

**Supporting Information-2 for  
Role of Ring *Ortho* Substituents on the Configuration of Carotenoid  
Polyene Chains**

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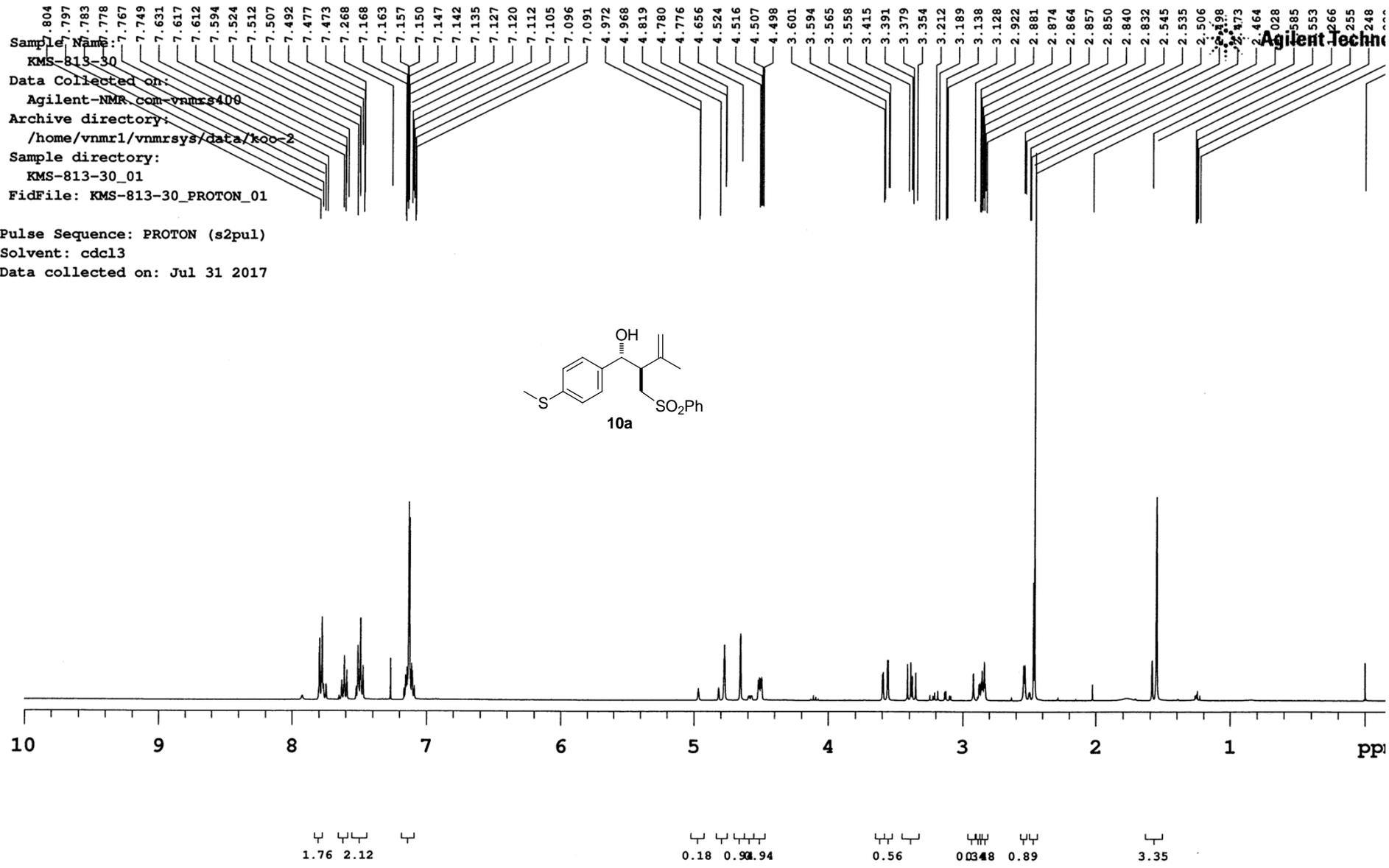
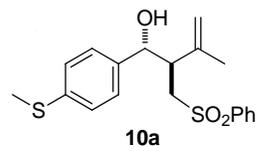
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<sup>3</sup>Department of Applied Chemistry, Kyung Hee University, Yongin, Gyeonggi-Do, 17104, Korea

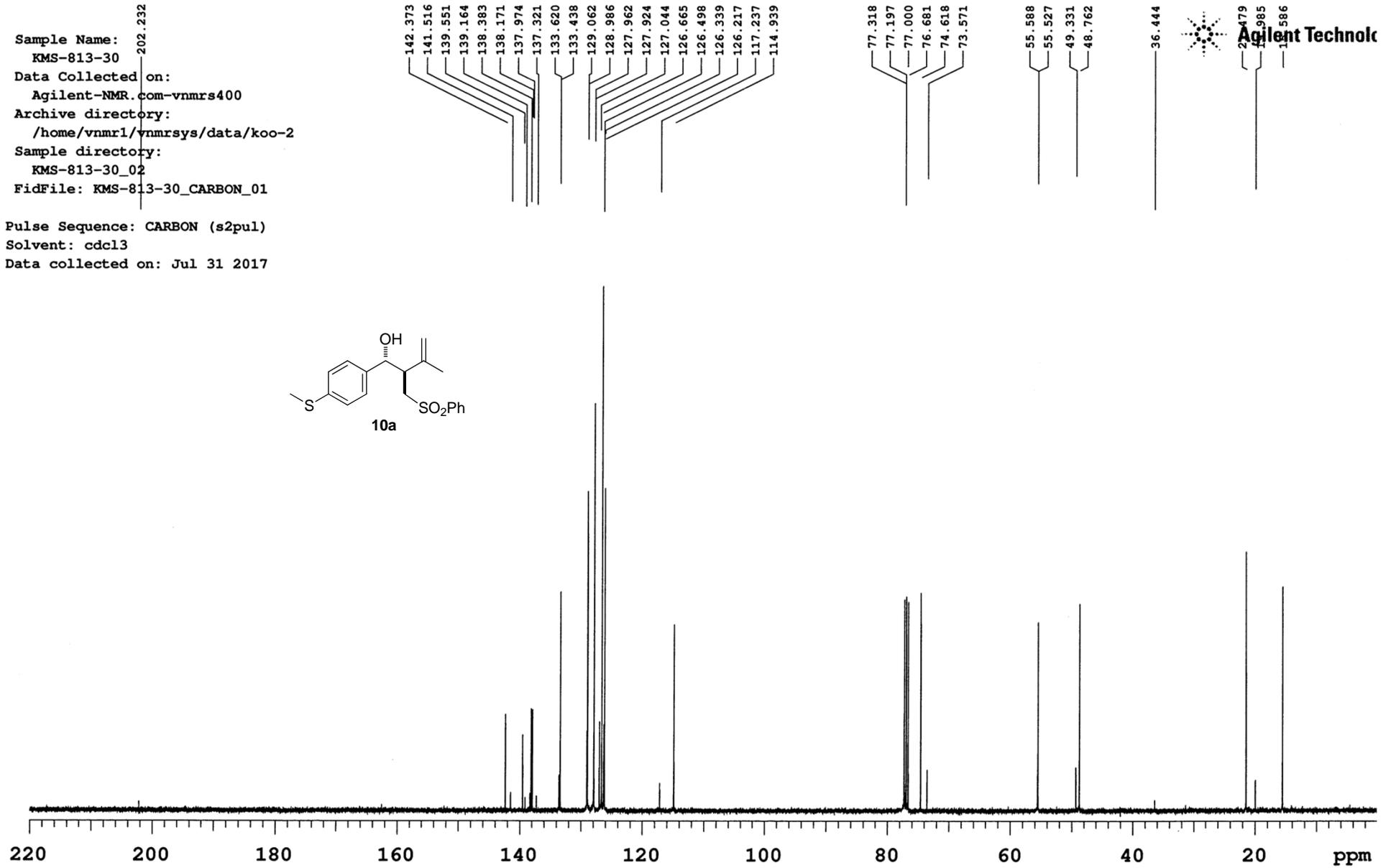
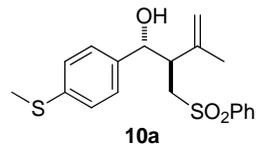
**NMR, UV, HPLC spectra of the compounds for the synthesis of 9-(*Z*)-9,9',13,13'-tetramethyl  
carotene 13 and all-(*E*)-9,9',13,13'-tetramethyl carotene 15**

Sample Name: KMS-813-30  
 Data Collected on: Agilent-NMR.com-vnmrs400  
 Archive directory: /home/vnmr1/vnmrsys/data/koo-2  
 Sample directory: KMS-813-30\_01  
 FidFile: KMS-813-30\_PROTON\_01  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Jul 31 2017



Sample Name: KMS-813-30  
 Data Collected on: Agilent-NMR.com-vnmrs400  
 Archive directory: /home/vnmr1/vnmrsys/data/koo-2  
 Sample directory: KMS-813-30\_02  
 FidFile: KMS-813-30\_CARBON\_01

Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Jul 31 2017



Sample: KMS-045-P  
Sample ID: s\_43\_KMS-045-P\_koo-2\_20150501\_01  
File: /home/waikup2/vnmrSYS/data/koo-2/KMS-045-P\_Proton\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdc13  
Temp. 25.0 C / 298.1 K  
Sample #43, Operator: walkup2  
File: KMS-045-P\_Proton\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340096 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

7.884  
7.864  
7.867  
7.649  
7.630  
7.562  
7.542  
7.523  
7.331  
7.310  
7.261  
7.213  
7.193  
7.176  
6.755  
6.715  
6.484  
6.444

5.582  
5.563  
5.541

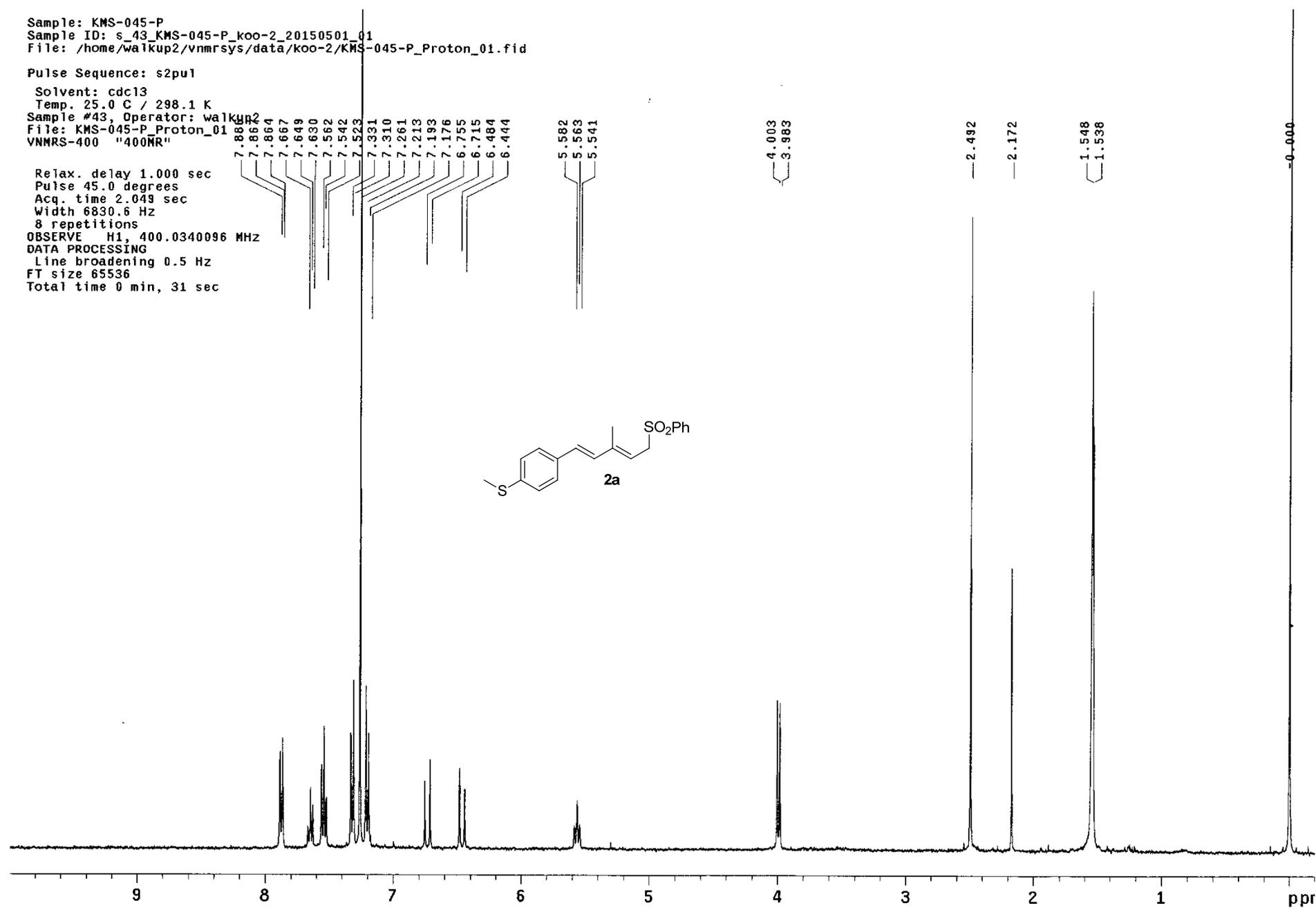
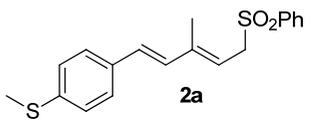
4.003  
3.983

2.492

2.172

1.548  
1.538

-0.000



1.78 2.02 2.10  
1.00 2.17

1.04 1.06

1.00

2.02

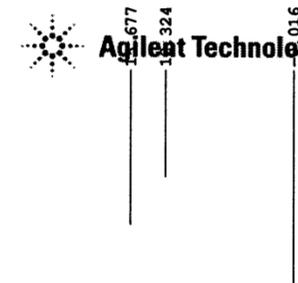
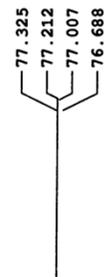
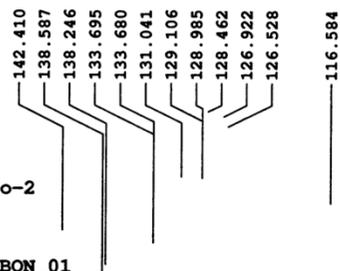
2.91

1.13

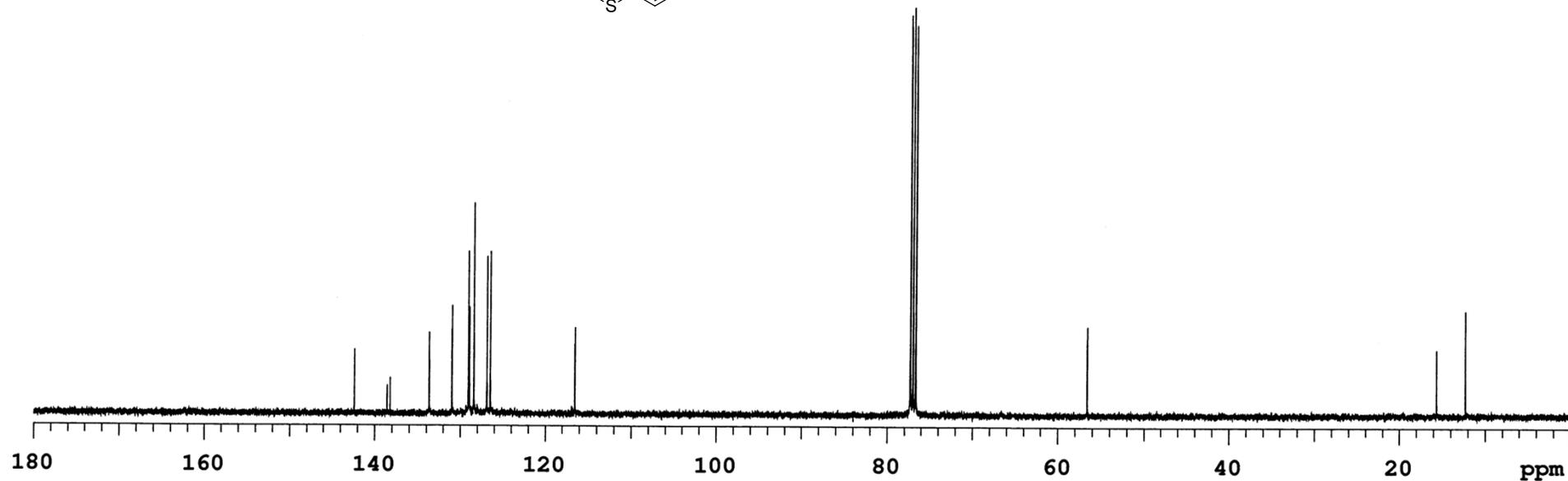
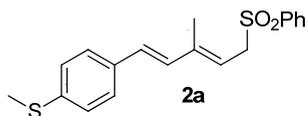
3.71  
4.75

S2-4

Sample Name:  
KDH-KMSSulfone-C  
Data Collected on:  
Agilent-NMR.com-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/koo-2  
Sample directory:  
KDH-KMSSulfone-C\_01  
FidFile: KDH-KMSSulfone-C\_CARBON\_01



Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 22 2017







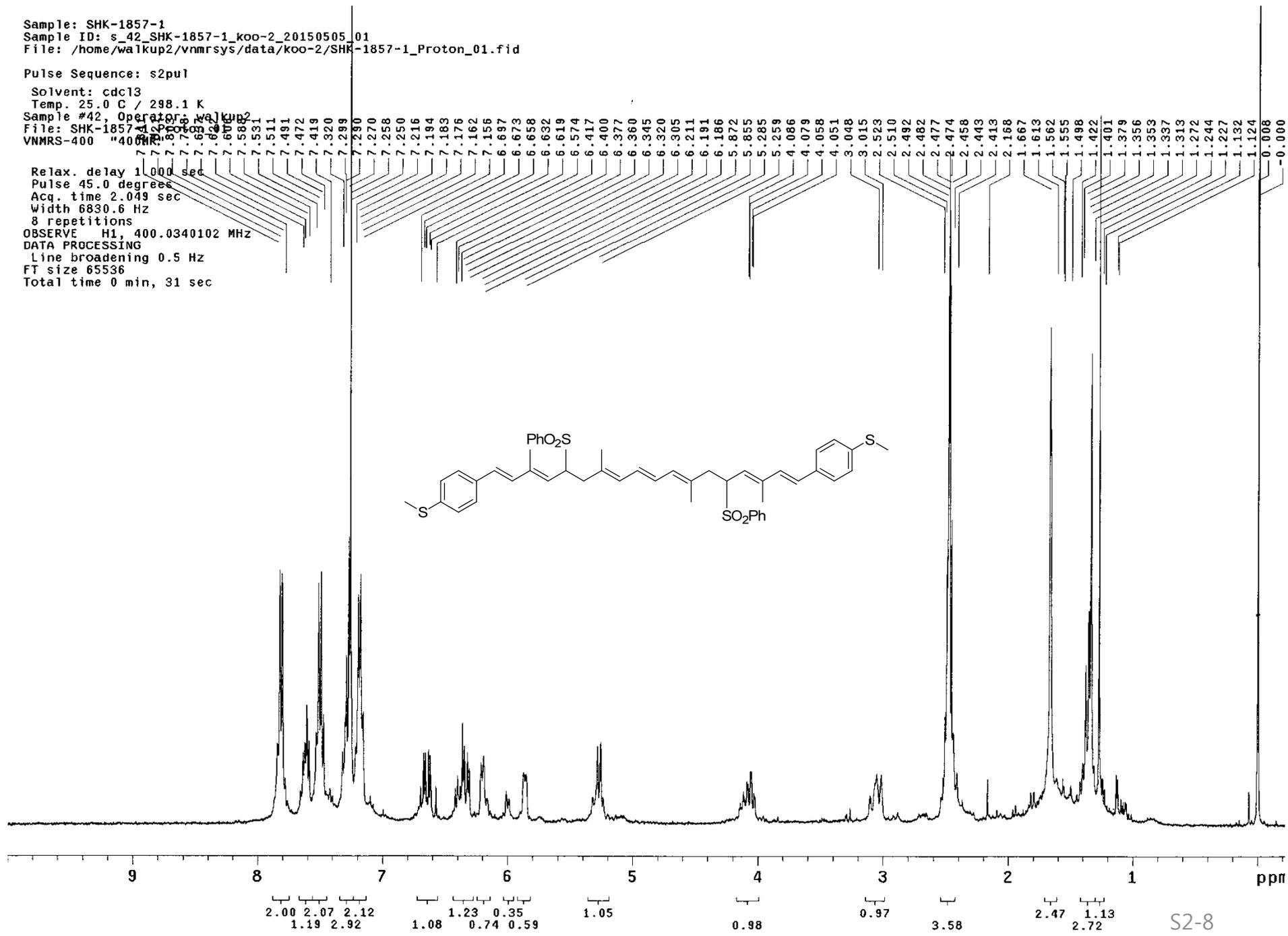
Sample: SHK-1857-1  
Sample ID: s\_42\_SHK-1857-1\_koo-2\_20150505\_01  
File: /home/walkup2/vnmrsvs/data/koo-2/SHK-1857-1\_Proton\_01.fid

Pulse Sequence: s2pul

Solvent: cdc13  
Temp. 25.0 C / 298.1 K

Sample #42, Operator: kjk  
File: SHK-1857-1\_koo-2\_20150505\_01  
VNMR-400 = 400.136360 MHz

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340102 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



SHK-1862-2R-re

Sample: SHK-1862-2R-re

Sample ID: s\_46\_SHK-1862-2R-re\_koo-2\_20150520\_01

File: /home/walkup2/vnmr/20150520/SHK-1862-2R-re\_Proton\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13

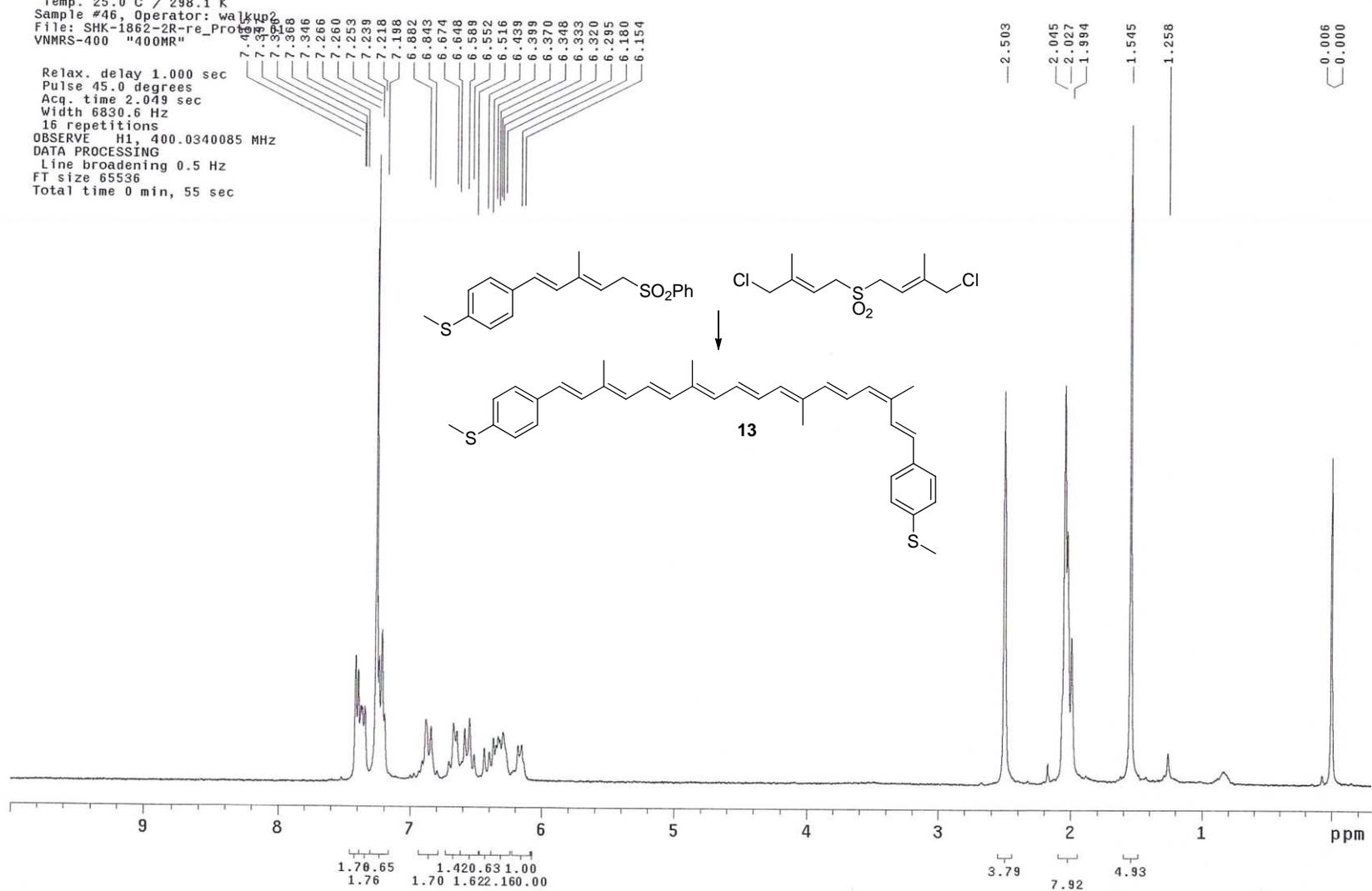
Temp: 25.0 C / 298.1 K

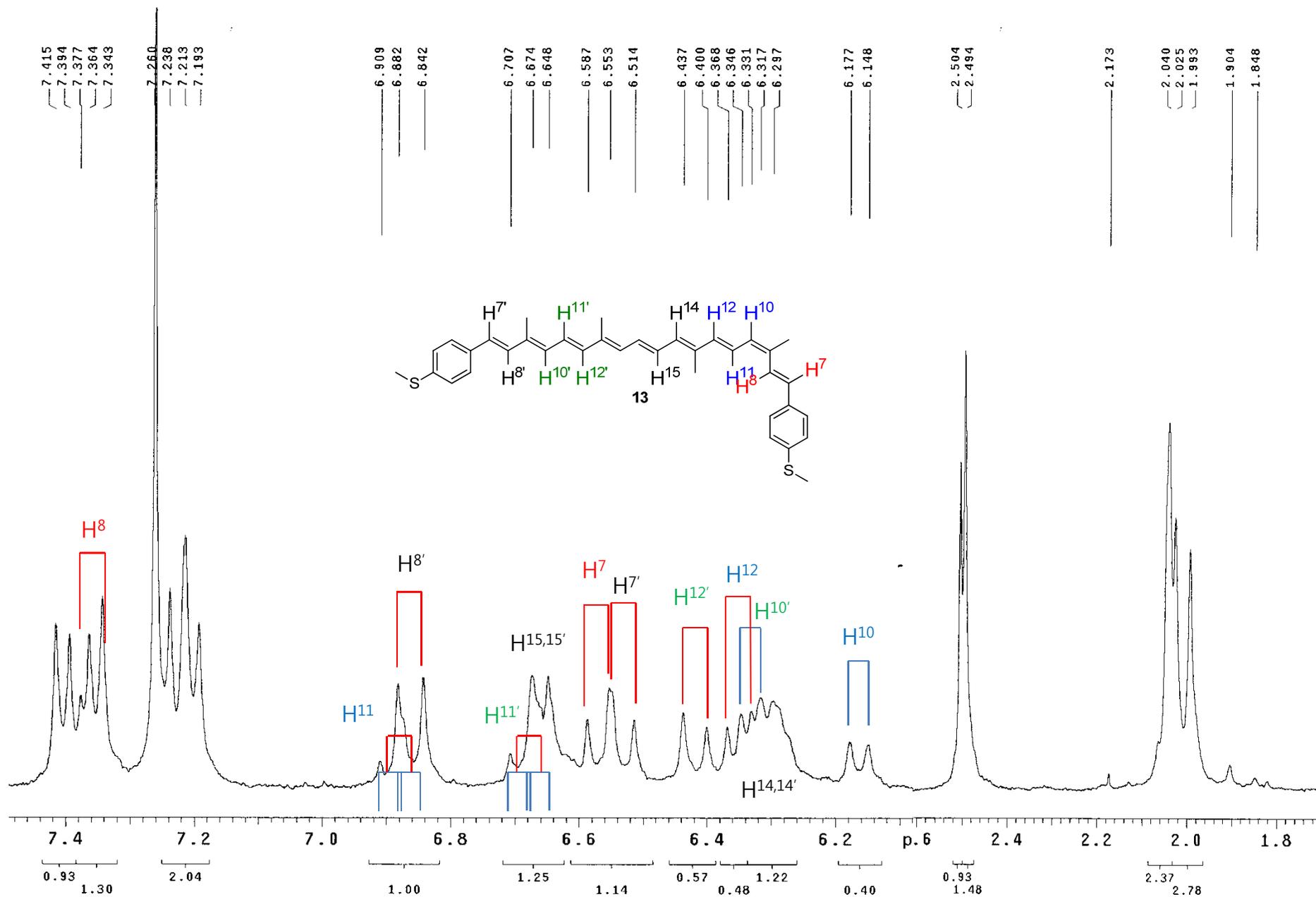
Sample #46, Operator: walkup2

File: SHK-1862-2R-re\_Proton\_01.fid

VNMRS-400 "400MR"

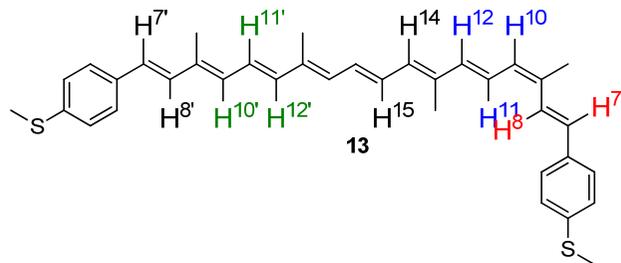
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
16 repetitions  
OBSERVE H1, 400.0340085 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 55 sec





