 :-179.816063

C4 -C3 -C2 -H8 :-179.990871

C4 -C5 -C6 -H12 : 179.981939

C4 -S12 -C13 -H14 : 179.858723

C4 -S12 -C13 -H15 : -62.000858

C4 -S12 -C13 -H16 : 61.729518

C5 -C4 -C3 -H9 :-179.975065

C5 -C4 -S12 -C13 : 0.205732

C5 -C6 -C1 -C17 : 179.962334

C6 -C1 -C2 -H8 : 179.993163

C6 -C1 -C17 -C16 : 179.980699

C6 -C1 -C17 -H19 : -0.049074

C6 -C5 -C4 -S12 :-179.999396

H8 -C2 -C1 -C17 : 0.030196

H8 -C2 -C3 -H9 : -0.019394

H9 -C3 -C4 -S12 : 0.045277

H11 -C5 -C4 -S12 : 0.001740

H11 -C5 -C6 -H12 : -0.019174

H12 -C6 -C1 -C17 : -0.039602

C16 -C21 -C20 -H24 : -0.037579

C16 -C21 -C20 -C25 : 179.959503

C17 -C16 -C21 -C20 : 179.957591

C17 -C16 -C21 -H23 : -0.052278

H19 -C17 -C16 -H20 : 179.972663

H19 -C17 -C16 -C21 : -0.047424

H20 -C16 -C21 -C20 : -0.061841

H20 -C16 -C21 -H23 : 179.928290

C20 -C25 -C24 -H28 : -0.031995

C20 -C25 -C24 -C29 : 179.986715

C21 -C20 -C25 -C24 : 179.902312

C21 -C20 -C25 -H27 : -0.091657

H23 -C21 -C20 -H24 : 179.972435

H23 -C21 -C20 -C25 : -0.030483

H24 -C20 -C25 -C24 : -0.100564

H24 -C20 -C25 -H27 : 179.905467

C24 -C29 -C28 -H32 : -0.118673

C24 -C29 -C28 -C35 :-179.999315

C25 -C24 -C29 -C28 : 179.841297

C25 -C24 -C29 -H31 : -0.093279

H27 -C25 -C24 -H28 : 179.961887

H27 -C25 -C24 -C29 : -0.019404

H28 -C24 -C29 -C28 : -0.140276

H28 -C24 -C29 -H31 : 179.925147

C28 -C35 -C34 -C33 :-179.954093

C28 -C35 -C34 -H40 : 0.027746

C28 -C35 -C36 -C37 : 179.987583

C28 -C35 -C36 -H41 : -0.111035

C29 -C28 -C35 -C34 : 179.111485

C29 -C28 -C35 -C36 : -0.914905

H31 -C29 -C28 -H32 : 179.813747

H31 -C29 -C28 -C35 : -0.066896

H32 -C28 -C35 -C34 : -0.771563

H32 -C28 -C35 -C36 : 179.202046

C32 -C33 -C34 -C35 : -0.059216

C32 -C33 -C34 -H40 : 179.958964

C32 -C37 -C36 -C35 : -0.004766

C32 -C37 -C36 -H41 :-179.907584

C32 -S42 -C43 -H44 :-179.801580

C32 -S42 -C43 -H45 : -61.697886

C32 -S42 -C43 -H46 : 62.115255

C33 -C32 -C37 -C36 : 0.018070

C33 -C32 -C37 -H42 :-179.953984

C33 -C32 -S42 -C43 : 179.944840

C33 -C34 -C35 -C36 : 0.070399

C34 -C33 -C32 -C37 : 0.013291

C34 -C33 -C32 -S42 : 179.989975

C34 -C35 -C36 -C37 : -0.038335

C34 -C35 -C36 -H41 : 179.863047

C35 -C34 -C33 -H39 : 179.974618

C35 -C36 -C37 -H42 : 179.967798

C36 -C35 -C34 -H40 :-179.947761

C36 -C37 -C32 -S42 :-179.956517

C37 -C32 -C33 -H39 : 179.979421

C37 -C32 -S42 -C43 : -0.080130

H39 -C33 -C32 -S42 : -0.043894

H39 -C33 -C34 -H40 : -0.007202

H41 -C36 -C37 -H42 : 0.064980

H42 -C37 -C32 -S42 : 0.071428

Nuclear repulsion energy: 1764.727438154 hartrees

Total energy: -1647.96862312329 hartrees

HOMO energy: -0.17263 hartrees

LUMO energy: -0.07160 hartrees

Orbital energies (hartrees):

