

Supporting Information

Sulfone-Mediated Syntheses of Crocetin Derivatives – Regioselectivity of Highly Functionalized Building Blocks

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¹H and ¹³C NMR Spectra for

Compounds **2**, **3a**, **5**, **7**, **8**, **9**, **10**, **11a**, **11b**, **12b**, **13a**, **15a**, **15b**, **16**, **17**, **18**, **19**.

Sample: OET-1040
 Sample ID: s_40_OET-1040_koo-3_20130620_01
 File: /home/walkup2/vnmrsys/data/koo-3/OET-1040_Proton_01.fid

Pulse Sequence: s2pul

Solvent: cdc13

Ambient temperature

Sample #40, Operator: walkup2

File: OET-1040_Proton_01

VNMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

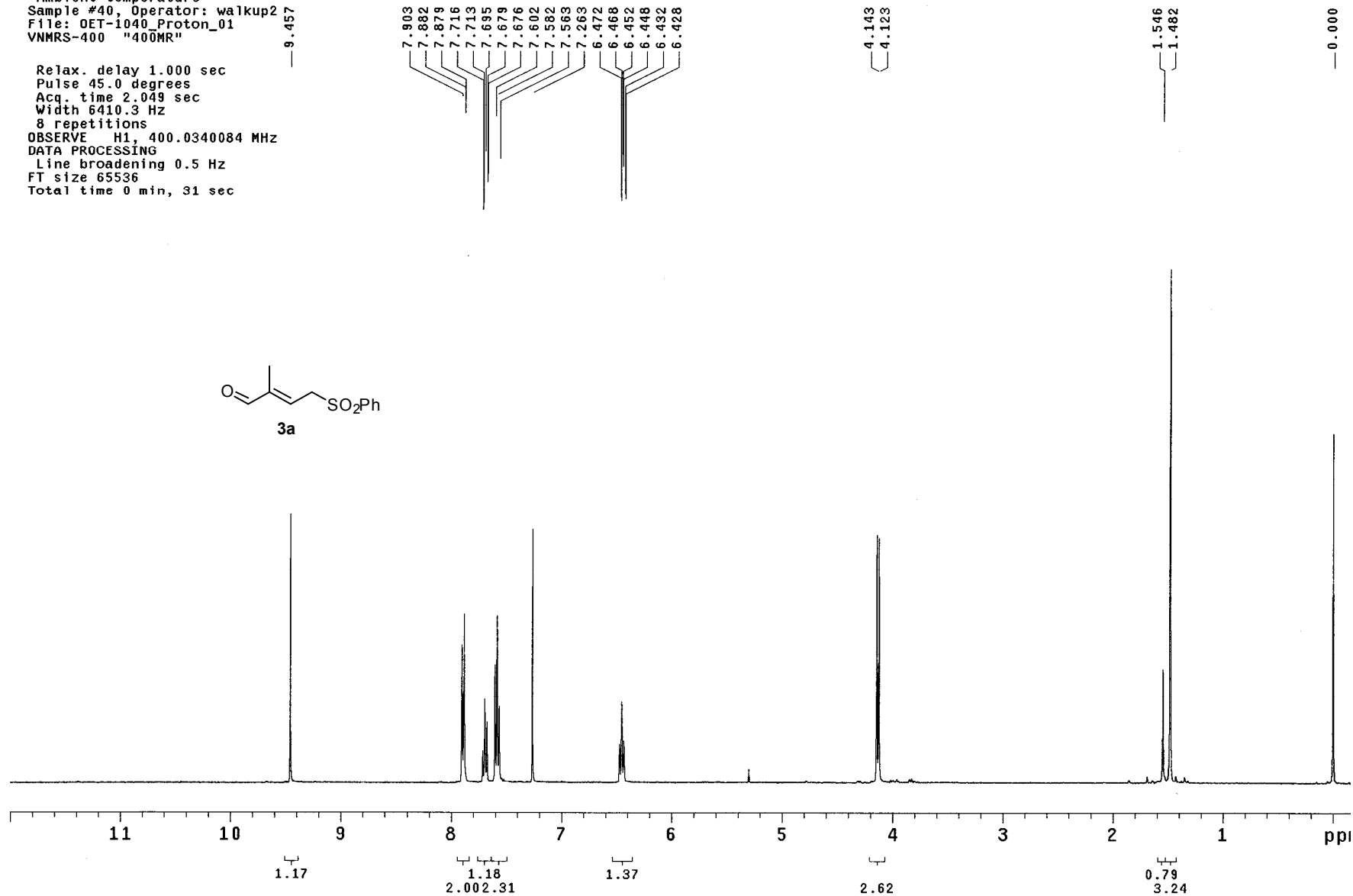
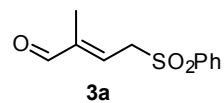
OBSERVE H1, 400.0340084 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec

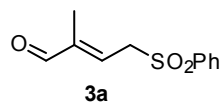


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Pulse Sequence: s2pu1
  Solvent: cdc13
  Ambient temperature
Sample #37, Operator: walkup2
File: OET-1076_Carbon_01
VNMRS-400 "400MR" 3
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Ambient temperature
 Sample #37, Operator: walkup2
 File: OET-1076_Carbon_01
 VNMRS-400 "400MR".
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 512 repetitions
 OBSERVE C13, 100.5886346 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

145.419
 138.265
 136.347
 134.294
 129.446
 128.212
 77.319
 77.000
 76.680
 56.253
 9.198
 -1.778
 -1.800

O=C(C=C(CS(=O)(=O)c1ccccc1)C)C
3a



Sample: OET-1025
 Sample ID: s_40_OET-1025_koo-3_20130529_01
 File: /home/walkup2/vnmrSys/data/koo-3/OET-1025_Proton_01.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Sample #40, Operator: walkup2

