

## Supplementary Materials-2 for

# Oxo-carotenoids as Efficient Superoxide Radical Scavengers

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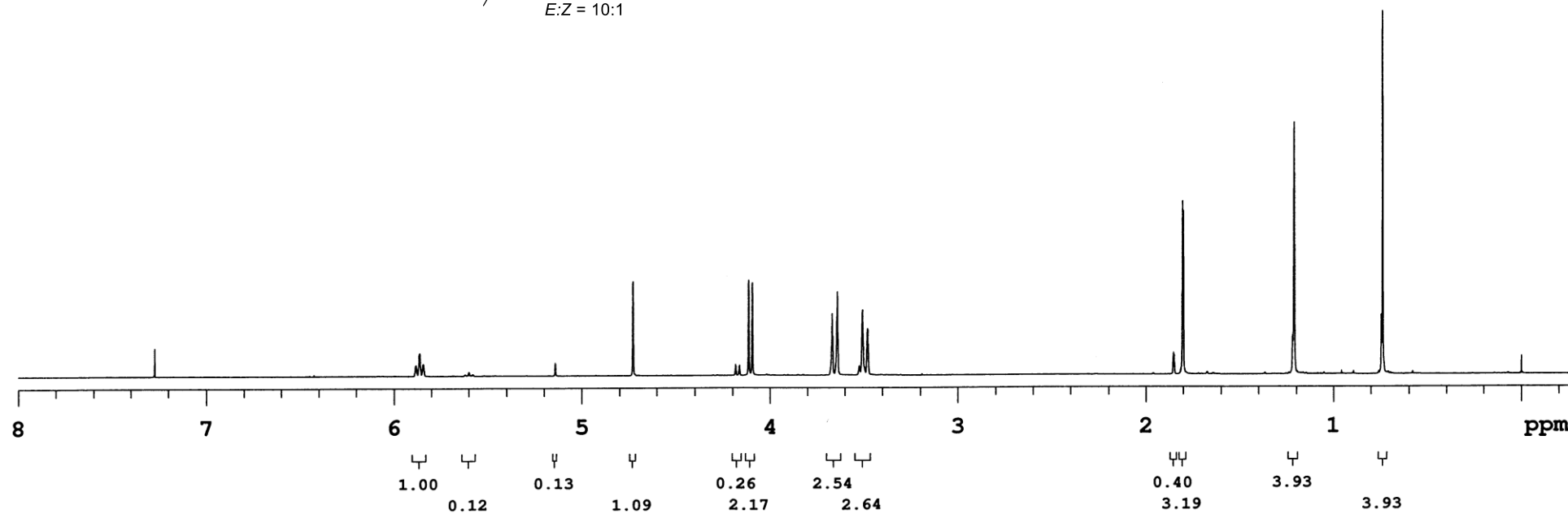
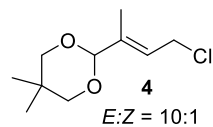
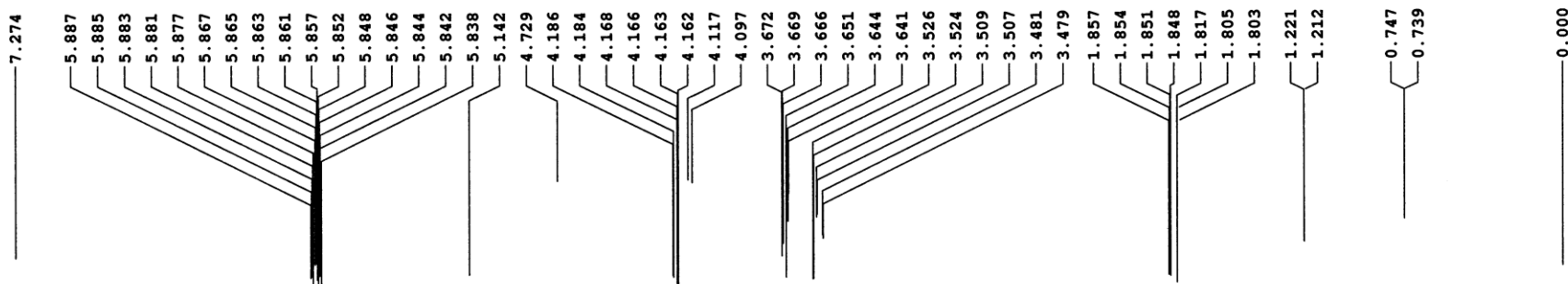
# (1) <sup>1</sup>H- and <sup>13</sup>C-NMR Spectra

SGS-1354-1

Sample Name **SGS-1354-1**  
Date collected **2021-05-13**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



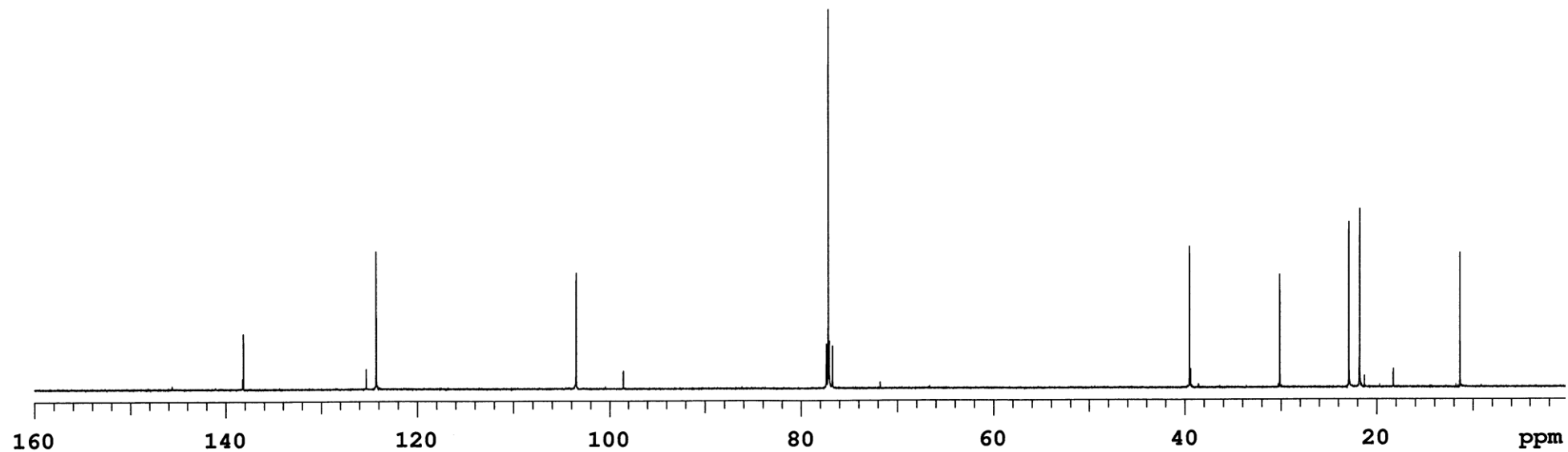
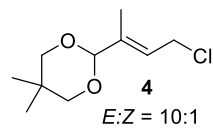
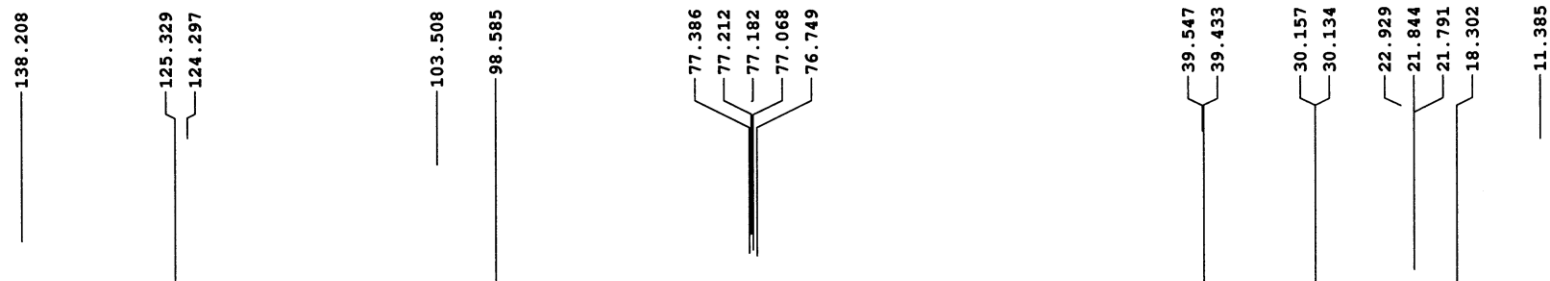
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Sample Name **SGS-1354-1-13C**  
Date collected **2021-05-17**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



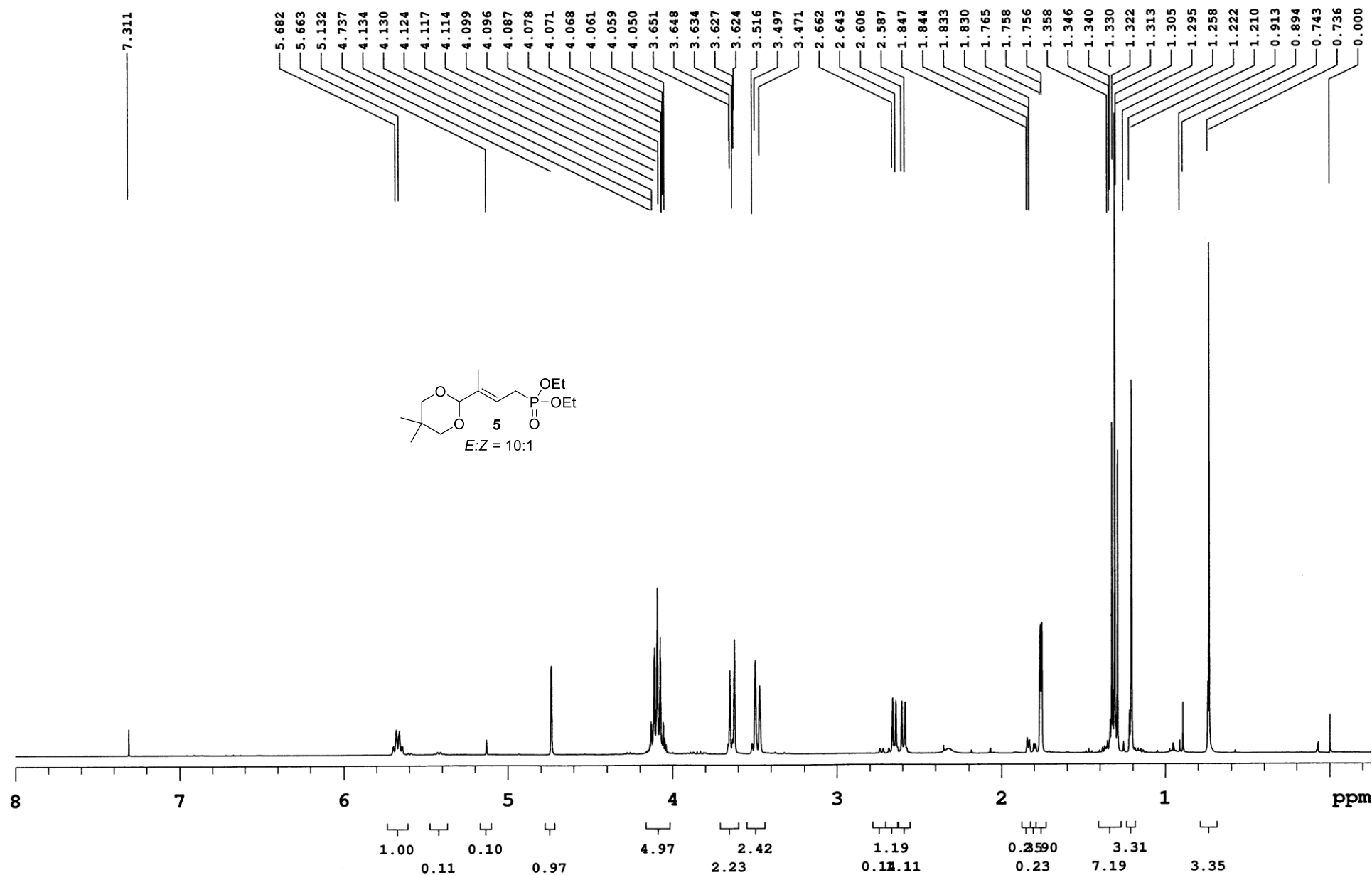
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Date collected **2021-11-09**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs4000**

Study owner **vnmr1**  
Operator **vnmr1**





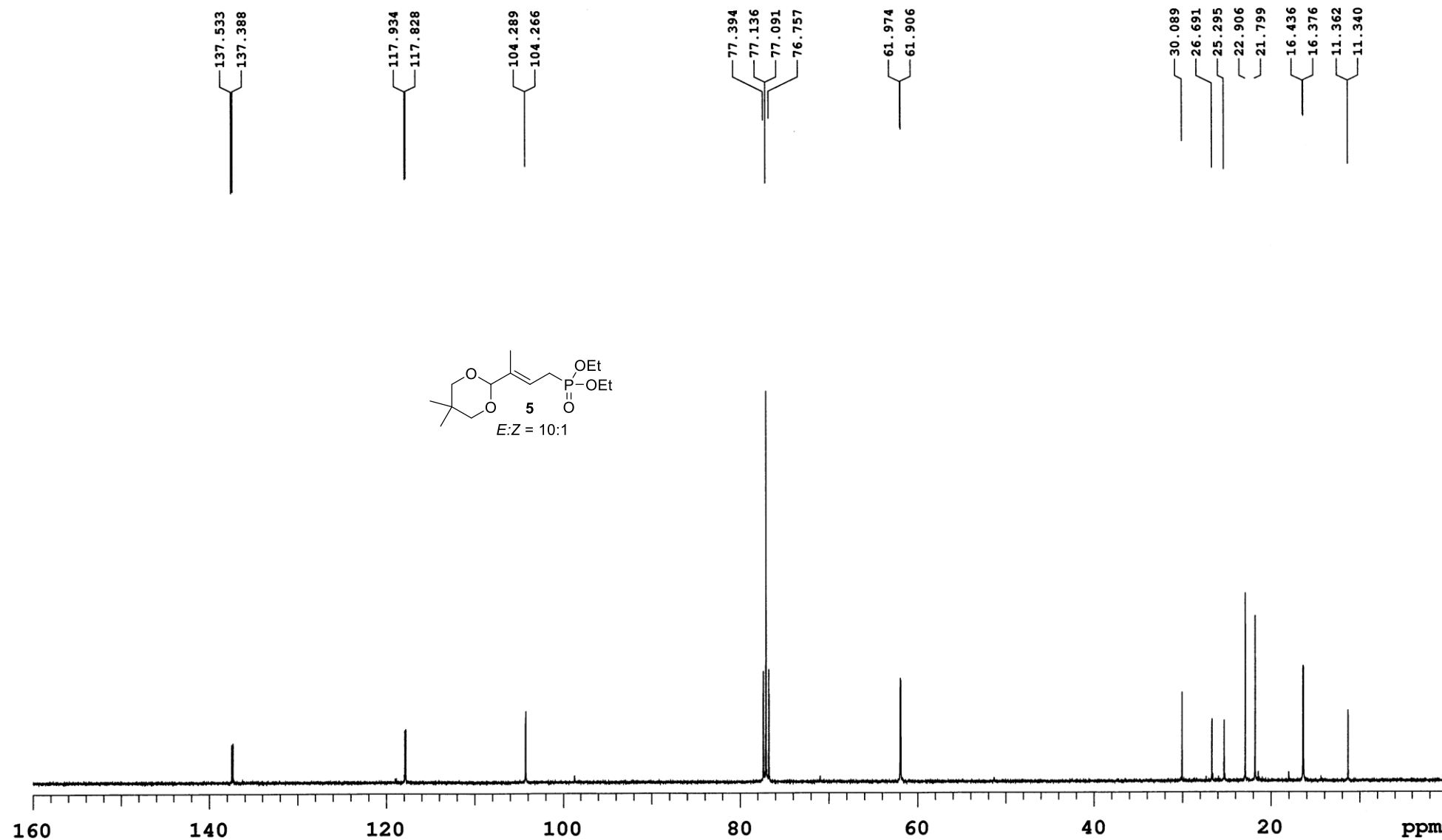
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Sample Name **SGS-1540-11-13C**  
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Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



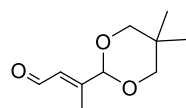
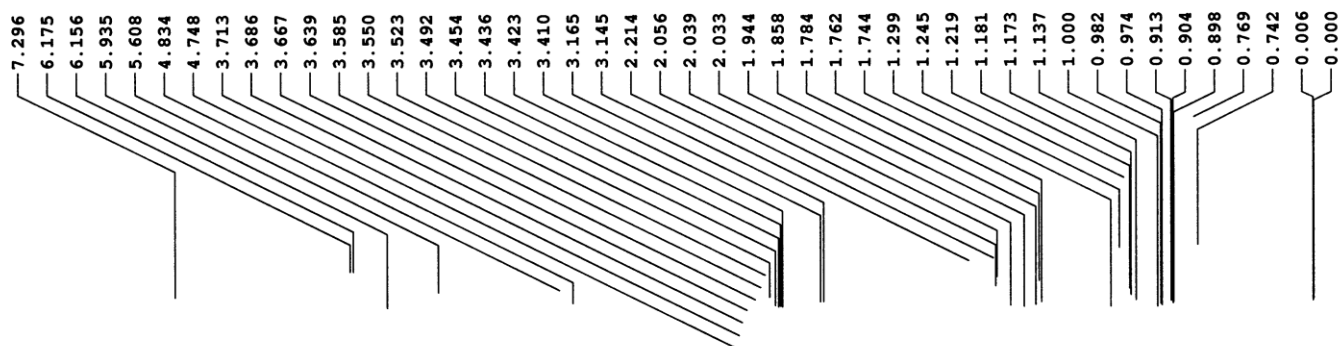
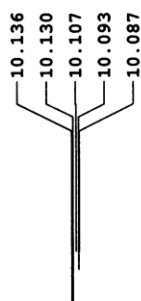
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Sample Name **SGS-1621-2**  
Date collected **2021-11-10**

Pulse sequence **PROTON**  
Solvent **cdcl3**

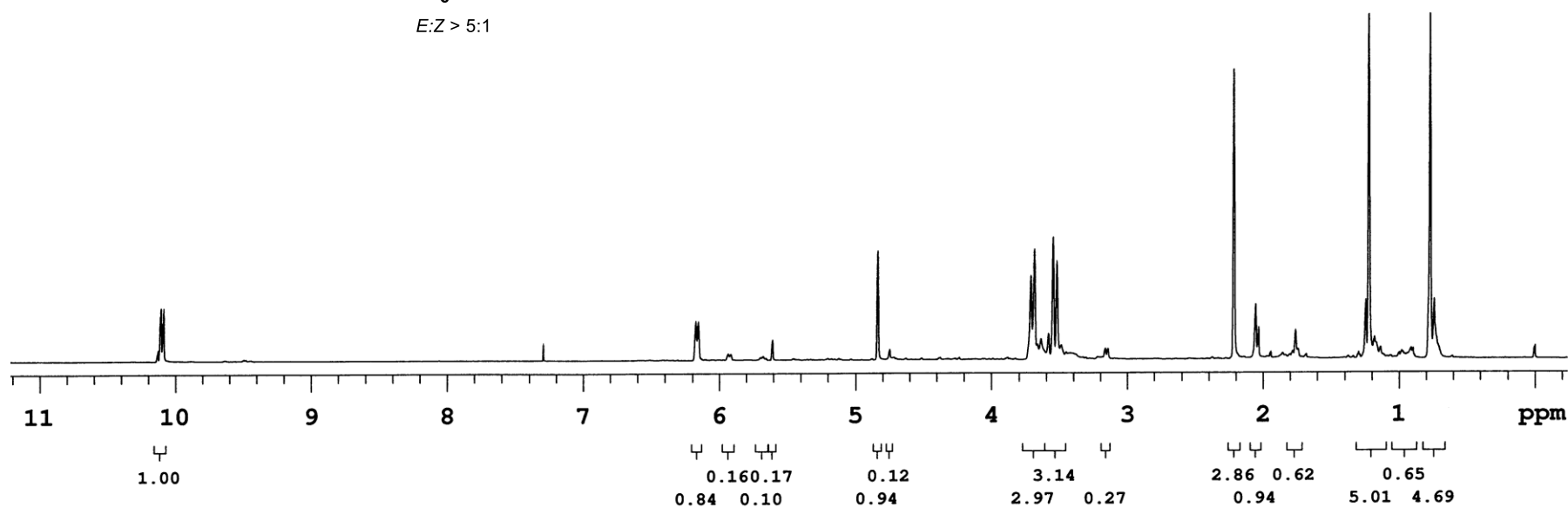
Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



**6**

*E:Z* > 5:1

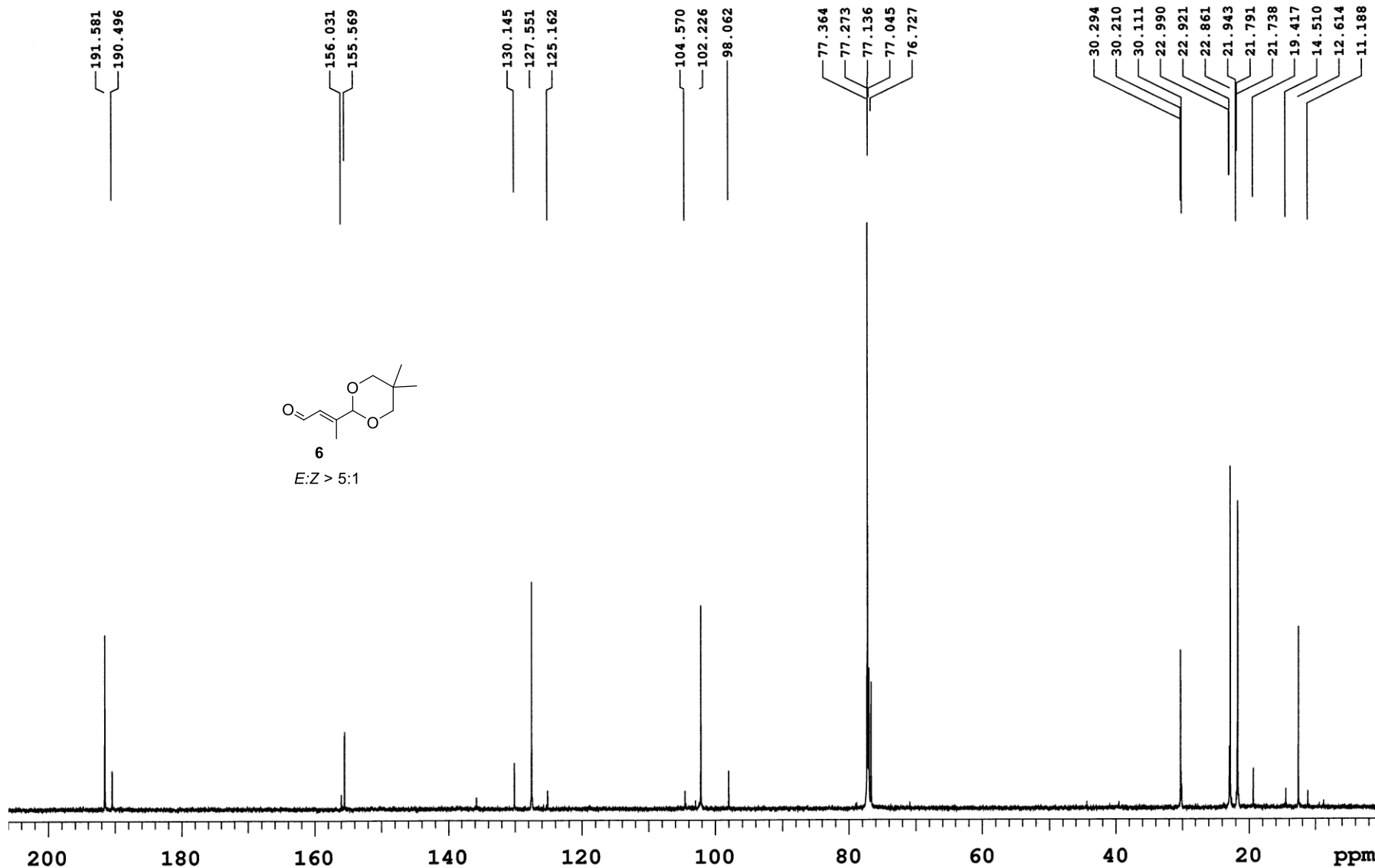


SGS-1621-2

Sample Name **SGS-1621-2**  
Date collected **2021-11-12**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**

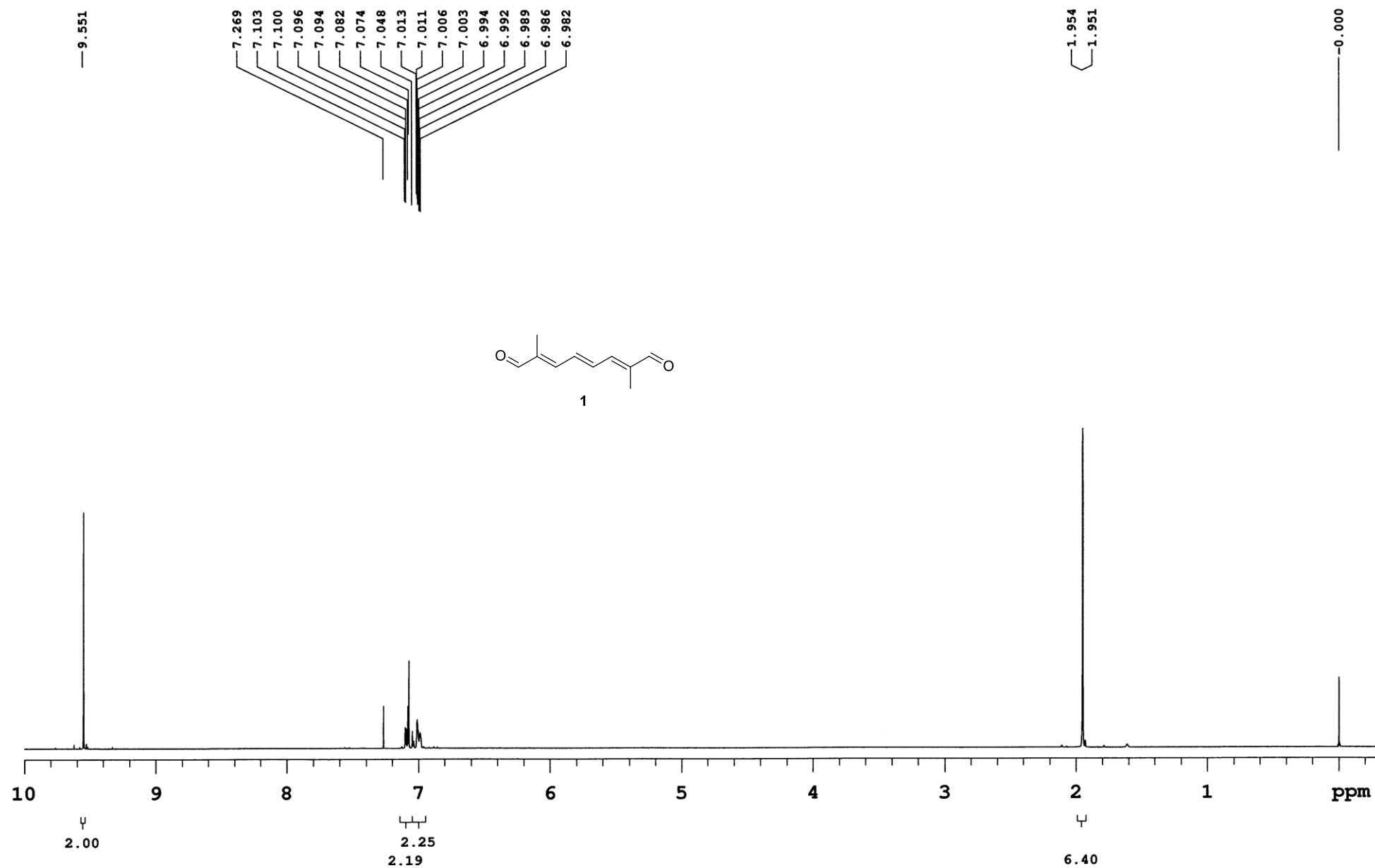


SGS-1541-21re

Sample Name **SGS-1541-21re**  
Date collected **2021-10-12**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**

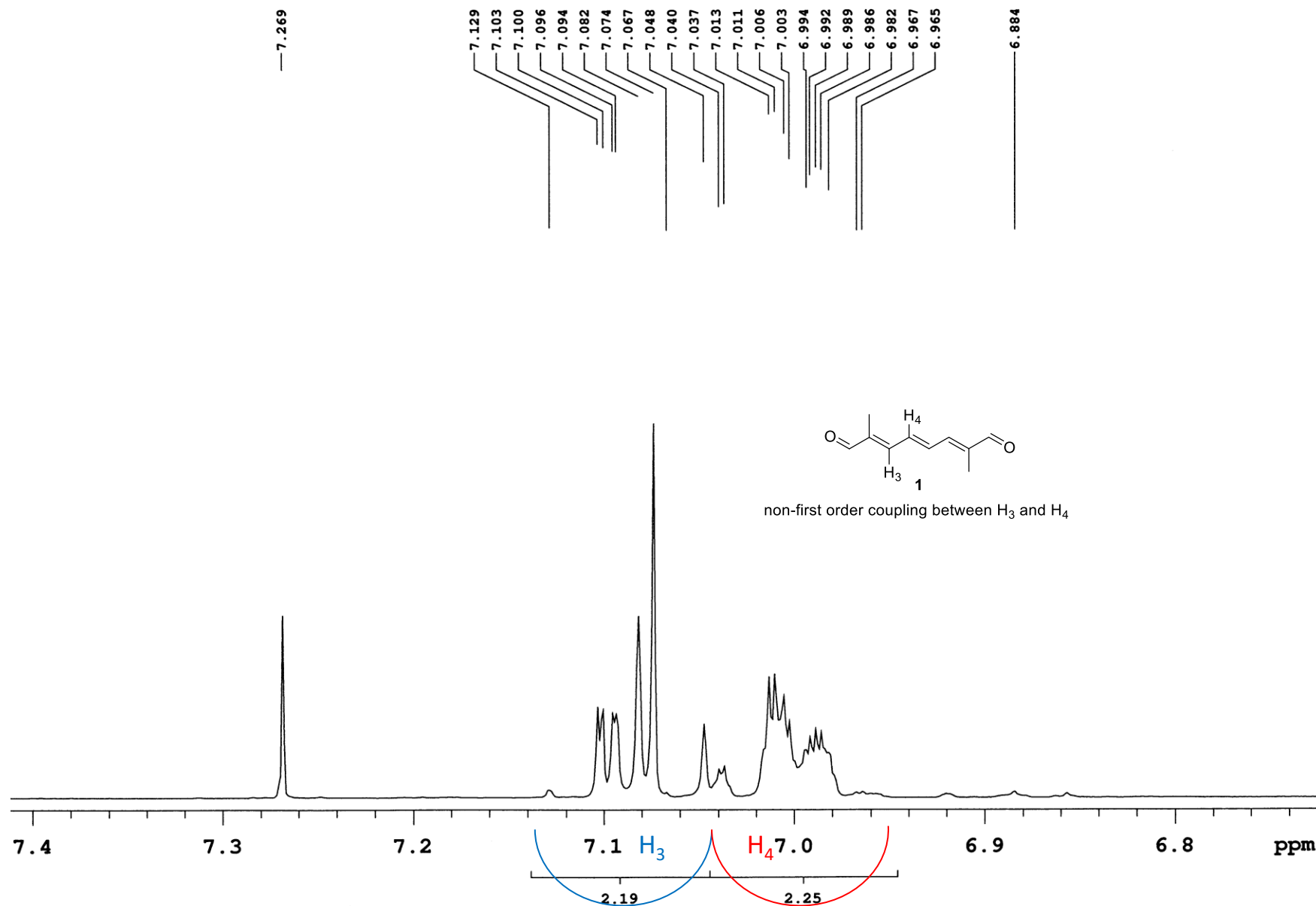


SGS-1541-21re

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Date collected **2021-10-12**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



SGS-1412-C20

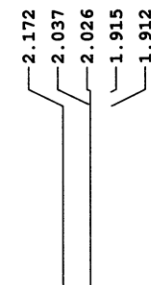
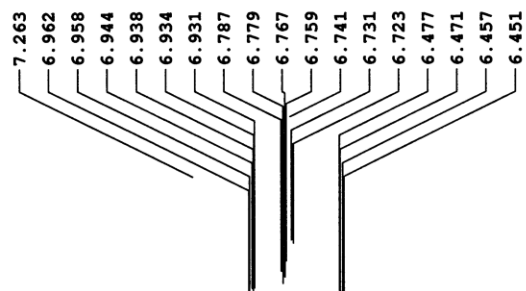
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Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

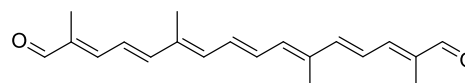
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Operator **vnmr1**

9.470

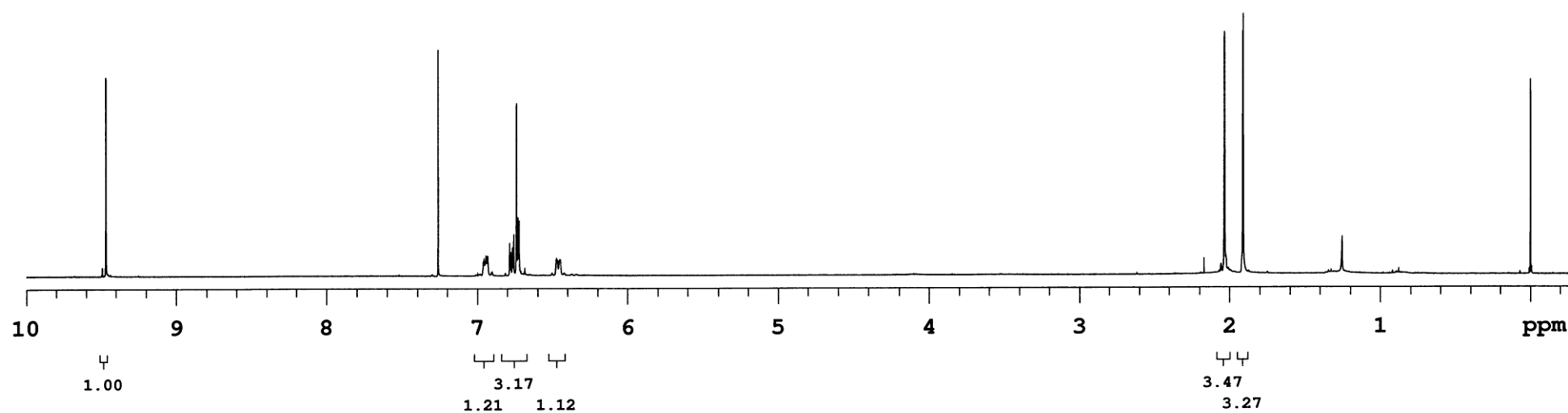


1.254

0.000



2



SGS-1412-C20

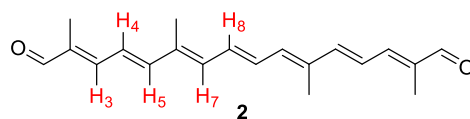
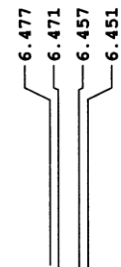
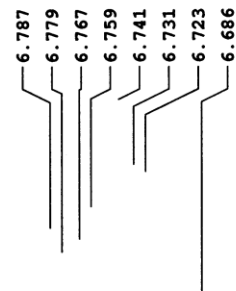
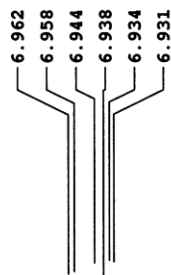
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Pulse sequence **PROTON**  
Solvent **cdcl3**

