12-2020

Chemical Investigation of Avocado (*Persea americana*) Seed Husk (Testa): A Waste of Waste

Orlando A. Castillo Scheren
The University of Texas Rio Grande Valley

CHEMICAL INVESTIGATION OF AVOCADO (*Persea americana*) SEED HUSK (TESTA): A WASTE OF WASTE

A Thesis

by

Orlando A. Castillo Scheren

Submitted to the Graduate College of
The University of Texas Rio Grande Valley
In partial fulfillment of the requirements for the degree of
MASTER OF SCIENCE

December 2020

Major Subject: Chemistry

CHEMICAL INVESTIGATION OF AVOCADO (PERSEA AMERICANA) SEED HUSK: A WASTE OF WASTE

A Thesis
by
ORLANDO A. CASTILLO SCHEREN

COMMITTEE MEMBERS

Dr. Debasish Bandyopadhyay
Chair of the Committee

Dr. Javier Macossay-Torres
Committee Member

Dr. Evangelia Kotsikorou
Committee Member

Dr. Frank Dean
Committee Member

December 2020

ABSTRACT

Castillo Scheren, Orlando A., A Chemical Investigation of Avocado (Persea Americana) Seed Husk (Testa): A Waste of Waste, Master of Science (MS), December 2020, 125pp., 6 tables, 84 figures, references 101 titles.

Food chemistry is a new field in the world and is currently still expanding into the types of market in which it can be tapped into. There are about 1.3 billion tons of food waste produced in 2016 in the world, and food chemistry is going to help get rid of that waste by finding new and exciting applications to the things currently considered as waste. In these products, there might be new and undiscovered drugs that can be used in the market to help treat diseases for which might not have a cure at the current moment. The avocado (*Persea americana*) is a widely adored fruit due to its nutritional properties and in the versatility of where it can be used. Though the seed is an untapped source of potential as it is one of the most underused parts of the avocado, accounting for about 13-18% of the fruit, mostly just heading to the trash as the avocado is processed for drinks, guacamole, and some medications. As production of the fruit increases the amount of waste that is produced unfortunately increases as well, to find a new use for the seed rather than just letting it rot inside a landfill or burning it for space, this study will focus on the untapped chemical sources of the avocado seed husk. In this way using the principles of Natural Product Chemistry is it a hope that new use is discovered for the husk of the seed that which is already considered a waste of waste.

ACKNOWLEDGMENT

Thank you to the Department of Chemistry for all the help and support that was given to me over the years, and to Dr. B. Connie Allen as she helped me and my lab out during these trying times of COVID-19.

Thank you to my thesis committee members for the advice that has been given to me professionally and informally I will forever enjoy the moments that we had together throughout the years.

Thank you to the C-Stem center for providing funding to me while I was working on my thesis, and to Dr. Villalobos and Idalia Mejia for all the help they have given me these past years.

Thank you to Dr. Debasish Bandyopadhyay for all the direction and help he's given to me during my undergrad and graduate career of college. I will remember the times in your laboratory very fondly.

TABLE OF CONTENTS

LIST OF TABLES

Page

LIST OF FIGURES

CHAPTER I

REVIEW

Food Chemistry is currently a brand-new field in the world that is being discussed; generally, it is to see if many plants that are used in people's daily life have any other uses whether it be medicinally or industrially. The reason for this is to tackle the increasing problem of food waste that is currently produced in the world. This is important since a lot of the food that is consumed is processed industrially, and as the industrial process goes, waste is generally produced. In 2016, about 31.4 million tons is produced in the US, 15 million tons in the United Kingdom, and 90 million tons in China; with the Food and Agriculture Organization (FAO) estimating about 1.3 billion tons of food waste produced annually.[1–3] Though a definition for food waste must be produced, the United States Department of Agriculture (USDA) defines it as anything that is either lost in the production, transportation, or spoilage from the farm to retail stores[4]. In finding, a new purpose for the parts of food that are not used and just discarded, it would be possible to reduce food waste, drastically and repurposed to something more useful.

The Avocado (*Perces americana*) fruit is a widely popular agricultural product that is mostly produced in tropical and Mediterranean trees and shrubs, with an origin in countries such as Mexico and South America[5]. The avocado is commonly/affectionally referred to as the "perfect fruit", due to its nutritional value and the healthy dietary effects that the fruit carries.[6] Containing mostly carbohydrates, it carries about 75% of total fat, with mostly mono- and

polyunsaturated, proven to be much healthier than saturated fats[6]. It has also been shown that the probability of cardiovascular diseases (CVD) is less likely to occur if it is incorporated into the daily diet. Looking at the normal Mediterranean diet, it is possible to see that it is a high-fat diet, but it is also important to note that it also consists of olive oil which is known to have many CVD preventative properties.[7] Which leads into what is called the French paradox, in which a high-fat diet, that is safe to assume would increase the chances of a CVD, does not occur.[6] Though it is also important to note, that the French diet involves the consumption of red wine which is said to also decrease CVD, this can be said that in the Mediterranean diet olive oil acts as the "red wine" which is why the French paradox is used to contrast this.[7] It is believed that the phenols inside of red wine are the cause of this phenomenon, so the question then becomes what is the substitute to red wine in the Mediterranean diet? So, an obvious substitute is olive oil, but avocados come in as a close second in the number of phenols that are produced[8] and it's also safe to assume that these phenols decrease the chances of CVD. Hence, gives more reason to study the avocado and see what is inside of it.

Currently, Americas produces about 73.4%, followed by Africa at 12.2%, and Asia at 11.5%, during the time frame of 2017 to 2018 according to the FAO; with the world producing 6,407,171 avocados during a year timeframe, with Mexico leading as the world producer of the fruit[4]. The U.S. demand for avocadoes has tripled when comparing 2001 to 2018 and producing about 364 million avocados with California being its major producer[9]; with some major products ranging from drinks, oils, and medication[10]. The Spanish produced about 77,000 tons in 2014, and Indonesia was the fifth largest producer in the world producing about 300,000 tons/year in 2016; producing about 51,000-93,000 tons/year of waste.[11,12] The Mediterranean region, consumption of avocados has been reported to increase 150% overall in the European Union[7],

meaning that with the increased consumption of avocados there is also an increase in production to meet the demand. Japan has reportedly imported about 30,000 tons of avocados from Mexico and is also working to cultivate a local production of avocados.[13] The majority of waste coming from the seed which accounts for 613 thousand tons of waste produced just by the seed[14]. The waste produce normally comes from the peel and the seed which is mostly discarded as a non-useable source of the fruit, with the seed being regarded especially as a dead-end source of applicable use.[12] While most of the waste that is produced is biodegradable, it is currently being reused as biomass fuel, or composting which generates greenhouse gases, mainly methane, which adds to the global warming crisis[1,5,15,16]; with the increased production there is also the issue of landfills which will lead to just burning the material so that it takes up less space. Therefore, an increase in the production of waste coming from the seed and overall contribute even more to the problem.

Due to the seed not being edible, it has become one of the most underused parts of the fruit, accounting on average for 13-18% and the most discarded part[5]. The possibility of using the seed as biomass fuel, it has been reported that it is a readily available source and can be used in industrial/business sectors to provide energy.[17] There is also evidence that it can be used to make biodiesel, which is a mixture of methyl esters from a transesterification reaction usually involving animal fats, vegetable oil, and alcohol with either a base or an acid catalyst; using eggshells as the catalyst it is possible to turn the seed oil that is produced into a source of biodiesel.[18] The seed has also been used as a source of fatty acid, even though its natural fatty acid content is low; by using the natural lipase enzyme abundant in the oil it's possible to increase its fatty acid content making it a good source for oleo food and chemicals.[11] The importance of this comes from being able to make different products from the fatty acids that are

produced such as tires, plastics, and soap diversifying, even more, the use for the seed[11]; and with these products coming from a natural plant, it's also much healthier for the environment since these products are more readily biodegradable.

It's also been previously reported that the seed does have some properties such as being able to relieve muscle pain, mycosis, and other parasites[17]. These properties are believed due to the nature of polyacids, phenols, and steroids present inside of the avocado[17]; in Japan some researchers and looking into how ripeness may affect the total lipid content from the fruit extract.[13] The findings that have been published suggest that lipid content inside of the avocado's seed and mesocarp changes with regards to where the avocado is cultivated. Looking at three regions, with two being in Japan and the other imported from Mexico, it shows that there is no significant difference in the types of lipids made by the avocado but, there is a difference in nutritional content with Japan's production being more nutritional; it was noted however that due to the cold storage transportation from Mexico there might be some lost content.[13] The seed has also been shown to contain anti-inflammatory, anti-oxidant, and anti-cancer properties; it was found that the avocado flesh (the green part of the avocado) and seed with chloroform/methanol extracts that are rich with saturated fatty acids and oleic acid.[19] The principal component being phytosterols which act just like cholesterols in animal cell membranes; it is also important to state that phytosterols can be used to decrease the amount of cholesterol in animals.[19] The water extract is reported to have an LC_{50} value of 13.3 $\mu g/mL$ in HepG-2 and 22 $\mu g/mL$ in HT-29 cell line respectably, which means that it's a favorable source for treating liver and colon cancer[19]; Meaning that the avocado and the seed might have anti-cancer properties that are worth researching in. There has been research into the leaf of the avocado tree, in which they tested

for alkaloids, flavonoids, saponin, tannin, and steroids finding that while alkaloids might not be present in the leaf, it did find presence of the other components.[20]

Even something as mundane as food coloring is presented with the utmost of care due to the safety regulations that are present worldwide, but it has also come to the attention of consumers that synthetic food coloring might not be good for the body.[21] The amount of testing to determined how safe and healthy a type of food coloring is astronomical, especially when it's touching a food industry that relies on color to make products more appealing. Though one thing that is common among all these findings is the number of phenolic compounds that are present in the fruit and the seed of the fruit. A study that focuses on the phenolic and polar compound content ran HPLC-DAD-ESI-QTOF-MF identifying 84 compounds in total with 45 being phenolic and the rest being a combination of phenolic acids and flavonoids, extracted in the ethanol-water mixture.[12] This gives rise to the idea that the seed husk might be a gold mine of natural product compounds in which it could be used in the industry.

The fact is that people just in general are trying to be more environmentally friendly and economical and if it is possible to reduce the waste whatever the source is then more than likely these practices should be looked into. More so for the seed husk as it is the waste of waste.

Previously, it was reported by our lab group in the American Chemical Society press release August 21st, 2017 the diethyl ether extract of the avocado seed husk, components found in wax and oil; both parts of the extracts were sent for GC-MS analysis. The wax of the diethyl ether extract is made up of 16 different components with Benzyl butyl phthalate being the major constituent, followed by Di-n-octyl phthalate, and Acetic acid (2.35%). The main constituent of the wax Benzyl butyl phthalate is used as a plasticizer for polyvinyl chloride

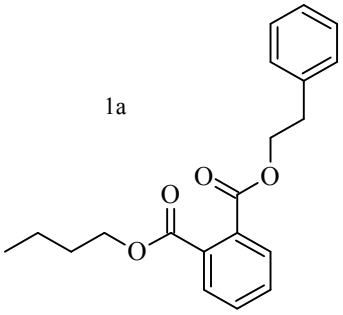
(PVC) and it is sold under the trade name Palatinol BB, Unimoll BB, Sicol 160, or Santicizer 160. The second highest component is Di-n-butyl phthalate, which is used as an insect repellent, which makes sense since the seed husk of the avocado seed acts as a protection against insects at the same time it's been used as a plasticizer for PVC, but due to being suspected as an endocrine disruptor and teratogen it's mostly now used for the manufacturing methods of phthalic anhydride with n-butyl alcohol.[22] This shows that the seed husk has a future in being used for plasticizers and different types of plastics.

Table 1. Wax GC-MS contents:

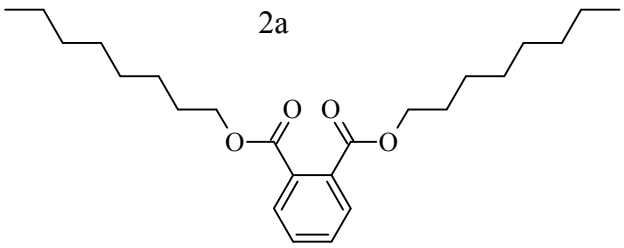
S.No.	Name	Retention Time	M.W.	Chemical Formula	Percentage	Common uses
1a	Benzyl Butyl phthalate	51.7	312.2	$C_{19}H_{20}O_4$	68.60	Plasticizer for polyvinyl chloride (PVC). Sold under trade names in Palatinol BB, Unimoll BB, Sicol 160, or Santicizer 160.
2a	Di-n-octyl phthalate	54.687	279.2	$C_{24}H_{38}O_4$	18.80	Plasticizer used to keep plastics soft or flexible
3a	Acetic acid	4.068	45.0	$C_2H_4O_2$	2.35	Vinegar. Antibacterial and antiseptic when diluted under 8%.
4a	Acetaldehyde	1.566	29.0	C_2H_4O	2.14	Manufacturing resin, used to produce polyvinyl acetate
5a	1,2-Benzenedicarboxylic acid	29.288	104.0	$C_{16}H_{22}O_4$	1.20	Plasticizer
6a	1,2-Benzenedicarboxylic acid, dinonyl ester	57.516	149.0	$C_8H_6O_4$	1.06	Plasticizer

7a	Phthalic acid bis (7-methyloctyl) ester	57.635	149.0	$C_{26}H_{42}O_4$	1.05	Plasticizer used to keep plastics soft or flexible
8a	Acetic anhydride	8.459	43.0	C_4H6O_3	0.96	Used to make pharmaceuticals, dyes, perfumes, explosives, and in food starch
9a	Dibutyl phthalate	44.317	149.0	$C_{16}H_{22}O_4$	0.84	Plasticizer to make plastic soft or flexible; also used for dental mold materials
10a	Bis(2-butoxyethyl) phthalate	53.384	149.0	$C_{20}H_{30}O_6$	0.73	Plasticizer
11a	Hexanedioic acid, bis(2-ethylhexyl) ester	51.989	129.0	$C_{22}H_{42}O_4$	0.44	Flavoring agent, and Plasticizer
12a	2,5-cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-4-hydroxy-4-methyl-	33.292	165.1	$C_{15}H_{24}O_2$	0.43	
13a	Hexanoic acid, 2-ethyl-, oxybis(2,1-ethanediyloxy-2,1-ethanediyl) ester	53.247	446.6	$C_{24}H_{46}O_7$	0.37	Adhesive
14a	Benzaldehyde	17.812	106.1	C_7H_6O	0.35	Used as a preservative for cosmetic, personal care products, and car detailing products
15a	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	42.413	149.0	$C_{26}H_{42}O_4$	0.33	Adhesive; Plasticizer
16a	Butylated hydroxytoluene	34.438	205.1	$C_{15}H_{24}O$	0.32	Preservative also used in food, cosmetics, inks, animal feeds, and other commercial products

1a

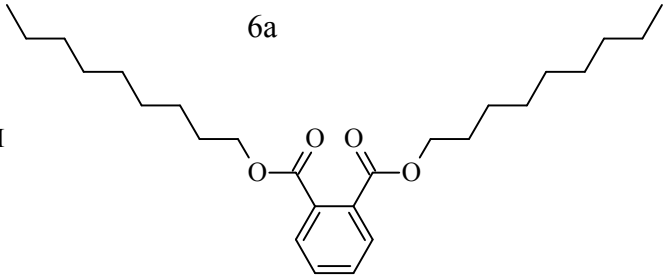


2a

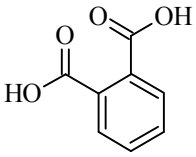


3a

6a

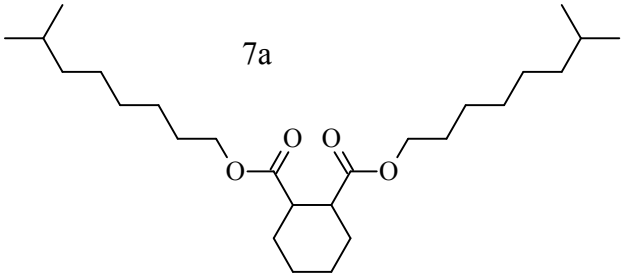


5a

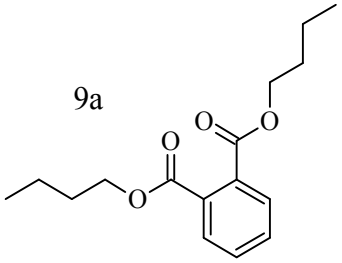


4a

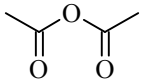
7a



9a



8a



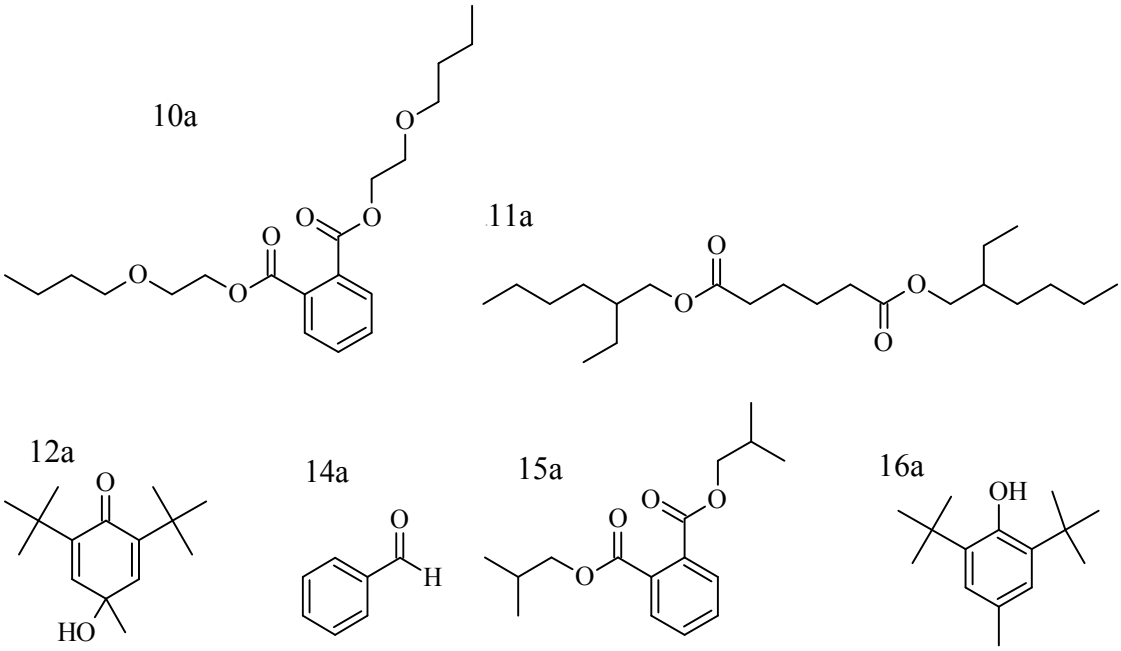


Figure 1. Structure of molecules present in the wax of DEE extract

The oil was found to have 116 compounds with the major component being Heptacosane, Docosane, n-Hexadecanoic acid (Palmitic Acid). Heptacosane is sold through different chemical vendors such as Sigma-Aldrich (Cat# 51560-1G cost 255.00) and is mostly used in the cosmetic industry to help retain the scent of different perfumes and cosmetics. Docosane has been used for adhesives, sealants, fuels, heat transfers, and lubricants.[23] Palmitic acid is used to produce soaps, cosmetics, and industrial mold release agents. This also shows that the seed husk has a future in anti-microbial soaps and different automotive industries.

Table 2. Oil GC-MS content:

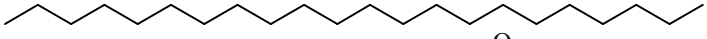
S.No.	**Name**	**Retention Time**	**M.W.**	**Chemical Formula**	**Percentage**	**Common Uses**
1b	Heptacosane	57.661	380.7	$C_{27}H_{56}$	10.23	Used in cosmetic and perfume industries
2b	Docosane	48.559	310.6	$C_{22}H_{46}$	6.12	Food additive, fragrance
3b	n-Hexadecanoic acid	44.079	256.4	$C_{16}H_{32}O_2$	4.21	Soap, lubricating oil, waterproofing materials, and food additive
4b	Hexacosane	55.427	366.7	$C_{26}H_{54}$	3.31	
5b	Tetracosane	51.971	338.7	$C_{24}H_{50}$	2.94	Plastics
6b	Behenic alcohol	48.449	326.6	$C_{22}H_{46}O$	1.64	Soaps, laundry products, consumer, and drugs for pets
7b	Tricosane	50.296	324.6	$C_{23}H_{48}$	1.56	Food additive flavoring, fragrance, and pesticide
8b	Cetene	36.249	224.4	$C_{16}H_{32}$	1.16	Soaps and industrial fluid (lubricating agent)
9b	Dodecane	25.587	170.3	$C_{12}H_{26}$	>1.00	Soaps, fragrance, and stain remover
10b	Tridecane	28.503	184.4	$C_{13}H_{28}$	>1.00	Clay, soap, stain remover, and food additive
11b	1-Tetradecene	31.037	196.4	$C_{14}H_{30}$	>1.00	Used for flooring insulation, and soaps
12b	Tetradecane	31.237	198.4	$C_{14}H_{30}$	>1.00	Stain remover and food additive

13b	Undec-10-ynoic acid, tetradecyl ester	32.691	378.6	$C_{25}H_{46}O_2$	>1.00	Flavoring agent and food additive
14b	Hexadecane, 2,6,10,14-tetramethyl-	32.876	282.5	$C_{20}H_{42}$	>1.00	Absorbent agent and plastics
15b	Pentadecane	33.813	212.4	$C_{15}H_{32}$	>1.00	Food additives
16b	2,4-Di-tert-butylphenol	34.22	206.3	$C_{14}H_{22}O$	>1.00	Antioxidant, automotive maintenance, and fuel additive
17b	Benzoic acid, 4-ethoxy-, ethyl ester	34.666	194.2	$C_{11}H_{14}O_3$	>1.00	Preservative, antioxidant, food additive, bactericide, fungicide, and medication
18b	Dodecanoic acid	35.226	200.3	$C_{12}H_{24}O_2$	>1.00	Food additive and flavoring agent
19b	Dodecane, 5,8-diethyl	35.565	226.4	$C_{16}H_{34}$	>1.00	
20b	Hexadecane	35.249	226.4	$C_{16}H_{34}$	>1.00	Absorbent and adhesive
21b	Cyclopentane, undecyl	37.716	236.2	$C_{16}H_{32}$	>1.00	
22b	Heptadecane	38.552	240.5	$C_{17}H_{36}$	>1.00	Food additive and fragrance
23b	Pentadecane, 2,6,10,14-tetramethyl	38.697	268.5	$C_{19}H_{40}$	>1.00	Lubricant
24b	Benzene, (1-methyldecyl)	38.876	232.4	$C_{17}H_{28}$	>1.00	
25b	Tetradecanoic acid	39.807	228.4	$C_{14}H_{28}O_2$	>1.00	Food flavoring, food additive, and cosmetic cleanser
26b	Heptadecane, 3-methyl	40.131	254.5	$C_{18}H_{38}$	>1.00	
27b	1-Nonadecene	40.607	266.5	$C_{19}H_{38}$	>1.00	Plastics
28b	Octadecane	40.741	254.5	$C_{18}H_{38}$	>1.00	Skin conditioner

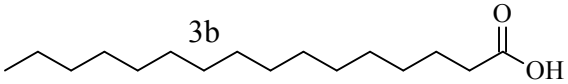
29b	5,5-Diethylpentadecane	40.952	268.5	$C_{19}H_{40}$	>1.00	
30b	1-Octadecene	42.21	252.5	$C_{18}H_{36}$	>1.00	Adhesive, cleaning automotive, flooring, and insulation
31b	Heptadecane, 9-hexyl	42.701	324.6	$C_{23}H_{48}$	>1.00	
32b	Nonadecane	42.826	268.5	$C_{19}H_{40}$	>1.00	Food additive, flavoring, and fragrance
33b	Benzene, (1-methyldodecyl)	43.272	260.5	$C_{19}H_{32}$	>1.00	
34b	17-Pentatriacontene	43.641	490.9	$C_{35}H_{70}$	>1.00	Dental
35b	Nonadecane, 2,3-dimethyl	44.284	296.6	$C_{21}H_{44}$	>1.00	Soaps and cosmetics
36b	1-Heneicosanol	44.703	312.6	$C_{21}H_{44}O$	>1.00	
37b	Eicosane	44.816	282.5	$C_{20}H_{42}$	>1.00	Food additive, food flavoring, and fragrance
38b	Octadecane, 3-ethyl-5-(2-ethylbutyl)	45.581	366.7	$C_{26}H_{54}$	>1.00	
39b	1-Eicosanol	46.28	298.5	$C_{20}H_{42}O$	>1.00	Adhesive, apparel, and detergent
40b	Heneicosane	46.717	296.6	$C_{21}H_{44}$	>1.00	Food additive, food flavoring, and fragrance
41b	Hexatriacontane	47.883	507.0	$C_{36}H_{74}$	>1.00	Detergent
42b	1-Dodecene	25.341	168.32	$C_{12}H_{24}$	>1.00	

1b

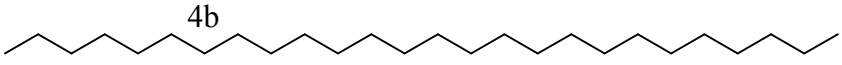
2b



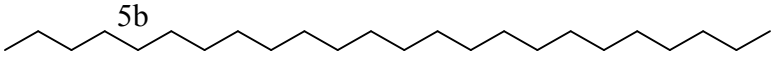
3b



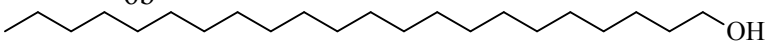
4b



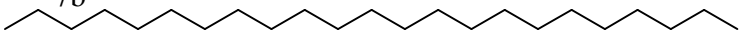
5b



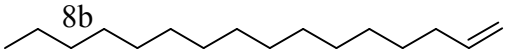
6b



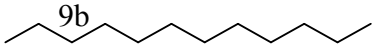
7b



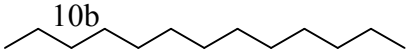
8b



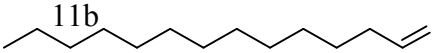
9b



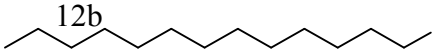
10b



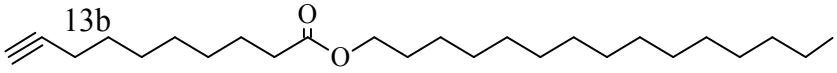
11b



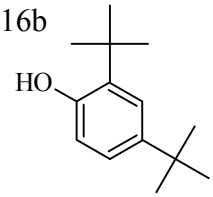
12b



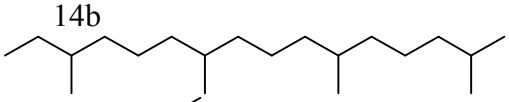
13b



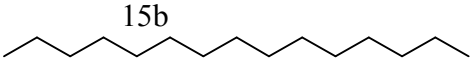
16b



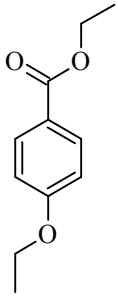
14b



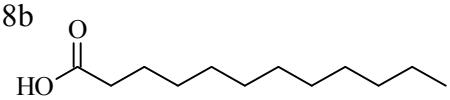
15b



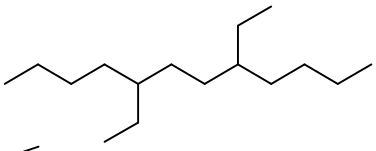
17b



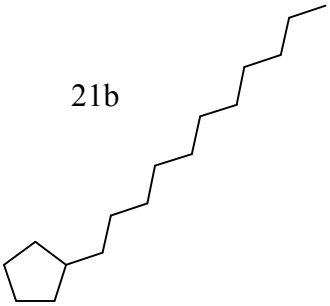
18b



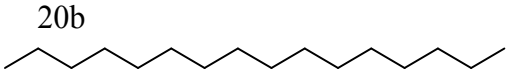
19b



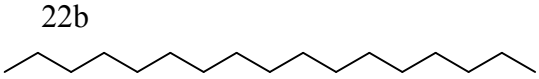
21b



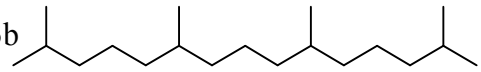
20b



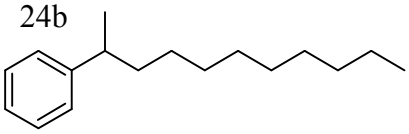
22b



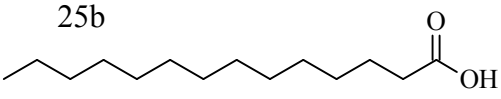
23b



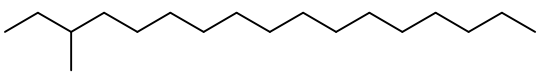
24b



25b

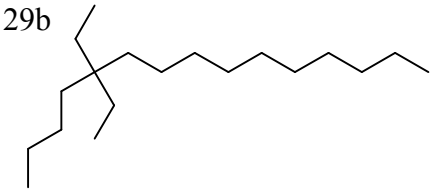


26b



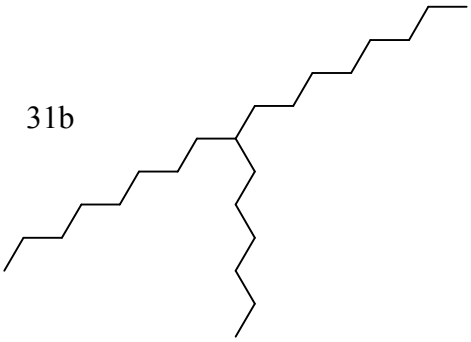
27b

29b

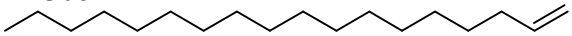


28b

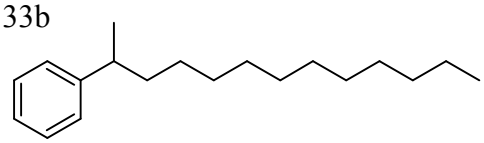
31b



30b

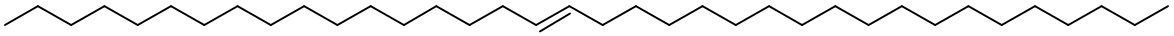


33b

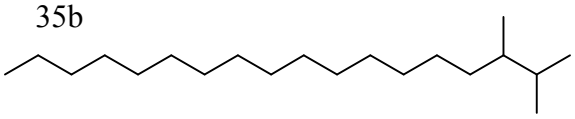


32b

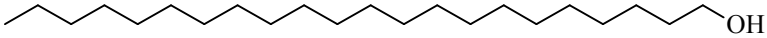
34b



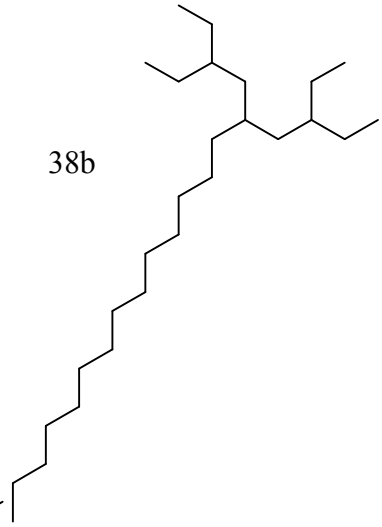
35b



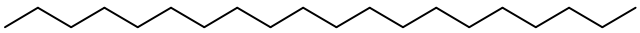
36b



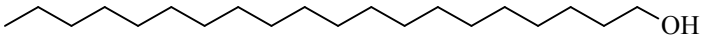
38b



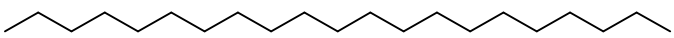
37b



39b



40b



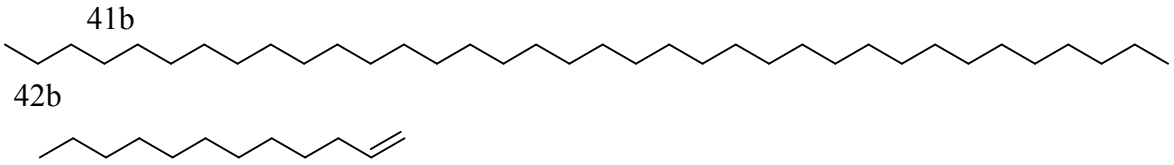


Figure 2. Structure of molecules present in the oil of DEE extract

This highlights just some of the different components that are available inside of the seed husk. These components were extracted from a 1 kg amount of avocado seed husk using so it piqued our interest, even more, when the active component for Abreva™ (Behenic alcohol) inside of the husk ready to be used.

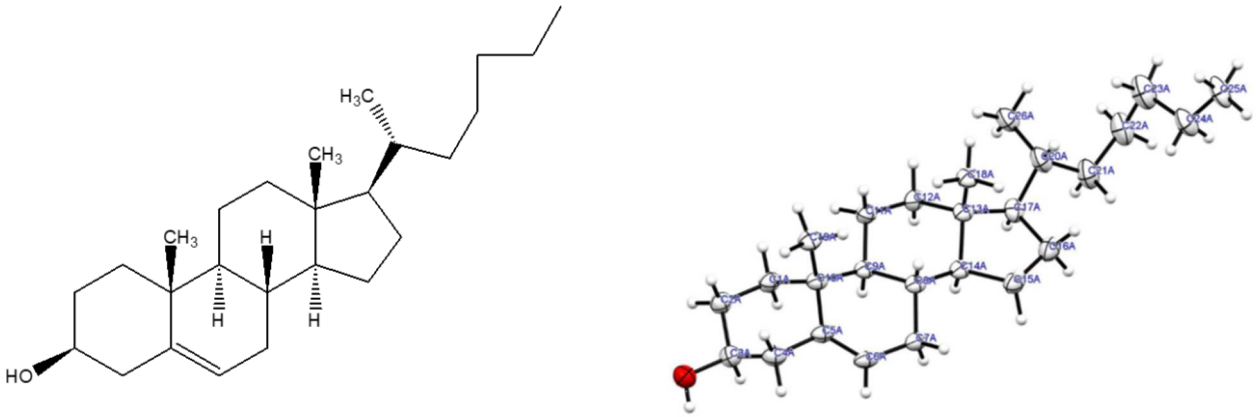


Figure 3. Structure and X-Ray of (3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol

It was also previously reported the existence of a new type of cholesterol called **(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((*R*)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-ol** (DBOC-1) the white crystalline powder was at extracted 10% ethyl acetate in hexane, and then put through a re-chromatography column at 5% ethyl acetate in hexane, elucidating 0.594 g of

the pure substance with a melting point of 135.2-137.7℃ with an RF value of 0.50 in 40% ethyl acetate in hexane, HRMS 300.213 m/z. Looking at the FT-IR, there is a range of 2850.05-2957.29 which is usually representative of an alkene, this could be representative of the functional group attached to C9. 1050.29 is representative of a primary alcohol group which is seen attached to C1. DBOC-1 ^{1}H NMR (500 MHz, $CDCl_3$ ppm δ 7.25) ^{1}H-NMR ppm δ5.3515 (2H, t, J=5.22), 3.5200 (1H, tq, J=31.56), 1.8473 (3H, q, J=3.60), 1.608 (3H, m), 1.4764(9H, m), 1.2501 (8H, m), 1.0964 (3H, m) 1.0772 (4H, s), 0.9220 (5H, d, J=6.54), 0.8303(6H, m), 0.6986 (2H, s), 0.6804 (3H, s), 0.0002 (1H, s); ^{13}C ppm δ140.77, 121.72, 71.82, 56.79, 56.09, 50.16, 50.16, 45.86, 42.34, 39.80, 37.27, 36.52, 36.15, 33.97, 31.92, 31.68, 29.19, 28.25, 26.12, 24.31, 23.09, 21.10, 19.82, 19.40, 19.05, 11.99. Looking at the HMQCGP, there is a relation between the signal ppm δ ^{1}H 5.3515, and ^{13}C 140.77, this relation seems to be the double bond relation between C13 and C14; 3.5200 and 71.82, which shows to be the C-OH; and the rest seems to be part of the steroid motif.

In summary, this is a continuation of the project, with the hope of finding a novel anti-cancer compound since the avocado itself is known to be a good anti-cancer preventative.

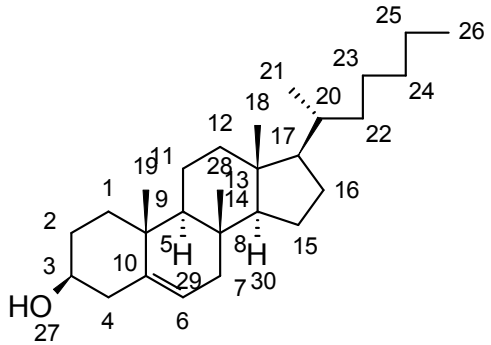


Figure 4. (3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol with numbered Carbons

CHAPTER II

METHODS

Figure 5. Avocado Seed Husk

The mature avocado fruits were gathered from a grove at 3 Mile Mission, TX. The seeds were separated and air-dried in the absence of sunlight as seen in Figure 4. The husks were separated from the dry seeds. The husks were then ground to a fine powder using a grinder and then immersed in diethyl ether for 21 days (cold extraction method). After the stipulated time, the extract was filtered and the solvent was removed by reduced pressure distillation using Buchi Rotary evaporator R114, with a water bath 50 °C with a Buchi B-480. A small part of the crude extract was saved at -20 °C for biological evaluation and the rest was used to make a slurry with silica gel in dichloromethane. The solvent was removed at reduced pressure and the slurry was dried in a vacuum liner for two hours. A gravity column was then prepared 38 mm x 300 mm, using silica as packing for the column. Hexane was used as an eluent, to increase the polarity ethyl acetate was used increasing by 2% until 10% ethyl acetate/hexane after checking the TLC for compound; the polarity was then increased by 5% after each time. A chamber with a developing eluent of hexane was used to check the TLC for the compound. The TLC plate was then transferred to an iodine chamber to dye the compound. The compound was originally collected in a round bottom flask with the eluent, and the solvent was removed under reduced pressure distillation at 35 °C which was then transferred to a test

tube after each charge. The test tube was then compared with the other test tubes in the rack for similar TLC spots. The

similar test tubes were then transferred into a round bottom flask. FT-IR spectra were recorded on a Bruker Alpha modular Platinum-ATR FT-IR spectrometer with OPUS software, using the samples directly (neat) without making pallets.

The resulting ethanol and water extracts were made from gathering the fine powder that was filtered out of the DEE extract and then immersed once again into ethanol using the same process (water extract repeats the same process).

HPLC/MS-MS was done by sending it off to a collaborating lab, where 25 mg of sample was weighed out and dissolved in 300 μL water. Mixed well and 100 μL sample was mixed with 300 μL methanol (containing 5 μg/mL 2-Chloro-L-phenylalanine as internal standard). The mixture was mixed by a vortex mixer for 1 min. Then the mixture was centrifuged at 13,000 rpm, 4°C for 10 min. The supernatant was transferred to sampler vials for detection. An in-house quality control (QC) was prepared by mixing an equal amount of each sample. Agilent 1290 Infinity II UHPLC system coupled to an Agilent 6545 UHD and Accurate-Mass Q-TOF/MS was used for LC-MS analysis. The chromatographic column used was Waters XSelect HSS T3 (2.5 μm 100*2.1 mm). Mass spectrometry was operated in both positive and negative ion modes. The parameters optimized were as follows. Capillary voltage: 3.5 kV. Drying gas flow: 10 L/min. Gas temperature: 325°C. Nebulizer pressure, 20 psi/g. Fragmentor voltage: 120 V. Skimmer voltage: 45 V. Mass range: m/z 50–3000.

NMR proton, carbon-13, COSY NMR experiment, and NOESY NMR experiments methods were recorded using the Bruker Ultrashield Plus 600 MHz NMR with Topspin software and with deuterated chloroform solvent. With 0.1 mg send to a collaborating lab to take the X-ray crystallographic structure of the compound

CHAPTER III

RESULTS

Ethanol Extract

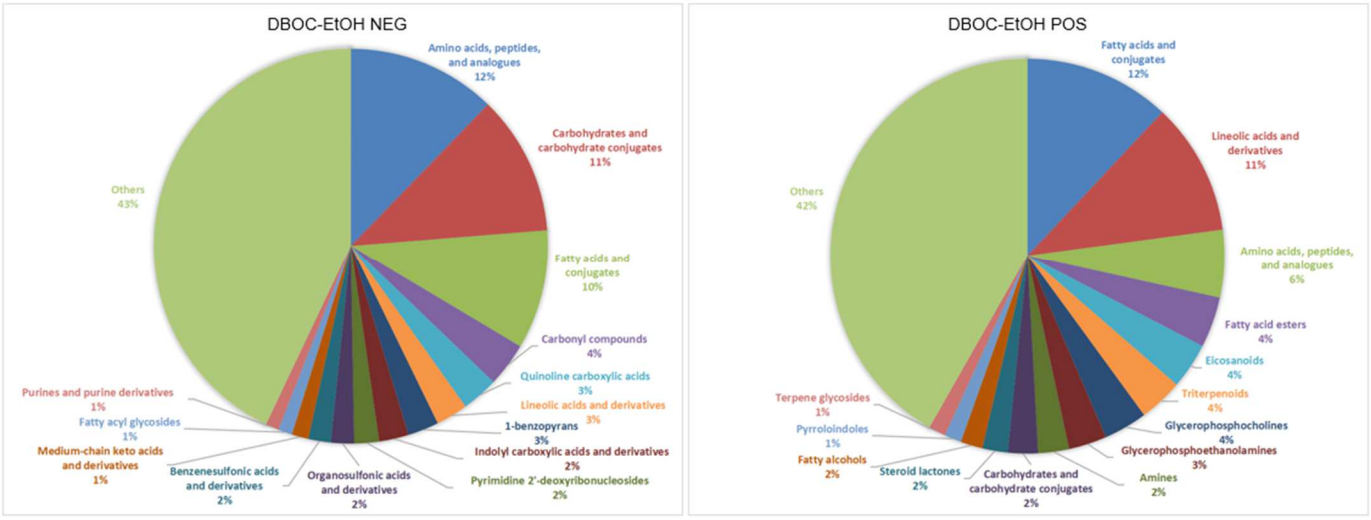


Figure 7. Ethanol extract type of components by percentage available; Left Negative; Right Positive

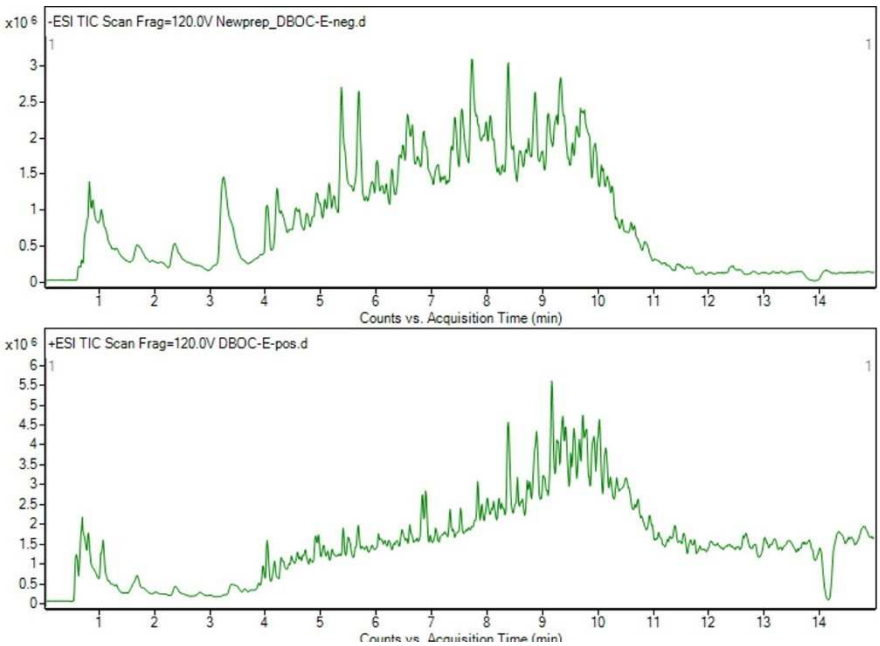


Figure 6. Ethanol extract scan; Top Negative; Bottom Positive

Table 3. Ethanol LC-MS extract Positive:

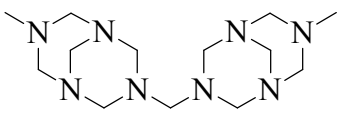
S.No.	Name	Retention Time	M.W.	Chemical Formula	Area under peak	Common uses
1c	1,3,5,7-Tetraazabicyclo[3.3.1]nonane, 3,3'-methylenebis[7-methyl-	10.017	296.2	$C_{13}H_{28}N_8$	10.47	General reactions
2c	3-[(Dibutylboranyl)imino]-2-methyl-1-phenylbut-1-en-1-amine	9.180	298.3	$C_{19}H_{31}BN_2$	4.59	General reactions
3c	4,4'-(Phenylmethylene)bis(5-methyl-2-undecyl-1H-imidazole)	9.774	560.5	$C_{37}H_{60}N_4$	4.47	Suspected hair conditioner, anti-microbial, fragrance, flame retardant[24]
4c	Methanesulfonic acid--heptadecan-1-ol (1/1)	9.543	352.3	$C_{18}H_{40}O_4S$	4.34	Suspected hair conditioner, anti-microbial, flame retardant, surfactant, emulsion stabilizer[24]
5c	2,2,6,6-Tetramethyl-1-phosphanylpiperidine	0.718	173.1	$C_9H_{20}NP$	4.34	Quinolinyl modulators of RORγT[25]
6c	1-Dodecyl-3-methylimidazolium tetrafluoroborate	9.180	338.3	$C_{16}H_{31}BF_4N_2$	4.03	Antimicrobial, androgen receptor; Sold by Sigma Aldrich 5g for $85.00[26]
7c	2,2'-(Ethane-1,2-diyl)bis(4,6-dimethyl-1,3,5,2,4,6-triazatriborinane)	8.381	244.2	$C_6H_{22}B_6N_6$	3.97	Suspected catalyst[24]
8c	3-{3-[Methyl(dipropyl)silyl]propoxy}-2-[(oxiran-2-yl)methoxy]propan-1-ol	10.017	318.2	$C_{16}H_{34}O_4Si$	3.67	General reactions
9c	Tetrakis(3-aminopropyl)ammonium	9.330	246.3	$C_{12}H_{32}N_5$	3.64	Buffer for RNA stabilization and enzymic properties,

						electrode manufacture for solar cells[27]
10c	DG(14:0/0:0/20:5n3)	14.933	586.5	$C_{37}H_{62}O_5$	3.61	Surfactant and Emulsifier[28]
11c	Methyl 12-[(methanesulfonyl)oxy]octadecanoate	9.544	392.3	$C_{20}H_{40}O_5S$	3.53	Mitochondria-Targeted Inhibitors of Cytochrome C Peroxidase for Protection from Apoptosis[29,30]
12c	L-Aminocarnityl-succinyl-leucyl-argininal-diethylacetal	9.389	587.4	$C_{27}H_{53}N7O_7$	3.19	C-101, also called Myodur, is developed for the treatment of Duchenne's muscular dystrophy (DMD), currently still in clinical trials; last update Oct. 16, 2018[31]
13c	N-(tetradecanoyl)-sphing-4-enine-1-(2-aminoethylphosphonate)	13.034	616.5	$C_{34}H_{69}N_2O_5P$	2.42	Used for production of glycoglycerolipids and glycosphingolipids from lipid phases[32]
14c	[([1,1'-Biphenyl]-4-yl)methyl](hydroxy)boranyl	1.129	195.1	$C_{13}H_{12}BO$	2.31	Vasodilating agent, type of boronic acid can be used in different reactions, can probably be used in treatment of HIV, obesity, diabetes, and cancer; Requires more study[33]
15c	2,4-Bis(methoxycarbonyl)-1-methylpyridin-1-ium	0.729	210.1	$C_{10}H_{12}NO_4$	2.25	Used for iFret prob[34]
16c	3-Benzyl-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one	6.902	321.2	$C_{20}H_{23}N_3O$	2.17	DDR1 inhibitor, used for reperfusion injury, sold through Key