File: OET-1025_Proton_01

VNMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

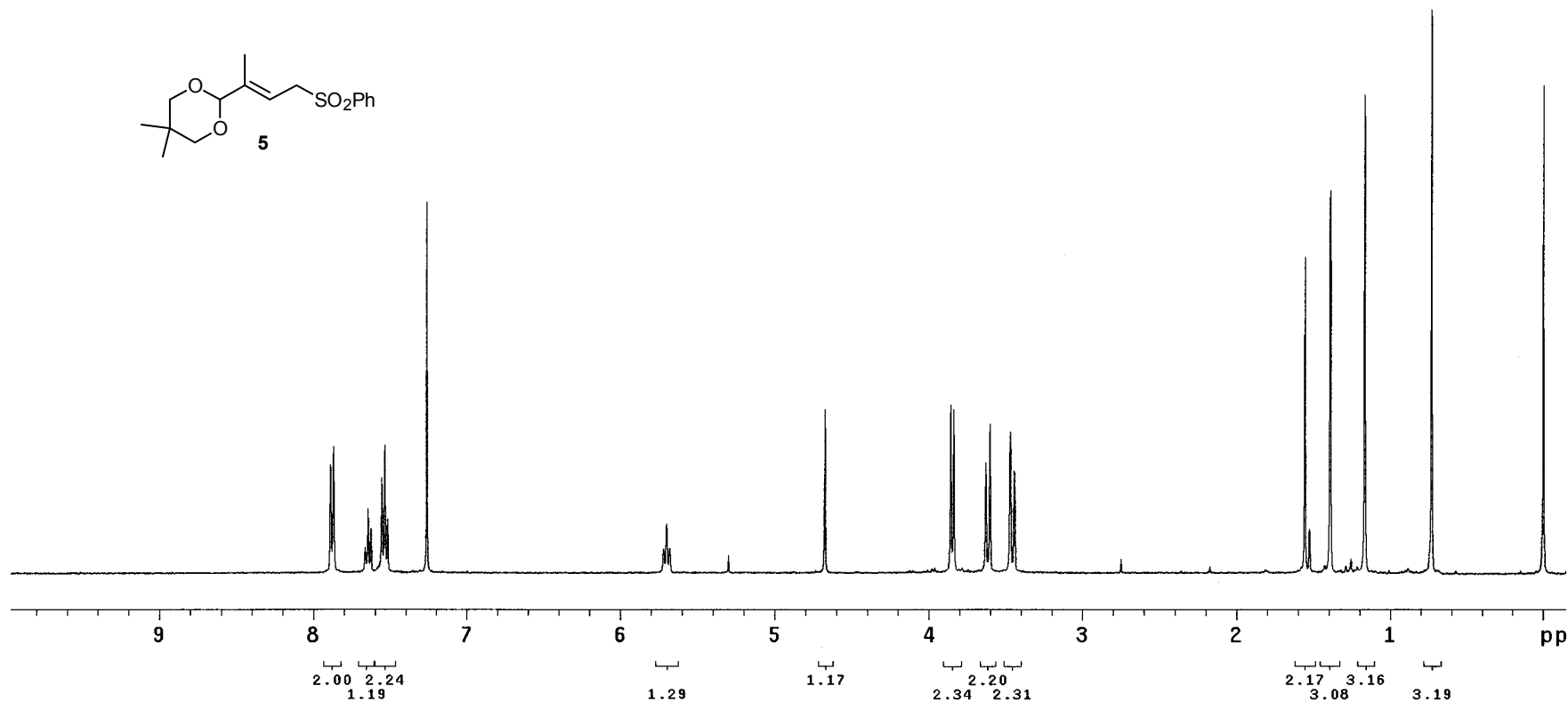
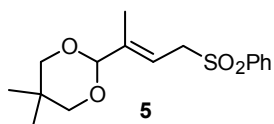
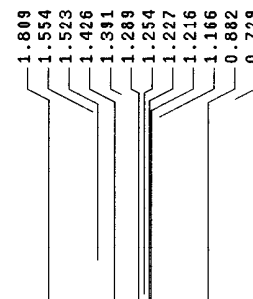
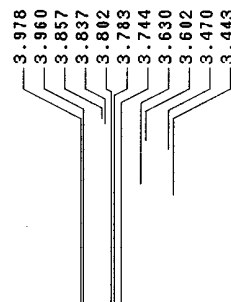
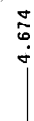
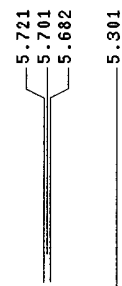
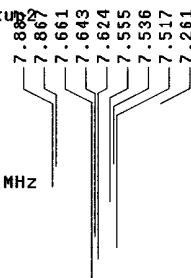
OBSERVE H1, 400.0340091 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