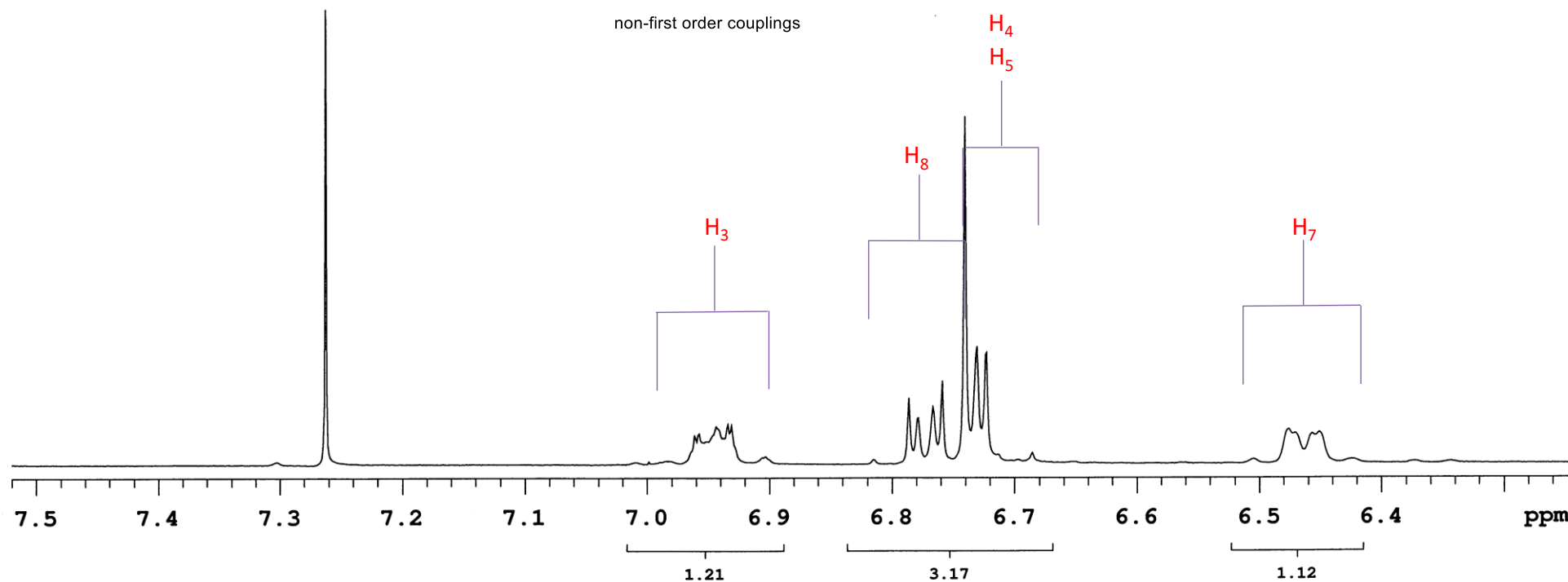
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Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**

— 7.263



non-first order couplings

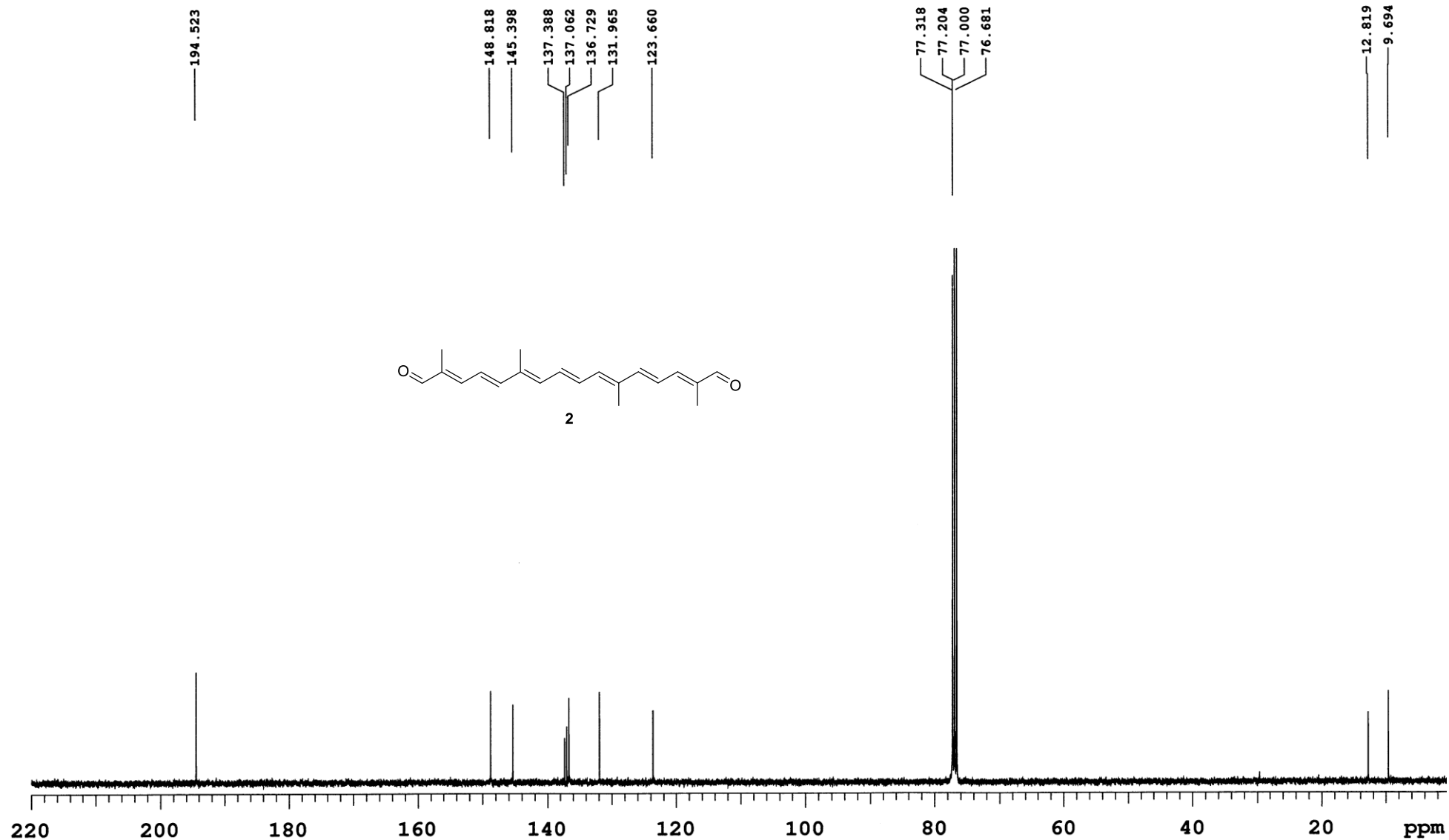


SGS-1412-C20-13C

Sample Name **SGS-1412-C20-13C**  
Date collected **2021-11-17**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**





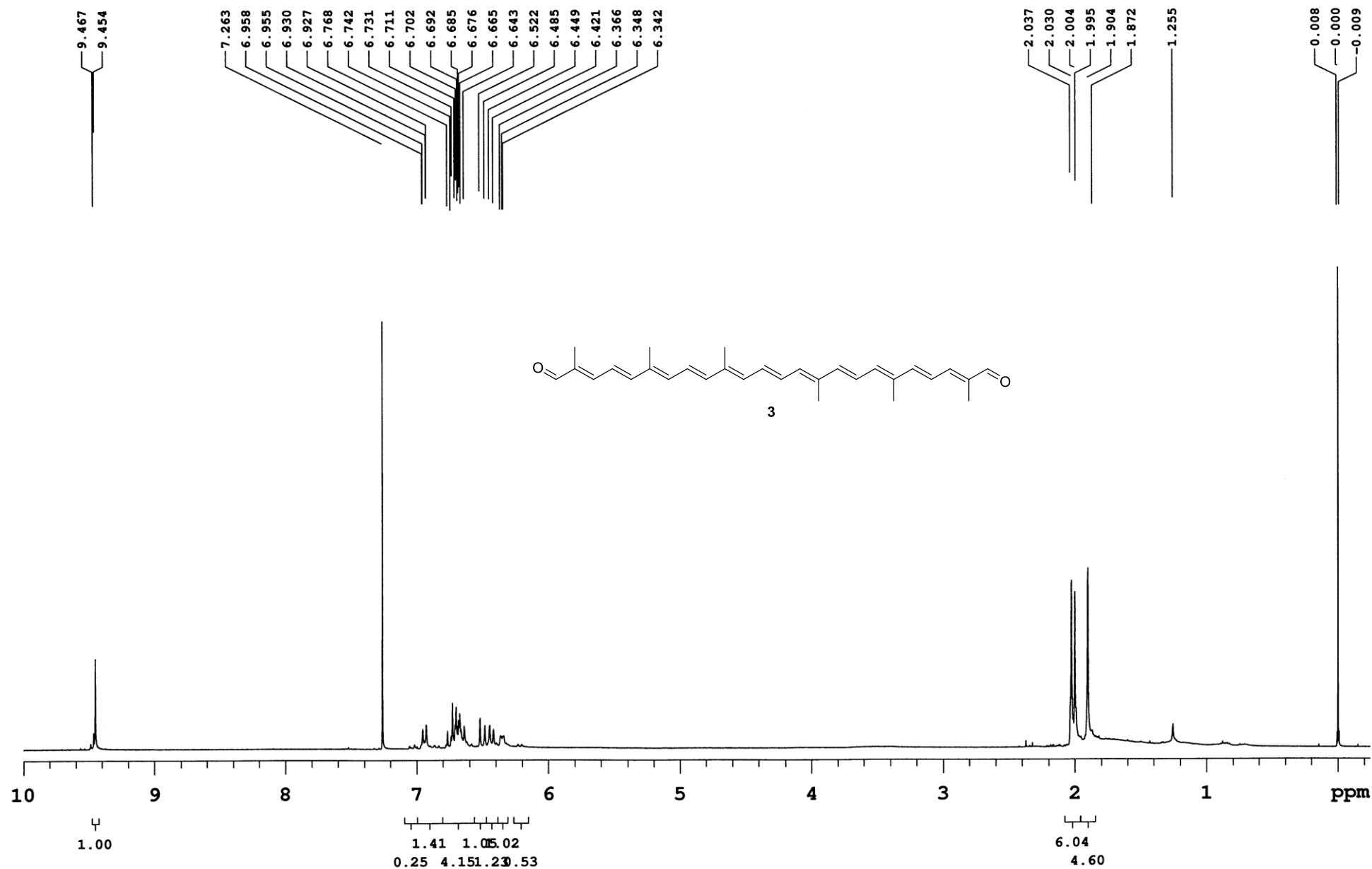
SGS-1492-23re

Sample Name **SGS-1492-23re**  
Date collected **2021-07-05**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**



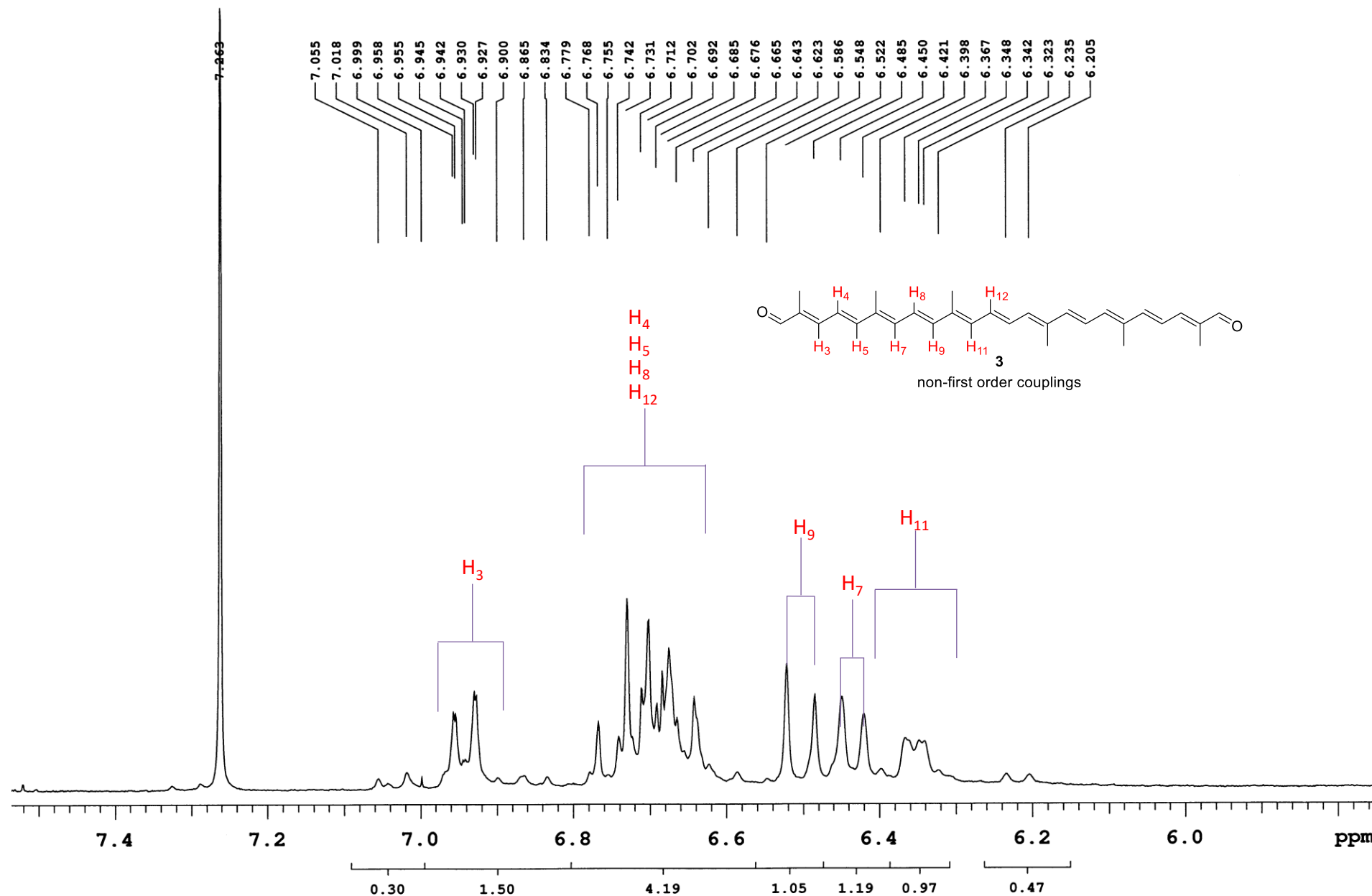
SGS-1492-23re

Sample Name **SGS-1492-23re**  
Date collected **2021-07-05**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**

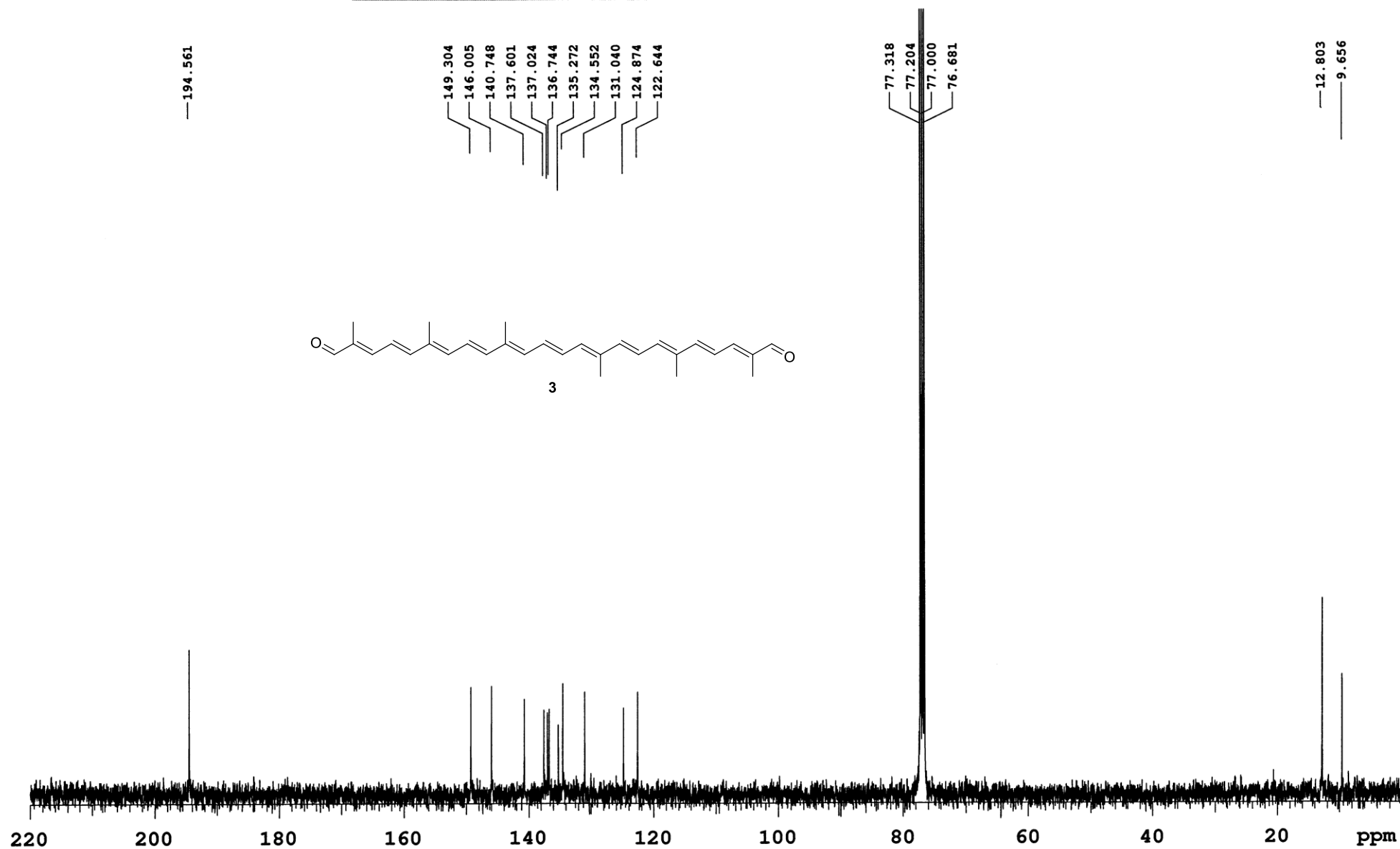


SGS-1492-23re

Sample Name **SGS-1492-23re**  
Date collected **2021-07-02**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs4000**  
Study owner **vnmr1**  
Operator **vnmr1**

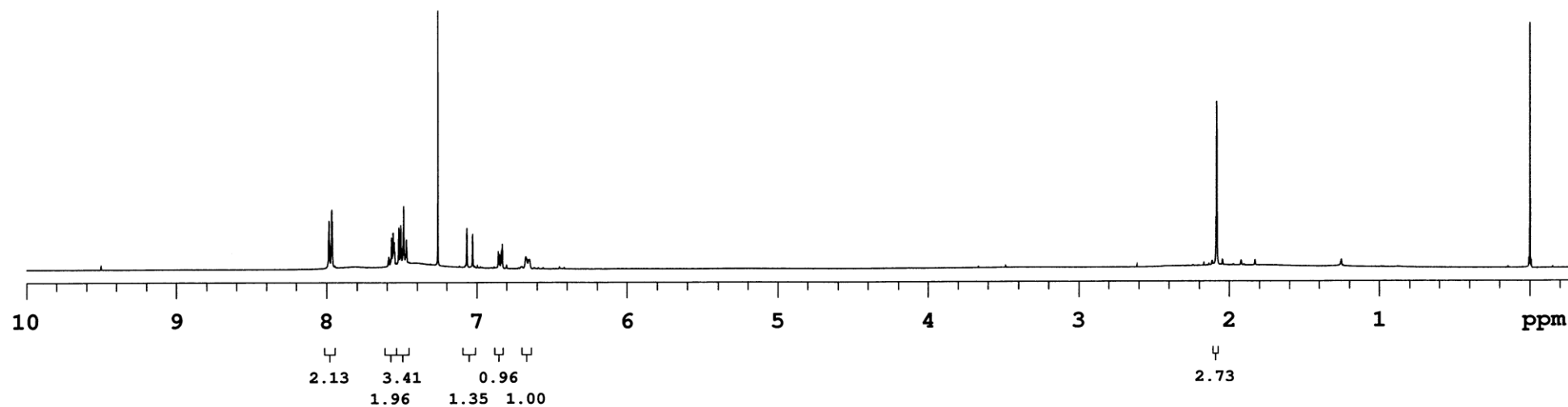
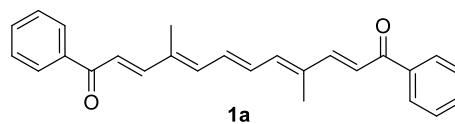
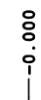
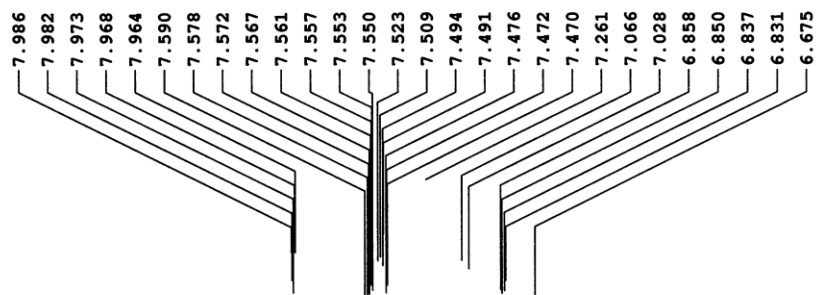


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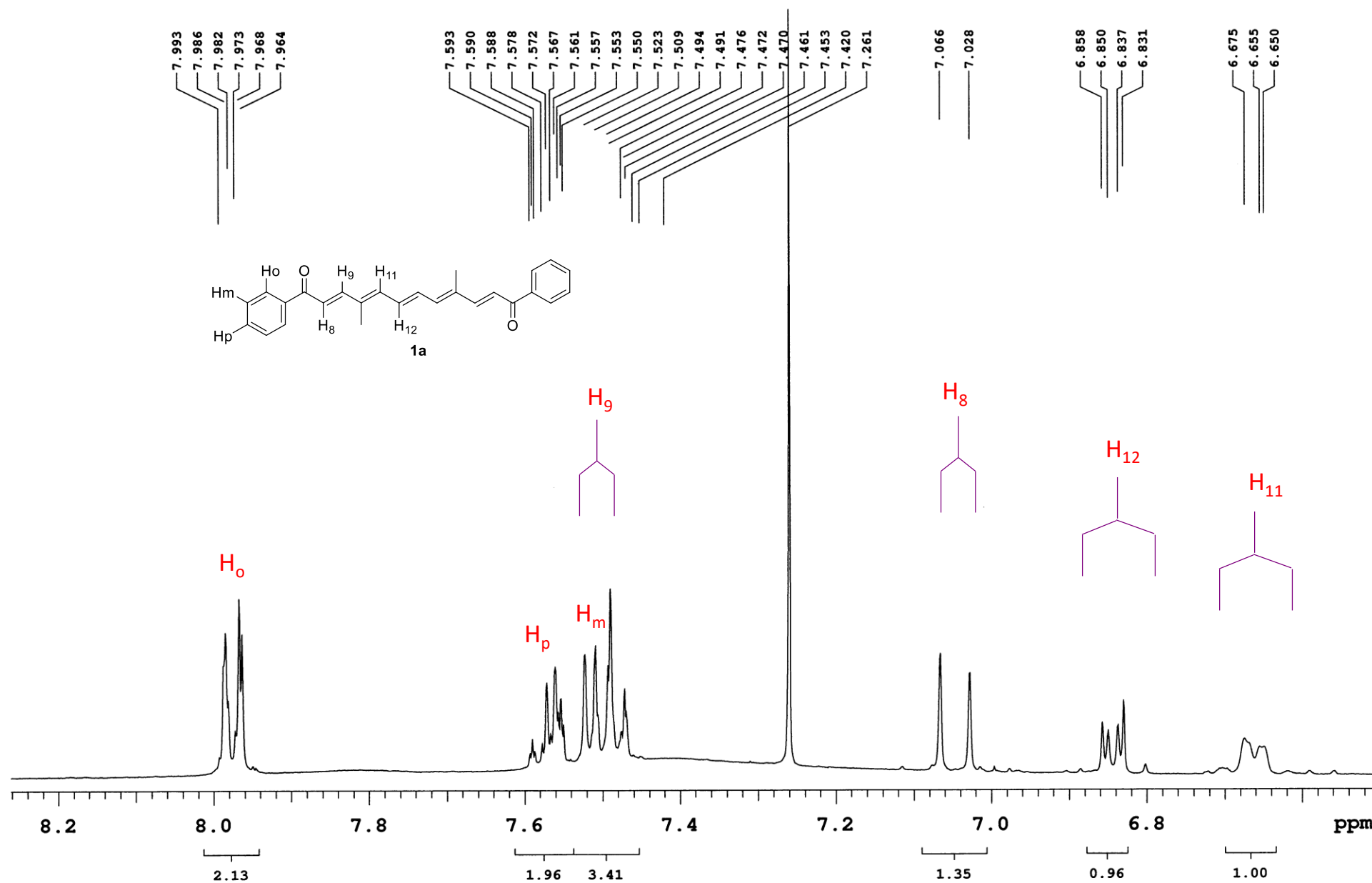
Sample Name **SGS-1332-1re**  
Date collected **2021-06-02**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



SGS-1332-1re

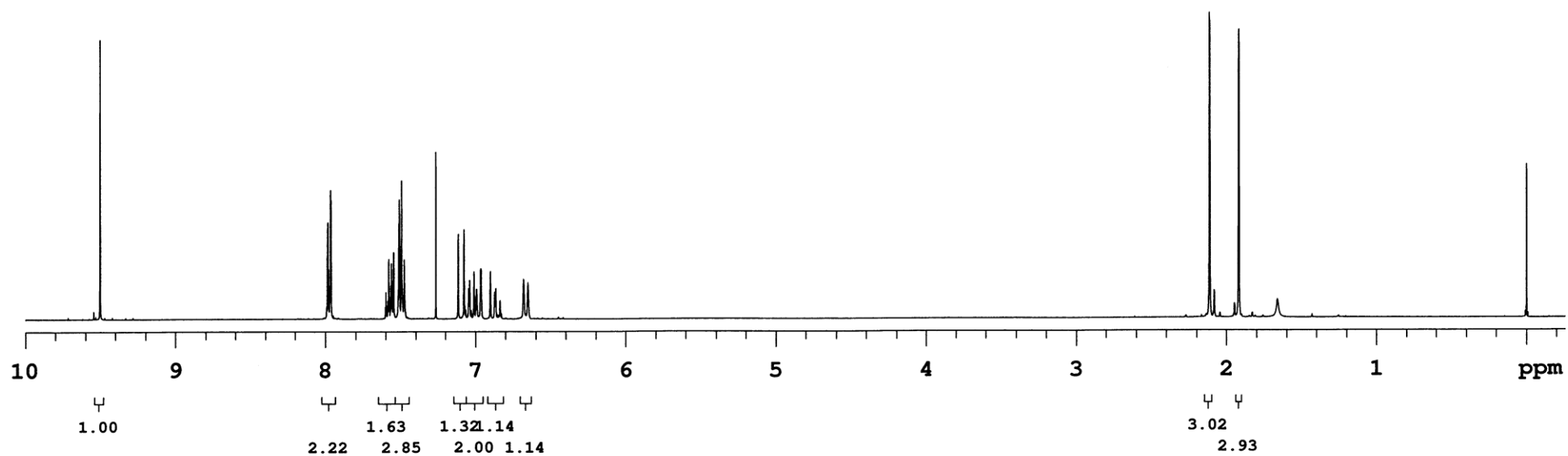
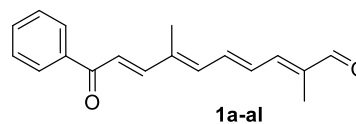
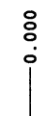
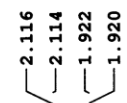
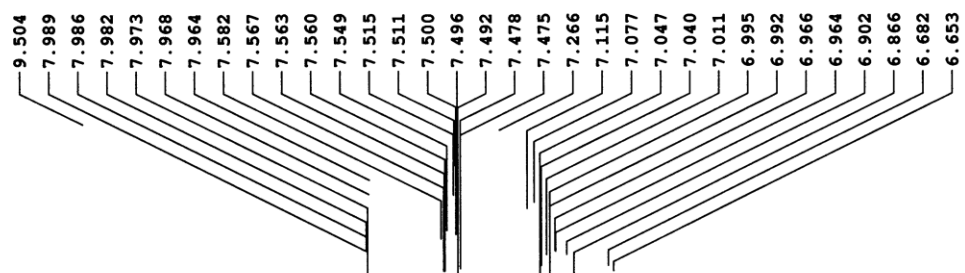
Sample Name **SGS-1332-1re**  
Date collected **2021-06-02**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**Study owner **vnmr1**  
Operator **vnmr1**

SGS-1396-2re

Sample Name **SGS-1396-2re**  
Date collected **2021-06-16**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**



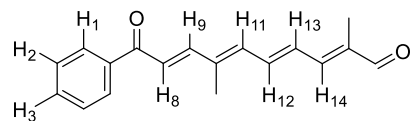
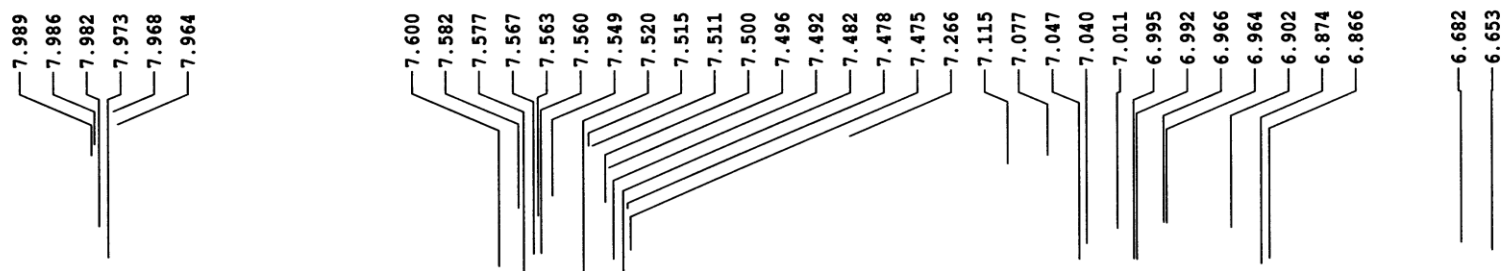
SGS-1396-2re

Sample Name **SGS-1396-2re**  
Date collected **2021-06-16**

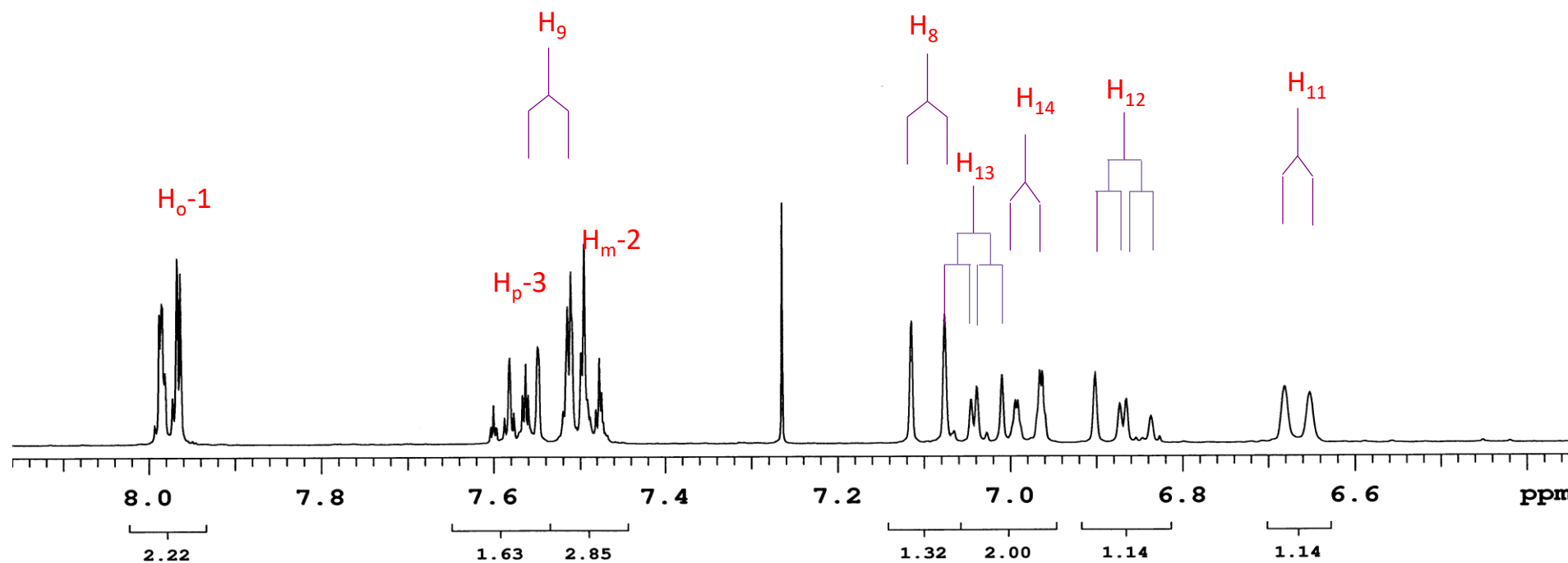
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**



1a-al



SGS-1396-2re-13C

Sample Name **SGS-1396-2re-13C**  
Date collected **2021-06-18**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

