Heterotetracenes: Flexible Synthesis and *in Silico* Assessment of the Hole Transport Properties

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Abstract: Thienoacenes and furoacenes are among the most frequent molecular units found in organic materials. The efficient synthesis of morphologically different heteroacenes and the rapid determination of their solid-state and electronic properties are still challenging tasks, which slow down progress in the development of new materials. Herein, we report a flexible and efficient synthesis of unprecedented heterotetracenes based on a platinum- and gold-catalyzed cyclization-alkynylation domino process using EthynylBenziodoXole (EBX) hypervalent iodine reagents as key step. The proof-of-principle *in silico* estimation of the synthesized tetracenes' charge transport properties reveals their strong dependence on both the position and nature of the heteroatoms in the ring system. A broad range of mobilities is predicted, with some compounds displaying performance potentially comparable to that of state-of-the art electronic organic materials.

Introduction

Acenes and heteroacenes are important compounds in material science.[1] Among them, thienoacenes and furoacenes were intensively studied due to their easily tuned electronic properties depending on their conjugation topology.[2] Especially successful examples are dibenzo[*b*,*b'*] thieno[2,3-*f*55,4-*f'*]bis[1]benzothiophene (DBTBT, **1**),[2b] benzo[1,2-b:4,5-b]bis[b]benzothiophene (BBBT, **2**),[2c] [1]benzothieno[3,2-b][1]benzothiophene (BTBT, **3**),[2e-f] dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]thiophene (DNTT, **4**),[2g-h] benzodifuran (BDF, **5**),[2j] and naphtho[2,1-*b*:6,5-*b'*]difuran (NDF, **6**)[2k] (Figure 1). Systematic studies of the influence of the sulfur and oxygen heteroatoms on the electronic properties in dependence on their position in the ring systems are limited.[1h,3] This is surprising, when considering that a broad diversity of building blocks and a good understanding of their electronic properties will be essential for the development of new organic materials.

One possible reason for this lack of diversity is that a rapid and flexible synthesis of novel and morphologically diverse building blocks remains difficult. To address this challenge, we envisioned a new synthesis of heterotetracenes derived from either dibenzofuran or dibenzothiophene starting from broadly available iodo- and alkynyl arenes in four steps only (Scheme 1, goal 1). This approach allows varying systematically the central and the last ring of the conjugated system to study their effect on the hole transport properties and to introduce selectively either an oxygen or a sulfur heteroatom at the desired position. It is interesting to note that despite their relative simplicity, most of the targeted compounds have not yet been reported.

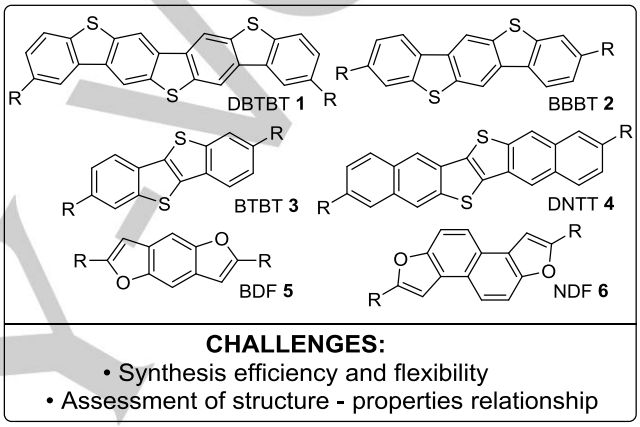

Figure 1. Thieno- and furo- acenes building blocks for organic materials

Improved synthesis methods are necessary but alone not sufficient for the development of new materials. Indeed, analyzing the relationship between structure and electronic properties is also required to guide the synthetic effort. Since measuring the hole transport properties under conditions relevant for the material applications can be highly resource and time-consuming, rapid computational pre-screening is valuable for identifying the most promising structures for subsequent experimental testing. Admittedly, highly accurate estimates of charge mobility require rigorous multiscale simulations, based on experimental crystal structures.[4] In the absence of the latter in this study we retreat to a much more limited and computationally inexpensive approach of applying the Marcus hopping model of the charge transport to the model dimers.[5] This approach ignores the crucial effects of disorder and specificity of crystal packing, but allows isolating the role of the nature and position of the heteroatoms in the π-conjugated cores (*via* the reorganization energy) and the extent of orbital overlap between them (*via* the transfer integral, see Scheme 1, goal 2), providing a hypothetical estimate of the core's charge transport capacity.

Overall, herein we present a method for the synthesis and assessment of heterotetracene building blocks with potential for applications in organic materials. A highly efficient synthetic approach based on a platinum-catalyzed domino cyclization-alkynylation process is first presented. Computational evaluation of the charge transport properties of the synthesized tetracenes

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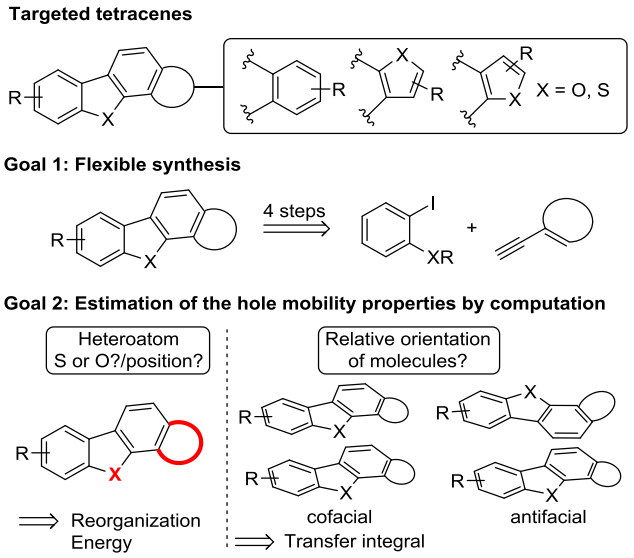
indicates that several of them can potentially compete with the current state-of-the art organic semiconducting materials.



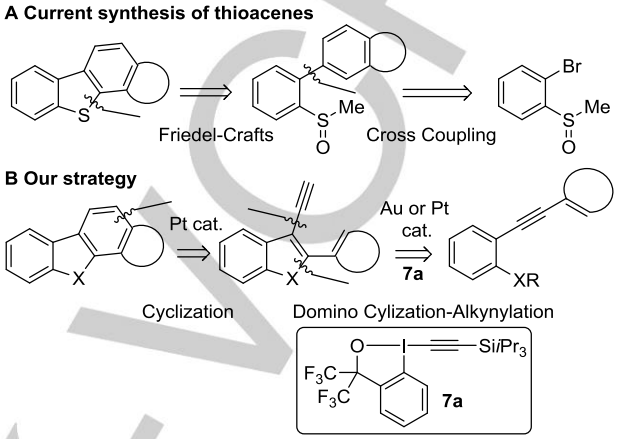
Scheme 1. Targeted tetracenes: flexible synthesis and hole mobility prediction.

Results and Discussion

Synthesis of Heterotetracenes

Most of the past efforts in the synthesis of heterotetracenes have focused on the synthesis of thioacenes bearing an external thiophene ring.[6] Only a few reports dealt with the installation of an internal thiophene ring. One of the most efficient approaches was introduced by Müllen and co-workers based on the intermolecular cross coupling with an aryl sulfoxide followed by a Friedel-Crafts annulation (Scheme 2, **A**).[2b] This convenient transformation has been limited so far to the introduction of only one heteroaryl ring into the π-conjugation system and cannot be used for the synthesis of benzofuran derivatives. Only a few methods were reported for furoacene synthesis.[2j-k] An improved approach to construct heteroaryl fused thienoacenes and furoacenes in a rapid way is consequently required to reach our goal of systematic structure modification.

In view of developing a more general synthesis, we envisaged to form the benzene ring of heterotetracenes using a platinum-catalyzed cyclization as the last step instead of forming the C-X bond (Scheme 2, **B**).[7] This disconnection leads to 2,3-disubstituted 3-alkynyl benzothiophenes and benzofurans as starting materials, which needed to be efficiently synthesized. Usually, a multi-step synthesis is employed to access these substrates, such as halogenation at C3 position starting from C2 substituted precursors, followed by functional group transformations.[8] In the last two decades, C-H functionalization has been developed as a more efficient method to introduce substituents to heterocycle rings, but it takes place at the C2 position for benzothiophenes and benzofurans or requires the introduction of directing groups.[9] To improve synthetic efficiency and allow functionalization at less reactive positions, domino reactions constitute an attractive strategy.[10] For example, the formation of the heterocycle and another C-C bond at *C3* position was employed to synthesize alkenyl-, aryl- or alkyl- C3-substituted benzofurans via Pd,[11] or Rh[12] catalysis, and C3 alkyl or aryl benzothiophenes and benzofurans via Au/Pt,[13] or Pd[14] catalysis. To our surprise, a cyclization-alkynylation domino process was unprecedented.[15,16]



Scheme 2. Current synthesis of thioacenes (**A**) and our new strategy for the synthesis of heterotetracenes (**B**).

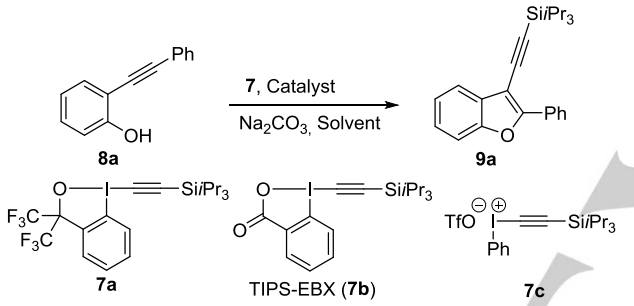
Recently, we developed cyclization-alkynylation domino reactions to access functionalized furans[17] and indoles[18] based on the use of ethynylbenziodoxole (EBX) hypervalent iodine reagents. We therefore envisaged that these reagents could be used to develop the unprecedented domino cyclization alkynylation process. Herein, we report the first intermolecular domino reactions to synthesize 2,3-disubstituted 3-alkynyl benzothiophenes and benzofurans, easily obtained via Sonogashira coupling of the corresponding iodo- and alkynyl-aryls, via gold- or platinum- catalyzed domino reactions using EBX reagent **7a** (Scheme 2, **B**).

We started our investigations on the cyclization-alkynylation domino reaction with 2-alkynyl phenol **8a**[11d] as substrate (Table 1). The conditions reported for Lautens's domino reaction[12] or Hashmi's benzofuran formation[19] didn't give any desired product, independently of the hypervalent iodine reagent used (Table 1, entries 1-6). $PtCl_2$[18] was not efficient for this domino process (Table 1, entry 7). When we turned our attention to Au(III) catalysts, we were pleased to observe the formation of the desired product with benziodoxole **7a** (Table 1, entries 8-10). Other hypervalent iodine reagents were not successful in this transformation (results not shown). $AuCl_3$ gave a better yield (83%) when compared to dichloro(pyridine-2-carboxylato)gold(III) ($PicAuCl_2$) and pyridine gold(III) trichloride ($PyAuCl_3$). The influence of the solvents was then examined, demonstrating that THF was optimal (Table 1, entries 11-12).

We continued our investigation with 2-ethynyl thioanisole **10a** (Table 2).[20] An iodide salt was added to the reaction, as it has been reported to promote demethylation.[16c] The conditions optimized for the cyclization-alkynylation of **8a** were not successful: neither $AuCl_3$ nor $AuBr_3$ could be used as catalyst (Table 2, entries 1-2). On the other hand, AuCl could promote

the desired transformation in 41% yield (Table 2, entry 3). The yield was improved to 61% when $PtCl_2$ was used (Table 2, entry 4). The effect of solvents was then examined. 41%, 28% and 19% of benzothiophene **11a** were obtained in toluene, ether and DCM respectively (Table 2, entries 5-7). 2-Phenyl benzothiophene was isolated as by-product in toluene and DCM. Initially, we used basic conditions to prevent proto-demetalation. However, as no proton is generated during the reaction, we wondered if the use of a base was really required. Indeed, in the absence of the base the yield could even be increased to 77% (Table 2, entry 8). This result is consistent with our previous observation with a platinum catalyst.[18] The reaction did not occur without NaI (Table 2, entry 9). The use of 2.0 equiv. of **7a** did not improve the yield (Table 2, entry 10). Under the optimized reaction conditions, it was therefore possible to obtain the desired 3-alkynyl benzo- furan and thiophene **9a** and **11a** at room temperature using open flasks, resulting in a highly practical procedure.

Table 1. Optimization of the Domino Cyclization- Alkynylation Reaction of 2-Alkynyl Phenol **8a**.

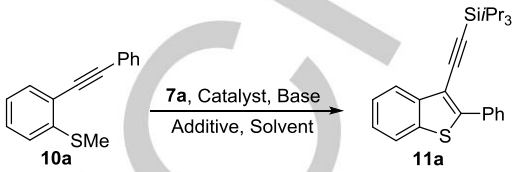


entry	catalyst	reagent	temp	solvent	yield[a]
1	$[Rh(cod)OH]_2$	**7a**	90 °C	dioxane	<5%
2	$[Rh(cod)OH]_2$	**7b**	90 °C	dioxane	<5%
3	$[Rh(cod)OH]_2$	**7c**	90 °C	dioxane	<5%
4	IPrAuCl/AgOTf	**7a**	rt	THF	<5%
5	IPrAuCl/AgOTf	**7b**	rt	THF	<5%
6	IPrAuCl/AgOTf	**7c**	rt	THF	<5%
7	$PtCl_2$	**7a**	rt	THF	<5%
8	$PyAuCl_3$	**7a**	rt	THF	53%
9	$PicAuCl_2$	**7a**	rt	THF	53%
10	$AuCl_3$	**7a**	rt	THF	83%
11	$AuCl_3$	**7a**	rt	DCM	53%
12	$AuCl_3$	**7a**	rt	toluene	<5%

[a] Reaction conditions: **8a** (0.10 mmol), catalyst (10 mol%), **7** (0.12 mmol), Na_2CO_3 (0.12 mmol), 0.1 M, overnight. Isolated yields after column chromatography.

We then explored the scope of the domino reaction for the synthesis of benzofurans (Scheme 3, **A**). The reaction was easily scaled up to 0.3 mmol. Phenyl and tolyl substituted alkynes gave the domino products **9a** and **9b** in 85% and 66% yield respectively. A cyclopropyl group was well tolerated (product **9c**). Benzofurans **9d** and **9e** bearing a C2- and C3-substituted thiophene substituent respectively could also be obtained in good yields.

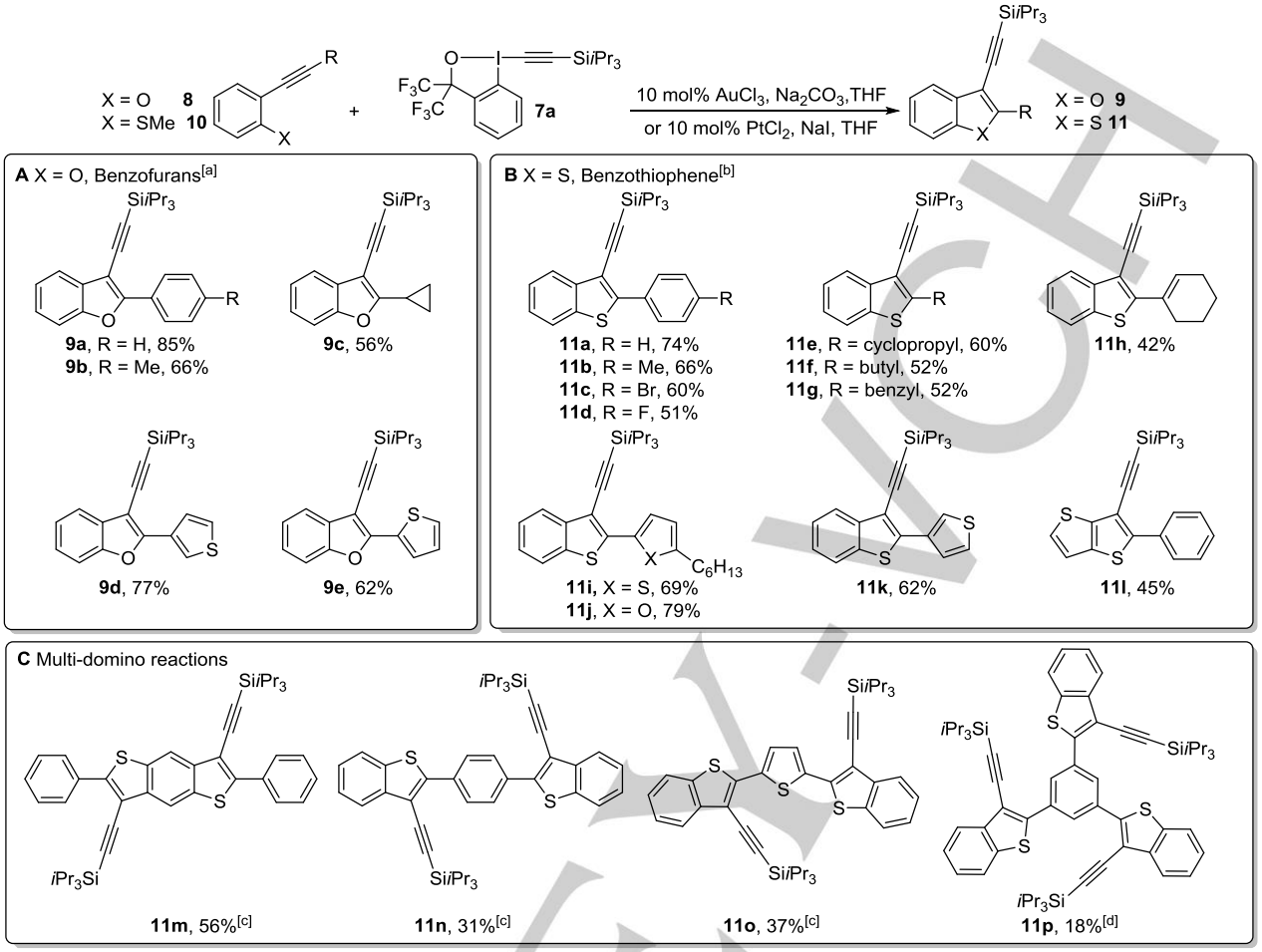
Table 2. Optimization of the Domino Cyclization- Alkynylation Reaction of 2-Alkynyl Thioanisole **10a**.



entry	catalyst	additive	base	solvent	yield[a]
1	$AuCl_3$	NaI	Na_2CO_3	THF	<5%
2	$AuBr_3$	NaI	Na_2CO_3	THF	<5%
3	AuCl	NaI	Na_2CO_3	THF	41%
4	$PtCl_2$	NaI	Na_2CO_3	THF	61%
5	$PtCl_2$	NaI	Na_2CO_3	toluene	41%[b]
6	$PtCl_2$	NaI	Na_2CO_3	Et_2O	28%
7	$PtCl_2$	NaI	Na_2CO_3	DCM	19%[c]
8	$PtCl_2$	NaI	-	THF	77%
9	$PtCl_2$	-	Na_2CO_3	THF	<5%
10[d]	$PtCl_2$	NaI	-	THF	54%

[a] Reaction conditions: **10a** (0.10 mmol), catalyst (10 mol%), **7a** (0.12 mmol), Na_2CO_3 (0.12 mmol), NaI (0.10 mmol), 0.1 M, overnight. Isolated yields after column chromatography. [b] 19% of 2-phenyl benzothiophene was isolated. [c] 11% of 2-phenyl benzothiophene was isolated [d] 0.20 mmol **7a** was used.

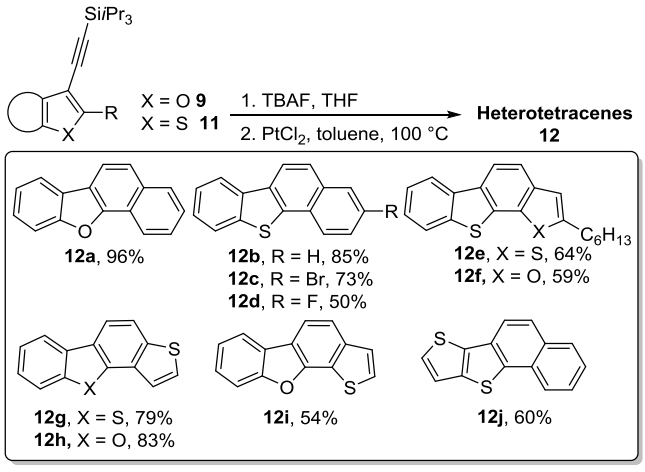
The synthesis of benzothiophene derivatives is then proposed in Scheme 3, **B**. A methyl, a bromide and a fluoride substituent were well tolerated on the phenyl ring linked to the alkyne (products **11b**-**11d**). C2 alkylated benzothiophenes **11e-g** could also be accessed using our method, as well as cyclohexene substituted product 11**h**. The reaction conditions were also applicable to substrates bearing furan or thiophene heterocycles (**11i**-**k**). Disubstituted thienothiophene **11l** was obtained in 45% yield. Even though the yield is moderate, it is usually challenging to synthesize *C3*-substituted thienothiophenes as the *C2* position is more reactive.[1i] Gratifyingly, double and triple domino reactions also took place (Scheme 3, **C**). Symmetric 2,3,5,6-tetrasubstituted benzodithiophene **5m** was synthesized in 56% yield. The multi domino reaction could also be performed when the thioanisoles units were linked by a benzene or a thiophene ring (products **5n-p**). The overall yields were moderate, but the yield for each domino reaction remains between 56% and 75%. Both thienothiophenes and benzodithiophenes are important building blocks in organic material science. They are used as donor fragments for small gap organic solar cell.[21] Moreover, benzodithiophenes showed remarkable properties for applications as field-effect transistors, such as high hole mobility and excellent on/off ratio.[2e]



Scheme 3. Scope of 3-alkynylated benzofurans and 3-alkynylated benzothiophenes.

With a series of 3-alkynylated benzofurans and benzothiophenes in hand, we then performed the envisaged sequence of transformations involving desilylation promoted by TBAF followed by $PtCl_2$ catalyzed cyclization to obtain the desired heterotetracenes **12** (Scheme 4).

Naphtho[1,2-b]benzofuran (**12a**) and naphtho[1,2-b]benzothiophene (**12b**) were obtained in excellent yields -96% and 85% respectively. When a halogen was introduced on the phenyl group, the cyclization step still occurred but with a decrease in yield (products **12c** and **12d**). Heteroacene **12c** can be further functionalized via conventional cross coupling methods. Notably, 3-halogenated naphtho[1,2-b]benzothiophenes such as **12c** are highly challenging to synthesize via Friedel-Crafts halogenation, as it usually takes place on the more nucleophilic *para*-position to the sulfur atom.[22] Two heteroatom-containing heteroacenes **12e-j**, which could not be yet synthesized using conventional approaches,[2b] were smoothly accessed with diverse and unprecedented morphologies. Heteroacenes **12e** and **12f** containing S,S and S,O heteroatoms *ortho* to each other and **12g** and **12h** containing S,S and S,O heteroatoms *meta* to each other were obtained in 59-83% yield.



Scheme 4. Synthesis of heterotetracenes; The yields of the $PtCl_2$-catalysed cyclization are given.

The structure of **12h** was further confirmed by X-ray analysis.[23] Heteroacene **12i** with an *ortho* O,S substitution was formed in 54% yield. Finally, the synthesis of naphtho[2,1-b]thienothiophene **12j** was also possible.[24]

Assessment of the hole mobility properties

In order to assess the potential of the novel heterotetracenes in molecular electronics applications, we have estimated their hole transport properties. Details of the computations[25] can be found in the Supporting Information. The following substrates were investigated: **12a**, **12b**, **12e** and **12f** (a C_6H_{13} group was replaced with a hydrogen atom in the calculations to facilitate the computational effort), **12g**, **12h**, **12i** and **12j** (Figure 2). In order to have a more complete analysis of the influence of introducing thiophene rings in the tetracene, we also examined compounds **13a** and **13b** (3 S atoms), as well as tetrabenzene (**TB**) and tetrathiophene (**TT**) (0 and 4 S atoms respectively). As a further reference point we have chosen a π-conjugated heteroaromatic core, namely the [1]benzothieno[3,2-*b*][1]benzothiophene (BTBT, **3**, also computed without substituent). This substrate has been shown to yield superior organic field effect transistor (OFET) characteristics, with experimentally measured mobilities in the range of 1.0-3.0 $cm^2V^{-1}s^{-1}$.[1h]

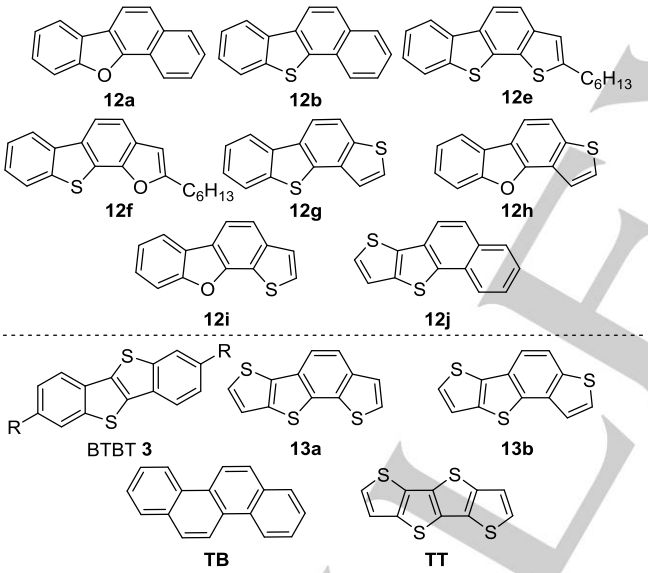


Figure 2. Tetracenes selected for *in silico* pre-screening.

To estimate the hole transport rates we utilise the Marcus-Hush theory for the hopping charge mechanism,[26] which affords an excellent agreement with the experimental results for various acene- and thiophene-based systems.[27] It relies upon two main parameters: the reorganization energy λ_+ of the monomer and the electronic coupling t_+ (hole transfer integral) in the dimer. Our results indicate the dependence of the reorganization energies λ_+ (evaluated as the energy difference between the charged and the neutral counterparts) on the type, number and mutual arrangement of the heteroatoms. Substitution of sulfur with oxygen in either the central or terminal ring (compare compounds **12a** with **12b, 12f** with **12e**, **12h** with **12g** and **12i** with **12e**) generally impedes the ionization and thus leads to higher λ_+ since smaller, less polarizable and more electronegative O atoms are less effective in stabilizing the positive charge (Figure 3, **A**). Adding more sulfur atoms tends to increase the reorganization energy. A clear correlation is also observed between λ_+ and the structural pattern of the heterocycles (Figure 3, **B**): species with the benzothiophene motif have the lowest reorganization energies, while molecules, which also comprise the thienothiophene moiety, have higher λ_+. Compounds with lower reorganization energies are expected to afford better charge transport properties. In this case, simple tetrabenzene (**TB**) should have a significant charge transfer rate. However, reorganization energies alone are insufficient to predict material properties – charge transport rates depend greatly on the crystallinity of the material, the extent of structural and energetic disorder, the type of crystal packing, etc.[4,5,28]

Reliable computational prediction of the charge transport properties is challenging[29] and necessitates (*i*) more sophisticated computational techniques, e.g. involving molecular dynamics and kinetic Monte-Carlo simulations,[30] and (*ii*) the pre-existing knowledge of the crystal structure. Since the determination of the crystal structure for each compound studied here is experimentally challenging and very time-consuming, we retreat to simplistic models based on π-stacked dimers. Such approach admittedly ignores the disorder and packing effects and the influence of substituents,[31] however it provides an insight into the range of transfer integrals that can potentially be expected in the materials comprising the investigated heterotetracene cores.[32] Furthermore, while in general the latter tend to favour the herringbone crystal packing,[33] π-stacking can be enforced *via* side-chain modification.[34]

Initially, we consider coplanar cofacial dimers in what we call a 'frozen' geometry, *i.e.* the geometry with fixed zero longitudinal and transversal shifts (as well as any rotations) and energetically optimal interplanar separation (at SAPT0/jun-cc-pVDZ level of theory)[35]. Their computed transfer integrals (red line in Figure 4) are fairly similar, in the range of 0.22-0.30 eV. However, once allowed to fully relax, such dimers tend to contract (interplanar distance decreasing from 3.7-3.8Å to ~3.3Å) and undergo lateral and/or transversal shifting and even minor rotations disturbing the cores' coplanarity (See Table S2 in the Supporting Information), leading to a much broader range of t_+ values. This range expands even further when non-cofacial mutual core orientations (antifacial, *i.e.* various disordermers,[36,37] Figure 4 top panel) are accounted for, and many more transfer integral values can be achievable for herringbone and other types of dimer assemblies. This complex behaviour of the electronic coupling is caused by an interplay of several factors, including the frontier orbital symmetries, proximity of the heteroatoms, mutual orientation of the monomers within a given crystal packing, contribution of exchange and charge penetration effects to their interaction energies, etc.[38] On average for the optimized π-stacked dimers (black line in Figure 4), we observe somewhat higher t_+ for sulfur-containing cores (*vs.* oxygen) and for systems with more heteroatoms (3- and 4- S atom cores *vs.* 0-2 S atoms).

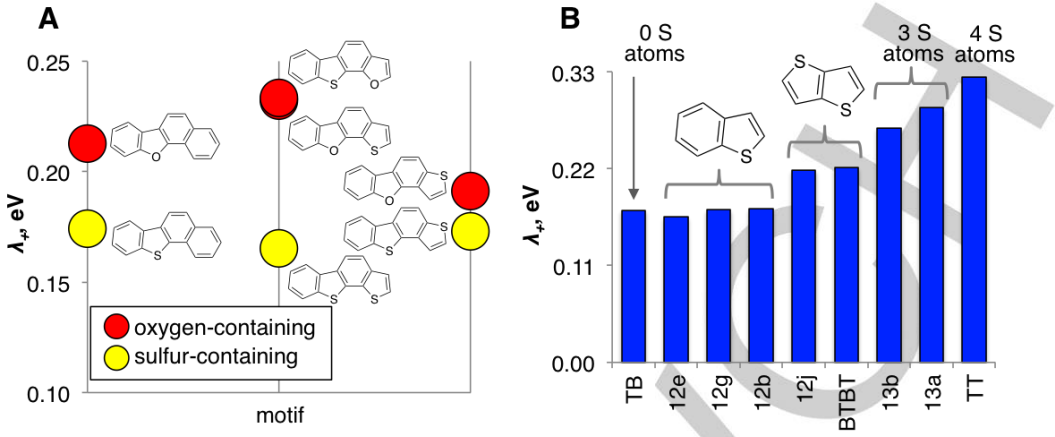


Figure 3. Reorganization energies depending of the type (**A**), number and mutual arrangement (**B**) of the heteroatoms in the core.

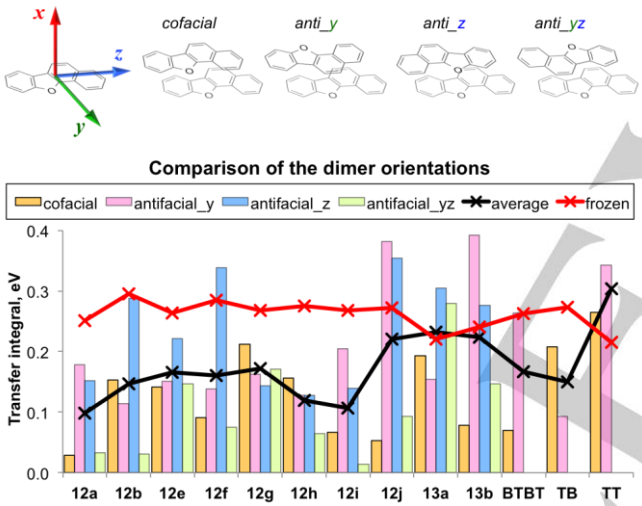


Figure 4. Various dimer geometries depending on the mutual orientation of two monomer cores (disordermer, illustrated here for **12a**) and the computed transfer integrals for the model 'frozen' and optimized dimers ('average' corresponds to the average value for the optimized disordermers).

The resulting hole mobilitites, computed for the studied dimers, are shown in Figure 5. Generally, higher mobilities are expected for systems with lower monomer reorganization energies and higher transfer integrals. Since the t_+ values in the 'frozen' model dimers are fairly similar, their mobilities are largely defined by their λ_+. Regarding the optimized dimers, the two "extreme" (from the reorganization energy perspective) compounds **TB** and **TT** give moderate mobilities: **TB** because of its average transfer integral, and **TT** because of its high λ_+. The chosen reference core, BTBT **3**, with its average t_+ and λ_+ displays a moderate computed mobility of 3.3 $cm^2V^{-1}s^{-1}$.[39] Several heterotetracenes bearing 1-3 sulfur atoms – **12b**, **12e**, **12g**, **12j** and **13b** – display comparable (μ_+ > 3.0 $cm^2V^{-1}s^{-1}$) hole transport characteristics. Considering various disordermers, the antifacial dimers afford the highest mobilities (See Table S3 in the Supporting Information), consistent with experimental observations.[36,40] Our results, based on a crude dimer model, illustrate the potential of the new heterotetracenes to achieve mobilities, comparable to or better than those already reported, and reveal that these properties depend on the type and arrangement of the heteroatoms within the monomer frame. As noted above, more sophisticated modelling based on the experimental crystal structures and, ultimately, experimental testing of these compounds in real life devices is necessary to exhaustively evaluate their performance in the molecular electronics applications.

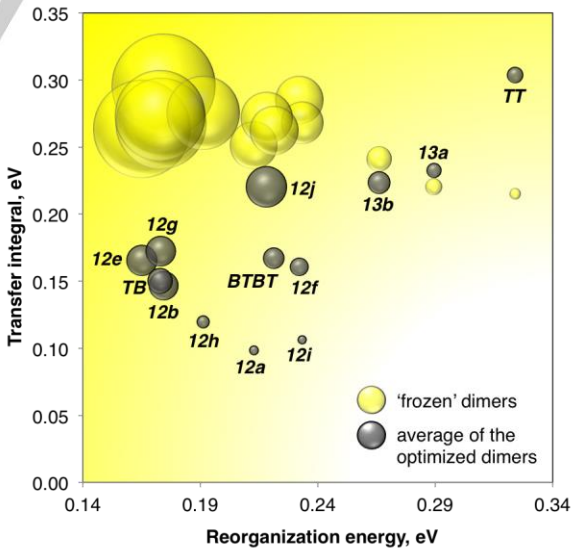


Figure 5. Computed hole mobilities (bubble sizes) for 'frozen' dimers and average between the optimized disordermers, plotted against the corresponding reorganization energies and transfer integrals. For each core, the average mobility bubble is labelled.

Conclusions

In conclusion, we have developed efficient gold- and platinum-catalyzed domino reactions to synthesize 3-alkynylated benzofurans and benzothiophenes based on the use of EBX hypervalent iodine reagents. Heterotetracenes containing two O, two S, or one O and one S heteroatoms were accessed in only four steps. Subsequent proof-of-principle computations suggest that some of the synthesized compounds and other heterotetracenes can potentially afford hole mobilities, comparable or superior to current state-of-the-art organic materials, provided they are not hampered by the crystal packing and disorder effects. The results confirmed that both the identity and position of the heteroatom in the conjugated system strongly affect the hole mobility. Our study combining improved synthetic methodologies and *in silico* analysis of the electronic structure leads to a better understanding of the relationships between the structure and charge transport properties of the heteroacenes. Further effort can now be focused on other factors (e.g. crystallization techniques, substitution patterns) that influence both the solid-state structure and the material performances of the most promising cores.[41]

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Keywords: Acenes • Domino Reactions • Hole Mobility Computation• Organic Materials • Hypervalent Iodine

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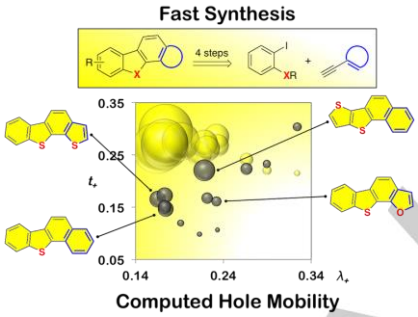
Entry for the Table of Contents (Please choose one layout)

Layout 1:

FULL PAPER

Thienoacenes and furoacenes are among the most frequent molecular units found in organic materials. Herein, we report a flexible and efficient synthesis of heterotetracenes based on a platinum- and gold- catalyzed cyclization-alkynylation domino process using EthynylBenziodoXole (EBX) hypervalent iodine reagents as key step, as well the *in silico* estimation of the synthesized tetracenes' charge transport mobilities.



Yifan Li, Ganna Gryn'ova, Felipe Saenz, Xavier Jeanbourquin, Kevin Sivula, Clémence Corminboeuf, Jérôme Waser**

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Heterotetracenes: Flexible Synthesis and *in Silico* Assessment of the Hole Transport Properties

Heterotetracenes: Flexible Synthesis and Hole Transport Assessment Based on Computations

Yifan Li,[a] Ganna Gryn'ova,[b] Felipe Saenz,[a] Xavier Jeanbourquin,[c] Kevin Sivula,[c] Clémence Corminboeuf[b]* and Jérôme Waser[a]*

(160 pages)

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1. Computational Details

Geometries of all heterotetracene and thienothiophene monomers were optimized at the PBE0/def2SVP level using Gaussian 09 software package.[1] Electronic energies of the monomers and the respective cation radicals in optimized and vertical geometries were computed at the same level of theory. Geometries of their parallel π-stacked dimers were optimized at the PBE0-dDsC[2]/def2SVP level using the development version of Q-Chem.[3] For systems with C_{2h} symmetry two dimer geometries were considered – co- and antifacial, whilst for monomers with lower symmetry four different monomer orientations in the dimer geometry were studied. For all species, vibrational frequencies analysis was performed to confirm they were the minima on the potential energy surfaces.

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The 'frozen' dimer geometry for a given core was obtained as follows: a coplanar cofacial dimer was generated from the optimized monomer geometry with zero longitudinal and transversal shifts, zero rotations and interplanar distances (*d*) in the range of 3.0-4.0Å with a step size of 0.1Å. The energy for each *d* was evaluated using the zeroth order symmetry adapted perturbation theory (SAPT0) with a jun-cc-pVDZ basis set[4] using the Psi4-Beta5 code.[5] For the lowest energy dimer, the energy decomposition analysis of the total interaction energy E_{tot} into the exchange E_{exch}, electrostatic E_{elst}, dispersion E_{disp} and induction E_{ind} components at the SAPT0/jun-cc-pVDZ level was complimented by distributed multipole analysis (DMA)[6] at the HF/6-311G** level using MOLPRO[7] and evaluation of the charge penetration, E_{CPen},[8] as the difference between E_{elst} and E_{DMA}. These analyses werfe also performed for the optimized cofacial disordermers.

The hole transport rates were estimated using the Marcus-Hush theory for the hopping charge transfer mechanism:[9]

$$\boldsymbol{k_+ = \frac{4\pi^2}{h}\frac{1}{\sqrt{4\pi\lambda_+ k_B T}} t_+^2 \exp(-\frac{\lambda_+}{4k_B T})}, \qquad \text{Eq. 1}$$

where λ_+ is the reorganization energy, t_+ is the electronic coupling (hole transfer integral), *h* is the Planck's constant, k_B is the Boltzmann constant and *T* is the absolute temperature. The reorganization energies were evaluated as

$$\boldsymbol{\lambda_+ = \left(E^{charge=0}_{cation\ geom.} - E^{charge=0}_{neutral\ geom.}\right) + \left(E^{charge=+1}_{neutral\ geom.} - E^{charge=+1}_{cation\ geom.}\right)}, \qquad \text{Eq. 2}$$

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where the electronic energies, *E*, of the charged and neutral counterparts in the optimized (adiabatic) and single-point (vertical) geometries were computed using the PBE0-D3BJ/def2SVP method. The corresponding effective transfer integrals, t_+, were computed for each dimer as

$$\boldsymbol{t_+ = \frac{J - S\frac{\varepsilon_1 + \varepsilon_2}{2}}{1 - S^2}},$$ Eq. 3

where *J* is the charge transfer integral, *S* is the overlap integral, ε_1 and ε_2 are the cite energies for the hole transport.[10] These quantities were obtained at the PBE0-dDsC/DZP level of theory using the direct quantum-mechanical approach, implemented in ADF2014,[11] which utilizes the orthogonalized orbitals of each monomer fragment as the basis for the dimer's Hamiltonian. The drift hole mobility, μ_+, were evaluated using the Einstein relation[12]

$$\boldsymbol{\mu_+ = \frac{D}{k_B T}},$$ Eq. 4

in which the diffusion coefficient of the charge carriers *D* is equal to

$$\boldsymbol{D = \frac{d^2 k_+}{2}},$$ Eq. 5

where *d* is the length of the hole transfer. This length was estimated as an average interplanar distance between the monomers in the optimized dimer geometry.

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[12] (a) Cornil, J.; Beljonne, D.; Calbert, J.-P.; Brédas, J.-L. Interchain Interactions in Organic p-Conjugated Materials: Impact on Electronic Structure, Optical Response, and Charge Transport. *Adv. Mater.* **2001**, *13*, 1053-1067. (b) Atkins, P. W. Physical Chemistry, 5th ed.; Oxford University Press: Oxford, U.K.; **1994**.

Table S1. Vertical and adiabatic ionization potentials and electron affinities, as well as the reorganization energies (all in eV), corresponding to the hole and electron transfer, computed from the PBE0/def2SVP electronic energies.

Core	*IP*		λ_+	*EA*		λ_-
	vertical	adiabatic		vertical	adiabatic	
			E_e			
12a	7.49	7.38	0.21	0.13	0.01	0.26
12b	7.43	7.34	0.17	-0.01	-0.13	0.24
12e	7.52	7.44	0.17	0.09	-0.05	0.28
12f	7.60	7.50	0.23	0.30	0.17	0.28
12g	7.49	7.41	0.17	0.29	0.18	0.24
12h	7.60	7.50	0.19	0.31	0.20	0.22
12i	7.55	7.44	0.23	0.17	0.04	0.26
12j	7.45	7.34	0.22	0.02	-0.09	0.24
13a	7.47	7.33	0.29	0.12	-0.02	0.28
13b	7.54	7.42	0.27	0.30	0.18	0.24
BTBT	7.43	7.32	0.22	-0.02	-0.17	0.29
TB	7.38	7.29	0.17	-0.12	-0.23	0.22
TT	7.33	7.17	0.32	0.06	-0.09	0.29

Table S2. Computed classical electrostatic interaction energies (E_{DMA} @ HF/6-311G**, eV), SAPT0/jun-cc-pVDZ total interaction energies and their components (eV), charge penetration energies (E_{CPen}, eV), geometrical parameters (interplanar distances d, longitudinal shifts r_{l} and transversal shifts r_{v}, Å) in the PBE0-dDsC/def2SVP optimized cofacial and 'frozen' cofacial dimer geometries.

Core	E_{DMA}	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{tot}	E_{CPen}	d	r_{l}	r_{v}
					optimized cofacial					
12a	0.11	-0.56	1.47	-0.12	-1.53	-0.75	-0.68	3.27	1.51	0.12
12b	0.09	-0.63	1.60	-0.14	-1.69	-0.86	-0.72	3.29	1.62	0.30
12e	0.08	-0.64	1.59	-0.13	-1.64	-0.81	-0.71	3.30	1.62	0.20
12f	0.09	-0.57	1.43	-0.12	-1.48	-0.74	-0.66	3.29	1.59	0.30
12g	0.09	-0.62	1.55	-0.13	-1.61	-0.81	-0.71	3.32	1.59	0.18
12h	0.11	-0.55	1.42	-0.12	-1.44	-0.70	-0.66	3.26	1.36	0.66
12i	0.10	-0.55	1.43	-0.12	-1.46	-0.70	-0.65	3.28	1.45	0.33
12j	0.06	-0.64	1.55	-0.13	-1.63	-0.85	-0.70	3.29	1.74	0.27
13a	0.10	-0.58	1.44	-0.12	-1.46	-0.72	-0.68	3.32	1.68	0.27
13b	0.05	-0.66	1.55	-0.12	-1.58	-0.81	-0.71	3.32	1.67	0.25
BTBT	0.06	-0.65	1.57	-0.13	-1.63	-0.84	-0.71	3.29	1.63	0.48
TB	0.13	-0.66	1.73	-0.16	-1.81	-0.89	-0.79	3.27	1.72	0.11
TT	0.00	-0.68	1.50	-0.11	-1.52	-0.81	-0.68	3.30	1.86	0.09
					'frozen'					
12a	0.14	-0.11	0.61	-0.02	-0.96	-0.48	-0.25	3.70	0.00	0.00
12b	0.17	-0.14	0.76	-0.03	-1.10	-0.52	-0.31	3.70	0.00	0.00
12e	0.15	-0.09	0.59	-0.03	-0.95	-0.48	-0.24	3.80	0.00	0.00
12f	0.16	-0.12	0.66	-0.03	-0.95	-0.44	-0.27	3.70	0.00	0.00

12g	0.15	-0.10	0.59	-0.03	-0.94	-0.48	-0.24	3.80	0.00	0.00
12h	0.14	-0.13	0.66	-0.03	-0.93	-0.43	-0.27	3.70	0.00	0.00
12i	0.14	-0.12	0.66	-0.03	-0.94	-0.43	-0.27	3.70	0.00	0.00
12j	0.16	-0.18	0.80	-0.03	-1.08	-0.49	-0.33	3.70	0.00	0.00
13a	0.14	-0.12	0.63	-0.03	-0.93	-0.46	-0.26	3.80	0.00	0.00
13b	0.14	-0.12	0.63	-0.03	-0.93	-0.46	-0.26	3.80	0.00	0.00
BTBT	0.14	-0.10	0.59	-0.03	-0.95	-0.49	-0.24	3.80	0.00	0.00
TB	0.18	-0.11	0.71	-0.03	-1.12	-0.55	-0.29	3.70	0.00	0.00
TT	0.13	-0.15	0.66	-0.03	-0.91	-0.44	-0.27	3.80	0.00	0.00

Table S3. Computed effective hole transfer integrals t_+ (PBE0-dDsC/DZP, in eV), hopping rates k_+ (in s^{-1}), hole mobilities μ_+ (in $cm^2V^{-1}s^{-1}$) and interplanar distances d (in Å) in the PBE0-dDsC/def2SVP optimized cofacial and various antifacial dimer geometries (disordermers), and in 'frozen' cofacial dimers.

Core	t_+	k_+	μ_+	d	t_+	k_+	μ_+	d
	cofacial				*antifacial_y*			
12a	0.029	3.84×10^{12}	0.080	3.273	0.179	1.47×10^{14}	3.030	3.254
12b	0.153	1.73×10^{14}	3.644	3.294	0.114	9.62×10^{13}	2.000	3.269
12e	0.142	1.66×10^{14}	3.529	3.303	0.152	1.90×10^{14}	3.960	3.270
12f	0.091	3.02×10^{13}	0.635	3.285	0.139	7.01×10^{13}	1.467	3.279
12g	0.213	3.38×10^{14}	7.268	3.323	0.162	1.98×10^{14}	4.266	3.332
12h	0.157	1.47×10^{14}	3.032	3.258	0.128	9.84×10^{13}	2.049	3.272
12i	0.067	1.61×10^{13}	0.339	3.282	0.204	1.50×10^{14}	3.131	3.273
12j	0.053	1.19×10^{13}	0.250	3.286	0.382	6.27×10^{14}	13.773	3.360
13a	0.193	6.93×10^{13}	1.485	3.317	0.154	4.43×10^{13}	0.955	3.330
13b	0.079	1.52×10^{13}	0.326	3.323	0.392	3.76×10^{14}	8.518	3.412
BTBT	0.070	2.04×10^{13}	0.431	3.293	0.264	2.89×10^{14}	6.182	3.316
TB	0.208	3.24×10^{14}	6.719	3.266	0.093	6.50×10^{13}	1.363	3.283
TT	0.265	8.83×10^{13}	1.869	3.298	0.343	1.48×10^{14}	3.195	3.329
	antifacial_z				*antifacial_yz*			
12a	0.153	1.07×10^{14}	2.201	3.253	0.033	5.03×10^{12}	0.102	3.226
12b	0.288	6.14×10^{14}	12.984	3.297	0.031	7.07×10^{12}	0.149	3.292
12e	0.222	4.08×10^{14}	8.609	3.293	0.147	1.79×10^{14}	3.899	3.346
12f	0.338	4.17×10^{14}	8.932	3.319	0.075	2.05×10^{13}	0.431	3.286
12g	0.144	1.54×10^{14}	3.259	3.294	0.171	2.19×10^{14}	4.803	3.358
12h	0.128	9.84×10^{13}	2.051	3.273	0.065	2.52×10^{13}	0.519	3.255
12i	0.140	6.99×10^{13}	1.456	3.271	0.014	7.47×10^{11}	0.015	3.238
12j	0.354	5.39×10^{14}	11.858	3.362	0.094	3.76×10^{13}	0.797	3.299
13a	0.305	1.73×10^{14}	3.715	3.320	0.279	1.46×10^{14}	3.035	3.271
13b	0.276	1.86×10^{14}	4.053	3.344	0.147	5.30×10^{13}	1.118	3.293
	'frozen' cofacial							
12a	0.252	2.91×10^{14}	7.747	3.700				
12b	0.296	6.45×10^{14}	17.183	3.700				
12e	0.264	5.75×10^{14}	16.171	3.800				

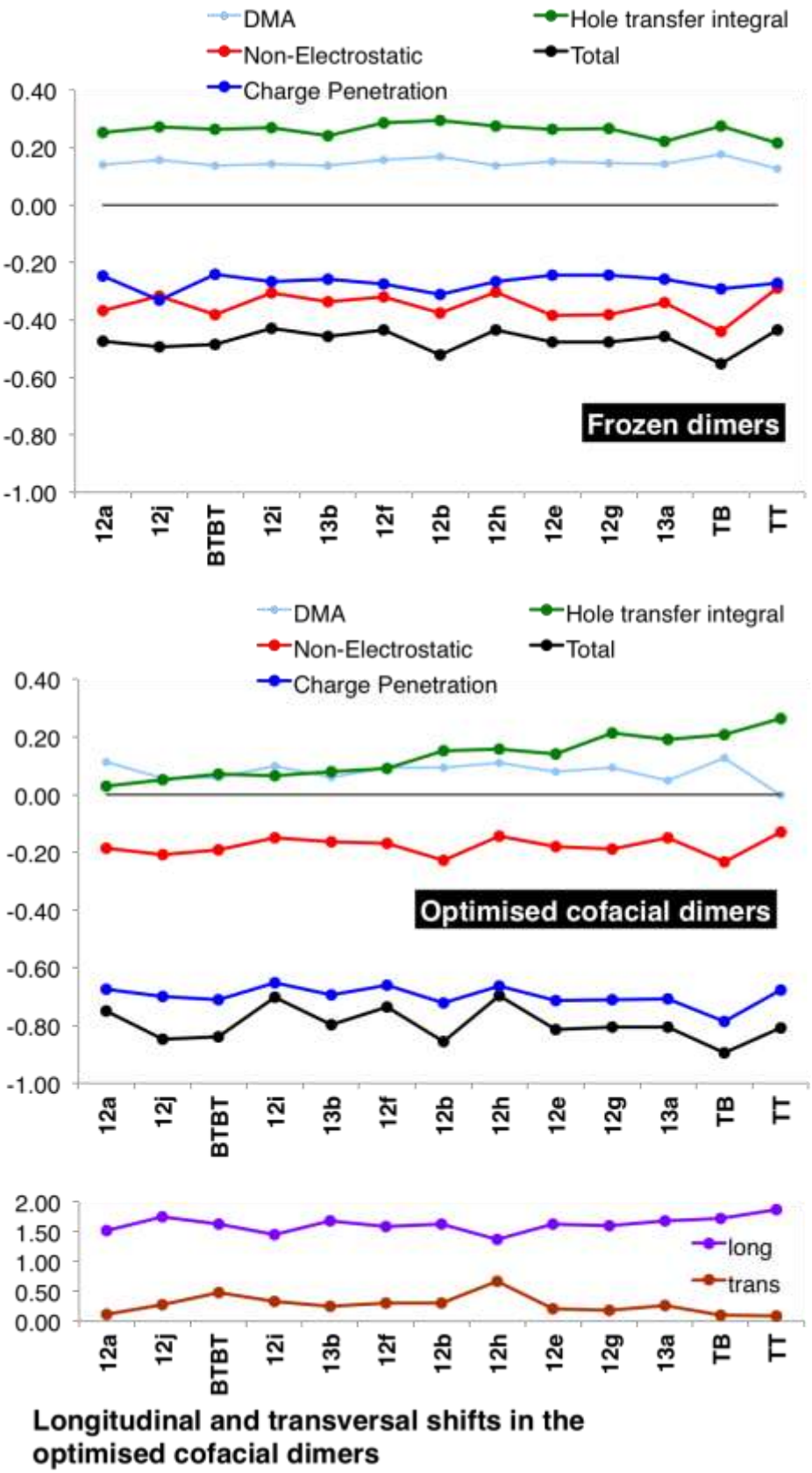
12f	0.285	2.96×10^{14}	7.876	3.700	
12g	0.267	5.36×10^{14}	15.050	3.800	
12h	0.276	4.53×10^{14}	12.081	3.700	
12i	0.268	2.58×10^{14}	6.885	3.700	
12j	0.272	3.18×10^{14}	8.462	3.700	
13a	0.221	9.08×10^{13}	2.553	3.800	
13b	0.241	1.42×10^{14}	3.989	3.800	
BTBT	0.262	2.85×10^{14}	8.016	3.800	
TB	0.274	5.62×10^{14}	14.976	3.700	
TT	0.215	5.84×10^{13}	1.641	3.800	

Table S4. Computed electronic energies and zero point vibrational energies (at the PBE0-D3BJ/def2SVP level, all in Hartrees) for the neutral, cation radical and anion radical cores in the optimized and single point neutral geometries.

geom.	0,1	0,1	+1,2	+1,2	0,1	–1,2	–1,2
c,m[a]	0,1	+1,2	+1,2	0,1	–1,2	–1,2	0,1
Core				E_e			
12a	-689.73391	-689.45881	-689.46268	-689.72996	-689.72896	-689.73370	-689.72909
12b	-1012.59053	-1012.31750	-1012.32064	-1012.58726	-1012.59085	-1012.59526	-1012.58600
12e	-1333.23795	-1332.96172	-1332.96464	-1333.23480	-1333.23455	-1333.23961	-1333.23287
12f	-1010.37952	-1010.10007	-1010.10404	-1010.37496	-1010.36835	-1010.37345	-1010.37440
12g	-1333.23865	-1332.96322	-1332.96629	-1333.23536	-1333.22789	-1333.23218	-1333.23426
12h	-1010.38146	-1010.10230	-1010.10573	-1010.37786	-1010.37012	-1010.37417	-1010.37736
12i	-1010.38045	-1010.10293	-1010.10716	-1010.37611	-1010.37408	-1010.37881	-1010.37565
12j	-1333.22718	-1332.95330	-1332.95731	-1333.22317	-1333.22638	-1333.23063	-1333.22265
13a	-1653.87435	-1653.59978	-1653.60507	-1653.86901	-1653.87005	-1653.87513	-1653.86922
13b	-1653.87506	-1653.59780	-1653.60243	-1653.86990	-1653.86418	-1653.86857	-1653.87058
BTBT	-1333.23387	-1332.96082	-1332.96484	-1333.22975	-1333.23477	-1333.24005	-1333.22855
TB	-691.87823	-691.60705	-691.61018	-691.87501	-691.88259	-691.88651	-691.87401
TT	-1974.46287	-1974.19332	-1974.19931	-1974.45696	-1974.46070	-1974.46601	-1974.45747

[a] charge, spin multiplicity

Figure S1. Results of the energy decomposition analysis and computed hole transfer integrals and geometric parameters for the optimized and 'frozen' cofacial dimers.



Longitudinal and transversal shifts in the optimised cofacial dimers

2. Hole Mobility Measurements.

To provide preliminary experimental verification of the ability of the synthesized heterotetracenes to transport holes, an estimation of the charge carrier mobility of selected molecules was performed on thin films using the space-charge limited current technique, which has been previously employed for acenes.[13] Molecules **12e** and **12f** were chosen due to the presence of the alkyl functionalization, which facilitated thin film formation. Hole-only devices were prepared on SiO_2 substrates with Au contacts in a lateral architecture.[14] Both molecules gave reproducible current-voltage behaviour, confirming the ability to conduct charges though the film (Figure S2, **A**). Correcting the current-voltage (I-V) data for contact resistance gave curves that showed the typical ohmic behaviour up to ca. 10 V,[13] and at higher voltages the data fit well to the space-charge limited currents model using the Mott-Gurney relation (Figure S2, **B**).[15]
The estimated mobility was 27.5 x 10^{-3} and 6.02 x 10^{-3} $cm^2V^{-1}s^{-1}$ for **12e** and **12f**, respectively. We note that the relative trend between the molecules corresponds well to mobility estimated by computation (Table S3). On the other hand, the measured values are nearly three orders of magnitude lower than estimated by the computational method. This is not surprising, when considering that computations were performed on well-ordered π-stacked dimers – an ideal case usually not occurring in real melt-processed thin films. Furthermore, extrinsic factors (e.g. defects and traps in the film, environment, etc.) also influence the transport efficiency.[16] When compared to BTBT (**3**), X-ray diffraction of thin films of **12e** and **12f** (See Section 9 of this supporting information) showed a smaller packing distance of the π-stacked lamella, which is probably also due to the different alkyl chain substitution. Indeed, the optimization of alkyl-side chain length and position is known to be important for thin-film charge carrier mobility, as it has a profound influence on solid-state structure.[17]

Experimental details:

Hole-only devices were fabricated using a lateral architecture with Au as hole-selective electrodes on a silicon oxide substrate. The space between the two electrodes was set to 20 µm and the contact thickness was 30 nm over a length of 1 cm. The active material was deposited by melting the materials at 140 °C before placing an OTS-treated SiO_2 substrate on top as a confining layer. Once cooled down to RT the confining layer was removed prior to measurements. Electronic testing of the device was carried out using a custom-built probe station and a Keithley 2612A unit. Device fabrication and testing was performed under inert atmosphere, respectively, in an argon and a nitrogen filled glovebox.

[13] J. E. Anthony, *Angew. Chem. Int. Ed.* **2008**, *47*, 452; c) *Handbook of Thiophene-Based Materials*, I. F. Perepichka, D. F. Perepichka, ed., Wiley-VCH, Weinheim, Germany, **2009.**
[14] O. D. Jurchescu, T. T. M. Palstra, *Appl. Phys. Lett.* **2006**, *88*, 122101.
[15] K. Takimiya, I. Osaka, T. Mori, M. Nakano, *Acc. Chem. Res.* **2014**, *47*, 1493.
[16] H. Sirringhaus, *Adv. Mater.* **2009**, *21*, 3859.
[17] J. E. Anthony, *Chem. Rev.* **2006**, *106*, 5028.

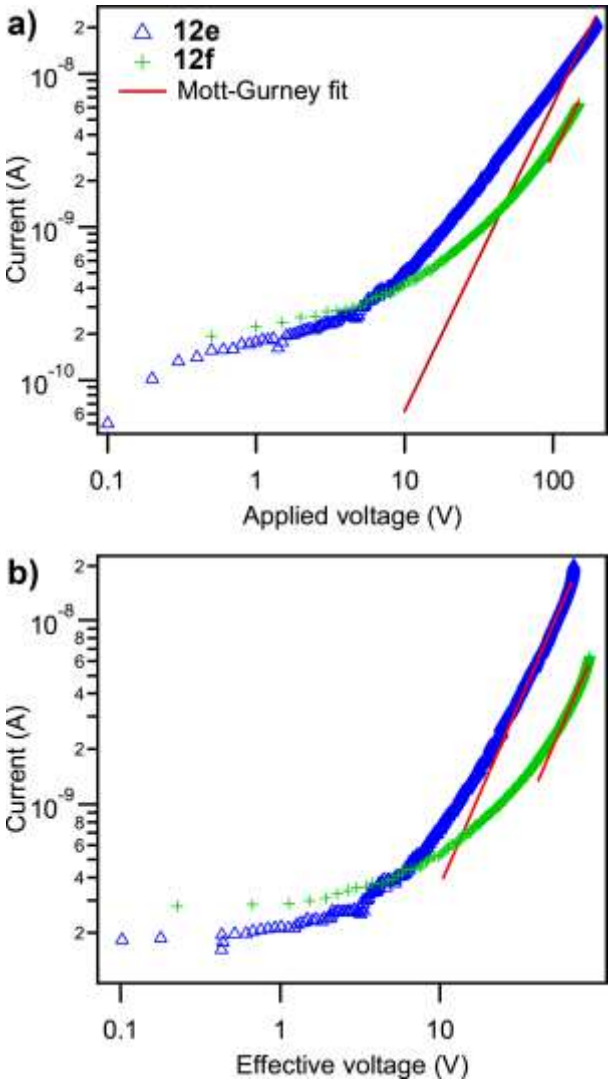


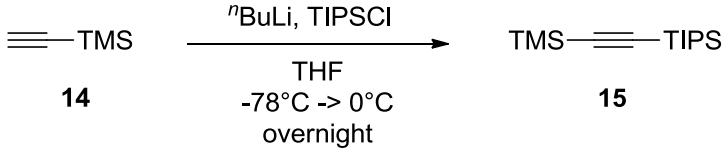
Figure S2. IV curves of hole-only diodes with **12e** and **12f** as the active layer. (a) Raw data and (b) data corrected for contact resistance. Red lines indicate the fitting.

3. General Synthetic Method.

All reactions were carried out in oven dried glassware under an atmosphere of nitrogen, unless stated otherwise. For quantitative flash chromatography technical grade solvents were used. For flash chromatography for analysis, HPLC grade solvents from Sigma-Aldrich were used. THF, Et_2O, CH_3CN, toluene, hexane and CH_2Cl_2 were dried by passage over activated alumina under nitrogen atmosphere (H_2O content < 10 ppm, *Karl-Fischer* titration). The solvents were degassed by Freeze-Pump-Thaw method when mentioned. All chemicals were purchased from Acros, Aldrich, Fluka, VWR, Aplichem or Merck and used as such unless stated otherwise. Chromatographic purification was performed as flash chromatography using Macherey-Nagel silica 40-63, 60 Å, using the solvents indicated as eluent with 0.1-0.5 bar pressure.TLC was performed on Merck silica gel 60 F_{254} TLC glass plates or aluminium plates and visualized with UV light, permanganate stain, CAN stain or Anisaldehyde stain. Melting points were measured on a Büchi B-540 melting point apparatus using open glass capillaries, the data is uncorrected. ^{1}H-NMR spectra were recorded on a Brucker DPX-400 400 MHz spectrometer in chloroform-d, DMSO-d_6 or CD_3OD, all signals are reported in ppm with the internal chloroform signal at 7.26 ppm, the internal DMSO signal at 2.50 ppm or the internal methanol signal at 3.30 ppm as standard. The data is being reported as (s = singlet, d = doublet, t = triplet, q = quadruplet, qi = quintet, m = multiplet or unresolved, br = broad signal, app = apparent, coupling constant(s) in Hz, integration, interpretation).^{13}C-NMR spectra were recorded with ^{1}H-decoupling on a Brucker DPX-400 100 MHz spectrometer in chloroform-d, DMSO-d_6 or CD_3OD, all signals are reported in ppm with the internal chloroform signal at 77.0 ppm, the internal DMSO signal at 39.5 ppm or the internal methanol signal at 49.0 ppm as standard. Infrared spectra were recorded on a JASCO FT-IR B4100 spectrophotometer with an ATR PRO410-S and a ZnSe prisma and are reported as cm^{-1} (w = weak, m = medium, s = strong, br = broad). Gas chromatographic and low resolution mass spectrometric measurements were performed on a Perkin-Elmer Clarus 600 gas chromatographer and mass spectrometer using a Perkin-Elemer Elite fused silica column (length: 30 m, diameter: 0.32 mm) and Helium as carrier gas. High resolution mass spectrometric measurements were performed by the mass spectrometry service of ISIC at the EPFL on a MICROMASS (ESI) Q-TOF Ultima API. HPLC measurement were done on a JASCO HPLC system with an AS2055 Autosampler, a PU 2089 Pump, a UV 2075 detector and a SEDEX 85 (SEDERE) detector using a CHIRALPAK IC column from DAICEL Chemical Industries Ltd. HPLC grade solvents from Sigma-Aldrich were used.

4. Preparation of Reagents.

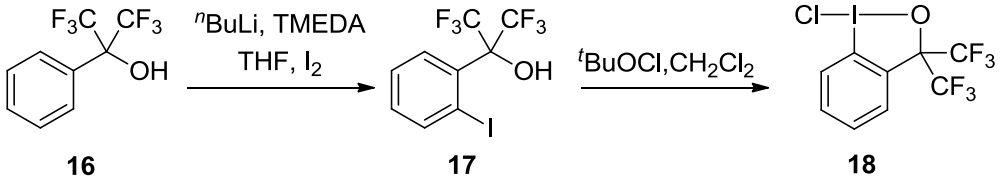
Tri*iso*propylsilyl trimethylsilylacetylene (15)



Following a reported procedure,[18] *n*-butyllithium (2.5 M in hexanes, 12.0 mL, 29.9 mmol, 0.98 equiv) was added dropwise to a stirred solution of ethynyltrimethylsilane (**14**) (3.0 g, 30 mmol, 1.0 equiv) in THF (48 mL) at -78 °C. The mixture was then warmed to 0 °C and stirred for 5 min. The mixture was then cooled back to -78 °C and chlorotri*iso*propylsilane (6.4 mL, 30 mmol, 1.0 equiv) was added dropwise. The mixture was then allowed to warm to room temperature and stirred overnight. A saturated solution of ammonium chloride (40 mL) was added, and the reaction mixture was extracted with diethyl ether (2 x 60 mL). The organic layer was washed with water and brine, then dried over $MgSO_4$, filtered and concentrated under reduced pressure to obtain a colorless liquid which was further purified by Kugelrohr distillation (56-57°C/0.25 mmHg) to yield **15** (7.16 g, 28.0 mmol, 92% yield) as colorless liquid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (m, 21 H, TIPS), 0.18 (s, 9 H, TMS). IR ν 2959 (m), 2944 (m), 2896 (w), 2867 (m), 1464 (w), 1385 (w), 1250 (m), 996 (w), 842 (s), 764 (s), 675 (m), 660 (m). Characterization data of **15** corresponded to the literature values.[18]

1-Chloro-1,3-dihydro-3,3-bis(trifluoromethyl)-1,2-benziodoxole (18)



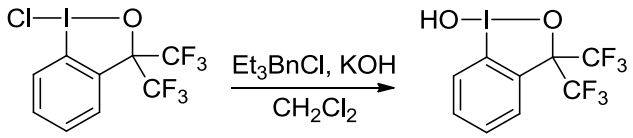
Following a reported procedure,[19] TMEDA (distilled over KOH) (1.26 mL, 8.20 mmol, 0.2 equiv) was added to a solution of ^{n}BuLi (2.5 M in hexanes, 36.6 mL, 91.6 mmol, 2.2 equiv). After 15 min, the cloudy solution was cooled to 0 °C and **16** (7.0 mL, 42 mmol, 1 equiv) in THF (6 mL) was added dropwise. The reaction was stirred 30 min at 0 °C and then at RT overnight. I_2 (11.2 g, 44.0 mmol, 1.06 equiv) was then added portion wise at 0 °C and the mixture stirred at 0 °C for 30 min and 4 h at RT. The reaction was quenched with saturated NH_4Cl. Et_2O (100 mL) was added and the layers were separated. The aqueous layer was then extracted twice with Et_2O (3 x 50 mL). The organic layers were combined, washed twice with saturated NaS_2O_3 (2 x 50 mL), dried over $MgSO_4$, filtered and reduced to afford 15.6 g of **17**as brown oil which was used without further purification.

The crude oil was dissolved in wet CH_2Cl_2 (40 mL) in the dark under air. ^{t}BuOCl (5.2 mL, 44 mmol, 1.05 equiv) was then added dropwise at 0 °C. After 30 min, the resulting suspension was filtered to afford **18** (7.30 g, 18.1 mmol, 43%) as a yellow solid. The mother liquors were carefully reduced to one third and filtered to afford **18** (3.51 g, 8.71 mmol, 21%) as a yellow

[18] C. J. Helal, P. A. Magriotis, E. J. Corey, *J. Am. Chem. Soc.***1996**, *118*, 10938.
[19] E. F. Perozzi, R. S Michalak, G. D. Figuly, W. H. Stevenson, D. Dess, M. Rose, J. C. Martin, *J. Org. Chem.* **1981**, *46*, 1049.

solid. Combined yield: 64%. Mp 167 – 169°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, 1 H, *J* = 8.4 Hz, ArH), 7.85 (m, 1 H, ArH), 7.73 (m, 2 H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.8, 132.1, 131.6, 129.7, 128.5, 122.8 (q, 289 Hz), 113.4, 84.8. Characterization data of **18** corresponded to the literature values.[19]

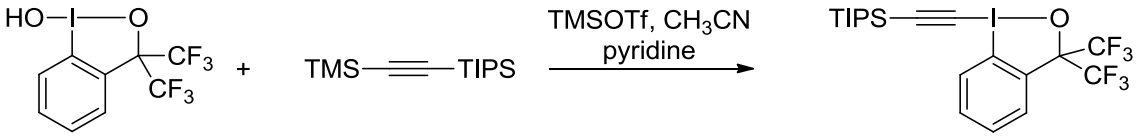
1-Hydroxy-3,3-bis(trifluoromethyl)-3-(*1H*)-1,2-benziodoxole (19)



18 **19**

Following a preported procedure,[20] Et_3BnNCl (83 mg, 0.36 mmol, 0.05 equiv) was added to a stirring solution of **18** (10.7 g, 26.5 mmol, 1 equiv) in CH_2Cl_2 (150 mL) and KOH (1.48 g, 26.5 mmol, 1 equiv) in water (28 mL). The reaction was kept under air until TLC indicated that all starting material was consumed. The organic layer was separated and dried over $MgSO_4$. The resulting solid was purified over a silica plug eluting with EtOAc, then recristallized in EtOAC and washed with pentane to afford **19** (7.42 g, 19.2 mmol, 73%) as white solid. ^{1}H NMR (400 MHz, DMSO) δ 7.96 (m, 2 H, ArH), 7.73 (m, 2 H, ArH). ^{13}C NMR (101 MHz, DMSO) δ 133.3, 131.0, 130.8, 128.9, 127.9, 123.4 (q, *J* = 290 Hz), 117.2, 83.7 (m). IR 1464 (w), 1435 (w), 1290 (w), 1263 (m), 1185 (s), 1139 (s), 1103 (m), 1041 (w), 1021 (w), 952 (s), 760 (m), 730 (m), 692 (m).

1-[(Tri*iso*propylsilyl)ethynyl]-3,3-bis(trifluoromethyl)-3(*1H*)-1,2-benziodoxole (7a)



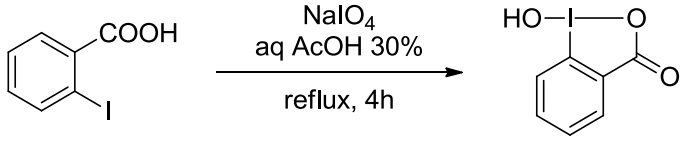
19 **15** **7a**

TMSOTf (3.80 g, 17.1 mmol, 1.1 equiv) was added to **19** (6.00 g, 15.5 mmol, 1.0 equiv) in CH_2Cl_2 (200 mL) at RT. After 20 min, the solution was concentrated at 0 °C under reduced pressure. After evaporation of the solvent, the reaction flask was directly filled with Ar, to prevent decomposition of the hygroscopic triflate intermediate. Then the resulting yellow solid was dissolved in CH_3CN (200 mL). (Trimethylsilyl)(tri*iso*-propylsilyl)acetylene (**15**) (5.14 g, 20.2 mmol, 1.3 equiv) was added and after 20 min several drops of pyridine was added. The reaction was then concentrated under vacuum, dissolved in Et_2O and filtered over a silica plug (eluant Et_2O). The resulting solid was recrystallized from pentane to afford **7a** (5.43 g, 9.87 mmol, 64%) as white crystals.

Rf (PET/Et_2O 95/5): 0.4. Mp 131 – 132°C. ^{1}H NMR (400 MHz, $CDCl_3$) (*ca* 0.10 mmol/mL) δ 8.36 (dd, 1 H, *J* = 7.9, 1.7 Hz, ArH), 7.84 (d, 1 H, *J* = 6.7 Hz, ArH), 7.68 (m, 2H, ArH), 1.15 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.7, 131.1, 129.9, 129.9 (m), 128.2, 123.6 (q, 288 Hz), 112.1, 110.8, 81.4 (m), 69.7, 18.5, 11.2. IR 2947 (m), 2868 (m), 2249 (w), 1566 (w), 1465 (m), 1438 (w), 1387 (w), 1264 (s), 1218 (m), 1184 (s), 1149 (s), 1071 (w), 994 (w), 951 (s), 910 (m), 873 (w), 732 (s), 696 (s), 655 (s), 655 (s). HRMS(ESI) calcd for $C_{20}H_{26}OF_6ISi^+$ (M+H) 551.0702, found 551.0723.

[20] A. J. Blake, A. Novak, M. Davies, R. I. Robinson, S. Woodward, *Synth. Commun.* **2009**, *39*, 1065.

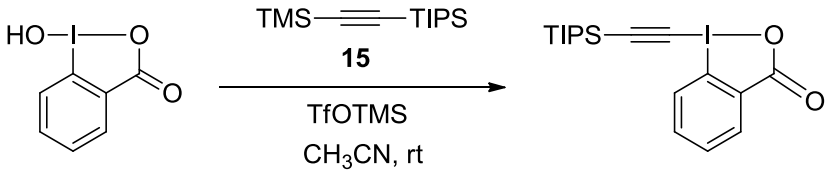
1-Hydroxy-1,2-benziodoxol-3-(1*H*)-one (21)



20 **21**

Following the reported procedure,[21] $NaIO_4$ (7.24 g, 33.8 mmol, 1.05 equiv) and 2-iodobenzoic acid (**20**) (8.00 g, 32.2 mmol, 1.00 equiv) were suspended in 30% (v:v) aq. AcOH (48 mL). The mixture was vigorously stirred and refluxed for 4 h. The reaction mixture was then diluted with cold water (180 mL) and allowed to cool to rt, protecting it from light. After 1 h, the crude product was collected by filtration, washed on the filter with ice water (3 x 20 mL) and acetone (3 x 20 mL), and air-dried in the dark to give the pure product **21** (8.3 g, 31 mmol, 98%) as colorless solid.
^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.02 (dd, 1 H, *J* = 7.7, 1.4 Hz, ArH), 7.97 (m, 1 H, ArH), 7.85 (dd, 1 H, *J* = 8.2, 0.7 Hz, ArH), 7.71 (td, 1 H, *J* = 7.6, 1.2 Hz, ArH); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 167.7, 134.5, 131.5, 131.1, 130.4, 126.3, 120.4; IR ν 3083 (w), 3060 (w), 2867 (w), 2402 (w), 1601 (m), 1585 (m), 1564 (m), 1440 (m), 1338 (s), 1302 (m), 1148 (m), 1018 (w), 834 (m), 798 (w), 740 (s), 694 (s), 674 (m), 649 (m); Characterization data of **16** corresponded to the literature values.[21]

1-[(Tri*iso*-propylsilyl)ethynyl]-1,2-benziodoxol-3(1*H*)-one (TIPS-EBX, 7b)



21 **7b**

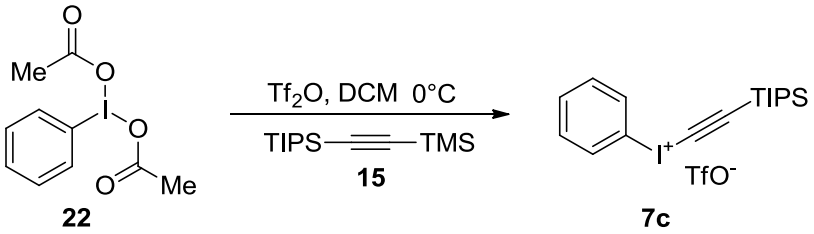
Following a reported procedure,[22] 2-iodosylbenzoic acid (**21**) (21.7 g, 82.0 mmol, 1.0 equiv) was charged in oven-dried three-neck 1L flask equipped with a magnetic stirrer. After 3 vacuum/nitrogen cycles, anhydrous acetonitrile (500 mL) was added via canula and cooled to 0 °C. Trimethylsilyltriflate (16.4 mL, 90.0 mmol, 1.1 equiv) was added dropwise via a dropping funnel over 30 min (no temperature increase was observed). After 15 min, (trimethylsilyl)(tri*iso*propylsilyl)acetylene (**15**) (23.0 g, 90.0 mmol, 1.1 equiv) was added via canula over 15 min (no temperature increase was observed). After 30 min, the suspension became an orange solution. After 10 min, pyridine (7.0 mL, 90 mmol, 1.1 equiv) was added via syringe. After 15 min, the reaction mixture was transferred in a one-neck 1L flask and reduced under vacuum until a solid was obtained. The solid was dissolved in DCM (200 mL) and transferred in a 1L separatory funnel. The organic layer was added and washed with 1 M HCl (200 mL) and the aqueous layer was extracted with CH_2Cl_2 (200 mL). The organic layers were combined, washed with a saturated solution of $NaHCO_3$ (2 x 200 mL), dried over $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. Recrystallization from acetonitrile (*ca* 120 mL) afforded **7b** (30.1 g, 70.2 mmol, 86%) as colorless crystals.

Melting point (Dec.) 170-176°C

[21] L. Kraszkiewicz, L. Skulski, *Arkivoc*, **2003**, *6*, 120.
[22] J. P. Brand. J. Waser, *Angew. Chem., Int. Ed.* **2009**, *49*, 7304.

^{1}H NMR (400 MHz, CDCl3) δ 8.44 (m, 1 H, ArH), 8.29 (m, 1 H, ArH), 7.77 (m, 2 H, ArH), 1.16 (m, 21 H, TIPS). ^{13}C NMR (100 MHz, CDCl3) δ 166.4, 134.6, 132.3, 131.4, 131.4, 126.1, 115.6, 114.1, 64.6, 18.4, 11.1. IR ν 2943 (m), 2865 (m), 1716 (m), 1618 (m), 1604 (s), 1584 (m), 1557 (m), 1465 (m), 1439 (w), 1349 (m), 1291 (m), 1270 (w), 1244 (m), 1140 (m), 1016 (m), 999 (m), 883 (m), 833 (m), 742 (m), 702 (s), 636 (m); Melting point (Dec.) 170-176°C; Characterization data of **7b** corresponded to the literature values.[22]

Phenyl(tri*iso*propylsilyl)iodonium triflate (7c)



22 **15** **7c**

Following a slight modification of the reported procedure,[23] phenyliodonium diacetate (**22**) (2.53 g, 7.85 mmol, 1.00 equiv) was diluted with DCM (7 mL) and the mixture was stirred for 5 minutes. Tf_2O (0.60 mL, 3.9 mmol, 0.50 equiv.) was added dropwise at 0 °C and the resulting yellow mixture was stirred 30 min. (Trimethylsilyl)(tri*iso*propylsilyl)acetylene (**15**) (2.00 g, 7.86 mmol, 1.00 equiv) was added and the mixture was then stirred 2 h. Water was then added (30 mL) followed by extraction of the aqueous layer with DCM (2 x 30 mL). The combined organic layers were dried over $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. The resulting solid was triturated in hexane (10 mL). Filtration and removal of solvent *in vacuo* afforded phenyl(tri*iso*propylsilyl)iodonium triflate (**7c**) (2.90 g, 11.2 mmol, 70% yield) as colorless solid.

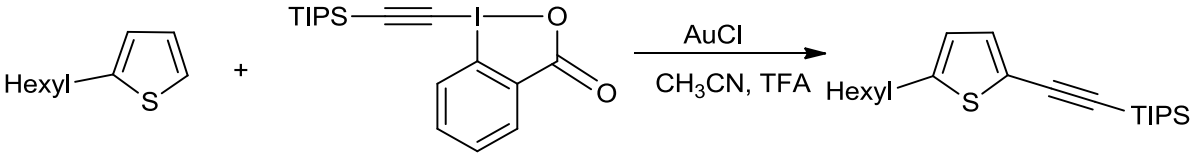
Melting point: 109 – 114°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (m, 2 H, ArH), 7.65 (m, 1 H, ArH), 7.52 (m, 2 H, ArH), 1.15-1.01 (m, 21 H, TIPS); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.7, 132.5, 132.4, 119.7, 117.6, 117.6, 44.9, 18.3, 11.1; IR ν 3288 (w), 3088 (m), 2949 (m), 2894 (m), 2869 (w), 1563 (m), 1467 (w), 1451 (w), 1388 (w), 1281 (s), 1236 (s), 1221 (s), 1174 (s), 1068 (w), 1028 (s), 988 (m), 916 (m), 884 (m), 736 (s), 679 (m), 639 (s); HRMS (ESI) calcd for $C_{17}H_{26}ISi^{+}$ (M-OTf) 385.0843; found 385.0812; Characterization data of **7c** corresponded to the literature values.[22]

[23] T. Kitamura, M. Kotani, Y. Fujiwara, Y, *Synthesis*, **1998**, *10*, 1416.

5. Synthesis of starting materials

((5-Hexylthiophen-2-yl)ethynyl)tri*iso*propylsilane (24)

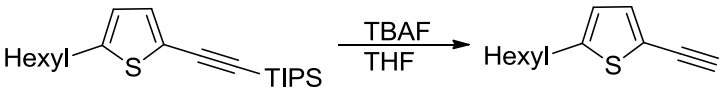


23 **7b** **24**

According to our previous report,[24] 2-hexylthiophene (**23**) (72 µL, 0.40 mmol, 1 equiv) was added to a stirring solution of AuCl (4.6 mg, 0.020 mmol, 0.05 equiv) in CH_3CN (2 mL) under air. After 2 min, TFA (36 µL, 0.48 mmol, 1.2 equiv) and **7b** (206 mg, 0.480 mmol, 1.2 equiv) were added. The reaction was sealed and stirred at RT for 14 h. Et_2O (10 mL) was added, the organic layer was washed twice with 0.1 M NaOH (15 mL). The aqueous layers were combined and extracted with Et_2O (20 mL). The organic layers were combined, washed with saturated $NaHCO_3$ (20 mL), brine (20 mL), dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (pentane) to afford **24** (116 mg, 0.333 mmol, 83%) as slightly yellow oil.

^{1}H NMR δ 7.08 (d, *J* = 3.5 Hz, 1 H, ArH), 6.65 (d, *J* = 3.5 Hz, 1 H, ArH), 2.80 (t, *J* = 7.5 Hz, 2 H, hexylH), 1.68 (m, 2 H, hexylH), 1.44-1.30 (m, 6 H, hexylH), 1.15 (m, 21 H, TIPS), 0.93 (t, *J* = 6.1 Hz, 3 H, hexylH). ^{13}C NMR δ 148.1, 132.4, 123.9, 121.0, 99.8, 94.3, 31.7, 31.6, 30.2, 28.7, 22.6, 18.7, 14.1, 11.4. Characterization data of **24** corresponded to the literature values.[24]

((5-Hexylthiophen-2-yl)ethynyl)tri*iso*propylsilane (25)



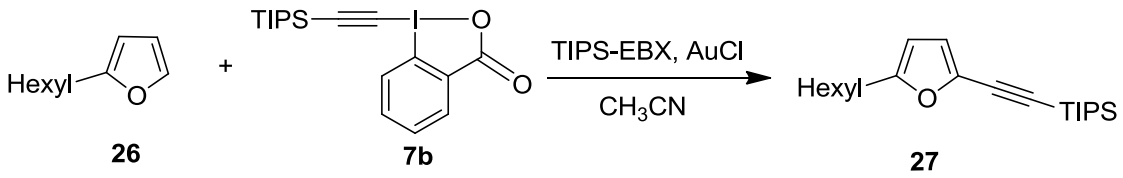
24 **25**

TBAF (1 M in THF, 0.98 mL, 0.98 mmol, 1.1 equiv) was added to a stirring solution of ((5-hexylthiophen-2-yl)ethynyl)tri*iso*propylsilane (**24**) (311 mg, 0.890 mmol, 1 equiv) in THF (10 mL) at 0 °C. After 1 h, a saturated solution of NH_4Cl (20 mL) was added. The mixture was extracted three times with Et_2O (3 x 20 mL). The organic layers were then combined, washed twice with saturated NH_4Cl, brine, dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (pentane) to afford **25** (157 mg, 0.816 mmol, 92 %) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.10 (d, *J* = 3.6 Hz, 1 H, ArH), 6.64 (td, *J* = 3.6 Hz, 0.8 Hz, 1 H, ArH), 3.30 (s, 1 H, CH), 2.78 (t, *J* = 7.6 Hz, 2 H, CH_2), 1.66 (m, 2 H, CH_2), 1.33 (m, 6 H, CH_2), 0.90 (m, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 148.6, 133.1, 124.0, 119.2, 80.4, 77.5, 31.5, 31.5, 30.2, 28.7, 22.6, 14.1. Characterization data of **25** corresponded to the literature values.[24]

((5-Hexylfuran-2-yl)ethynyl)triisopropylsilane (27)

[24] J. P. Brand, J. Waser, *Angew. Chem., Int. Ed.* **2010**, *49*, 7304.