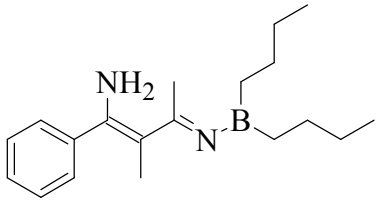
						Organics (5g for 591.02)[35]
17c	N-Nitroso-N-methyl-N-tetradecylamine	9.344	256.3	$C_{15}H_{32}N_2O$	2.16	Found in liquid dishwashing detergents, and hair products as a contaminate[36]
18c	4-oxo 2-Nonenal-d3	1.082	157.1	$C_9H_{11}D_3O_2$	2.14	Used for the std. of 4-ONE through GC-, LC-MS, 50µg cost $78.00[37]
19c	N~1~,N~3~,N~5~-Trioctylbenzene-1,3,5-tricarboxamide	9.410	543.4	$C_{33}H_{57}N_3O_3$	2.07	Polypropylene resin, electret material[38]
20c	4-Aminobutanoic acid--water (1/5)	2.312	193.1	$C_4H_{19}NO_7$	2.07	Suspected flavoring agent, flavor additive, preservative, common inhibitor neurotransmitter in central nervous system[24]
21c	DG(11D3/9D3/0:0)	13.530	672.5	$C_{41}H_{68}O_7$	2.06	Metabolite
22c	Petroselinic acid	10.141	282.3	$C_{18}H_{34}O_2$	2.05	Cosmetic agent, used in packaging and coloring of products, used in the treatment of Alzheimer, sold through Sigma Aldrich 25µg for $99.00 (CAS#593-39-5)[39]
23c	L-Lysyl-N~2~-(12-aminododecanoyl)-L-lysine	8.548	471.4	$C_{24}H_{49}N_5O_4$	2.02	Type of lysine amino acid
24c	Tetrabutylphosphonium chloride	9.713	294.2	$C_{16}H_{36}ClP$	2.01	A catalyst for pharmaceuticals, seal material, and printing wiring boards; sold by Sigma Aldrich 10g for 217.00 (CAS#2304-30-5)[40]

25c	Oleyldimethylamine	7.823	295.3	$C_{20}H_{41}N$	1.96	Antimicrobial, antistatic agent, oil and gas field corrosion inhibitor and detergent; sold through Ochem incorporation 5g for $1765.00 (CAS#061O690)[41]
26c	Ethanesulfonic acid, 2-[cyclohexyl(1-oxooctadecyl)amino]-, sodium salt	9.169	495.3	$C_{26}H_{50}NNaO_4S$	1.91	Suspected surfactant, lubricating agent, heat stabilizer, skin conditioner[24]
27c	1-Ethyl-6-fluoro-3-formyl-1,4-dihydro-7-(4-methyl-1-piperazinyl)-4-oxoquinoline	4.037	317.2	$C_{17}H_{20}FN_3O_2$	1.81	Pefloxacin aldehyde thiosemicarbazone derivatives and its preparation method and application (redox drug derivative)[42]
28c	Ethanesulfonic acid, 2-[cyclohexyl(1-oxooctadecyl)amino]-, sodium salt	9.169	496.3	$C_{26}H_{50}NNaO_4S$	1.91	Dental pre-treatment agent meant for detin [patent pretreatment agent]

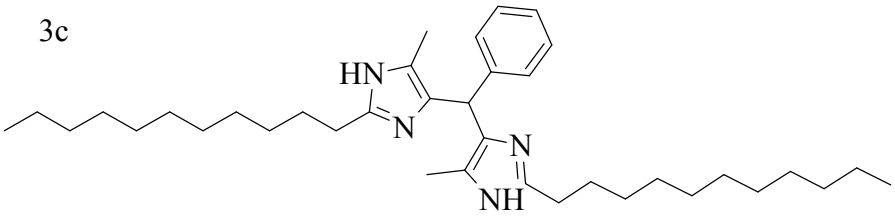
1c



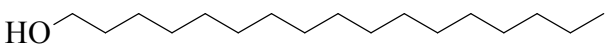
2c



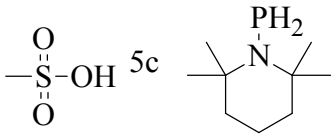
3c



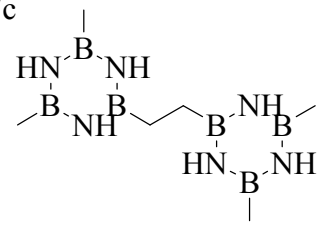
4c



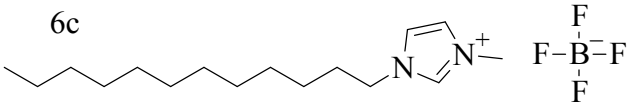
5c



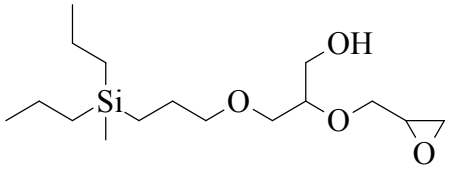
7c



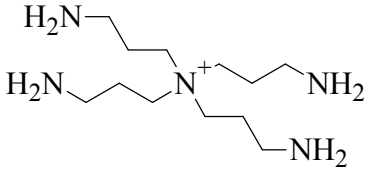
6c



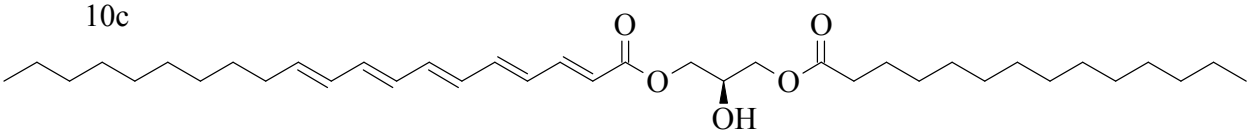
8c



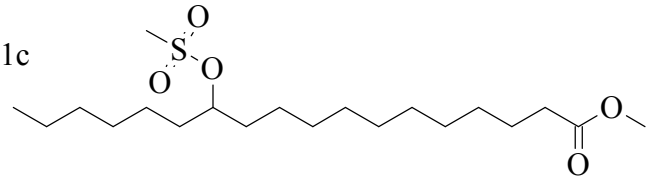
9c



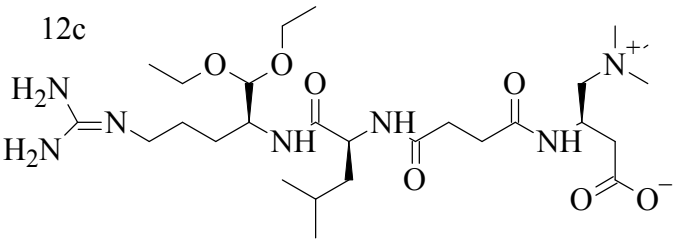
10c



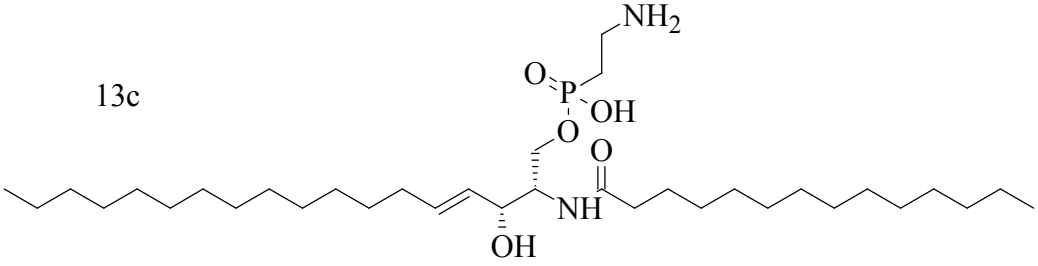
11c



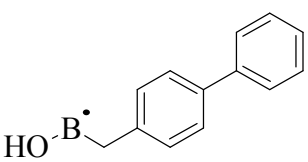
12c



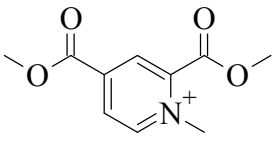
13c



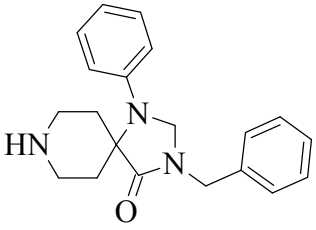
14c



15c



16c



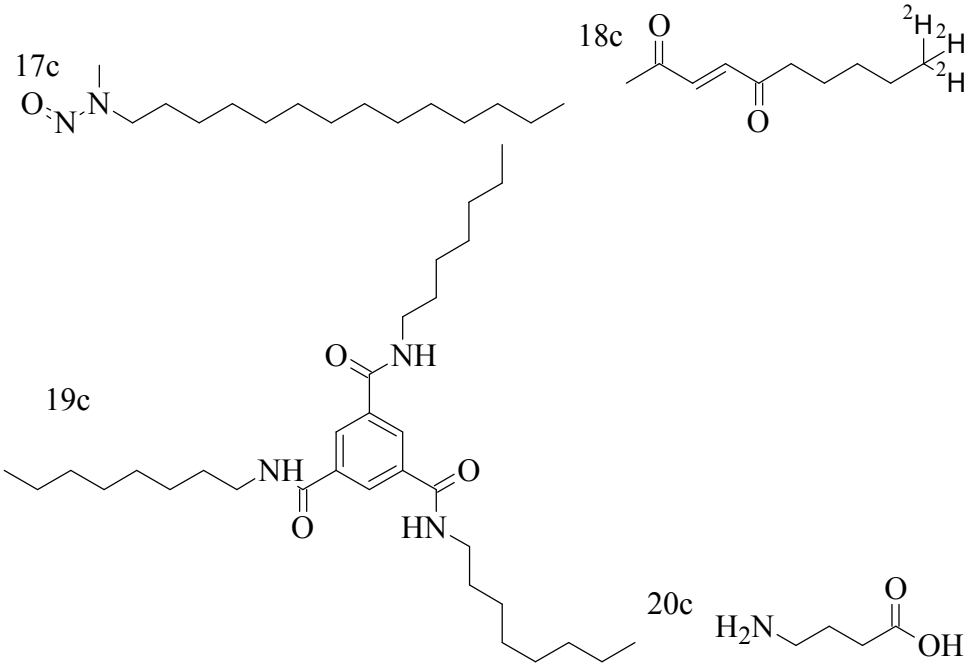


Figure 8. Top 20 structures from Ethanol extract Positive

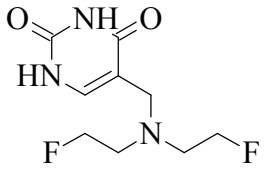
Table 4. Ethanol LC-MS extract Negative:

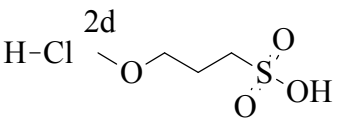
S.No.	Name	Retention Time	M.W.	Chemical Formula	Area under peak	Common uses
1d	Uracil, 5-((bis(2-fluoroethyl)amino)methyl)-, monohydrochloride	7.828	268.1	$C_9H_{14}ClF_2N_3O_2$	462.2	Looked at as a possible anti-cancer, the toxicity of 275 mg/kg in mouse[43]
2d	3-Methoxypropanesulphonic acid	3.258	153.0	$C_4H_{10}O_4S$	356.1	The nonaqueous electrolyte used in a battery for high storage temperatures, a cyanine dye, photosensitive resin, also used in a method to produce perfluorosulfonic acid, sold by Accelera 5g for $750 (CAS#51980-59-7)[44]
3d	Cgp 4718A	8.148	284.1	$C_{14}H_{17}C_{l2}NO$	340.2	Studied in 1980 as a possible anti-depressant under the name Sercloremine, never came out to market[45]
4d	2-Amino-9-[(1S,3R)-4-[hydroxy(dimethyl)silyl]-3-(hydroxymethyl)-2-methylidenecyclopentyl]-3,9-dihydro-6H-purin-6-one	7.484	334.1	$C_{14}H_{21}N_5O_3Si$	225.2	Intermediate for carbon-silicon oxidations, ingredient for making Entecavir anti-viral drug for hepatitis B; Sold by Chem Space 1mg for $176 (CAS#870614-82-7)[46]
5d	NSC400216	7.794	350.1	$C_{15}H_{21}N_5O_3S$	182.6	Studied as a diuretic, does not exhibit any diuretic activity[47]
6d	1-Pyrrolidinecarbonyl chloride	2.340	132.0	C_5H_8ClNO	173.1	Used for pneumatic tires, sold by Sigma Aldrich 5 g for $91.92 (CAS#1192-63-8)[48]
7d	Nitric acid--3-ethoxypropane-1,2-diol (2/1)	6.040	245.1	$C_5H_{14}N_2O_9$	170.4	Nitric acid salt meant for multiple types of reactions, but mostly used as a polymer additive ranging from

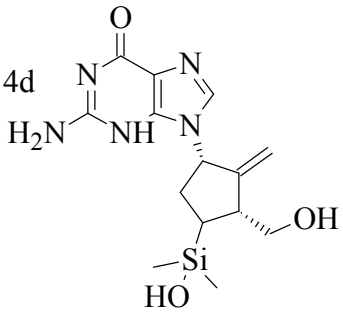
						reinforcing polyurethanes thermoplastic, to also being used in aqueous solution in inkjet ink for printers[49]
8d	Allylamine, N,N-bis(2-chloroethyl)-	6.153	180.0	$C_7H_{13}Cl_2N$	158.7	Used in the synthesis of macrocyclic polyether, sold by Aurora Fine Chemicals starting at 1,290.00 up to 25g (Catalog#A21.117.715)[50]
9d	N,N'-[(3,6-Dioxopiperazine-2,5-diyl)di(propane-3,1-diyl)]diacetamide	9.304	311.2	$C_{14}H_{24}N_4O_4$	149.6	General reactions
10d	2-oxoindole-3-acetic acid	5.704	236.1	$C_{10}H_9NO_3$	147.5	Researched as a possibility to help plant growth. Sold by Achemblocks 5g for $750(CAS#2971-31-5)[51]
11d	N,N'-[(Methylazanediyl)di(propane-3,1-diyl)]bis(2,2,2-trifluoroacetamide)	7.497	336.1	$C_{11}H_{17}F_6N_3O_2$	146.8	Used for making a compound by forming a polymer from a template drug[52]
12d	N-(N'-Pentylcarbamimidoyl)thiourea	5.698	187.1	$C_7H_{16}N_4S$	138.4	Improves anti-inflammatory composition and method of treating inflammation when pairing with an anti-inflammatory agent[53]
13d	3(2H)-Pyridazinone, 4-isopropoxy-2-(2-morpholinoethyl)-6-phenyl-, hydrochloride	8.457	378.2	$C_{19}H_{26}ClN_3O_3$	133.3	General reactions
14d	3-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(trifluoromethyl)aniline	6.314	286.1	$C_{13}H_{17}BF_3NO_2$	126.5	Used for multiple substituted isoxazolopyridazinones and isothiazolopyridazinones, sold by Sigma Aldrich 5g for

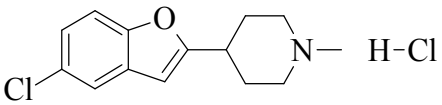
						$1250(CAS# 510771-54-7)[54]
15d	Pyrazinecarbothioamide, N-(4-morpholinylmethyl)-6-(1-piperidinyl)-	10.521	320.2	$C_{15}H_{23}N_5OS$	121.2	General reactions
16d	Calcium propan-2-olate	4.234	157.1	$C_6H_{14}CaO_2$	109.8	Used as a thermoelectric material[55]
17d	AGN-PC-00FD32	9.681	293.2	$C_{15}H_{28}B_2O_4$	103.3	Meant for Diboronation type of reactions
18d	1-Methyl-1-{2-[(1-phenylcyclohexane-1-carbonyl)oxy]ethyl}piperidin-1-ium	6.879	329.2	$C_{21}H_{32}NO_2$	102.1	General reactions
19d	Methyl {6-[(pyrazin-2-yl)sulfanyl]-1H-benzimidazol-2-yl}carbamate	6.478	300.1	$C_{13}H_{11}N_5O_2S$	97.7	Useful as an anthelmintic[56]
20d	5-(4-Hydroxy-3-methoxyphenyl)-5-phenylhydantoin	1.030	297.1	$C_{16}H_{14}N_2O_4$	87.9	Used for infections, and for detecting patters in hereditary disease[57,58]
21d	2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(trifluoromethoxy)aniline	6.532	302.1	$C_{13}H_{17}BF_3NO_3$	87.2	Substituted isoxazolopyridazinones and isothiazolopyridazinones, synthesis method of phosphorescent material including DMP ligands using microwave, compound for voltage-gated sodium channel modulators, pharmaceutical containing sodium-dependent phosphate transporter inhibitor[54]
22d	PS(21:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	9.361	876.6	$C_{49}H_{84}NO_{10}P$	85.7	Type of Glycerophospholipids
23d	3(2H)-Pyridazinone, 4-isopropoxy-2-(2-morpholinoethyl)-6-phenyl-, hydrochloride	9.241	378.2	$C_{19}H_{26}ClN_3O_3$	83.9	General reactions

24d	{[Isothiocyanato(phenyl)silyl]methanetriyl}tris(trimethylsilane)	6.621	394.1	$C_{17}H_{33}NSSi_4$	82.5	General reactions
25d	Inosine, 2-fluoro-	6.623	285.1	$C_{10}H_{11}FN_4O_5$	79.9	Used in methods involving quantifying methylglyoxal induced nucleic acid adducts, in production of 2-chloradenosine, and other DNA based methods[59]
26d	2'-Deoxy-2'-fluoroinosine	7.824	269.1	$C_{10}H_{11}FN_4O_4$	78.6	Used in methods of synthesis involving phosphorylated molecules, cyclopentane-based molecule for stimulator of interferon genes, and sold by Combi-Blocks 1g for $750.00 (CAS#80049-87-2)[60]
27d	Hydroxy(oxo)(2-phenylethenyl)phosphanium	7.327	166.0	$C_8H_8O_2P$	75.5	Weathering improver resin for coating metal nanowires[61]
28d	3-[2-(Diphenylphosphanyl)anilino]-1,3-diphenylprop-2-en-1-one	5.254	482.2	$C_{33}H_{26}NOP$	73.4	General reactions

1d 

2d 

4d 

3d 

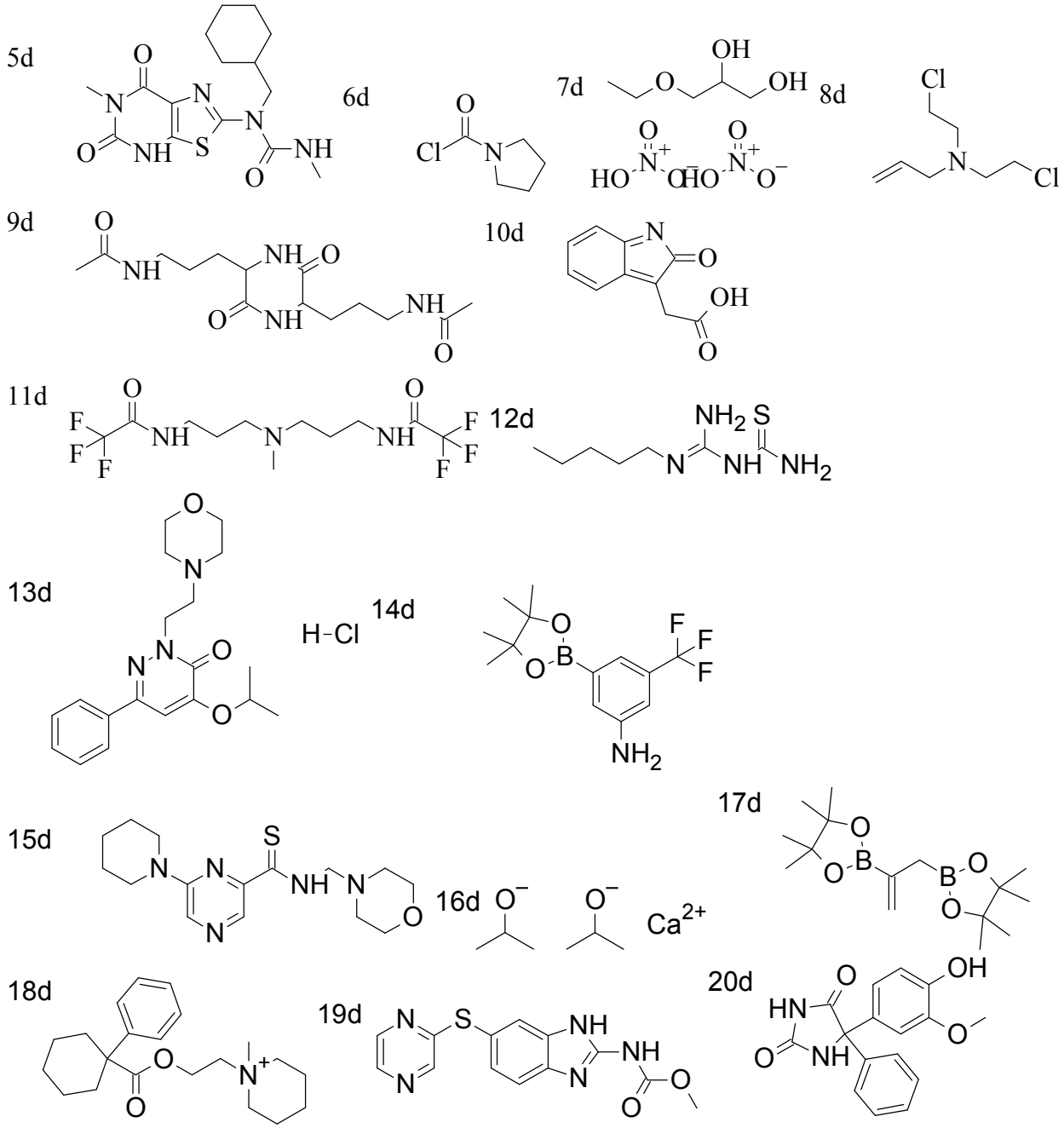


Figure 9. Top 20 structures from Ethanol extract Negative

Water Extract

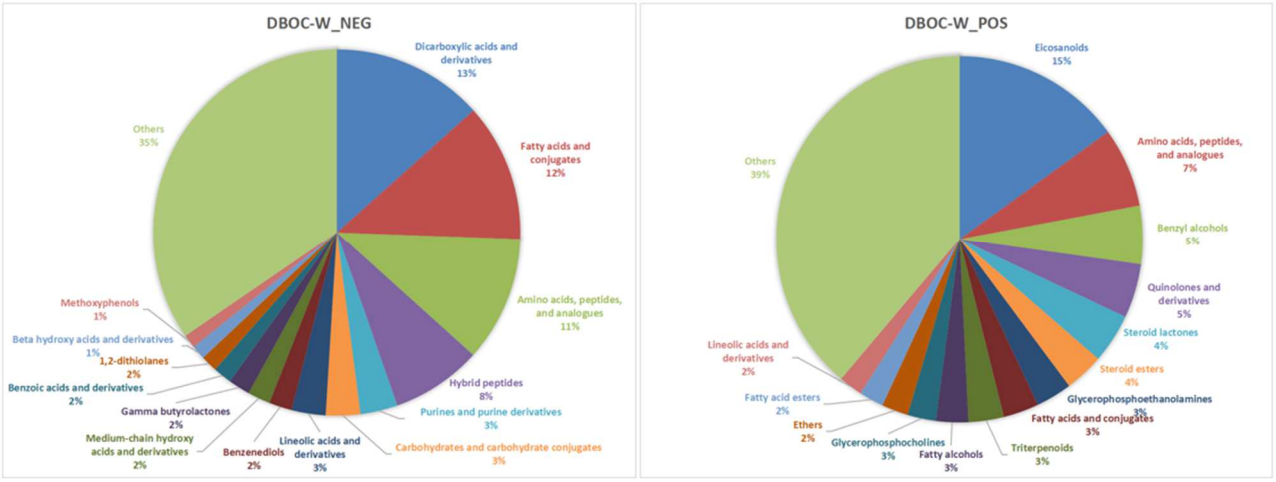


Figure 10. Water extract scan; Top Negative; Bottom Positive

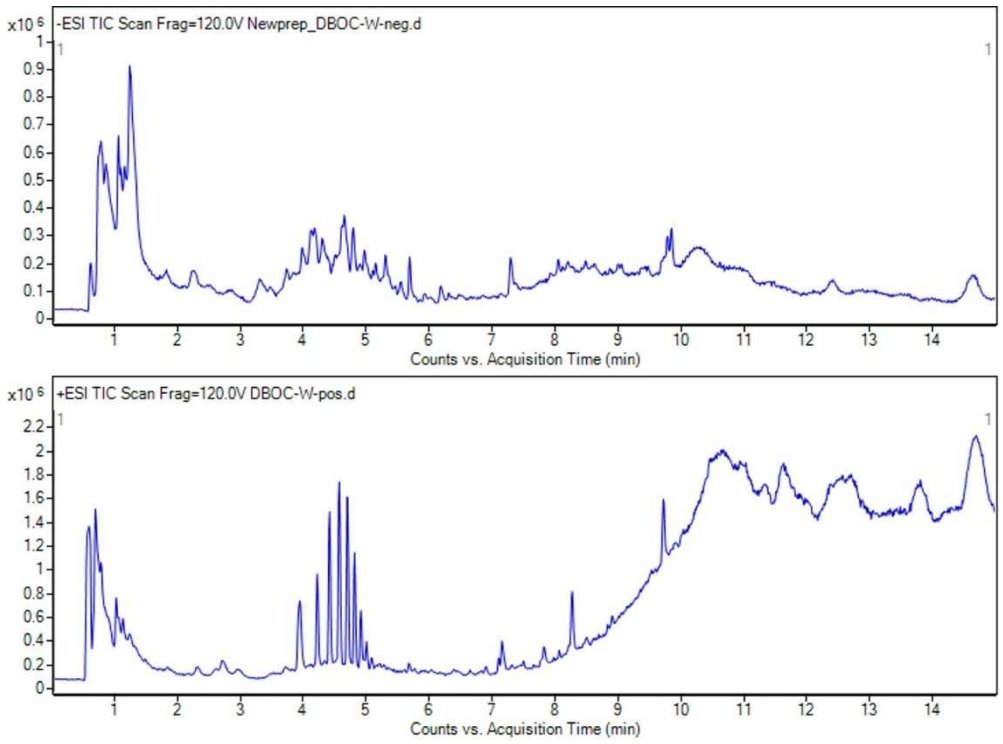


Figure 11. Water extract type of components by percentage available; Left Negative; Right Positive

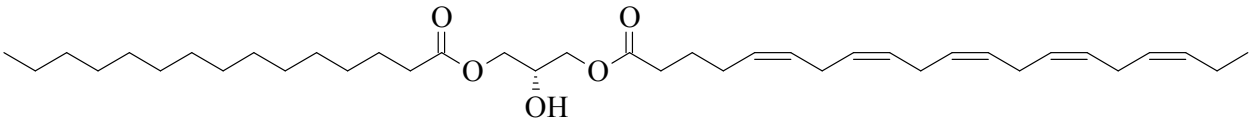
Table 5. Water LC-MS extract Positive:

S.No.	Name	Retention Time	M. W.	Chemical Formula	Area under peak	Common uses
1e	DG(15:0/0:0/20:5n3)	14.690	601.5	$C_{38}H_{64}O_5$	10.39	Metabolite
2e	Pentabromo(2-bromoethyl)benzene	14.679	596.5	$C_8H_4Br_6$	5.14	Used in methods to produce styrene monomer, selective dehydrobromation, penta-bromostyrene polymers, and flameproofing additive for thermoplastic resins[62,63]
3e	Benzenamine, N-[[4-(nonyloxy)phenyl]methylene]-4-propyl-	4.574	388.3	$C_{25}H_{35}NO$	4.35	Used for fixing two solids together using a liquid crystal compound[64]
4e	Sulfuric acid--N''-octadecylguanidine (1/1)	4.704	432.3	$C_{19}H_{43}N_3O_4S$	4.06	Sulfiric acid salt of octadecylguanidine normally used for reactions
5e	N-(hexadecanoyl)-deoxysphing-4-enine-1-sulfonate	14.690	602.5	$C_{34}H_{67}NO_5S$	3.78	Sphingolipids[65]
6e	2-(Methoxycarbonyl)-1,2,3,4-tetrahydroisoquinoline-1-carboxylate	0.715	235.1	$C_{12}H_{12}NO_4$	3.70	General reactions
7e	6-chloro-n,n'-bis[2-(diethylamino)ethyl]-1,3,5-triazine-2,4-diamine	4.417	344.2	$C_{15}H_{30}ClN_7$	3.47	Suspected antimicrobial[24]
8e	Asp Glu Arg Arg	14.540	575.3	$C_{21}H_{38}N_{10}O_9$	3.32	Combination of Amino Acids
9e	Methanone, [4-(hexadecyloxy)-2-hydroxyphenyl]phenyl-, oxime	4.817	476.3	$C_{29}H_{43}NO_3$	2.56	Used in methods for process accelerator for copper extraction from waessress

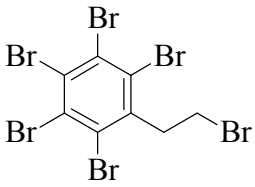
						solutions; sold by Sigma Aldrich 100 mg for $55.10 (SKU# R739154)[66]
10e	DG(13:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	10.956	573.5	$C_{36}H_{60}O_5$	1.92	Diradylglycerols [sub class GL0201][67]
11e	1-tert-Butyl-3,5-bis(4-chloro-2,4-dimethylpentan-2-yl)benzene	9.719	399.3	$C_{24}H_{40}Cl_2$	1.91	Sterically hindered binifer telechelic polymer[68]
12e	{[(2R)-2,3-Bis(tetradecyloxy)propoxy]methyl}benzene	14.679	597.5	$C_{38}H_{70}O_3$	1.76	Suspected surfactant, hair conditioner[24]
13e	Phosphoric acid--N~2~-(3-aminopropyl)-2,5-dimethylhexane-2,5-diamine (1/1)	4.231	300.2	$C_{11}H_{30}N_3O_4P$	1.73	Suspected crosslinker, hair conditioner, buffer, skin conditioner[24]
14e	PE-Cer(d14:2(4E,6E)/19:0)	11.231	645.5	$C_{35}H_{69}N_2O_6P$	1.52	Sphingolipids
15e	2-Cyanoethylphosphine	0.587	110.0	C_3H_6NP	1.37	Adhesive composition using polyamideimide resin, polycarbonate mold, protective film[69–71]
16e	N-{4-[(E)-(Hydrazinylmethylidene)amino]phenyl}methanesulfonamide	0.717	251.1	$C_8H_{12}N_4O_2S$	1.33	Suspected former[24]
17e	Methanesulfonic acid--2,3-bis(tetradecyloxy)propan-1-ol (1/1)	11.559	603.5	$C_{32}H_{68}O_6S$	1.29	Suspected surfactant[24]
18e	3-{[(Benzyloxy)carbonyl]amino}-N-(tert-butoxycarbonyl)-L-alanine--N-cyclohexylcyclohexanamine (1/1)	4.915	520.3	$C_{28}H_{45}N_3O_6$	1.22	Antibacterial amide-macrocycles IV, V sold by Sigma Aldrich 2.5g for $285.00 (CAS#65710-58-9)[72]
19e	10,12-Pentacosadiynoyl chloride	8.272	393.3	$C_{25}H_{41}ClO$	1.09	Fluorescent material that can be used in

						art, plastics and for thermoplastics
20e	Hexabromobenzene	11.0325	545.5	C_6Br_6	1.08	Flame retardant[73]

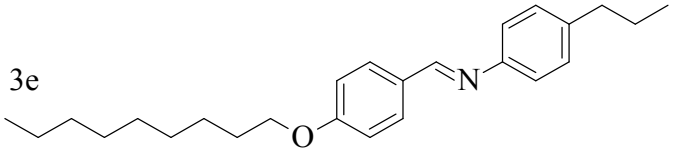
1e



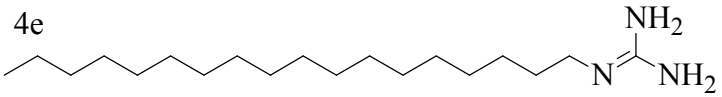
2e



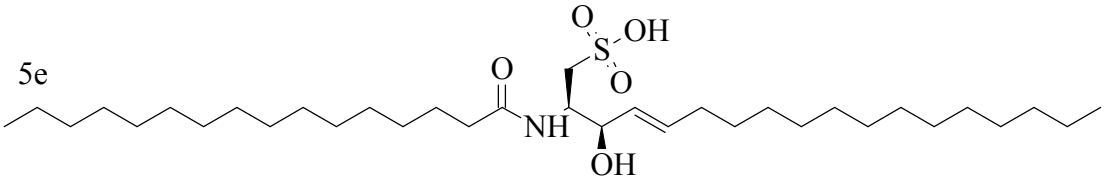
3e



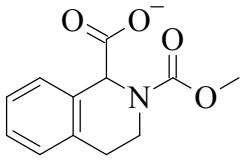
4e



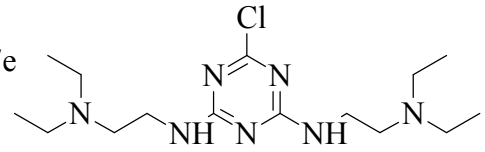
5e



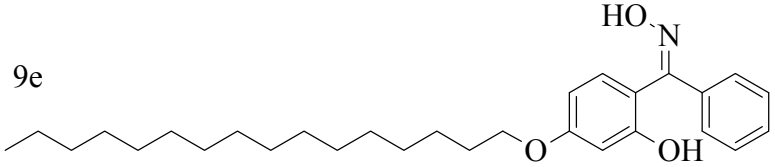
6e



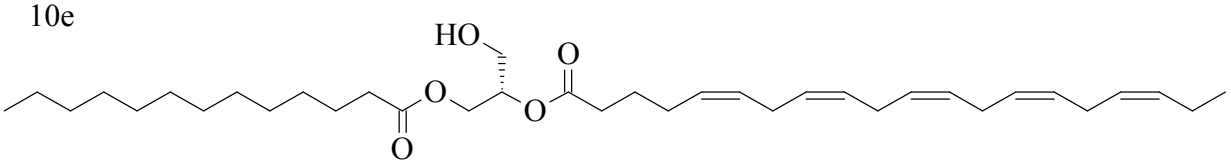
7e



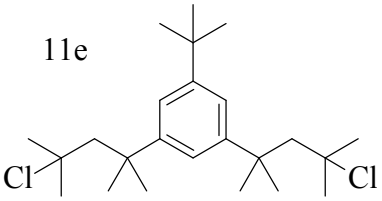
9e



10e



11e



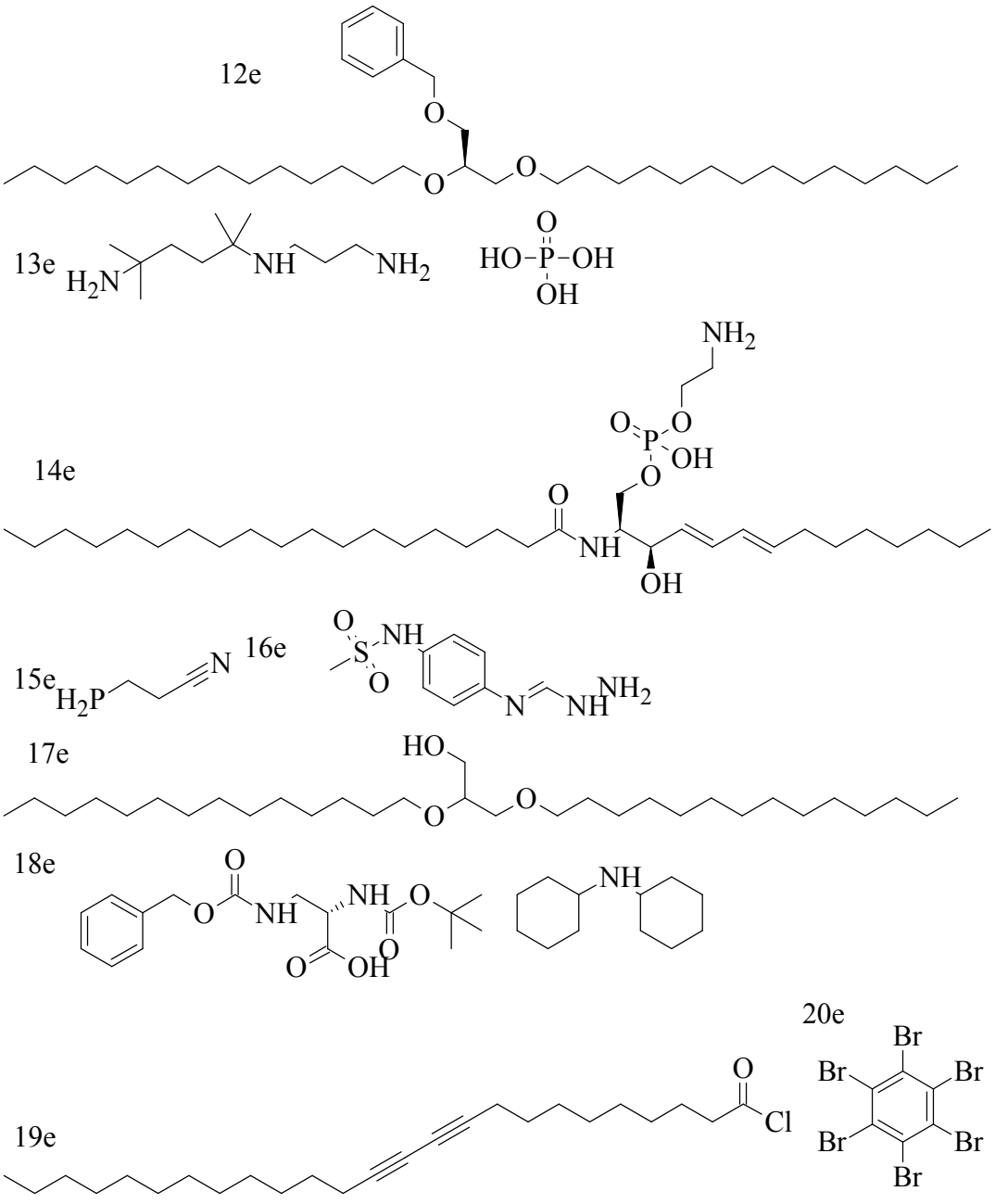


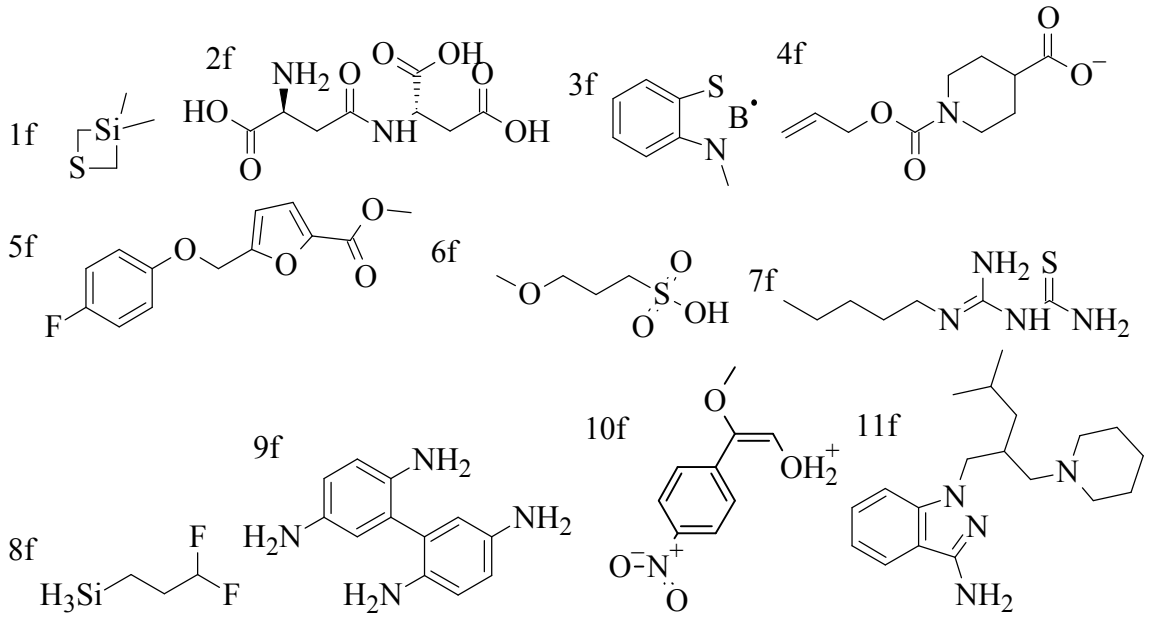
Figure 12. Top 20 structures from Water extract Positive

Table 6. Water LC-MS extract Negative:

S.No.	Name	Retention Time	M. W.	Chemical Formula	Area under peak	Common uses
1f	3,3-Dimethyl-3-silathietane	1.270	117.0	$C_4H_{10}SSi$	53.531	Investigated intensively mass spec, NMR, and other methods due to its unique structure[74]
2f	beta-Aspartylaspartic acid	0.757	247.1	$C_8H_{12}N_2O_7$	37.962	Drug carrier for liver targeting synthesis; sold by Ark Pharma Scientific, Ltd. 1g for $1300.00 (CAS#60079-22-3)[75,76]
3f	3-Methyl-1,3,2-benzothiazaborol-2(3H)-yl	1.258	147.0	C_7H_7BNS	33.141	General reactions
4f	1-{[(Prop-2-en-1-yl)oxy]carbonyl}piperidine-4-carboxylate	0.721	211.1	$C_{10}H_{14}NO_4$	30.712	Suspected fragrance[24]
5f	Methyl 5-((4-fluorophenoxy)methyl)furan-2-carboxylate	0.747	249.1	$C_{13}H_{11}FO_4$	10.887	Sold by AK Scientific, Inc. 1g for $1593.00 (CAS#438220-96-3)
6f	3-Methoxypropanesulphonic acid	3.258	153.0	$C_4H_{10}O_4S$	10.828	Used in non-aqueous electroylte secondary battery[77]
7f	N-(N'-Pentylcarbamimidoyl)thiourea	5.698	187.1	$C_7H_{16}N_4S$	9.601	Improves anti-inflammatory composition and method of treating inflammation when pairing with an anti-inflammatory agent[78]
8f	(3,3-Difluoropropyl)silane	4.135	109.0	$C_3H_8F_2Si$	8.776	Suspected hair conditioner[24]
9f	[1,1'-Biphenyl]-2,2',5,5'-tetramine	7.300	213.1	$C_{12}H_{14}N_4$	8.587	Composition for coloring keratin fibers, long lasting cosmetic

						composition, silicone resin-linear copolymer[79]
10f	[2-Methoxy-2-(4-nitrophenyl)ethenyl]oxidanium	0.784	195.1	$C_9H_{10}NO_4$	8.199	Pharmacutical for erectile-dysfunction and for deep vein thrombosis, and extremity edema
11f	1-{4-Methyl-2-[(piperidin-1-yl)methyl]pentyl}-1H-indazol-3-amine	9.812	313.2	$C_{19}H_{30}N_4$	7.857	General reactions
12f	Phosphinic acid, bis(1-aziridinyl)-, methyl ester	1.359	161.0	$C_5H_{11}N_2O_2P$	7.825	Prodrug that can be used to treat cancer when administered alone or in combination with one or more anti-neoplastic agents[80]
13f	6H-Purin-6-one	0.984	133.0	$C_5H_2N_4O$	6.929	Stimulator of interferon genes (STING) modulators/agonists, for the treatment of cancer and other STING related diseases; used for treating conditions that TRPA1 receptor uses
14f	Salicylic acid	4.320	137.0	$C_7H_6O_3$	6.037	Treats acne caused by causing skin cells to slough off more daily, which in turn prevents pores from clogging up, flavoring agent; sold by Fisher Scientific 500g for $210.00[81–83]
15f	(3-Methylbuta-1,2-diene-1,1-diyl)bis[tert-butyl(dimethyl)silane]	9.948	295.2	$C_{17}H_{36}Si_2$	5.664	General reactions

16f	4-hydroxy-valeric acid	3.498	117.1	$C_5H_{10}O_3$	5.523	Used in various reactions involving catalyst applications, green chemistry, polymers; sold by MolPort 1mg for $61.00[84,85]
17f	2,3,3-Trimethyl-1,3-thiasilinane	1.181	159.1	$C_7H_{16}SSi$	5.418	Used in multiple reactions to study rearrangement and structure analysis[86,87]
18f	{(But-2-yn-1-yl)[(2R)-1-(3-hydroxyphenyl)propan-2-yl]amino}oxidanide	5.303	217.1	$C_{13}H_{16}NO_2$	5.129	General reactions
19f	Triethyl{5-[(triethylsilyl)oxy]pent-1-yn-1-yl}silane	8.037	311.2	$C_{17}H_{36}OSi_2$	4.770	Substituted piperdine derivative useful as 5-HT1 receptor agonist[88]
20f	Pyridine, 2-(1-piperidinylmethyl)-, dihydrochloride	4.956	247.1	$C_{11}H_{18}Cl_2N_2$	3.989	General reactions



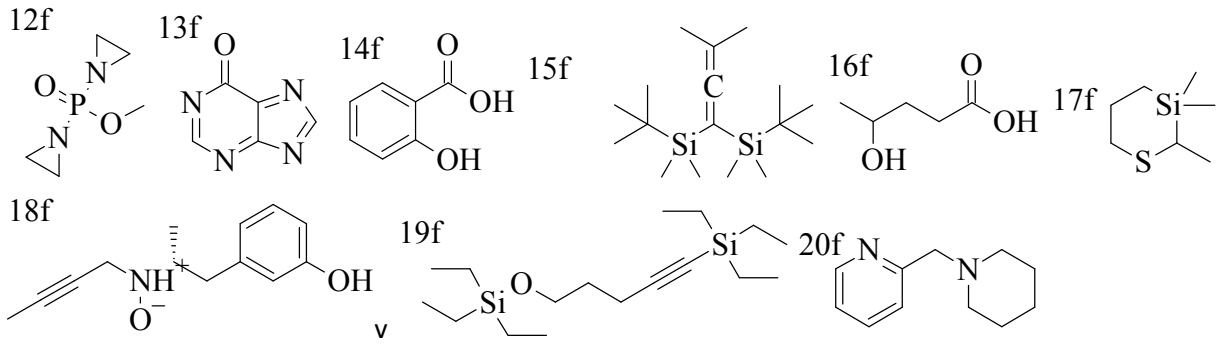


Figure 13. Top 20 structures from Water extract Negative

12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one

12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one (DBOC-2), white powder, elucidated from mother column at 10% ethyl acetate in hexane, then re-chromatography at 3% ethyl acetate in hexane, with a melting point range of 56.9-59.2°C. HRMS weight of 255.0879 m/z. FTIR cm^{-1} 2953.90-2847.63 aldehyde, 1698.03 conjugated aldehyde, ^{1}H NMR (600 MHz, $CDCl_3$ ppm δ 7.25) ^{1}H-NMR ppm δ5.3470 (s), 2.3452 (3H, t, J = 7.50), 2.0109 (1H, d, J = 5.40), 1.6299 (2H, q, J = 7.56), 1.2923 (15H, m), 0.8798 (3H, t, J = 7.14); ^{13}C ppm δ180.12, 130.02, 34.06, 31.93, 29.70, 29.68, 29.67, 29.64, 29.59, 29.36, 29.24, 29.07, 27.22, 27.16, 24.68, 22.69, 14.10. HMQCGP shows that the signal ppm ^{1}H and ^{13}C δ5.3470 and 130.02 this shows a relationship between the two probably a carbonyl.