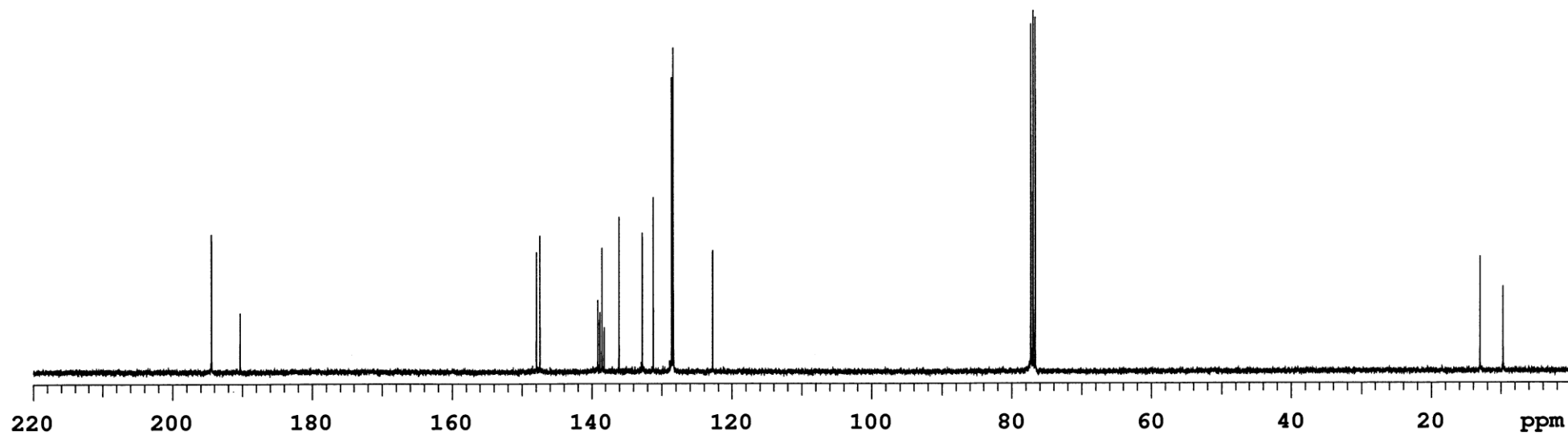
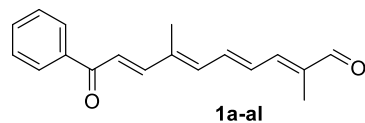
Study owner **vnmr1**  
Operator **vnmr1**

194.470  
190.375

147.977  
147.476  
139.156  
138.867  
138.564  
138.238  
136.099  
132.777  
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128.621  
128.401  
122.811

77.341  
77.022  
76.704

13.061  
9.777





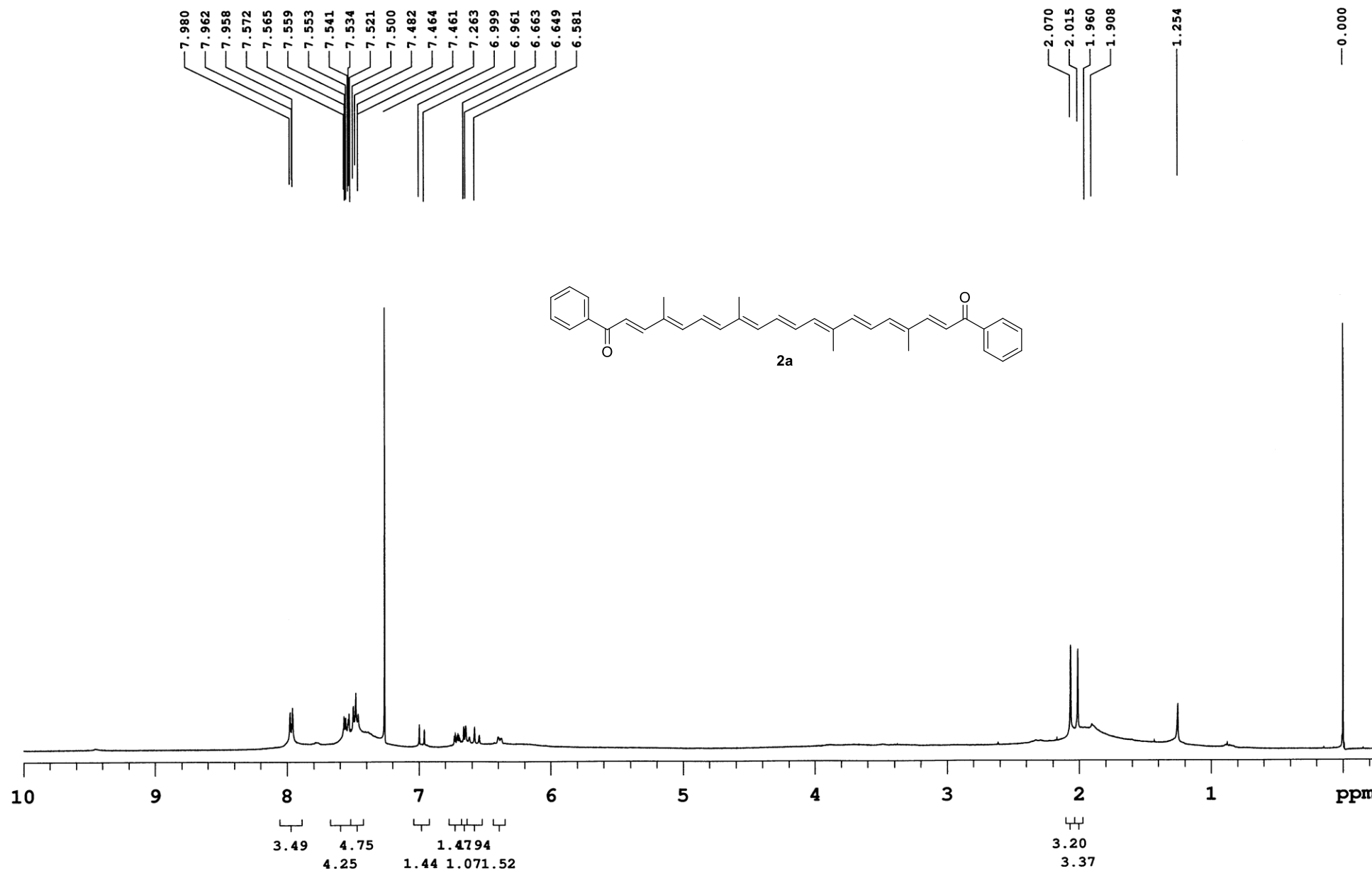
SGS-1420-12re

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Date collected **2021-06-14**

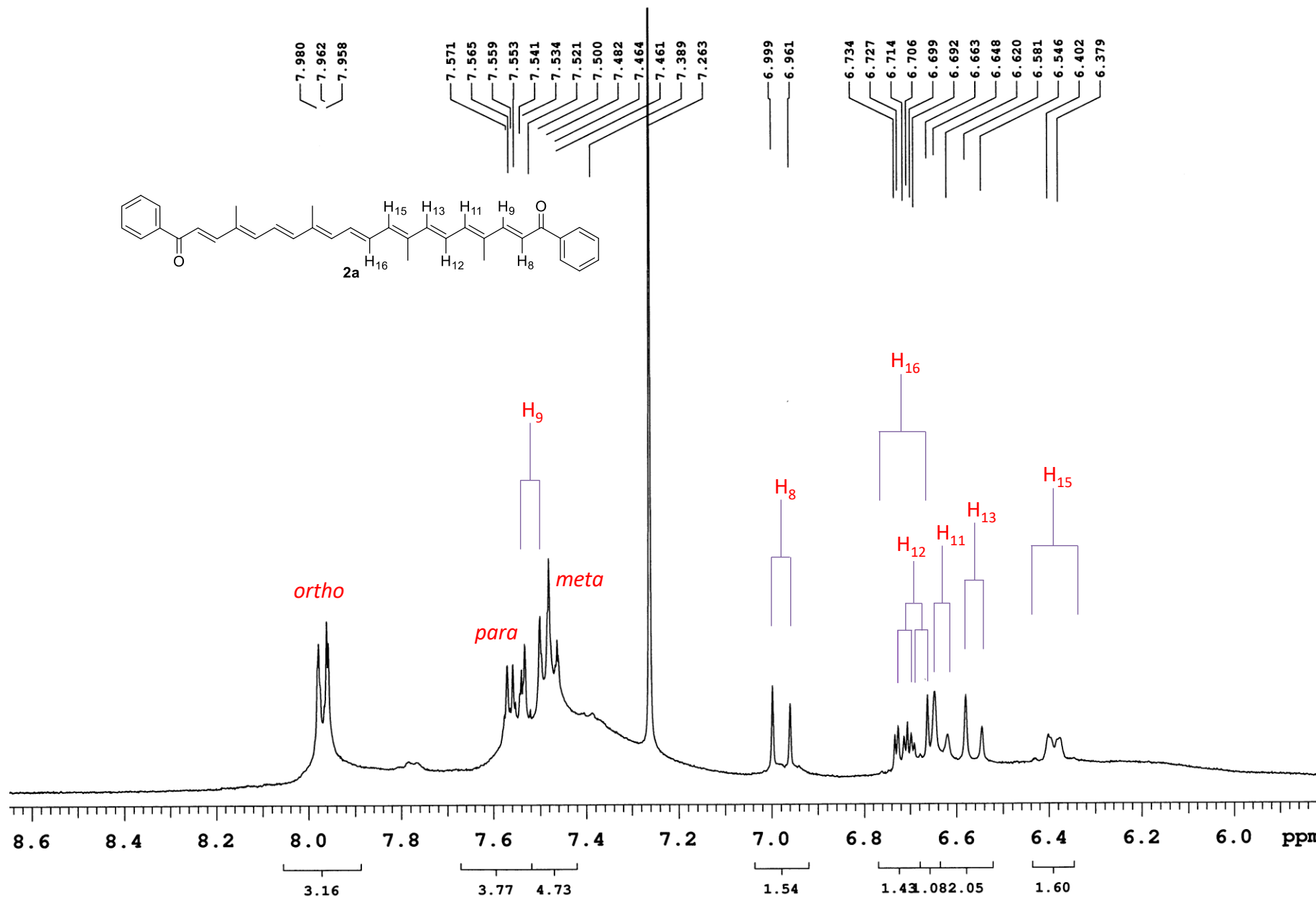
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

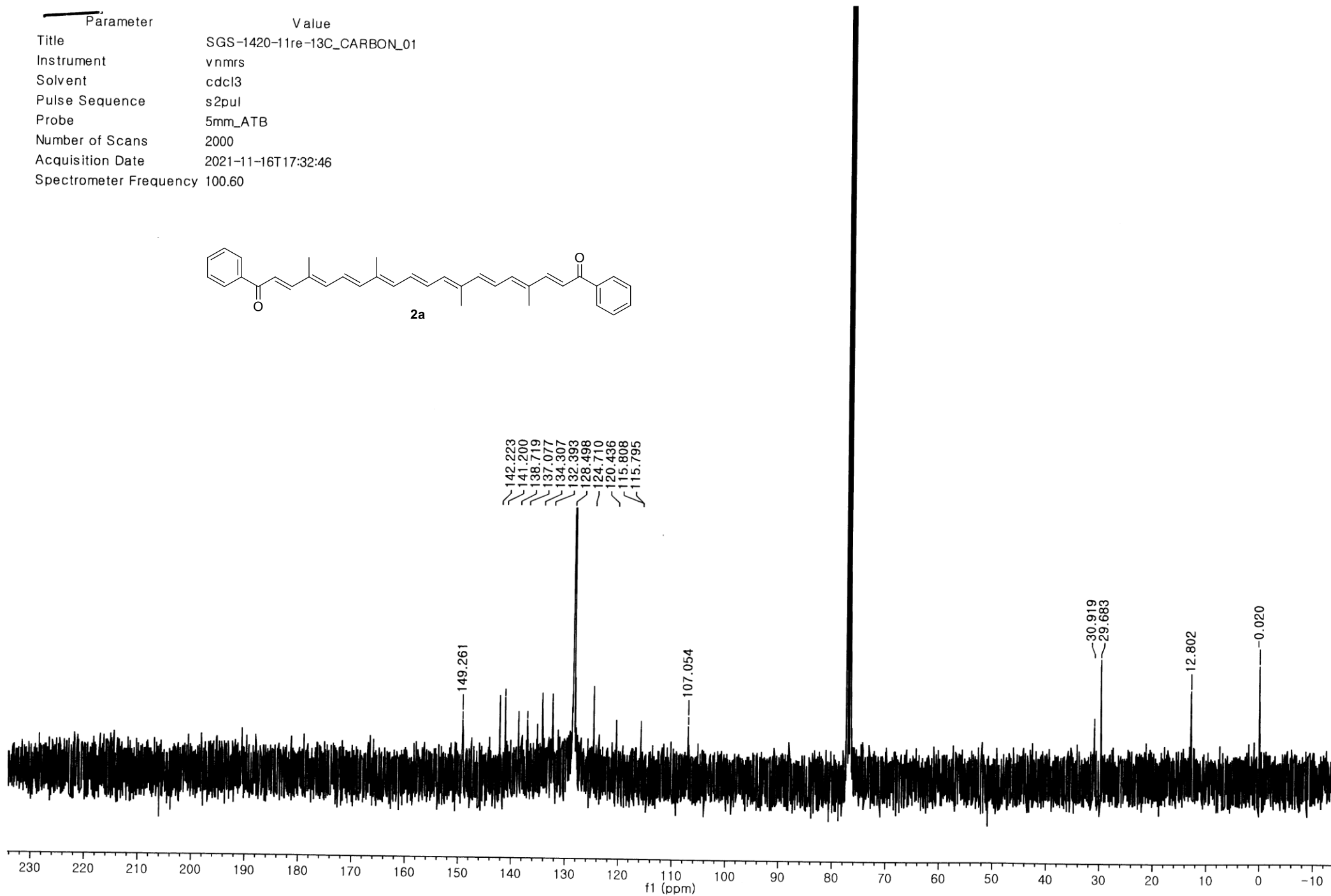
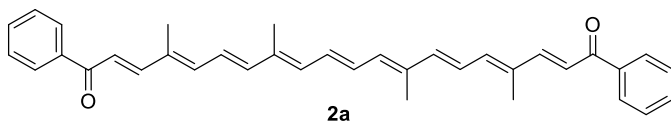
Study owner **vnmr1**  
Operator **vnmr1**



SGS-1420-12re

Sample Name **SGS-1420-12re**  
Date collected **2021-06-14**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**

Parameter	Value
Title	SGS-1420-11re-13C_CARBO_01
Instrument	vnmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Probe	5mm_ATB
Number of Scans	2000
Acquisition Date	2021-11-16T17:32:46
Spectrometer Frequency	100.60



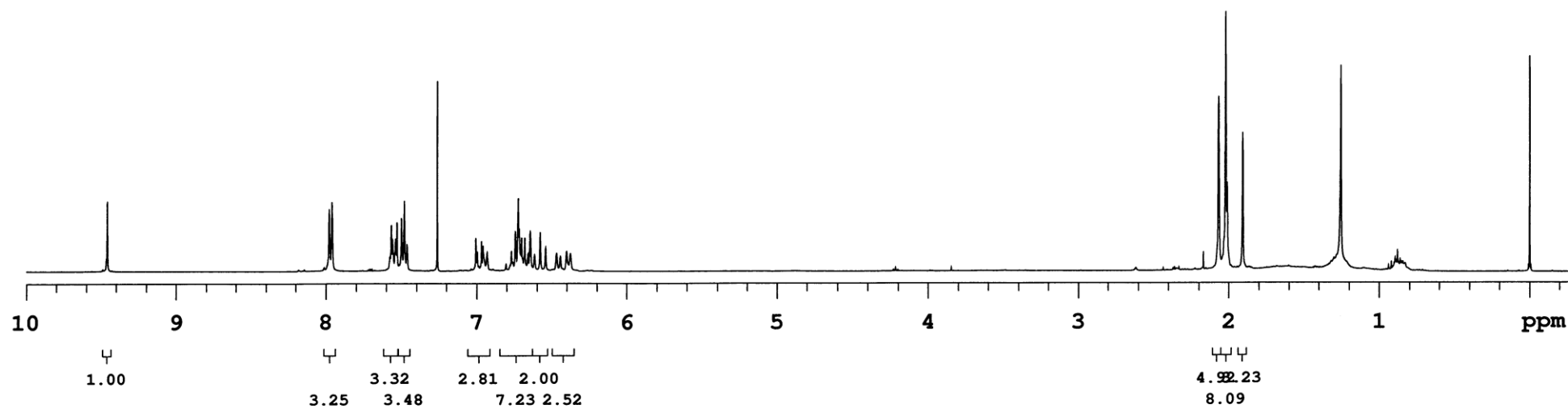
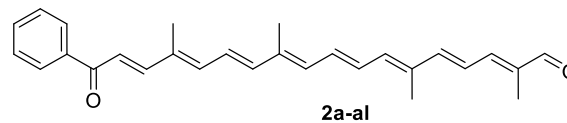
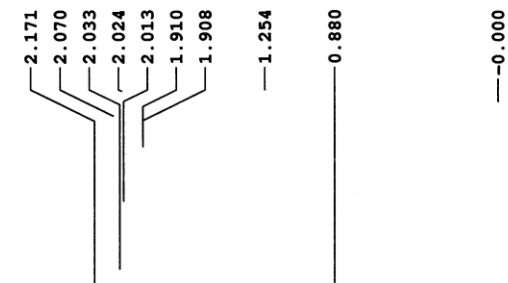
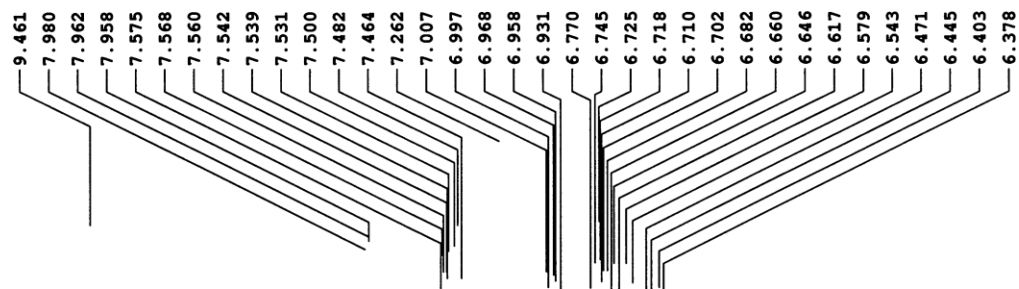
SGS-1421-11re

Sample Name **SGS-1421-11re**  
Date collected **2021-11-16**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



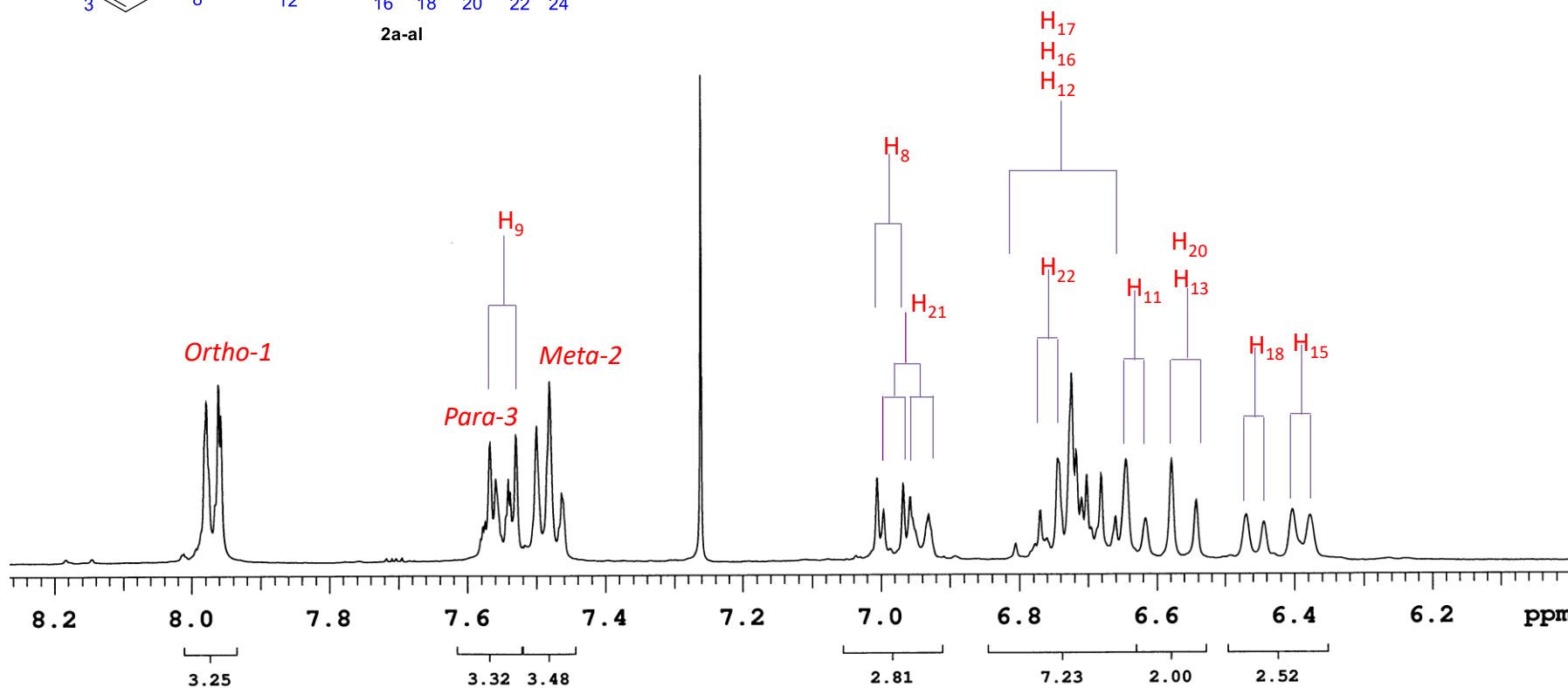
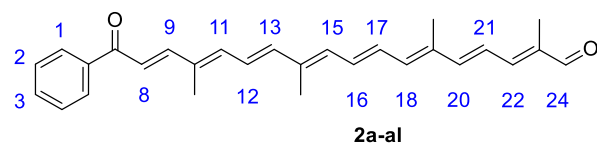
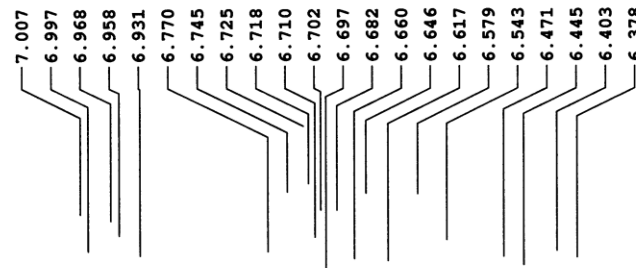
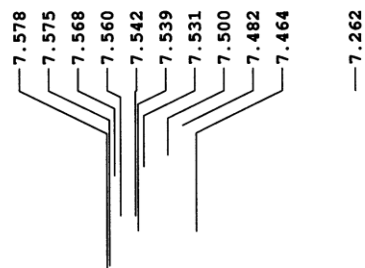
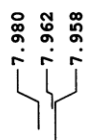
SGS-1421-11re

Sample Name **SGS-1421-11re**  
Date collected **2021-11-16**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**



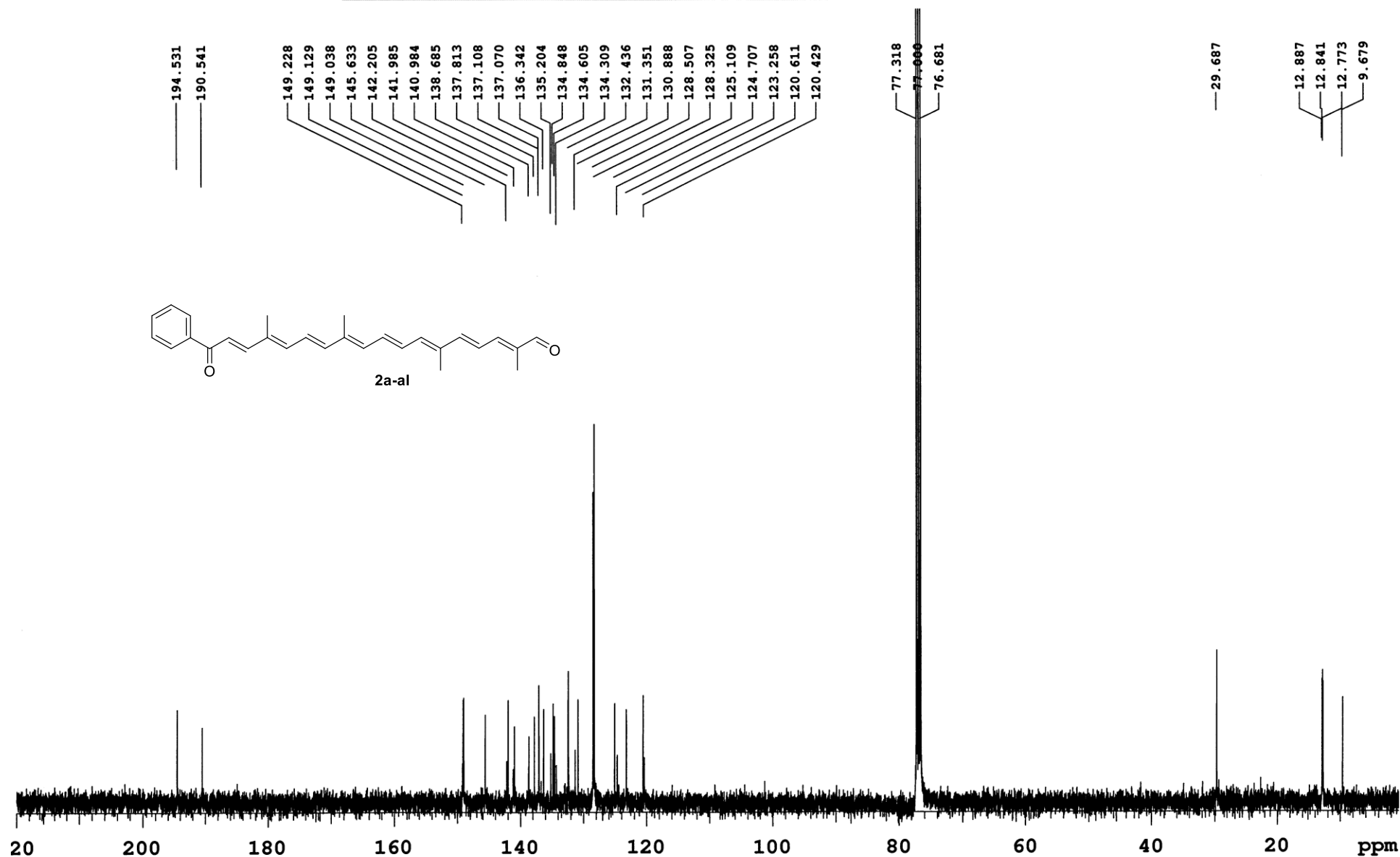
SGS-1421-11re

Sample Name **SGS-1421-11re**  
Date collected **2021-11-17**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**



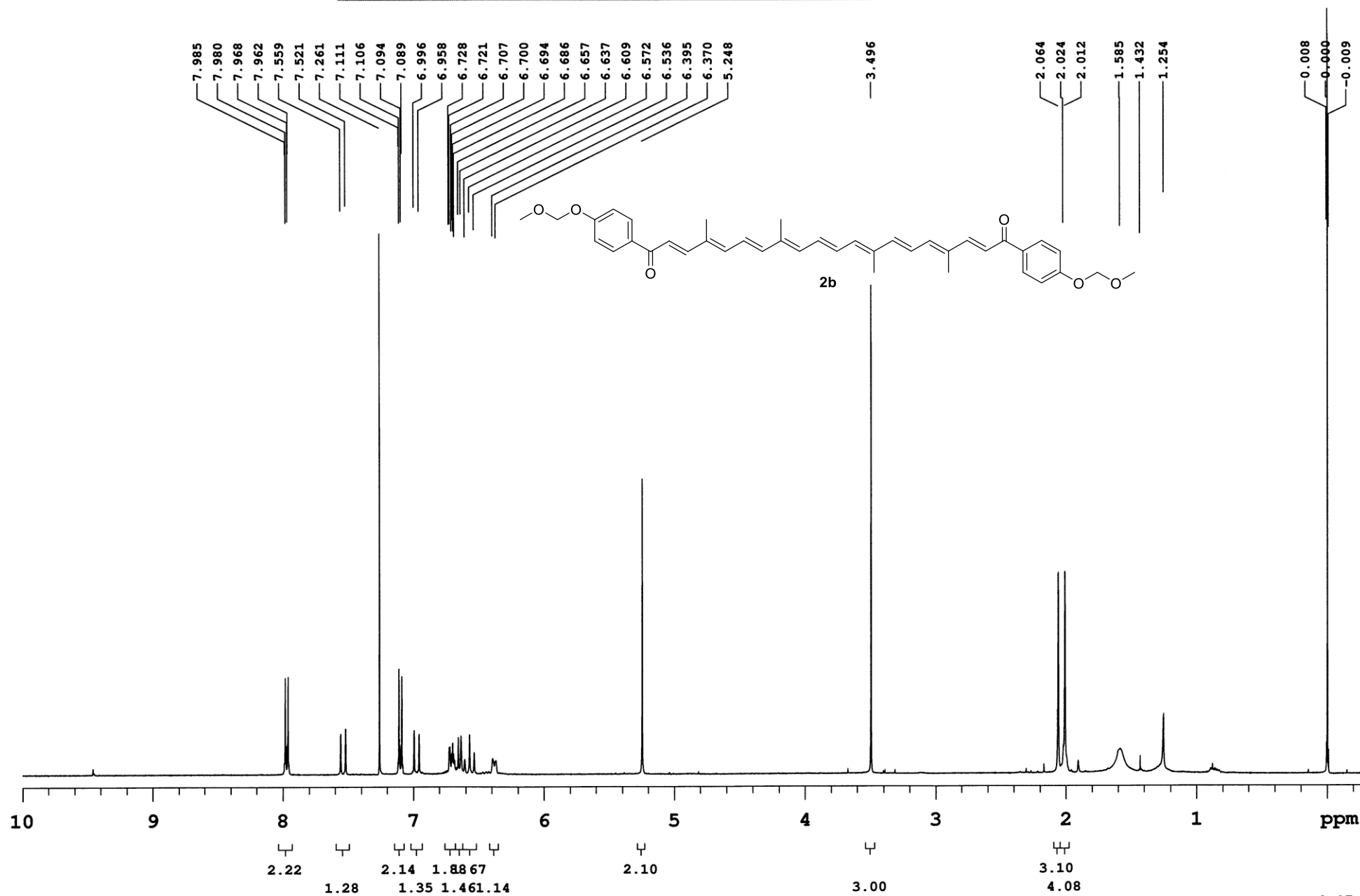
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Sample Name **SGS-1557-3re**  
Date collected **2021-09-07**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



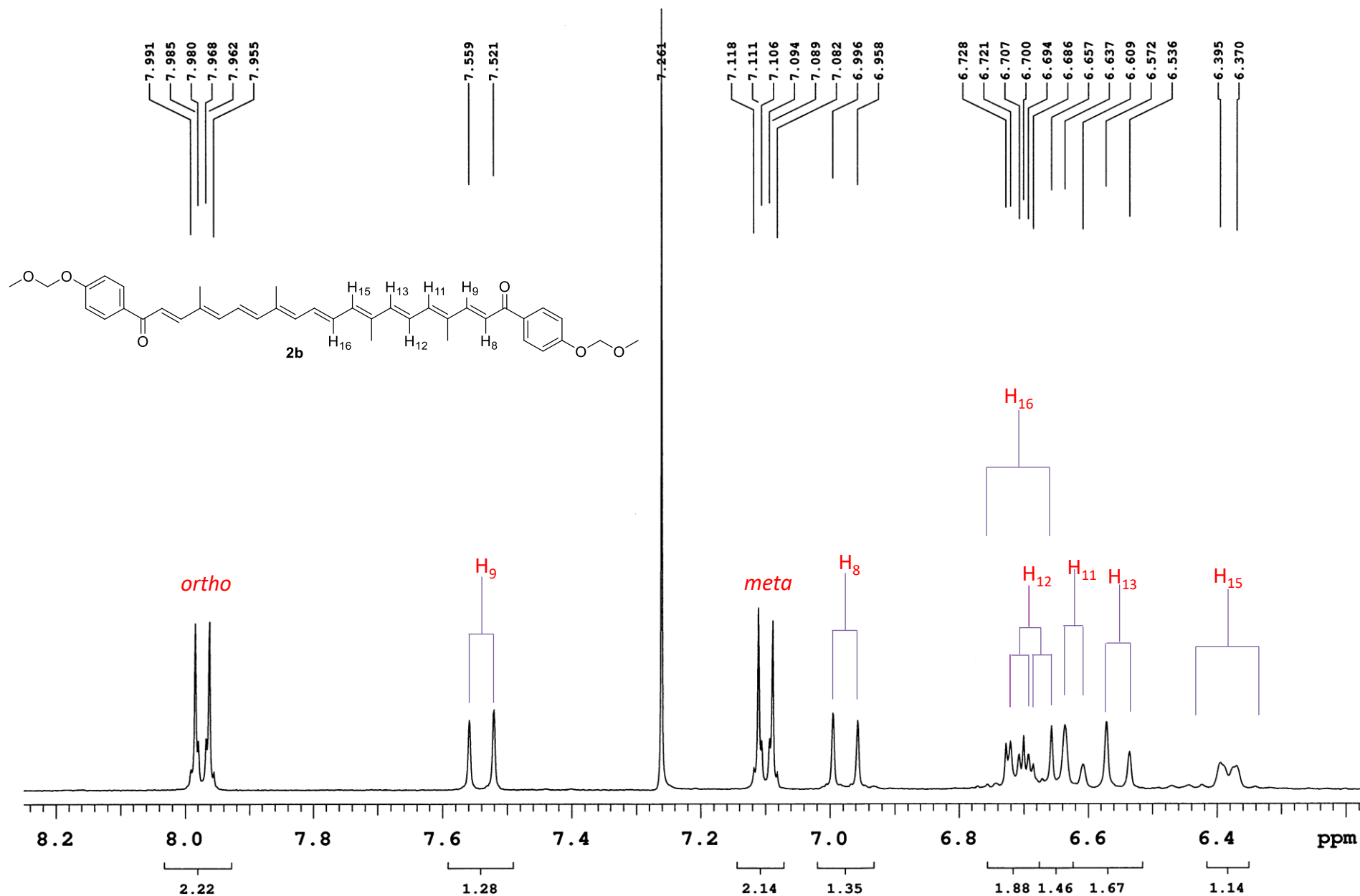
SGS-1557-3re

Sample Name **SGS-1557-3re**  
Date collected **2021-09-07**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**