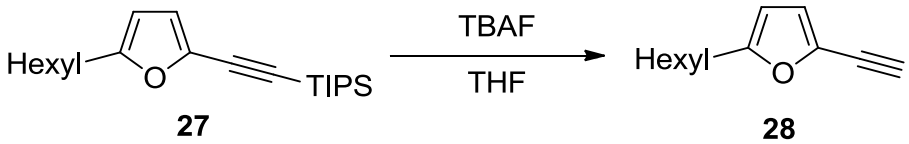


26 **7b** **27**

According to our previous report.[25] **7b** (206 mg, 0.480 mmol, 1.20 equiv), AuCl (4.6 mg, 0.020 mmol, 0.050 equiv) and **26** (0.40 mmol, 1.0 equiv) were added into CH_3CN (1.0 mL) under air. The mixture was stirred for 26 hours at room temperature. The organic layer was washed with 1 M HCl (20 mL), the aqueous layer was extracted with CH_2Cl_2 (20 mL). The combined organic layers were washed with saturated Na_2CO_3 aqueous solution (20 mL), brine (20 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash column chromatography (SiO_2; Pentane) to afford **27** as yellow oil (119 mg, 0.360 mmol, 90%).

^{1}H NMR (400MHz, $CDCl_3$) δ 6.50 (d, 1 H, *J* = 3.3 Hz, furanH), 5.95 (d, 1 H, *J* = 3.2 Hz, furanH), 2.60 (t, 2 H, *J* = 7.6 Hz, hexylH), 1.63 (t, 2 H, *J* = 6.9 Hz, hexylH), 1.32 (m, 6 H, hexylH), 1.12 (m, 21 H, TIPS), 0.89 (m, 3 H, hexylH); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 135.4, 116.7, 105.9, 96.7, 95.3, 31.5, 28.8, 28.3, 27.8, 22.5, 18.6, 14.0, 11.3. Characterization data of **27** corresponded to the literature values.[25]

2-Ethynyl-5-hexylfuran (28)

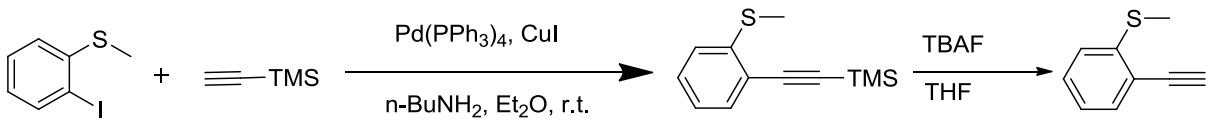


27 **28**

TBAF (1 M in THF, 0.48 mL, 0.48 mmol, 1.2 equiv) was added into a solution of **27** (133 mg, 0.400 mmol, 1.0 equiv) and dry THF (5 mL) at 0 °C. A saturated solution of NH_4Cl (20 mL) was added into the solution after 1 h. The aqueous layer was extracted with Et_2O (3 x 10 mL). The combined organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (pentane) to afford **28** (55 mg, 0.31 mmol, 78%) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (d, 1 H, *J* = 3.3, furanH), 5.96 (dt, 1 H, *J* = 3.3, 0.8 Hz, furanH), 3.39 (s, 1 H, CH), 2.60 (t, 2 H, *J* = 7.6 Hz, hexylH), 1.64 (m, 2 H, hexylH), 1.31 (m, 6 H, hexylH), 0.89 (m, 3 H, hexylH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 134.3, 117.1, 106.0, 81.3, 74.5, 31.5, 28.8, 28.2, 27.8, 22.5, 14.0. Characterization data of **28** corresponded to the literature values. [25]

(2-Ethynylphenyl)(methyl)sulfane (27)



29 **14** **30** **31**

Following a modified procedure,[26] **14** (0.68 mL, 4.8 mmol, 1.2 equiv.) was added into a solution of $Pd(PPh_3)_4$ (0.23 g, 0.20 mmol, 0.05 equiv.), butan-1-amine (0.47 mL, 4.8 mmol,

[25] Y. Li, J. P. Brand. J. Waser, *Angew. Chem., Int. Ed.* **2013**, *52*, 6743.
[26] C. Chen, C. Chen, M. Wu, *J. Org. Chem.* **2014**, *79*, 4704.

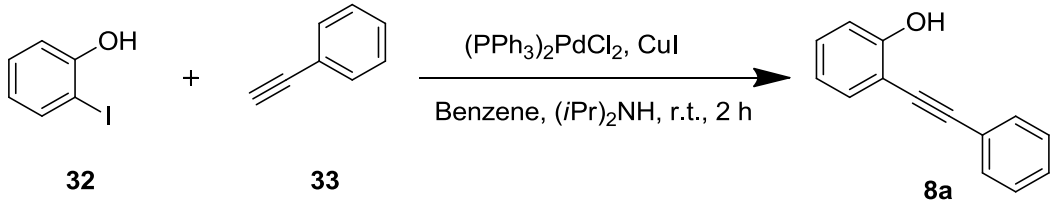
1.2 equiv.), CuI (0.076 g, 0.40 mmol, 0.1 equiv.) and **29** (1.0 g, 4.0 mmol, 1.0 equiv.) in degased Et_2O (9 mL) and the mixture was stirred overnight. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with EtOAc (2 x 10 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **30** as yellow oil (0.61 g, 2.7 mmol, 69%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (dd, 1 H, *J* = 7.6, 1.2 Hz, ArH), 7.05 (m, 1 H, ArH), 6.90 (d, 1 H, *J* = 8.0 Hz, ArH), 6.84 (td, 1 H, *J* = 7.6, 1.2 Hz, ArH), 2.24 (s, 3 H, CH_3), 0.12 (s, 9 H, TMS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 132.5, 128.9, 124.0, 123.8, 121.0, 102.2, 101.2, 14.8, 0.01.

TBAF (1 M in THF, 5.1 mL, 5.1 mmol, 1.2 equiv) was added into a solution of **30** (994 mg, 0.426 mmol, 1.0 equiv) and dry THF (4 mL) at 0 °C. A saturated solution of NH_4Cl (20 mL) was added into the solution after 1 h. The aqueous layer was extracted with Et_2O (3 x 10 mL). The combined organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (Pentane/DCM= 15:1) to afford **31** (505 mg, 3.41 mmol, 80%) as brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, 1 H, *J* = 7.6, 1.4 Hz, ArH), 7.29 (td, 1 H, *J* = 7.9, 1.5 Hz, ArH), 7.15-7.13 (m, 1 H, ArH), 7.07 (td, 1 H, *J* = 7.6, 1.4 Hz), 3.49 (s, 1 H, CH), 2.47 (s, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 132.9, 129.1, 124.0, 124.0, 120.0, 83.4, 80.9, 14.9. Characterization data of **31** corresponded to the literature values.[26]

2-(Phenylethynyl)phenol (8a)

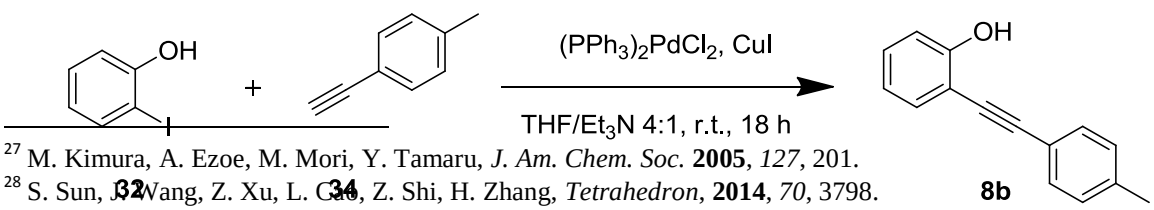


32 **33** **8a**

Following a modified procedure,[27] **33** (0.76 g, 7.5 mmol, 1.5 equiv) was added into a solution of $Pd(PPh_3)_2Cl_2$ (0.11 g, 0.15 mmol, 0.03 equiv.) , CuI (0.09 g, 0.5 mmol, 0.1 equiv), **32** (1.10 g, 5.00 mmol, 1.0 equiv) and diisopropylamine (0.71 mL, 5.0 mmol, 1.0 equiv) in degased benzene (25 mL) and the mixture was stirred for 2 h. Then, the reaction mixture was filtered on a celite pad and the solvent was removed under vacuum. The residue was dissolved in EtOAc and the resulting solution was washed with water (3 x 30 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to give **8a** as yellow oil (0.91 g, 4.7 mmol, 93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.50 (m, 2 H, ArH), 7.46-7.42 (m, 1 H, ArH), 7.39-7.35 (m, 3 H, ArH), 7.32-7.28 (m, 1 H, ArH), 7.03-6.98 (m, 1 H, ArH), 6.92 (t, 1 H, *J* = 7.6 Hz, ArH), 5.84 (s, 1 H, OH).^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 131.8, 131.8, 130.6, 129.0, 128.7, 122.5, 120.6, 114.9, 109.7, 96.5, 83.2. Characterization data of **8a** corresponded to the literature values except one carbon at 131.8 ppm was missing in the literature.[28]

2-(p-Tolylethynyl)phenol (8b)



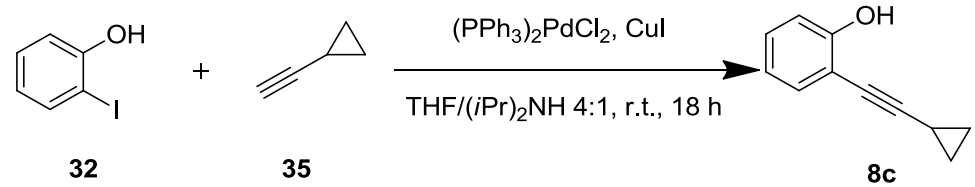
32 **34** **8b**

[27] M. Kimura, A. Ezoe, M. Mori, Y. Tamaru, *J. Am. Chem. Soc.* **2005**, *127*, 201.

[28] S. Sun, J. Wang, Z. Xu, L. Gao, Z. Shi, H. Zhang, *Tetrahedron*, **2014**, *70*, 3798.

Following a reported procedure,[29] **34** (0.23 g, 2.0 mmol, 2.0 equiv.) was added into a solution of $Pd(PPh_3)_2Cl_2$ (15 mg, 20 µmol, 0.05 equiv.), CuI (8 mg, 0.04 mmol, 0.01 equiv.) and **32** (0.22 g, 1.0 mmol, 1.0 equiv.) in degased THF (10 mL) and Et_3N (2.5 mL). The reaction mixture was stirred for 18 h. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with DCM (2 x 10 mL). The combined organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **8b** as yellow solid (0.14 g, 0.69 mmol, 69%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (m, 3 H, ArH), 7.25 (m, 1 H, ArH), 7.15 (d, 2 H, *J* = 8.0 Hz, ArH), 7.03 (d, 1 H, *J* = 8.2 Hz, ArH), 6.91 (m, 1 H, ArH), 6.12 (s, 1 H, OH), 2.35 (s, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8, 139.2, 132.0, 131.8, 130.6, 129.5, 120.7, 119.6, 115.1, 110.2, 96.8, 82.9, 21.8. Characterization data of **8b** corresponded to the literature values except one carbon at 110.2 ppm was missing in the literature.[30]

2-(Cyclopropylethynyl)phenol (8c).

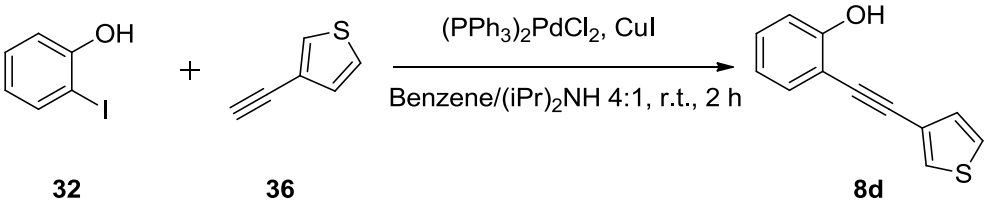


32 **35** **8c**

Following a reported procedure,[29] **32** (0.35 mL, 4.0 mmol, 2.0 equiv.) was added into a solution of $Pd(PPh_3)_2Cl_2$ (30 mg, 40 µmol, 0.02 equiv.), CuI (15 mg, 80 µmol, 0.04 equiv.) and **35** (0.44 g, 2.0 mmol, 1.0 equiv.) in degased THF (16 mL) and $(iPr)_2NH$ (4 mL) . The reaction mixture was stirred for 18 h. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with DCM (2 x 10 mL). The combined organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **8c** as yellow oil (0.11 g, 0.72 mmol, 36%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dd, 1 H, *J* = 7.7, 1.6 Hz, ArH), 7.21 (m, 1 H, ArH), 6.96 (dd, 1 H, *J* = 8.2 Hz, ArH), 6.85 (m, 1 H, ArH), 5.95 (s, 1 H, OH), 1.55-1.48 (m, 1 H, CH), 0.95-0.84 (m, 4 H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8, 131.7, 129.6, 120.2, 114.4, 110.2, 101.0, 69.7, 9.0, 0.3. Characterization data of **8c** corresponded to the literature values.[31]

2-(Thiophen-3-ylethynyl)phenol (8d)



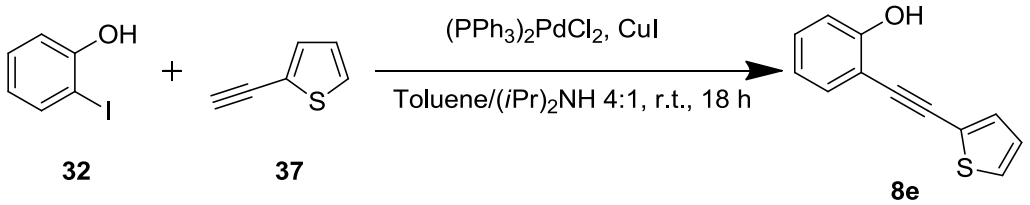
32 **36** **8d**

Following a modified procedure,[29] **36** (0.16 g, 1.5 mmol, 1.5 equiv.) was added into a solution of $Pd(PPh_3)_2Cl_2$ (0.35 g, 0.10 mmol, 0.05 equiv.), CuI (0.019 g, 0.10 mmol, 0.1 equiv.), **32** (0.22 g, 1.0 mmol, 1.0 equiv.) and diisopropylamine (0.14 mL, 1.0 mmol, 1.0 equiv.) in degased benzene (5 mL) and the mixture was stirred for 2 h. Then, the reaction mixture was

[29] R. Alvarez, C. Martinez, Y. Madich, J. G. Denis, J. M. Aurrecoechea, A. R. De Lera, *Chem. Eur. J.* **2010**, *16*, 12746.
[30] C. Martinez, R. Alvarez, J. M. Aurrecoechea, *Org. Lett*, **2009**, *11*, 1083.
[31] A. Fürstner, P. W. Davies, *J. Am. Chem. Soc.* **2005**, *127*, 15024.

filtered on a celite pad and the solvent was removed under vacuum. The residue was dissolved in EtOAc and the resulting solution was washed with water (3 x 30 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to give **8d** as brown solid (90 mg, 0.45 mmol, 45%).
Rf (Pentane / EtOAc= 10 / 1): 0.5. Melting point 113-115 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, 1 H, *J* = 2.9, 1.1 Hz, thiopheneH), 7.31 (dd, 1 H, *J* = 7.7, 1.5 Hz, ArH), δ 7.20 (dd, 1 H, *J* = 5.0, 3.0 Hz, thiopheneH). δ 7.15 (m, 1 H, ArH), δ 7.10 (dd, 1 H, *J* = 5.0, 1.1 Hz, thiopheneH), 6.88 (d, 1 H, *J* = 8.3 Hz, ArH), 6.80 (td, 1 H, *J* =7.7, 1.0 Hz, ArH), 5.77 (s, 1 H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 131.6, 130.4, 129.7, 129.2, 125.7, 121.3, 120.4, 114.7, 109.5, 91.3, 82.6. IR 3509 (w), 1578 (w), 1487 (m), 1456 (w), 1351 (w), 1029 (w), 853 (w), 784 (s), 755 (s). HRMS (ESI) calcd for $C_{12}H_9OS^+$ $[M+H]^+$ 201.0369; found 201.0371.

2-(Thiophen-2-ylethynyl)phenol (8e)



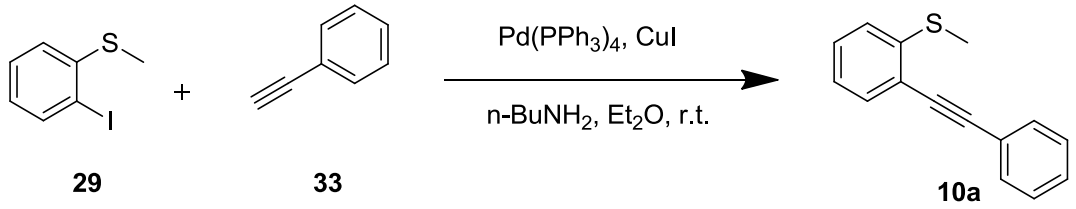
32 **37** **8e**

Following a modified procedure, [29] **37** (0.26 g, 2.4 mmol, 1.2 equiv.) was added into a solution of $Pd(PPh_3)_2Cl_2$ (0.07 g, 0.1 mmol, 0.05 equiv.), CuI (0.038 g, 0.20 mmol, 0.1 equiv.), **32** (0.44 g, 2.0 mmol, 1.0 equiv.) and diisopropylamine (0.34 mL, 2.4 mmol, 1.2 equiv.) in degased toluene (6 mL) and the mixture was stirred for 18 h. Then, the reaction mixture was filtered on a celite pad and the solvent was removed under vacuum. The residue was dissolved in EtOAc and the resulting solution was washed with water (3 x 30 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to **8e** as yellow oil (90 mg, 0.45 mmol, 45%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, 1 H, *J* = 7.7, 1.4 Hz, ArH), 7.37 (dd, 1 H, *J* = 5.2, 1.1 Hz, thiopheneH), 7.35 (dd, 1 H, *J* = 3.7. 1.1 Hz, thiopheneH), 7.30-7.27 (m, 1 H, ArH), 7.04 (dd, 1 H, *J* = 5.1, 3.7 Hz, thiopheneH), 6.98 (dd, 1 H, *J* = 8.3, 0.7 Hz, ArH), 6.91 (td, 1 H, *J* = 7.6, 1.1 Hz, ArH), 5.80 (s, 1 H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 132.5, 131.7, 130.7, 128.0, 127.2, 122.2, 120.5, 114.9, 109.3, 89.3, 86.7. Characterization data of **8e** corresponded to the literature values.[32]

<u>The procedure for the synthesis of 10a represents the general procedure for 10b-10k</u>

Methyl(2-(phenylethynyl)phenyl)sulfane (10a)



29 **33** **10a**

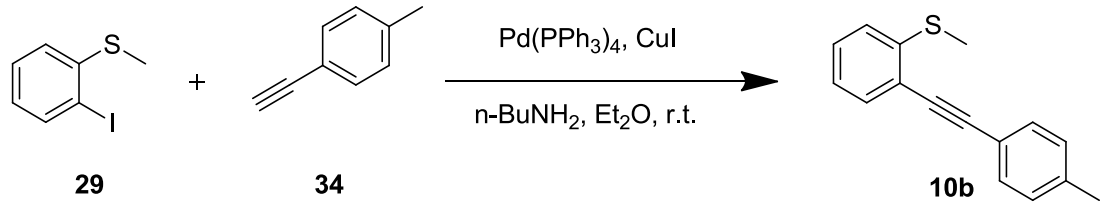
29 (0.70 mL, 5.0 mmol, 1.0 equiv.) was added into a solution of $Pd(PPh_3)_4$ (0.29 g, 0.25 mmol, 0.05 equiv.), butan-1-amine (0.59 mL, 6.0 mmol, 1.2 equiv.), CuI (0.10 g, 0.50 mmol, 0.1

[32] M. Nakamura, L. Ilies, S. Otsubo, E. Nakamura, *Angew. Chem., Int. Ed.* **2006**, *45*, 944.

equiv.) and **33** (0.66 g, 6.0 mmol, 1.2 equiv.) in degased Et_2O (15 mL) and the mixture was stirred overnight. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with EtOAc (2 x 10 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 95:5) to afford **10a** as yellow oil (1.07 g, 4.80 mmol, 95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.66 (m, 2 H, ArH), 7.56 (dd, 1 H, *J* = 7.6, 1.1 Hz, ArH), 7.46-7.32 (m, 4 H, ArH), 7.21 (d, 1 H, *J* = 7.8 Hz, ArH), 7.17-7.11 (m, 1 H, ArH), 2.56 (s, 3 H, Me).^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 132.3, 131.7, 128.9, 128.5, 128.4, 124.3, 124.2, 123.3, 121.4, 96.0, 87.0, 15.2. Characterization data of **10a** corresponded to the literature values.[33]

Methyl(2-(p-tolylethynyl)phenyl)sulfane (10b)

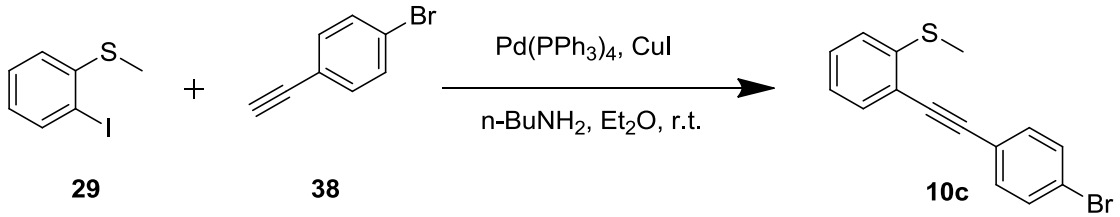


29 **34** **10b**

Following the conditions described for **10a**. Starting from **29** (0.28 mL, 2.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **10b** as yellow oil (0.28 g, 1.2 mmol, 60%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (m, 3 H, ArH), 7.29 (td, *J* = 7.5, 1.5 Hz, 1 H, ArH), 7.17 (m, 3 H, ArH), 7.11 (td, *J* = 7.5, 1.0 Hz, 1 H, ArH), 2.51 (s, 3 H, Me), 2.37 (s, 3 H, Me). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 138.7, 132.2, 131.6, 129.2, 128.7, 124.3, 124.2, 121.7, 120.2, 96.2, 86.4, 21.7, 15.2. Characterization data of **10b** corresponded to the literature values.[33]

(2-((4-Bromophenyl)ethynyl)phenyl)(methyl)sulfane (10c)



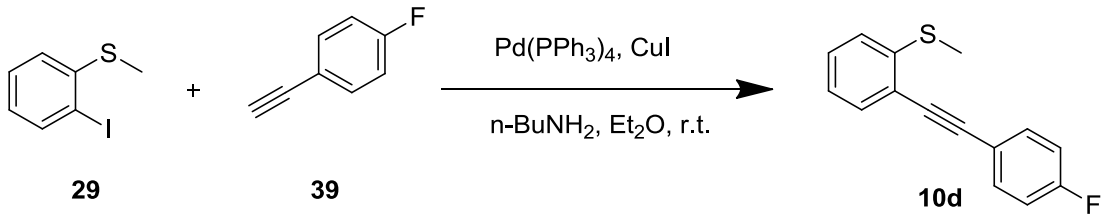
29 **38** **10c**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **10c** as yellow oil (0.26 g, 0.84 mmol, 84%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.37 (m, 5 H, ArH), 7.24 (td, *J* = 8.0, 1.5 Hz, 1 H, ArH), 7.10 (d, *J* = 8.0, 1 H, ArH), 7.05 (m, 1 H, ArH), 2.44 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 132.8, 132.0, 131.4, 128.8, 124.0, 123.8, 122.4, 121.9, 120.6, 94.6, 87.9, 14.8. Characterization data of **4c** corresponded to the literature values.[33]

[33] C. Lin, C. Chen, M. Wu, *Chem. Eur. J.* **2013**, *19*, 2578.

(2-((4-Fluorophenyl)ethynyl)phenyl)(methyl)sulfane (10d)

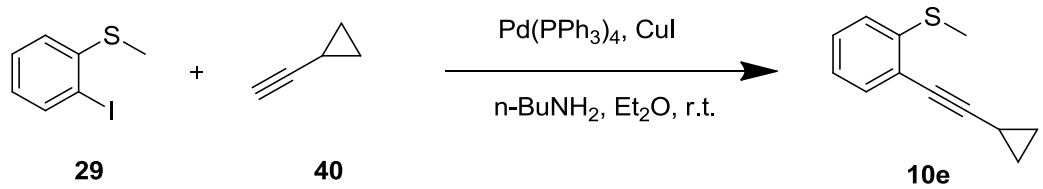


29 **39** **10d**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc 20:1) to afford **10d** as yellow oil (0.096 g, 0.40 mmol, 40%).

Rf (Pentane / EtOAc= 50 / 1): 0.1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (m, 2 H, ArH), 7.49 (dd, *J* = 7.6, 1.2 Hz, 1 H, ArH), 7.31 (m, 1 H, ArH), 7.18 (d, *J* = 7.9 Hz, 1 H, ArH), 7.12 (dd, *J* = 7.6, 0.9 Hz, 1 H, ArH), 7.06 (m, 2 H, ArH), 2.51 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5 (d, *J* = 249.6), 141.6, 133.4 (d, *J* = 8.4), 132.0, 128.7, 124.3, 124.1, 121.0, 119.2, 115.5 (d, *J* = 22.1), 94.7, 86.5, 14.9. IR 3056 (w), 2922 (w), 1598 (w), 1506 (m), 1464 (w), 1264 (w), 1228 (m), 1156 (w), 1068 (w), 836 (s), 803 (w), 741 (s). HRMS (ESI) calcd for $C_{15}H_{12}FS^{+}$ $[M+H]^{+}$ 243.0638; found 243.0638.

(2-(Cyclopropylethynyl)phenyl)(methyl)sulfane (10e)

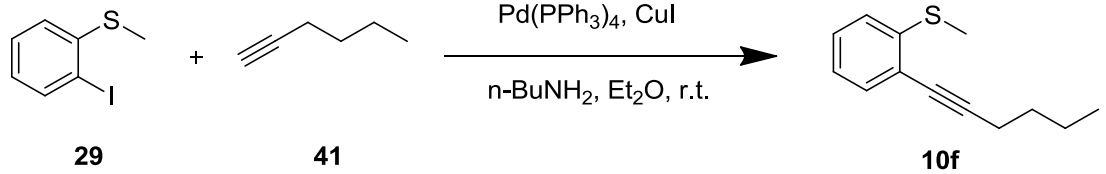


29 **40** **10e**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc/Toluene 20:1:1) to afford **10e** as yellow oil (0.10 g, 0.53 mmol, 53%).

Rf (Pentane / EtOAc/Toluene= 20 / 1/1): 0.2. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.33 (m, 1 H, ArH), 7.22 (td, 1 H, *J* = 7.9, 1.4 Hz, ArH), 7.10 (d, 1 H, *J* = 7.8 Hz, ArH), 7.04 (td, 1 H, *J* = 7.5, 1.1 Hz, ArH), 2.45 (s, 3 H, CH_3), 1.57-1.50 (m, 1 H, CH), 0.92-0.87 (m, 4 H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 132.0, 127.8, 123.9, 123.5, 121.7, 100.3, 73.0, 14.7, 8.8, 0.3. IR 3012 (w), 2958 (w), 2921 (m), 2853 (w), 2226 (w), 1464 (w), 1434 (w), 1263 (m), 1093 (w), 1064 (w), 1030 (m), 1029 (m), 954 (w), 803 (m), 745 (s). HRMS (ESI) calcd for $C_{12}H_{13}S^{+}$ $[M+H]^{+}$ 189.0732; found 189.0737.

(2-(Hex-1-yn-1-yl)phenyl)(methyl)sulfane (10f)

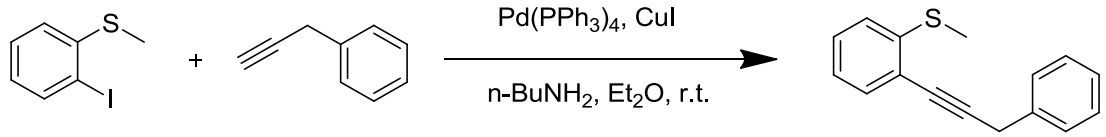


29 **41** **10f**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc/Toluene 20:1:1) to afford **10f** as yellow oil (0.096 g, 0.47 mmol, 47%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (dd, 1 H, *J* = 7.6, 1.3 Hz, ArH), 7.13 (m, 1 H, ArH) 7.00 (d, 1 H, *J* = 7.9 Hz, ArH), 6.94 (td, 1 H, *J* = 7.6, 1.3 Hz, ArH), 2.40 (t, 2 H, *J* = 6.9 Hz, C≡C*CH*$_2$), 2.35 (s, 3 H, SCH_3), 1.56-1.40 (m, 4 H, *CH*$_2$-*CH*$_2$-CH_3), 0.86 (t, 3 H, *J* = 7.3 Hz, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 132.1, 127.9, 123.9, 123.6, 121.9, 97.2, 78.0, 30.7, 21.9, 19.3, 14.8, 13.6. Characterization data of **10f** corresponded to the literature values.[34]

Methyl(2-(3-phenylprop-1-yn-1-yl)phenyl)sulfane (10g)

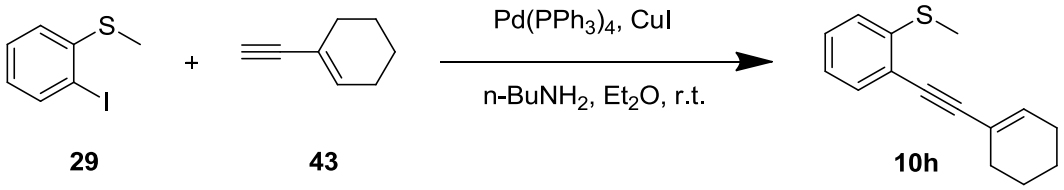


29 **42** **10g**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/DCM= 10:1) to afford **10g** as yellow oil (0.12 g, 0.49 mmol, 49%).

Rf(Pentane/DCM= 10:1):0.3. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (m, 2 H, ArH), 7.41 (dd, 1 H, *J* = 7.5, 1.1 Hz, ArH) 7.35 (t, 2 H, *J* = 7.4 Hz, ArH), 7.30-7.23 (m, 2 H, ArH), 7.15 (d, 1 H, *J* = 7.9 Hz, ArH), 7.08 (td, 1 H, *J* = 7.5, 1.1 Hz, ArH), 3.94 (s, 2 H, CH_2), 2.49 (s, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.3, 136.5, 132.4, 128.5, 128.3, 128.0, 126.6, 124.1, 123.9, 121.7, 94.2, 80.2, 26.0, 15.1. IR 3059 (w), 3033 (w), 2918 (w), 1593 (w), 1491 (w), 1460 (m), 1432 (m), 1329 (w), 1186 (w), 1077 (w), 1037 (w), 960 (w), 949 (w), 746 (s). HRMS (ESI) calcd for $C_{16}H_{15}S^+$ $[M+H]^+$ 239.0889; found 239.0896.

(2-(Cyclohex-1-en-1-ylethynyl)phenyl)(methyl)sulfane (10h)



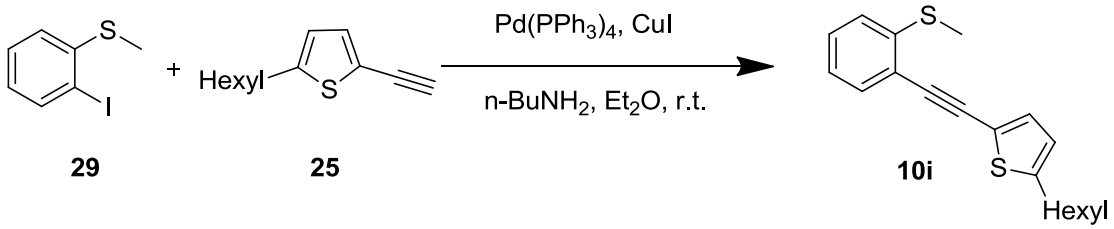
29 **43** **10h**

Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc= 10:1) to afford **10h** as yellow oil (0.11 g, 0.50 mmol, 50%).

Rf(Pentane/EtOAc= 10:1):0.3. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, 1 H, *J* = 7.6, 1.3 Hz, ArH), 7.21-7.16 (m, 1 H, ArH), 7.07 (m, 1 H, ArH), 7.00 (dd, 1 H, *J* = 7.6, 1.3 Hz, ArH), 6.21 (m, 1 H, CH), 2.41 (s, 3 H, CH_3), 2.25-2.21 (m, 2 H, CH_2), 2.12-2.08 (m, 2 H, CH_2), 1.65-1.55 (m, 4 H, CH_2-CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8, 135.0, 131.5, 127.8, 123.7, 123.5, 121.4, 120.3, 97.5, 83.9, 28.7, 25.4, 21.9, 21.1, 14.6. IR 3055 (w), 2927 (s), 2862 (m), 2361 (w), 2353 (w), 2336 (w), 2200 (w), 1581 (w), 1456 (s), 1434 (s), 1349 (w), 1272 (w), 1070 (m), 1042 (w), 791 (w). HRMS (ESI) calcd for $C_{15}H_{17}S^+$ $[M+H]^+$ 229.1045; found 229.1045.

2-Hexyl-5-((2-(methylthio)phenyl)ethynyl)thiophene (10i)

[34] S. Kim, N. Dahal, T. Kasharwani, *Tetrahedron Lett.* **2013**, *54*, 4373.

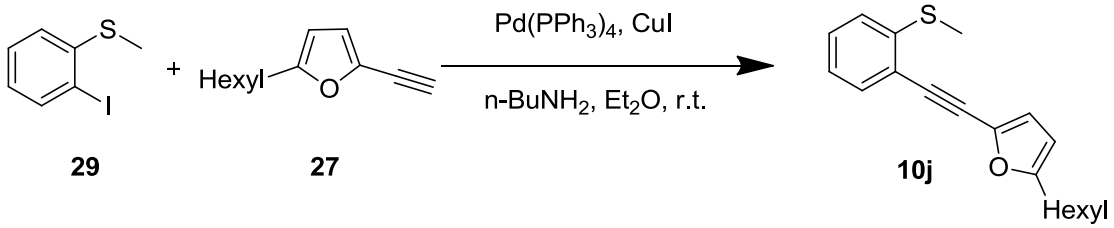


29 **25** **10i**

Following the conditions described for **10a**. Starting from **29** (0.15 g, 0.79 mmol, 1.0 equiv.) The crude product was purified by column chromatography (eluent: Pentane/EtOAc/Toluene= 23:2:1) to afford **10i** as green oil (0.10 g, 0.32 mmol, 41%).

Rf(Pentane/EtOAc/Toluene= 23:2:1):0.3. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, 1 H, *J* = 7.6, 1.2 Hz, ArH), 7.23-7.17 (m, 1 H, ArH), 7.10-7.07 (m, 2 H, ArH + ThiopheneH), 7.03 (m, 1 H, ArH), 6.62 (d, 1 H, *J* = 3.6 Hz, ThiopheneH), 2.73 (t, 2 H, *J* = 7.5 Hz, HexylH), 2.42 (s, 3 H, SCH_3), 1.61 (m, 2 H, HexylH), 1.31-1.22 (m, 6 H, HexylH), 0.84 (t, 3 H, *J* = 6.7 Hz, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 141.4, 132.1, 132.0, 128.6, 124.2, 124.2, 124.2, 121.4, 120.2, 89.8, 89.6, 31.5 (Two carbons overlap), 30.2, 28.7, 22.6, 15.1, 14.1. IR 3062 (w), 2926 (s), 2858 (m), 2201 (w), 1444 (m), 1277 (w), 1215 (w), 1071 (w), 1033 (w), 803 (m), 752 (s). HRMS (ESI) calcd for $C_{19}H_{23}S_2^+$ $[M+H]^+$ 315.1236; found 315.1236.

2-Hexyl-5-((2-(methylthio)phenyl)ethynyl)furan (10j)

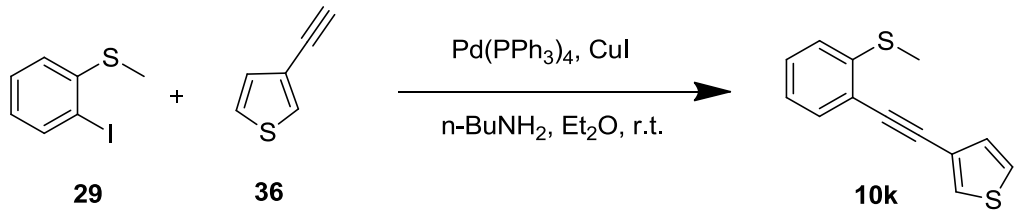


29 **27** **10j**

Following the conditions described for **10a**. Starting from **27** (0.25 g, 1.4 mmol, 1.0 equiv.) the crude product was purified by column chromatography (eluent: Pentane/DCM= 20:1) to afford **10j** as yellow oil (0.10 g, 0.34 mmol, 24%).

Rf(Pentane/DCM= 20:1):0.2. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, 1 H, *J* = 7.7, 1.3 Hz, ArH), 7.29 (td, 1 H, *J* = 7.5, 1.1 Hz, ArH), 7.18 (d, 1 H, *J* = 7.7 Hz, ArH), 7.10 (td, 1 H, *J* = 7.5, 1.1 Hz, ArH), 6.61 (d, 1 H, *J* = 3.3 Hz, FuranH), 6.02 (d, 1 H, *J* = 3.3 Hz, Furan H), 2.64 (t, 2 H, *J* = 7.5 Hz, HexylH), 2.51 (s, 3 H, SCH_3), 1.65 (m, 2 H, HexylH), 1.37-1.26 (m, 6 H, HexylH), 0.89 (t, 3 H, *J* = 6.7 Hz CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 141.4, 135.0, 132.2, 128.9, 124.3, 124.3, 120.9, 116.8, 106.4, 90.3, 86.2, 31.5, 28.8, 28.3, 27.8, 22.5, 15.2, 14.1. IR 2954 (s), 2929 (s), 2861 (m), 1698 (w), 1558 (w), 1539 (m), 1508 (w), 1461 (s), 1436 (m), 1384 (w), 1306 (w), 1305 (w), 1250 (w), 1196 (w), 1162 (w), 1070 (w), 1039 (w), 1017 (m), 960 (w), 911 (w), 883 (w). HRMS (ESI) calcd for $C_{19}H_{23}OS^+$ $[M+H]^+$ 299.1464; found 299.1467.

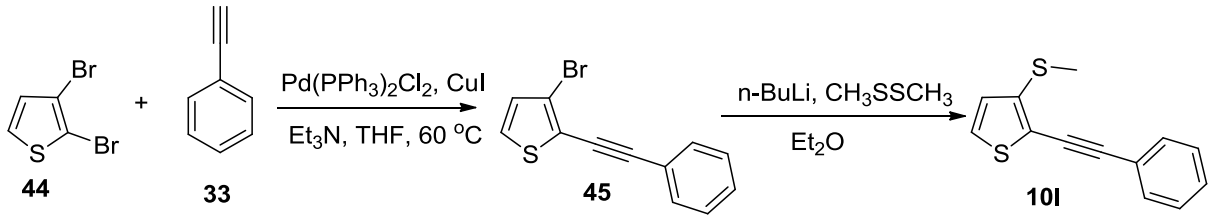
3-((2-(Methylthio)phenyl)ethynyl)thiophene (10k)



Following the conditions described for **10a**. Starting from **29** (0.14 mL, 1.0 mmol, 1.0 equiv.), the crude product was purified by column chromatography (eluent: Pentane/EtOAc= 10:1) to afford **10k** as yellow oil (0.12 g, 0.53 mmol, 53%).

Rf(Pentane/EtOAc= 10:1):0.4. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, 1 H, *J* = 3.0, 1.2 Hz, ThiopheneH), 7.34 (dd, 1 H, *J* = 7.6, 1.4 Hz, ArH), 7.16-7.13 (m, 2 H, ArH+ThiopheneH), 7.11 (td, 1 H, *J* = 5.1, 1.5 Hz, ThiopheneH), 7.01 (d, 1 H, *J* = 7.3 Hz, ArH), 6.96 (td, 1 H, *J* = 7.6, 1.4 Hz, ArH), 2.34 (s, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 132.0, 129.7, 128.6, 128.6, 125.3, 124.1, 123.9, 122.0, 121.0, 90.9, 86.3, 14.8. IR 3109 (w), 3061 (w), 2988 (w), 1731 (w), 1464 (w), 1433 (w), 1073 (w), 907 (s), 784 (m). HRMS (ESI) calcd for $C_{13}H_{11}S_2^+$ $[M+H]^+$ 231.0297; found 231.0300.

3-(Methylthio)-2-(phenylethynyl)thiophene (10l)



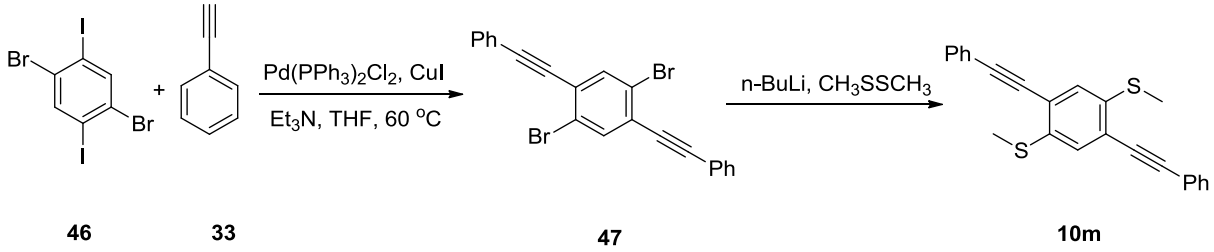
33 (0.56 g, 5.5 mmol, 1.2 equiv) was added into a solution of **44** (1.1 g, 4.6 mmol, 1.0 equiv), $Pd(PPh_3)Cl_2$ (105 mg, 0.150 mmol, 0.03 equiv) and CuI (57 mg, 0.30 mmol, 0.06 equiv) in degased Et_3N (6 mL). The mixture was kept overnight at 60 °C. The reaction was filtered through a plug of celite and the crude was purified by column chromatography (Pentane/DCM= 20:1,) to afford **45** as brown oil (0.79 g, 3.0 mmol, 65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.55 (m, 2 H, ArH), 7.38-7.36 (m, 3 H, ArH), 7.23 (d, 1 H, *J* = 5.4 Hz, ThiopheneH), 7.00 (d, 1 H, *J* = 5.4 Hz, ThiopheneH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.5, 131.5, 130.1, 128.8, 128.4, 127.0, 122.5, 116.1, 97.0, 81.0.

BuLi (0.48 mL, 1.2 mmol, 1.2 equiv) was added dropwise into a solution of **45** (0.26 g, 1.0 mmol, 1.0 equiv) in dry ether (100 mL) at -78 °C. The mixture was kept at -78 °C for 10 minutes and 0 °C for 1 hour. Then dimethyl sulfide (0.1 mL, 1.7 mmol, 1.7 equiv) was added dropwise to the mixture at 0 °C. The reaction was stirred at room temperature for 1 h and quenched with sat NH_4Cl (30 mL). The aqueous layer was extracted with Et_2O (3 x 20 mL). The organic layers were combined, washed with saturated $NaHCO_3$ (20 mL), brine (20 mL), dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (pentane/DCM=20:1) to afford **10l** (125 mg, 0.543 mmol, 54%) as yellow oil.

Rf(pentane/DCM=20:1): 0.3. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.53 (m, 2 H, ArH), 7.36-7.34 (m, 3 H, ArH), 7.26 (d, 1 H, *J* = 5.3 Hz), 6.95 (d, 1 H, *J* = 5.3 Hz), 2.57 (s, 3 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9, 131.4, 128.5, 128.3, 127.8, 126.5, 122.9, 118.6, 97.8, 81.4, 17.3. IR 3104 (w), 3082 (w), 2922 (w), 2877 (w), 2849 (w), 2199 (w), 1687 (s), 1645 (w), 1597 (w), 1503 (m), 1482 (m), 1440 (m), 1424 (m), 1403 (w), 1350 (w), 1319 (w), 1299 (w), 1266 (w), 1172 (w), 1115 (w), 1069 (w), 1027 (w), 974 (w), 916 (w), 883 (s). HRMS (ESI) calcd for $C_{13}H_{11}S_2^+$ $[M+H]^+$ 231.0297; found 231.0298.

(2,5-Bis(phenylethynyl)-1,4-phenylene)bis(methylsulfane) (10m)



46 **33** **47** **10m**

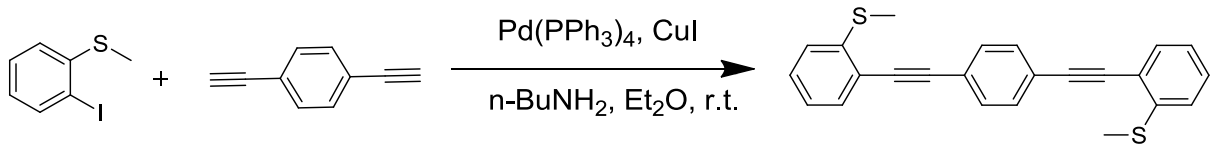
33 (0.21 g, 2.1 mmol, 2.1 equiv) was added into a solution of **46** (0.49 g, 1.0 mmol, 1.0 equiv), $Pd(PPh_3)Cl_2$ (140 mg, 0.200 mmol, 0.2 equiv) and CuI (19 mg, 0.10 mmol, 0.1 equiv) in degased Et_3N (2 mL) and THF (2 mL). The mixture was kept overnight at 60 ˚C. The reaction was filtered through a plug of celite and the crude was purified by column chromatography (Pentane) to afford **47** as white solid (0.20 g, 0.45 mmol, 45%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 2 H, ArH), 7.60-7.58 (m, 4 H, ArH), 7.40-7.37 (m, 6 H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.1, 131.9, 129.2, 128.5, 126.5, 123.8, 122.4, 96.7, 86.9.

BuLi (0.45 mL, 1.1 mmol, 2.5 equiv) was added dropwise into a solution of **47** (0.20 g, 0.45 mmol, 1.0 equiv) in dry ether (100 mL) at -78 ^{o}C. The mixture was kept at -78 ^{o}C for 10 minutes and 0 ^{o}C for 1 hour. Then dimethyl sulfide (0.12 mL, 1.3 mmol, 3.0 equiv) was added dropwise to the mixture at 0 ^{o}C. The reaction was stirred at room temperature for 1 h and quenched with sat NH_4Cl (30 mL). The aqueous layer was extracted with Et_2O (3 x 20 mL). The organic layers were combined, washed with saturated $NaHCO_3$ (20 mL), brine (20 mL), dried with $MgSO_4$ and concentrated under reduced pressure. The resulting oil was purified by flash chromatography (pentane/DCM=5:1) to afford **10m** (139 mg, 0.375 mmol, 84%) as yellow solid.

Rf(pentane/DCM=5:1): 0.4. Melting point : 162-164 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.50 (m, 4 H, ArH), 7.28-7.26 (m, 6 H, ArH), 7.20 (s, 2 H, ArH), 2.42 (s, 6 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 131.5, 128.6, 128.3, 127.8, 122.7, 121.9, 97.4, 86.7, 15.3. IR 2953 (w), 2922 (w), 2363 (m), 2343 (w), 2331 (m), 1597 (w), 1508 (w), 1494 (s), 1462 (w), 1437 (m), 1364 (w), 1265 (w), 1105 (w), 874 (w). HRMS (ESI) calcd for $C_{24}H_{19}S_2^+$ $[M+H]^+$ 371.0923; found 371.0916.

1,4-Bis((2-(methylthio)phenyl)ethynyl)benzene (10n)

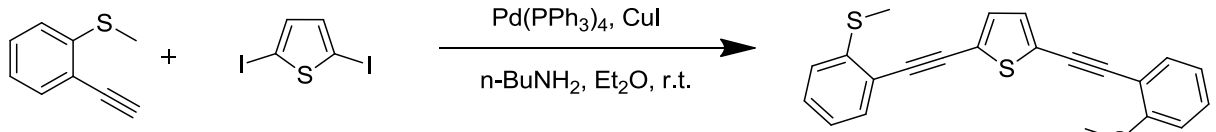


29 **48** **10n**

48 (0.13 g, 1.0 mmol, 1.0 equiv.) was added into a solution of $Pd(PPh_3)_4$ (0.12 g, 0.10 mmol, 0.1 equiv.), butan-1-amine (0.24 mL, 2.4 mmol, 2.4 equiv.), CuI (0.04 g, 0.2 mmol, 0.2 equiv.) and **29** (0.34 mL, 2.4 mmol, 2.4 equiv.) in degased Et_2O (5 mL) and the mixture was stirred overnight. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with EtOAc (2 x 10 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 5:1) to afford **10n** as green solid (0.083 g, 0.22 mmol, 22%).

Rf(pentane/DCM=5:1): 0.6. Melting point: 158-159 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 4 H, ArH), 7.49 (dd, 2 H, *J* = 7.6, 1.3 Hz, ArH), 7.34-7.30 (m, 2 H, ArH), 7.19 (d, 2 H, *J* = 7.8 Hz, ArH), 7.13 (td, 2 H, *J* = 7.6, 1.3 Hz, ArH), 2.50 (s, 6 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 132.2, 131.4, 128.9, 124.2, 124.1, 123.1, 121.0, 95.5, 88.7, 15.0. IR 2923 (m), 2858 (w), 1510 (m), 1460 (w), 1435 (m), 1164 (w), 1125 (w), 1068 (w), 1041 (w), 839 (m), 752 (s), 722 (w). HRMS (ESI) calcd for $C_{24}H_{19}S_2^+$ $[M+H]^+$ 371.0923; found 371.0925.

2,5-Bis((2-(methylthio)phenyl)ethynyl)thiophene (10o)

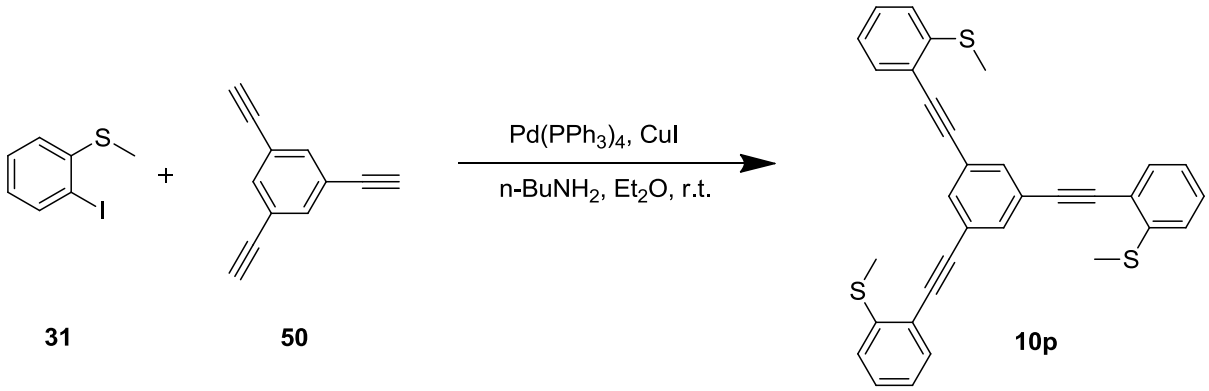


31 **49** **10o**

31 (0.13 g, 1.0 mmol, 1.0 equiv.) was added into a solution of $Pd(PPh_3)_4$ (0.085 g, 0.074 mmol, 0.1 equiv.), butan-1-amine (0.17 mL, 1.7 mmol, 2.4 equiv.), CuI (0.028 g, 0.15 mmol, 0.2 equiv.) and **49** (0.14 g, 0.40 mmol, 0.55 equiv.) in degased Et_2O (5 mL) and the mixture was stirred overnight. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with EtOAc (2 x 10 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/DCM/Toluene=10:1:1) to afford **10o** as brown solid (0.065 g, 0.17 mmol, 23%).

Rf(Pentane/DCM/Toluene=10:1:1):0.2. Melting point: 112-113 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, 2 H, *J* = 7.6, 1.2 Hz, ArH), 7.31 (td, 2 H, *J* = 7.9, 1.4 Hz, ArH), 7.19 (m, 4 H, ArH+ThiopheneH), 7.12 (td, 2 H, *J* = 7.5, 0.9 Hz, ArH), 2.42 (s, 6 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 132.2, 131.9, 129.1, 124.7, 124.3, 124.3, 120.7, 91.7, 88.5, 15.1. IR 3059 (w), 2921 (w), 2199 (w), 1587 (w), 1521 (w), 1435 (m), 1315 (w), 1274 (w), 1126 (w), 1068 (w), 1032 (w), 962 (w), 806 (m), 752 (s). HRMS (ESI) calcd for $C_{22}H_{17}S_3^+$ $[M+H]^+$ 377.0487; found 377.0488.

1,3,5-Tris((2-(methylthio)phenyl)ethynyl)benzene (10p)



50 (0.15 g, 1.0 mmol, 1.0 equiv.) was added into a solution of $Pd(PPh_3)_4$ (0.17 g, 0.15 mmol, 0.15 equiv.), butan-1-amine (0.26 mL, 3.6 mmol, 3.6 equiv.), CuI (0.06 g, 0.3 mmol, 0.3 equiv.) and **31** (0.45 mL, 3.2 mmol, 3.2 equiv.) in degased Et_2O (6 mL) and the mixture was stirred overnight. The reaction was quenched with sat. NH_4Cl (20 mL) and the aqueous layer was extracted with EtOAc (2 x 10 mL). The organic layers were dried with $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluent: Pentane/EtOAc 5:1) to afford **10p** as green solid (0.11 g, 0.22 mmol, 21%).

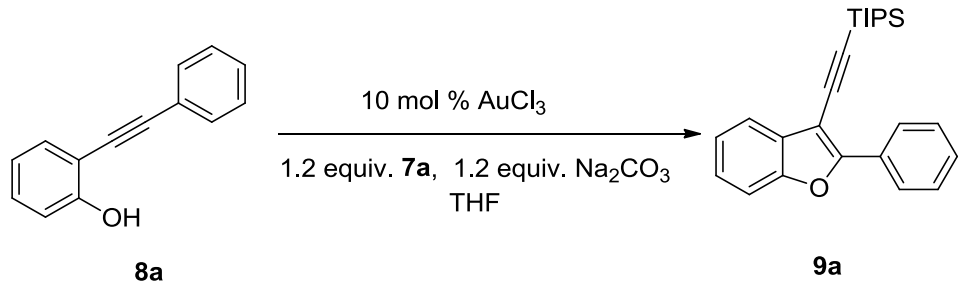
Rf(pentane/EtOAc=5:1): 0.5. Melting point: 176-177 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 3 H, ArH), 7.50 (dd, 3 H, *J* = 7.6, 1.4 Hz, ArH), 7.33 (td, 3 H, *J* = 7.8, 1.4 Hz, ArH), 7.20 (d, 3 H, *J* = 8.1 Hz, ArH), 7.13 (td, 3 H, *J* = 7.5, 1.0 Hz, ArH), 2.53 (s, 9 H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 134.1, 132.4, 129.1, 124.2, 124.1, 123.9, 120.8, 94.2, 88.0, 15.1. IR 3054 (w), 2963 (w), 2925 (s), 2858 (w), 1581 (w), 1465 (w), 1185 (w), 1154 (w), 1117 (m), 1097 (s), 1074 (w), 1025 (w), 878 (w), (w), 749 (s). HRMS (ESI) calcd for $C_{33}H_{25}S_3^+$ $[M+H]^+$ 517.1113; found 517.1125.

6. Domino Cyclization Alkynylation

General procedure 1 for the domino reaction to 3-alkynylated benzofurans-(GP1).

7a (198 mg, 0.320 mmol, 1.2 equiv)**,** Na_2CO_3 (38 mg, 0.36 mmol, 1.2 equiv) and $AuCl_3$ (9 mg, 0.03 mmol, 0.1 equiv) were added into a solution of **8** (0.3 mmol, 1 equiv) and THF (3 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up.

Triisopropyl((2-phenylbenzofuran-3-yl)ethynyl)silane (9a)

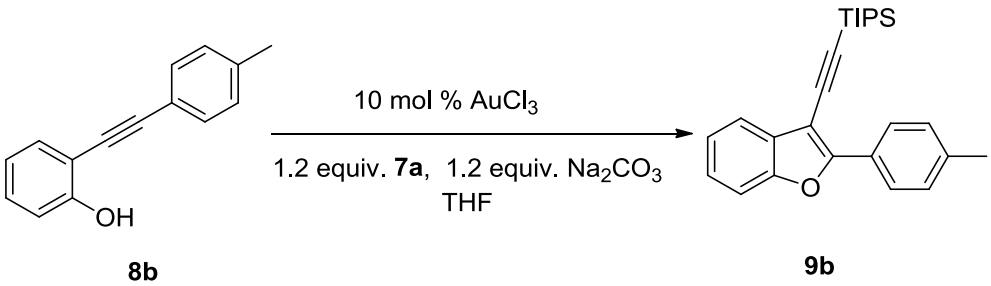


8a **9a**

Following the general procedure **GP1**, starting from **8a** (58 mg, 0.30 mmol), **9a** was obtained as yellow oil (96 mg, 0.26 mmol, 85%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40-8.33 (m, 2 H, ArH), 7.69-7.63 (m, 1 H, ArH), 7.56-7.28 (m, 6 H, ArH), 1.31 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 153.5, 130.4, 130.3, 129.3, 128.7, 126.2, 125.4, 123.5, 120.5, 111.3, 99.8, 99.7, 98.5, 18.9, 11.5. IR 2942 (s), 2865 (s), 2361 (m), 2337 (m), 2157 (w), 2063 (w), 1949 (w), 1746 (w), 1462 (m), 1373 (w), 1258 (w), 1204 (w), 1138 (m), 1071 (w), 1002 (w), 916 (w), 885 (m), 825 (w), 748 (s). HRMS (ESI) calcd for $C_{25}H_{31}OSi^+$ $[M+H]^+$ 375.2139; found 375.2139.

Triisopropyl((2-(p-tolyl)benzofuran-3-yl)ethynyl)silane (9b)



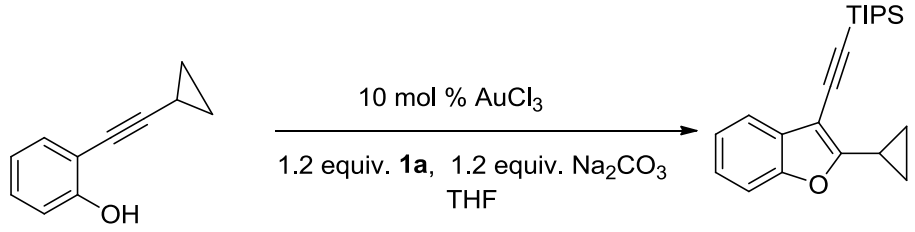
8b **9b**

Following the general procedure **GP1**, starting from **8b** (62 mg, 0.30 mmol), **9b** was obtained as yellow oil (77 mg, 0.20 mmol, 66%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, 2 H, *J* = 8.3 Hz, ArH), 7.58-7.51 (m, 1 H, ArH), 7.41-7.36 (m, 1 H, ArH), 7.23-7.15 (m, 4 H, ArH), 2.31 (s, 3 H, CH_3), 1.13 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 153.4, 139.5, 130.5, 129.4, 127.6, 126.1, 125.2, 123.4, 120.3, 111.2, 99.4, 98.9, 98.7, 21.7, 18.9, 11.5. IR 3669 (w), 2974 (m), 2966 (s),

2949 (s), 2866 (m), 2252 (w), 2155 (w), 1907 (w), 1738 (w), 1507 (w), 1456 (m), 1376 (w), 1292 (w), 1254 (m), 1205 (w), 1111 (m), 1070 (m), 1016 (m), 906 (m), 822 (m), 742 (s). HRMS (ESI) calcd for $C_{26}H_{33}OSi^+$ $[M+H]^+$ 389.2295; found 389.2301.

((2-Cyclopropylbenzofuran-3-yl)ethynyl)triisopropylsilane (9c)

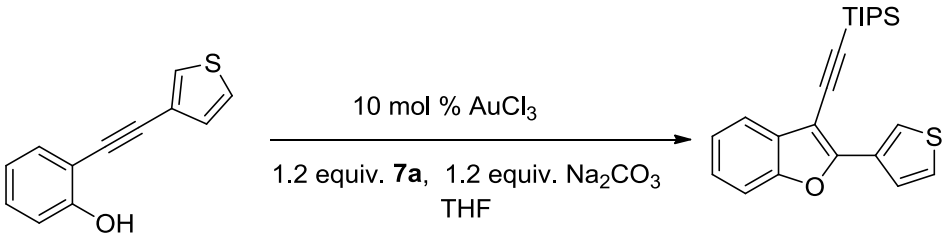


8c **9c**

Following the general procedure **GP1**, starting from **8c** (47 mg, 0.30 mmol), **9c** was obtained as yellow oil (44 mg, 0.13 mmol, 56%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.47 (m, 1 H, ArH), 7.34-7.30 (m, 1 H, ArH), 7.23-7.18 (m, 2 H, ArH), 2.31-2.21 (m, 1 H, CH), 1.27-1.07 (m, 25 H, TIPS/CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 153.0, 129.7, 124.0, 123.2, 119.5, 110.8, 99.2, 97.4, 96.5, 18.9, 11.5, 9.7, 8.1. IR 2945 (m), 2866 (m), 2254 (w), 2150 (w), 1741 (w), 1594 (w), 1461 (m), 1384 (w), 1262 (w), 1186 (w), 1134 (w), 1062 (w), 999 (w), 945 (w), 910 (m), 888 (w), 833 (w), 773 (w), 741 (s). HRMS (ESI) calcd for $C_{22}H_{31}OSi^+$ $[M+H]^+$ 339.2139; found 339.2145.

Triisopropyl((2-(thiophen-3-yl)benzofuran-3-yl)ethynyl)silane (9d)

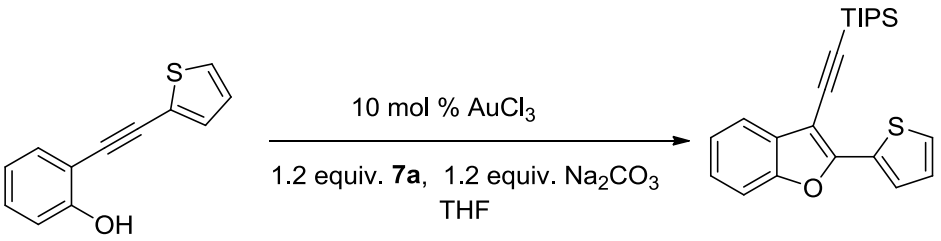


8d **9d**

Following the general procedure **GP1**, starting from **8d** (60 mg, 0.30 mmol), **9d** was obtained as yellow oil (88 mg, 0.23 mmol, 77%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, 1 H, *J* = 3.0, 1.2 Hz, ThiopheneH), 8.03 (dd, 1 H, *J* = 5.1, 1.2 Hz, ThiopheneH), 7.69-7.66 (m, 1 H), 7.51-7.49 (m, 1 H), 7.43 (dd, 1 H, *J* = 5.1, 3.0 Hz, ThiopheneH), 7.37-7.31 (m, 2 H), 1.25 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.3, 153.2, 131.7, 129.9, 125.9, 125.6, 125.1, 123.7, 123.4, 120.2, 111.0, 99.3, 98.6, 98.2, 18.8, 11.4. IR 2949 (s), 2865 (m), 2350 (w), 2337 (w), 2152 (m), 2151 (m), 1460 (m), 1341 (w), 1203 (w), 1189 (w), 1136 (w), 1067 (w), 1005 (w), 876 (s), 784 (s), 750 (s). HRMS (ESI) calcd for $C_{23}H_{29}OSSi^+$ $[M+H]^+$ 381.1703; found 381.1704.

Triisopropyl((2-(thiophen-2-yl)benzofuran-3-yl)ethynyl)silane (9e)



8e **9e**

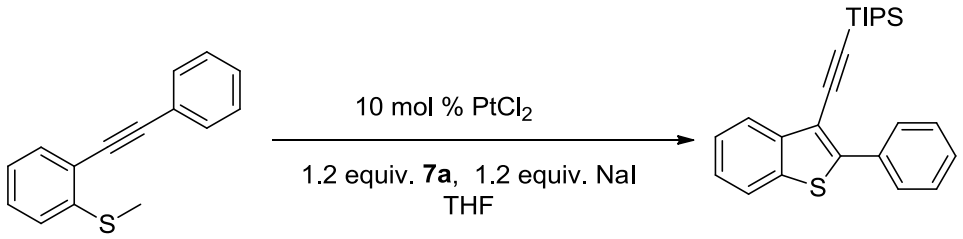
Following the general procedure **GP1**, starting from **8e** (60 mg, 0.30 mmol), **9e** was obtained as yellow oil (71 mg, 0.19 mmol, 62%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, 1 H, *J* = 3.8, 1.1 Hz, ThiopheneH), 7.63-7.61 (m, 1 H, ArH), 7.48-7.43 (m, 2 H, ArH+ThiopheneH), 7.34-7.28 (m, 2 H, ArH), 7.15 (dd, 1 H, *J* = 5.1, 3.9 Hz, ThiopheneH), 1.25 (m, 21H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 153.3, 132.4, 130.0, 127.6, 127.1, 126.6, 125.2, 123.6, 120.2, 111.1, 101.1, 98.5, 97.6, 18.8, 11.1. IR 2943 (s), 2942 (s), 2892 (m), 2865 (s), 2149 (m), 1455 (s), 1382 (w), 1368 (w), 1260 (w), 1220 (w), 1198 (m), 1181 (w), 1149 (w), 1134 (s), 1102 (w), 1073 (w), 1058 (w), 1019 (w), 998 (w), 920 (w), 909 (w), 884 (m), 854 (m), 831 (w), 830 (w). HRMS (ESI) calcd for $C_{23}H_{29}OSSi$ [M+] 381.1708; found 381.1701.

General procedure 2 for the domino reaction to 3-alkynylated benzothiophenes (GP2).

7a (198 mg, 0.360 mmol, 1.2 equiv), NaI (54 mg, 0.36 mmol, 1.2 equiv) and $PtCl_2$ (8 mg, 0.03 mmol, 0.1 equiv) were added into a solution of **10** (0.30 mmol, 1 equiv) and THF (3 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up.

Triisopropyl((2-phenylbenzo[b]thiophen-3-yl)ethynyl)silane (11a)

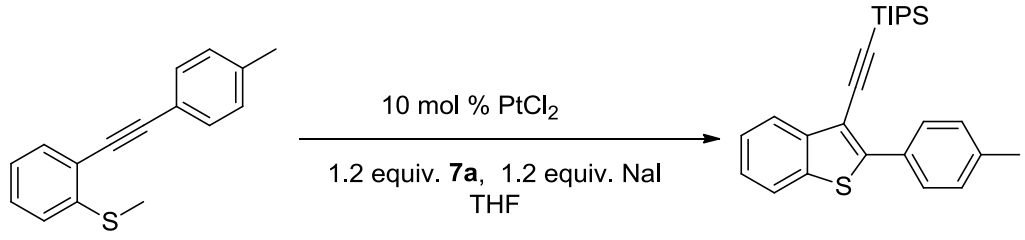


10a **11a**

Following the general procedure **GP2**, starting from **10a** (67 mg, 0.30 mmol), **11a** was obtained as yellow oil (87 mg, 0.22 mmol, 74%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.10 (m, 2 H, ArH), 7.96 (d, 1 H, *J* = 7.9 Hz, ArH), 7.80 (d, 1 H, *J* = 8.0 Hz, ArH), 7.48-7.36 (m, 5 H, ArH), 1.05 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 141.7, 137.5, 133.9, 128.9, 128.7, 128.5, 125.3, 125.1, 123.4, 122.1, 114.2, 101.2, 97.3, 18.9, 11.6. IR 3062 (w), 2940 (s), 2864 (s), 2723 (w), 2146 (m), 1748 (w), 1600 (w), 1464 (m), 1381 (w), 1285 (w), 1247 (w), 1074 (w), 997 (w), 956 (w), 885 (m), 758 (s). HRMS (APCI) calcd for $C_{25}H_{31}SSi^{+}$ $[M+H]^{+}$ 391.1910; found 391.1916.

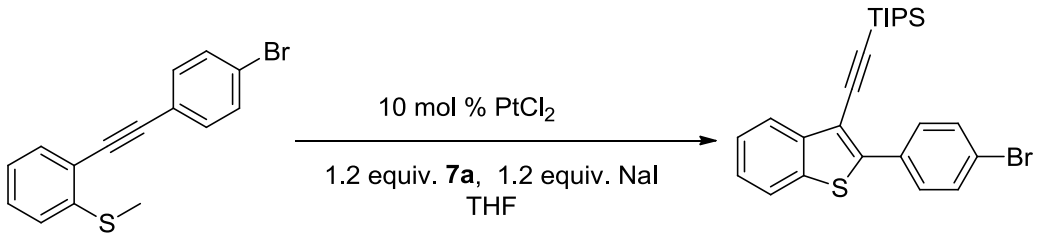
Triisopropyl((2-(p-tolyl)benzo[b]thiophen-3-yl)ethynyl)silane (11b)



10b **11b**

Following the general procedure **GP2**, starting from **10b** (72 mg, 0.30 mmol), **11b** was obtained as yellow oil (80 mg, 0.20 mmol, 66%). Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, 2 H, *J* = 8.2 Hz, ArH), 7.95 (d, 1 H, *J* = 7.9 Hz, ArH), 7.79 (d, 1 H, *J* = 8.0 Hz, ArH), 7.45 (m, 1 H, ArH), 7.37 (m, 1 H, ArH), 7.24 (d, 2 H, *J* = 8.2 Hz, ArH), 2.42 (s, 3H, CH_3), 1.20 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 141.6, 138.9, 137.2, 130.9, 129.2, 128.2, 125.0, 124.9, 123.1, 121.9, 113.4, 101.2, 97.1, 21.4, 18.8, 11.4. IR 3669 (w), 2961 (s), 2946 (s), 2867 (s), 2145 (w), 1463 (m), 1439 (w), 1400 (w), 1387 (w), 1236 (w), 1071 (s), 1054 (s), 1023 (m), 955 (w), 908 (w), 885 (m), 816 (w), 759 (w), 734 (m). HRMS (ESI) calcd for $C_{26}H_{33}SSi^{+}$ $[M+H]^{+}$ 405.2067; found 405.2068.

((2-(4-Bromophenyl)benzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11c)

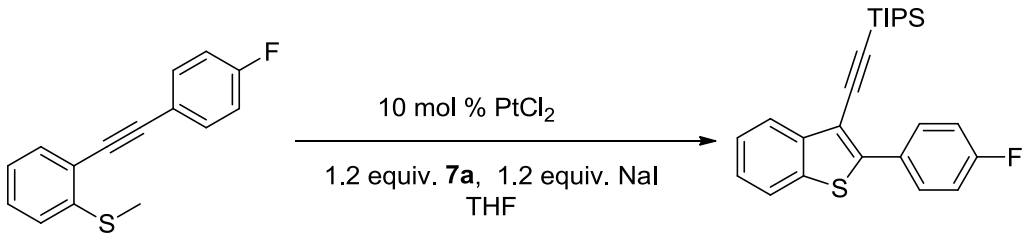


10c **11c**

Following the general procedure **GP2**, starting from **10c** (91 mg, 0.30 mmol), **11c** was obtained as yellow oil (85 mg, 0.18 mmol, 60%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.85 (m, 3 H, ArH), 7.79 (d, 1 H, *J* = 7.9 Hz, ArH), 7.56 (m, 2 H, ArH), 7.47 (m, 1 H, ArH), 7.40 (m, 1 H, ArH), 1.21 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 141.4, 137.2, 132.6, 131.6, 129.7, 125.4, 125.1, 123.3, 122.8, 122.0, 114.4, 100.6, 98.0, 18.7, 11.4. IR 2944 (s), 2893 (m), 2866 (s), 2362 (w), 2338 (w), 2148 (w), 1604 (w), 1527 (m), 1497 (m), 1464 (m), 1237 (s), 1164 (w), 1053 (w), 1016 (w), 997 (w), 961 (w), 884 (w), 833 (s), 808 (w), 761 (m), 732 (m). HRMS (ESI) calcd for $C_{25}H_{30}{}^{79}BrSSi^{+}$ $[M+H]^{+}$ 469.1015; found 469.1029.

((2-(4-Fluorophenyl)benzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11d)

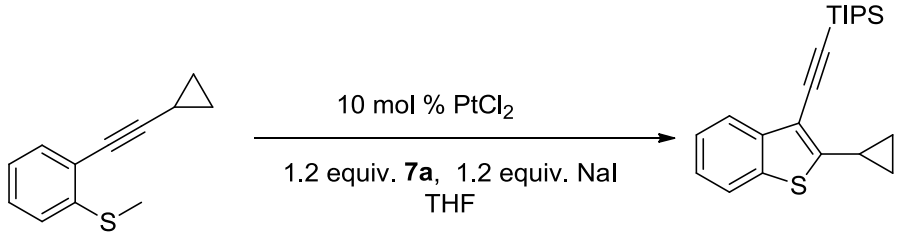


10d **11d**

Following the general procedure **GP2**, starting from **10d** (73 mg, 0.30 mmol), **11d** was obtained as yellow oil (62 mg, 0.15 mmol, 51%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (m, 2 H, ArH), 7.96 (d, 1 H, *J* = 7.9 Hz, ArH), 7.79 (d, 1 H, *J* = 7.9 Hz, ArH), 7.47 (m, 1 H, ArH), 7.39 (m, 1 H, ArH), 7.13 (t, 2 H, *J* = 8.7 Hz, ArH), 1.21 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9 (d, *J* = 249.5 Hz), 145.6, 141.3, 137.2, 130.2 (d, *J* = 8.1 Hz), 130.0, 125.3, 125.2, 123.3, 122.0, 115.6 (d, *J* = 21.7 Hz), 114.0, 100.7, 97.2, 18.7, 11.4. IR 2940 (s), 2889 (m), 2862 (s), 2361 (w), 2338 (w), 2143 (w), 1514 (w), 1463 (m), 1436 (w), 1233 (w), 1075 (m), 1050 (w), 1013 (m), 956 (m), 883 (m), 821 (m), 756 (m), 732 (m), 705 (m). HRMS (ESI) calcd for $C_{25}H_{30}FSSi^{+}$ $[M+H]^{+}$ 409.1816; found 409.1822.

((2-Cyclopropylbenzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11e)

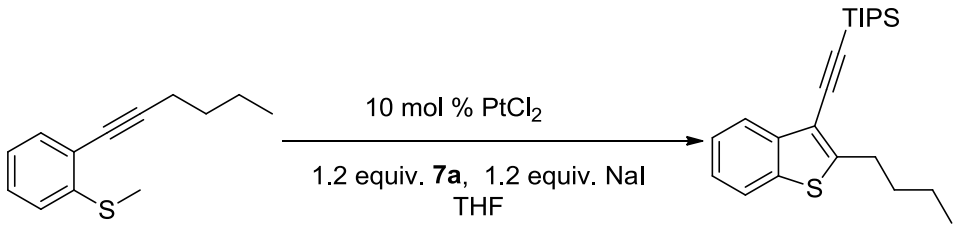


10e **11e**

Following the general procedure **GP2**, starting from **10e** (56 mg, 0.30 mmol), **11e** was obtained as yellow oil (64 mg, 0.18 mmol, 60%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, 1 H, *J* = 7.9 Hz, ArH), 7.68 (d, 1 H, *J* = 7.9 Hz, ArH), 7.39 (m, 1 H, ArH), 7.28 (m, 1 H, ArH), 2.43 (m, 1 H, CH), 1.19 (m, 21 H, TIPS), 0.99 (m, 4 H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 140.5, 135.9, 124.7, 124.2, 122.0, 115.4, 100.1, 95.9, 18.8, 12.3, 11.4, 10.8 (One aromatic carbon was not resolved). IR 2947 (s), 2895 (m), 2866 (s), 2349 (w), 2145 (m), 1693 (w), 1464 (m), 1441 (w), 1335 (w), 1308 (m), 1263 (m), 1250 (m), 1249 (m), 1225 (m), 1090 (m), 1056 (s), 1002 (m), 916 (w), 905 (w), 886 (w), 759 (m), 736 (m). HRMS (ESI) calcd for $C_{22}H_{31}SSi^{+}$ $[M+H]^{+}$ 355.1910; found 355.1905.

((2-Butylbenzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11f)

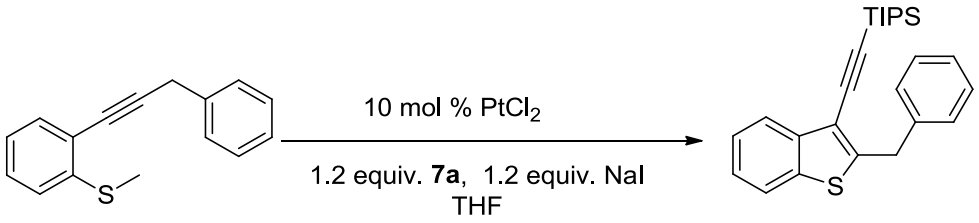


10f **11f**

Following the general procedure **GP2**, starting from **10f** (62 mg, 0.30 mmol), **11f** was obtained as yellow oil (58 mg, 0.16 mmol, 52%).

Rf(pentane): 0.7. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, 1 H, *J* = 7.9 Hz, ArH), 7.75 (d, 1 H, *J* = 7.9 Hz, ArH), 7.42 (m, 1 H, ArH), 7.32(m, 1 H, ArH), 2.98 (t, 2 H, *J* = 7.6 Hz, Butyl), 1.67 (m, 2 H, Butyl), 1.35 (m, 2 H, Butyl), 1.10 (m, 21 H, TIPS), 0.86 (t, 3 H, *J* = 7.4 Hz, Butyl) ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.8, 140.1, 137.3, 124.6, 124.3, 122.5, 122.0, 115.7, 99.9, 95.7, 33.1, 29.7, 22.3, 18.7, 13.8, 11.3. IR 3061 (w), 2938 (s), 2864 (s), 2362 (w), 1463 (s), 1439 (m), 1260 (w), 1216 (w), 1070 (m), 1015 (m), 883 (m), 848 (w), 804 (w), 756 (m), 732 (m). HRMS (ESI) calcd for $C_{23}H_{35}SSi^+$ $[M+H]^+$ 371.2223; found 371.2227.

((2-Benzylbenzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11g)

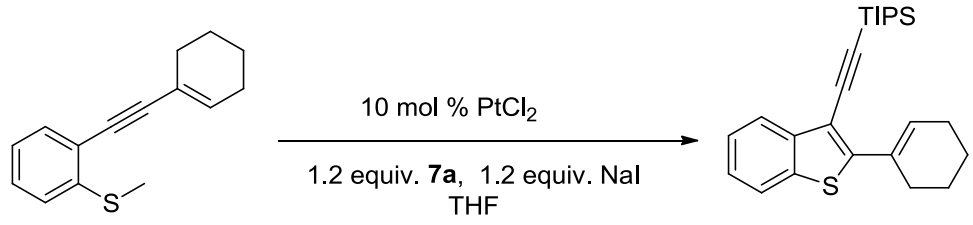


10g **11g**

Following the general procedure **GP2**, starting from **10g** (72 mg, 0.30 mmol), **11g** was obtained as yellow oil (63 mg, 0.16 mmol, 52%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, 1 H, *J* = 8.0 Hz, ArH), 7.57 (d, 1 H, *J* = 8.0 Hz, ArH), 7.32-7.25 (m, 3 H, ArH), 7.22-7.16 (m, 3 H, ArH), 7.14-7.10 (m, 1 H, ArH), 4.29 (s, 2 H, CH_2), 1.09 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.0, 140.0, 139.5, 137.9, 128.9, 128.8, 126.8, 124.9, 124.7, 122.9, 122.2, 116.3, 100.0, 96.3, 36.2, 18.9, 11.4. IR 3061 (w), 3030 (w), 2944 (s), 2864 (s), 2146 (m), 1487 (w), 1461 (m), 1253 (w), 1241 (w), 1073 (w), 1024 (m), 1008 (w), 915 (w), 886 (m), 818 (w), 756 (m), 733 (m). HRMS (ESI) calcd for $C_{26}H_{33}SSi^+$ $[M+H]^+$ 405.2067; found 405.2066.

((2-(Cyclohex-1-en-1-yl)benzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11h)

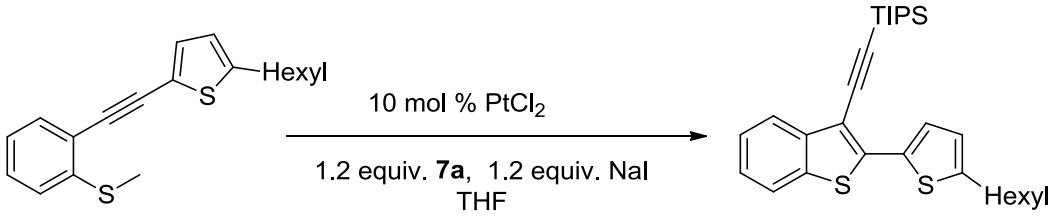


10h **11h**

Following the general procedure **GP2**, starting from **10h** (69 mg, 0.30 mmol), **11h** was obtained as yellow oil (50 mg, 0.13 mmol, 42%).

Rf(pentane/DCM= 10:1): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, 1 H, *J* = 7.9 Hz, ArH), 7.72 (d, 1 H, *J* = 7.9 Hz, ArH), 7.42-7.39 (m, 1 H, ArH), 7.34-7.30 (m, 1 H, ArH), 6.77 (t, 1 H, *J* = 3.8 Hz, CH), 2.71 (m, 2 H, Cyclohexene), 2.29-2.28 (m, 2 H, Cyclohexene), 1.82-1.69 (m, 4 H, Cyclohexene), 1.20 (m, 2 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 141.4, 136.4, 131.6, 130.5, 124.7, 124.7, 122.8, 121.8, 112.1, 101.7, 97.1, 29.1, 26.0, 22.9, 21.8, 18.8, 11.5. IR 2936 (s), 2866 (s), 2376 (w), 2349 (m), 2143 (m), 1459 (m), 1330 (w), 1044 (m), 887 (w), 742 (w). HRMS (ESI) calcd for $C_{25}H_{35}SSi^{+}$ $[M+H]^{+}$ 395.2223; found 395.2229.

((2-(5-Hexylthiophen-2-yl)benzo[b]thiophen-3-yl)ethynyl)triisopropylsilane (11i)

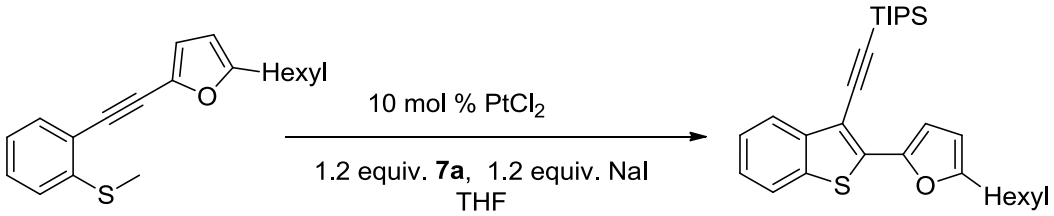


10i **11i**

Following the general procedure **GP2**, starting from **10i** (94 mg, 0.30 mmol), **11i** was obtained as yellow oil (99 mg, 0.21 mmol, 69%).

Rf(pentane): 0.6. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, 1 H, *J* = 7.9 Hz, ArH), 7.70 (d, 1 H, *J* = 7.9 Hz, ArH), 7.50 (d, 1 H, *J* = 3.7 Hz, ThiopheneH), 7.43 (m, 1 H, ArH), 7.32 (m, 1 H, ArH), 6.75 (d, 1 H, *J* = 3.7 Hz, ThiopheneH), 2.84 (t, 2 H, *J* = 7.6 Hz, Hexyl), 1.71 (m, 2 H, Hexyl), 1.66-1.34 (m, 27 H, Hexyl+TIPS), 0.90 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 141.3, 141.0, 136.5, 133.6, 126.9, 125.1, 125.0, 124.3, 122.9, 121.8, 112.1, 100.8, 100.2, 31.6, 31.5, 30.3, 28.8, 22.5, 18.8, 14.1, 11.5. IR 2933 (s), 2863 (s), 2349 (w), 2142 (w), 1463 (m), 1462 (m), 1007 (w), 894 (w), 799 (w), 752 (w). HRMS (ESI) calcd for $C_{29}H_{41}S_2Si^{+}$ $[M+H]^{+}$ 481.2413; found 481.2422.

Triisopropyl((2-(5-hexylfuran-2-yl)benzo[b]thiophen-3-yl)ethynyl)silane (11j)



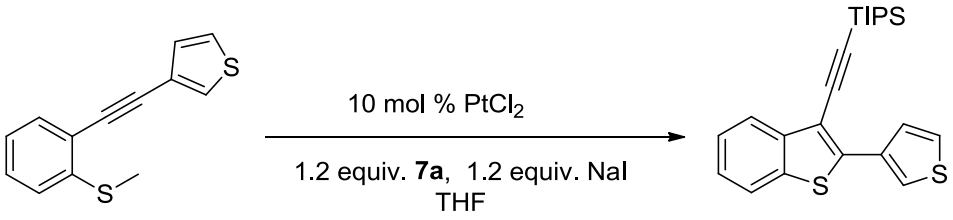
10j **11j**

Following the general procedure **GP2**, starting from **10j** (90 mg, 0.30 mmol), **11j** was obtained as yellow oil (110 mg, 0.237 mmol, 79%).