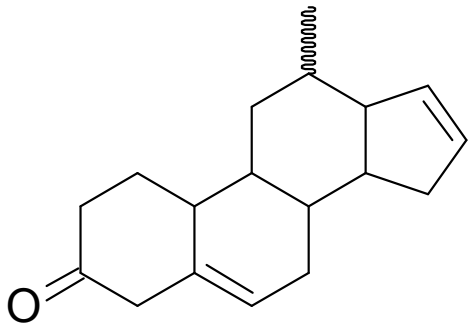


Figure 14. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one proposed structure

(4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol

(4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol (DBVC-1), white powder, elucidated from column in ethanol, has a weight of 232.0775 m/z, melting point 184.6-185.7. FT-IR shorth broad band at cm^{-1} 3100-3500, which is probably representative of -OH, 1310.05 is a phenol, 1092.70 amine; ^{1}H NMR (600 MHz, DMSO-d6, 2.50 ppm δ 7.25) ^{1}H-NMR ppm δ4.4093 (1H, q, J = 22.56), 4.3345 (1H, t, J = 11.34), 4.1083 (3H, d, J = 6.72), 4.0497 (2H, q, J = 21.48), 3.9457 (3H, d, J=7.80), 3.7167 (2H, m), 3.6228 (3H, q, J = 19.98), 3.5727 (5H, t, J = 8.04);); ^{13}C ppm δ 72.07, 70.67, 70.15, 69.61, 68.97, 64.40, 63.73, 40.42, 40.28,40.14, 40.00.

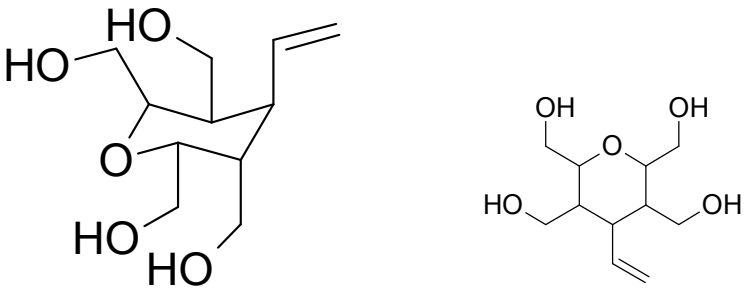


Figure 15. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol proposed structure

CHAPTER IV

DISCUSSION

It is important to note that some molecules are stated as "suspected" on the table; this is due to the only available information as to what these molecules could be for come from the Environmental Protective Agency (EPA), in which these molecules are put through a high-throughput screening which labeled the chances of what it uses cold be.[89] It is also important to note that some of these molecules are currently found in commercial products as byproducts, but show to have no relative harmful interaction with humans.

Then there are molecules such as **2d** and **6f** which are the same but have a different label these molecules both appeared in the water and ethanol extract, but **2d** has a higher peak area and therefore would be better to extract in ethanol; the same goes for **12d** and **7f**.

Interesting Molecules in Ethanol Extract Positive and Negative

Molecule **5c** can be used as a quinolyl modulator for retinoic acid-related nuclear receptor gamma t(RORyT), which essentially means that it can be used to prevent/treat inflammatory-related diseases.[25] **6c** can be used when complexed with β-cyclodextrin to make an antimicrobial; also when used with Triton X-100 surfactant, it can increase the critical micelle concentration of the product.[90,91] **9c** can be used in manufacturing to make solar cells, as a buffer for RNA strands, and can be used in combination with Heparin anticoagulant for blood to create a sustainable release of the medication increasing its therapeutic nature; as a bonus due to the recent strains of the novel COVID-19 virus, it has been shown that Herapin can inhibit it's

binding to glycoproteins further helping manage the strain of the virus.[27,92] **11c** can be used to prevent cell death through apoptosis that results from Ischemia/Reperfusion injury.[29,30] **12c** is a drug that is still not on the market and is currently going through clinical trials for Duchenne Muscular Dystrophy; if the drug comes out positive out of the clinical trials it could very well be that the seed husk as a natural source of the drug, and since the drug is considered an orphan drug and could lower the cost of manufacturing it drastically.[31,93] **14c** is a type of peripheral vasodilating agent which can be used to widen blood vessels, and in conjunction to it being a type of boronic acid (which have been widely been known to treat other diseases) it could warrant an investigation to see if there is any bioactivity into this molecule.[33,94] 1**5c** is used as induced fluorescence resonance energy transfer (iFRET), which can be used to study DNA hybridization/denaturing through the intensity of fluorescence.[95] **15c** can be used as a Discoidin Domain Receptors (DDRs) inhibitor, specifically DDR1 which has been linked to inflammation and any resulting fibrosis.[58,96] **18c** is commonly used as a GC-,LC-MS standardization through 4-ONE where 50µg for $78.00 making it astronomically expensive; a new source of collecting this molecule can make this cheaper.[37] **22c** is a naturally occurring fatty acid, that is used in the cosmetic industry to help with the anti-aging of the skin; as a side note it's also been studied to help with Alzheimer's disease which is essentially a neurological degradation, it's been shown that with the use of other metabolites it's possible to slow this degradation down. **24c** can be used for general reactions, but it is mostly used for pharmaceuticals; a new source of this constituent could bring the price down. **25c** has multiple uses starting as just a general substituent for multiple reactions, as a corrosion inhibitor[97], and acts as an antimicrobial[98]; coupled with the extravagant expense for just 5g this could also be a new source for it.

Molecule **2d** has usage for non-aqueous batteries and is used in the process to make perfluorosulfonic acid, which for the most part is used in fuel cells.[99] **3d** is an interesting one as it is a drug called Sercloremine which was studied in the 1980s, but for some reason never came out to market, there does seem to be some use for it androgen-mediated cancers, and it seems that is still being studied as a patent dated 2008 has been placed on it.[100,101] **4d** is a substituent in making Entecavir, which is a drug used for the virus hepatitis B halting its DNA elongation by adding a few more bases into the chain; the drug cost about $90.12 for a supply of 30 tablets, apart from that **4d** is relatively expensive to 1mg for $175.00, which could potentially lower the price on the drug overall if the seed husk is added into the supply chain.[46,102,103] **8d**, **14d**, and **26d** has an astronomical price of 25g for $1290.00, 5g for $1250.00, and 1g for $750.00 respectively, while the uses are for general reactions the avocado seed husk could prove to be a natural source for researches who don't wish to pay such a price.

Interesting Molecules in Water Extract Positive and Negative

2e, **3e**, **4e**, **6e**, and **11e** are generally used for reactions, with **2e** and **3e** showing some use in the polymer industry and acting a sort of adhesive; and **11e** being used to produce binifer telechelic polymers at higher degrees such as -30°C. **9e** is used to accelerate the extraction of copper from aqueous solutions more economical, with 1 mg costing about $55.00 on Sigma Aldrich™.[66] **15e** is used for general molds and resin, used in the plastic industry, as a protective film and adhesive; it's and cost of 1g for $22.80 (Alfa Aesar) could drop the price down even further. **18e** looks promising due to it being an antimicrobial which is sold through Sigma Aldrich (and other companies) 2.5g for $285.00. This antimicrobial for which there is a patent explaining that derivatives such as this can be useful against *Staphylococcus aureus (S. aureus)* bacteria and its derivatives of this molecule can be used to combat the different strains of it.[91]

1f, **5f**, and **17f** are used to study their structures and the further advancement of science through different methods such as GC-MS, NMR, and IR; these can generally be used for a multitude of reactions. **2f** is interesting both for its cost on the market, but also because it uses as a drug carrier for the liver make it a promising component to be extracted from the seed husk.[104] **9f** and **16f** is used for multiple polymer reactions, with **16f** having the bonus of being used for green chemistry reactions. **12f** is a prodrug used in cancer chemotherapy treatments in combination with other medications.[80] **14f** is an amazing find as firstly it's used for skin care treatments, to prevent build up on skin pores and this shows that the seed husk is definitely another source for such a versatile type of drug.[81–83] **19f** is used as a receptor agonist, that might show vasoconstriction, which is the constriction of blood vessels, treating things such as migraines.[88]

12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one

DBOC-2 has a very similar motif as DBOC-1, sharing some common ^{13}C peaks from DBOC-1, there seem to be two smaller peaks indicative of the double bond present in the steroid, and DBOC-2 ppm δ 130.02, shows a greater peak, but still not as intense in a similar range. ^{13}C peak ppm δ180.12, shows the carbonyl group present inside of the steroid and is also indicative of a quaternary carbon present. Looking at the HMBGCP ^{13}C peak ppm δ27.22 and 27.16 and H peak 1.6299 quintuplets are related leaving me to suspect that it is a double bond too.

(4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol

The physical properties of the compound show that it's relatively pure as it has a melting point range that is 1.1°C; inputting the proposed structure into Scifinder™, ScienceDirect™, and Google Scholar™ doesn't bring up any information on this molecule. Leaving to believe this is a newly discovered molecule and as such its uses are still unknown; as such it will be sent for biological testing to further explore what a possible use for this compound could be.

CHAPTER V

CONCLUSION

This investigation shows that the avocado seed husk is ripped full of chemical components that are already on the market and some of which are extremely expensive and/or difficult to make. Some of which are already used as medication on the market such as salicylic acid, but also medication such as Myodur which is still going through clinical trials. This is also not discounting the use of polymers that can be gathered from just harvesting a part that is right now disappointingly going to waste. I do not doubt that if the seed husk is implemented industrially it would reduce not only waste, it will also increase the productivity of materials and medication that are desperately needed on the market.

REFERENCES

(1) Ahamed, A.; Yin, K.; Ng, B. J. H.; Ren, F.; Chang, V. W. C.; Wang, J. Y. *Journal of Cleaner Production* **2016**, *131*, 607–614.

(2) Lin, C. S. K.; Koutinas, A. A.; Stamatelatou, K.; Mubofu, E. B.; Matharu, A. S.; Kopsahelis, N.; Pfaltzgraff, L. A.; Clark, J. H.; Papanikolaou, S.; Kwan, T. H.; Luque, R. *Biofuels, Bioproducts and Biorefining* **2014**, *8* (5), 686–715.

(3) Salemdeeb, R.; zu Ermgassen, E. K. H. J.; Kim, M. H.; Balmford, A.; Al-Tabbaa, A. *Journal of Cleaner Production* **2017**, *140*, 871–880.

(4) Key facts on food loss and waste you should know! | SAVE FOOD: Global Initiative on Food Loss and Waste Reduction | Food and Agriculture Organization of the United Nations http://www.fao.org/save-food/resources/keyfindings/en/ (accessed Dec 6, 2017).

(5) Bahru, T. B.; Tadele, Z. H.; Ajebe, E. G. *Chemical Science International Journal* **2019**, 1–10.

(6) Lin, X.; Zhang, H.; Hu, L.; Zhao, G.; Svanberg, S.; Svanberg, K. *Journal of Biophotonics* **2020**, *13* (8).

(7) Ford, N. A.; Liu, A. G. *Frontiers in Nutrition* **2020**, *7*, 78.

(8) Haiyan, Z.; Bedgood, D. R.; Bishop, A. G.; Prenzler, P. D.; Robards, K. *Food Chemistry* **2007**, *100* (4), 1544–1551.

(9) USDA ERS - Charts of Note https://www.ers.usda.gov/data-products/charts-of-note/charts-of-note/?topicId=14849 (accessed Nov 6, 2020).

(10) Dennis; Cut Nurliza; Wulandari Savitri. *International Journal of Applied Dental Sciences* **2016**, *3* (1), 89–93.

(11) Tambun, R.; Tambun, J. O. A.; Tarigan, I. A. A. In *IOP Conference Series: Materials Science and Engineering*; Institute of Physics Publishing, 2020; Vol. 725, p 012075.

(12) Figueroa, J. G.; Borrás-Linares, I.; Lozano-Sánchez, J.; Segura-Carretero, A. *Food Research International* **2018**, *105*, 752–763.

(13) Takenaga, F.; Matsuyama, K.; Abe, S.; Torii, Y.; Itoh, S. *Journal of Oleo Science* **2008**, *57* (11), 591–597.

(14) Food Waste FAQs | USDA https://www.usda.gov/foodwaste/faqs (accessed Nov 6, 2020).

(15) Salemdeeb, R.; zu Ermgassen, E. K. H. J.; Kim, M. H.; Balmford, A.; Al-Tabbaa, A. *Journal of Cleaner Production* **2017**, *140*, 871–880.

(16) Sze, C.; Lin, K.; Papanikolaou, S.; Luque, R. **2014**.

(17) Perea-Moreno, A. J.; Aguilera-Ureña, M. J.; Manzano-Agugliaro, F. *Fuel* **2016**, *186*, 358–364.

(18) Valensya, D.; Rozalia, I.; Syamsuddin, Y. .

(19) Alkhalaf, M. I.; Alansari, W. S.; Ibrahim, E. A.; ELhalwagy, M. E. A. *Journal of King Saud University - Science* **2019**, *31* (4), 1358–1362.

(20) Rahman, N.; Dewi, N. U.; Bohari. *Asian Journal of Scientific Research* **2018**, *11* (3), 357–363.

(21) Hatzakis, E.; Mazzola, E. P.; Shegog, R. M.; Ziegler, G. R.; Lambert, J. D. *Food Chemistry* **2019**, *293*, 15–22.

(22) Di-n-butyl phthalate - American Chemical Society https://www.acs.org/content/acs/en/molecule-of-the-week/archive/d/di-n-butyl-phthalate.html (accessed Nov 8, 2020).

(23) Docosane - Substance Information - ECHA https://echa.europa.eu/substance-information/-/substanceinfo/100.010.111 (accessed Nov 8, 2020).

(24) CompTox Chemicals Dashboard | Home https://comptox.epa.gov/dashboard (accessed Nov 25, 2020).

(25) WO2015057626A1 - QUINOLINYL MODULATORS OF RORyT - Google Patents https://patents.google.com/patent/WO2015057626A1 (accessed Nov 27, 2020).

(26) 1-Dodecyl-3-methylimidazolium tetrafluoroborate | C16H31BF4N2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/1-Dodecyl-3-methylimidazolium-tetrafluoroborate#section=Drug-Gene-Interactions (accessed Nov 23, 2020).

(27) Tetrakis(3-aminopropyl)ammonium | C12H32N5+ - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Tetrakis_3-aminopropyl_ammonium#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 23, 2020).

(28) Human Metabolome Database: Showing metabocard for DG(14:0/0:0/20:5n3) (HMDB0055978) https://hmdb.ca/metabolites/HMDB0055978 (accessed Nov 24, 2020).

(29) Methyl 12-[(methanesulfonyl)oxy]octadecanoate | C20H40O5S - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Methyl-12-_methanesulfonyl_oxy_octadecanoate#section=Patents (accessed Nov 25, 2020).

(30) Stuart, J. *(54) MITOCHONDRIA-TARGETED INHIBITORS OF CYTOCHROME C PEROXIDASE FOR PROTECTION FROMAPOPTOSIS (71) (72) (21) (22) (60) Applicants: Jeffrey Atkinson, St. Catharines (CA); (30) Foreign Application Priority Data*;

2013.

(31) L-aminocarnityl-succinyl-leucyl-argininal-diethylacetal | DrugBank Online https://go.drugbank.com/drugs/DB06124 (accessed Nov 25, 2020).

(32) N-(Tetradecanoyl)-sphing-4-enine-1-(2-aminoethylphosphonate) | C34H69N2O5P - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/5283605#section=Patents (accessed Nov 24, 2020).

(33) Cambre, J. N.; Sumerlin, B. S. *Polymer*. Elsevier Ltd September 29, 2011, pp 4631–4643.

(34) 3,5-Bis(methoxycarbonyl)-1-methylpyridinium | C10H12NO4+ - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/3_5-Bis_methoxycarbonyl_-1-methylpyridinium#section=Patents (accessed Nov 24, 2020).

(35) 8-Benzyl-1-phenyl-1,3,8-triaza-spiro[4.5]decan-4-one | C20H23N3O - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/70419#section=Literature (accessed Nov 25, 2020).

(36) Morrison, J. B.; Hecht, S. S. *Food and Chemical Toxicology* **1982**, *20* (5), 583–586.

(37) Szarka, S.; Prokai-Tatrai, K.; Prokai, L. *Analytical Chemistry* **2014**, *86* (14), 7033–7040.

(38) N1,N3,N5-Trioctylbenzene-1,3,5-tricarboxamide | C33H57N3O3 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/N1_N3_N5-Trioctylbenzene-1_3_5-tricarboxamide#section=Patents (accessed Nov 25, 2020).

(39) Petroselinic acid | C18H34O2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/5281125#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(40) Tetrabutylphosphonium chloride | C16H36ClP - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/75311#section=Patents (accessed Nov 25, 2020).

(41) Oleyldimethylamine | C20H41N - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/5357010#section=Patents (accessed Nov 25, 2020).

(42) 1-Ethyl-6-fluoro-3-formyl-1,4-dihydro-7-(4-methyl-1-piperazinyl)-4-oxoquinoline | C17H20FN3O2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/3082580#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(43) Sprinzl, M.; Farkaš, J.; Šorm, F. *Collection of Czechoslovak Chemical Communications* **1967**, *32* (4), 1649–1652.

(44) 51980-59-7,3-Methoxypropane-1-sulfonic Acid-AccelaChem|AccelaChemBio|Accela design, synthesis, manufacture and market advanced R&D chemicals http://www.accelachem.com/cn/productview_goodsid_13098_goodscode_SY011651.html (accessed Nov 24, 2020).

(45) Waldmeier, P. C.; Tipton, K. F.; Bernasconi, R.; Felner, A. E.; Baumann, P. A.; Maitre, L. *European Journal of Pharmacology* **1984**, *107* (1), 79–89.

(46) Zhou, M. X.; Pendri, R.; Glastonbury, S.; Davis, S. B.; Hn, O. H.; Ny X Hn M N O, N. *(54) (76) (21) (22) PROCESS FOR THE PREPARATION OF ENTECAVIR AND NOVELINTERMEDIATES THEREOF WIA CARBON-SILICON OXIDATION BRISTOL-MYERS SQUIBB COMPANY PATENT DEPARTMENT PO BOX 4000 Processes for preparing entecavir and novel intermediates thereof using carbon-Silicon oxidation. 1 (entecavir) OH PROCESS FOR THE PREPARATION OF ENTECAVIR AND NOVELINTERMEDIATES THEREOF WIA CARBON-SILICON OXIDATION RELATED APPLICATION*; 2005.

(47) Blicke, F. F.; Schaaf, R. L. *Journal of the American Chemical Society* **1956**, *78* (22), 5857–5863.

(48) 1-Pyrrolidinecarbonyl chloride | C5H8ClNO - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/70937#section=Patents (accessed Nov 25, 2020).

(49) 3-Ethoxy-1,2-propanediol | C5H12O3 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/3-Ethoxy-1_2-propanediol#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 28, 2020).

(50) Allylamine, N,N-bis(2-chloroethyl)- | C7H13Cl2N - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/45077#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(51) Aremu, A. O.; Masondo, N. A.; Rengasamy, K. R. R.; Amoo, S. O.; Gruz, J.; Bíba, O.; Šubrtová, M.; Pěnčík, A.; Novák, O.; Doležal, K.; Van Staden, J. *Planta* **2015**, *241* (6), 1313–1324.

(52) Acetamide, N,N'-[(methylimino)di-3,1-propanediyl]bis[2,2,2-trifluoro- | C11H17F6N3O2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/54519756#section=Patents (accessed Nov 24, 2020).

(53) *United States Patent o Hill et al. (54 PROCESSES FOR 2-(1-PENTYL-3-GUANIDINO)-4-(2-METHYL 4-MIDAZOLYL) THAZOLE AND*; 1989.

(54) 2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-YL)-4-(trifluoromethyl)aniline | C13H17BF3NO2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/1058062-64-8#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 24, 2020).

(55) Diisopropoxycalcium | C6H14CaO2 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/13766994#section=Patents (accessed Nov 24, 2020).

(56) Kingsbury, W. D. *Application Data 63 Continuation-in-part of Ser*; 1974; Vol. 841.

(57) 5-(4-Hydroxy-3-methoxyphenyl)-5-phenylhydantoin | C16H14N2O4 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/3080785#section=Patents (accessed Nov 25, 2020).

(58) Chen, Z.; Kolokoltsov, A. A.; Wang, J.; Adhikary, S.; Lorinczi, M.; Elferink, L. A.; Davey, R. A. **2012**.

(59) Inosine, 2-fluoro- | C10H11FN4O5 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Inosine_-2-fluoro#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(60) 2'-Deoxy-2'-fluoroinosine | C10H11FN4O4 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/135435172#section=Patents (accessed Nov 25, 2020).

(61) Hydroxy(oxo)(2-phenylethenyl)phosphanium | C8H8O2P+ - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Hydroxy_oxo_2-phenylethenyl_phosphanium#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(62) Pullheim, Herbert, Cologne, Robert, Rosrath, P. POLYPENTABROMOSTYRENE, PROCESS FOR THE PRODUCTION AND USE BACKGROUND OF THE INVENTION, July 7, 1981.

(63) Pentabromo(2-bromoethyl)benzene | C8H4Br6 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Pentabromo_2-bromoethyl_benzene#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 25, 2020).

(64) Yokoyama, Yasuaki, Bessho, Nobuo, Hanamura, M. COMPOSITION AND METHOD FOR TEMPORARLY FIXING SOLID, May 12, 2003.

(65) N-(3E-Hexadecenoyl)-deoxysphing-4-enine-1-sulfonate | C34H65NO5S - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/42608341#section=LIPID-MAPS-Classification (accessed Nov 28, 2020).

(66) Peter Muehl, Karsten Gloe, Joerg Beger, H. J. B. **1982**.

(67) 1-Tridecanoyl-2-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycerol | C36H60O5 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/56936336#section=Information-Sources (accessed Nov 29, 2020).

(68) Kennedy, J. The present invention relates to sterically hindered binifers and to polyisobutylene telechelic polymers made therefrom. BACKGROUND ART, August 6, 1984.

(69) **家根武久小柳英之**, **大類學**, **海老原智**. Adhesive composition using polyamidoximine resin, March 3, 2017.

(70) Nobuhiro, W. Polycarbonatharz-Zusammensetzung und Formprodukt daraus, November 8, 2016.

(71) **田 完 二田 完 二**, **藤 和 也 佐**, **藤 和 也 佐**. Protective film forming film, September 15, 2016.

(72) Endermann, R.; Ehlert, K.; Raddatz, S.; Michels, M.; Cancho-Grande, Y.; Weigand, S.;

Fischer, K. Antibacterial amide-macrocycles v.

(73) Venier, M.; Ma, Y.; Hites, R. A. *Environmental Science and Technology* **2012**, *46* (16), 8653–8660.

(74) Gusel'nikov, L. E.; Volkova, V. V.; Zaikin, V. G.; Tarasenko, N. A.; Tishenkov, A. A.; Nametkin, N. S.; Voronkov, M. G.; Kirpichenko, S. V. *Journal of Organometallic Chemistry* **1981**, *215* (1), 9–17.

(75) Reiko, T. L.; Yuan-Chuan, L.; Mei-Hui, W.; Wuu-Jyh, L. Novel liver-targeting agents and their synthesis, September 27, 2010.

(76) L-beta-Aspartyl-L-aspartic acid | C8H12N2O7 - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/274178#section=Depositor-Supplied-Patent-Identifiers (accessed Nov 27, 2020).

(77) Shuhei, S.; Kunihisa, S.; Yasuyuki, S.; Masamichi, O.; Atsushi, W. Non-aqueous electrolyte solution and non-aqueous electrolyte secondary battery employing the same, July 31, 2013.

(78) John, L. Formulation of antiinflammatory drugs, October 9, 1985.

(79) Antonio, C.; Massimo, F.; Katiuscia, G. Composition for colouring keratin fibres, October 17, 2019.

(80) Matteucci, Mark, Duan, Jian-xin, Jiao, Hailong, Kaizerman, J. Phosphoramidate alkylator prodrugs, June 29, 2006.

(81) Salicylic acid | DrugBank Online https://go.drugbank.com/drugs/DB00936 (accessed Nov 27, 2020).

(82) Salicylic acid | HOC6H4COOH - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/Salicylic-acid#section=Patents (accessed Nov 27, 2020).

(83) Cartron, A. M.; Blaszczak, A.; Trinidad, J. C. *Dermatologic Therapy* **2020**, *33* (2).

(84) Horváth, I. T.; Mehdi, H.; Fábos, V.; Boda, L.; Mika, L. T. *Green Chemistry* **2008**, *10* (2), 238–24.

(85) Valentin, H. E.; Schönebaum, A.; Steinbüchel, A. *Applied Microbiology and Biotechnology* **1992**, *36* (4), 507–514.

(86) Suslova, E. N.; Ushakov, I. A.; Shainyan, B. A. *Russian Journal of General Chemistry* **2007**, *77* (2), 253–263.

(87) 2,3,3-Trimethyl-1,3-thiasilinane | C7H16SSi - PubChem https://pubchem.ncbi.nlm.nih.gov/compound/2_3_3-Trimethyl-1_3-thiasilinane#section=Information-Sources (accessed Nov 27, 2020).

(88) Baker, R.; Madin, A.; Guilio Matassa, V.; Joseph Street, L. *PIPERAZINE, PIPERIDINE AND TETRAHYDROPYRIDINE DERVATIVES USEFUL AS 5-HT1 RECEPTERAGONSTS*; 1997; Vol. 102.

(89) Phillips, K. A.; Wambaugh, J. F.; Grulke, C. M.; Dionisio, K. L.; Isaacs, K. K. *Green Chemistry* **2017**, *19* (4), 1063–1074.

(90) Zhang, S.; Gao, Y.; Dong, B.; Zheng, L. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **2010**, *372* (1–3), 182–189.

(91) Hodyna, D.; Bardeau, J. F.; Metelytsia, L.; Riabov, S.; Kobrina, L.; Laptiy, S.; Kalashnikova, L.; Parkhomenko, V.; Tarasyuk, O.; Rogalsky, S. *Chemical Engineering Journal* **2016**, *284*, 1136–1145.

(92) Ito, D.; Ge, D.; Kogure, N.; Manaka, H.; Terui, Y.; Takayama, H.; Linhardt, R. J.; Toida, T.; Higashi, K. *Heliyon* **2020**, *6* (10), e05168.

(93) Radley, H. G.; De Luca, A.; Lynch, G. S.; Grounds, M. D. *International Journal of Biochemistry and Cell Biology*. Pergamon January 1, 2007, pp 469–477.

(94) US5656642A - Peripheral vasodilating agent containing piperidine derivative as active ingredient - Google Patents https://patents.google.com/patent/US5656642A/en (accessed Nov 27, 2020).

(95) Howell, W. M.; Jobs, M.; Brookes, A. J. *Genome Research* **2002**, *12* (9), 1401–1407.

(96) US10239876B2 - Triaza-spirodecanones as DDR1 inhibitors - Google Patents https://patents.google.com/patent/US10239876B2 (accessed Nov 27, 2020).

(97) WO2020046967A1 - Oil and gas field corrosion inhibitor compositions - Google Patents https://patents.google.com/patent/WO2020046967A1 (accessed Nov 27, 2020).

(98) WO2020043269A1 - Antimicrobial mixtures comprising at least one hydroxyphenone derivative - Google Patents https://patents.google.com/patent/WO2020043269A1 (accessed Nov 27, 2020).

(99) *Non-aqueous electrolyte solution and non-aqueous electrolyte secondary battery employing the same*; 2013.

(100) BRAND, B. S.; BURCH, D. J.; KRISHNAN, R. **2012**.

(101) Delini-Stula, A.; Fischbach, R.; Gnirss, F.; Bures, E.; Pöldinger, W. *Drug Development Research* **1985**, *6* (4), 371–384.

(102) Langley, D. R.; Walsh, A. W.; Baldick, C. J.; Eggers, B. J.; Rose, R. E.; Levine, S. M.; Kapur, A. J.; Colonno, R. J.; Tenney, D. J. *Journal of Virology* **2007**, *81* (8), 3992–4001.

(103) Entecavir Prices, Coupons & Patient Assistance Programs - Drugs.com https://www.drugs.com/price-guide/entecavir (accessed Nov 28, 2020).

(104) Kazunori, Kataoka, Yasutaka, Anraku, Nobuhiro, Nishiyma, Kanjiro, Miyata, Takehiko, ISHII, Yu, Matsumoto, Yu, Fukusato, Akihiro, Mizoguchi, Takanori, Yokota, Hiroya, Kuwahara, Kazutaka, Nishina, Hedehiro, M. *Carrier for use in delivering drug, conjugate, composition comprising same, and method for administrating same*; 2014.

APPENDIX

(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((*R*)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-*1H*-cyclopenta[a]phenanthren-3-ol Spectras

Figure 16. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras FTIR

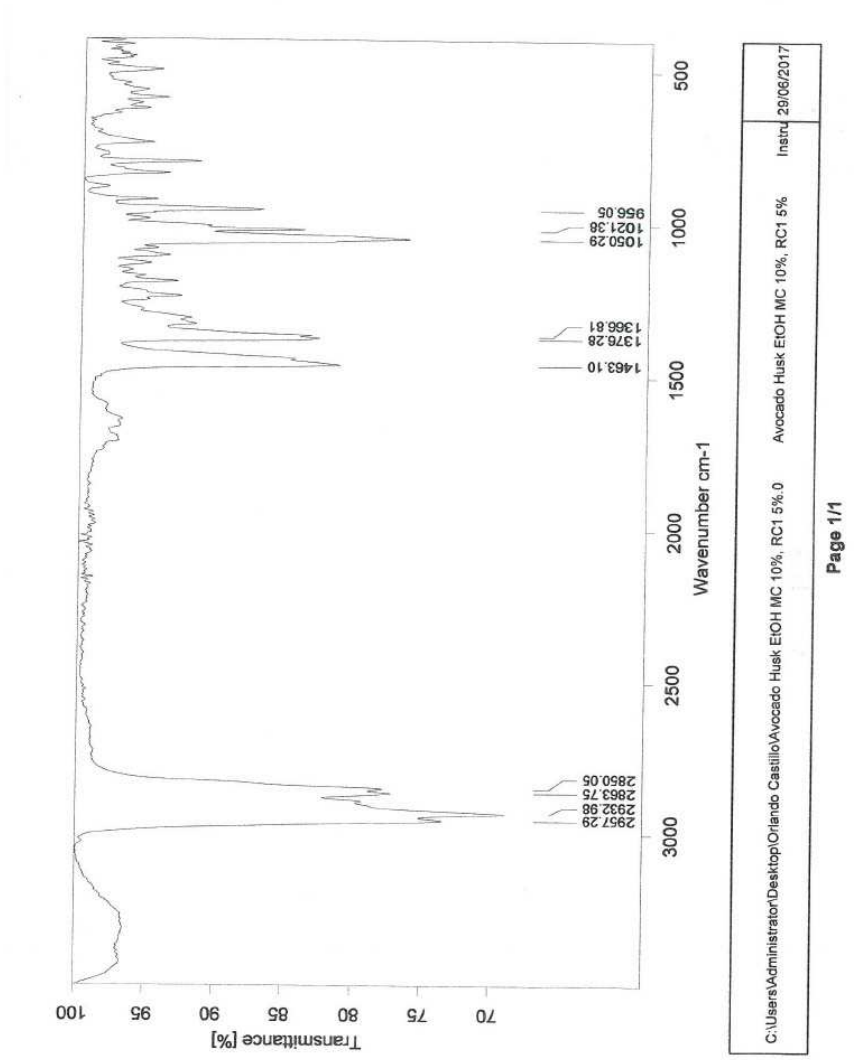


Figure 17. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Proton NMR 1

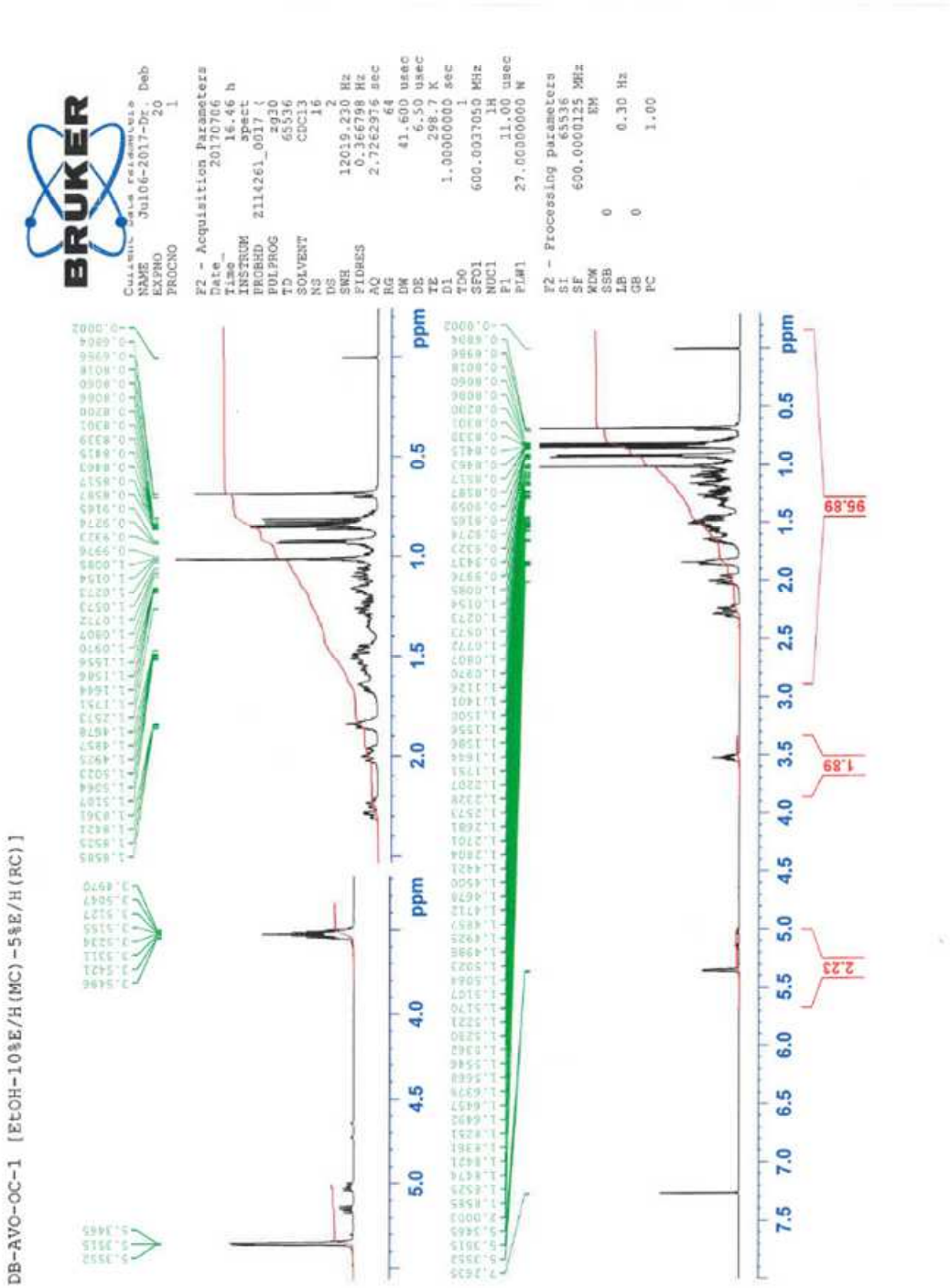


Figure 18. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Proton NMR 2

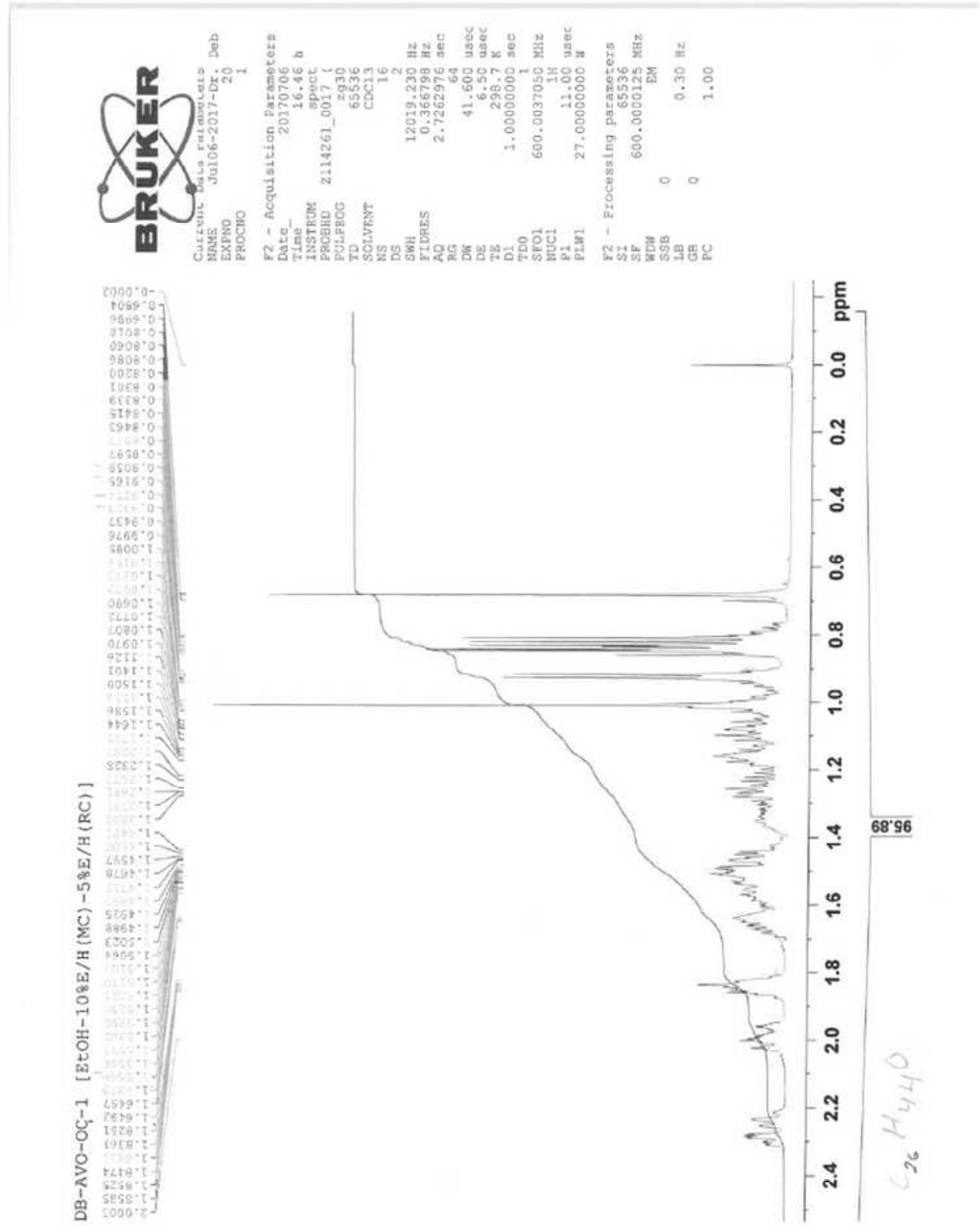


Figure 19. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Proton NMR 3

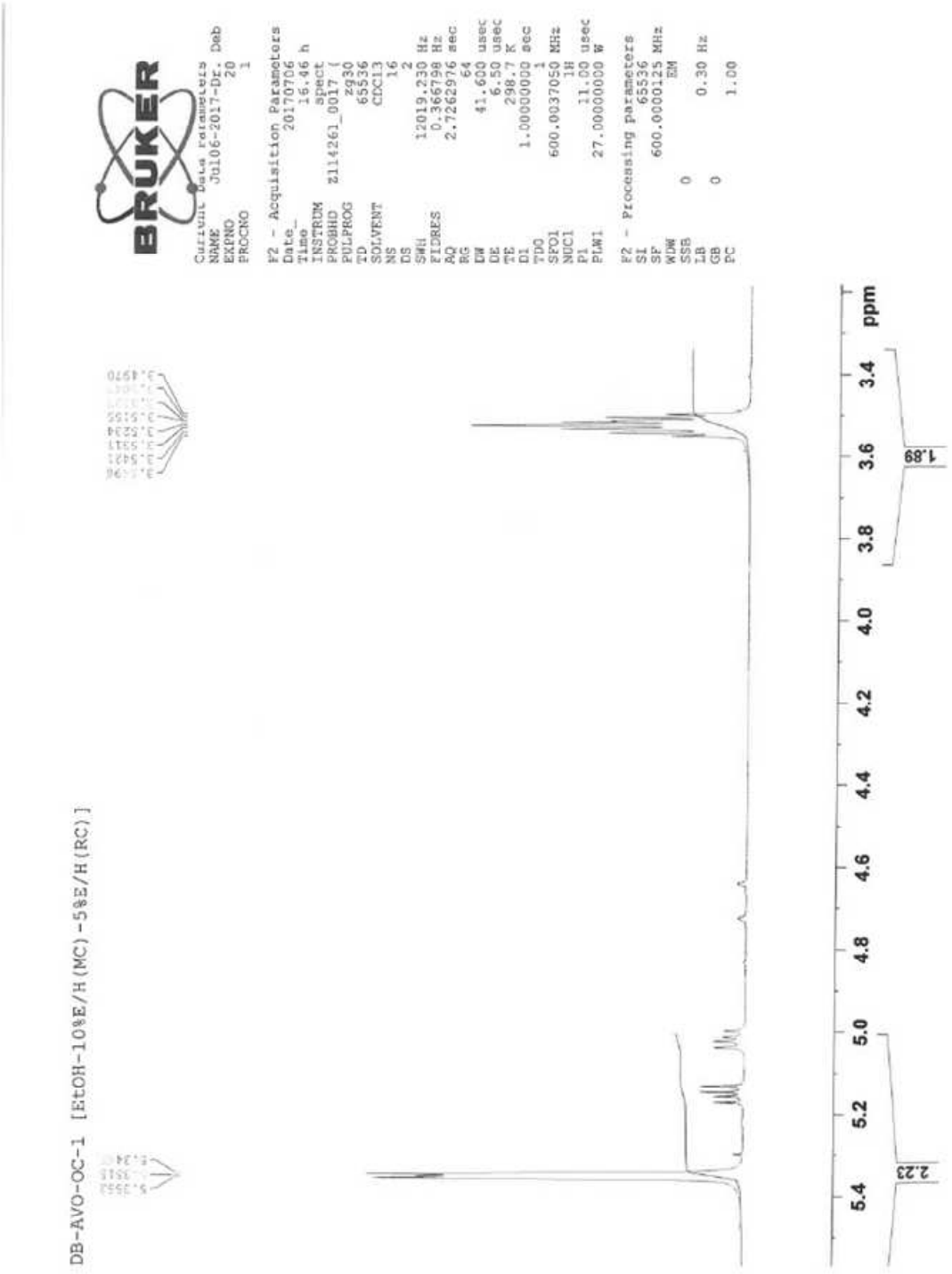


Figure 20. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Carbon NMR

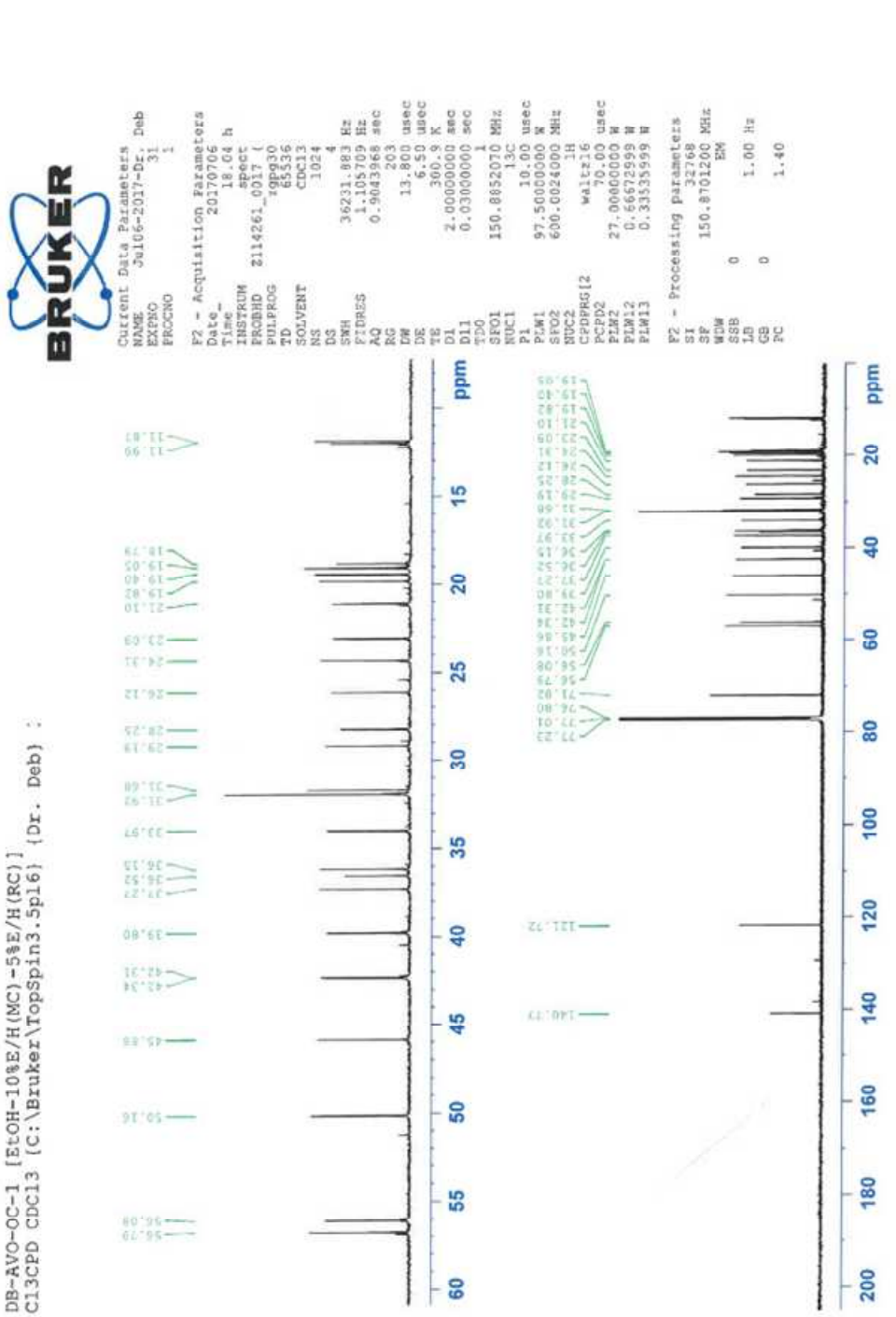


Figure 21. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras. Carbon DEPT90 NMR