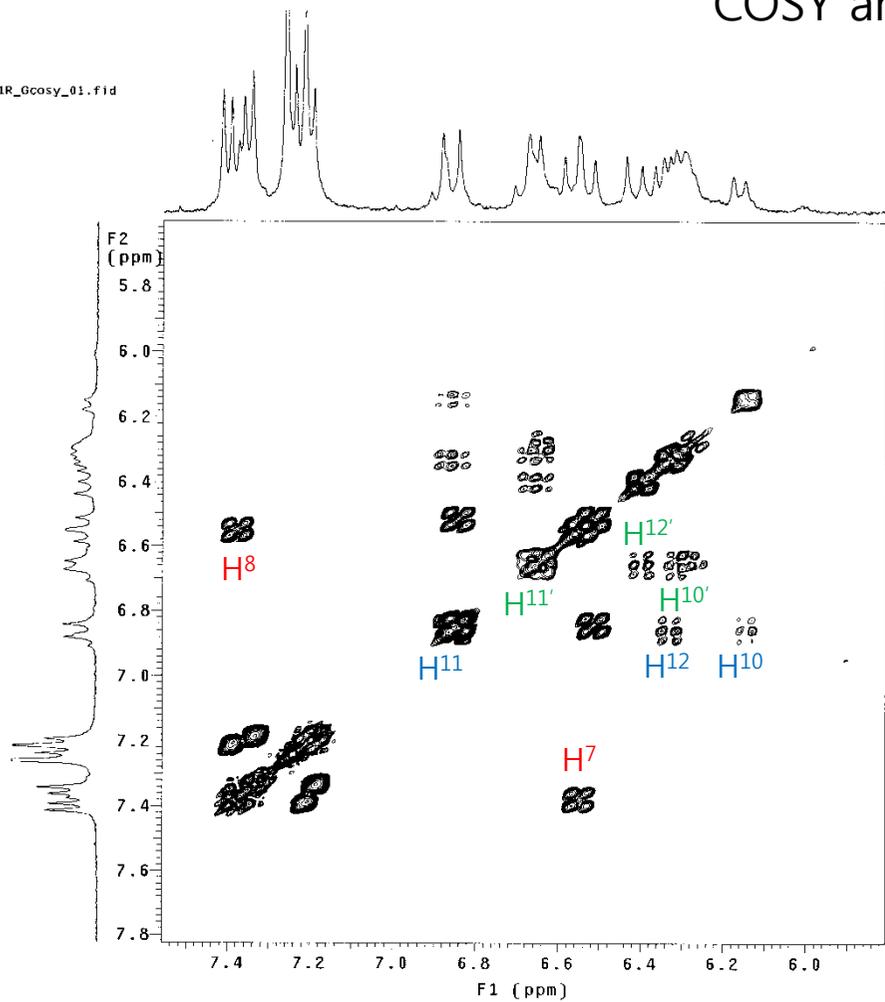




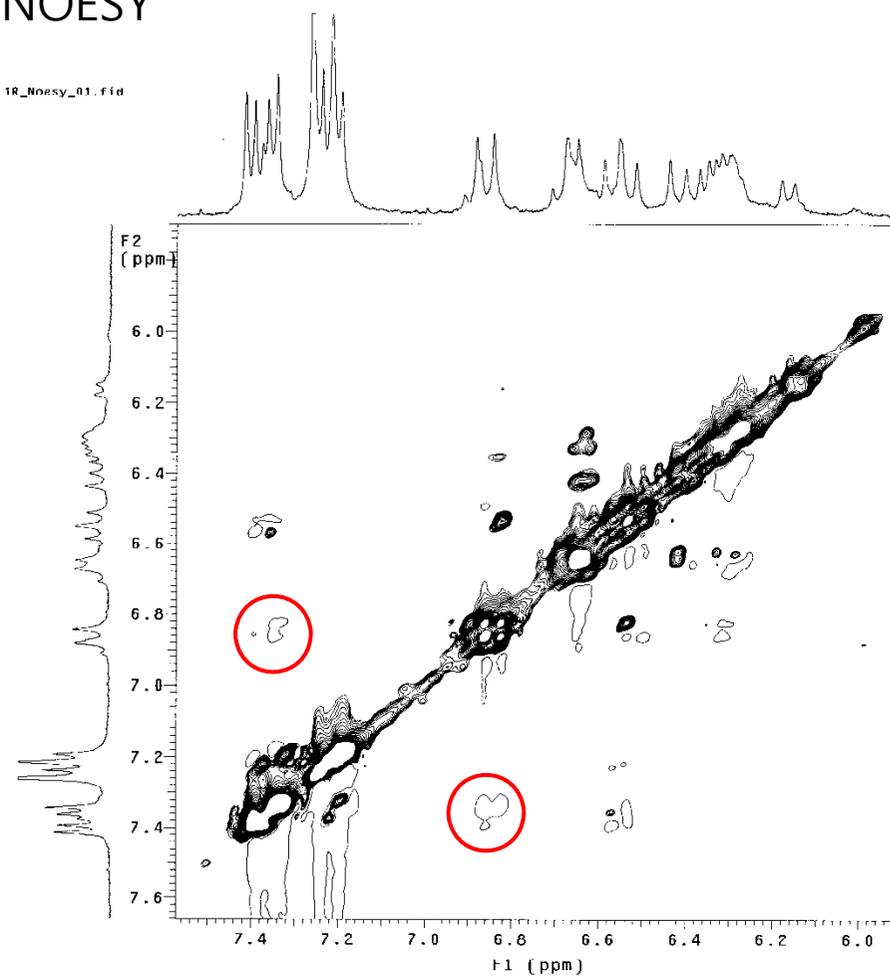


## COSY and NOESY

-1R\_gcosy\_01.fid

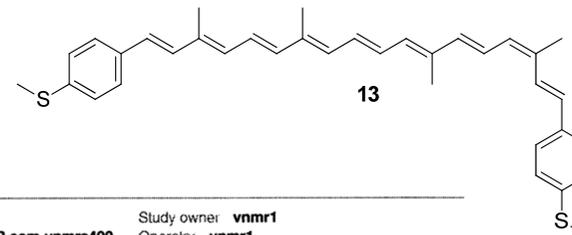


1R\_Noesy\_01.fid





# HMQC (C-H correlation)



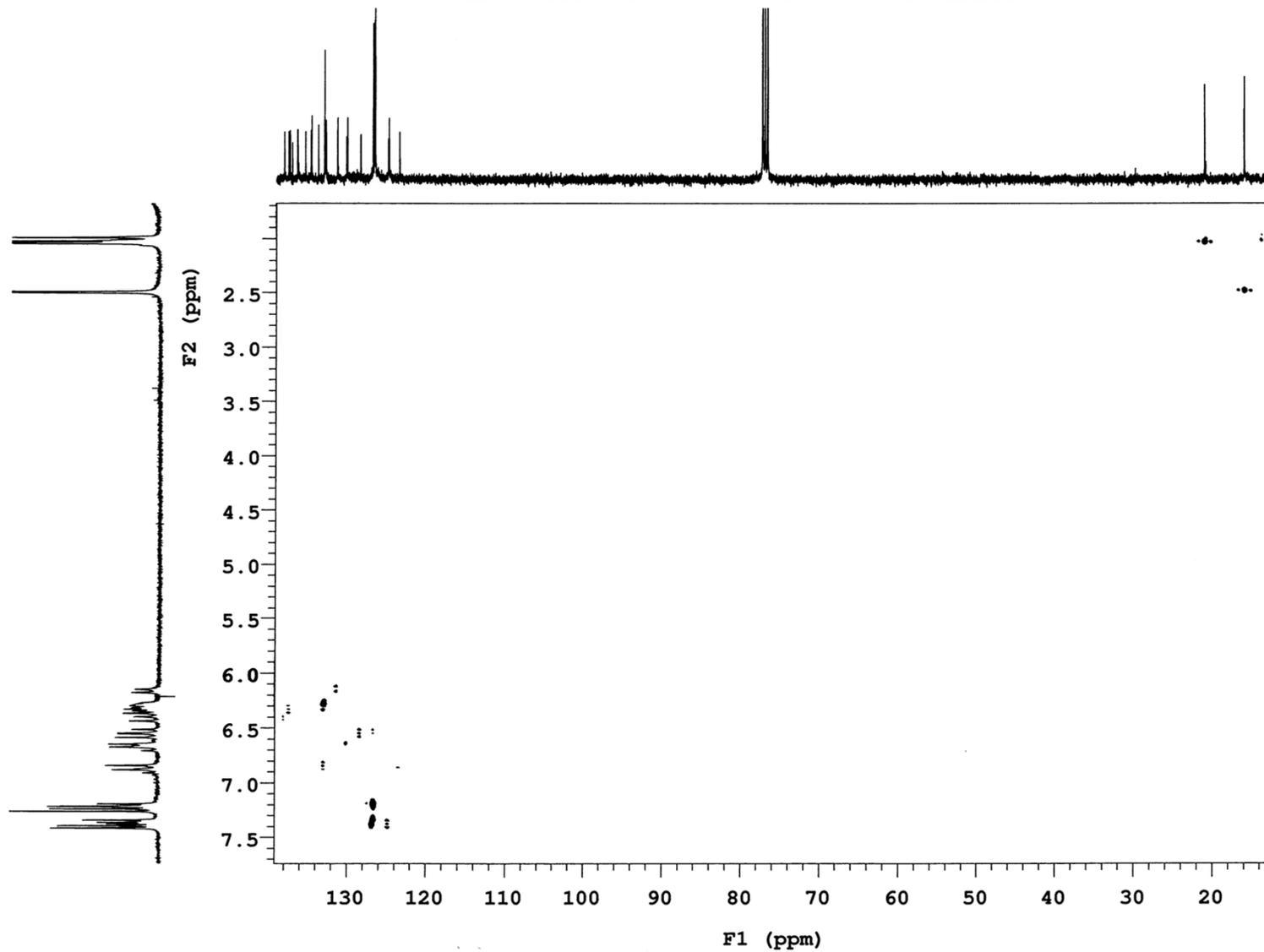
KDH-510-1204-HMQC

Sample Name **KDH-510-1204-HMQC**  
Date collected **2017-12-04**

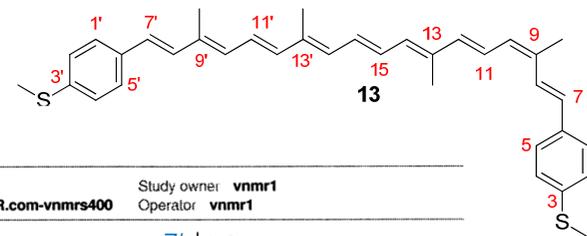
Pulse sequence **gHMQC**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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



# HMQC (C-H correlation)



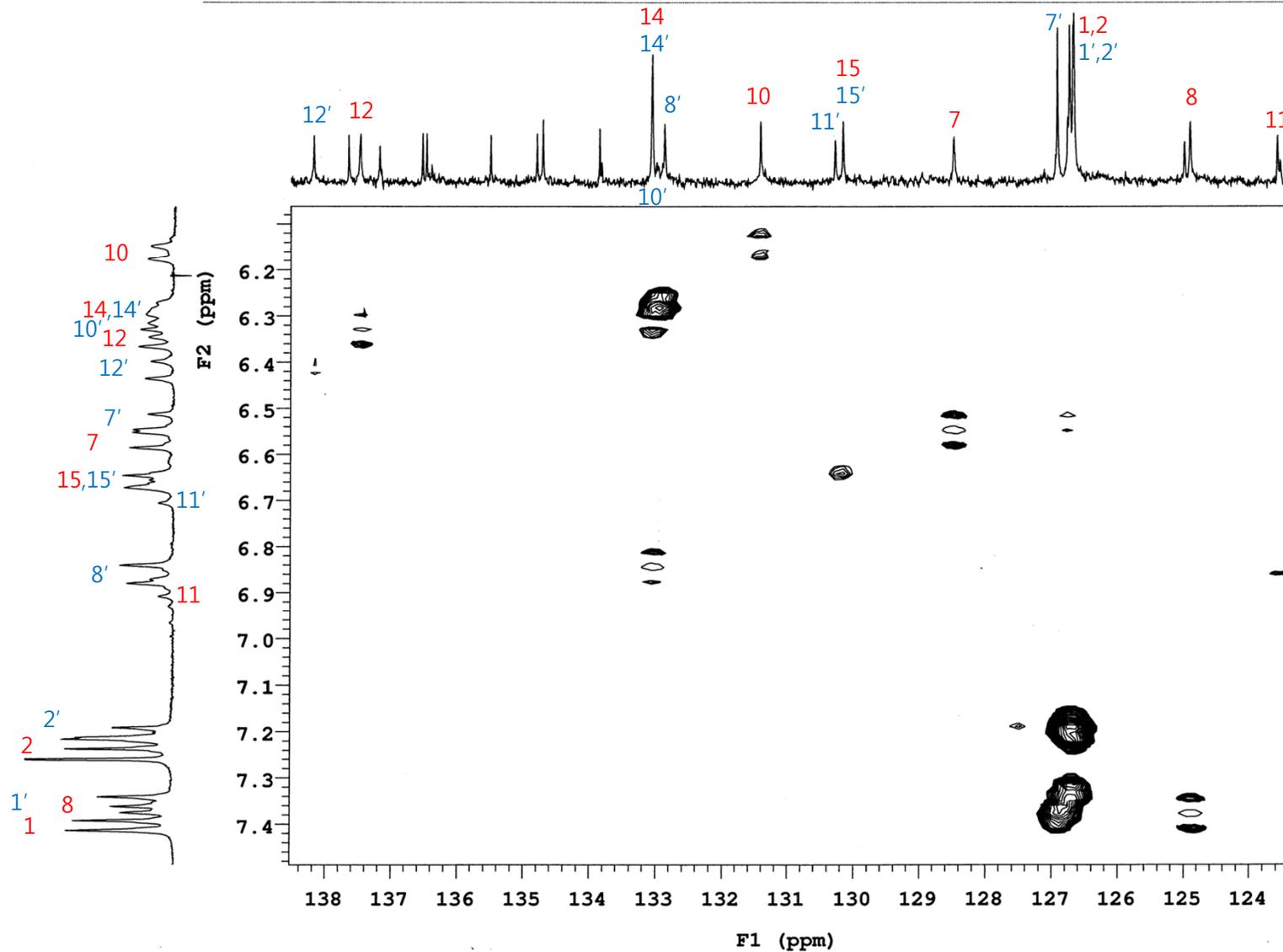
KDH-510-1204-HMQC

Sample Name **KDH-510-1204-HMQC**  
Date collected **2017-12-04**

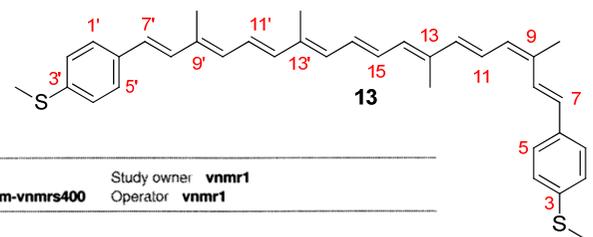
Pulse sequence **gHMQC**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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



# HMQC (C-H correlation)



KDH-510-1204-HMQC

Sample Name **KDH-510-1204-HMQC**

Pulse sequence **gHMQC**

Temperature **24**

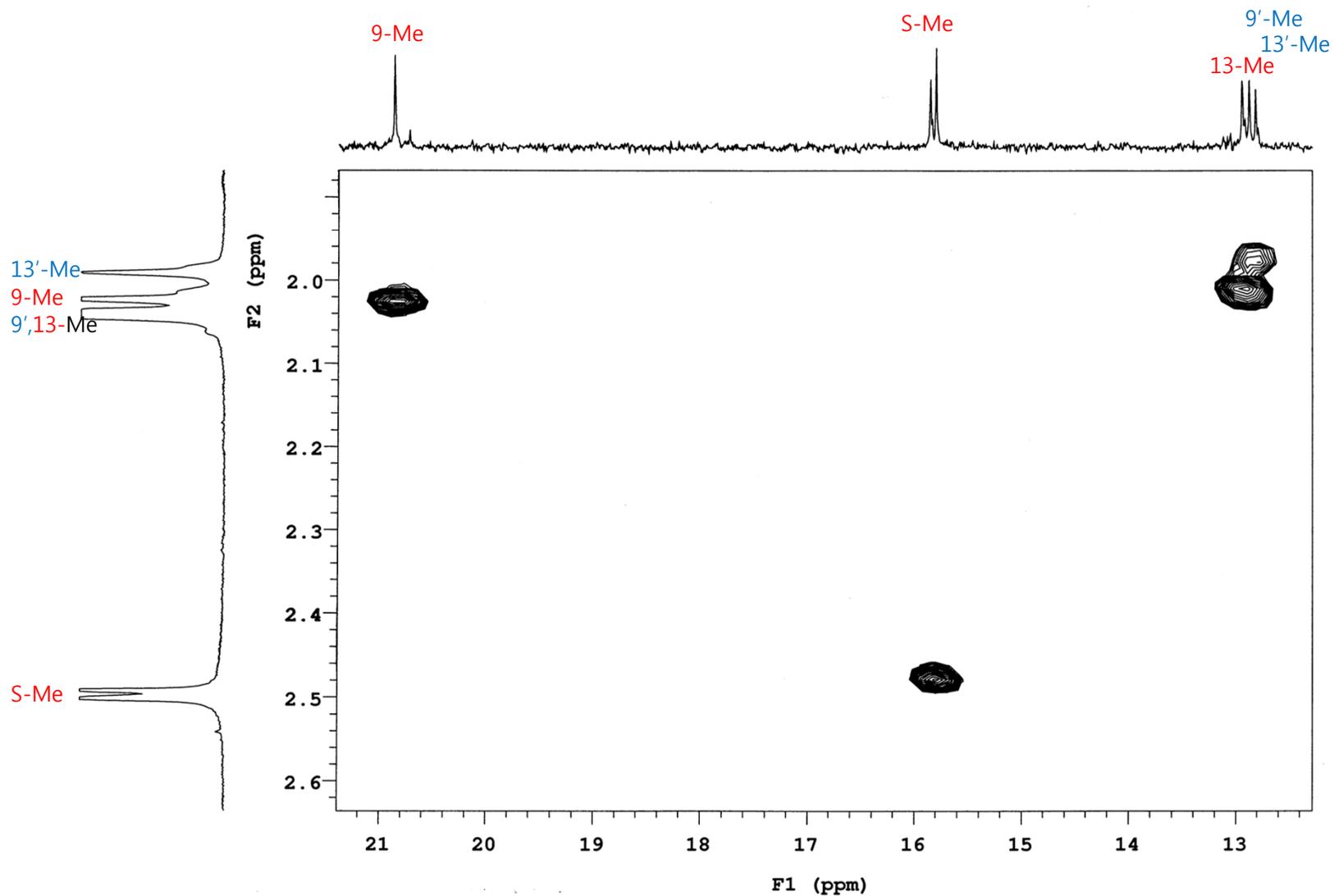
Study owner **vnmr1**

Date collected **2017-12-04**

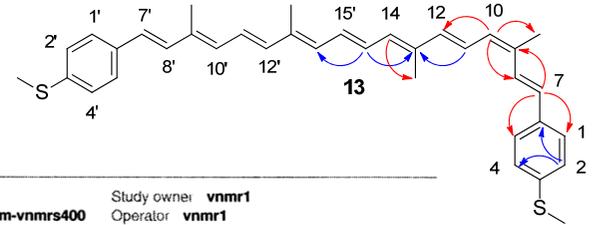
Solvent **cdcl3**

Spectrometer **Agilent-NMR.com-vnmrs400**

Operator **vnmr1**



# HMBC (C-H correlation)



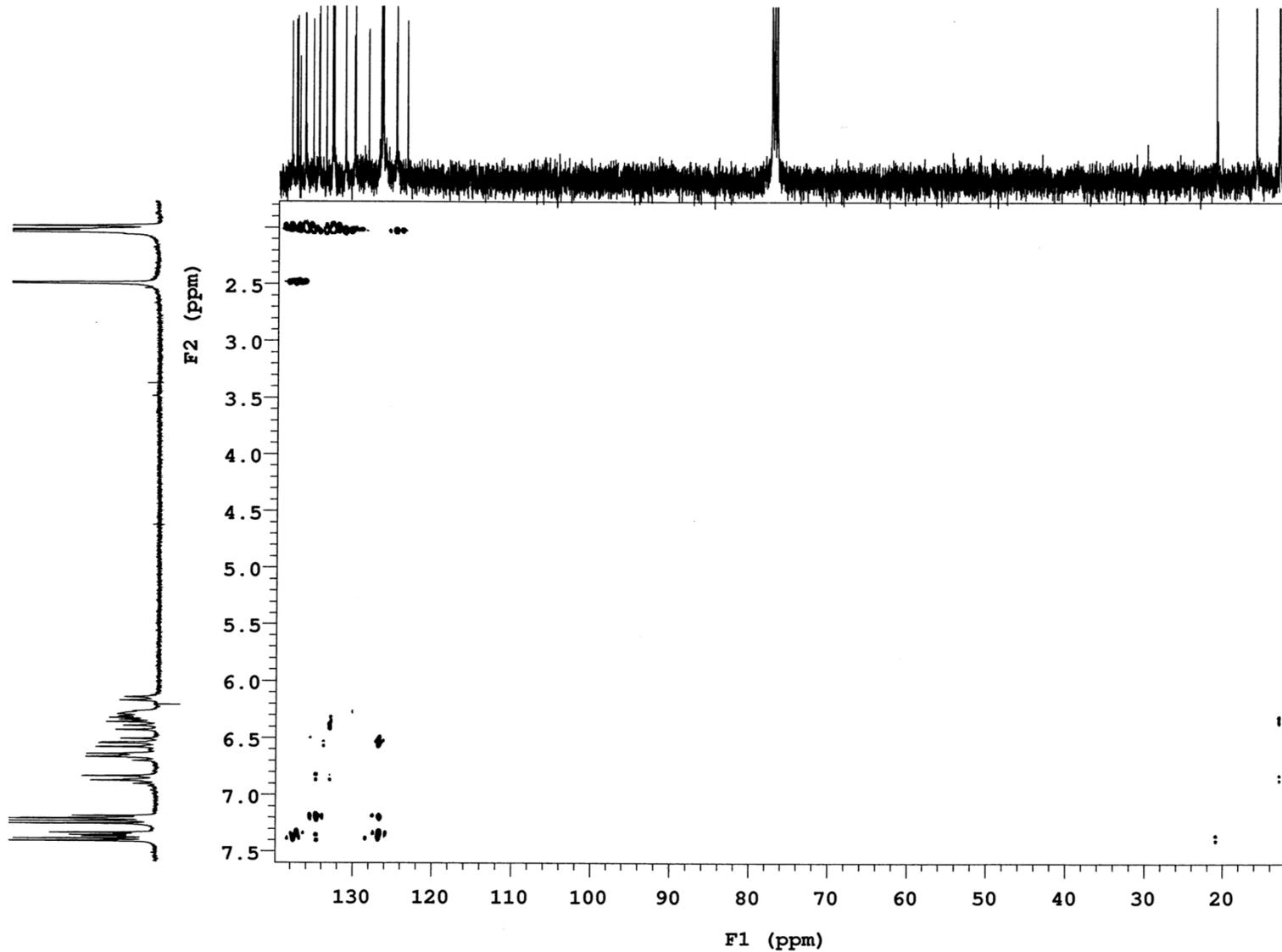
KDH-510-MC-1206-HMBC2

Sample Name **KDH-510-MC-1206-HMBC2**  
Date collected **2017-12-06**

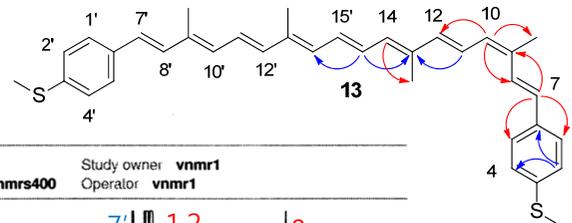
Pulse sequence **gHMBCAD**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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

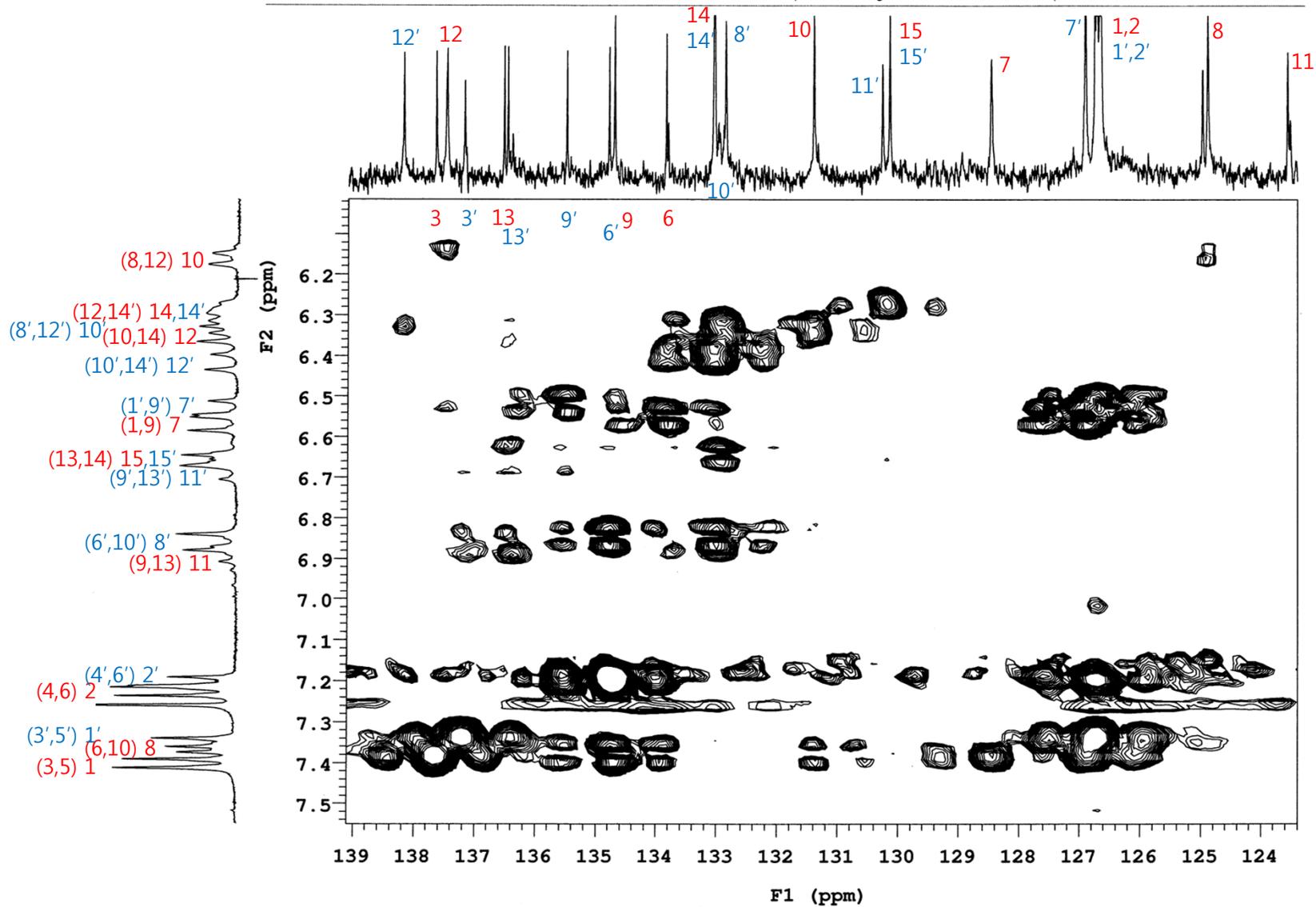


# HMBC (C-H correlation)

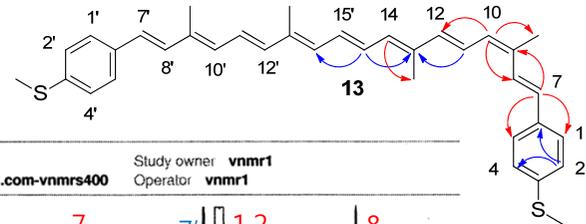


KDH-510-MC-1206-HMBC2

Sample Name	KDH-510-MC-1206-HMBC2	Pulse sequence	gHMBCAD	Temperature	24	Study owner	vnmr1
Date collected	2017-12-06	Solvent	cdcl3	Spectrometer	Agilent-NMR.com-vnmrs400	Operator	vnmr1



# HMBC (C-H correlation)



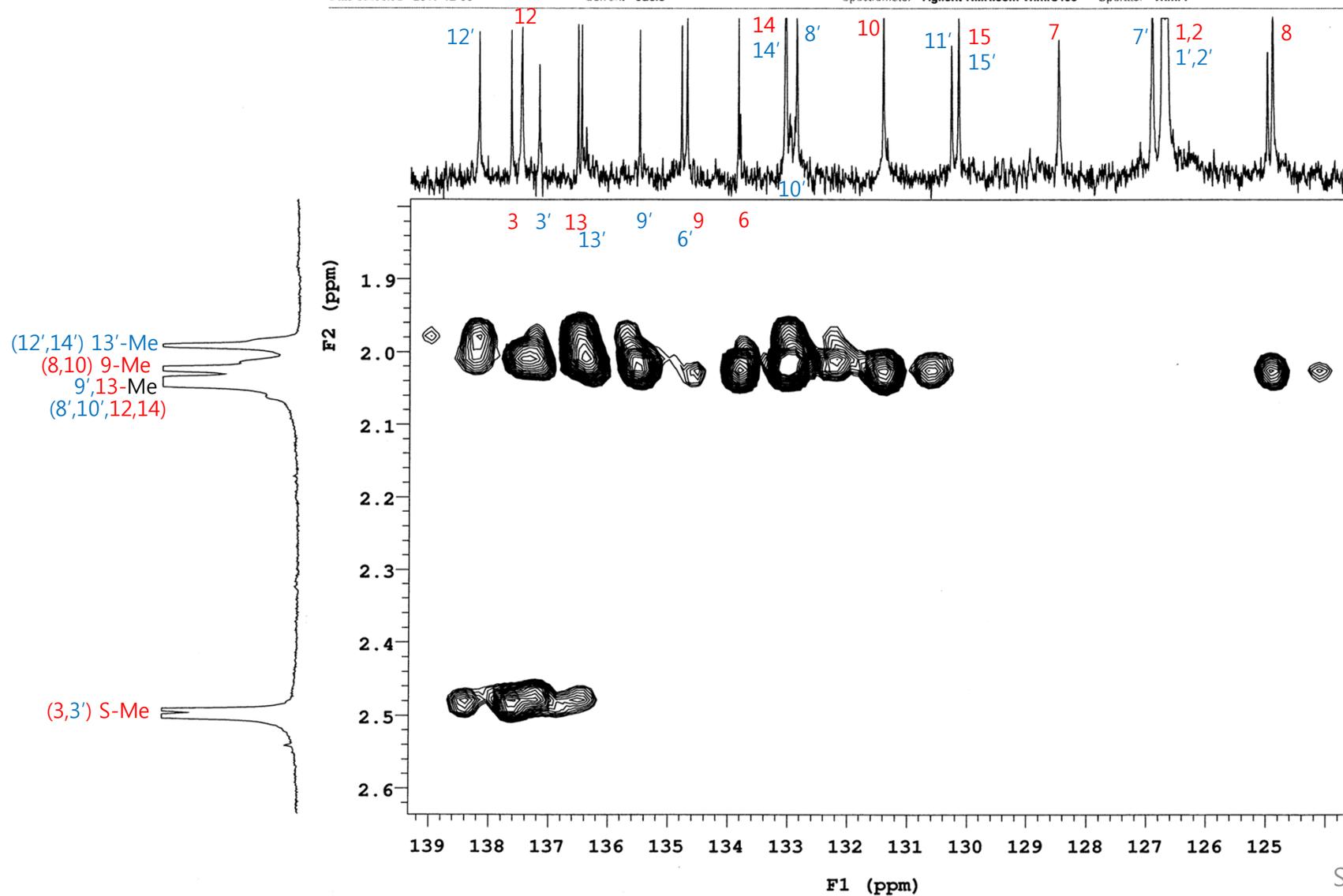
KDH-510-MC-1206-HMBC2

Sample Name **KDH-510-MC-1206-HMBC2**  
Date collected **2017-12-06**

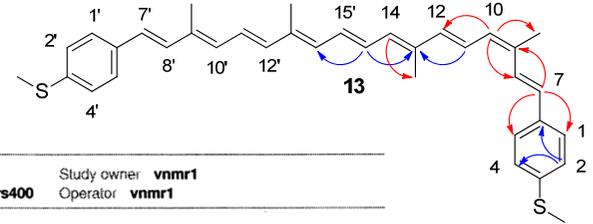
Pulse sequence **gHMBCAD**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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