Study owner **vnmr1**  
Operator **vnmr1**



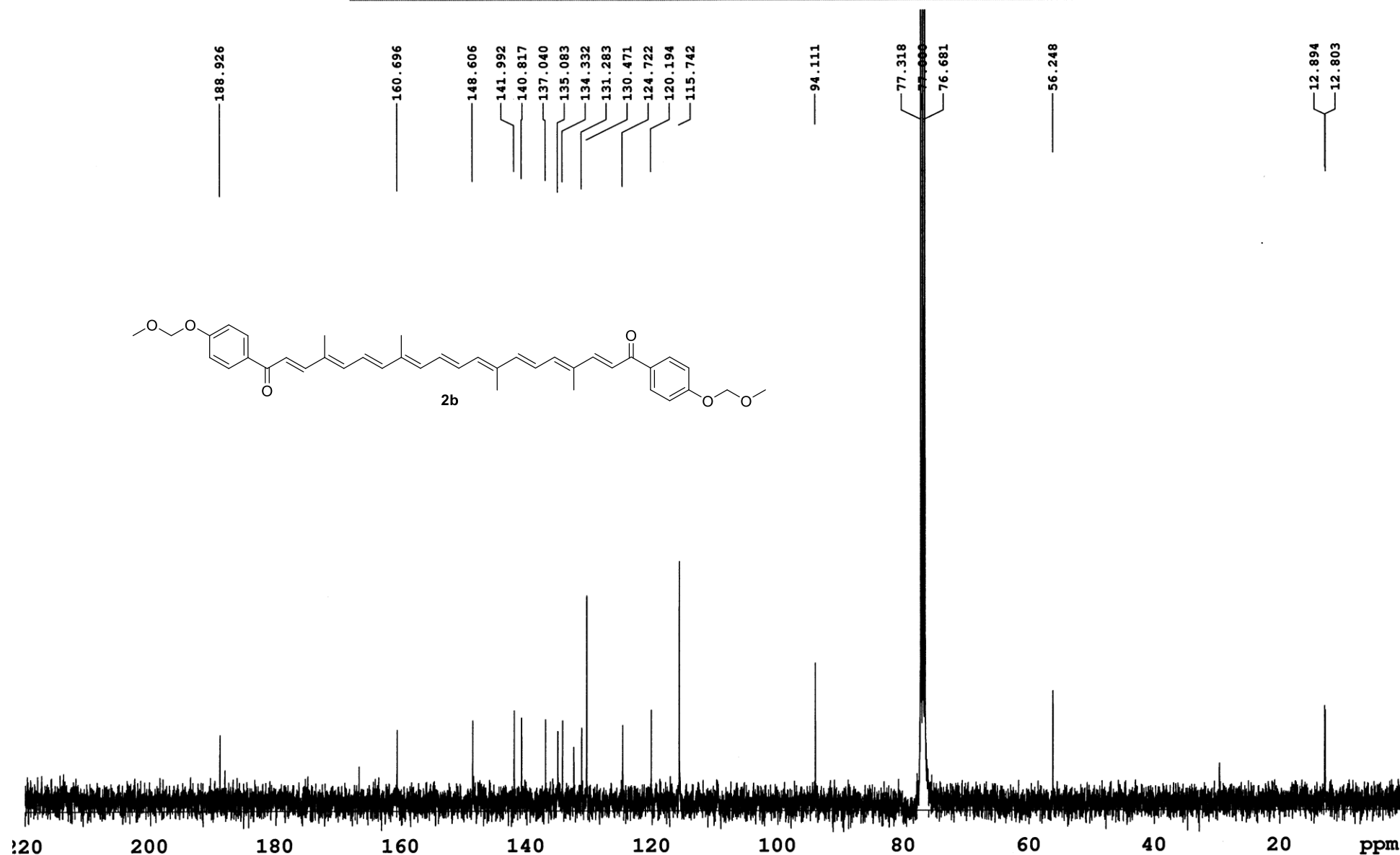


SGS-1557-3re-13C

Sample Name **SGS-1557-3re-13C**  
Date collected **2021-09-09**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



SGS-1557-3re-13C

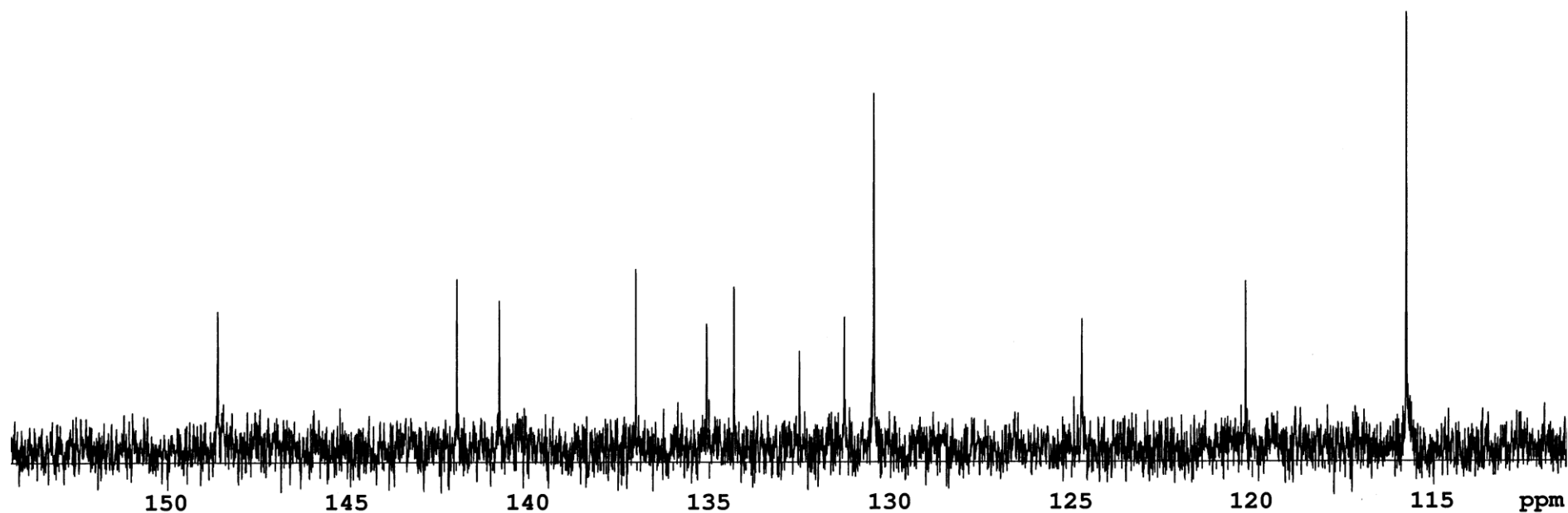
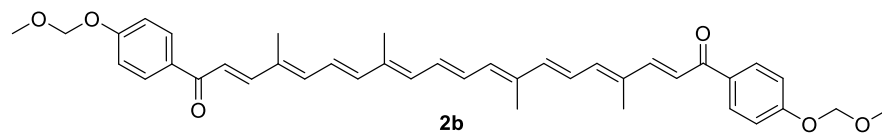
Sample Name **SGS-1557-3re-13C**  
Date collected **2021-09-09**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**

148.606  
141.992  
140.817  
137.040  
135.083  
134.332  
132.527  
131.283  
130.471  
124.722  
120.194  
115.742



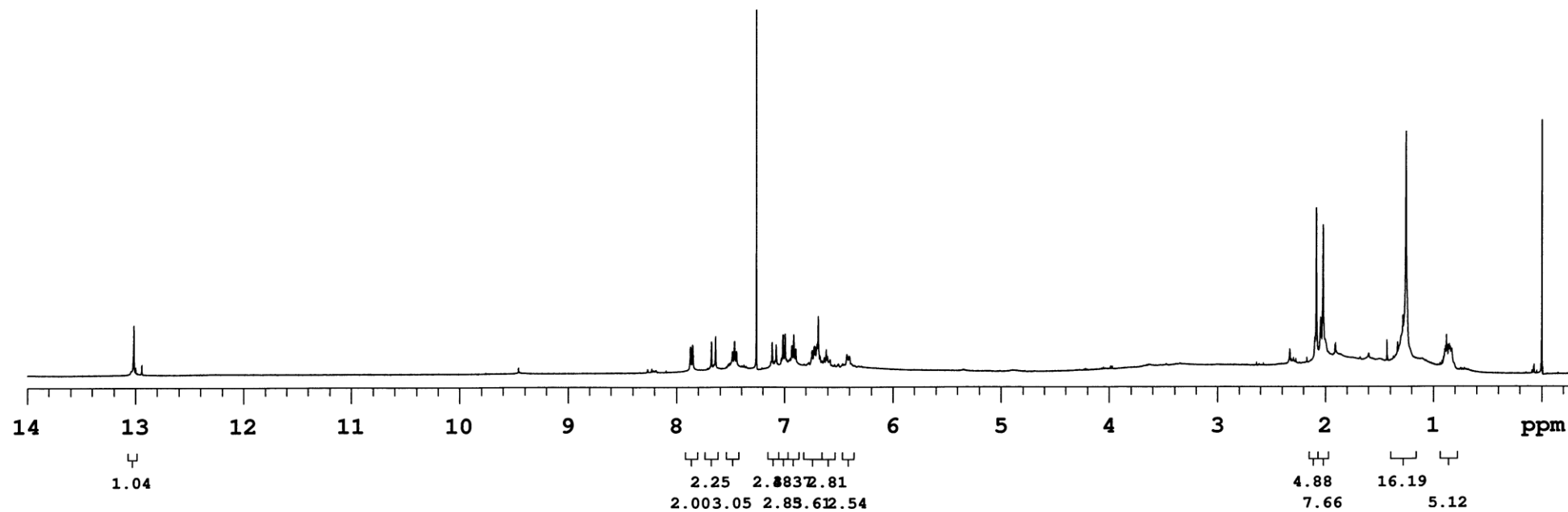
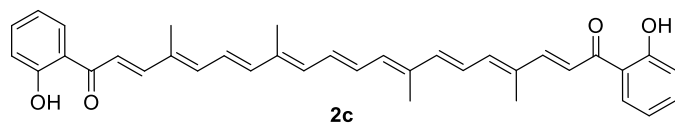
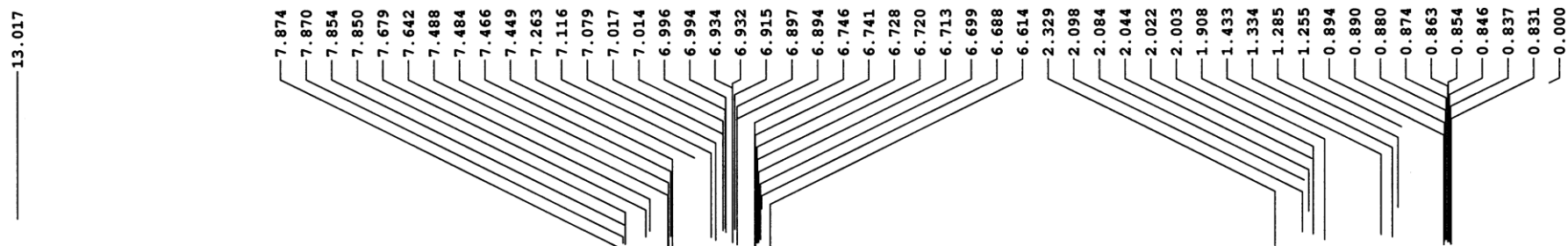
SGS-1521-EA2

Sample Name **SGS-1521-EA2**  
Date collected **2021-09-01**

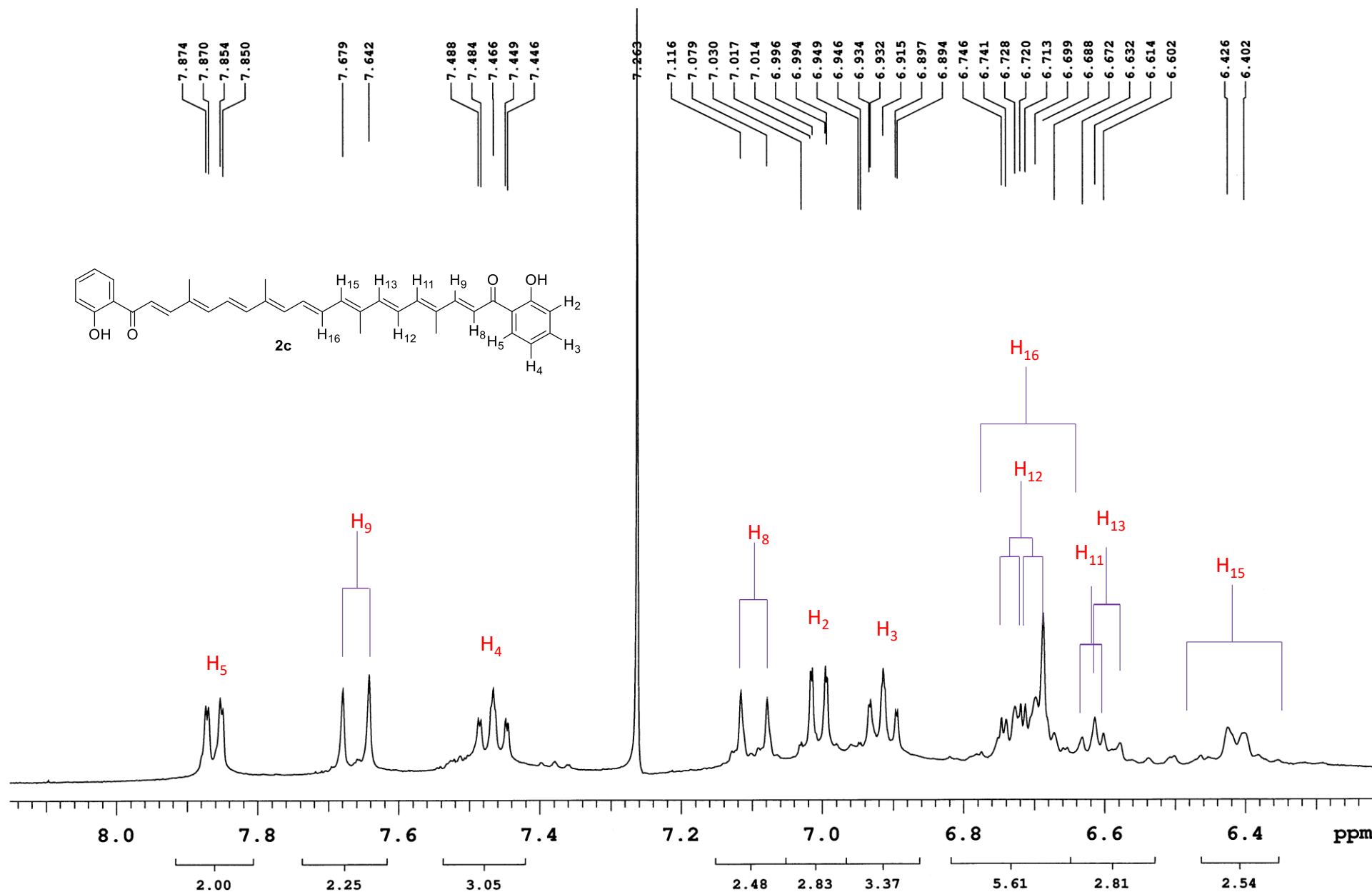
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



SGS-1521-EA2

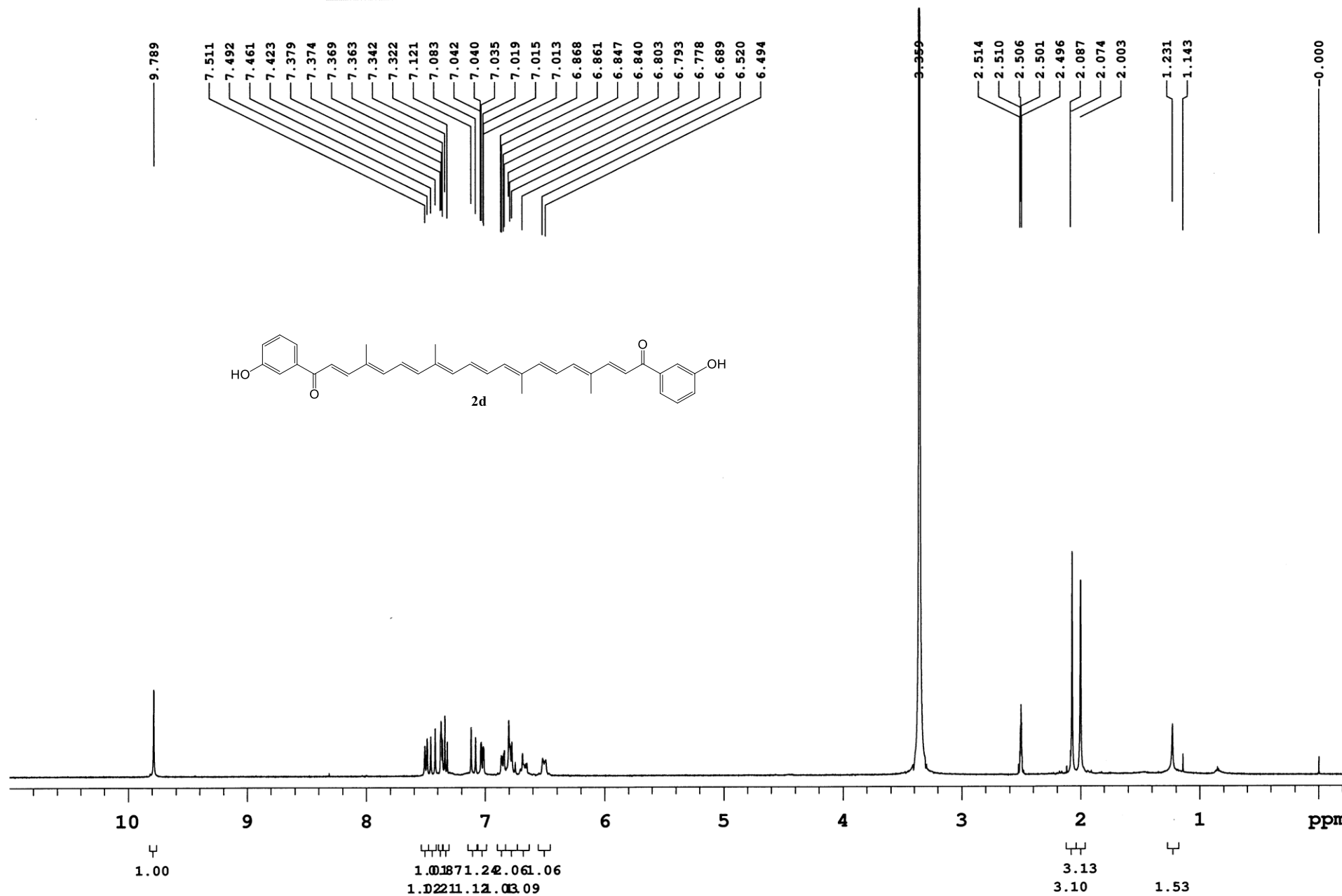
Sample Name **SGS-1521-EA2**  
Date collected **2021-09-01**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**

SGS-1597-EA1

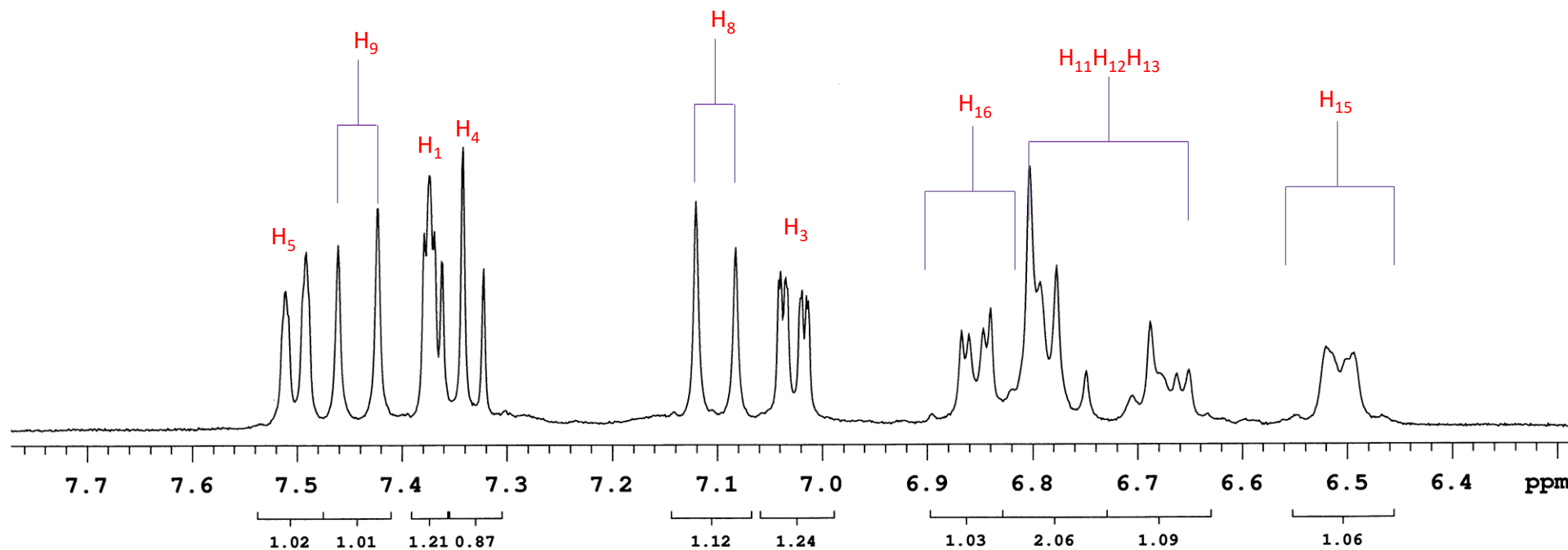
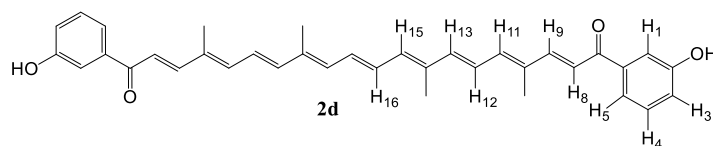
Sample Name **SGS-1597-EA1**  
Date collected **2021-10-05**

Pulse sequence **PROTON**  
Solvent **dms**

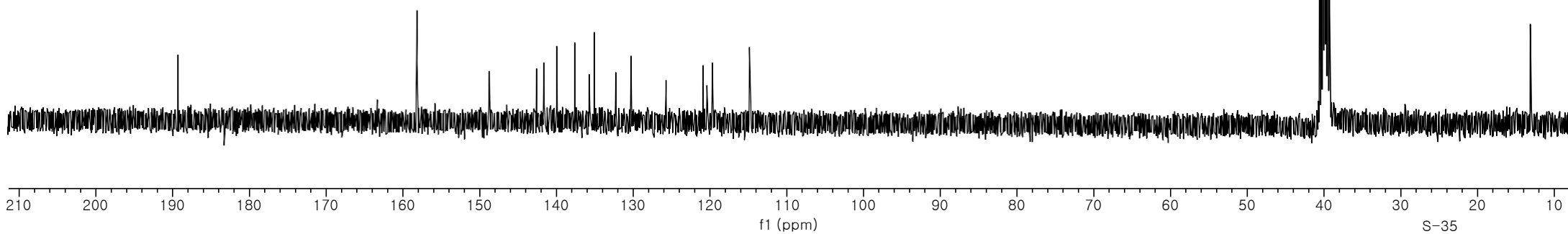
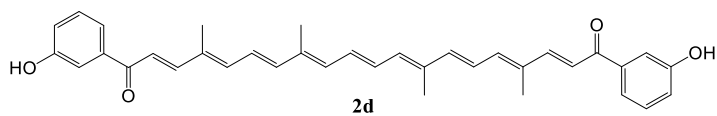
Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**



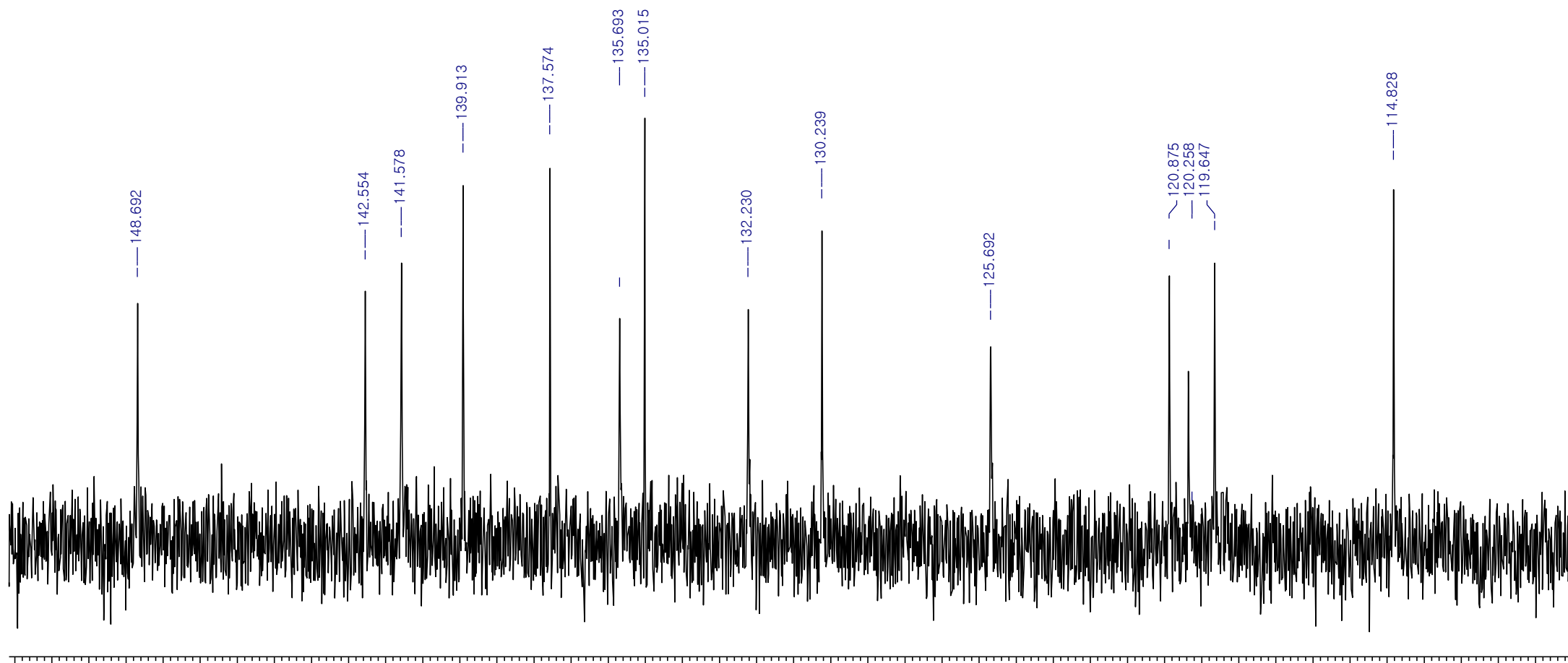
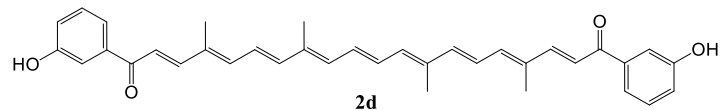
SGS-1597-EA1

Sample Name **SGS-1597-EA1**  
Date collected **2021-10-05**Pulse sequence **PROTON**  
Solvent **dms**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**7.511  
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7.461  
7.423  
7.379  
7.374  
7.369  
7.363  
7.342  
7.3227.121  
7.083  
7.042  
7.040  
7.035  
7.019  
7.015  
7.0136.868  
6.861  
6.847  
6.840  
6.803  
6.793  
6.778  
6.749  
6.689  
6.663  
6.6526.520  
6.494

Parameter	Value
Data File Name	F:/NMR/ 2110-koo-4-06/ SGS-1597-EA1_01/ SGS-1597-EA1_CARBO1_01.fid/ fid
Instrument	vnmrs
Solvent	dmso
Probe	5mm_ATB
Number of Scans	2000
Acquisition Date	2021-10-06T01:45:21
Spectrometer Frequency	100.60



Parameter	Value
Data File Name	F:/NMR/ 2110-koo-4-06/ SGS-1597-EA1_01/ SGS-1597-EA1_CARBON_01.fid/ fid
Instrument	vnmrs
Solvent	dmso
Probe	5mm_ATB
Number of Scans	2000
Acquisition Date	2021-10-06T01:45:21
Spectrometer Frequency	100.60



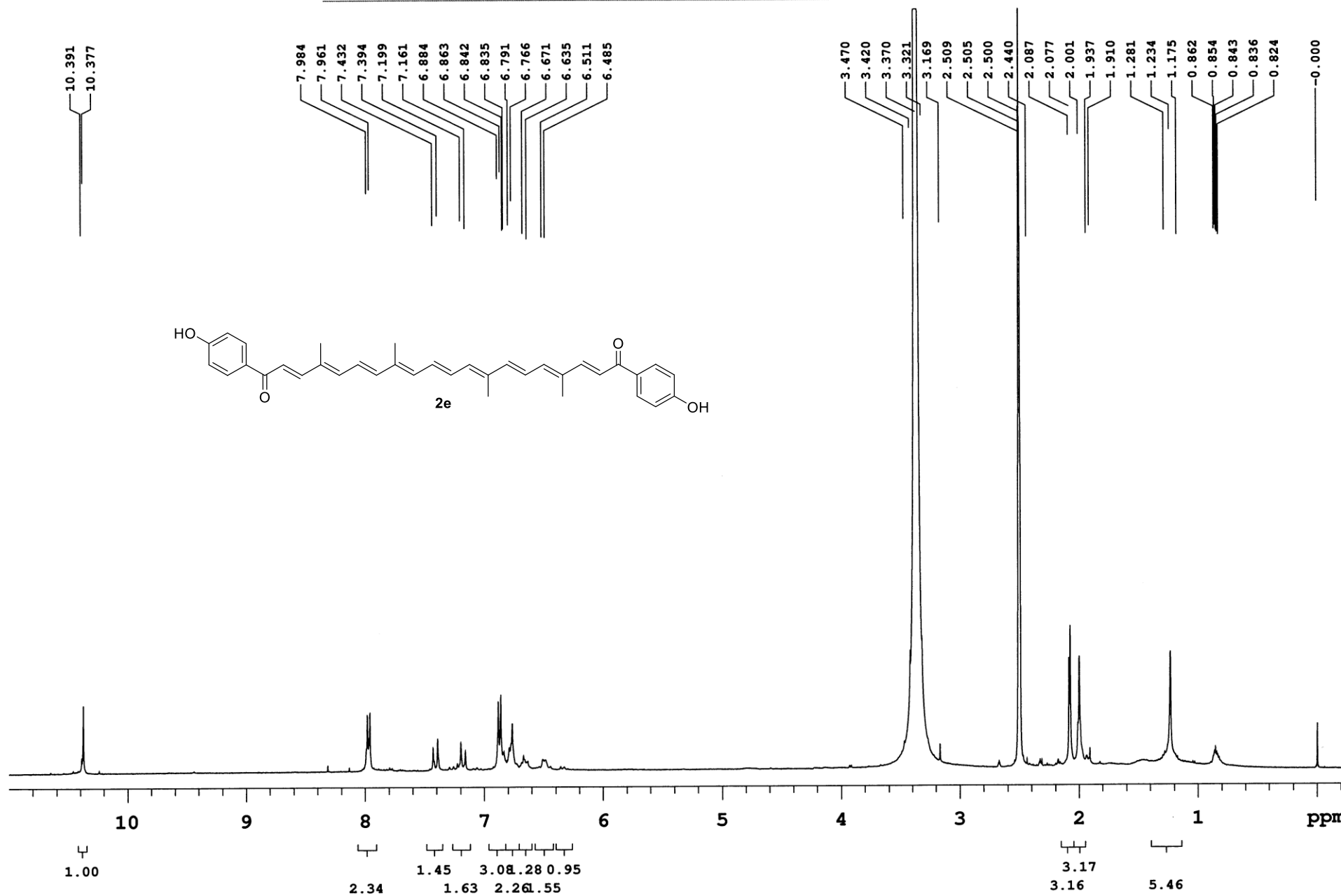


SGS-2022-2re-1

Sample Name **SGS-2022-2re-1**  
Date collected **2022-01-04**

Pulse sequence **PROTON**  
Solvent **dms**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**

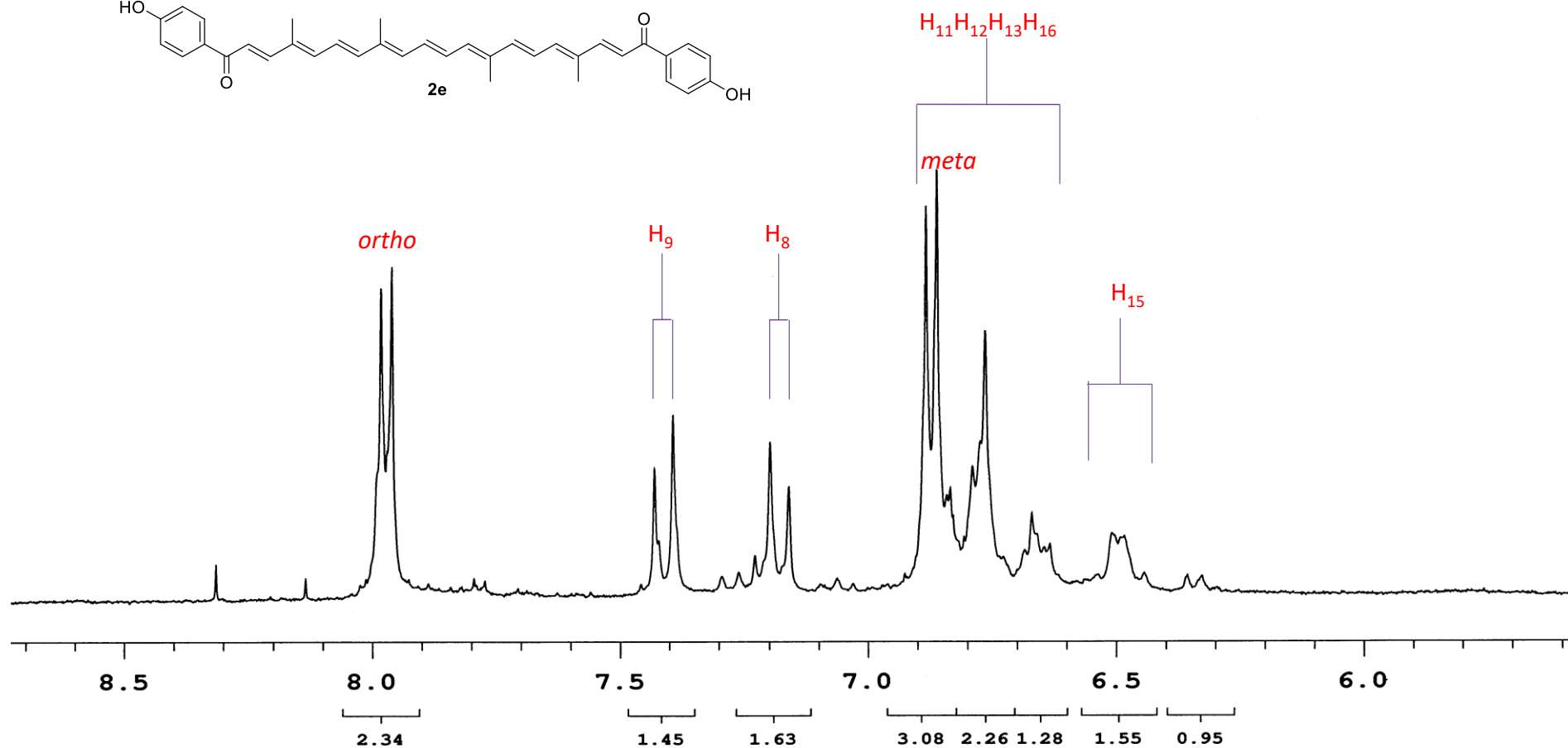
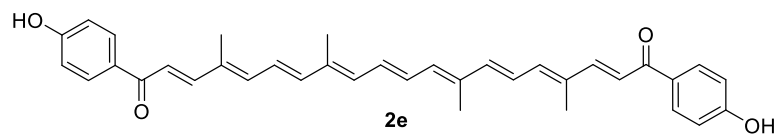
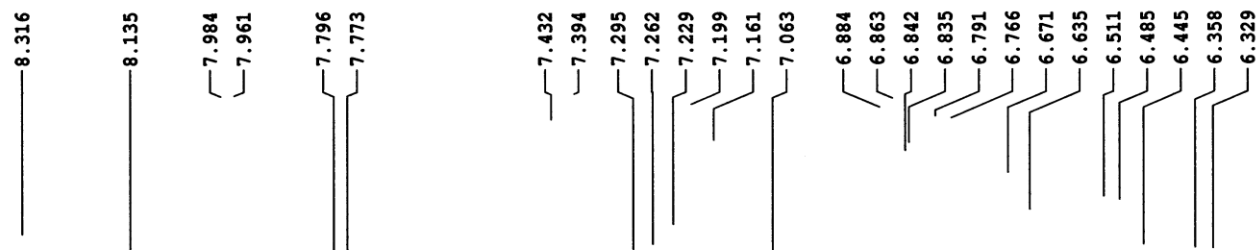