Rf(pentane): 0.7. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, 1 H, *J* = 7.7 Hz, ArH), 7.77 (d, 1 H, *J* = 7.7 Hz, ArH), 7.43 (m, 1 H, ArH), 7.36-7.32 (m, 2 H, FuranH+ArH), 6.19 (d, 1 H, *J* = 3.4

Hz, FuranH), 2.72 (t, 2 H, *J* = 7.6 Hz, Hexyl), 1.72 (m, 2 H, Hexyl), 1.44-1.19 (m, 27 H, Hexyl+TIPS), 0.93 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2, 147.2, 141.0, 136.7, 136.7, 124.9, 124.8, 122.7, 122.0, 110.8, 110.4, 107.6, 100.9, 98.9, 31.6, 28.9, 28.1, 27.9, 22.6, 18.8, 14.1, 11.4. IR 2936 (w), 2864 (w), 2140 (w), 1545 (w), 1462 (w), 1006 (w), 1005 (w), 917 (w), 727 (s), 690 (s), 655 (s), 648 (s), 647 (s), 621 (s), 559 (s). HRMS (ESI) calcd for $C_{29}H_{41}OSSi^+$ $[M+H]^+$ 465.2642; found 465.2638.

Triisopropyl((2-(thiophen-3-yl)benzo[b]thiophen-3-yl)ethynyl)silane (11k)

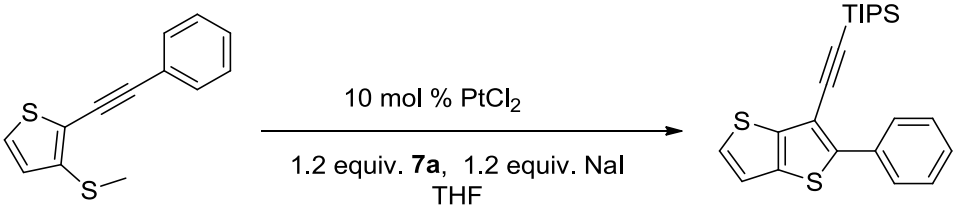


10k **11k**

Following the general procedure **GP2**, starting from **10k** (69 mg, 0.30 mmol), **11k** was obtained as yellow oil (74 mg, 0.19 mmol, 62%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, 1 H, *J* = 2.9, 1.3 Hz, ThiopheneH), 7.92 (d, 1 H, *J* = 8.0 Hz, ArH), 7.81 (d, 1 H, *J* = 5.0 Hz, ThiopheneH), 7.76 (d, 1 H, *J* = 7.9 Hz, ArH), 7.44 (t, 1 H, *J* = 7.7 Hz, ArH), 7.39-7.34 (m, 2 H, ArH+ThiopheneH), 1.21 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 141.3, 136.8, 134.6, 127.3, 125.6, 125.1, 125.0, 123.9, 123.1, 122.0, 113.3, 101.3, 98.0, 18.8, 11.4. IR 3062 (w), 2944 (s), 2866 (s), 2143 (m), 1460 (m), 1280 (w), 1232 (m), 1198 (m), 1116 (w), 1067 (w), 998 (m), 939 (w), 879 (m), 770 (s). HRMS (ESI) calcd for $C_{23}H_{29}S_2Si^+$ $[M+H]^+$ 397.1474; found 397.1477.

Triisopropyl((2-phenylthieno[3,2-b]thiophen-3-yl)ethynyl)silane (11l)

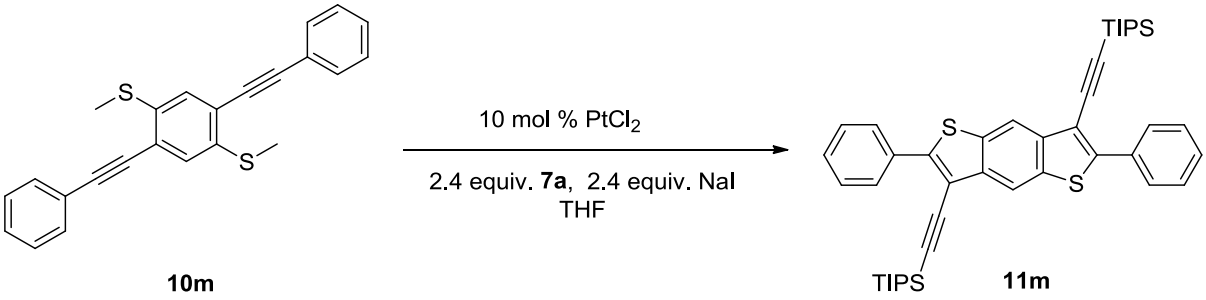


10l **11l**

Following the general procedure **GP2**, starting from **10e** (69 mg, 0.30 mmol), **11l** was obtained as brown oil (53 mg, 0.13 mmol, 45%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.99 (m, 2 H, ArH+ThiopheneH), 7.42-7.34 (m, 4 H, ArH), 7.23 (d, 1 H, *J* = 5.2 Hz, ThiopheneH), 1.16 (m, 21 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 143.6, 135.3, 134.2, 128.6, 128.3, 127.5, 127.2, 119.7, 111.1, 100.4, 97.2, 18.7, 11.3. IR 2925 (s), 2863 (s), 2360 (w), 2340 (w), 2151 (w), 1464 (m), 1382 (w), 1359 (w), 1244 (w), 1222 (w), 1191 (w), 1190 (w), 1066 (w), 1016 (w), 997 (w), 955 (w), 913 (w), 884 (m). HRMS (ESI) calcd for $C_{23}H_{29}S_2Si^+$ $[M+H]^+$ 397.1474; found 397.1467.

((2,6-Diphenylbenzo[1,2-b:4,5-b']dithiophene-3,7-diyl)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (11m)

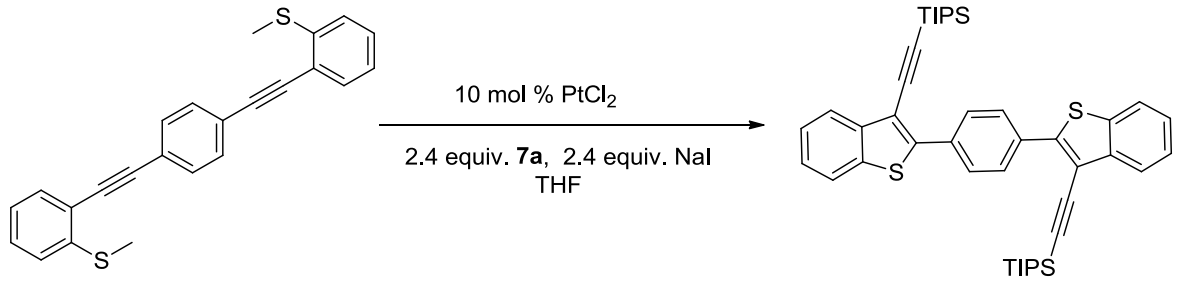


10m **11m**

7a (132 mg, 0.240 mmol, 2.4 equiv), NaI (36 mg, 0.24 mmol, 2.4 equiv) and $PtCl_2$ (5 mg, 0.02 mmol, 0.2 equiv) were added into a solution of **10m** (37 mg, 0.10 mmol, 1 equiv) and THF (1 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up. **11m** was obtained as brown oil (39 mg, 0.055 mmol, 56%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 2 H, ArH), 8.15 (d, 4 H, *J* = 7.3 Hz, ArH), 7.44 (m, 6 H, ArH), 1.22 (m, 42 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 139.9, 135.2, 133.7, 128.9, 128.6, 128.4, 116.2, 113.0, 100.8, 97.7, 18.8, 11.5. IR 2942 (s), 2925 (m), 2890 (w), 2864 (s), 2343 (m), 2140 (w), 1519 (w), 1491 (w), 1462 (m), 1444 (w), 1389 (w), 1214 (w), 1073 (w), 1062 (w), 1018 (w), 997 (w), 953 (w), 910 (w), 883 (m), 864 (w), 857 (w). HRMS (ESI) calcd for $C_{44}H_{55}S_2Si_2^+$ $[M+H]^+$ 703.3278; found 703.3277.

1,4-Bis(3-((triisopropylsilyl)ethynyl)benzo[b]thiophen-2-yl)benzene (11n)

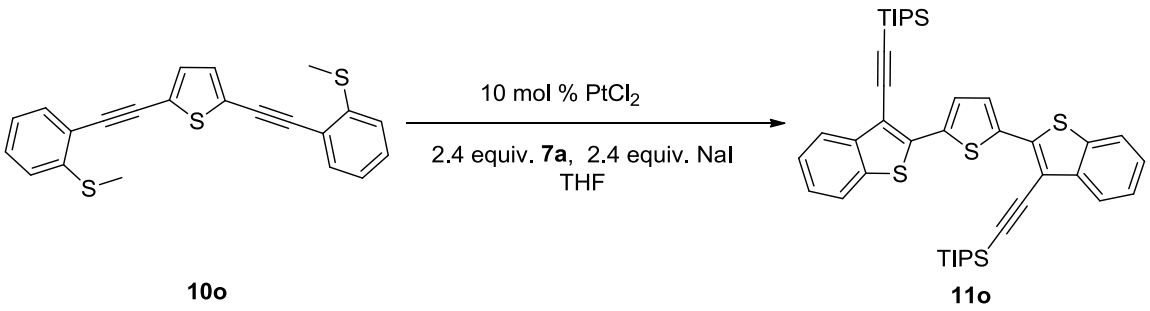


10n **11n**

7a (132 mg, 0.240 mmol, 2.4 equiv), NaI (36 mg, 0.24 mmol, 2.4 equiv) and $PtCl_2$ (5 mg, 0.02 mmol, 0.2 equiv) were added into a solution of **10n** (37 mg, 0.10 mmol, 1 equiv) and THF (1 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up. **11n** was obtained as yellow solid (22 mg, 0.031 mmol, 31%).

Rf(pentane): 0.4. Melting point: 142-143 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 4 H, ArH), 7.96 (d, 2 H, *J* = 7.9 Hz, ArH), 7.81 (d, 2 H, *J* = 7.9 Hz, ArH), 7.46 (td, 2 H, *J* = 7.9, 0.8 Hz, ArH), 7.40 (td, 2 H, *J* = 7.9, 0.8 Hz, ArH), 1.19 (m, 42 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 141.5, 137.4, 134.0, 128.4, 125.4, 125.1, 123.4, 122.0, 114.4, 100.8, 98.0, 18.8, 11.5. IR 2942 (s), 2925 (m), 2890 (w), 2864 (s), 2361 (s), 2343 (m), 2330 (m), 2140 (w), 1519 (w), 1518 (w), 1509 (w), 1491 (w), 1462 (m), 1444 (w), 1389 (w), 1214 (w), 1073 (w), 1062 (w), 1018 (w), 997 (w), 953 (w), 910 (w), 883 (m), 864 (w), 857 (w). HRMS (ESI) calcd for $C_{44}H_{55}S_2Si_2^+$ $[M+H]^+$ 703.3278; found 703.3271.

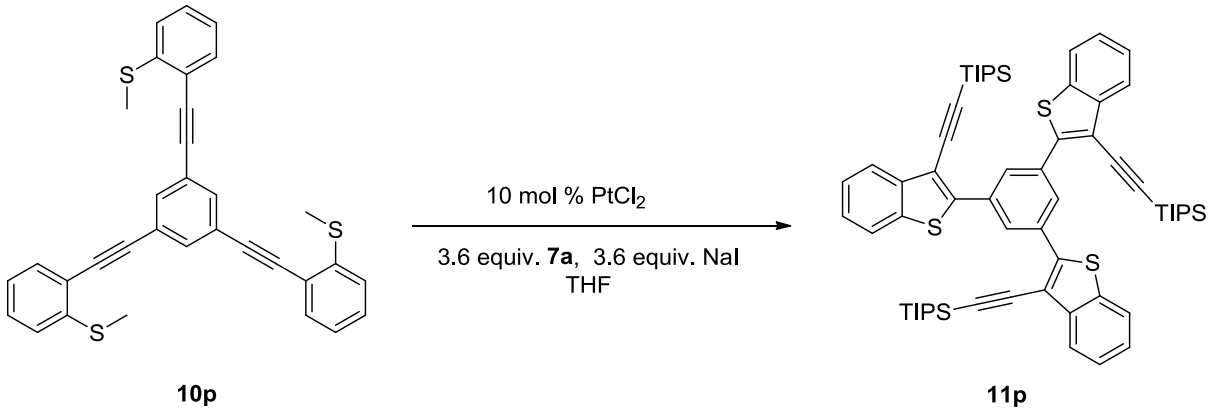
2,5-Bis(3-((triisopropylsilyl)ethynyl)benzo[b]thiophen-2-yl)thiophene (11o)



7a (132 mg, 0.240 mmol, 2.4 equiv), NaI (36 mg, 0.24 mmol, 2.4 equiv) and $PtCl_2$ (5 mg, 0.02 mmol, 0.2 equiv) were added into a solution of **10o** (38 mg, 0.10 mmol, 1 equiv) and THF (1 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up. **11o** was obtained as green oil (26 mg, 0.037 mmol, 37%).

Rf(pentane): 0.5. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 2 H, Thiophene), 7.90 (d, 2 H, *J* = 8.1 Hz, ArH), 7.75 (d, 2 H, *J* = 8.1 Hz, ArH), 7.44 (td, 2 H, *J* = 7.2, 1.0 Hz, ArH), 7.37 (td, 2 H, *J* = 7.2, 1.0 Hz, ArH), 1.25 (m, 42 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 139.4, 136.9, 127.3, 125.5, 125.3, 123.2, 121.9, 113.7, 101.2, 100.7, 18.9, 11.4 (One carbon was not resolved). IR 3062 (w), 2947 (s), 2866 (s), 2141 (m), 1732 (w), 1502 (w), 1463 (m), 1265 (w), 1239 (w), 1238 (w), 1081 (w), 1021 (m), 959 (w), 909 (m), 887 (m), 803 (m), 733 (s). HRMS (ESI) calcd for $C_{42}H_{53}S_3Si_2^+$ $[M+H]^+$ 709.2842; found 709.2831.

1,3,5-Tris(3-((triisopropylsilyl)ethynyl)benzo[b]thiophen-2-yl)benzene (11p)



7a (198 mg, 0.360 mmol, 3.6 equiv), NaI (54 mg, 0.36 mmol, 3.6 equiv) and $PtCl_2$ (9 mg, 0.03 mmol, 0.3 equiv) were added into a solution of **10p** (52 mg, 0.10 mmol, 1 equiv) and THF (1 mL). The reaction was stopped after stirring during 12 h, the solvent was removed under vacuum, and the crude product was purified by column chromatography directly (SiO_2, Pentane) without any further work-up. **11p** was obtained as yellow solid (18 mg, 0.018 mmol, 18%).

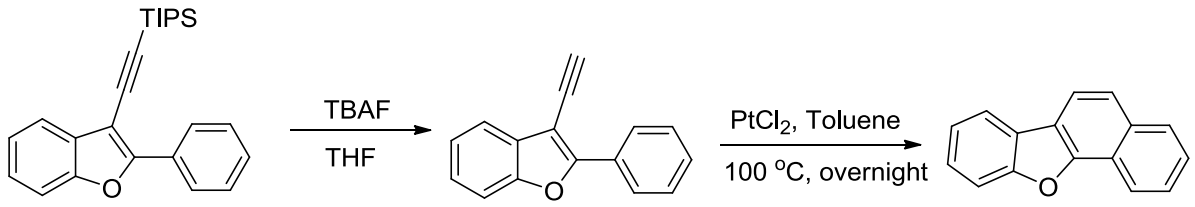
Rf(pentane): 0.3. Melting point: 123-124 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 3 H, ArH), 7.97-7.95 (d, 3 H, *J* = 7.9 Hz, ArH), 7.83 (d, 3 H, *J* = 7.9 Hz, ArH), 7.47 (td, 3 H, *J* = 7.3, 1.0 Hz, ArH), 7.41 (td, 3 H, *J* = 7.3, 1.0 Hz, ArH), 0.91 (m, 62 H, TIPS). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.8, 141.2, 137.8, 134.6, 129.4, 125.3, 125.0, 123.4, 122.0, 115.5, 100.1,

97.1, 18.5, 11.2. IR 2930 (s), 2861 (m), 2349 (w), 1463 (w), 1462 (w), 1016 (w), 1015 (w), 1014 (w), 884 (w), 753 (w), 740 (w). HRMS (ESI) calcd for $C_{63}H_{79}S_3Si_3^+$ $[M+H]^+$ 1015.4646; found 1015.4639.

7. Tetracene Synthesis

The protocol for the synthesis of 12a represents the general procedure 3 for the synthesis of 12b-6j

Naphtho[1,2-b]benzofuran (12a)



9a **51** **12a**

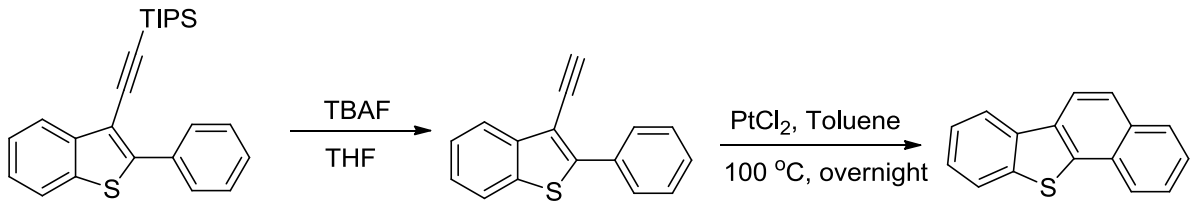
TBAF (1 M in THF, 0.45 mL, 0.45 mmol, 1.2 equiv) was added slowly into a solution of **9a** (0.14 g, 0.37 mmol, 1.0 equiv) in THF (4 mL) at 0 °C. The reaction was quenched with sat NH_4Cl solution (20 mL) after 30 min. The aqueous and organic layers were separated and the aqueous layer was extracted with ether (3 x 10 mL). After drying over $MgSO_4$ and concentrating under vacuum, the crude product was purified by column chromatography (Pentane) to afford **51** as yellow oil (53 mg, 0.24 mmol, 65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.14 (m, 2 H, ArH), 7.60-7.55 (m, 1 H, ArH), 7.42-7.33 (m, 3 H, ArH), 7.32-7.28 (m, 1 H, ArH), 7.26-7.17 (m, 2 H, ArH), 3.48 (s, 1 H, CH, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 153.4, 130.1, 130.0, 129.5, 128.8, 126.2, 125.5, 123.6, 120.3, 111.3, 98.2, 85.2, 75.8.

$PtCl_2$ (3 mg, 0.01 mmol, 0.1 equiv) was added into a solution of **51** (23 mg, 0.11 mmol, 1.0 equiv) in toluene (1 mL). The mixture was kept at 100 ^{o}C during 12 h. The crude product was purified by column chromatography (Pentane/DCM= 10:1) directly to afford **12a** as white solid (22 mg, 0.10 mmol, 96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52-8.42 (m, 1 H, ArH), 8.09-7.97 (m, 3 H, ArH), 7.79 (d, 1 H, *J* = 8.5 Hz, ArH), 7.73 (d, 1 H, *J* = 8.2 Hz, ArH), 7.68-7.39 (m, 4 H, ArH).^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1, 152.2, 133.2, 128.6, 126.6, 126.3, 126.2, 125.2, 123.4, 123.1, 121.6, 121.0, 120.4, 119.3, 118.6, 112.0. Characterization data of **12a** corresponded to the literature values.[35]

Benzo[b]naphtho[2,1-d]thiophene (12b)



11a **52** **12b**

[35] S. Maetani, T. Fukuyama, I. Ryu, *Org. Lett.* **2013**, *15*, 2754.

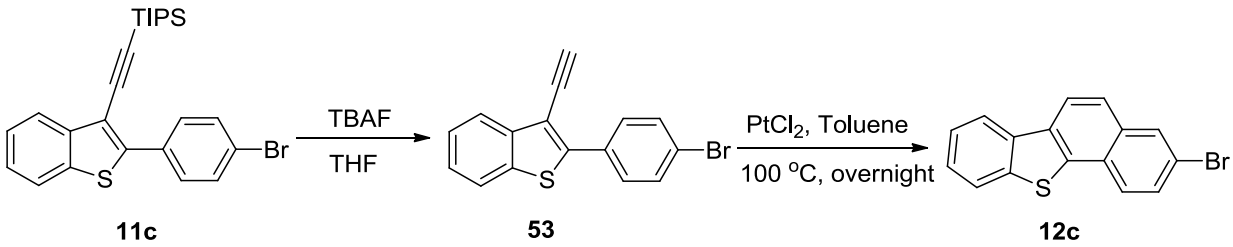
Following the general procedure **GP3,** starting from **11a** (0.14 g, 0.36 mmol), **52** was obtained as colorless oil (57 mg, 0.24 mmol, 68%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.96 (m, 3 H), 7.81 (d, 1 H, *J* = 7.9 Hz), 7.50-7.37 (m, 5 H), 3.47 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 141.4, 137.6, 133.6, 129.1, 128.8, 128.6, 125.4, 125.2, 123.4, 122.2, 112.6, 82.8, 78.3.

Starting from **52** (23 mg, 0.10 mmol), **12b** was obtained as white solid (20 mg, 0.085 mmol, 85%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.14 (m, 3 H, ArH), 8.02-7.95 (m, 2 H, ArH), 7.87 (d, 1 H, *J* = 8.6 Hz, ArH), 7.68-7.47 (m, 4 H, ArH).^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2, 137.4, 136.7, 132.8, 132.5, 129.1, 129.0, 126.9, 126.4, 126.3, 125.6, 124.7, 124.6, 123.1, 121.7, 119.8. Characterization data of **12b** corresponded to the literature values.[36]

3-Bromobenzo[b]naphtho[2,1-d]thiophene (12c)



11c **53** **12c**

Following the general procedure **GP3,** starting from **11c** (40 mg, 0.085 mmol), **53** was obtained as white solid (22 mg, 0.070 mmol, 82%).

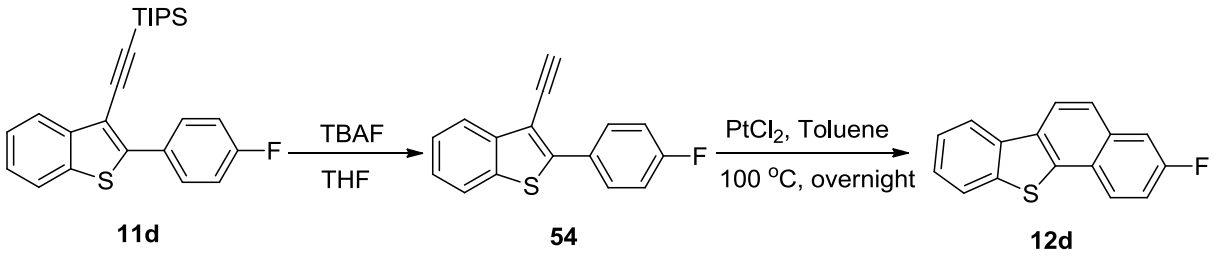
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, 1 H, *J* = 7.9 Hz, ArH), 7.86 (d, 2 H, *J* = 8.5 Hz, ArH), 7.80 (d, 1 H, *J* = 7.9 Hz), 7.59 (d, 2 H, *J* = 8.5 Hz, ArH)), 7.46 (td, 1 H, *J* = 8.0 Hz, 1.0 ArH), 7.40 (td, 1 H, *J* = 8.0 Hz, 1.0 ArH), 3.49 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 141.2, 137.4, 132.4, 131.9, 129.9, 125.6, 125.2, 123.3, 123.2, 122.1, 113.0, 83.2, 77.9.

Starting from **53** (22 mg, 0.070 mmol), **12c** was obtained as white solid (16 mg, 0.051 mmol, 73%).

Rf(pentane): 0.7. Melting point: 201-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21-8.12 (m, 3 H, ArH), 8.00-7.95 (m, 2 H, ArH), 7.76 (d, 1 H, *J* = 8.6 Hz, ArH), 7.68 (dd, 1 H, *J* = 8.7, 1.9 Hz, ArH), 7.51 (m, 2 H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0, 137.3, 136.3, 133.5, 133.0, 131.0, 130.0, 127.5, 126.5, 126.1, 124.8, 124.5, 123.0, 121.7, 120.8, 120.1. IR 2966 (w), 2368 (w), 2349 (s), 2335 (m), 2318 (w), 2305 (w), 2052 (m), 1727 (w), 1257 (w), 1203 (w), 1202 (w), 1077 (w), 912 (w), 886 (w), 883 (w). HRMS (ESI) calcd for $C_{16}H_9Ag^{79}BrS^+$ $[M+Ag]^+$ 418.8654; found 418.8657.

3-Fluorobenzo[b]naphtho[2,1-d]thiophene (12d)

[36] R. Che, Z. Wu, Z. Li, H, Xiang, X. Zhou *Chem. Eur. J.* **2014**, *20*, 7258.



11d **54** **12d**

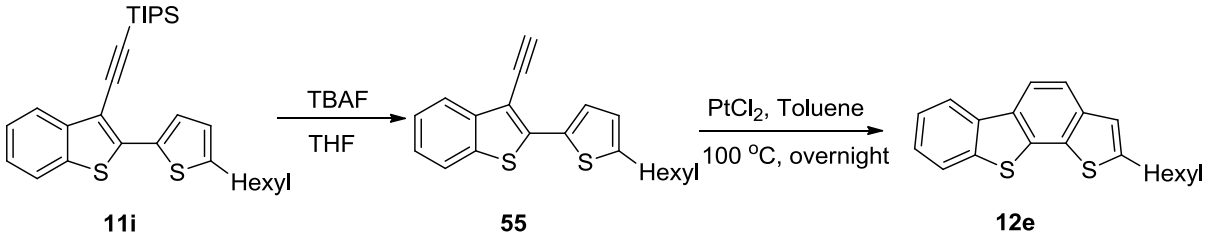
Following the general procedure **GP3,** starting from **11d** (40 mg, 0.098 mmol), **54** was obtained as white solid (21 mg, 0.079 mmol, 85%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (m, 3 H, ArH), 7.80 (d, 1 H, *J* = 7.9 Hz, ArH), 7.46 (td, 1 H, *J* = 8.0 Hz, 1.0 ArH), 7.40 (td, 1 H, *J* = 8.0 Hz, 1.0 ArH), 7.16 (t, 2 H, *J* = 7.6 Hz, ArH), 3.47 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5 (d, *J* = 243.6 Hz), 146.7, 141.1, 137.3, 130.3 (d, *J* = 8.2 Hz) 129.6, 125.4, 125.1, 123.2, 122.0, 115.6 (d, *J* = 21.7 Hz), 112.5, 82.7, 77.9.

Starting from **54** (21 mg, 0.079 mmol), **12d** was obtained as white solid (10 mg, 0.040 mmol, 50%).

Rf(pentane) =0.7. Melting point: 204-205 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 2 H, ArH), 8.13 (dd, 1 H, *J* = 9.0, 5.4 Hz, ArH), 7.96 (m, 1 H, ArH), 7.81 (d, 1 H, *J* = 8.6 Hz, ArH), 7.61 (dd, 1 H, *J* = 9.7, 2.5 Hz, ArH), 7.57-7.54 (m, 2 H, ArH), 7.39 (td, 1 H, *J* = 8.6, 2.6 Hz, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5 (d, *J* = 246.5 Hz), 138.8, 137.4, 136.4, 133.4 (d, *J* = 9.2 Hz), 132.1, 126.7 (d, *J* = 9.2 Hz), 126.2, 125.8, 124.8, 124.7, 122.9, 121.6, 120.8, 116.7 (d, *J* = 25.2 Hz), 112.5 (d, *J* = 20.6 Hz). IR 2931 (m), 2354 (m), 2345 (m), 2052 (s), 1457 (w), 1255 (m), 1206 (m), 961 (w), 817 (w). HRMS (ESI) calcd for $C_{16}H_{10}FS^{+}$ $[M+H]^{+}$ 253.0482; found 253.0481.

2-Hexylbenzo[4,5]thieno[3,2-g]benzothiophene (12e)



11i **55** **12e**

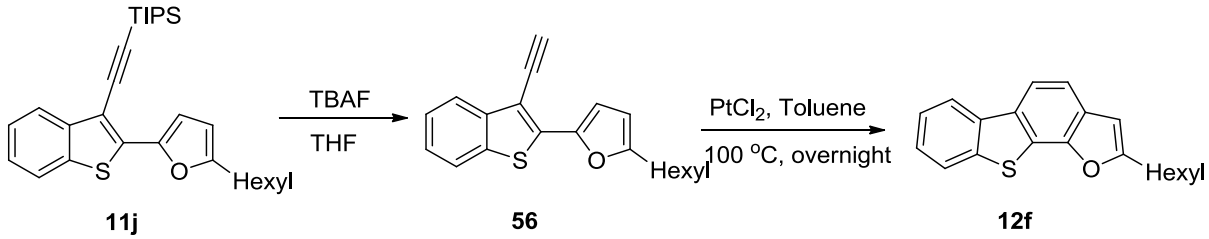
Following the general procedure **GP3,** starting from **11i** (83 mg, 0.17 mmol), **55** was obtained as brown oil (45 mg, 0.14 mmol, 80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, 1 H, *J* = 7.9 Hz, ArH), 7.72 (d, 1 H, *J* = 7.9 Hz, ArH), 7.53 (d, 1 H, *J* = 3.6 Hz, ThiopheneH), 7.42 (t, 1 H, *J* = 7.2 Hz, ArH), 7.35 (dd, 1 H, *J* = 8.1, 1.0 Hz, ArH), 6.79 (d, 1 H, *J* = 3.6 Hz, ThiopheneH), 3.69 (s, 1 H, Alkyne H), 2.86 (t, 2 H, *J* = 7.6 Hz, Hexyl), 1.73 (m, 2 H, Hexyl), 1.36-1.28 (m, 6 H, Hexyl), 0.92 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 141.9, 141.0, 136.5, 133.2, 127.1, 125.2, 125.0, 124.5, 122.8, 121.8, 110.5, 85.2, 78.2, 31.5, 30.2, 29.7, 28.8, 22.6, 14.1.

Starting from **55** (45 mg, 0.14 mmol), **12e** was obtained as brown solid (29 mg, 0.089 mmol, 64%).

Rf(pentane) =0.5. Melting point: 105-106 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (m, 1 H, ArH), 8.06 (d, 1 H, *J* = 8.4 Hz, ArH), 7.88 (m, 1 H, ArH), 7.73 (d, 1 H, *J* = 8.4 Hz, ArH), 7.46 (m, 2 H, ArH), 7.14 (s, 1 H, ArH), 2.96 (t, 2 H, *J* = 7.3 Hz, Hexyl), 1.80 (m, 2 H, Hexyl), 1.44 (m, 2 H, Hexyl), 1.34 (m, 4 H, Hexyl),0.92 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 139.4, 138.5, 136.4, 132.8, 132.8, 131.7, 126.1, 124.6, 122.9, 121.5, 121.4, 119.7, 117.9, 31.6, 31.2, 30.8, 28.8, 22.6, 14.1. IR 3056 (w), 2922 (m), 2349 (m), 2335 (w), 2318 (w), 1416 (w), 1390 (m), 909 (w), 838 (m), 767 (m), 735 (s). HRMS (ESI) calcd for $C_{20}H_{21}S_2^+$ $[M+H]^+$ 325.1079; found 325.1082.

2-Hexylbenzo[4,5]thieno[3,2-g]benzofuran (12f)



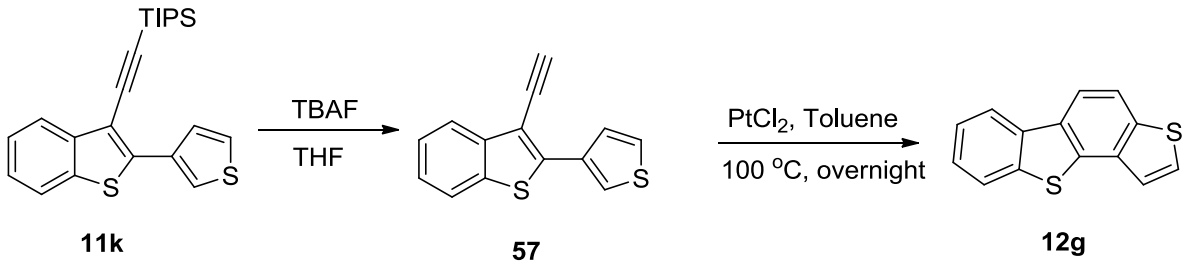
Following the general procedure **GP3,** starting from **11j** (0.11 g, 0.24 mmol), **56** was obtained as brown oil (51 mg, 0.17 mmol, 70%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, 1 H, *J* = 7.9 Hz, ArH), 7.77 (d, 1 H, *J* = 7.9 Hz, ArH), 7.42 (td, 1 H, *J* = 7.4, 1.1 Hz, ArH), 7.34 (td, 1 H, *J* = 8.2, 1.2 Hz, ArH), 7.27 (d, 1 H, *J* = 3.4 Hz, FuranH), 6.18 (d, 1 H, *J* = 3.4 Hz, FuranH), 3.68 (s, 1 H, Alkyne H), 2.72 (t, 2 H, *J* = 7.5 Hz, Hexyl), 1.72 (m, 2 H, Hexyl), 1.43-1.32 (m, 6 H, Hexyl), 0.92 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 146.8, 140.6, 137.7, 136.7, 125.0, 124.9, 122.6, 122.0, 110.8, 108.8, 107.7, 84.5, 78.2, 31.5, 28.8, 28.1, 27.9, 22.6, 14.1.

Starting from **56** (51 mg, 0.17 mmol), **12f** was obtained as white solid (30 mg, 0.097 mmol, 59%).

Rf(pentane) =0.7. Melting point: 72 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (m, 1 H, ArH), 7.98 (d, 1 H, *J* = 8.2 Hz, ArH), 7.90 (m, 1 H, ArH), 7.56 (d, 1 H, *J* = 8.2 Hz, ArH), 7.46 (m, 2 H, ArH), 6.53 (s, 1 H, ArH), 2.86 (t, 2 H, *J* = 7.3 Hz, Hexyl), 1.81 (m, 2 H, Hexyl), 1.47 (m, 2 H, Hexyl), 1.33 (m, 4 H, Hexyl), 0.92 (t, 3 H, *J* = 7.4 Hz, Hexyl). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 149.2, 138.7, 136.3, 132.8, 127.3, 125.9, 124.5, 123.0, 121.7, 121.4, 117.2, 116.2, 102.7, 31.6, 28.9, 28.5, 27.8, 22.6, 14.1. IR 3061 (w), 3017 (w), 2954 (s), 2927 (s), 2856 (s), 1777 (w), 1735 (w), 1672 (w), 1657 (w), 1599 (m), 1465 (m), 1459 (m), 1430 (s), 1417 (s), 1378 (w), 1322 (w), 1316 (w), 1303 (m), 1251 (w), 1184 (w), 1127 (w), 1053 (m), 1021 (w937 (s), 911 (m), 890 (w), 859 (w), 853 (w), 817 (s). HRMS (ESI) calcd for $C_{20}H_{21}OS^+$ $[M+H]^+$ 309.1308; found 309.1309.

Benzo[4,5]thieno[2,3-e]benzothiophene (12g)



11k **57** **12g**

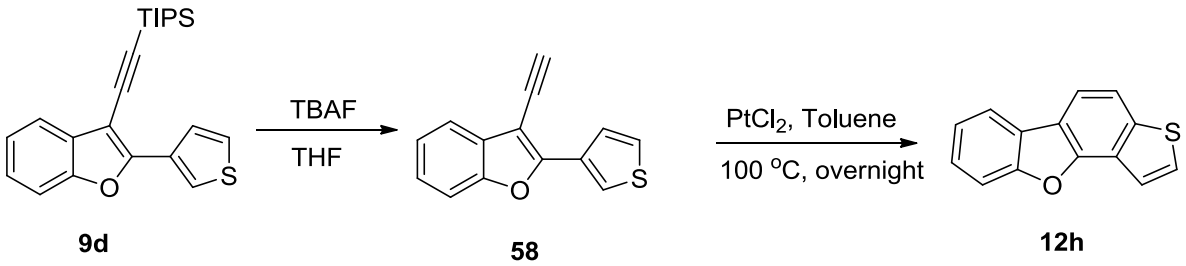
Following the general procedure **GP3,** starting from **11k** (74 mg, 0.18 mmol), **57** was obtained as brown oil (38 mg, 0.16 mmol, 85%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, 1 H, *J* =3.0, 1.3 Hz, ThiopheneH), 7.94 (d, 1 H, *J* = 8.0 Hz, ArH), 7.78 (d, 1 H, *J* = 8.0 Hz, ArH), 7.76 (dd, 1 H, *J* = 5.3, 1.4 Hz, ThiopheneH), 7.47-7.36 (m, 3 H, ArH+ThiopheneH), 3.60 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5, 141.0, 136.8, 134.3, 127.1, 125.9, 125.2, 125.0, 124.0, 123.0, 121.9, 111.6, 83.6, 78.5.

Starting from **57** (38 mg, 0.16 mmol), **12g** was obtained as white solid (30 mg, 0.13 mmol, 79%).

Rf(pentane): 0.5. Melting point: 222-223 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 1 H, ArH), 8.11 (d, 1 H, *J* = 8.5 Hz, ArH), 7.93 (m, 2 H, ArH), 7.62 (d, 1 H, *J* = 5.4 Hz, ArH), 7.58 (d, 1 H, *J* = 5.4 Hz, ArH), 7.52-7.46 (m, 2 H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7, 138.4, 136.2, 134.1, 133.8, 132.2, 127.5, 126.1, 124.6, 123.0, 121.9, 121.5, 119.1, 117.9. IR 2360 (m), 2336 (m), 1448 (w), 1395 (w), 1201 (w), 1025 (w), 777 (w), 749 (s). HRMS (ESI) calcd for $C_{14}H_9S_2^+$ $[M+H]^+$ 241.0140; found 241.0138.

Benzo[b]thieno[2,3-g]benzofuran (12h)



9d **58** **12h**

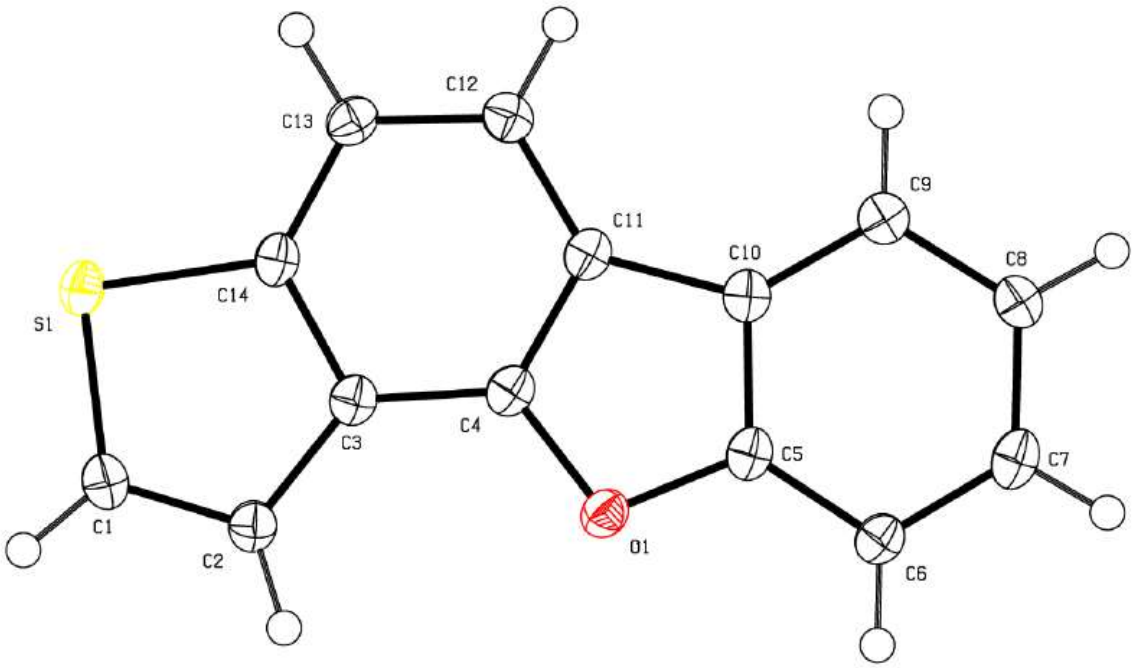
Following the general procedure **GP3,** starting from **9d** (88 mg, 0.23 mmol), **58** was obtained as brown oil (40 mg, 0.18 mmol, 77%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, 1 H, *J* =3.0, 1.2 Hz, ThiopheneH), 7.95 (dd, 1 H, *J* = 5.1. 1.2 Hz, ThiopheneH), 7.67 (m, 1H, ArH), 7.50 (m, 1H, ArH), 7.43 (dd, 1 H, *J* = 5.1. 3.0 Hz, ThiopheneH), 7.39-7.26 (m, 2 H, ArH), 3.61 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9, 153.1, 131.3, 129.5, 126.1, 125.6, 125.2, 124.1, 123.5, 120.1, 111.1, 97.0, 84.8, 75.6.

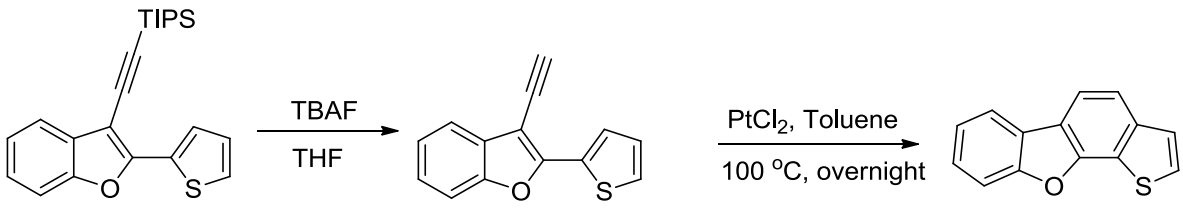
Starting from **58** (40 mg, 0.18 mmol), **12h** was obtained as white solid (33 mg, 0.15 mmol, 83%).

Rf(pentane): 0.5. Melting point: 129-130 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, 1 H, *J* = 7.6 Hz, ArH), 7.92 (d, 1 H, *J* = 8.2 Hz, ArH), 7.84 (d, 1 H, *J* = 8.4 Hz, ArH), 7.78 (d, 1 H, *J* = 5.5 Hz, ArH), 7.67 (d, 1 H, *J* = 8,2 Hz, ArH), 7.59 (d, 1 H, *J* = 5.5 Hz, ArH), 7.47 (td, 1 H, *J* = 7.4, 1.3 Hz, ArH), 7.39 (td, 1 H, *J* = 7.4, 1.3 Hz, ArH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.6, 150.9, 139.9, 127.1, 126.3, 125.6, 124.8, 122.9, 120.3, 119.5, 119.2, 117.2, 116.8, 111.7. IR 1191 (w), 926 (w), 745 (w), 641 (m), 631 (m), 621 (m), 612 (m), 604 (m), 508 (s), 474 (s), 468 (s), 433 (s), 425 (s). HRMS (ESI) calcd for $C_{14}H_9OS^+$ $[M+H]^+$ 225.0369; found 225.0367.
Crystal data of **12h** has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1420341).



Benzo[b]thieno[3,2-g]benzofuran (12i)



Following the general procedure **GP3,** starting from **9e** (72 mg, 0.19 mmol), **59** was obtained as brown oil (30 mg, 0.13 mmol, 71%).

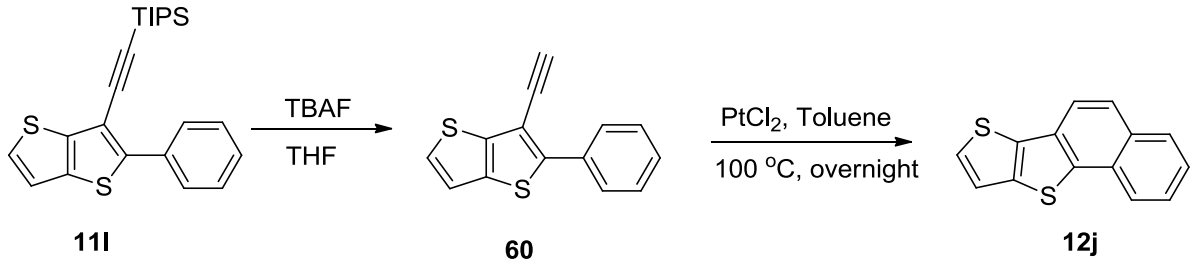
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, 1 H, *J* = 3.7 Hz, thiopheneH), 7.65 (m, 1 H, ArH), 7.48 (d, 1 H, *J* = 7.2 Hz, ArH), 7.45 (d, 1 H, *J* = 4.5 Hz, thiopheneH), 7.35-7.28 (m, 2 H, ArH), 7.95 (dd, 1 H, *J* =4.5, 3.7 Hz, thiopheneH), 3.67 (s, 1 H, Alkyne H). ^{13}C NMR (101

MHz, $CDCl_3$) δ 154.2, 153.2, 132.0, 129.5, 127.8, 127.2, 126.8, 125.3, 123.6, 120.1, 111.1, 96.9, 86.1, 75.2.

Starting from **59** (30 mg, 0.13 mmol), **12i** was obtained as white solid (14 mg, 0.062 mmol, 54%).

Rf(pentane): 0.7. Melting point: 108-109 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, 1 H, *J* = 7.5 Hz, ArH), 7.93 (d, 1 H, *J* = 8.2 Hz, ArH), 7.81 (d, 1 H, *J* = 8.2 Hz, ArH), 7.66 (d, 1 H, *J* = 8.2 Hz, ArH), 7.51 (s, 2 H, ArH), 7.47(m, 1 H, ArH), 7.39 (t, 1 H, *J* = 7.5 Hz, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.0, 151.0, 140.8, 126.4, 126.0, 124.9, 124.9, 123.1, 123.0, 120.5, 119.6, 118.7, 117.1, 111.8. IR 2922 (w), 2388 (m), 2301 (s), 1781 (w), 1706 (m), 1688 (s), 1677 (s), 1658 (s), 1646 (s), 1565 (s), 1550 (s), 1532 (s), 1516 (m), 1448 (s), 1414 (m), 1408 (m), 1321 (m), 1244 (m), 1231 (m), 1207 (m), 1189 (s), 1176 (m), 1046 (w), 880 (m). HRMS (ESI) calcd for $C_{14}H_8OS$ [M+] 224.0290; found 224.0289.

Naphtho[1,2-b]thieno[2,3-d]thiophene (12j)



11l **60** **12j**

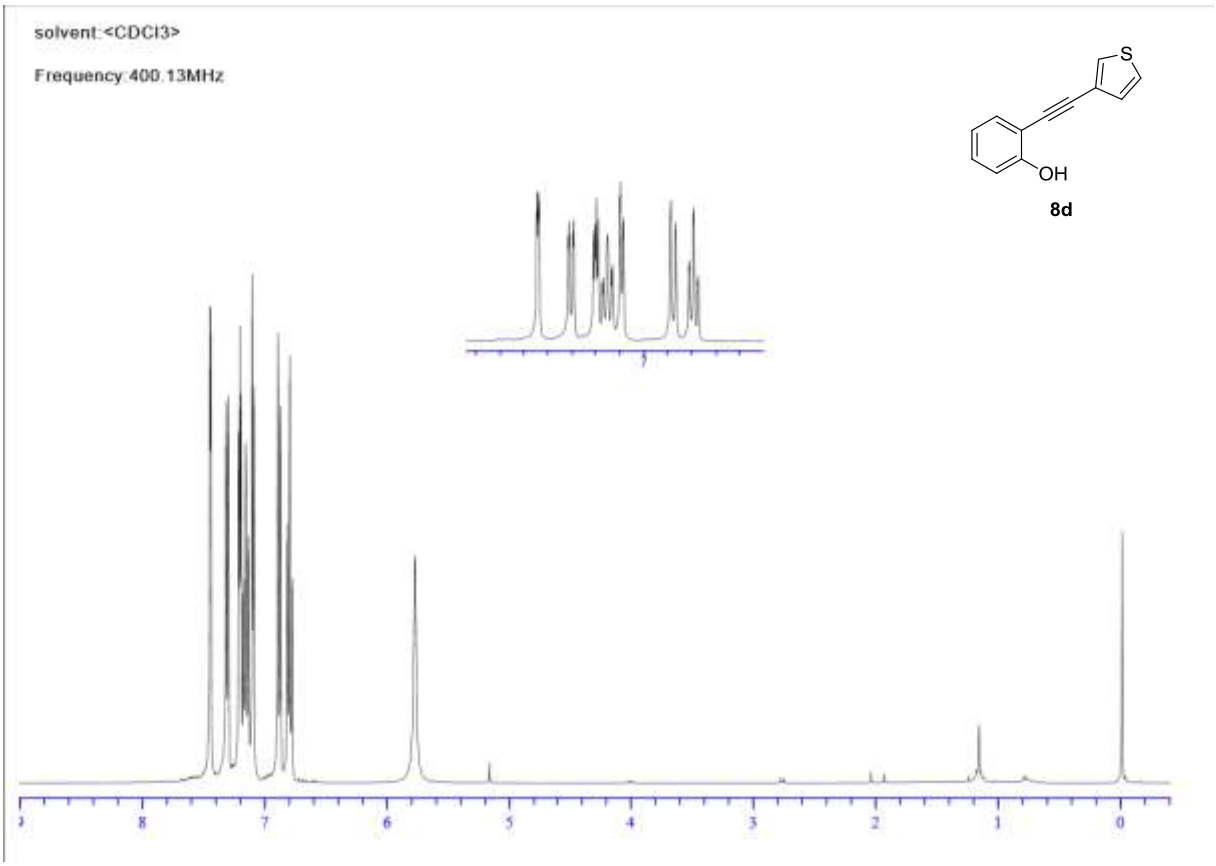
Following the general procedure **GP3,** starting from **11l** (43 mg, 0.11 mmol), **60** was obtained as brown oil (15 mg, 0.062 mmol, 58%).

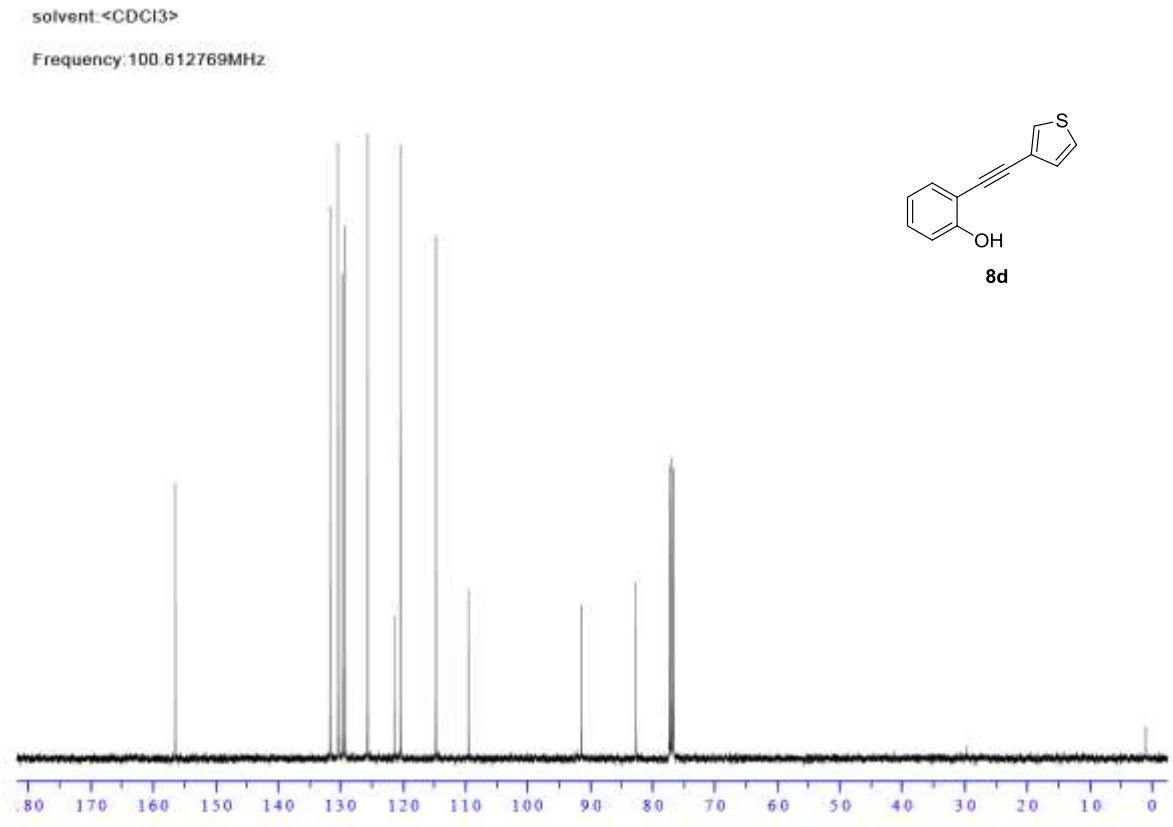
^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (t, 2 H, *J* = 7.5 Hz, ArH), 7.35 (t, 2 H, *J* = 7.2 Hz, ArH), 7.31 (d, 1 H, *J* = 5.1 Hz, ThiopheneH), 7.28 (d, 1 H, *J* = 7.4 Hz, ArH), 7.15 (t, 1 H, *J* = 4.3 Hz, ThiopheneH), 3.32 (s, 1 H, Alkyne H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 143.0, 135.8, 133.9, 128.8, 128.6, 127.8, 127.3, 119.7, 109.6, 82.4, 77.7.

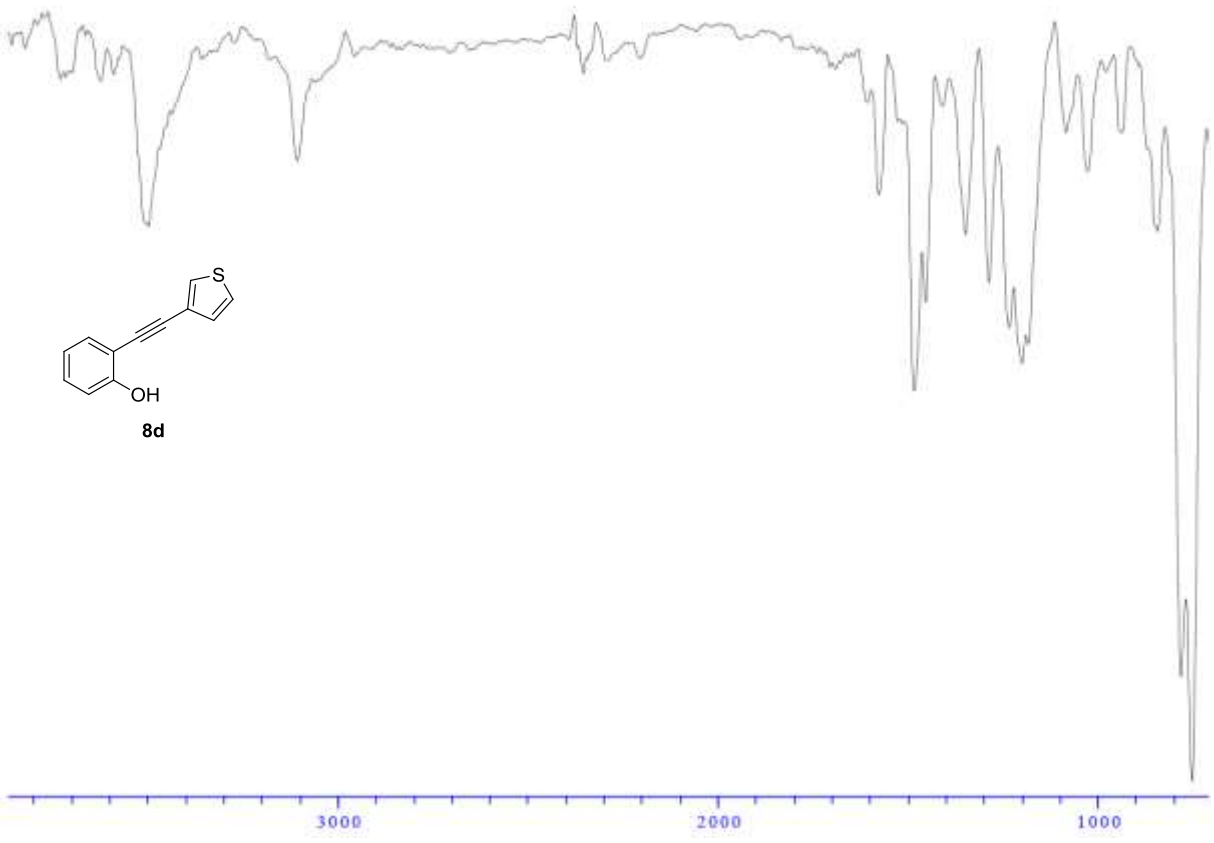
Starting from **60** (15 mg, 0.062 mmol), **12j** was obtained as white solid (9 mg, 0.04 mmol, 60%).

Rf(pentane): 0.5. Melting point: 153-154 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, 1 H, *J* = 8.1 Hz, ArH), 7.95 (d, 1 H, *J* = 8.1 Hz, ArH), 7.88 (d, 1 H, *J* = 8.6 Hz, ArH), 7.82 (d, 1 H, *J* = 8.6 Hz, ArH), 7.59 (t, 1 H, *J* = 7.0 Hz, ArH), 7.52 (m, 2 H, ArH), 7.41 (d, 1 H, *J* = 5.2 Hz, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.8, 137.3, 136.3, 130.9, 130.1, 129.9, 129.0, 127.5, 126.9, 125.8, 125.7, 123.2, 120.3, 119.7. IR 3095 (w), 3055 (w), 3008 (w), 2927 (s), 2860 (m), 2394 (w), 2352 (w), 2338 (w), 2292 (w), 2273 (w), 2051 (w), 1803 (w), 1726 (w), 1707 (w), 1689 (w), 1658 (w), 1628 (w), 1549 (w), 1532 (w), 1517 (w), 1464 (w), 1380 (w), 1330 (m), 1259 (m), 1083 (w), 981 (w), 910 (w). HRMS (ESI) calcd for $C_{14}H_9S_2^+$ $[M+H]^+$ 241.0140; found 241.0144.

8. Spectra for new compounds







8d

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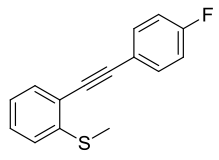
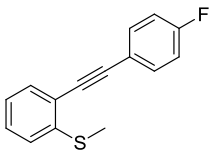
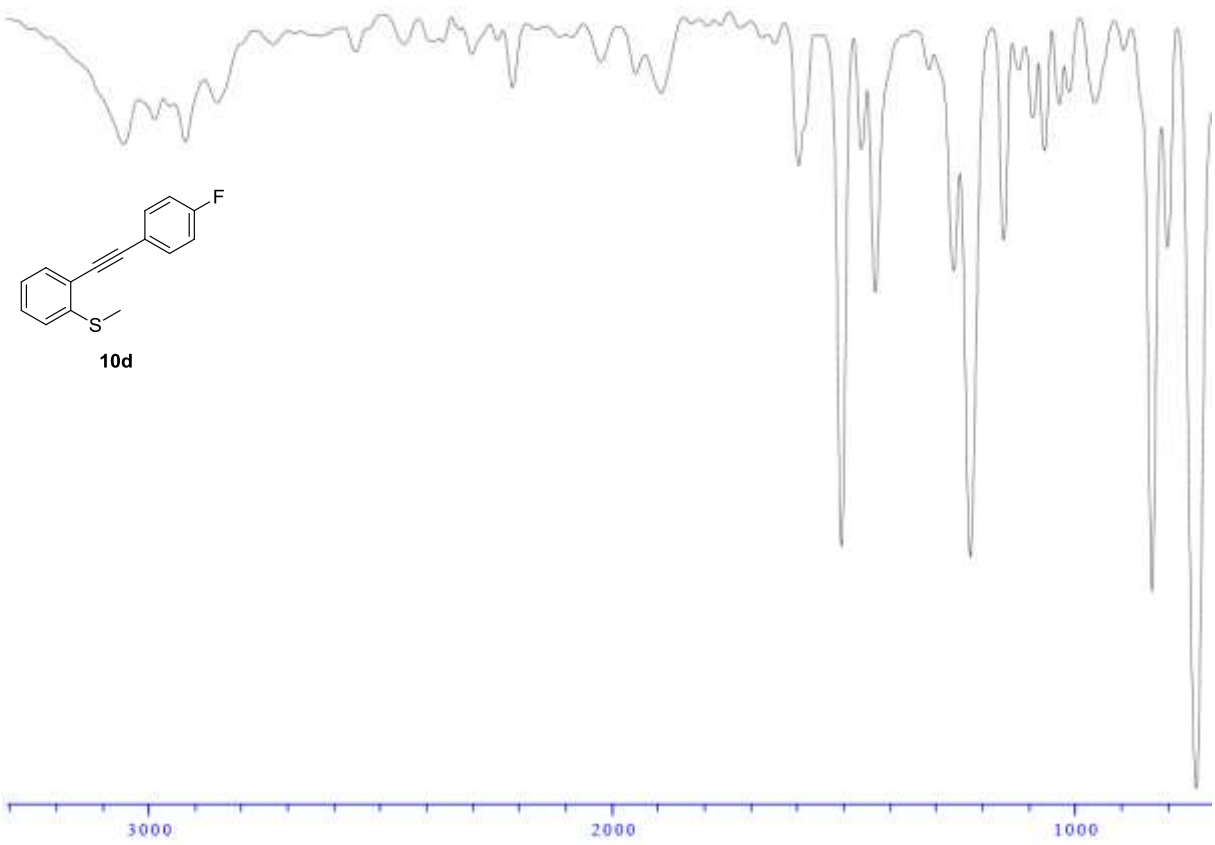


10d

solvent:<CDCl3>
Frequency:100.612769MHz



10d



10d

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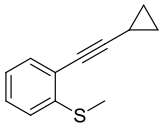
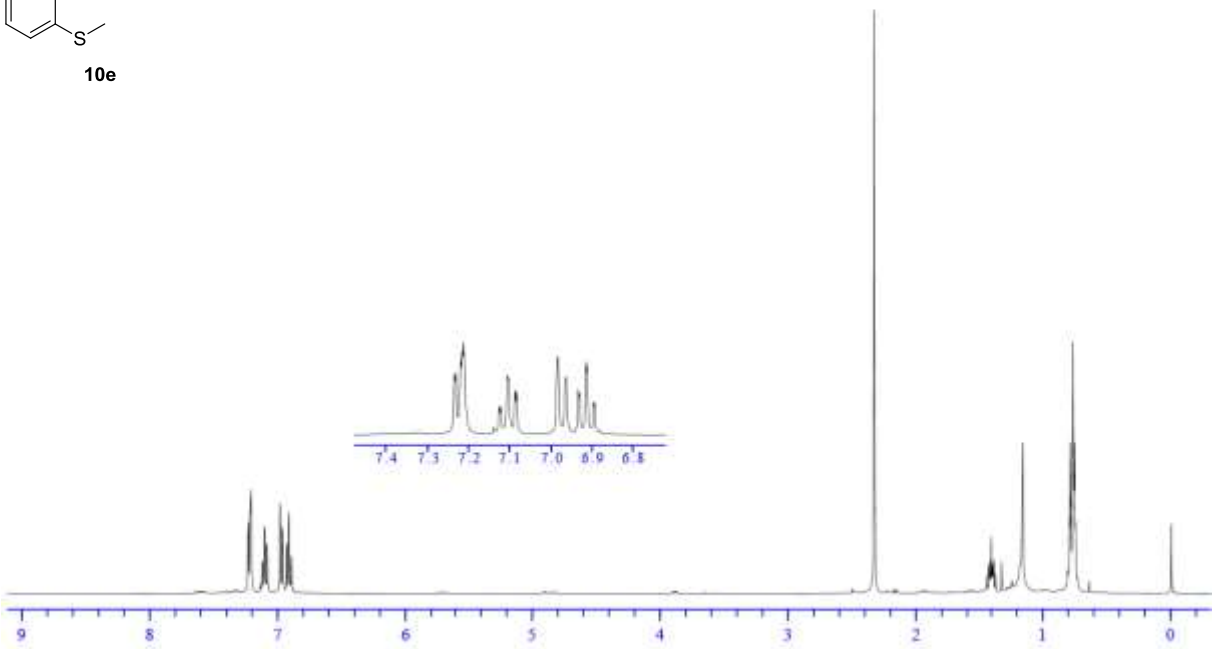


10e



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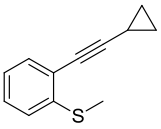

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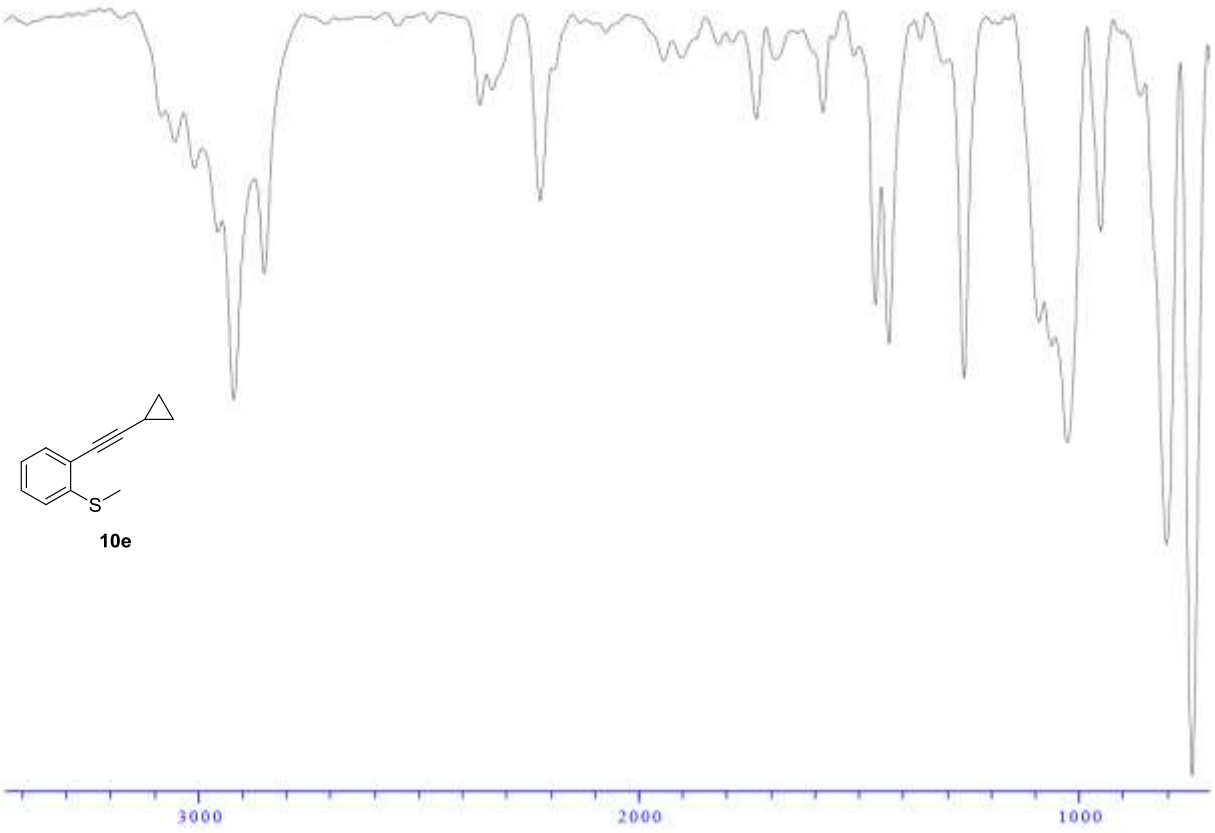

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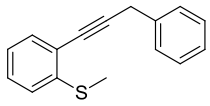

10g

solvent:<CDCl3>
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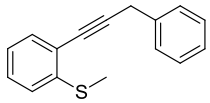
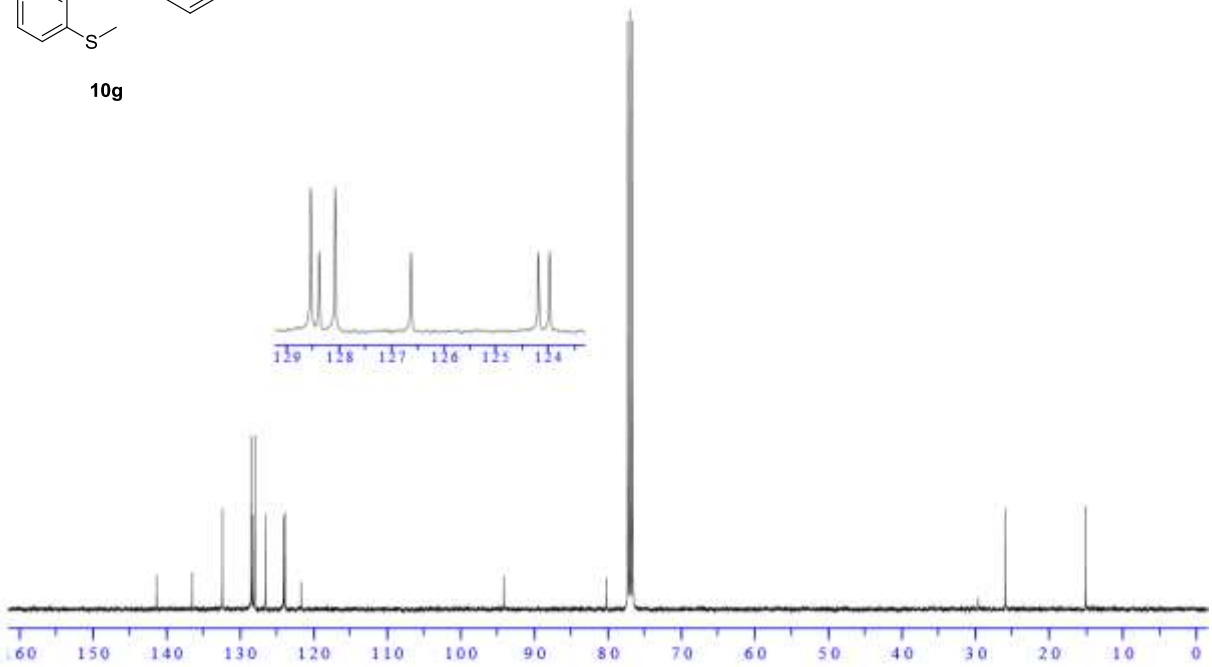
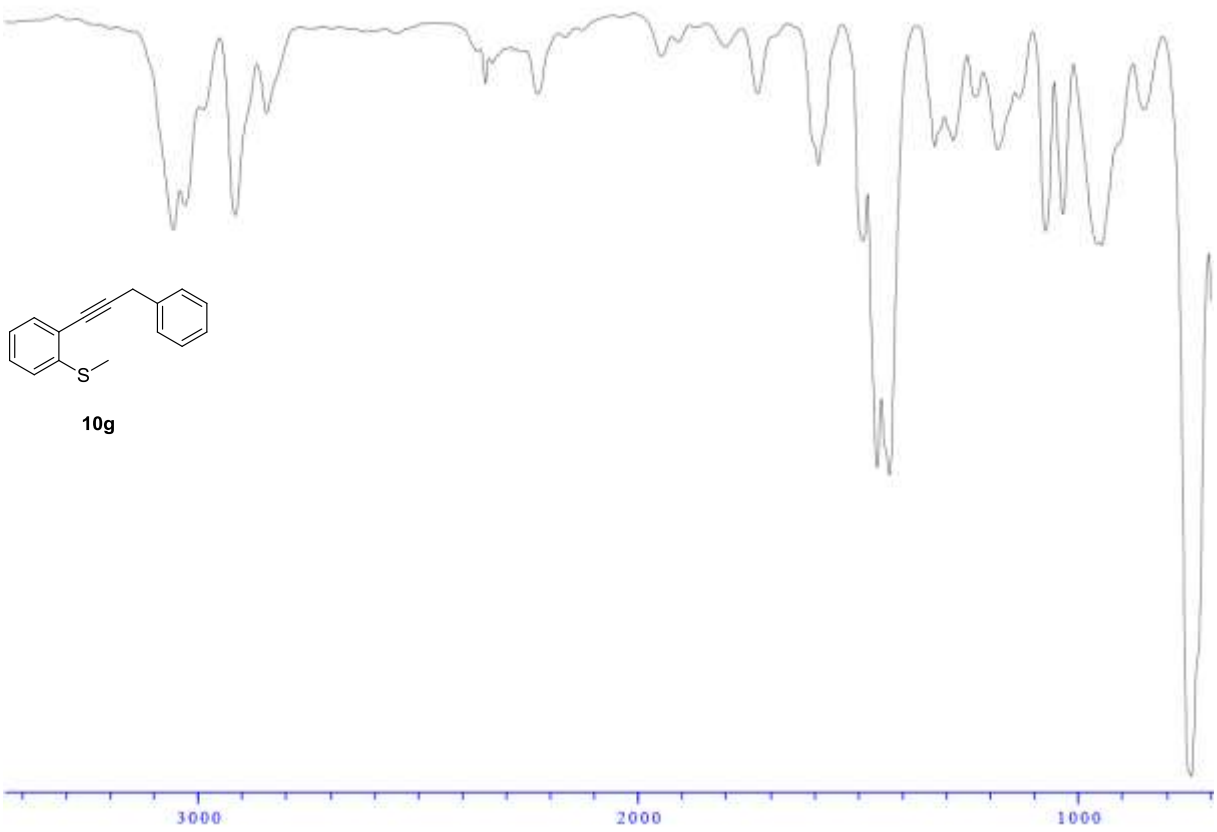


10g





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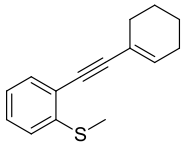

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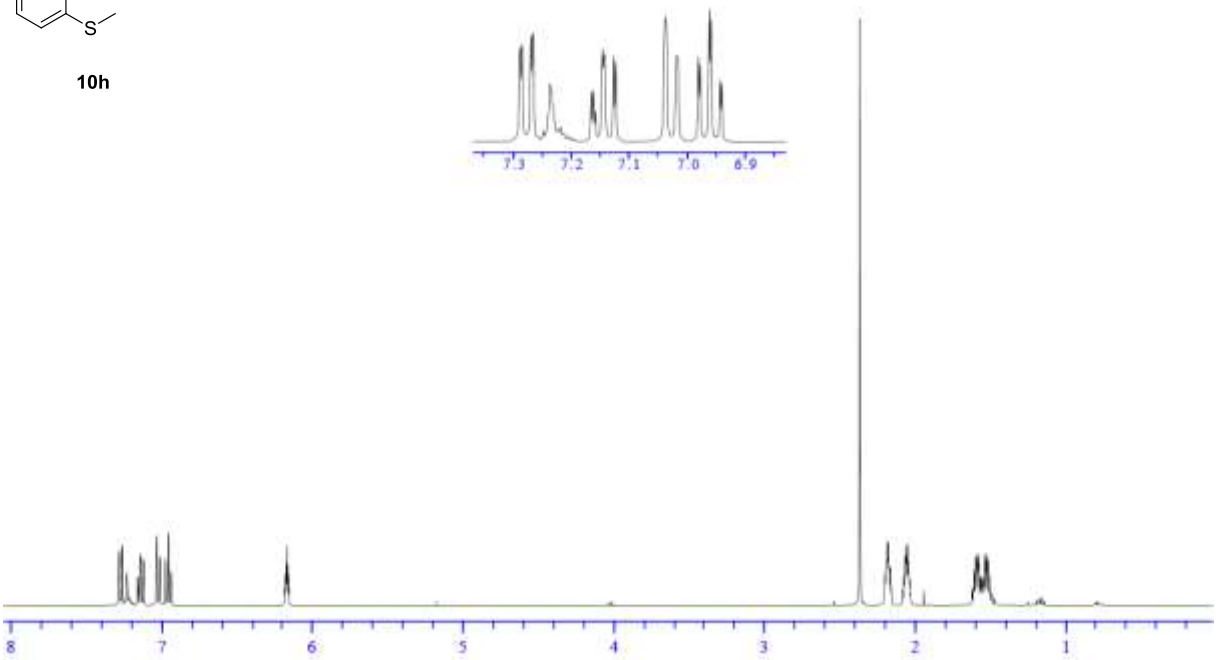

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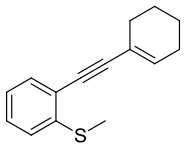
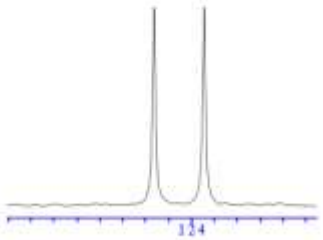
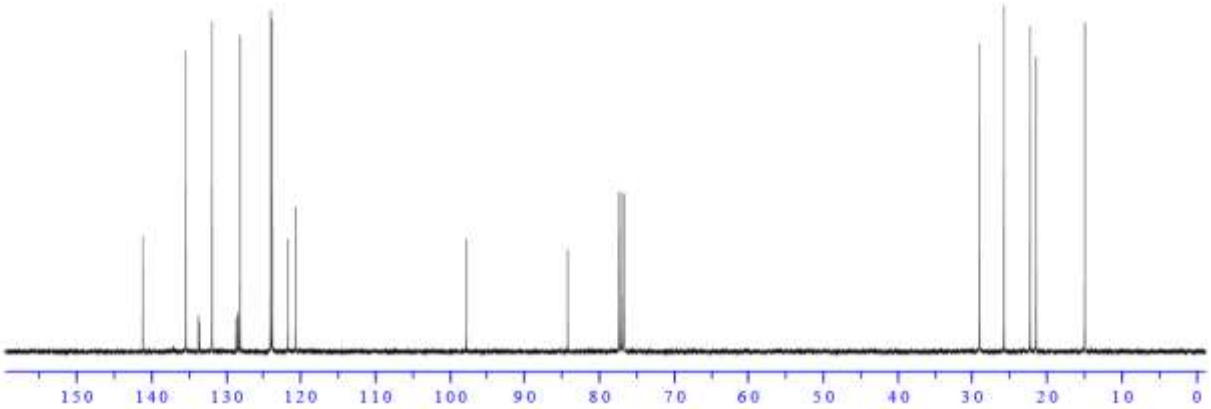
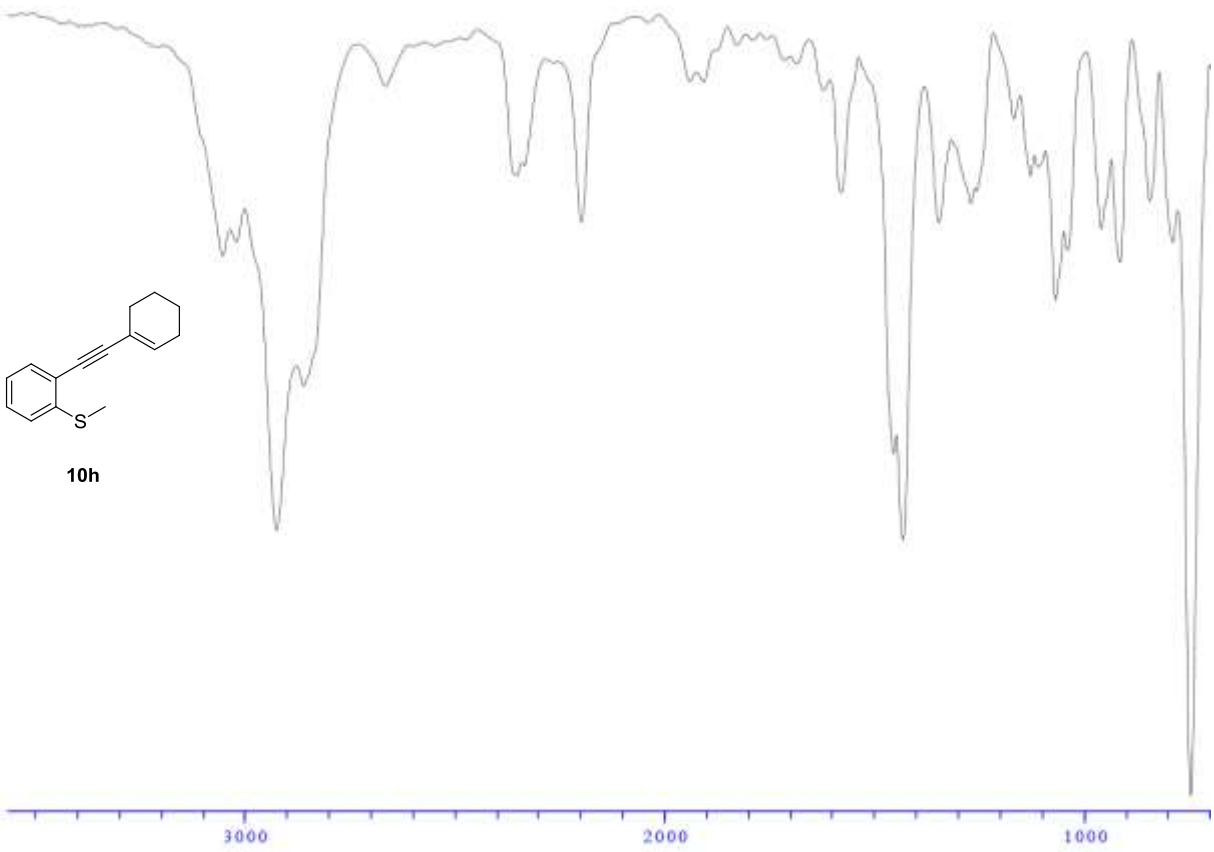


10h







10h

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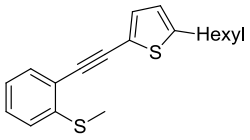
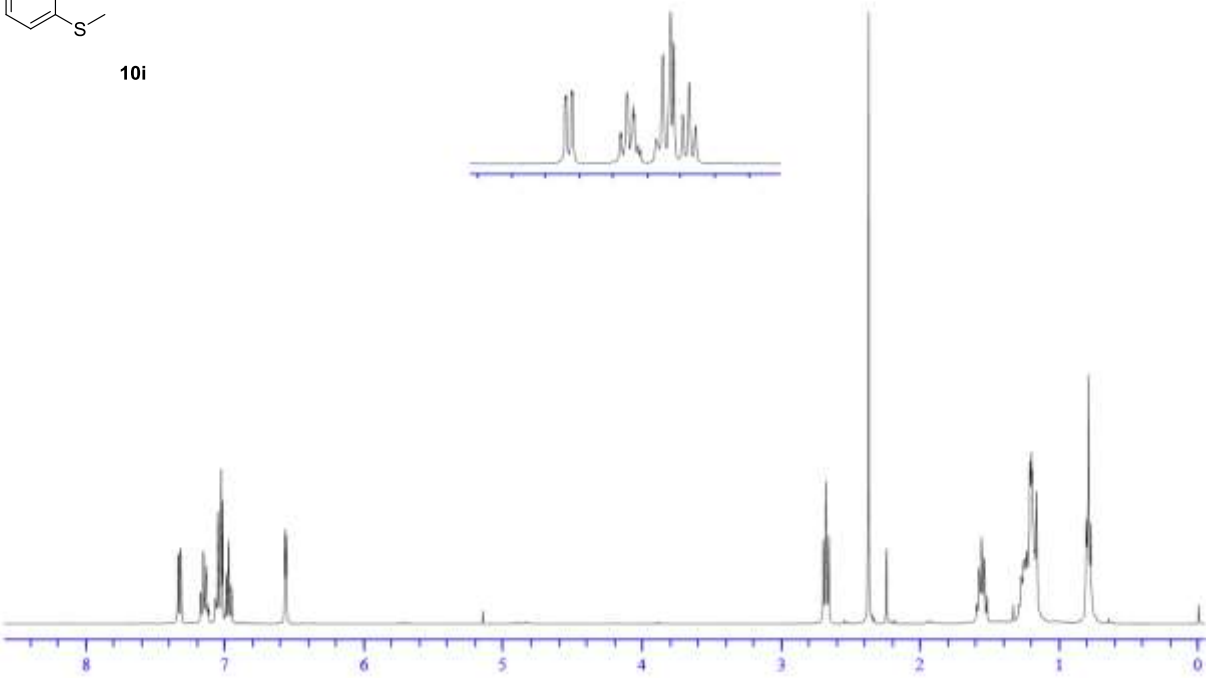


10i



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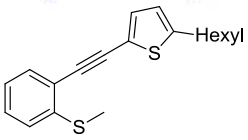