# HMBC (C-H correlation)



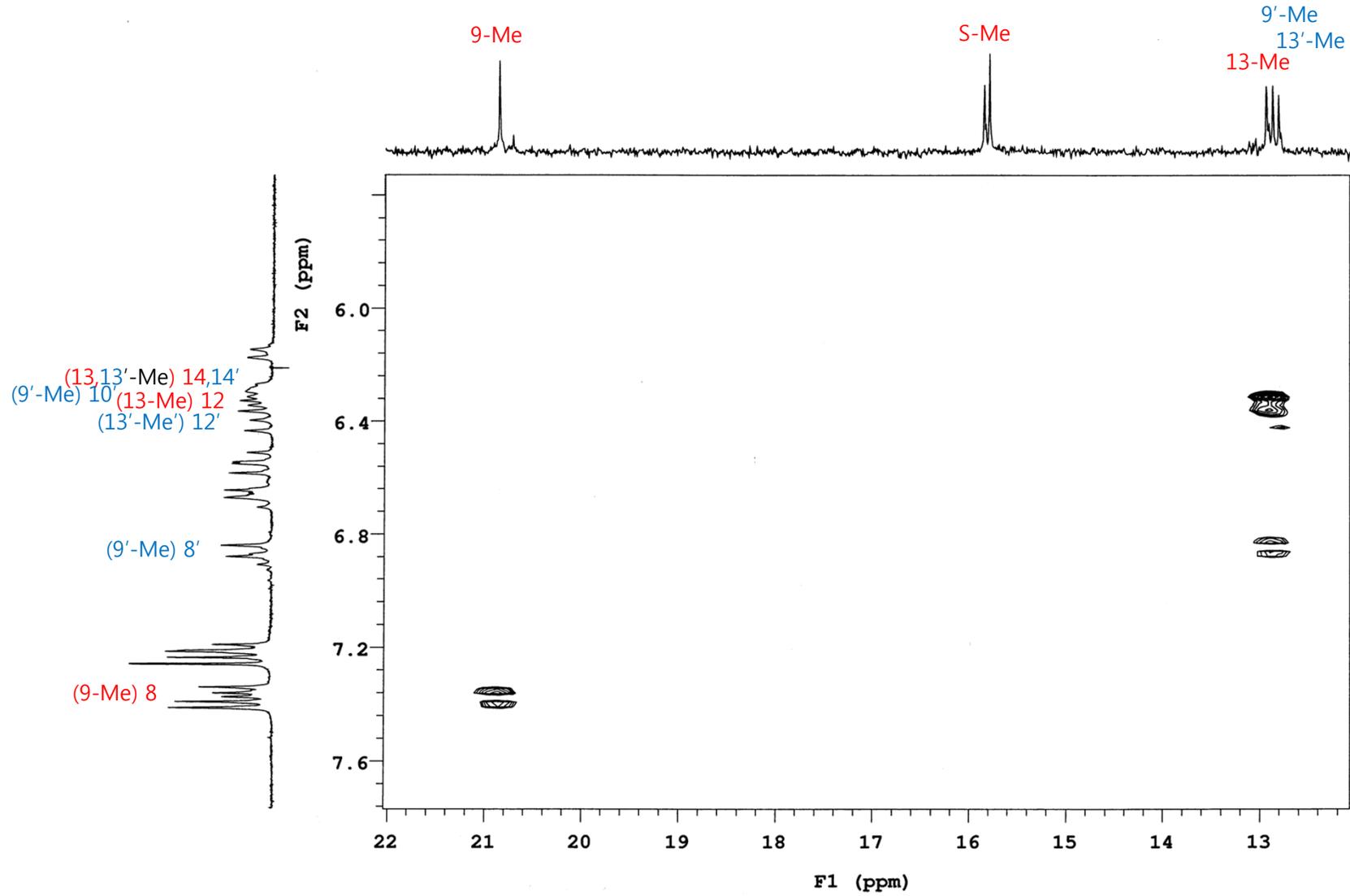
KDH-510-MC-1206-HMBC2

Sample Name **KDH-510-MC-1206-HMBC2**  
Date collected **2017-12-06**

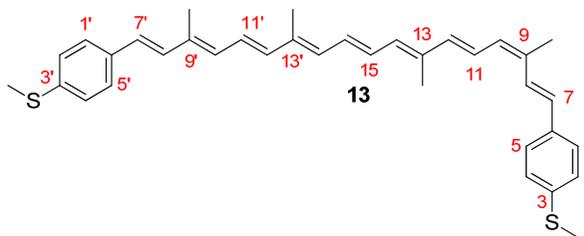
Pulse sequence **gHMBCAD**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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

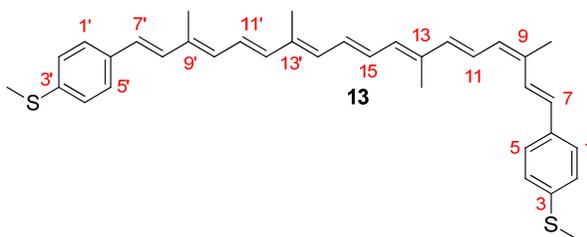


## Assignment of $^1\text{H}$ and $^{13}\text{C}$ NMR peaks of 9-*Z*-carotene **13** (based on HMQC and HMBC)



Numbering	$^1\text{H}$ NMR		$^{13}\text{C}$ NMR	
	Shift (ppm)	Multiplicity (Hz)	Shift (ppm)	DEPT
1	7.40	d (8.0)	126.7	CH
2	7.25	d (8.0)	126.8	CH
3	-	-	137.6	q
3-SMe	2.50	s	15.8	CH <sub>3</sub>
4	7.25	d (8.0)	126.8	CH
5	7.40	d (8.0)	126.7	CH
6	-	-	133.8	q
7	6.57	d (14.8)	128.5	CH
8	7.36	d (14.8)	124.9	CH
9	-	-	134.7	q
9-Me	2.04	s	20.8	CH <sub>3</sub>
10	6.16	d (11.6)	131.4	CH
11	6.88	dd (14.8)	123.5	CH
12	6.33	d (11.6)	137.5	CH
13	-	-	136.5	q
13-Me	2.03	s	12.9	CH <sub>3</sub>
14	6.26-6.36	m	133.1	CH
15	6.60-6.70	m	130.2	CH

## Assignment of $^1\text{H}$ and $^{13}\text{C}$ NMR peaks of 9-cis-carotene **13** (based on HMQC and HMBC)

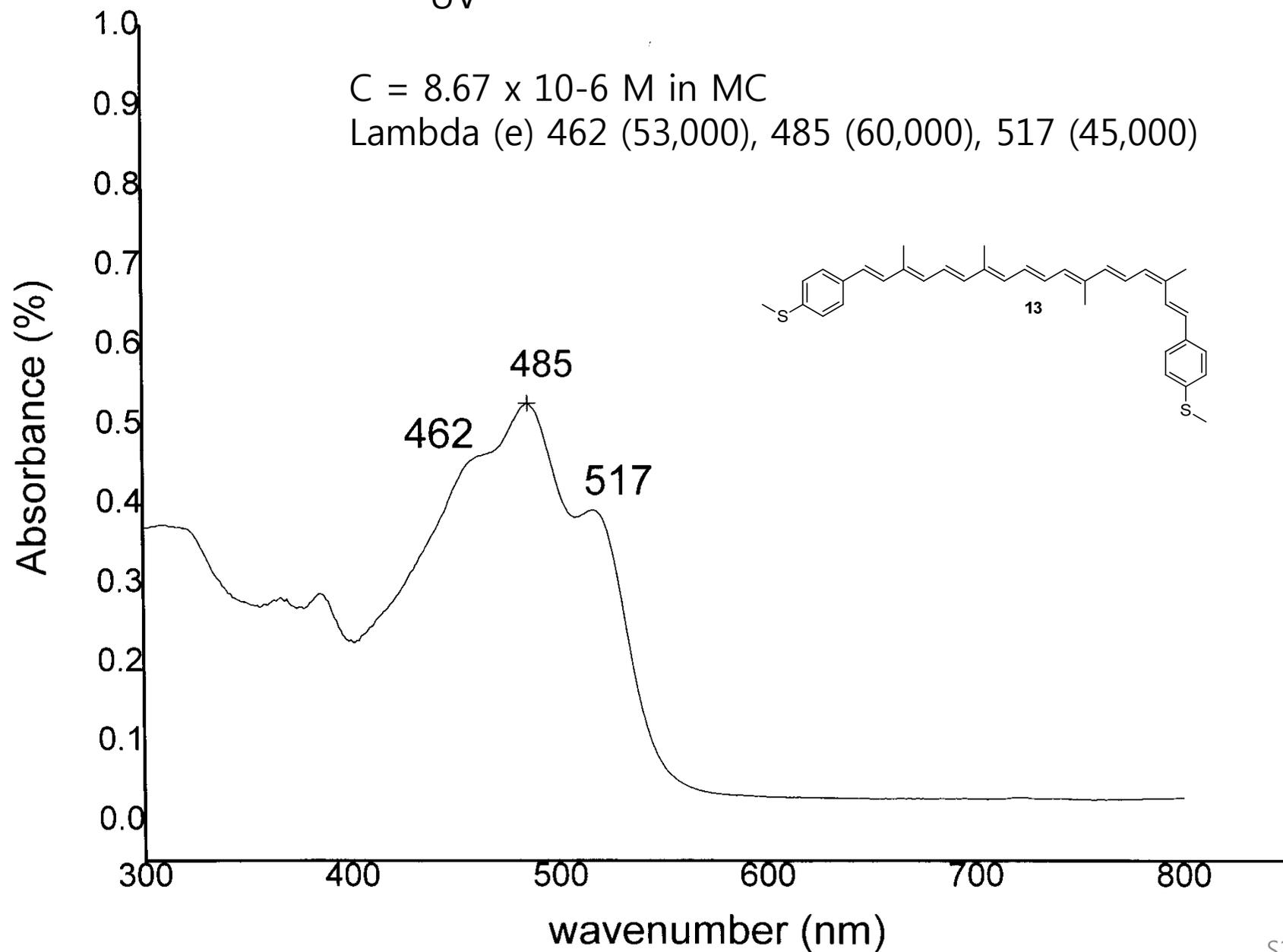


Numbering	$^1\text{H}$ NMR		$^{13}\text{C}$ NMR	
	Shift (ppm)	Multiplicity (Hz)	Shift (ppm)	DEPT
1'	7.35	d (8.0)	126.6	CH
2'	7.20	d (8.0)	126.8	CH
3'	-	-	137.2	q
3'-SMe	2.49	s	15.8	CH <sub>3</sub>
4'	7.20	d (8.0)	126.8	CH
5'	7.35	d (8.0)	126.6	CH
6'	-	-	134.8	q
7'	6.53	d (14.8)	126.9	CH
8'	6.86	d (14.8)	132.9	CH
9'	-	-	135.5	q
9'-Me	2.04	s	12.9	CH <sub>3</sub>
10'	6.35	d (14.8)	133.0	CH
11'	6.67	dd (14.8)	130.3	CH
12'	6.42	d (14.8)	138.2	CH
13'	-	-	136.5	q
13'-Me	1.99	s	12.8	CH <sub>3</sub>
14'	6.26-6.36	m	133.1	CH
15'	6.60-6.70	m	130.2	CH

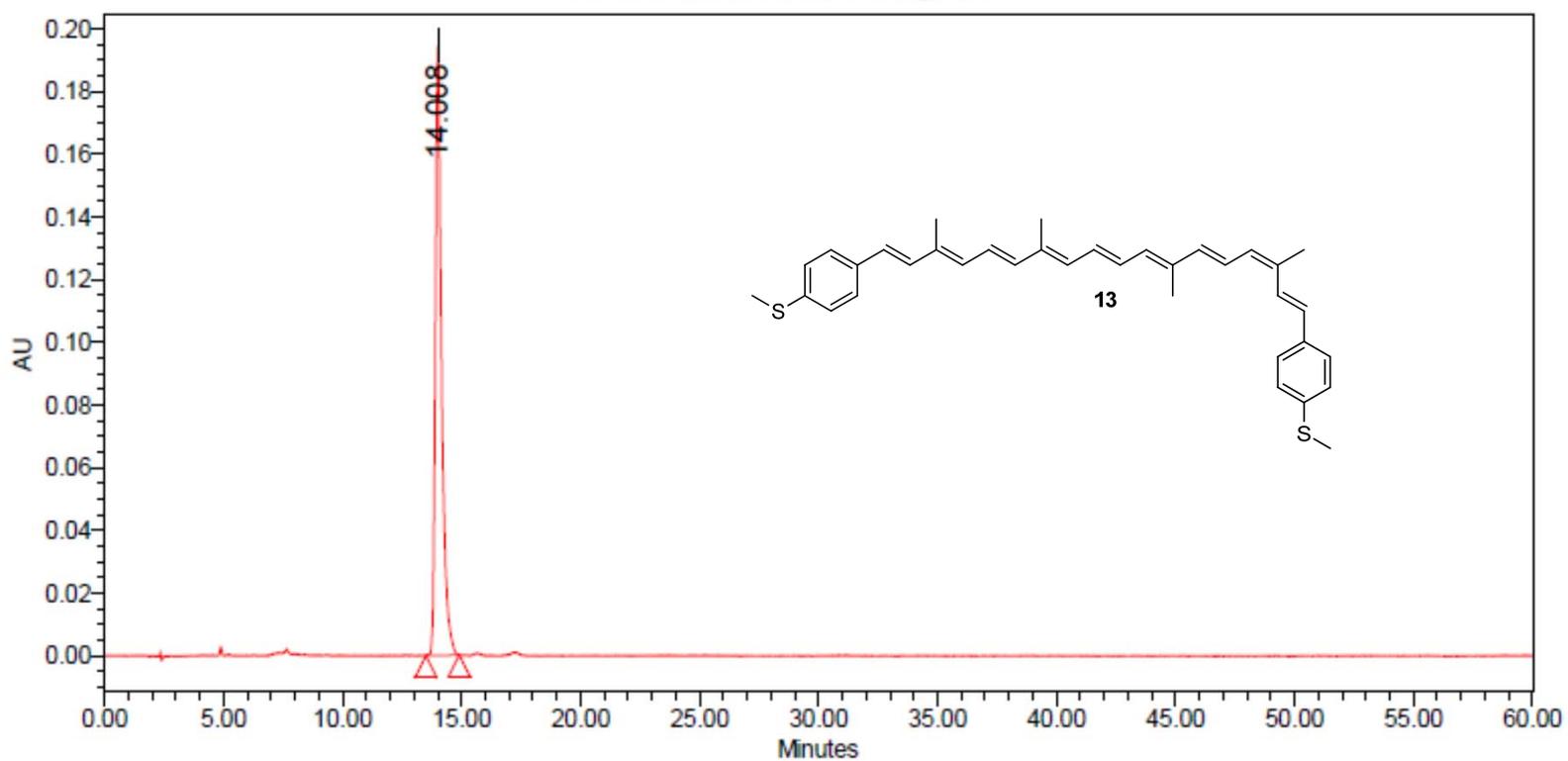
UV

 $C = 8.67 \times 10^{-6} \text{ M}$  in MC

Lambda (e) 462 (53,000), 485 (60,000), 517 (45,000)



### Auto-Scaled Chromatogram



### Peak Results

Name	RT(min)	Area(uv*sec)	%Area	Height(uv)	Amount	Units
1	14.008	3547027	100	194458		

Column: Hypersil BDS C18 250 x 4 mm 5 µm, Part No: 28105-254030

Mobile phase: 100% MeCN Flow rate: 1.0 mL/min

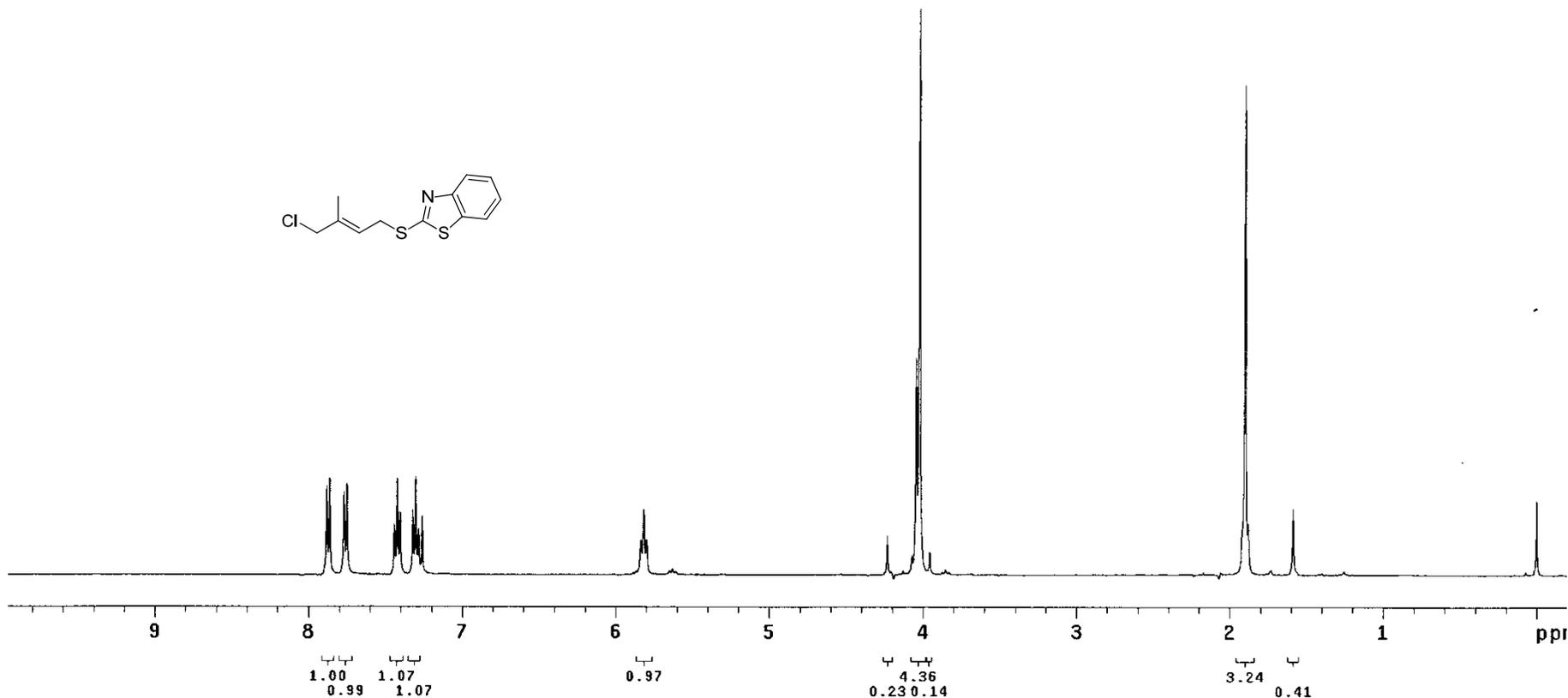
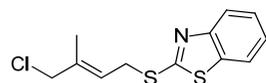
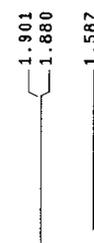
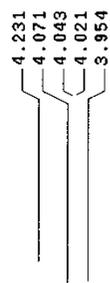
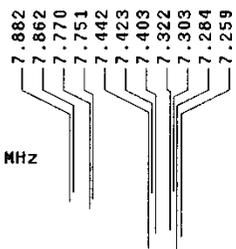
Detection: UV @ 506nm Temperature: 25°C

Sample: SHK-1728-1  
File: /home/waikup2/vnmrsvs/data/koo-2/SHK-1728-1\_proton.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Operator: waikup2  
File: SHK-1728-1\_proton  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340098 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

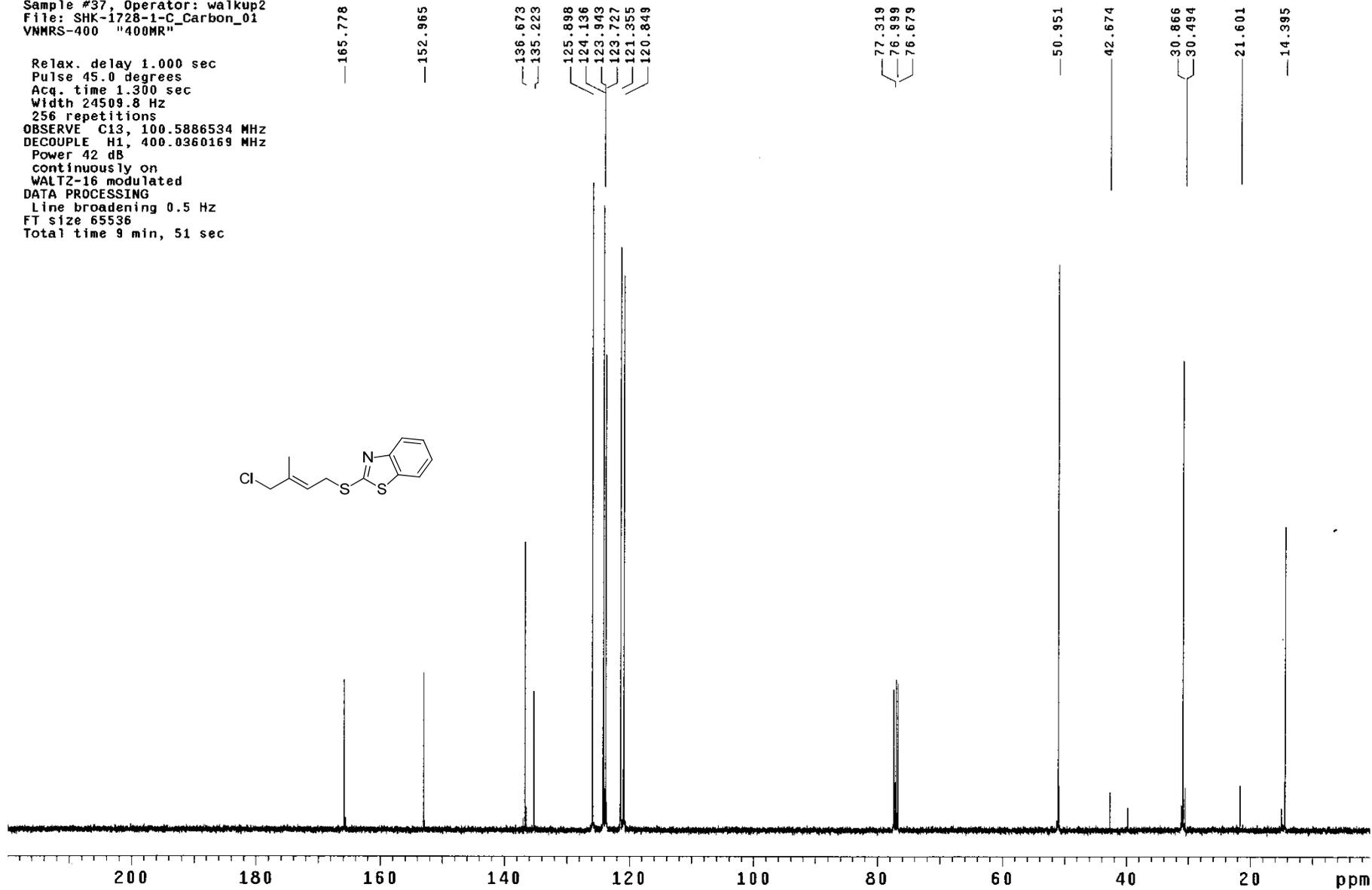
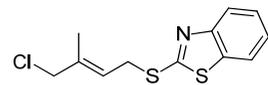


Sample: SHK-1728-1-C  
Sample ID: s\_37\_SHK-1728-1-C\_koo-2\_20140207\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1728-1-C\_Carbon\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Sample #37, Operator: walkup2  
File: SHK-1728-1-C\_Carbon\_01  
VNMRS-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886534 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

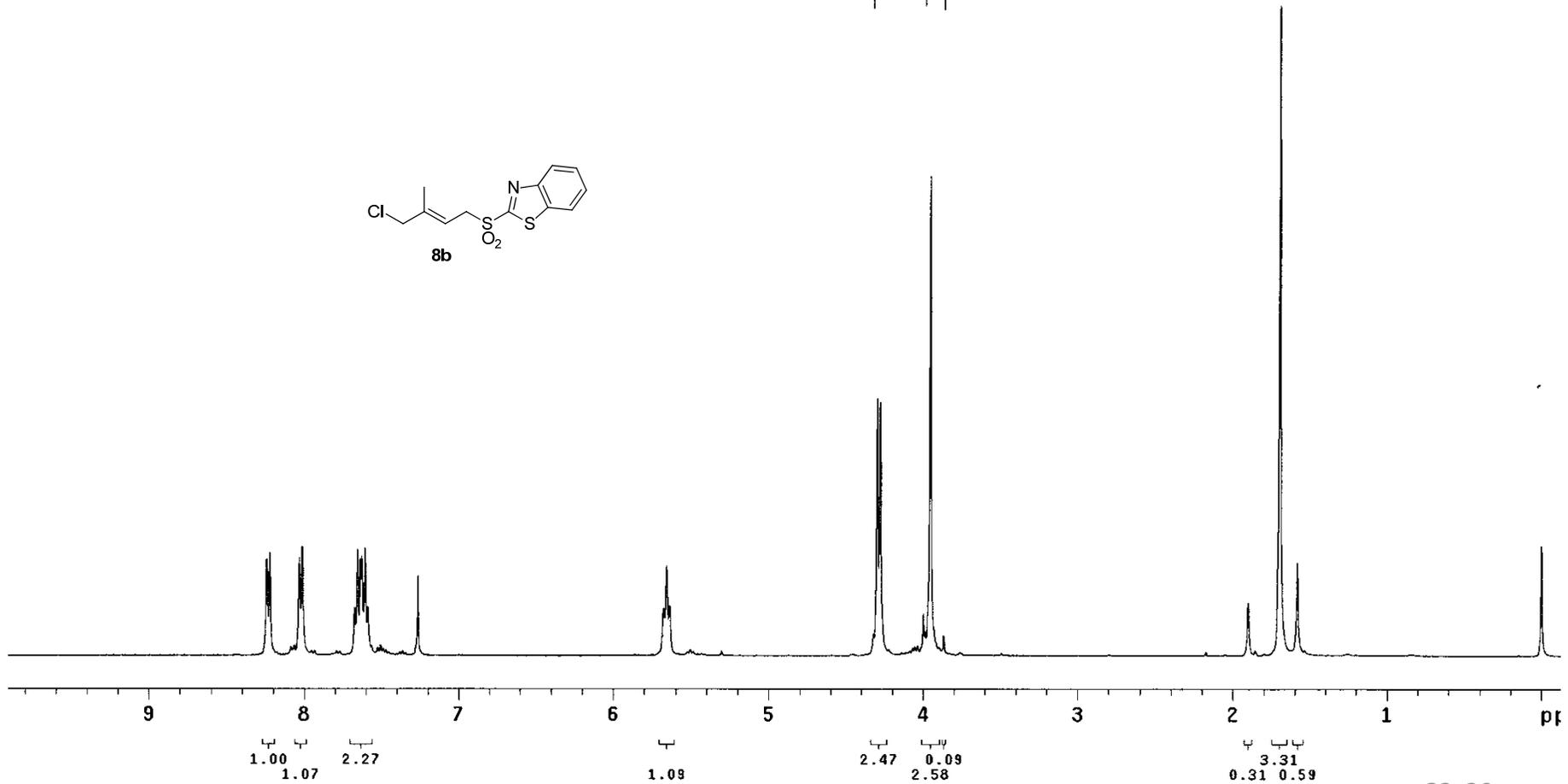
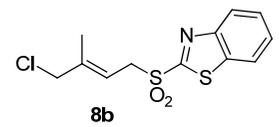
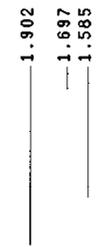
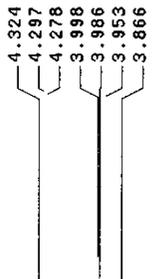
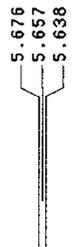
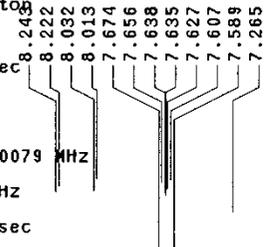


Sample: SHK-1736-R1  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1736-R1\_proton.fid

Pulse Sequence: s2pu1

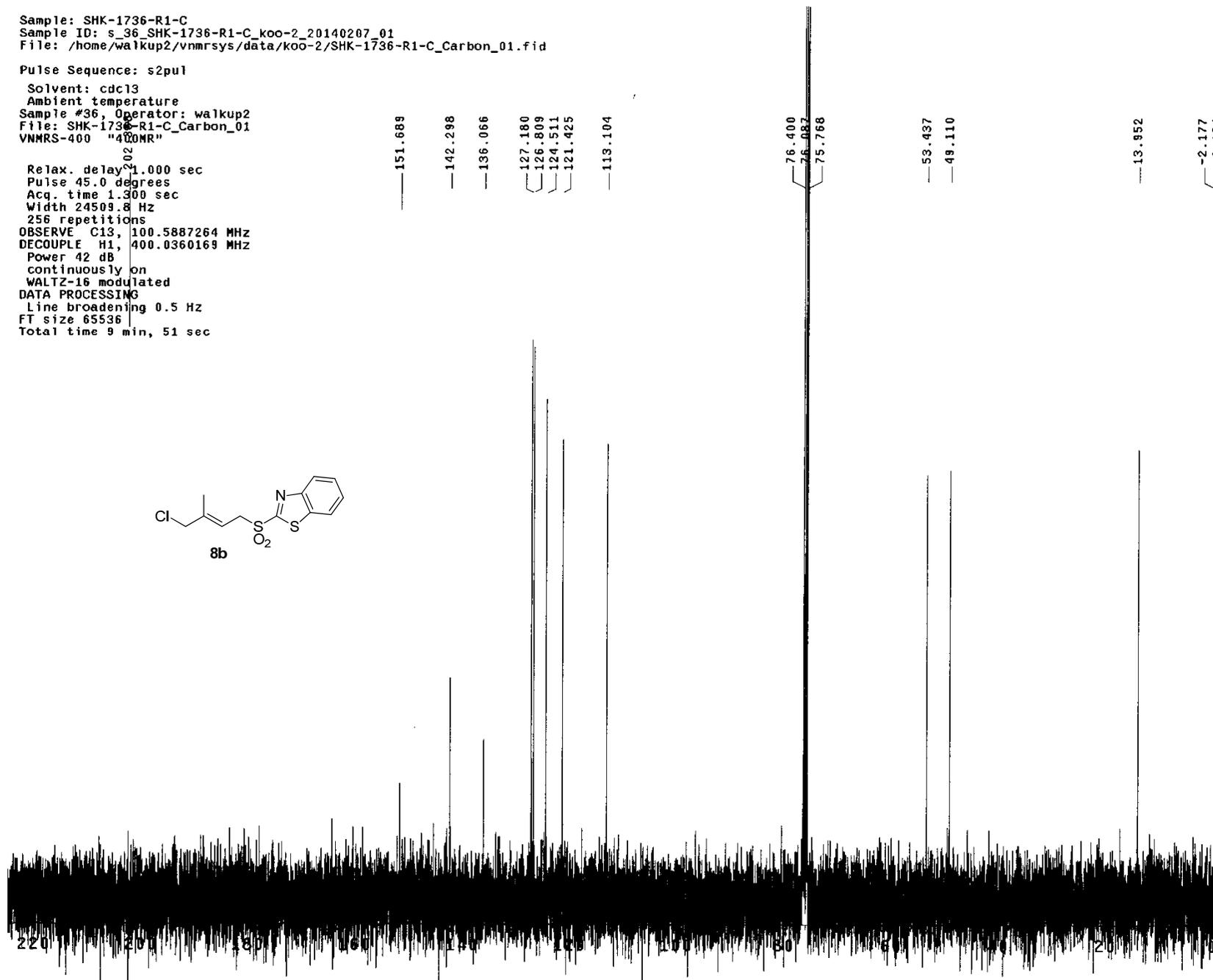
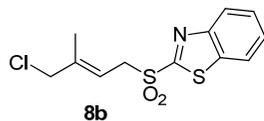
Solvent: cdc13  
Ambient temperature  
Operator: walkup2  
File: SHK-1736-R1\_proton.fid  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340079 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-1736-R1-C  
Sample ID: s\_36\_SHK-1736-R1-C\_koo-2\_20140207\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1736-R1-C\_Carbon\_01.fid

Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
Sample #36, Operator: walkup2  
File: SHK-1736-R1-C\_Carbon\_01  
VNMR5-400 "400MR"  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5887264 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec