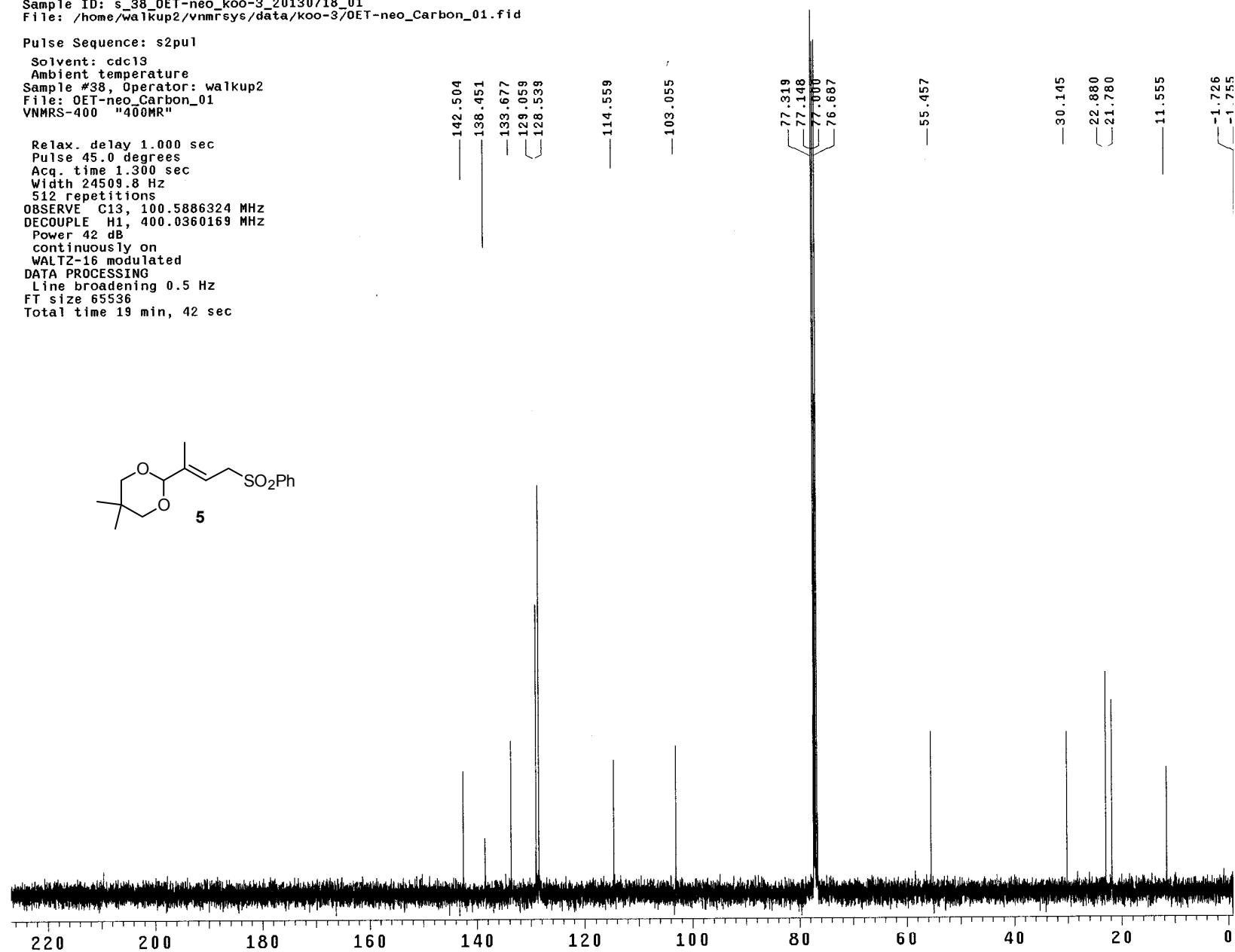
Total time 0 min, 31 sec



Sample: OET-neo
 Sample ID: s_38_OET-neo_koo-3_20130718_01
 File: /home/walkup2/vnmrsys/data/koo-3/OET-neo_Carbon_01.fid

Pulse Sequence: s2pul
 Solvent: cdc13
 Ambient temperature
 Sample #38, Operator: walkup2
 File: OET-neo_Carbon_01
 VNMRS-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 512 repetitions
 OBSERVE C13, 100.5886324 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



Sample: SHK-1507
 Sample ID: s_30_SHK-1507_koo-2_20130403_01
 File: /home/walkup2/vnmr5sys/data/koo-2/SHK-1507_Proton_01.fid

Pulse Sequence: s2pul

Solvent: cdc13

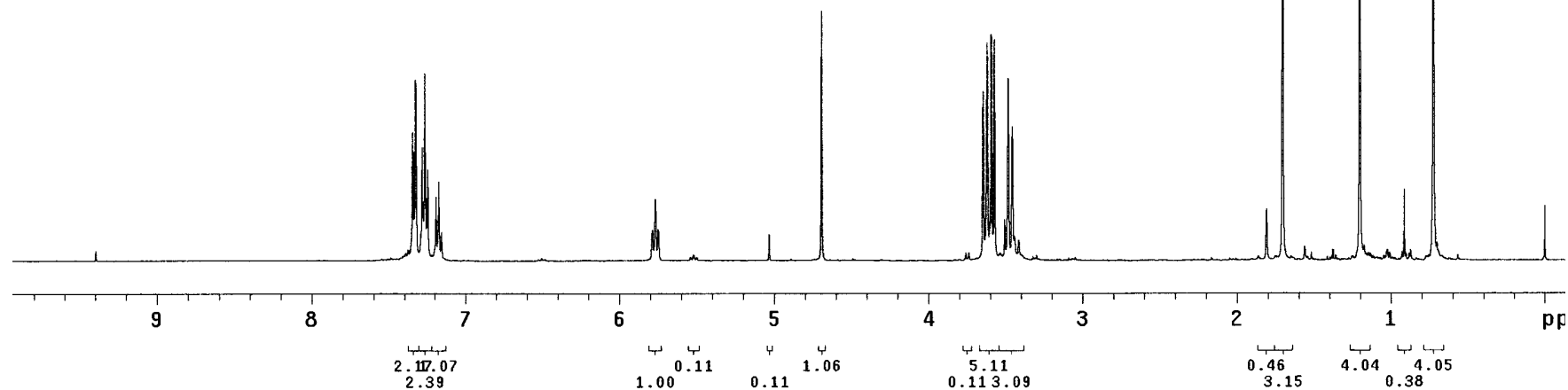
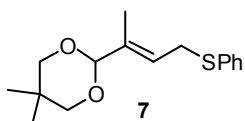
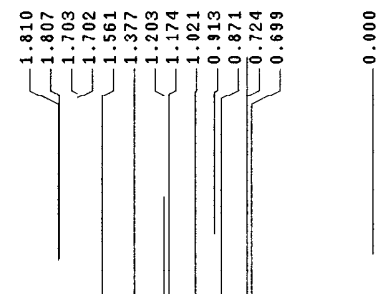
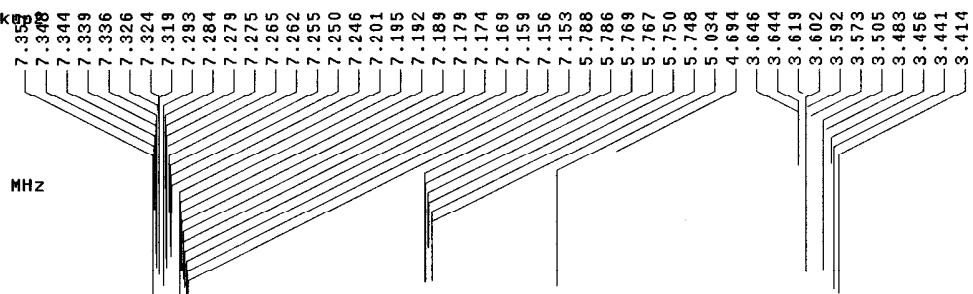
Ambient temperature

Sample #30, Operator: walkup

File: SHK-1507_Proton_01

VNMR5-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.0340119 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec