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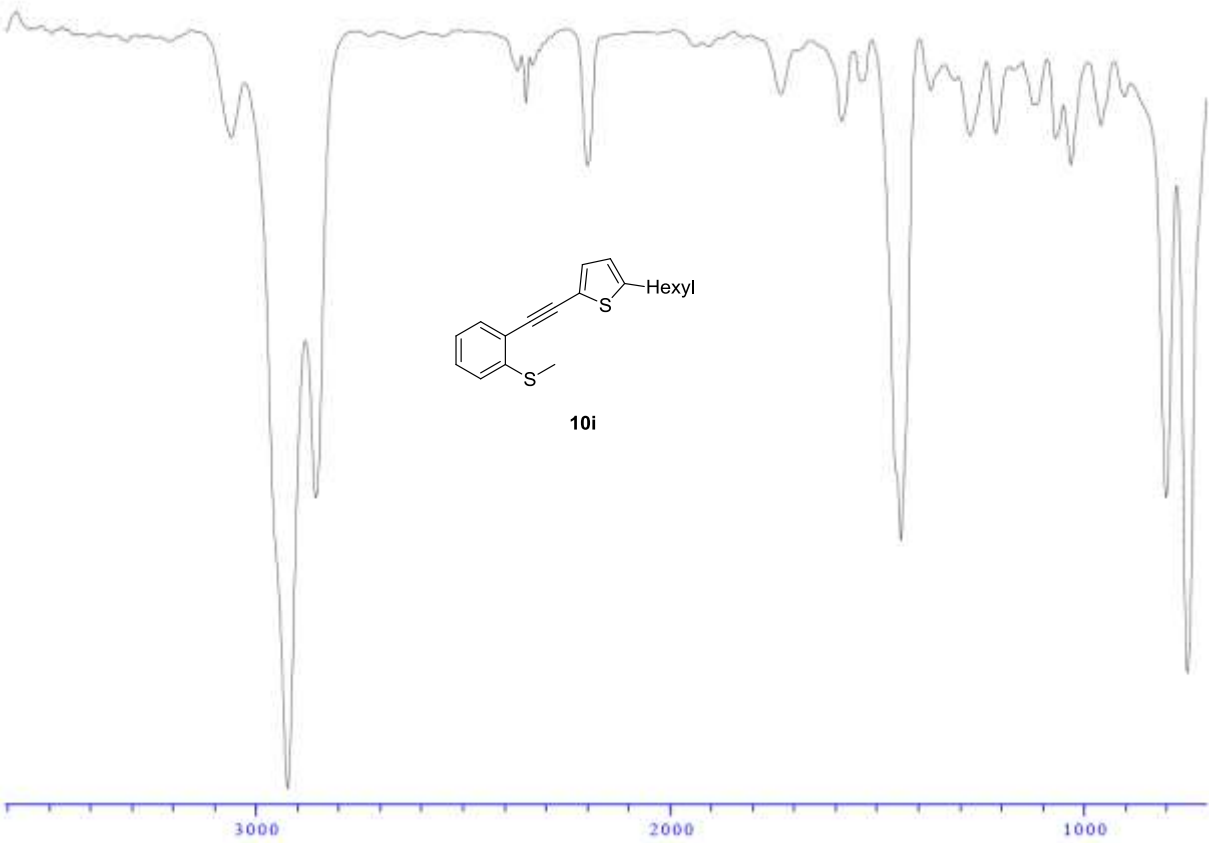

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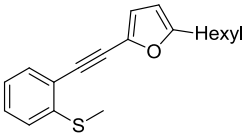

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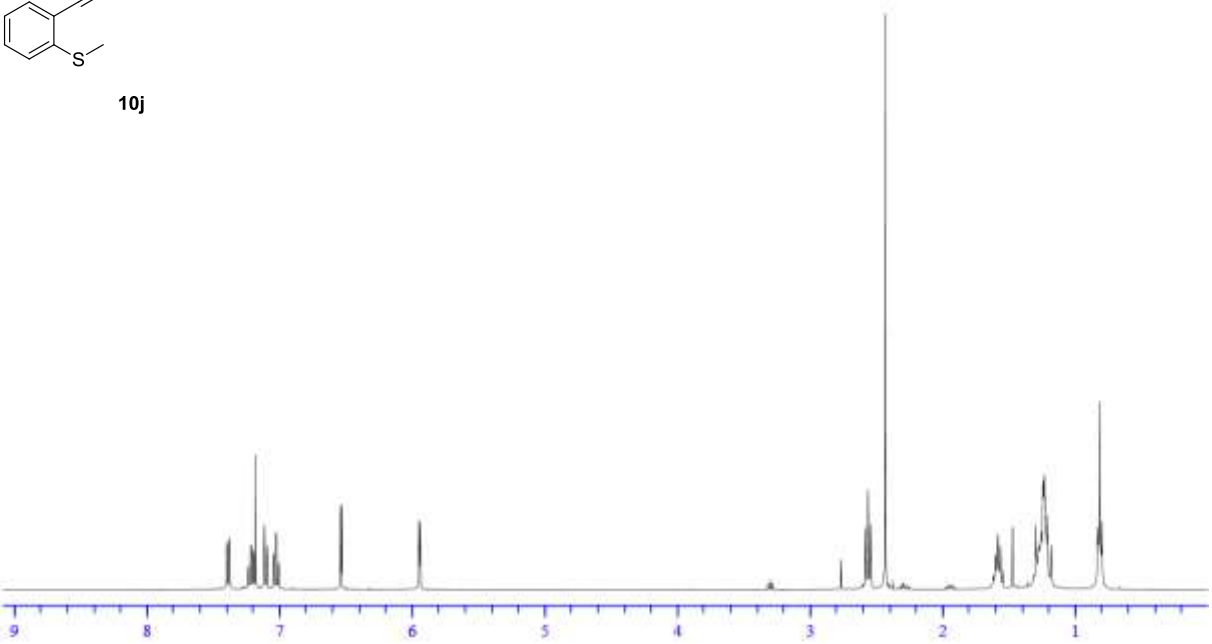

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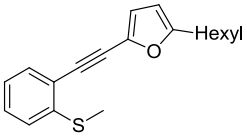

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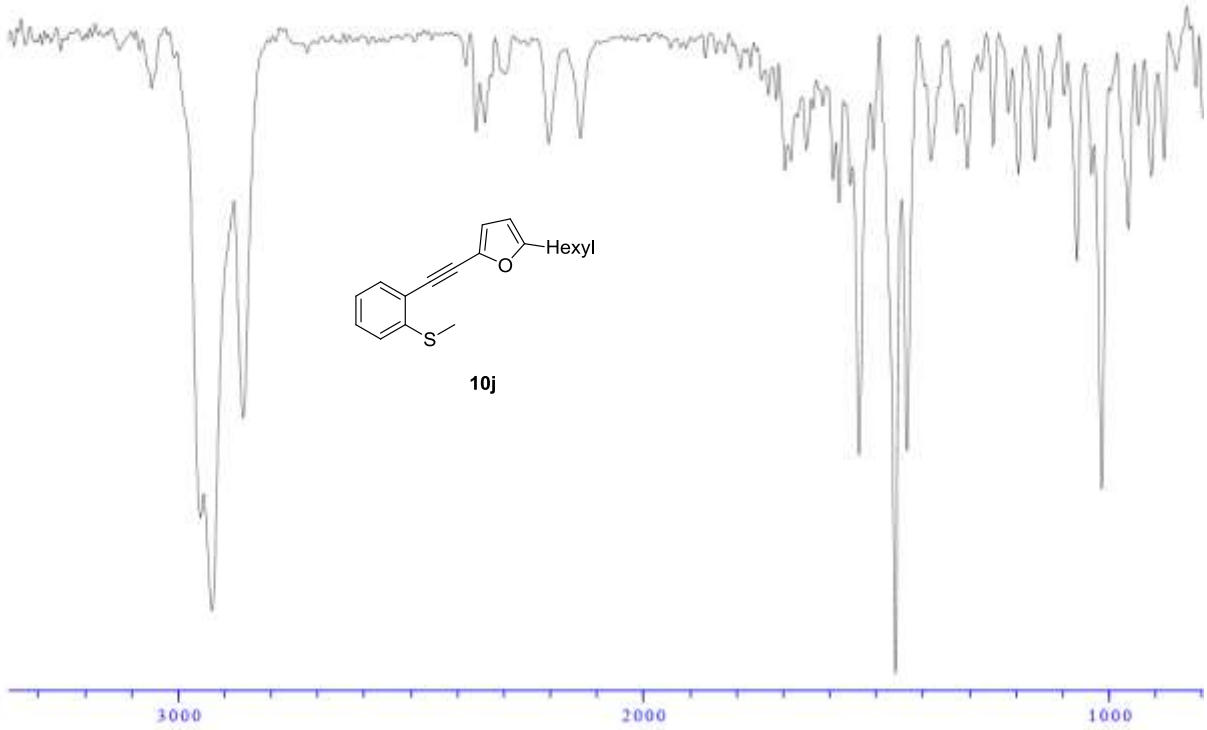

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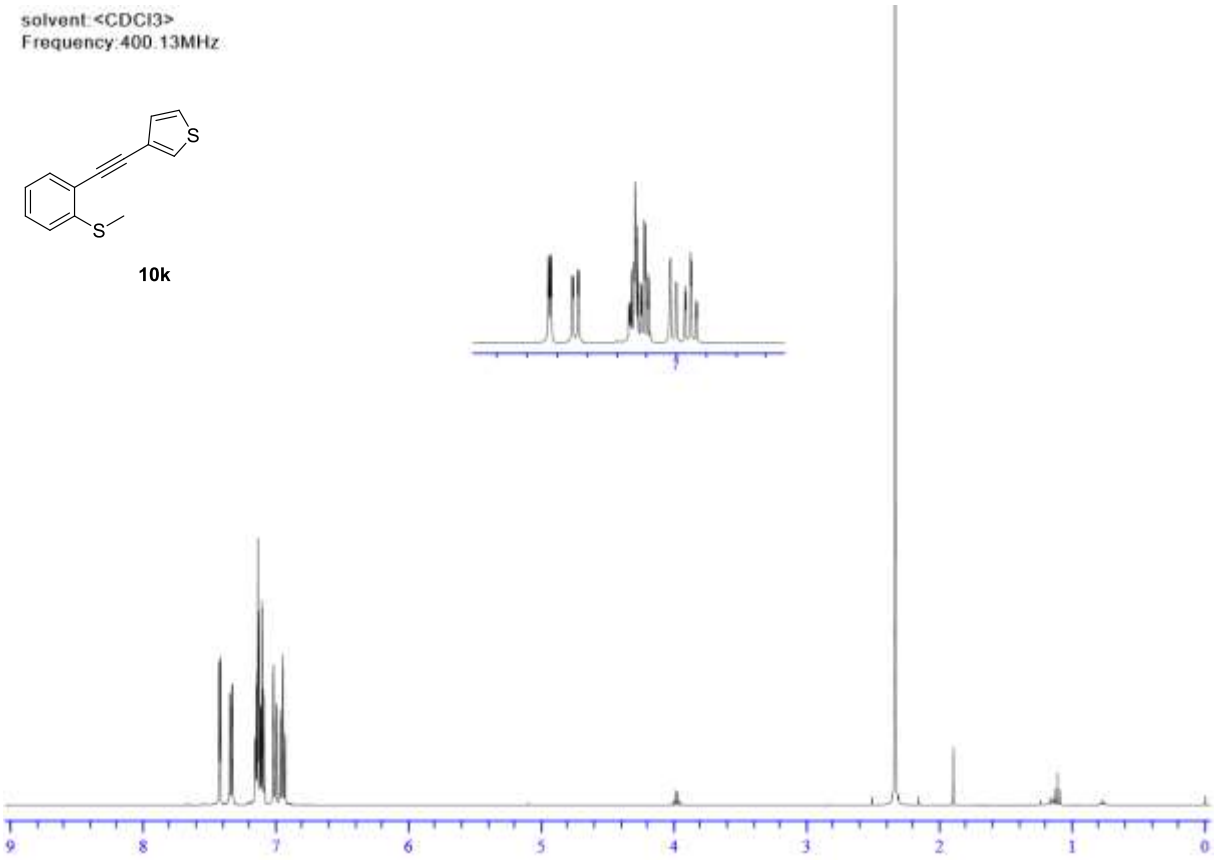
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10k
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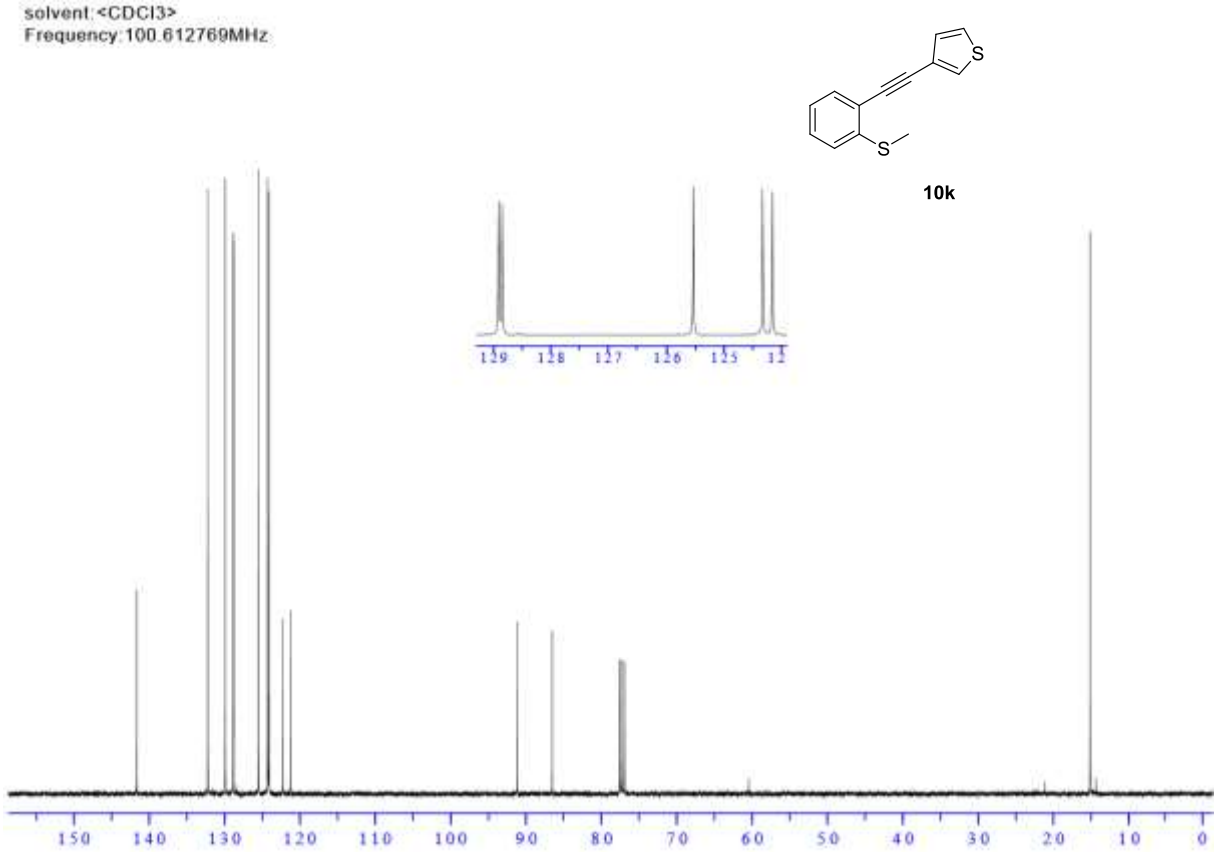
5
4
3
2
1
0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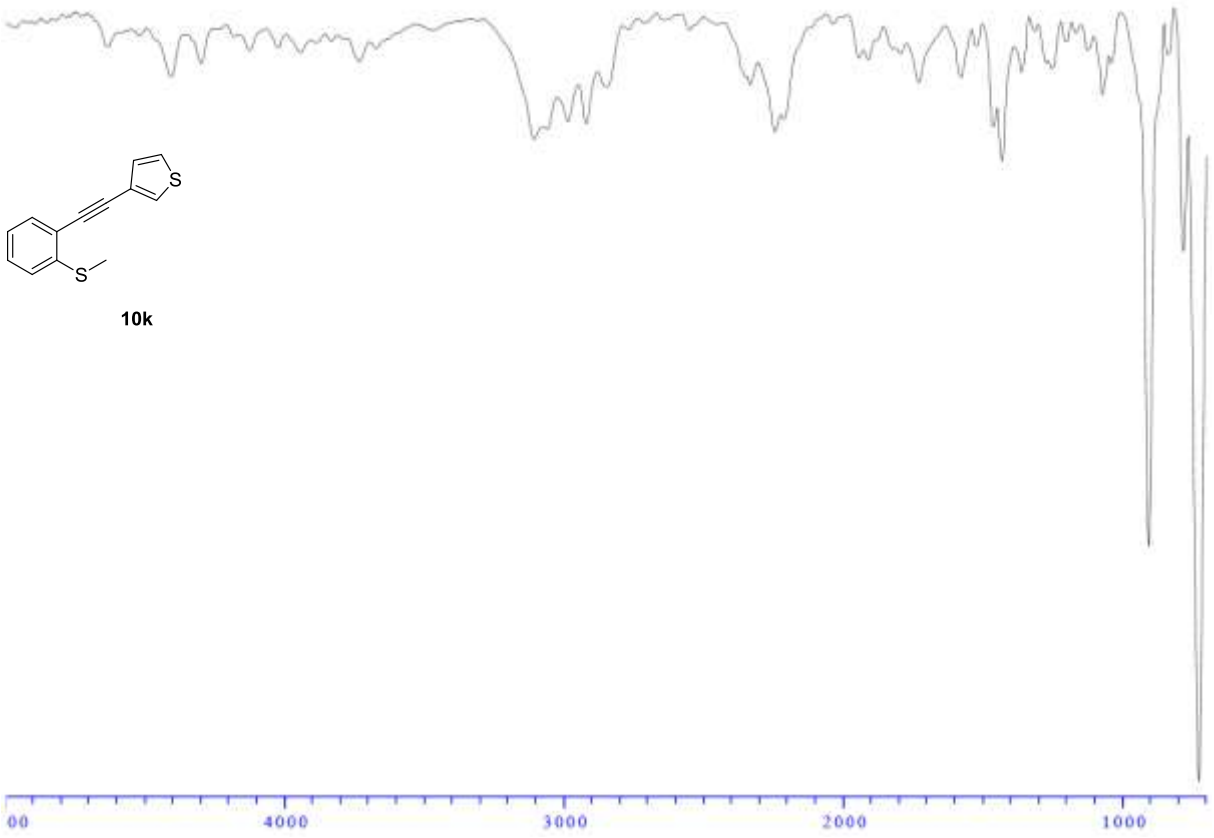
10
0



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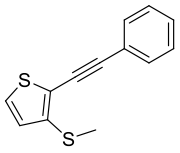

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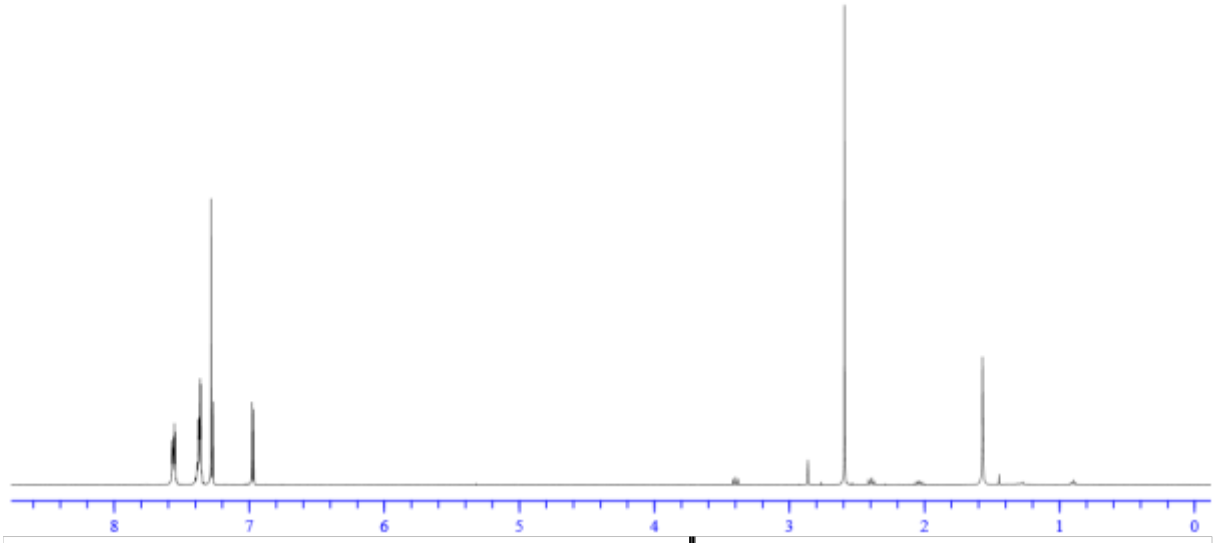

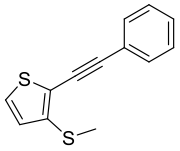

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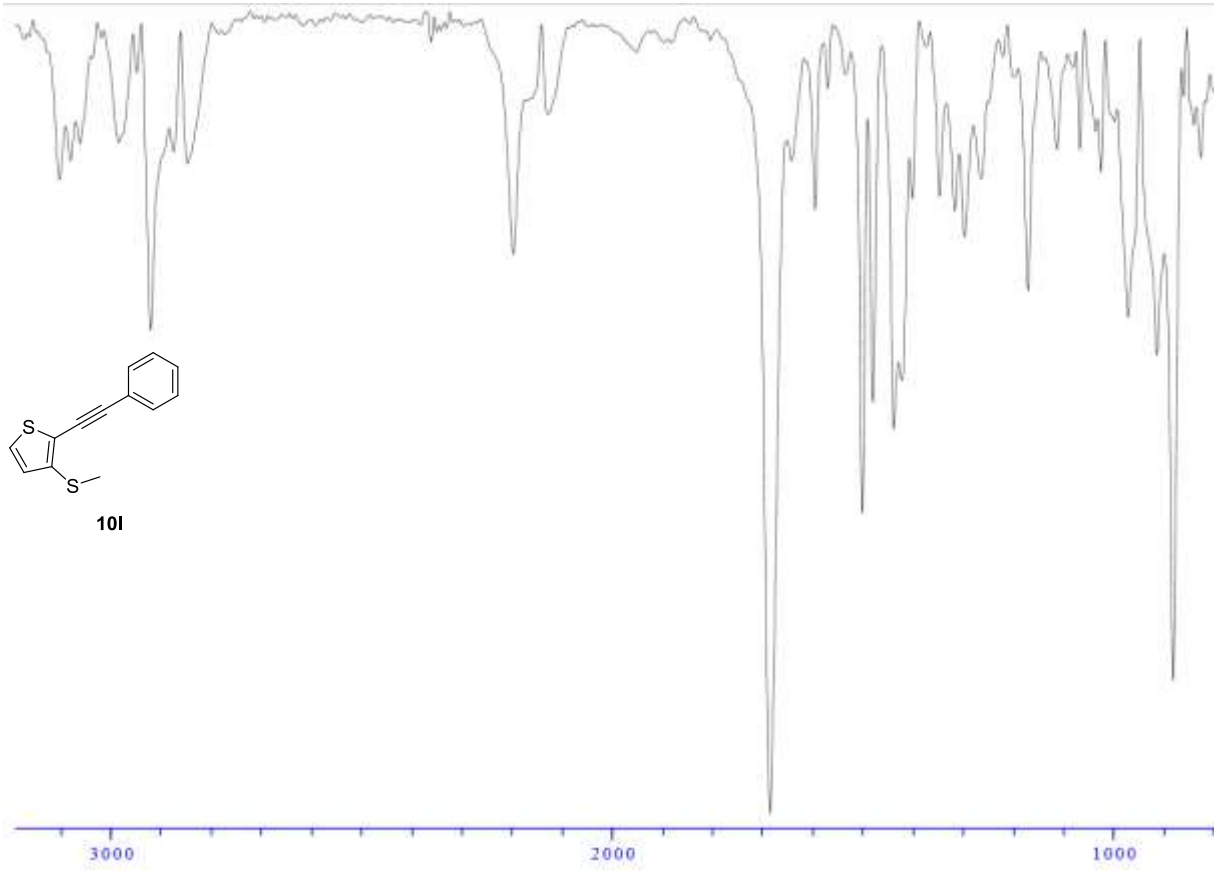

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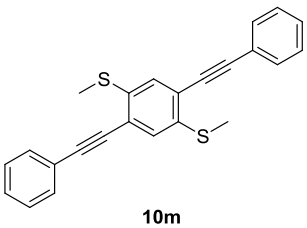

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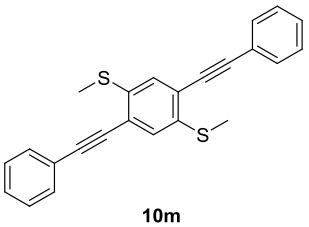
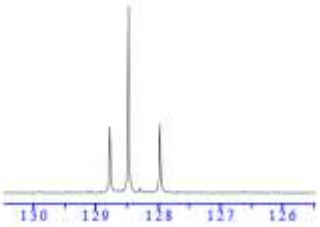
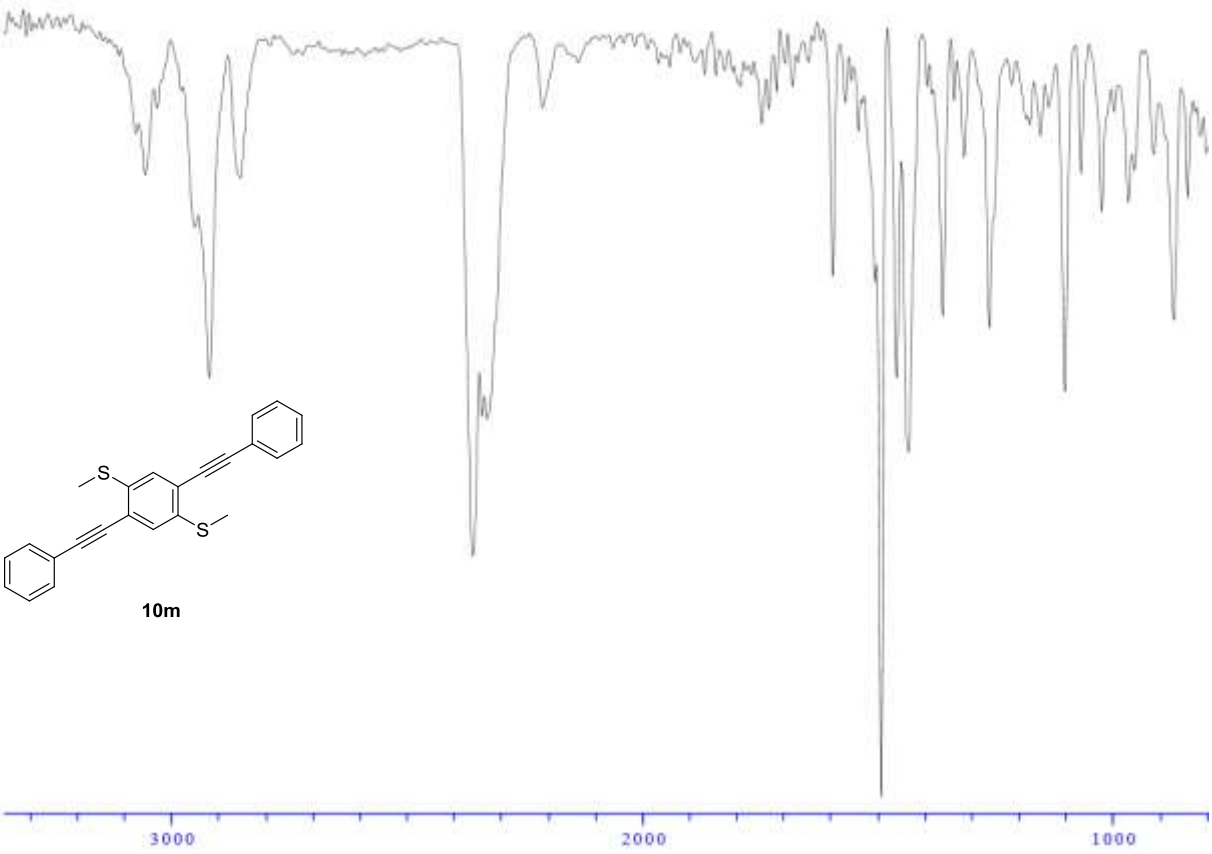


10m





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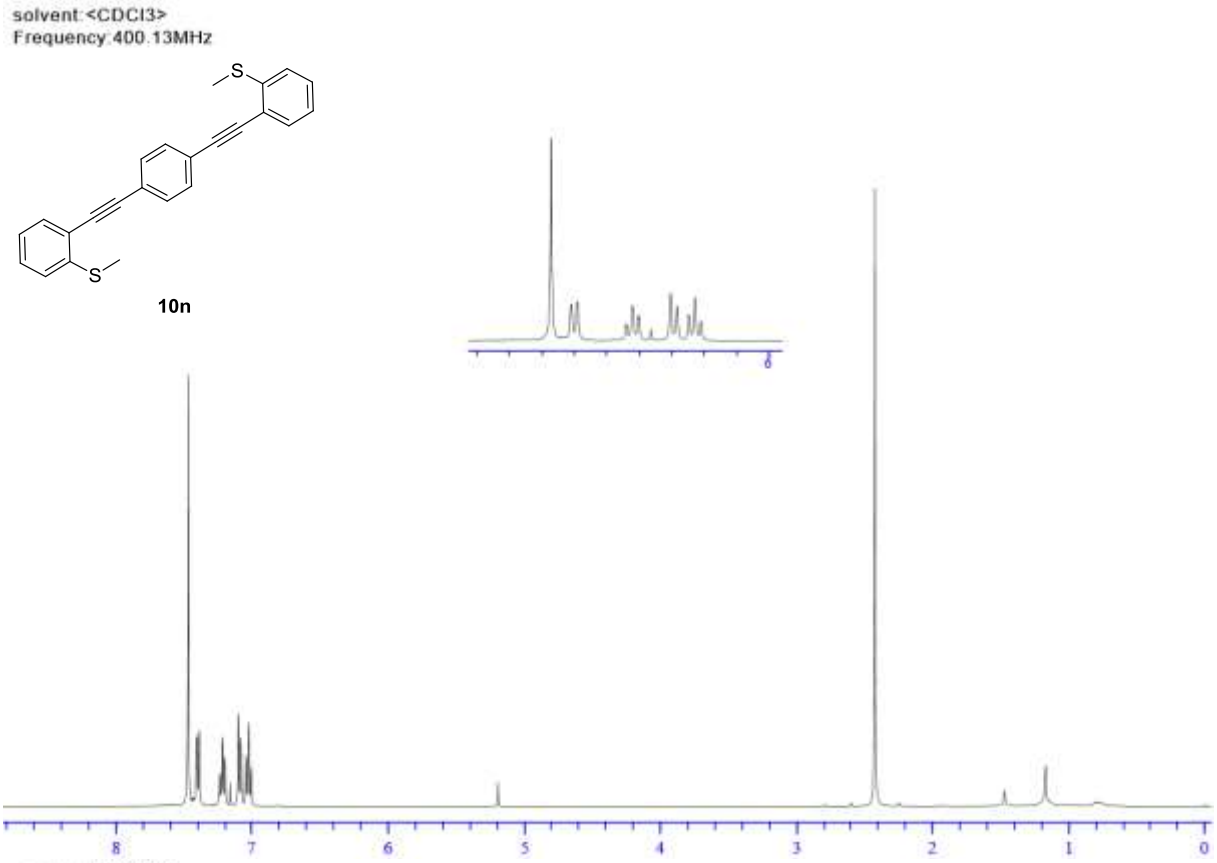
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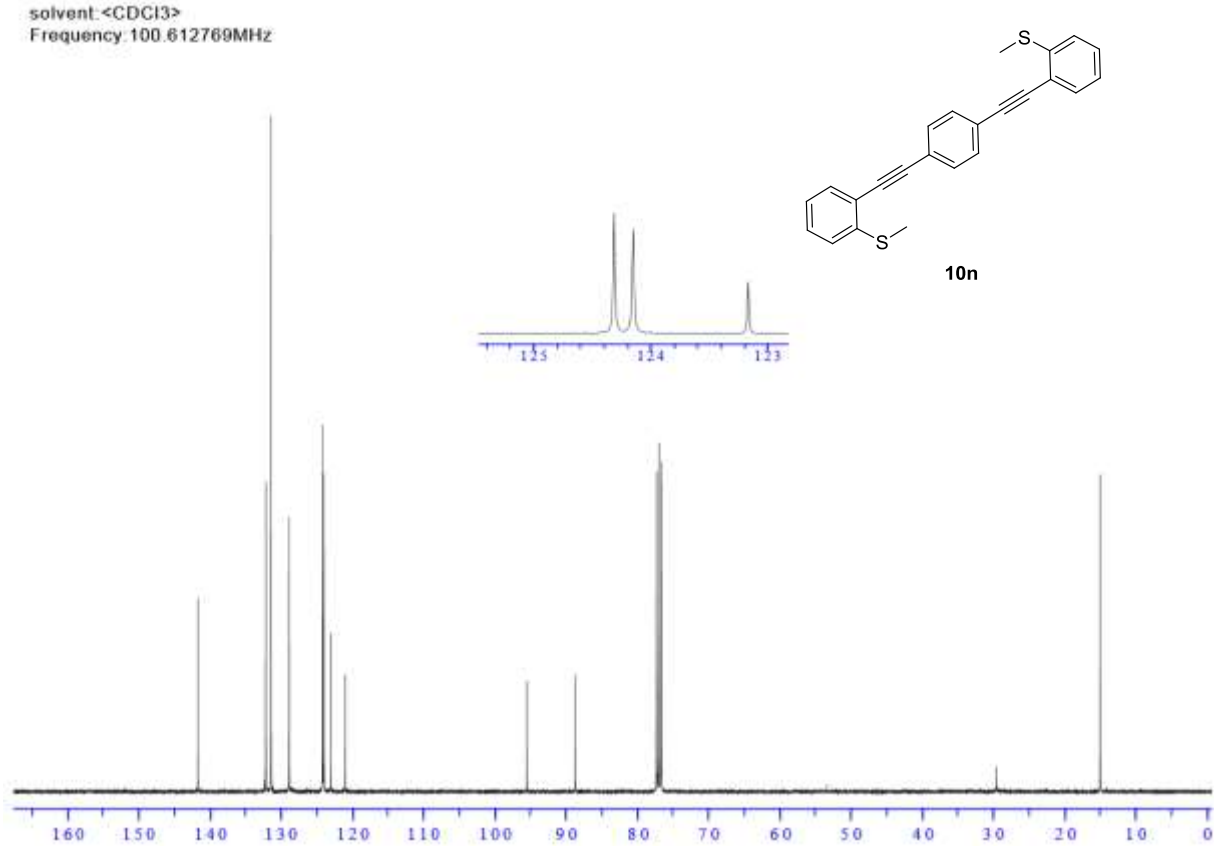
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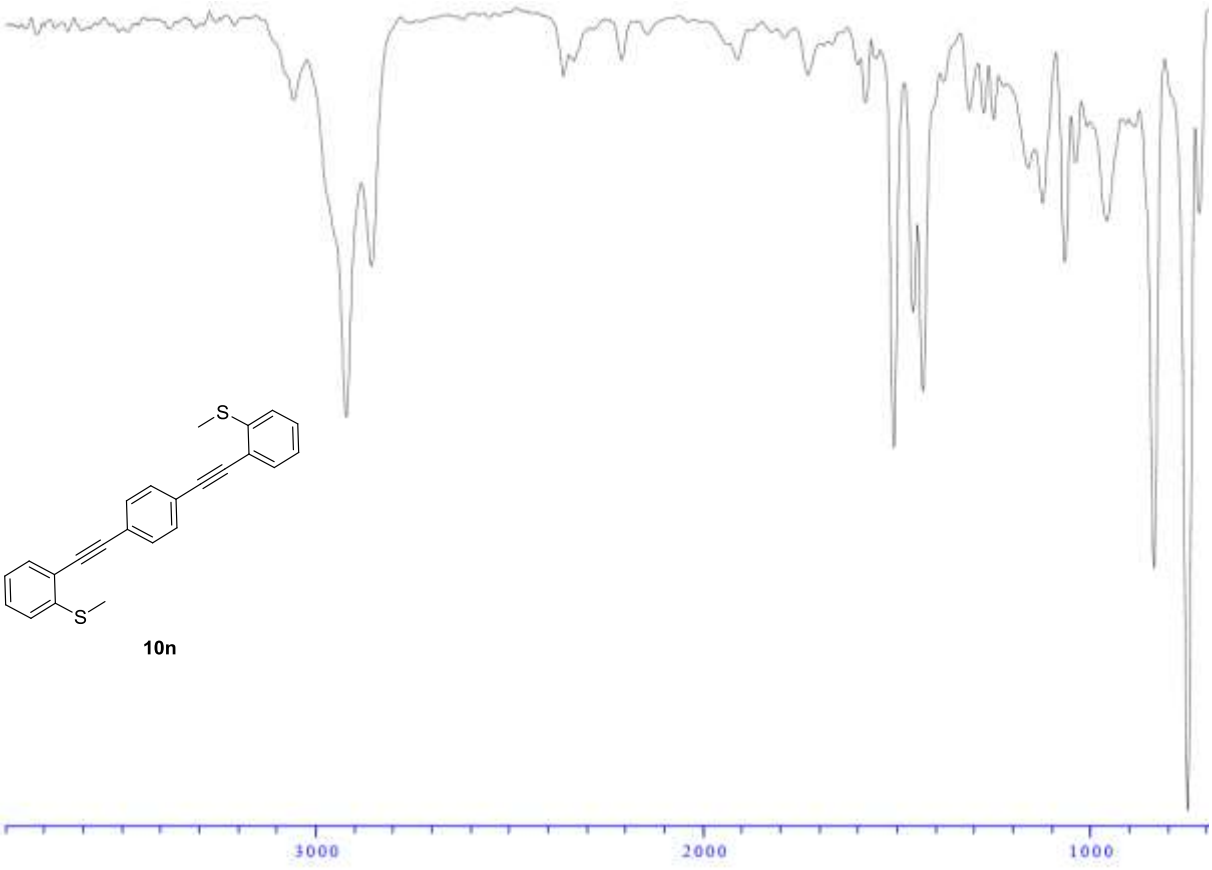
10
0



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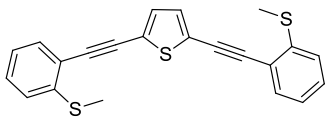

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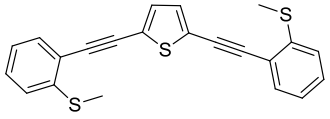

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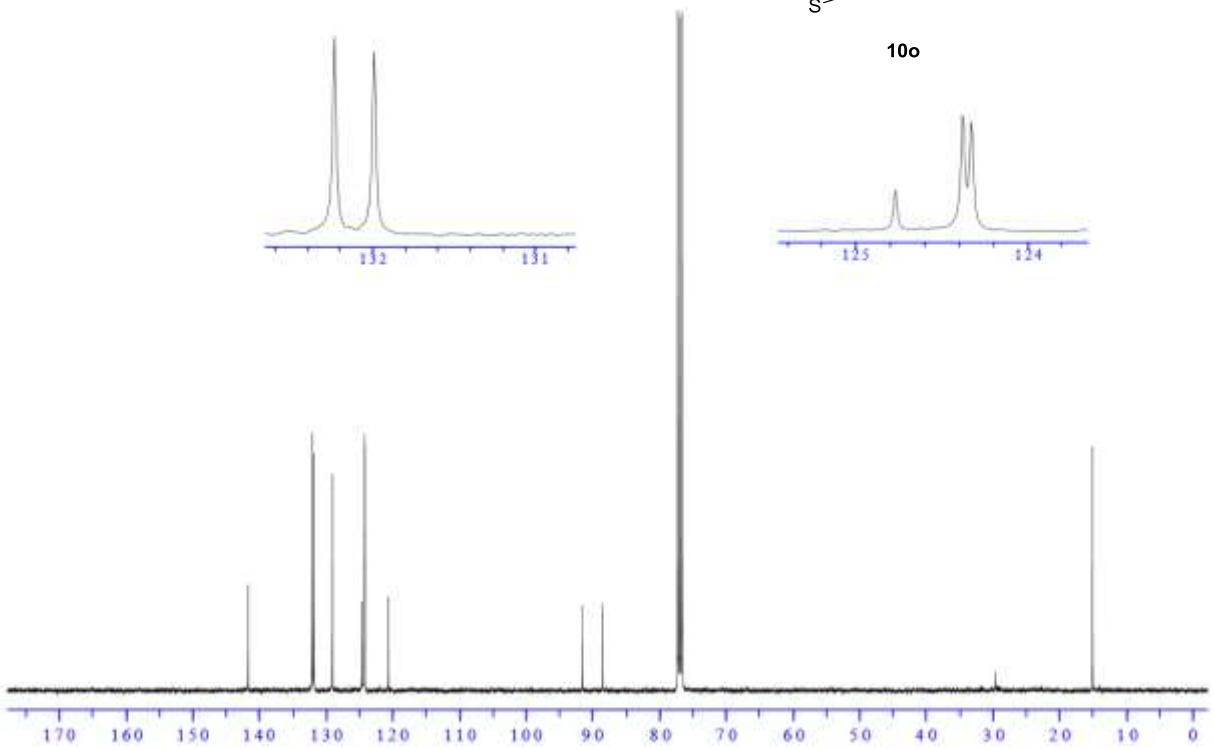

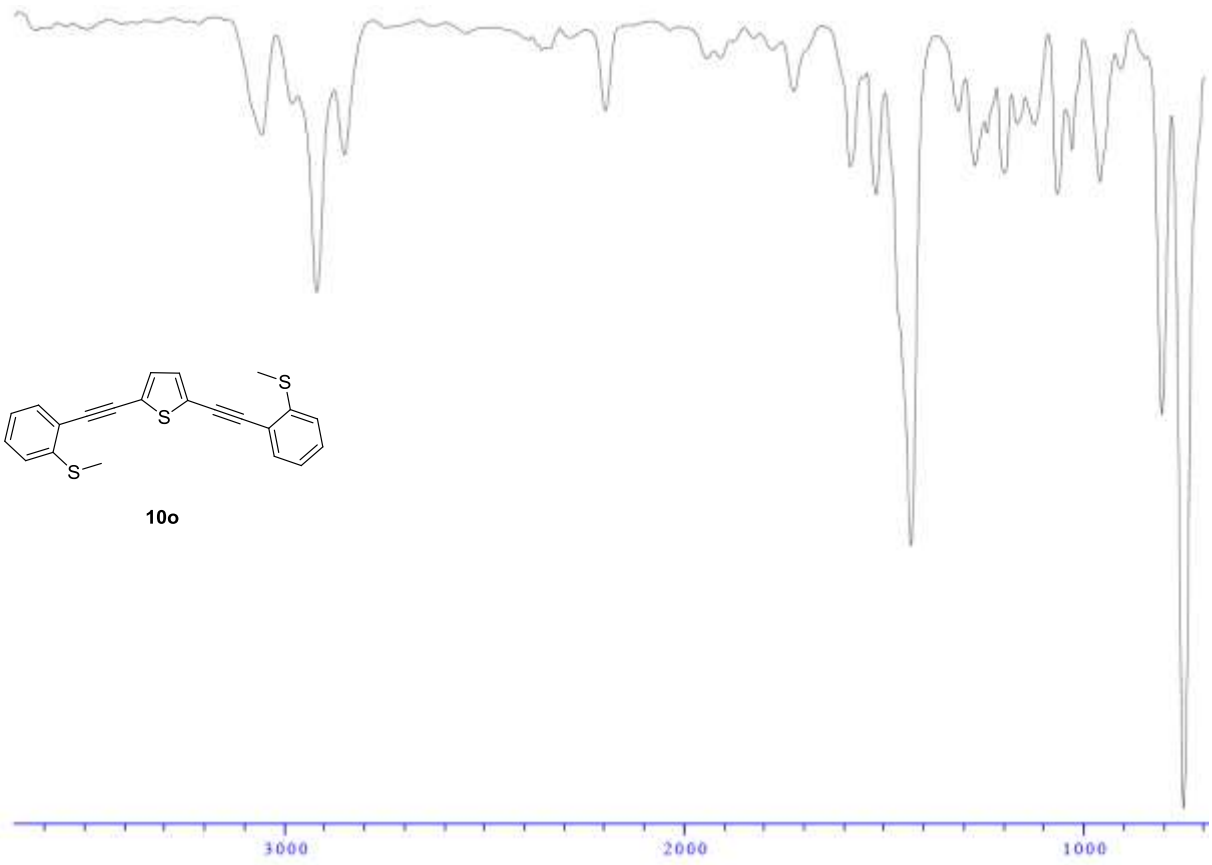

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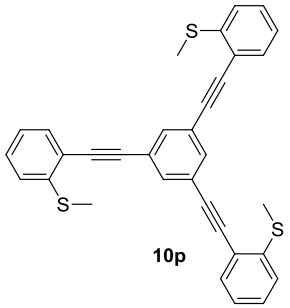

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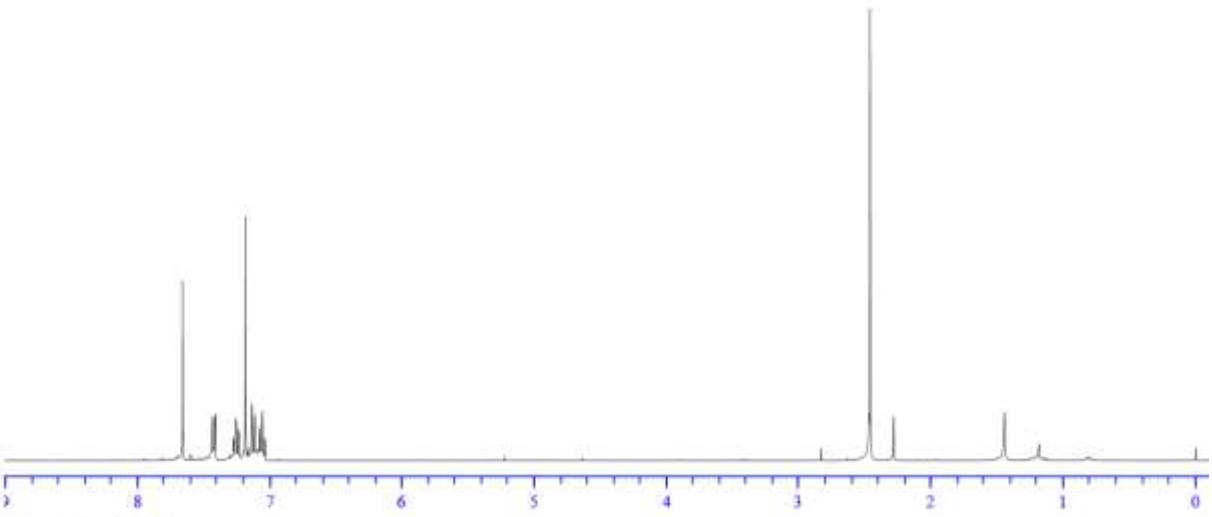

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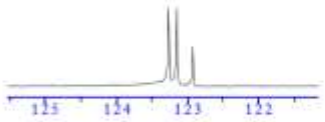
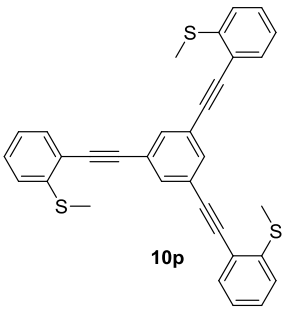
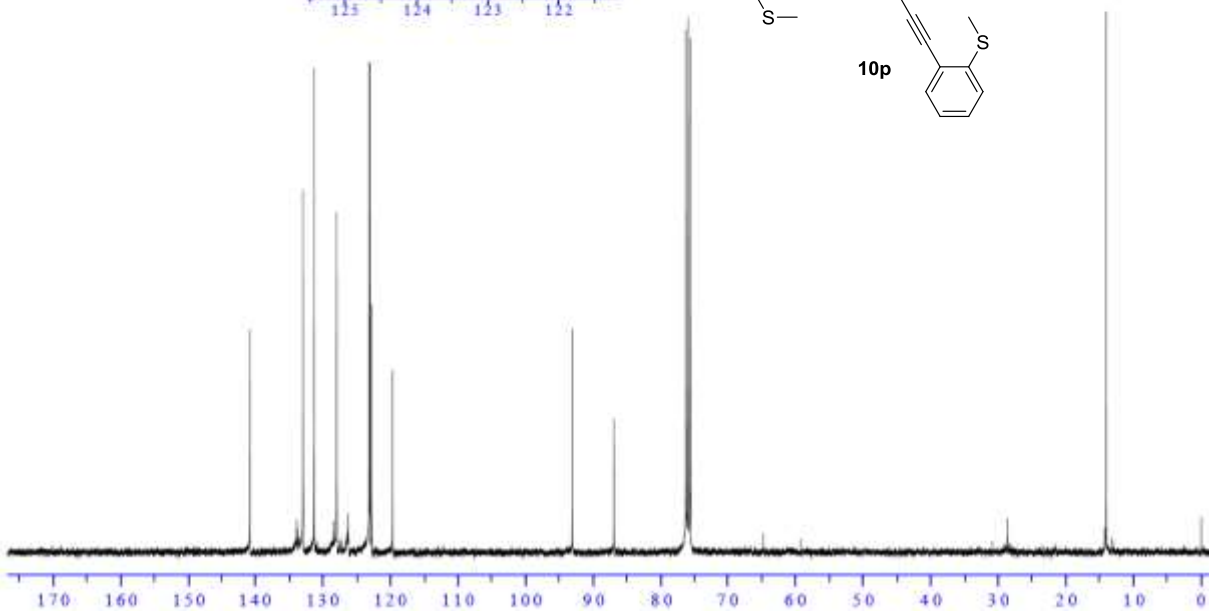
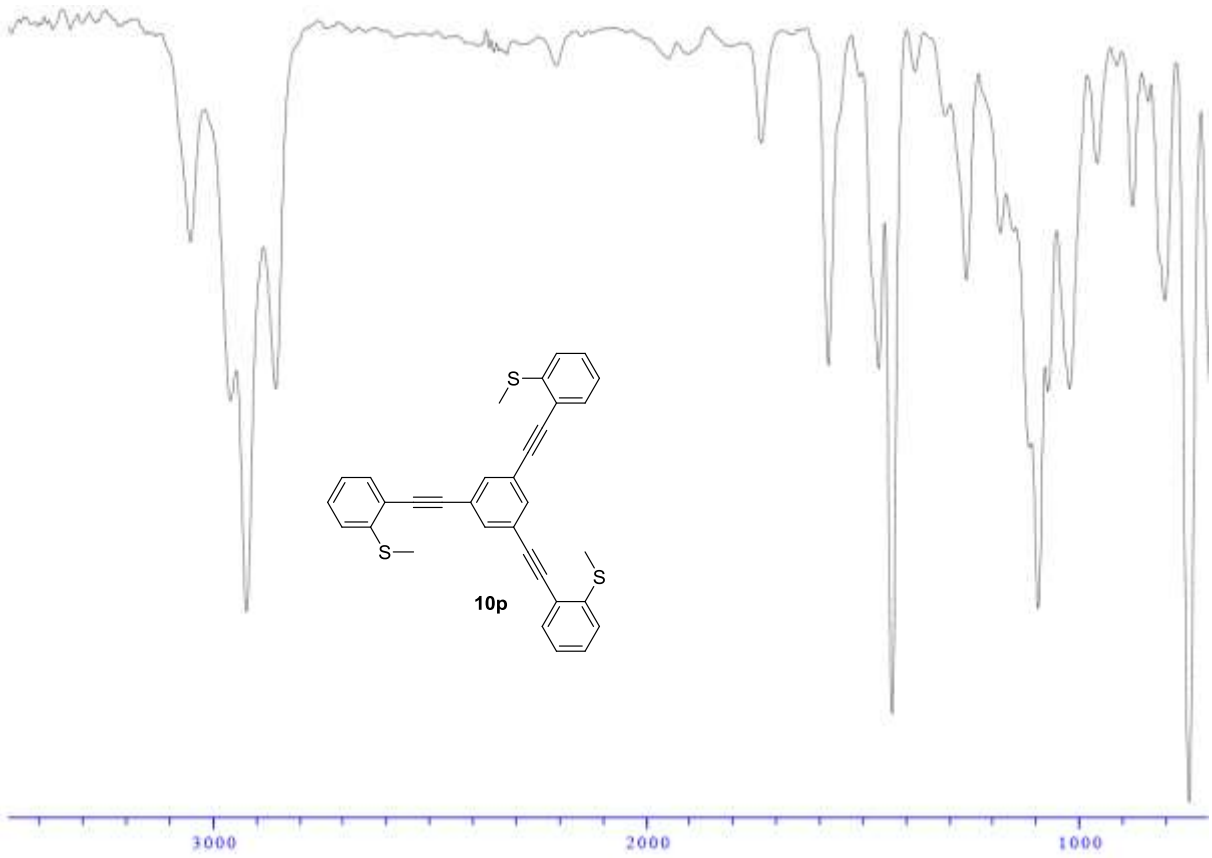




10p




S
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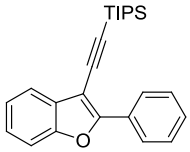
2000
1000

solvent:<CDCl3>
Frequency:400.13MHz



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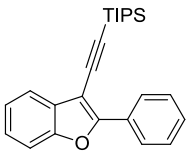
solvent:<CDCl3>
Frequency:100.612769MHz



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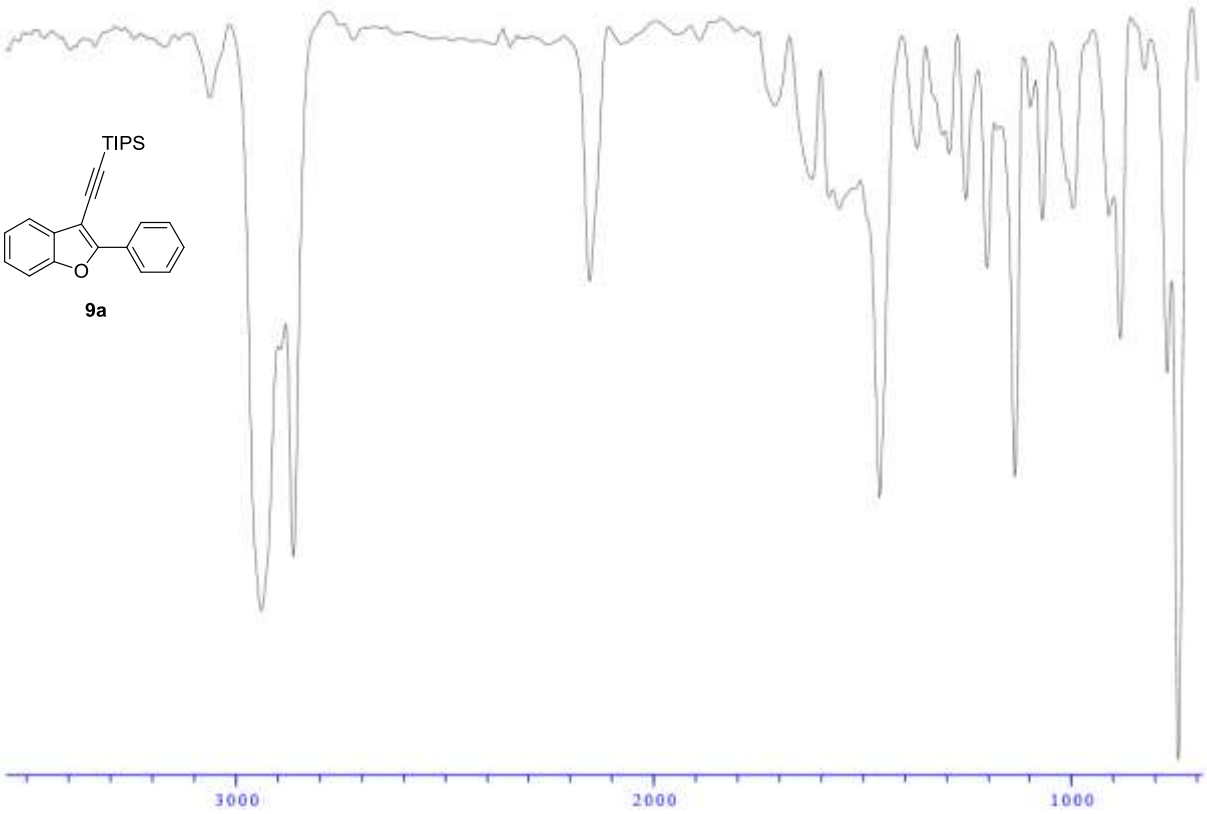

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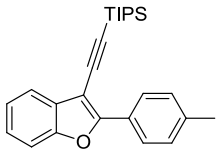

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solvent:<CDCl3>
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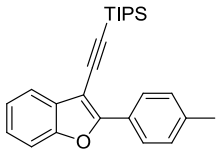

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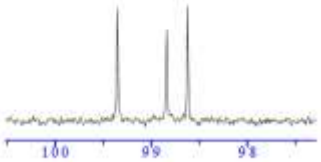

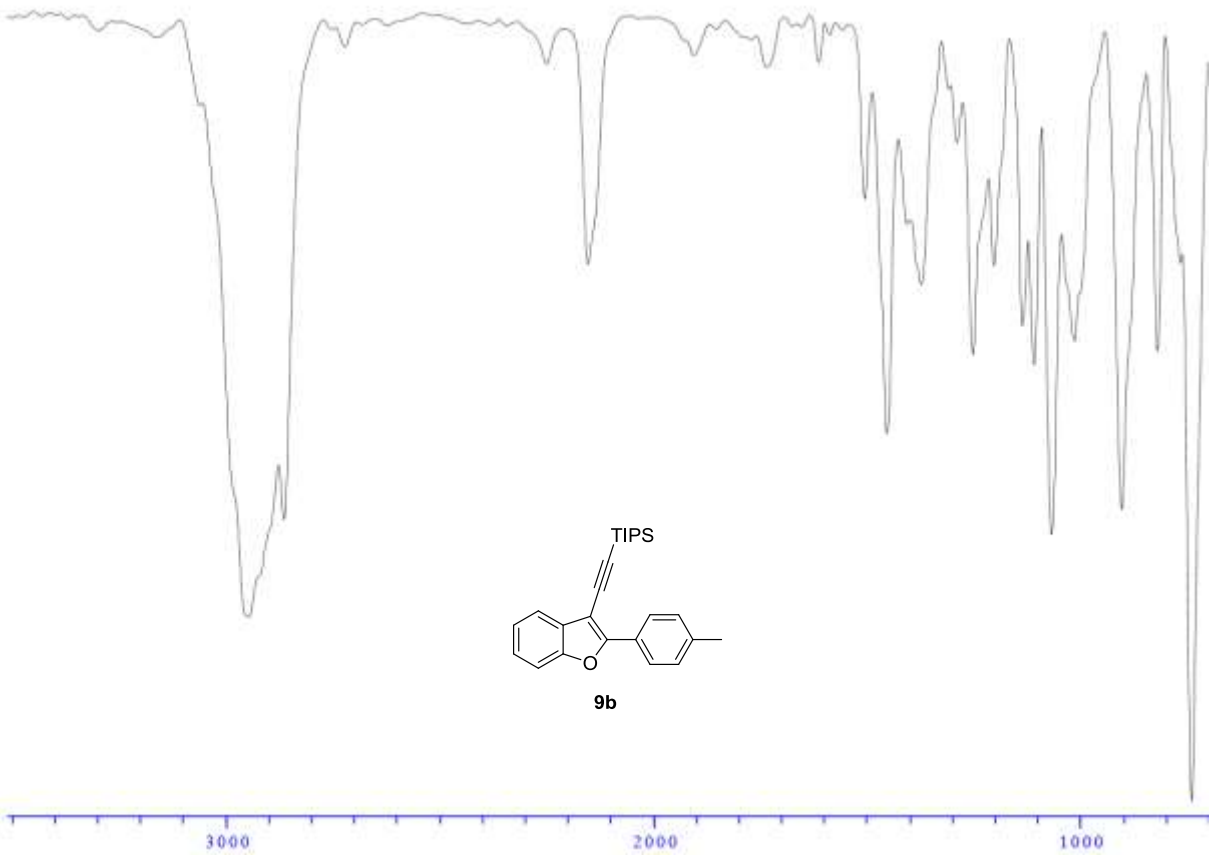

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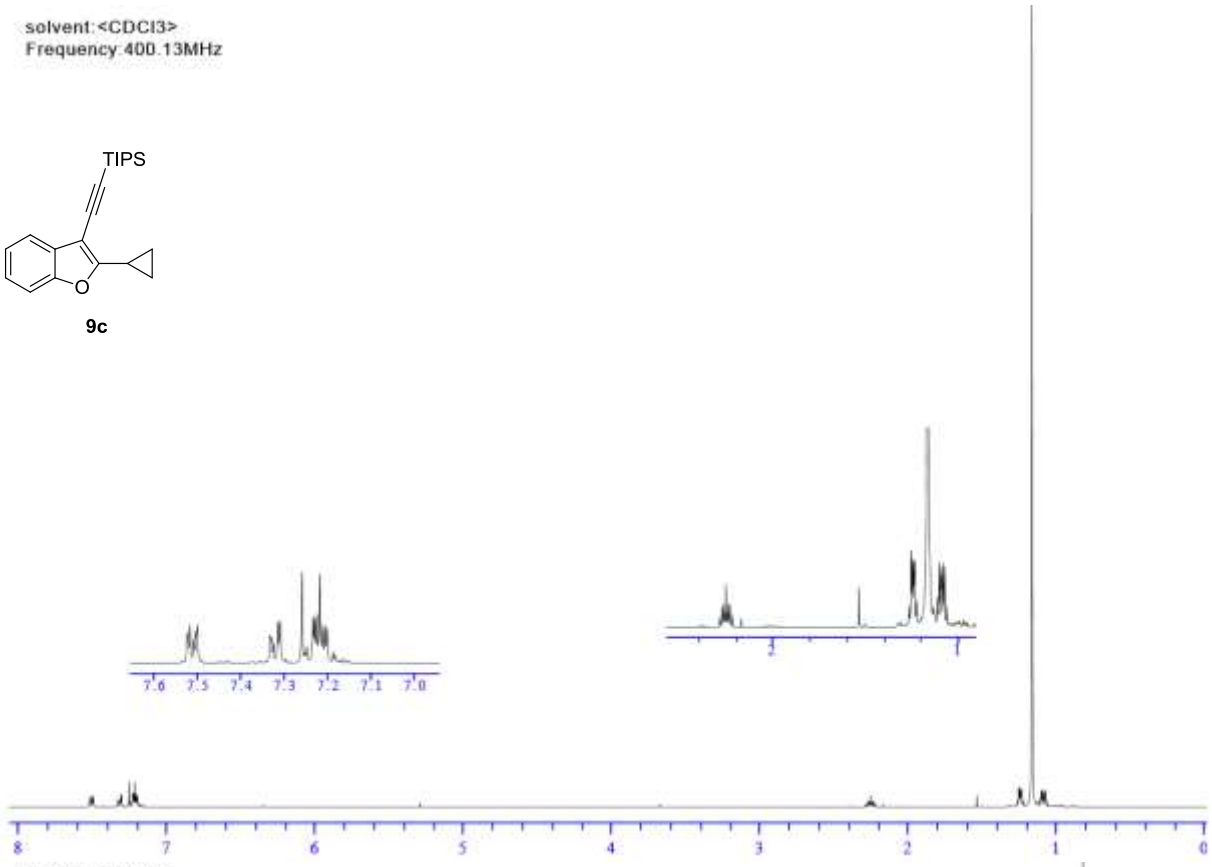
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TIPS
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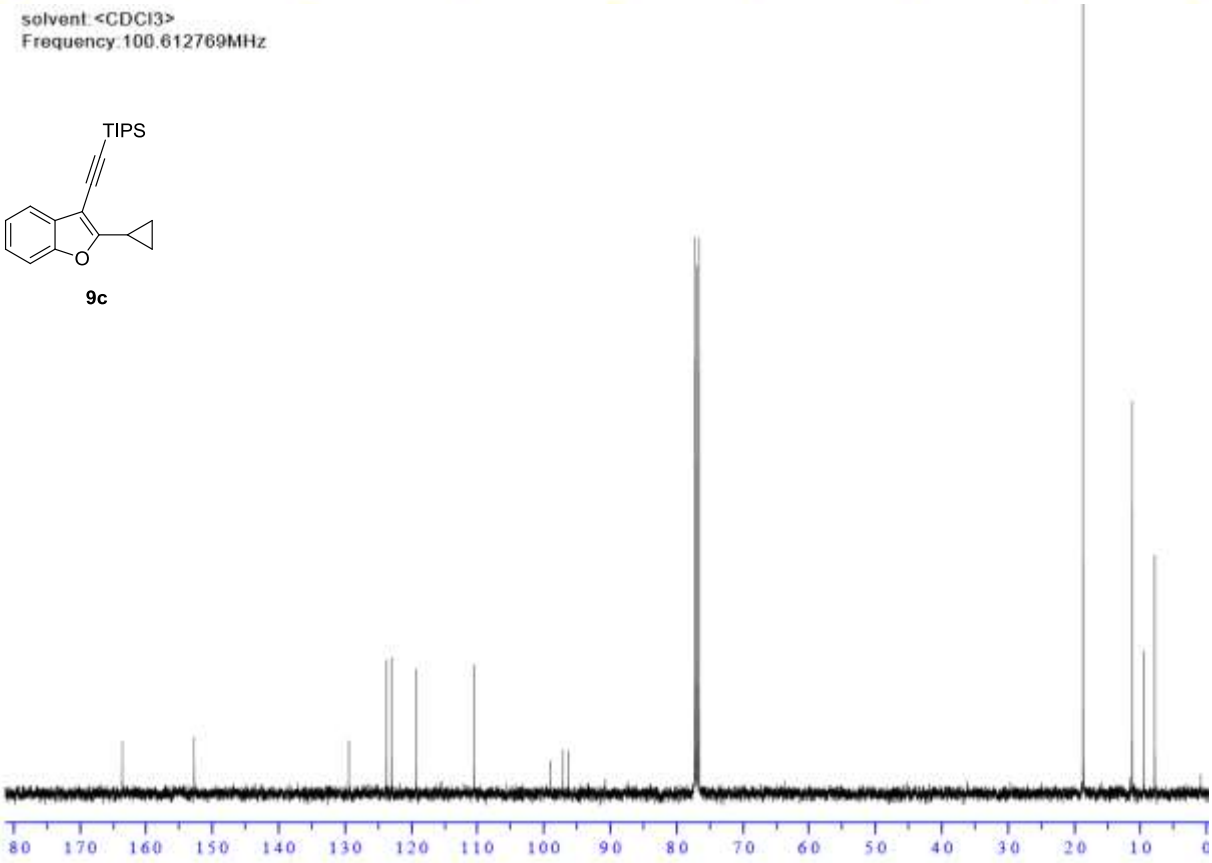
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TIPS
O
9c
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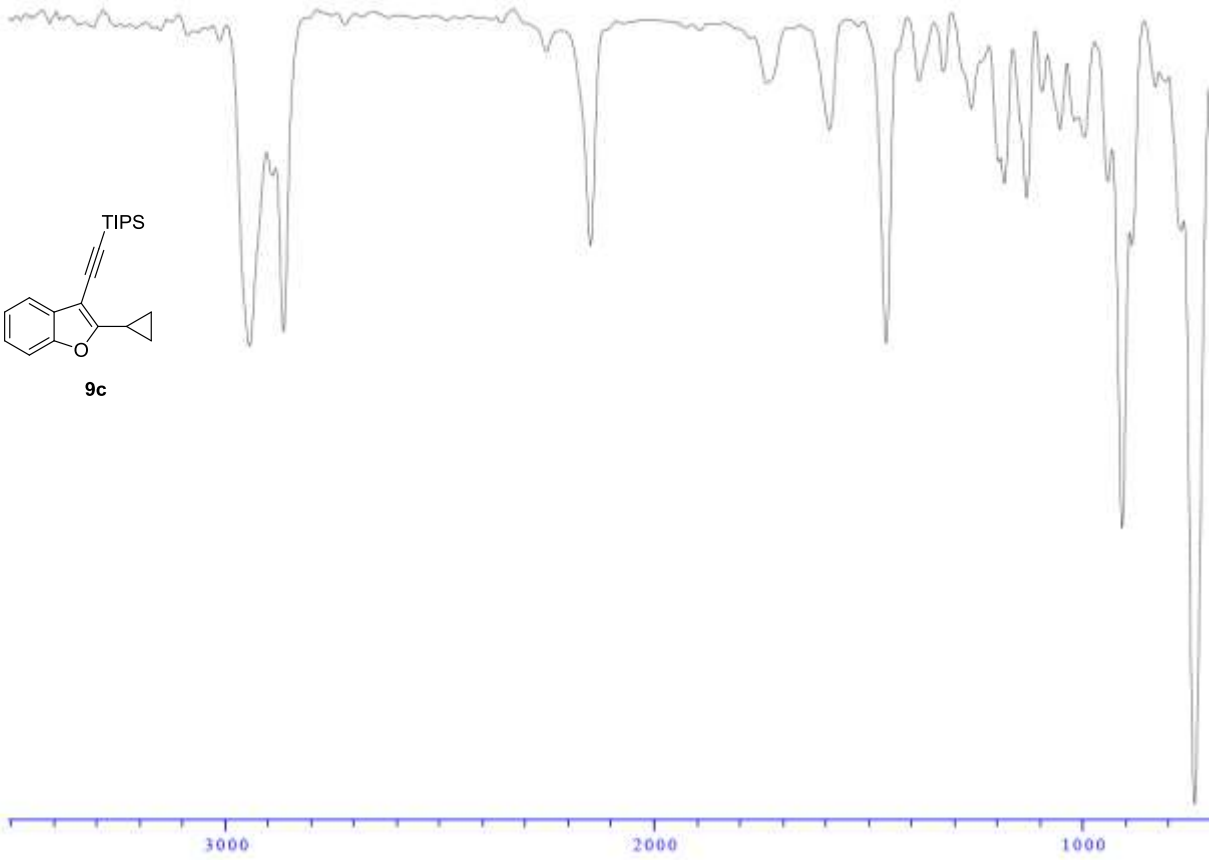

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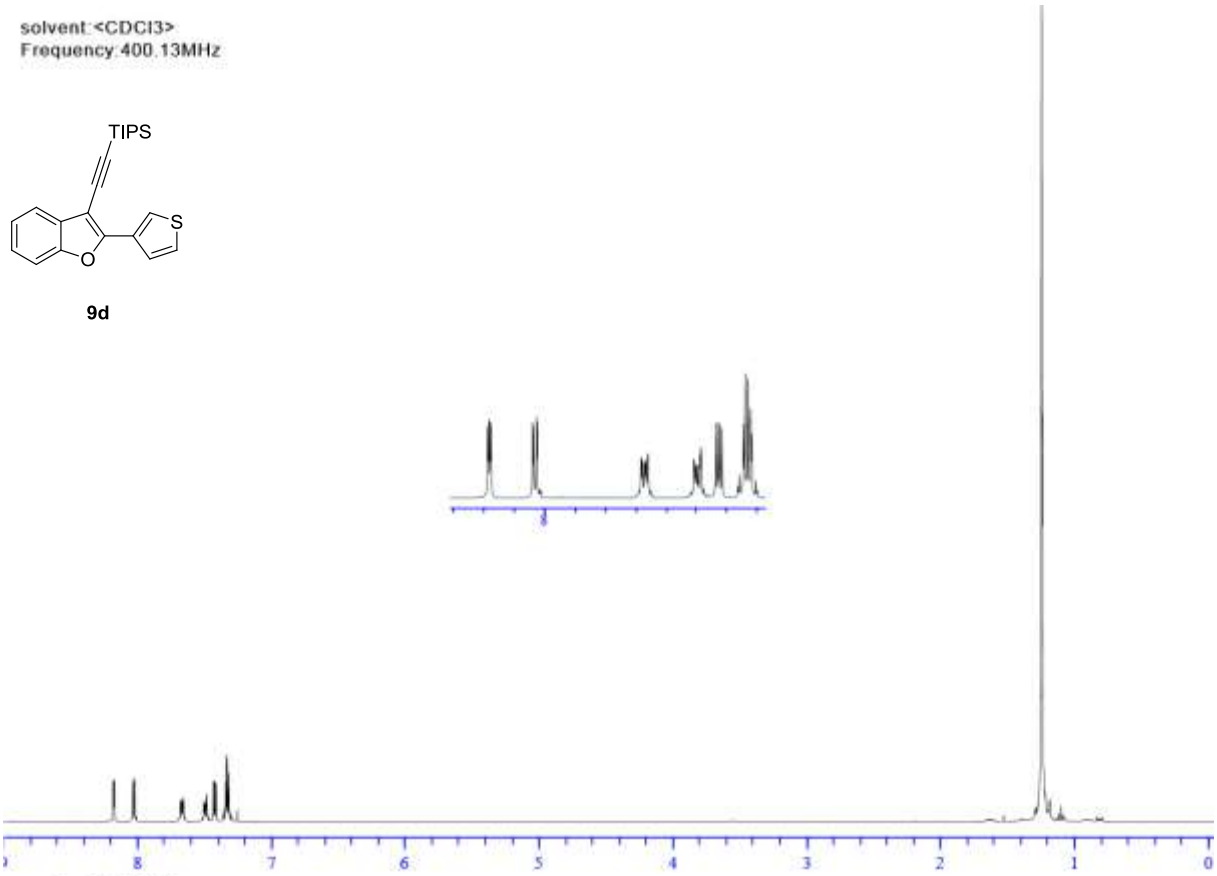
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TIPS
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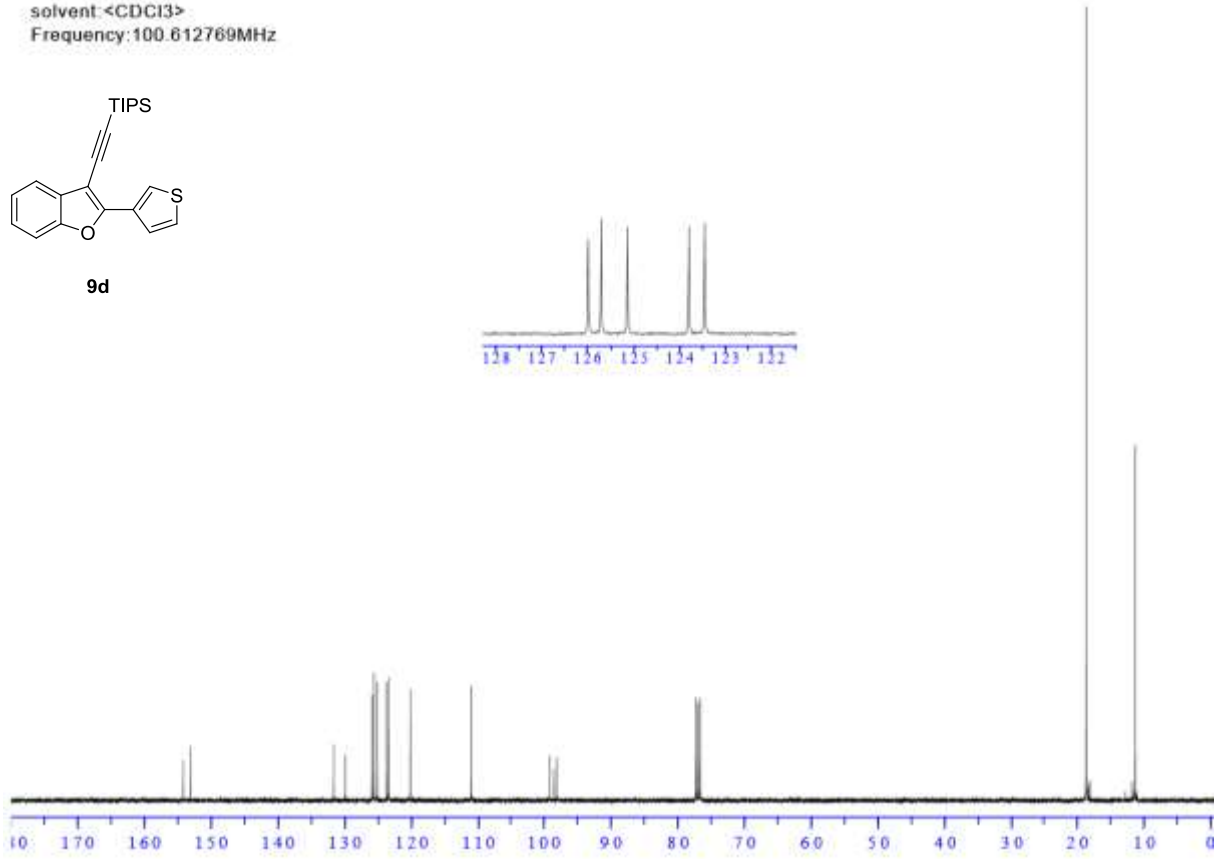
9d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TIPS
S
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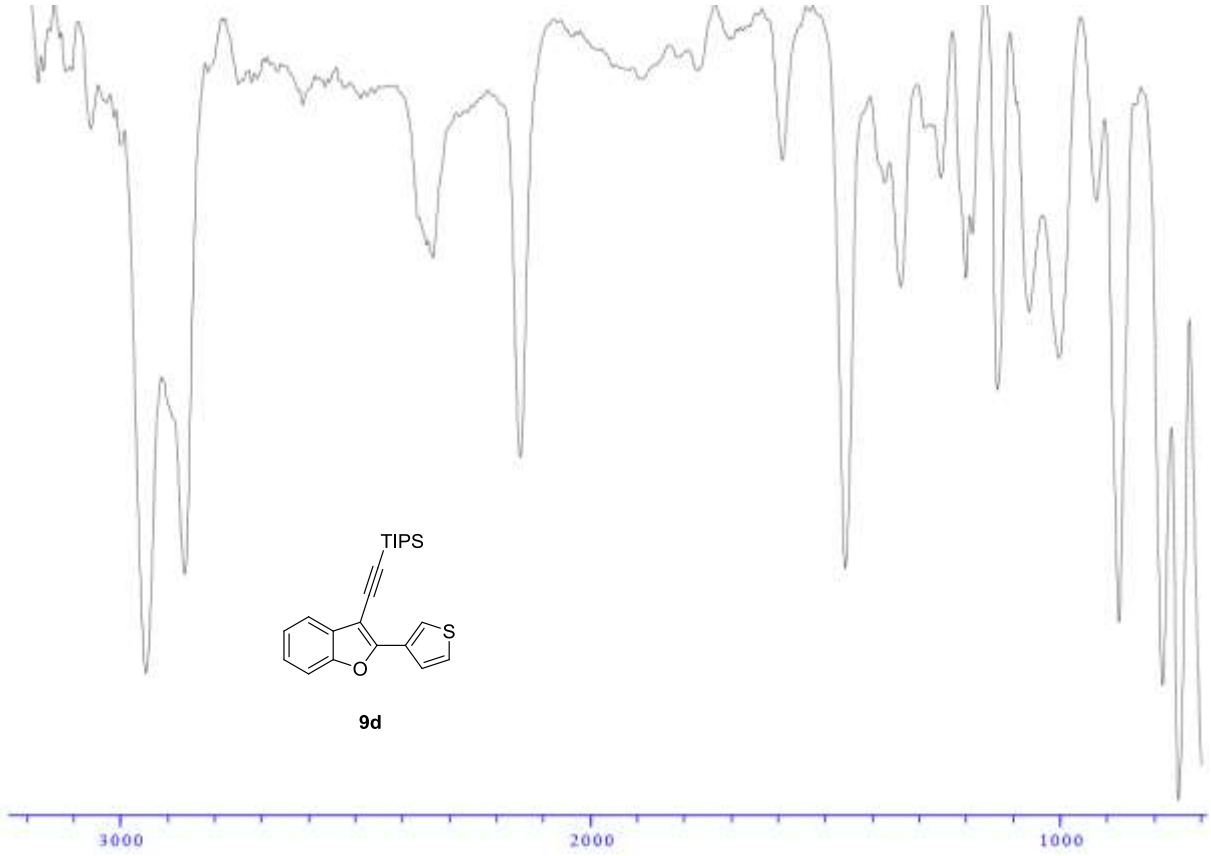
9d



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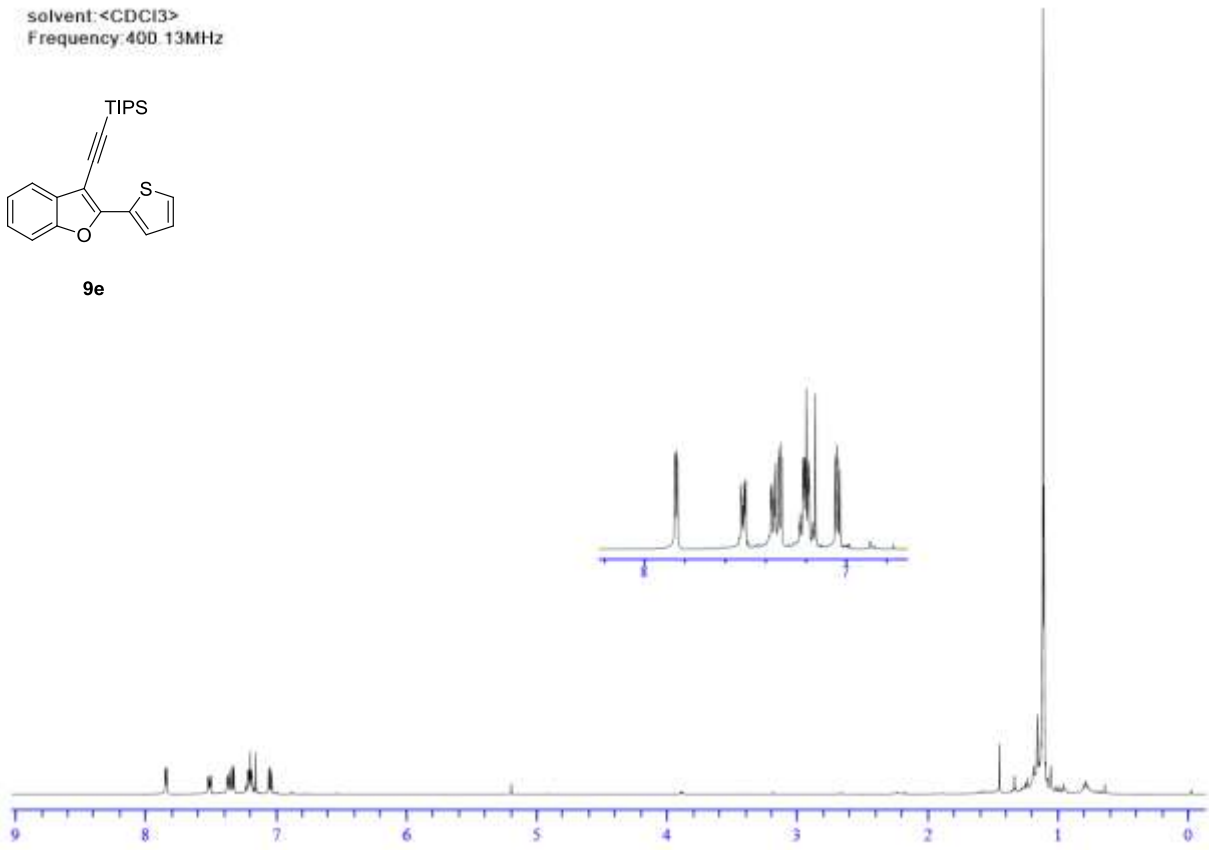
solvent:<CDCl3>
Frequency:400.13MHz
TIPS
S
O
9e
9
8
7
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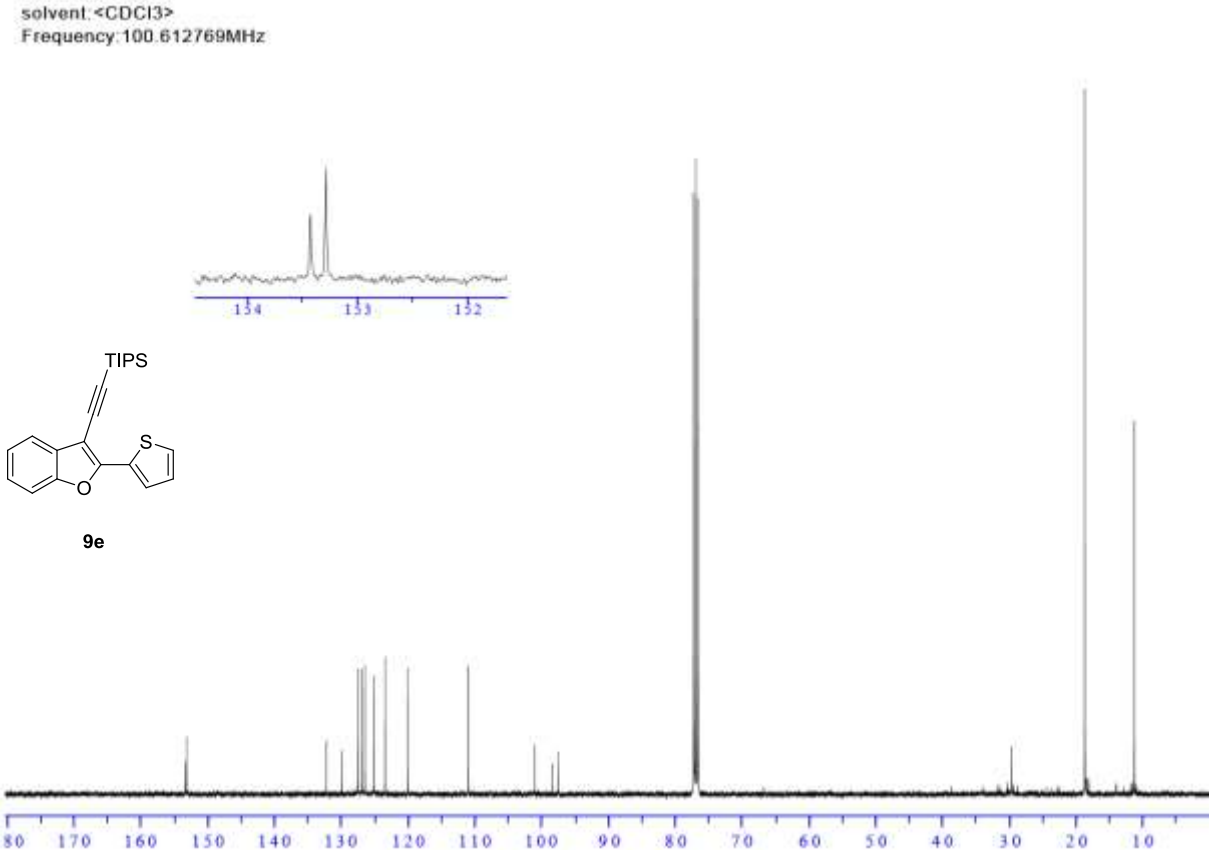
3
2
1
0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TIPS
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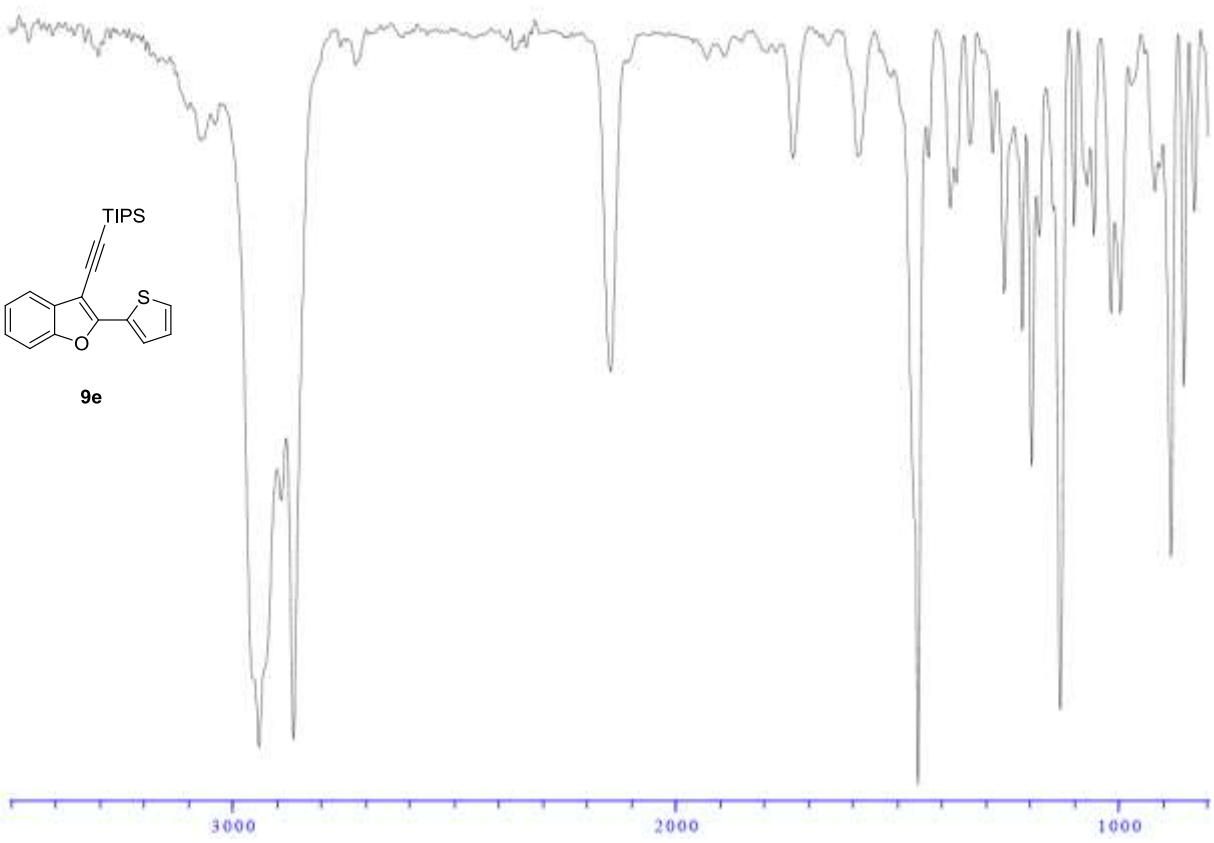
20
10