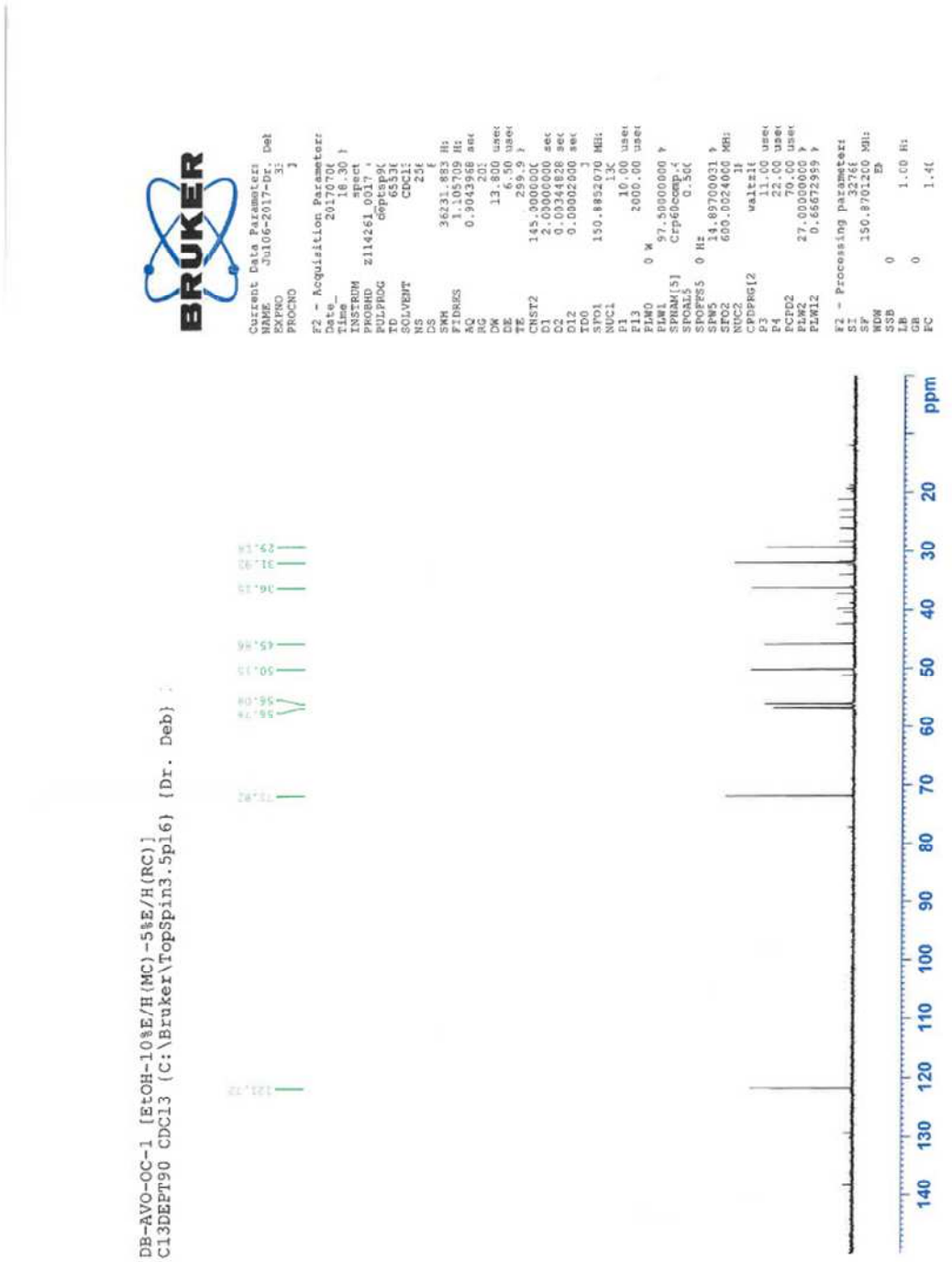


Figure 22. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Carbon DEPT135

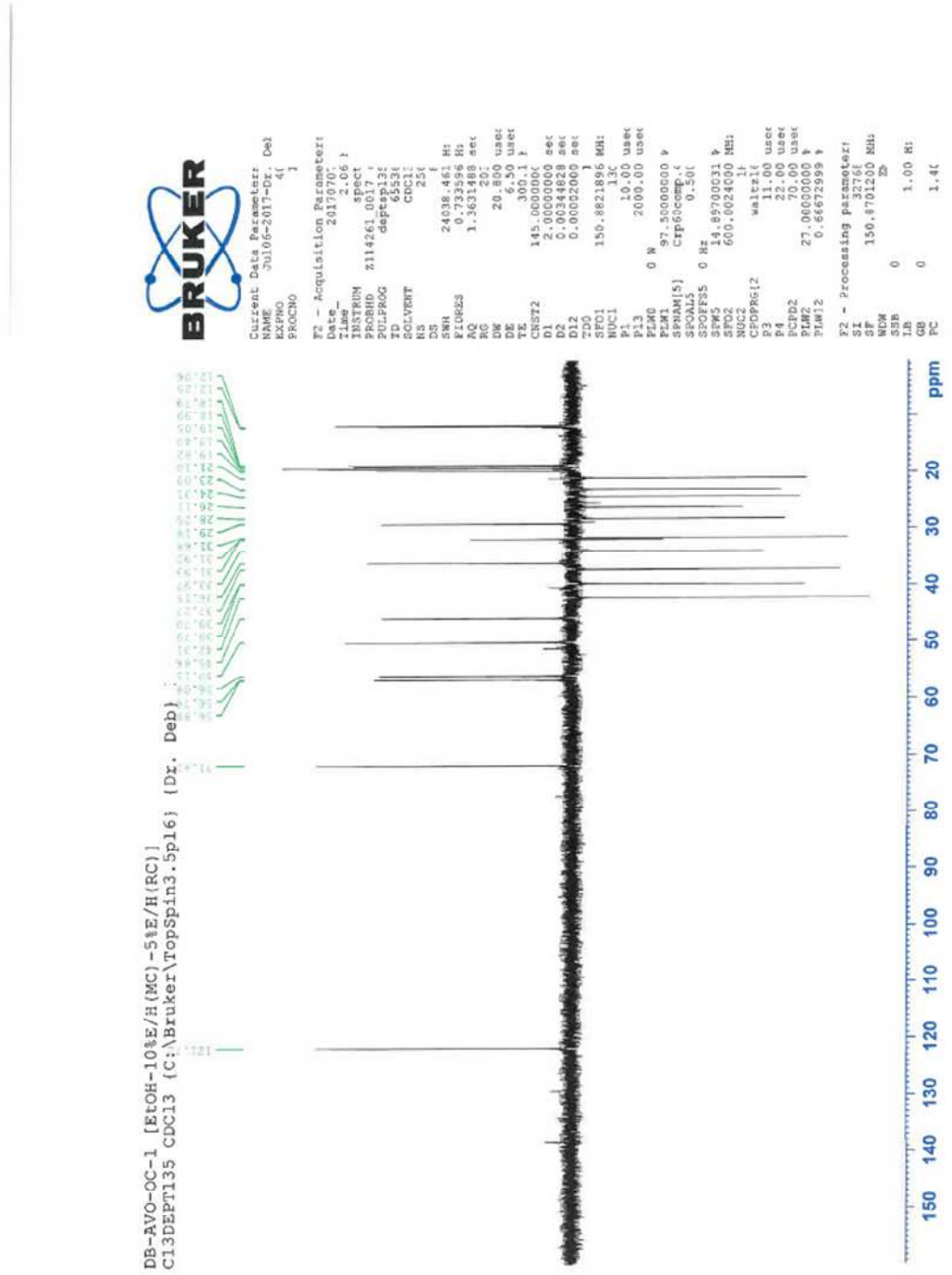


Figure 23. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Carbon APT NMR 1

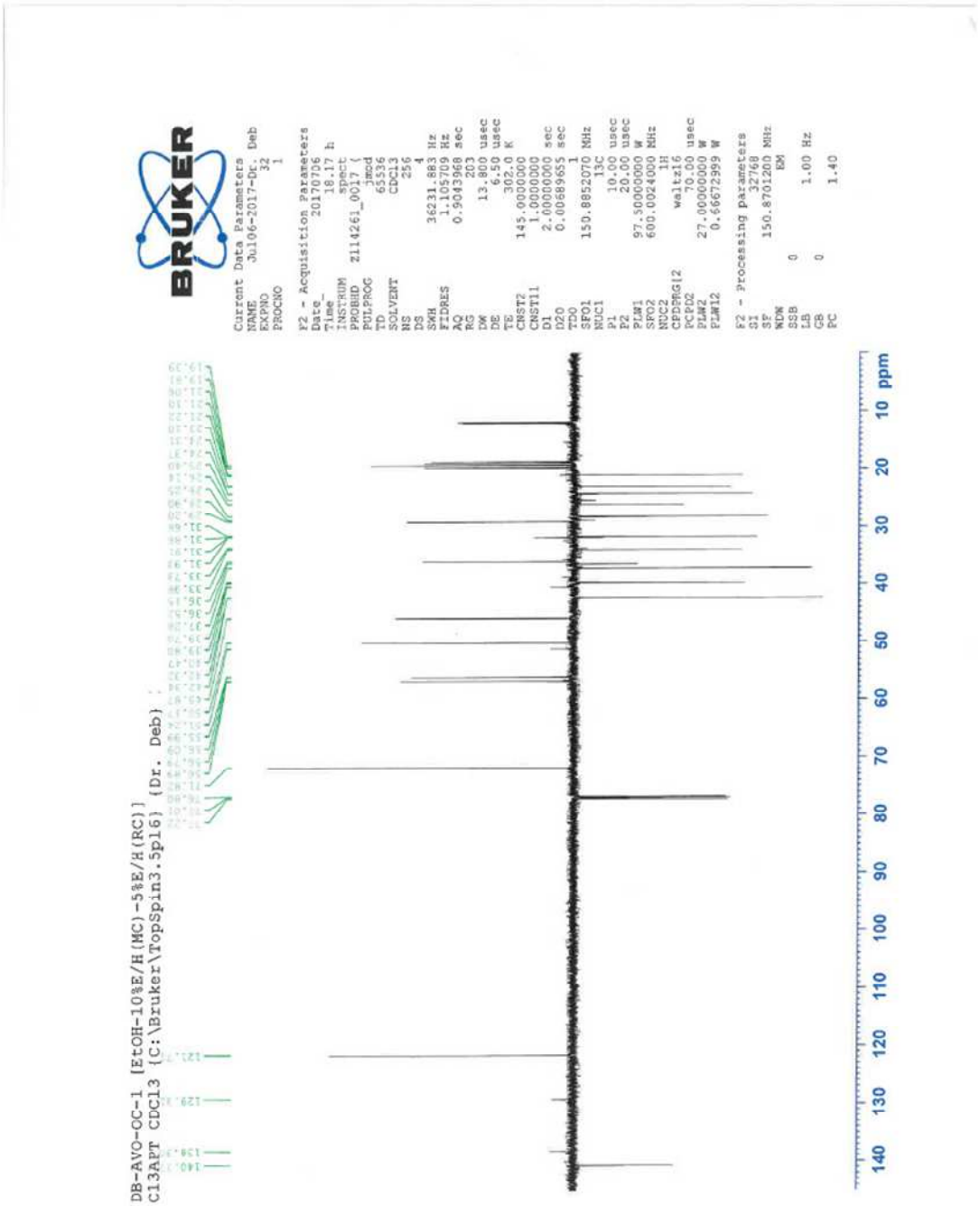


Figure 24. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Carbon APT NMR 2

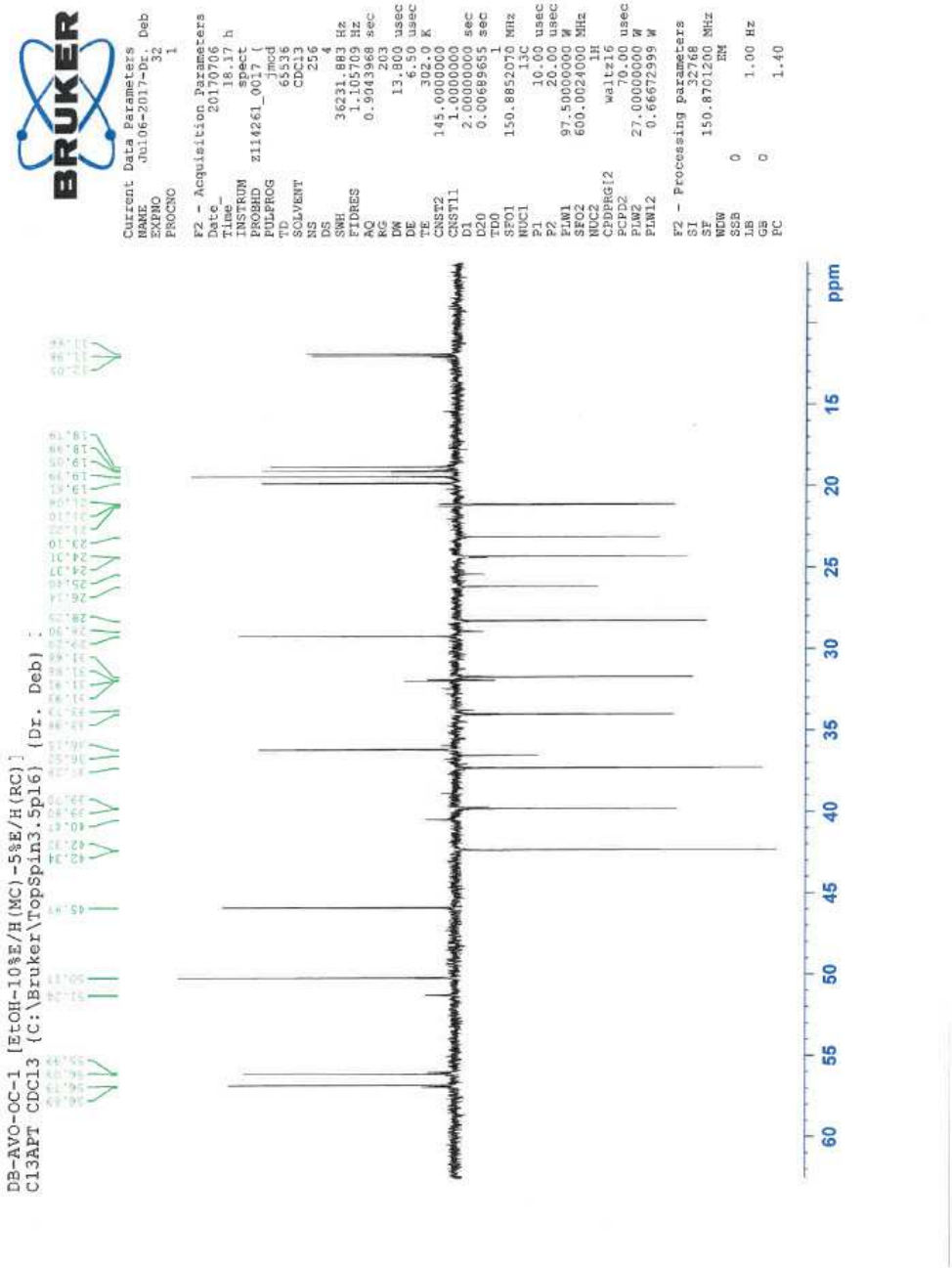


Figure 25. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras Carbon APT NMR 3