-88.88664 -88.88662 -10.22527 -10.22501 -10.22118 -10.22107

-10.19802 -10.19782 -10.19596 -10.19474 -10.19449 -10.19425

-10.19373 -10.19341 -10.19296 -10.19273 -10.19207 -10.19169

-10.19104 -10.19085 -10.19036 -10.19017 -10.18991 -10.18980

-7.94756 -7.94755 -5.91283 -5.91280 -5.90869 -5.90867

-5.90248 -5.90247 -0.86617 -0.86596 -0.82532 -0.81635

-0.80658 -0.79180 -0.77116 -0.75242 -0.74954 -0.74811

-0.72855 -0.70079 -0.66686 -0.65277 -0.62254 -0.61230

-0.61121 -0.59016 -0.57428 -0.55961 -0.55540 -0.54615

-0.50806 -0.50232 -0.47652 -0.47483 -0.45956 -0.45770

-0.45357 -0.44797 -0.43818 -0.43805 -0.43702 -0.43520

-0.42319 -0.41986 -0.41123 -0.40515 -0.39266 -0.38400

-0.37977 -0.37941 -0.37565 -0.36327 -0.35838 -0.35448

-0.34608 -0.34527 -0.33997 -0.33958 -0.32650 -0.32139

-0.32112 -0.30656 -0.28375 -0.25593 -0.25513 -0.25235

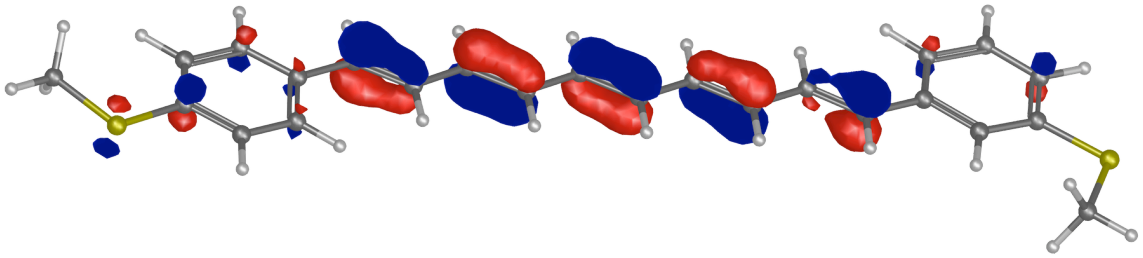
-0.22517 -0.20365 -0.17263 -0.07160 -0.02598 -0.00359

-0.00300 0.01629 0.03479 0.03483 0.05453 0.07291

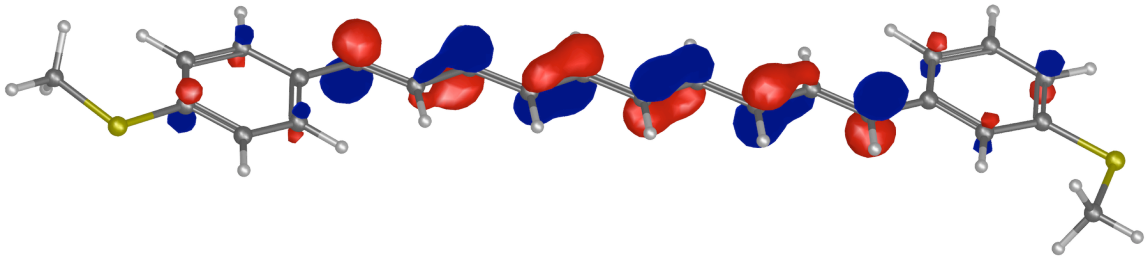
0.07298

1-(3-(methylthio)phenyl)-10-(4-(methylthio)phenyl)-deca-1,3,5,7,9-pentaene (**5**):