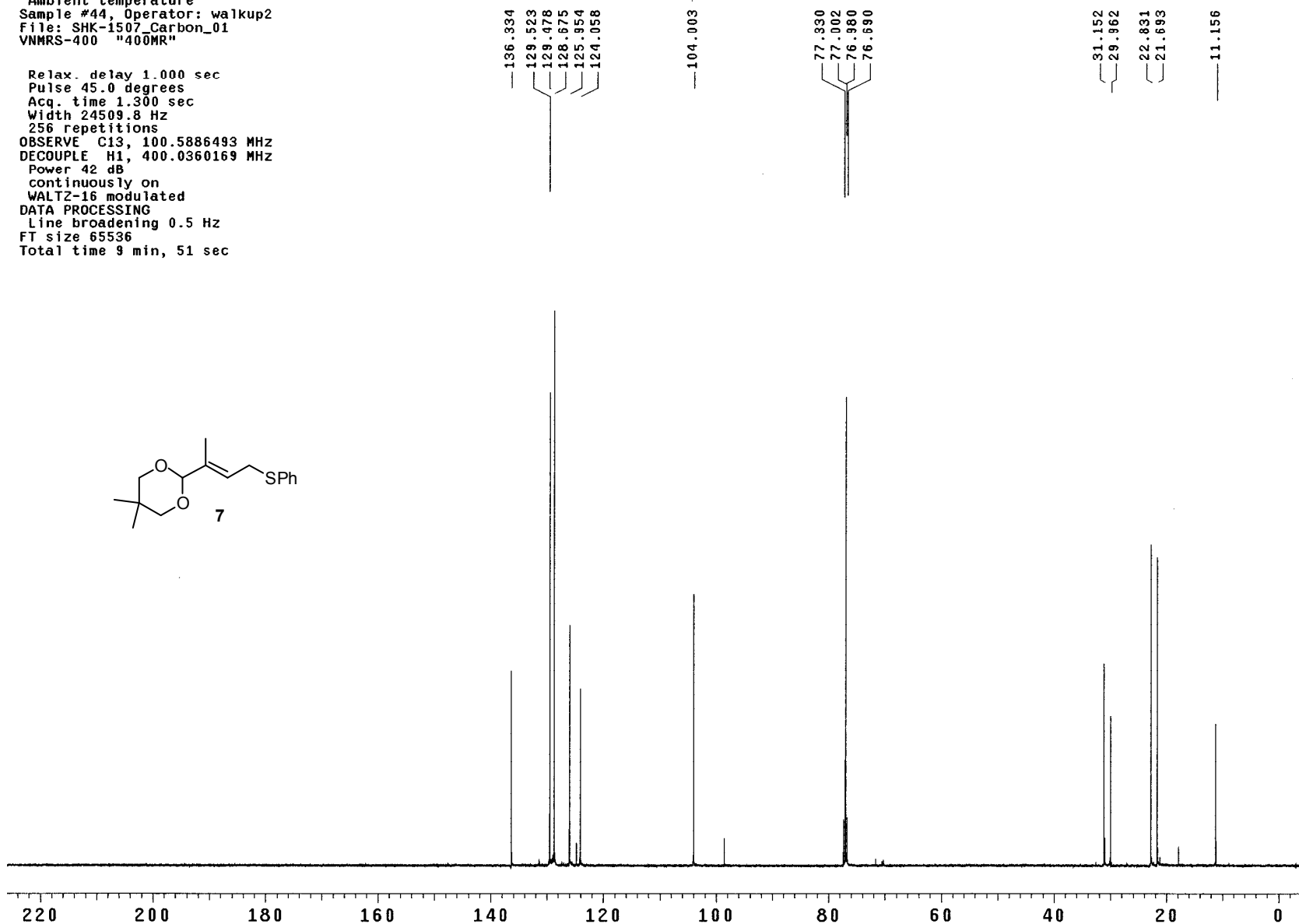


Sample: SHK-1507
 Sample ID: s_44_SHK-1507_koo-2_20130404_01
 File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1507_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: cdc13
 Ambient temperature
 Sample #44, Operator: walkup2
 File: SHK-1507_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, 100.5886493 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: OET-927
 Sample ID: s_40_OET-927_koo-3_20130131_01
 File: /home/waikup2/vnmrsys/data/koo-3/OET-927_Proton_01.fid