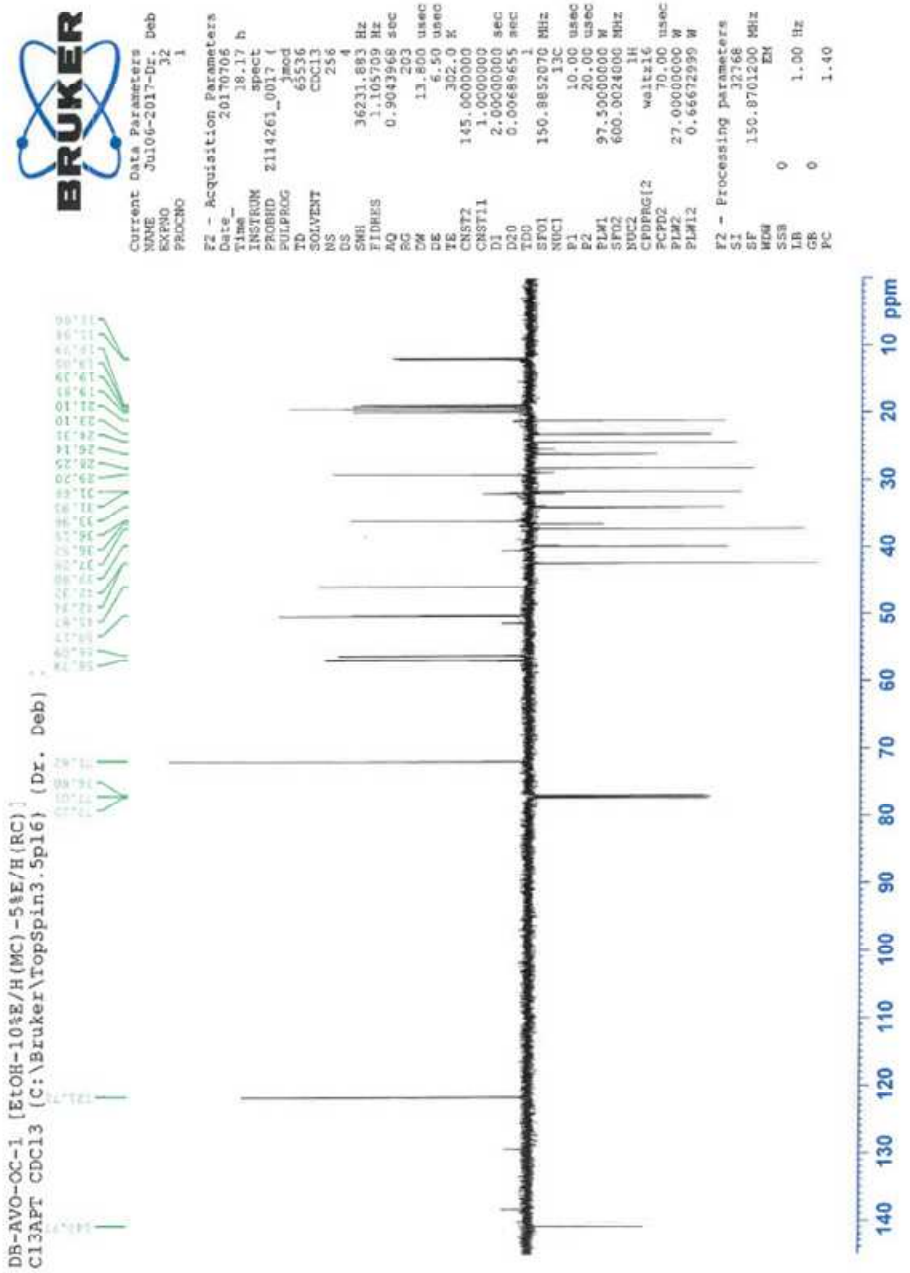


Figure 26. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D COSY NMR 1

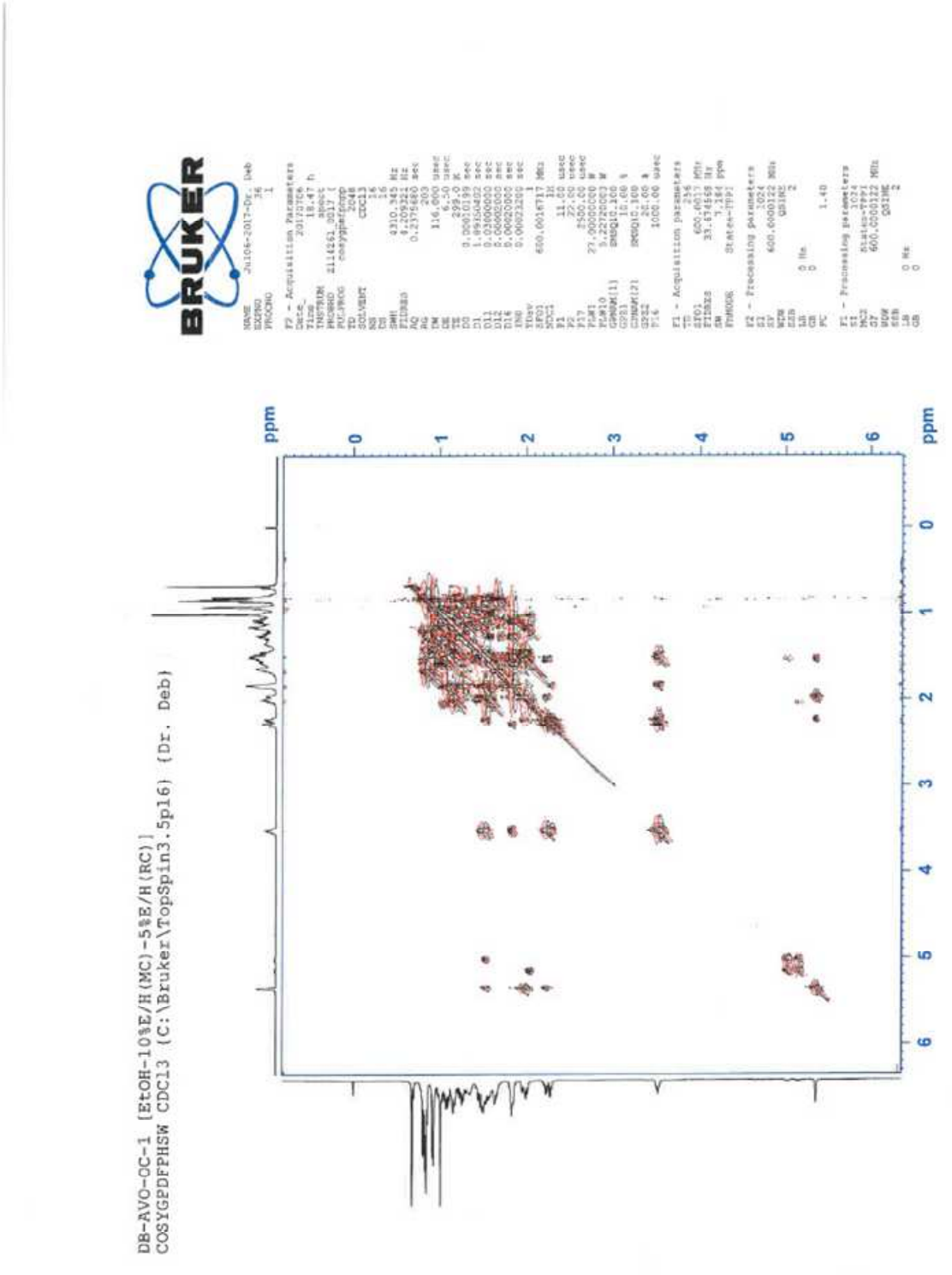


Figure 27. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D COSY NMR 2

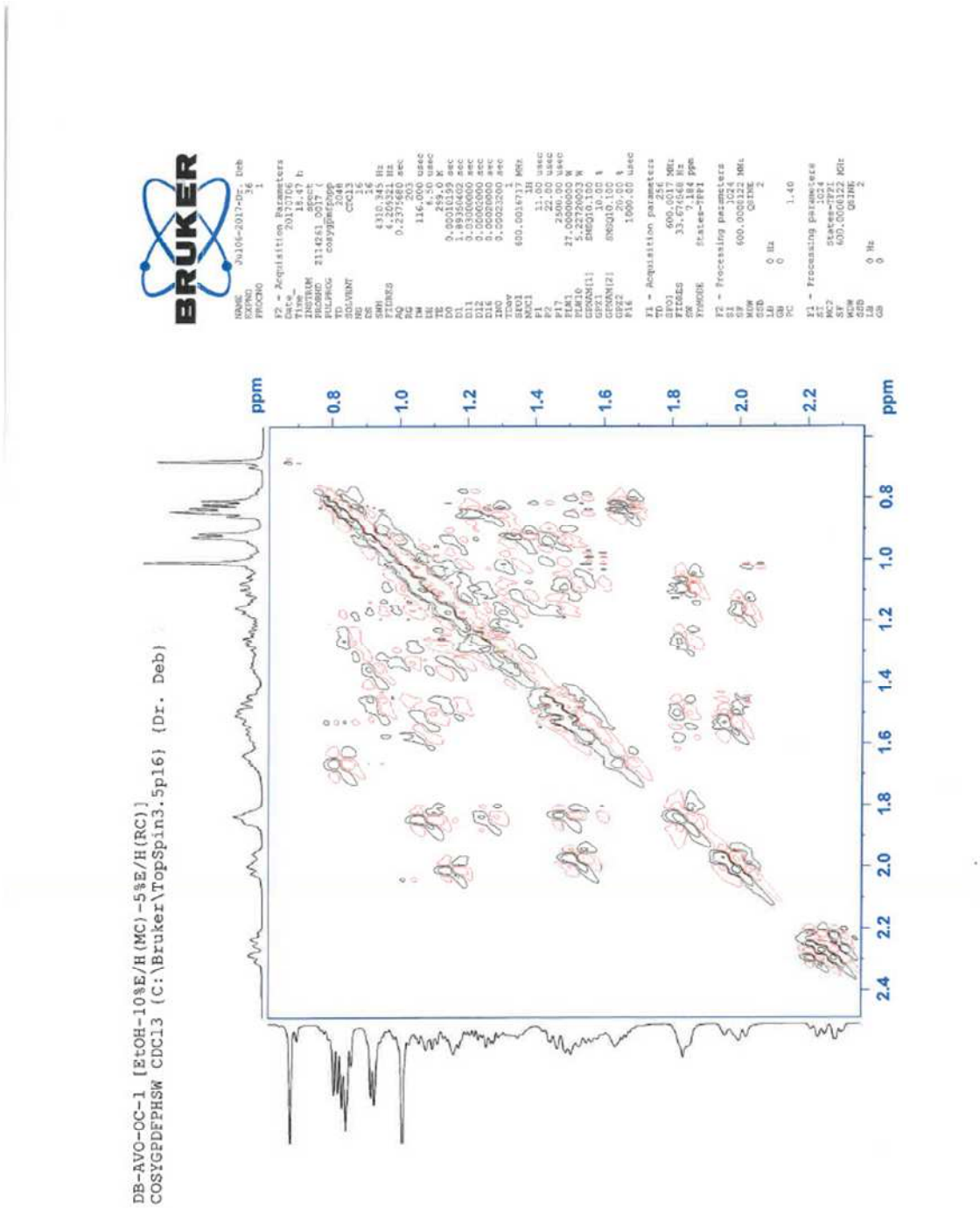


Figure 28. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D ROSEY NMR 1

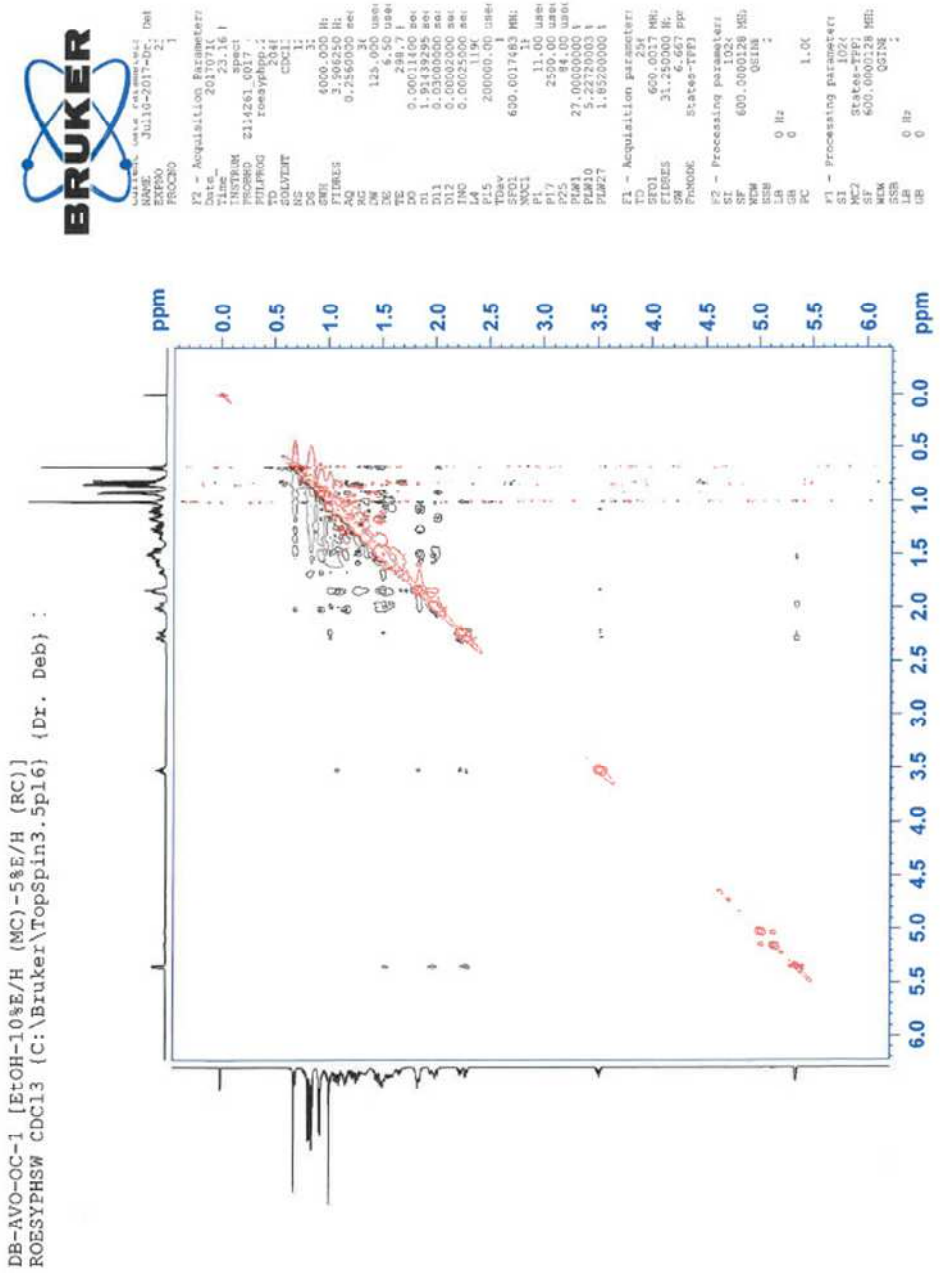


Figure 29. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D ROESY NMR 2

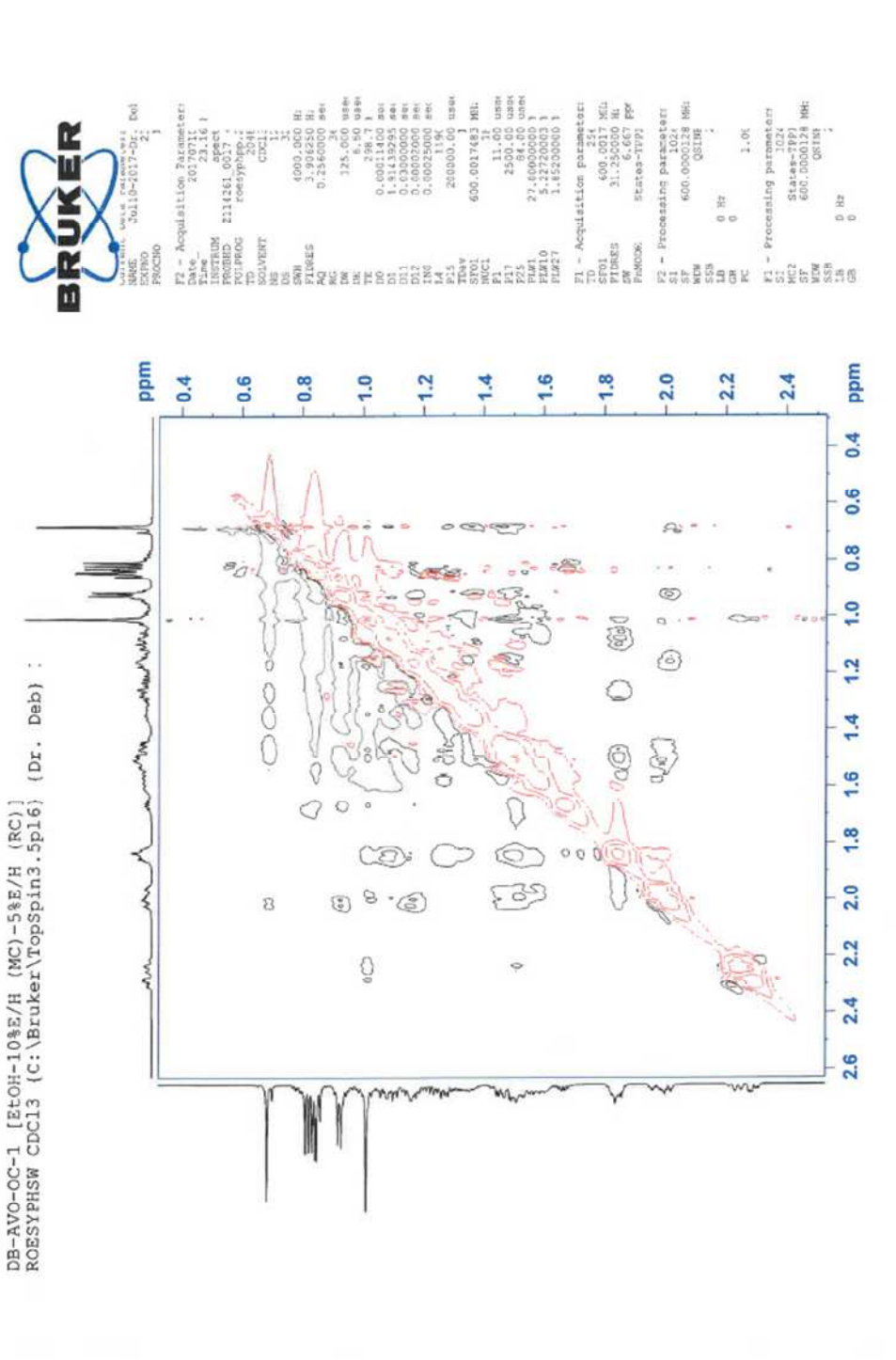


Figure 30. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D NOESY NMR

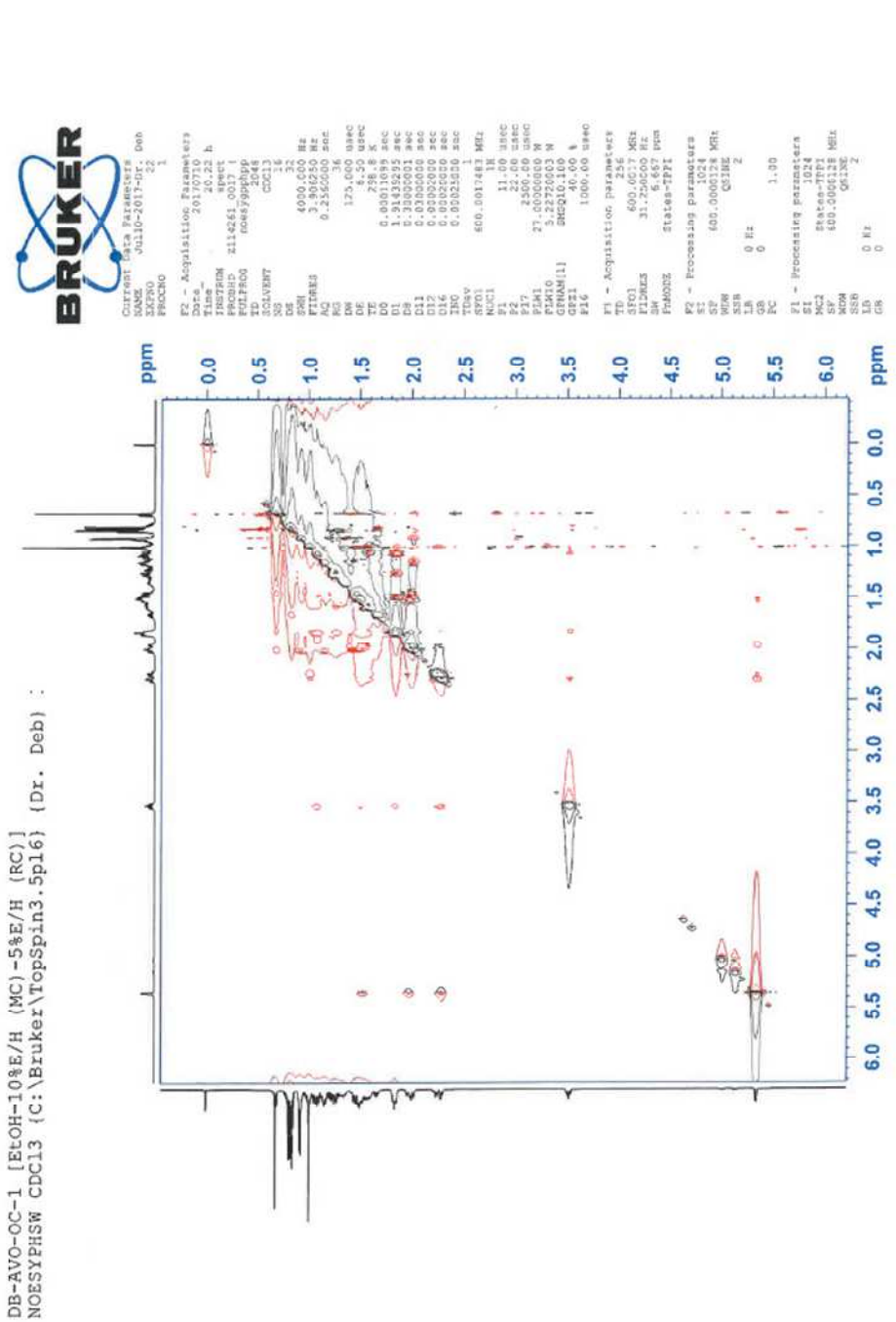


Figure 31. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D NMR HMBCGP 1

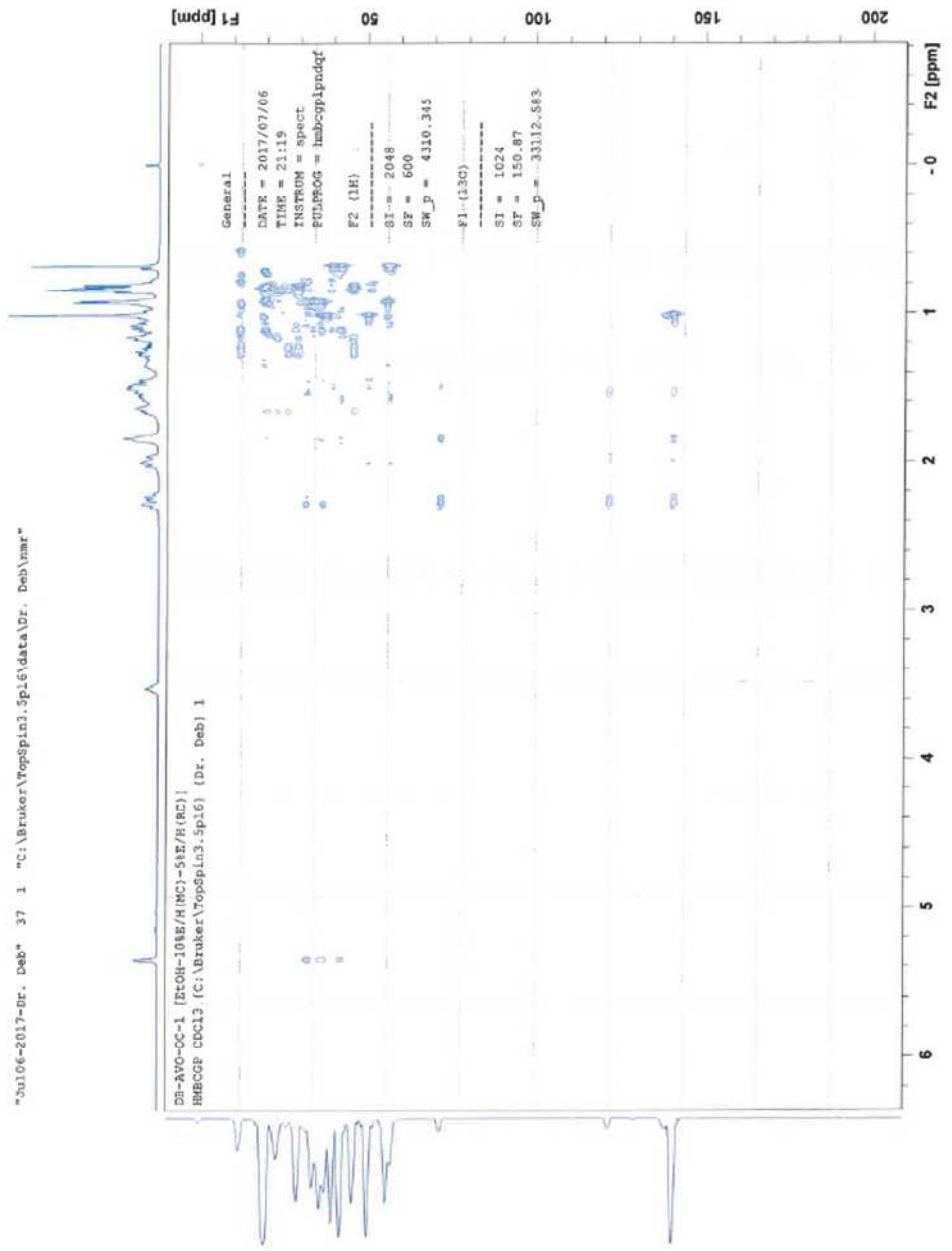


Figure 32. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D HMQCGP NMR 2

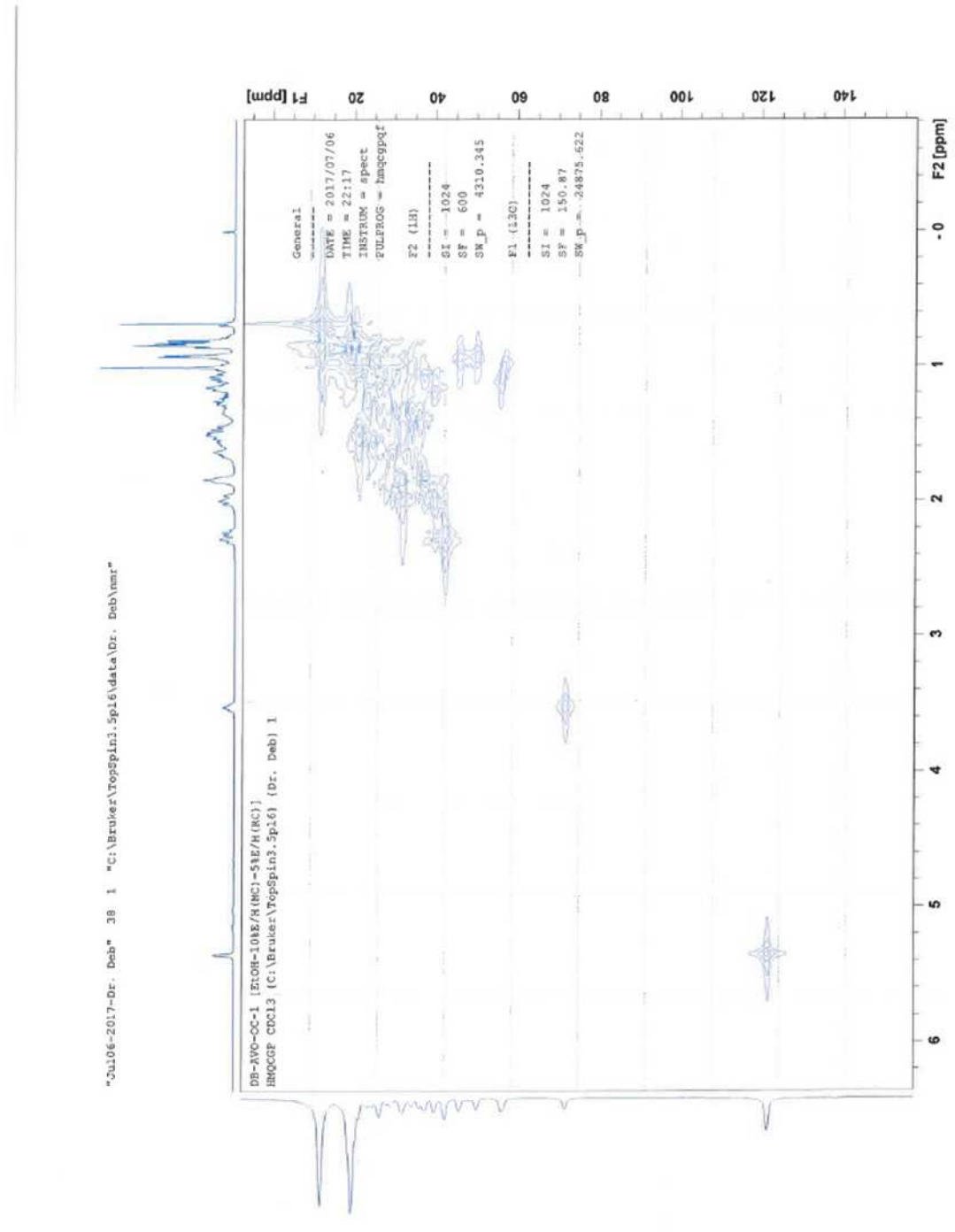


Figure 33. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D HMQCGP NMR 3

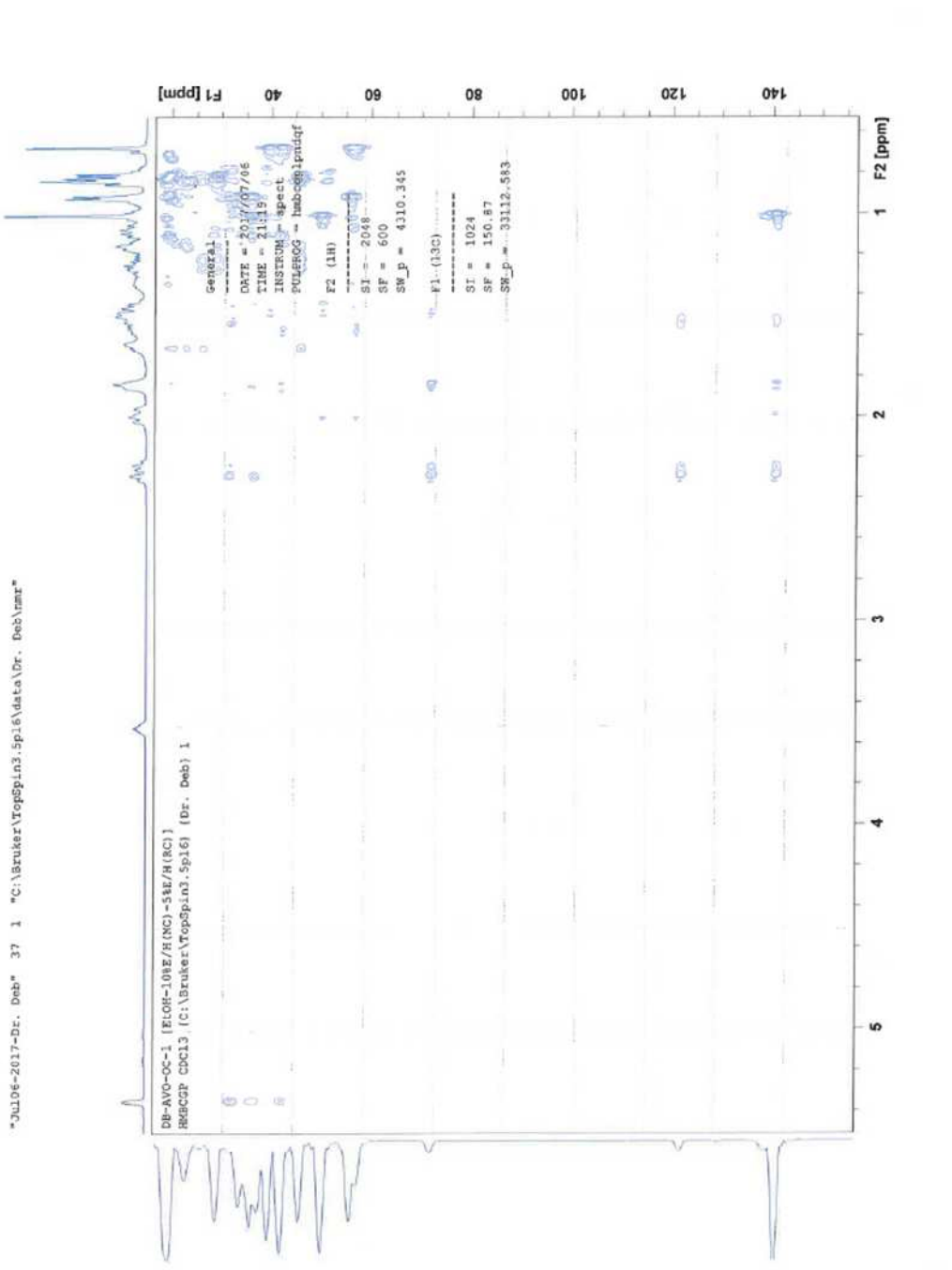


Figure 34. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D HMQCGP NMR 4

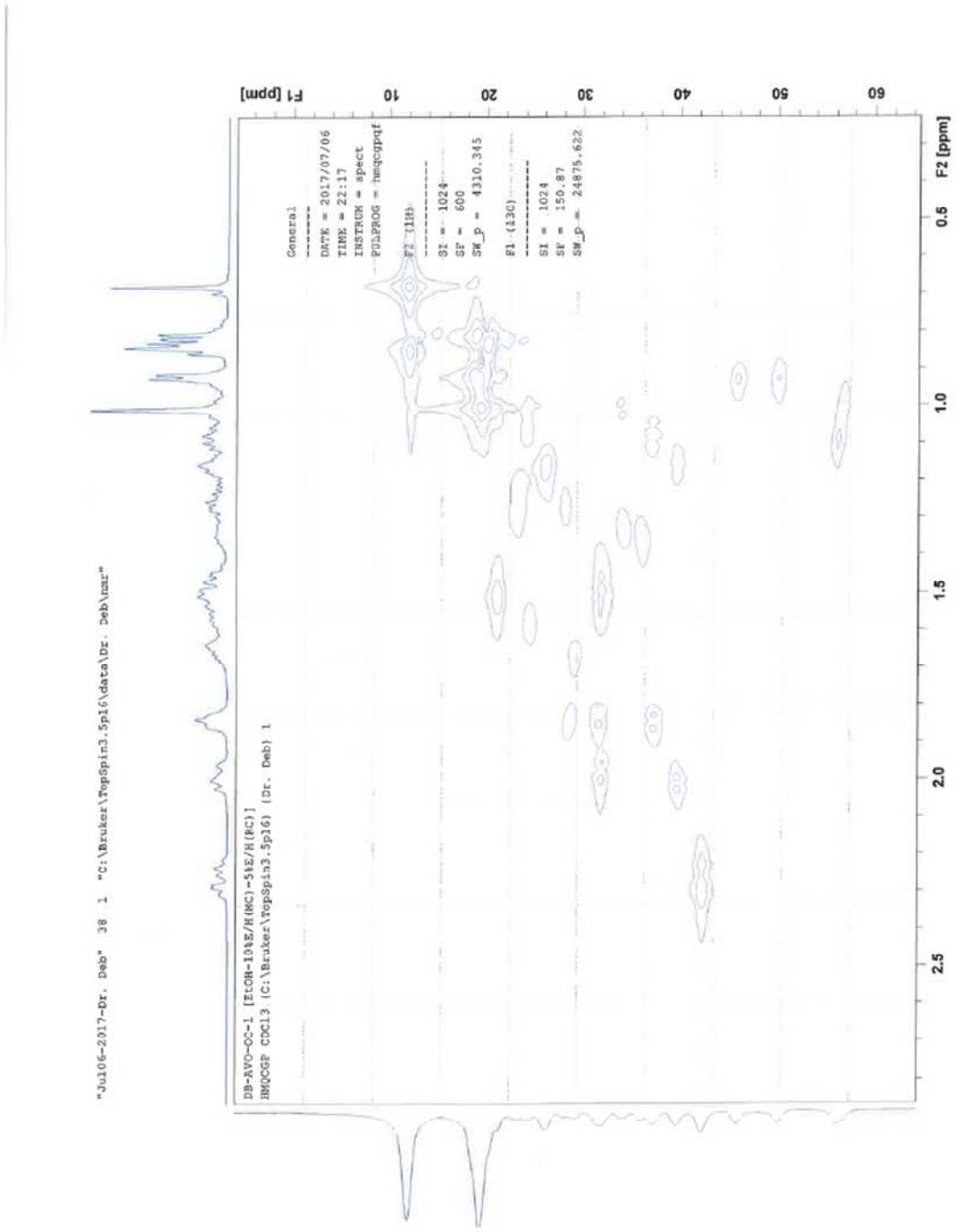


Figure 35. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D MLEVPHS NMR 1

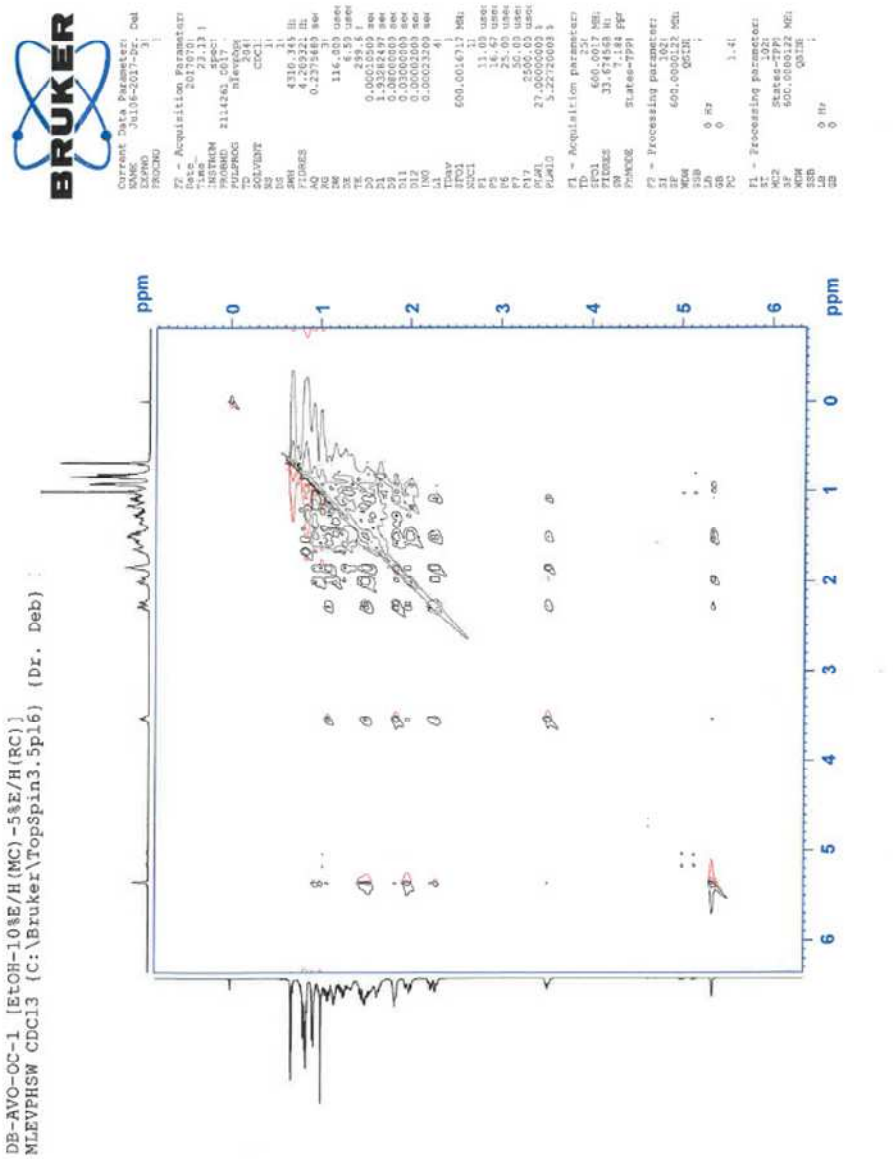


Figure 36. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D MLEVPHSW NMR 2

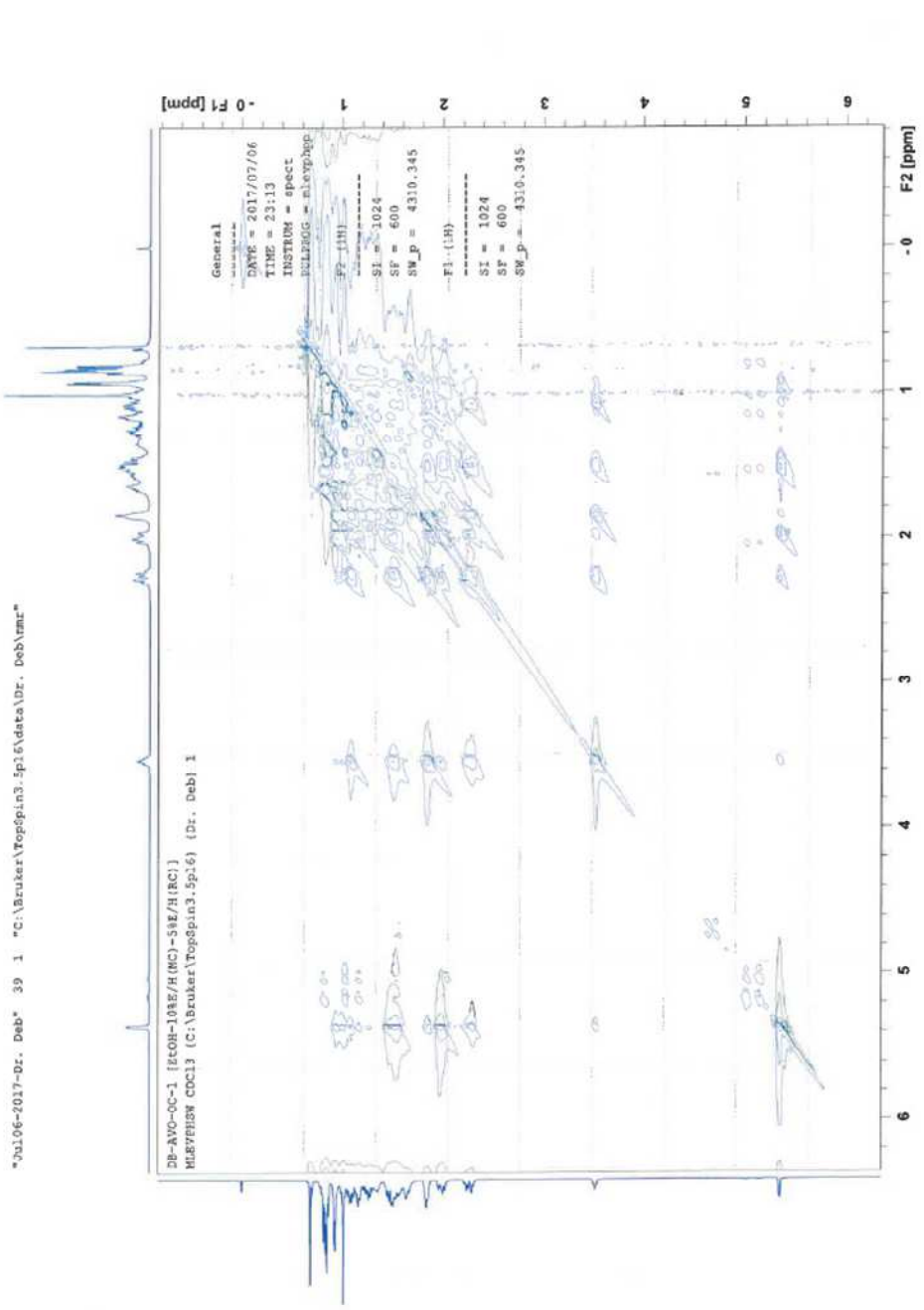


Figure 37. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D MLEVPHSW NMR 3

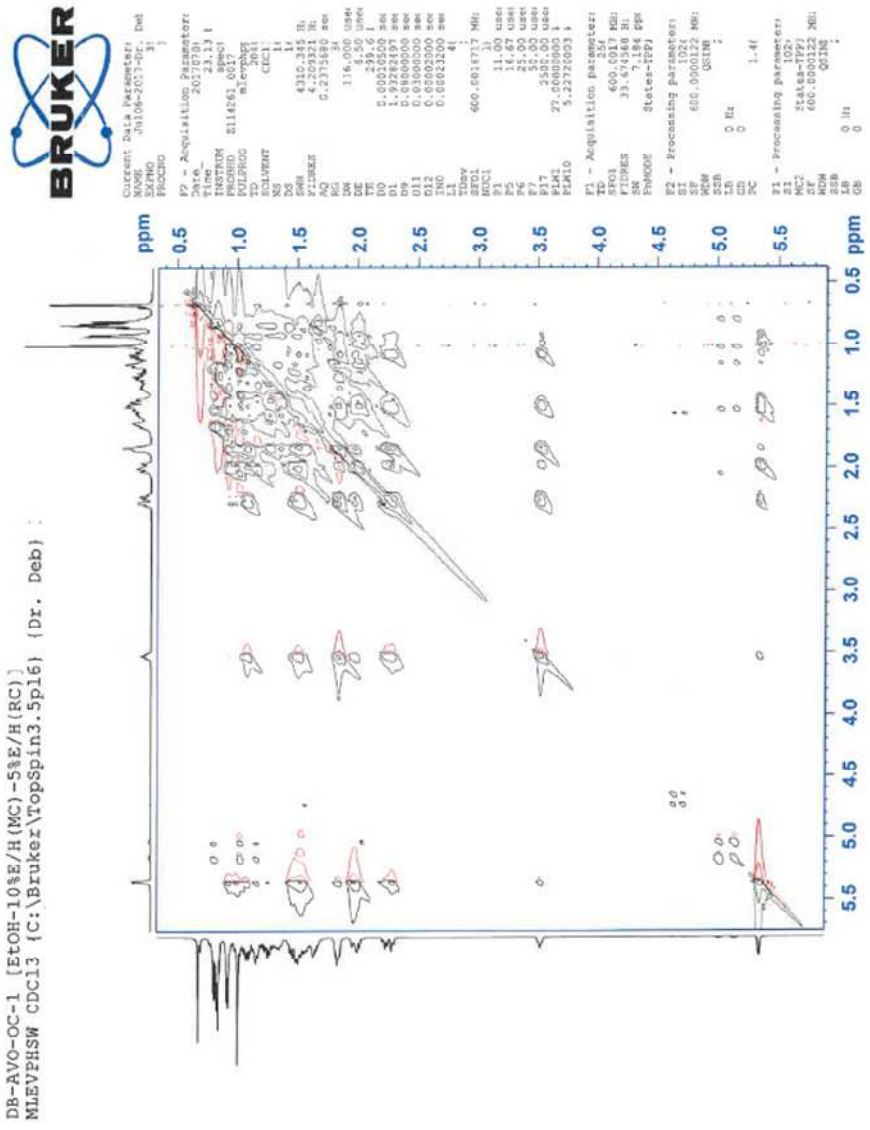


Figure 38. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D MLEVPHSW NMR 4

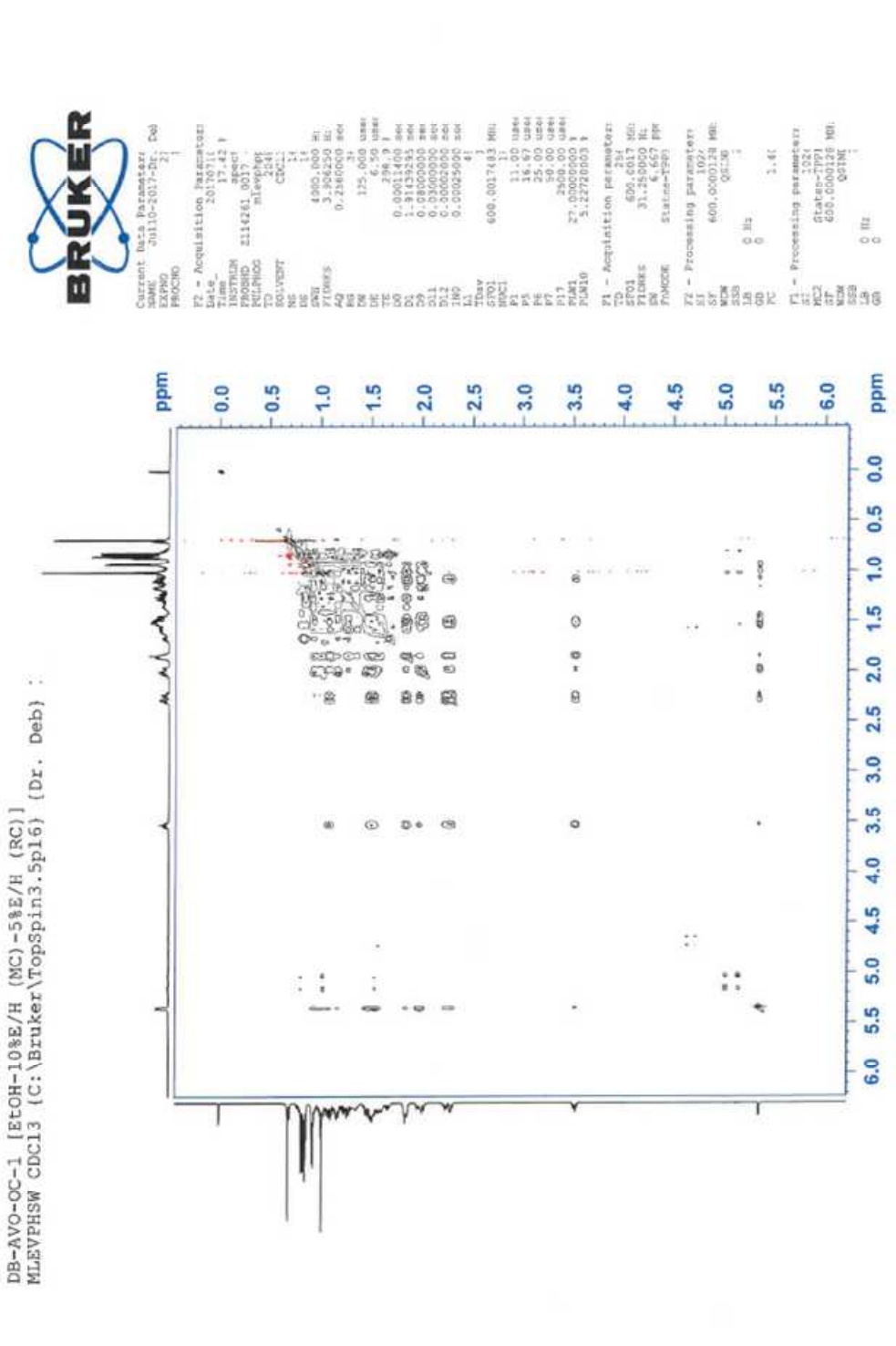


Figure 39. 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras 2-D MLEVPHSW NMR

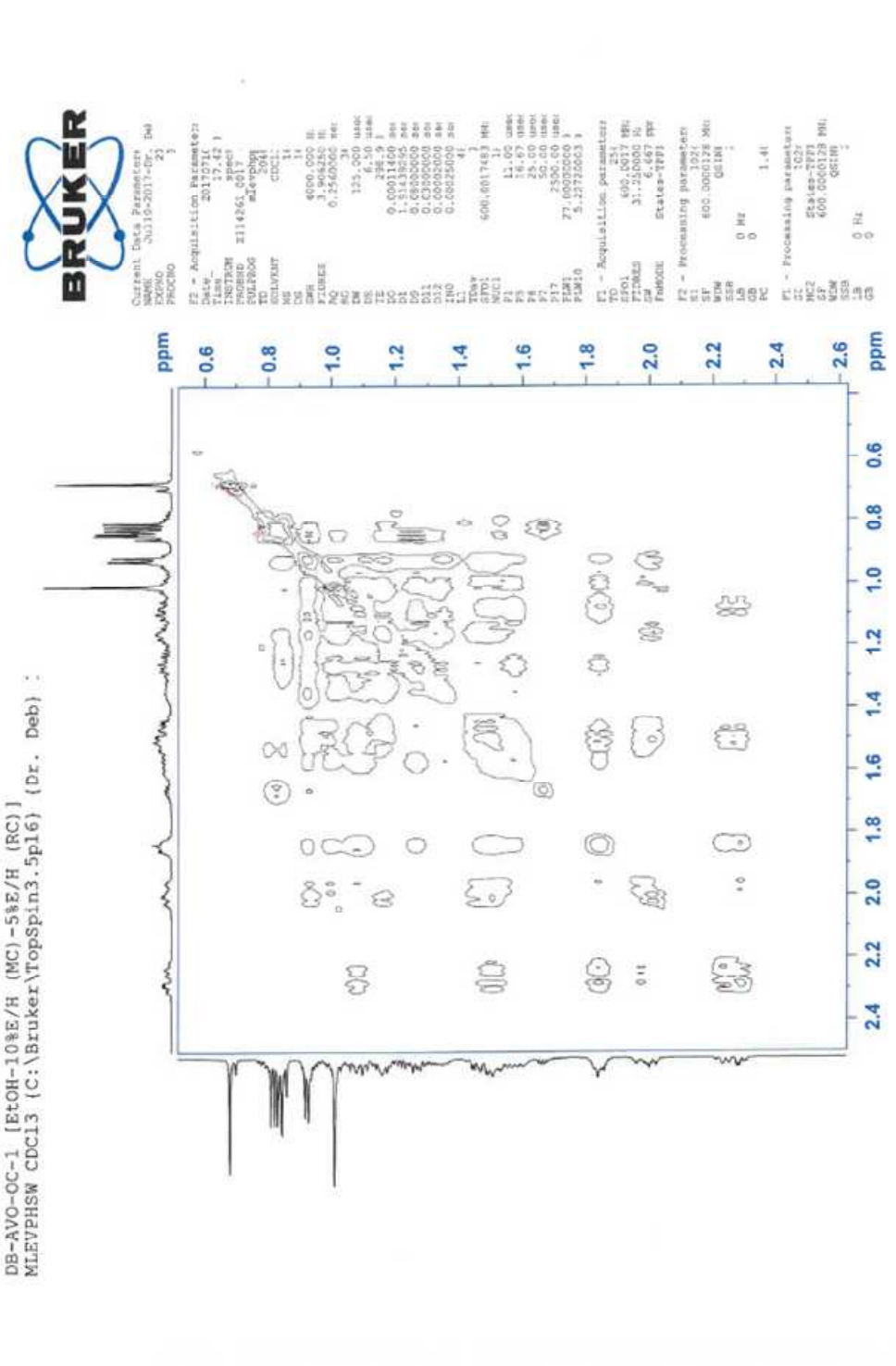
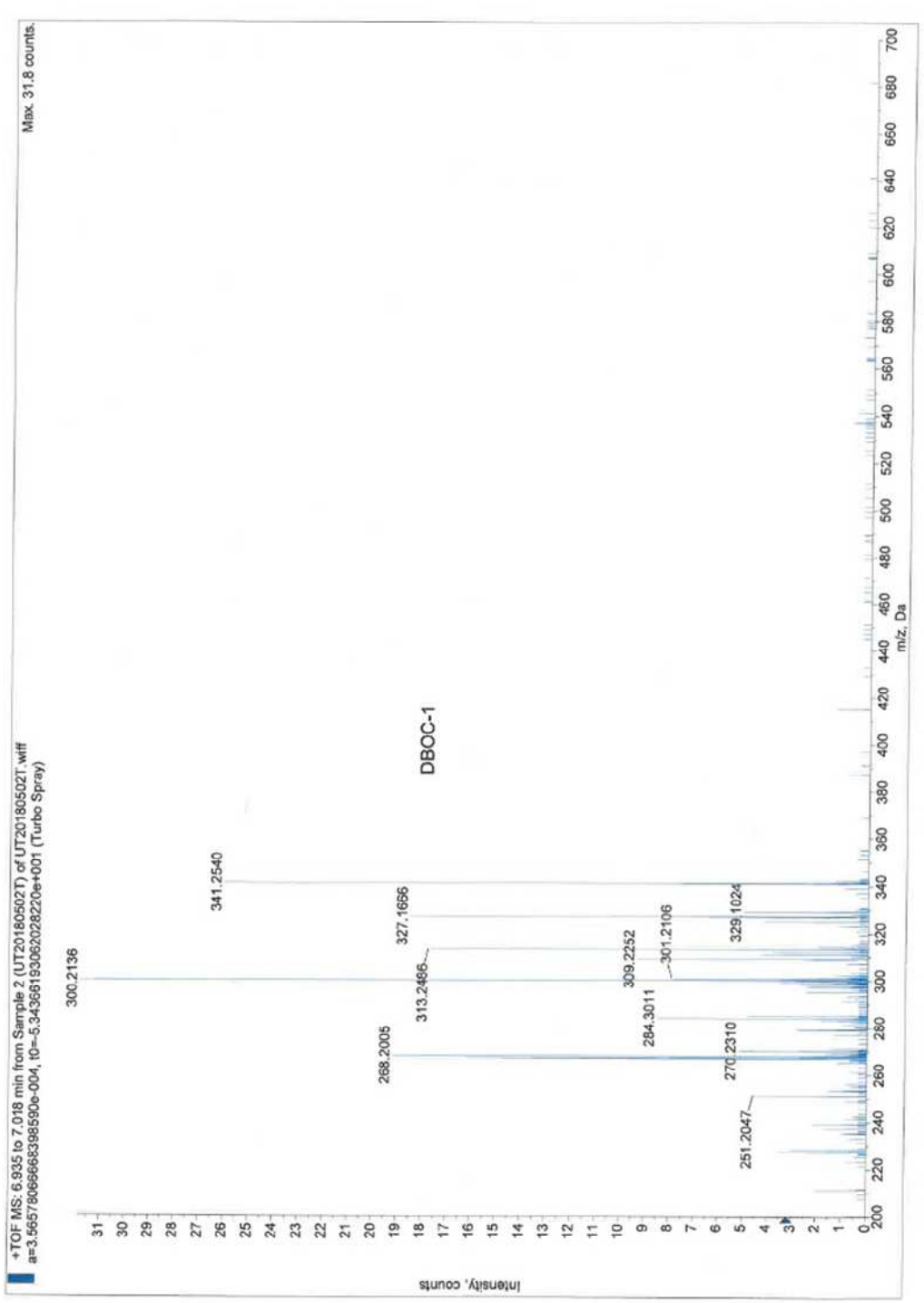


Figure 40 3S,8S,9S,10R,13R,14S,17R)-17-((R)-heptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol Spectras HRMS