SGS-2022-2re-1

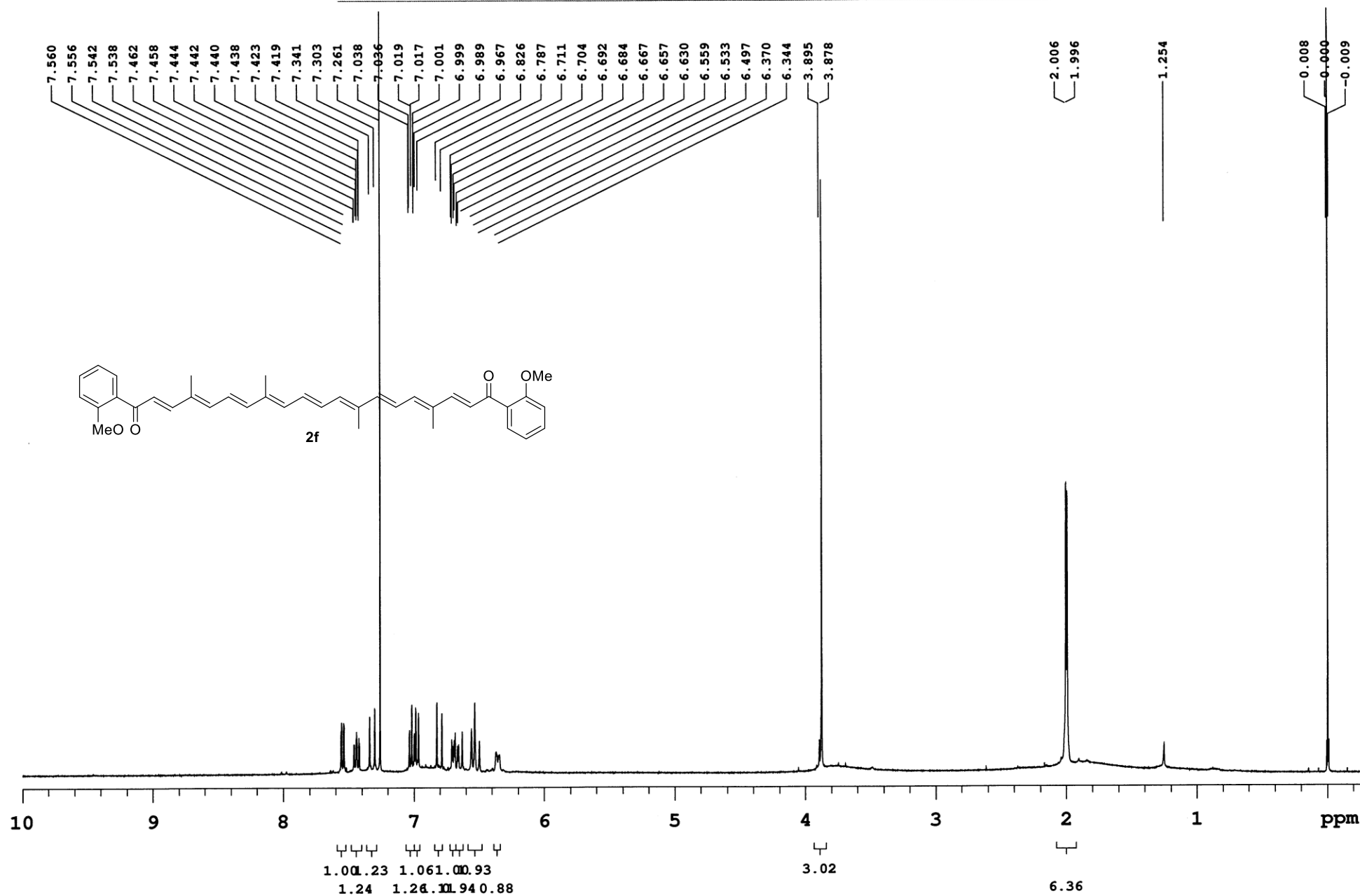
Sample Name **SGS-2022-2re-1**  
Date collected **2022-01-04**

Pulse sequence **PROTON**  
Solvent **dms**

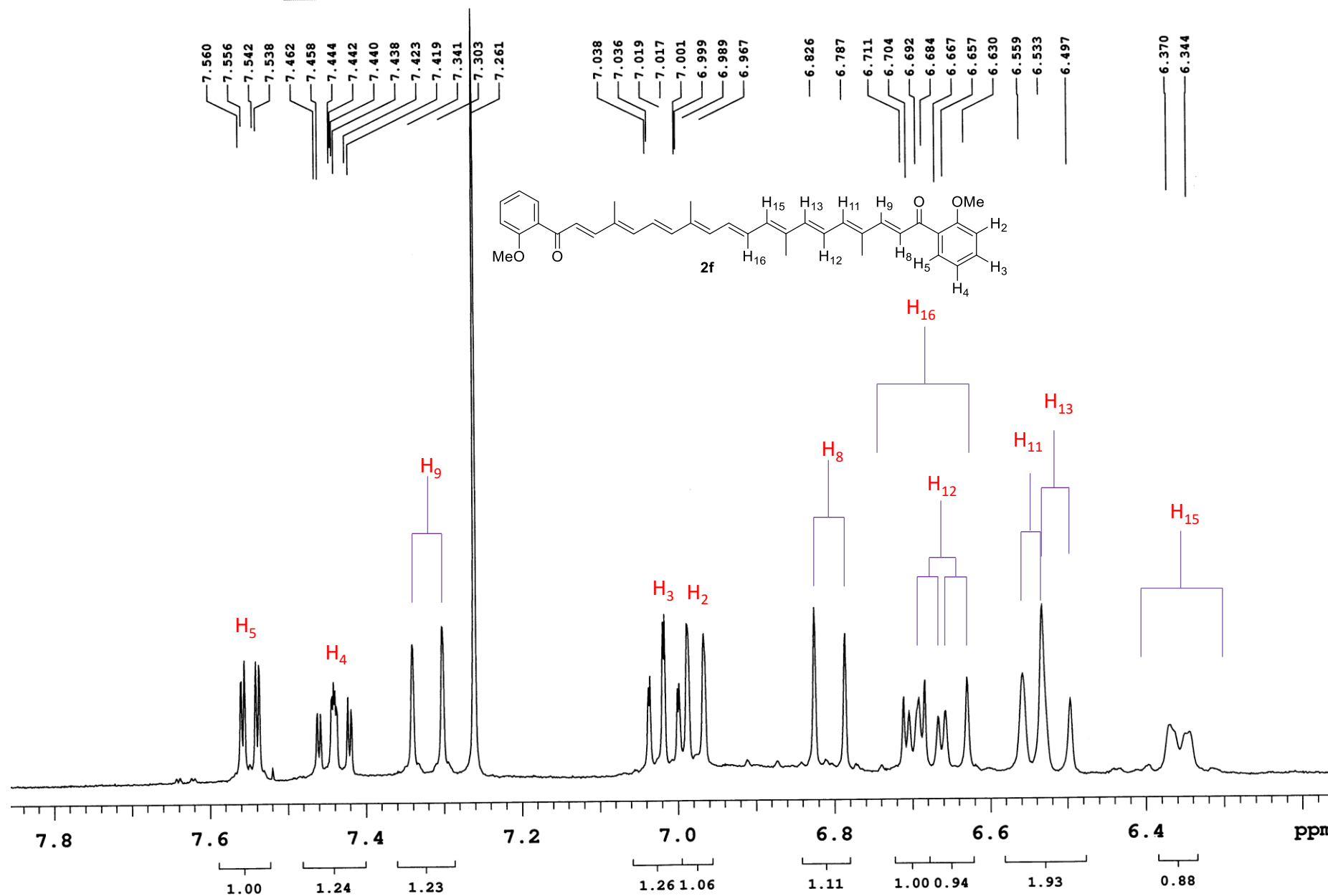
Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



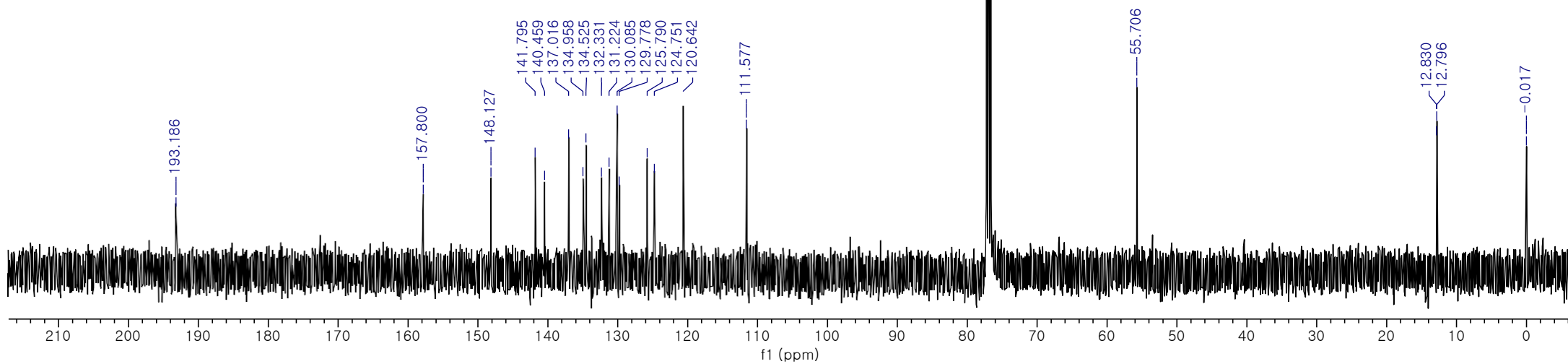
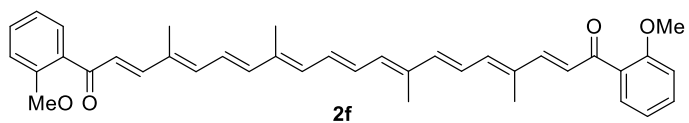
SGS-1547-1

Sample Name **SGS-1547-1**  
Date collected **2021-08-31**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**Study owner **vnmr1**  
Operator **vnmr1**

SGS-1547-1

Sample Name **SGS-1547-1**  
Date collected **2021-08-31**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**

Parameter	Value
Data File Name	F:/NMR/ 2109-koo-4-01/ SGS-1547-1_01/SGS-1547-1_CARBON_01.fid/ fid
Instrument	vnmr5
Solvent	cdcl3
Probe	5mm_ATB
Number of Scans	3000
Acquisition Date	2021-09-01T10:36:07
Spectrometer Frequency	100.60

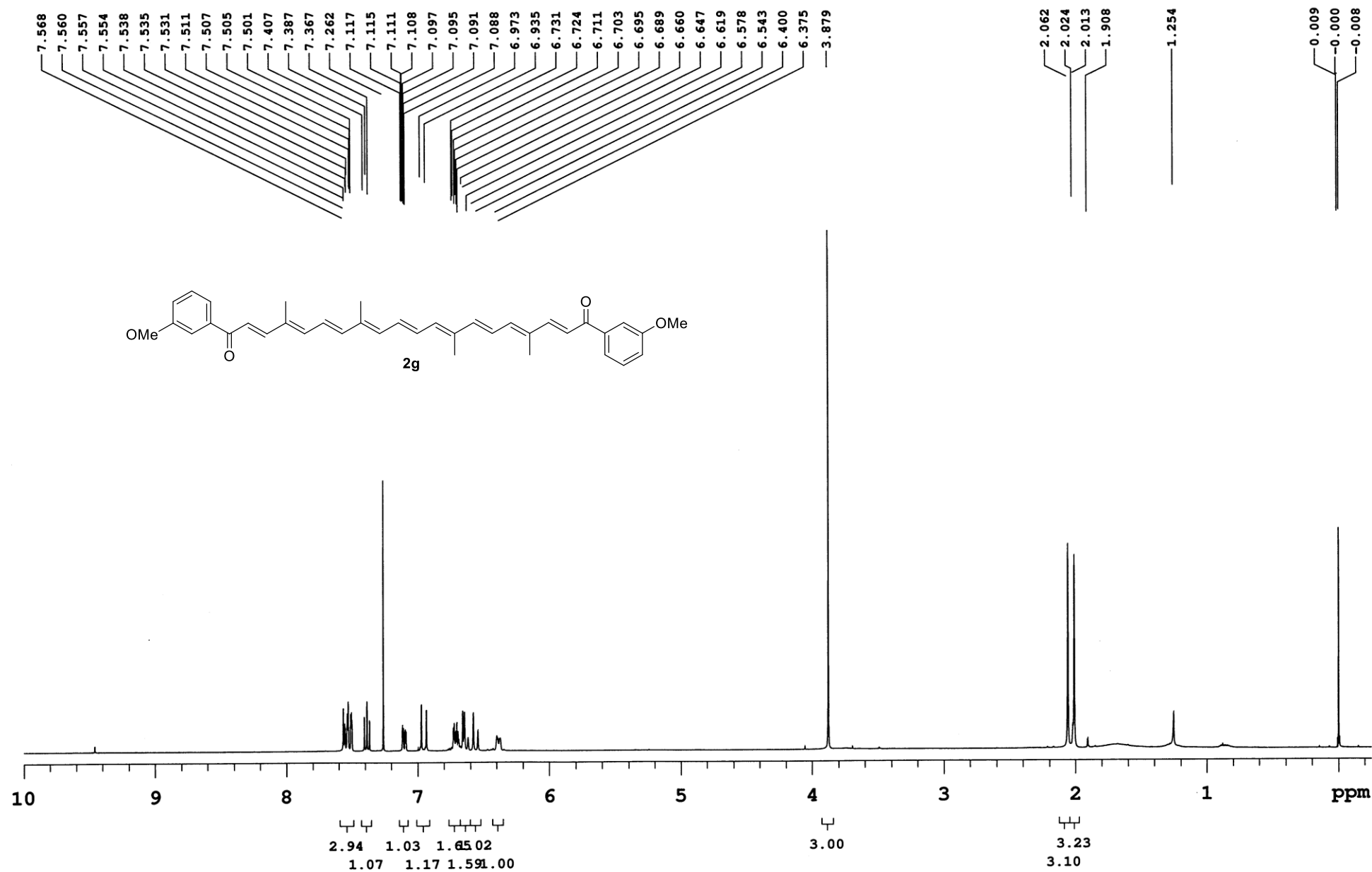


SGS-1600-2re

Sample Name **SGS-1600-2re**  
Date collected **2021-10-08**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**



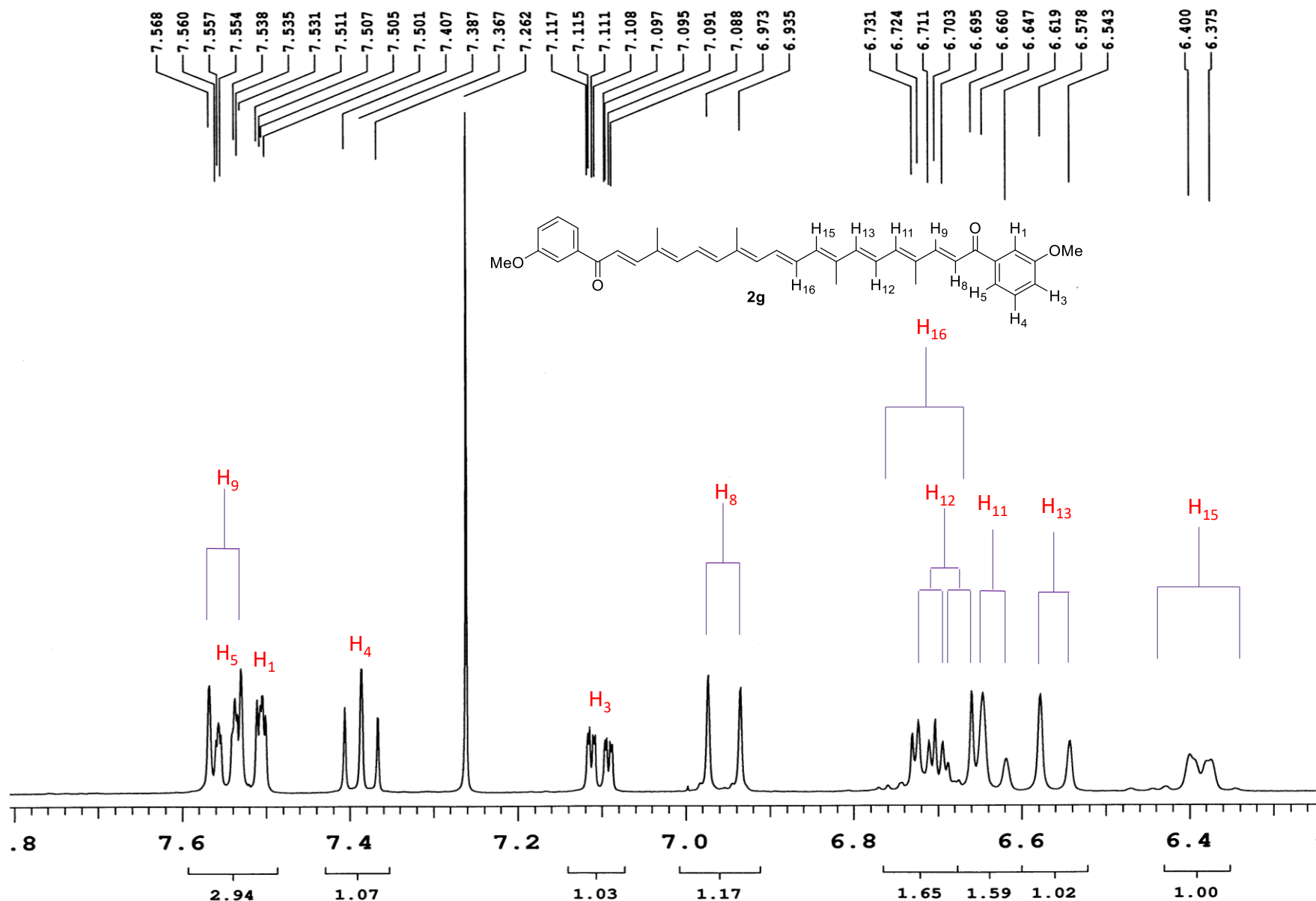
SGS-1600-2re

Sample Name **SGS-1600-2re**  
Date collected **2021-10-08**

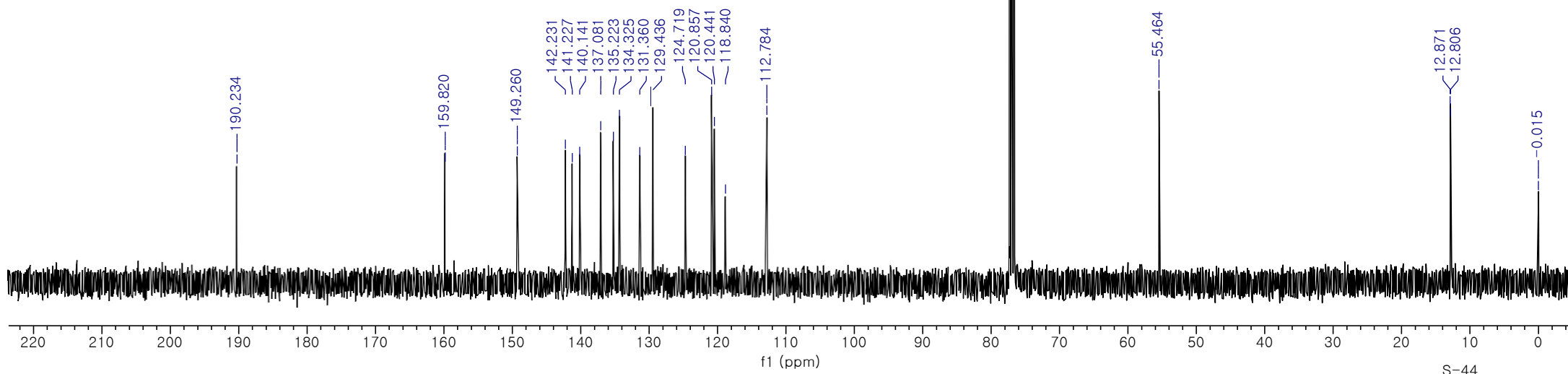
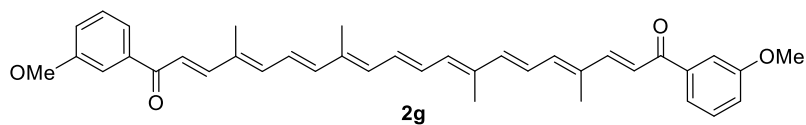
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study own  
Operator

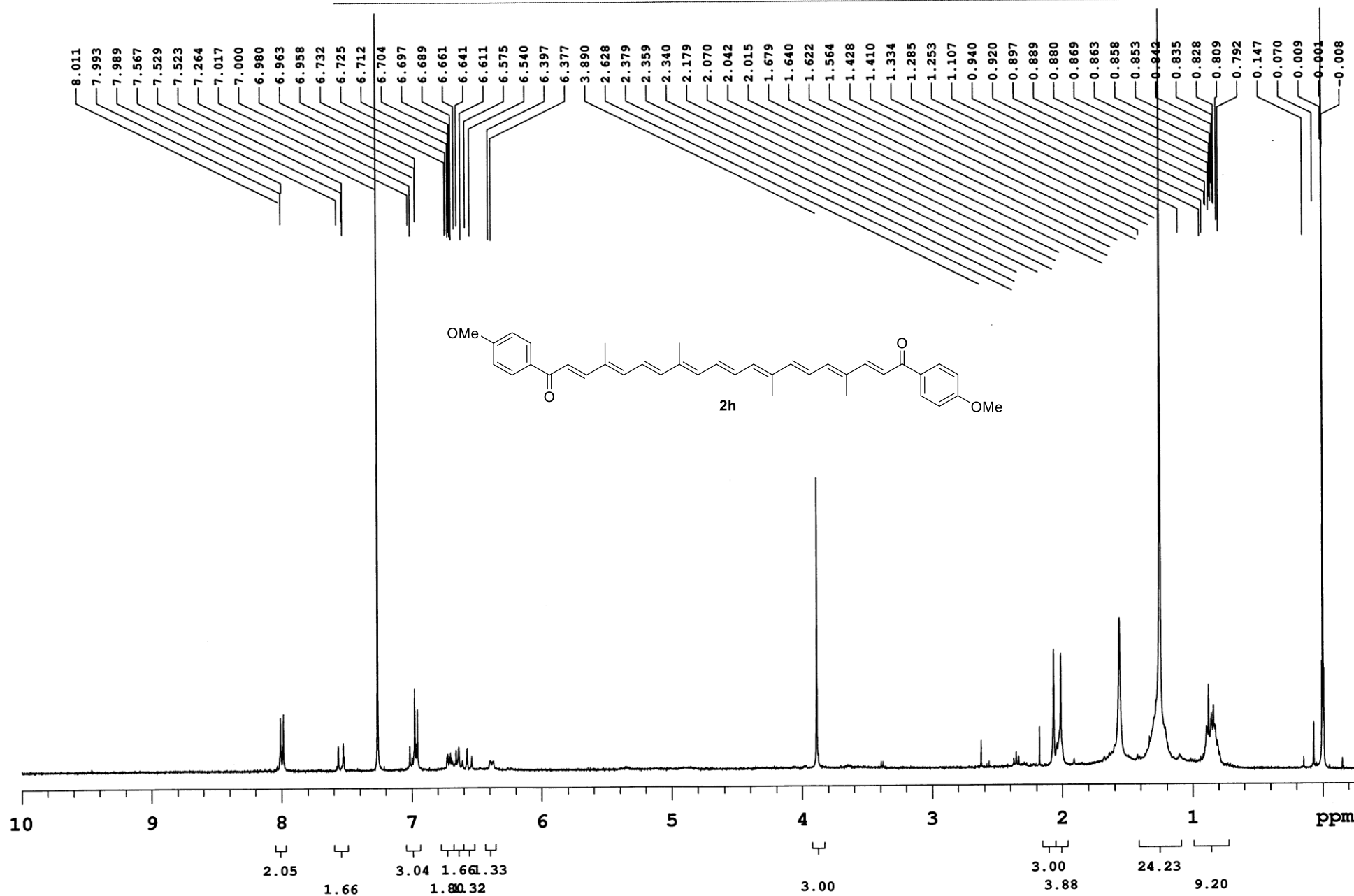


Parameter	Value
Data File Name	F:/NMR/ 2110-koo-4-12/ SGS-1600-2re-13C_01/ SGS-1600-2re-13C_CARBON_01.fid/fid
Instrument	vnmrs
Solvent	cdcl3
Probe	5mm_ATB
Number of Scans	2000
Acquisition Date	2021-10-08T20:33:05
Spectrometer Frequency	100.60





SGS-1629-3re

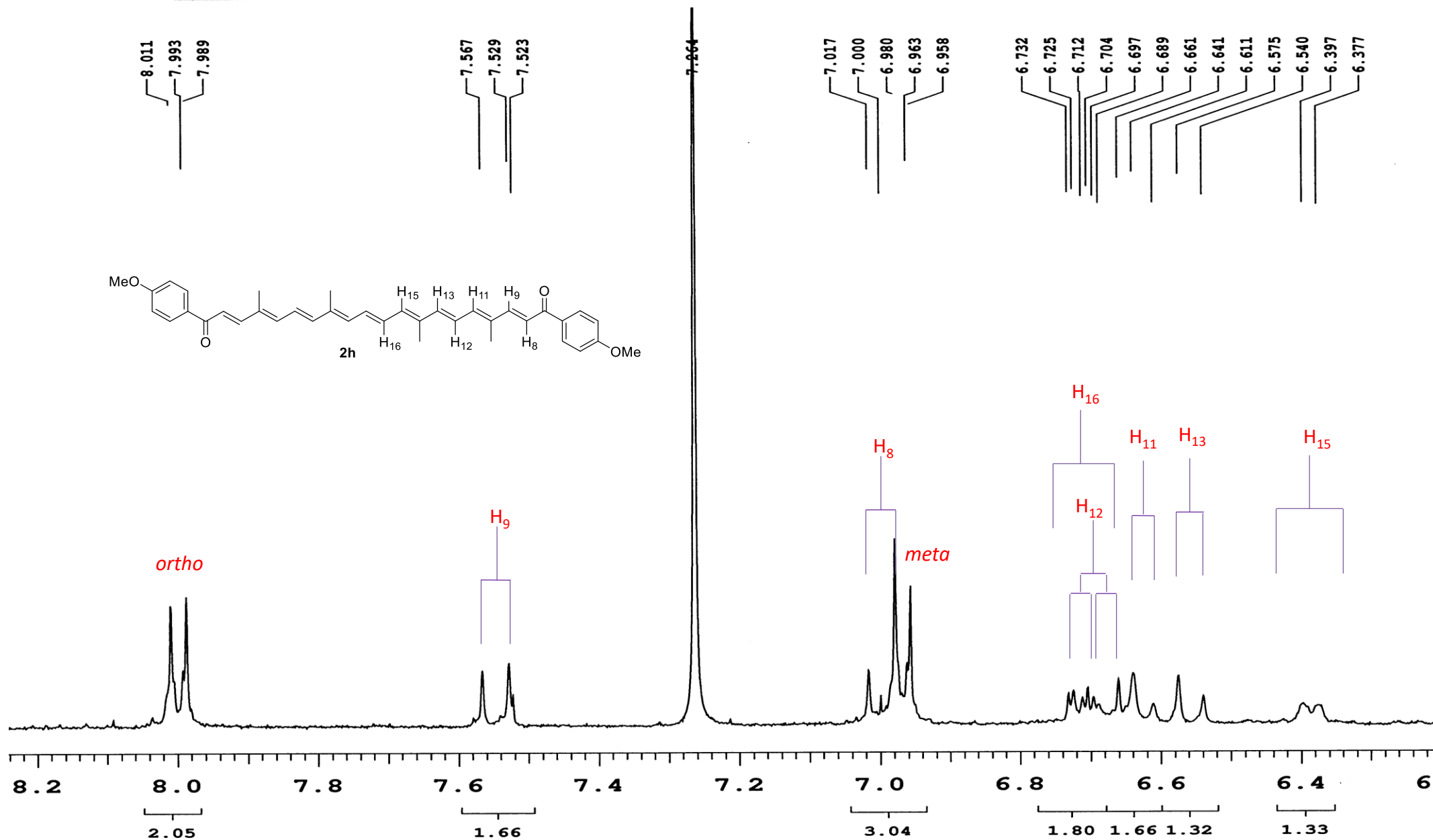
Sample Name **SGS-1629-3re**  
Date collected **2022-01-05**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**Study owner **vnmr1**  
Operator **vnmr1**

SGS-1629-3re

Sample Name **SGS-1629-3re**  
Date collected **2022-01-05**

Pulse sequence **PROTON**  
Solvent **cdcl3**

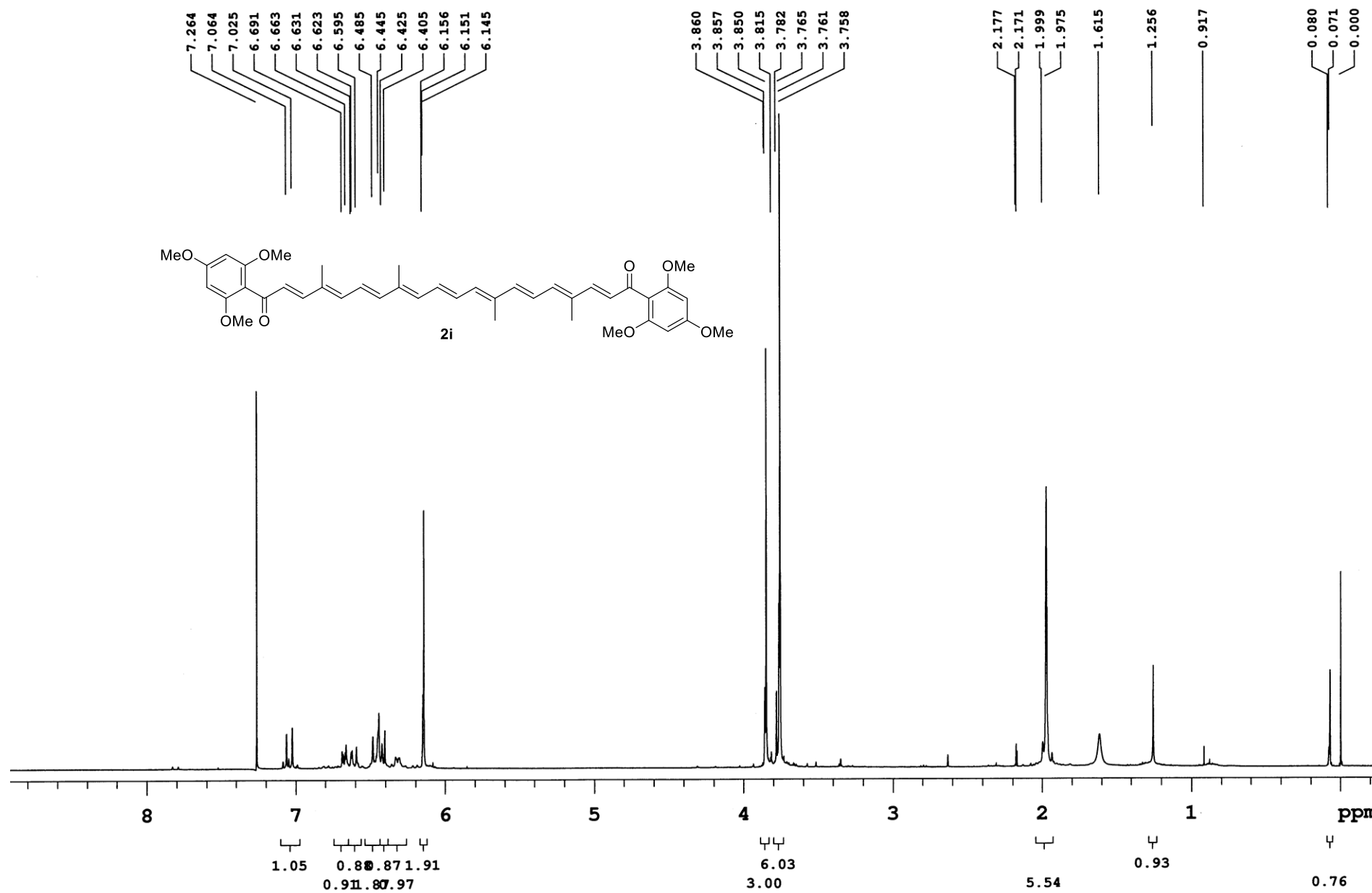
Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



Sample Name **SGS-1573-4t**  
Date collected **2021-09-24**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature 25 Study owner vnmr1  
Spectrometer Agilent-NMR.chem.com-vnmrs409 Operator vnmr1

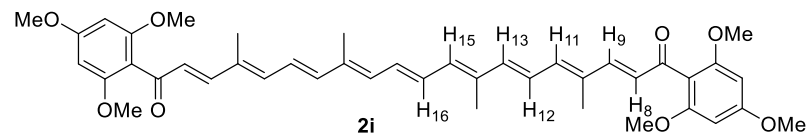


Sample Name **SGS-1573-4t**  
Date collected **2021-09-24**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature 25  
Spectrometer Ag