Pulse Sequence: s2pul

Solvent: cdcl3

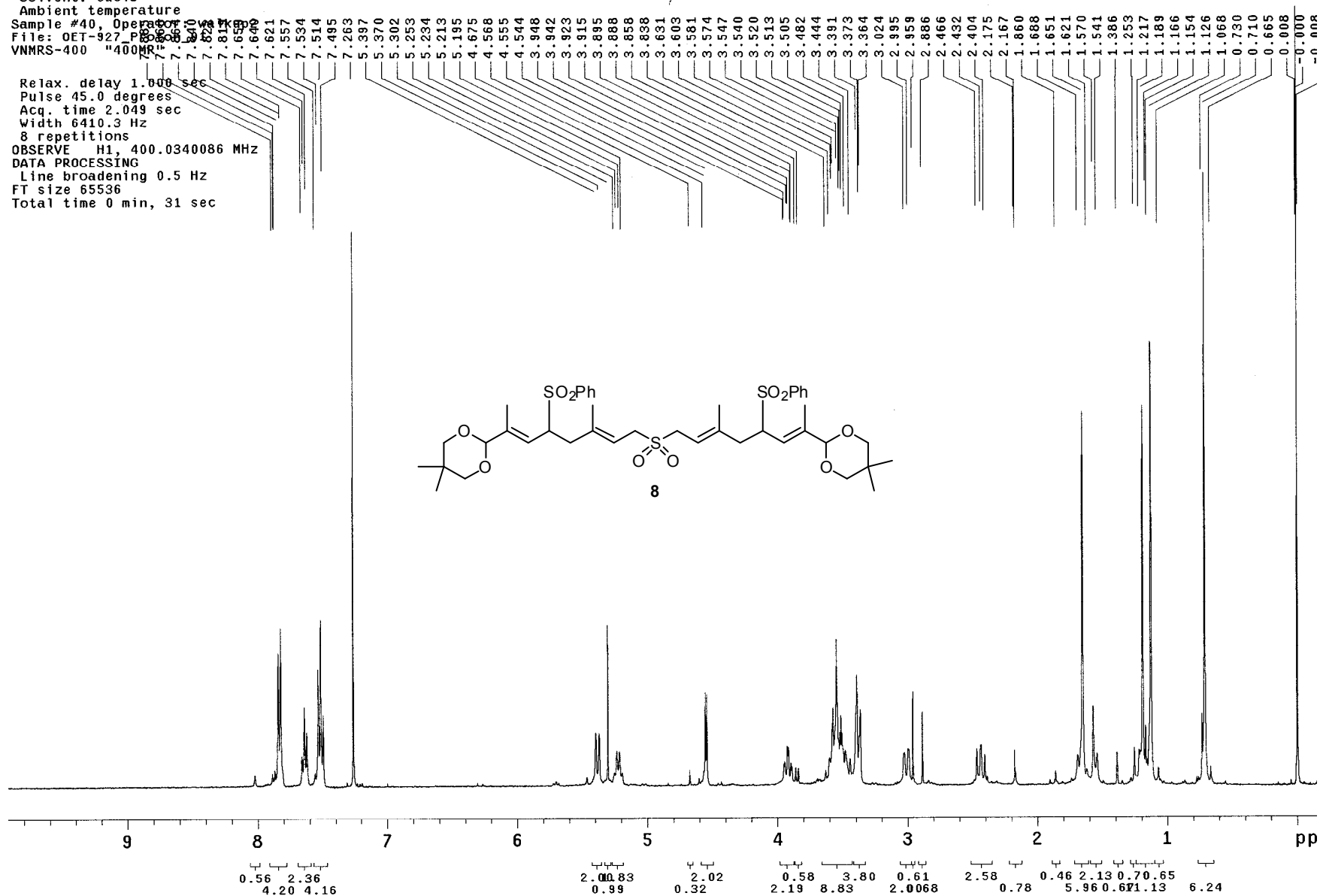
Ambient temperature

Sample #40, Operator

File: OET-927_P808086.fid

VNMR-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.0340086 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec



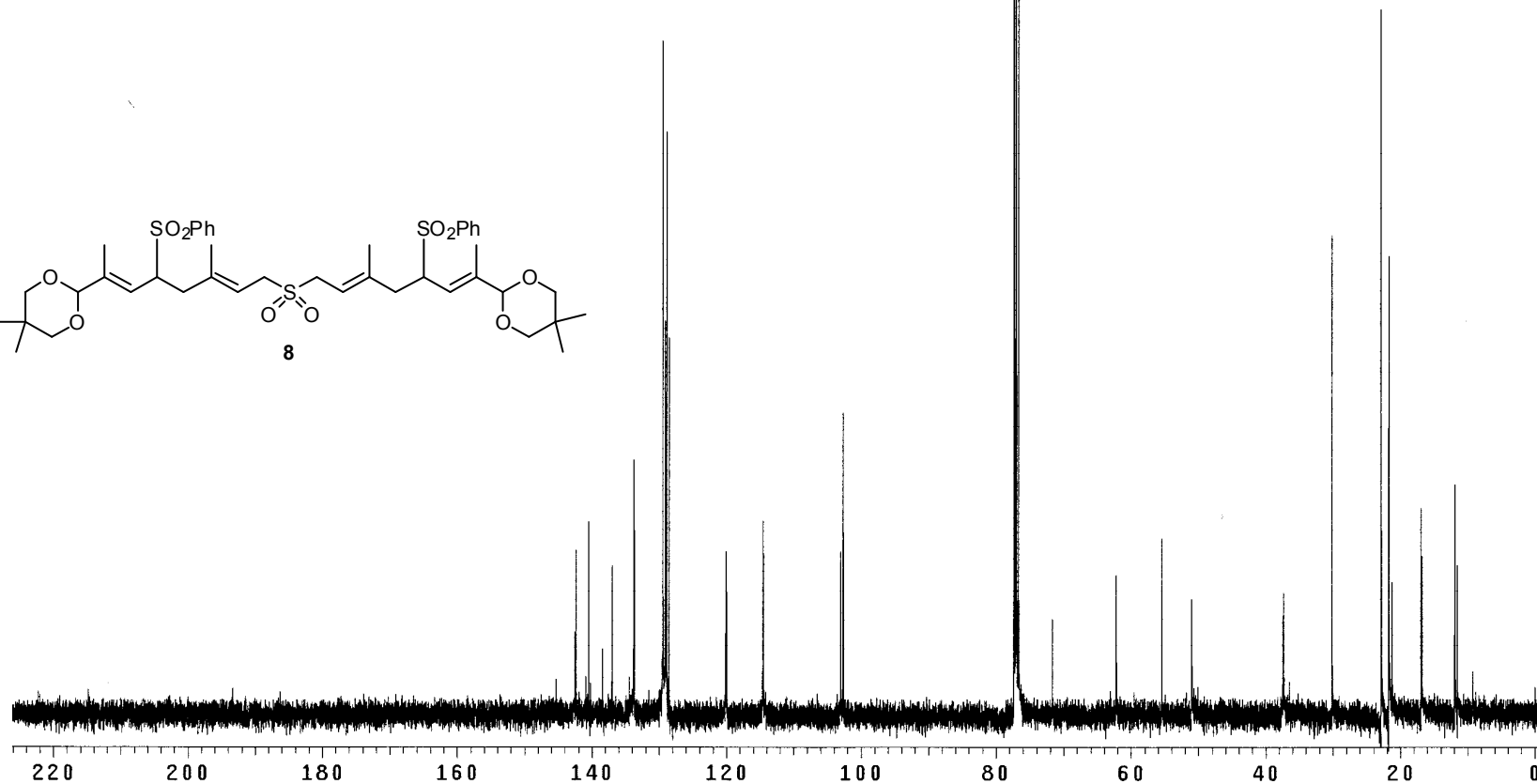
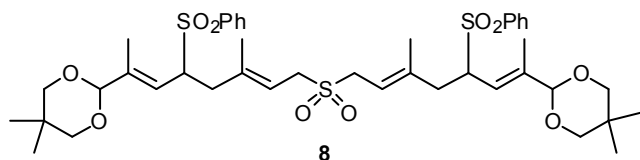
Sample: OET-neo-2
 Sample ID: s_33_OET-neo-2_koo-3_20130729_01
 File: /home/walkup2/vnmrsys/data/koo-3/OET-neo-2_Carbon_02.fid

Pulse Sequence: s2pul

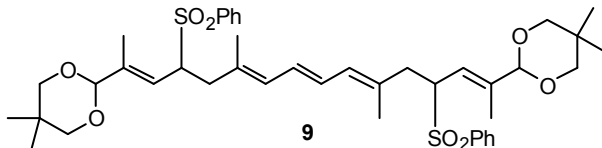
Solvent: cdc13
 Ambient temperature
 Sample #33, Operator: walkup2
 File: OET-neo-2_Carbon_02
 VNMR-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 2048 repetitions
 OBSERVE C13, 100.5886346 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