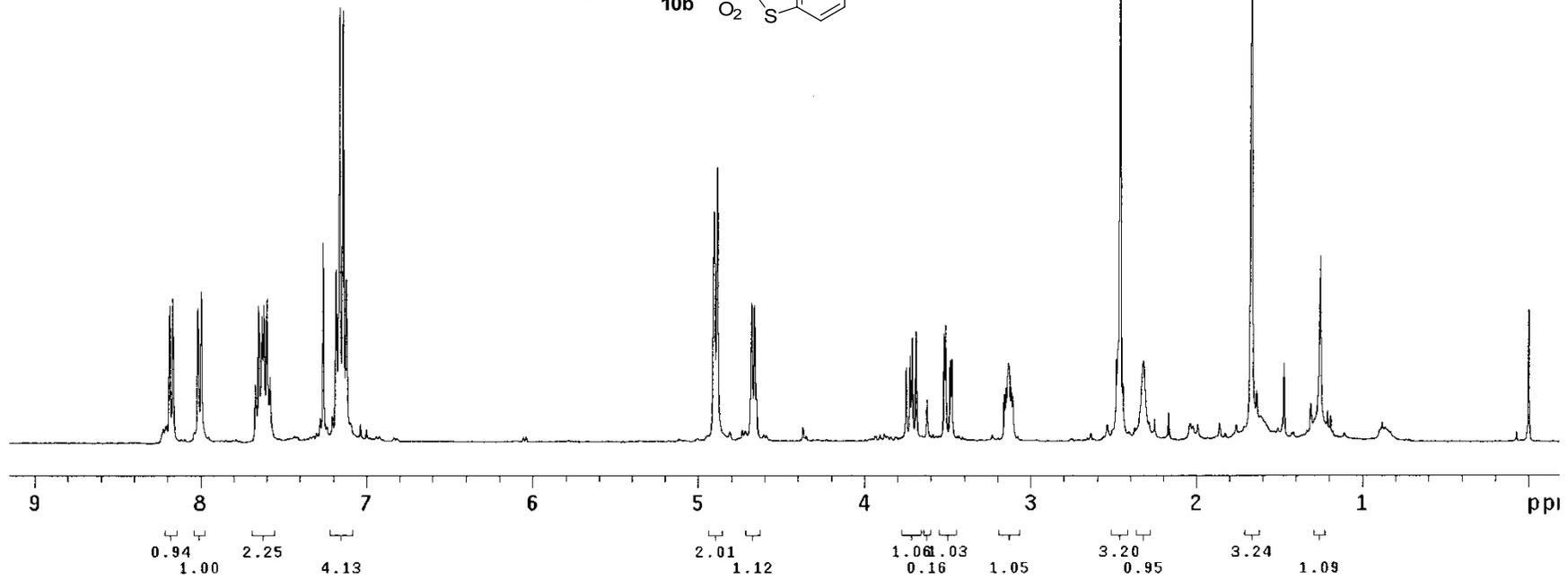
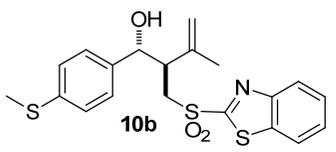
TIC13  
 Temperature  
 Operator: [unclear]  
 18-P\_Proc: [unclear]  
 400MR = 400.0340089 MHz  
 8.110 sec  
 8.045 sec  
 7.996 sec  
 7.668 sec  
 7.650 sec  
 7.630 sec  
 7.627 sec  
 7.619 sec  
 7.616 sec  
 7.599 sec  
 7.581 sec  
 7.261 sec  
 7.184 sec  
 7.163 sec  
 7.142 sec  
 7.121 sec  
 1.000 sec  
 degrees  
 0.049 sec  
 6 Hz  
 ns  
 400.0340089 MHz  
 SING  
 0.5 Hz  
 36  
 ) min, 31 sec

4.904  
 4.886  
 4.680  
 4.662  
 4.650

3.749  
 3.725  
 3.712  
 3.688  
 3.624  
 3.521  
 3.512  
 3.484  
 3.475  
 3.159  
 3.149  
 3.134  
 3.117  
 3.107  
 2.483  
 2.476  
 2.464  
 2.445  
 2.323

1.669  
 1.636  
 1.472  
 1.311  
 1.255

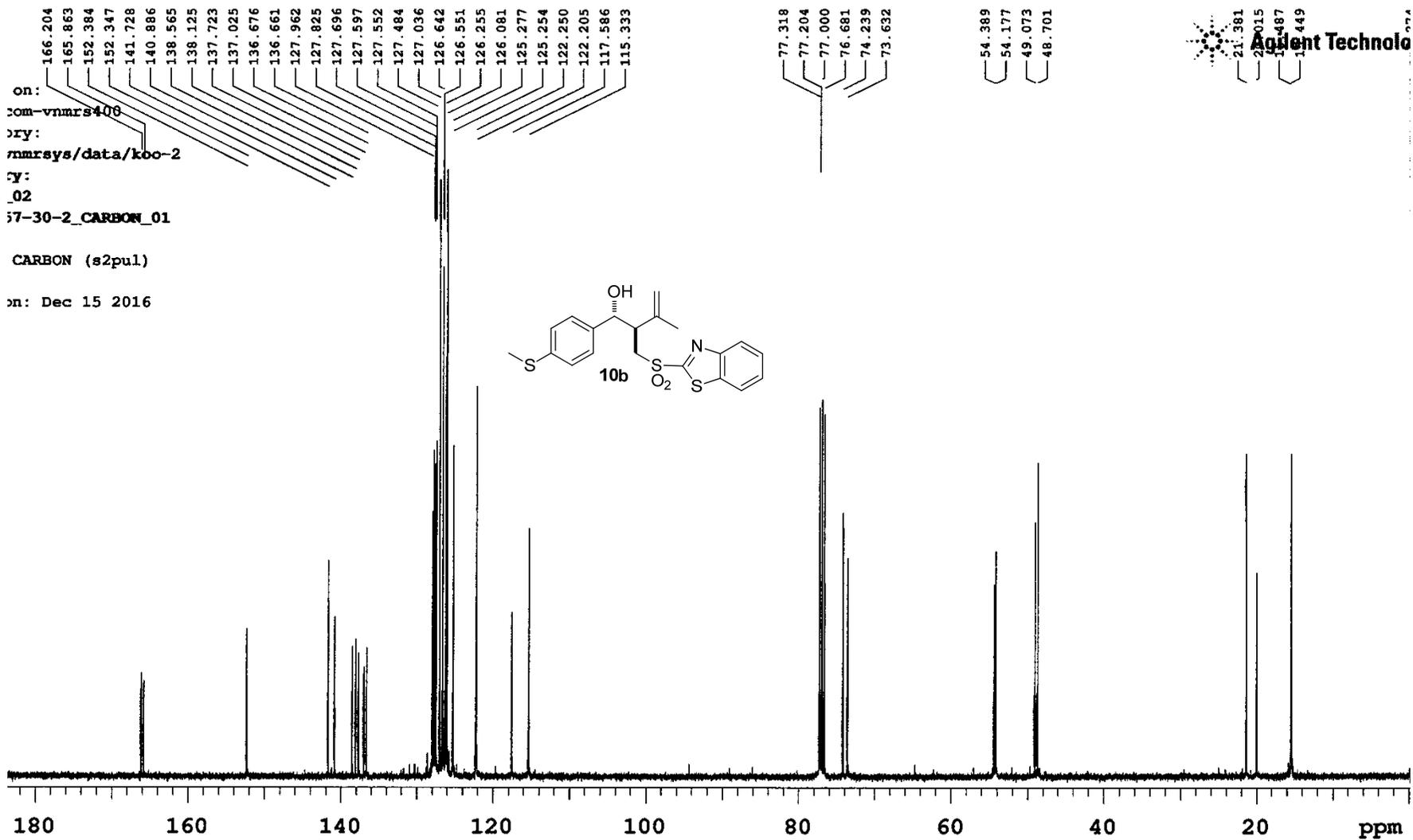
0.002  
 -0.001

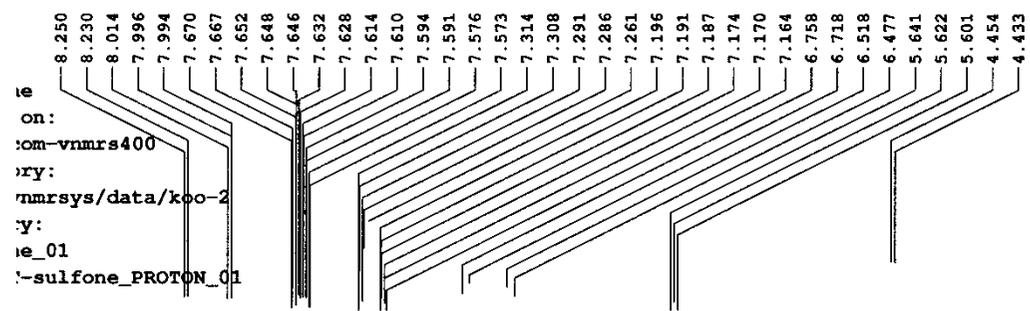


on:  
 :om-vnmrs400  
 >ry:  
 nmrsys/data/koc-2  
 y:  
 \_02  
 i7-30-2 CARBON\_01

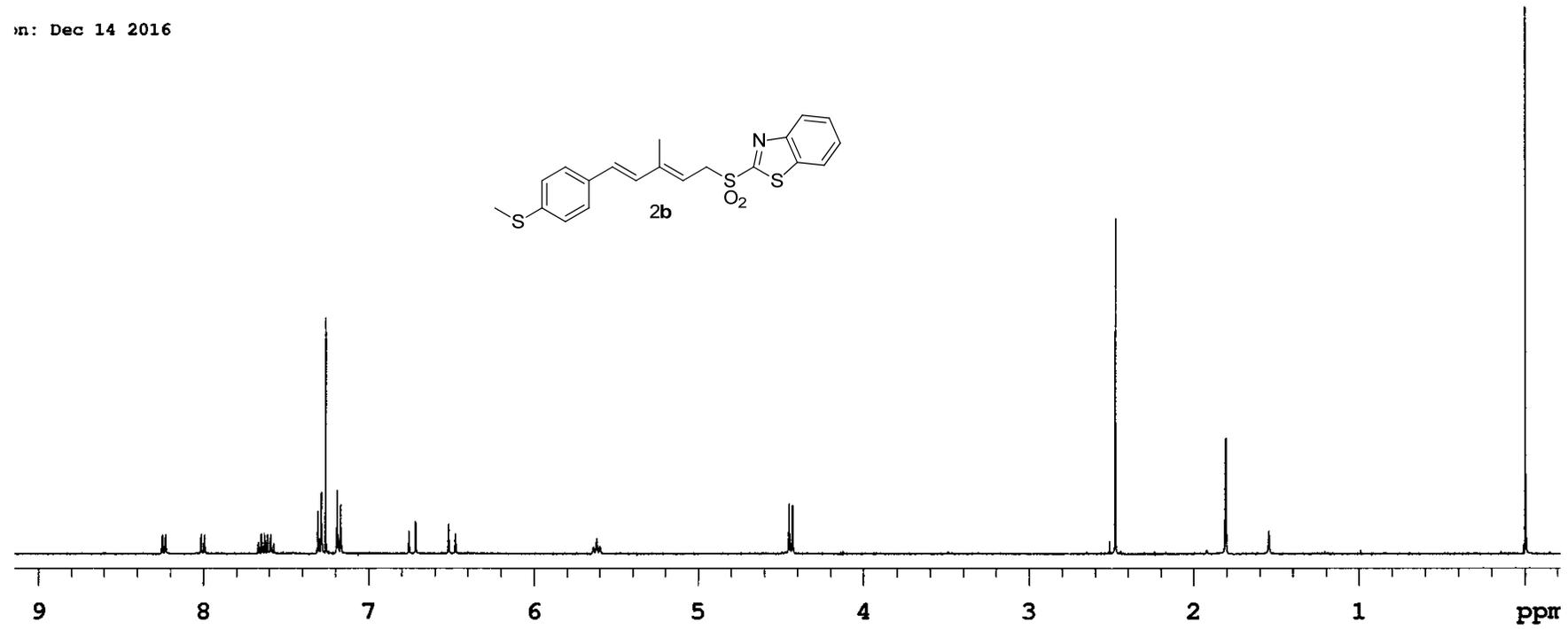
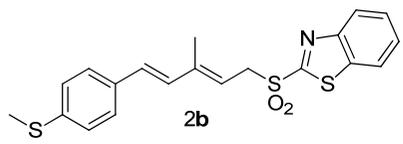
CARBON (s2pul)

on: Dec 15 2016





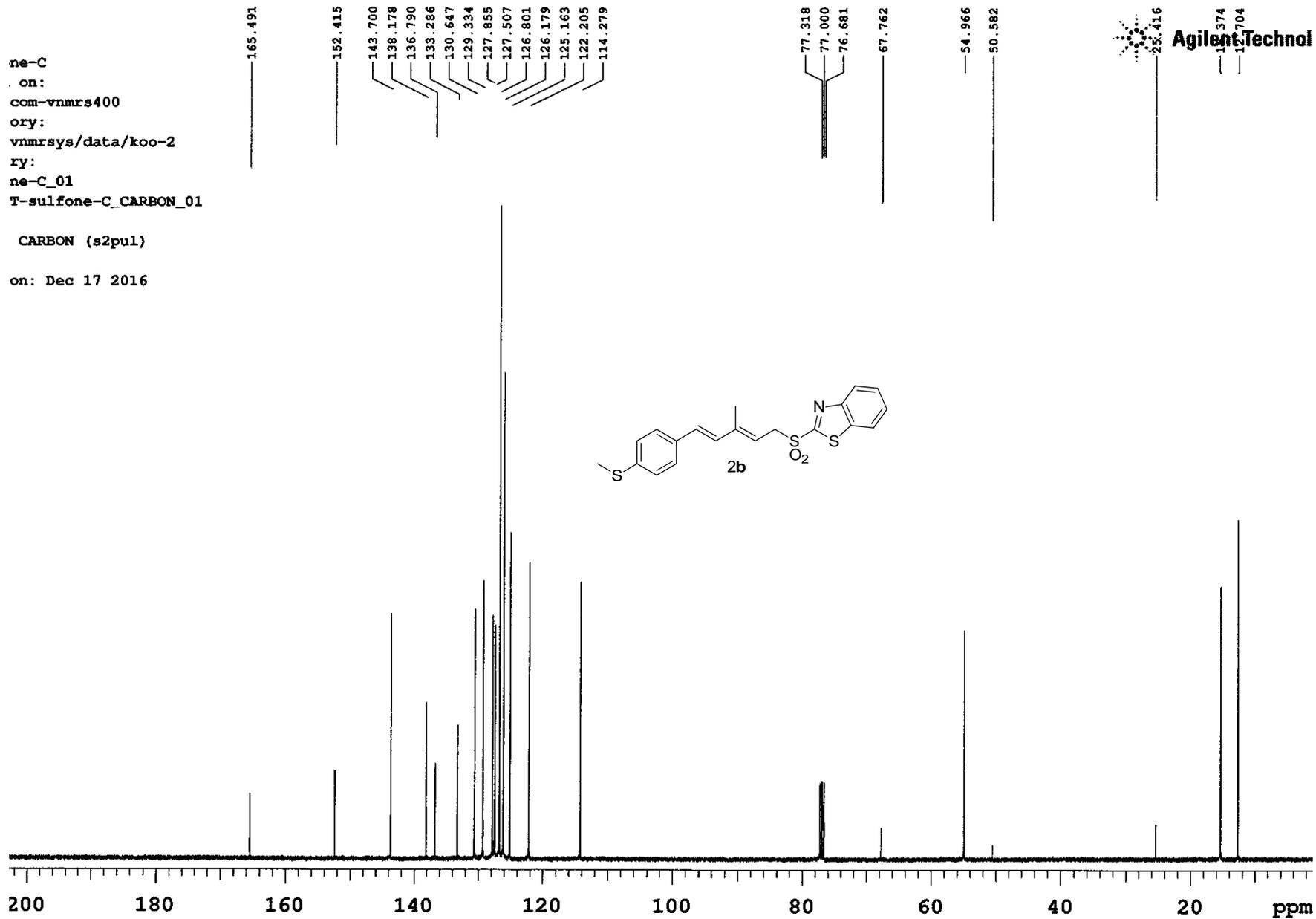
PROTON (s2pul)  
 Date: Dec 14 2016



ne-C  
on:  
com-vnmrs400  
ory:  
vnmrsys/data/koo-2  
ry:  
ne-C\_01  
T-sulfone-C CARBON\_01

CARBON (s2pul)

on: Dec 17 2016

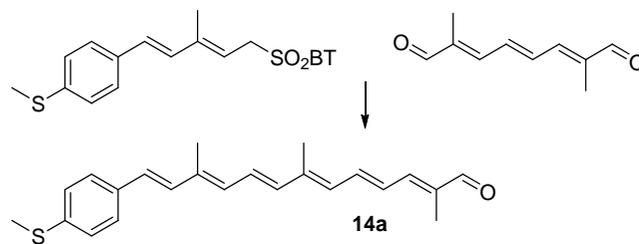
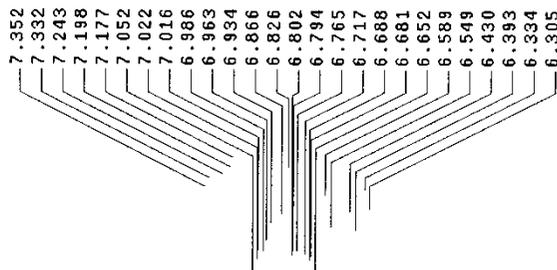


Sample: SHK-1885-3  
Sample ID: s\_44\_SHK-1885-3\_koo-2\_20151013\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1885-3\_Proton\_02.fid

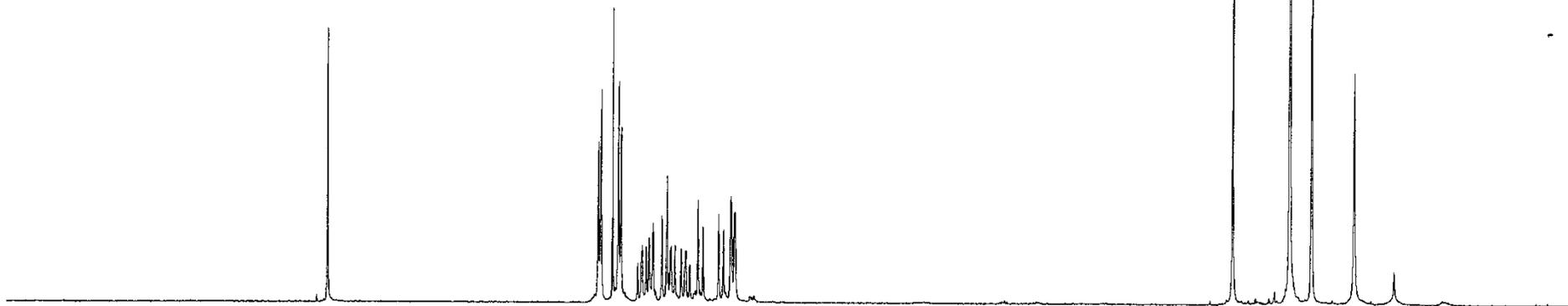
Pulse Sequence: s2pu1  
Solvent: cdcl3  
Ambient temperature  
Sample #44, Operator: walkup2  
File: SHK-1885-3\_Proton\_02  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340167 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

9.442



2.428  
2.041  
1.873  
1.545  
1.235

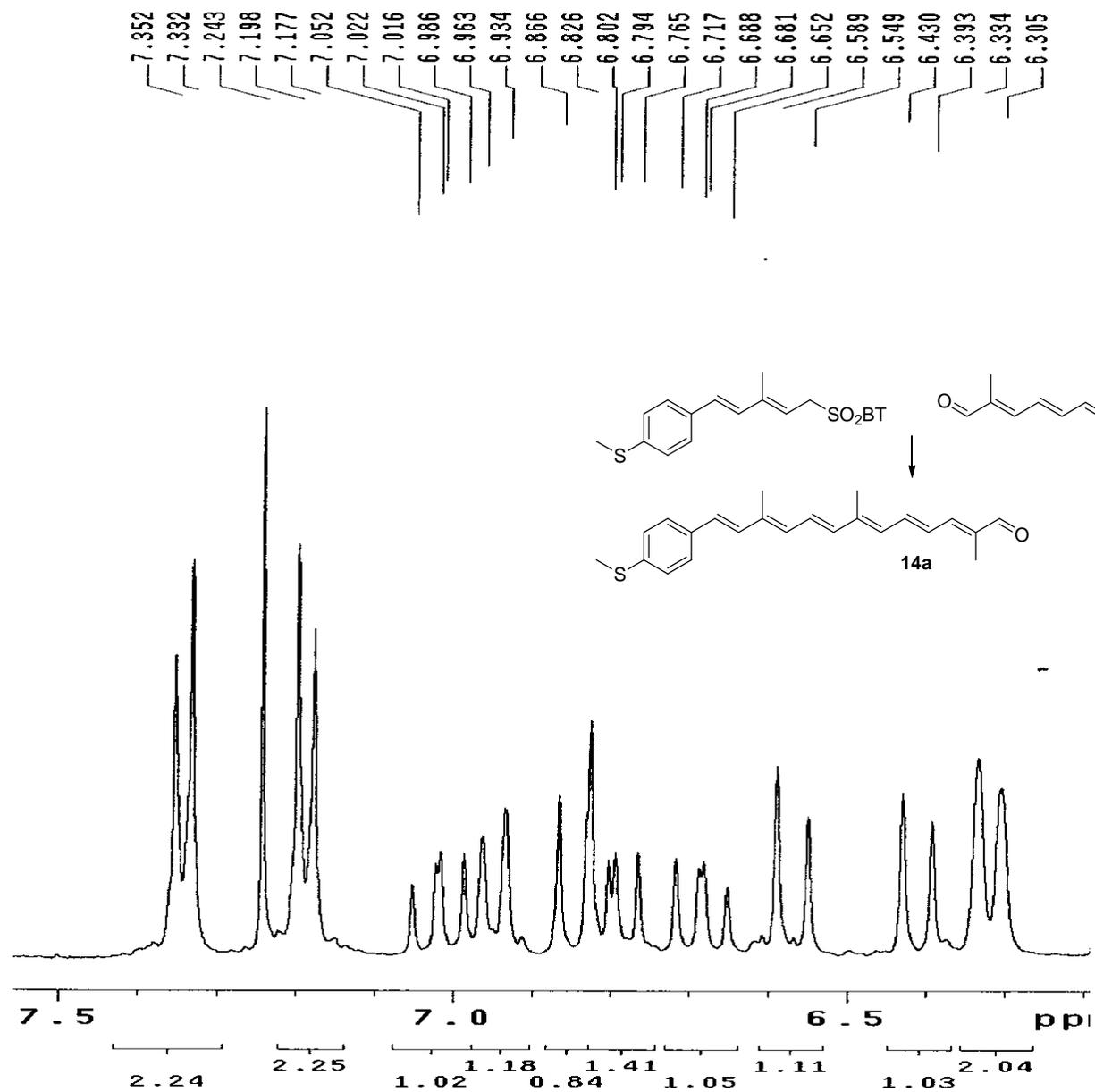


11 10 9 8 7 6 5 4 3 2 1 pp

1.00

2.29 1.84 1.12 0.04  
2.24 1.02 2.84 0.51 0.03

3.26 6.68 3.27 2.21 0.62



Sample: SHK-1885-3R  
Sample ID: s\_41\_SHK-1885-3R\_koo-2\_20151013\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1885-3R\_Carbon\_01.fid

Pulse Sequence: s2pu1

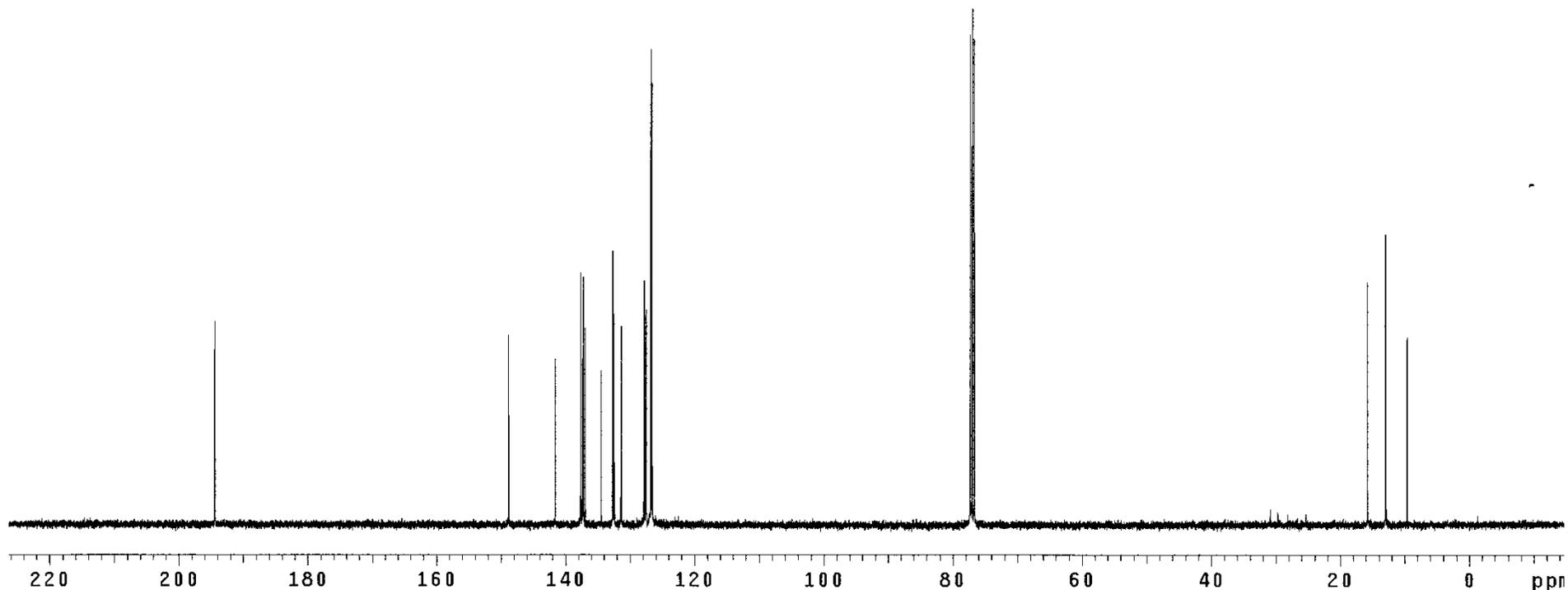
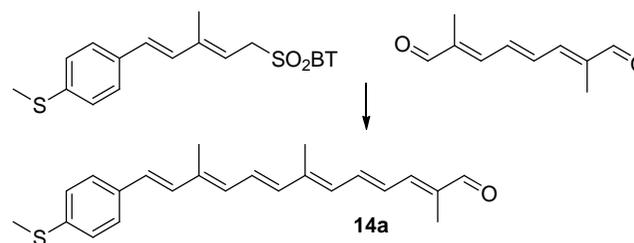
Solvent: cdcl3  
Ambient temperature  
Sample #41, Operator: walkup2  
File: SHK-1885-3R\_Carbon\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
2048 repetitions  
OBSERVE C13, 100.5886362 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 18 min, 50 sec

148.816  
141.558  
137.640  
137.595  
137.327  
137.201  
136.918  
134.449  
132.680  
132.457  
131.364  
127.794  
127.556  
127.460  
126.761  
126.597

77.318  
76.999  
76.679

15.718  
13.004  
12.930  
9.576

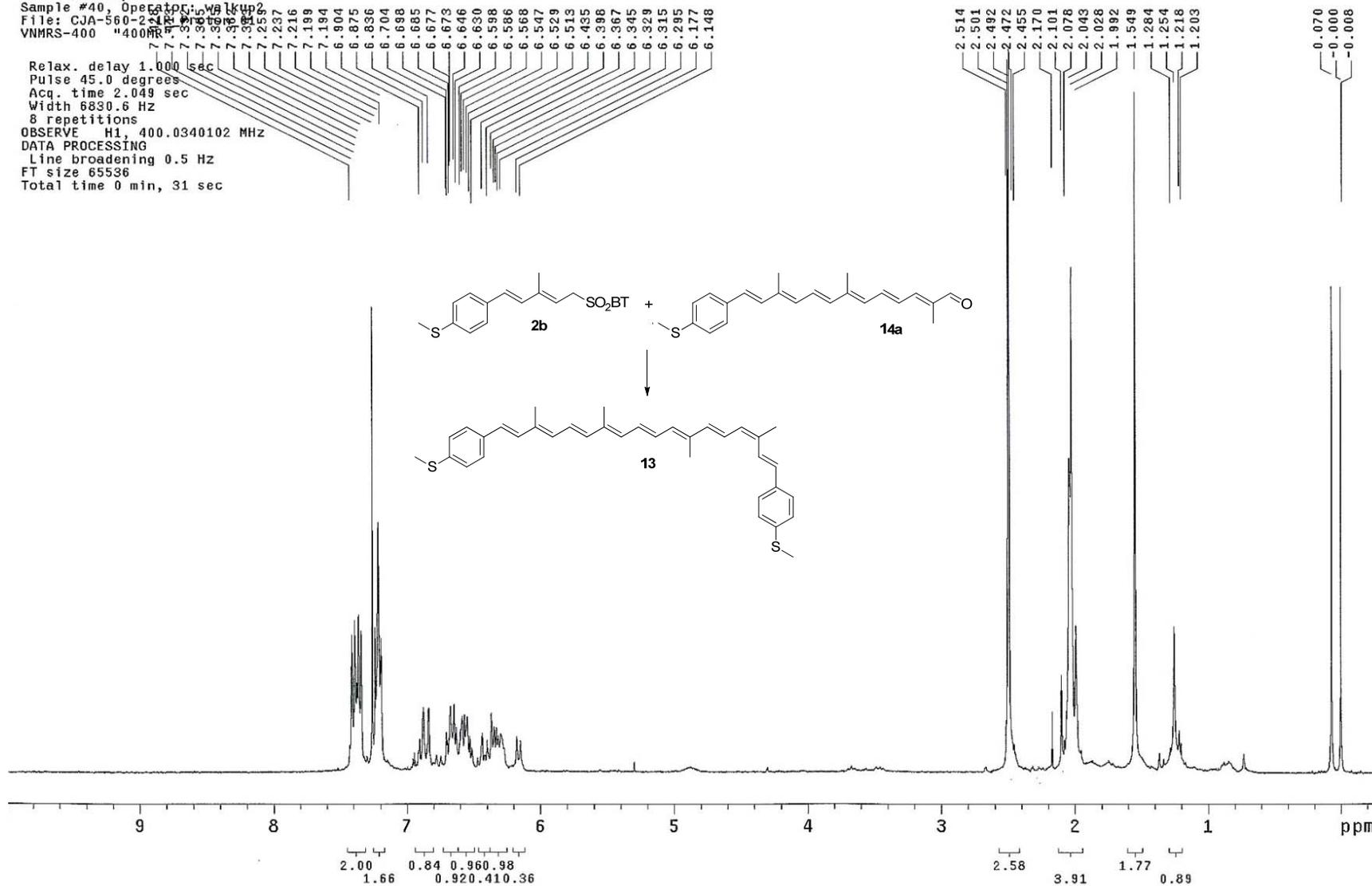


Sample: CJA-560-2-1R  
 Sample ID: s\_40\_CJA-560-2-1R\_koo-2\_20140603\_01  
 File: /home/walkup2/vnmrsys/data/koo-2/CJA-560-2-1R\_Proton\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
 Ambient temperature  
 Sample #40, Operator: walkup2  
 File: CJA-560-2-1R\_Proton\_01  
 VNMR5-400 "400MHz"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.049 sec  
 Width 6830.6 Hz  
 8 repetitions  
 OBSERVE H1, 400.0340102 MHz  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 0 min, 31 sec

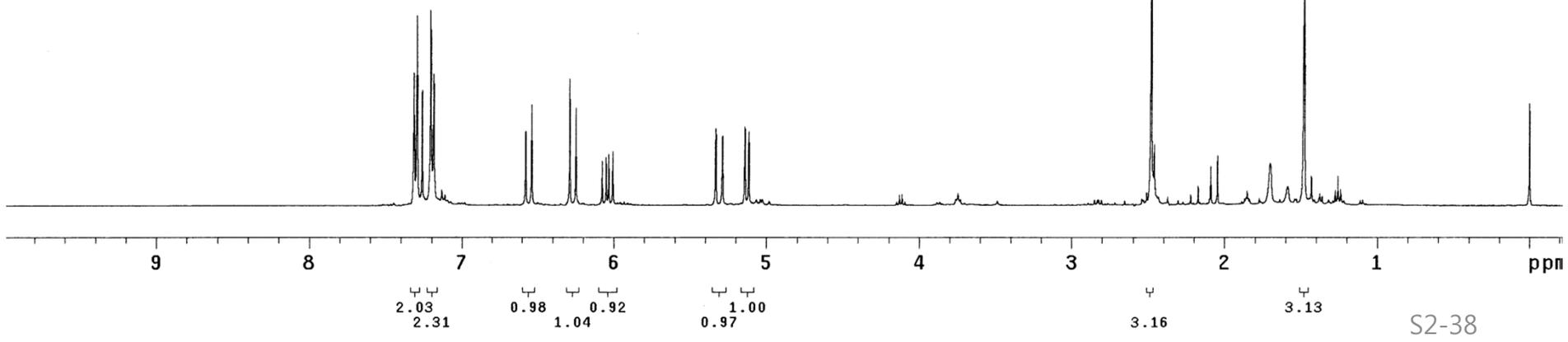
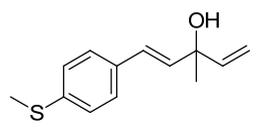