Study owner vnmr1  
rs409 Operator vnmr1



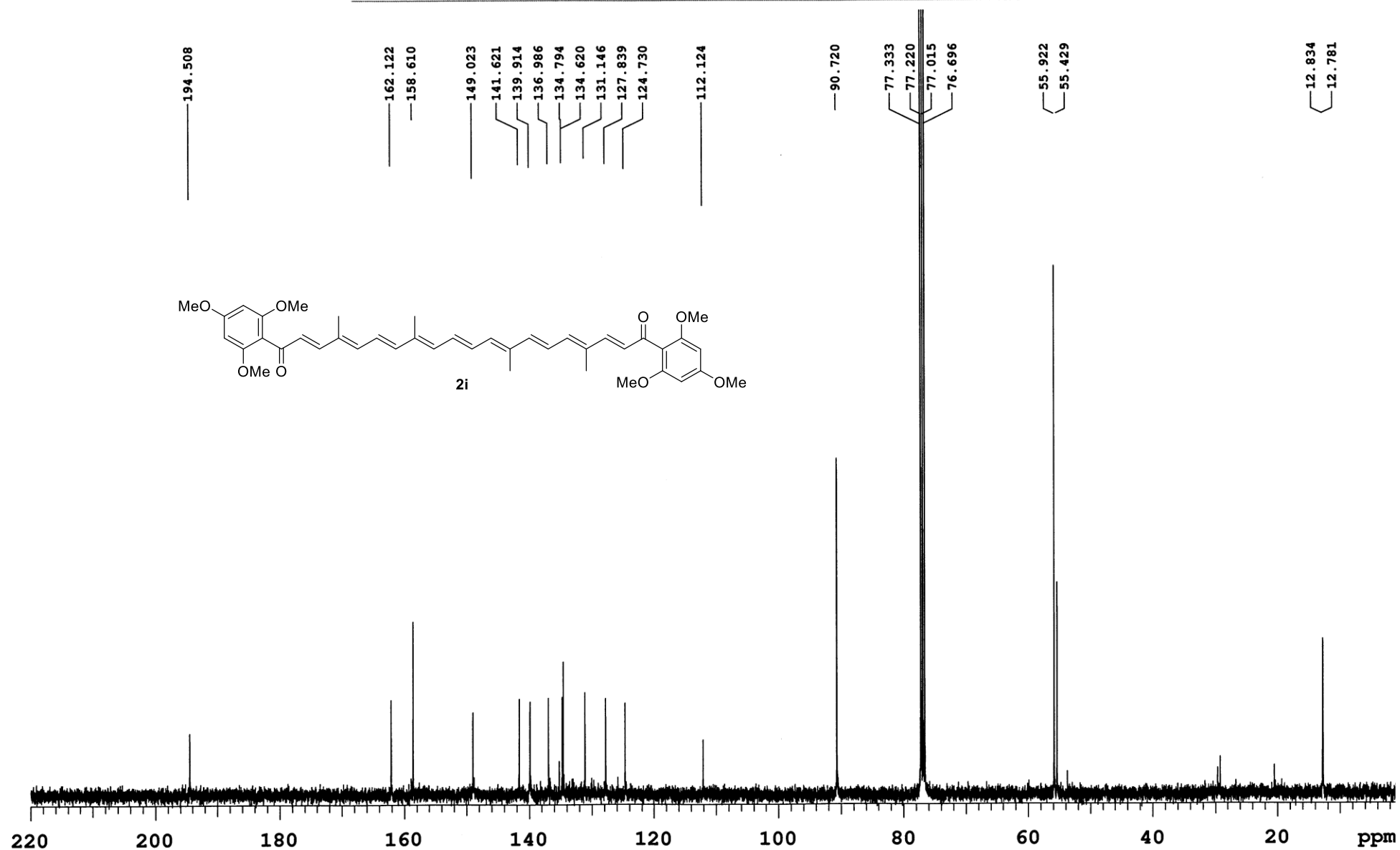
SGS-1573-4t

Sample Name **SGS-1573-4t**  
Date collected **2021-09-29**

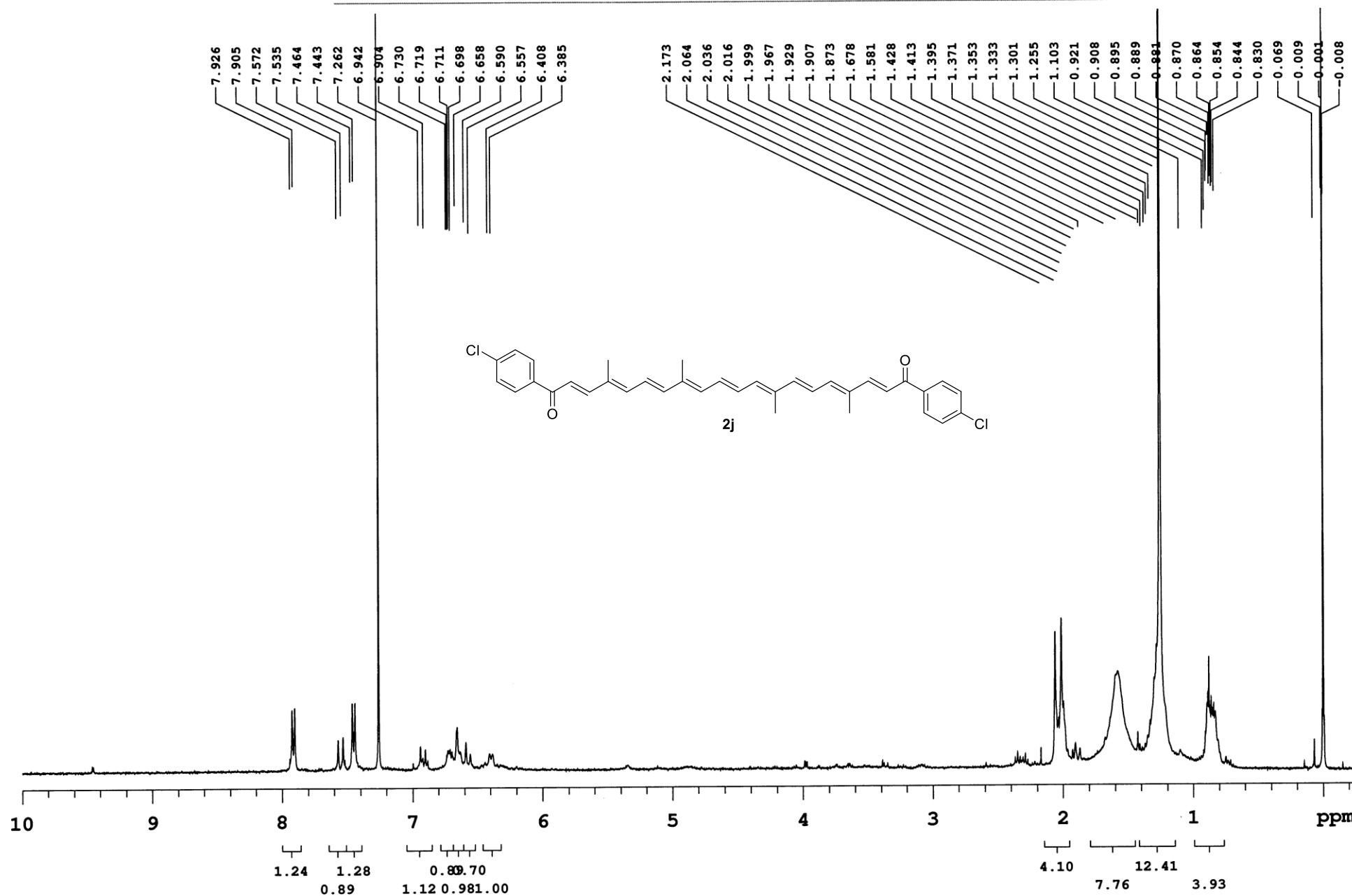
Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**



SGS-1570-EA2

Sample Name **SGS-1570-EA2**  
Date collected **2021-09-16**Pulse sequence **PROTON**  
Solvent **cdcl3**Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**

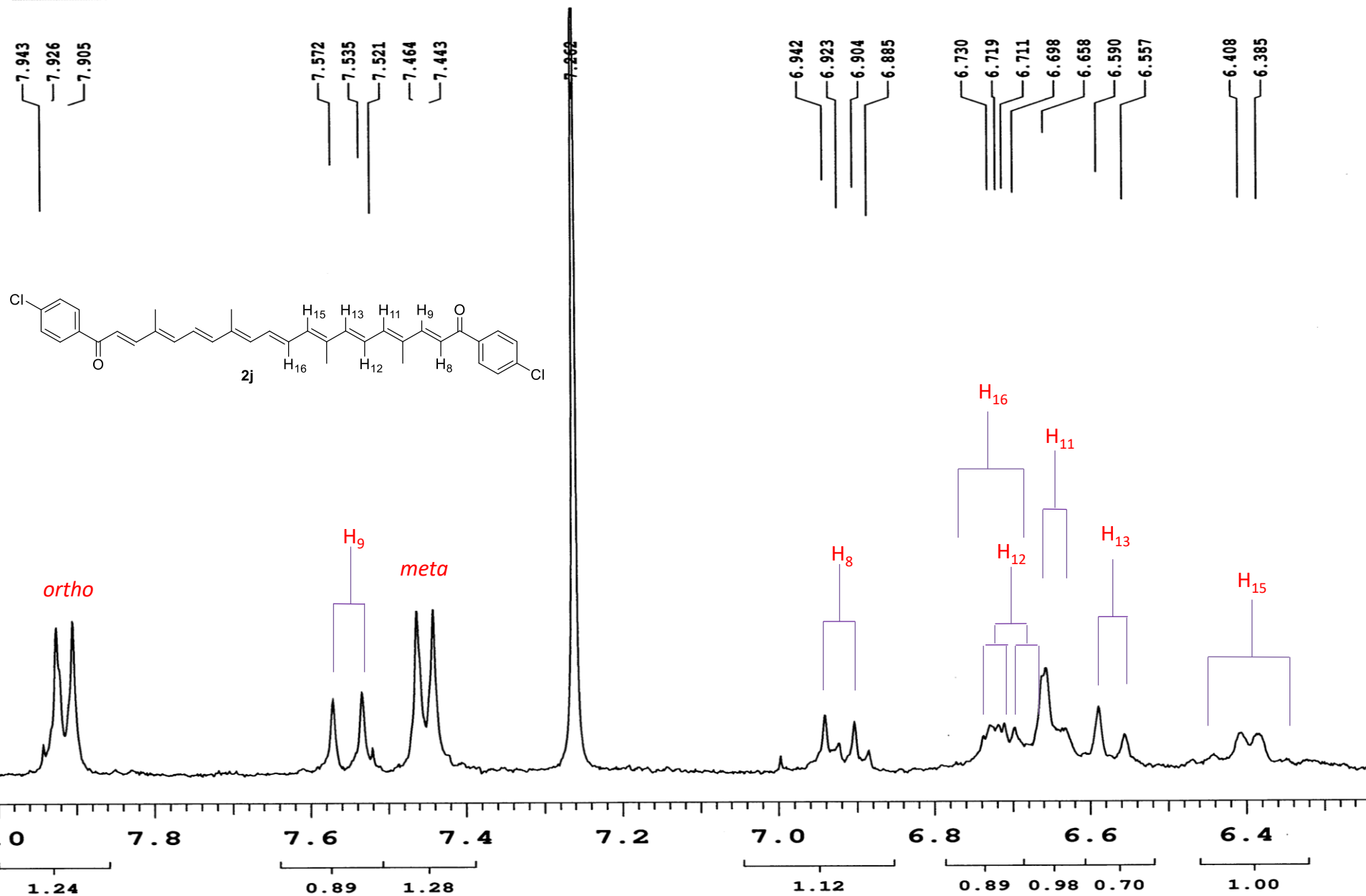
SGS-1570-EA2

Sample Name **SGS-1570-EA2**  
Date collected **2021-09-16**

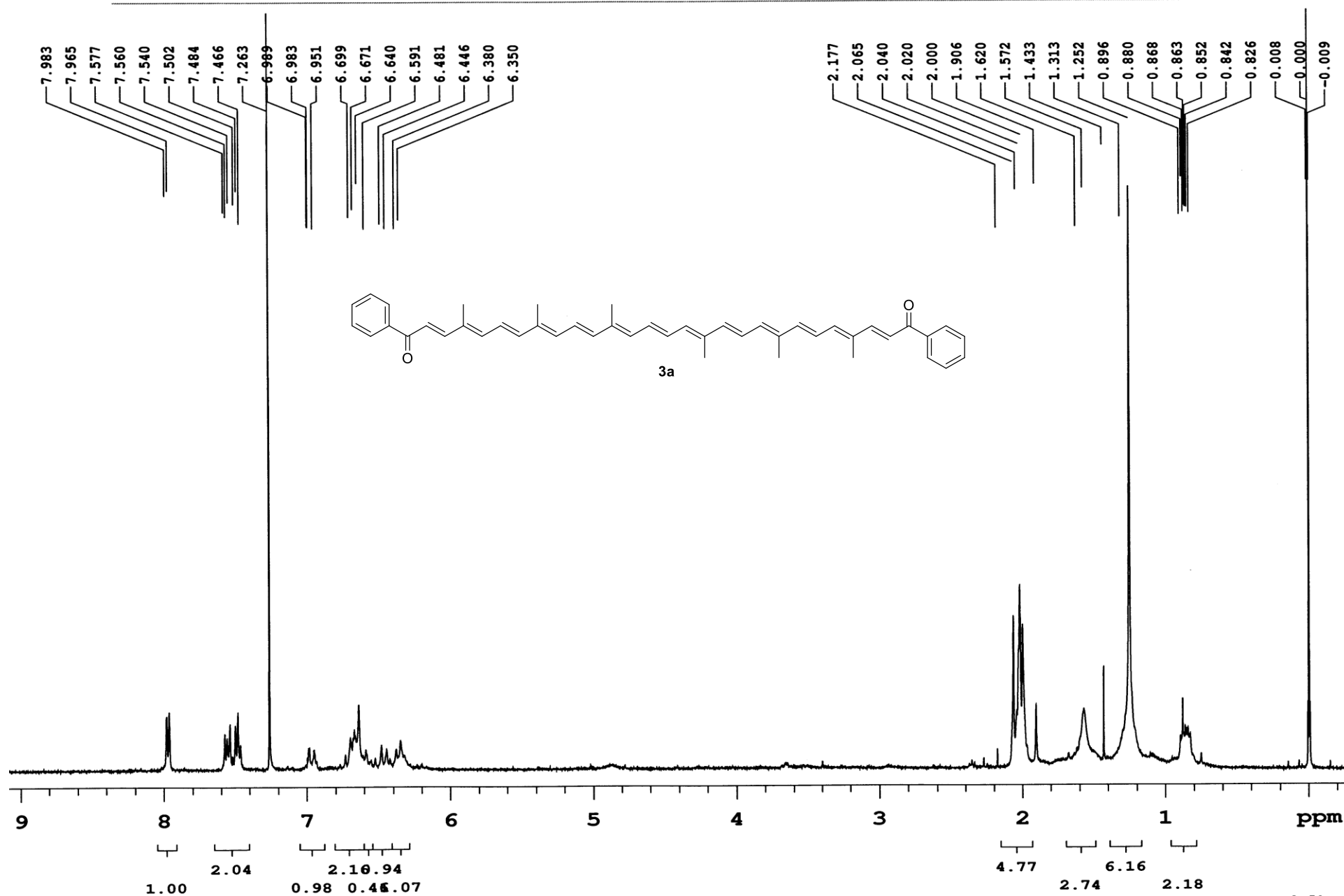
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnn**  
Operator **vnmr1**



Temperature 20 Study owner vnmr1  
Spectrometer Agilent-NMR.chem.com-vnmrs400 Operator vnmr1



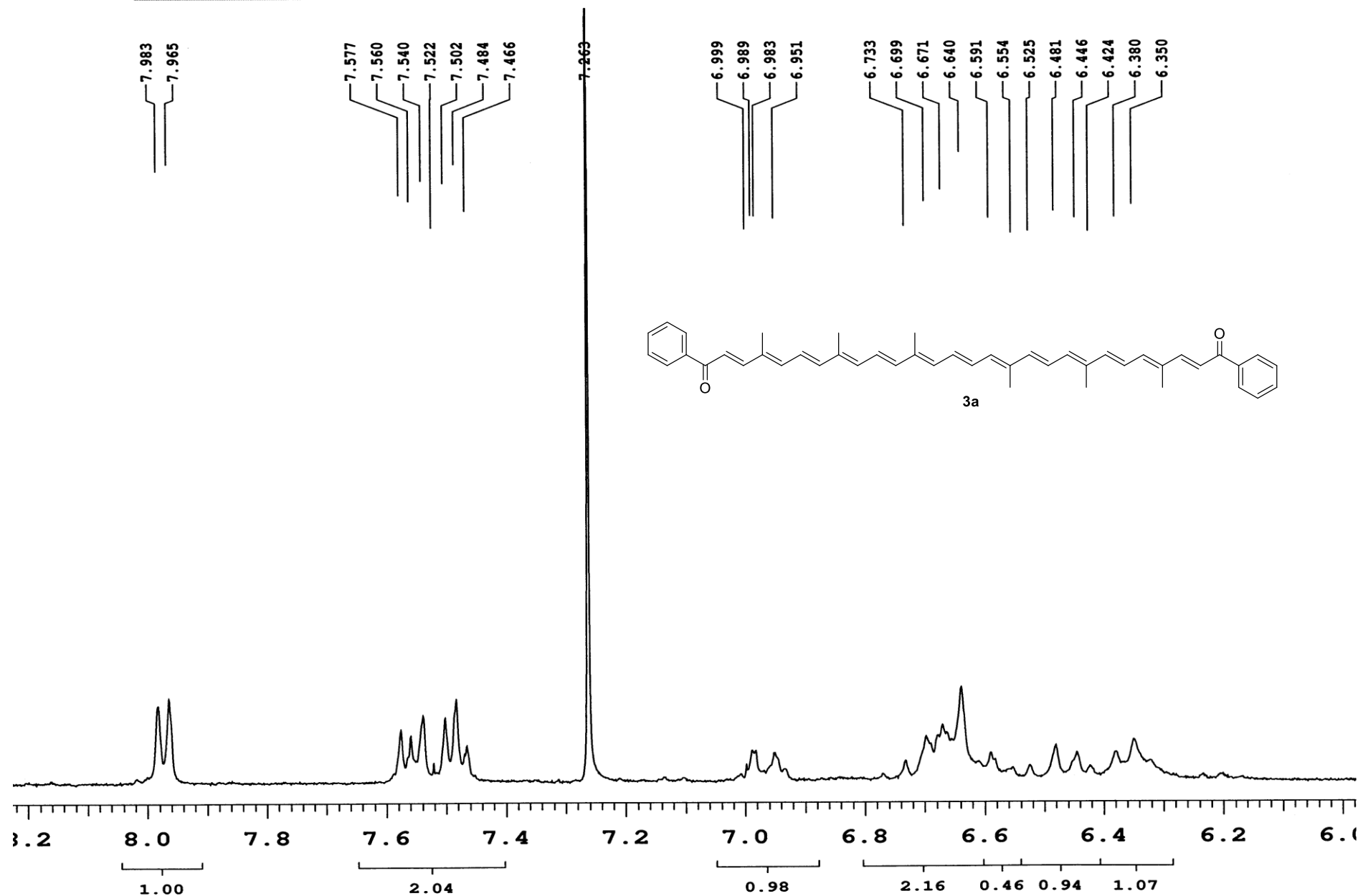


Sample Name **SGS-2130-CI-3re**  
Date collected **2022-02-16**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature 20 Spectrometer Agilent-NMR.chem.com-vnmrs400

Study owner vnmr1  
Operator vnmr1

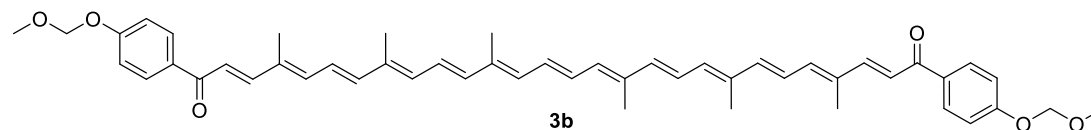


Sample Name **SGS-1590-32**  
Date collected **2021-10-05**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25** Stu  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
rs400 operator **vnmr1**

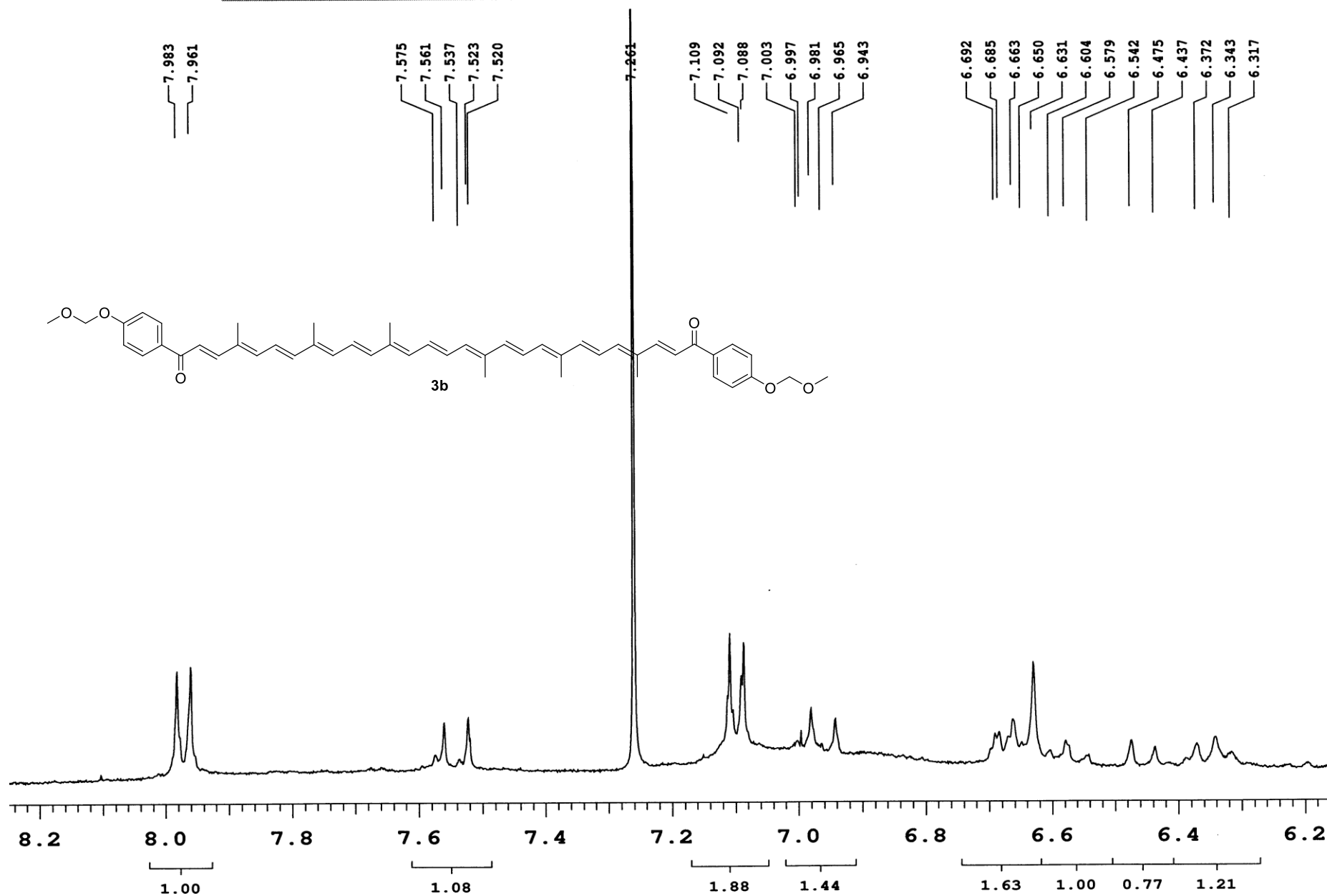


Sample Name **SGS-1590-32**  
Date collected **2021-10-05**

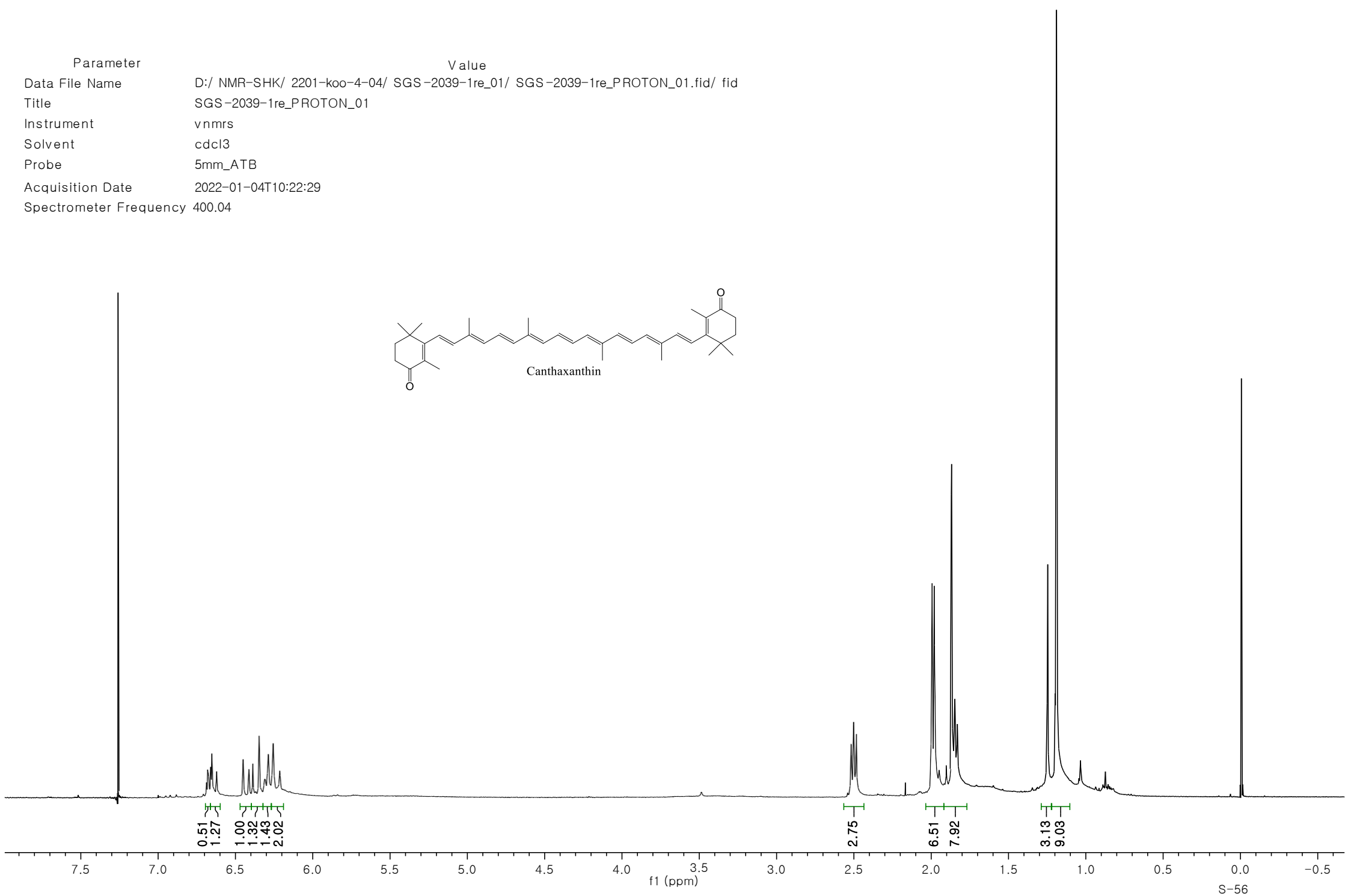
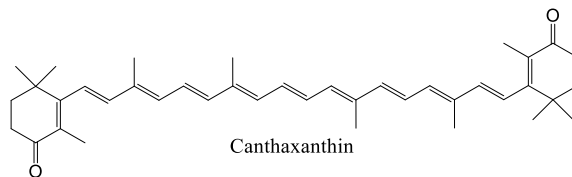
Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Ag**

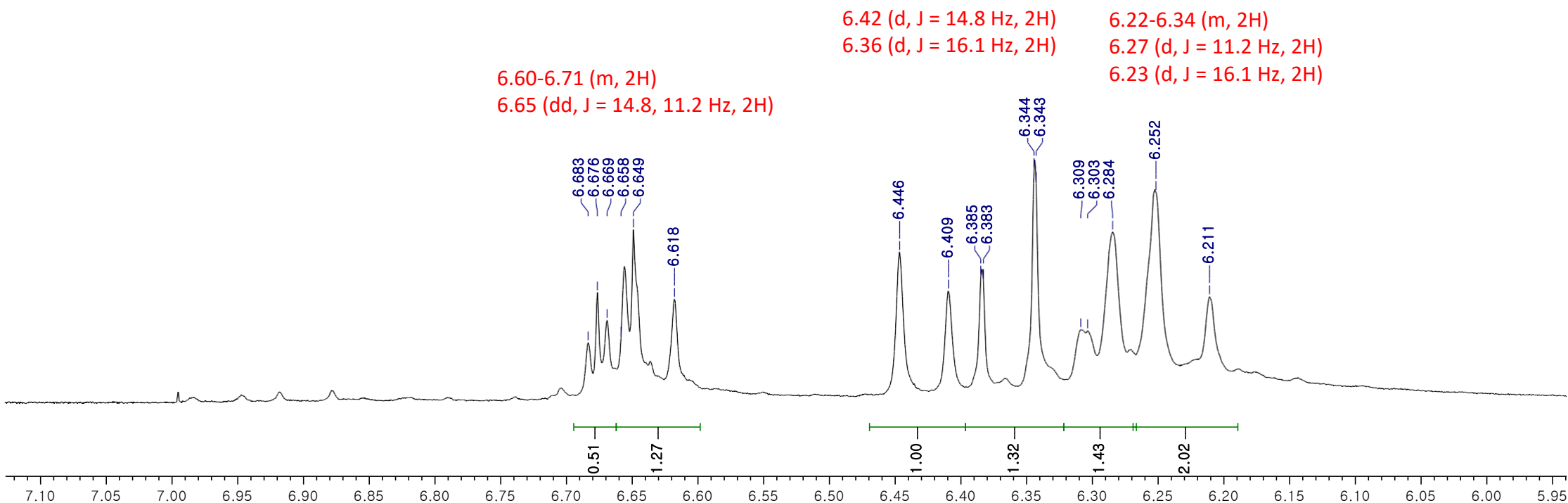
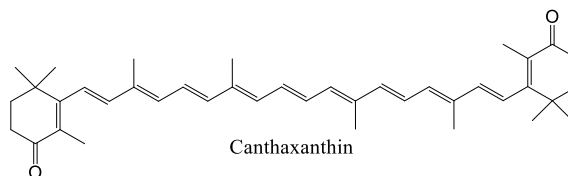
Study owner **vnmr1**  
 s400 operator **vnmr1**



Parameter	Value
Data File Name	D:/ NMR-SHK/ 2201-koo-4-04/ SGS-2039-1re_01/ SGS-2039-1re_PROTON_01.fid/ fid
Title	SGS-2039-1re_PROTON_01
Instrument	vnmrs
Solvent	cdcl3
Probe	5mm_ATB
Acquisition Date	2022-01-04T10:22:29
Spectrometer Frequency	400.04

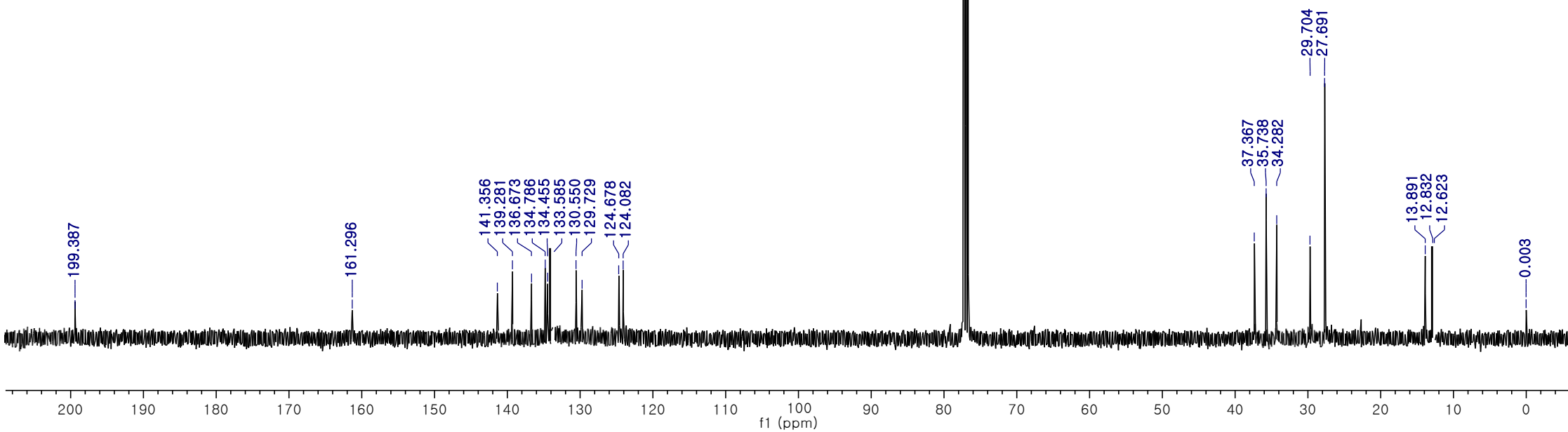
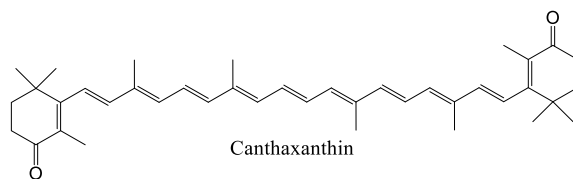


Parameter	Value
Data File Name	D:/ NMR-SHK/ 2201-koo-4-04/ SGS-2039-1re_01/ SGS-2039-1re_PROTON_01.fid/ fid
Title	SGS-2039-1re_PROTON_01
Instrument	vnmr5
Solvent	cdcl3
Probe	5mm_ATB
Acquisition Date	2022-01-04T10:22:29
Spectrometer Frequency	400.04



Parameter	Value
Data File Name	D:/ NMR-SHK/ 2201-koo-4-05/ SGS-2039-1re_01/ SGS-2039-1re_CARBON_01.fid/ fid
Title	SGS-2039-1re_CARBON_01
Instrument	vnmrs
Solvent	cdcl3
Probe	5mm_ATB
Acquisition Date	2022-01-05T13:35:39
Spectrometer Frequency	100.60

$^{13}\text{C}$  NMR (101 MHz,  $\text{cdcl}_3$ )  $\delta$  199.39, 161.30, 141.36, 139.28, 136.67, 134.79, 134.46, 133.58, 130.55, 129.73, 124.68, 124.08, 37.37, 35.74, 34.28, 29.70, 27.69, 13.89, 12.83, 12.62, 0.00.