142.489
 142.363
 142.326
 140.430
 138.414
 136.949
 133.752
 133.678
 129.417
 129.328
 129.052
 128.926
 128.867
 128.502
 120.092
 119.980
 114.574
 114.522
 114.426
 103.026
 102.647
 102.610
 77.320
 77.208
 77.119
 77.000
 76.680
 71.898
 62.217
 62.195
 55.421
 51.034
 50.996
 37.403
 37.322
 30.116
 30.094
 22.851
 21.751
 21.706
 21.267
 16.939
 16.806
 11.898
 11.883
 11.533
 -1.851
 -1.881



Total time 0 min, 31 sec

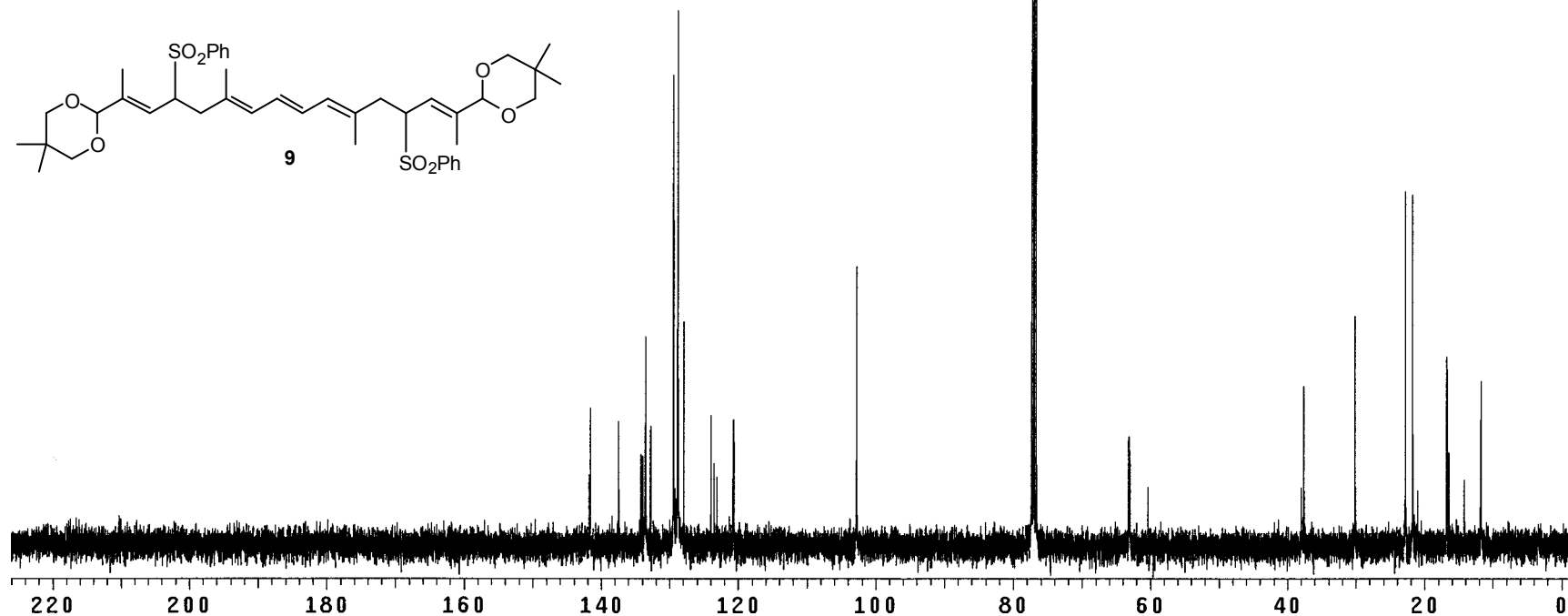
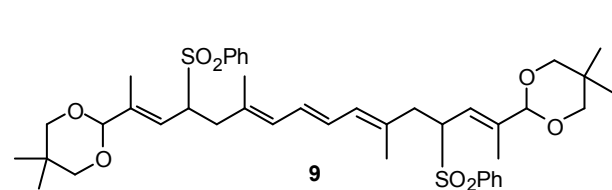
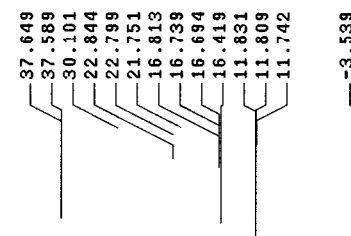
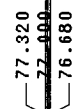
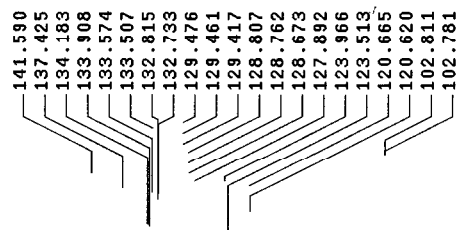


Sample: OET-1028-1
 Sample ID: s_45_OET-1028-1_koo-4_20130603_01
 File: /home/walkup2/vnmrsys/data/koo-4/OET-1028-1_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: cdc13
 Ambient temperature
 Sample #45, Operator: walkup2
 File: OET-1028-1_Carbon_01
 VNMRS-400 "400MR"

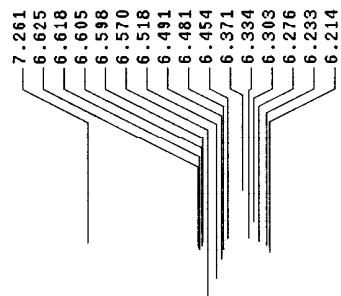
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 512 repetitions
 OBSERVE C13, 100.5886323 MHz
 DECOUPLE H1, 400.0360169 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 19 min, 42 sec



Sample: SHK-1570-0-1
 Sample ID: s_45_SHK-1570-0-1_koo-2_20130606_01
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1570-0-1_Proton_01.fid

Pulse Sequence: s2pu1
 Solvent: cdc13
 Ambient temperature
 Sample #45, Operator: walkup2
 File: SHK-1570-0-1_Proton_01
 VNMR5-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.0340093 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec



4.774

3.681
 3.654
 3.528
 3.501

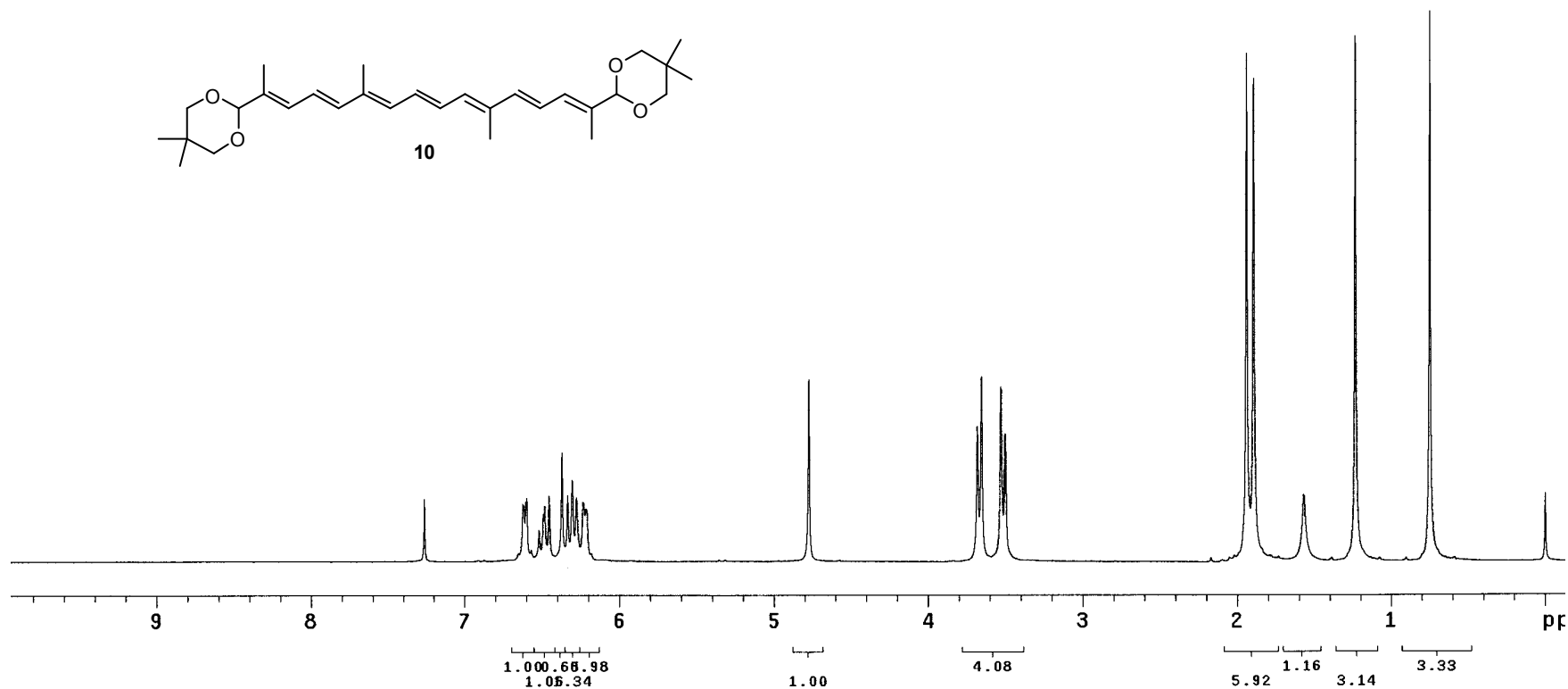
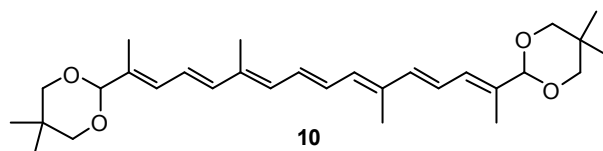
1.938
 1.893

1.568

1.231

0.745

0.000



Sample: SHK-1570-0-1
 Sample ID: s_45_SHK-1570-0-1_koo-2_20130606_02
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1570-0-1_Carbon_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13
 Ambient temperature
 Sample #45, Operator: walkup2
 File: SHK-1570-0-1_Carbon_01
 VNMR-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 1000 repetitions
 OBSERVE C13, 100.5886319 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 38 min, 29 sec

138.917
 136.166
 134.054
 132.708
 130.090
 128.581
 123.651

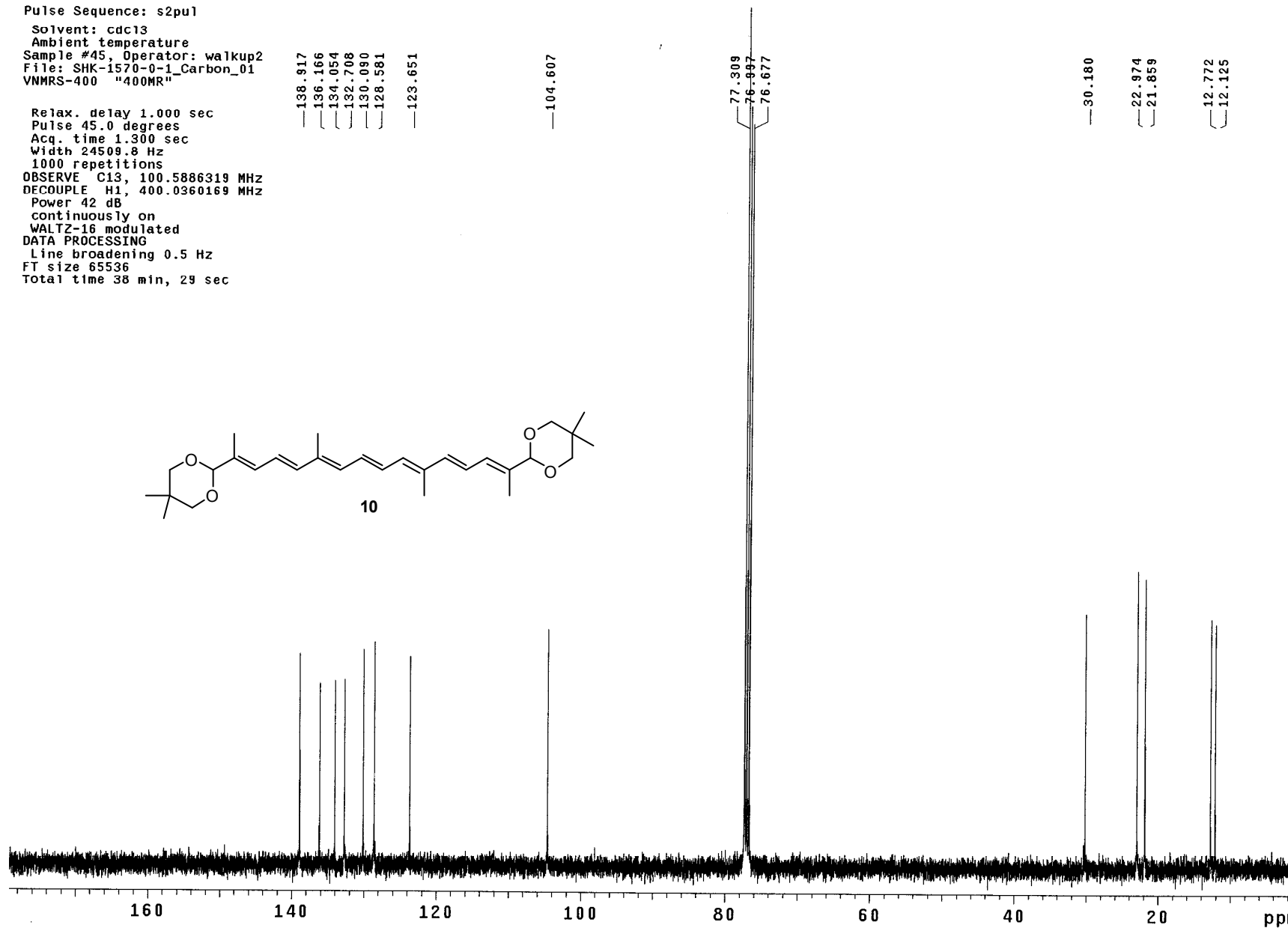
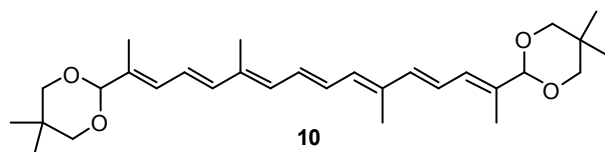
104.607