HOMO:



LUMO:



Final Geometry:

		angstroms	
atom	x	y	z
C1	-1.2685483096	-0.5232818274	-0.1741804875
C2	-1.9792472266	-1.7432042485	-0.1844324071
C3	-3.3634919748	-1.7718377283	-0.2091844483
C4	-4.1108090872	-0.5794189701	-0.2251672053
C5	-3.4239587808	0.6397315968	-0.2157256438
C6	-2.0318917221	0.6576095905	-0.1907349026
H8	-1.4405272218	-2.6857048685	-0.1723392490
H9	-3.8792507160	-2.7281728092	-0.2159774678
H11	-3.9609761890	1.5812642582	-0.2275377093
H12	-1.5192734494	1.6165106158	-0.1836371183
S12	-5.8835248777	-0.7502446407	-0.2563815512

C13	-6.4808669862	0.9703004921	-0.2670290909
H14	-7.5705258724	0.9025396510	-0.2832936138
H15	-6.1732570339	1.5069041237	0.6332445861
H16	-6.1465420406	1.5052968932	-1.1586961432
C16	1.0868017945	-1.4448560680	-0.1272563633
C17	0.1859789246	-0.4294491090	-0.1469668459
H19	0.5794399871	0.5871869929	-0.1415554208
H20	0.7397658423	-2.4769632963	-0.1316328835
C20	3.4247501182	-2.2612294771	-0.0765768600
C21	2.5092387323	-1.2521600868	-0.0989909199
H23	2.8687413565	-0.2226526971	-0.0943353152
H24	3.0643009576	-3.2904989360	-0.0808128156
C24	5.7571122792	-3.0837785610	-0.0206874179
C25	4.8443015169	-2.0711175217	-0.0459816170
H27	5.2069098775	-1.0427175989	-0.0416767966
H28	5.3913840367	-4.1112041210	-0.0245118238
C28	8.0799698726	-3.9230528956	0.0410882561
C29	7.1778311343	-2.9023551393	0.0124775555
H31	7.5481279425	-1.8766666767	0.0159794904
H32	7.7037093103	-4.9463791481	0.0381457785
C32	10.3764267035	-4.8018392175	0.1097661505
C33	9.5058659047	-3.7606539435	0.0770503314
H35	9.8798085368	-2.7379206284	0.0793874495
H36	9.9497691694	-5.8050633092	0.1093730483
C36	14.6741269991	-4.8154937179	0.2343456067
C37	13.9331904083	-6.0081172814	0.2419424167
C38	12.5479587435	-5.9749037572	0.1999921573
C39	11.8330545021	-4.7602023439	0.1499237255
C40	12.5913207418	-3.5743975337	0.1421839950
C41	13.9814010569	-3.5967948788	0.1833030027

H43	14.4481426442	-6.9640684011	0.2808573413
H44	11.9960805730	-6.9115444231	0.2066884962
H45	12.0913223329	-2.6117557189	0.1014487585
H46	14.5191223146	-2.6555017915	0.1745415410
S46	16.4471948646	-4.9771965985	0.2918107100
C47	17.0407481622	-3.2556403314	0.2671630450
H48	18.1301269227	-3.3212820239	0.3027989976
H49	16.7474293982	-2.7431686699	-0.6517371552
H50	16.6915822130	-2.6983545951	1.1392099966

bond lengths (angstroms):

C1	-C2	:	1.411881	C1	-C6	:	1.406226
C1	-C17	:	1.457805	C2	-C3	:	1.384762
C2	-H8	:	1.085667	C3	-C4	:	1.407338
C3	-H9	:	1.086568	C4	-C5	:	1.399350
C4	-S12	:	1.781201	C5	-C6	:	1.392406
C5	-H11	:	1.083979	C6	-H12	:	1.087345
S12	-C13	:	1.821320	C13	-H14	:	1.091885
C13	-H15	:	1.092273	C13	-H16	:	1.092275
C16	-C17	:	1.357542	C16	-H20	:	1.088898
C16	-C21	:	1.435708	C17	-H19	:	1.090133
C20	-C21	:	1.362676	C20	-H24	:	1.090567
C20	-C25	:	1.432552	C21	-H23	:	1.090481
C24	-C25	:	1.363578	C24	-H28	:	1.090585
C24	-C29	:	1.432640	C25	-H27	:	1.090463
C28	-C29	:	1.362533	C28	-H32	:	1.090311
C28	-C33	:	1.435565	C29	-H31	:	1.090490
C32	-C33	:	1.357576	C32	-H36	:	1.090181