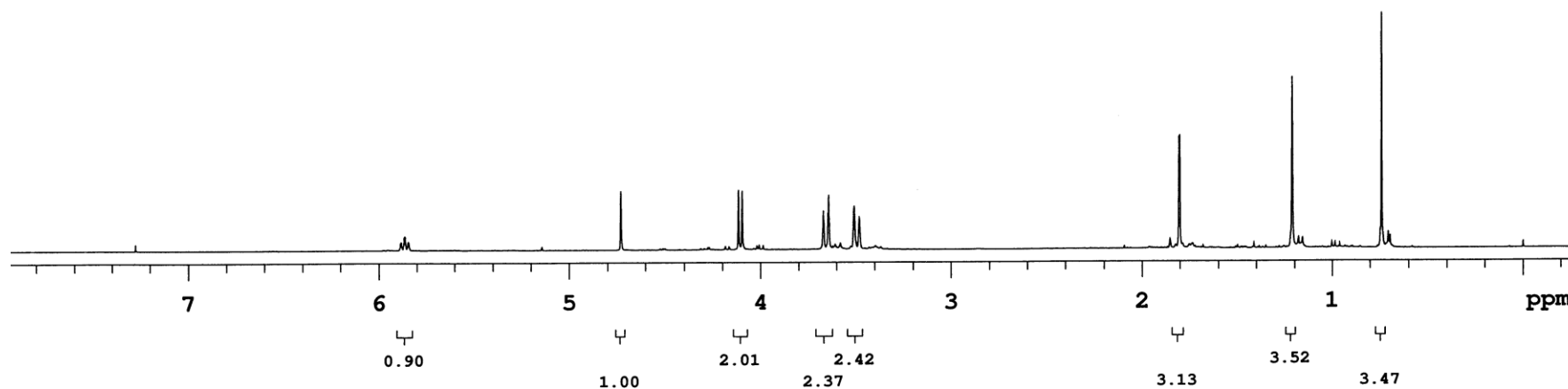
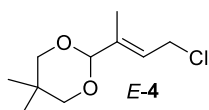
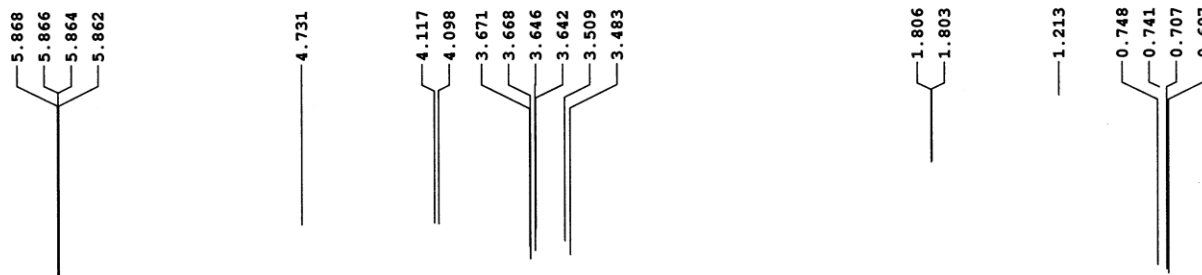
## (2) Assignment of *E*-stereochemistry for **4** by N.O.E.

SGS-2207-2

Sample Name **SGS-2207-2**  
Date collected **2022-06-20**

Pulse sequence **PROTON**  
Solvent **cdcl3**

Temperature **20**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**



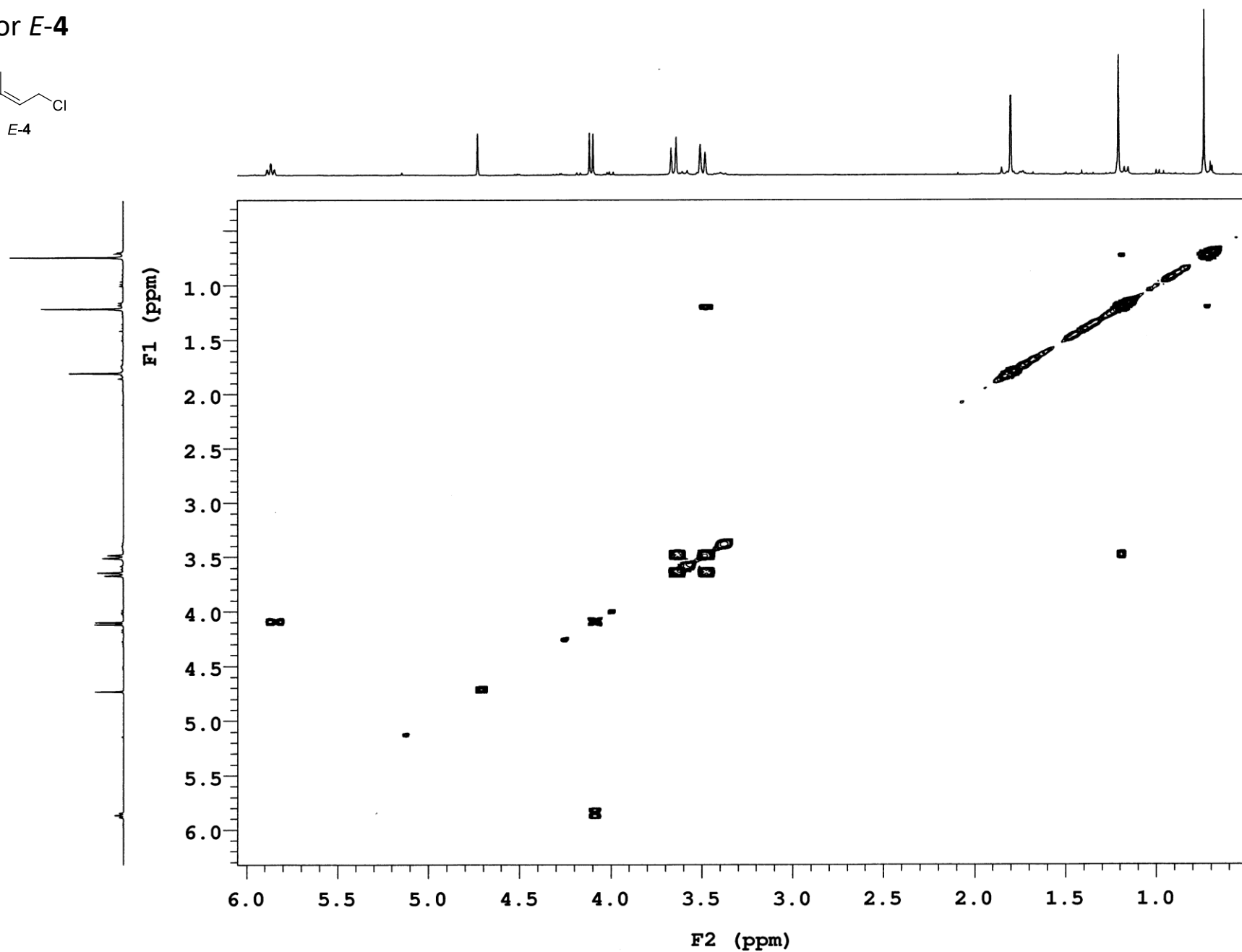
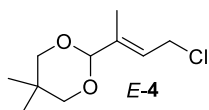
SGS-2207-2

Sample Name **SGS-2207-2**  
Date collected **2022-06-21**

Pulse sequence **gCOSY**  
Solvent **cdcl3**

Temperature **20**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**  
Study owner **vnmr1**  
Operator **vnmr1**

# COSY for *E*-4





SGS-2207-2

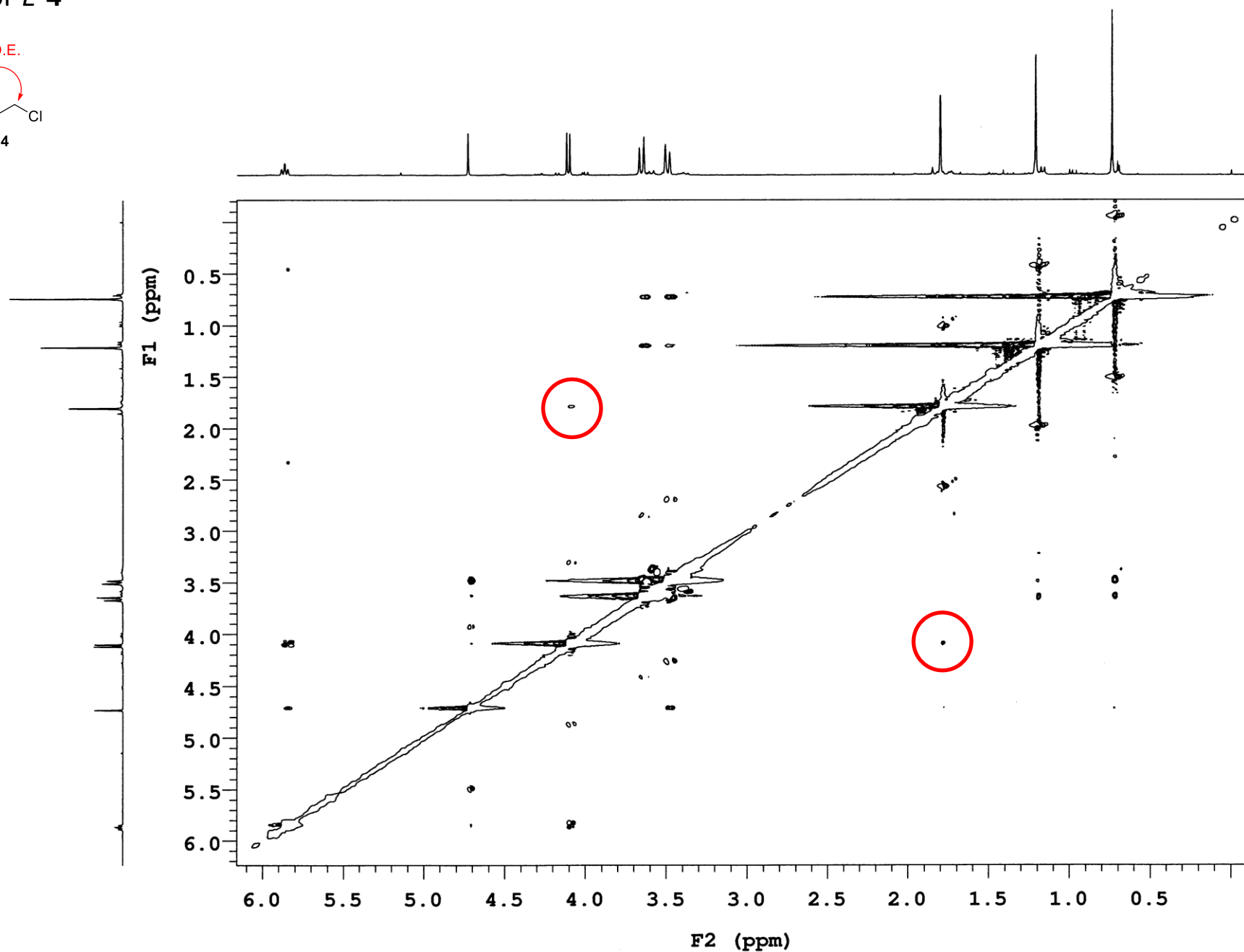
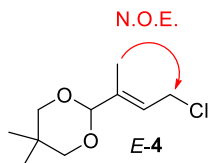
Sample Name **SGS-2207-2**  
Date collected **2022-06-21**

Pulse sequence **NOESY**  
Solvent **cdcl3**

Temperature **20**  
Spectrometer **Agilent-NMR.chem.com-vnmrs400**

Study owner **vnmr1**  
Operator **vnmr1**

# NOSEY for *E*-4

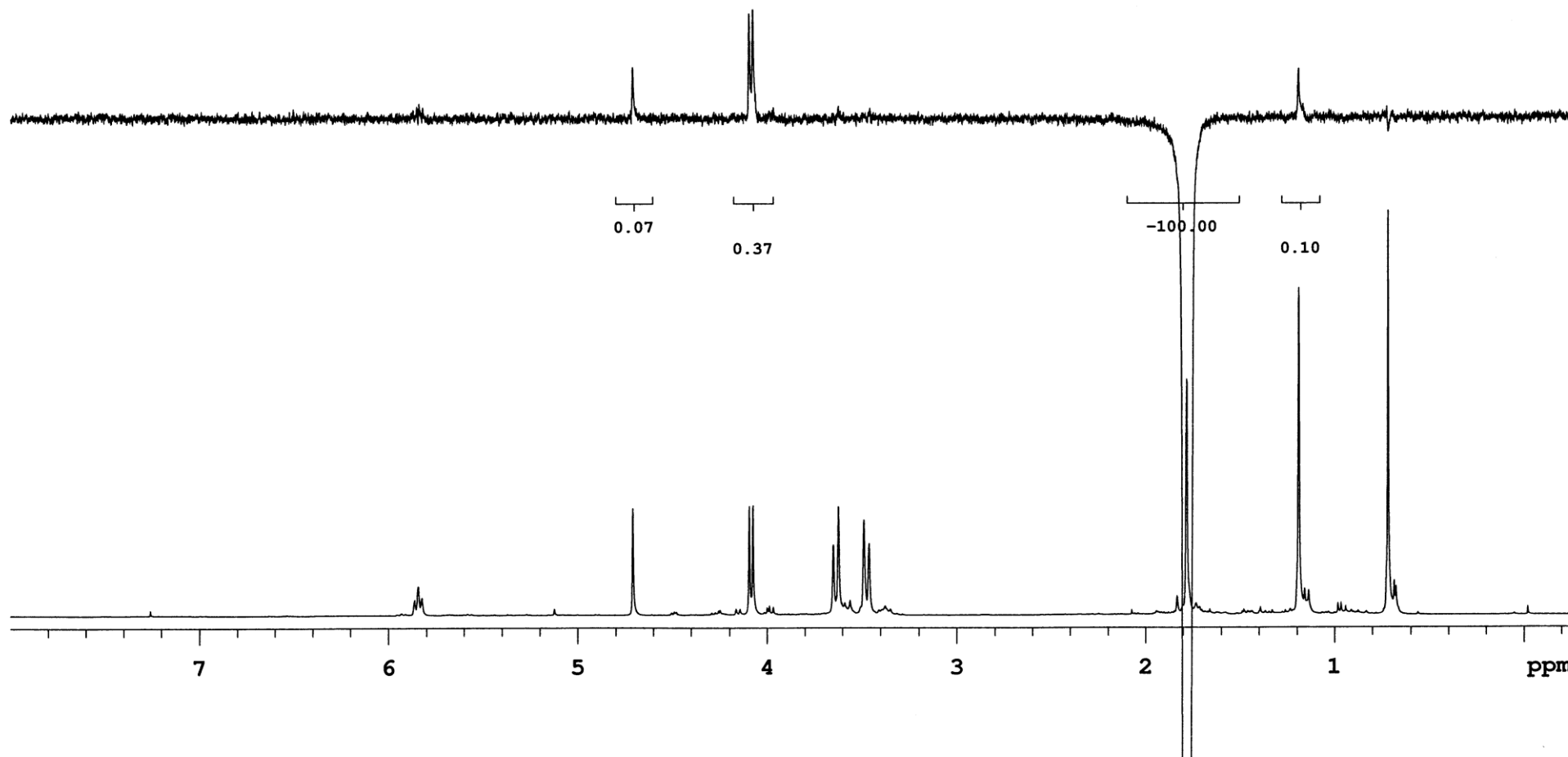
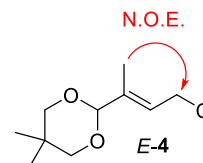


# 1D N.O.E. of *E*-4

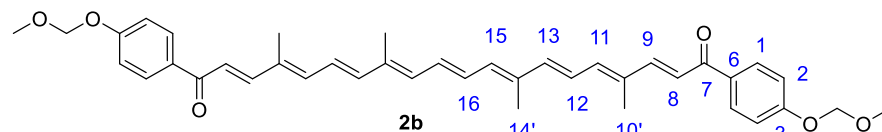


Sample Name:  
SGS-2207-2  
Data Collected on:  
Agilent-NMR.chem.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/2206-koo-4  
Sample directory:  
SGS-2207-2\_01  
FidFile: SGS-2207-2\_PROTON\_01

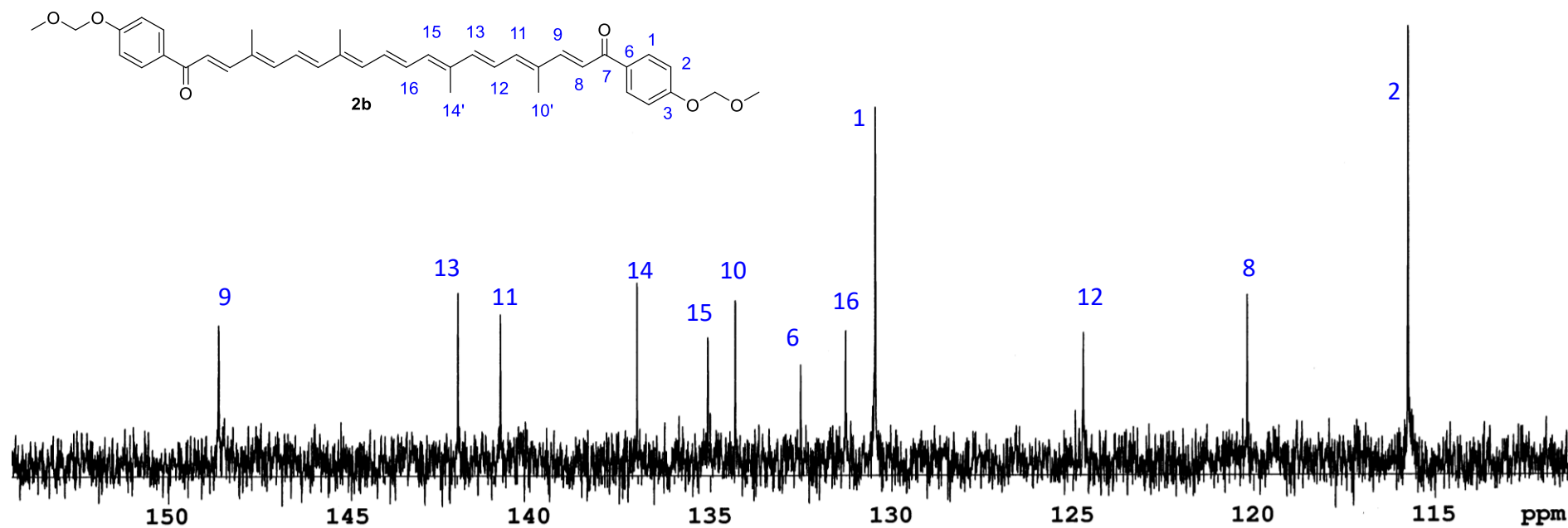
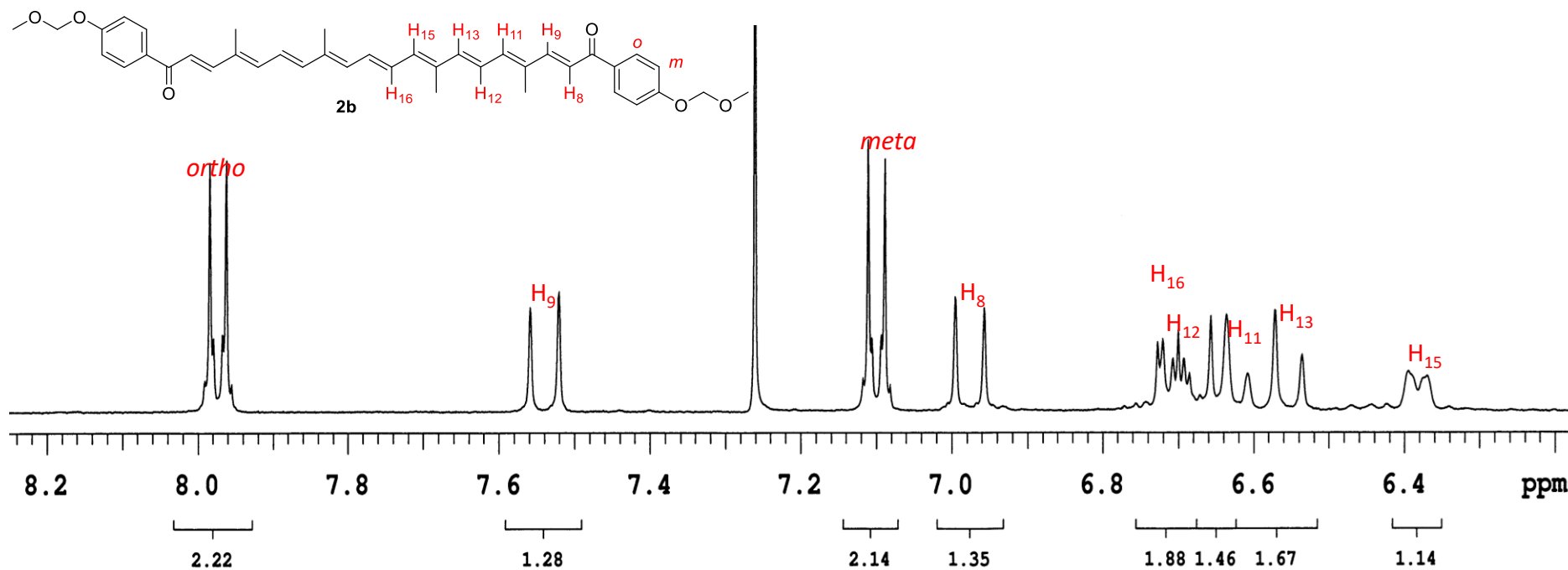
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 22 2022



### (3) Peak assignment for **2b** by COSY, HMBC, and DEPT



Numbering	<sup>1</sup> H NMR		<sup>13</sup> C NMR	
	Shift (ppm)	Multiplicity (Hz)	Shift (ppm)	DEPT
<b>1</b>	7.97	d (8.8)	130.5	CH
<b>2</b>	7.10	d (8.8)	115.7	CH
<b>3</b>	-	-	160.7	C
<b>3-OCH<sub>2</sub>O</b>	5.25	s	94.1	CH <sub>2</sub>
<b>3-OMe</b>	3.50	s	56.2	CH <sub>3</sub>
<b>6</b>	-	-	132.5	C
<b>7</b>	-	-	188.9	C
<b>8</b>	6.97	d (15.2)	120.2	CH
<b>9</b>	7.54	d (15.2)	148.6	CH
<b>10</b>	-	-	134.3	C
<b>10'(Me)</b>	2.06	s	12.9	CH <sub>3</sub>
<b>11</b>	6.62	d (11.2)	140.8	CH
<b>12</b>	6.69	dd (14.4, 11.2)	124.7	CH
<b>13</b>	6.55	d (14.4)	142.0	CH
<b>14</b>	-	-	137.0	C
<b>14'(Me)</b>	2.01	s	12.8	CH <sub>3</sub>
<b>15</b>	6.33-6.43	m	135.1	CH
<b>16</b>	6.66-6.76	m	131.3	CH



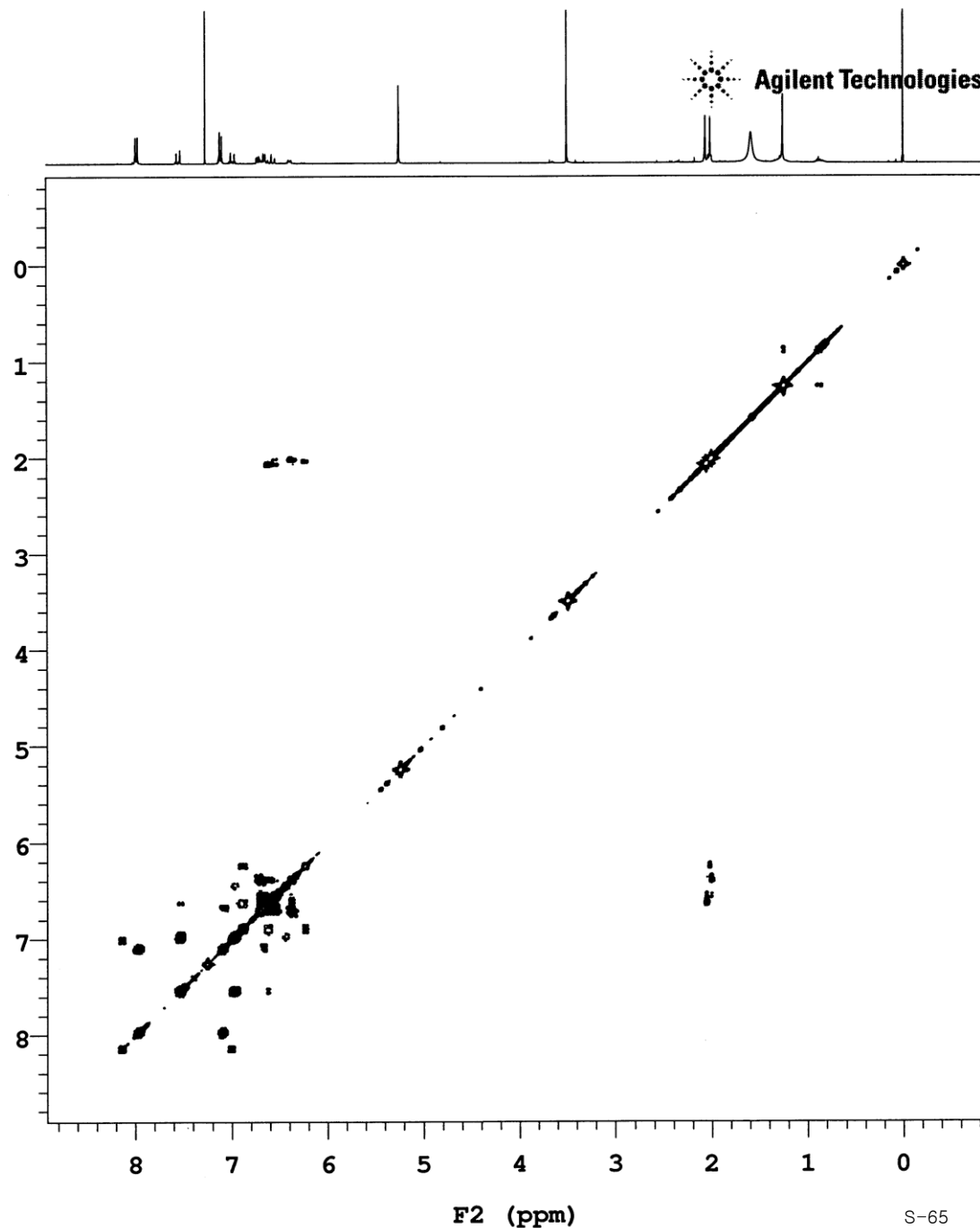
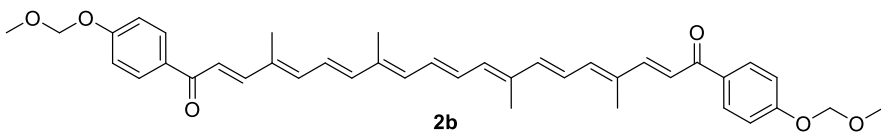
# COSY for 2b

Sample Name:  
SGS-1586-3re-2D\_NMR  
Data Collected on:  
Agilent-NMR.chem.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/2206-koo-4-25  
Sample directory:  
SGS-1586-3re-2D\_NMR\_01  
FidFile: SGS-1586-3re-2D\_NMR\_gCOSY\_01

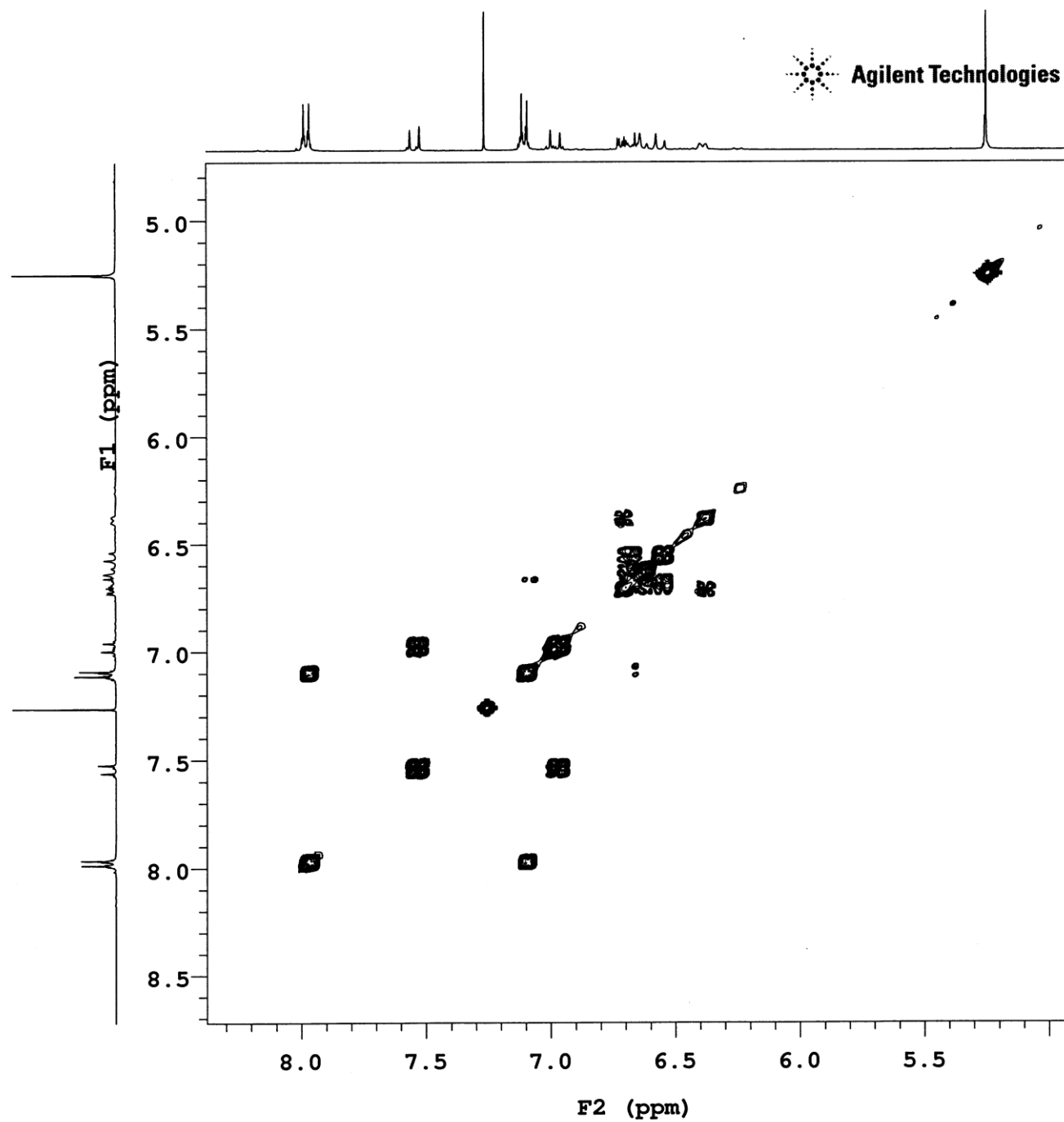
Pulse Sequence: gCOSY  
Solvent: cdcl3  
Data collected on: Jun 25 2022

Sample #21, Operator: vnmr1

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 3930.8 Hz  
2D Width 3930.8 Hz  
16 repetitions  
512 increments  
OBSERVE H1, 400.0405310 MHz  
DATA PROCESSING  
Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Sq. sine bell 0.080 sec  
FT size 4096 x 4096  
Total time 2 hr, 50 min



# COSY for 2b



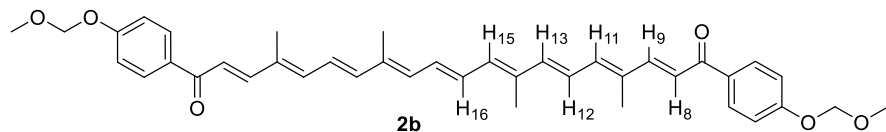
# COSY for 2b

Sample Name:  
SGS-1586-3re-2D\_NMR  
Data Collected on:  
Agilent-NMR.chem.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/2206-koo-4-25  
Sample directory:  
SGS-1586-3re-2D\_NMR\_01  
FidFile: SGS-1586-3re-2D\_NMR\_gCOSY\_01