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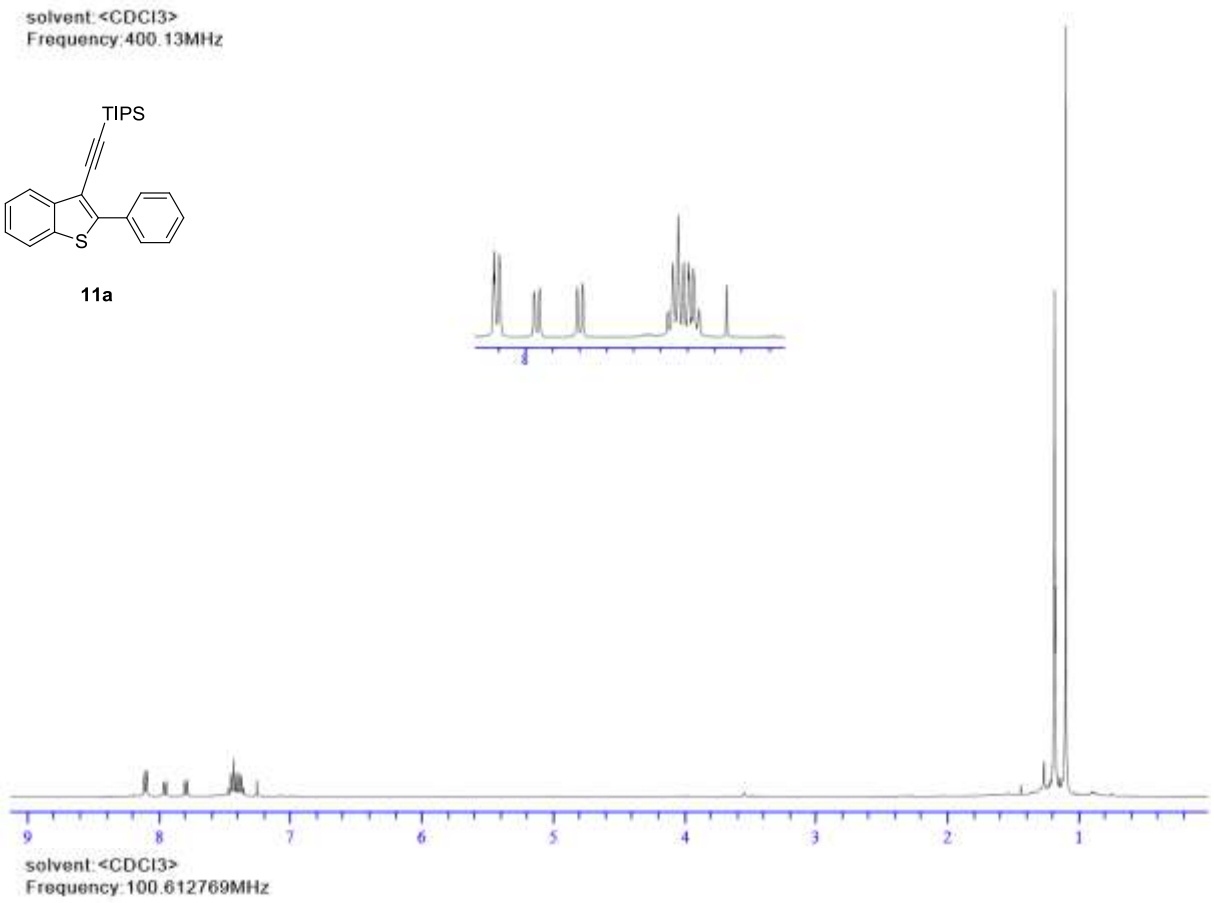
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TIPS
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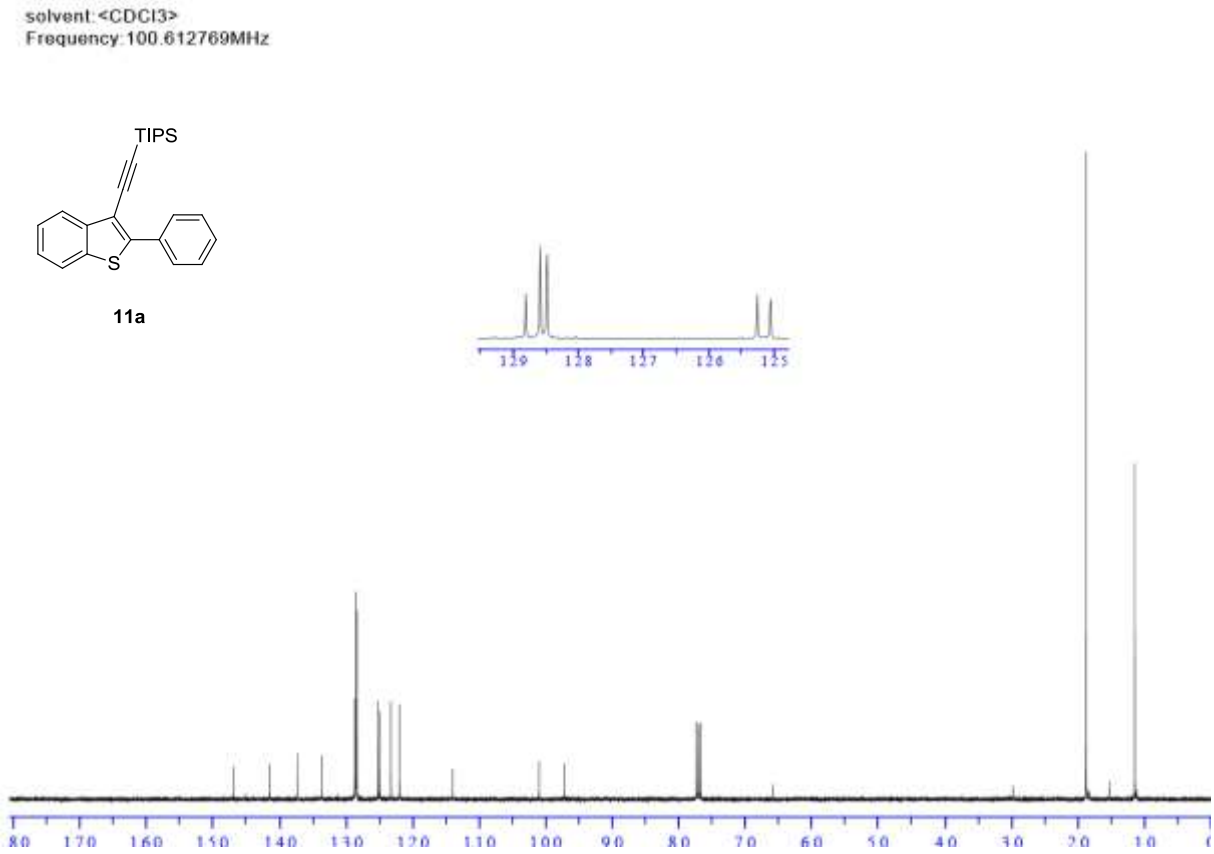
1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TIPS
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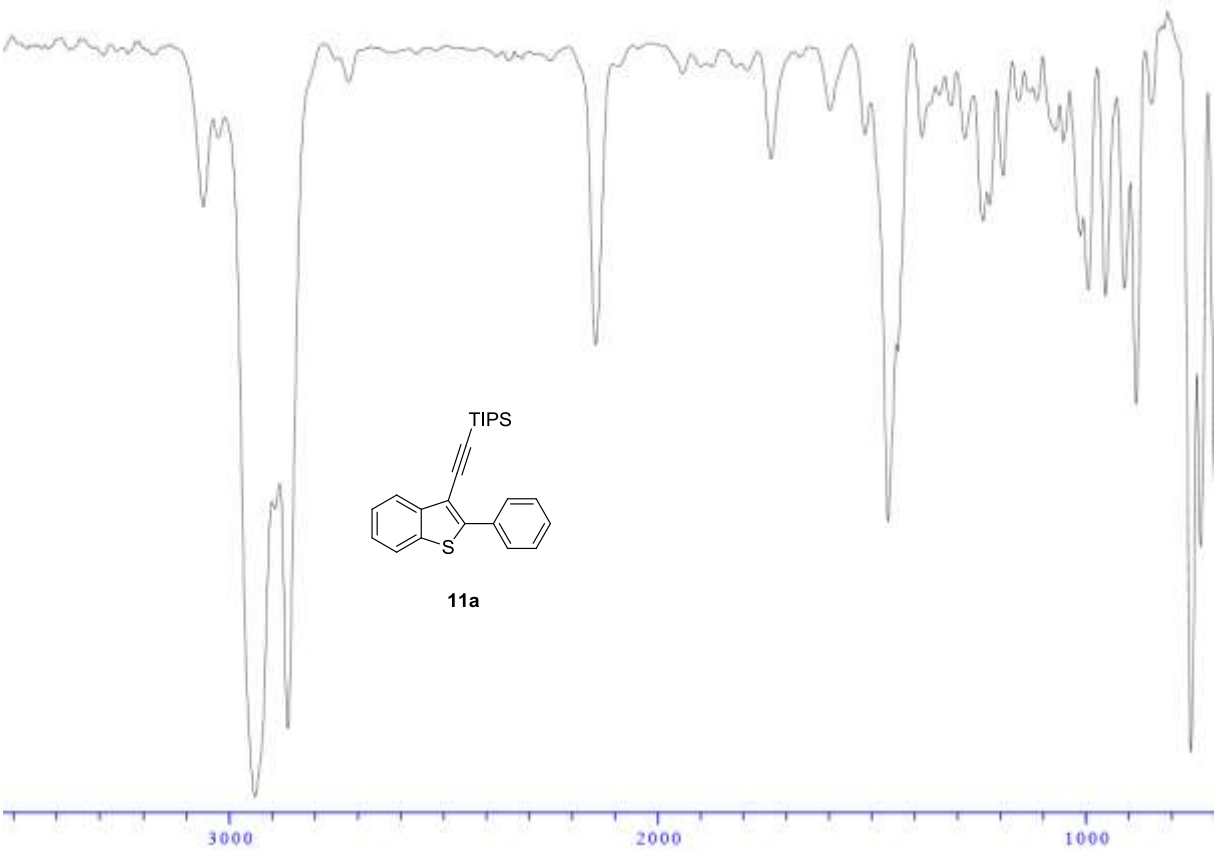
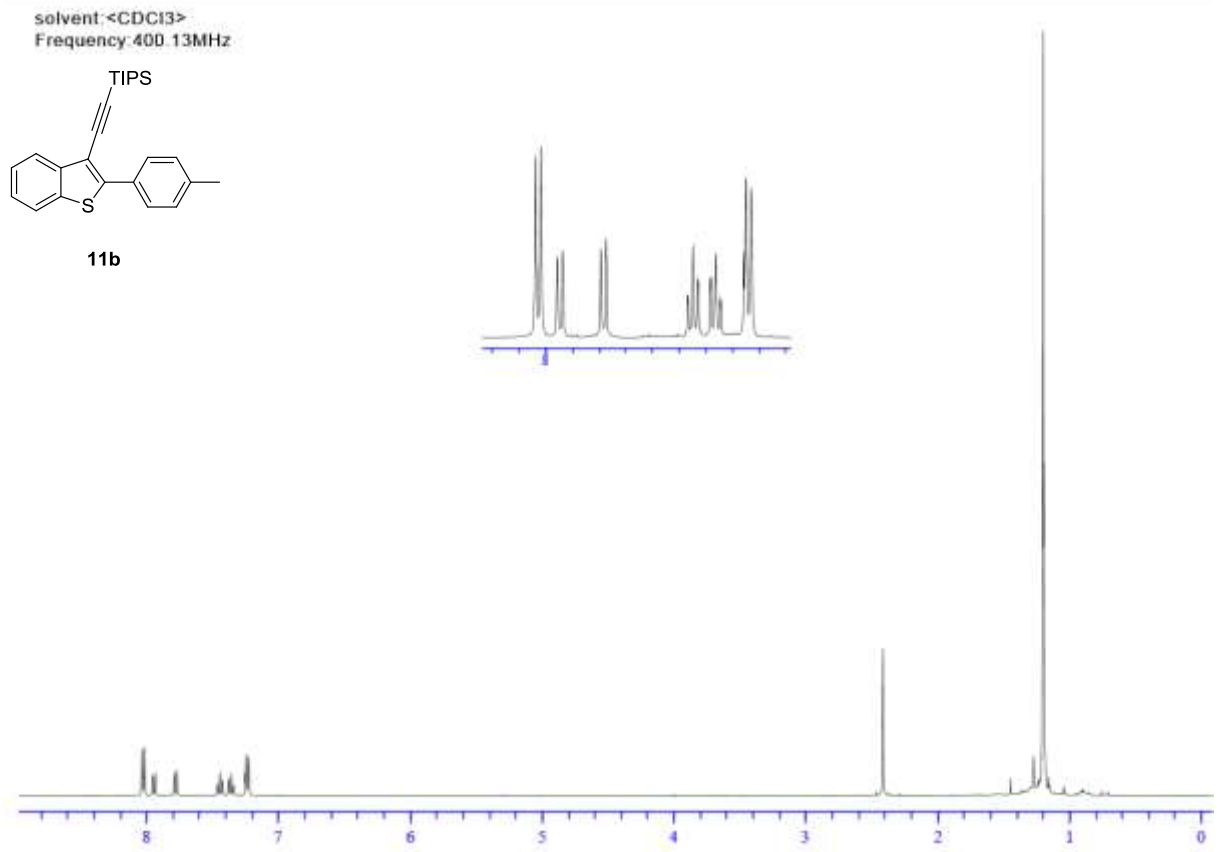


11a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TIPS
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11b
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6
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3
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1
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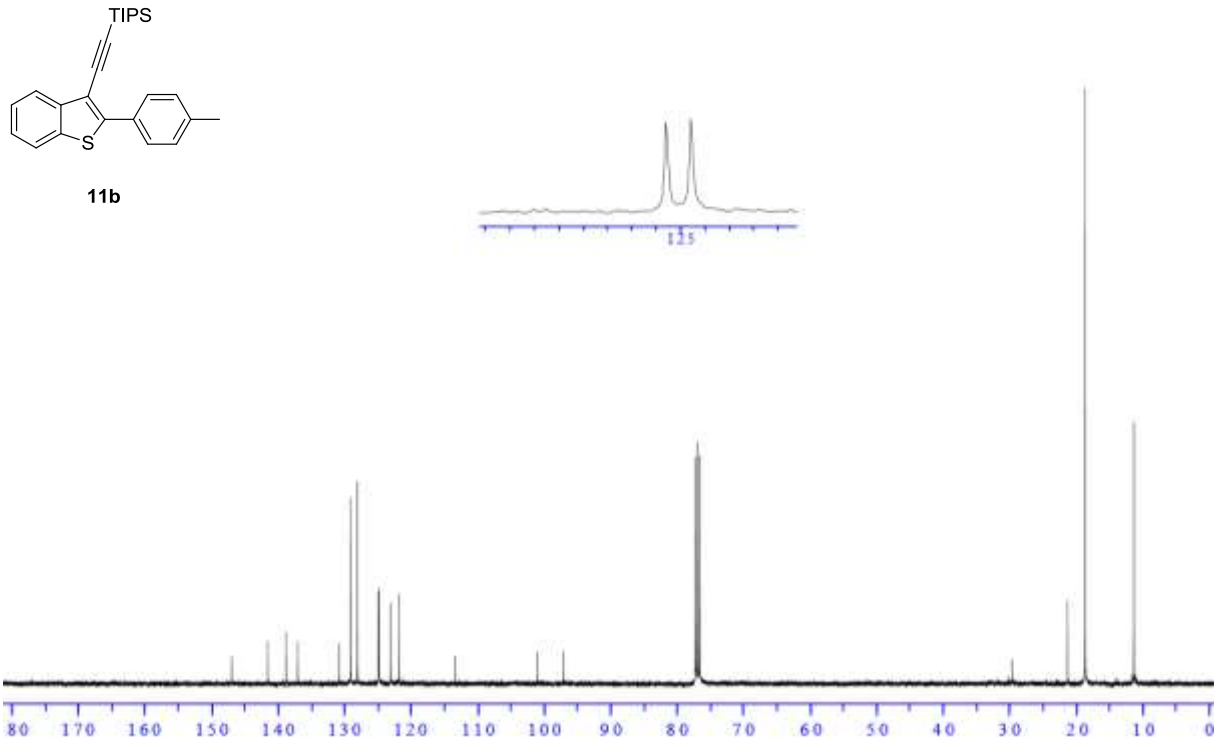
solvent:<CDCl3>
Frequency:100.612769MHz
TIPS
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10
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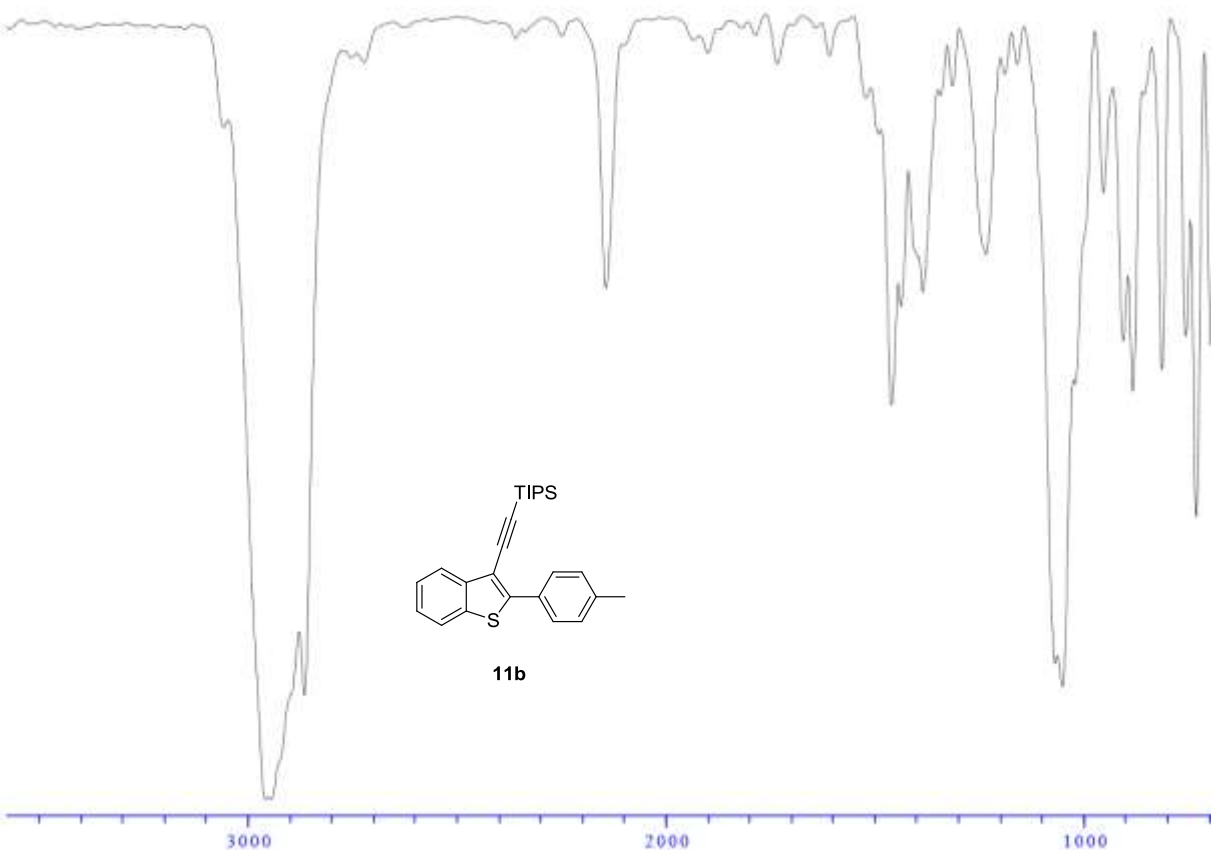
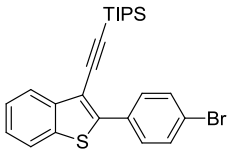


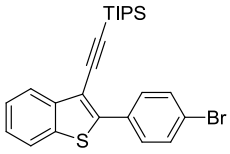
11b

solvent:<CDCl3>
Frequency:400.13MHz

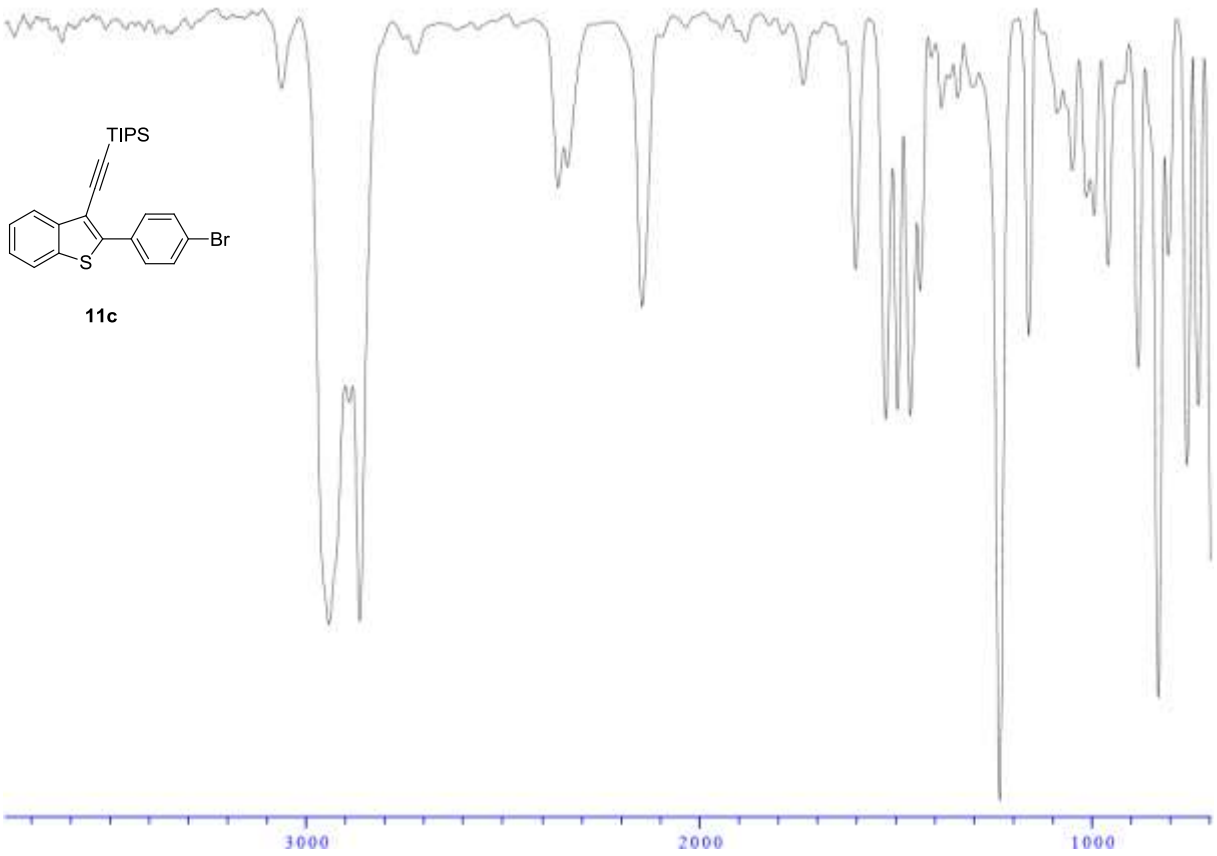


11c

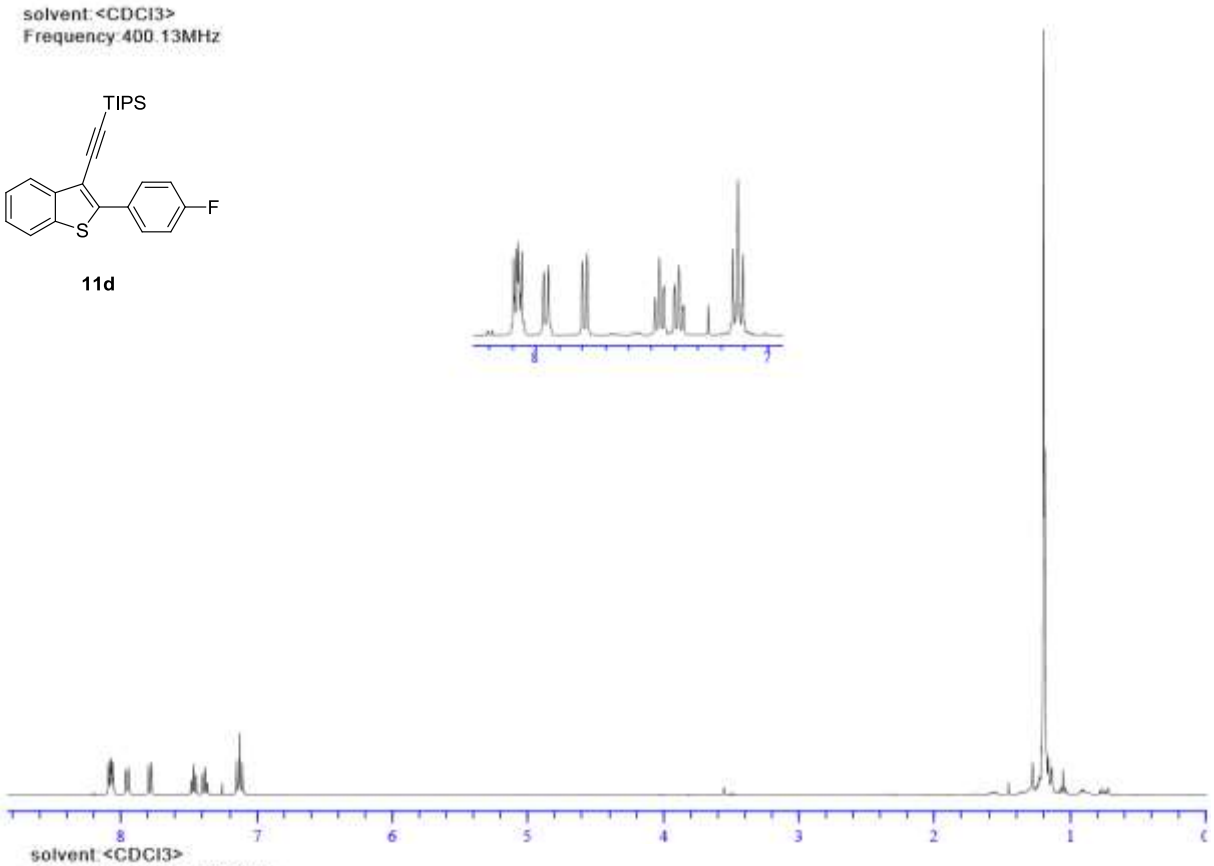
solvent:<CDCl3>
Frequency:100.612769MHz

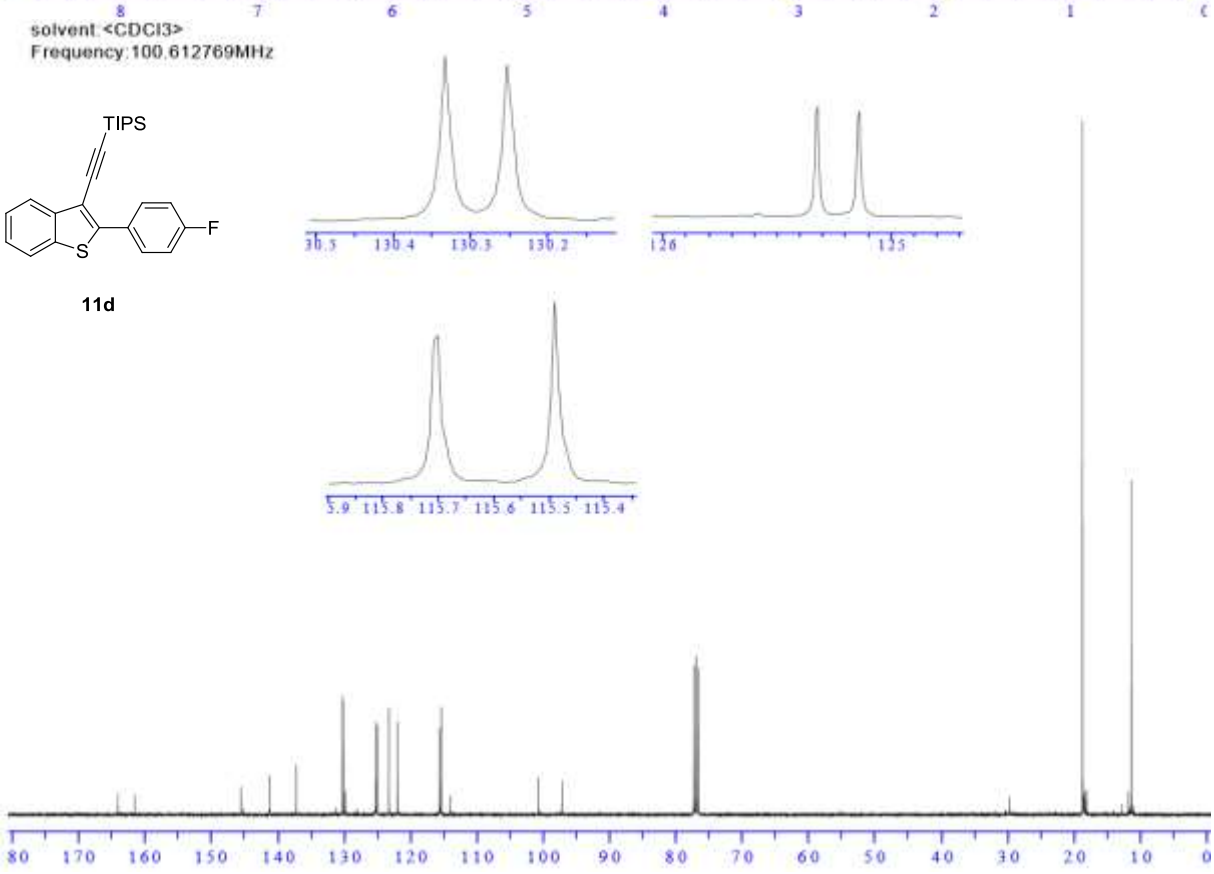


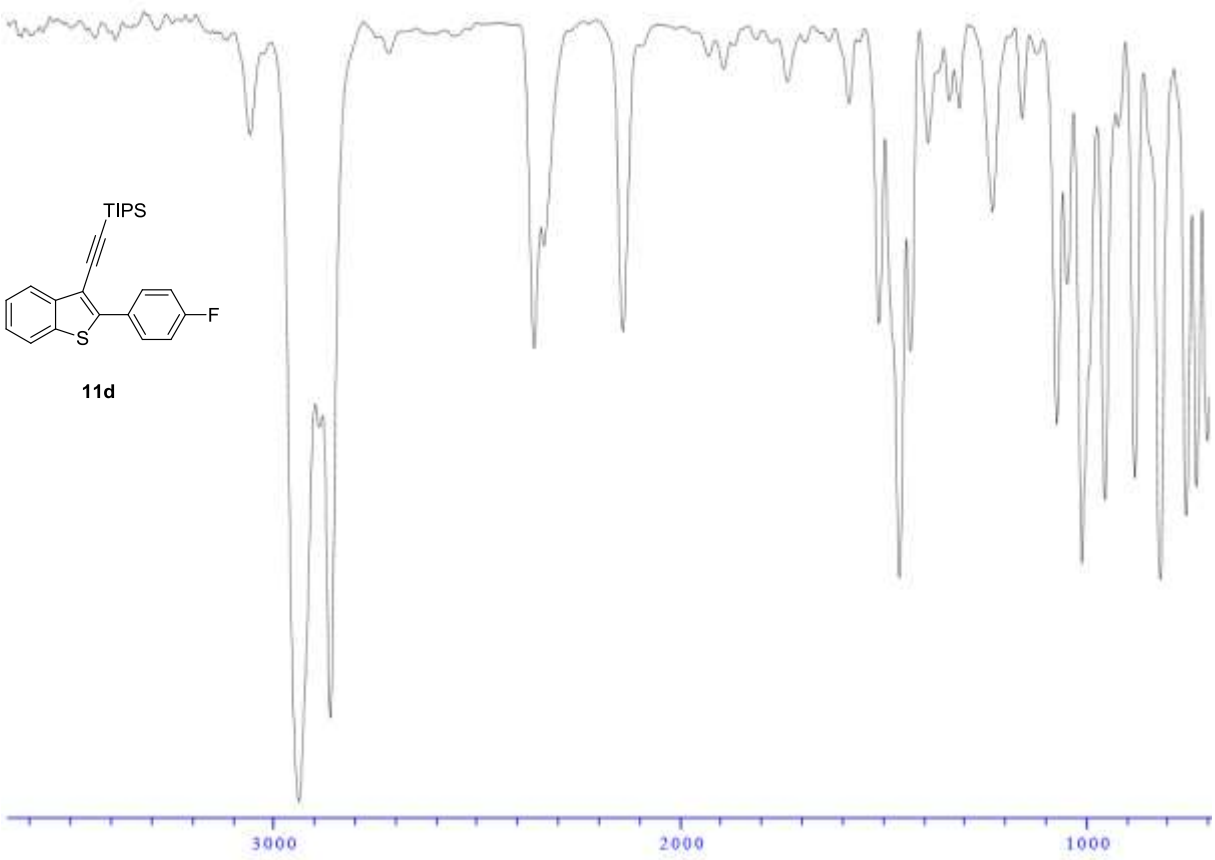
11c



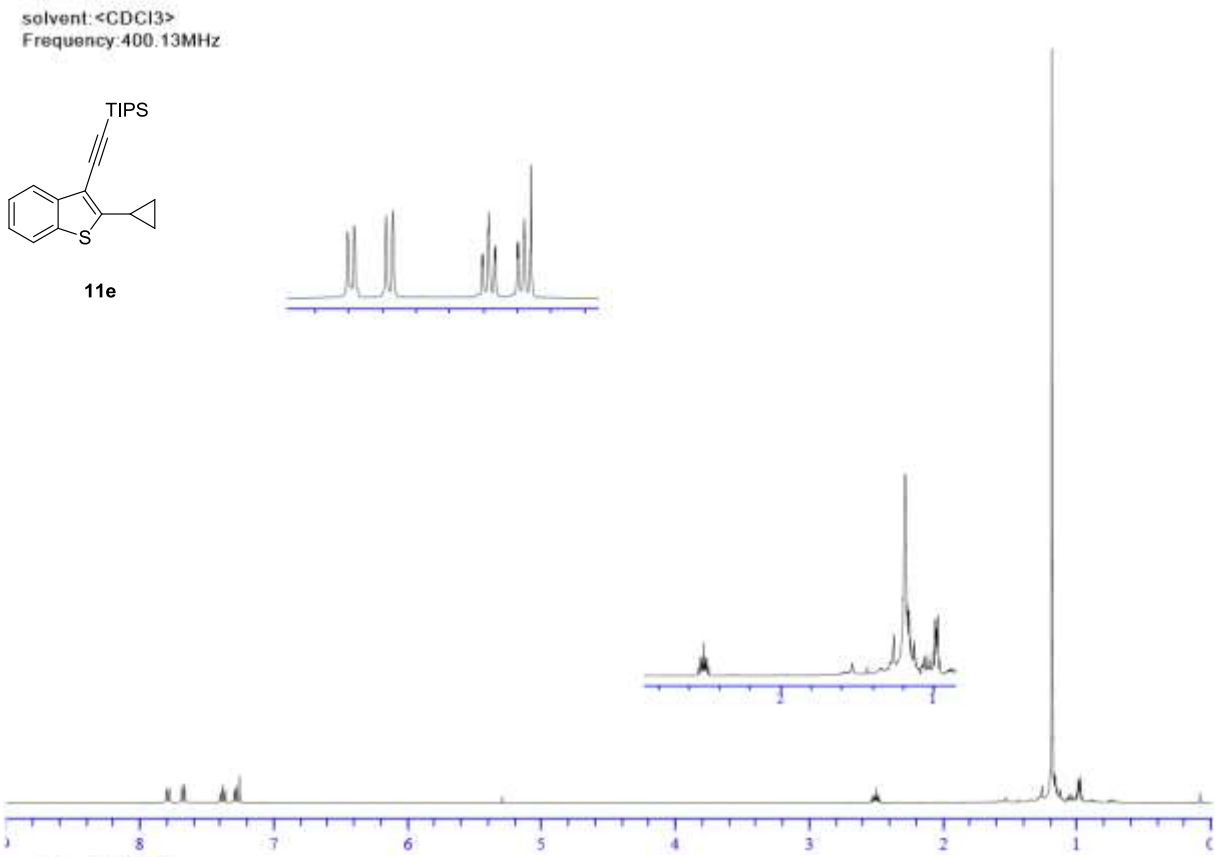
11c


solvent:<CDCl3>
Frequency:400.13MHz
TIPS
F
S
11d


solvent:<CDCl3>
Frequency:100.612769MHz
TIPS
F
S
11d



11d


solvent:<CDCl3>
Frequency:400.13MHz
TIPS
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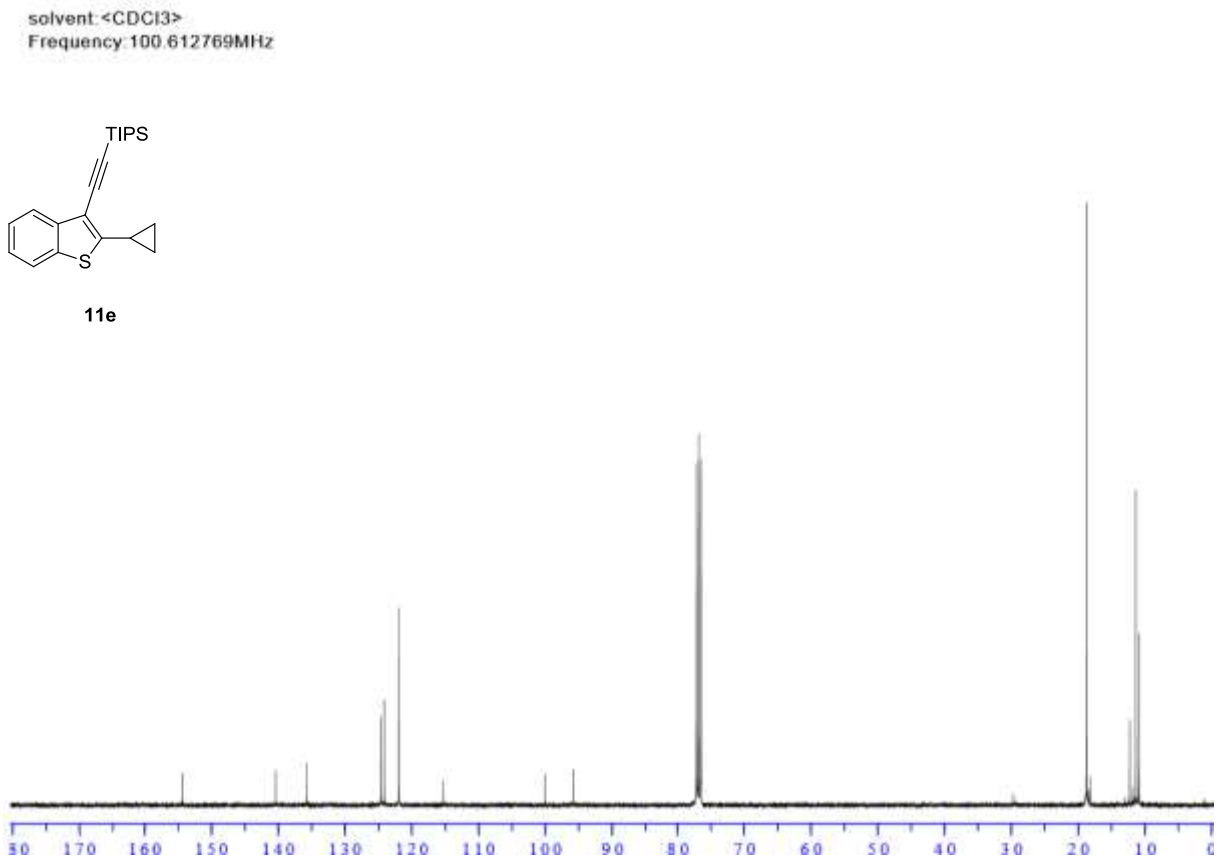
11e
8
7
6
5
4
3
2
1
0


solvent:<CDCl3>
Frequency:100.612769MHz
TIPS
S
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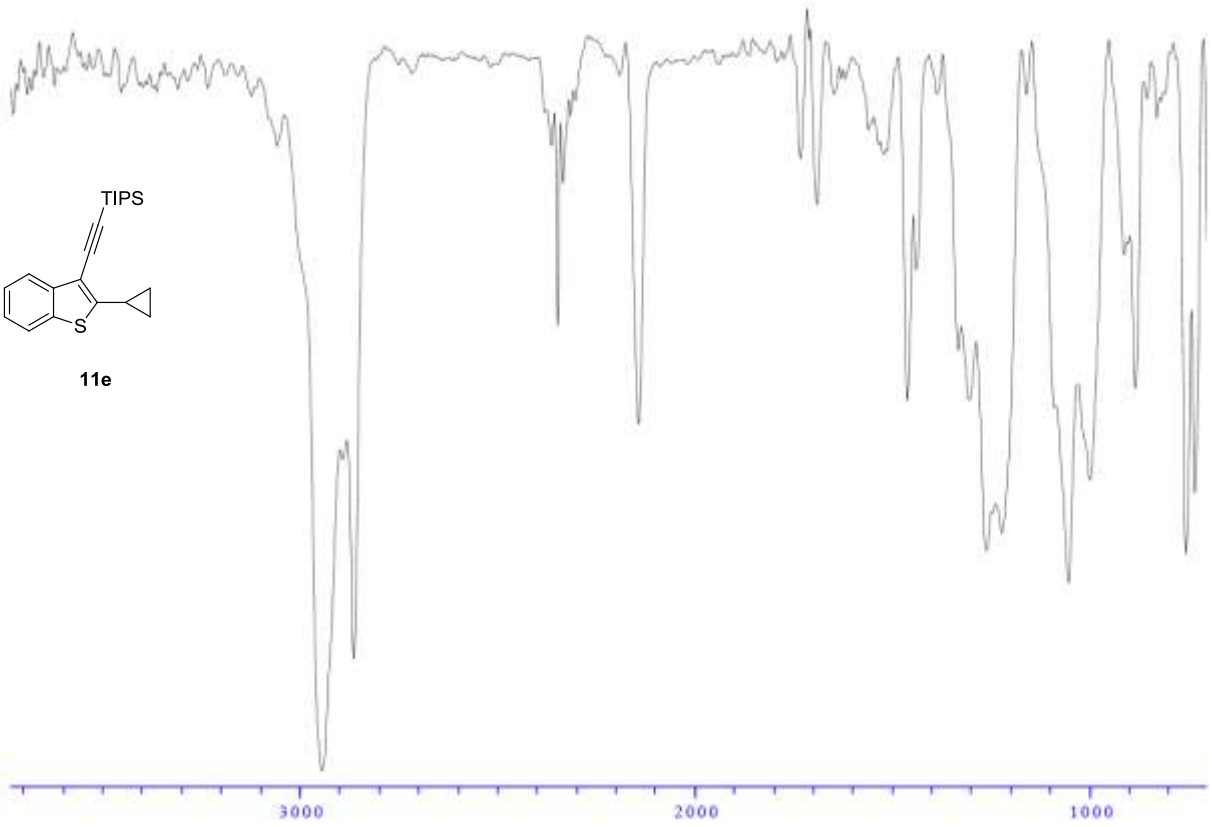
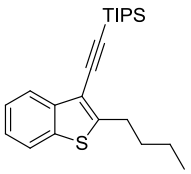
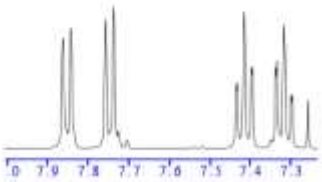


11e

solvent:<CDCl3>
Frequency:400.13MHz



11f



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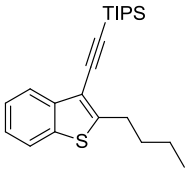

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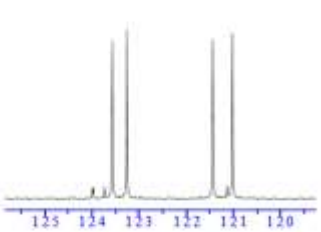

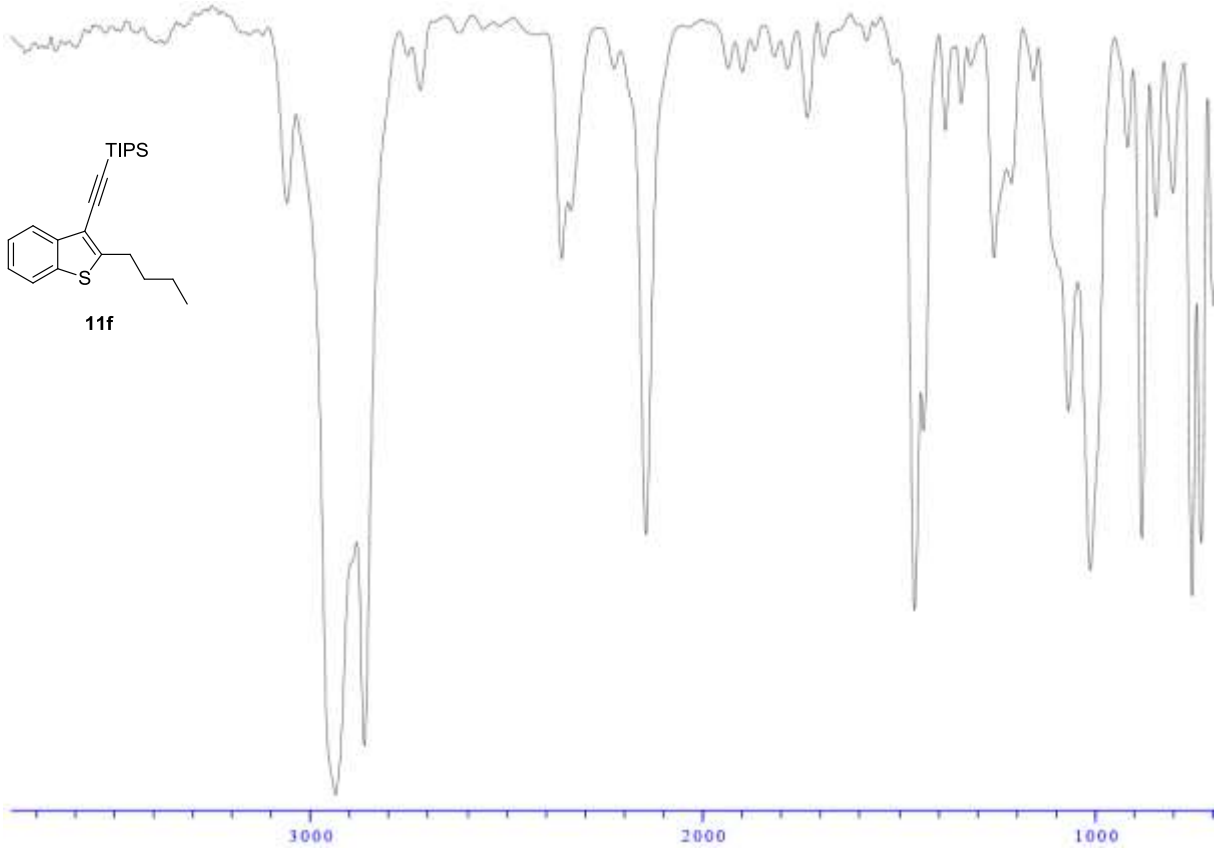

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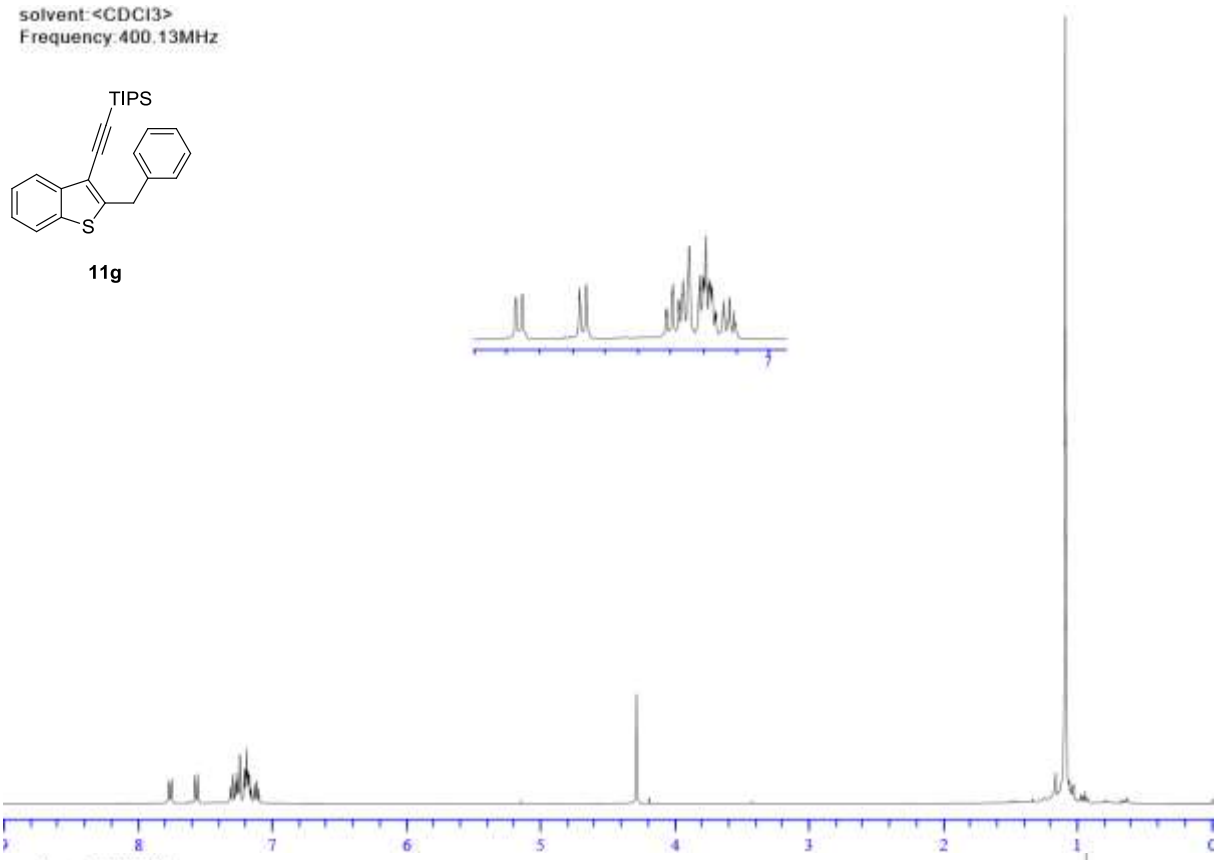
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TIPS
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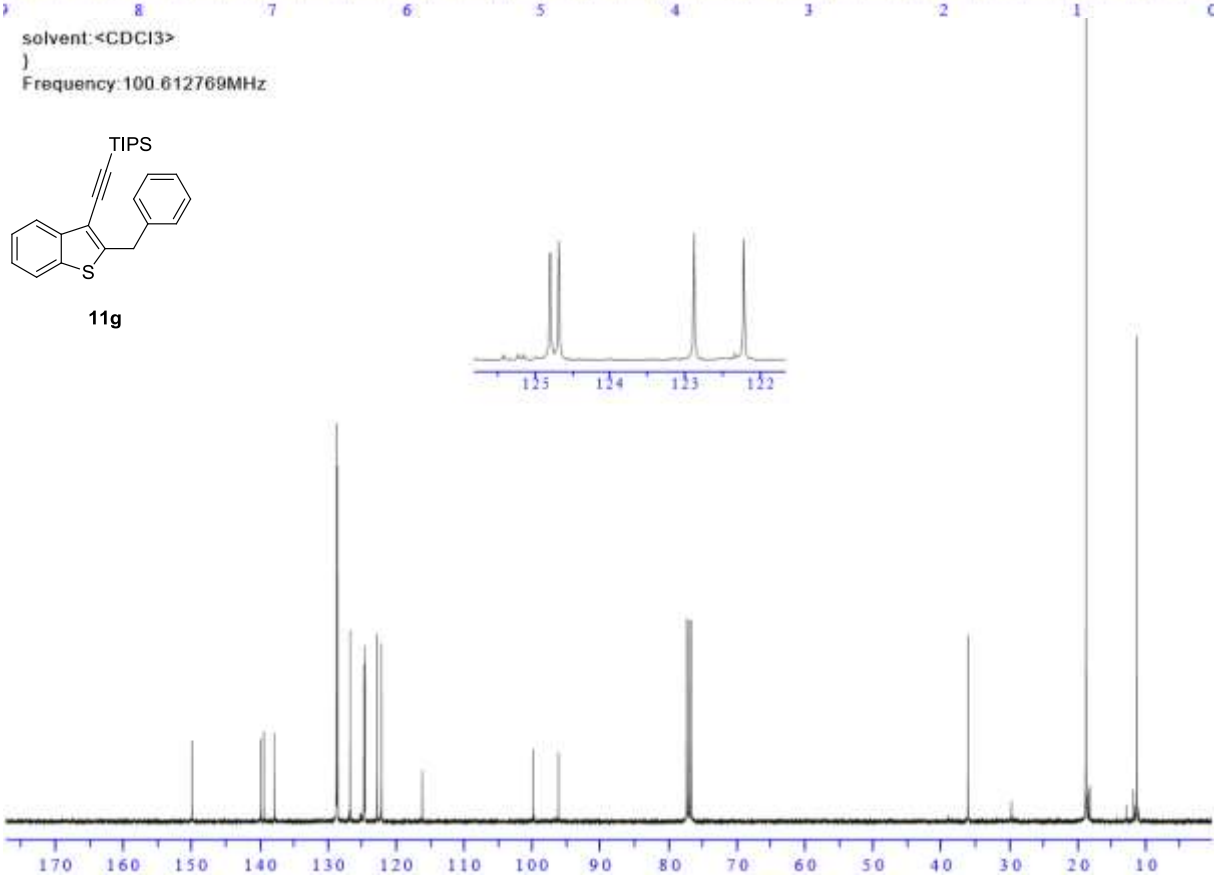
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TIPS
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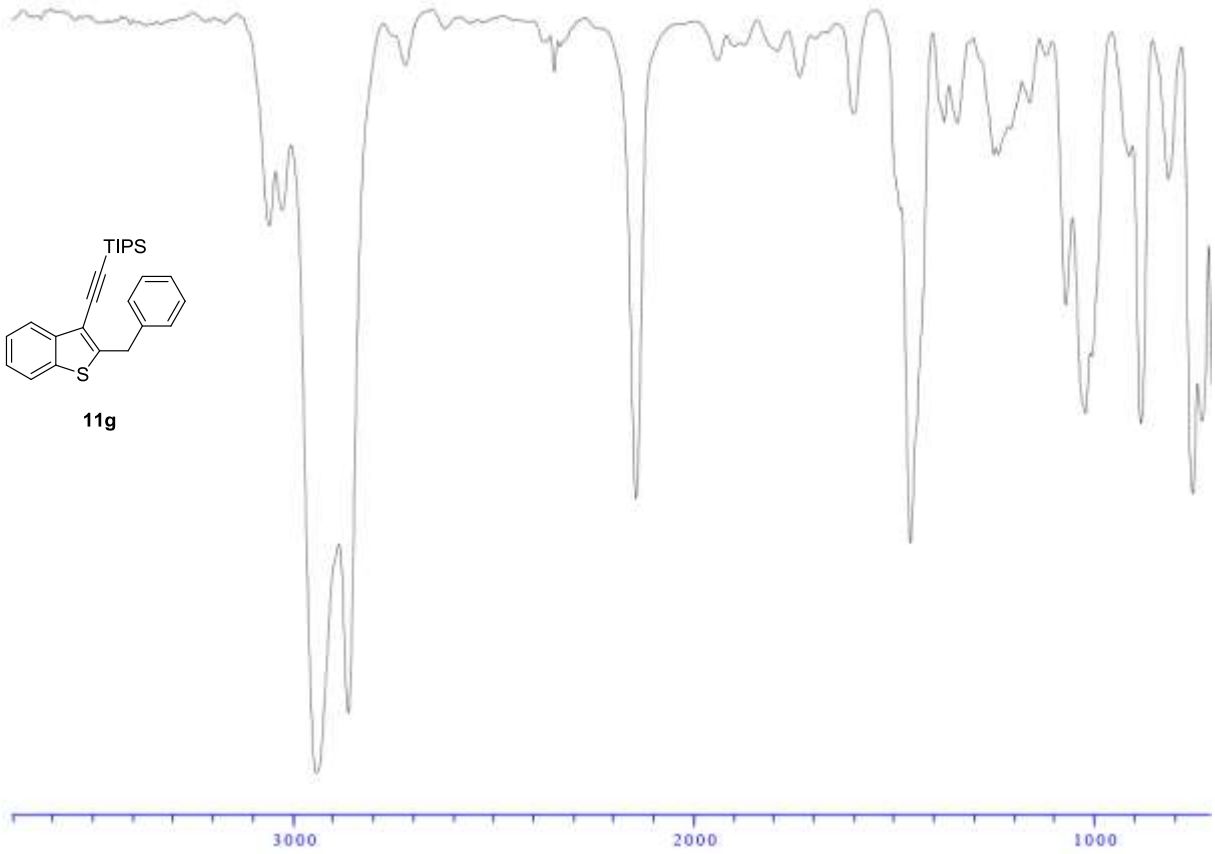

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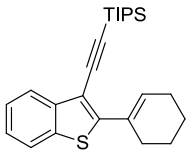

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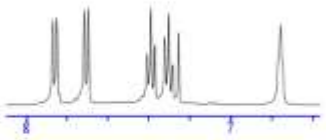

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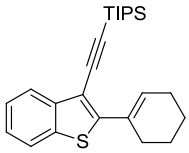

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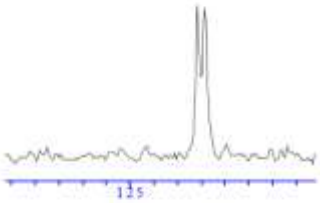

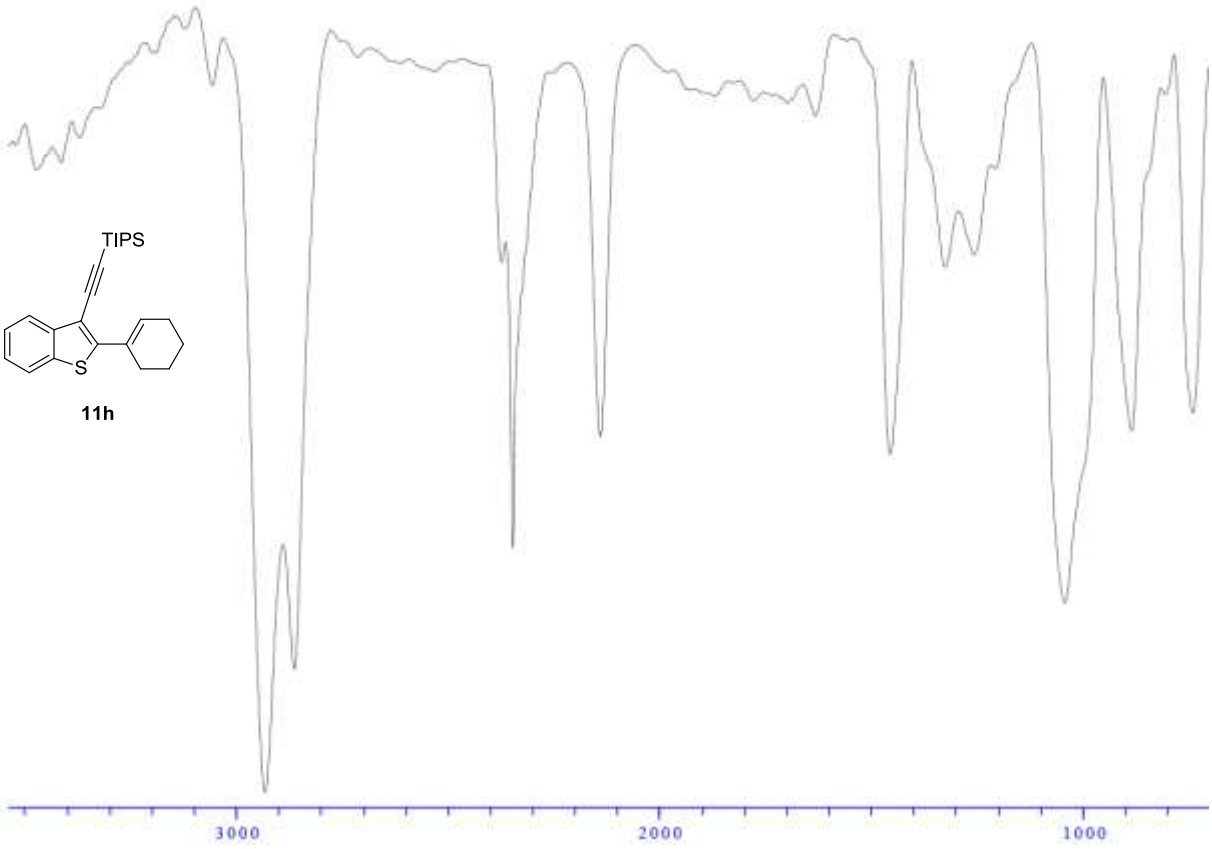

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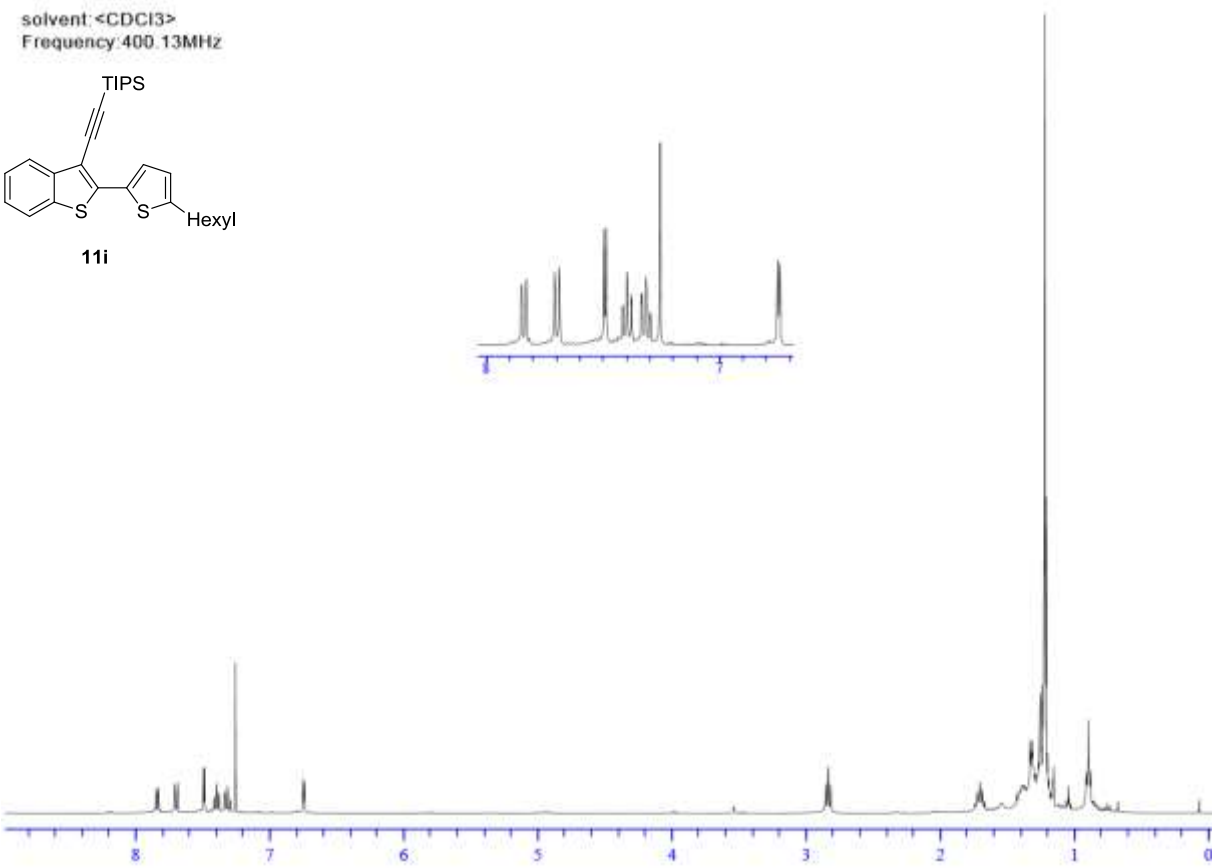
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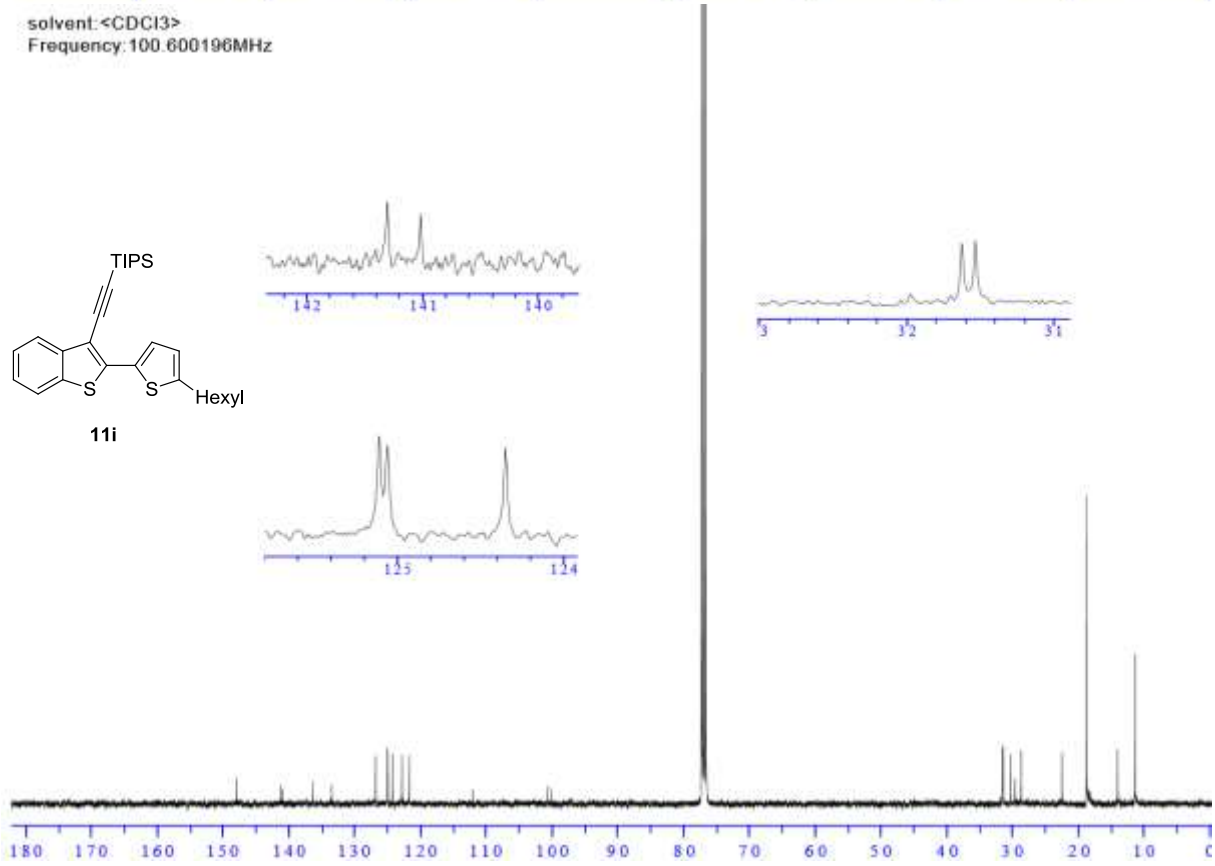
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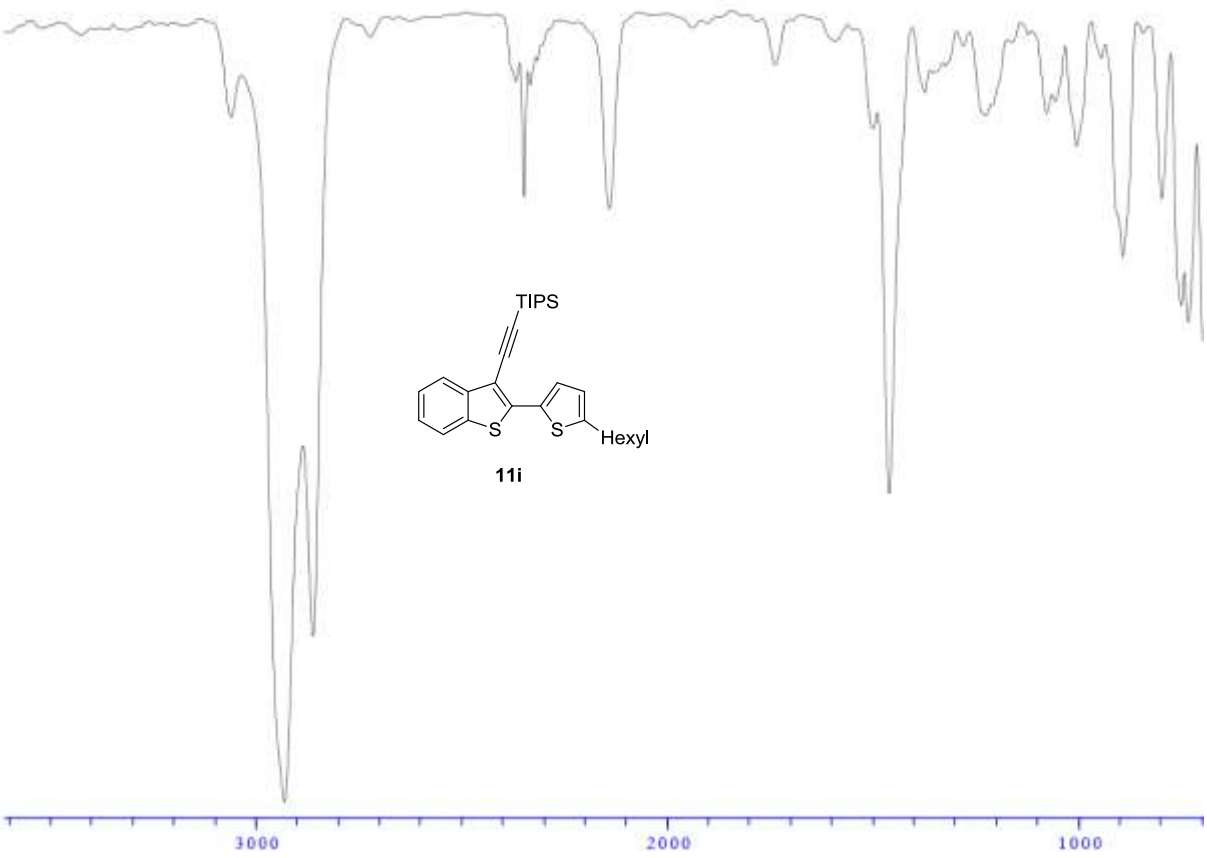

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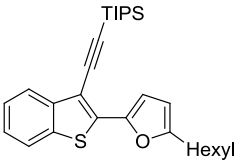

11j

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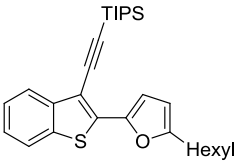

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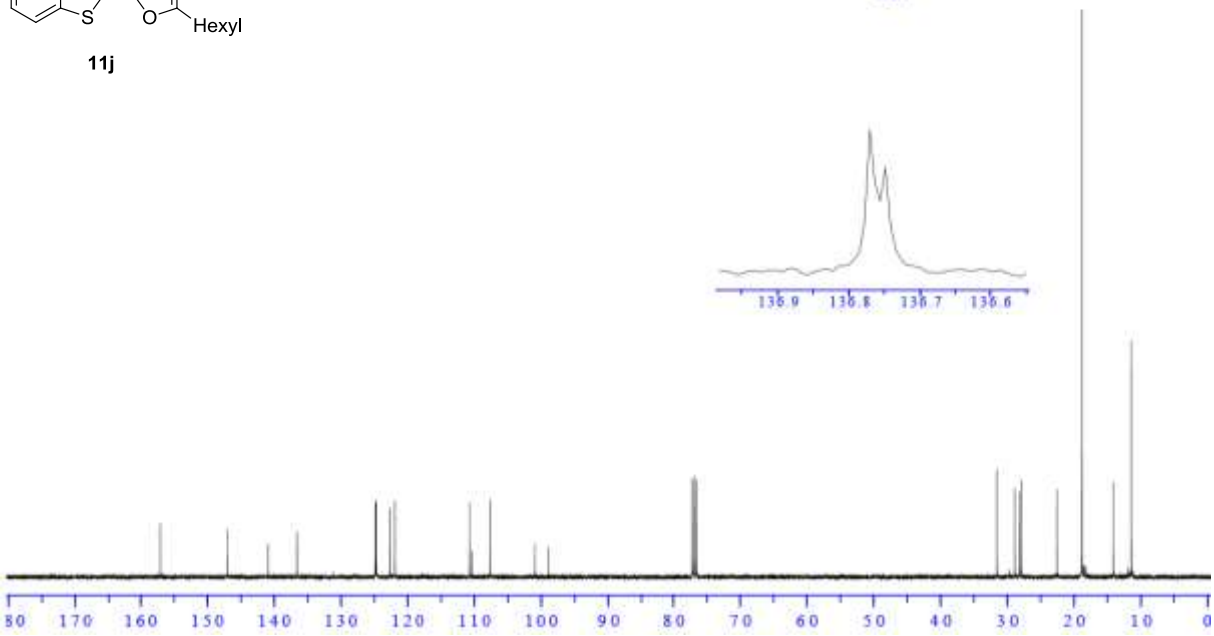

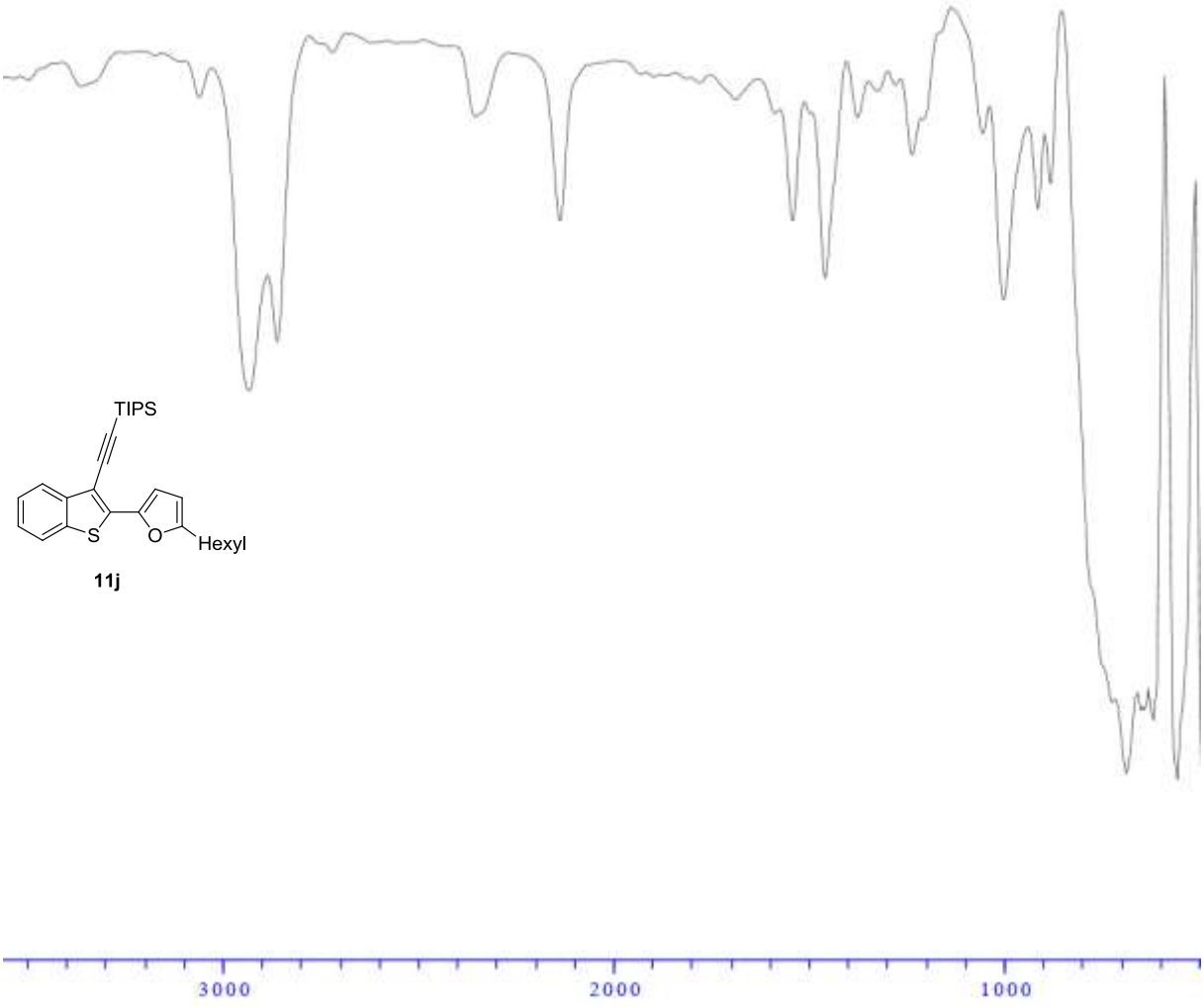

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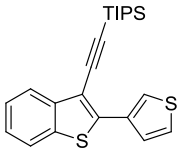