Sample: SHK-1969  
Sample ID: s\_45\_SHK-1969\_koo-2\_20160301\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1969\_Proton\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Sample #45, Operator: walkup2  
File: SHK-1969\_Proton\_01  
VNMR5-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340087 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-2007-1  
Sample ID: s\_40\_SHK-2007-1\_koo-2\_20160415\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-2007-1\_Proton\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

Sample 740 Operator: walkup2

File 30 SHK-2007-1\_Proton\_01

VNMR 400.130056 MHz

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6830.6 Hz

8 repetitions

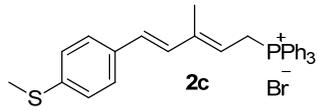
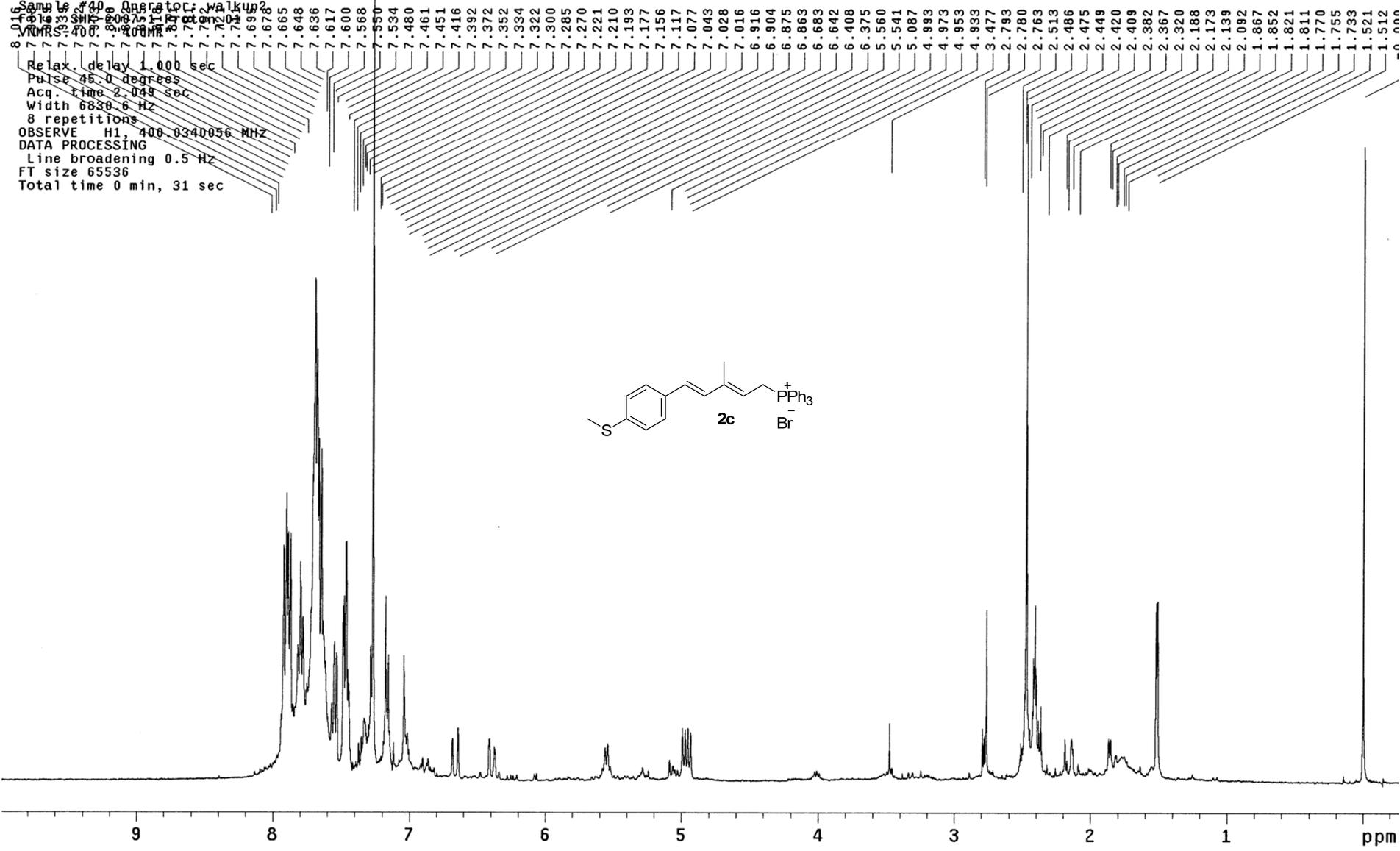
OBSERVE H1, 400.130056 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec



5.0888.98.91 3.23  
4.18.13016.052.39 1.17 1.15 1.34 2.00 0.85 0.57 1.59 2.960.72 1.27 2.84

Sample: SHK-2010-1-1R  
 Sample ID: s\_41\_SHK-2010-1-1R\_koo-2\_20160421\_01  
 File: /home/walkup2/vnmrSYS/data/koo-2/SHK-2010-1-1R\_Proton\_01.fid

Pulse Sequence: s2pul

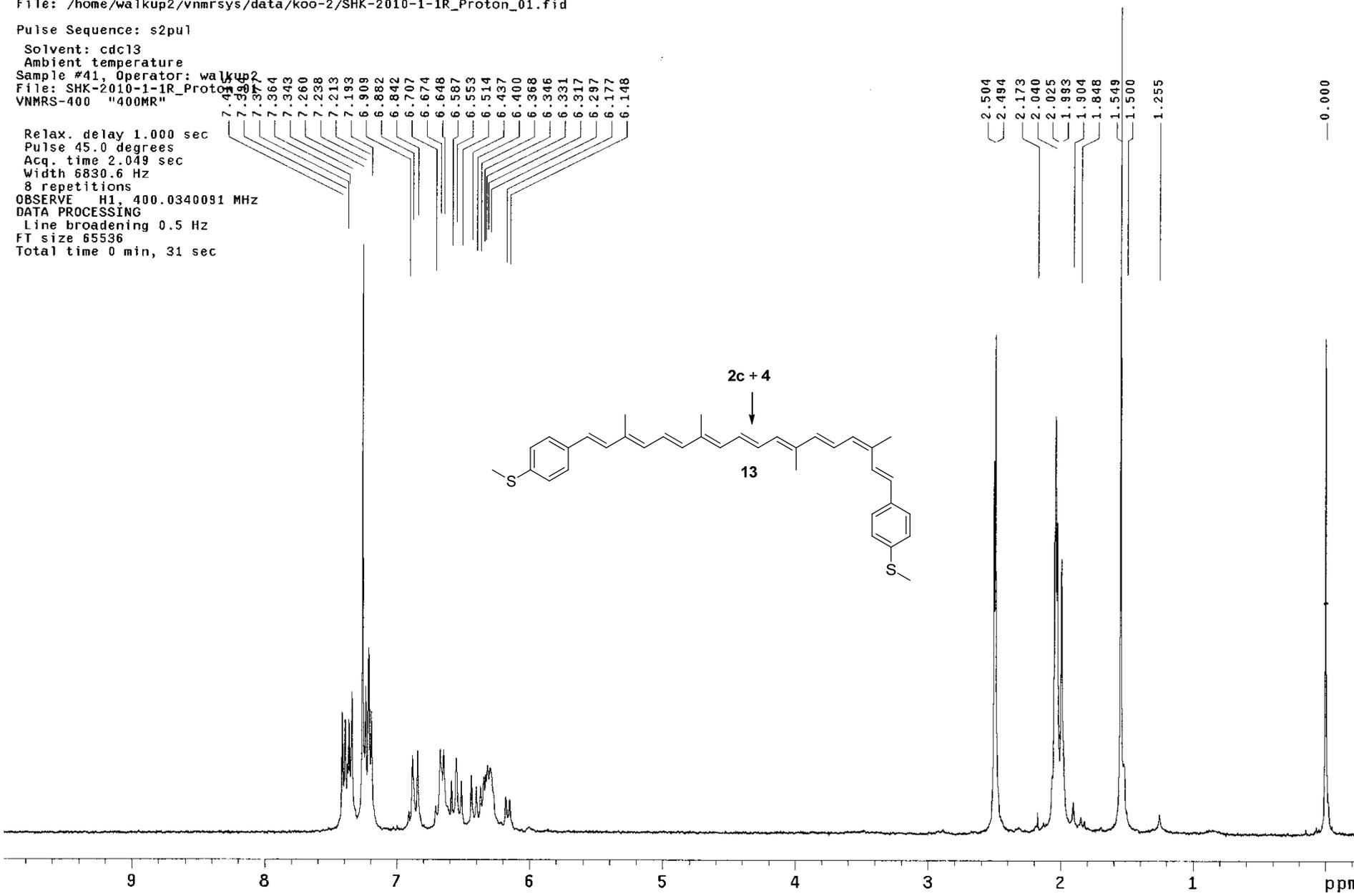
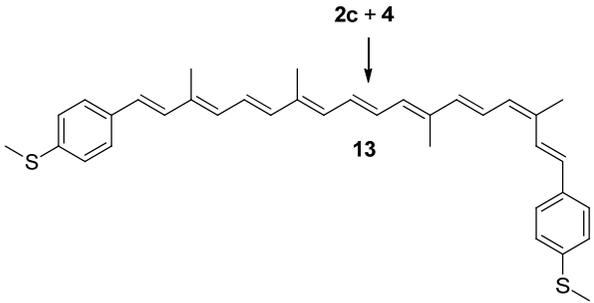
Solvent: cdcl3  
 Ambient temperature  
 Sample #41, Operator: walkup2  
 File: SHK-2010-1-1R\_Proton\_01  
 VNMR-400 "400MR"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.049 sec  
 Width 6830.6 Hz  
 8 repetitions  
 OBSERVE H1, 400.0340091 MHz  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 0 min, 31 sec

7.407  
7.397  
7.377  
7.364  
7.343  
7.260  
7.238  
7.213  
7.193  
6.909  
6.882  
6.842  
6.707  
6.674  
6.648  
6.587  
6.553  
6.514  
6.437  
6.400  
6.368  
6.346  
6.331  
6.317  
6.297  
6.177  
6.148

2.504  
2.494  
2.173  
2.040  
2.025  
1.993  
1.904  
1.848  
1.549  
1.500  
1.255

0.000



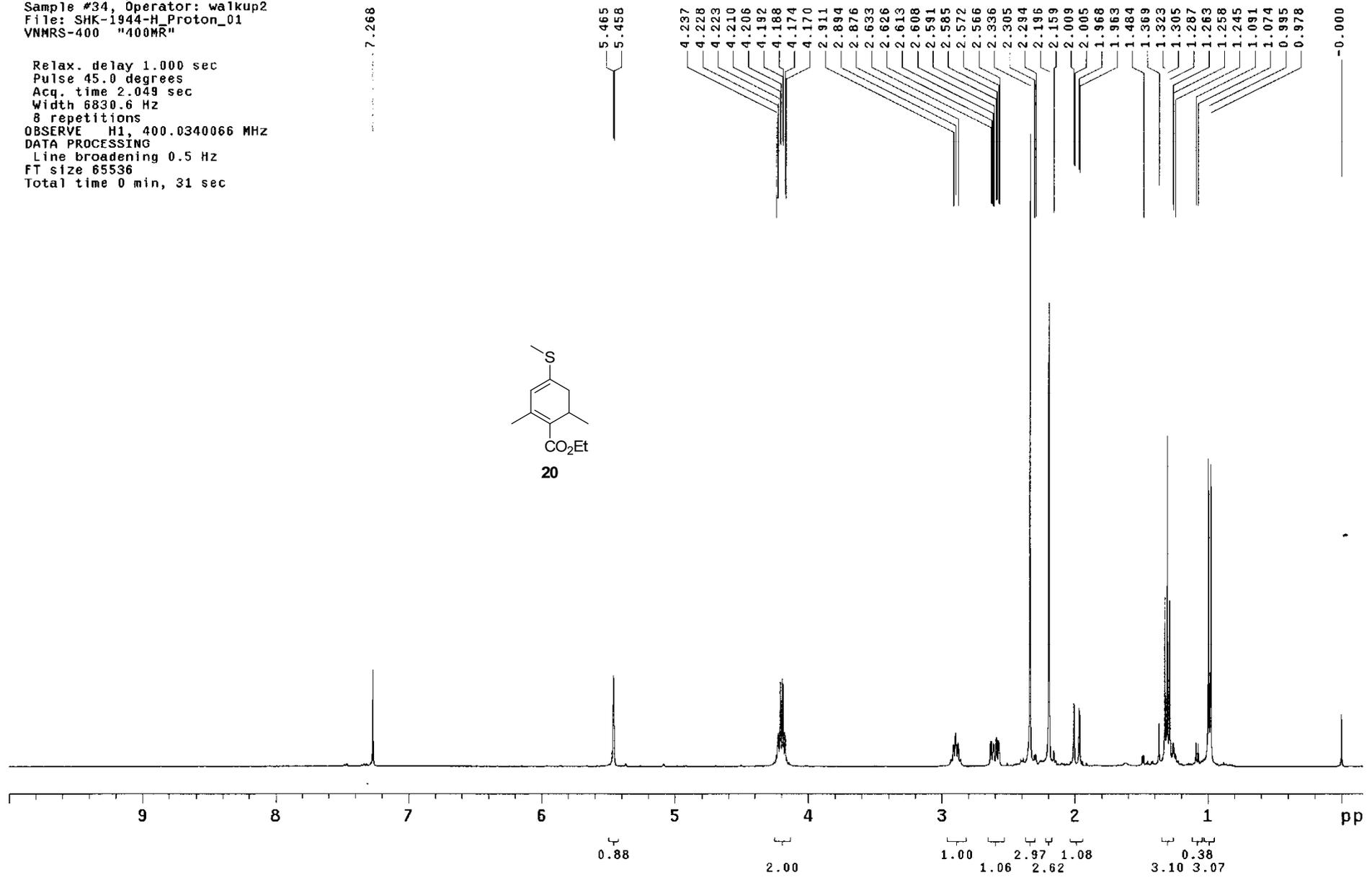
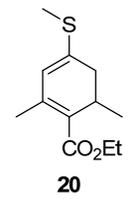
0.92 0.04  
1.30 1.00 1.10 1.40 1.40

0.93 2.37 2.81  
1.48 2.78

Sample: SHK-1944-H  
Sample ID: s\_34\_SHK-1944-H\_koo-2\_20160113\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1944-H\_Proton\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdcl3  
Ambient temperature  
Sample #34, Operator: walkup2  
File: SHK-1944-H\_Proton\_01  
VNMRS-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340066 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-1944-C  
Sample ID: s\_37\_SHK-1944-C\_koo-2\_20160114\_01  
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1944-C\_Carbon\_02.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Sample #37, Operator: walkup2  
File: SHK-1944-C\_Carbon\_02  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886373 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

142.150  
142.083

123.017  
118.563

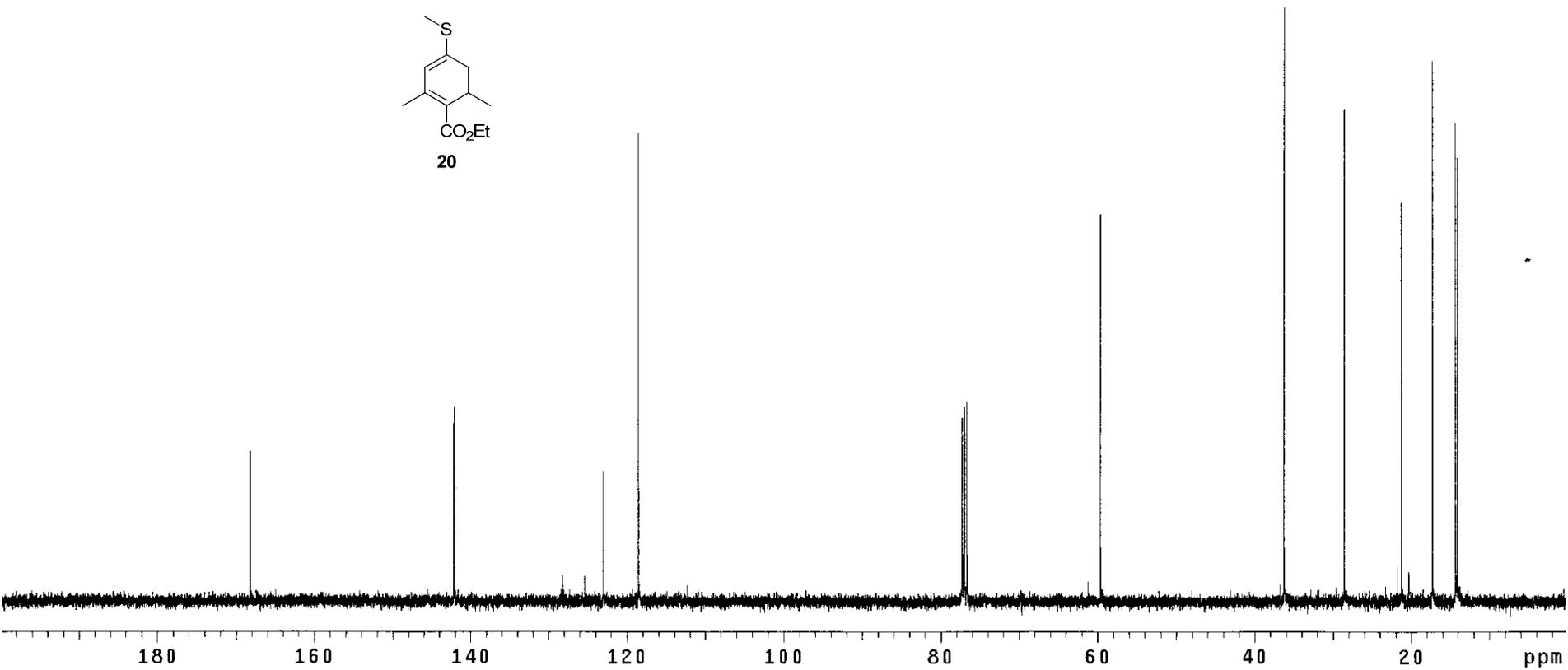
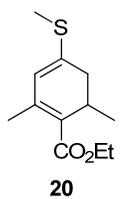
77.300  
76.988  
76.668

59.617

36.253

28.594

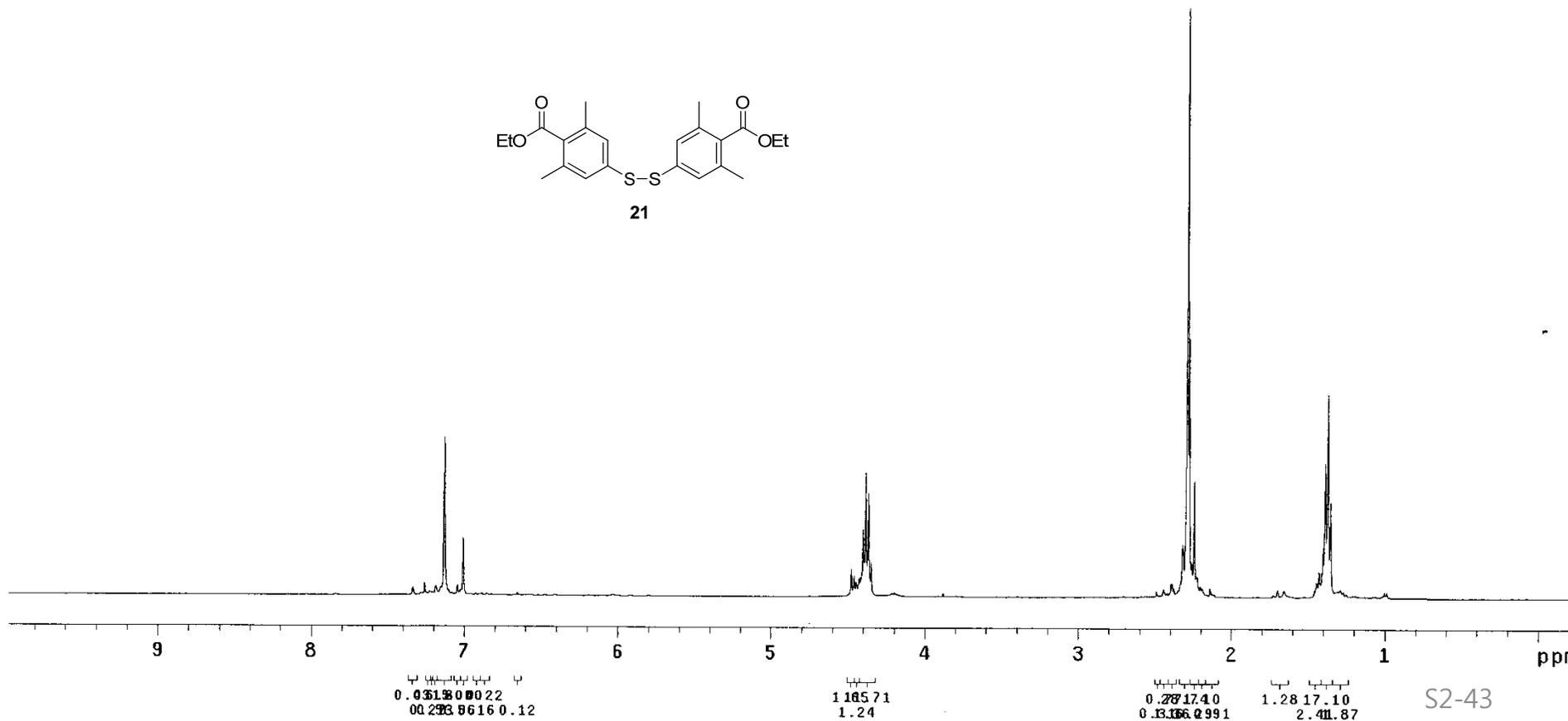
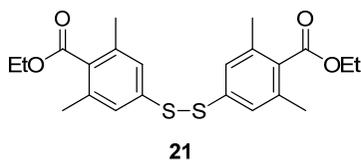
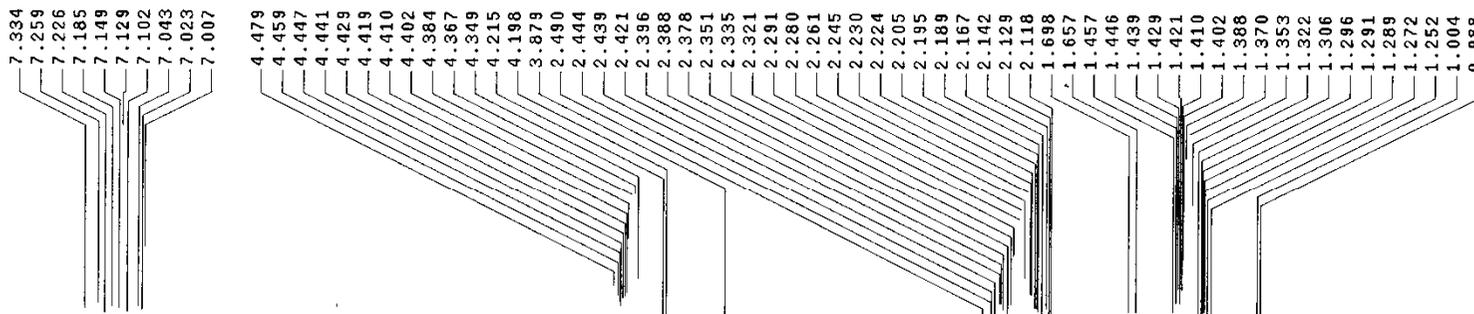
21.232  
17.269  
14.332  
14.057



Sample: SHK-1931-2-1  
 Sample ID: s\_41\_SHK-1931-2-1\_koo-2\_20151214\_01  
 File: /home/walkup2/vnmrsvs/data/koo-2/SHK-1931-2-1\_Proton\_01.fid

Pulse Sequence: s2pu1  
 Solvent: cdc13  
 Ambient temperature  
 Sample #41, Operator: walkup2  
 File: SHK-1931-2-1\_Proton\_01  
 VNMR5-400 "400MR"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.049 sec  
 Width 6830.6 Hz  
 8 repetitions  
 OBSERVE H1, 400.0340098 MHz  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 0 min, 31 sec



Sample: SHK-1931-2-1-c  
Sample ID: s\_46\_SHK-1931-2-1-c\_koo-2\_20151215\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1931-2-1-c\_Carbon\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

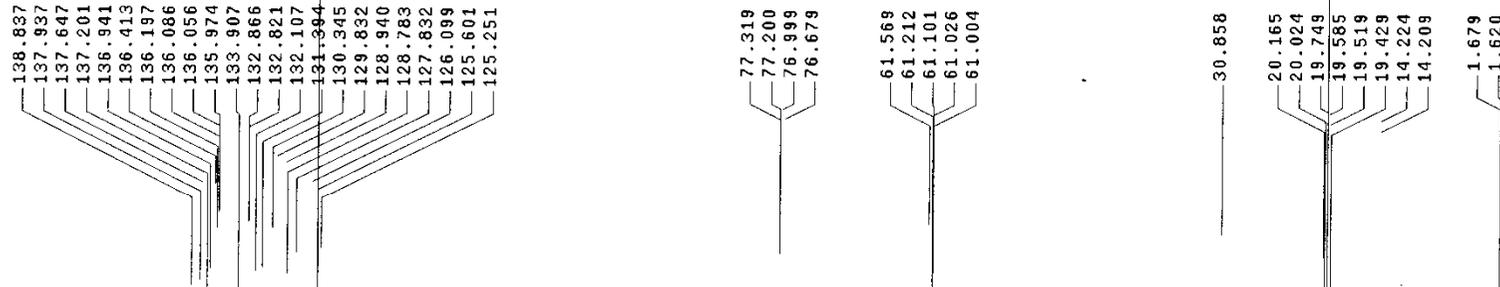
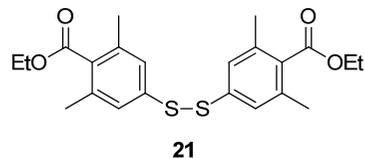
Sample #46, Operator: walkup2

File: SHK-1931-2-1-c\_Carbon\_01

VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
512 repetitions  
OBSERVE C13, 100.5886377 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 19 min, 42 sec

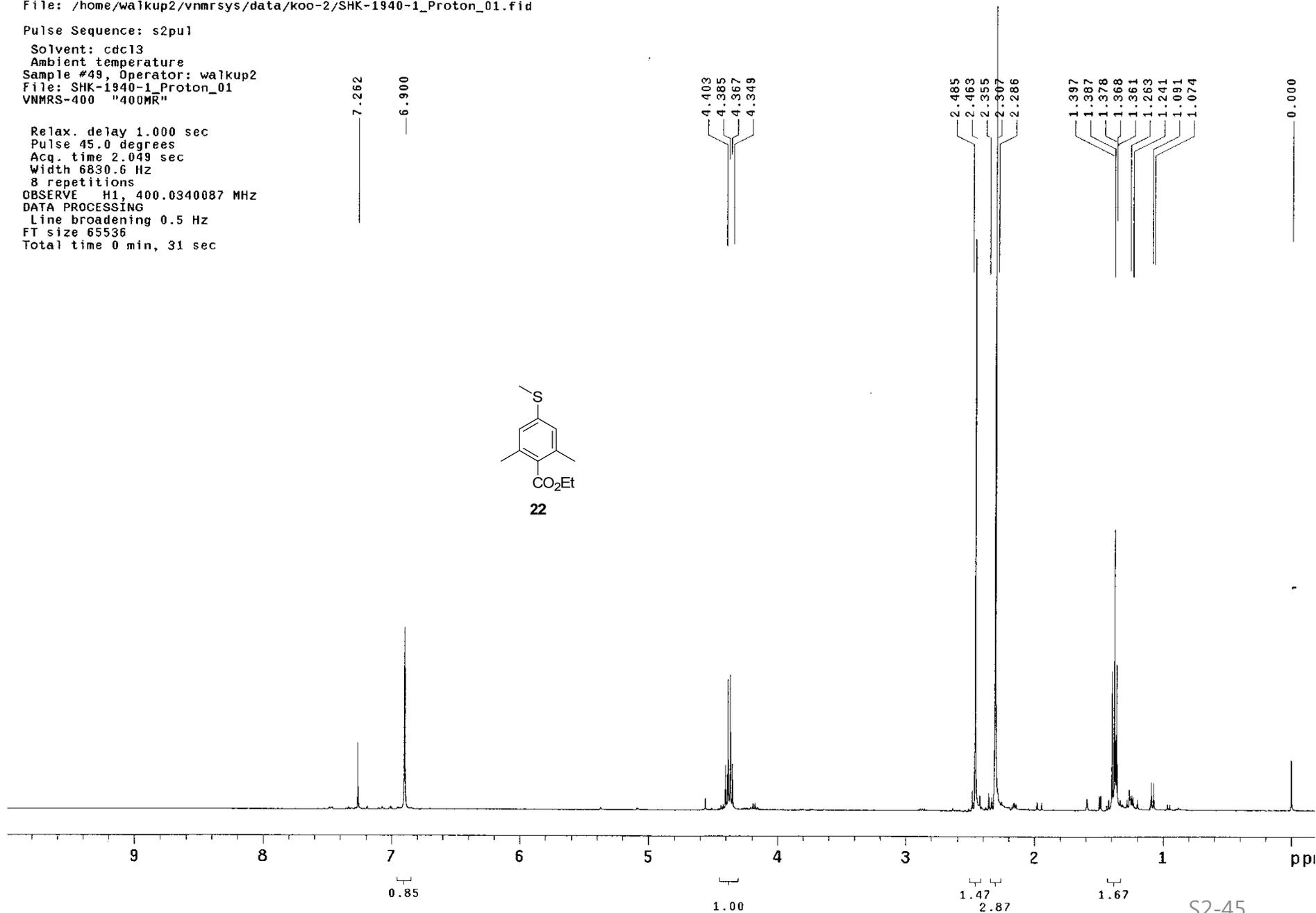
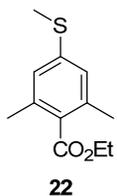
180 160 140 120 100 80 60 40 20 ppm



Sample: SHK-1940-1  
Sample ID: s\_49\_SHK-1940-1\_koo-2\_20160111\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1940-1\_Proton\_01.fid

Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
Sample #49, Operator: walkup2  
File: SHK-1940-1\_Proton\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340087 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-1940-1  
Sample ID: s\_33\_SHK-1940-1\_koo-2\_20160112\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1940-1\_Carbon\_01.fid

Pulse Sequence: s2pu1

Solvent: cdcl3  
Ambient temperature  
Sample #33, Operator: walkup2  
File: SHK-1940-1\_Carbon\_01  
VNMRS-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
2048 repetitions  
OBSERVE C13, 100.5886430 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 18 min, 50 sec