12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one

Figure 41. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one FTIR

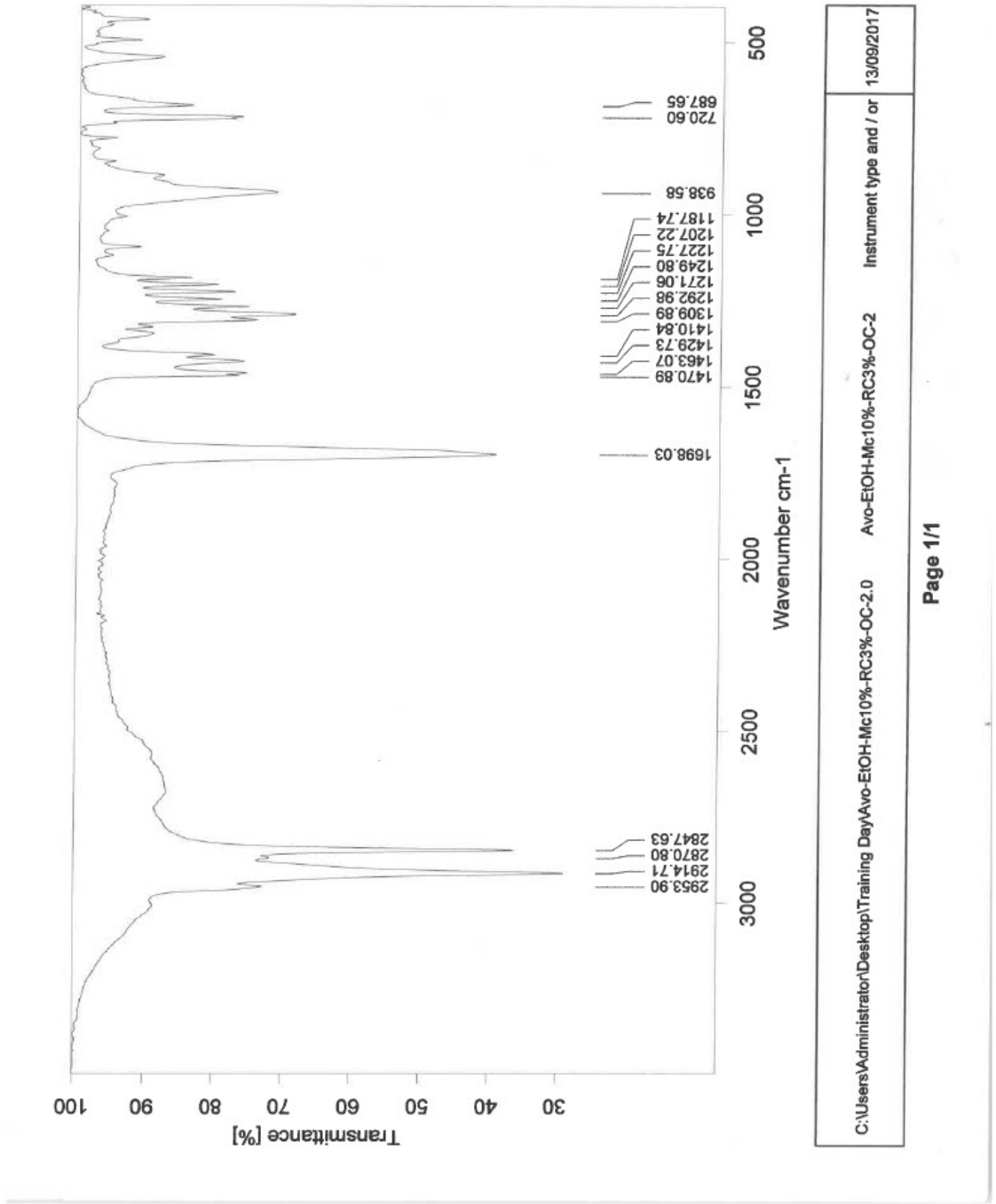


Figure 42. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Proton NMR 1

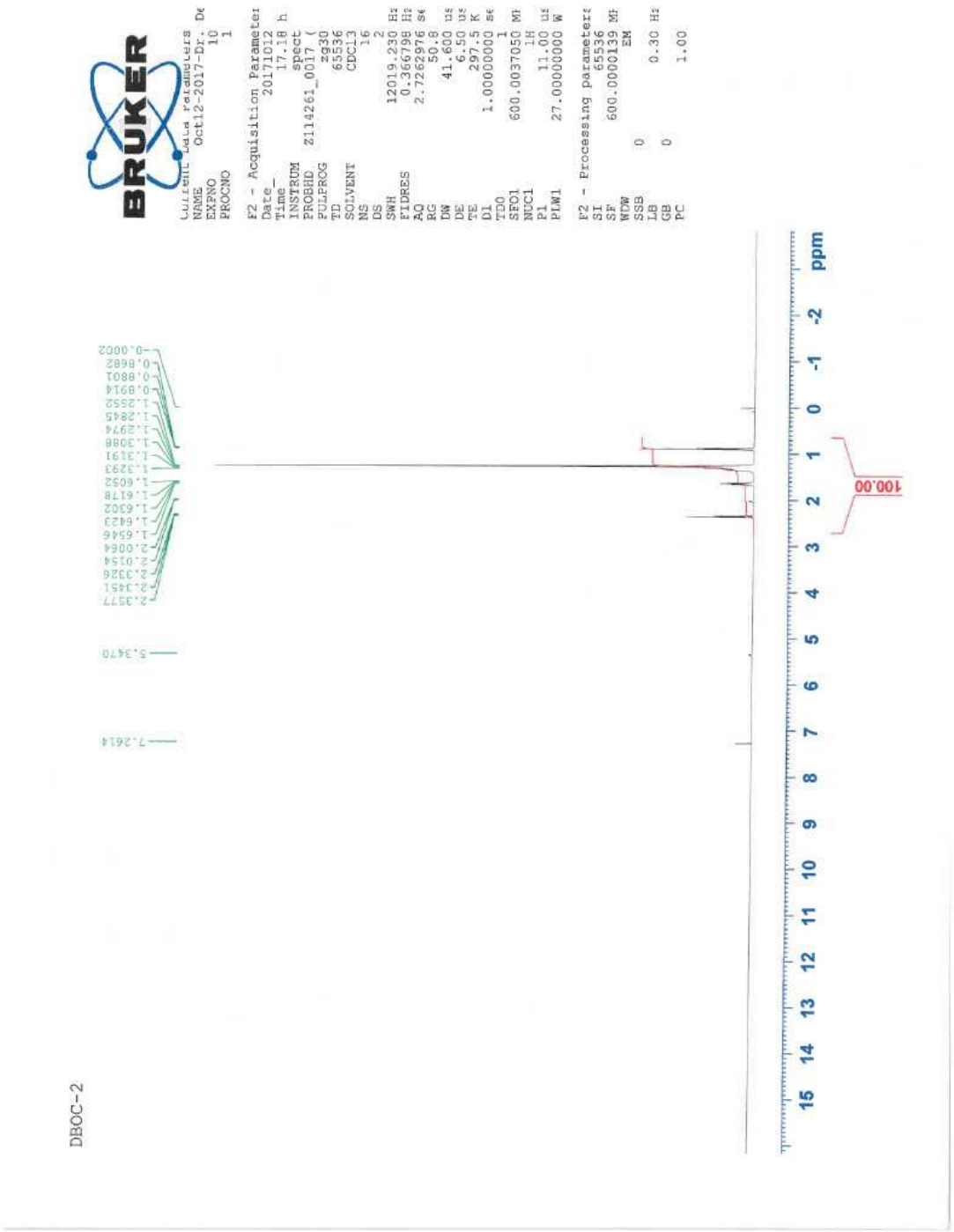


Figure 43. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Proton NMR 2

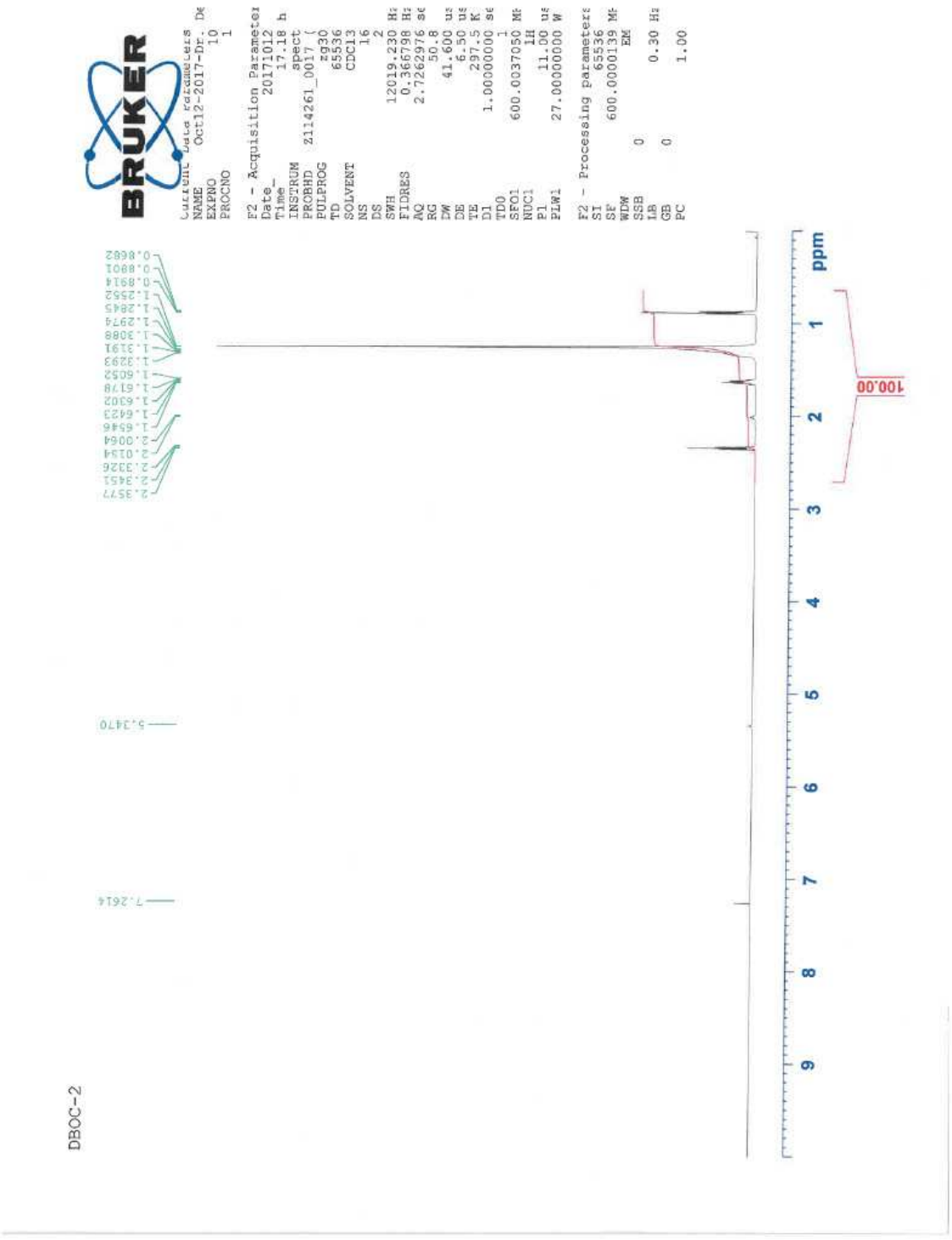


Figure 44. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Proton NMR 3

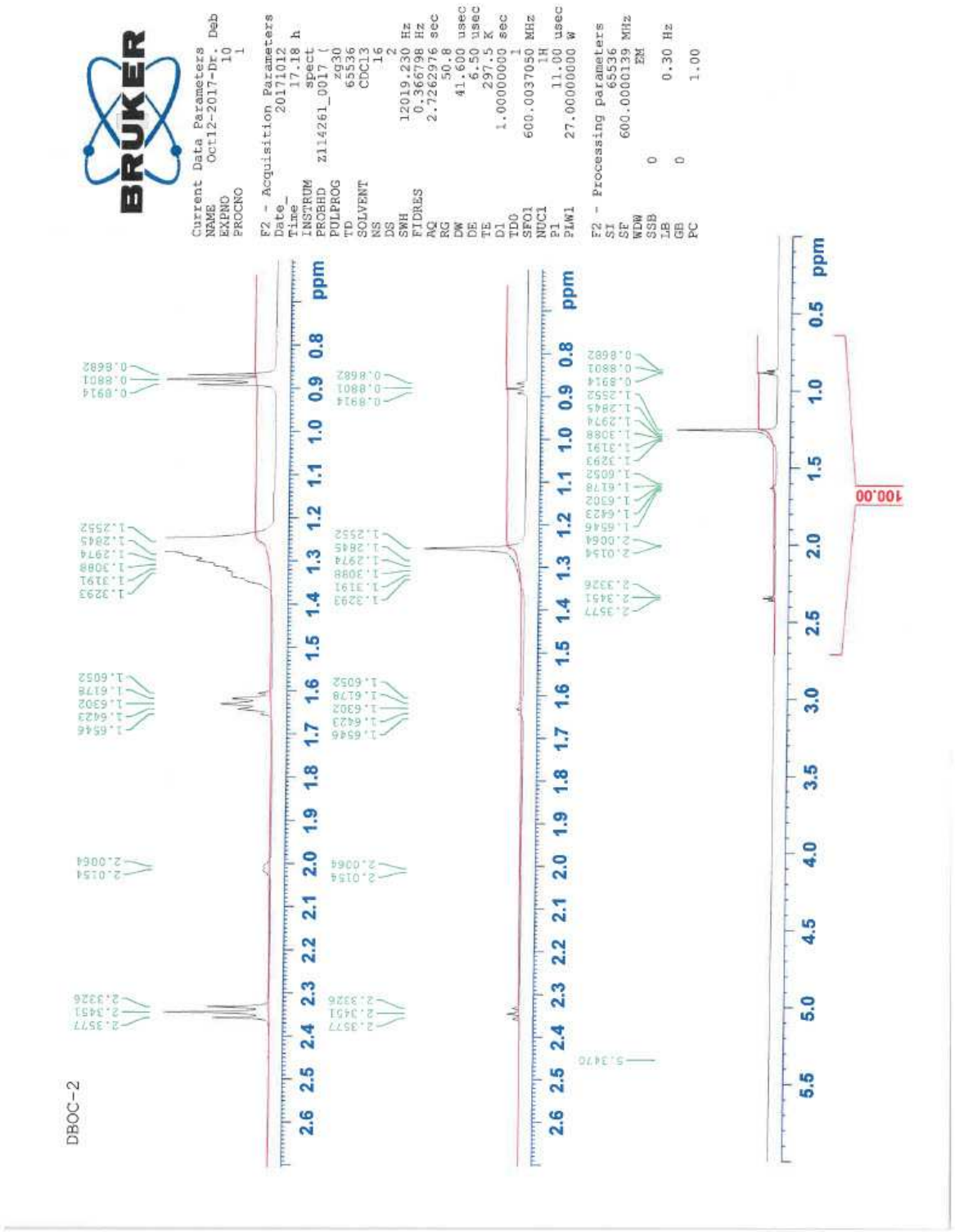


Figure 45. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Proton NMR 4

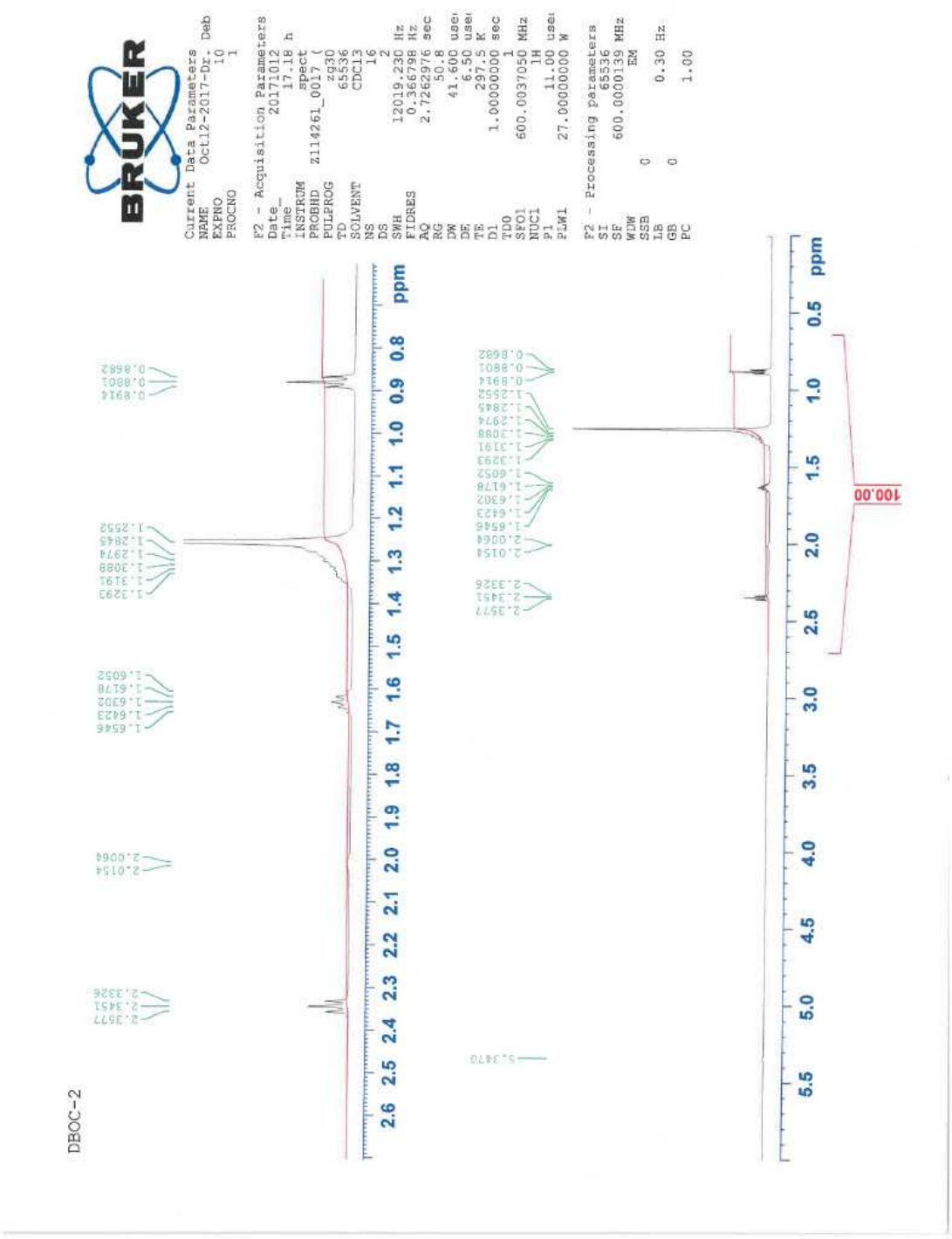


Figure 46. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon NMR 1

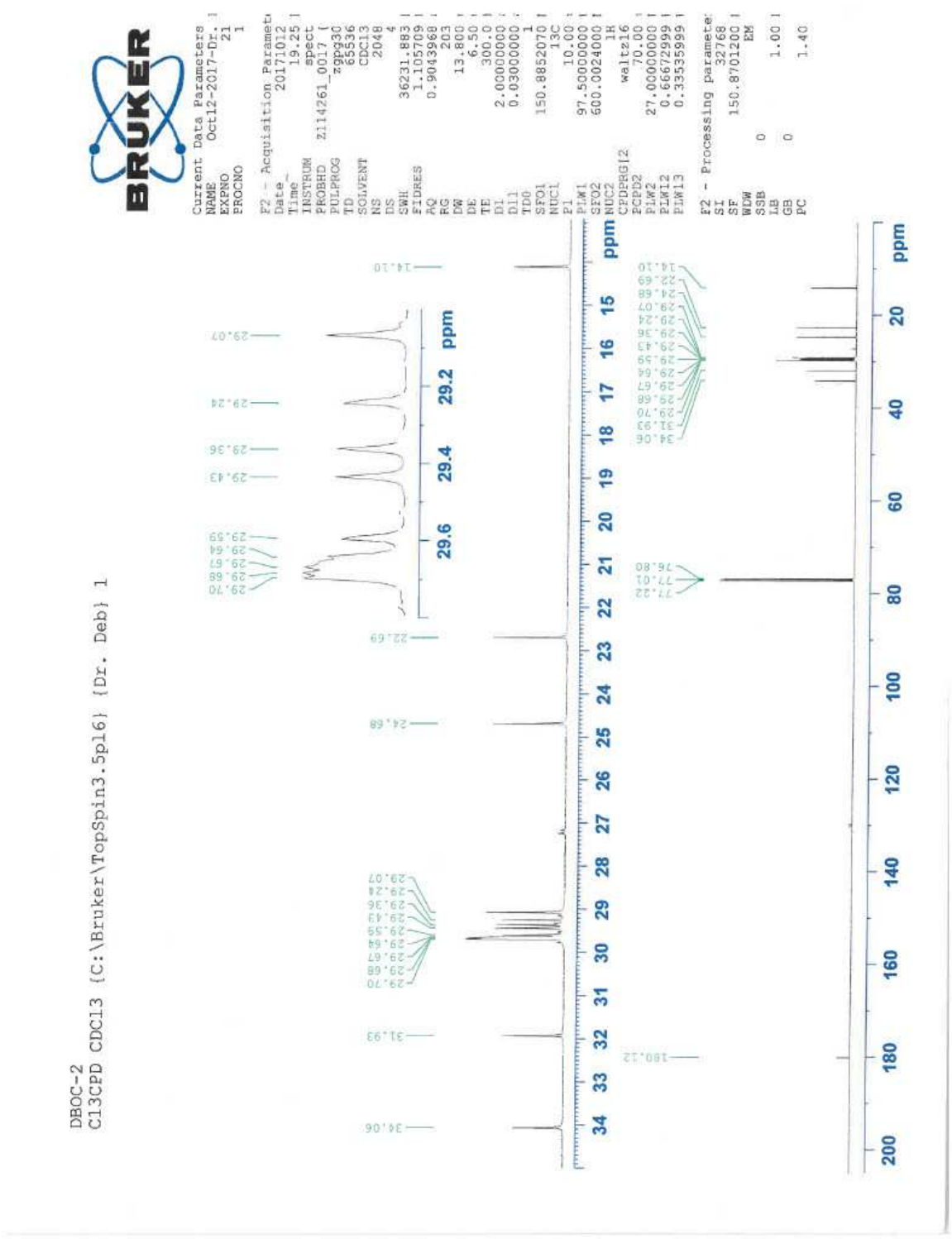


Figure 47. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon NMR 2

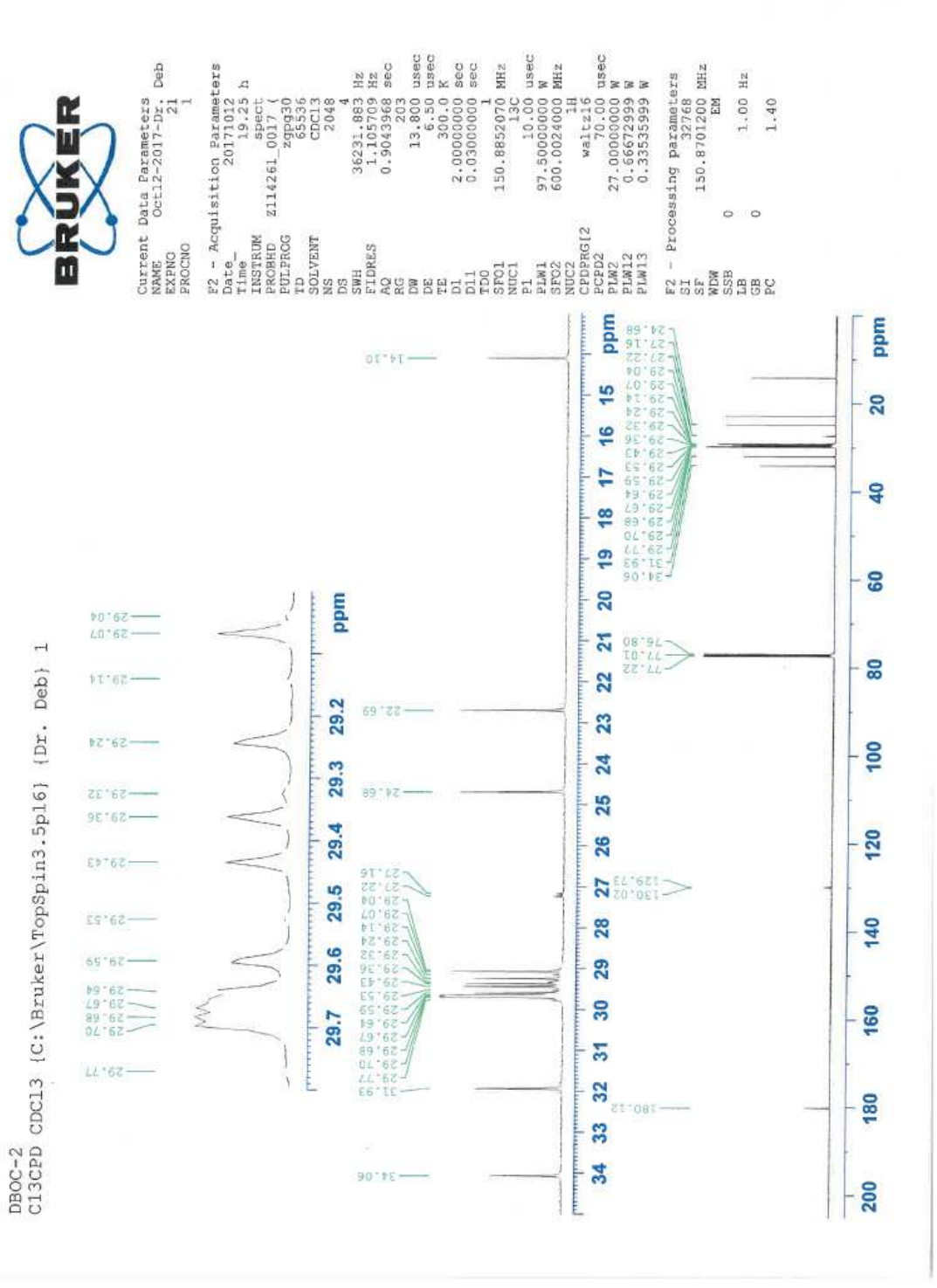


Figure 48. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon NMR 3

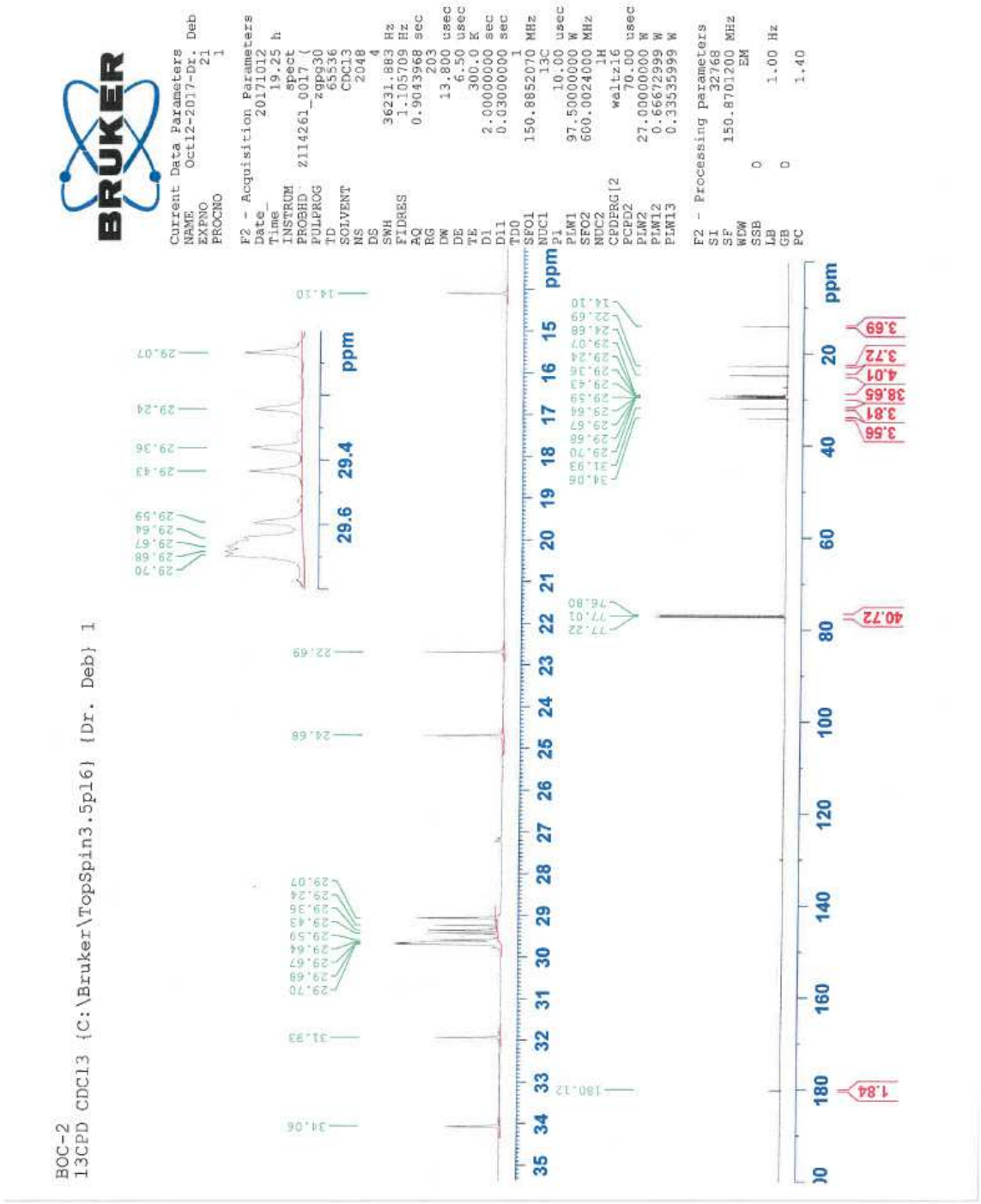


Figure 49. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon NMR 4

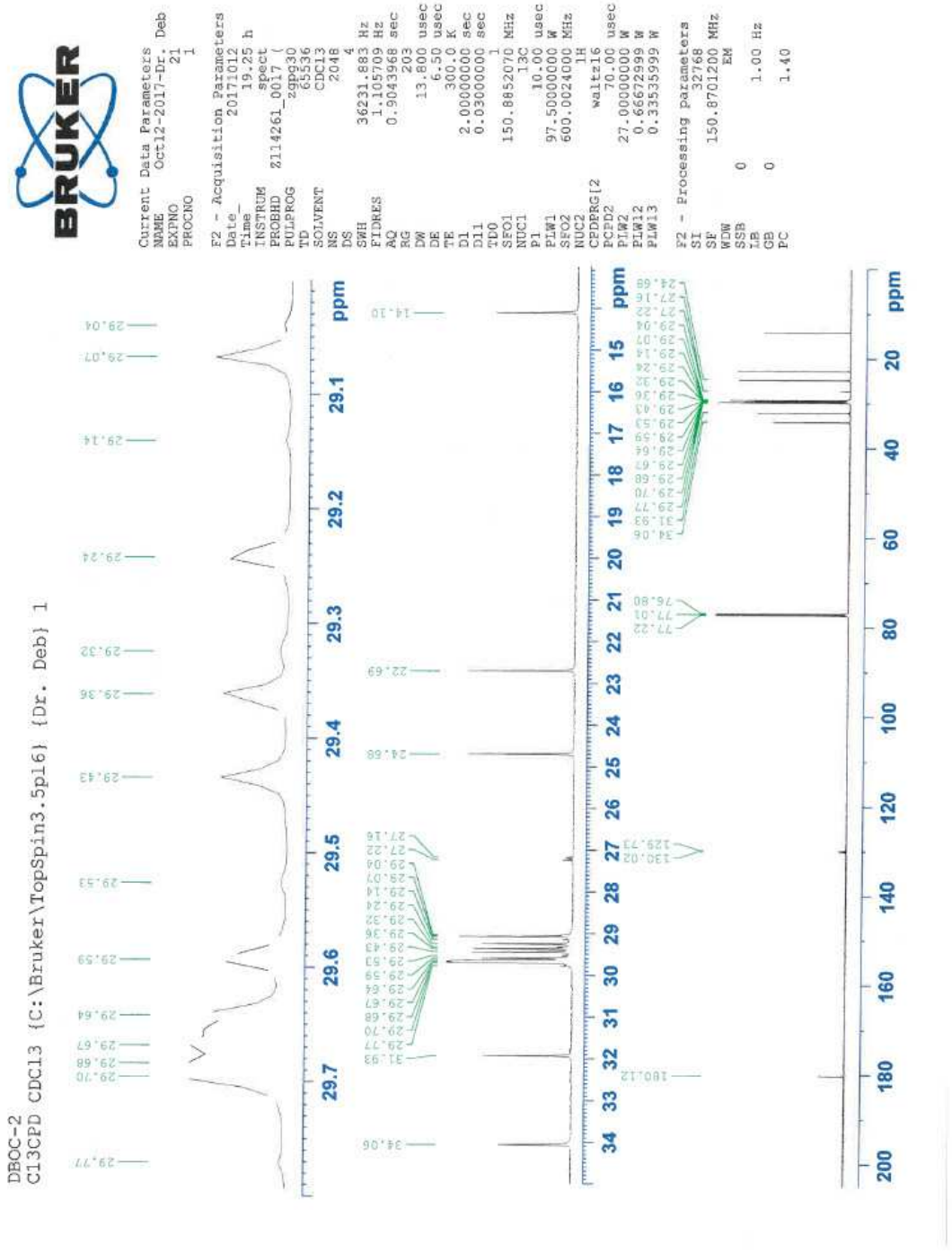


Figure 50. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon NMR 5

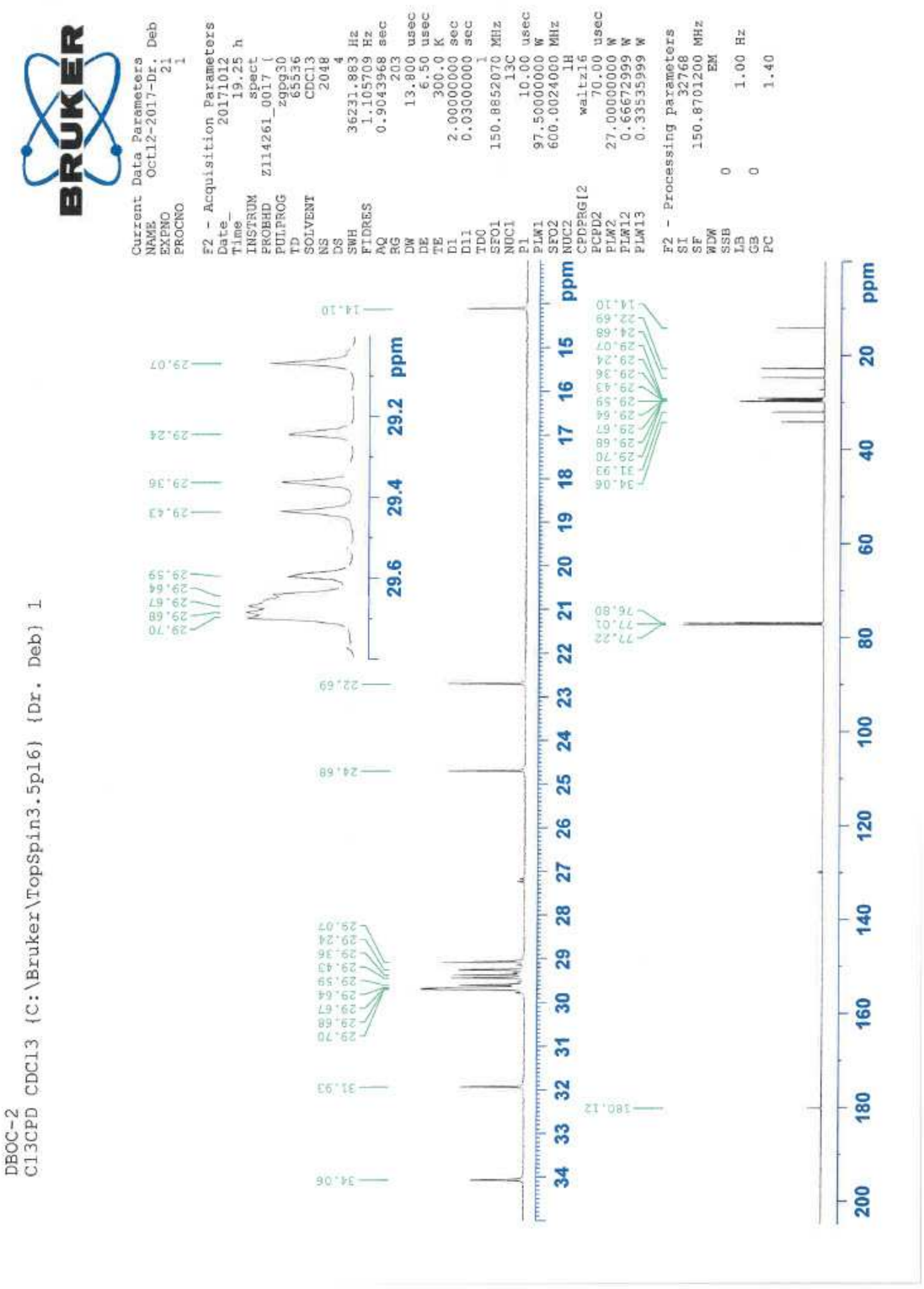


Figure 51. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon Dept90

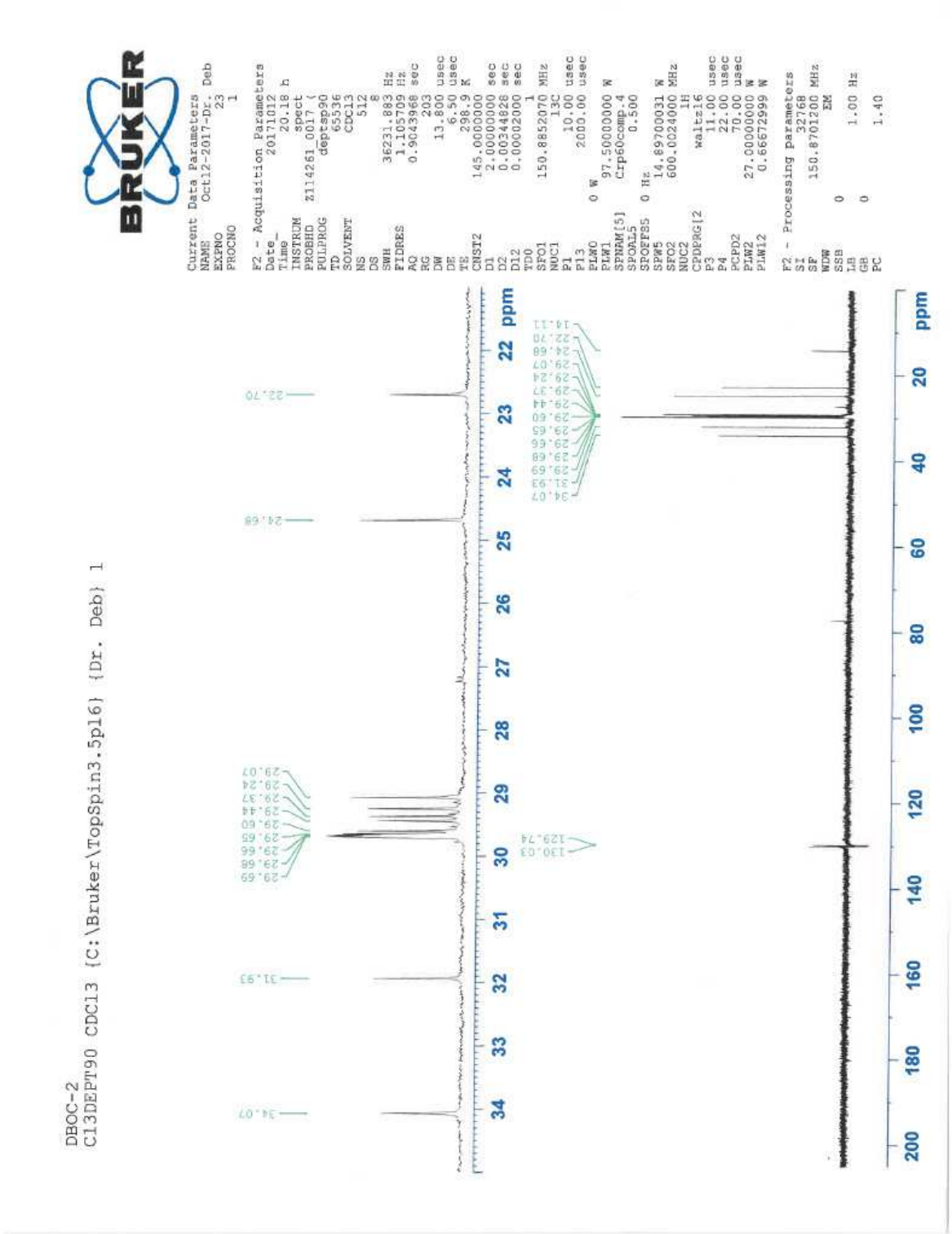


Figure 52. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon Dept135 NMR

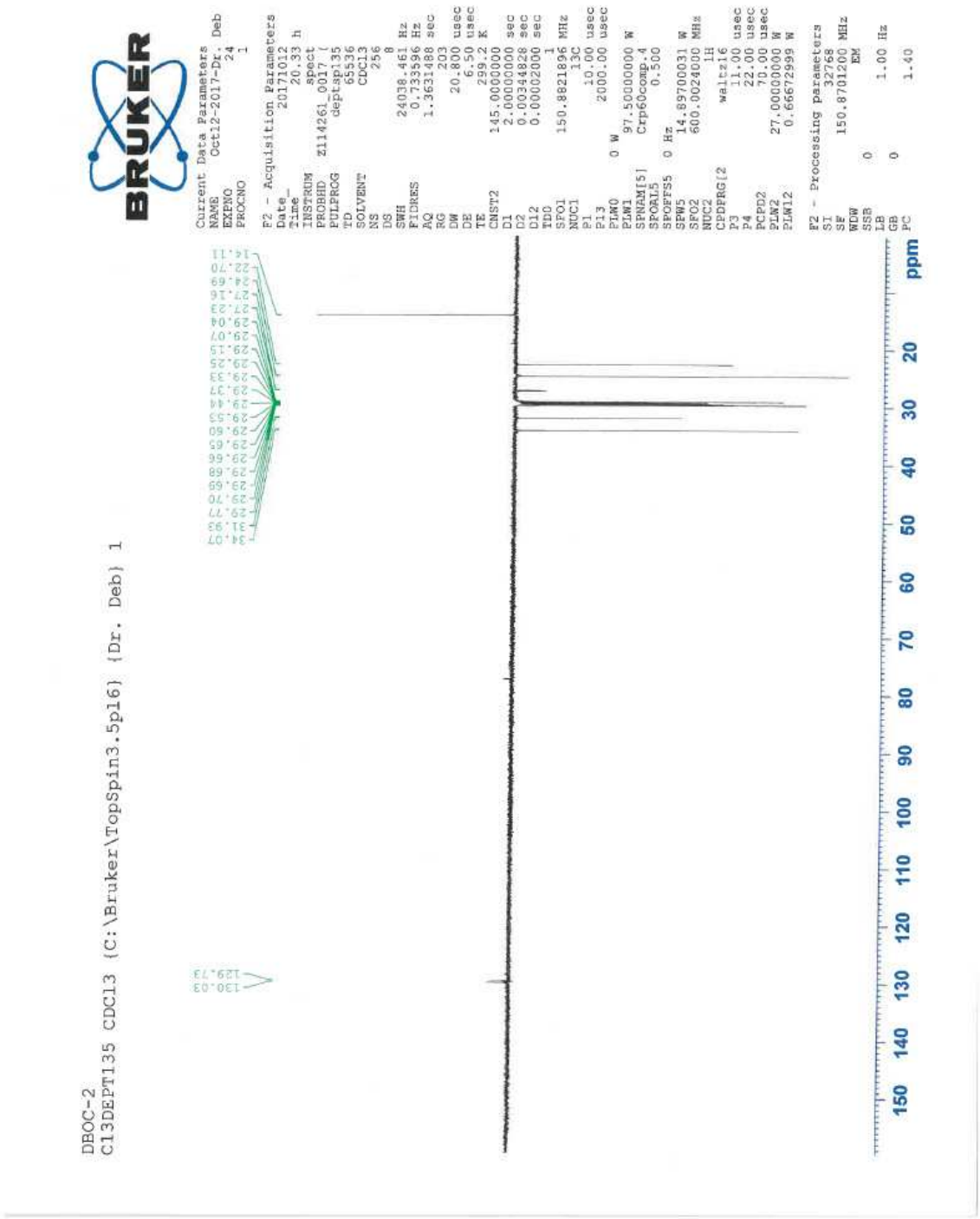


Figure 53. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one Carbon APT NMR