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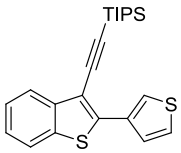
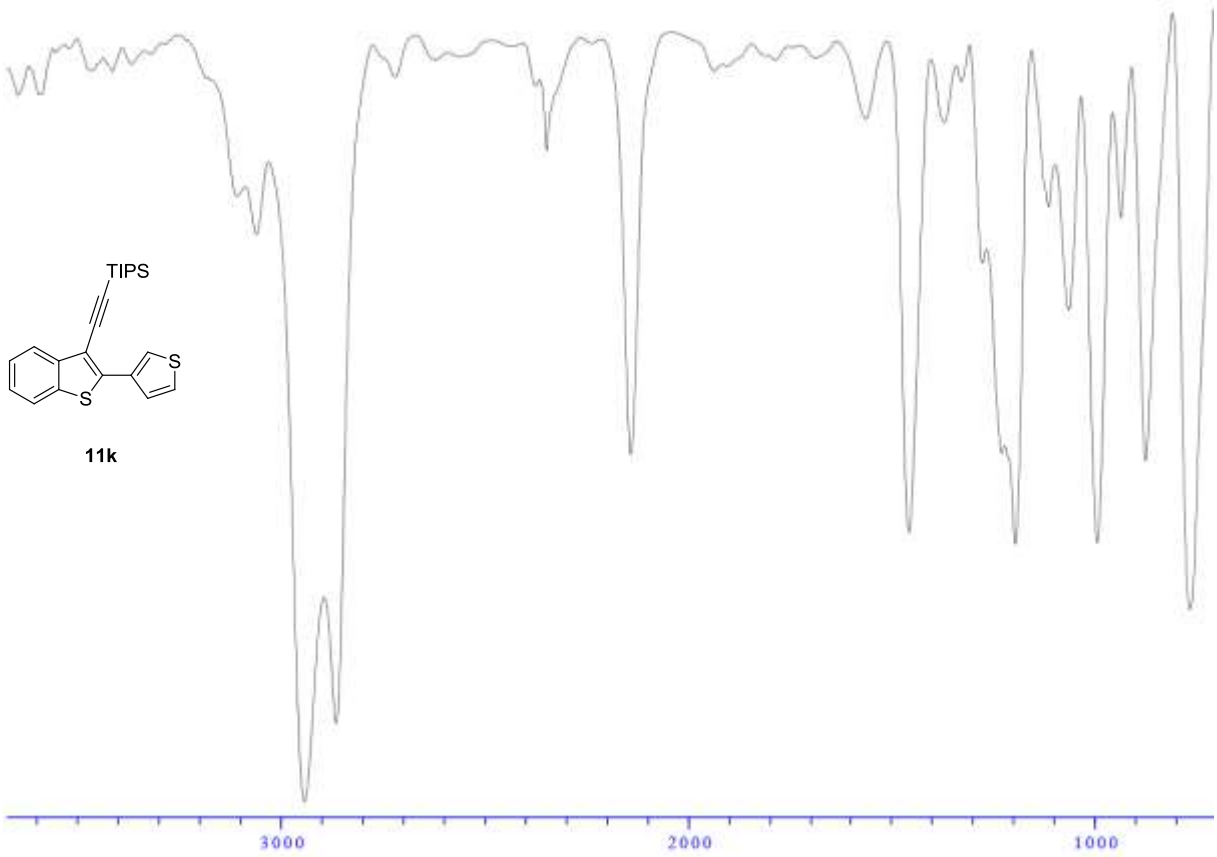
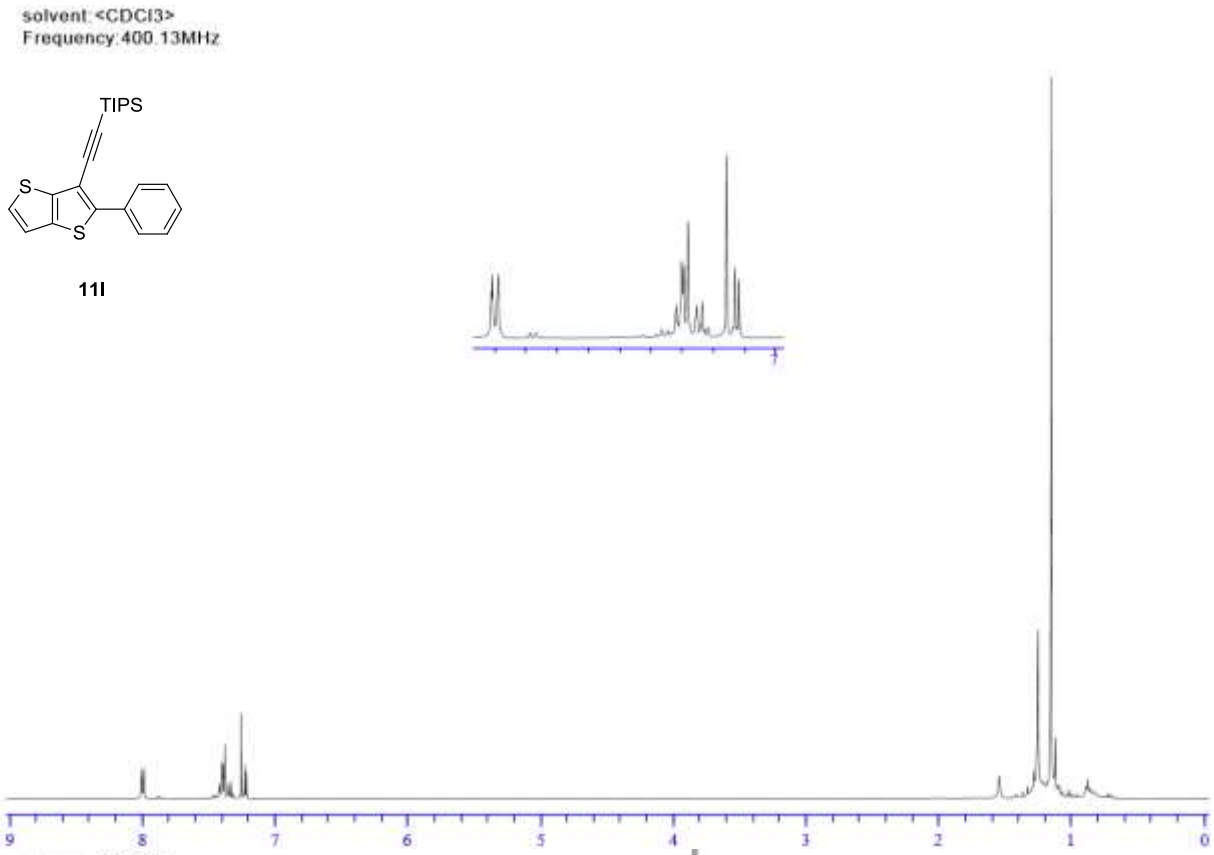


11k



11k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TIPS
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S
11l
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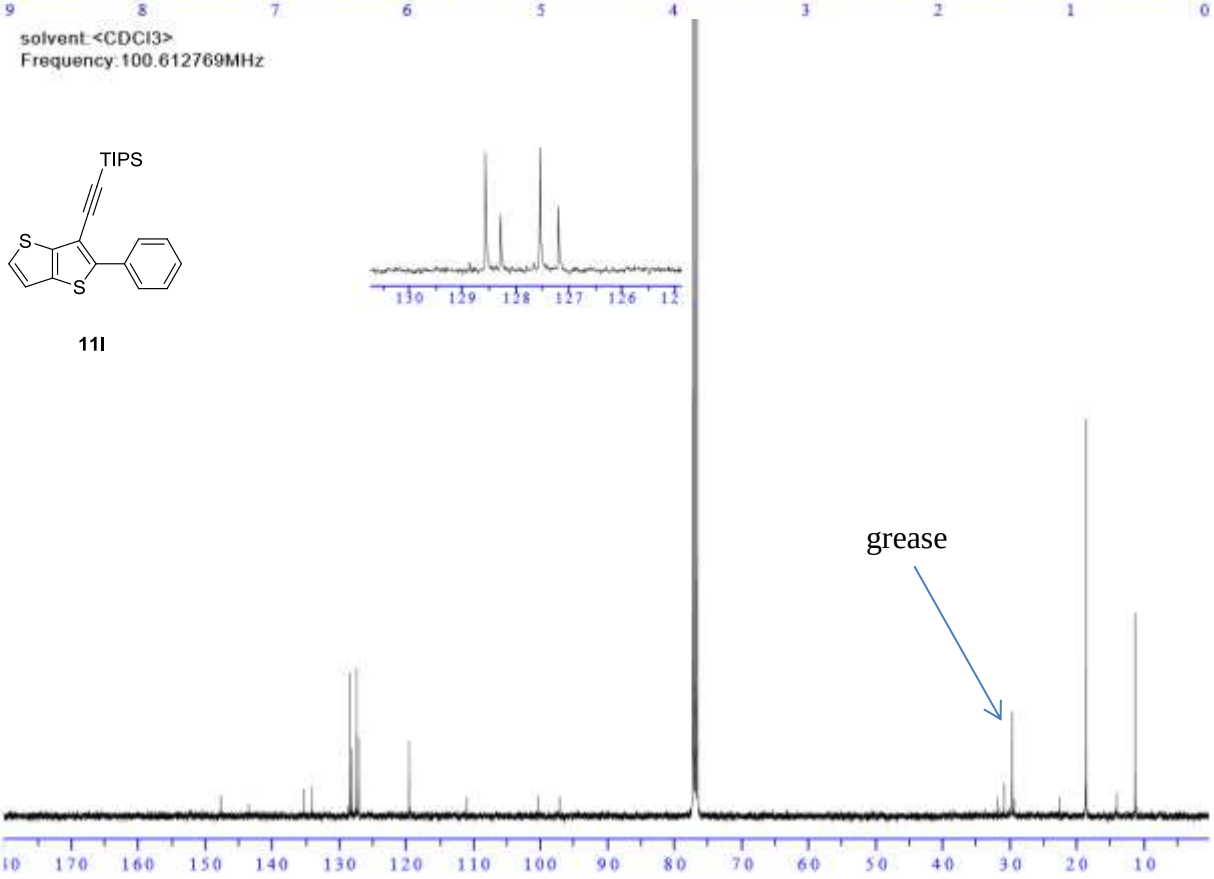
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TIPS
S
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grease
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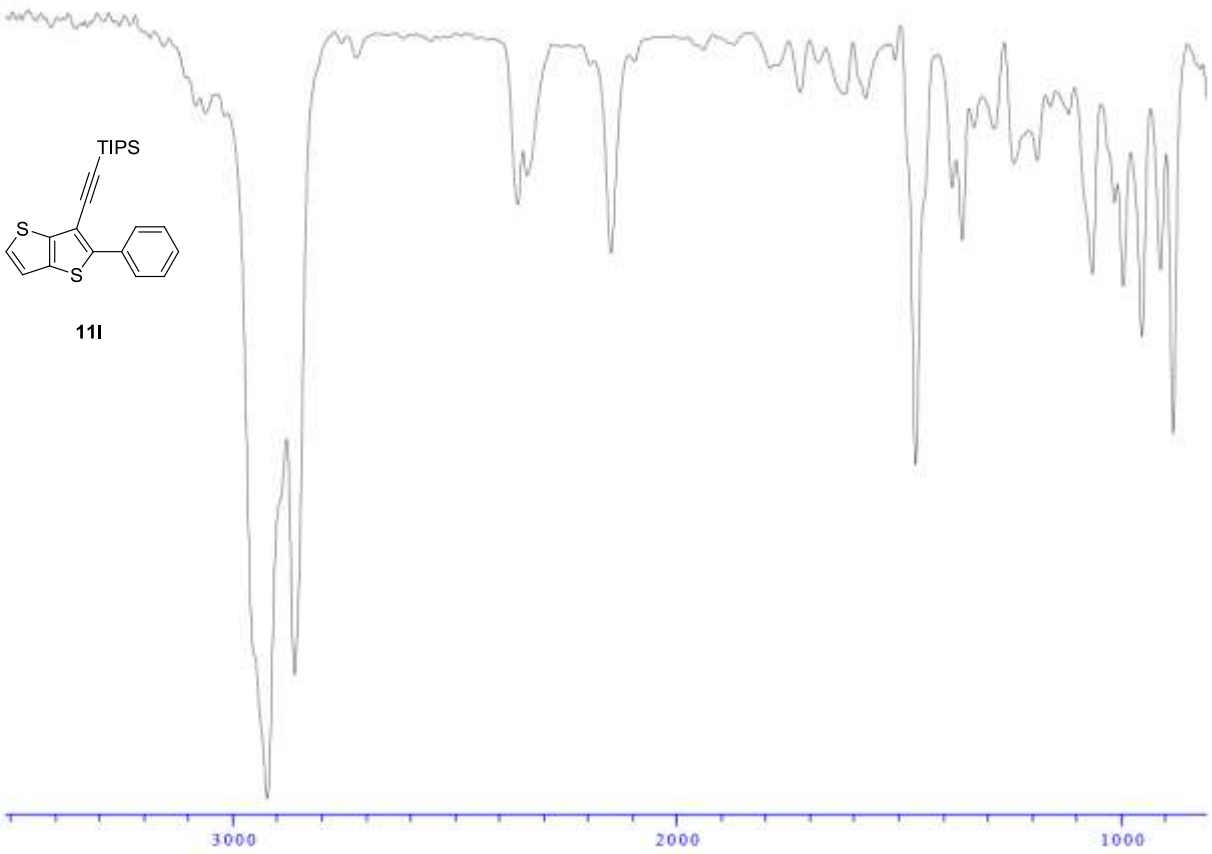

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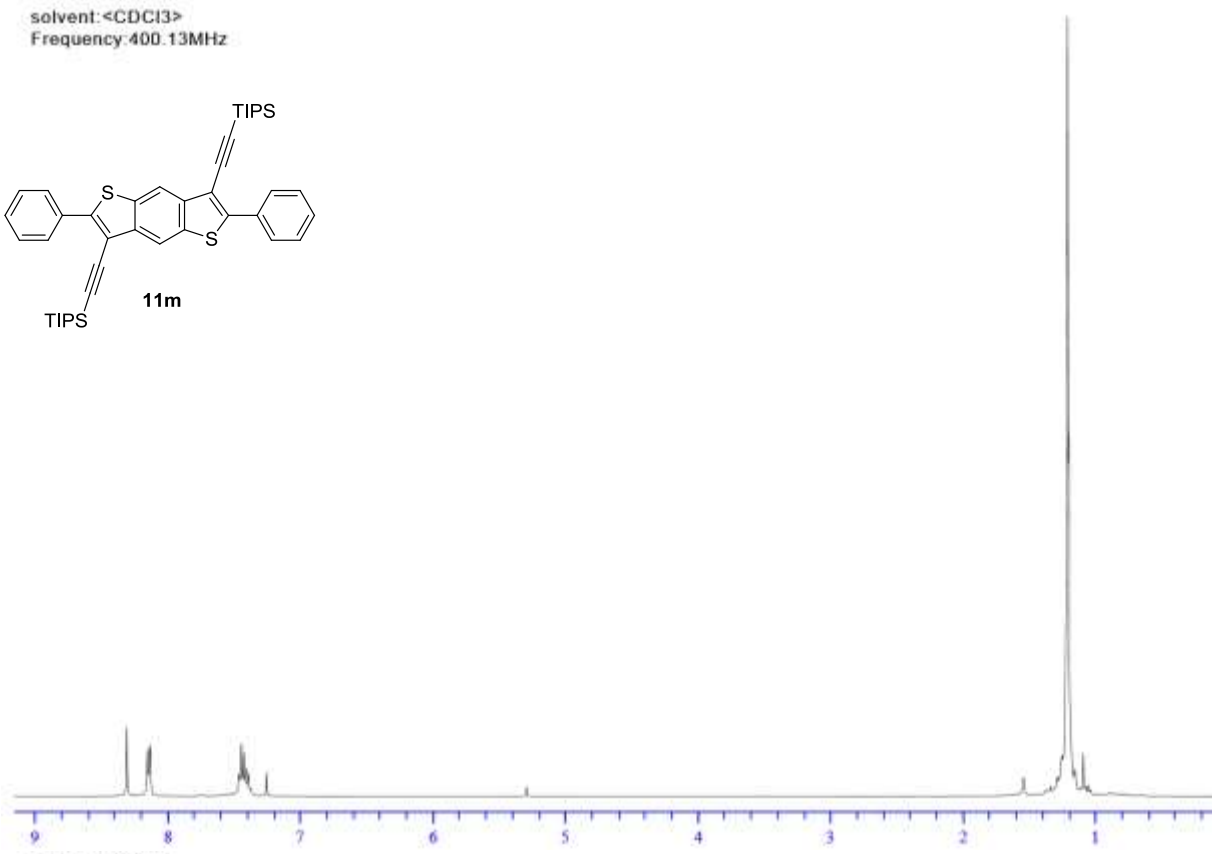
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TIPS
S
S
TIPS
11m
9
8
7
6
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4
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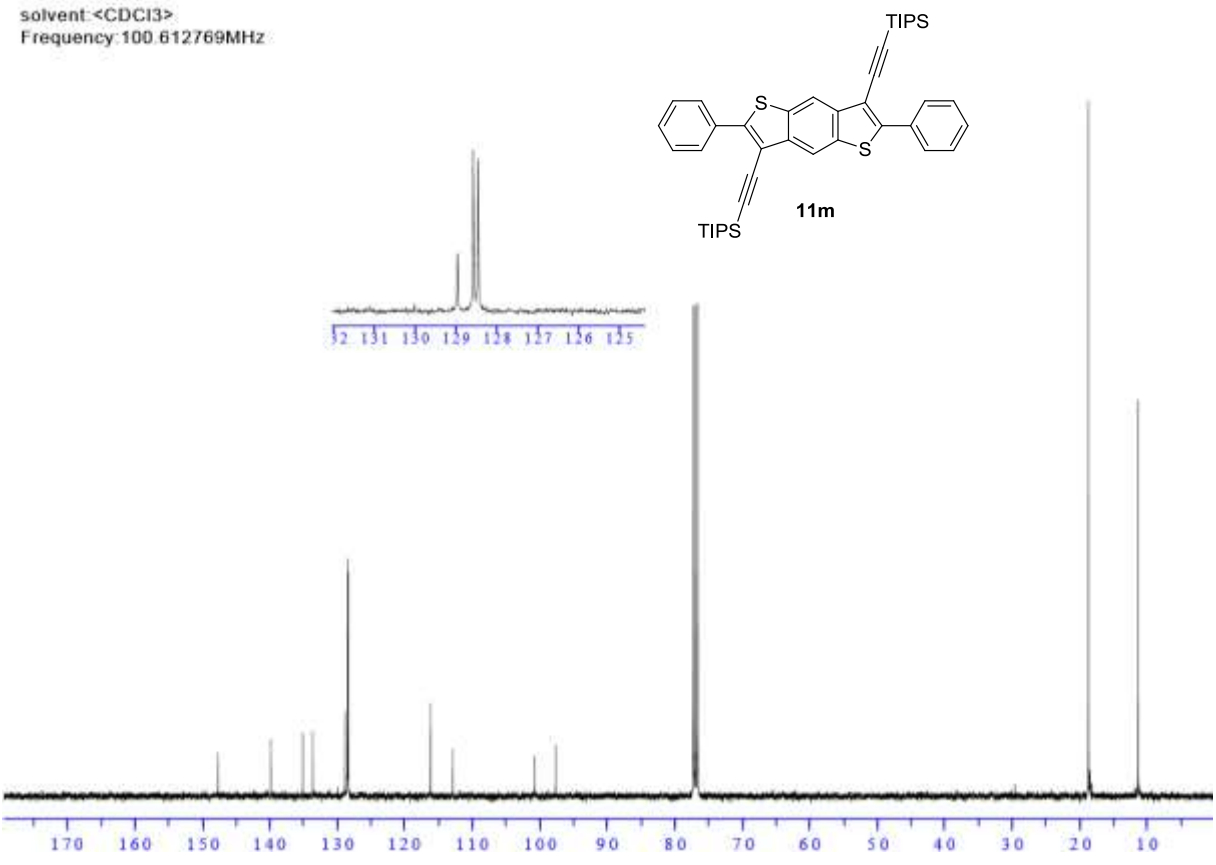
2
1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TIPS
S
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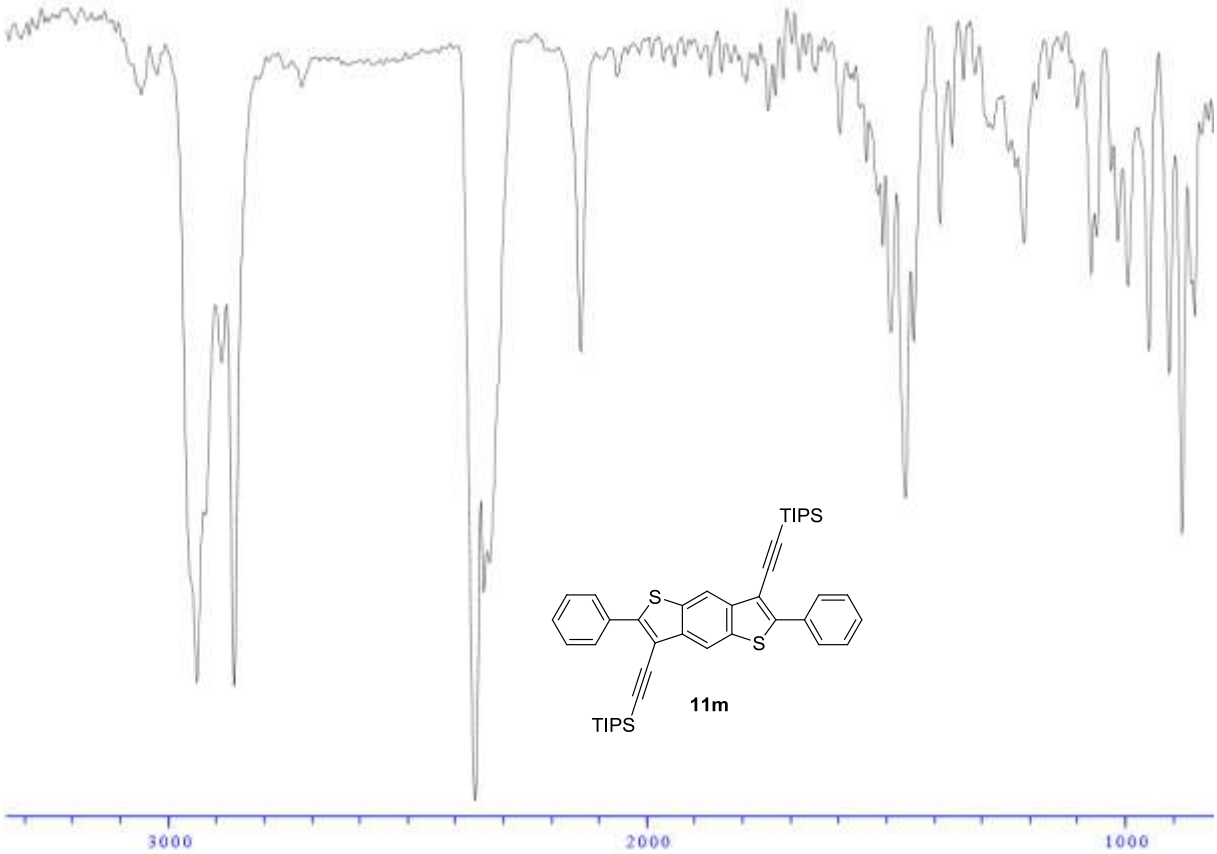
TIPS
11m
132 131 130 129 128 127 126 125
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


TIPS
S
S
TIPS
11m
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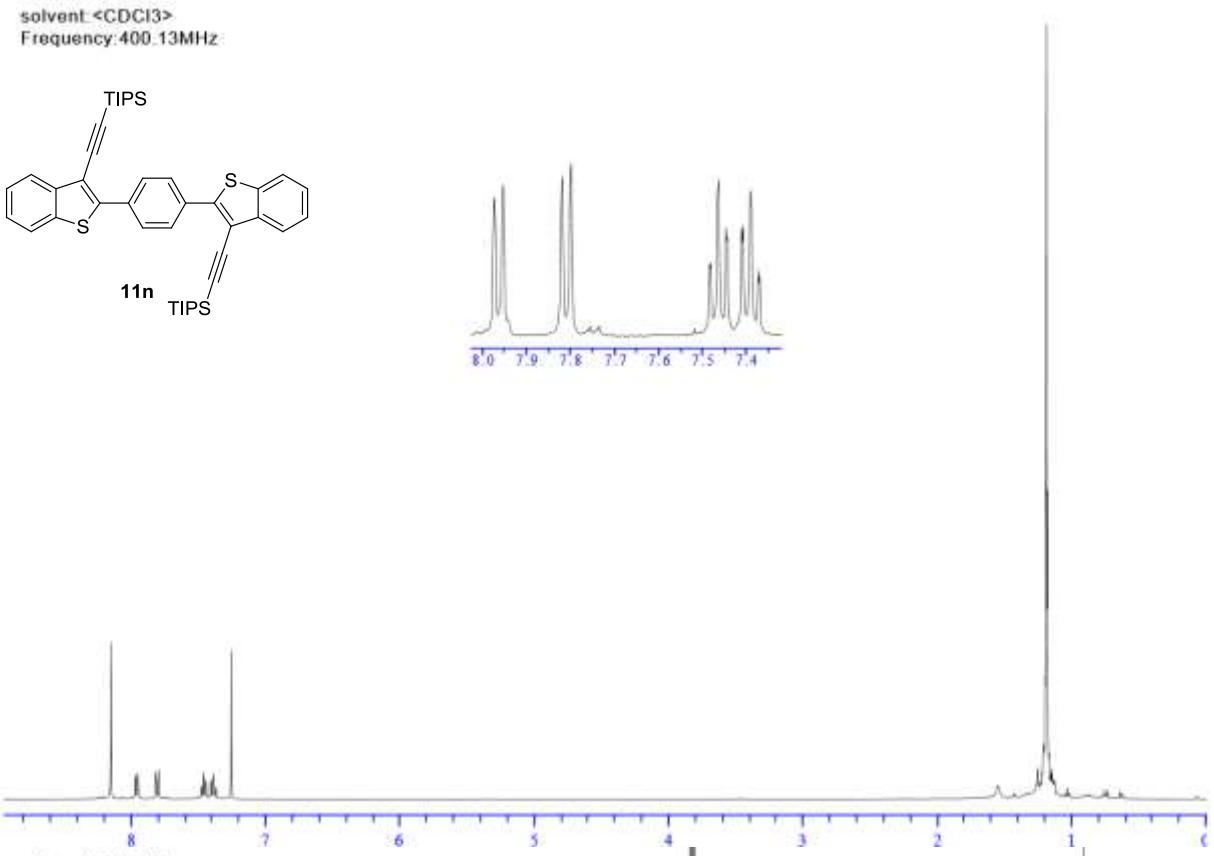
2000
1000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TIPS
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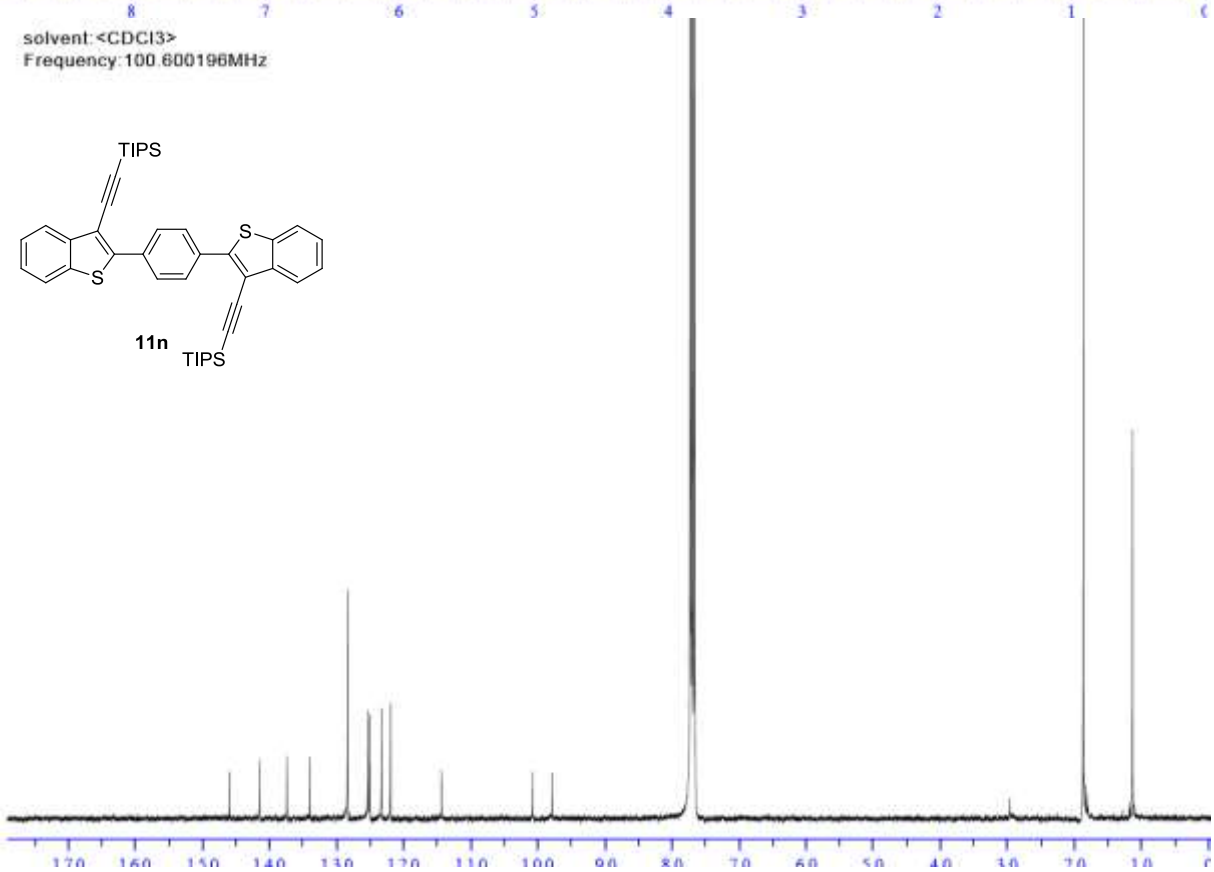
S
11n
TIPS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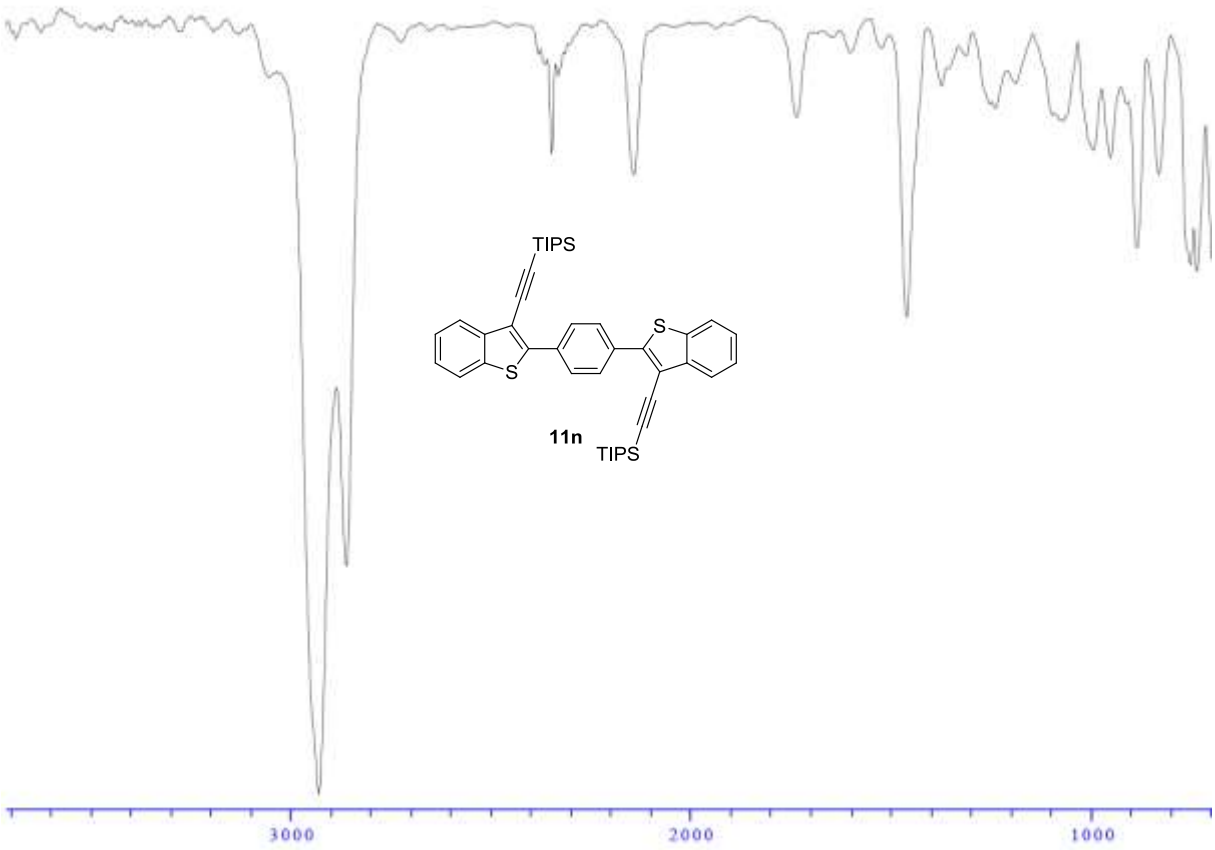
S
11n
TIPS



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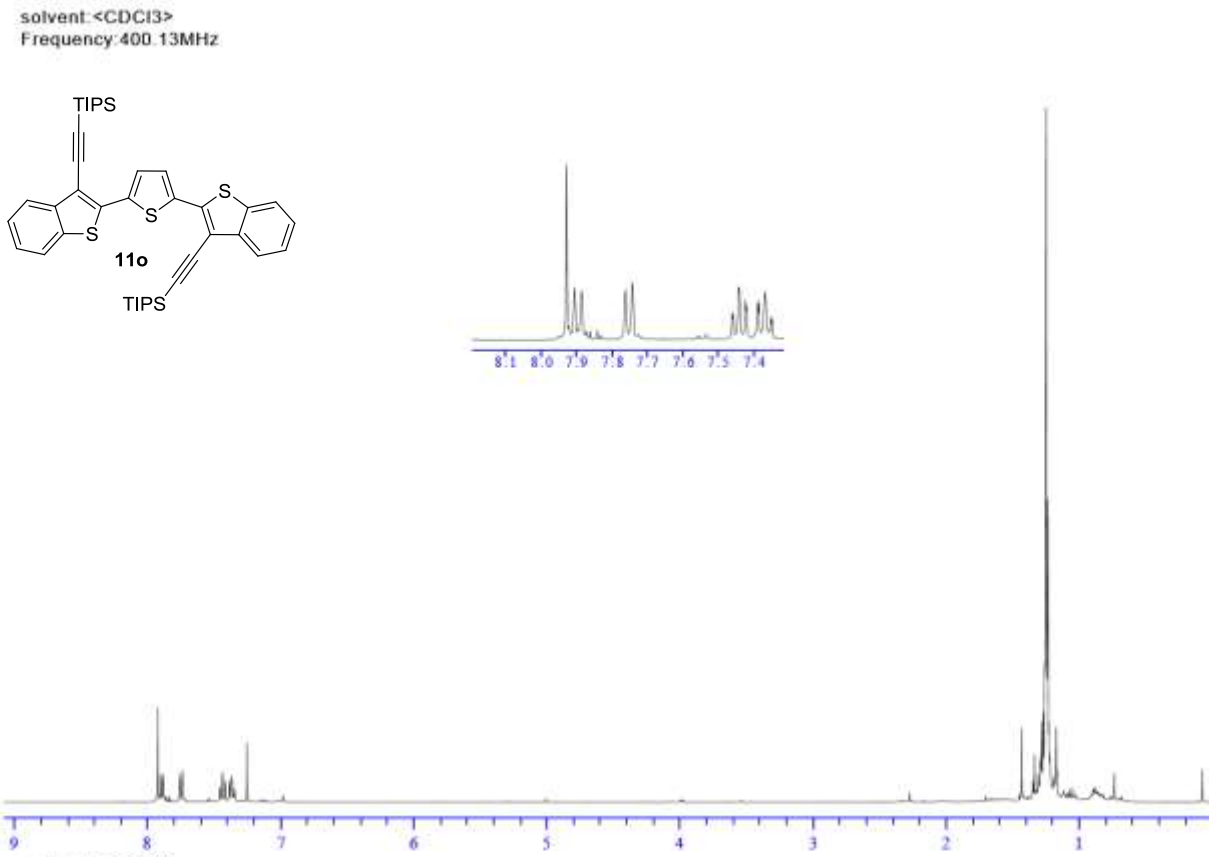
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TIPS
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S
S
11o
TIPS
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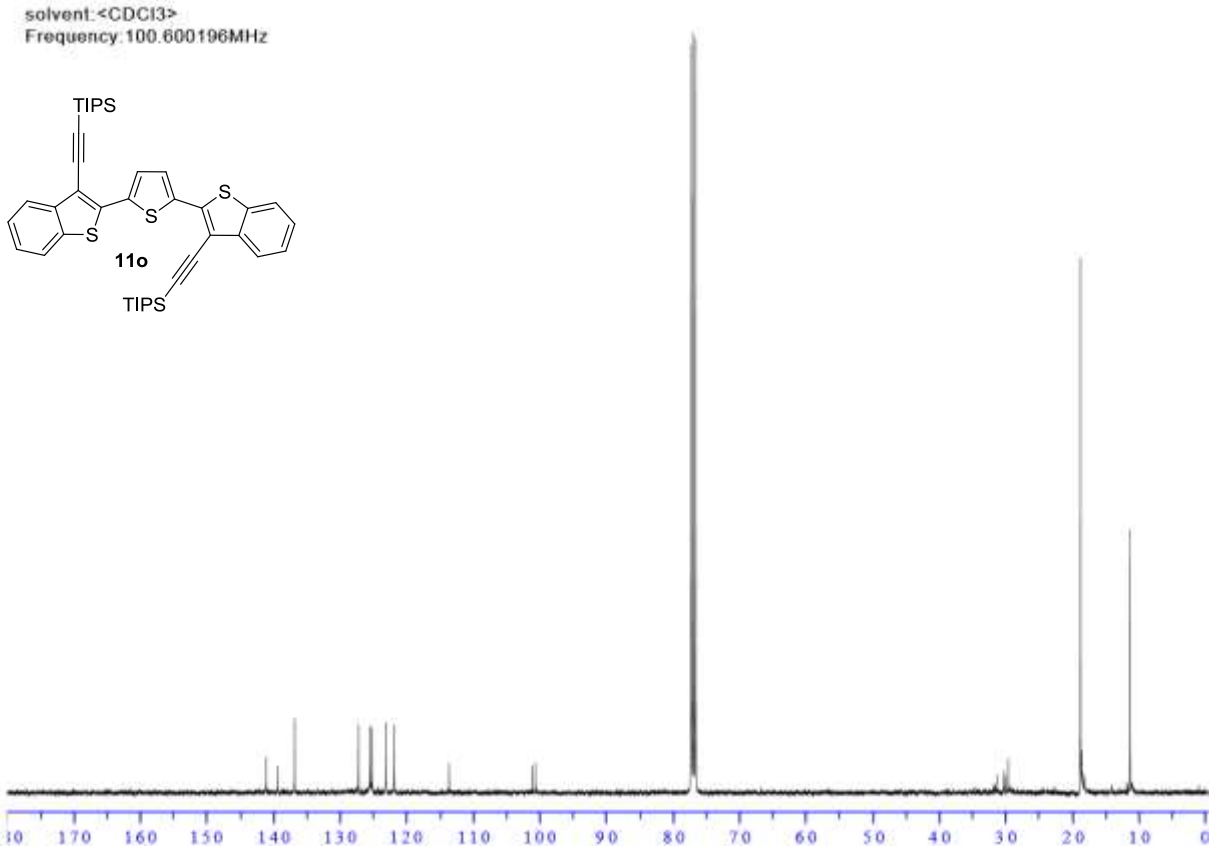
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TIPS
S
S
S
11o
TIPS
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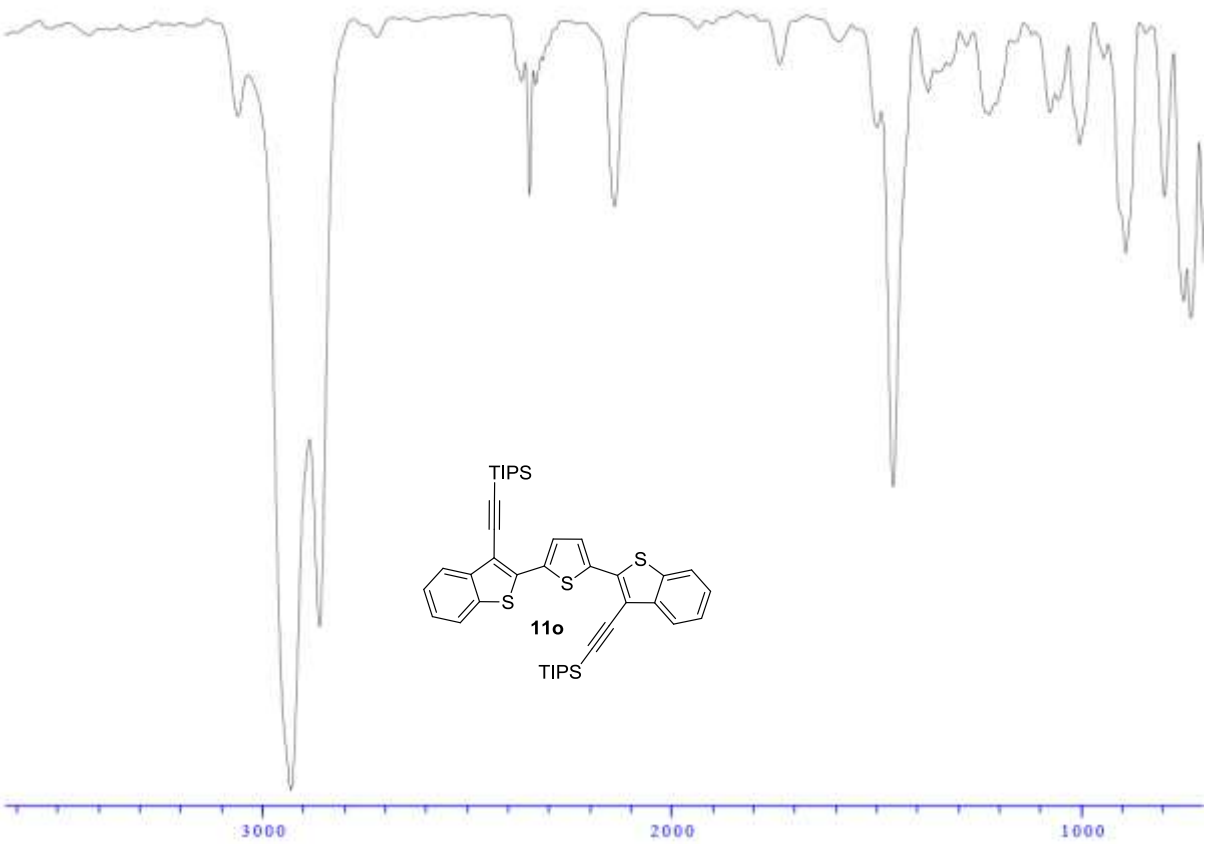

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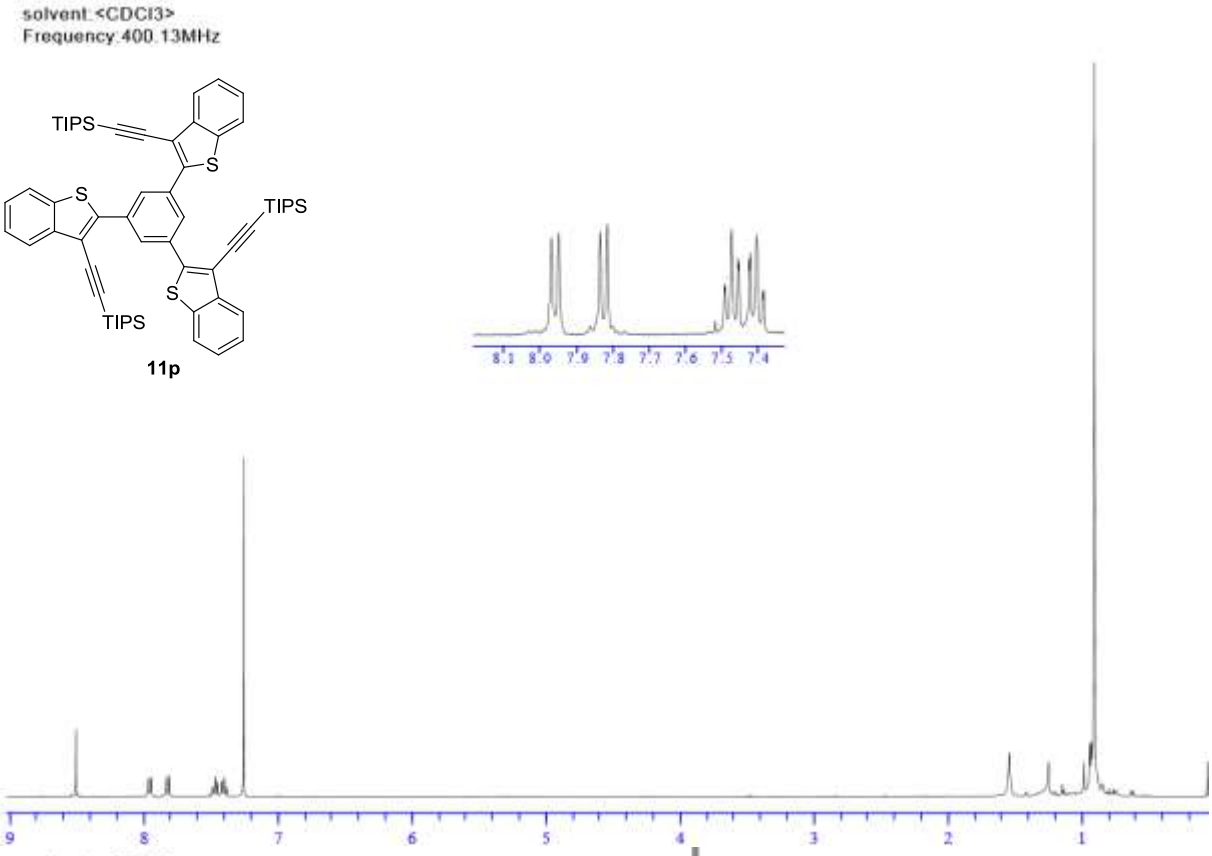
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Frequency:400.13MHz
TIPS
TIPS
TIPS
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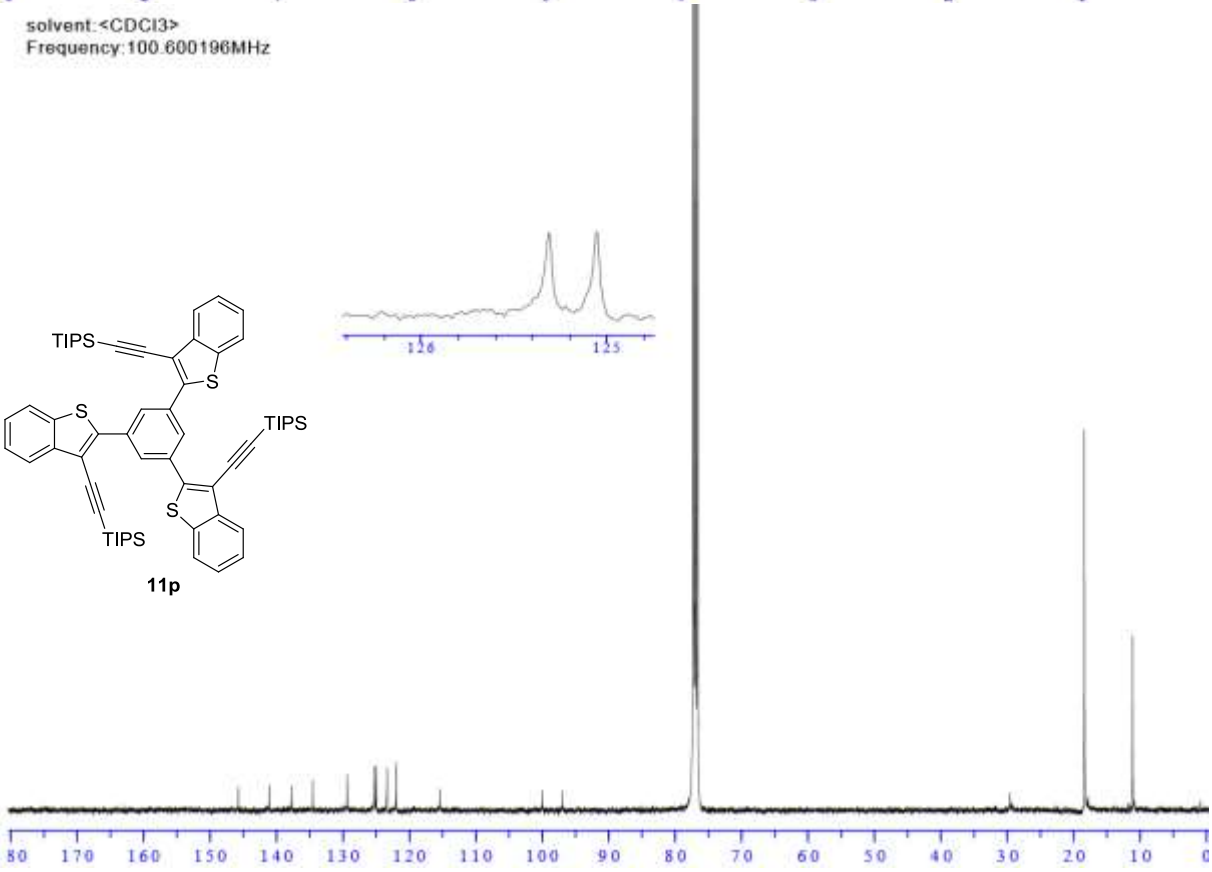
S
S
S
11p
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
9 8 7 6 5 4 3 2 1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TIPS
TIPS
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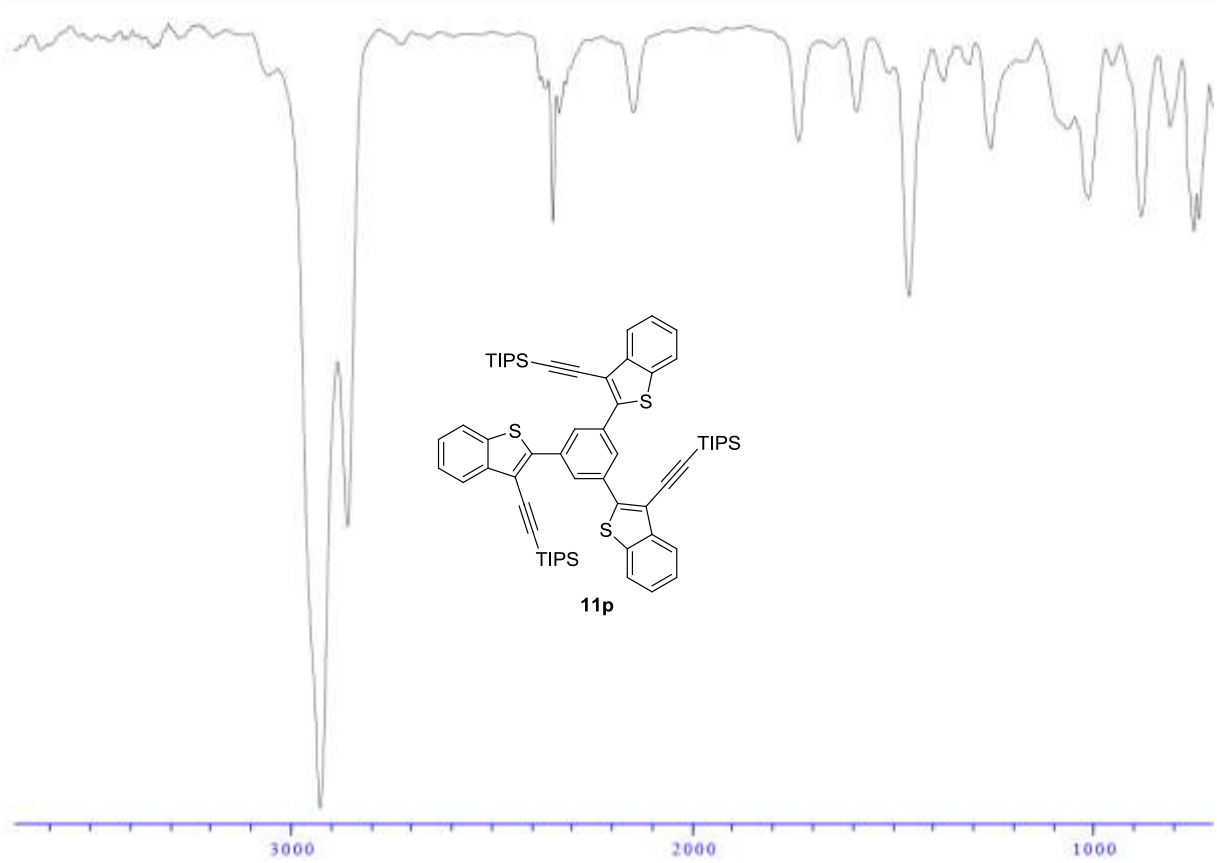
S
S
S
11p
126 125
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



11p

solvent:<CDCl3>
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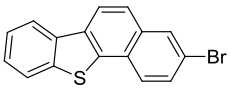
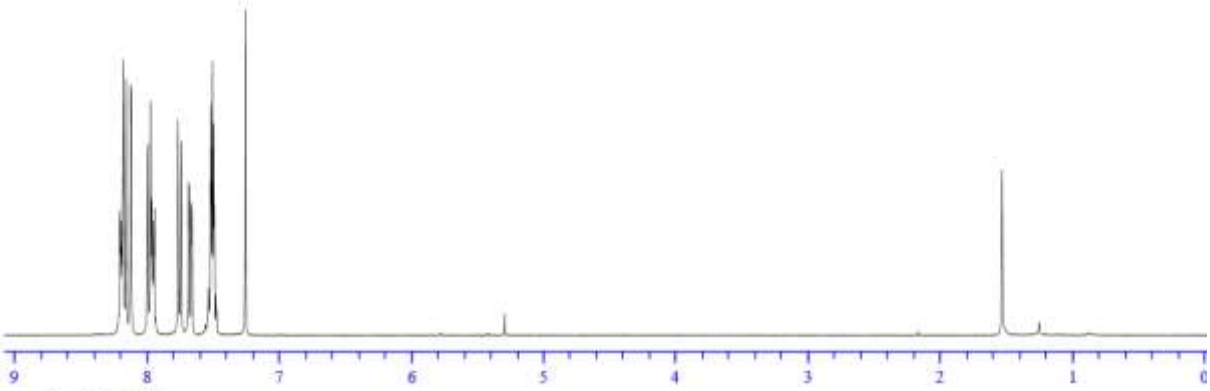


12c



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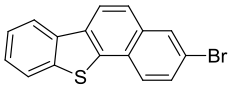
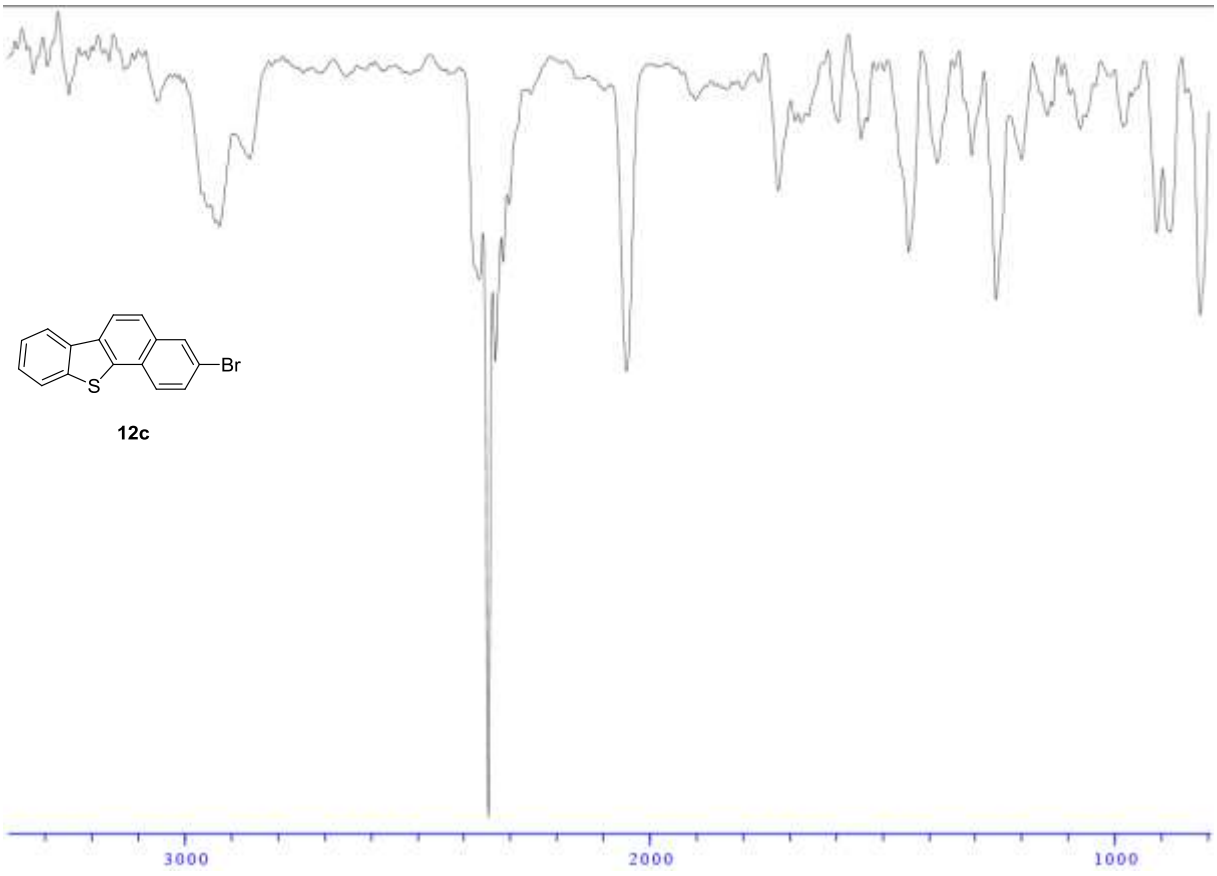
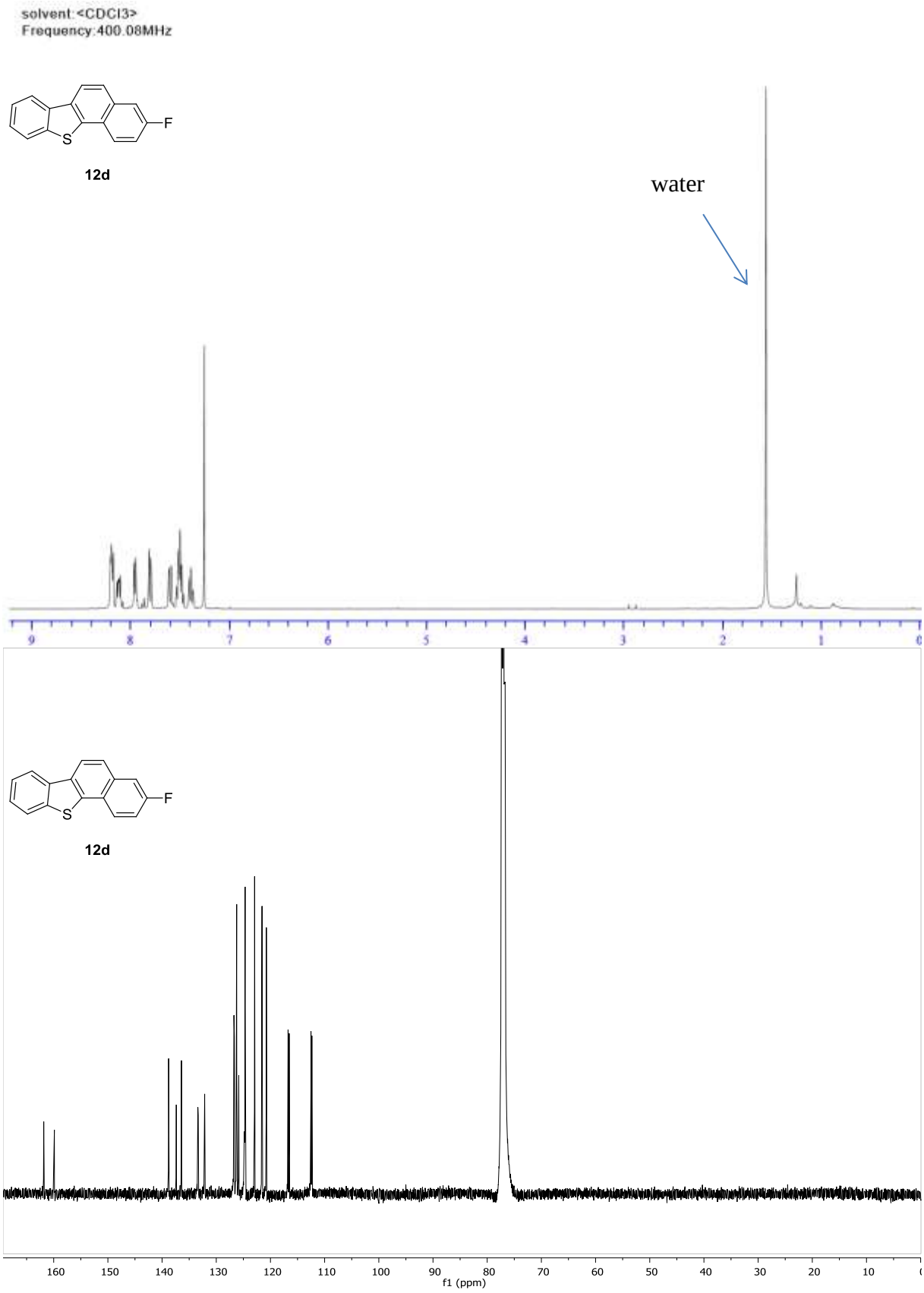


12c



12c


solvent:<CDCl3>
Frequency:400.08MHz
F
S
12d
water
9
8
7
6
5
4
3
2
1
0
F
S
12d
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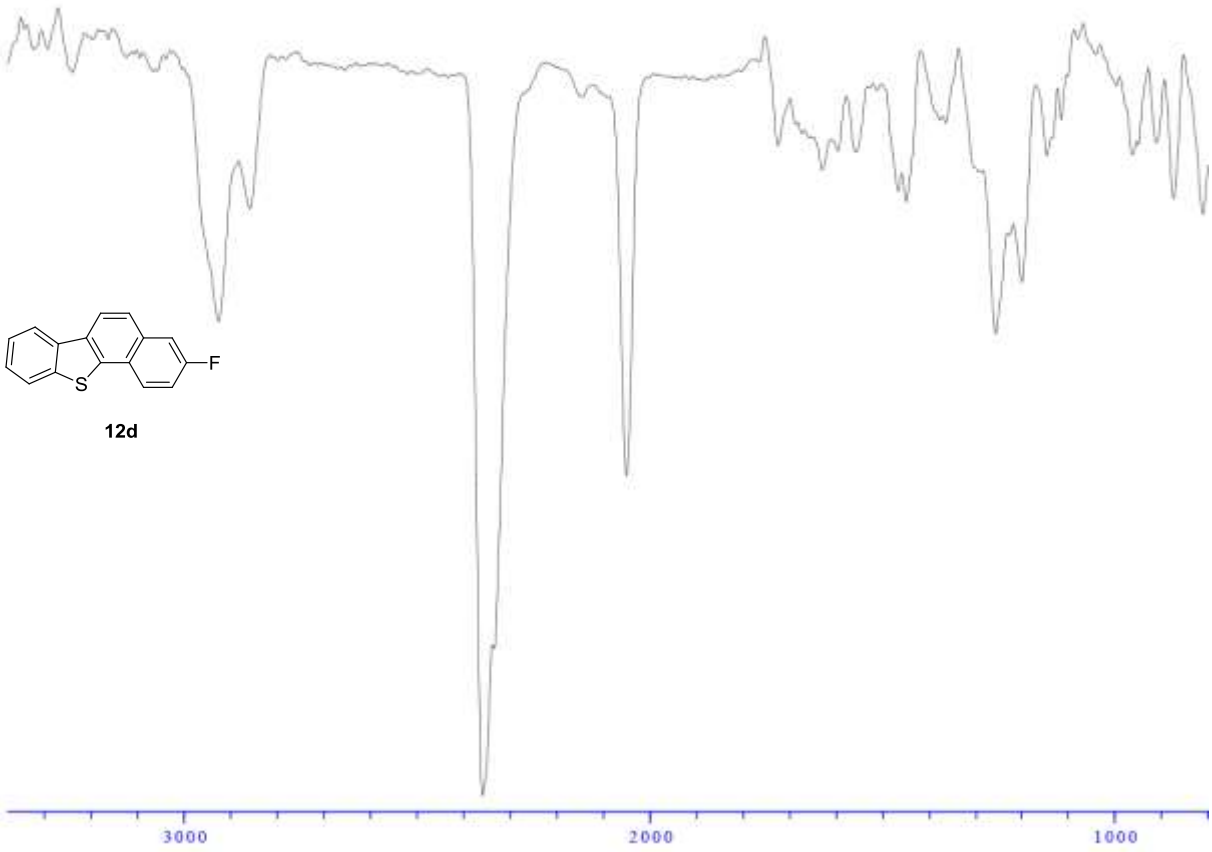
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



12d

solvent:<CDCl3>

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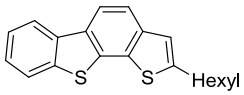
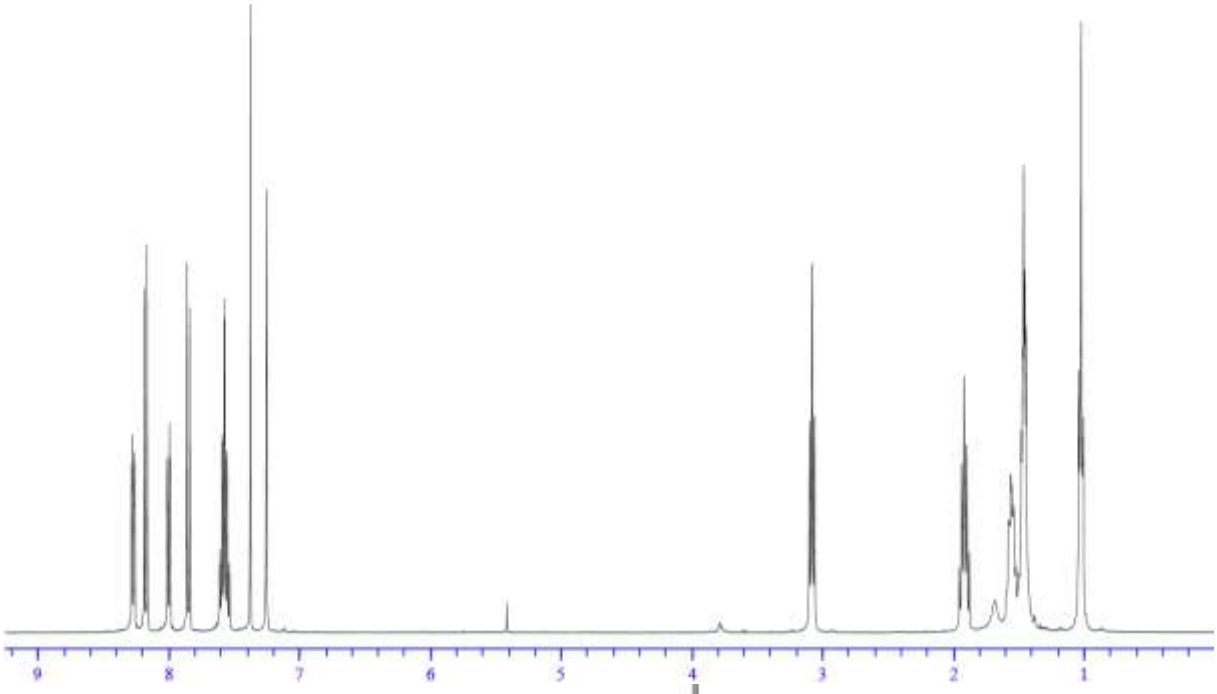


12e



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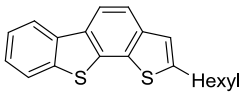
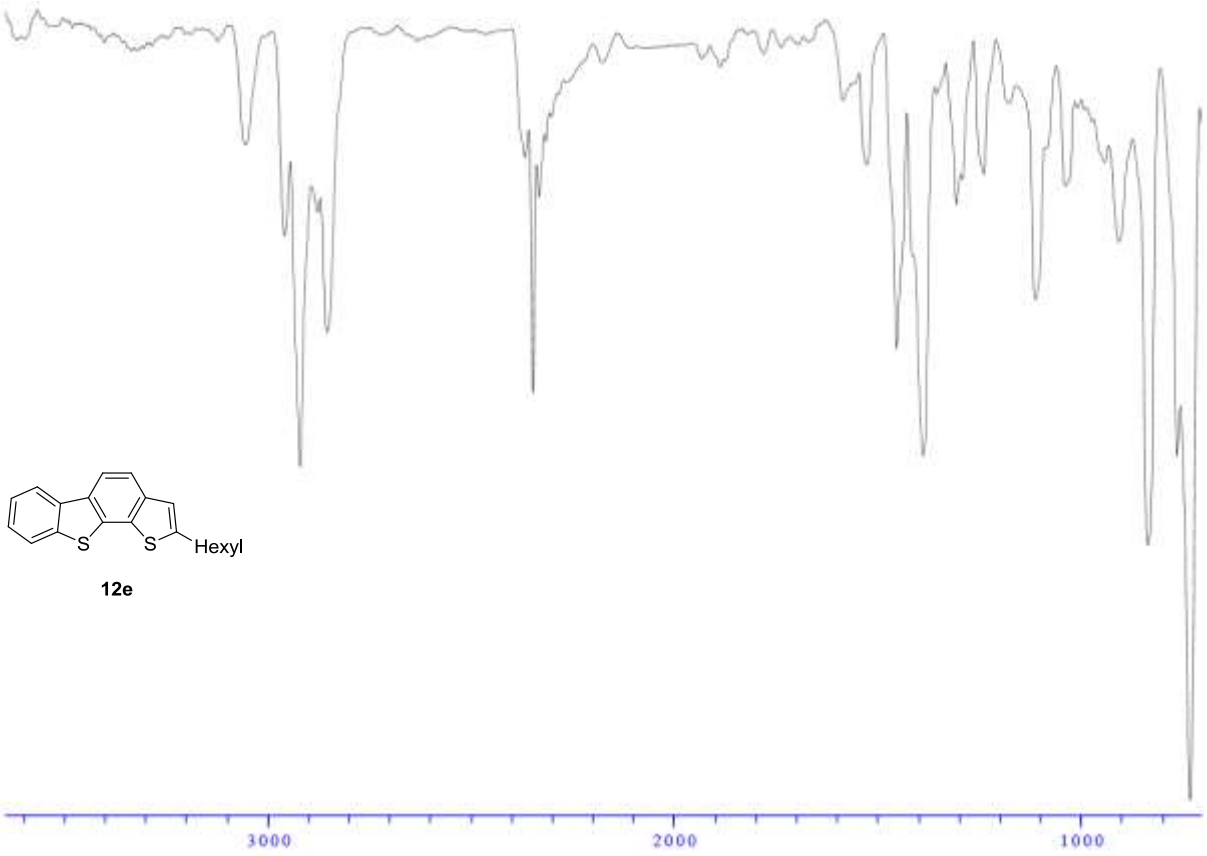


12e



12e

solvent:<CDCl3>
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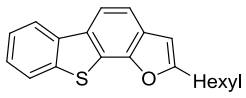
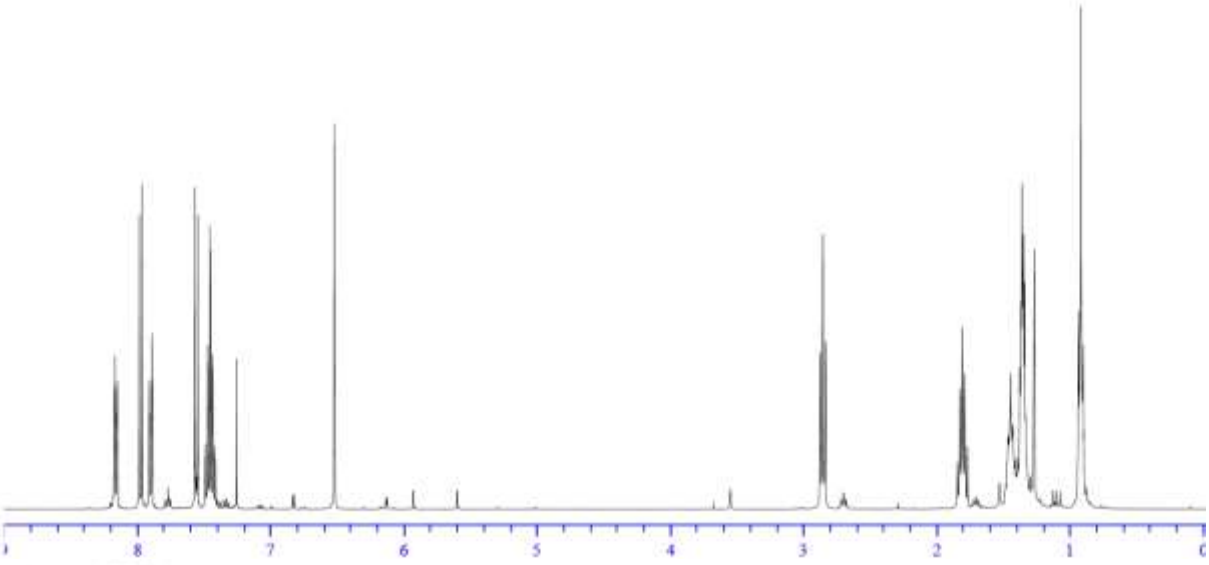


12f



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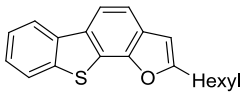
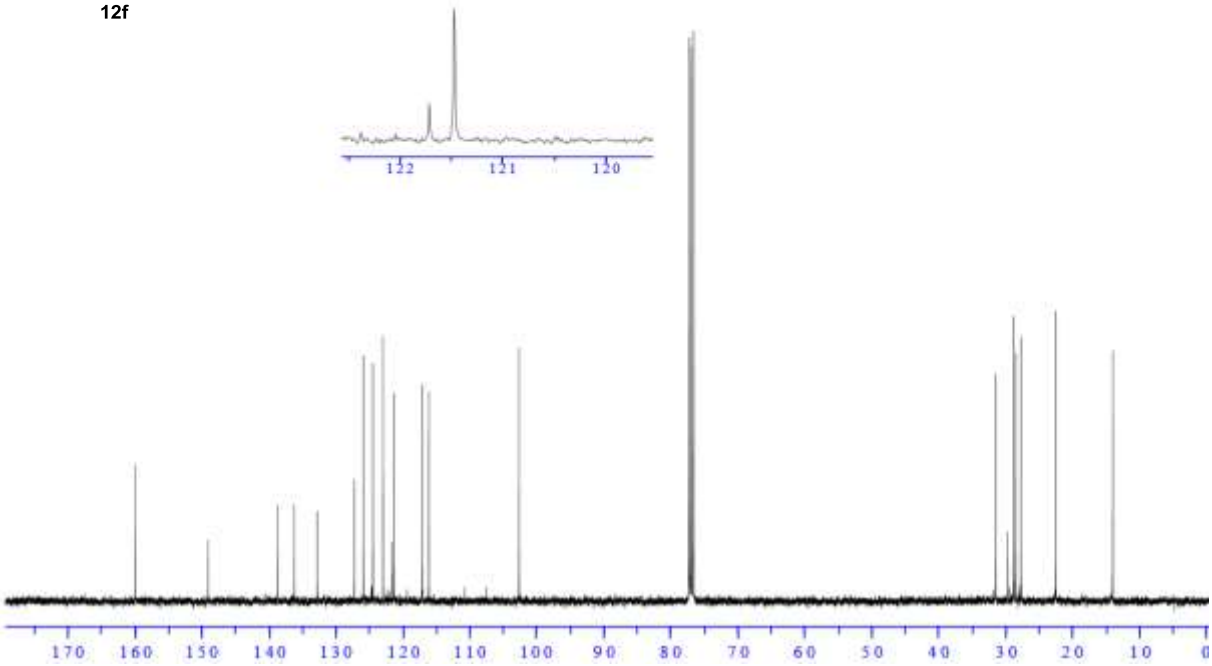
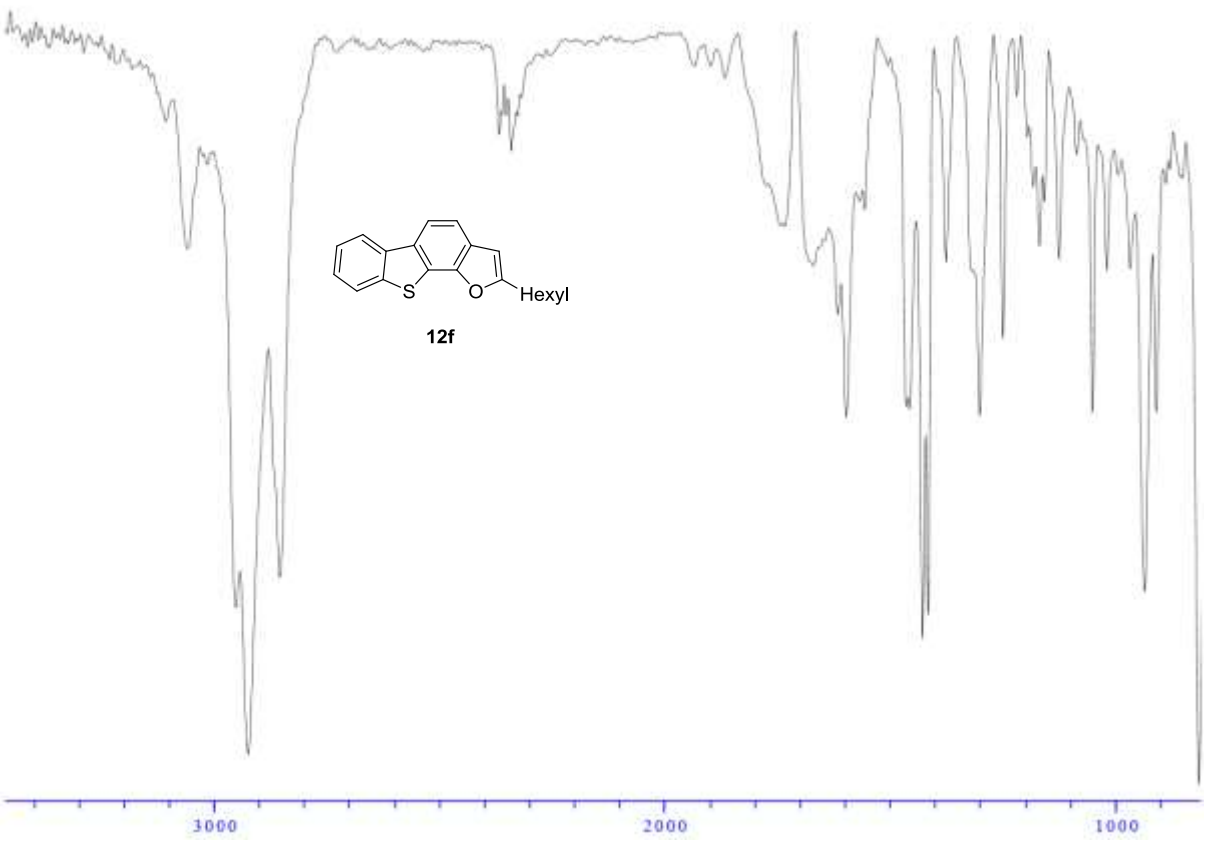


12f





12f

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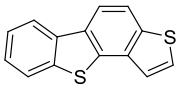
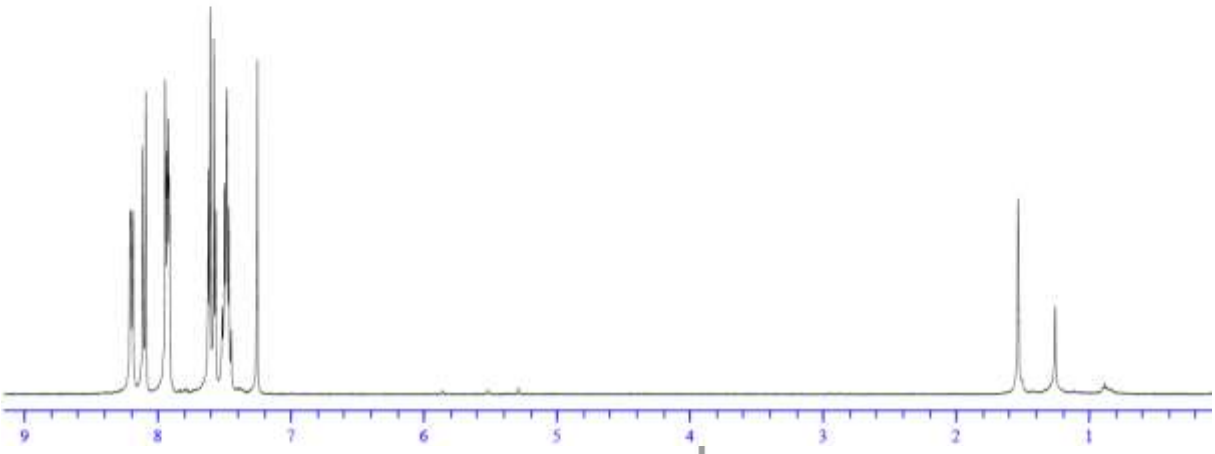
Frequency:400.13MHz



12g



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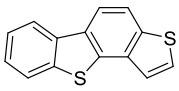
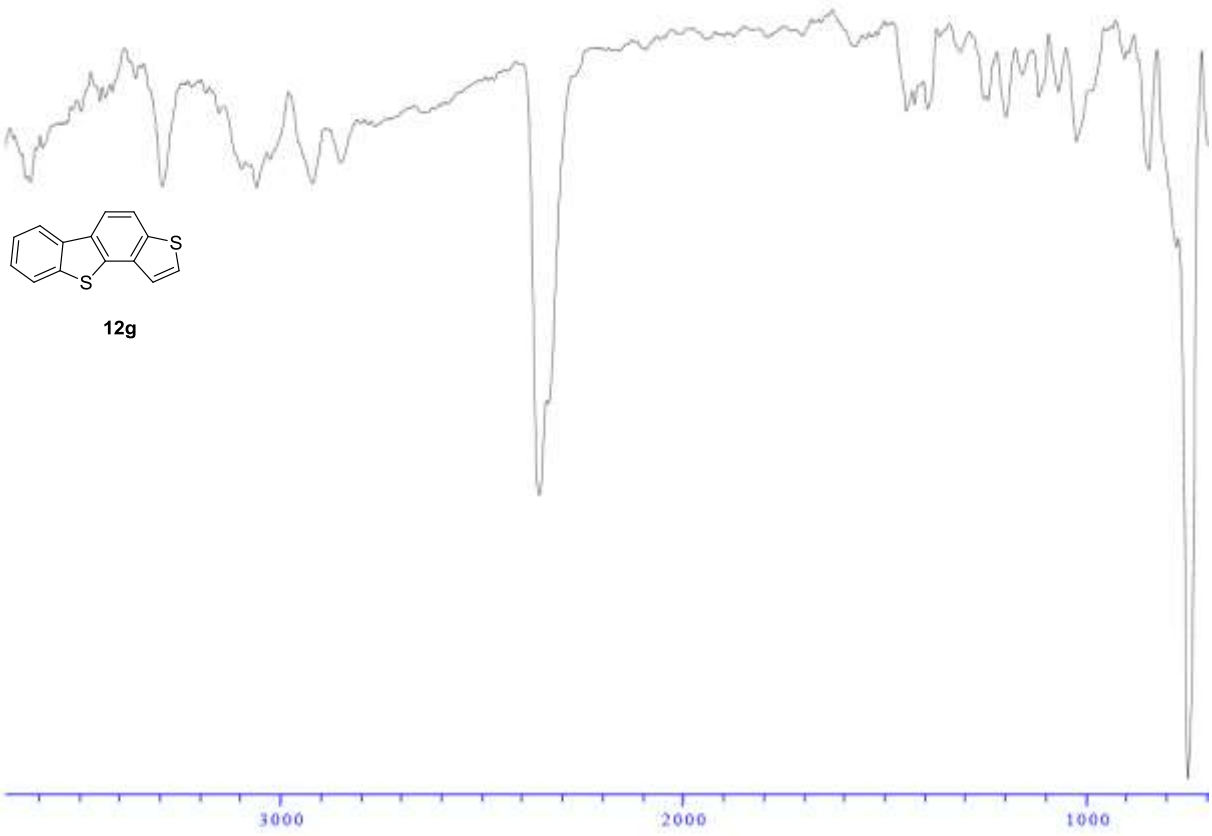
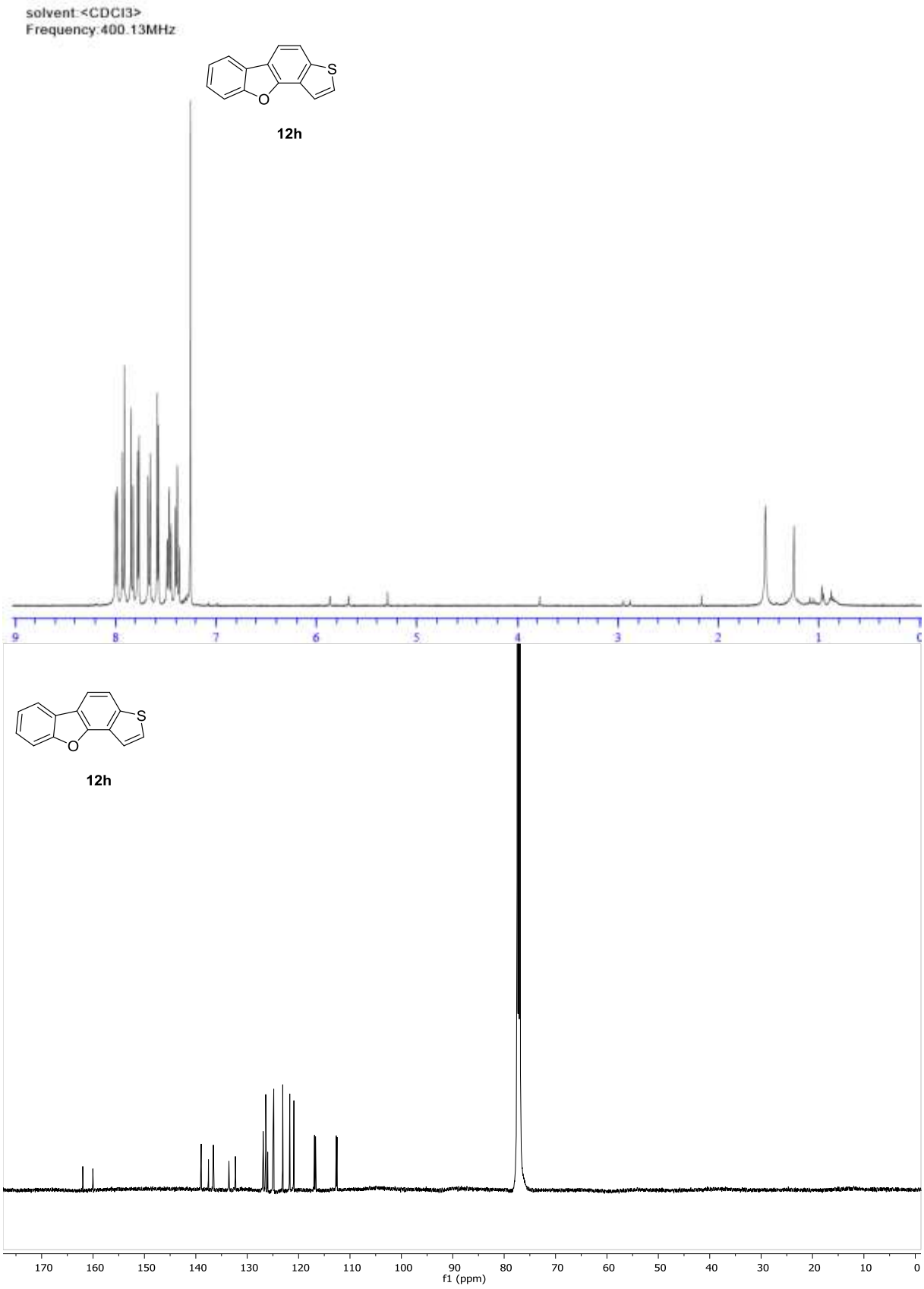
Frequency:100.612769MHz