169.480

139.929

135.705

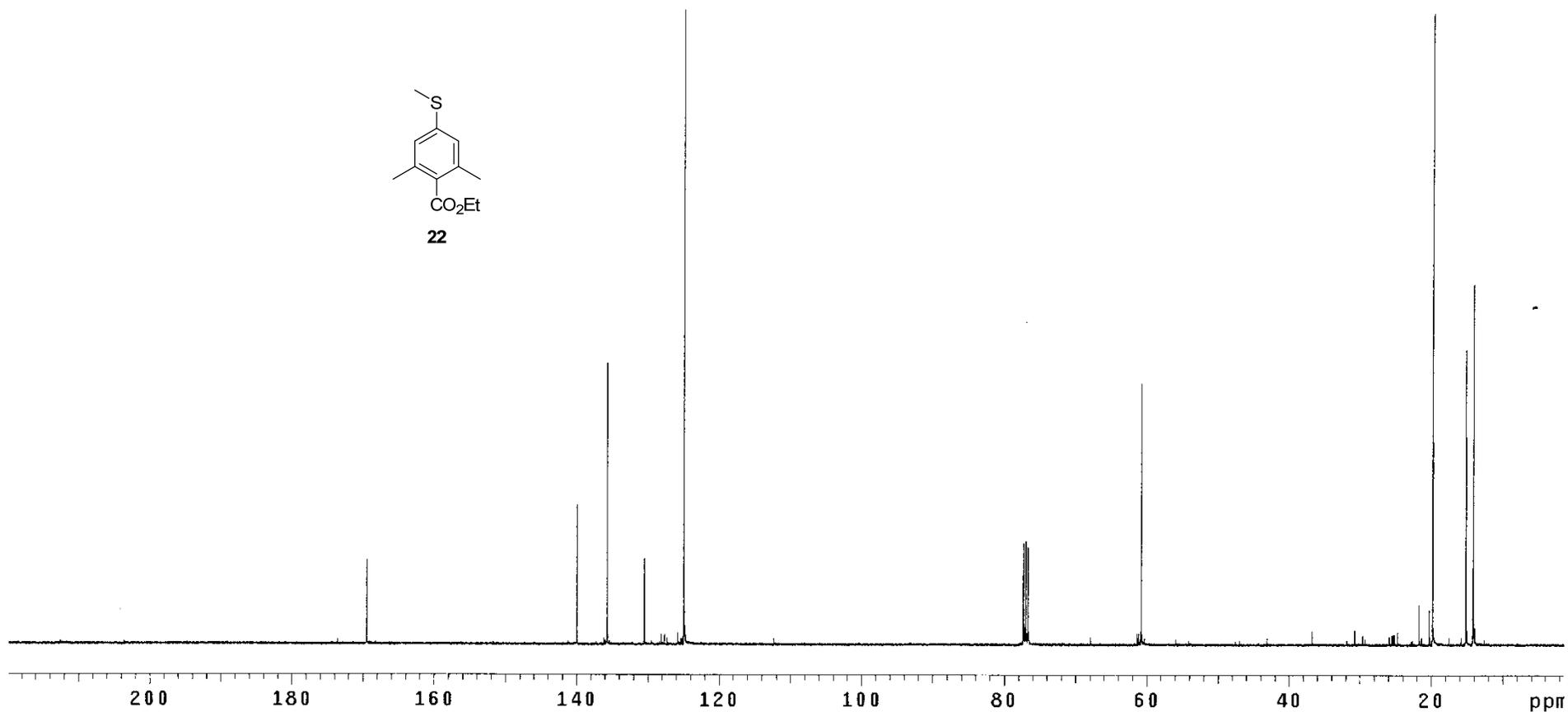
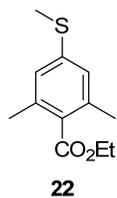
130.470

124.923

77.303  
77.184  
76.983  
76.663

60.765

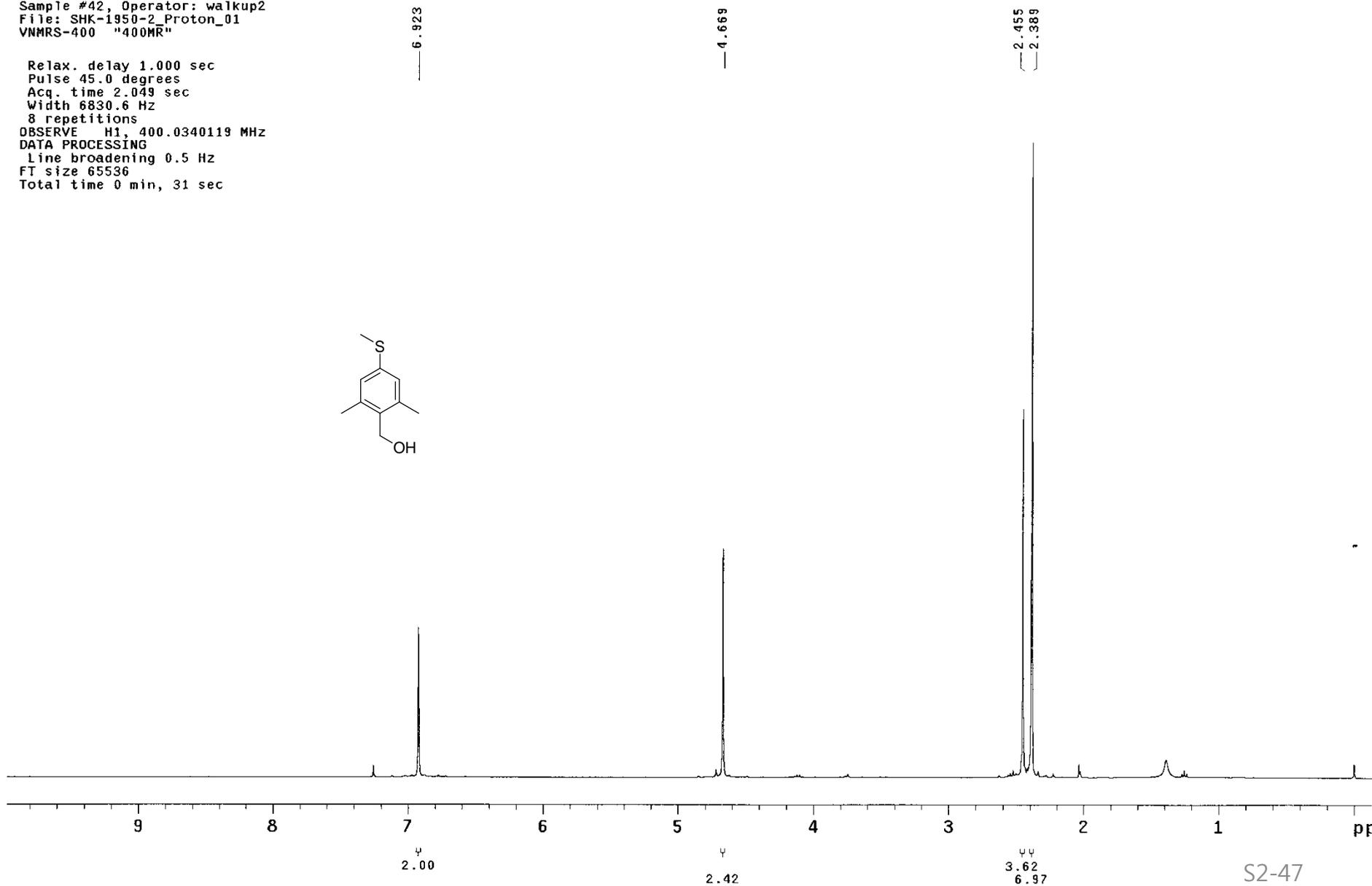
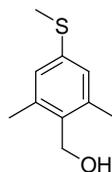
21.659  
20.276  
19.785  
19.711  
15.152  
14.171  
14.096



Sample: SHK-1950-2  
Sample ID: s\_42\_SHK-1950-2\_koo-2\_20160202\_01  
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1950-2\_Proton\_01.fid

Pulse Sequence: s2pul  
Solvent: cdc13  
Ambient temperature  
Sample #42, Operator: walkup2  
File: SHK-1950-2\_Proton\_01  
VNMRS-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340119 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-1950-2  
Sample ID: s\_34\_SHK-1950-2\_koo-2\_20160203\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1950-2\_Carbon\_01.fid

Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
Sample #34, Operator: walkup2  
File: SHK-1950-2\_Carbon\_01  
VNMRS-400 "400MR"

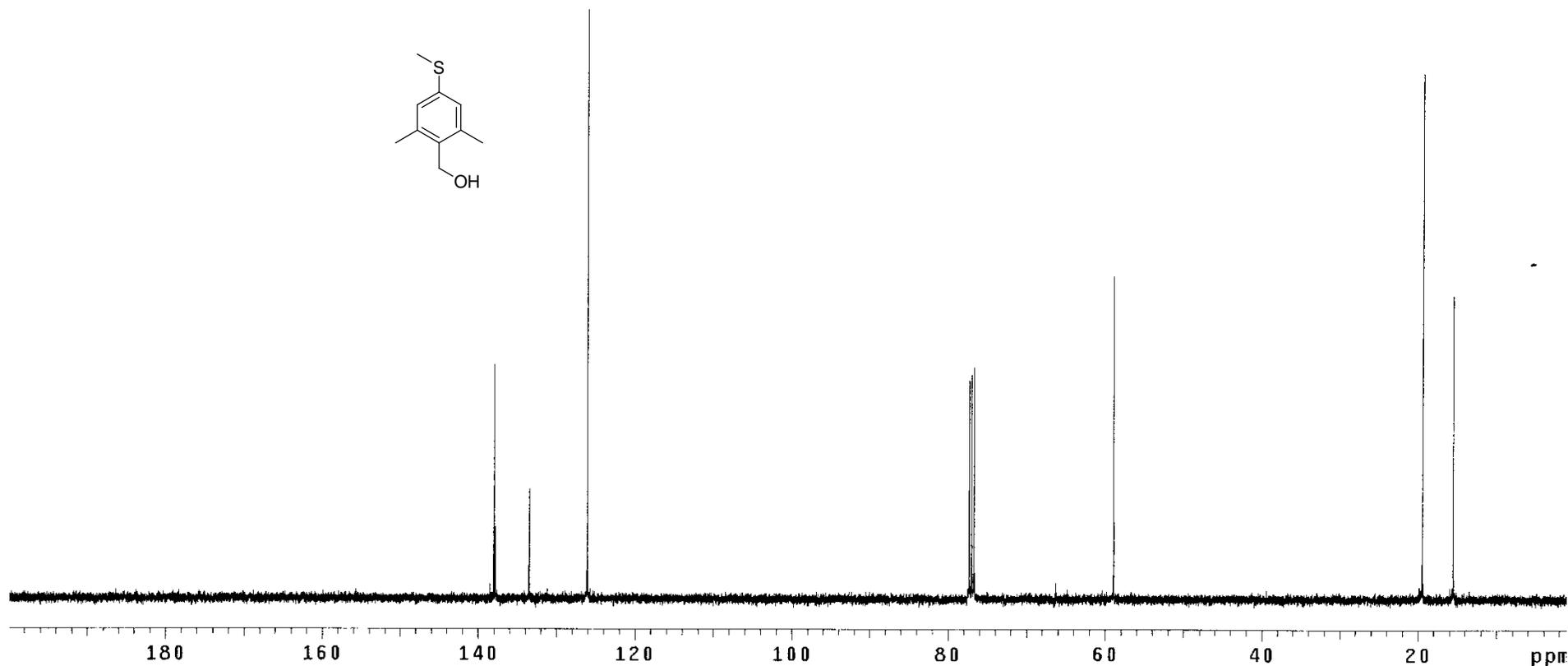
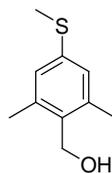
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886391 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

137.975  
137.789  
133.491  
126.062

77.312  
76.999  
76.680

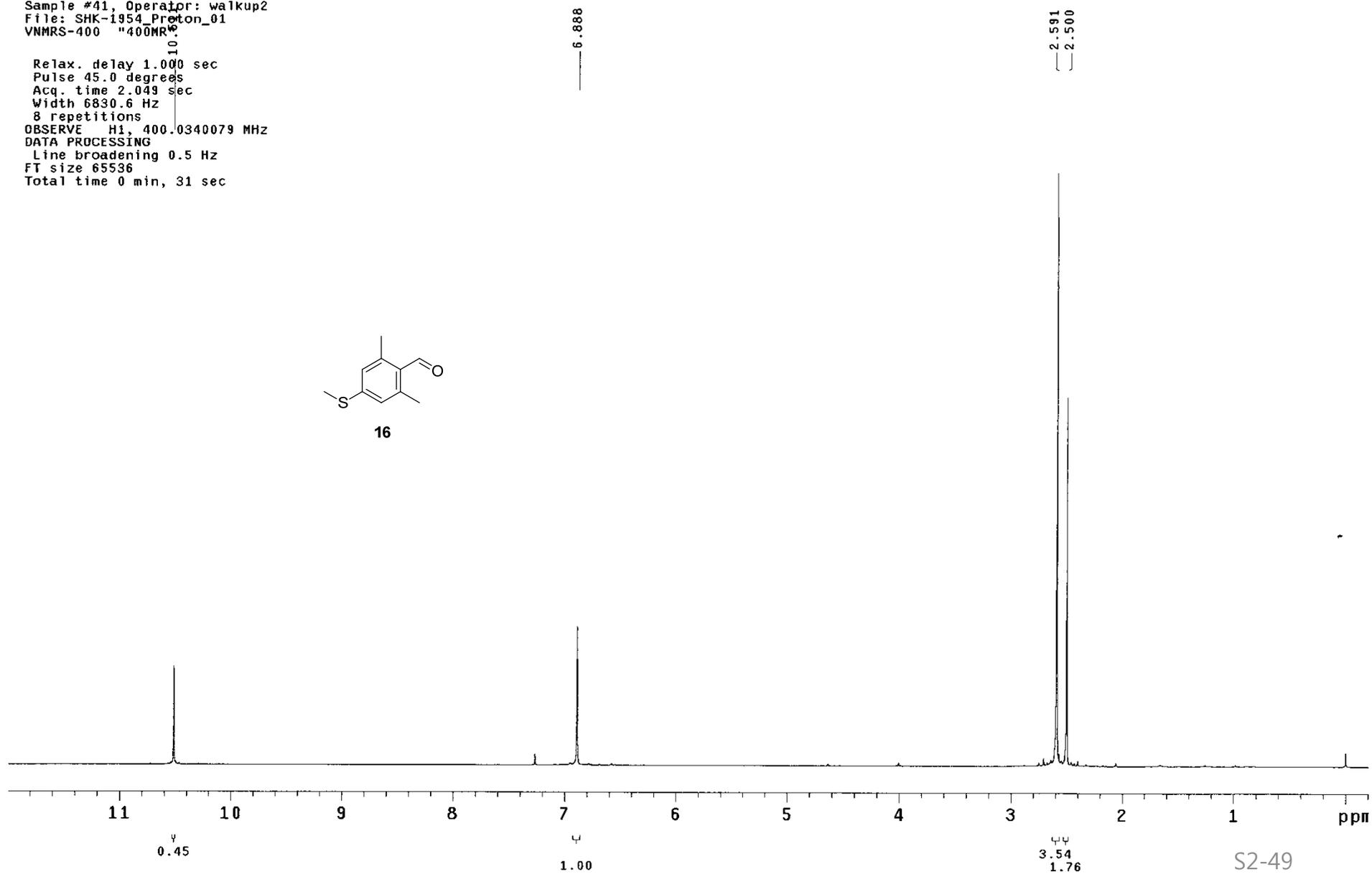
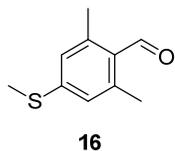
58.922

19.415  
15.533



Sample: SHK-1954  
Sample ID: s\_41\_SHK-1954\_koo-2\_20160204\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1954\_Proton\_01.fid

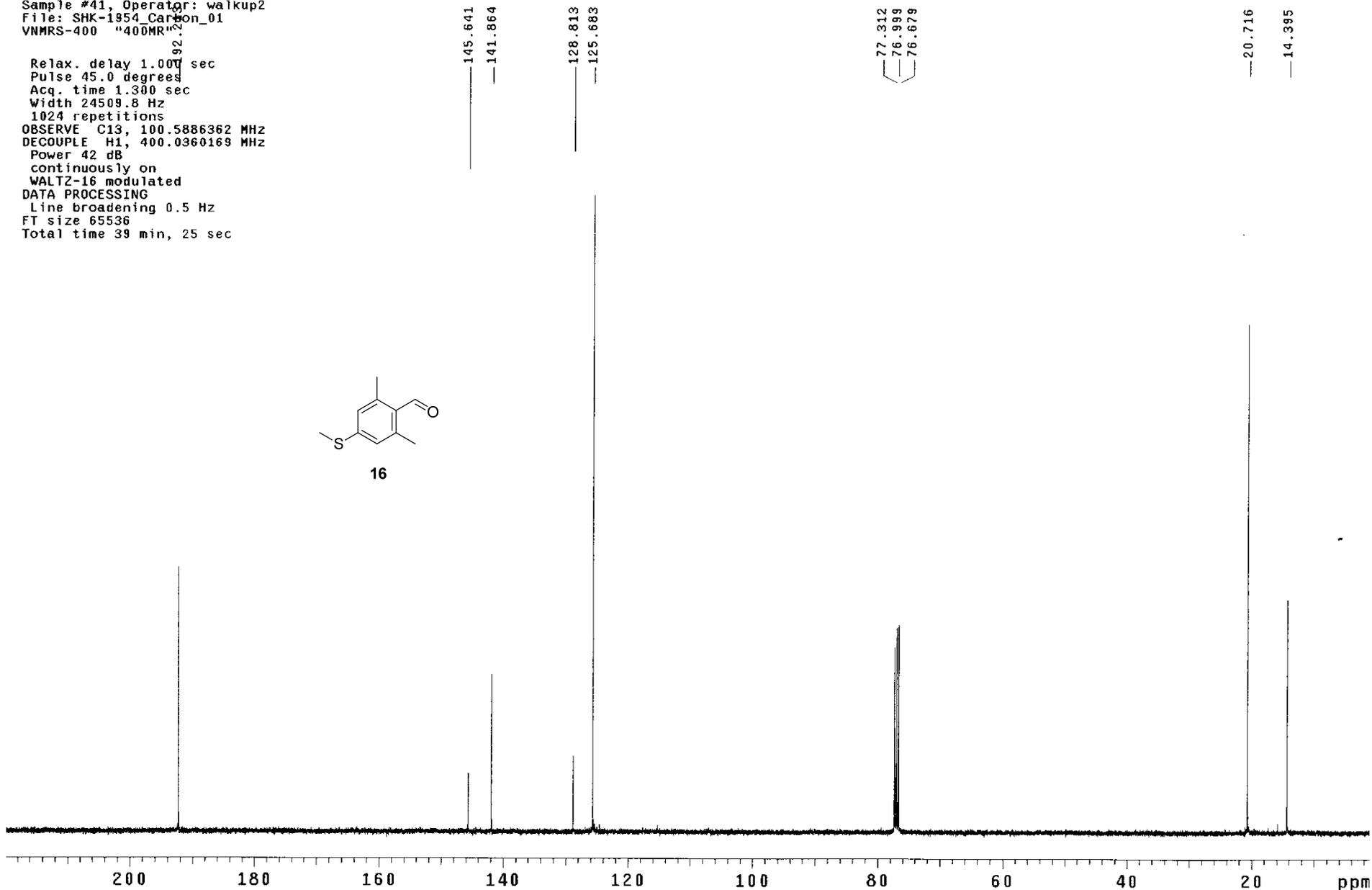
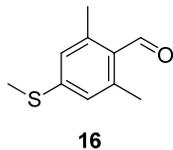
Pulse Sequence: s2pu1  
Solvent: cdcl3  
Ambient temperature  
Sample #41, Operator: walkup2  
File: SHK-1954\_Proton\_01  
VNMRS-400 "400MR"  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340079 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



Sample: SHK-1954  
Sample ID: s\_41\_SHK-1954\_koo-2\_20160204\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1954\_Carbon\_01.fid

Pulse Sequence: s2pul  
Solvent: cdc13  
Ambient temperature  
Sample #41, Operator: walkup2  
File: SHK-1954\_Carbon\_01  
VNMRS-400 "400MR"

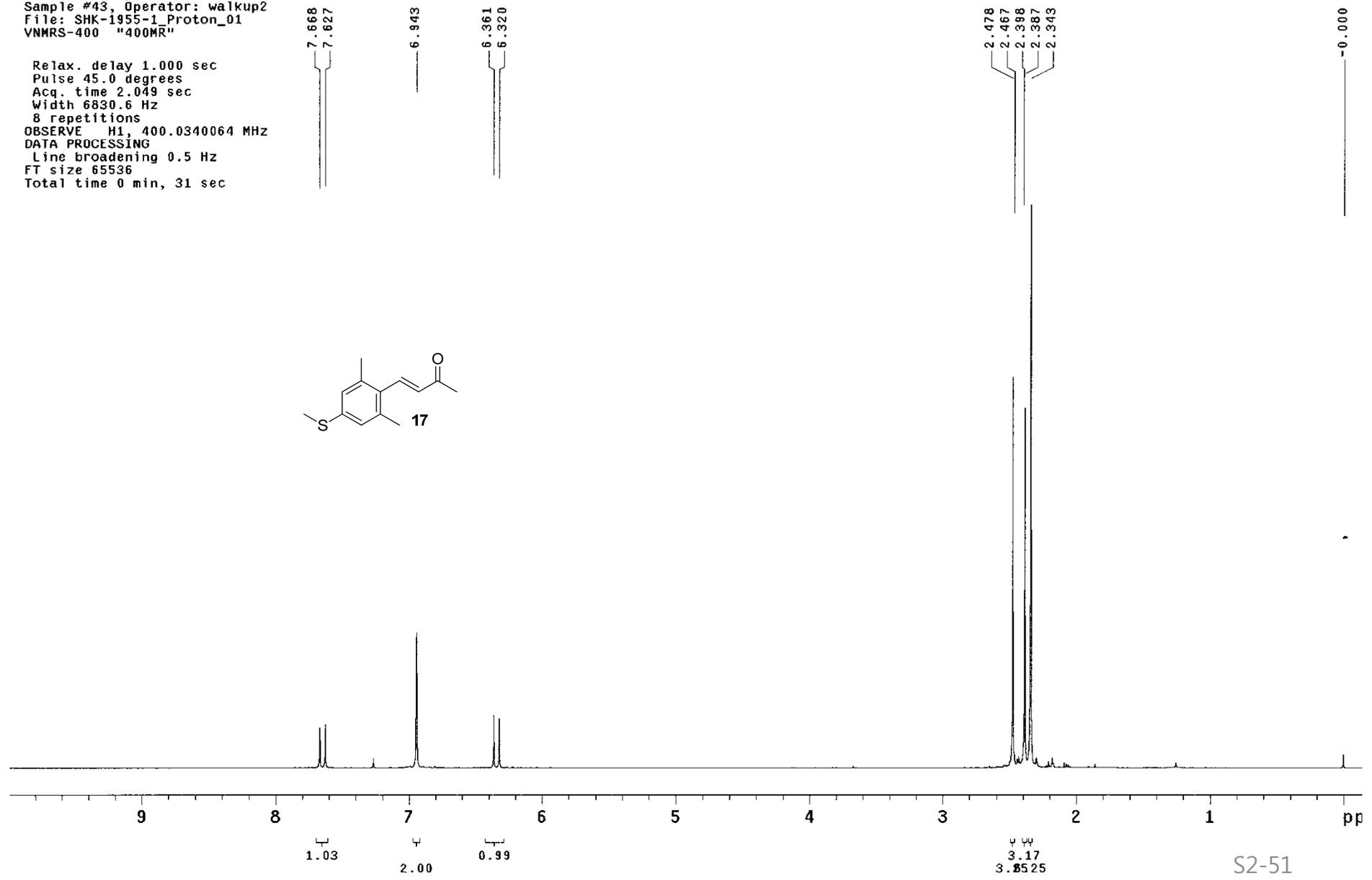
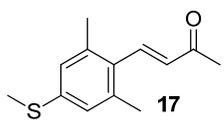
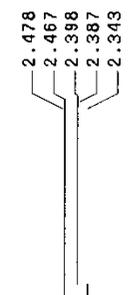
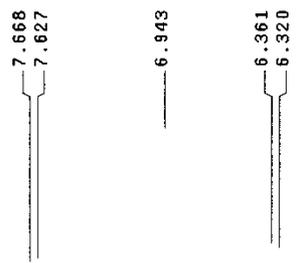
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
1024 repetitions  
OBSERVE C13, 100.5886362 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 39 min, 25 sec



Sample: SHK-1955-1  
Sample ID: s\_43\_SHK-1955-1\_koo-2\_20160212\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1955-1\_Proton\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdc13  
Ambient temperature  
Sample #43, Operator: walkup2  
File: SHK-1955-1\_Proton\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340064 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

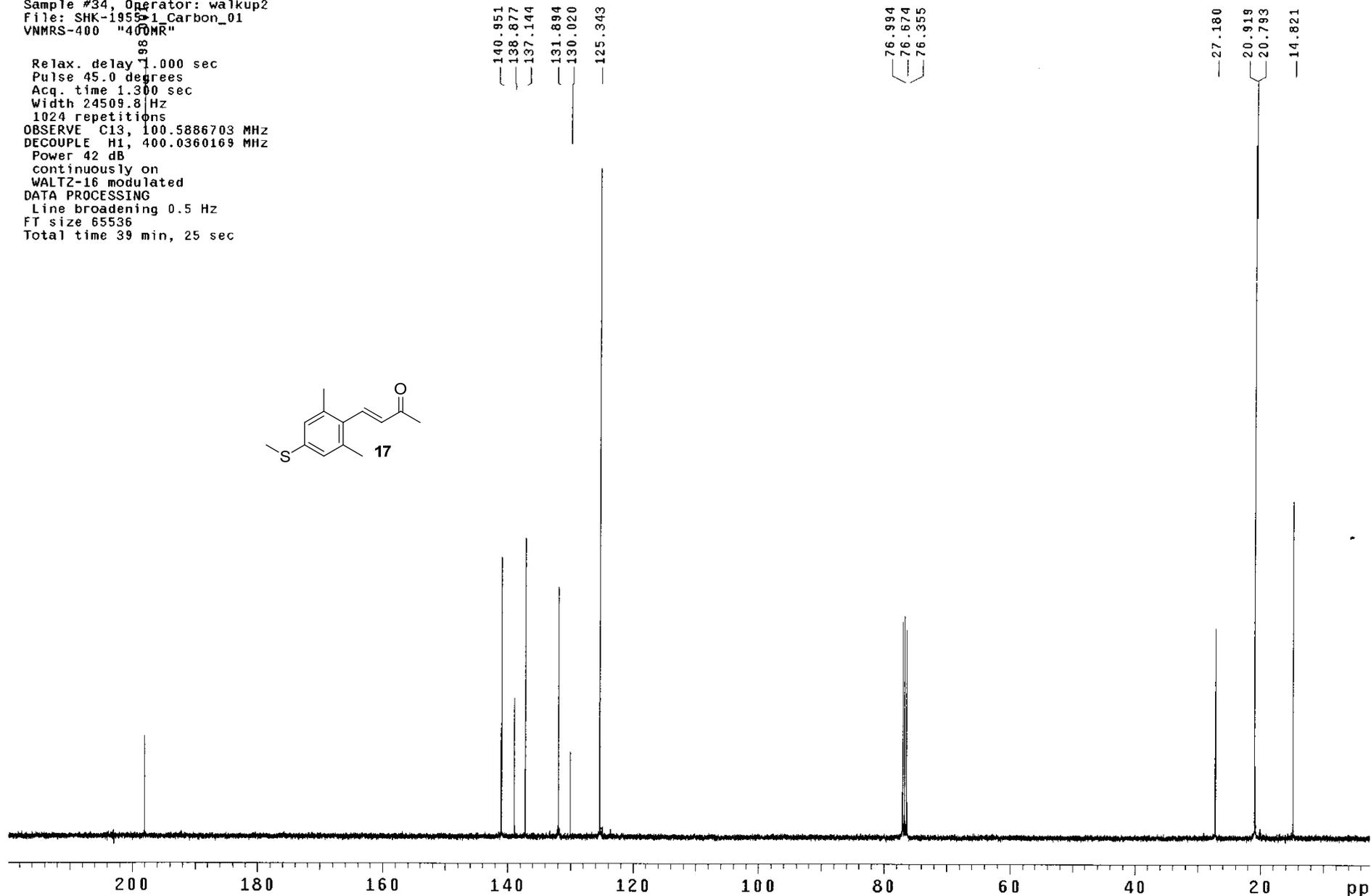
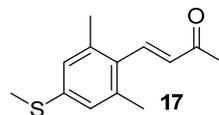


Sample: SHK-1955-1  
Sample ID: s\_34\_SHK-1955-1\_koo-2\_20160212\_01  
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1955-1\_Carbon\_01.fid

Pulse Sequence: s2pul

Solvent: cdc13  
Ambient temperature  
Sample #34, Operator: walkup2  
File: SHK-1955-1\_Carbon\_01  
VNMR-400 "400MR"

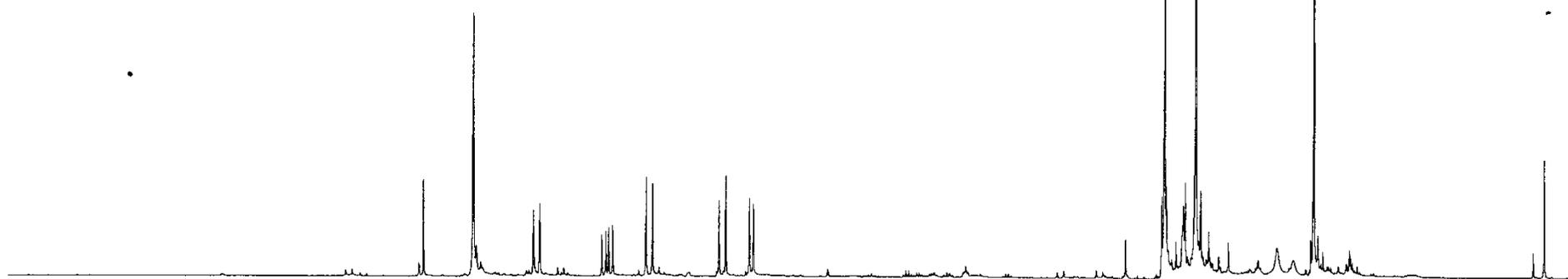
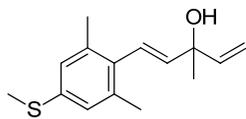
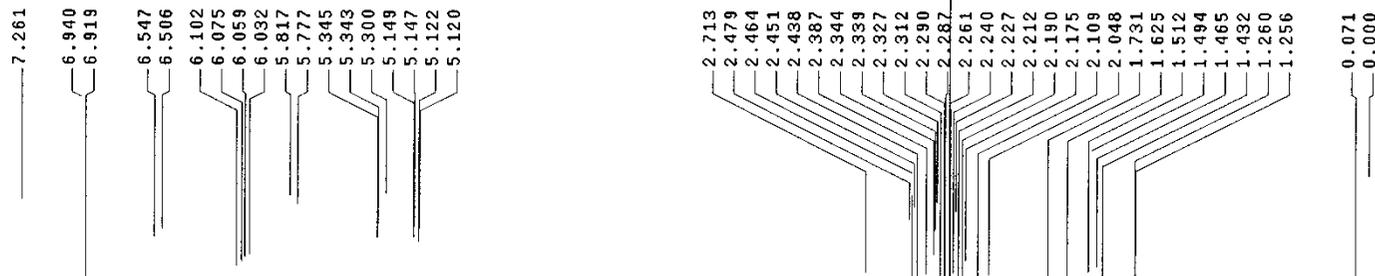
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
1024 repetitions  
OBSERVE C13, 100.5886703 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 39 min, 25 sec



Sample: SHK-1959  
Sample ID: s\_41\_SHK-1959\_koo-2\_20160215\_01  
File: /home/walkup2/vnmr/sys/data/koo-2/SHK-1959\_Proton\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdc13  
Ambient temperature  
Sample #41, Operator: walkup2  
File: SHK-1959\_Proton\_01  
VNMRs-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340087 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec



9 8 7 6 5 4 3 2 1 pp

Integration values: 2.52, 1.00, 0.86, 0.93, 1.02, 0.95, 4.37, 1.87, 0.02, 3.92

Sample: SHK-1960-2  
 Sample ID: s\_42\_SHK-1960-2\_koo-2\_20160216\_01  
 File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1960-2\_Proton\_01.fid