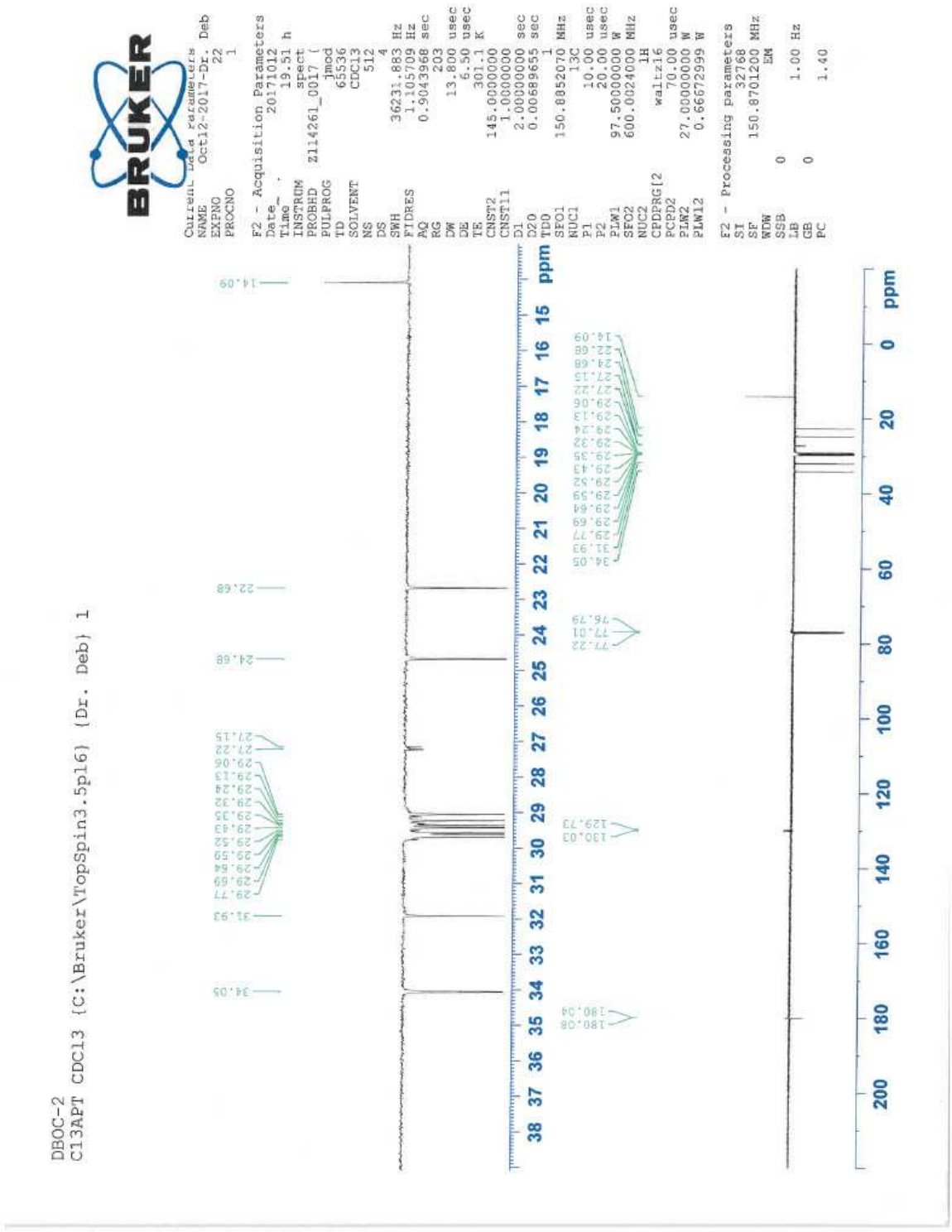


Figure 54. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one COSY NMR 1

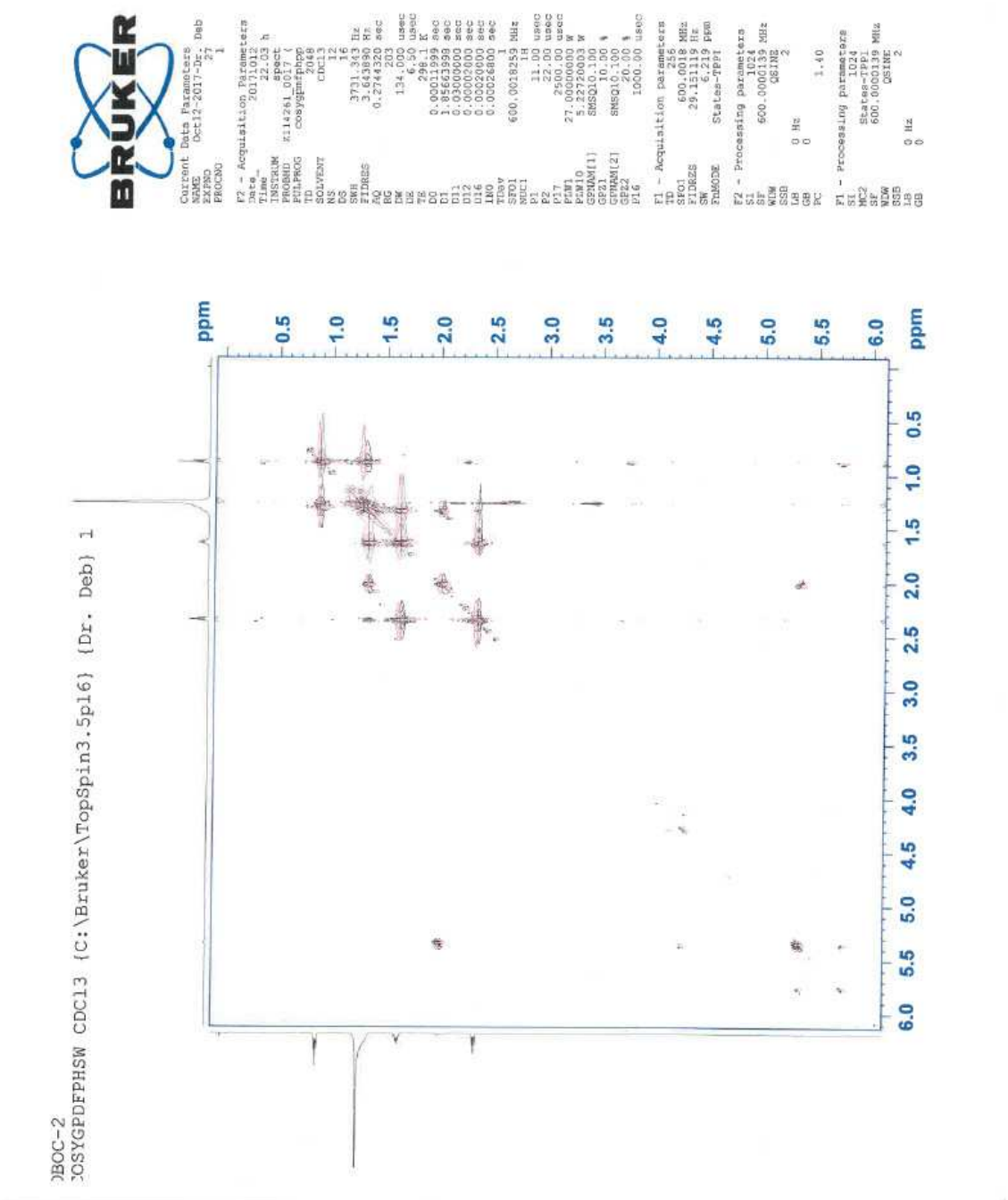


Figure 55. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one COSY NMR 2

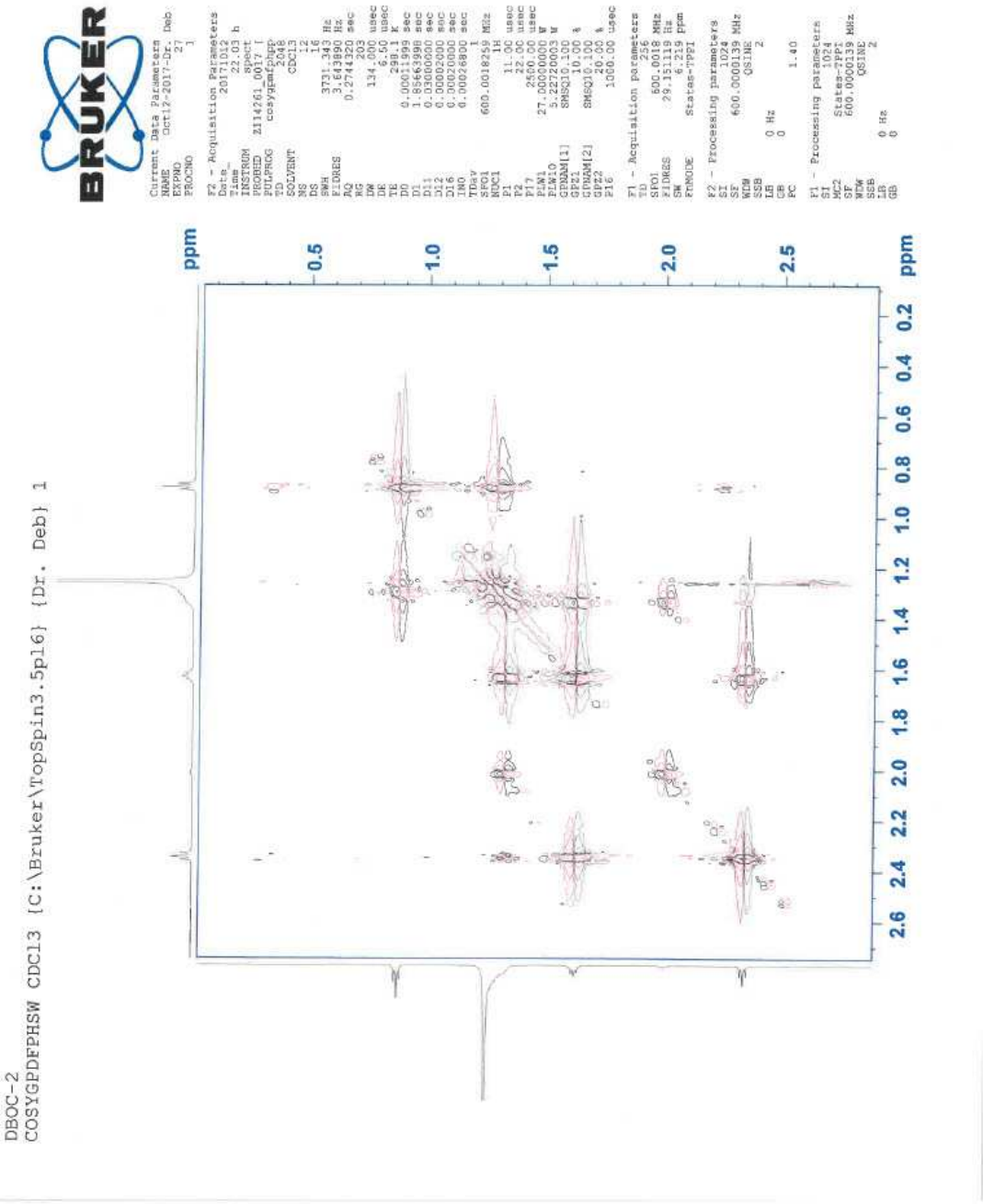


Figure 56. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one COSY NMR 3

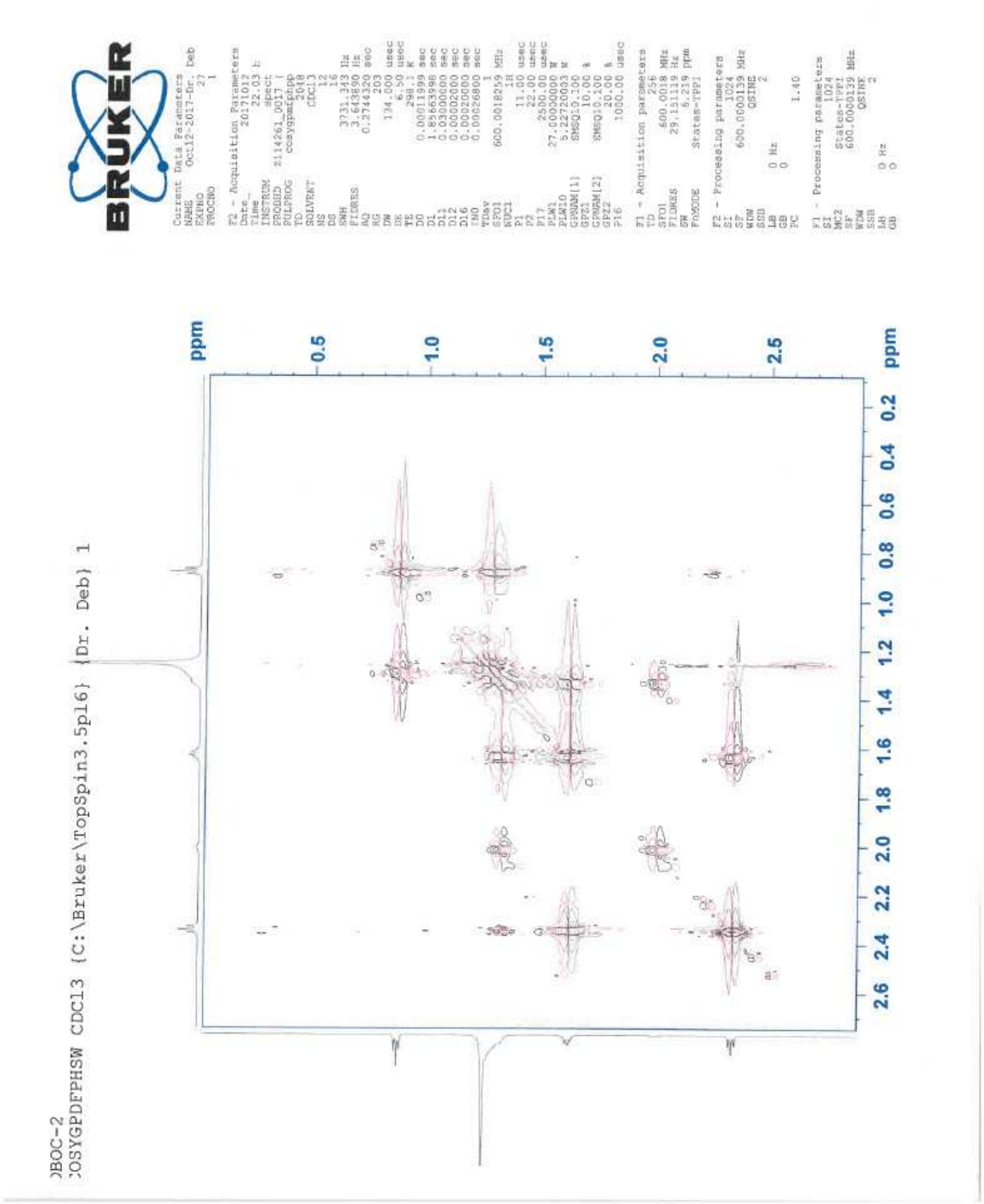


Figure 57. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMQCGP NMR

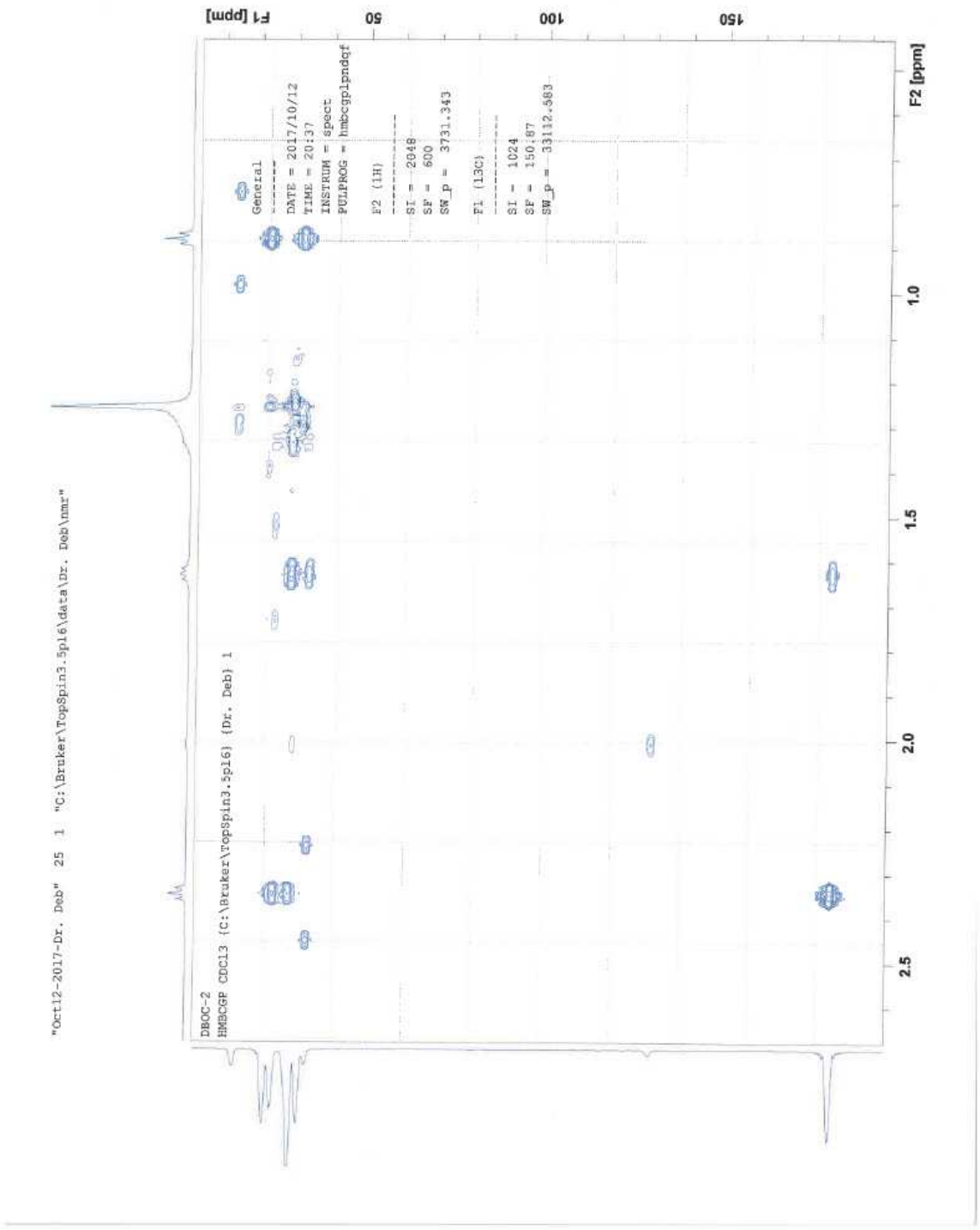


Figure 58. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMBCGP NMR 1

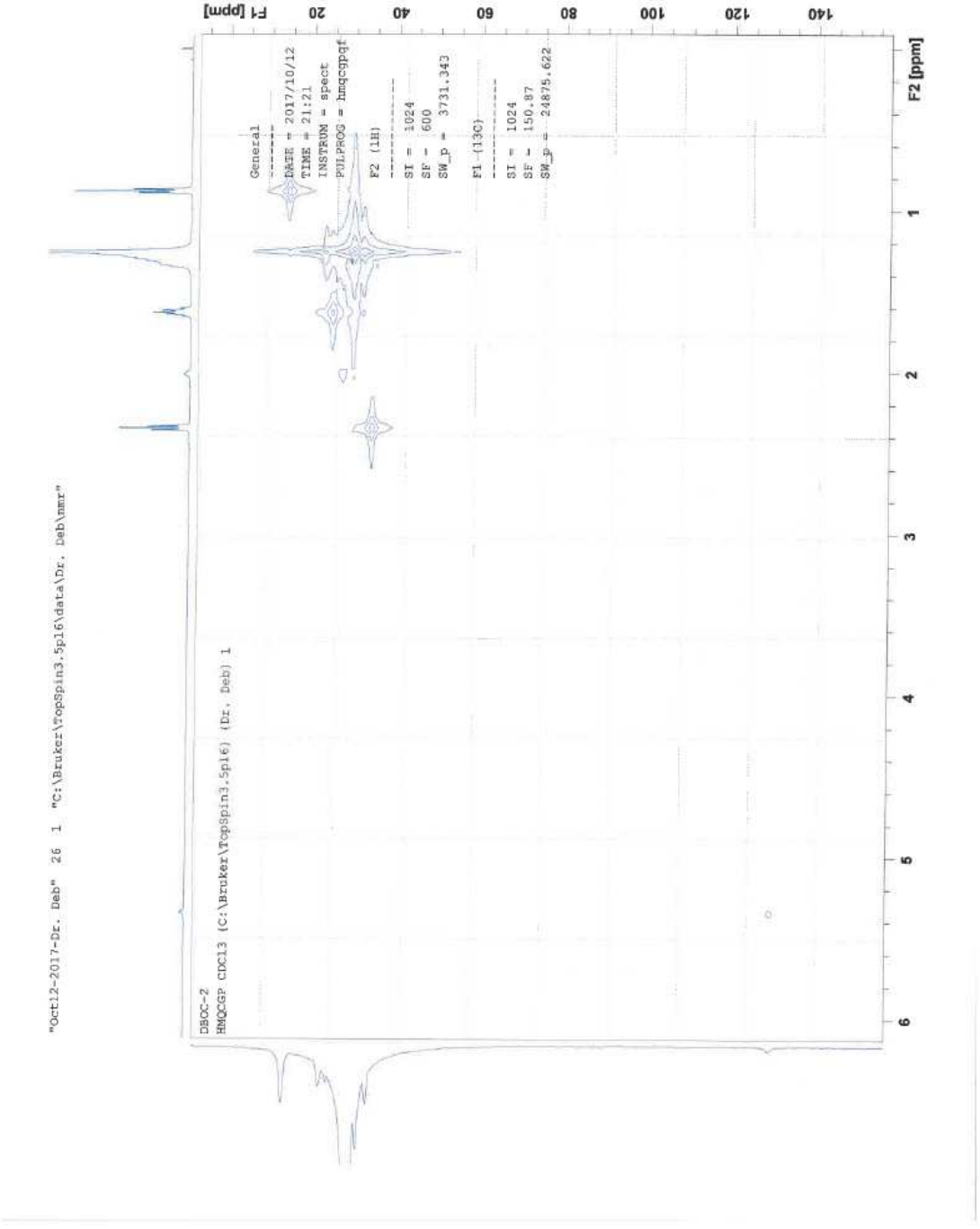


Figure 59. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMBCGP NMR 2

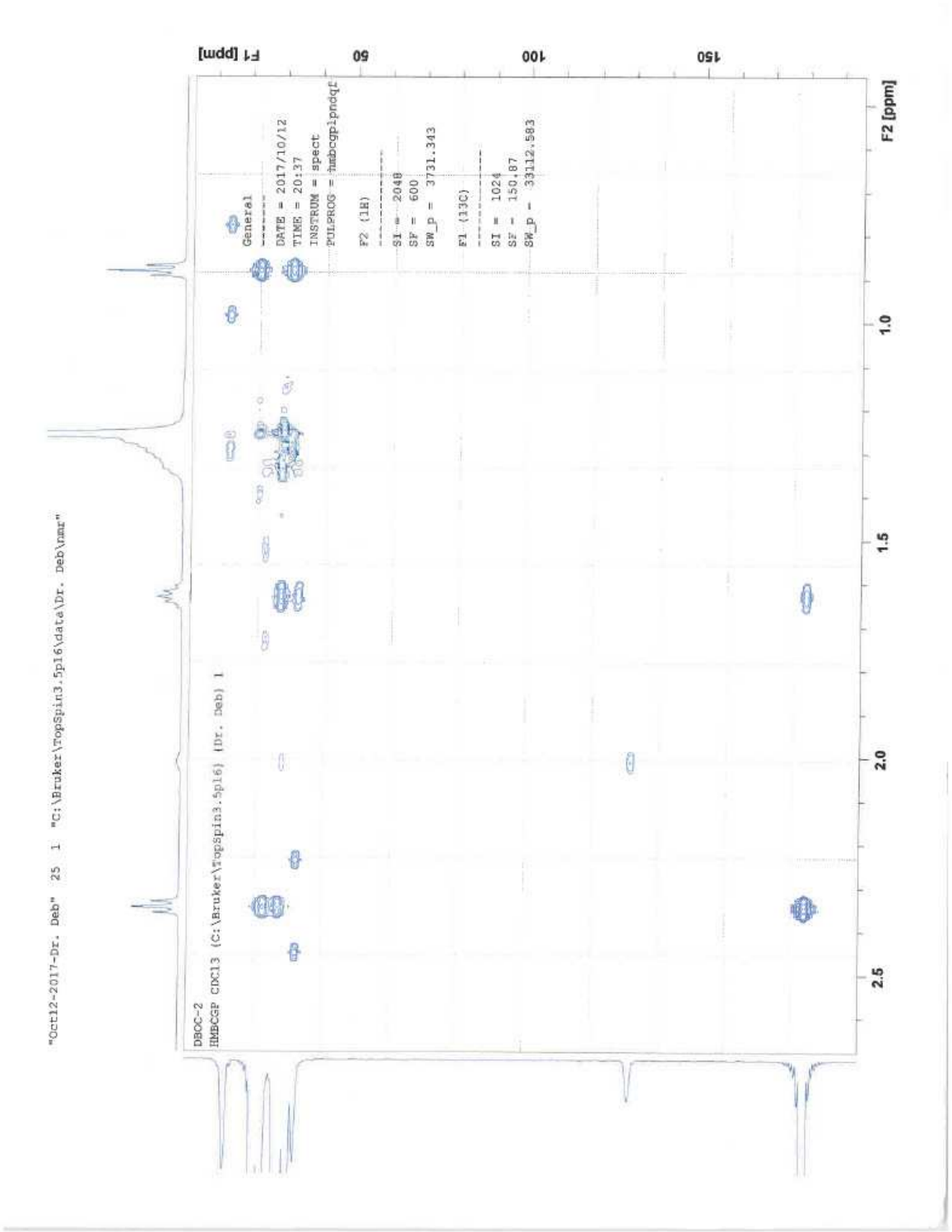


Figure 60. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMBCGP NMR 3

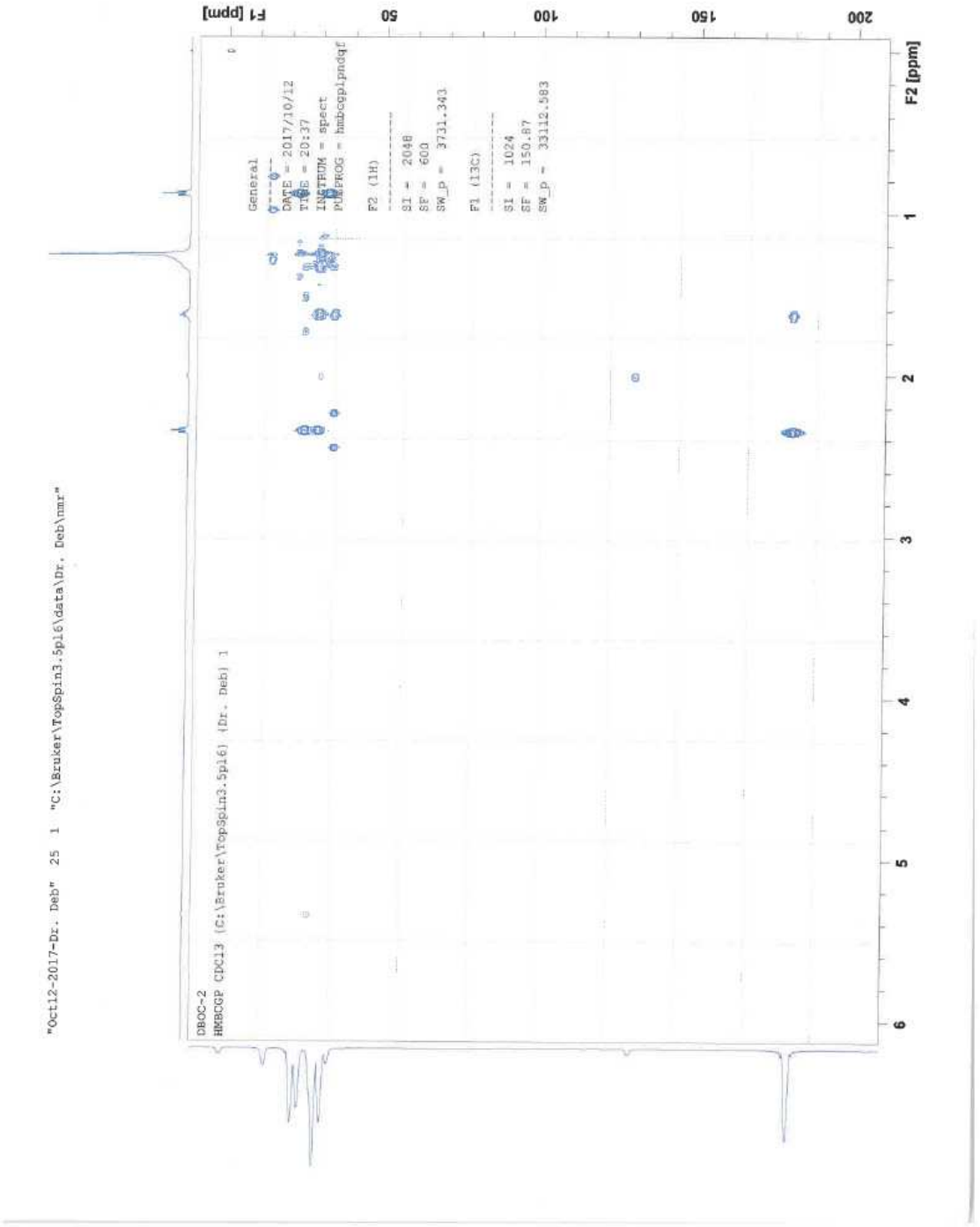


Figure 61. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMQCGP NMR 4

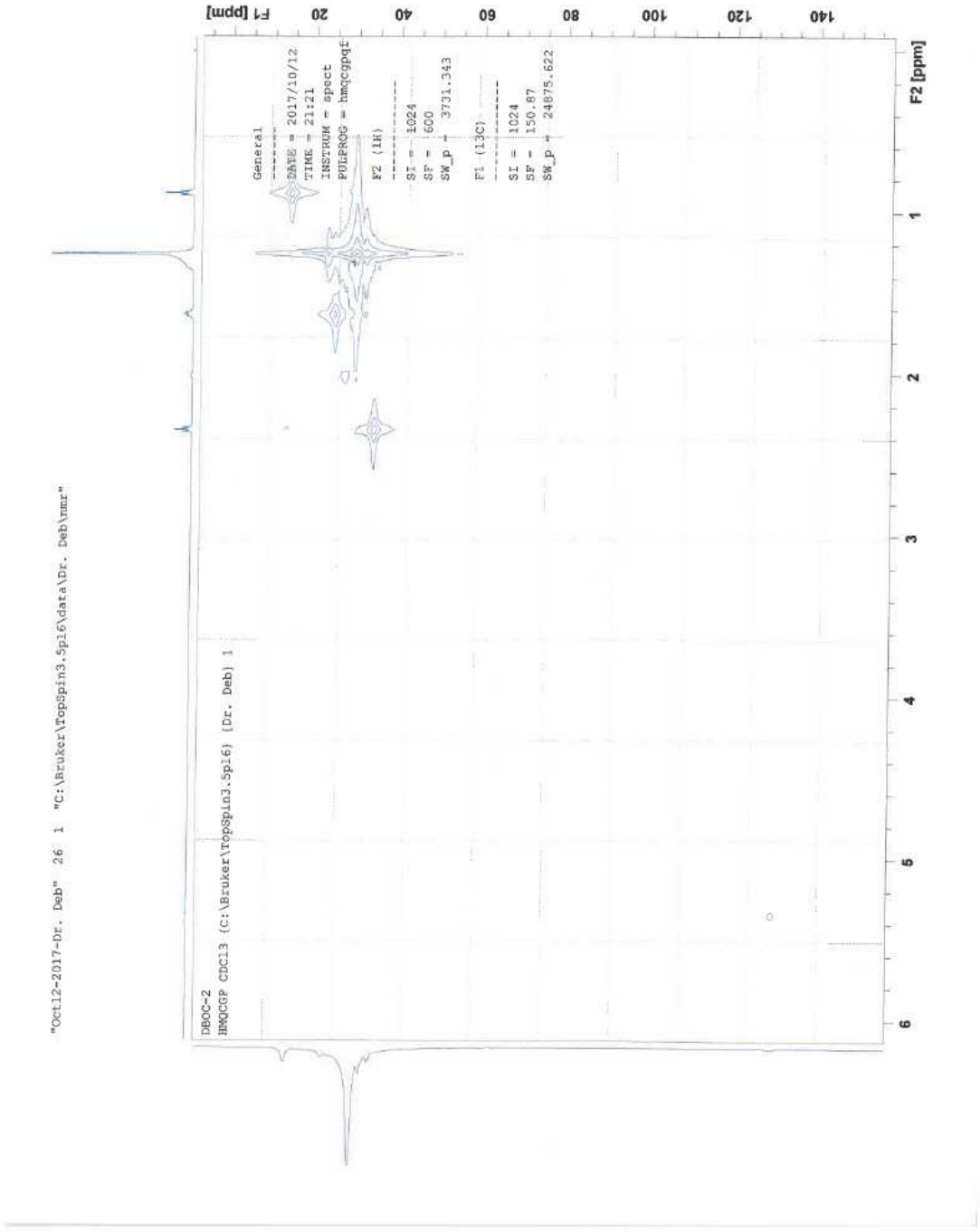


Figure 62. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HMQCGP NMR 5

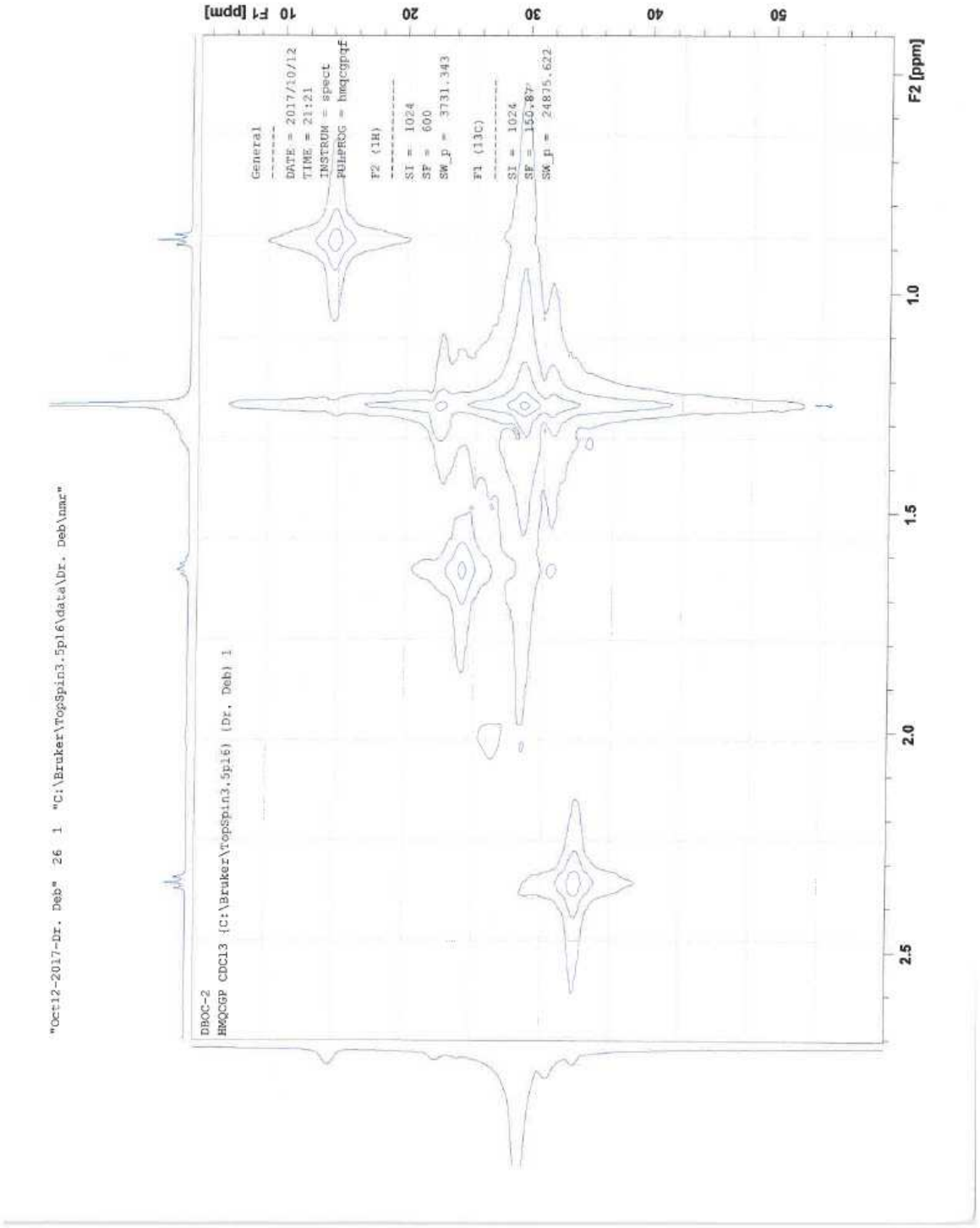
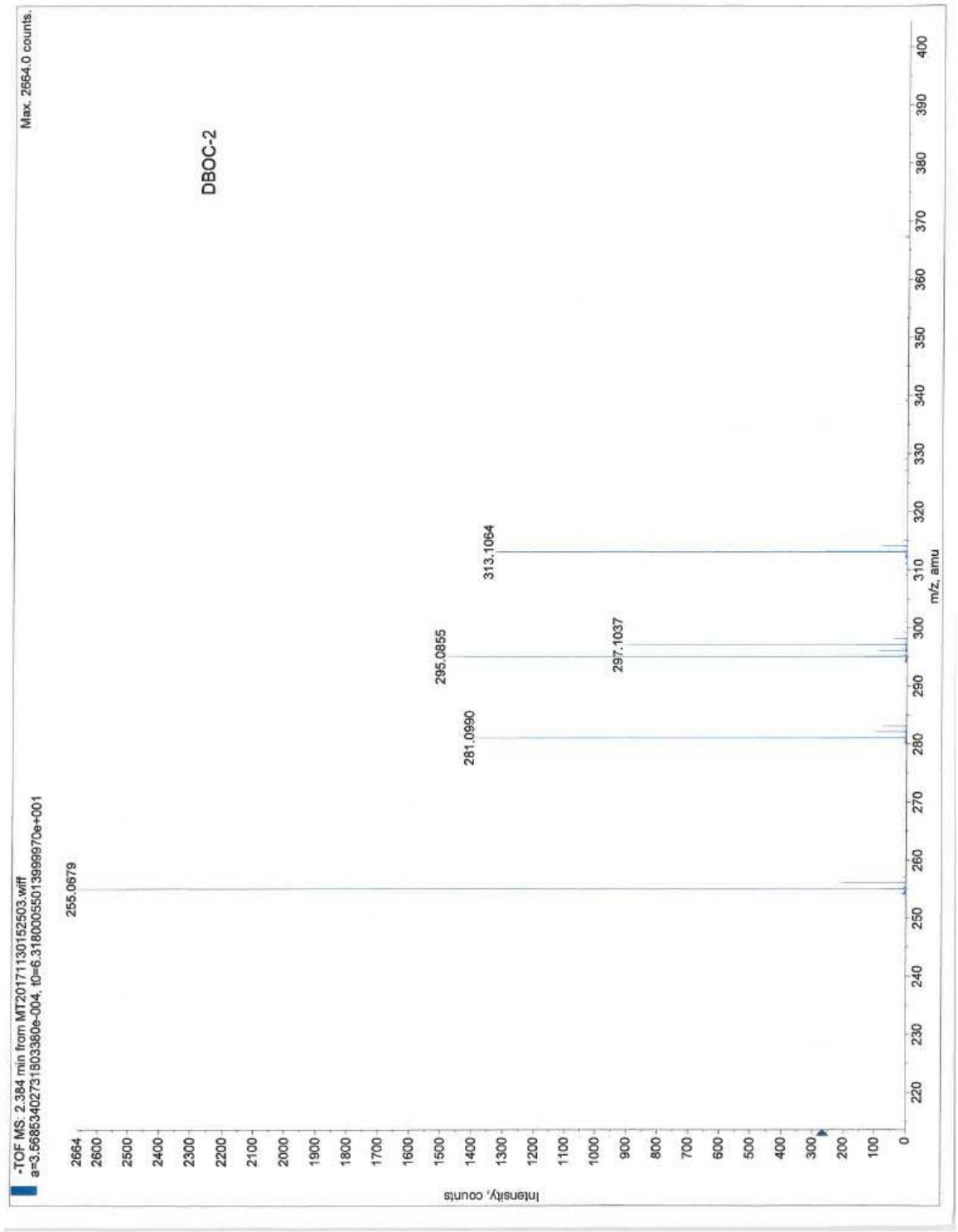


Figure 63. 12-methyl-4,7,8,9,10,11,12,13,14,15-decahydro-1H-cyclopenta[a]phenanthren-3(2H)-one HRMS



(4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol

Figure 64. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol FTIR

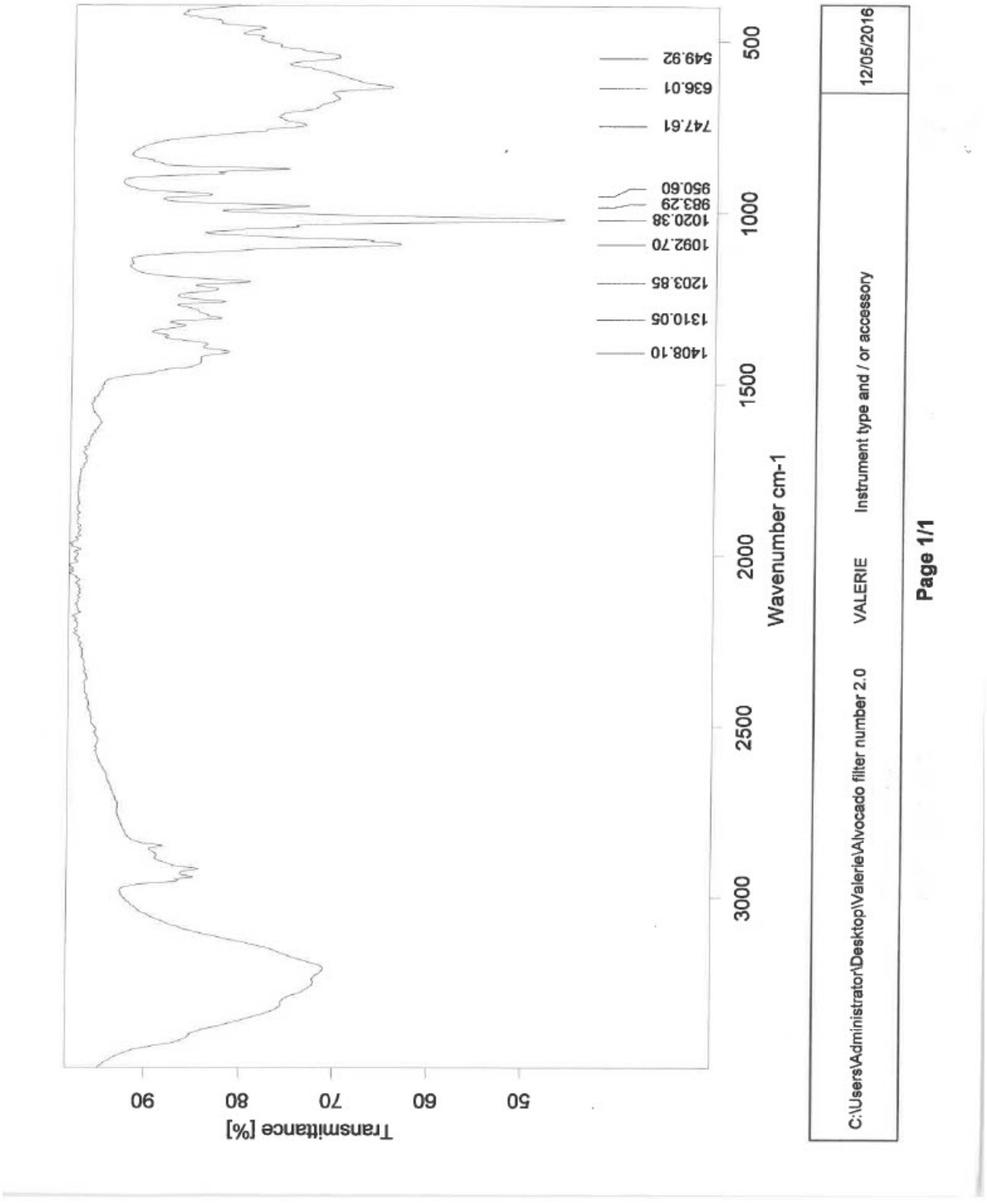


Figure 65. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Proton NMR 1

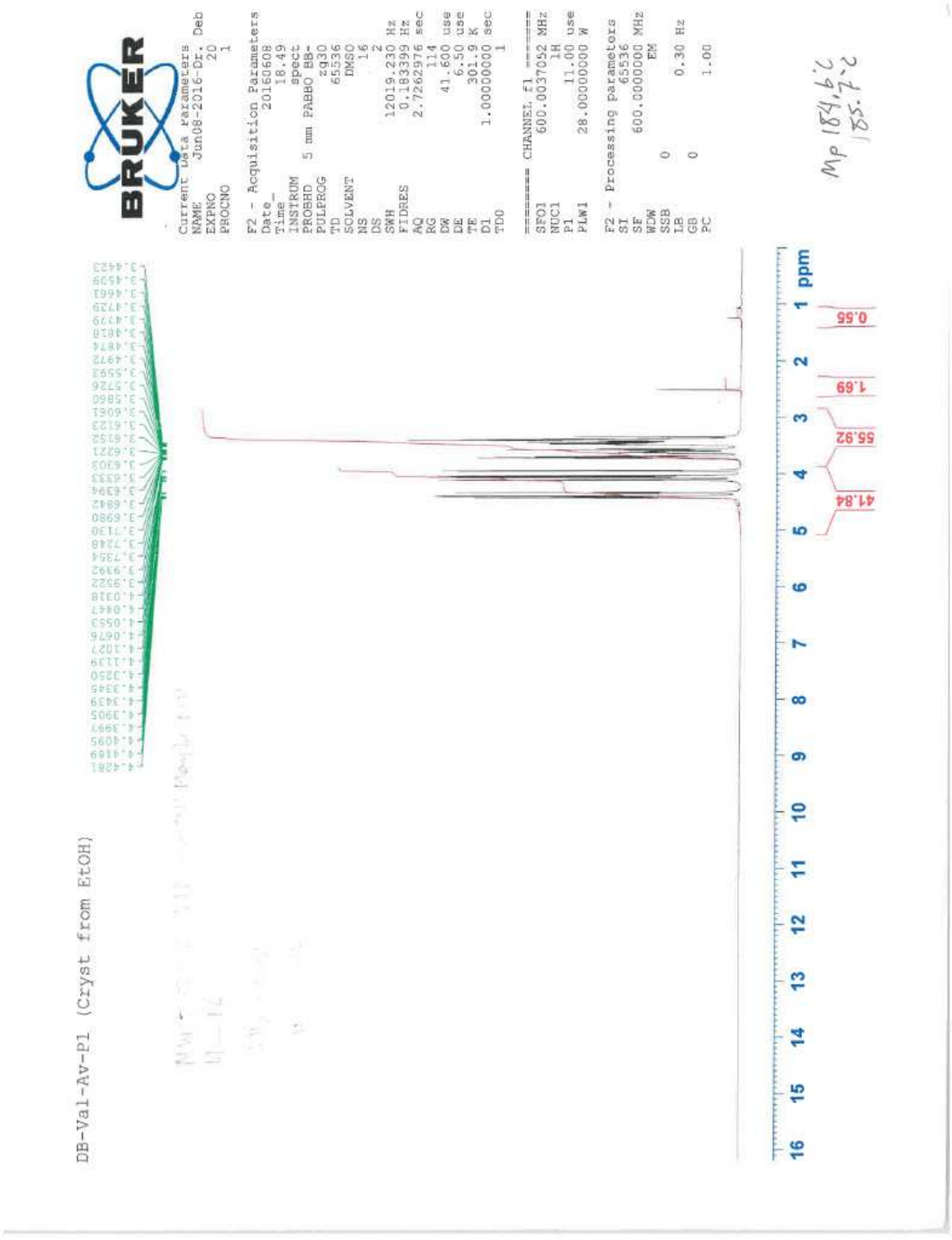


Figure 66. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Proton NMR 2

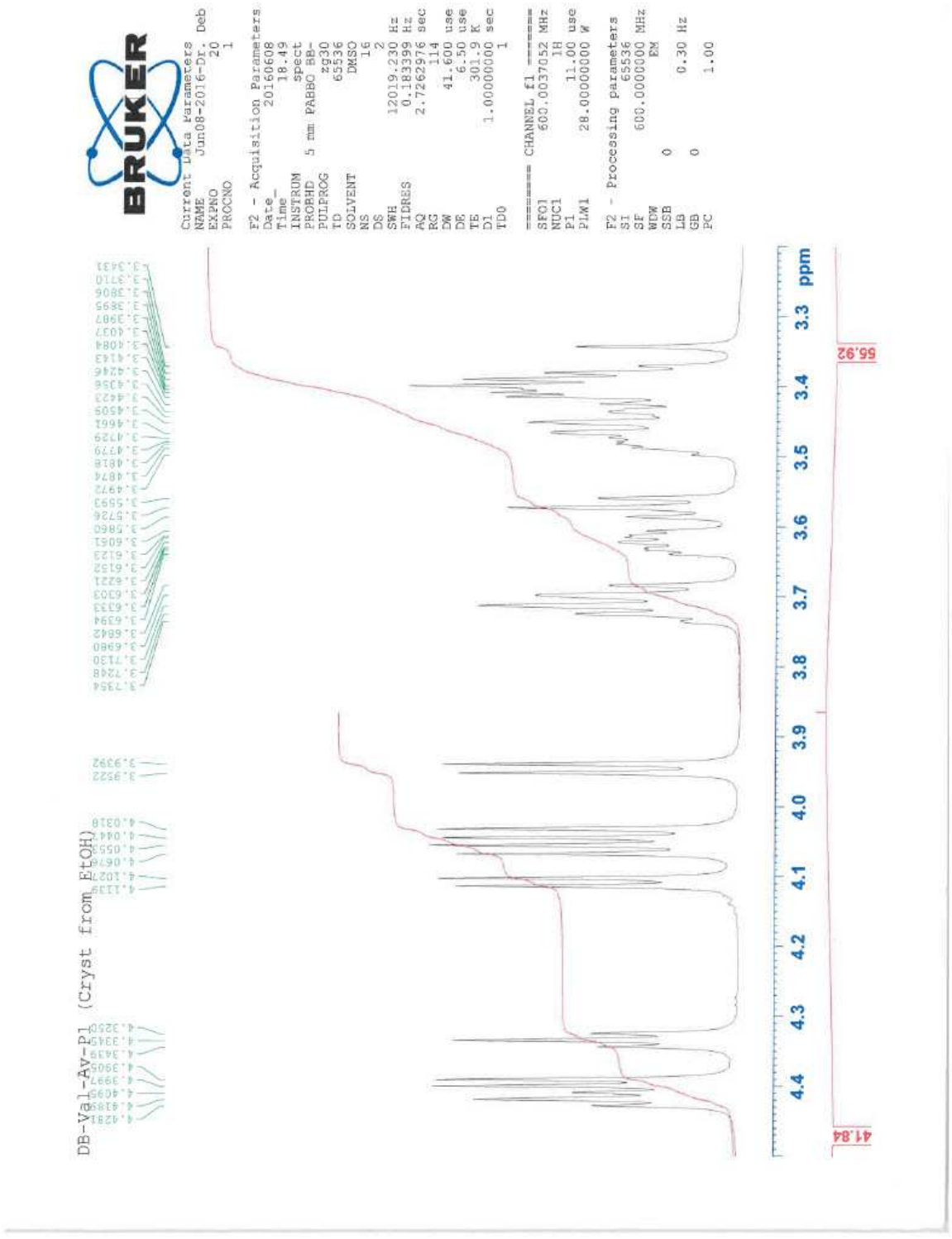


Figure 67. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Proton NMR 3

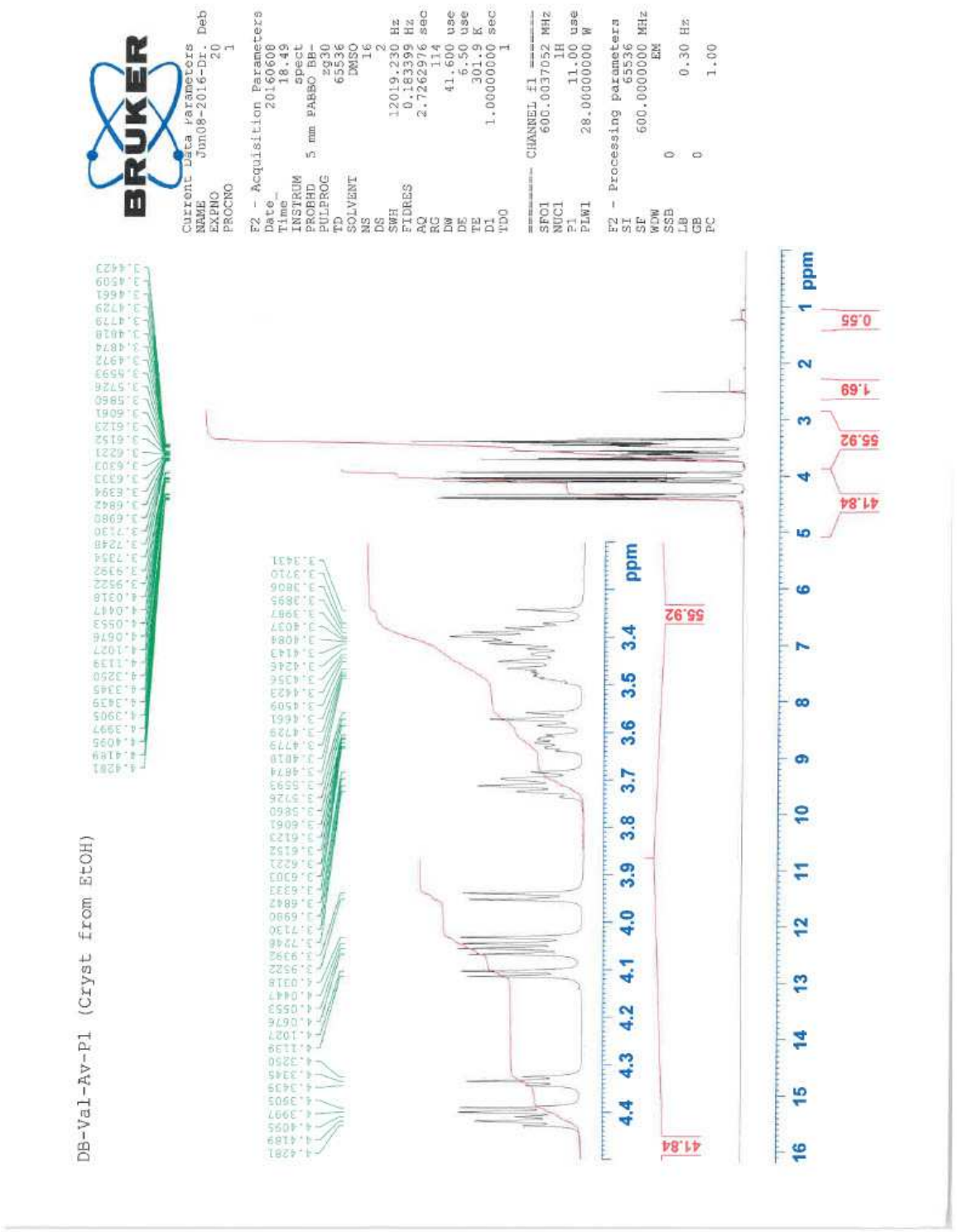


Figure 68. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon NMR 1

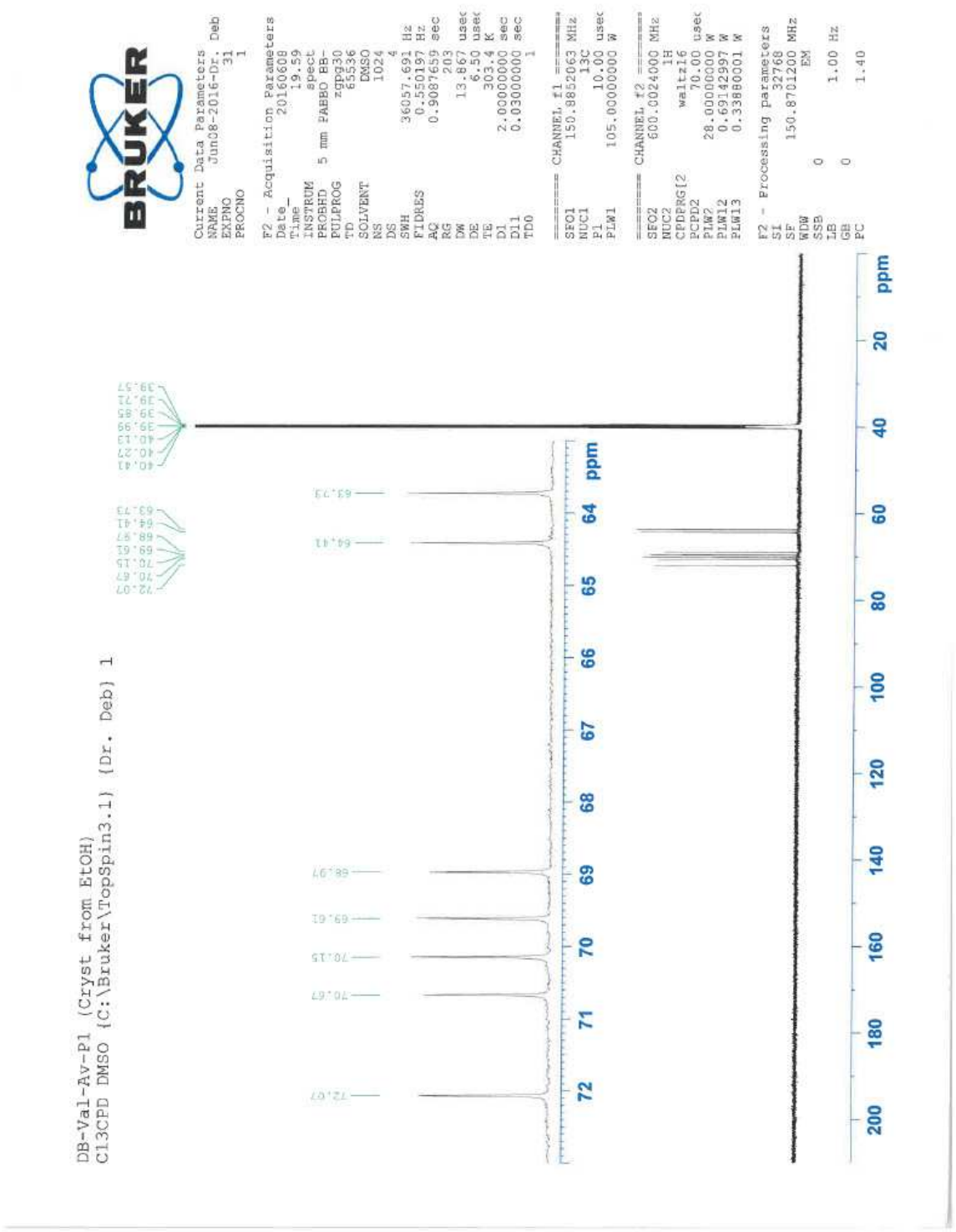


Figure 69. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon NMR 2

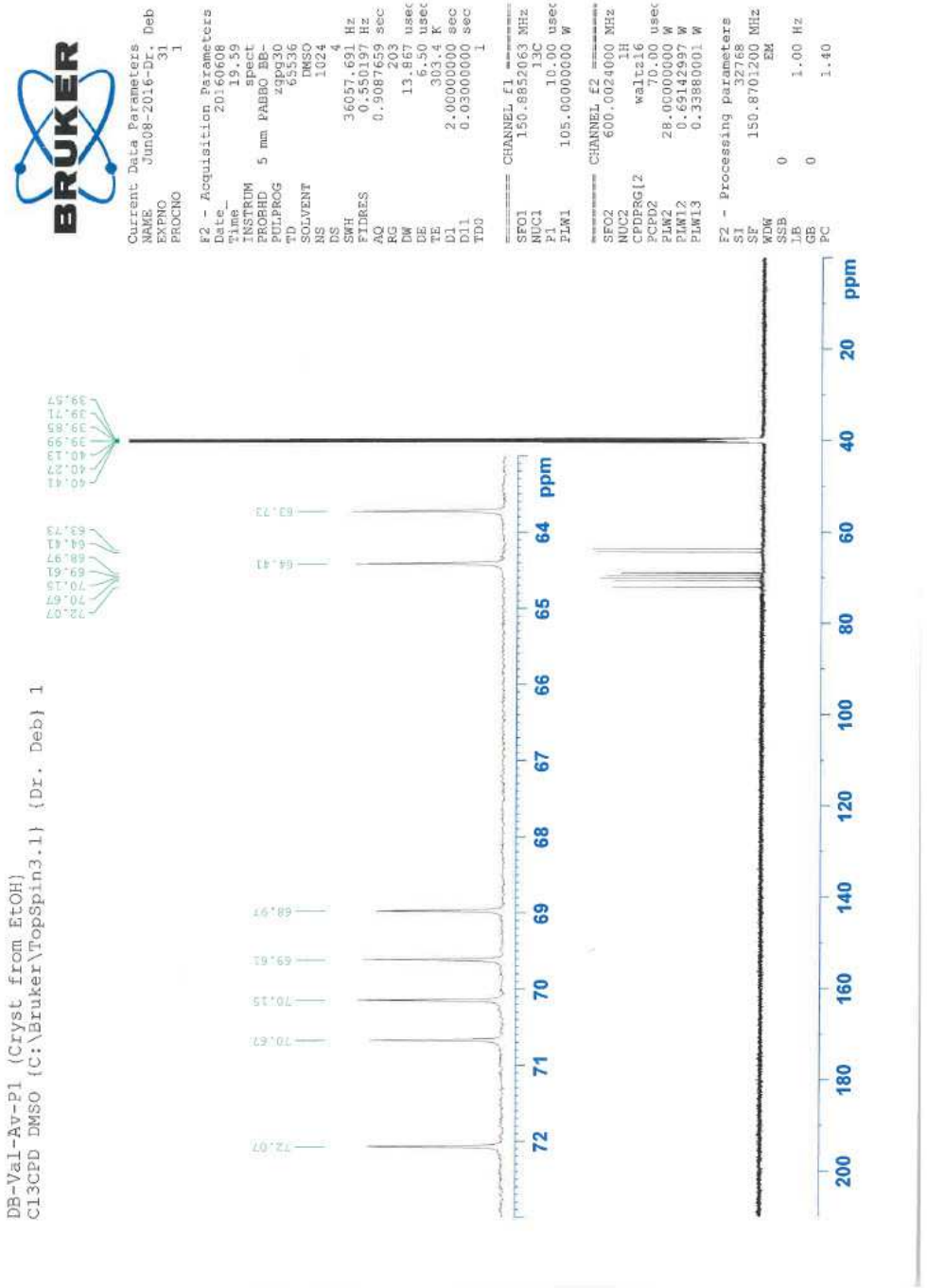


Figure 70. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon DEPT45

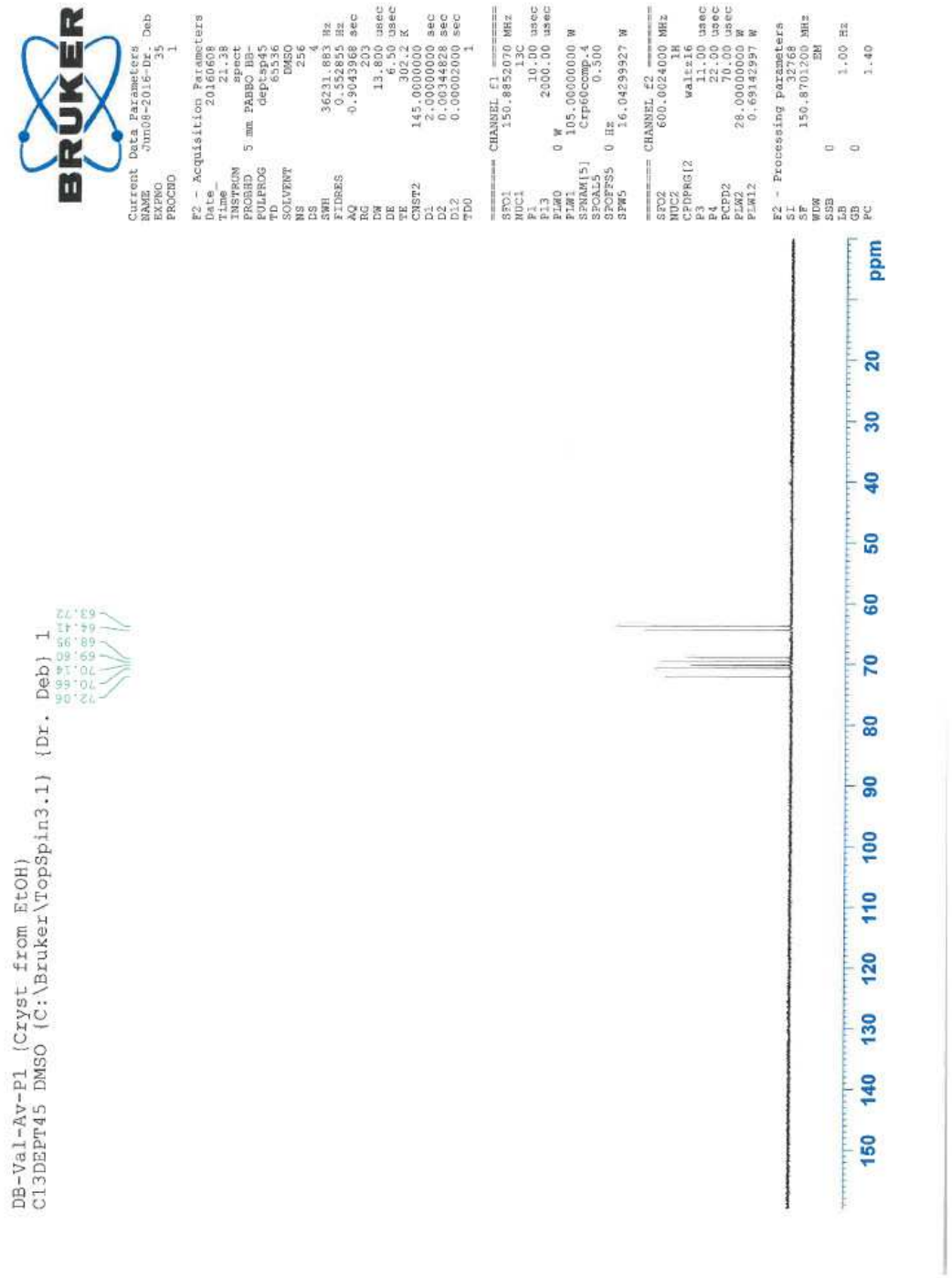


Figure 71. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon DEPT90

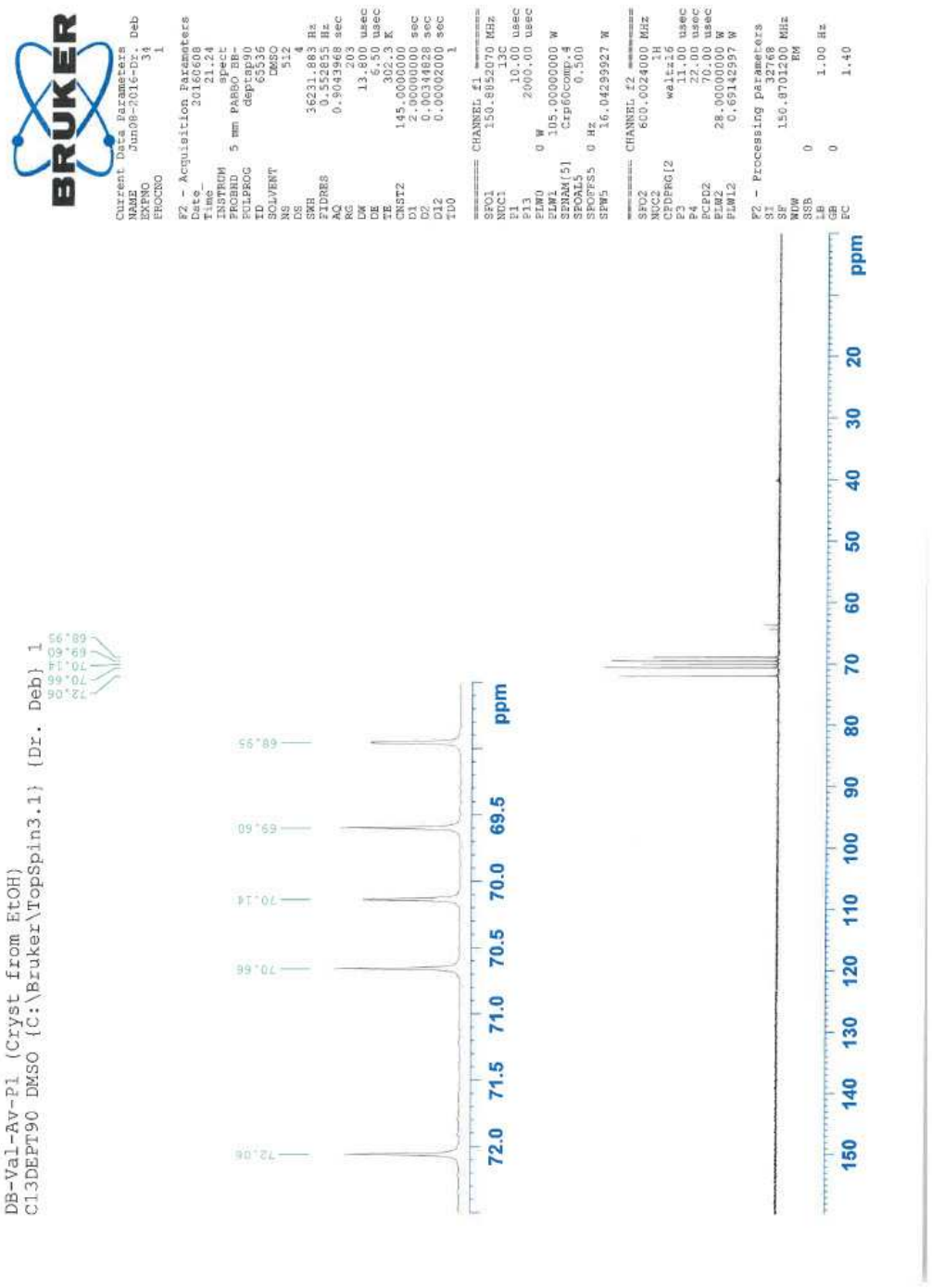


Figure 72. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon DEPT135

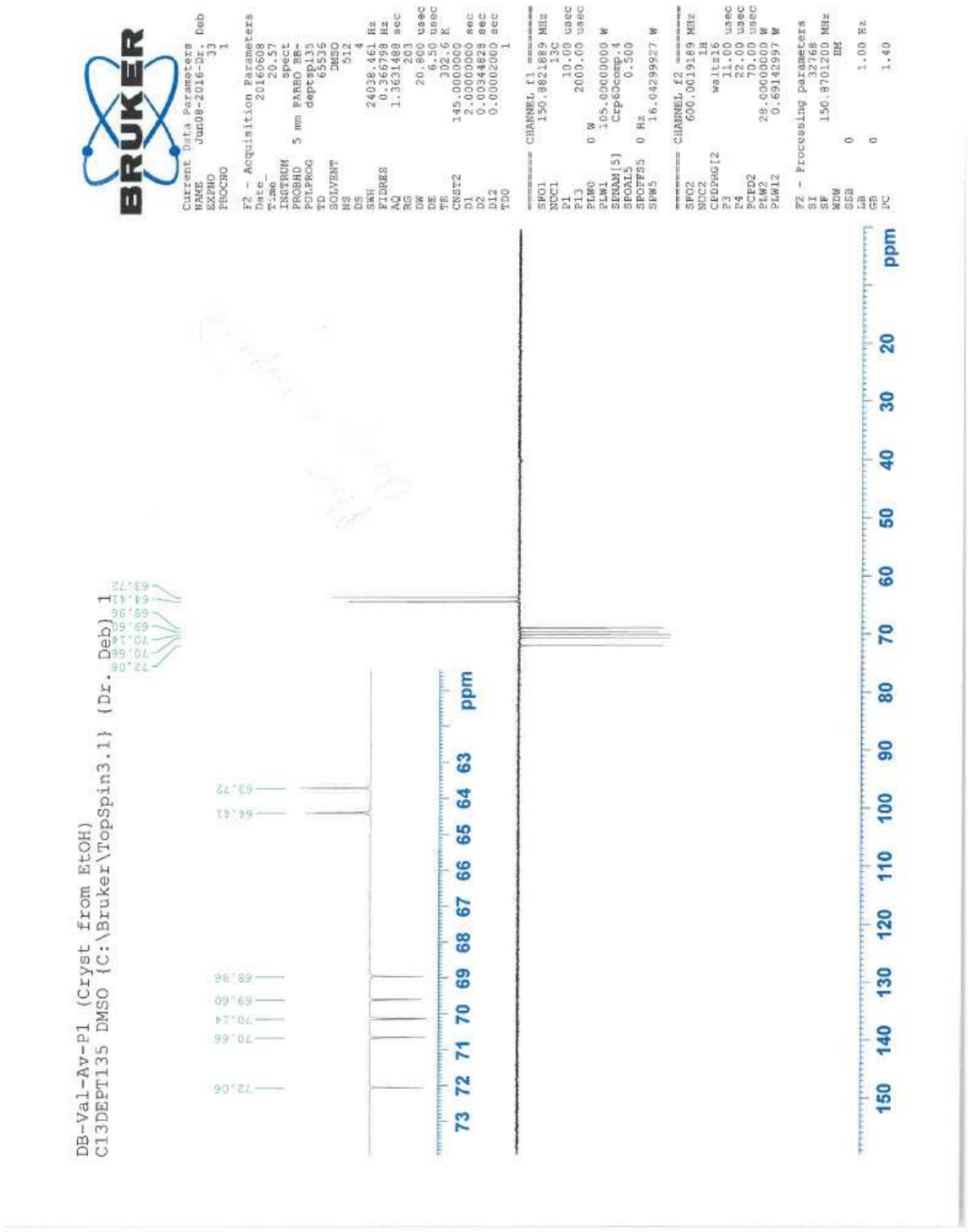


Figure 73. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol. Carbon APT NMR 1