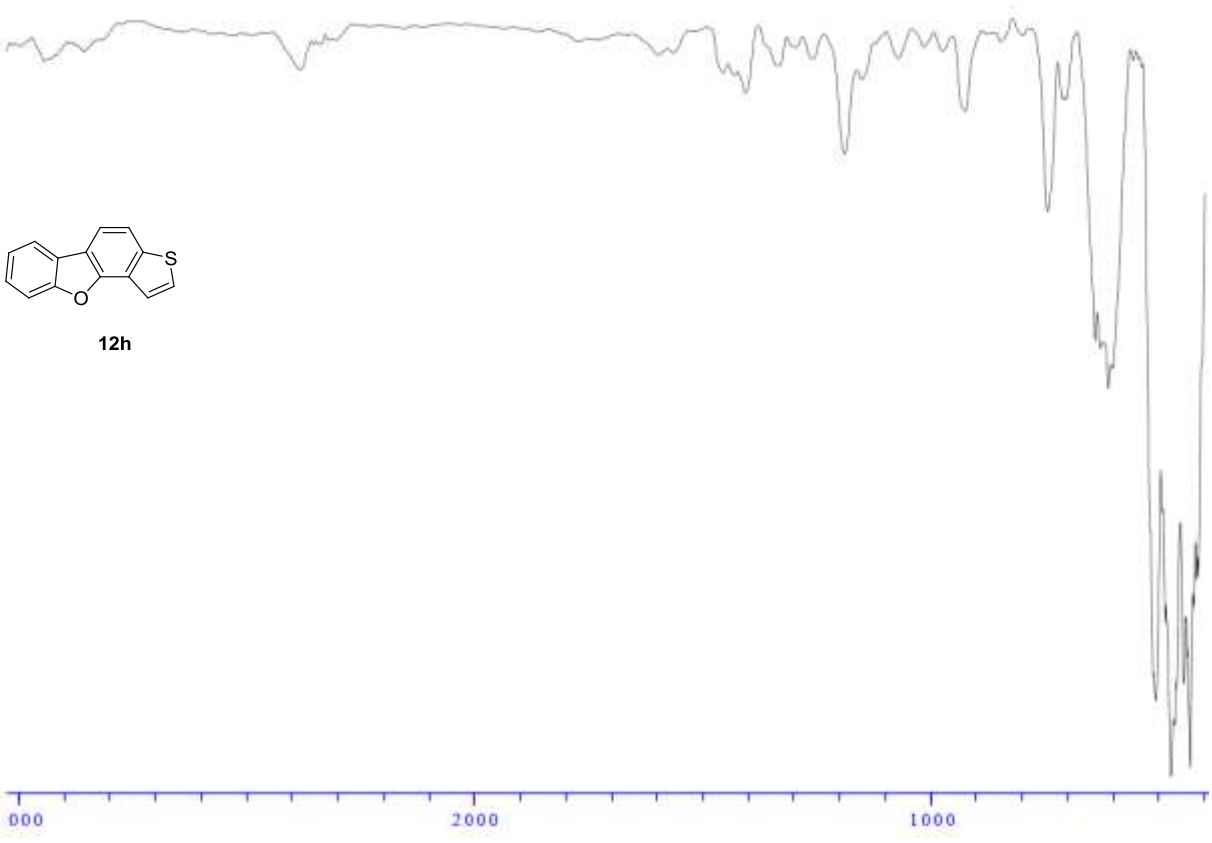


12g



12g


solvent:<CDCl3>
Frequency:400.13MHz
S
O
12h
9
8
7
6
5
4
3
2
1
S
O
12h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



12h

solvent:<CDCl3>
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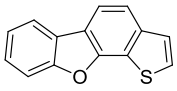
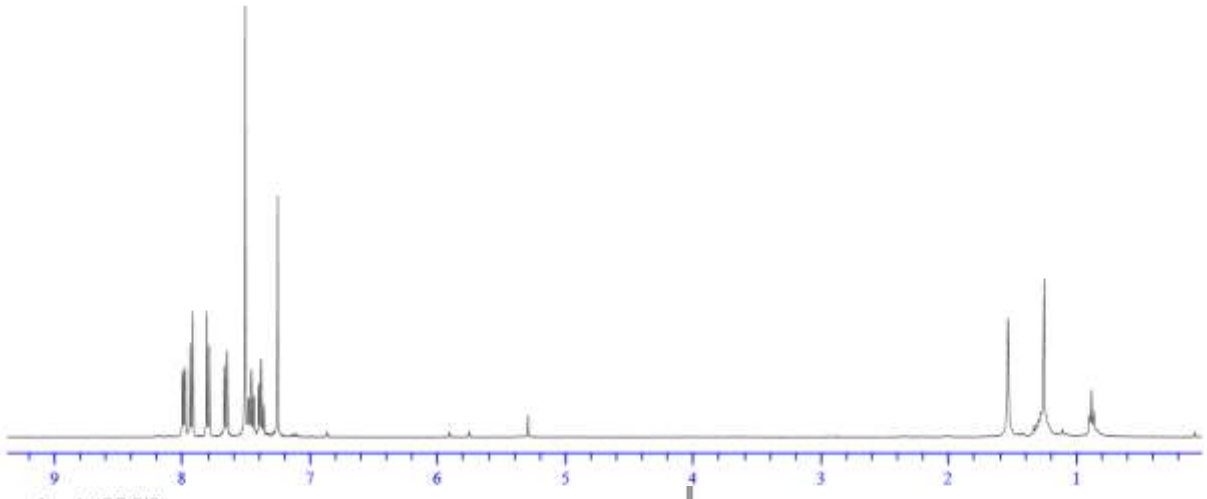


12i



solvent:<CDCl3>
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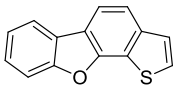
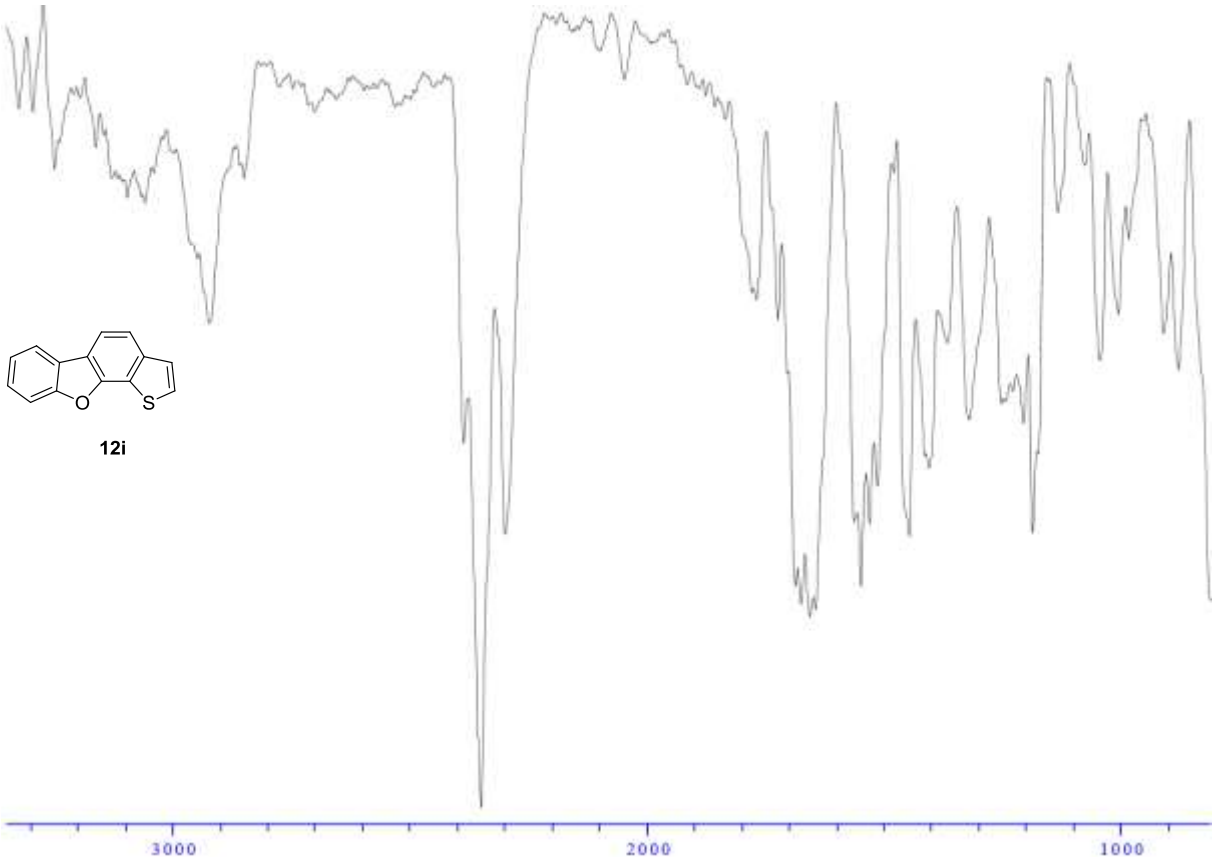
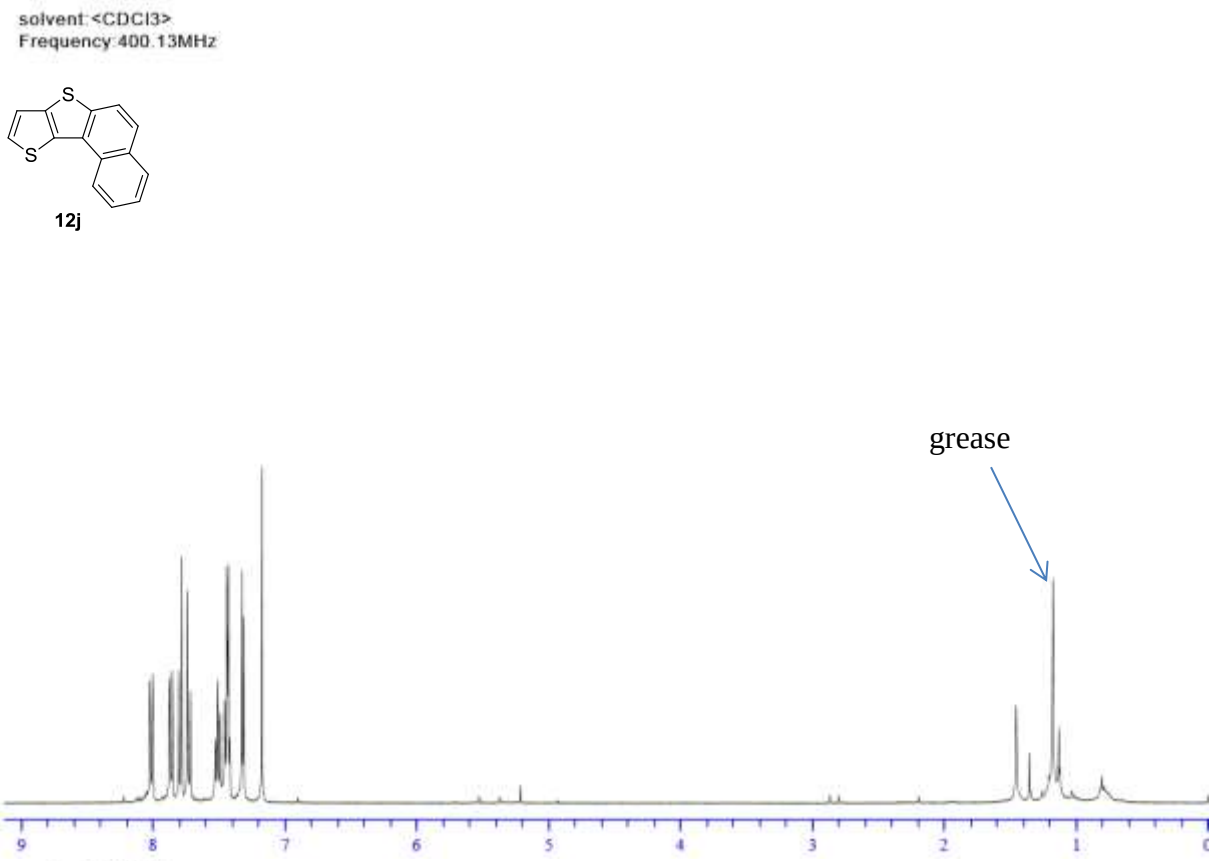
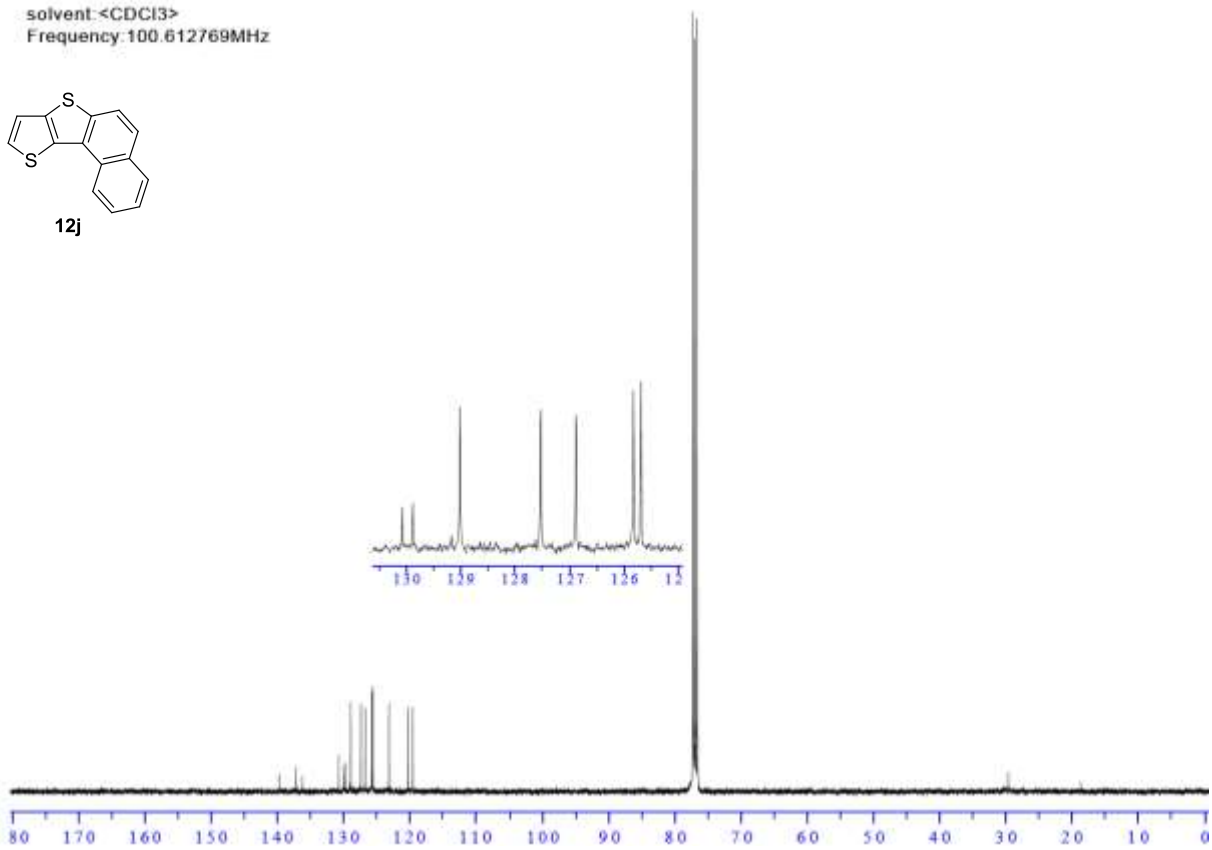
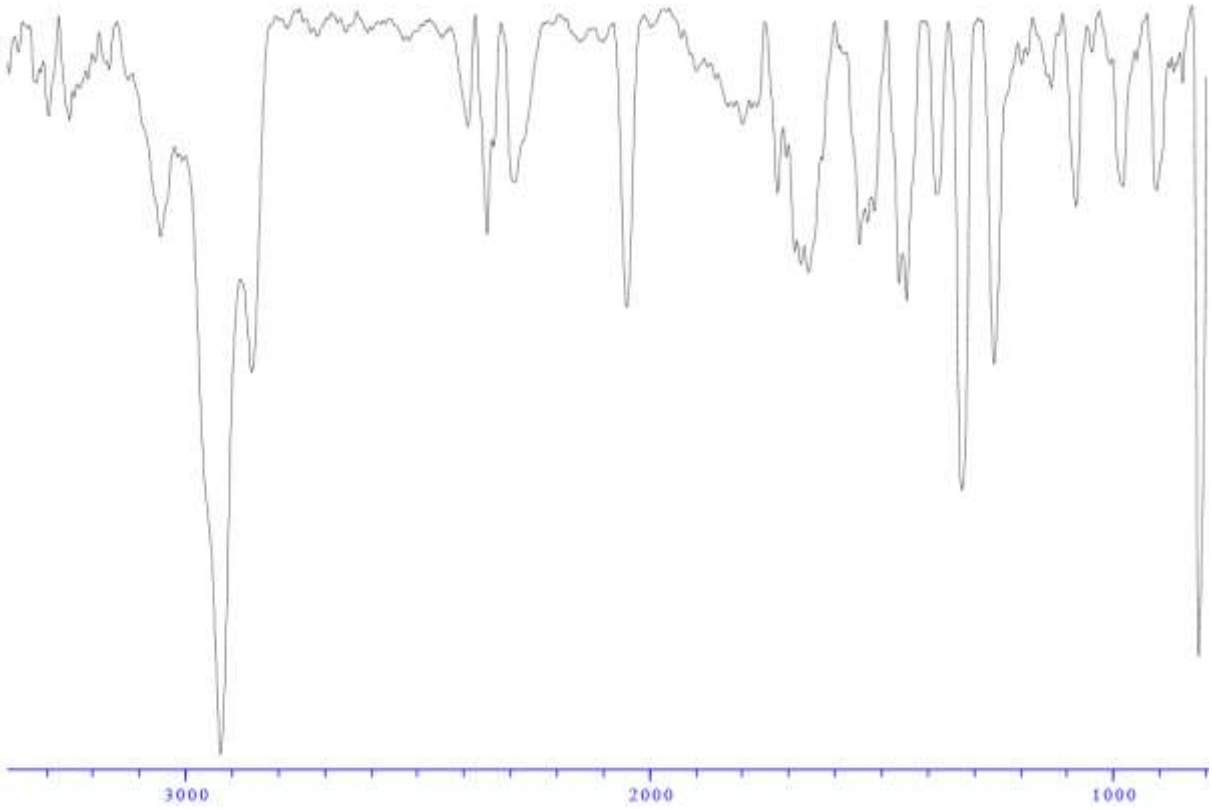


12i

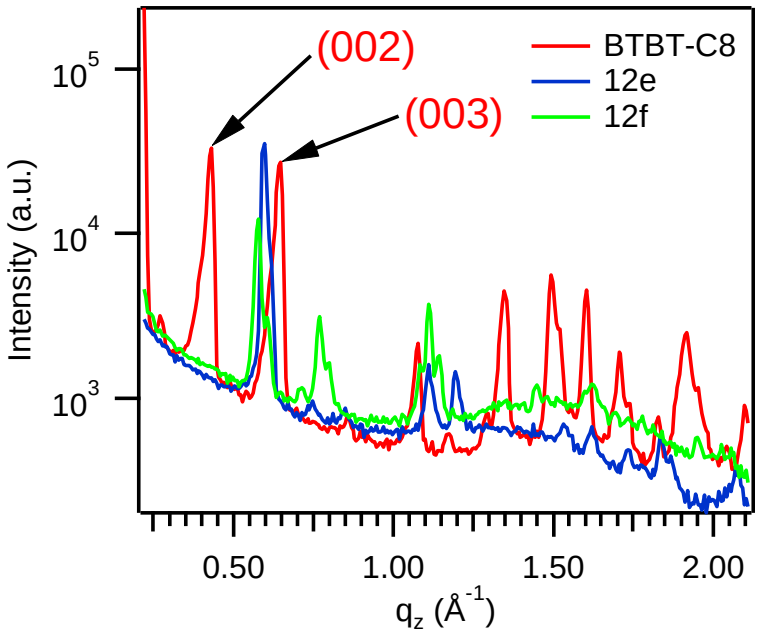

O
S
12i
3000
2000
1000


solvent:<CDCl3>
Frequency:400.13MHz
S
S
12j
grease
9
8
7
6
5
4
3
2
1
0


solvent:<CDCl3>
Frequency:100.612769MHz
S
S
12j
130
129
128
127
126
125
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


3000
2000
1000

9. Thin film X-ray diffraction of selected compounds



Out-of-plane GIXRD pattern of melt-processed films of BTBT, 12e and 12f on SiO_2 substrate. The two first peaks of the BTBT (control) diffractogram exhibit a scattering vector of 0.43 and 0.64 $Å^{-1}$, which correspond to Bragg spacing of 14.6 and 9.8 Å respectively, and can be attributed to packing of the BTBT molecules without interdigitating of the side chains as proposed by Collela et al. (ChemPlusChem **2014**, *79*, 371-374.). The smaller distances observed in this work with molecules 12e and 12f is likely caused by the shorter alkyl side-chains of the molecule (C8 vs. C12) and the presence of only one alkyl chain instead of two.

APPENDIX 1

Optimised geometries of all monomers (PBE0-D3BJ/def2SVP) and dimers (PBE0-dDsC/def2SVP) in the form of Cartesian coordinates.

12a

0 1
C 0.0000000009 -0.5773046315 -1.9048150124
C 0.0000000009 -0.9301122491 -0.5023339578
C -0.0000000001 0.2815147715 0.1809681993
O 0.0000000015 1.3429268282 -0.6673066595
C 0.0000000008 0.8312177294 -1.9291095687
C 0.0000000015 -1.2786697495 -3.1148212885
C 0.0000000014 -2.1426467812 0.2278807229
C -0.0000000005 0.3892747029 1.5872885666
C 0.0000000015 1.5709026467 -3.1025108423
C -0.0000000018 -0.553232416 -4.3018786654
C -0.0000000013 0.8506342209 -4.2953718542
C 0. -0.8484225527 2.3058760646
C -0.0000000006 -2.0894829422 1.6000597056
H 0.0000000007 -2.3706656583 -3.1269587795
H 0.0000000018 -3.1015822553 -0.294199175
C -0.0000000002 1.6189011334 2.2852668989
H 0.0000000014 2.6614758306 -3.0811666462
H -0.0000000027 -1.082218084 -5.2572748184
H -0.000000002 1.3909449019 -5.2445827115
C -0.0000000009 -0.7918353498 3.7208569183
H -0.0000000002 -3.0128023486 2.1839836627
C 0.0000000003 1.6293355367 3.66187519
C -0.0000000009 0.4155966604 4.3838523262
H 0.0000000003 2.5486215171 1.7133326667
H -0.000000001 -1.7293739924 4.2826474674
H 0.0000000002 2.579610249 4.2004443537
H -0.000000001 0.4369122819 5.4760072366

1 2
C 0.000000009 -0.5822040555 -1.9019580232
C 0.0000000102 -0.9417750903 -0.5187007768
C 0.0000000018 0.3085814766 0.1872403801
O 0.000000017 1.3393960574 -0.6452271529
C 0.0000000005 0.8274451317 -1.9296895784
C 0.0000000091 -1.2937330417 -3.1146215102
C 0.0000000091 -2.143741186 0.2026879332
C 0.000000008 0.4065811125 1.5916862611
C 0.0000000016 1.5704261814 -3.086200779
C -0.0000000064 -0.566123306 -4.2983234598
C -0.0000000181 0.8367850164 -4.2841929674
C 0.0000000077 -0.8355600796 2.2992573276
C -0.0000000076 -2.0798907557 1.5838445028
H 0.0000000168 -2.3852092615 -3.1250497694
H 0.000000006 -3.1057522193 -0.3116809903
C 0.0000000067 1.6309676143 2.288403435
H 0.0000000035 2.6607818163 -3.073200664
H -0.000000013 -1.0895055023 -5.2558177398

-1 2
C -0.0000000017 -0.5946486139 -1.9055432685
C 0.0000000132 -0.9400714057 -0.5238789656
C -0.0000000003 0.2840996562 0.1978100964
O 0.0000000052 1.3492848598 -0.6824732683
C 0.0000000173 0.828446437 -1.9397076436
C -0.0000000154 -1.2877502506 -3.1369991438
C 0.0000000298 -2.141359157 0.2243761693
C 0.0000000015 0.3998336859 1.5803653441
C 0.0000000234 1.5626538301 -3.1092075812
C -0.0000000257 -0.5512490111 -4.3267473783
C -0.0000000023 0.844992111 -4.3296611468
C 0.0000000244 -0.8440678039 2.3267929102
C 0.0000000168 -2.0879191843 1.5974515226
H -0.0000000221 -2.3803974318 -3.1584408589
H 0.0000000293 -3.1079236675 -0.2889306229
C -0.000000008 1.6355026973 2.3086873663
H 0.0000000435 2.6540146588 -3.0786301845
H -0.0000000517 -1.0853985111 -5.2824801067

H	-0.0000000219	1.379176757	-5.232191133
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H	-0.0000000112	-3.0040674898	2.1665877184
C	0.0000000102	1.6331648888	3.6797492265
C	-0.0000000123	0.4251170083	4.3803686693
H	0.0000000048	2.5673049204	1.7269286432
H	-0.0000000045	-1.7327476025	4.2633638565
H	0.0000000045	2.5801585538	4.2225787919
H	-0.0000000235	0.4308750925	5.472414896

H	-0.0000000012	1.3903264688	-5.2769769175
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H	0.0000000058	-3.0154329732	2.1784809473
C	0.0000000053	1.6286772935	3.6942322237
C	-0.0000000136	0.4295988013	4.4218988567
H	-0.0000000197	2.5730647926	1.7492852979
H	-0.0000000141	-1.7386308209	4.2777729389
H	-0.0000000075	2.5837908416	4.2312280805
H	-0.000000033	0.4435988196	5.5148175289

cofacial

0 1

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C	-0.682597	-1.776549	0.594733
C	-1.232563	-1.276724	-0.576518
O	-0.312212	-1.161519	-1.564278
C	0.864901	-1.597488	-1.041102
C	1.818180	-2.477570	0.996180
C	-1.504457	-1.953636	1.729758
C	-2.593332	-0.949338	-0.724407
C	2.075269	-1.649345	-1.712469
C	3.039408	-2.542041	0.337092
C	3.166586	-2.132416	-0.997419
C	-3.408315	-1.141001	0.430863
C	-2.835783	-1.635841	1.638982
H	1.725150	-2.792041	2.037525
H	-1.081931	-2.335500	2.660801
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H	2.159386	-1.315986	-2.747067
H	3.921502	-2.905930	0.867213
H	4.144803	-2.174102	-1.479252
C	-4.781968	-0.823146	0.330566
H	-3.491385	-1.762982	2.503315
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H	-2.510129	-0.337831	-2.792247
H	-5.416512	-0.959232	1.209726
H	-4.939378	0.193283	-2.913867
H	-6.381205	-0.112656	-0.904221
C	2.984530	0.918810	0.638027
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C	0.903144	1.532361	0.054374
O	1.665743	1.683786	-1.057040
C	2.924476	1.314093	-0.708209
C	4.204684	0.496460	1.168783
C	0.995703	0.842333	2.371367
C	-0.474841	1.815572	0.108648
C	4.024079	1.310458	-1.551002
C	5.318759	0.481478	0.339155
C	5.229228	0.882448	-1.002453
C	-1.105933	1.585021	1.367335
C	-0.348165	1.096194	2.471504
H	4.277521	0.177297	2.210085
H	1.561431	0.469341	3.227098
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H	3.936370	1.625759	-2.591327
H	6.282245	0.152931	0.734251
H	6.123801	0.861417	-1.628635
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H	-0.872326	0.921423	3.413166

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0 1

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C	-1.103534	-1.053195	-1.230371
C	-0.371667	-1.659208	-0.219539
O	-1.160079	-2.068903	0.805097
C	-2.434832	-1.748213	0.458412
C	-3.709617	-0.723164	-1.317638
C	-0.432519	-0.538436	-2.361860
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C	-3.563553	-2.003163	1.218926
C	-4.855303	-0.974562	-0.571852
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H	-0.992155	-0.036800	-3.153157
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H	-5.829509	-0.673937	-0.962668
H	-5.701709	-1.786066	1.240806
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C	3.124008	-2.634937	0.619014
C	3.788095	-2.115513	-0.511579
H	1.232140	-2.882371	1.618887
H	3.600125	-1.067930	-2.375020
H	3.697275	-3.143357	1.397284
H	4.871841	-2.218094	-0.595452
C	-1.374339	1.552806	0.899768
C	-0.030147	1.173307	1.253970
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C	0.565868	0.511790	2.350053
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C	2.747657	0.811913	1.289616
C	1.926337	0.338446	2.353619
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H	4.610793	0.151086	2.160712
H	4.969104	2.136497	-1.644539
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0 1

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C	0.466973	1.553297	0.301143
O	1.410261	1.435400	1.265909
C	2.599524	1.303232	0.623135
C	3.551711	1.204634	-1.593565
C	0.167899	1.621360	-2.098453
C	-0.905680	1.736142	0.558928
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C	4.938282	1.053999	0.399149
C	-1.739997	1.864568	-0.590428
C	-1.176923	1.799220	-1.898581
H	3.449324	1.216876	-2.680537
H	0.583098	1.569744	-3.106407
C	-1.460491	1.799218	1.855048
H	3.921050	1.155998	2.323279
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H	-1.853078	1.892288	-2.751145
C	-2.812881	1.994005	2.012673
C	-3.649637	2.122656	0.884345
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H	-3.777613	2.139876	-1.256962
H	-3.244450	2.043991	3.014677
H	-4.723777	2.261768	1.021526
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C	-1.013227	-1.499641	-0.973269
C	-0.467000	-1.553513	0.301006
O	-1.410289	-1.435739	1.265773
C	-2.599534	-1.303355	0.623003
C	-3.551676	-1.204340	-1.593697
C	-0.167909	-1.621170	-2.098618
C	0.905654	-1.736383	0.558763
C	-3.833836	-1.171796	1.236671
C	-4.798932	-1.064945	-0.996453
C	-4.938249	-1.053731	0.399015
C	1.739970	-1.864576	-0.590617
C	1.176913	-1.799044	-1.898767
H	-3.449278	-1.216448	-2.680669
H	-0.583120	-1.569326	-3.106556
C	1.460475	-1.799618	1.854871
H	-3.921060	-1.156143	2.323147
H	-5.688636	-0.967072	-1.622050
H	-5.932536	-0.945464	0.837463
C	3.125450	-2.055120	-0.385597
H	1.853105	-1.891884	-2.751324
C	2.812887	-1.994281	2.012459
C	3.649648	-2.122674	0.884105
H	0.798393	-1.693177	2.715343

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0 1

C	-2.737077	-0.930731	-0.859949
C	-1.349896	-1.015002	-1.240062
C	-0.709965	-1.602887	-0.159042
O	-1.570696	-1.885855	0.850572
C	-2.794677	-1.473969	0.434227
C	-3.909567	-0.460280	-1.452910
C	-0.595999	-0.629687	-2.370615
C	0.669260	-1.877468	-0.120266
C	-3.965313	-1.559596	1.170596
C	-5.094547	-0.539197	-0.731668
C	-5.121316	-1.078244	0.562955
C	1.411866	-1.491737	-1.275362
C	0.755323	-0.864315	-2.373891
H	-3.892025	-0.030050	-2.455793
H	-1.083484	-0.145912	-3.218676
C	1.318801	-2.488251	0.973861
H	-3.968826	-1.985395	2.174652
H	-6.022320	-0.172664	-1.175806
H	-6.068591	-1.125012	1.104467
C	2.802457	-1.751766	-1.286901
H	1.362477	-0.567702	-3.231603
C	2.672369	-2.725021	0.922880
C	3.418472	-2.356218	-0.216764
H	0.726265	-2.764279	1.847370
H	3.384155	-1.454437	-2.161833
H	3.176187	-3.198617	1.768392
H	4.494290	-2.538614	-0.240680
C	2.737010	0.930535	0.860040
C	1.349803	1.014866	1.240051
C	0.709960	1.602725	0.158961
O	1.570779	1.885660	-0.850587
C	2.794708	1.473692	-0.434166
C	3.909504	0.460325	1.453192
C	0.595788	0.629492	2.370507
C	-0.669244	1.877425	0.120103
C	3.965452	1.559586	-1.170334
C	5.094564	0.539368	0.732092
C	5.121437	1.078398	-0.562536
C	-1.411947	1.491748	1.275154
C	-0.755535	0.864123	2.373652
H	3.891895	0.030089	2.456073
H	1.083193	0.145791	3.218656
C	-1.318695	2.488260	-0.974053
H	3.969028	1.985361	-2.174399
H	6.022321	0.172939	1.176352
H	6.068783	1.125305	-1.103912
C	-2.802490	1.752031	1.286702
H	-1.362743	0.567628	3.231369
C	-2.672230	2.725240	-0.923085
C	-3.418407	2.356555	0.216550
H	-0.726117	2.764214	-1.847557

H	3.777611	-2.139530	-1.257204	H	-3.384245	1.454713	2.161600
H	3.244470	-2.044353	3.014452	H	-3.175950	3.198966	-1.768582
H	4.723810	-2.261646	1.021247	H	-4.494175	2.539243	0.240509

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C	0.0000000065	-0.5993318447	-1.8447099726
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C	0.0000000158	0.313203316	0.3304457737
S	-0.0000000019	1.749058383	-0.6628800666
C	-0.0000000055	0.787083504	-2.1195315335
C	0.0000000111	-1.5017702616	-2.9175424488
C	0.0000000023	-2.1150011658	0.2443920839
C	0.0000000131	0.3025751623	1.7514034026
C	-0.0000000162	1.2728980701	-3.4283413065
C	-0.0000000019	-1.0224637502	-4.2197404411
C	-0.0000000035	0.3574224367	-4.473397126
C	0.000000008	-0.9720487013	2.3975696619
C	-0.0000000012	-2.1626552644	1.6134553857
H	0.0000000169	-2.577170333	-2.7258011602
H	-0.0000000027	-3.0375421446	-0.3401264897
C	0.0000000172	1.4777734076	2.5392161747
H	-0.000000025	2.3468627845	-3.6252598951
H	0.0000000048	-1.7247571642	-5.0560080191
H	-0.0000000091	0.7186262289	-5.5042079058
C	-0.0000000014	-1.0123983958	3.8127814703
H	-0.0000000087	-3.1248720476	2.1307932598
C	0.0000000093	1.4021969222	3.9140137512
C	-0.0000000158	0.146185736	4.5571795958
H	0.0000000221	2.4515332994	2.0424912827
H	-0.0000000143	-1.9868997469	4.3077738458
H	0.0000000066	2.3175977188	4.5098282158
H	-0.0000000286	0.0954834321	5.6482811668

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C	0.0000000018	-0.6156414761	-1.8553870678
C	0.0000000225	-0.8821694474	-0.4364431367
C	0.0000000031	0.3307860811	0.331833243
S	0.0000000103	1.7248777853	-0.6506612633
C	0.0000000036	0.7678179143	-2.1260929147
C	-0.000000017	-1.5153932813	-2.9274379039
C	0.0000000194	-2.1119912713	0.227319432
C	-0.000000002	0.3205573893	1.7588902174
C	0.000000003	1.2710666767	-3.4171395142
C	-0.0000000172	-1.0228054503	-4.2333175895
C	-0.0000000076	0.3504909729	-4.4751697415
C	-0.0000000022	-0.9549602054	2.3996060804
C	0.0000000156	-2.1435695346	1.6139948339
H	-0.0000000137	-2.5923848566	-2.7473828285
H	0.0000000197	-3.0435198615	-0.3410212377
C	-0.0000000059	1.4859865726	2.5440863376
H	0.0000000096	2.3449754722	-3.6128128682
H	-0.0000000059	-1.71998255	-5.0729627713
H	-0.0000000009	0.7207917681	-5.5023428286
C	-0.0000000186	-1.0128603726	3.8062658591
H	0.000000005	-3.1065153286	2.1303927921
C	-0.0000000102	1.4005892922	3.9330787514
C	-0.0000000082	0.1535185772	4.5646038475
H	0.0000000029	2.4678753385	2.0638418291
H	-0.0000000134	-1.9878373588	4.2989891636

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C	0.0000000013	-0.6161905968	-1.844008628
C	-0.0000000054	-0.8770890641	-0.4441109774
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S	-0.0000000057	1.7539204187	-0.6690763531
C	-0.0000000239	0.7828630802	-2.1353275987
C	0.0000000097	-1.5091054557	-2.9439011587
C	-0.0000000016	-2.1154300453	0.2409551531
C	0.0000000132	0.3113439208	1.7500070776
C	-0.0000000175	1.2654390439	-3.4354426605
C	0.0000000128	-1.0200462811	-4.2460899716
C	-0.0000000049	0.3551927741	-4.5084612466
C	0.0000000191	-0.9704232505	2.4203011979
C	-0.0000000056	-2.1625180031	1.6130667265
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C	0.0000000176	1.4902546565	2.5596929043
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H	0.0000000171	-1.7270860908	-5.081839001
H	0.0000000002	0.7231833145	-5.5374817601
C	-0.0000000027	-1.0109568186	3.8195252834
H	-0.0000000089	-3.128482915	2.127291239
C	0.0000000133	1.402718578	3.9462643431
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H	0.0000000175	2.467172326	2.0683838236
H	-0.0000000114	-1.9901090351	4.309848574

H	0.0000000034	2.314427894	4.530398407
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H	-0.0000000017	2.3239582319	4.5387603714
H	-0.0000000183	0.1063267902	5.6855690439

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C	0.611859	-1.997635	0.077343
C	-0.784504	-1.779681	0.366078
C	-1.457576	-1.195912	-0.704844
S	-0.417345	-0.896139	-2.068408
C	0.952387	-1.557653	-1.217180
C	1.608007	-2.555001	0.886624
C	-1.493805	-2.075697	1.554243
C	-2.841413	-0.890671	-0.650370
C	2.254070	-1.660474	-1.704992
C	2.902367	-2.664465	0.402798
C	3.224121	-2.220476	-0.886255
C	-3.533173	-1.198753	0.557006
C	-2.829471	-1.790391	1.643390
H	1.363023	-2.895602	1.894762
H	-0.967275	-2.528028	2.396716
C	-3.548913	-0.305041	-1.722931
H	2.504564	-1.302391	-2.704890
H	3.683779	-3.089421	1.035579
H	4.252088	-2.296905	-1.244584
C	-4.911189	-0.896456	0.642029
H	-3.381904	-2.014624	2.558644
C	-4.890958	-0.024997	-1.609800
C	-5.577996	-0.319319	-0.414508
H	-3.013801	-0.071689	-2.646318
H	-5.440826	-1.129729	1.569022
H	-5.426176	0.428282	-2.446875
H	-6.643307	-0.093006	-0.331519
C	2.974884	0.809283	0.785234
C	1.592989	0.989266	1.155338
C	0.849156	1.582404	0.138691
S	1.807500	1.935858	-1.273753
C	3.232809	1.280053	-0.517810
C	4.021789	0.243474	1.521138
C	0.955554	0.633102	2.368072
C	-0.537597	1.847875	0.273610
C	4.501335	1.187801	-1.089341
C	5.284647	0.148901	0.958253
C	5.522105	0.615932	-0.342176
C	-1.156574	1.479384	1.503247
C	-0.381499	0.872783	2.531331
H	3.837266	-0.130048	2.530287
H	1.536374	0.162913	3.163843
C	-1.317380	2.442252	-0.742389
H	4.686095	1.553535	-2.101219
H	6.102297	-0.294693	1.530079
H	6.522672	0.534852	-0.772539
C	-2.539023	1.722872	1.663624
H	-0.882877	0.593340	3.460095
C	-2.660903	2.669216	-0.551089
C	-3.278433	2.307887	0.662130
H	-0.841211	2.714651	-1.687132
H	-3.015235	1.426789	2.600954
H	-3.255564	3.123062	-1.346315
H	-4.348505	2.474052	0.797030

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C	-2.267952	-0.370520	-1.433754
C	-0.863317	-0.697209	-1.429130
C	-0.570381	-1.737701	-0.550464
S	-1.984741	-2.347085	0.264123
C	-3.000301	-1.192416	-0.553693
C	-2.943359	0.615315	-2.161424
C	0.179967	-0.102836	-2.178642
C	0.750659	-2.216004	-0.361498
C	-4.378080	-1.049434	-0.398067
C	-4.313507	0.762010	-2.008995
C	-5.027521	-0.068390	-1.134284
C	1.783842	-1.595585	-1.121841
C	1.466108	-0.543434	-2.025173
H	-2.388152	1.266181	-2.839871
H	-0.047530	0.713561	-2.865675
C	1.082551	-3.245940	0.546218
H	-4.931411	-1.691455	0.289568
H	-4.843182	1.529597	-2.577141
H	-6.106743	0.059160	-1.025964
C	3.113953	-2.036416	-0.940814
H	2.280556	-0.077395	-2.583035
C	2.388595	-3.650524	0.701400
C	3.414110	-3.040983	-0.049718
H	0.287662	-3.718037	1.129044
H	3.905081	-1.549156	-1.514881
H	2.632174	-4.447242	1.407632
H	4.448392	-3.367363	0.079455
C	-0.910203	0.895322	1.662370
C	0.514948	0.770380	1.469948
C	0.995717	1.659511	0.512560
S	-0.263322	2.651498	-0.172152
C	-1.465274	1.889923	0.833499
C	-1.752811	0.186275	2.526338
C	1.416055	-0.111540	2.114255
C	2.364235	1.707336	0.146665
C	-2.827223	2.184919	0.853257
C	-3.107577	0.476988	2.552346
C	-3.641167	1.468568	1.718474
C	3.250592	0.810979	0.811064
C	2.746013	-0.083737	1.795389
H	-1.340925	-0.592237	3.170743
H	1.040474	-0.818538	2.855888
C	2.872768	2.574858	-0.846196
H	-3.244411	2.950160	0.197490
H	-3.767909	-0.076596	3.222892
H	-4.712356	1.677456	1.741973
C	4.616688	0.818157	0.447132
H	3.442404	-0.772520	2.276827
C	4.206845	2.552952	-1.181677
C	5.088268	1.665278	-0.529479
H	2.189454	3.261117	-1.352547
H	5.293171	0.125669	0.953855
H	4.586590	3.225687	-1.953665
H	6.146214	1.654714	-0.800485

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C	1.335019	-1.764976	0.881030
C	-0.102350	-1.644727	0.904203
C	-0.646776	-1.590160	-0.377047
S	0.567468	-1.690944	-1.624100
C	1.834844	-1.799452	-0.435785
C	2.234380	-1.847604	1.949726
C	-0.959169	-1.582982	2.028122
C	-2.042158	-1.473501	-0.598929
C	3.199978	-1.903443	-0.697347
C	3.592245	-1.959083	1.695837
C	4.071222	-1.983004	0.378993
C	-2.885304	-1.424119	0.549362
C	-2.312056	-1.476744	1.850054
H	1.864077	-1.820782	2.976449
H	-0.532962	-1.621894	3.032452
C	-2.621647	-1.404362	-1.885374
H	3.573792	-1.910157	-1.722023
H	4.296569	-2.023732	2.527789
H	5.144794	-2.057027	0.194589
C	-4.282562	-1.328079	0.359296
H	-2.980163	-1.427438	2.712234
C	-3.986078	-1.306933	-2.035067
C	-4.825800	-1.276526	-0.903119
H	-1.970895	-1.429094	-2.762548
H	-4.926259	-1.290980	1.241131
H	-4.421625	-1.257958	-3.035539
H	-5.907793	-1.203087	-1.031806
C	-1.334979	1.766488	0.878707
C	0.102383	1.646227	0.902019
C	0.646751	1.589431	-0.379158
S	-0.567545	1.688110	-1.626326
C	-1.834868	1.798689	-0.438145
C	-2.234279	1.851014	1.947304
C	0.959242	1.586376	2.026006
C	2.042129	1.472423	-0.600892
C	-3.200014	1.902247	-0.699822
C	-3.592154	1.962079	1.693285
C	-4.071198	1.983704	0.376426
C	2.885323	1.425018	0.547447
C	2.312123	1.479831	1.848070
H	-1.863928	1.825977	2.974054
H	0.533054	1.626977	3.030278
C	2.621574	1.401160	-1.887242
H	-3.573883	1.907163	-1.724487
H	-4.296434	2.028200	2.525160
H	-5.144779	2.057421	0.191956
C	4.282581	1.328695	0.357490
H	2.980253	1.431966	2.710315
C	3.986002	1.303562	-2.036823
C	4.825770	1.275074	-0.904861
H	1.970796	1.424403	-2.764437
H	4.926315	1.293054	1.239362
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C	1.249754	-2.050216	0.470051
C	-0.180969	-1.901095	0.359662
C	-0.559448	-1.393013	-0.880790
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C	1.907990	-1.671160	-0.718082
C	2.014531	-2.490845	1.556308
C	-1.175598	-2.202324	1.321017
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C	3.294340	-1.742118	-0.841124
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C	4.029422	-2.192358	0.245900
C	-2.898713	-1.465618	-0.231243
C	-2.495735	-1.996173	1.026574
H	1.522217	-2.776434	2.488127
H	-0.879853	-2.597014	2.294828
C	-2.322624	-0.581274	-2.441207
H	3.789648	-1.432388	-1.762649
H	3.993289	-2.905601	2.285583
H	5.117544	-2.246481	0.171910
C	-4.258957	-1.240780	-0.539765
H	-3.268353	-2.225460	1.762943
C	-3.656539	-0.365888	-2.706787
C	-4.634607	-0.706413	-1.751224
H	-1.563647	-0.321992	-3.183485
H	-5.011279	-1.493568	0.210927
H	-3.958983	0.064934	-3.663829
H	-5.690882	-0.538360	-1.972073
C	-1.584956	1.687526	0.535858
C	-0.306731	1.832179	-0.116240
C	0.748810	1.441930	0.704752
S	0.215706	0.906709	2.274177
C	-1.448717	1.196283	1.849368
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C	-0.036967	2.303361	-1.423133
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C	-2.557994	0.980601	2.665574
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C	2.345210	1.970470	-1.046914
C	1.254984	2.368774	-1.870713
H	-2.988209	2.324970	-0.980431
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H	-2.438653	0.597374	3.680634
H	-4.969412	1.949987	0.460109
H	-4.699321	1.099010	2.777539
C	3.681448	2.025068	-1.505188
H	1.471767	2.726142	-2.879746
C	4.474861	1.178691	0.612175
C	4.726160	1.640529	-0.695207
H	2.990892	0.726869	2.091664
H	3.871293	2.385181	-2.519382
H	5.305689	0.863655	1.246579
H	5.752615	1.691952	-1.064844

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C 0.0000000018 -0.9086161237 -0.4624644723
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C -0.0000000002 -1.0094414337 3.7673729194
H -0.0000000005 -3.2679527211 2.0090837849
C -0.0000000025 0.2836053606 4.1917214428
H -0.0000000009 -1.8652393946 4.4433047237
H -0.0000000045 0.6457218267 5.2191848224
S 0.0000000019 1.4294678203 2.8921105959

1 2

C -0.000000001 -0.5968206462 -1.8744705956
C 0.0000000275 -0.9193146736 -0.4736177634
C 0.0000000052 0.2835344165 0.3358030567
S 0.0000000532 1.7183311383 -0.5958935919
C 0.0000000138 0.7966877216 -2.1003369206
C -0.0000000155 -1.4638527265 -2.9785357203
C 0.0000000341 -2.178275619 0.1411147504
C 0.0000000255 0.1681050765 1.727786563
C 0.0000000043 1.3364576128 -3.3733056462
C -0.0000000332 -0.9328179277 -4.2670565247
C -0.0000000198 0.4480819089 -4.4623752941
C 0.0000000295 -1.1084633176 2.3338550782
C 0.0000000316 -2.2775767389 1.5226832087
H -0.0000000195 -2.5457434724 -2.8308359289
H 0.000000023 -3.0821093515 -0.4697571286
H 0.0000000035 2.4155648855 -3.5378967584
H -0.0000000333 -1.6026935968 -5.1284890084
H -0.0000000343 0.8531579532 -5.4764848684
C -0.0000000025 -1.0146682696 3.7494432636
H 0.0000000269 -3.2590868384 2.0015672488
C -0.0000000655 0.2948020541 4.1845737946
H -0.0000000329 -1.8704314708 4.4254813024
H -0.0000001358 0.6468684435 5.2169019181
S 0.0000001151 1.4318734383 2.912485565

-1 2

C -0.0000000043 -0.6008827286 -1.8665850805
C 0.0000000025 -0.9106633144 -0.4828185927
C 0.0000000022 0.2587756153 0.3480099412
S 0.000000019 1.7309888807 -0.6164618779
C 0.0000000109 0.8079241036 -2.1196945764
C -0.0000000088 -1.4592151157 -3.0018615193
C 0.0000000064 -2.1826139117 0.1660750458
C 0.0000000068 0.1565976004 1.7219857844
C 0.0000000178 1.3362966759 -3.3975771926
C -0.0000000187 -0.923284937 -4.2844700928
C -0.0000000064 0.4600999611 -4.5055486162
C 0.0000000146 -1.1278024166 2.3657192871
C 0.0000000196 -2.2877240525 1.536700008
H -0.0000000201 -2.5429775175 -2.8586056959
H 0.0000000077 -3.0882516857 -0.4473462253
H 0.0000000287 2.4197536472 -3.5458772609
H -0.0000000297 -1.6024860403 -5.1436228454
H -0.0000000098 0.8613633792 -5.5218239425
C 0.0000000124 -1.0084827269 3.7764021046
H 0.0000000242 -3.275236011 2.0087122877
C -0.000000029 0.2918020202 4.2329009379
H 0.0000000109 -1.8713482534 4.4473318067
H -0.0000000595 0.6490463391 5.2608800363
S 0.0000000025 1.4499304885 2.9102162786

cofacial

0 1

C	0.620626	-2.011870	0.041297
C	-0.761809	-1.803369	0.404679
C	-1.482334	-1.198645	-0.636920
S	-0.507800	-0.868627	-2.039675
C	0.898892	-1.551026	-1.260442
C	1.654016	-2.581809	0.792267
C	-1.406608	-2.119238	1.615783
C	-2.841878	-0.925963	-0.469795

antifacial_y

0 1

C	-0.983707	0.894977	1.681436
C	0.446226	0.770585	1.512116
C	0.927093	1.663041	0.542996
S	-0.325002	2.645559	-0.163122
C	-1.532854	1.880692	0.838987
C	-1.834417	0.188873	2.539178
C	1.336327	-0.102850	2.167246
C	2.286154	1.676811	0.227513

C	2.175892	-1.641569	-1.809705
C	2.925706	-2.678179	0.248115
C	3.185683	-2.209718	-1.045312
C	-3.482366	-1.240964	0.746879
C	-2.745115	-1.841210	1.789323
H	1.456099	-2.940828	1.804372
H	-0.833250	-2.581873	2.420980
H	2.379162	-1.265981	-2.813923
H	3.736565	-3.113160	0.835191
H	4.196237	-2.274894	-1.452073
C	-4.866303	-0.872970	0.717513
H	-3.244809	-2.083618	2.729339
C	-5.236773	-0.318156	-0.467947
H	-5.550539	-1.026531	1.552449
H	-6.225561	0.037709	-0.754647
S	-3.937171	-0.212443	-1.604544
C	2.944025	0.759472	0.828420
C	1.564310	0.953747	1.208385
C	0.829008	1.562690	0.180591
S	1.786607	1.906525	-1.233124
C	3.204882	1.229808	-0.473739
C	3.986603	0.182072	1.560509
C	0.930883	0.609612	2.418504
C	-0.530052	1.825326	0.363627
C	4.470518	1.125364	-1.047636
C	5.247974	0.074671	0.995316
C	5.487587	0.541182	-0.303988
C	-1.160425	1.479777	1.576859
C	-0.410403	0.867225	2.601934
H	3.799838	-0.188612	2.570317
H	1.511985	0.131799	3.209335
H	4.657325	1.491254	-2.059102
H	6.061756	-0.378315	1.565269
H	6.486050	0.450460	-0.737243
C	-2.550279	1.827516	1.558050
H	-0.904743	0.596001	3.536280
C	-2.930806	2.407032	0.389569
H	-3.232672	1.636305	2.385762
H	-3.924987	2.753474	0.113007
S	-1.635210	2.552792	-0.750041

C	-2.895307	2.171973	0.841268
C	-3.190904	0.473396	2.546581
C	-3.717478	1.458667	1.701439
C	3.172417	0.800058	0.884773
C	2.679941	-0.087956	1.862955
H	-1.426968	-0.584517	3.192389
H	0.950540	-0.805295	2.907627
H	-3.306041	2.934828	0.178513
H	-3.856838	-0.077900	3.213456
H	-4.789174	1.666258	1.713335
C	4.508786	0.941958	0.387047
H	3.368041	-0.774317	2.358746
C	4.609405	1.878651	-0.593427
H	5.353180	0.357538	0.753231
H	5.505005	2.185234	-1.132244
S	3.097800	2.644083	-0.958366
C	-2.136086	-0.380436	-1.468486
C	-0.724751	-0.686919	-1.454330
C	-0.436143	-1.729611	-0.561232
S	-1.846532	-2.346173	0.251170
C	-2.865833	-1.204122	-0.588394
C	-2.820049	0.584400	-2.215337
C	0.312035	-0.090976	-2.199743
C	0.881623	-2.163374	-0.406057
C	-4.247286	-1.085310	-0.452225
C	-4.194865	0.708283	-2.081729
C	-4.905789	-0.126102	-1.209605
C	1.915255	-1.563533	-1.152964
C	1.612545	-0.520010	-2.052465
H	-2.267941	1.238343	-2.893224
H	0.078494	0.724813	-2.885305
H	-4.797444	-1.730950	0.234516
H	-4.729697	1.462025	-2.663365
H	-5.988672	-0.018592	-1.118110
C	3.186503	-2.146814	-0.844034
H	2.419566	-0.045493	-2.612963
C	3.100045	-3.131206	0.089845
H	4.121937	-1.827476	-1.303445
H	3.910063	-3.735157	0.496634
S	1.481397	-3.406483	0.639075

antifacial_z

0 1

C	2.306734	1.385549	-0.730229
C	0.884603	1.540253	-0.929971
C	0.201058	1.632003	0.292654
S	1.251448	1.512207	1.673707
C	2.647901	1.360401	0.636605
C	3.326131	1.279941	-1.682371
C	0.168562	1.615444	-2.140106
C	-1.184169	1.806278	0.303330
C	3.970205	1.233106	1.057458
C	4.644548	1.159021	-1.269514
C	4.965293	1.137338	0.093776
C	-1.895837	1.875571	-0.911775
C	-1.199969	1.776140	-2.134324
H	3.079182	1.297516	-2.745893
H	0.707857	1.539264	-3.085820
H	4.216547	1.212672	2.120603
H	5.440600	1.083104	-2.013191

antifacial_yz

0 1

C	2.402166	1.710942	-0.334699
C	0.981144	1.969777	-0.346436
C	0.360772	1.470833	0.810065
S	1.472426	0.719992	1.915797
C	2.805630	1.035605	0.835181
C	3.362763	2.012320	-1.306213
C	0.210579	2.612752	-1.334902
C	-1.019827	1.600754	0.967081
C	4.132056	0.665584	1.044917
C	4.683440	1.640464	-1.105741
C	5.066436	0.971280	0.064525
C	-1.788537	2.233362	-0.031215
C	-1.152721	2.744314	-1.182167
H	3.067258	2.529179	-2.221529
H	0.701574	2.997877	-2.230495
H	4.424914	0.135154	1.952433
H	5.432815	1.871663	-1.865563

H	6.007886	1.042426	0.404725	H	6.111021	0.686971	0.209279
C	-3.298570	2.051546	-0.684396	C	-3.178997	2.245024	0.313214
H	-1.755605	1.830059	-3.072506	H	-1.751810	3.235317	-1.951483
C	-3.609377	2.124631	0.636417	C	-3.426680	1.658848	1.513493
H	-4.038413	2.109569	-1.482085	H	-3.956337	2.666241	-0.323612
H	-4.596757	2.245063	1.079290	H	-4.391882	1.523724	1.998503
S	-2.231372	1.979681	1.671647	S	-1.999079	1.060371	2.287714
C	-2.306736	-1.385826	-0.729614	C	-2.564841	-1.376337	-0.176838
C	-0.884610	-1.540661	-0.929308	C	-1.255451	-1.806472	0.257206
C	-0.201033	-1.631661	0.293356	C	-0.272426	-1.499089	-0.696148
S	-1.251383	-1.511053	1.674366	S	-0.909682	-0.687970	-2.096932
C	-2.647870	-1.359904	0.637215	C	-2.523302	-0.747378	-1.437213
C	-3.326167	-1.280806	-1.681789	C	-3.799726	-1.515450	0.466289
C	-0.168601	-1.616670	-2.139414	C	-0.894594	-2.463965	1.450387
C	1.184180	-1.806065	0.304106	C	1.058037	-1.853909	-0.461593
C	-3.970177	-1.232491	1.058030	C	-3.676445	-0.259190	-2.049743
C	-4.644581	-1.159738	-1.268966	C	-4.951442	-1.038800	-0.141229
C	-4.965300	-1.137353	0.094319	C	-4.889729	-0.410912	-1.392006
C	1.895807	-1.876255	-0.910972	C	1.411425	-2.521701	0.729593
C	1.199910	-1.777551	-2.133567	C	0.415787	-2.820978	1.683265
H	-3.079244	-1.298943	-2.745307	H	-3.850757	-2.000769	1.443030
H	-0.707919	-1.541112	-3.085166	H	-1.664138	-2.690638	2.190448
H	-4.216492	-1.211504	2.121170	H	-3.625424	0.226751	-3.025924
H	-5.440654	-1.084273	-2.012667	H	-5.915280	-1.152353	0.359370
H	-6.007896	-1.042384	0.405238	H	-5.804658	-0.038983	-1.858275
C	3.298519	-2.052309	-0.683516	C	2.817898	-2.787476	0.777706
H	1.755501	-1.832213	-3.071732	H	0.694664	-3.329338	2.608183
C	3.609355	-2.124541	0.637338	C	3.474133	-2.340553	-0.327110
H	4.038320	-2.111056	-1.481192	H	3.309768	-3.292116	1.609599
H	4.596721	-2.244897	1.080259	H	4.539983	-2.403324	-0.540251
S	2.231401	-1.978688	1.672509	S	2.433397	-1.576346	-1.474812

12f

0 1

C 0.0000000065 -0.583114528 -1.6003683931
C 0.0000000051 -0.8220688663 -0.170780528
C 0.0000000036 0.3944648578 0.5424474088
S 0.0000000061 1.8060213108 -0.476824178
C -0.0000000024 0.7964214094 -1.9071395474
C 0.0000000038 -1.5084216765 -2.6529263207
C 0.0000000018 -2.0546991509 0.5185398671
C 0.0000000036 0.3336071705 1.9319787314
C -0.0000000041 1.2516193217 -3.2264096359
C 0.000000001 -1.0596279223 -3.9664184846
C -0.0000000022 0.3132544079 -4.2515905166
C -0.0000000043 -0.8885151584 2.6219932468
C -0.0000000061 -2.0996302586 1.9010178523
H 0.0000000079 -2.5791061396 -2.4365897002
H -0.0000000011 -2.9839687211 -0.054925748
H -0.0000000058 2.3209246807 -3.4476028073
H 0.0000000022 -1.7815641041 -4.7857840335
H -0.0000000059 0.6517898405 -5.2900274391
C -0.0000000012 -0.5223608198 4.0146086604
H -0.0000000094 -3.0565706707 2.4259994476
C 0.0000000057 0.8357596425 4.0440050794
H -0.0000000021 -1.186252399 4.8757720319
H 0.0000000071 1.5528796589 4.8608979435
O -0.0000000098 1.3713481147 2.7950070631

1 2 -1 2

C	0.0000002158	-0.5783332295	-1.5833057009
C	0.0000003254	-0.8151569001	-0.181834222
C	-0.000000189	0.4371914425	0.5456491883
S	0.00000008	1.8335282802	-0.4613578253
C	-0.000000251	0.8094906447	-1.8937829318
C	0.0000003241	-1.5220769483	-2.6367699411
C	0.0000005642	-2.061865852	0.5057839104
C	-0.0000002725	0.3579932779	1.9199099086
C	-0.0000004521	1.2565170806	-3.2013306284
C	0.0000000785	-1.0775096981	-3.9477487081
C	-0.0000002908	0.2969633691	-4.2269966648
C	-0.0000000075	-0.8748394992	2.6065327208
C	0.0000004057	-2.1057058951	1.8755698663
H	0.0000005417	-2.591078037	-2.4153021748
H	0.0000005845	-2.9872761794	-0.0716589925
H	-0.0000006235	2.3215789581	-3.4404078241
H	0.0000002072	-1.7961722662	-4.7686672857
H	-0.0000003989	0.6349358373	-5.2657989826
C	-0.0000014229	-0.5397661539	3.9775707707
H	0.0000001274	-3.0583566264	2.4076265968
C	0.0000013199	0.8439040295	4.0235629121
H	-0.0000025478	-1.2094725944	4.835183095
H	0.0000018196	1.5419594927	4.8595471529
O	-0.0000001381	1.3857374671	2.8029057602

C	0.0000000083	-0.5934278902	-1.5889383135
C	0.0000000086	-0.8208226166	-0.1903878205
C	0.0000000087	0.4053454225	0.5672681547
S	0.0000000104	1.8165172218	-0.4812789466
C	-0.0000000028	0.7986773829	-1.9266452522
C	-0.0000000012	-1.5191251249	-2.6748424873
C	0.0000000018	-2.0555013497	0.5268151458
C	0.0000000075	0.3453729486	1.9411216968
C	-0.0000000036	1.2512259441	-3.23252426
C	-0.0000000061	-1.0577862232	-3.9865997804
C	-0.0000000051	0.3089709329	-4.2907022029
C	0.000000003	-0.8880550865	2.649216275
C	0.0000000002	-2.0995935164	1.9042819861
H	-0.0000000036	-2.5928190691	-2.4692064372
H	0.000000009	-2.9898231116	-0.0422071223
H	0.0000000017	2.3242685101	-3.4439058993
H	-0.0000000089	-1.7870464193	-4.8042489668
H	-0.0000000004	0.6495002643	-5.3289611894
C	-0.0000000008	-0.5252283926	4.0269674769
H	0.0000000009	-3.0623238974	2.4238543816
C	-0.0000000014	0.8445384053	4.0826135415
H	-0.0000000131	-1.1977989068	4.8841046402
H	-0.0000000072	1.5573528596	4.9021572517
O	-0.0000000061	1.3897717123	2.8169281281

cofacial

0 1

C	0.332404	-1.962279	0.067223
C	-1.058282	-1.706355	0.366795
C	-1.701241	-1.090650	-0.721582
S	-0.665753	-0.826143	-2.089653
C	0.681097	-1.533995	-1.229221
C	1.316558	-2.541804	0.874972
C	-1.767523	-1.985132	1.552363
C	-3.043277	-0.764859	-0.580548
C	1.978846	-1.669244	-1.718042
C	2.608713	-2.679408	0.391781
C	2.938597	-2.245680	-0.897918
C	-3.753727	-1.036332	0.594521
C	-3.104442	-1.659935	1.676630
H	1.064852	-2.874388	1.884092
H	-1.243338	-2.461806	2.382621
H	2.236697	-1.317477	-2.718328
H	3.381325	-3.119933	1.024590
H	3.964430	-2.343986	-1.257011
C	-5.077413	-0.537523	0.344200
H	-3.647551	-1.877922	2.597811
C	-5.050036	-0.024036	-0.912076
H	-5.934503	-0.560513	1.012570
H	-5.810892	0.450322	-1.526253
O	-3.829987	-0.155838	-1.489557
C	2.681838	0.807825	0.837389
C	1.288413	1.057206	1.129374
C	0.639048	1.634181	0.024439
S	1.680720	1.892060	-1.342873
C	3.030185	1.211301	-0.467240
C	3.663193	0.233666	1.651909
C	0.579053	0.790300	2.317971
C	-0.714064	1.921466	0.144926
C	4.322559	1.044975	-0.961502

antifacial_y

0 1

C	1.074201	-1.365677	1.319343
C	-0.364939	-1.275551	1.215981
C	-0.808269	-1.741951	-0.033426
S	0.473848	-2.281978	-1.074641
C	1.657917	-1.888683	0.149010
C	1.903482	-1.005346	2.386848
C	-1.284524	-0.789959	2.167507
C	-2.170487	-1.702297	-0.292922
C	3.036626	-2.054115	0.030837
C	3.275256	-1.171277	2.276520
C	3.837769	-1.691756	1.103835
C	-3.090805	-1.228808	0.649215
C	-2.639435	-0.765749	1.898346
H	1.467256	-0.592298	3.298055
H	-0.911853	-0.419335	3.123852
H	3.475871	-2.446924	-0.887159
H	3.924283	-0.890101	3.108423
H	4.920984	-1.804496	1.026085
C	-4.365411	-1.326730	-0.005198
H	-3.347033	-0.381371	2.634286
C	-4.112757	-1.830309	-1.239942
H	-5.338630	-1.053085	0.393846
H	-4.760011	-2.079557	-2.076629
O	-2.790550	-2.068557	-1.432069
C	1.737041	1.115678	-1.256767
C	0.298884	1.250659	-1.205425
C	-0.109520	1.801891	0.021060
S	1.203516	2.163809	1.099241
C	2.355110	1.572710	-0.075322
C	2.536621	0.608966	-2.286451
C	-0.651784	0.905580	-2.188034
C	-1.469569	1.988171	0.227642
C	3.738719	1.538968	0.084463

C	4.950628	0.065294	1.165735
C	5.277824	0.466187	-0.136208
C	-1.423670	1.665505	1.324191
C	-0.765041	1.089751	2.425923
H	3.408933	-0.085964	2.664376
H	1.106314	0.335113	3.158390
H	4.576880	1.359040	-1.975725
H	5.716265	-0.384951	1.800874
H	6.295715	0.327156	-0.506918
C	-2.764886	2.096913	1.044723
H	-1.312264	0.875195	3.344821
C	-2.749670	2.554574	-0.232022
H	-3.627676	2.054711	1.703334
H	-3.524836	2.966437	-0.871638
O	-1.518002	2.454940	-0.794120

C	3.914606	0.573239	-2.131769
C	4.512463	1.039634	-0.954365
C	-2.418095	1.657964	-0.747112
C	-2.001132	1.105730	-1.972919
H	2.072278	0.243569	-3.204428
H	-0.308208	0.467554	-3.126410
H	4.201783	1.891423	1.007573
H	4.540131	0.180496	-2.936162
H	5.598594	1.003957	-0.846514
C	-3.681469	2.000760	-0.157687
H	-2.733519	0.831478	-2.733486
C	-3.396531	2.483798	1.077982
H	-4.668819	1.890185	-0.597470
H	-4.024893	2.863569	1.879130
O	-2.063182	2.487607	1.329058

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C	1.450943	-1.652183	0.814158
C	0.005742	-1.641867	0.823210
C	-0.504996	-1.623773	-0.486348
S	0.722871	-1.628487	-1.716671
C	1.971606	-1.647302	-0.496479
C	2.339303	-1.674377	1.893404
C	-0.864964	-1.658450	1.931656
C	-1.884841	-1.621818	-0.643632
C	3.343827	-1.662815	-0.736644
C	3.706393	-1.692707	1.660007
C	4.205151	-1.686722	0.351709
C	-2.755521	-1.657769	0.452078
C	-2.235126	-1.670341	1.758970
H	1.953365	-1.673911	2.914616
H	-0.441512	-1.665068	2.937682
H	3.731577	-1.652430	-1.756720
H	4.400244	-1.711468	2.502979
H	5.283900	-1.695964	0.182328
C	-4.069961	-1.677769	-0.125619
H	-2.905211	-1.683535	2.619782
C	-3.886467	-1.645972	-1.468932
H	-5.022977	-1.699327	0.396000
H	-4.580669	-1.640816	-2.304851
O	-2.570386	-1.607163	-1.802487
C	-1.450949	1.651691	0.814661
C	-0.005746	1.641194	0.823711
C	0.504998	1.623650	-0.485852
S	-0.722875	1.629085	-1.716174
C	-1.971615	1.647580	-0.495978
C	-2.339302	1.673565	1.893920
C	0.864959	1.657299	1.932166
C	1.884849	1.621856	-0.643132
C	-3.343838	1.663602	-0.736130
C	-3.706388	1.692385	1.660537
C	-4.205153	1.687216	0.352237
C	2.755524	1.657435	0.452594
C	2.235121	1.669357	1.759488
H	-1.953361	1.672501	2.915129
H	0.441509	1.663470	2.938195
H	-3.731597	1.653870	-1.756209
H	-4.400232	1.710922	2.503520
H	-5.283901	1.696896	0.182866

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C	0.621165	-1.764750	0.667173
C	-0.776210	-1.466942	0.886349
C	-1.474727	-1.407682	-0.331496
S	-0.483842	-1.722234	-1.723274
C	0.918801	-1.932054	-0.700146
C	1.652018	-1.885892	1.604284
C	-1.445351	-1.247169	2.107468
C	-2.831927	-1.119489	-0.287359
C	2.209230	-2.223468	-1.135048
C	2.938878	-2.175139	1.175867
C	3.215289	-2.345882	-0.185478
C	-3.505291	-0.909065	0.921340
C	-2.798945	-0.973961	2.137126
H	1.441126	-1.745049	2.665922
H	-0.877179	-1.294136	3.037902
H	2.426207	-2.341899	-2.197822
H	3.745637	-2.264574	1.905722
H	4.234969	-2.564562	-0.507486
C	-4.863630	-0.642140	0.540706
H	-3.312514	-0.807387	3.085543
C	-4.890267	-0.710811	-0.814819
H	-5.706428	-0.426222	1.192354
H	-5.690195	-0.583245	-1.539247
O	-3.672685	-1.002896	-1.334068
C	-0.621181	1.764862	-0.667065
C	0.776171	1.467047	-0.886345
C	1.474801	1.407910	0.331441
S	0.484076	1.722722	1.723275
C	-0.918684	1.932311	0.700265
C	-1.652138	1.885784	-1.604089
C	1.445173	1.247069	-2.107503
C	2.831958	1.119540	0.287216
C	-2.209091	2.223663	1.135271
C	-2.939000	2.174837	-1.175555
C	-3.215278	2.345753	0.185796
C	3.505171	0.908848	-0.921519
C	2.798728	0.973694	-2.137251
H	-1.441351	1.744794	-2.665727
H	0.876901	1.293920	-3.037881
H	-2.425960	2.342237	2.198051
H	-3.745886	2.263920	-1.905310
H	-4.234957	2.564316	0.507883

C	4.069962	1.677972	-0.125091	C	4.863486	0.641685	-0.540974
H	2.905204	1.682224	2.620307	H	3.312181	0.806870	-3.085686
C	3.886478	1.646749	-1.468418	C	4.890264	0.710536	0.814537
H	5.022971	1.699545	0.396542	H	5.706157	0.425415	-1.192669
H	4.580682	1.642139	-2.304340	H	5.690209	0.582815	1.538917
O	2.570402	1.607824	-1.801992	O	3.672793	1.002946	1.333861

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C	0.0000000103	0.5913851963	1.9368011918
C	-0.0000000034	0.7880219964	0.5009972369
C	0.000000004	-0.4360160409	-0.1894959336
S	0.0000000148	-1.8180465758	0.8744811355
C	-0.0000000064	-0.7789211847	2.2809807262
C	0.0000000218	1.545030477	2.9635810918
C	-0.0000000158	2.0004840933	-0.2208087226
C	-0.0000000037	-0.475055583	-1.5963444979
C	-0.0000000125	-1.1989849375	3.6119309459
C	0.0000000124	1.1317876091	4.2887481056
C	0.0000000021	-0.2329617269	4.6110208075
C	-0.0000000147	0.7637540827	-2.2776311131
C	-0.0000000296	1.996362649	-1.6024092866
H	0.0000000261	2.6096076674	2.7187594914
H	-0.0000000136	2.9497050447	0.3189000763
H	-0.0000000171	-2.2618675855	3.861906312
H	0.0000000207	1.8755023711	5.0884123101
H	0.0000000003	-0.5429424236	5.6583649314
S	0.0000000207	0.5237144842	-3.9974724787
H	-0.0000000318	2.933754499	-2.1613385932
C	0.0000000115	-1.1957674524	-3.8029293849
H	0.000000029	-1.8337346799	-4.6860224027
C	-0.0000000103	-1.5884682309	-2.4991825177
H	-0.0000000148	-2.6317237491	-2.1813994312

1 2			
C	0.0000000285	0.6116509472	1.9495237632
C	0.0000000189	0.8090918996	0.5102312541
C	0.0000000313	-0.4453556138	-0.1860377623
S	0.0000000556	-1.7839792628	0.8673592839
C	0.0000000126	-0.7557869142	2.2894019216
C	0.0000000023	1.5565143187	2.9757390758
C	-0.000000006	1.9954442707	-0.2124499446
C	0.0000000173	-0.4935685485	-1.6042665511
C	-0.0000000005	-1.1999071328	3.6058212604
C	-0.000000014	1.1251799947	4.3064389029
C	-0.0000000144	-0.2332440262	4.6181439267
C	-0.0000000102	0.747911417	-2.2857744309
C	-0.0000000152	1.9724828963	-1.6169837795
H	-0.0000000107	2.6245167652	2.7481143458
H	-0.0000000081	2.9558294825	0.3058635621
H	0.0000000187	-2.2640690893	3.8492937815
H	-0.0000000158	1.8641754144	5.1097486927
H	-0.0000000232	-0.5527212782	5.6620076581
S	0.0000000644	0.5113415356	-4.004439484
H	-0.0000000068	2.9114103296	-2.17489306
C	-0.0000000444	-1.1828501163	-3.8158487291
H	-0.0000000793	-1.8236526244	-4.6985506843
C	0.0000000092	-1.593129452	-2.4978591091
H	-0.0000000102	-2.6426652131	-2.2007338935

-1 2			
C	0.0000000244	0.5921686716	1.9240396199
C	0.0000000196	0.7939434018	0.5153936259
C	0.0000000149	-0.4263467014	-0.2021184676
S	0.0000000272	-1.8158588621	0.8705422169
C	0.0000000008	-0.7866330514	2.2946078345
C	0.0000000249	1.5488595301	2.9807606819
C	-0.0000000005	2.0268887421	-0.2246333216
C	0.0000000007	-0.4734678732	-1.5993872359
C	-0.0000000251	-1.2102255328	3.6119664753
C	0.0000000067	1.1214937785	4.3022265013
C	-0.0000000028	-0.2403137934	4.6399642307
C	-0.0000000146	0.7874483983	-2.2997713558
C	-0.0000000178	2.0011770821	-1.6203704702
H	0.0000000269	2.6155431338	2.7433511177
H	-0.0000000063	2.9789756072	0.3092459375
H	-0.0000000319	-2.2772175575	3.8508616705
H	-0.0000000055	1.8690078046	5.1028347026
H	-0.0000000019	-0.5522661453	5.6871771306
S	-0.0000000338	0.5204615463	-4.0455643281
H	-0.0000000318	2.9411629517	-2.1805805897
C	0.0000000069	-1.2190214966	-3.8138518576
H	0.0000000119	-1.8753601554	-4.6833320511
C	-0.0000000066	-1.582485393	-2.4975941137
H	0.0000000136	-2.623314086	-2.1659179537

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S	-0.56204	-0.86816	-2.00685
C	-1.52311	-1.20827	-0.59709
C	-0.78804	-1.81114	0.43210
C	0.59389	-2.00737	0.05830
C	0.85842	-1.54023	-1.24389
C	-2.89265	-0.93585	-0.44297
C	-3.48880	-1.29656	0.78272
C	-2.76591	-1.89291	1.82725
C	-1.42096	-2.14353	1.64490
C	-3.82711	-0.33010	-1.34096
C	-5.07424	-0.23993	-0.80574
S	-5.17059	-0.87848	0.79872
C	1.63600	-2.57561	0.79792
C	2.90273	-2.66700	0.24158
C	3.14946	-2.19324	-1.05246
C	2.13101	-1.62470	-1.80490
H	-0.83894	-2.60045	2.44715
H	-3.25892	-2.14975	2.76614
H	-5.96760	0.17181	-1.27352
H	-3.56906	0.02051	-2.34029
H	2.32438	-1.24515	-2.80961
H	4.15603	-2.25536	-1.46938
H	3.72006	-3.10125	0.82020
H	1.44883	-2.93768	1.81104
C	2.92155	0.76777	0.81161
C	1.55143	0.94929	1.23224
C	0.77876	1.55344	0.23241
S	1.69144	1.91030	-1.20716
C	3.13903	1.24669	-0.49545
C	3.99114	0.19828	1.50984
C	0.95913	0.59801	2.46119
C	-0.58579	1.81972	0.43375
C	4.38859	1.15827	-1.10658
C	5.23657	0.10700	0.90760
C	5.43314	0.58208	-0.39583
C	-1.13624	1.46135	1.68129
C	-0.37746	0.85136	2.69202
H	3.83838	-0.17980	2.52261
H	1.56503	0.12046	3.23338
H	4.54167	1.53099	-2.12123
H	6.07143	-0.33966	1.45146
H	6.41959	0.50463	-0.85824
S	-2.81936	1.86917	1.75159
H	-0.83989	0.57776	3.64138
C	-2.78162	2.49574	0.14349
H	-3.69533	2.89380	-0.29450
C	-1.55353	2.41071	-0.43639
H	-1.33555	2.74658	-1.45014

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C	1.239738	-1.806982	0.758057
C	-0.188909	-1.620635	0.852344
C	-0.795308	-1.599041	-0.410956
S	0.344033	-1.822232	-1.709207
C	1.668268	-1.924167	-0.577438
C	2.189226	-1.876172	1.784114
C	-0.972911	-1.472036	2.012526
C	-2.184697	-1.433591	-0.541148
C	3.014830	-2.092784	-0.899744
C	3.526515	-2.052270	1.469727
C	3.937259	-2.154262	0.133514
C	-2.935132	-1.313783	0.646987
C	-2.341249	-1.324194	1.917867
H	1.872396	-1.786318	2.824789
H	-0.490559	-1.480774	2.991542
H	3.336613	-2.162385	-1.939953
H	4.269908	-2.104048	2.267740
H	4.996897	-2.274157	-0.099573
S	-4.627609	-1.169242	0.298196
H	-2.952739	-1.211940	2.814341
C	-4.328508	-1.235351	-1.401660
H	-5.164816	-1.168626	-2.096191
C	-3.009911	-1.374790	-1.708102
H	-2.627002	-1.436894	-2.726849
C	2.400299	1.348178	-0.747953
C	0.968542	1.509682	-0.850228
C	0.368088	1.635693	0.408883
S	1.515262	1.556033	1.715789
C	2.836148	1.355626	0.592000
C	3.347375	1.206732	-1.767540
C	0.177278	1.561125	-2.015282
C	-1.019091	1.827728	0.533077
C	4.184063	1.226716	0.920136
C	4.690844	1.083779	-1.446087
C	5.106741	1.094784	-0.108901
C	-1.769584	1.883448	-0.658711
C	-1.185901	1.745367	-1.928219
H	3.025282	1.197299	-2.810949
H	0.651320	1.450412	-2.991837
H	4.506923	1.228868	1.962686
H	5.431588	0.978094	-2.241423
H	6.167640	0.994938	0.130133
S	-3.445857	2.147432	-0.322204
H	-1.803764	1.781618	-2.826613
C	-3.147363	2.182972	1.378885
H	-3.979413	2.333199	2.065228
C	-1.836544	1.999531	1.694063
H	-1.454202	1.981040	2.714499

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C	2.314085	1.426122	-0.660049
C	0.881387	1.548892	-0.803432
C	0.239607	1.607902	0.440573
S	1.343946	1.489288	1.779563
C	2.705667	1.385718	0.692926
C	3.300411	1.367827	-1.650339
C	0.121766	1.628310	-1.986607

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C	2.427089	1.709678	-0.420058
C	1.001105	1.915765	-0.311720
C	0.496972	1.409768	0.894230
S	1.731368	0.732118	1.915212
C	2.956222	1.080935	0.725050
C	3.287814	2.021861	-1.478316
C	0.130383	2.528834	-1.234340

C	-1.152843	1.764486	0.533514	C	-0.874847	1.471472	1.187380
C	4.046085	1.292240	1.063289	C	4.311395	0.773815	0.830046
C	4.635795	1.278207	-1.287343	C	4.635508	1.708871	-1.383947
C	5.007227	1.243425	0.062727	C	5.145116	1.090687	-0.233660
C	-1.872338	1.849838	-0.675765	C	-1.711709	2.084114	0.232242
C	-1.248898	1.777398	-1.930966	C	-1.219667	2.622180	-0.967437
H	3.015060	1.397025	-2.704053	H	2.894896	2.505605	-2.375202
H	0.625107	1.570473	-2.953251	H	0.528777	2.926999	-2.169310
H	4.332096	1.261031	2.116216	H	4.703365	0.281498	1.721546
H	5.405764	1.234516	-2.060227	H	5.307572	1.950081	-2.210156
H	6.062886	1.172593	0.333082	H	6.209694	0.854495	-0.171620
S	-3.564475	2.058695	-0.373762	S	-3.362714	2.062517	0.755621
H	-1.840590	1.838511	-2.845648	H	-1.897991	3.090652	-1.682079
C	-3.309180	2.032267	1.334857	C	-2.936754	1.247416	2.216788
H	-4.162263	2.132306	2.004263	H	-3.718163	0.984294	2.928178
C	-2.003120	1.871482	1.678851	C	-1.603868	0.995383	2.321581
H	-1.647023	1.822895	2.707539	H	-1.146435	0.478448	3.164961
C	-2.314087	-1.426386	-0.659528	C	-2.610186	-1.397792	-0.163621
C	-0.881391	-1.549212	-0.802869	C	-1.261616	-1.764801	0.202207
C	-0.239581	-1.607517	0.441154	C	-0.344464	-1.434760	-0.804917
S	-1.343906	-1.488191	1.780099	S	-1.094750	-0.693813	-2.188348
C	-2.705657	-1.385294	0.693429	C	-2.665924	-0.802234	-1.439934
C	-3.300428	-1.368655	-1.649837	C	-3.798436	-1.563478	0.556011
C	-0.121809	-1.629297	-1.986024	C	-0.810682	-2.388446	1.382292
C	1.152870	-1.764112	0.534140	C	1.024699	-1.713039	-0.659541
C	-4.046079	-1.291730	1.063760	C	-3.871373	-0.374375	-1.994919
C	-4.635813	-1.278938	-1.286870	C	-5.000646	-1.143217	0.007843
C	-5.007237	-1.243511	0.063185	C	-5.036373	-0.549858	-1.260841
C	1.872318	-1.850211	-0.675117	C	1.428922	-2.353740	0.529073
C	1.248848	-1.778435	-1.930342	C	0.525662	-2.691864	1.548428
H	-3.015091	-1.398375	-2.703540	H	-3.773208	-2.021130	1.547009
H	-0.625182	-1.571973	-2.952682	H	-1.527787	-2.639246	2.166192
H	-4.332082	-1.259987	2.116673	H	-3.897841	0.085865	-2.984485
H	-5.405792	-1.235692	-2.059769	H	-5.928180	-1.274037	0.568986
H	-6.062899	-1.172629	0.333515	H	-5.990042	-0.220835	-1.678905
S	3.564439	-2.059108	-0.373057	S	3.143457	-2.608370	0.536603
H	1.840510	-1.840100	-2.845007	H	0.876950	-3.177659	2.460033
C	3.309210	-2.031708	1.335552	C	3.308492	-1.872012	-1.019007
H	4.162300	-2.131532	2.004981	H	4.297151	-1.769531	-1.462925
C	2.003184	-1.870547	1.679504	C	2.125598	-1.443991	-1.533241
H	1.647131	-1.821371	2.708179	H	2.032861	-0.937743	-2.493675

12h

0 1

C -0.0000000013 0.5831916029 1.9943120886
C -0.000000002 0.8617072483 0.5731028147
C -0.0000000002 -0.3963082431 -0.0412503552
O 0.0000000032 -1.406598706 0.8655202368
C -0.0000000066 -0.821099185 2.09710359
C -0.0000000044 1.3500361188 3.1631355735
C -0.0000000036 2.0312576472 -0.2107896679
C 0.0000000002 -0.5541840885 -1.4312768972
C -0.0000000059 -1.494305377 3.3093667941
C -0.0000000002 0.692159208 4.3894815871
C 0.0000000057 -0.7092046245 4.4611023781
C -0.0000000032 0.64670837 -2.1829317053
C 0.0000000007 1.9233680159 -1.591060895
H -0.0000000017 2.4410525809 3.114557366
H -0.0000000044 3.0142659368 0.2640321067
H -0.0000000041 -2.5843944151 3.3481922109