Pulse Sequence: s2pu1

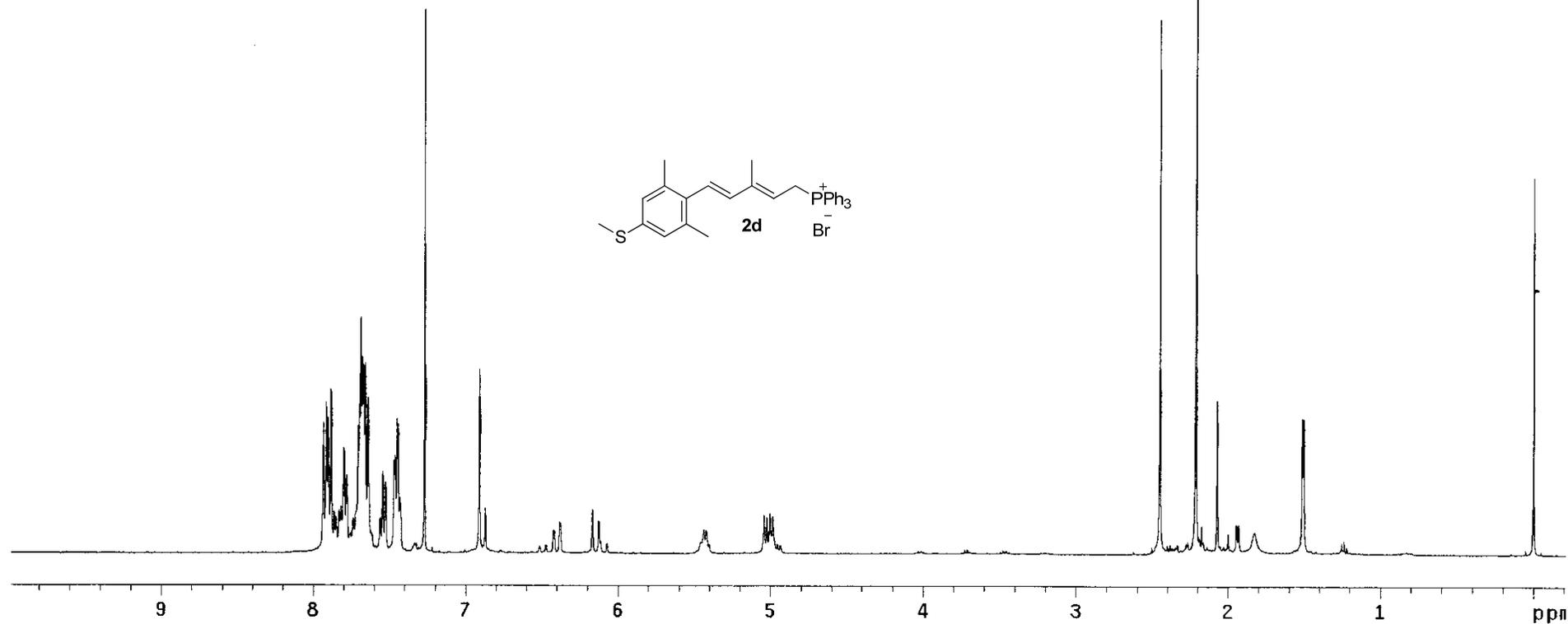
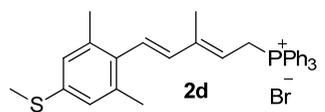
Solvent: cdc13  
 Ambient temperature  
 Sample #42 Operator: walkup2  
 File: s\_42\_SHK-1960-2\_koo-2\_20160216\_01  
 VNMR5 7.000 MHz

Relax delay 1.000 sec  
 Pulse 95.0 degrees  
 Acq. time 2.049 sec  
 Width 6830.6 Hz  
 8 repetitions  
 OBSERVE H1, 400.034056 MHz  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 0 min, 31 sec

7.740 7.736 7.706 7.697 7.687 7.678 7.672 7.668 7.659 7.642 7.638 7.622 7.614 7.611 7.564 7.560 7.545 7.542 7.527 7.523 7.470 7.463 7.451 7.444 7.433 7.426 7.268 6.911 6.872 6.422 6.416 6.382 6.376 6.166 6.125 6.114 5.938 5.420 5.043 5.023 5.004 4.984

2.452 2.265 2.214 2.189 2.175 2.164 2.072 1.998 1.944 1.931 1.826 1.513 1.504 1.237

0.008 -0.000 -0.008



108.582 106.357  
 200.812 192.5

0.35 0.320.31 0.52 0.58  
 1.00 0.230.33 0.52 0.63

2.05 0.76 1.65  
 3.12 0.42

Sample: SHK-1962-2R  
Sample ID: s\_42\_SHK-1962-2R\_koo-2\_20160222\_01  
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1962-2R\_Proton\_01.fid

Pulse Sequence: s2pu1

Solvent: cdcl3  
Ambient temperature  
Sample #42, Operator: walkup2  
File: SHK-1962-2R\_Proton\_01  
VNMR-400 "400MR"

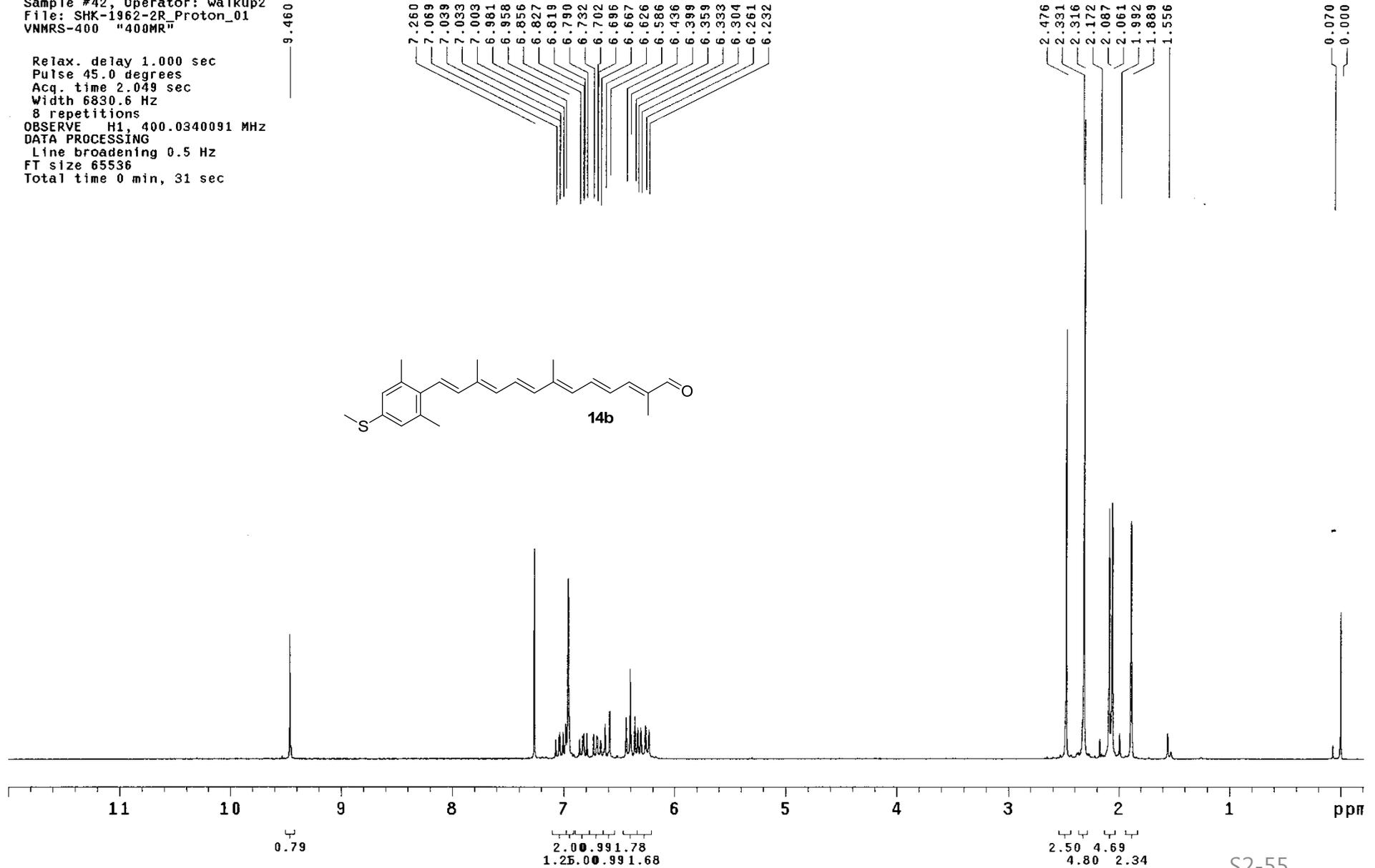
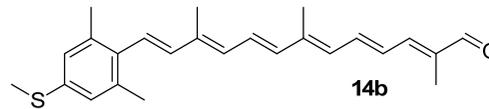
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340091 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

9.460

7.260  
7.069  
7.039  
7.033  
7.003  
6.981  
6.958  
6.856  
6.827  
6.819  
6.790  
6.732  
6.702  
6.696  
6.667  
6.626  
6.586  
6.436  
6.399  
6.359  
6.333  
6.304  
6.261  
6.232

2.476  
2.331  
2.316  
2.172  
2.087  
2.061  
1.992  
1.889  
1.556

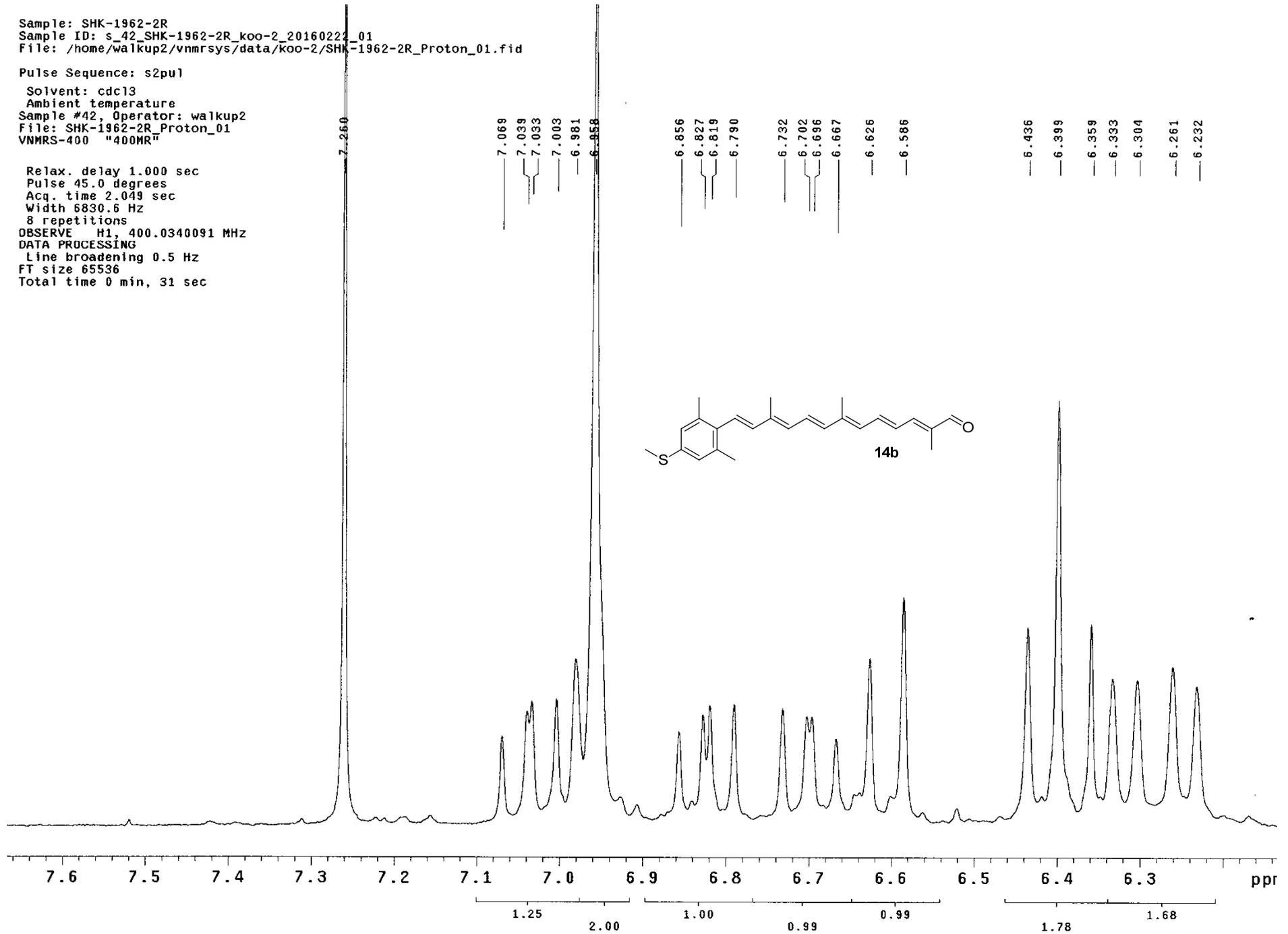
0.070  
0.000



Sample: SHK-1962-2R  
Sample ID: s\_42\_SHK-1962-2R\_koo-2\_20160222\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1962-2R\_Proton\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdcl3  
Ambient temperature  
Sample #42, Operator: walkup2  
File: SHK-1962-2R\_Proton\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6830.6 Hz  
8 repetitions  
OBSERVE H1, 400.0340091 MHz  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 0 min, 31 sec

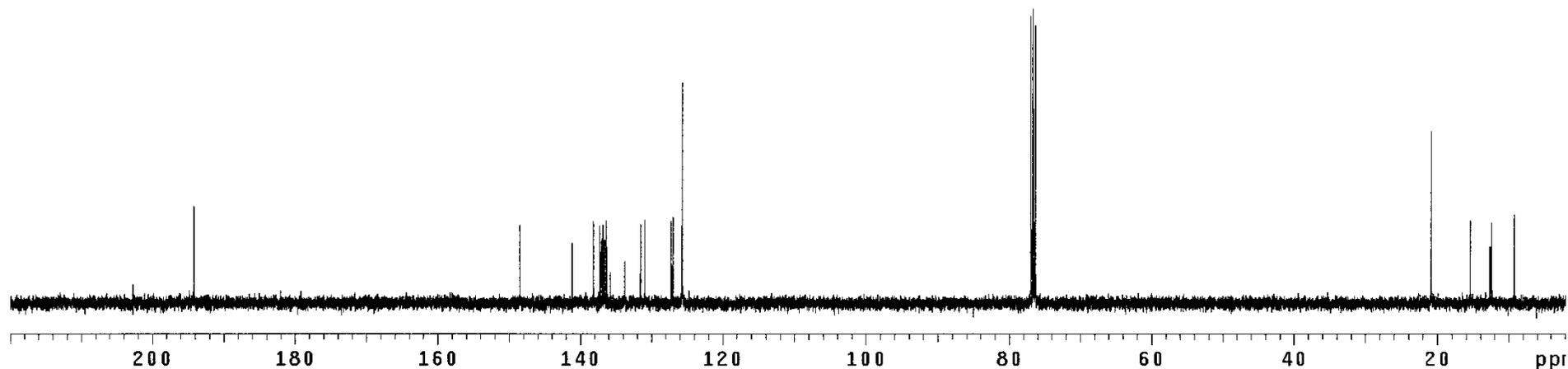
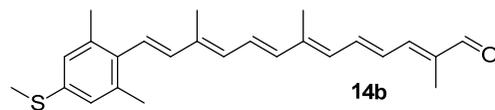
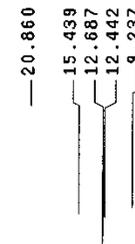
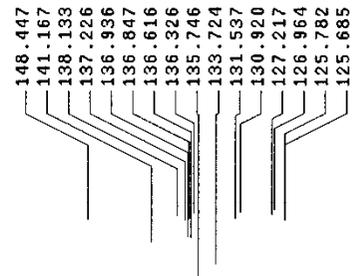


Sample: SHK-1962-2R  
Sample ID: s\_43\_SHK-1962-2R\_koo-2\_20160222\_01  
File: /home/walkup2/vnmrSYS/data/Koo-2/SHK-1962-2R\_Carbon\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Sample #43, Operator: walkup2  
File: SHK-1962-2R\_Carbon\_01  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886703 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec



Sample: SHK-1962-2R  
Sample ID: s\_43\_SHK-1962-2R\_koo-2\_20160222\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1962-2R\_Carbon\_01.fid

Pulse Sequence: s2pu1  
Solvent: cdcl3  
Ambient temperature  
Sample #43, Operator: walkup2  
File: SHK-1962-2R\_Carbon\_01  
VNMRS-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886703 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec

141.167

138.133

137.226

136.936

136.847

136.616

136.326

135.746

133.724

131.537

130.920

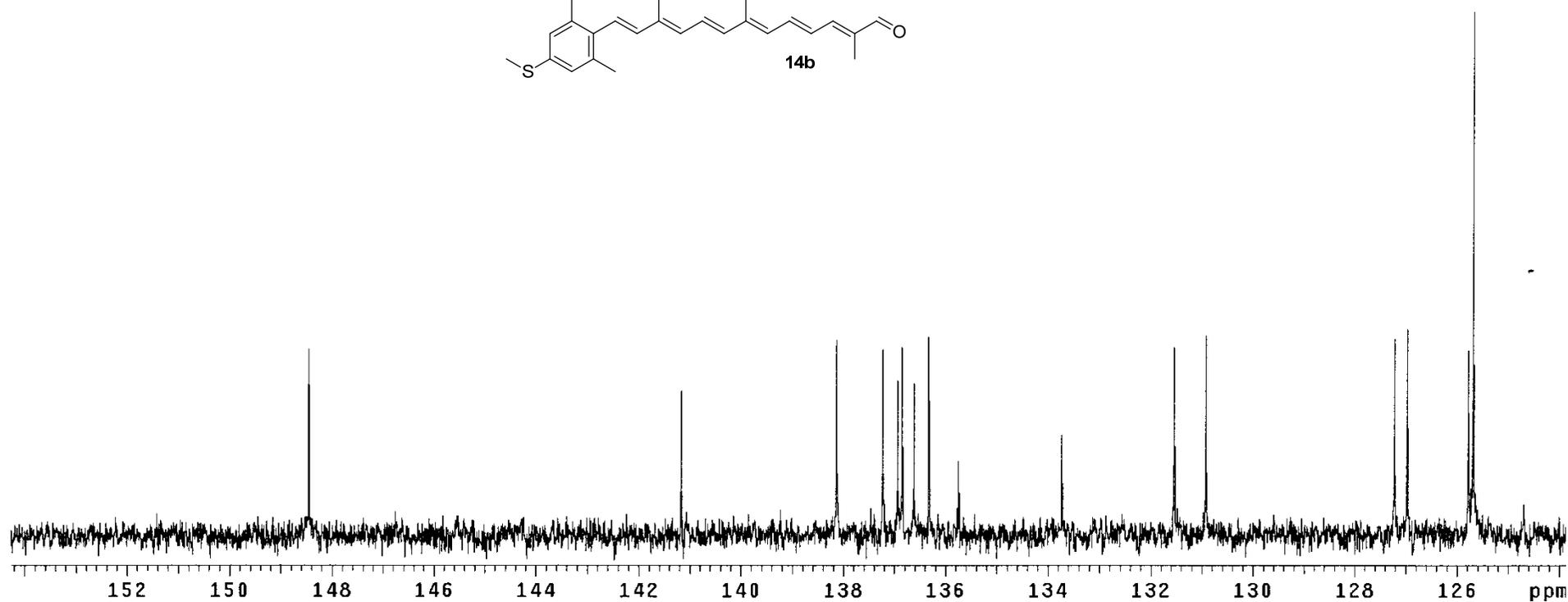
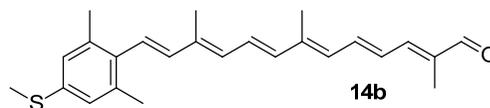
127.217

126.964

125.782

125.685

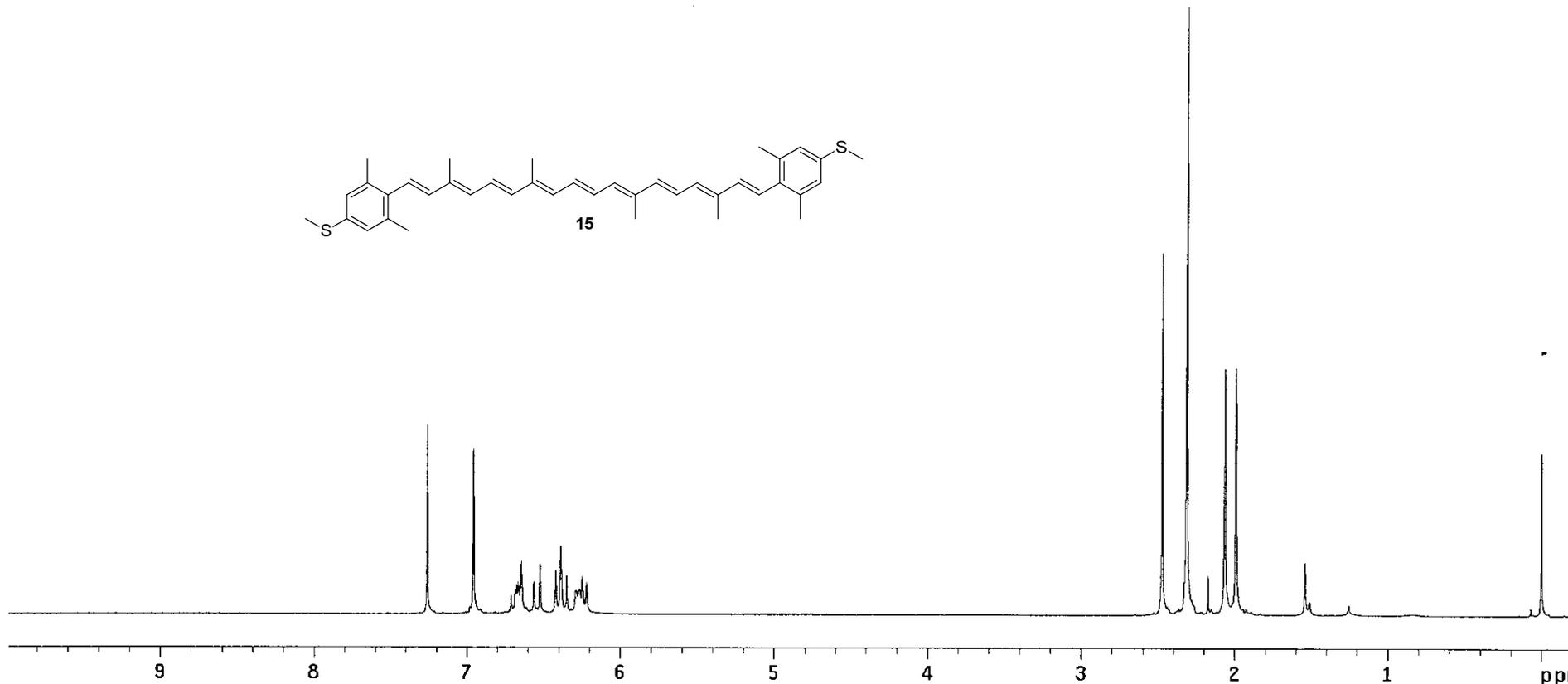
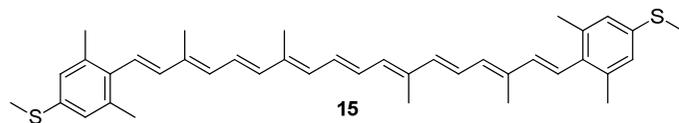
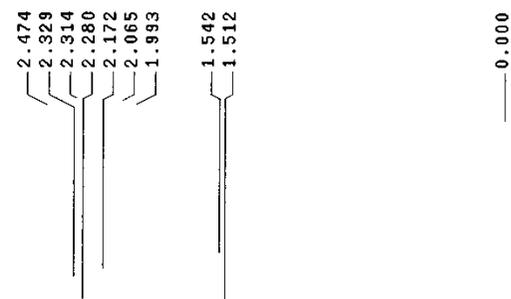
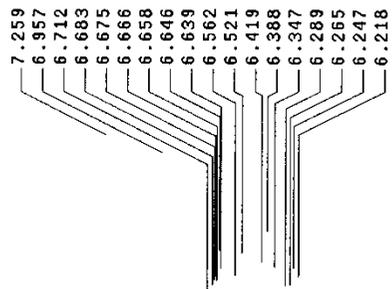
148.447



Sample: SHK-1962-1-2R  
 Sample ID: s\_41\_SHK-1962-1-2R\_koo-2\_20160223\_01  
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1962-1-2R\_Proton\_02.fid

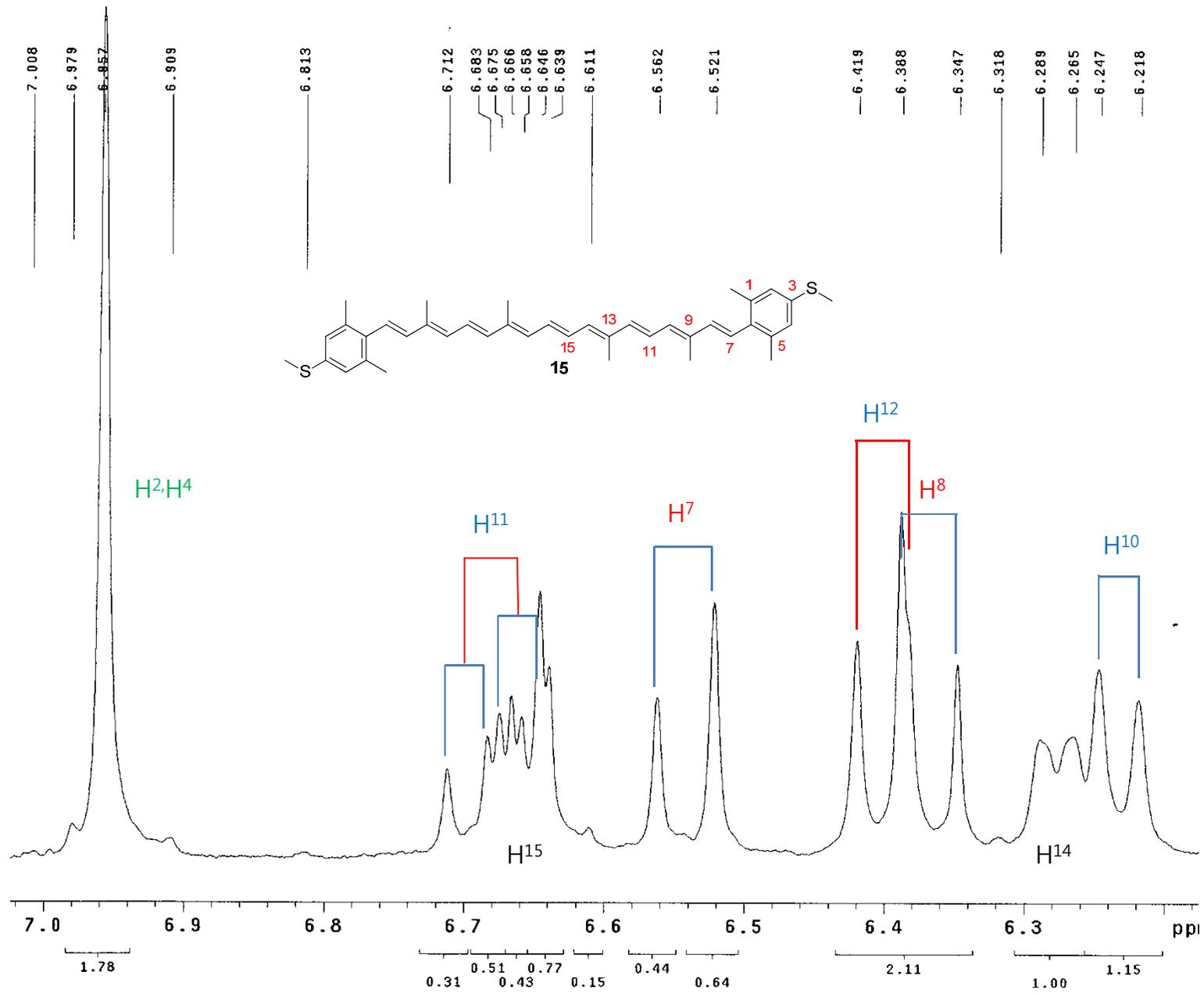
Pulse Sequence: s2pul  
 Solvent: cdcl3  
 Ambient temperature  
 Sample #41, Operator: walkup2  
 File: SHK-1962-1-2R\_Proton\_02  
 VNMR-400 "400MR"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.049 sec  
 Width 6830.6 Hz  
 8 repetitions  
 OBSERVE H1, 400.0340091 MHz  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 0 min, 31 sec



1.78 00.8772 11.15  
 00846541.00

6.16 0.69 0.31  
 3.07 6.27 0.34



Sample: SHK-1967-R  
 Sample ID: s\_44\_SHK-1967-R\_koo-2\_20160227\_01  
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1967-R\_Carbon\_01.fid

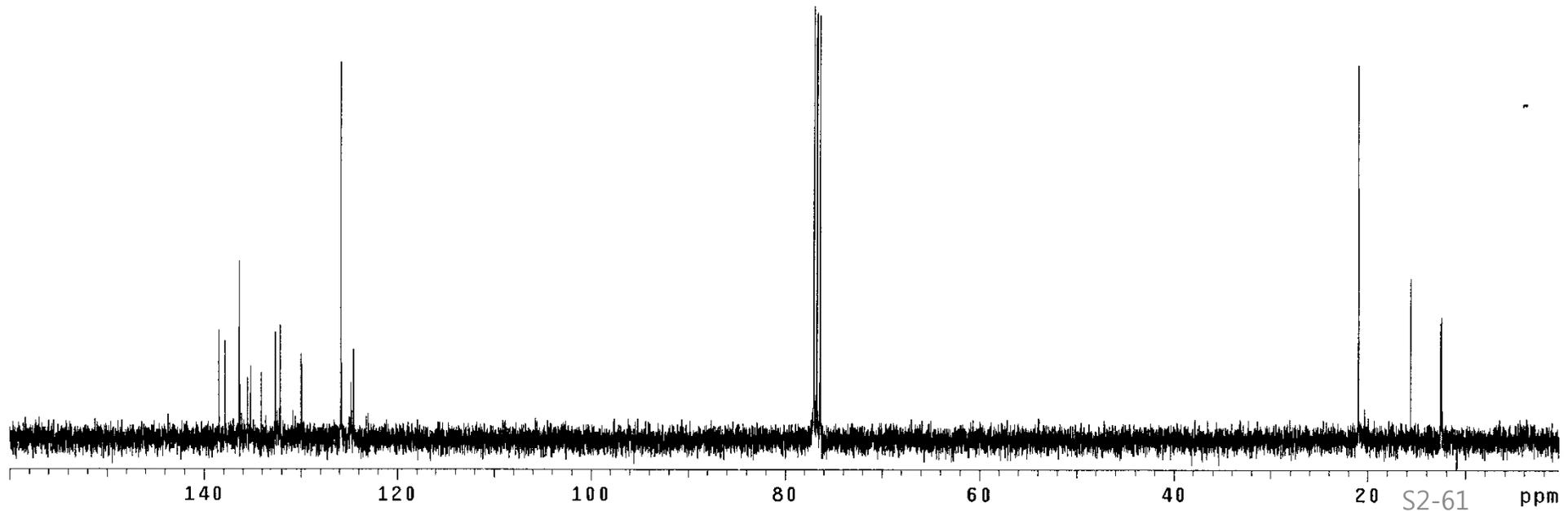
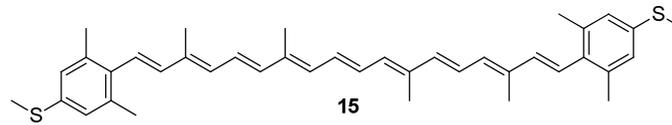
Pulse Sequence: s2pu1  
 Solvent: cdcl3  
 Ambient temperature  
 Sample #44, Operator: [unclear]  
 File: SHK-1967-R\_Carbon\_01.fid  
 VNMRS-400 "400MHz"

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 24509.8 Hz  
 256 repetitions  
 OBSERVE C13, 100.5886622 MHz  
 DECOUPLE H1, 400.0360169 MHz  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 9 min, 51 sec

137.264  
 136.388  
 136.280  
 135.514  
 135.202  
 134.094  
 132.629  
 132.138  
 129.937  
 125.818  
 125.773  
 124.784  
 124.546