C32 -C39 : 1.457776 C33 -H35 : 1.088955

C36 -C37 : 1.404064 C36 -C41 : 1.402748

C36 -S46 : 1.781353 C37 -C38 : 1.386265

C37 -H43 : 1.086523 C38 -C39 : 1.410353

C38 -H44 : 1.087157 C39 -C40 : 1.407537

C40 -C41 : 1.390869 C40 -H45 : 1.085512

C41 -H46 : 1.084091 S46 -C47 : 1.821172

C47 -H48 : 1.091936 C47 -H49 : 1.092264

C47 -H50 : 1.092223

bond angles:

C6 -C1 -C2 : 116.888481 C17 -C1 -C2 : 123.916812

C17 -C1 -C6 : 119.194694 C3 -C2 -C1 : 121.411311

H8 -C2 -C1 : 120.015947 H8 -C2 -C3 : 118.572734

C4 -C3 -C2 : 120.897205 H9 -C3 -C2 : 119.524871

H9 -C3 -C4 : 119.577921 C5 -C4 -C3 : 118.519710

S12 -C4 -C3 : 116.578604 S12 -C4 -C5 : 124.901686

C6 -C5 -C4 : 120.133933 H11 -C5 -C4 : 120.897117

H11 -C5 -C6 : 118.968950 C5 -C6 -C1 : 122.149356

H12 -C6 -C1 : 118.984457 H12 -C6 -C5 : 118.866186

C13 -S12 -C4 : 103.645498 H14 -C13 -S12 : 105.590831

H15 -C13 -S12 : 111.524984 H15 -C13 -H14 : 108.893780

H16 -C13 -S12 : 111.535979 H16 -C13 -H14 : 108.886445

H16 -C13 -H15 : 110.243985 H20 -C16 -C17 : 119.829722

C21 -C16 -C17 : 123.871368 C21 -C16 -H20 : 116.298887

C16 -C17 -C1 : 127.894108 H19 -C17 -C1 : 114.849542

H19 -C17 -C16 : 117.256339 H24 -C20 -C21 : 118.474271

C25 -C20 -C21 : 124.599124 C25 -C20 -H24 : 116.926568

C20 -C21 -C16 : 124.511643 H23 -C21 -C16 : 116.963454

H23 -C21 -C20 : 118.524868 H28 -C24 -C25 : 118.364825

C29 -C24 -C25 : 124.766705 C29 -C24 -H28 : 116.868430

C24 -C25 -C20 : 124.415362 H27 -C25 -C20 : 117.048794

H27 -C25 -C24 : 118.535799 H32 -C28 -C29 : 118.330023

C33 -C28 -C29 : 124.989506 C33 -C28 -H32 : 116.680420

C28 -C29 -C24 : 124.209170 H31 -C29 -C24 : 117.124690

H31 -C29 -C28 : 118.666092 H36 -C32 -C33 : 117.051720

C39 -C32 -C33 : 128.280687 C39 -C32 -H36 : 114.667344

C32 -C33 -C28 : 123.420874 H35 -C33 -C28 : 116.575908

H35 -C33 -C32 : 120.003098 C41 -C36 -C37 : 118.525948

S46 -C36 -C37 : 116.613787 S46 -C36 -C41 : 124.860262

C38 -C37 -C36 : 120.450955 H43 -C37 -C36 : 119.829470

H43 -C37 -C38 : 119.719575 C39 -C38 -C37 : 121.885900

H44 -C38 -C37 : 119.106059 H44 -C38 -C39 : 119.008021

C38 -C39 -C32 : 118.873444 C40 -C39 -C32 : 124.208439

C40 -C39 -C38 : 116.918117 C41 -C40 -C39 : 121.646985

H45 -C40 -C39 : 119.945422 H45 -C40 -C41 : 118.407494

C40 -C41 -C36 : 120.572027 H46 -C41 -C36 : 120.643956

H46 -C41 -C40 : 118.784006 C47 -S46 -C36 : 103.777716

H48 -C47 -S46 : 105.538537 H49 -C47 -S46 : 111.554266

H49 -C47 -H48 : 108.879179 H50 -C47 -S46 : 111.550758

H50 -C47 -H48 : 108.877805 H50 -C47 -H49 : 110.270375

torsional angles:

C1 -C2 -C3 -C4 : 0.007500

C1 -C2 -C3 -H9 :-179.969577

C1 -C6 -C5 -C4 : -0.000414

C1 -C6 -C5 -H11 : 179.994003

C1 -C17 -C16 -H20 : 0.034584

C1 -C17 -C16 -C21 :-179.907696

C2 -C1 -C6 -C5 : 0.017837

C2 -C1 -C6 -H12 :-179.992710

C2 -C1 -C17 -C16 : -0.003863

C2 -C1 -C17 -H19 :-179.964052

C2 -C3 -C4 -C5 : 0.010565

C2 -C3 -C4 -S12 :-179.993057

C3 -C2 -C1 -C6 : -0.021285

C3 -C2 -C1 -C17 : 179.936793

C3 -C4 -C5 -C6 : -0.014008

C3 -C4 -C5 -H11 : 179.991684

C3 -C4 -S12 -C13 : 179.875659

C4 -C3 -C2 -H8 : 179.976460

C4 -C5 -C6 -H12 :-179.989879

C4 -S12 -C13 -H14 :-179.840667

C4 -S12 -C13 -H15 : -61.712667

C4 -S12 -C13 -H16 : 62.034318

C5 -C4 -C3 -H9 : 179.987630

C5 -C4 -S12 -C13 : -0.128222

C5 -C6 -C1 -C17 :-179.942313

C6 -C1 -C2 -H8 :-179.989803

C6 -C1 -C17 -C16 : 179.953307

C6 -C1 -C17 -H19 : -0.006882

C6 -C5 -C4 -S12 : 179.989942

H8 -C2 -C1 -C17 : -0.031725

H8 -C2 -C3 -H9 : -0.000617

H9 -C3 -C4 -S12 : -0.015992

H11 -C5 -C4 -S12 : -0.004366

H11 -C5 -C6 -H12 : 0.004538

H12 -C6 -C1 -C17 : 0.047141

C16 -C21 -C20 -H24 : 0.043409

C16 -C21 -C20 -C25 :-179.884434

C17 -C16 -C21 -C20 : 179.876611

C17 -C16 -C21 -H23 : -0.054652

H19 -C17 -C16 -H20 : 179.993947

H19 -C17 -C16 -C21 : 0.051667

H20 -C16 -C21 -C20 : -0.067535

H20 -C16 -C21 -H23 :-179.998798

C20 -C25 -C24 -H28 : 0.047017

C20 -C25 -C24 -C29 :-179.878284

C21 -C20 -C25 -C24 : 179.850764

C21 -C20 -C25 -H27 : -0.070070

H23 -C21 -C20 -H24 : 179.973680

H23 -C21 -C20 -C25 : 0.045837

H24 -C20 -C25 -C24 : -0.078095

H24 -C20 -C25 -H27 :-179.998929

C24 -C29 -C28 -H32 : 0.038357

C24 -C29 -C28 -C33 :-179.876036

C25 -C24 -C29 -C28 : 179.819944

C25 -C24 -C29 -H31 : -0.099669

H27 -C25 -C24 -H28 : 179.966761

H27 -C25 -C24 -C29 : 0.041460

H28 -C24 -C29 -C28 : -0.106370

H28 -C24 -C29 -H31 : 179.974017

C28 -C33 -C32 -H36 : -0.080228

C28 -C33 -C32 -C39 :-179.887491

C29 -C28 -C33 -C32 : 179.756688

C29 -C28 -C33 -H35 : -0.116626

H31 -C29 -C28 -H32 : 179.956817

H31 -C29 -C28 -C33 : 0.042424

H32 -C28 -C33 -C32 : -0.158978

H32 -C28 -C33 -H35 : 179.967708

C32 -C39 -C38 -C37 :-179.904109

C32 -C39 -C38 -H44 : 0.043578

C32 -C39 -C40 -C41 : 179.938720

C32 -C39 -C40 -H45 : -0.177299

C33 -C32 -C39 -C38 : 179.060366