H 0.0000000055 1.2741089824 5.3135691071
H 0.000000009 -1.1964079495 5.4386305264
S 0.0000000139 0.294852621 -3.8842448345
H 0.0000000044 2.8177621021 -2.2165262262
C -0.0000000061 -1.4102606781 -3.5825415527
H -0.0000000016 -2.0999735582 -4.4259447157
C 0.0000000011 -1.724035074 -2.2578252348
H 0.0000000018 -2.7421485353 -1.8697242956

1 2

C 0.0000000023 0.5858248599 1.9922422328
C -0.0000000034 0.8711185159 0.5903140911
C 0.0000000205 -0.42810677 -0.04209638
O 0.0000000199 -1.4076983207 0.8469865563
C -0.000000006 -0.8192599884 2.1010630475
C -0.0000000109 1.3644095603 3.1629104013
C -0.0000000266 2.0322012468 -0.187310754
C 0.0000000295 -0.5779458924 -1.432795553
C -0.0000000102 -1.4945590857 3.2968996454
C 0.0000000017 0.7060886473 4.387869661
C -0.0000000033 -0.6936852131 4.4537799336
C 0.0000000085 0.6280315183 -2.1708735481
C -0.0000000187 1.9107222977 -1.5734907701
H -0.0000000123 2.4547518956 3.1110090346
H -0.0000000181 3.0183015729 0.2787952442
H -0.0000000017 -2.5839379979 3.3459699662
H 0.0000000009 1.284187599 5.3133409407
H 0.0000000191 -1.1823958577 5.4305122144
S 0.0000001121 0.2951458584 -3.8561278006
H 0. 2.8040814661 -2.2017146129
C -0.0000000331 -1.3996845307 -3.5954697489
H -0.000000088 -2.0748917592 -4.4515793579
C 0.0000000208 -1.737534764 -2.2651238573
H -0.0000000029 -2.7636148583 -1.8971205863

-1 2

C 0.0000000038 0.59078631 1.9836123455
C -0.0000000134 0.8737797271 0.5858000524
C 0.0000000001 -0.3835277141 -0.0470912877
O -0.0000000032 -1.403020525 0.8615554014
C -0.0000000178 -0.8245166158 2.1007492241
C 0.0000000202 1.3527907483 3.1816712789
C -0.0000000195 2.062124538 -0.2139442316
C 0.0000000169 -0.5515528279 -1.4311393376
C -0.0000000224 -1.5030418446 3.2998224194
C 0.0000000163 0.6778221632 4.4020048492
C -0.0000000154 -0.7215560781 4.4828677938
C -0.000000002 0.6709393335 -2.2028467258
C -0.0000000155 1.9285189418 -1.6104042349
H 0.0000000351 2.4447506651 3.1451835664
H -0.0000000217 3.0482374123 0.2533914417
H -0.0000000312 -2.594679791 3.3237980137
H 0.0000000355 1.2597499393 5.3299263805
H -0.0000000201 -1.2140666463 5.4584166743
S 0.0000000102 0.2868881866 -3.9289371357
H -0.0000000149 2.8234056003 -2.2401860744
C -0.000000002 -1.4380708549 -3.5877074777
H -0.0000000331 -2.1469805646 -4.4147562393
C 0.00000004 -1.7166352274 -2.2487865129
H 0.0000000543 -2.7305948755 -1.8450101839

cofacial

0 1

O	1.70898	0.90556	1.47556
C	2.92555	0.80805	0.87638
C	2.87537	1.24205	-0.45789
C	1.50531	1.63881	-0.67725
C	0.86416	1.40136	0.53942
C	4.08198	0.34301	1.47874
C	5.22732	0.30562	0.68887
C	5.20451	0.72300	-0.64946
C	4.03484	1.19621	-1.23323
C	0.78323	2.15217	-1.76843
C	-0.56552	2.41909	-1.62162
C	-1.18594	2.16943	-0.38635
C	-0.49552	1.65088	0.73190
S	-2.85295	2.43648	0.00635
C	-2.61898	1.85381	1.61499
C	-1.33823	1.47395	1.87193
H	4.08175	0.01364	2.51801
H	6.16204	-0.05816	1.12096
H	6.12316	0.67993	-1.23818
H	4.02262	1.52545	-2.27423
H	1.28009	2.33395	-2.72307
H	-1.14729	2.81370	-2.45577
H	-3.46961	1.81630	2.29336

antifacial_y

0 1

C	-2.534048	-1.197464	-0.634444
C	-1.155526	-1.197869	-1.064237
C	-0.439909	-1.703343	0.022155
O	-1.242637	-1.985383	1.076972
C	-2.510652	-1.686633	0.681646
C	-3.756543	-0.848552	-1.207711
C	-0.481724	-0.820190	-2.238480
C	0.942314	-1.894426	-0.010861
C	-3.648961	-1.841981	1.454397
C	-4.912428	-1.001122	-0.450096
C	-4.859305	-1.488136	0.862256
C	1.579987	-1.517997	-1.212965
C	0.889974	-0.977569	-2.311605
H	-3.801555	-0.457989	-2.225618
H	-1.035266	-0.401056	-3.080208
H	-3.589978	-2.227091	2.473082
H	-5.878845	-0.731946	-0.881065
H	-5.784419	-1.596330	1.432546
S	3.282595	-1.824064	-1.112725
H	1.435016	-0.684916	-3.210205
C	3.129939	-2.437540	0.496382
H	4.020423	-2.777585	1.023074
C	1.851099	-2.418766	0.959481

H	-0.99470	1.06876	2.82236
C	0.78930	-1.68800	-0.78727
C	-0.50671	-1.24797	-1.24835
C	-1.34022	-1.35363	-0.13327
O	-0.67649	-1.79759	0.96084
C	0.60934	-2.01107	0.56660
C	2.05221	-1.84635	-1.36118
C	-1.02718	-0.80948	-2.47706
C	-2.70223	-1.05216	-0.18179
C	1.62585	-2.49401	1.37376
C	3.08492	-2.33336	-0.57025
C	2.87346	-2.65283	0.77766
C	-3.18736	-0.61952	-1.43581
C	-2.37067	-0.49457	-2.57191
H	2.22546	-1.58693	-2.40713
H	-0.37827	-0.71868	-3.34958
H	1.44669	-2.72877	2.42337
H	4.08236	-2.45085	-0.99669
H	3.70840	-3.02140	1.37673
S	-4.88981	-0.29809	-1.34648
H	-2.79493	-0.15457	-3.51796
C	-4.93548	-0.73621	0.32662
H	-5.88133	-0.69105	0.86508
C	-3.72385	-1.11343	0.81632
H	-3.54827	-1.42831	1.84400

H	1.551138	-2.758067	1.949708
C	-1.419010	1.650079	0.709267
C	-0.062925	1.322854	1.079602
C	0.706577	1.667811	-0.032710
O	-0.047142	2.164577	-1.041921
C	-1.332628	2.153713	-0.597929
C	-2.667258	1.572388	1.329226
C	0.549665	0.788178	2.226150
C	2.096445	1.531676	-0.054469
C	-2.434613	2.584450	-1.318810
C	-3.783928	2.003665	0.625123
C	-3.668578	2.501547	-0.680358
C	2.676266	1.008855	1.121824
C	1.922802	0.629198	2.245630
H	-2.763877	1.173304	2.340191
H	-0.053355	0.498904	3.088203
H	-2.328104	2.971896	-2.332725
H	-4.770278	1.939117	1.087305
H	-4.566453	2.827136	-1.209923
S	4.401966	0.934121	0.961319
H	2.420880	0.213923	3.122856
C	4.331762	1.576971	-0.641158
H	5.255262	1.718752	-1.200929
C	3.064691	1.847025	-1.057210
H	2.813752	2.256528	-2.034779

antifacial_z

0 1

C	2.364295	1.404289	-0.715262
C	0.938411	1.530301	-0.899012
C	0.411849	1.571544	0.392384
O	1.374263	1.477397	1.341119
C	2.556892	1.383806	0.675564
C	3.475725	1.327090	-1.555964
C	0.085632	1.629394	-2.012034
C	-0.953456	1.725506	0.643156
C	3.805598	1.298725	1.268207
C	4.737790	1.237437	-0.980163
C	4.900484	1.227406	0.412043
C	-1.774127	1.839389	-0.500704
C	-1.272920	1.787281	-1.812757
H	3.355352	1.340038	-2.641069
H	0.493302	1.584917	-3.023268
H	3.912023	1.290107	2.353237
H	5.619797	1.176099	-1.620840
H	5.905489	1.159432	0.833773
S	-3.429890	2.051458	-0.036655
H	-1.953899	1.868078	-2.661386
C	-3.021298	1.976377	1.640616
H	-3.811552	2.060898	2.385229
C	-1.690742	1.802205	1.864636
H	-1.238973	1.723919	2.852285
C	-2.364834	-1.415033	-0.702310
C	-0.939144	-1.544538	-0.885307
C	-0.411606	-1.566193	0.406189
O	-1.373190	-1.457522	1.354156
C	-2.556309	-1.373550	0.688222
C	-3.476939	-1.349646	-1.543113
C	-0.087147	-1.660670	-1.997315
C	0.953855	-1.716400	0.658302

antifacial_yz

0 1

C	2.644429	1.096067	-0.774961
C	1.237817	1.209128	-1.075495
C	0.652001	1.654805	0.109898
O	1.562200	1.819570	1.100685
C	2.766826	1.480205	0.570395
C	3.787356	0.719505	-1.481111
C	0.442775	0.969304	-2.209584
C	-0.716968	1.902136	0.223558
C	3.975366	1.502351	1.246477
C	5.010471	0.735609	-0.820977
C	5.101987	1.118747	0.524362
C	-1.479767	1.665882	-0.941562
C	-0.918867	1.197757	-2.142210
H	3.719503	0.416875	-2.527668
H	0.895662	0.600982	-3.131457
H	4.030020	1.806006	2.292482
H	5.916910	0.444199	-1.355579
H	6.076797	1.118972	1.016565
S	-3.149833	2.035872	-0.656118
H	-1.556002	1.013080	-3.008242
C	-2.822659	2.473745	0.981991
H	-3.644623	2.794131	1.620702
C	-1.509511	2.359605	1.320620
H	-1.106477	2.587608	2.306366
C	-2.644377	-1.096098	0.775181
C	-1.237750	-1.209253	1.075597
C	-0.652047	-1.654822	-0.109891
O	-1.562332	-1.819456	-1.100621
C	-2.766909	-1.480137	-0.570189
C	-3.787213	-0.719481	1.481446
C	-0.442594	-0.969571	2.209636
C	0.716905	-1.902162	-0.223704

C	-3.804438	-1.278871	1.280549
C	-4.738484	-1.250477	-0.967679
C	-4.899980	-1.219580	0.424348
C	1.773824	-1.847128	-0.484241
C	1.271623	-1.815083	-1.796583
H	-3.357543	-1.379117	-2.628006
H	-0.495531	-1.632127	-3.008852
H	-3.909895	-1.253757	2.365402
H	-5.620977	-1.198144	-1.608481
H	-5.904571	-1.144544	0.845863
S	3.429943	-2.051607	-0.017979
H	1.951959	-1.908938	-2.644393
C	3.022275	-1.951850	1.658199
H	3.813136	-2.024221	2.403432
C	1.691808	-1.774713	1.880370
H	1.240630	-1.681373	2.866973

C	-3.975514	-1.502219	-1.246156
C	-5.010388	-0.735480	0.821418
C	-5.102049	-1.118588	-0.523921
C	1.479824	-1.666055	0.941370
C	0.919034	-1.198081	2.142126
H	-3.719239	-0.416897	2.528008
H	-0.895377	-0.601361	3.131606
H	-4.030281	-1.805826	-2.292168
H	-5.916762	-0.444024	1.356106
H	-6.076906	-1.118752	-1.016032
S	3.149874	-2.035921	0.655683
H	1.556242	-1.013534	3.008132
C	2.822533	-2.473543	-0.982462
H	3.644456	-2.793687	-1.621345
C	1.509335	-2.359466	-1.320912
H	1.106210	-2.587250	-2.306670

12i

0 1

C 0.0000000025 -0.5900146372 -1.9149140118
C -0.0000000001 -0.9814517117 -0.5208411458
C 0.0000000013 0.2271042449 0.1886141823
O -0.0000000002 1.3057622677 -0.6334352292
C -0.0000000009 0.8181276768 -1.9075854647
C 0.0000000051 -1.2628426244 -3.1404447473
C -0.0000000013 -2.2085171096 0.1701361381
C 0.0000000012 0.2492570753 1.5792395144
C -0.0000000025 1.5844901868 -3.0628644155
C 0.0000000023 -0.5106636553 -4.3112930947
C -0.0000000019 0.8920132448 -4.2726668543
C -0.000000002 -0.9875996112 2.2711200175
C -0.0000000042 -2.2062201361 1.5527072908
H 0.0000000064 -2.3542675535 -3.1772006707
H -0.0000000022 -3.1498926289 -0.3826521686
H -0.000000005 2.6742213968 -3.0157504748
H 0.000000003 -1.0181246737 -5.2782686412
H -0.0000000033 1.4544353717 -5.2089231532
C -0.000000001 -0.7736572224 3.6909186047
H -0.0000000058 -3.1482028253 2.1050053923
C 0.0000000042 0.5456197321 4.0258146631
H -0.0000000022 -1.5807909116 4.4242507167
H 0.000000007 0.9744469319 5.0273663451
S -0.0000000005 1.6061871721 2.6549072066

1 2

C -0.0000000038 -0.5858407203 -1.8983813218
C -0.0000000194 -0.9778398786 -0.5312228268
C -0.0000000105 0.2647613264 0.2007462903
O -0.0000000184 1.3210223297 -0.611854453
C -0.000000027 0.8298274343 -1.898235457
C 0.0000000181 -1.2774553971 -3.1274854713
C -0.0000000211 -2.2120156772 0.1507757078
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C -0.0000000216 1.5895827531 -3.0434731337
C 0.0000000259 -0.5307910604 -4.2943973702
C 0.0000000042 0.8755910121 -4.2528595335
C -0.000000023 -0.9759226352 2.2593463751
C -0.0000000281 -2.2080111322 1.527764018
H 0.0000000335 -2.3685522329 -3.1552569633
H -0.000000018 -3.150352864 -0.4052198671

-1 2

C 0.0000000089 -0.6038561079 -1.907804442
C -0.0000000087 -0.9839145283 -0.5398643686
C 0.0000000029 0.2322858037 0.202901137
O -0.0000000191 1.312452808 -0.6392638548
C -0.0000000233 0.8200040072 -1.9172653606
C 0.0000000239 -1.2702861699 -3.160779306
C -0.000000014 -2.2148856641 0.1790243533
C 0.0000000091 0.2576235782 1.5746427746
C -0.0000000233 1.5835795603 -3.062766351
C 0.0000000226 -0.5036842682 -4.3296146094
C 0.0000000026 0.8935799109 -4.3046224312
C -0.000000005 -0.9913405123 2.2974341489
C -0.0000000235 -2.2077213656 1.5576129737
H 0.0000000337 -2.3619268632 -3.2090101916
H -0.0000000185 -3.1624389431 -0.366560733

H	-0.000000031	2.6795650866	-3.0129358446
H	0.0000000486	-1.0345612032	-5.2623092441
H	0.0000000202	1.4342687176	-5.1915405775
C	0.0000000055	-0.7867103015	3.656776169
H	-0.0000000266	-3.148238367	2.0828338096
C	0.0000000446	0.5569965284	4.0056438286
H	0.0000000153	-1.5928927759	4.3913390084
H	0.0000000839	0.9661954426	5.0173529478
S	-0.0000000406	1.619063837	2.676662146

H	-0.0000000487	2.6738024849	-3.0042798038
H	0.0000000401	-1.0157513225	-5.2978841419
H	0.	1.459861388	-5.2393080318
C	-0.0000000056	-0.7741905896	3.6970268698
H	-0.0000000323	-3.1545898105	2.1069708739
C	0.0000000313	0.5535610247	4.0636659767
H	-0.0000000177	-1.5889666256	4.4256505336
H	0.0000000584	0.9759101715	5.0669248249
S	0.0000000061	1.6303120335	2.6704091592

cofacial

0 1

C	2.895530	1.234495	-0.459552
C	1.523957	1.629786	-0.670059
C	0.896295	1.396636	0.556634
O	1.747683	0.905874	1.487406
C	2.958365	0.804783	0.875736
C	4.048369	1.183710	-1.244631
C	0.789572	2.134985	-1.756836
C	-0.456192	1.649506	0.735204
C	4.117993	0.338166	1.469426
C	5.221910	0.709398	-0.669750
C	5.256149	0.295395	0.669286
C	-1.194428	2.149620	-0.361069
C	-0.558580	2.388780	-1.598335
H	4.027450	1.507862	-2.287062
H	1.280830	2.318881	-2.714035
H	4.124527	0.013002	2.509982
H	6.134734	0.661448	-1.267099
H	6.194071	-0.068626	1.094079
C	-2.567616	2.345034	0.000093
H	-1.150735	2.770516	-2.431806
C	-2.824012	2.015106	1.293127
H	-3.328226	2.709977	-0.689560
H	-3.781481	2.055707	1.809311
S	-1.429991	1.442709	2.146924
C	0.817895	-1.688938	-0.793419
C	-0.494520	-1.256197	-1.210553
C	-1.295379	-1.402863	-0.073821
O	-0.599633	-1.867985	0.988959
C	0.679038	-2.049536	0.555949
C	2.066431	-1.813984	-1.405370
C	-1.049223	-0.784853	-2.411619
C	-2.649986	-1.100652	-0.102803
C	1.724080	-2.535996	1.323112
C	3.127444	-2.304324	-0.655156
C	2.957435	-2.660384	0.689366
C	-3.204207	-0.623632	-1.312219
C	-2.392918	-0.470395	-2.457364
H	2.206001	-1.525972	-2.448844
H	-0.419609	-0.665274	-3.294569
H	1.576562	-2.802037	2.370122
H	4.114437	-2.395073	-1.111358
H	3.813217	-3.033372	1.255394
C	-4.606078	-0.364731	-1.161150
H	-2.841960	-0.100200	-3.381060
C	-5.062669	-0.646617	0.088511
H	-5.240173	0.011391	-1.964456
H	-6.081831	-0.546057	0.459817
S	-3.830018	-1.233276	1.153314

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C	-2.416462	-1.085357	-0.831777
C	-1.043262	-0.998033	-1.267401
C	-0.317918	-1.700648	-0.301368
O	-1.107913	-2.182470	0.687057
C	-2.379890	-1.813769	0.368636
C	-3.645012	-0.640122	-1.318699
C	-0.381936	-0.394967	-2.351148
C	1.057692	-1.854210	-0.401692
C	-3.508995	-2.111443	1.111618
C	-4.792671	-0.934768	-0.591351
C	-4.725618	-1.655624	0.607849
C	1.718611	-1.250254	-1.494366
C	0.988893	-0.516952	-2.455603
H	-3.701465	-0.067001	-2.245419
H	-0.948659	0.173324	-3.090356
H	-3.439059	-2.680377	2.039434
H	-5.763722	-0.593064	-0.955255
H	-5.644628	-1.869643	1.157707
C	3.127844	-1.499876	-1.436957
H	1.525616	-0.044162	-3.279821
C	3.483603	-2.261049	-0.368158
H	3.837865	-1.114438	-2.167948
H	4.485495	-2.587420	-0.093285
S	2.144853	-2.714716	0.630274
C	-1.400263	1.541184	0.936536
C	-0.065670	1.127213	1.294268
C	0.748357	1.631093	0.275769
O	0.041910	2.301517	-0.663790
C	-1.259106	2.245897	-0.269291
C	-2.670836	1.392844	1.495186
C	0.495662	0.405116	2.361557
C	2.125321	1.453351	0.300811
C	-2.326859	2.808663	-0.948319
C	-3.754262	1.952983	0.831233
C	-3.584569	2.651291	-0.372284
C	2.689407	0.744204	1.384006
C	1.862363	0.217784	2.400768
H	-2.810289	0.839701	2.425353
H	-0.144684	-0.001452	3.145740
H	-2.177173	3.351405	-1.882359
H	-4.757378	1.837257	1.244907
H	-4.457200	3.077677	-0.871640
C	4.116892	0.684647	1.265093
H	2.319189	-0.340028	3.219852
C	4.581300	1.318602	0.156257
H	4.760715	0.185005	1.989118
H	5.616666	1.419003	-0.166615
S	3.323335	2.009407	-0.814187

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C	2.394287	1.330353	-0.772111
C	0.983491	1.510185	-1.016544
C	0.409712	1.582171	0.255524
O	1.327141	1.466372	1.242285
C	2.530616	1.318842	0.625220
C	3.533817	1.187300	-1.566071
C	0.177891	1.621409	-2.163498
C	-0.956778	1.768188	0.422665
C	3.749045	1.184139	1.269185
C	4.766369	1.046092	-0.938810
C	4.872679	1.048792	0.459103
C	-1.762168	1.882323	-0.731771
C	-1.181986	1.806378	-2.017616
H	3.456168	1.188169	-2.655132
H	0.627265	1.556602	-3.155735
H	3.810263	1.181649	2.357723
H	5.669481	0.935106	-1.542639
H	5.855526	0.939594	0.922575
C	-3.137465	2.068008	-0.376278
H	-1.826509	1.891700	-2.894544
C	-3.332754	2.094893	0.968371
H	-3.942347	2.160093	-1.104689
H	-4.278554	2.206440	1.496171
S	-1.874786	1.897922	1.881195
C	-2.394305	-1.330783	-0.771596
C	-0.983521	-1.510781	-1.015963
C	-0.409713	-1.582093	0.256129
O	-1.327099	-1.465626	1.242848
C	-2.530585	-1.318364	0.625731
C	-3.533866	-1.188244	-1.565602
C	-0.177953	-1.622541	-2.162884
C	0.956776	-1.768059	0.423332
C	-3.748984	-1.183224	1.269657
C	-4.766401	-1.046658	-0.938388
C	-4.872650	-1.048398	0.459531
C	1.762138	-1.882731	-0.731072
C	1.181936	-1.807372	-2.016941
H	-3.456274	-1.189927	-2.654664
H	-0.627350	-1.558175	-3.155140
H	-3.810151	-1.180014	2.358195
H	-5.669544	-0.936161	-1.542261
H	-5.855476	-0.938887	0.922974
C	3.137456	-2.068163	-0.375527
H	1.826467	-1.893006	-2.893833
C	3.332778	-2.094430	0.969129
H	3.942326	-2.160505	-1.103919
H	4.278589	-2.205709	1.496966
S	1.874826	-1.897068	1.881897

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C	-2.626595	-0.930957	-0.893430
C	-1.242073	-0.984401	-1.294503
C	-0.589397	-1.620811	-0.235437
O	-1.437786	-1.954017	0.766316
C	-2.669289	-1.531570	0.374967
C	-3.807404	-0.445690	-1.456587
C	-0.516787	-0.543911	-2.414956
C	0.778979	-1.853136	-0.267914
C	-3.833156	-1.660705	1.114502
C	-4.987410	-0.568592	-0.732243
C	-4.999118	-1.164730	0.536553
C	1.504563	-1.418094	-1.399413
C	0.845655	-0.758939	-2.460491
H	-3.799639	0.026814	-2.440503
H	-1.027207	-0.029139	-3.230239
H	-3.825293	-2.131860	2.098040
H	-5.922178	-0.194403	-1.154946
H	-5.941847	-1.246901	1.081833
C	2.895453	-1.739868	-1.268712
H	1.431076	-0.416820	-3.315745
C	3.179978	-2.377046	-0.103783
H	3.647179	-1.483722	-2.014482
H	4.155443	-2.711301	0.245517
S	1.790340	-2.625984	0.901466
C	2.626629	0.931007	0.893320
C	1.242155	0.984527	1.294532
C	0.589415	1.620995	0.235544
O	1.437732	1.954213	-0.766268
C	2.669242	1.531662	-0.375060
C	3.807432	0.445552	1.456318
C	0.516938	0.543963	2.415000
C	-0.778958	1.853312	0.268105
C	3.833039	1.660673	-1.114726
C	4.987361	0.568292	0.731822
C	4.998996	1.164492	-0.536944
C	-1.504482	1.418141	1.399592
C	-0.845510	0.758938	2.460601
H	3.799703	-0.027007	2.440207
H	1.027420	0.029192	3.230245
H	3.825134	2.131881	-2.098238
H	5.922121	0.193919	1.154374
H	5.941669	1.246544	-1.082337
C	-2.895410	1.739747	1.268901
H	-1.430889	0.416731	3.315848
C	-3.180015	2.376889	0.103971
H	-3.647111	1.483457	2.014649
H	-4.155533	2.710933	-0.245375
S	-1.790402	2.626089	-0.901242

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C	0.0000000003	0.3858558419	1.8047956298
C	-0.0000000007	-0.9875314222	2.0172493049
C	-0.0000000009	-1.3540496133	3.3904026681
C	0.000000002	-0.2420014337	4.1908132648
S	0.0000000045	1.2420932699	3.3016797106
C	-0.0000000015	0.7617027854	0.4249387744

C -0.0000000013 -0.38046997 -0.3913686356
S -0.0000000035 -1.8717316016 0.5220181053
H -0.0000000027 -2.3750033099 3.7710827656
H 0.0000000027 -0.210926362 5.2796045911
C -0.0000000009 2.0496984211 -0.1716051324
C -0.0000000014 2.1668834961 -1.5354679745
C -0.0000000009 1.0197143342 -2.3833849229
C -0.0000000005 -0.289340919 -1.8092373275
C -0.0000000005 1.1399761338 -3.7936746401
C 0.0000000009 0.0258747376 -4.6034293572
C 0.0000000014 -1.2638836751 -4.0314705592
C 0.0000000001 -1.4174846184 -2.663134159
H -0.0000000003 2.9369245851 0.4654511865
H -0.000000001 3.1551114082 -2.0011468838
H -0.0000000006 2.1412676556 -4.2319788132
H 0.0000000018 0.1382833242 -5.6898289669
H 0.0000000025 -2.1444960749 -4.6776726426
H 0.0000000003 -2.418316993 -2.2234659864

1 2

C	0.0000000246	0.4022236595	1.791924027
C	0.0000000278	-0.9901434442	2.0021383507
C	0.0000000056	-1.3567970479	3.3504872192
C	-0.0000000427	-0.2219722017	4.1561174803
S	0.0000000335	1.2591722204	3.2983504868
C	0.0000000277	0.7788598804	0.4410366696
C	0.0000000049	-0.4001164631	-0.3952586742
S	0.0000000436	-1.8845644592	0.5025028161
H	-0.0000000093	-2.3734911323	3.7426911069
H	-0.0000000844	-0.2049887081	5.2473853951
C	0.0000000166	2.0653173301	-0.153599895
C	-0.0000000035	2.170288653	-1.5165684675
C	0.0000000005	1.0134008031	-2.3702864866
C	0.0000000113	-0.3001685426	-1.8034263955
C	-0.0000000267	1.1412077862	-3.7632422923
C	-0.0000000055	0.0123741667	-4.5860972038
C	0.0000000009	-1.2731408987	-4.0322980506
C	-0.0000000034	-1.4307544646	-2.6561784222
H	0.0000000175	2.9546894343	0.4787594384
H	0.0000000132	3.1558348547	-1.9873504942
H	-0.0000000294	2.1387178483	-4.2084302031
H	-0.000000033	0.1366373162	-5.6710826826
H	-0.0000000047	-2.1496829672	-4.6824603817
H	0.0000000149	-2.4347536234	-2.2239433409

-1 2

C	-0.0000000203	0.3960322457	1.8083822903
C	-0.0000000089	-0.9902327657	2.0359242278
C	-0.000000009	-1.348227586	3.3979462782
C	0.0000000174	-0.243200313	4.2300970561
S	0.0000000049	1.2529783668	3.3232488268
C	-0.0000000112	0.7765633979	0.4496984516
C	-0.0000000083	-0.3750312429	-0.4069976588
S	-0.0000000167	-1.8871874771	0.5241160494
H	-0.0000000202	-2.3746261571	3.7693645541
H	0.0000000381	-0.217389943	5.3179375098
C	0.0000000085	2.0515946022	-0.1635985771
C	0.0000000027	2.168876904	-1.5314710313
C	0.0000000133	1.0223881173	-2.4014442792
C	-0.0000000032	-0.2948476183	-1.8034230849
C	-0.000000002	1.1409577923	-3.7968412089
C	0.000000004	0.0116893659	-4.6348427109
C	0.0000000102	-1.2613281053	-4.0572271251
C	0.000000002	-1.4266260118	-2.6773495837
H	0.0000000023	2.9469706992	0.4660696759
H	-0.0000000172	3.1603624498	-1.9944863356
H	-0.0000000112	2.1461438272	-4.2312746535
H	0.0000000032	0.1296780282	-5.7216760772
H	0.0000000158	-2.1482096347	-4.7000364576
H	0.000000006	-2.4291789413	-2.2409461362

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C	-0.40723	0.19850	2.40772
C	-0.47275	-1.17829	2.55078
C	-0.60606	-1.60849	3.89596
C	-0.64170	-0.53694	4.74776
S	-0.51991	0.98347	3.93508
C	-0.23646	0.63634	1.06092
C	-0.18217	-0.46279	0.19606
S	-0.33547	-1.99041	1.02591
H	-0.67629	-2.64534	4.22313
H	-0.75079	-0.55736	5.83122
C	-0.10972	1.94748	0.53817
C	0.06418	2.12426	-0.80647

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C	-0.01096	0.76117	1.68729
C	-0.09066	-0.53227	2.17629
C	-0.12161	-0.60717	3.59299
C	-0.06914	0.64276	4.14643
S	0.02758	1.90635	2.97101
C	0.01056	0.84631	0.26425
C	-0.05550	-0.43214	-0.30092
S	-0.13372	-1.70086	0.89613
H	-0.17411	-1.52676	4.17389
H	-0.07309	0.89683	5.20522
C	0.08099	1.98480	-0.57619
C	0.07254	1.82381	-1.93351

C	0.11665	1.01966	-1.70372
C	-0.00796	-0.30866	-1.20277
C	0.30163	1.20433	-3.09195
C	0.35601	0.13179	-3.95151
C	0.23415	-1.17844	-3.44986
C	0.05581	-1.39483	-2.10281
H	-0.14294	2.80146	1.21740
H	0.17175	3.12893	-1.22019
H	0.41046	2.22270	-3.47168
H	0.51557	0.29197	-5.01904
H	0.29108	-2.02687	-4.13462
H	-0.03152	-2.41259	-1.71544
C	3.11266	0.62778	1.06009
C	3.03011	-0.73332	1.30390
C	2.84791	-1.05927	2.67303
C	2.80488	0.07165	3.44059
S	2.97151	1.52606	2.52128
C	3.28342	0.96318	-0.31548
C	3.33037	-0.19766	-1.09716
S	3.16626	-1.65721	-0.15710
H	2.74293	-2.06616	3.07391
H	2.65669	0.13363	4.51706
C	3.39487	2.23129	-0.93644
C	3.54651	2.31113	-2.29324
C	3.59751	1.14253	-3.10579
C	3.49062	-0.14566	-2.50502
C	3.74271	1.22418	-4.50871
C	3.78167	0.08957	-5.28716
C	3.68349	-1.18196	-4.68723
C	3.54067	-1.29523	-3.32359
H	3.35447	3.13362	-0.32323
H	3.63215	3.28466	-2.78113
H	3.82180	2.21249	-4.96840
H	3.89492	0.17180	-6.37032
H	3.71880	-2.07992	-5.30782
H	3.45678	-2.28078	-2.85975

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C	-0.06358	0.81412	1.73595
C	-0.07232	-0.49486	2.19024
C	-0.10701	-0.61069	3.60334
C	-0.13555	0.62422	4.19080
S	-0.11257	1.92336	3.05128
C	-0.03442	0.93574	0.31543
C	-0.03293	-0.33031	-0.28195
S	-0.04909	-1.63060	0.88171
H	-0.10536	-1.54724	4.15865
H	-0.16145	0.84847	5.25596
C	0.00266	2.09506	-0.49775
C	0.01791	1.96665	-1.85910
C	-0.00625	0.68803	-2.48623
C	-0.02483	-0.49409	-1.69046
C	-0.01717	0.55700	-3.89287
C	-0.05250	-0.68146	-4.49132
C	-0.06260	-1.84710	-3.69999
C	-0.04560	-1.75477	-2.32682
H	0.01980	3.07987	-0.02684
H	0.05123	2.85293	-2.49575
H	-0.00098	1.46541	-4.49942

C	-0.00788	0.53301	-2.52928
C	-0.06821	-0.62851	-1.70513
C	-0.03769	0.36966	-3.93180
C	-0.12228	-0.88030	-4.50034
C	-0.17444	-2.02595	-3.68143
C	-0.14772	-1.90149	-2.31140
H	0.14128	2.97873	-0.12900
H	0.12922	2.69228	-2.59245
H	0.01316	1.26118	-4.56064
H	-0.14525	-0.98772	-5.58683
H	-0.23937	-3.01661	-4.13688
H	-0.18805	-2.78964	-1.67657
C	3.26096	-0.76117	1.68729
C	3.34066	0.53227	2.17629
C	3.37161	0.60717	3.59299
C	3.31914	-0.64276	4.14643
S	3.22242	-1.90635	2.97101
C	3.23944	-0.84631	0.26425
C	3.30550	0.43214	-0.30092
S	3.38372	1.70086	0.89613
H	3.42411	1.52676	4.17389
H	3.32309	-0.89683	5.20522
C	3.16901	-1.98480	-0.57619
C	3.17746	-1.82381	-1.93351
C	3.25788	-0.53301	-2.52927
C	3.31821	0.62851	-1.70513
C	3.28769	-0.36966	-3.93179
C	3.37228	0.88030	-4.50033
C	3.42444	2.02595	-3.68143
C	3.39772	1.90149	-2.31140
H	3.10872	-2.97873	-0.12900
H	3.12078	-2.69228	-2.59244
H	3.23684	-1.26118	-4.56064
H	3.39526	0.98772	-5.58683
H	3.48937	3.01661	-4.13688
H	3.43805	2.78963	-1.67656

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C	0.04909	0.48038	1.17806
C	0.11955	-0.88655	1.39239
C	0.28739	-1.24257	2.75502
C	0.33557	-0.12781	3.54679
S	0.18685	1.34568	2.65777
C	-0.10177	0.84849	-0.19132
C	-0.14738	-0.29289	-1.00063
S	-0.00539	-1.77613	-0.09155
H	0.37882	-2.25892	3.13466
H	0.48504	-0.08841	4.62435
C	-0.18951	2.13225	-0.78259
C	-0.32466	2.24555	-2.13909
C	-0.38056	1.09730	-2.97938
C	-0.29169	-0.20602	-2.40827
C	-0.50659	1.21379	-4.38172
C	-0.54288	0.09851	-5.18808
C	-0.46232	-1.18816	-4.61765
C	-0.34015	-1.33553	-3.25526
H	-0.14467	3.01904	-0.14759
H	-0.39274	3.23130	-2.60471
H	-0.57395	2.21337	-4.81836

H	-0.06374	-0.76394	-5.58019	H	-0.64172	0.20779	-6.27028
H	-0.08686	-2.82858	-4.17868	H	-0.49676	-2.07071	-5.25999
H	-0.05376	-2.65907	-1.71403	H	-0.27348	-2.33281	-2.81459
C	3.31358	0.81412	-1.73595	C	3.20091	-0.48038	-1.17806
C	3.32232	-0.49486	-2.19024	C	3.13045	0.88655	-1.39239
C	3.35701	-0.61069	-3.60334	C	2.96261	1.24257	-2.75503
C	3.38555	0.62422	-4.19080	C	2.91443	0.12781	-3.54679
S	3.36257	1.92336	-3.05128	S	3.06315	-1.34569	-2.65777
C	3.28442	0.93574	-0.31543	C	3.35177	-0.84849	0.19133
C	3.28293	-0.33031	0.28195	C	3.39738	0.29289	1.00063
S	3.29909	-1.63060	-0.88171	S	3.25538	1.77613	0.09155
H	3.35536	-1.54724	-4.15865	H	2.87119	2.25892	-3.13466
H	3.41145	0.84847	-5.25596	H	2.76495	0.08841	-4.62435
C	3.24734	2.09506	0.49775	C	3.43951	-2.13225	0.78259
C	3.23209	1.96665	1.85910	C	3.57466	-2.24554	2.13909
C	3.25625	0.68803	2.48623	C	3.63056	-1.09730	2.97938
C	3.27483	-0.49409	1.69046	C	3.54169	0.20603	2.40827
C	3.26717	0.55700	3.89287	C	3.75660	-1.21379	4.38172
C	3.30250	-0.68146	4.49132	C	3.79288	-0.09851	5.18808
C	3.31260	-1.84710	3.69999	C	3.71232	1.18816	4.61765
C	3.29560	-1.75477	2.32682	C	3.59014	1.33553	3.25526
H	3.23020	3.07987	0.02684	H	3.39467	-3.01904	0.14759
H	3.19877	2.85293	2.49575	H	3.64274	-3.23130	2.60471
H	3.25098	1.46541	4.49942	H	3.82396	-2.21337	4.81836
H	3.31374	-0.76394	5.58019	H	3.89172	-0.20779	6.27028
H	3.33686	-2.82858	4.17868	H	3.74676	2.07071	5.25999
H	3.30376	-2.65907	1.71403	H	3.52348	2.33282	2.81459

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H	-0.0000000131	-2.9718345022	-0.5975797448
C	-0.0000000011	-2.1127038556	0.0765838485
C	-0.0000000101	-0.8085578755	-0.4659205119
C	-0.0000000224	-0.3723868536	-1.8301798871
C	0.0000000032	0.3165022689	0.3915147702
S	-0.0000000174	1.8419923119	-0.4611783849
C	0.0000000128	0.125108534	1.7773088551
S	0.0000000252	1.3305592025	3.0237635674
C	0.0000000113	-1.1834374884	2.3139369063
C	0.000000015	-1.1563632846	3.7491603034
C	0.0000000131	-2.296921317	1.4430738609
H	0.0000000057	-3.3049363691	1.8630033091
C	-0.0000000132	1.0072931871	-1.9894057899
C	0.0000000008	1.4276518564	-3.3464889503
C	0.0000000157	0.3478263375	-4.1903331263
S	-0.0000000403	-1.1688617647	-3.359006988
C	-0.0000000111	0.1077308202	4.2523990477
H	0.0000000135	-2.052193825	4.3711061097
H	0.0000000048	2.4629171863	-3.6863496249
H	0.0000000378	0.3591266998	-5.2794723403
H	-0.0000000304	0.4072087312	5.29975477

1 2

H	-0.0000000115	-2.9857481027	-0.609561592
C	-0.0000000007	-2.1303310208	0.0682778
C	0.0000000003	-0.8113312712	-0.4729919577
C	-0.0000000115	-0.3867859372	-1.8053928519
C	-0.0000000047	0.3392990999	0.3966409312
S	-0.0000000427	1.871126779	-0.4526965125
C	-0.0000000074	0.1442119743	1.7626368487

-1 2

H	-0.0000000005	-2.9842880769	-0.5880534355
C	-0.0000000007	-2.1193901302	0.0813595292
C	-0.0000000008	-0.8100914065	-0.4889117512
C	-0.0000000005	-0.3782406563	-1.8255948272
C	-0.0000000013	0.3175019848	0.4074695948
S	-0.0000000022	1.8569685218	-0.4602073878
C	0.0000000002	0.1282926934	1.7727159404

S	-0.0000000691	1.3499945891	3.0216964074
C	-0.0000000123	-1.1800928551	2.2980753738
C	-0.0000000015	-1.1603994046	3.7070348026
C	-0.0000000052	-2.3101221142	1.4228884968
H	-0.0000000067	-3.3139245548	1.8512986624
C	-0.0000000337	1.0247795359	-1.9673001449
C	-0.0000000173	1.4312496163	-3.3049837974
C	0.0000000506	0.3254436704	-4.1445940315
S	-0.0000000655	-1.193584913	-3.3371485063
C	0.0000000463	0.1268631178	4.2155833935
H	0.0000000112	-2.0503670251	4.3371736747
H	-0.0000000001	2.4600541312	-3.6641385961
H	0.0000001048	0.3444398547	-5.2361068783
H	0.0000000765	0.4109448298	5.2692984777

S	-0.0000000003	1.3476430746	3.0364240563
C	-0.0000000007	-1.1925212223	2.3379772378
C	0.0000000006	-1.157353329	3.7547477594
C	-0.0000000018	-2.3006292644	1.4443754931
H	-0.0000000013	-3.3136958455	1.8586635149
C	-0.0000000022	1.0208154756	-2.0106474347
C	-0.0000000021	1.4285409454	-3.3520407977
C	0.0000000033	0.3515332667	-4.2293747774
S	-0.0000000001	-1.183411791	-3.3755902302
C	0.0000000022	0.1119798624	4.2871626254
H	0.0000000008	-2.0586996027	4.3729915351
H	-0.0000000025	2.4680385254	-3.6853640302
H	0.0000000066	0.3660544611	-5.3171956109
H	0.0000000034	0.4066725137	5.3347829963

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S	0.34097	-0.98160	-2.20688
C	1.41327	-1.16910	-0.84579
C	0.78120	-1.70128	0.29767
C	-0.98091	-1.61734	-1.27486
C	-0.59576	-1.95058	0.01236
C	-2.35317	-1.85715	-1.54260
C	-2.97976	-2.37573	-0.44289
S	-1.92513	-2.56858	0.91256
C	2.77183	-0.84820	-0.79122
C	3.49745	-1.03950	0.40325
C	2.84958	-1.56981	1.53986
C	1.51355	-1.89882	1.48585
S	3.76836	-0.20201	-2.04932
C	5.13895	-0.16676	-0.99371
C	4.86212	-0.63075	0.25462
H	-2.85717	-1.65116	-2.48560
H	-4.03129	-2.63858	-0.34409
H	6.09354	0.19638	-1.37227
H	5.60105	-0.68916	1.05428
H	3.41845	-1.71801	2.45995
H	1.00687	-2.30641	2.36260
S	-2.00577	1.81979	-1.57776
C	-0.97586	1.61486	-0.18468
C	-1.64547	1.07980	0.93506
C	-3.36007	1.19168	-0.68925
C	-3.01775	0.85150	0.60880
H	-1.47460	0.42251	2.99009
C	-0.94383	0.84664	2.13576
C	0.38413	1.91766	-0.09218
C	1.08124	1.68330	1.11088
C	2.46055	2.05297	0.99389
C	0.39864	1.14236	2.22067
H	0.94818	0.95665	3.14503
C	-4.71634	0.93252	-1.01165
C	-5.37833	0.40044	0.06281
S	-4.37377	0.21616	1.45606
C	2.77085	2.54510	-0.23350
H	-5.18431	1.12807	-1.97589
H	-6.42773	0.11427	0.11773
H	3.74329	2.88151	-0.58842
S	1.41751	2.57347	-1.31473
H	3.18619	1.94105	1.79897

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H	1.049098	0.304205	-2.833133
C	0.450284	-0.338720	-2.186011
C	1.081005	-1.051189	-1.147118
C	2.457247	-1.094606	-0.765514
C	0.322480	-1.866065	-0.281305
S	1.276146	-2.628149	0.966381
C	-1.054614	-1.979256	-0.477683
S	-2.191729	-2.927416	0.419835
C	-1.680533	-1.264098	-1.519868
C	-3.091377	-1.508313	-1.546741
C	-0.910861	-0.440054	-2.366573
H	-1.406820	0.124678	-3.157882
C	2.720405	-1.885391	0.340571
C	4.087958	-1.913552	0.712211
C	4.836965	-1.139378	-0.134335
S	3.899765	-0.382424	-1.370614
C	-3.493418	-2.369848	-0.576528
H	-3.769860	-1.044338	-2.261966
H	4.502943	-2.469834	1.551867
H	5.912707	-0.973547	-0.100180
H	-4.505166	-2.717237	-0.373904
H	0.173867	-0.150634	2.835303
C	-0.559347	0.280727	2.152188
C	-0.126585	1.175583	1.152147
C	1.181347	1.676941	0.870987
C	-1.052696	1.730573	0.245145
S	-0.329803	2.836428	-0.894682
C	-2.401781	1.382264	0.345594
S	-3.721136	1.918160	-0.639232
C	-2.831704	0.499816	1.356648
C	-4.249298	0.298246	1.304648
C	-1.891375	-0.049284	2.254705
H	-2.230970	-0.741864	3.026404
C	1.235657	2.570274	-0.186522
C	2.534355	3.083621	-0.435818
C	3.439538	2.560199	0.448447
S	2.736447	1.454137	1.570725
C	-4.845442	0.994117	0.301428
H	-4.790543	-0.347018	1.996788
H	2.793446	3.794562	-1.219387
H	4.509568	2.756239	0.492234
H	-5.902591	1.017376	0.041036

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H	0.662852	-1.560726	-3.021934
C	0.135406	-1.630879	-2.069043
C	0.867053	-1.542218	-0.867342
C	2.269820	-1.379932	-0.647794
C	0.201980	-1.631164	0.373707
S	1.269380	-1.504425	1.744780
C	-1.182027	-1.816067	0.401368
S	-2.213130	-1.984750	1.782268
C	-1.906950	-1.904249	-0.804501
C	-3.304794	-2.096231	-0.560273
C	-1.229732	-1.807661	-2.038583
H	-1.799854	-1.875419	-2.966999
C	2.638808	-1.347725	0.686251
C	4.036037	-1.216020	0.893078
C	4.701445	-1.155863	-0.300824
S	3.648860	-1.245969	-1.668868
C	-3.601078	-2.160357	0.764336
H	-4.049308	-2.176350	-1.351897
H	4.525628	-1.171024	1.864988
H	5.773862	-1.051750	-0.457966
H	-4.580954	-2.291181	1.220660
H	-0.662852	1.560726	-3.021934
C	-0.135406	1.630879	-2.069043
C	-0.867053	1.542218	-0.867342
C	-2.269820	1.379932	-0.647794
C	-0.201980	1.631164	0.373707
S	-1.269380	1.504425	1.744780
C	1.182027	1.816067	0.401368
S	2.213130	1.984750	1.782268
C	1.906950	1.904249	-0.804501
C	3.304794	2.096231	-0.560273
C	1.229732	1.807661	-2.038583
H	1.799854	1.875419	-2.966999
C	-2.638808	1.347725	0.686251
C	-4.036037	1.216020	0.893078
C	-4.701445	1.155863	-0.300824
S	-3.648860	1.245969	-1.668868
C	3.601078	2.160357	0.764336
H	4.049308	2.176350	-1.351897
H	-4.525628	1.171024	1.864988
H	-5.773862	1.051750	-0.457966
H	4.580954	2.291181	1.220660

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H	0.988321	-2.253831	2.493953
C	1.612634	-1.833268	1.703483
C	1.055734	-1.622689	0.425810
C	-0.267478	-1.868160	-0.052769
C	1.840992	-1.073832	-0.609541
S	0.970440	-0.873972	-2.107791
C	3.173094	-0.740862	-0.356587
S	4.321531	-0.034390	-1.442248
C	3.724577	-0.949147	0.924942
C	5.085752	-0.506336	0.984005
C	2.927350	-1.502390	1.949177
H	3.360489	-1.658393	2.939271
C	-0.467709	-1.521481	-1.378216
C	-1.789566	-1.748117	-1.837386
C	-2.566734	-2.267421	-0.838034
S	-1.712918	-2.483997	0.647320
C	5.526743	0.000774	-0.198609
H	5.703080	-0.568264	1.880734
H	-2.156113	-1.524828	-2.837831
H	-3.626916	-2.511965	-0.882881
H	6.516529	0.393364	-0.427836
H	-0.988321	2.253831	-2.493953
C	-1.612634	1.833268	-1.703483
C	-1.055734	1.622689	-0.425810
C	0.267478	1.868160	0.052769
C	-1.840992	1.073832	0.609541
S	-0.970440	0.873972	2.107791
C	-3.173094	0.740862	0.356587
S	-4.321531	0.034390	1.442248
C	-3.724577	0.949147	-0.924942
C	-5.085752	0.506336	-0.984005
C	-2.927350	1.502390	-1.949177
H	-3.360489	1.658393	-2.939271
C	0.467709	1.521481	1.378216
C	1.789566	1.748117	1.837386
C	2.566734	2.267421	0.838034
S	1.712918	2.483997	-0.647320
C	-5.526743	-0.000774	0.198609
H	-5.703080	0.568264	-1.880734
H	2.156113	1.524828	2.837831
H	3.626916	2.511965	0.882881
H	-6.516529	-0.393364	0.427836

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H	-0.0000000082	-2.8597681752	-0.4141298303
C	-0.0000000042	-1.9390312796	0.173069922
C	-0.0000000017	-0.6919006325	-0.4897120346
C	-0.0000000049	-0.3901419785	-1.8904237079
C	0.0000000033	0.5068556547	0.2578604379
S	-0.0000000013	1.9420537903	-0.7388268295
C	0.0000000055	0.4755945925	1.6650808659
C	0.000000004	-0.7949354931	2.2851499226
S	0.000000023	-0.6394493121	4.0151908013
C	0.0000000028	-1.9951254394	1.5525732039
H	0.0000000053	-2.9570947047	2.0681461736
C	-0.0000000079	0.9677776799	-2.1809694925
C	-0.0000000038	1.2558613302	-3.5725995262

C	0.0000000095	0.100288941	-4.308900338
S	-0.0000000252	-1.3297557763	-3.3356713883
C	-0.0000000091	1.0865523456	3.9049247629
H	0.0000000014	2.2537266117	-4.0103183236
H	0.0000000207	0.0069114918	-5.3940758154
H	-0.000000017	1.6809800607	4.8179078523
C	0.0000000047	1.5430322838	2.6218170705
H	0.0000000033	2.600818009	2.3563462733

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H	-0.0000001231	-2.8778022638	-0.4278152532
C	-0.0000000896	-1.9590731508	0.1611607675
C	-0.0000000507	-0.6981362494	-0.5020496345
C	-0.0000001107	-0.4037727779	-1.8681795898
C	0.0000000136	0.5299420142	0.2553573444
S	-0.0000000971	1.9727866048	-0.734929614
C	0.0000000795	0.4955578212	1.6449617561
C	0.000000084	-0.7887171185	2.2631097102
S	0.0000004262	-0.6453223554	3.9629845747
C	0.0000000003	-2.0057439119	1.5289988651
H	0.0000000821	-2.9621557527	2.0547426949
C	-0.0000001385	0.9878611786	-2.1646938464
C	-0.0000000895	1.2629092592	-3.5328752568
C	0.0000002363	0.0790465753	-4.2643433639
S	-0.0000004394	-1.3552267765	-3.3161426955
C	-0.0000001188	1.0917913766	3.8842224882
H	-0.0000000046	2.252066541	-3.9903332303
H	0.0000004315	-0.0050901474	-5.3529650452
H	-0.0000002646	1.6653817212	4.8112070416
C	0.0000001086	1.5630317961	2.611387752
H	0.0000000645	2.623915616	2.3586345348

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H	0.0000000011	-2.8846797952	-0.4153931174
C	0.0000000004	-1.9627694539	0.1688783648
C	0.0000000004	-0.6963893916	-0.504594105
C	0.0000000003	-0.3840114274	-1.8825557753
C	-0.0000000007	0.4981593959	0.2656806192
S	0.0000000003	1.9435616922	-0.7344062934
C	-0.0000000008	0.4737564162	1.6675210329
C	-0.0000000003	-0.8220397932	2.3014946546
S	-0.0000000008	-0.6428583136	4.0593497005
C	-0.0000000009	-2.0006851245	1.5680200332
H	-0.0000000005	-2.9653475903	2.0842050267
C	0.0000000011	0.9885180082	-2.1998623477
C	0.0000000011	1.2683076289	-3.575103002
C	-0.0000000012	0.108703388	-4.3397320967
S	0.0000000021	-1.3382276108	-3.3446510529
C	0.0000000007	1.1068629068	3.9181220979
H	0.0000000008	2.2702174879	-4.0080453044
H	-0.0000000028	0.0191242534	-5.4241756364
H	0.0000000014	1.7183841333	4.8193859444
C	-0.0000000008	1.5343052693	2.6190342008
H	-0.0000000009	2.5903579207	2.3392670563

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H	0.945864	-2.388357	2.384619
C	1.475418	-1.966622	1.528260
C	0.774153	-1.730739	0.328641
C	-0.599173	-1.959653	0.007097
C	1.440194	-1.181339	-0.783845
S	0.402186	-0.958163	-2.165959
C	2.807563	-0.865759	-0.714920
C	3.470890	-1.121294	0.502511
S	5.136933	-0.651850	0.408880
C	2.818019	-1.664245	1.620697
H	3.365322	-1.843651	2.547507
C	-0.949976	-1.598596	-1.282154
C	-2.318151	-1.819561	-1.586180
C	-2.975658	-2.353499	-0.512442
S	-1.955151	-2.580895	0.863873
C	4.946171	-0.132843	-1.228316
H	-2.797905	-1.590606	-2.536452
H	-4.031994	-2.606405	-0.443675
H	5.802721	0.271194	-1.766442
C	3.679714	-0.298973	-1.696840
H	3.365221	-0.026615	-2.704240
H	-1.527935	0.415578	3.018927
C	-0.979434	0.840449	2.176257
C	-1.651865	1.078285	0.959680
C	-3.017720	0.852935	0.603216
C	-0.954184	1.612818	-0.139917

antifacial_y

0 1

H	2.891194	-1.629941	-0.006909
C	1.898304	-1.652516	-0.459464
C	0.758966	-1.659268	0.371002
C	0.665263	-1.669296	1.796410
C	-0.530317	-1.662317	-0.193760
S	-1.803025	-1.670956	0.999968
C	-0.700359	-1.680555	-1.588796
C	0.465782	-1.702301	-2.380877
S	0.069013	-1.779814	-4.065737
C	1.756940	-1.677125	-1.830111
H	2.632980	-1.671223	-2.480031
C	-0.630635	-1.682989	2.281937
C	-0.711410	-1.711992	3.698187
C	0.537787	-1.726551	4.255684
S	1.806728	-1.693906	3.083003
C	-1.621172	-1.753587	-3.715033
H	-1.634669	-1.718154	4.275644
H	0.788778	-1.742912	5.315036
H	-2.339058	-1.782134	-4.533628
C	-1.890539	-1.703392	-2.381597
H	-2.898612	-1.683959	-1.967347
H	-2.891194	1.629941	-0.006909
C	-1.898304	1.652516	-0.459464
C	-0.758966	1.659268	0.371002
C	-0.665263	1.669296	1.796410
C	0.530317	1.662317	-0.193760

S	-1.953110	1.823746	-1.554014
C	0.412671	1.921819	-0.041646
C	1.044255	1.675804	1.194514
S	2.719240	2.118529	1.130215
C	0.362200	1.136124	2.296533
H	0.889441	0.949138	3.233009
C	-3.330901	1.200695	-0.700153
C	-4.681318	0.948522	-1.052577
C	-5.367425	0.411700	0.004072
S	-4.393085	0.216262	1.417231
C	2.571674	2.613540	-0.515586
H	-5.128325	1.151384	-2.025233
H	-6.418577	0.128418	0.035070
H	3.447770	2.993698	-1.038224
C	1.314001	2.459102	-1.012661
H	1.029494	2.712126	-2.033931

S	1.803025	1.670956	0.999968
C	0.700359	1.680555	-1.588796
C	-0.465782	1.702301	-2.380877
S	-0.069013	1.779814	-4.065737
C	-1.756940	1.677125	-1.830111
H	-2.632980	1.671223	-2.480031
C	0.630635	1.682989	2.281937
C	0.711410	1.711992	3.698187
C	-0.537787	1.726551	4.255684
S	-1.806728	1.693906	3.083003
C	1.621172	1.753587	-3.715033
H	1.634669	1.718154	4.275644
H	-0.788778	1.742912	5.315036
H	2.339058	1.782134	-4.533628
C	1.890539	1.703392	-2.381597
H	2.898612	1.683959	-1.967347

antifacial_z

0 1

H	0.59271	-1.52854	-2.88742
C	0.10554	-1.60163	-1.91355
C	0.88596	-1.52689	-0.74192
C	2.30043	-1.39276	-0.58450
C	0.27114	-1.60918	0.52179
S	1.40124	-1.51503	1.84485
C	-1.11928	-1.77616	0.63501
C	-1.85867	-1.85410	-0.56265
S	-3.54322	-2.08616	-0.23479
C	-1.26064	-1.76664	-1.82996
H	-1.87076	-1.82322	-2.73267
C	2.72896	-1.38227	0.73202
C	4.13788	-1.29021	0.87567
C	4.74884	-1.23060	-0.34698
S	3.63341	-1.27869	-1.66598
C	-3.26001	-2.07648	1.46854
H	4.67509	-1.26684	1.82294
H	5.81506	-1.14641	-0.55087
H	-4.09843	-2.19917	2.15272
C	-1.94963	-1.90467	1.79221
H	-1.57783	-1.86513	2.81583
H	-0.59271	1.52854	-2.88742
C	-0.10554	1.60163	-1.91355
C	-0.88596	1.52689	-0.74192
C	-2.30043	1.39276	-0.58450
C	-0.27114	1.60918	0.52179
S	-1.40124	1.51503	1.84485
C	1.11928	1.77616	0.63501
C	1.85867	1.85410	-0.56265
S	3.54322	2.08616	-0.23479
C	1.26064	1.76664	-1.82996
H	1.87076	1.82322	-2.73267
C	-2.72896	1.38227	0.73202
C	-4.13788	1.29021	0.87567
C	-4.74884	1.23060	-0.34698
S	-3.63341	1.27869	-1.66598
C	3.26001	2.07648	1.46854
H	-4.67509	1.26684	1.82294
H	-5.81506	1.14641	-0.55087
H	4.09843	2.19917	2.15272
C	1.94963	1.90467	1.79221

antifacial_yz

0 1

H	0.996735	-2.315286	2.399023
C	1.539772	-1.902671	1.546945
C	0.861978	-1.694817	0.329008
C	-0.504560	-1.933384	-0.013472
C	1.545102	-1.155002	-0.777662
S	0.530403	-0.955299	-2.181741
C	2.907235	-0.823628	-0.686538
C	3.544919	-1.044015	0.550824
S	5.203656	-0.542242	0.488132
C	2.875795	-1.579373	1.662772
H	3.404634	-1.734753	2.604638
C	-0.835045	-1.587911	-1.312737
C	-2.198840	-1.807978	-1.633795
C	-2.874284	-2.323761	-0.561795
S	-1.874972	-2.537626	0.830988
C	5.044194	-0.062183	-1.165699
H	-2.665046	-1.587942	-2.592874
H	-3.933752	-2.566781	-0.504034
H	5.905954	0.347159	-1.691254
C	3.793111	-0.261955	-1.659979
H	3.498652	-0.016350	-2.680212
H	-0.996735	2.315286	-2.399023
C	-1.539772	1.902671	-1.546945
C	-0.861978	1.694817	-0.329008
C	0.504560	1.933384	0.013472
C	-1.545102	1.155002	0.777662
S	-0.530403	0.955299	2.181741
C	-2.907235	0.823628	0.686538
C	-3.544919	1.044015	-0.550824
S	-5.203656	0.542242	-0.488132
C	-2.875795	1.579373	-1.662772
H	-3.404634	1.734753	-2.604638
C	0.835045	1.587911	1.312737
C	2.198840	1.807978	1.633795
C	2.874284	2.323761	0.561795
S	1.874972	2.537626	-0.830988
C	-5.044194	0.062183	1.165699
H	2.665046	1.587942	2.592874
H	3.933752	2.566781	0.504034
H	-5.905954	-0.347159	1.691254
C	-3.793111	0.261955	1.659979

H	1.57783	1.86513	2.81583	H	-3.498652	0.016350	2.680212

BTBT

0 1
C -0.0000000003 -0.5387413693 1.7434577448
C -0.0000000004 0.8195700531 2.1578925297
S 0. 1.9388646326 0.8120835837
C 0.0000000008 0.614816035 -0.3138082902
C 0.0000000003 -0.614816035 0.3138082902
C 0.000000001 0.5387413693 -1.7434577448
C 0.0000000009 -0.8195700531 -2.1578925297
S 0.000000001 -1.9388646326 -0.8120835837
C -0.0000000006 -1.5509263169 2.7151491689
C -0.0000000005 1.1607547618 3.5114113159
C 0.0000000009 1.5509263169 -2.7151491689
C 0.0000000004 -1.1607547618 -3.5114113159
C -0.0000000002 -1.2068638234 4.0582273069
C 0. 0.1401812216 4.4539253624
C -0.0000000003 1.2068638234 -4.0582273069
C -0.0000000007 -0.1401812216 -4.4539253624
H -0.0000000005 -2.5988750893 2.4068010392
H -0.0000000004 2.207757505 3.8214978231
H 0.0000000008 2.5988750893 -2.4068010392
H 0.0000000002 -2.207757505 -3.8214978231
H 0. -1.9913679571 4.8178735035
H 0.0000000003 0.3914697472 5.5167691227
H -0.000000001 1.9913679571 -4.8178735035
H -0.0000000016 -0.3914697472 -5.5167691227

1 2			-1 2		
C	0.0000000057	-0.5530739041 1.7420154561	C	0.0000000007	-0.5512070645 1.7365738346
C	-0.0000000057	0.8066142699 2.1497772762	C	-0.0000000005	0.8184335864 2.1787019092
S	-0.0000000153	1.9324317873 0.7834331974	S	-0.0000000087	1.945204213 0.8177230329
C	-0.0000000143	0.6385916289 -0.3221949289	C	-0.0000000072	0.6204185626 -0.3362124575
C	-0.0000000004	-0.6385916289 0.3221949289	C	-0.0000000019	-0.6204185626 0.3362124575
C	-0.0000000192	0.5530739041 -1.7420154561	C	-0.0000000042	0.5512070645 -1.7365738346
C	-0.0000000152	-0.8066142699 -2.1497772762	C	-0.0000000042	-0.8184335864 -2.1787019092
S	-0.0000000153	-1.9324317873 -0.7834331974	S	-0.00000001	-1.945204213 -0.8177230329
C	0.0000000125	-1.5672263379 2.7151068076	C	0.0000000048	-1.5627694427 2.7394062665
C	-0.0000000006	1.1624820418 3.4853476404	C	0.0000000042	1.1573074269 3.5189348756
C	-0.0000000105	1.5672263379 -2.7151068076	C	0.0000000012	1.5627694427 -2.7394062665
C	-0.0000000089	-1.1624820418 -3.4853476404	C	-0.0000000009	-1.1573074269 -3.5189348756
C	0.0000000028	-1.2129183792 4.0599352416	C	0.000000003	-1.2061426049 4.0822006156
C	0.0000000035	0.1319095856 4.4393784647	C	0.0000000005	0.1338788249 4.4924510211
C	0.0000000134	1.2129183792 -4.0599352416	C	0.0000000043	1.2061426049 -4.0822006156
C	0.0000000104	-0.1319095856 -4.4393784647	C	0.0000000038	-0.1338788249 -4.4924510211
H	0.0000000117	-2.6173106278 2.4147201834	H	0.0000000044	-2.6141752659 2.4409026265
H	-0.0000000018	2.2082461565 3.7985226098	H	0.0000000021	2.208925508 3.8193772972
H	0.0000000024	2.6173106278 -2.4147201834	H	-0.0000000015	2.6141752659 -2.4409026265
H	-0.0000000046	-2.2082461565 -3.7985226098	H	-0.0000000029	-2.208925508 -3.8193772972
H	0.0000000033	-1.990754206 4.8252727882	H	0.0000000024	-1.996230831 4.8405489055
H	0.0000000092	0.3935912277 5.4996635522	H	-0.0000000015	0.3892380722 5.5547104933
H	0.0000000272	1.990754206 -4.8252727882	H	0.0000000058	1.996230831 -4.8405489055
H	0.0000000099	-0.3935912277 -5.4996635522	H	0.0000000063	-0.3892380722 -5.5547104933

cofacial

0 1

C	-0.498985	1.953275	-0.021217
C	-0.930063	1.565908	1.270482
S	0.356587	0.881243	2.235348

antifacial

0 1

C	-2.099278	-1.441848	0.747980
C	-2.675599	-1.410477	-0.545602
S	-1.485782	-1.547083	-1.817717

C	1.477665	1.104973	0.932307	C	-0.214501	-1.646185	-0.644012
C	0.892163	1.668369	-0.178959	C	-0.681147	-1.578766	0.649634
C	2.866848	0.814838	0.773705	C	1.202791	-1.793950	-0.745775
C	3.296538	1.188006	-0.522618	C	1.779594	-1.834252	0.545478
S	2.012271	1.873622	-1.487580	S	0.594679	-1.695806	1.820404
C	-1.422052	2.516887	-0.911111	C	-2.931749	-1.342193	1.869886
C	-2.254983	1.732888	1.669047	C	-4.052729	-1.290807	-0.719774
C	3.786021	0.243278	1.662558	C	2.031548	-1.894821	-1.870674
C	4.614348	0.987619	-0.930681	C	3.156338	-1.967698	0.717791
C	-2.736676	2.685403	-0.508794	C	-4.300813	-1.224012	1.692580
C	-3.151057	2.297472	0.772666	C	-4.858623	-1.202619	0.406359
C	5.094151	0.044358	1.254611	C	3.398076	-2.034005	-1.696786
C	5.504948	0.410716	-0.035915	C	3.956134	-2.068049	-0.410366
H	-1.099242	2.812751	-1.911368	H	-2.495493	-1.358940	2.870709
H	-2.580720	1.418568	2.661987	H	-4.485742	-1.264015	-1.721152
H	3.460951	-0.048464	2.663189	H	1.594845	-1.859848	-2.870556
H	4.937244	1.275671	-1.933064	H	3.594218	-1.983967	1.716733
H	-3.463870	3.115915	-1.199668	H	-4.954346	-1.150916	2.564403
H	-4.195421	2.422147	1.063517	H	-5.939925	-1.108924	0.286713
H	5.814274	-0.404020	1.942063	H	4.049494	-2.113958	-2.569404
H	6.540807	0.246656	-0.340475	H	5.037099	-2.164897	-0.292299
C	-2.866628	-0.814674	-0.774343	C	-1.202788	1.793914	-0.745929
C	-3.296858	-1.187752	0.521825	C	-1.779589	1.834315	0.545322
S	-2.013041	-1.873542	1.487276	S	-0.594669	1.696032	1.820260
C	-0.892410	-1.668455	0.179073	C	0.681157	1.578917	0.649501
C	-1.477429	-1.104995	-0.932415	C	0.214507	1.646197	-0.644150
C	0.498764	-1.953500	0.021836	C	2.099284	1.441979	0.747858
C	0.930403	-1.566053	-1.269647	C	2.675594	1.410392	-0.545725
S	-0.355842	-0.881332	-2.235022	S	1.485778	1.546888	-1.817850
C	-3.785381	-0.243013	-1.663568	C	-2.031554	1.894674	-1.870830
C	-4.614803	-0.987186	0.929358	C	-3.156339	1.967684	0.717631
C	1.421397	-2.517315	0.912055	C	2.931760	1.342476	1.869772
C	2.255492	-1.733076	-1.667659	C	4.052715	1.290601	-0.719884
C	-5.093643	-0.043908	-1.256141	C	-3.398086	2.033822	-1.696947
C	-5.504983	-0.410189	0.034234	C	-3.956144	2.067918	-0.410529
C	2.736155	-2.685964	0.510247	C	4.300819	1.224219	1.692475
C	3.151118	-2.297896	-0.770985	C	4.858616	1.202570	0.406254
H	-3.459867	0.048668	-2.664074	H	-1.594857	1.859639	-2.870712
H	-4.938126	-1.275153	1.931628	H	-3.594222	1.983949	1.716571
H	1.098112	-2.813330	1.912115	H	2.495521	1.359401	2.870601
H	2.581676	-1.418613	-2.660404	H	4.485712	1.263573	-1.721263
H	-5.813434	0.404560	-1.943881	H	-4.049507	2.113703	-2.569569
H	-6.540935	-0.245987	0.338401	H	-5.037114	2.164691	-0.292466
H	3.463011	-3.116702	1.201336	H	4.954354	1.151254	2.564308
H	4.195603	-2.422593	-1.061387	H	5.939910	1.108780	0.286612

TB

0 1

C 0.0000000005 0.5623681609 0.4288355793
C -0.0000000075 1.8683233519 -0.1508955939
H -0.000000009 2.7447311974 0.4971519654
C -0.0000000068 2.053319674 -1.5013158394
H -0.000000003 3.064165674 -1.9174411377
C -0.0000000049 0.9457905546 -2.39843792
C -0.0000000087 1.1411428864 -3.7994778152
C -0.0000000098 -0.3755864387 -1.8663773018
C 0. -1.4537342379 -2.7843370064
C 0.0000000048 -0.5623681609 -0.4288355793
C -0.0000000016 -1.8683233519 0.1508955939
C 0.0000000142 0.3755864387 1.8663773018

C -0.0000000036 -0.9457905546 2.39843792
C -0.0000000007 -2.053319674 1.5013158394
C -0.0000000105 -1.1411428864 3.7994778152
H -0.0000000083 -2.1646336994 4.1840501616
C -0.0000000012 -0.0694556725 4.6649262081
H -0.000000004 -0.2318413957 5.7453294634
C 0.0000000047 1.2396822054 4.14752337
H 0.0000000184 2.093989529 4.8287604105
C 0.0000000081 1.4537342379 2.7843370064
H 0.0000000159 2.4810589916 2.4192483649
C -0.0000000085 0.0694556725 -4.6649262081
C 0.000000007 -1.2396822054 -4.14752337
H -0.0000000113 2.1646336994 -4.1840501616
H 0.0000000196 -2.4810589916 -2.4192483649
H -0.000000011 -2.7447311974 -0.4971519654
H -0.0000000128 -3.064165674 1.9174411377
H 0.0000000046 0.2318413957 -5.7453294634
H 0.0000000251 -2.093989529 -4.8287604105

1 2

C	0.0000000052	0.5752238116	0.4366766234
C	0.0000000047	1.853960776	-0.1406497152
H	0.0000000048	2.7412585276	0.4917985993
C	0.0000000042	2.0306261886	-1.5151394987
H	0.0000000029	3.0446048341	-1.9238844551
C	0.0000000021	0.9334973551	-2.4102511592
C	-0.0000000014	1.1434445706	-3.8072875698
C	0.000000003	-0.3896553519	-1.8815570714
C	0.0000000006	-1.4572325227	-2.7922480525
C	0.0000000053	-0.5752238116	-0.4366766234
C	0.0000000046	-1.853960776	0.1406497152
C	0.000000003	0.3896553519	1.8815570714
C	0.0000000021	-0.9334973551	2.4102511592
C	0.0000000044	-2.0306261886	1.5151394987
C	-0.0000000013	-1.1434445707	3.8072875698
H	-0.0000000024	-2.1674456696	4.1888058994
C	-0.000000005	-0.0679608935	4.6822720311
H	-0.0000000085	-0.2342540423	5.7612467864
C	-0.0000000042	1.2317918637	4.1688460508
H	-0.0000000067	2.0863201388	4.8491953624
C	0.0000000006	1.4572325227	2.7922480525
H	0.0000000005	2.4896726457	2.4419171226
C	-0.000000005	0.0679608935	-4.6822720311
C	-0.0000000041	-1.2317918637	-4.1688460508
H	-0.0000000025	2.1674456696	-4.1888058994
H	0.0000000005	-2.4896726457	-2.4419171226
H	0.0000000047	-2.7412585276	-0.4917985993
H	0.0000000028	-3.0446048341	1.9238844551
H	-0.0000000083	0.2342540423	-5.7612467864
H	-0.0000000066	-2.0863201388	-4.8491953624

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C	-0.0000000277	0.5783227334	0.4381033236
C	-0.0000000319	1.8554032154	-0.143691027
H	-0.0000000184	2.7370197806	0.5021083928
C	-0.0000000067	2.0551343326	-1.5156578843
H	0.0000000183	3.0690787242	-1.9261374063
C	-0.0000000129	0.9520481434	-2.4166062837
C	0.0000000138	1.1355878163	-3.8200136699
C	-0.0000000347	-0.3830073916	-1.8859036568
C	-0.0000000101	-1.4476090953	-2.809449577
C	-0.0000000185	-0.5783227334	-0.4381033236
C	-0.0000000093	-1.8554032154	0.143691027
C	-0.0000000098	0.3830073916	1.8859036568
C	-0.0000000201	-0.9520481434	2.4166062837
C	0.0000000021	-2.0551343326	1.5156578843
C	-0.0000000012	-1.1355878163	3.8200136699
H	-0.000000005	-2.160107612	4.2061917325
C	0.0000000177	-0.0577216898	4.7002008392
H	0.0000000274	-0.2307006927	5.7810356976
C	0.000000011	1.2415329152	4.1913551866
H	0.0000000185	2.1021045361	4.8671188637
C	-0.0000000024	1.4476090953	2.809449577
H	0.0000000007	2.4753304685	2.440611747
C	0.0000000109	0.0577216898	-4.7002008392
C	-0.0000000026	-1.2415329152	-4.1913551866
H	0.0000000249	2.160107612	-4.2061917326
H	0.0000000072	-2.4753304685	-2.440611747
H	-0.0000000061	-2.7370197806	-0.5021083928
H	0.0000000263	-3.0690787241	1.9261374063
H	0.0000000267	0.2307006927	-5.7810356976
H	0.0000000117	-2.1021045362	-4.8671188637

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C	-0.76409	-1.65995	0.08469
C	-1.35441	-2.03502	1.32547
C	-2.67646	-1.83123	1.57976
C	-3.52562	-1.23127	0.60990
C	-2.97915	-0.84363	-0.64246
C	-1.57537	-1.06098	-0.90060
C	-0.98226	-0.67398	-2.13716

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C	-0.052897	0.099270	-0.327592
C	-0.169342	1.308647	-1.070448
H	-0.180289	2.260990	-0.542834
C	-0.258502	1.307610	-2.428742
H	-0.345932	2.247635	-2.977210
C	-0.215623	0.092749	-3.164980
C	-0.285808	0.096500	-4.574849

C	0.34164	-0.87149	-2.38472	C	-0.076632	-1.135442	-2.465959
C	1.18955	-1.47937	-1.41804	C	0.014909	-2.320441	-3.230554
C	0.64007	-1.87964	-0.17206	C	-0.017093	-1.126556	-1.023541
C	-4.89295	-1.00802	0.88029	C	0.081306	-2.337375	-0.278152
C	-5.71232	-0.41984	-0.05603	C	0.025149	0.112339	1.114901
C	-5.18106	-0.04253	-1.30209	C	0.130462	-1.117157	1.817287
C	-3.84829	-0.25033	-1.58401	C	0.152692	-2.334665	1.081394
C	1.50776	-2.47607	0.76890	C	0.213339	-1.117405	3.225790
C	2.84372	-2.66865	0.49083	H	0.303220	-2.075259	3.743287
C	3.38109	-2.27048	-0.74485	C	0.192635	0.061055	3.935442
C	2.56151	-1.68187	-1.67931	H	0.271719	0.051988	5.023968
H	-0.73518	-2.49206	2.09564	C	0.084188	1.280399	3.247002
H	-3.10564	-2.12481	2.54072	H	0.079103	2.219519	3.804227
H	-5.28863	-1.31157	1.85272	C	0.003176	1.303797	1.871698
H	-6.76911	-0.25155	0.16262	H	-0.066539	2.267089	1.369204
H	-5.82711	0.42000	-2.05147	C	-0.200832	-1.074454	-5.291426
H	-3.46577	0.05974	-2.55547	C	-0.041014	-2.293635	-4.607798
H	-1.59743	-0.20450	-2.90325	H	-0.394465	1.055758	-5.086297
H	0.77804	-0.56038	-3.33628	H	0.134430	-3.281651	-2.731313
H	2.96348	-1.35116	-2.63960	H	0.098046	-3.291051	-0.804123
H	4.44409	-2.40678	-0.94998	H	0.226085	-3.275547	1.632179
H	3.49198	-3.12595	1.24117	H	-0.250849	-1.060686	-6.382306
H	1.12481	-2.79163	1.73870	H	0.032278	-3.227185	-5.170138
C	1.57086	1.07778	0.91008	C	3.302064	0.010181	0.638454
C	0.97851	0.68597	2.14559	C	3.310032	-1.227029	-0.066458
C	-0.34500	0.88335	2.39533	H	3.369292	-2.161228	0.488689
C	-1.19381	1.49432	1.43129	C	3.225007	-1.273912	-1.424013
C	-0.64501	1.89923	0.18645	H	3.212395	-2.234178	-1.944151
C	0.75915	1.68128	-0.07200	C	3.141623	-0.084872	-2.198370
C	2.97458	0.86186	0.65034	C	3.060235	-0.141342	-3.605996
C	3.52016	1.25377	-0.60108	C	3.138824	1.171964	-1.537525
C	3.84507	0.26851	1.59063	C	3.068866	2.334900	-2.335888
C	4.88789	1.03354	-0.87204	C	3.203492	1.210830	-0.095582
C	5.17865	0.06559	1.30902	C	3.167356	2.446550	0.612864
C	5.70889	0.44636	0.06356	C	3.394336	0.051500	2.079372
H	3.46269	-0.04457	2.56118	C	3.373043	1.306604	2.743138
H	1.59398	0.21232	2.90883	C	3.247742	2.494622	1.971707
C	-1.51338	2.49868	-0.75185	C	3.469289	1.359052	4.150011
H	5.28303	1.34006	-1.84377	H	3.444262	2.336420	4.638230
H	5.82604	-0.39544	2.05817	C	3.593288	0.208107	4.894778
H	6.76633	0.28220	-0.15503	H	3.671391	0.260209	5.982889
C	-2.56567	1.69558	1.69393	C	3.617081	-1.037586	4.244813
H	-0.78055	0.56876	3.34614	H	3.711927	-1.955168	4.829567
C	-2.84935	2.68979	-0.47248	C	3.513302	-1.110692	2.872503
C	-3.38601	2.28754	0.76212	H	3.520626	-2.091538	2.398739
H	-1.13109	2.81815	-1.72065	C	2.991242	1.009451	-4.355585
H	-2.96718	1.36066	2.65295	C	2.998289	2.258652	-3.710261
H	-3.49741	3.15023	-1.22106	H	3.031543	-1.121196	-4.087550
H	-4.44886	2.42396	0.96822	H	3.070938	3.318368	-1.866735
C	1.34870	2.06152	-1.31159	H	3.075236	3.379504	0.058213
C	2.67035	1.85765	-1.56801	H	3.219716	3.454723	2.492369
H	0.72936	2.52308	-2.07899	H	2.920796	0.953890	-5.443610
H	3.09907	2.15565	-2.52780	H	2.949844	3.176376	-4.300756

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S	0.0000000019	-1.8589616741	0.9812356477
C	0.0000000011	-0.6391290423	-0.2573111984
C	0.000000001	0.6574985478	0.2576748123
C	0.000000002	0.6615855663	1.6766398132

C -0.0000000005 -0.6267358852 2.2118267372
C 0.0000000004 -0.6438805933 -1.6765663653
C -0.0000000037 0.644390116 -2.2114896623
S -0.0000000005 1.8771684085 -0.9812599057
S 0.0000000006 1.849103531 2.9273749426
C -0.0000000006 0.6182508347 4.1447168792
C 0.0000000004 -0.6513392466 3.6322113756
S -0.0000000061 -1.8311801703 -2.927607709
C 0.0000000012 -0.600061256 -4.14488474
C -0.0000000009 0.6694765288 -3.6321158856
H 0.0000000036 -0.8910517294 -5.1946998428
H 0.0000000011 1.5698934676 -4.2463420809
H -0.0000000019 0.909209264 5.1944844872
H 0.000000001 -1.5517166675 4.246552695

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S 0.0000000014 -1.8849662424 0.9683024522
C 0.0000000059 -0.6590237473 -0.2623312393
C 0.0000000022 0.6775618464 0.2621487819
C 0.0000000072 0.6773774244 1.6498507117
C -0.0000000131 -0.6382074051 2.1889840493
C 0.0000000078 -0.6594297498 -1.6500852479
C -0.0000000178 0.6559807 -2.1886782127
S -0.0000000022 1.9031971094 -0.9685322172
S -0.0000000105 1.8691977317 2.9072534182
C 0.0000000061 0.6276168638 4.0943046868
C -0.0000000093 -0.6639483642 3.5865006801
S -0.0000000046 -1.85137432 -2.9070886026
C 0.0000000074 -0.6094440148 -4.0942077172
C -0.0000000059 0.6820494094 -3.5864487835
H 0.0000000107 -0.8894397018 -5.1495548387
H 0.0000000006 1.5746273454 -4.2123237831
H 0.0000000216 0.907137133 5.1497696752
H -0.0000000073 -1.556392018 4.2125761869

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S -0.000000017 -1.8755833331 0.9821460896
C -0.0000000157 -0.6458015959 -0.2763296953
C -0.0000000182 0.6645273964 0.2764035894
C -0.000000008 0.6652234267 1.6700879292
C 0.0000000028 -0.6345001338 2.2352837876
C -0.0000000174 -0.6471447942 -1.6701305192
C -0.0000000012 0.6523549761 -2.2351323661
S -0.0000000266 1.8940938215 -0.9827749603
S -0.0000000172 1.8656282955 2.9374664675
C 0.0000000046 0.6254101256 4.1829263207
C 0.0000000242 -0.6501465818 3.6375896593
S -0.0000000373 -1.8477390138 -2.9371089853
C 0.0000000103 -0.6075139899 -4.1828671109
C 0.0000000176 0.6682298964 -3.6374477655
H 0.000000019 -0.8959628639 -5.2319797546
H 0.0000000396 1.5743805129 -4.2468901359
H 0.0000000023 0.9133802709 5.2321548282
H 0.0000000383 -1.5563164157 4.2470426216

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S	0.109920	-1.792871	0.447007
C	-0.104390	-0.599113	-0.792671
C	-0.140316	0.700422	-0.294074
C	-0.000290	0.728820	1.113819
C	0.144484	-0.545139	1.656333
C	-0.235994	-0.625469	-2.201571
C	-0.364113	0.649530	-2.746284
S	-0.328565	1.896645	-1.535739
S	0.054076	1.933157	2.341374
C	0.261454	0.726480	3.563634
C	0.298577	-0.546380	3.066138
S	-0.244373	-1.827662	-3.432258
C	-0.403239	-0.618904	-4.660478
C	-0.457817	0.654465	-4.160880
H	-0.467369	-0.924048	-5.703847
H	-0.563512	1.543699	-4.781550
H	0.375955	1.034240	4.601334
H	0.439082	-1.432822	3.682655
S	3.577823	-1.636184	2.021285
C	3.391965	-0.430094	0.788949
C	3.357328	0.865575	1.297547
C	3.487714	0.880800	2.706708
C	3.613546	-0.398651	3.241521

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S	0.086245	-1.799530	1.023594
C	0.026167	-0.602868	-0.232161
C	-0.062573	0.695950	0.262220
C	-0.083418	0.721928	1.677263
C	-0.011790	-0.554074	2.229583
C	0.029052	-0.626145	-1.647358
C	-0.060146	0.649088	-2.199719
S	-0.135034	1.893602	-0.988589
S	-0.189531	1.921436	2.906893
C	-0.132224	0.710219	4.139630
C	-0.035599	-0.561800	3.646975
S	0.087718	-1.828154	-2.877321
C	-0.021994	-0.620587	-4.113002
C	-0.088992	0.652235	-3.617753
H	-0.021628	-0.926452	-5.157889
H	-0.154897	1.542860	-4.241358
H	-0.162593	1.013366	5.184795
H	0.024681	-1.451826	4.271176
S	3.198203	2.052484	1.485717
C	3.248054	0.851732	0.236700
C	3.291310	-0.448588	0.733308
C	3.289630	-0.469906	2.148475
C	3.248105	0.808655	2.698798

C	3.251852	-0.447593	-0.619161	C	3.266345	0.877169	-1.178448
C	3.109993	0.830721	-1.152011	C	3.323889	-0.400539	-1.728378
S	3.144555	2.069071	0.066849	S	3.351586	-1.647490	-0.520337
S	3.495453	2.073036	3.947001	S	3.351783	-1.669869	3.380258
C	3.651489	0.854430	5.165788	C	3.337583	-0.455416	4.614049
C	3.705609	-0.414947	4.656184	C	3.275027	0.816844	4.116863
S	3.193043	-1.642686	-1.855467	S	3.250902	2.078953	-2.410344
C	2.985831	-0.426503	-3.068327	C	3.315969	0.865898	-3.640845
C	2.953646	0.842780	-2.561434	C	3.347929	-0.408492	-3.145757
H	2.867686	-0.726138	-4.108015	H	3.315847	1.168399	-4.686643
H	2.814579	1.734312	-3.170930	H	3.378417	-1.301296	-3.768143
H	3.714382	1.151266	6.211625	H	3.366399	-0.758213	5.659433
H	3.809937	-1.309208	5.269828	H	3.249577	1.710428	4.739198