77.030  
 76.710  
 76.398

20.948  
 15.594  
 12.537  
 12.426



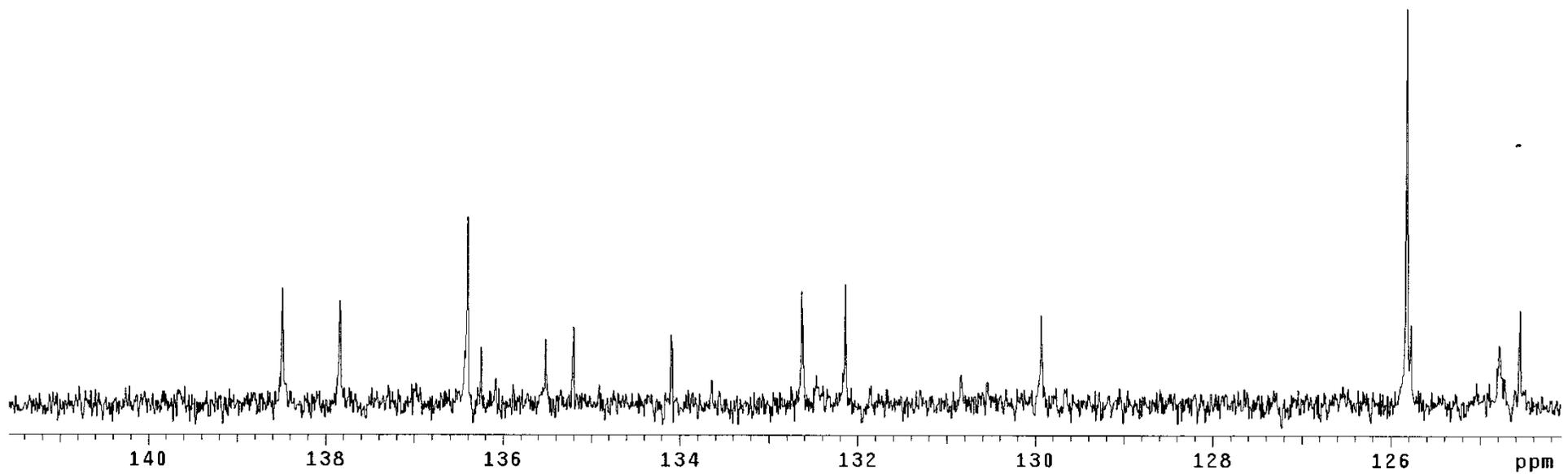
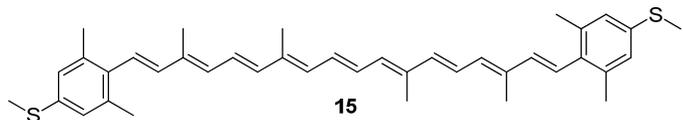
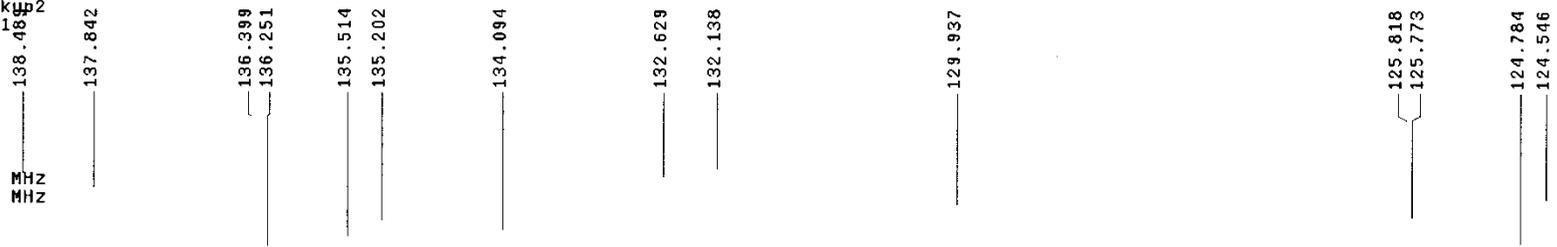
SHK-1967-R

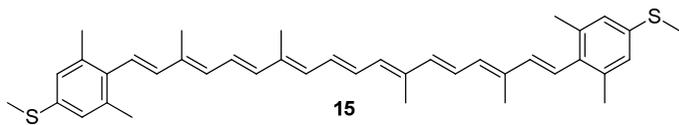
Sample: SHK-1967-R  
Sample ID: s\_44\_SHK-1967-R\_koo-2\_20160227\_01  
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1967-R\_Carbon\_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13  
Ambient temperature  
Sample #44, Operator: walkup2  
File: SHK-1967-R\_Carbon\_01.fid  
VNMR-400 "400MR"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 24509.8 Hz  
256 repetitions  
OBSERVE C13, 100.5886622 MHz  
DECOUPLE H1, 400.0360169 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9 min, 51 sec





# HMQC (C-H correlation)

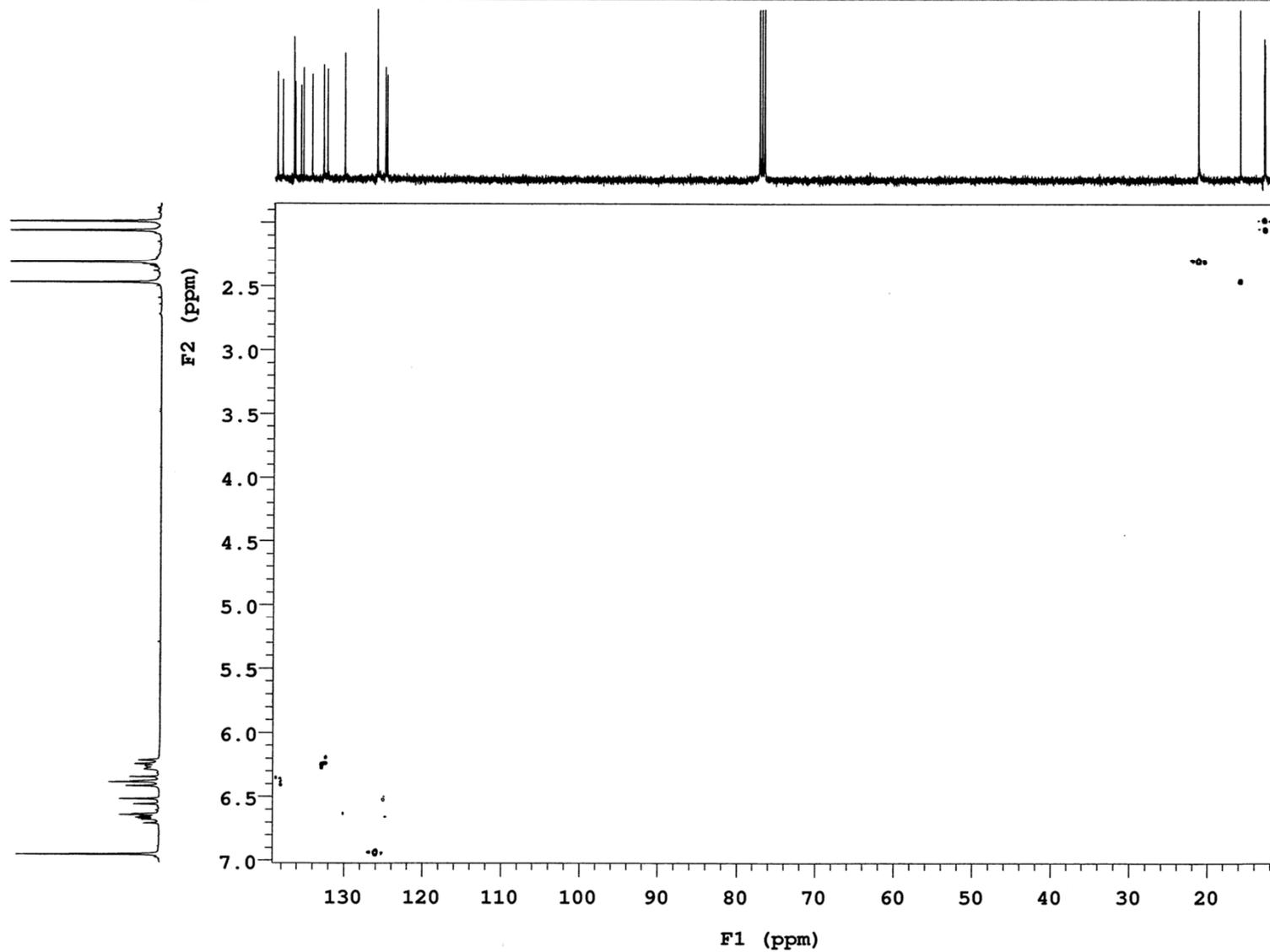
KDH-SHK1967data

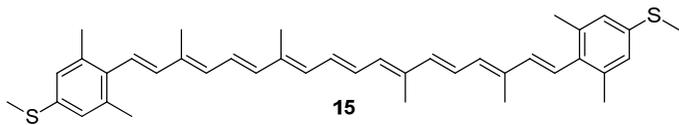
Sample Name **KDH-SHK1967data**  
Date collected **2017-12-07**

Pulse sequence **gHMQC**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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





# HMQC (C-H correlation)

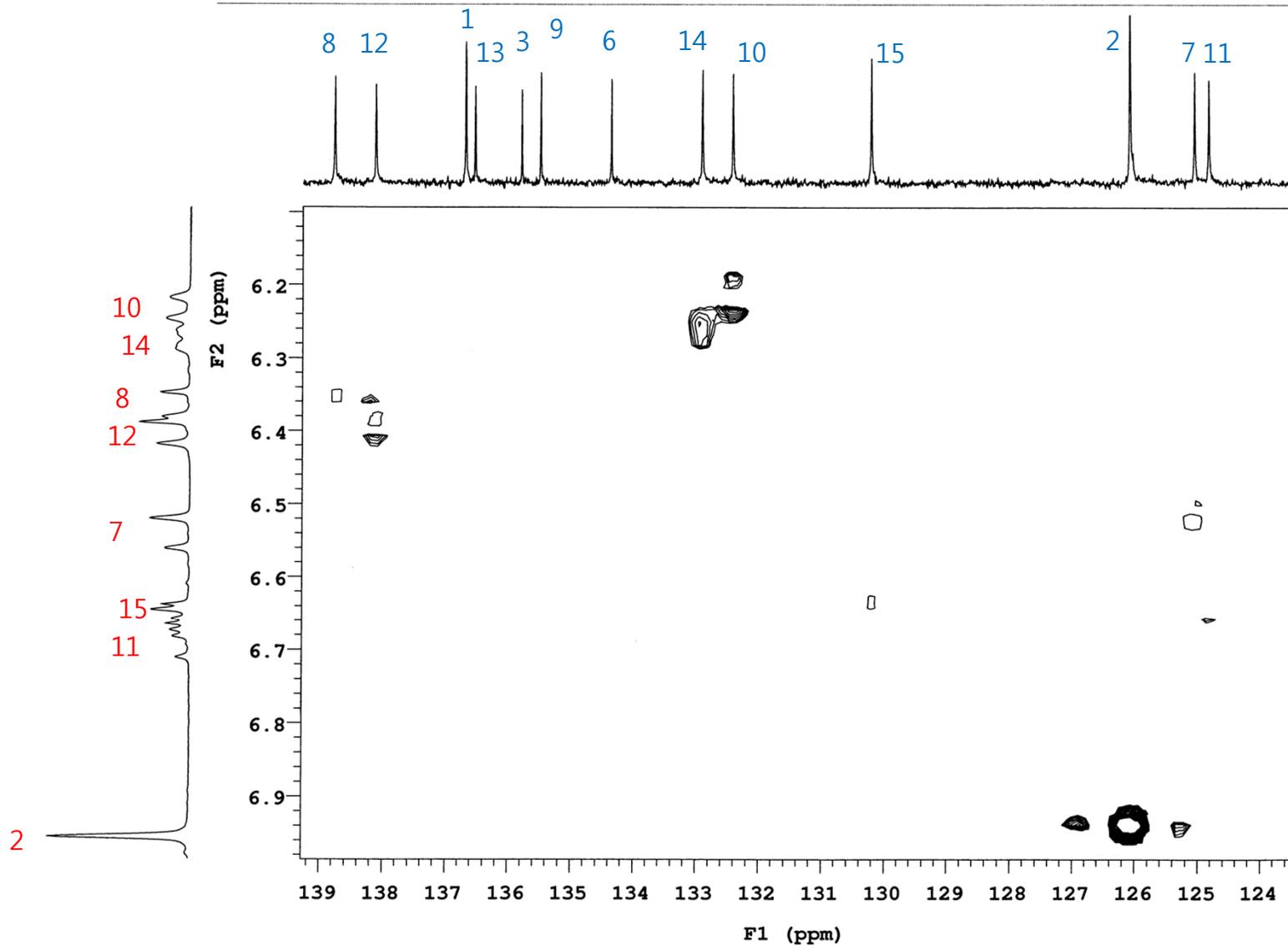
KDH-SHK1967data

Sample Name **KDH-SHK1967data**  
Date collected **2017-12-07**

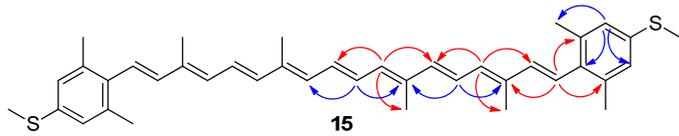
Pulse sequence **gHMQC**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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







# HMBC (C-H correlation)

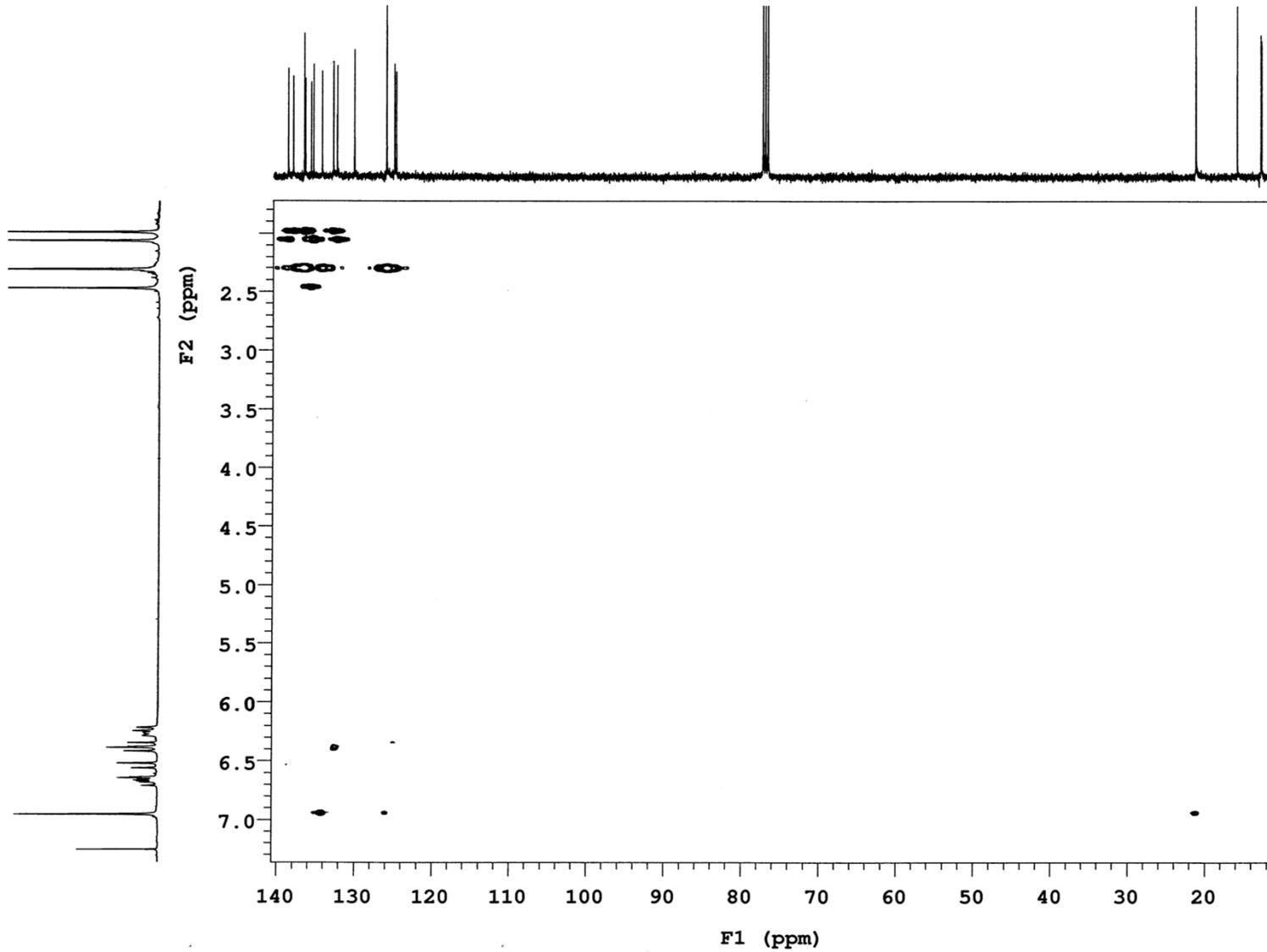
KDH-SHK1967data

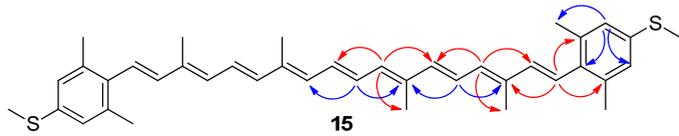
Sample Name **KDH-SHK1967data**  
Date collected **2017-12-08**

Pulse sequence **gHMBCAD**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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





# HMBC (C-H correlation)

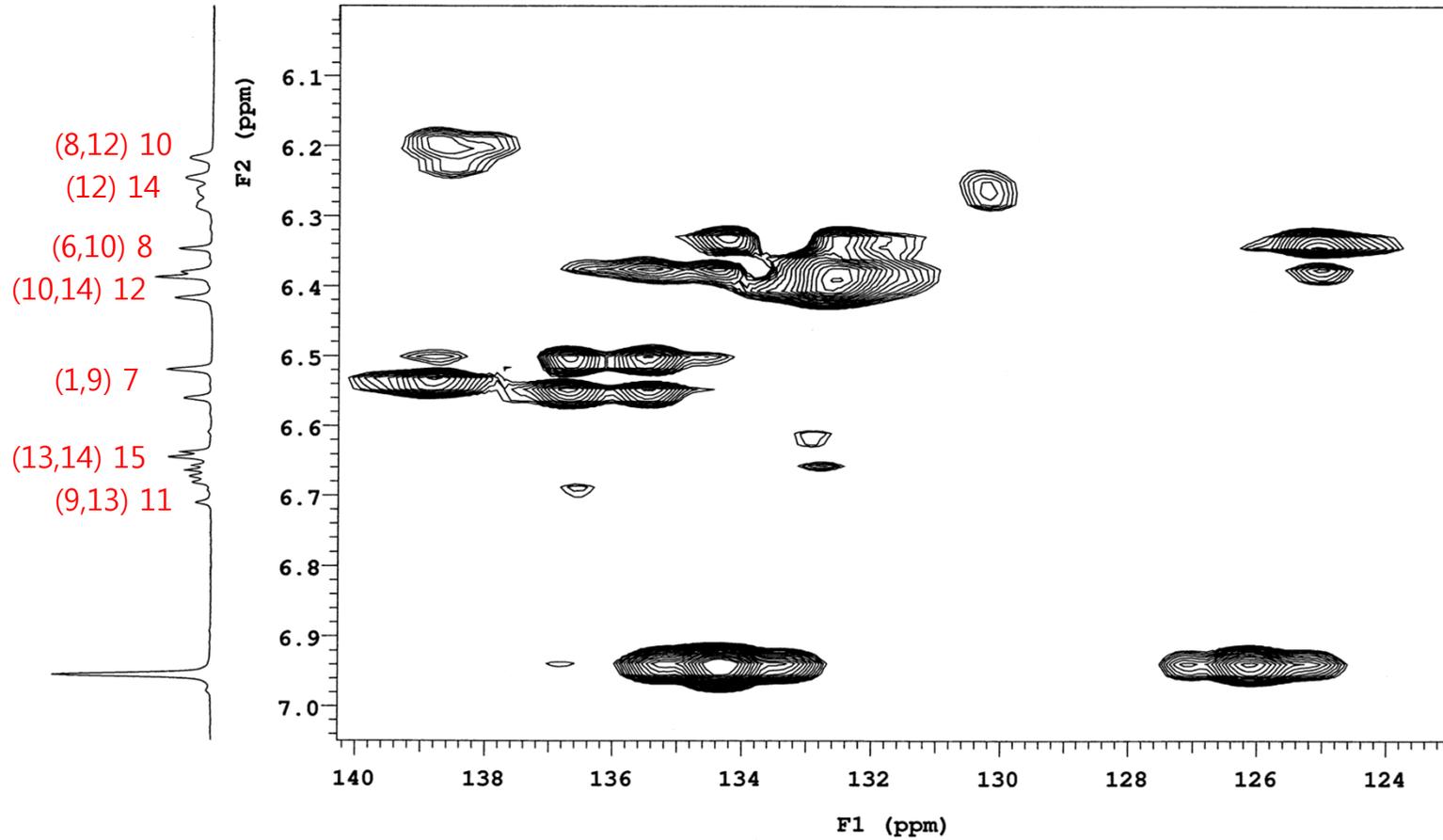
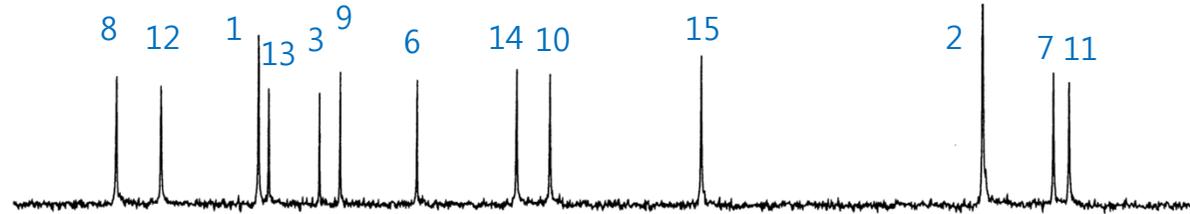
KDH-SHK1967data

Sample Name **KDH-SHK1967data**  
Date collected **2017-12-08**

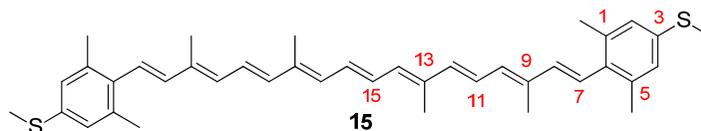
Pulse sequence **gHMBCAD**  
Solvent **cdcl3**

Temperature **24**  
Spectrometer **Agilent-NMR.com-vnmrs400**

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



## Assignment of $^1\text{H}$ and $^{13}\text{C}$ NMR peaks of all-*(E)*-carotene **15** (based on HMQC and HMBC)



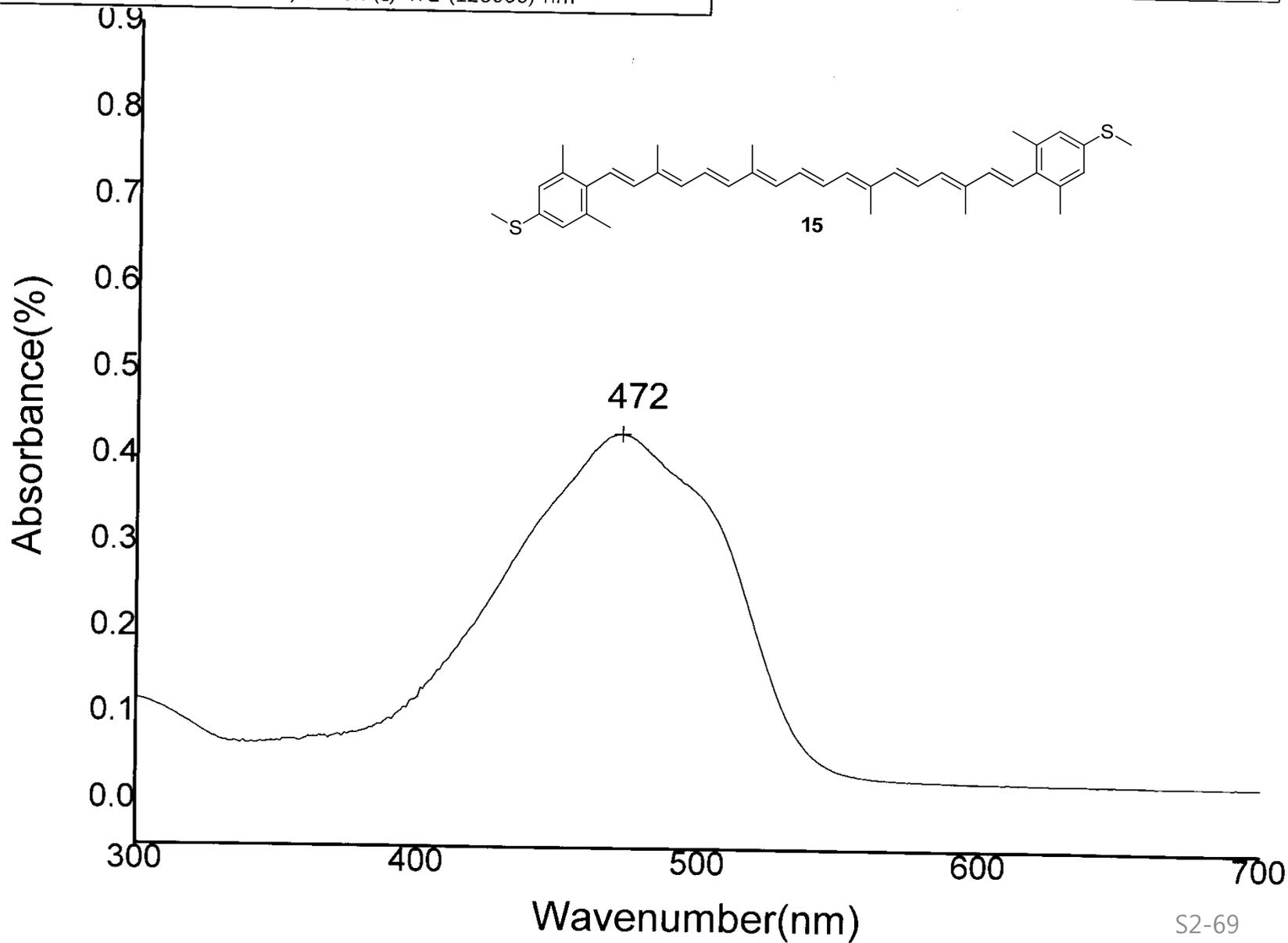
Numbering	$^1\text{H}$ NMR		$^{13}\text{C}$ NMR	
	Shift (ppm)	Multiplicity (Hz)	Shift (ppm)	DEPT
<b>1</b>	-	-	136.4	q
<b>1-Me</b>	2.31 ( $\text{CH}_3$ )	s	20.9	$\text{CH}_3$
<b>2</b>	6.96	s	125.8	CH
<b>3</b>	-	-	135.5	q
<b>3-SMe</b>	2.47 ( $\text{CH}_3$ )	s	15.6	$\text{CH}_3$
<b>4</b>	6.96	s	125.8	CH
<b>5</b>	-	-	136.4	q
<b>5-Me</b>	2.31 ( $\text{CH}_3$ )	s	20.9	$\text{CH}_3$
<b>6</b>	-	-	134.1	q
<b>7</b>	6.54	d (16.4)	124.8	CH
<b>8</b>	6.37	d (16.4)	138.5	CH
<b>9</b>	-	-	135.2	q
<b>9-Me</b>	2.07	s	12.4	$\text{CH}_3$
<b>10</b>	6.23	d (11.6)	132.1	CH
<b>11</b>	6.68	dd (14.8, 11.6)	124.5	CH
<b>12</b>	6.40	d (14.8)	137.8	CH
<b>13</b>	-	-	136.3	q
<b>13-Me</b>	1.99	s	12.5	$\text{CH}_3$
<b>14</b>	6.23–6.33	m	132.6	CH
<b>15</b>	6.60–6.70	m	129.9	CH

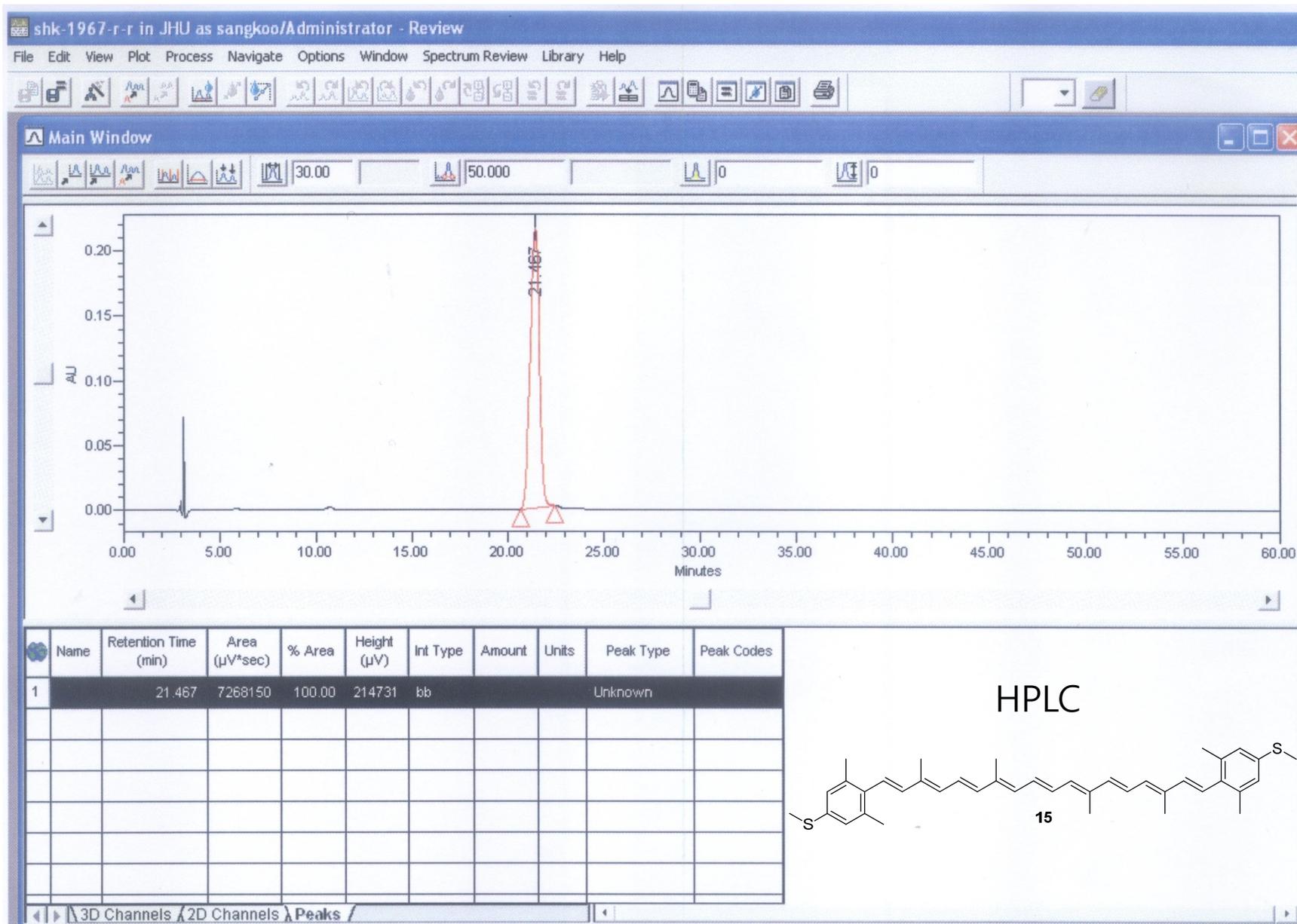
SHK-1967-re	
M	0.0000033499 M
$\epsilon$	128434

UV

SHK-1967

UV ( $c=3.35 \times 10^{-5}$  M in  $\text{CH}_2\text{Cl}_2$ )  $\lambda$  max ( $\epsilon$ ) 472 (128000) nm





Waters 2998 (PDA) , 1525 Binary HPLC Pump, Solvent (MeCN : MeOH : EtOAc = 7 : 2.4 : 0.6),  
Flow Rate 0.7 : 0.3 mL/min, Pressure = 353 psi, Temp = 25 °C