C33 -C32 -C39 -C40 : -0.941122

H35 -C33 -C32 -H36 : 179.788940

H35 -C33 -C32 -C39 : -0.018324

H36 -C32 -C39 -C38 : -0.750747

H36 -C32 -C39 -C40 : 179.247765

C36 -C37 -C38 -C39 : -0.062086

C36 -C37 -C38 -H44 : 179.990277

C36 -C41 -C40 -C39 : -0.006753

C36 -C41 -C40 -H45 :-179.892460

C36 -S46 -C47 -H48 : 179.936747

C36 -S46 -C47 -H49 : -61.968495

C36 -S46 -C47 -H50 : 61.845478

C37 -C36 -C41 -C40 : 0.044662

C37 -C36 -C41 -H46 :-179.916491

C37 -C36 -S46 -C47 :-179.978756

C37 -C38 -C39 -C40 : 0.097271

C38 -C37 -C36 -C41 : -0.010908

C38 -C37 -C36 -S46 : 179.970810

C38 -C39 -C40 -C41 : -0.062742

C38 -C39 -C40 -H45 : 179.821239

C39 -C38 -C37 -H43 : 179.943677

C39 -C40 -C41 -H46 : 179.955114

C40 -C39 -C38 -H44 :-179.955042

C40 -C41 -C36 -S46 :-179.935418

C41 -C36 -C37 -H43 : 179.983323

C41 -C36 -S46 -C47 : 0.001668

H43 -C37 -C36 -S46 : -0.034960

H43 -C37 -C38 -H44 : -0.003960

H45 -C40 -C41 -H46 : 0.069407

H46 -C41 -C36 -S46 : 0.103429

Nuclear repulsion energy: 1926.234326193 hartrees

Total energy: -1725.37955583703 hartrees

HOMO energy: -0.16991 hartrees

LUMO energy: -0.07610 hartrees

Orbital energies (hartrees):

-88.88692 -88.88690 -10.22570 -10.22547 -10.22135 -10.22125

-10.19836 -10.19823 -10.19624 -10.19509 -10.19478 -10.19444

-10.19401 -10.19379 -10.19335 -10.19308 -10.19260 -10.19226

-10.19139 -10.19122 -10.19088 -10.19062 -10.19036 -10.19021

-10.19009 -10.18994 -7.94785 -7.94783 -5.91311 -5.91308

-5.90897 -5.90895 -5.90277 -5.90275 -0.86647 -0.86629

-0.82666 -0.81906 -0.81048 -0.79944 -0.78284 -0.76403

-0.75067 -0.74976 -0.74469 -0.72404 -0.69844 -0.66682

-0.65437 -0.62594 -0.61470 -0.61160 -0.59506 -0.57878

-0.56292 -0.56148 -0.54998 -0.54567 -0.50899 -0.50119

-0.48304 -0.47122 -0.46694 -0.45680 -0.45507 -0.45203

-0.44373 -0.43838 -0.43825 -0.43812 -0.42736 -0.42209

-0.41913 -0.41268 -0.39867 -0.39735 -0.38070 -0.37998

-0.37979	-0.37962	-0.36778	-0.35993	-0.35684	-0.35226
-0.34807	-0.34559	-0.34021	-0.34000	-0.33304	-0.32165
-0.32138	-0.31525	-0.29654	-0.27289	-0.25563	-0.25525
-0.24411	-0.22058	-0.19992	-0.16991	-0.07610	-0.03471
-0.00442	-0.00349	0.00485	0.03458	0.03461	0.03961
0.07179	0.07269				

C6. References

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