Pulse Sequence: gCOSY  
Solvent: cdcl3  
Data collected on: Jun 25 2022

Sample #21, Operator: vnmr1

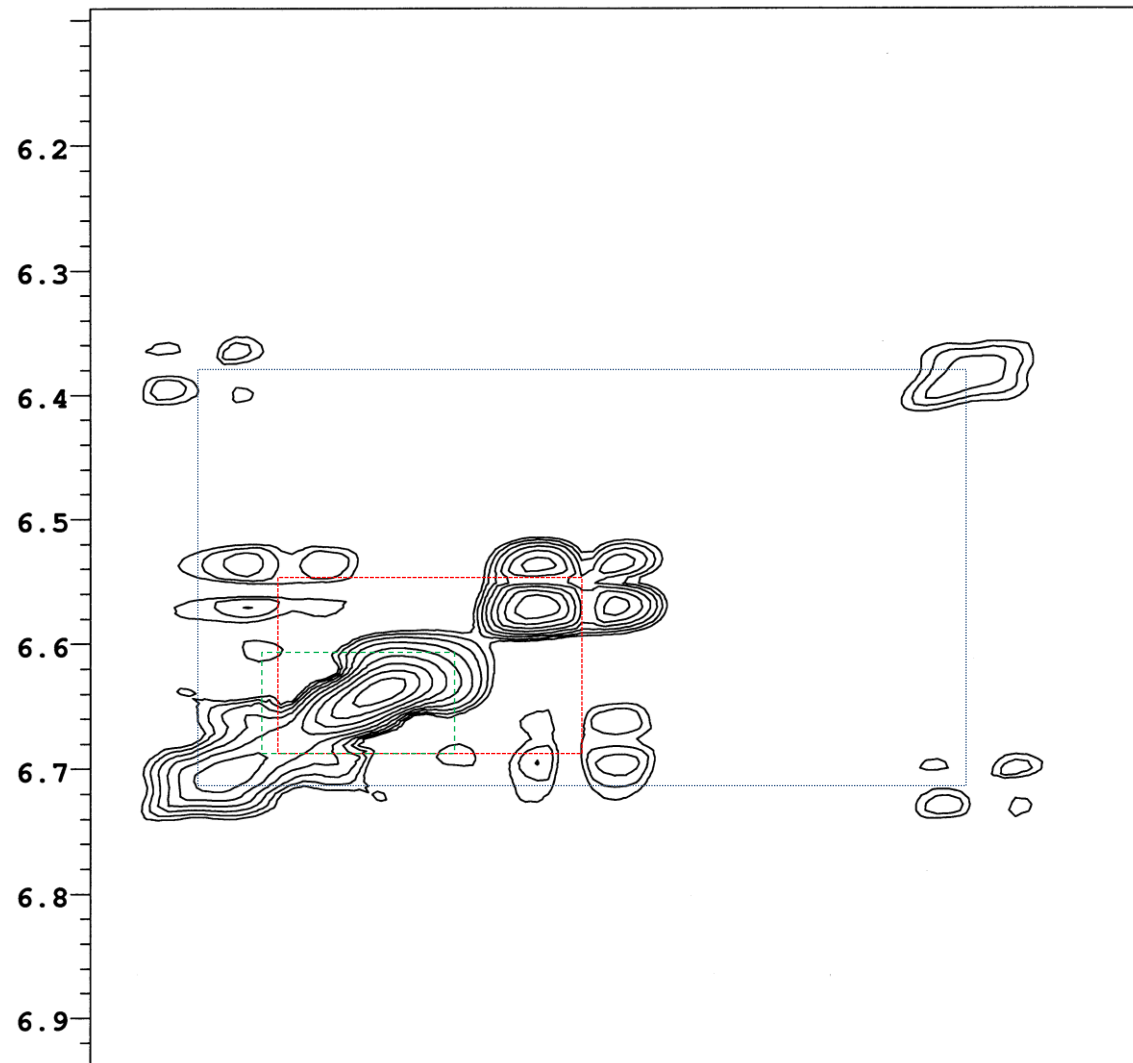
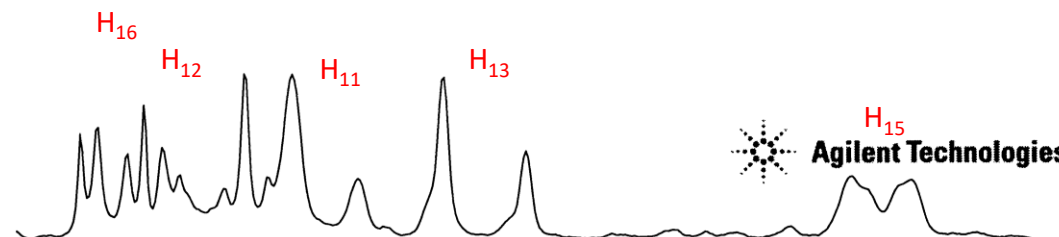
Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 3930.8 Hz  
2D Width 3930.8 Hz  
16 repetitions  
512 increments  
OBSERVE H1, 400.0405310 MHz  
DATA PROCESSING  
Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Sq. sine bell 0.080 sec  
FT size 4096 x 4096  
Total time 2 hr, 50 min



F1 (ppm)

H<sub>15</sub>  
H<sub>13</sub>  
H<sub>11</sub>  
H<sub>12</sub>  
H<sub>16</sub>

6.2  
6.3  
6.4  
6.5  
6.6  
6.7  
6.8  
6.9



6.7

6.6

6.5

6.4

F2 (ppm)

# NOSEY for 2b

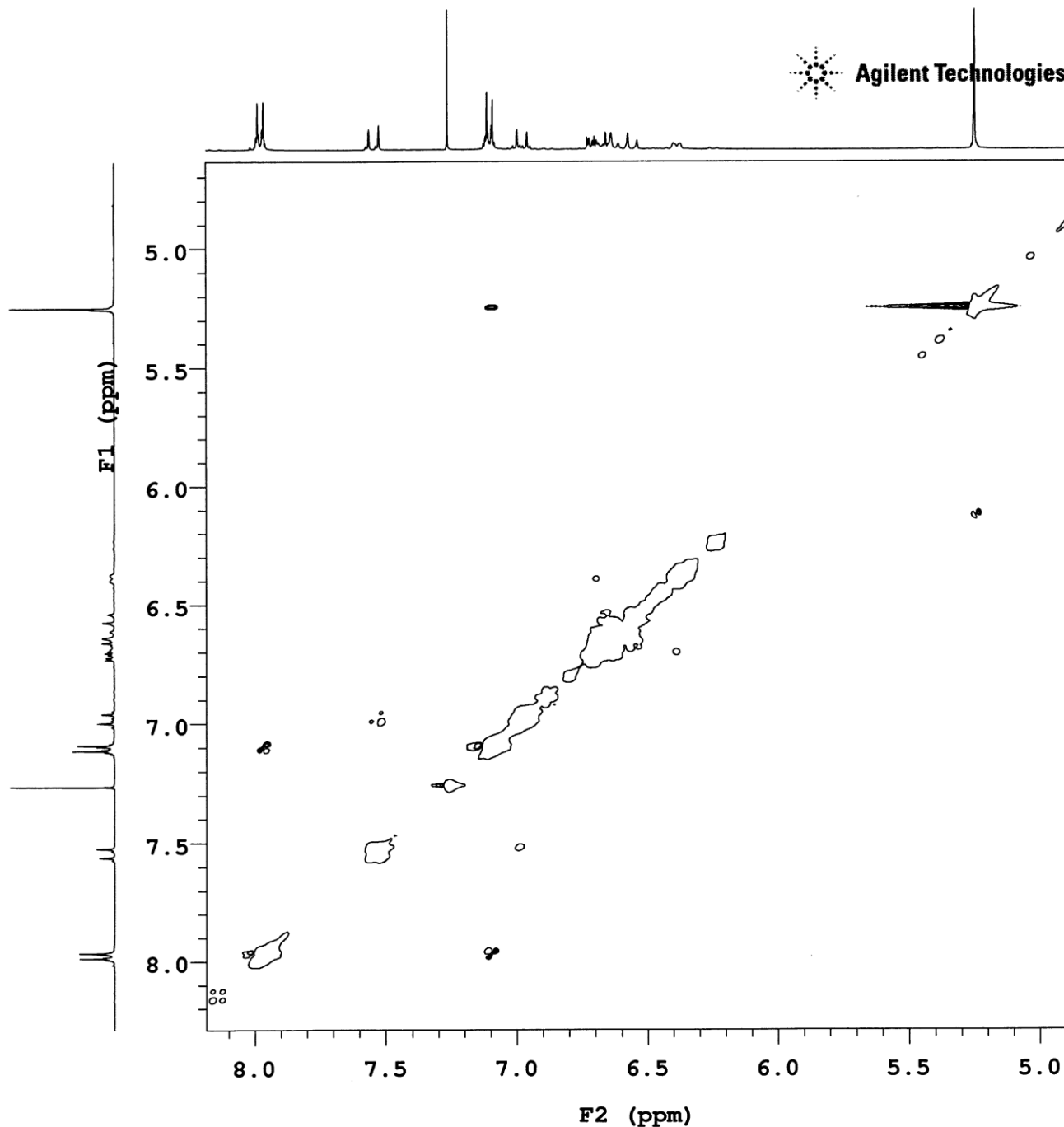


Sample Name:  
SGS-1586-3re-2D\_NMR  
Data Collected on:  
Agilent-NMR.chem.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/2206-koo-4-25  
Sample directory:  
SGS-1586-3re-2D\_NMR\_01  
FidFile: SGS-1586-3re-2D\_NMR\_NOESY\_01

Pulse Sequence: NOESY  
Solvent: cdcl3  
Data collected on: Jun 25 2022

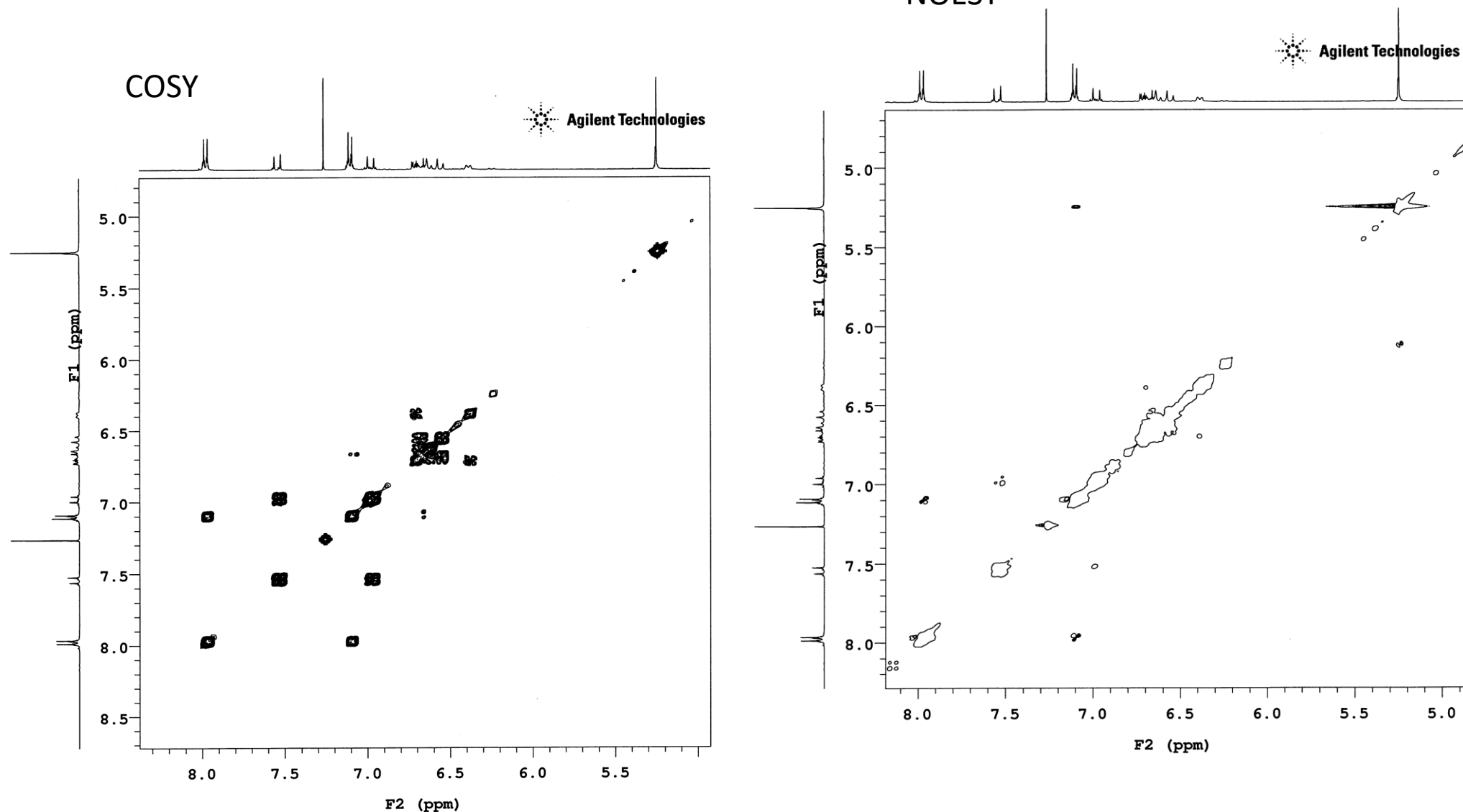
Sample #21, Operator: vnmr1

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 3930.8 Hz  
2D Width 3930.8 Hz  
16 repetitions  
2 x 512 increments  
OBSERVE H1, 400.0405310 MHz  
DATA PROCESSING  
Gauss apodization 0.069 sec  
F1 DATA PROCESSING  
Gauss apodization 0.074 sec  
FT size 4096 x 4096  
Total time 6 hr, 28 min



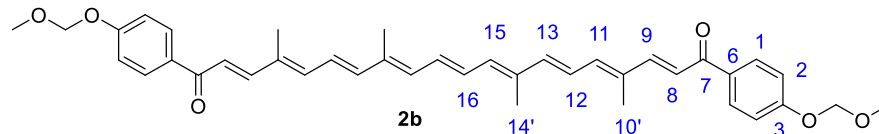


## Comparison of COSY and NOESY for **2b**



No further correlation in NOESY spectra (compared with COSY) confirmed all-*E* stereochemistry for **2b**

# HMBC for 2b

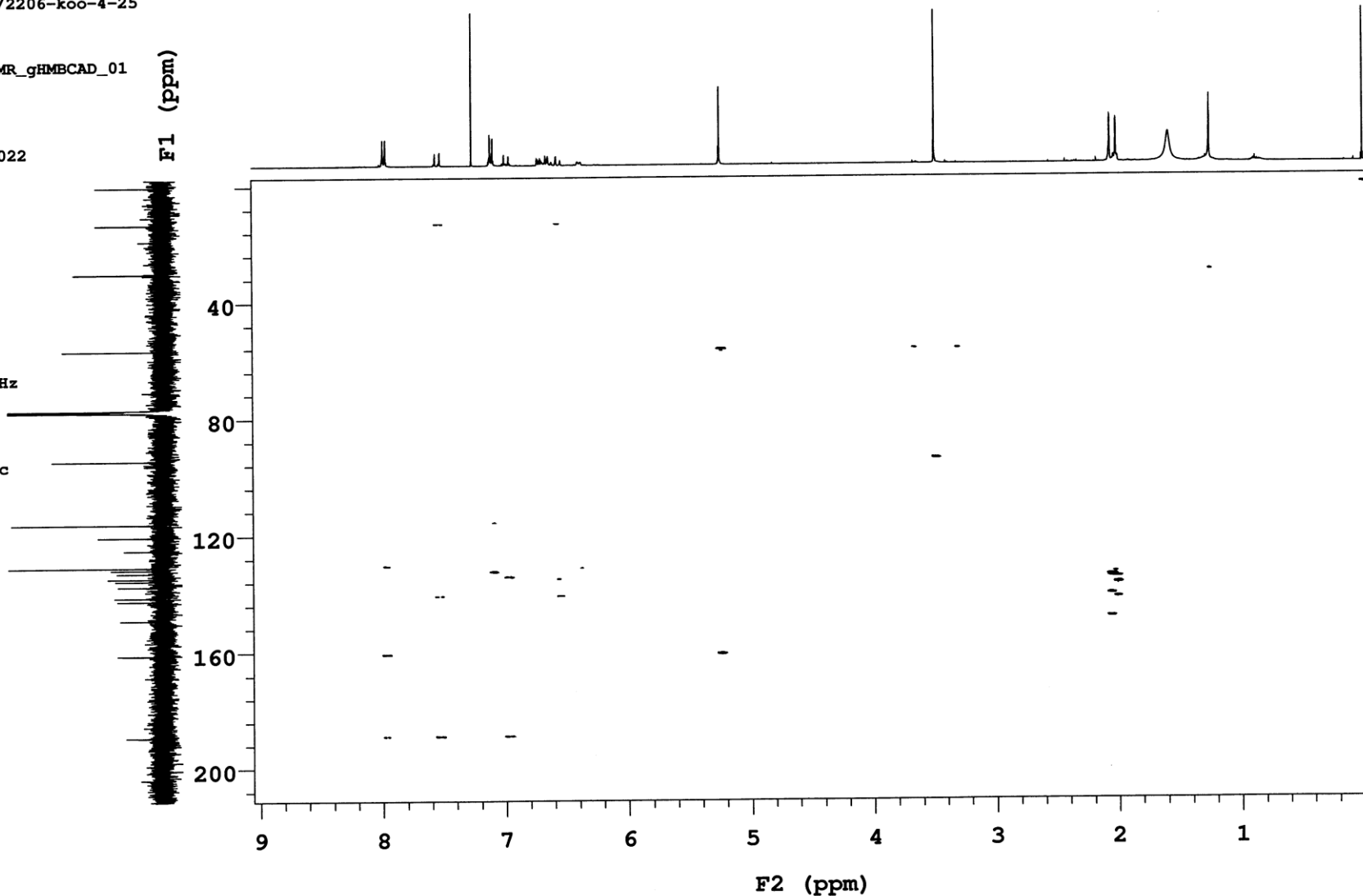


Sample Name:  
SGS-1586-3re-2D\_NMR  
Data Collected on:  
Agilent-NMR.chem.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/2206-koo-4-25  
Sample directory:  
SGS-1586-3re-2D\_NMR\_01  
FidFile: SGS-1586-3re-2D\_NMR\_gHMBCAD\_01

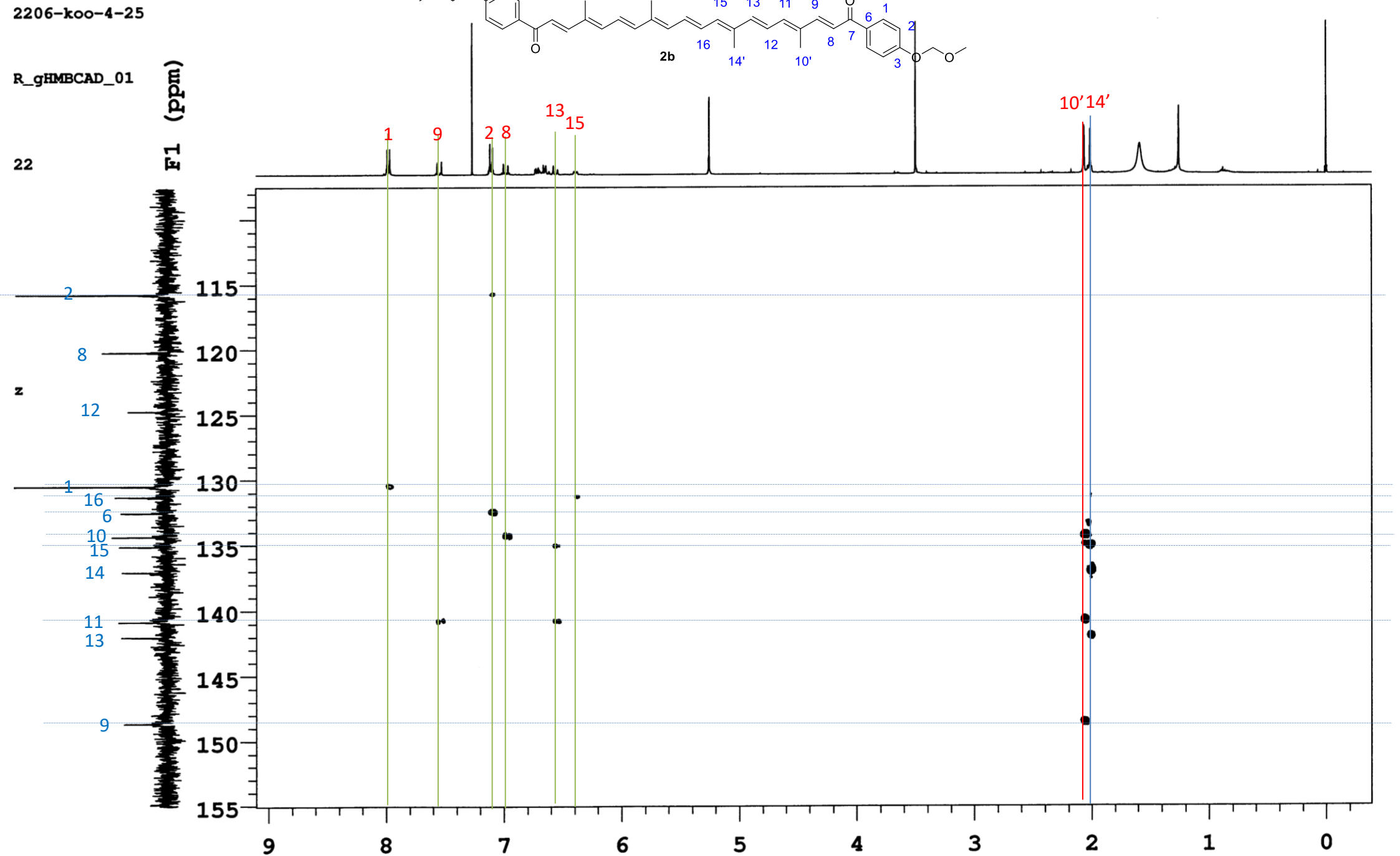
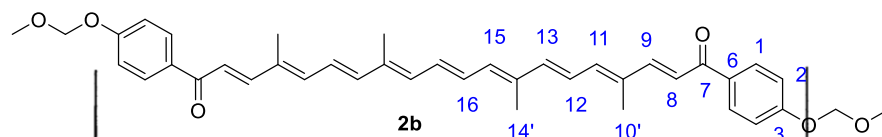
Pulse Sequence: gHMBCAD  
Solvent: cdcl3  
Data collected on: Jun 25 2022

Sample #21, Operator: vnmr1

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 6410.3 Hz  
2D Width 24140.0 Hz  
16 repetitions  
2 x 512 increments  
OBSERVE H1, 400.0405310 MHz  
DATA PROCESSING  
Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Gauss apodization 0.020 sec  
FT size 2048 x 4096  
Total time 5 hr, 39 min

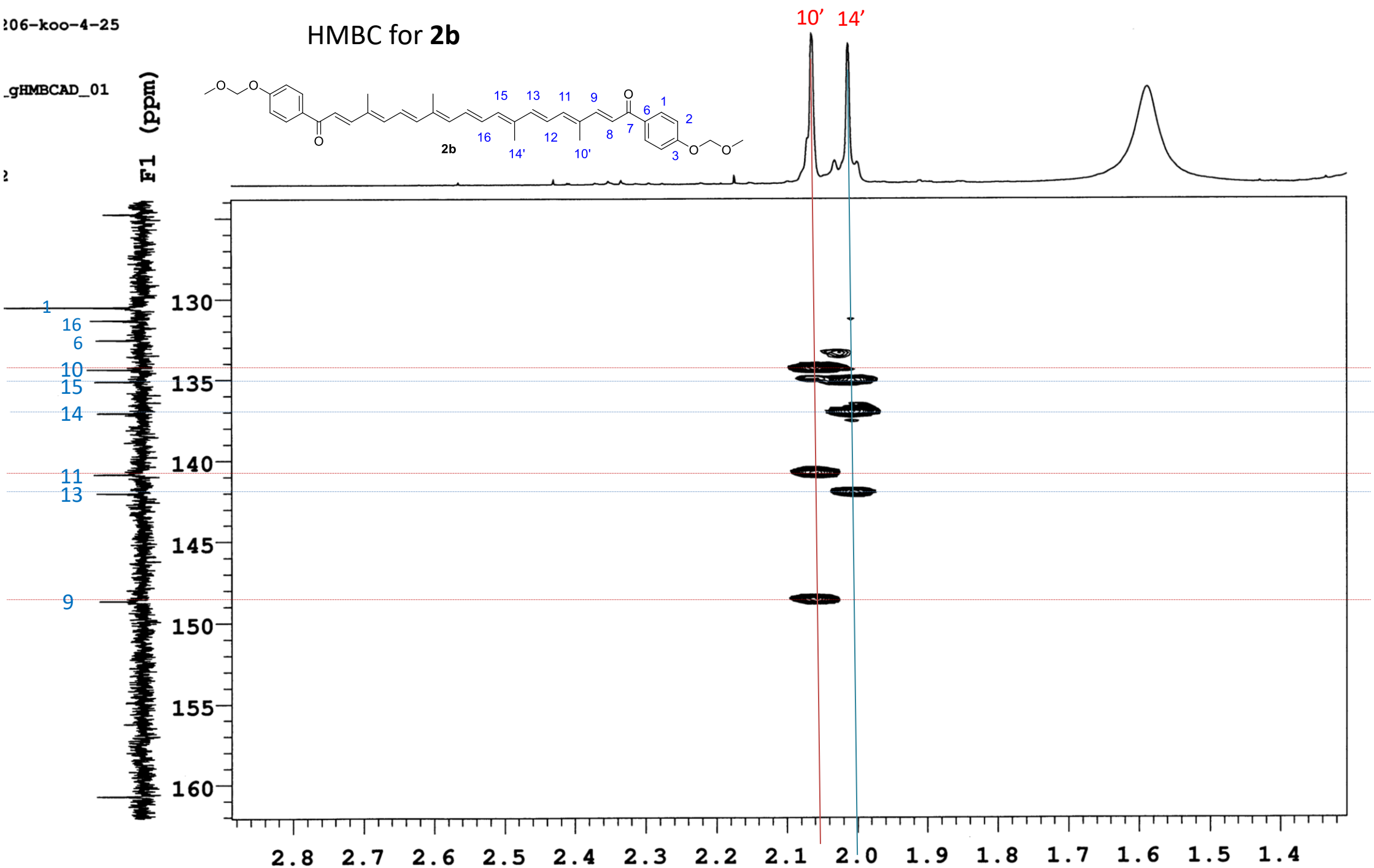


# HMBC for **2b**



HMBC for **2b**

\_gHMBCAD\_01



# HMBC for **2b**

'2206-koo-4-25

IR\_gHMBCAD\_01

122

F1 (ppm)

1z

:

132

136

140

144

148

6.8

6.7

6.6

6.5

6.4

6.3

6.2

F2 (ppm)

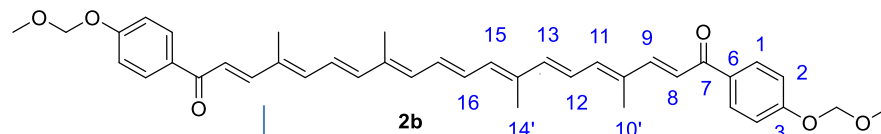
H<sub>16</sub>

H<sub>12</sub>

H<sub>11</sub>

H<sub>13</sub>

H<sub>15</sub>



**2b**

HMBC for **2b**

IMR\_gHMBCAD\_01

2022

meta

ortho

4Hz

13C

F1 (ppm)

120  
130  
140  
150  
160  
170  
180  
190

8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0

F2 (ppm)

Ortho

Meta

1

2

H<sub>9</sub>

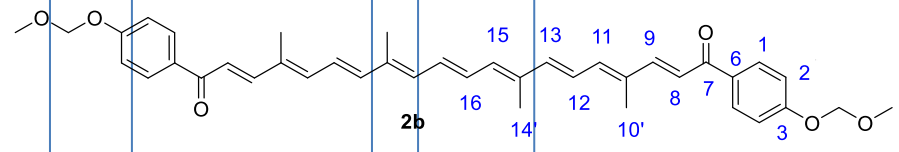
H<sub>8</sub>

H<sub>16</sub>  
H<sub>12</sub>

H<sub>11</sub>

H<sub>13</sub>

H<sub>15</sub>



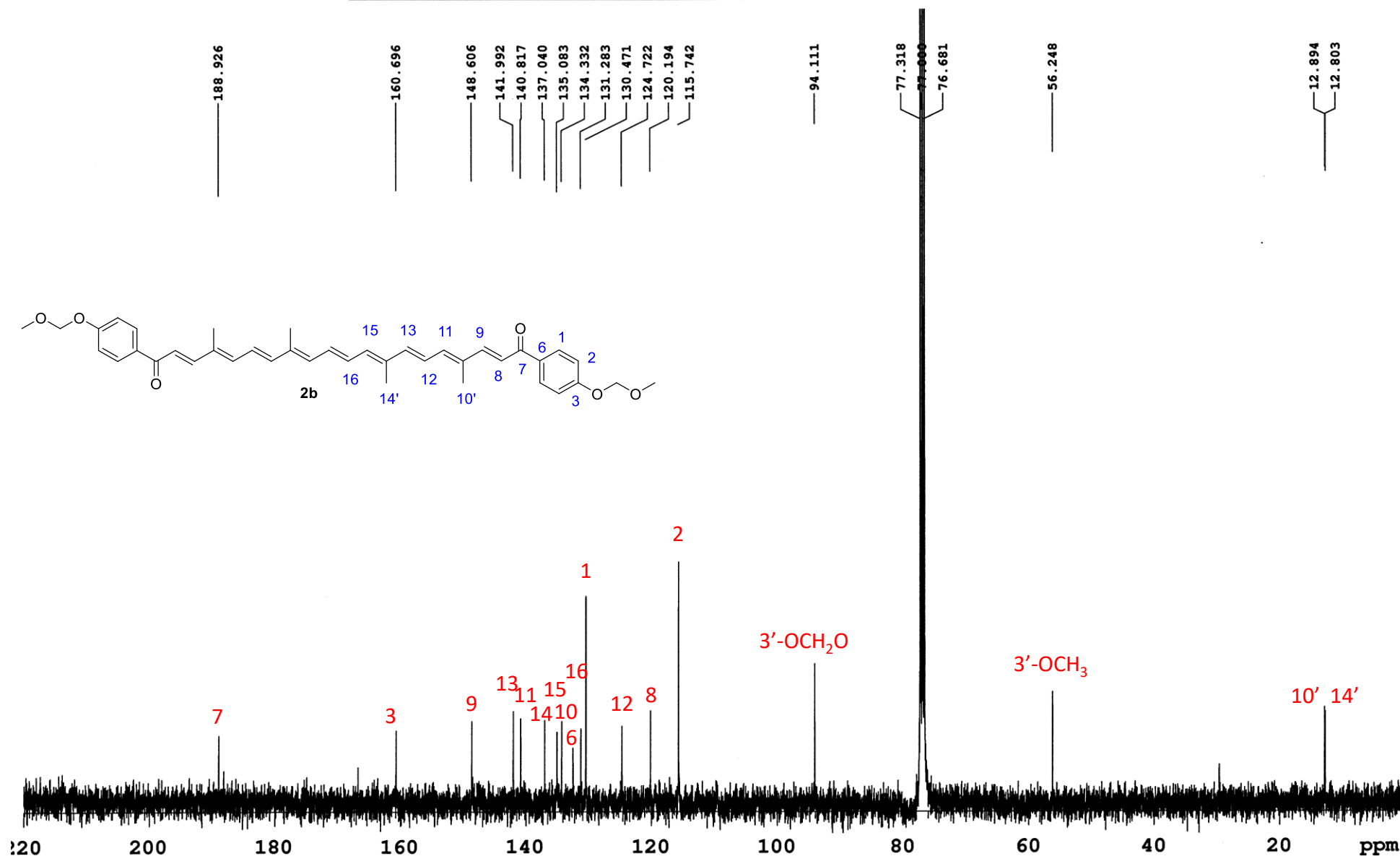
# <sup>13</sup>C-NMR for **2b**

SGS-1557-3re-13C

Sample Name **SGS-1557-3re-13C**  
Date collected **2021-09-09**

Pulse sequence **CARBON**  
Solvent **cdcl3**

Temperature **25**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**



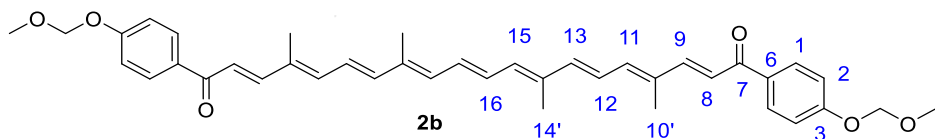
# DEPT for 2b

SGS-1586-3re-DEPT

Sample Name **SGS-1586-3re-DEPT**  
Date collected **2022-06-30**

Pulse sequence **DEPT**  
Solvent **cdcl3**

Temperature **20**  
Spectrometer **Agilent-NMR.chem.com-vnmr400**  
Study owner **vnmr1**  
Operator **vnmr1**



CH3 carbons

3'-OCH<sub>3</sub>

10' 14'

CH2 carbons

3'-OCH<sub>2</sub>O

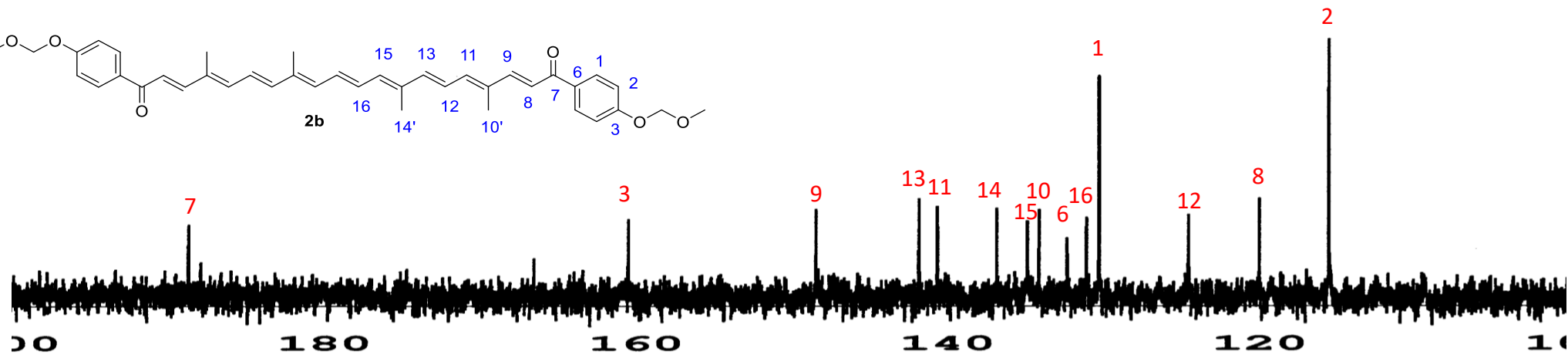
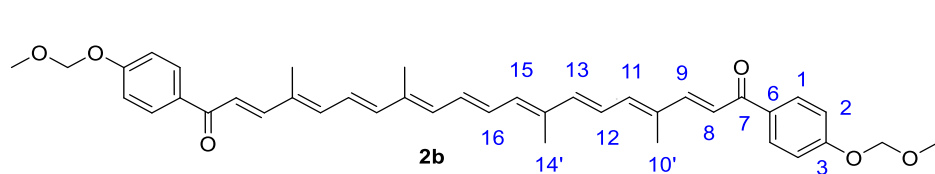
CH carbons

quaternary carbons

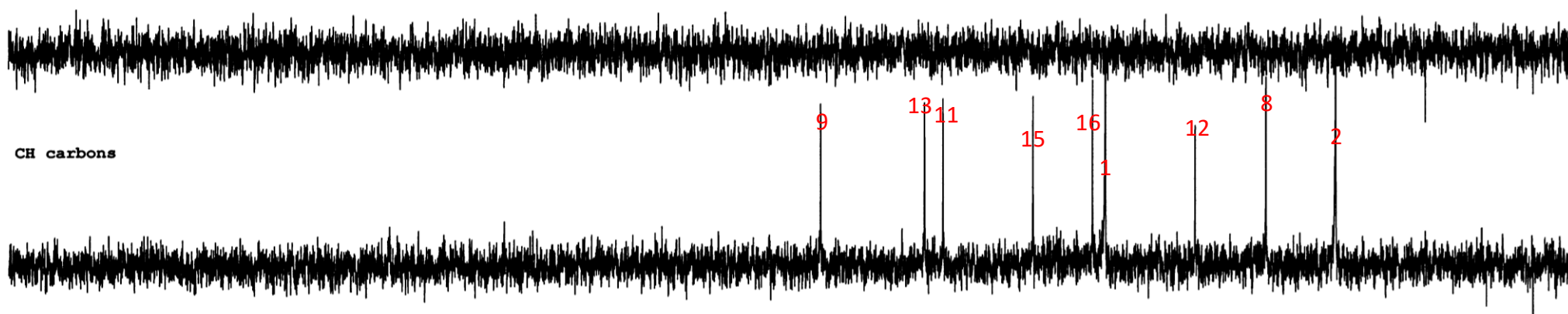
200 180 160 140 120 100 80 60 40 20 ppm



# DEPT for 2b



CH<sub>2</sub> carbons



CH carbons

quaternary carbons