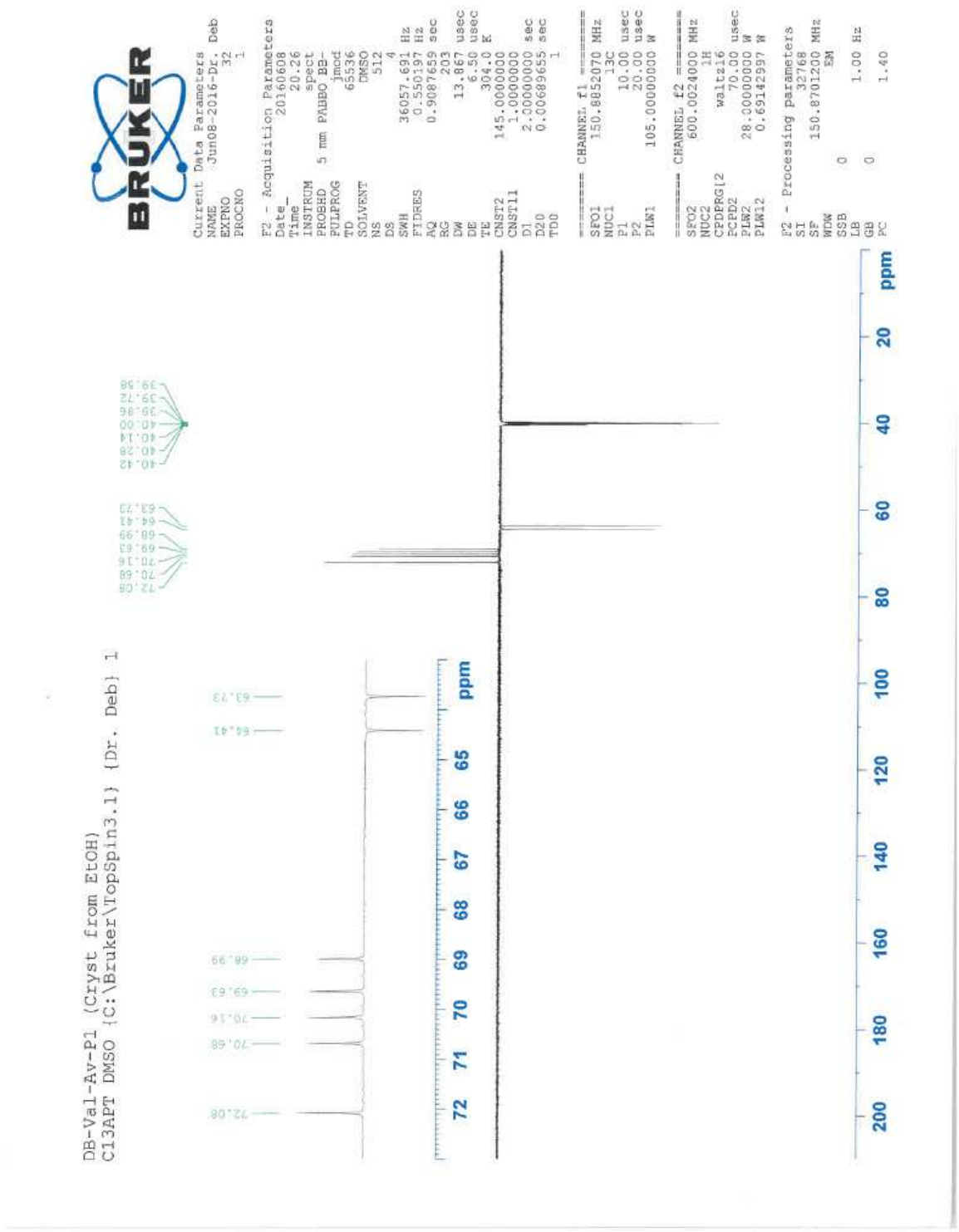


Figure 74. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol Carbon APT NMR 2

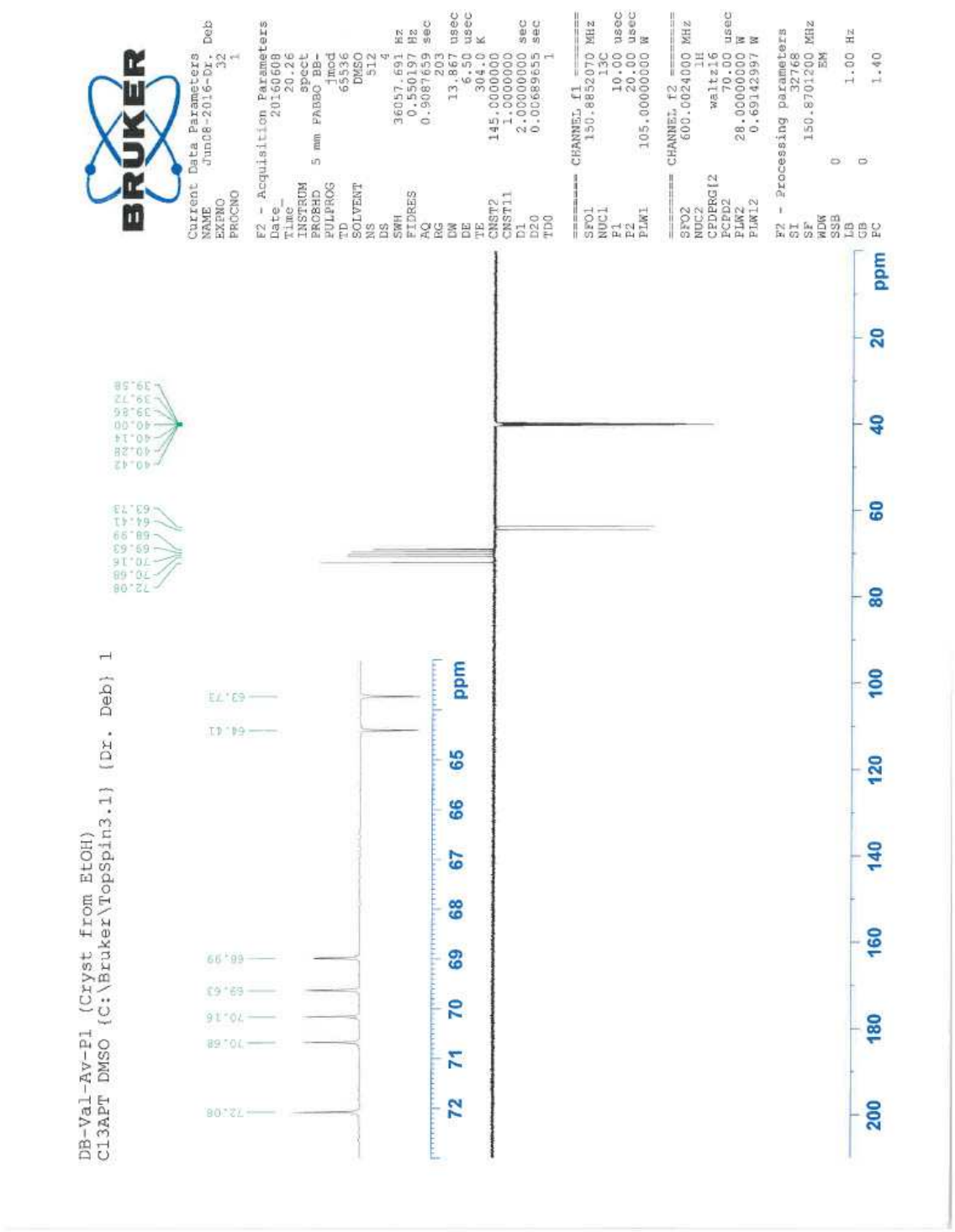


Figure 75. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol COSY NMR 1

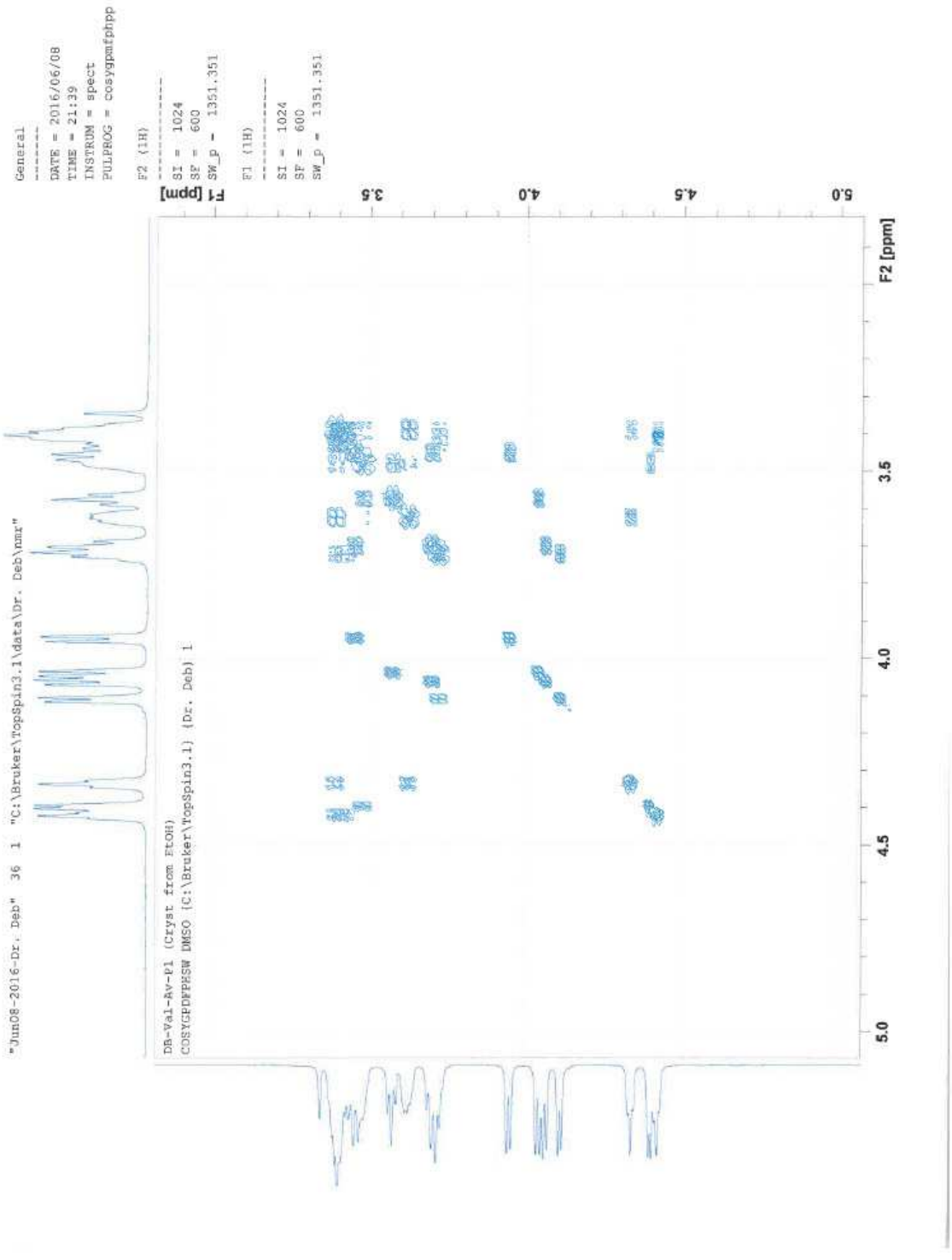


Figure 76. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol COSY NMR 2

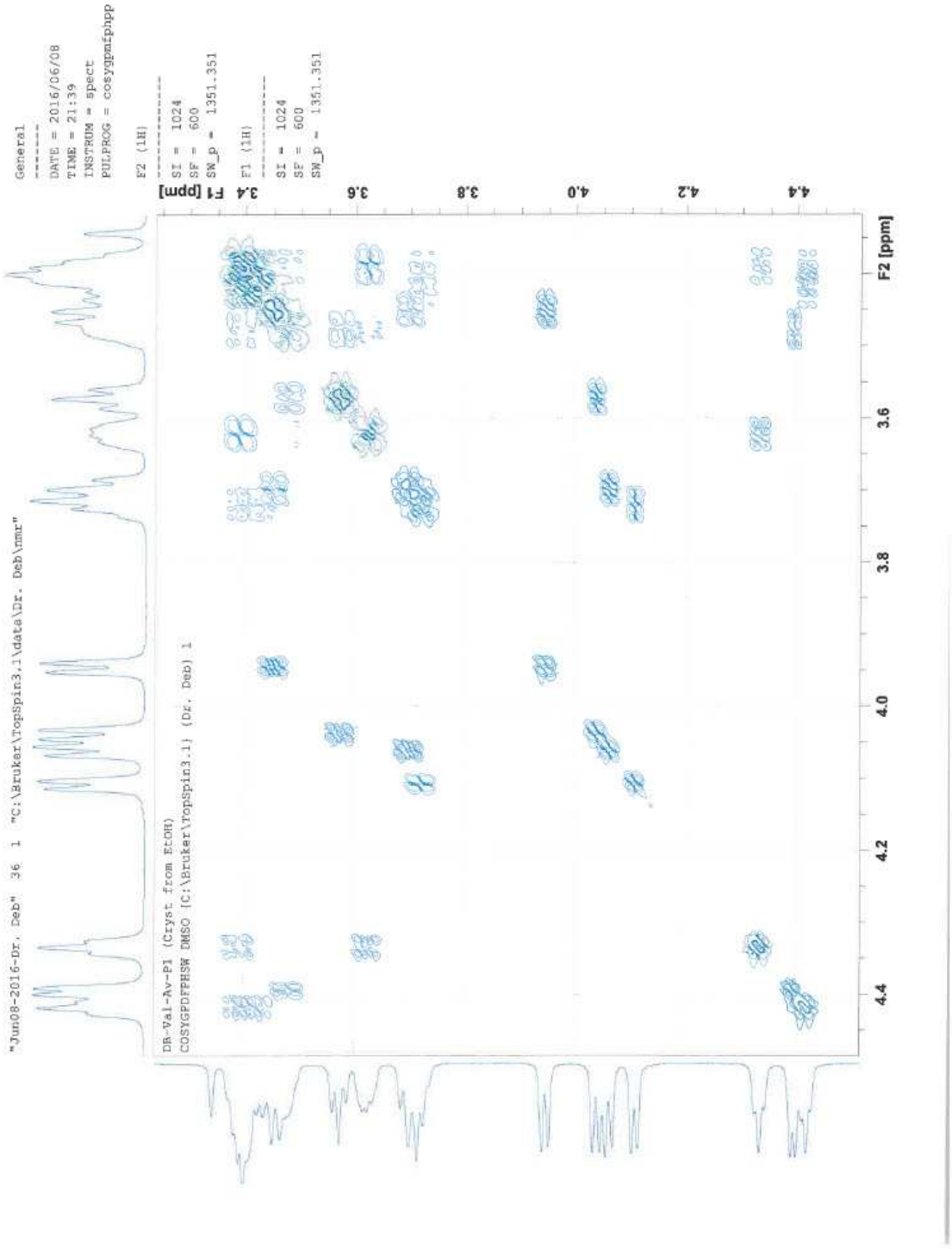


Figure 77. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol COSY NMR 3

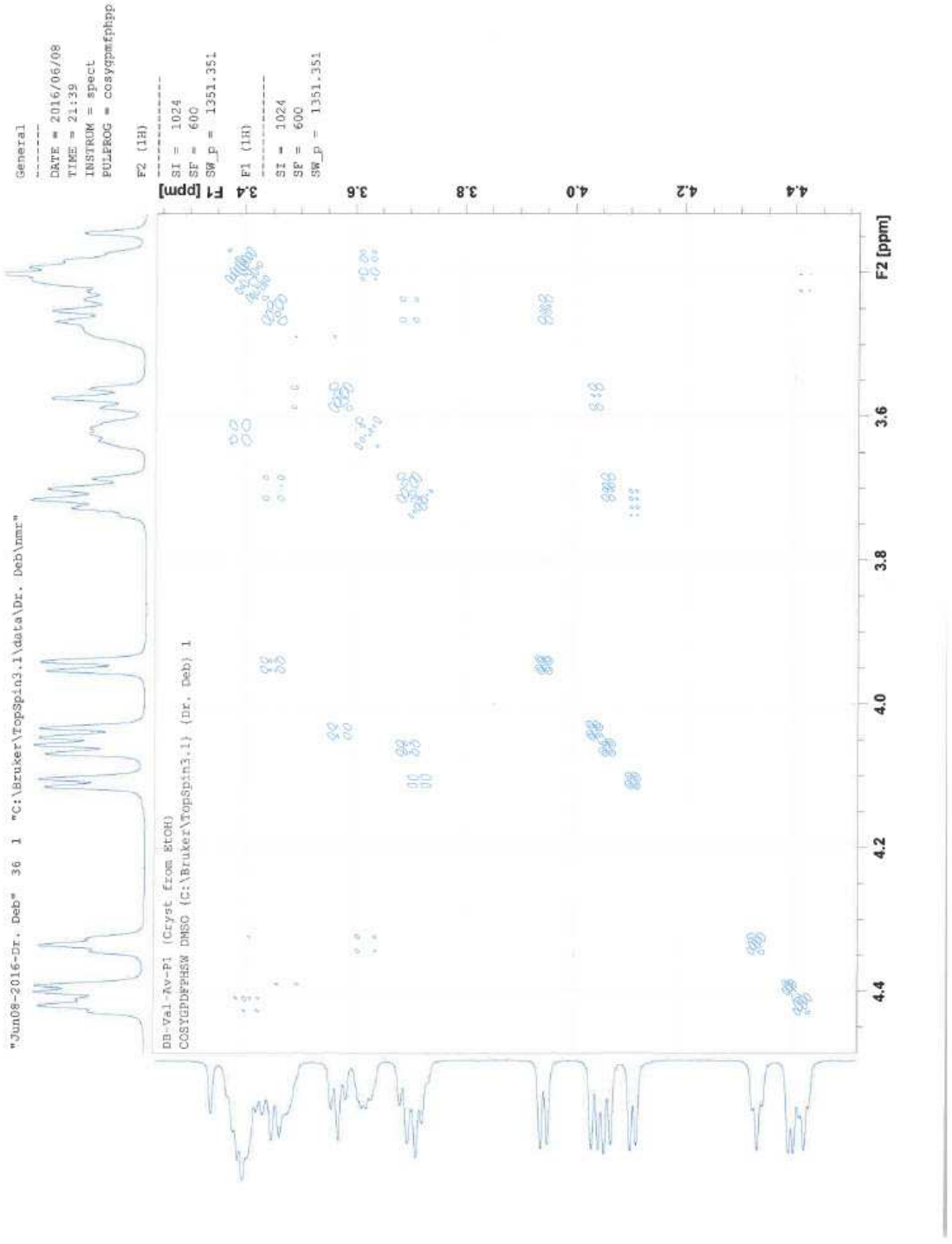


Figure 78. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMBCGP NMR 1

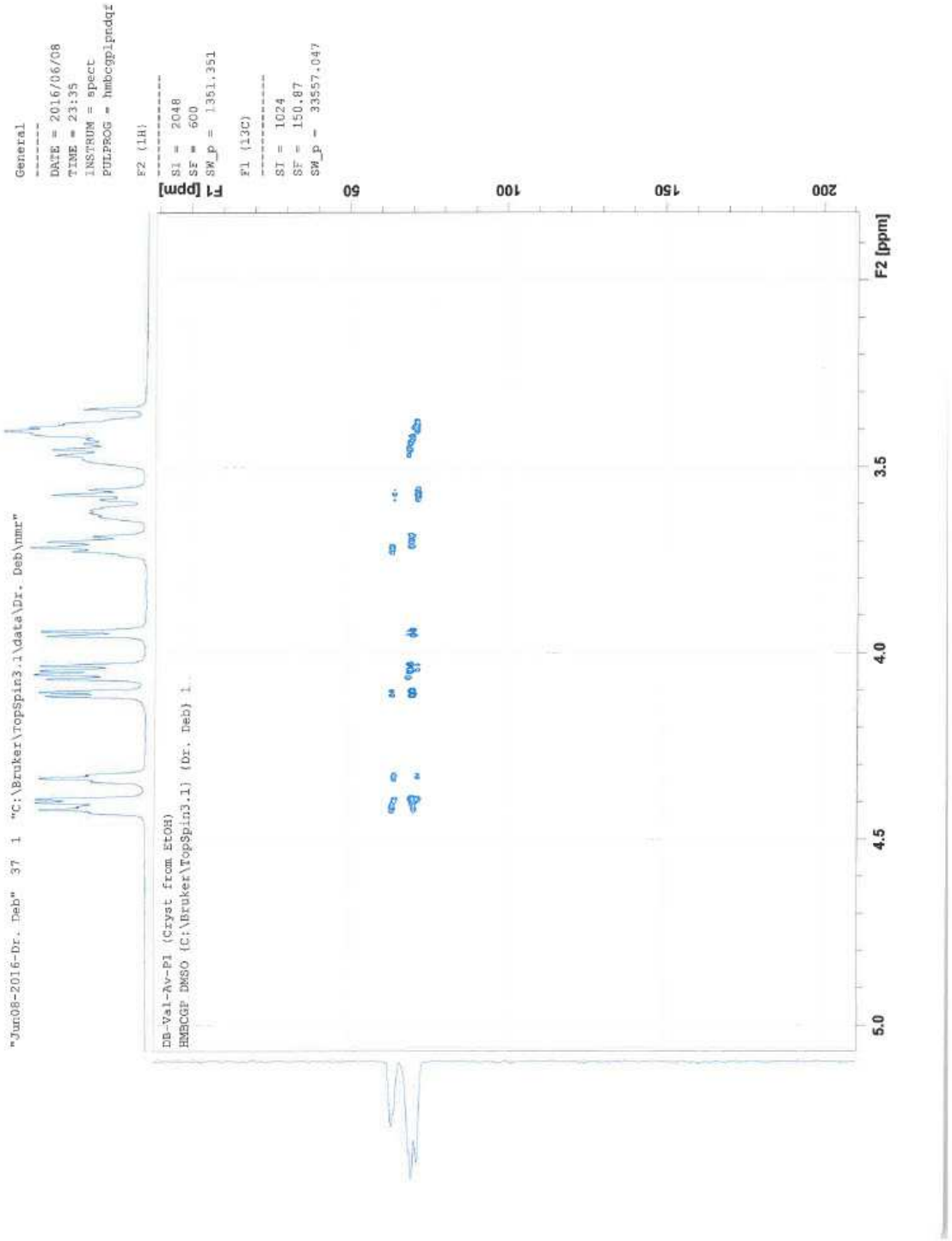


Figure 79. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMBCGP NMR 2

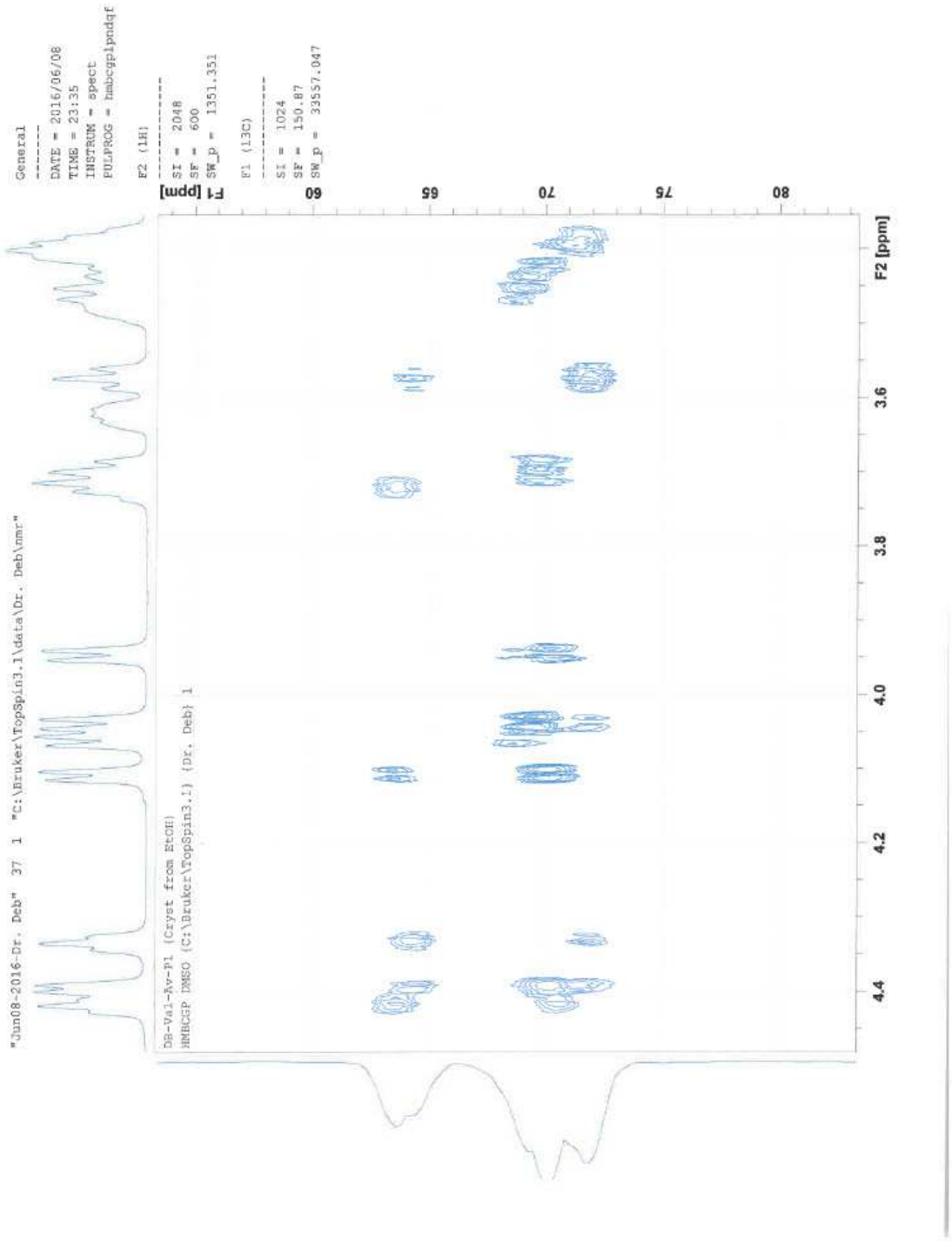


Figure 80. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMBCGP NMR 3

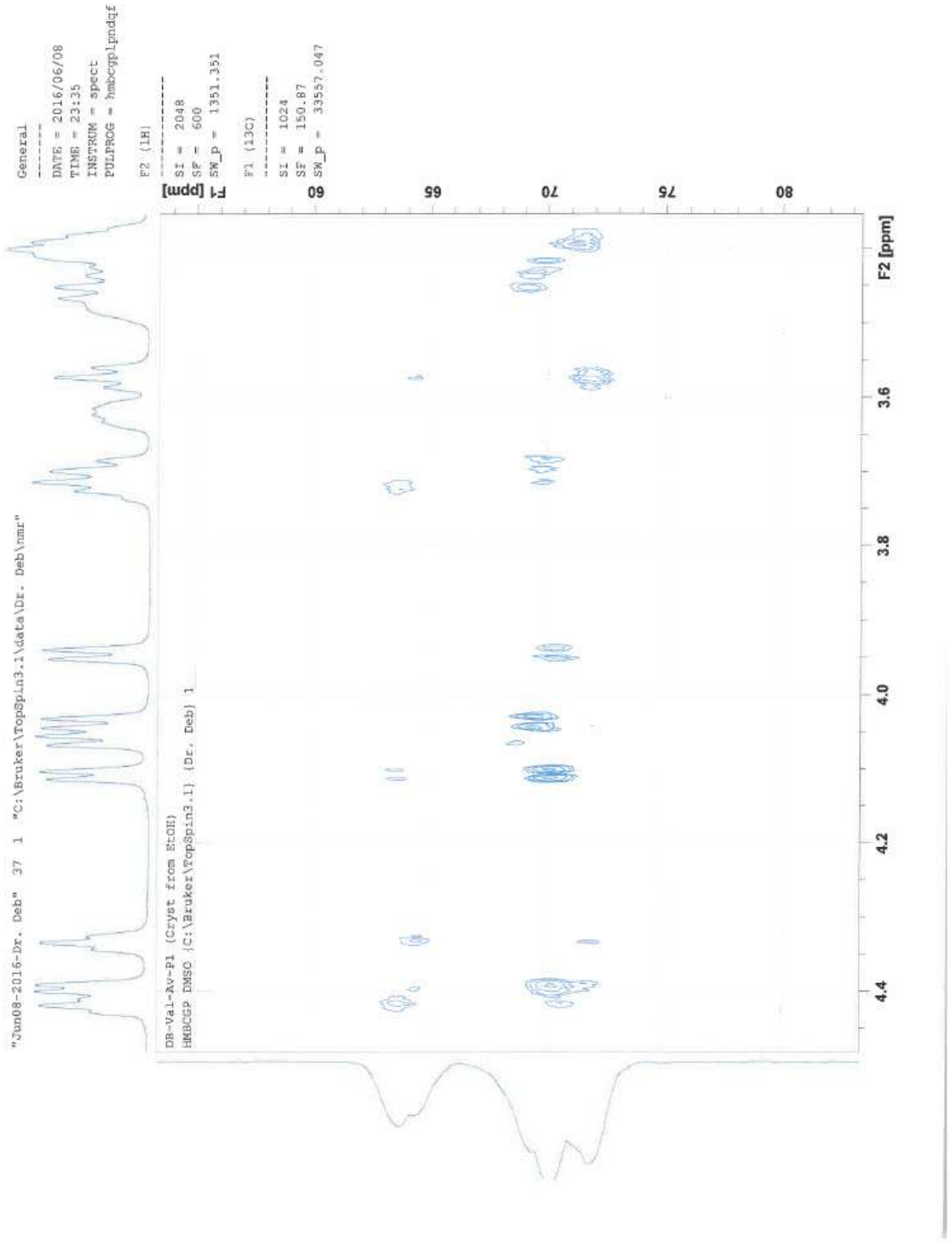


Figure 81. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMQCGP NMR 4

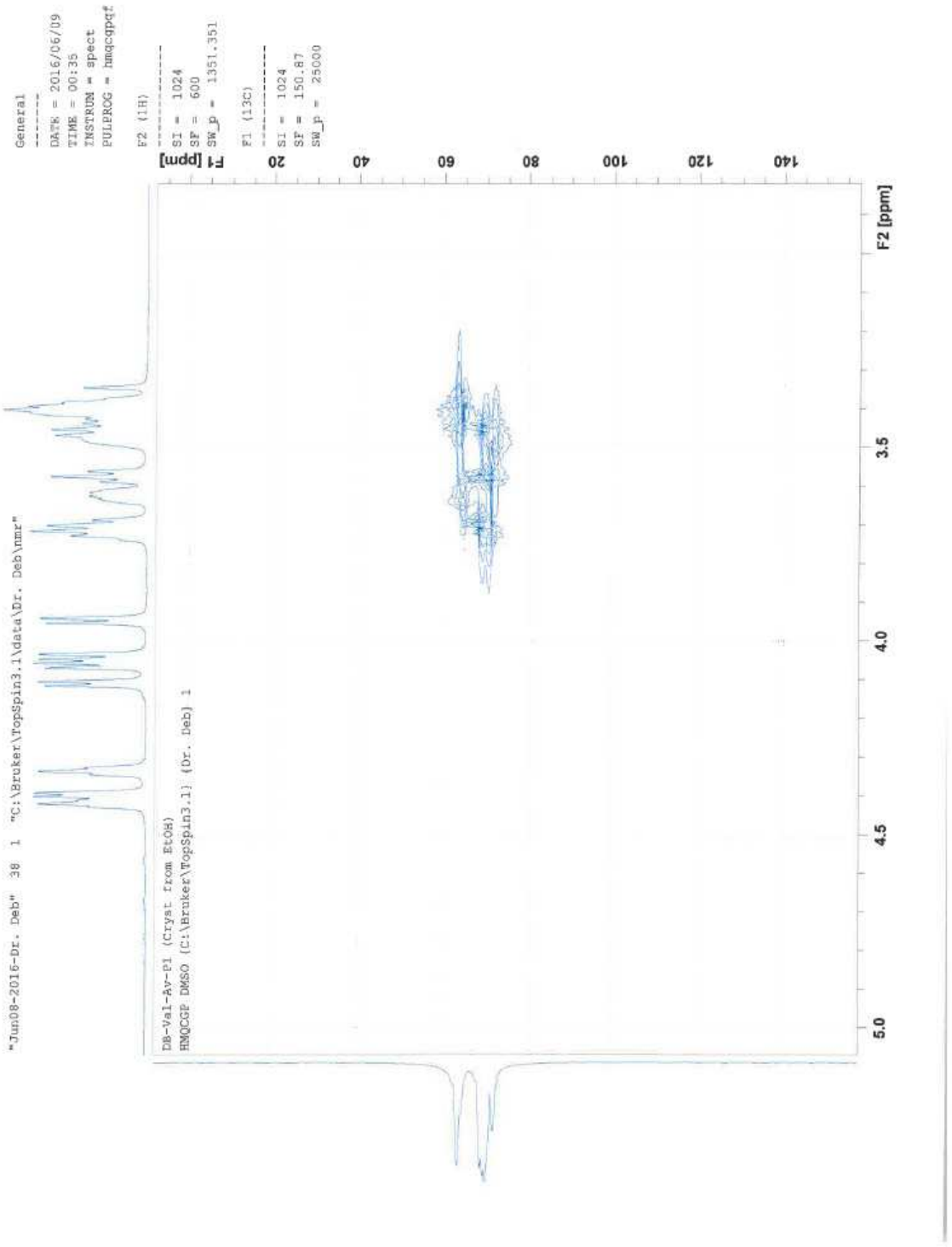


Figure 82. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMQCGP NMR 5

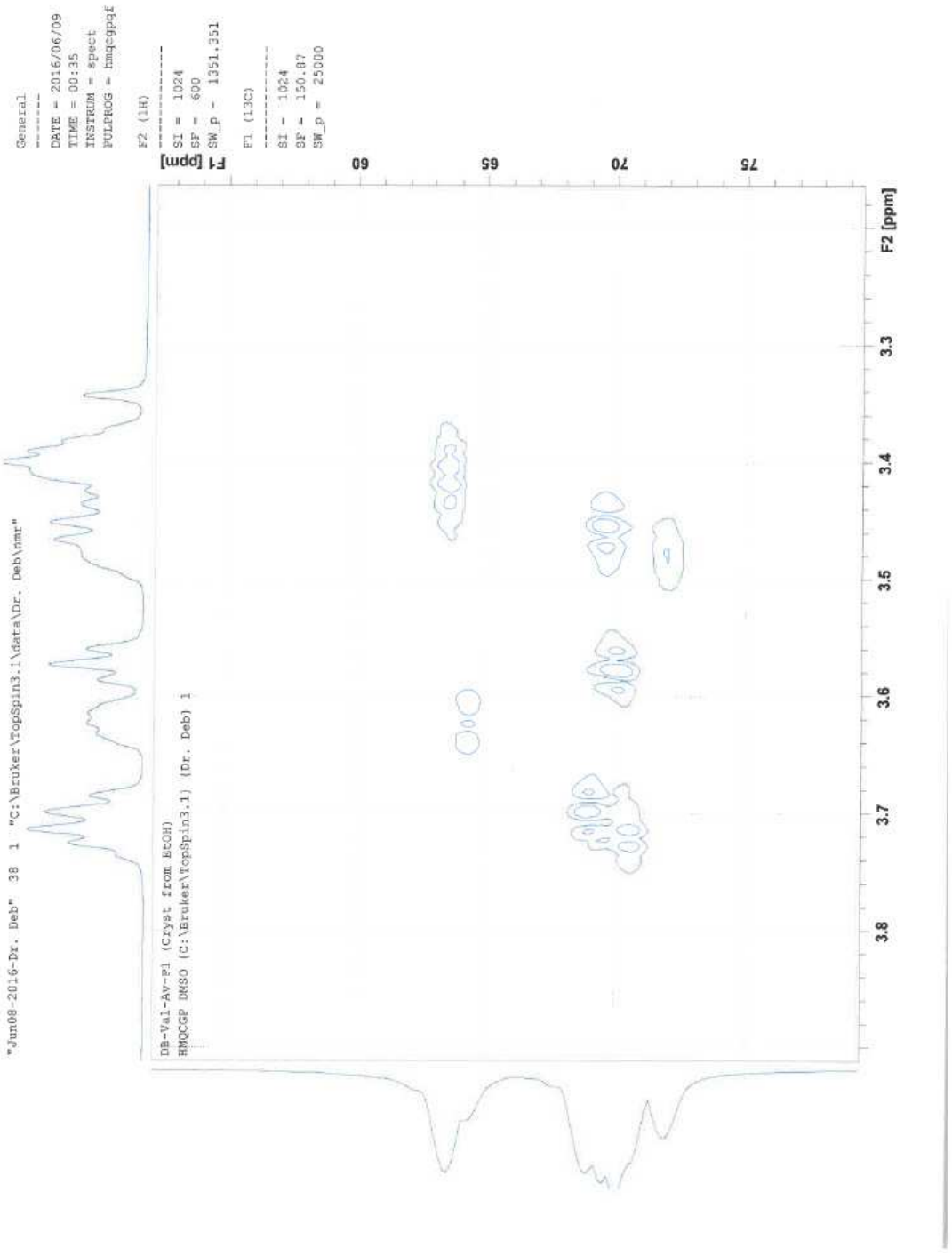


Figure 83. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HMQCGP NMR 6

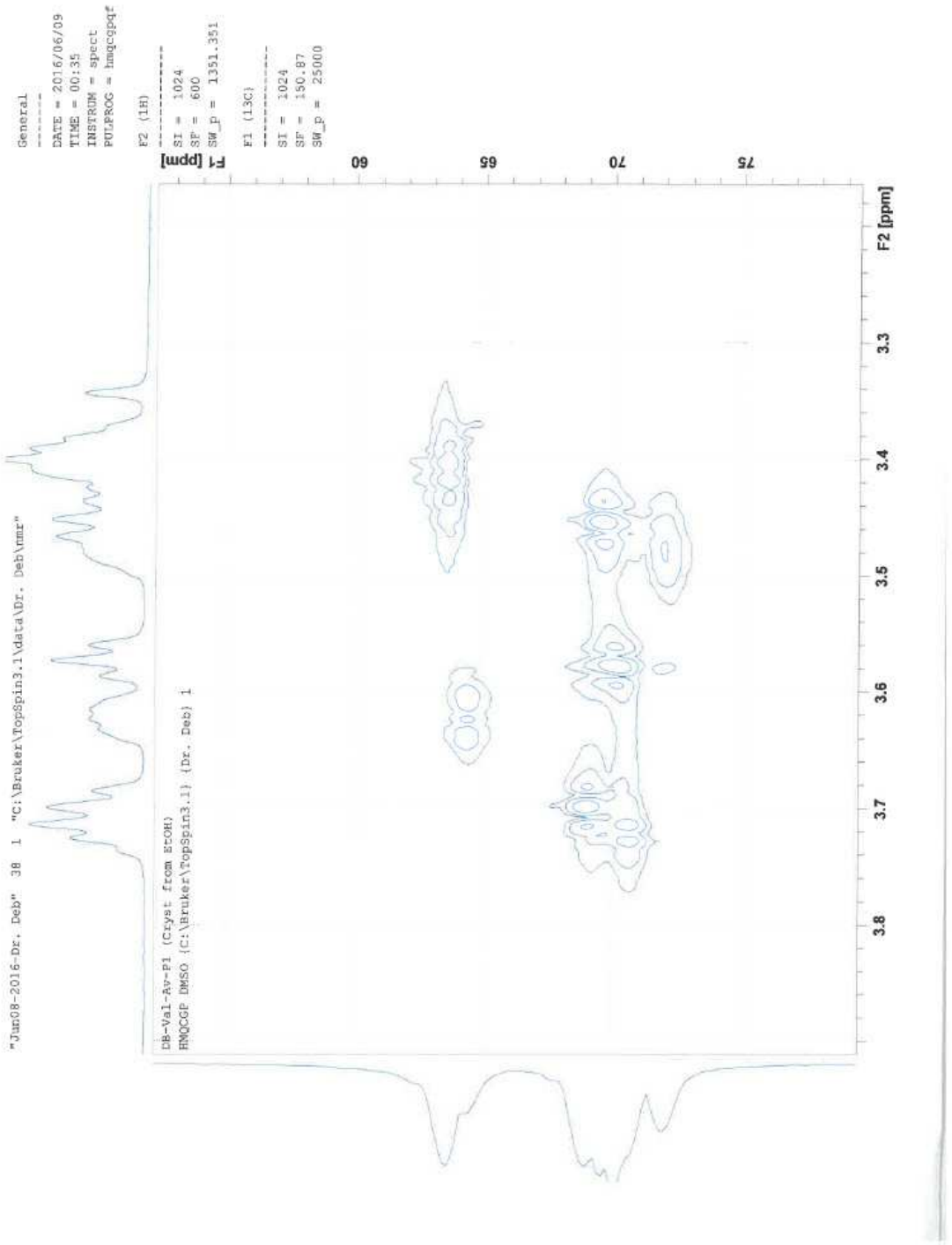
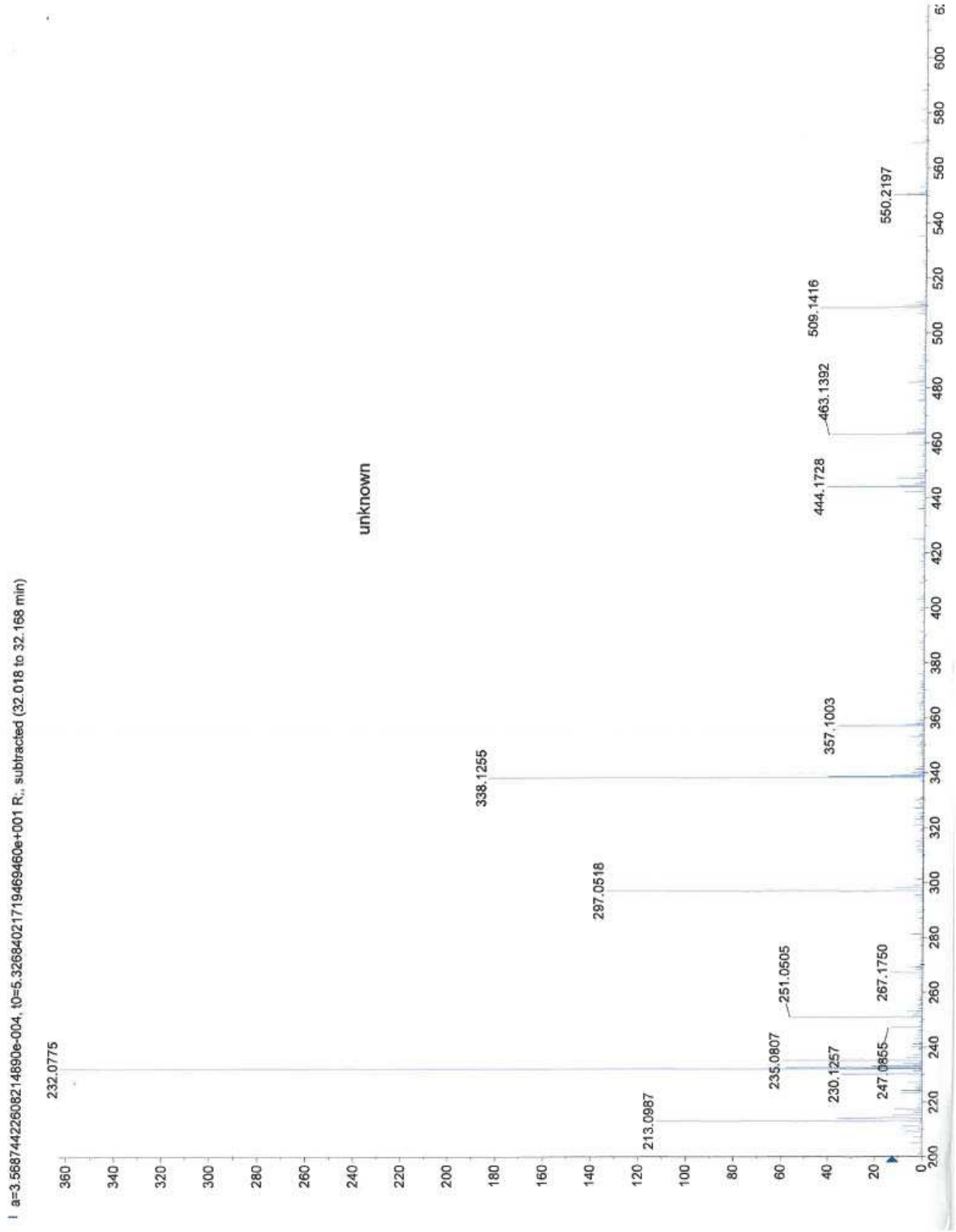


Figure 84. (4-ethenyloxane-2,3,5,6-tetrayl)tetramethanol HRMS



BIOGRAPHICAL SKETCH

Orlando A. Castillo Scheren finished high school at the Science Academy of South Texas Independent School District in the spring of 2013 in which he started his undergrad during the fall of 2013 at the University of Texas-Pan America. In 2015, he later enrolled in the University of Texas Rio Grande Valley in which he completed his B.S. Chemistry in the Fall of 2018. During this time Orlando A. Castillo Scheren joined the Elliott Chemical Society (ECS) in which he later became the Vice President of the Club; while in ECS he would go to different schools/charity events around the Valley and perform "magic shows" for children at the expense of the society. In 2017 he would proceed to do a press release at the American Chemical Society on his project "Chemical Investigation of the Avocado (*Persea americana*) Seed Husk: A Waste of Waste" in which he would show his initial findings on the project. In 2020, Orlando A. Castillo Scheren would complete his Thesis project "Chemical Investigation of the Avocado (*Persea americana*) Seed Husk (Testa): A Waste of Waste" and be awarded his M.S. Chemistry.

Email: orlando.castillo21@gmail.com

3001 Iris Avenue, McAllen Tx 78501