77.309
 76.997
 76.677

30.180

22.974
 21.859

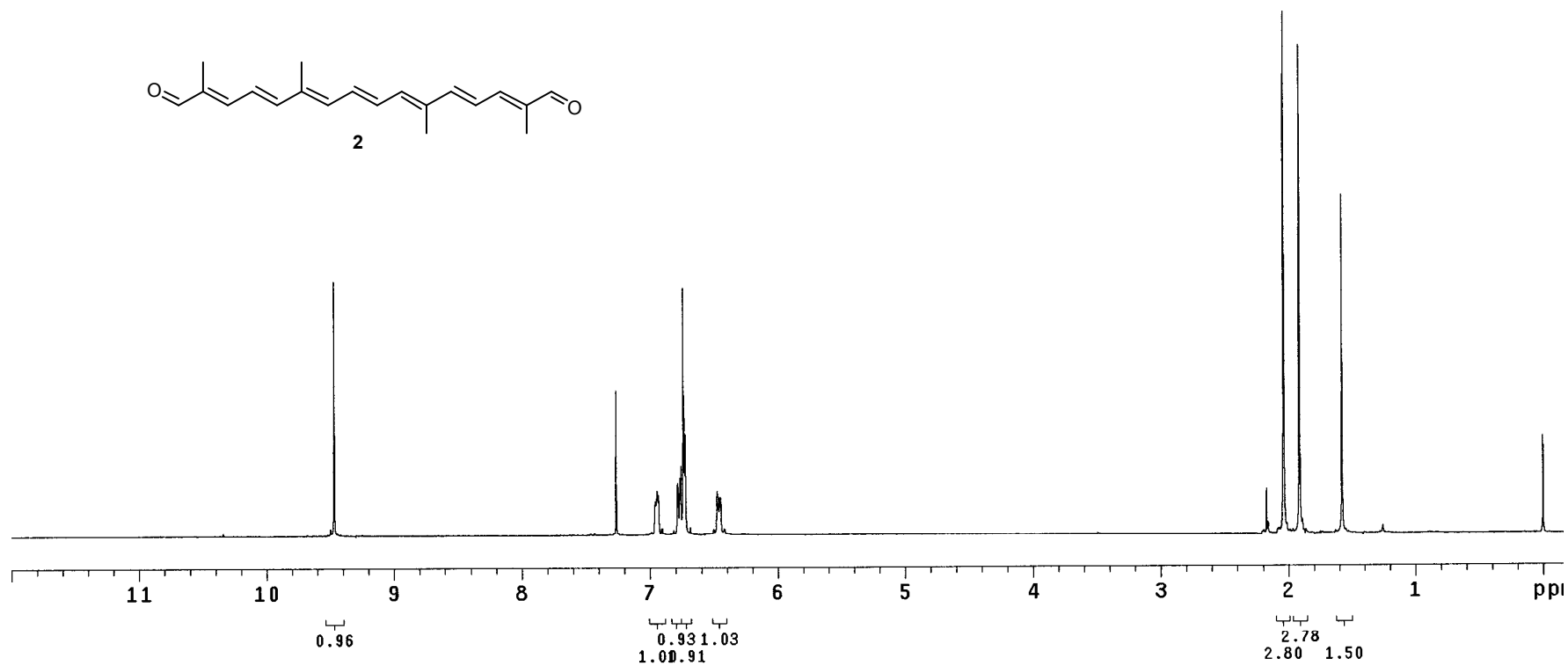
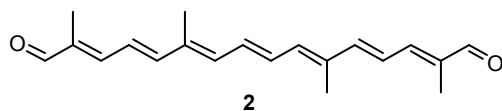
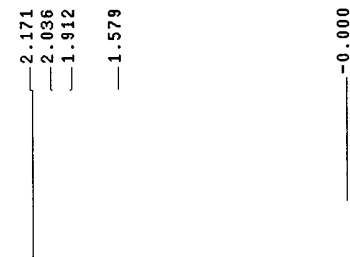
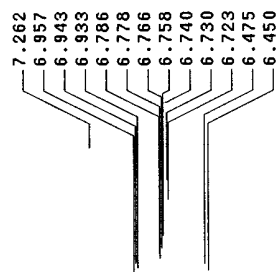
12.772
 12.125



Sample: SHK-1570-3-1
 Sample ID: s_46_SHK-1570-3-1_koo-2_20130606_01
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1570-3-1_Proton_01.fid

Pulse Sequence: s2pul
 Solvent: cdc13
 Ambient temperature
 Sample #46, Operator: walkup2
 File: SHK-1570-3-1_Proton_01
 VNMR-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.0340088 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec

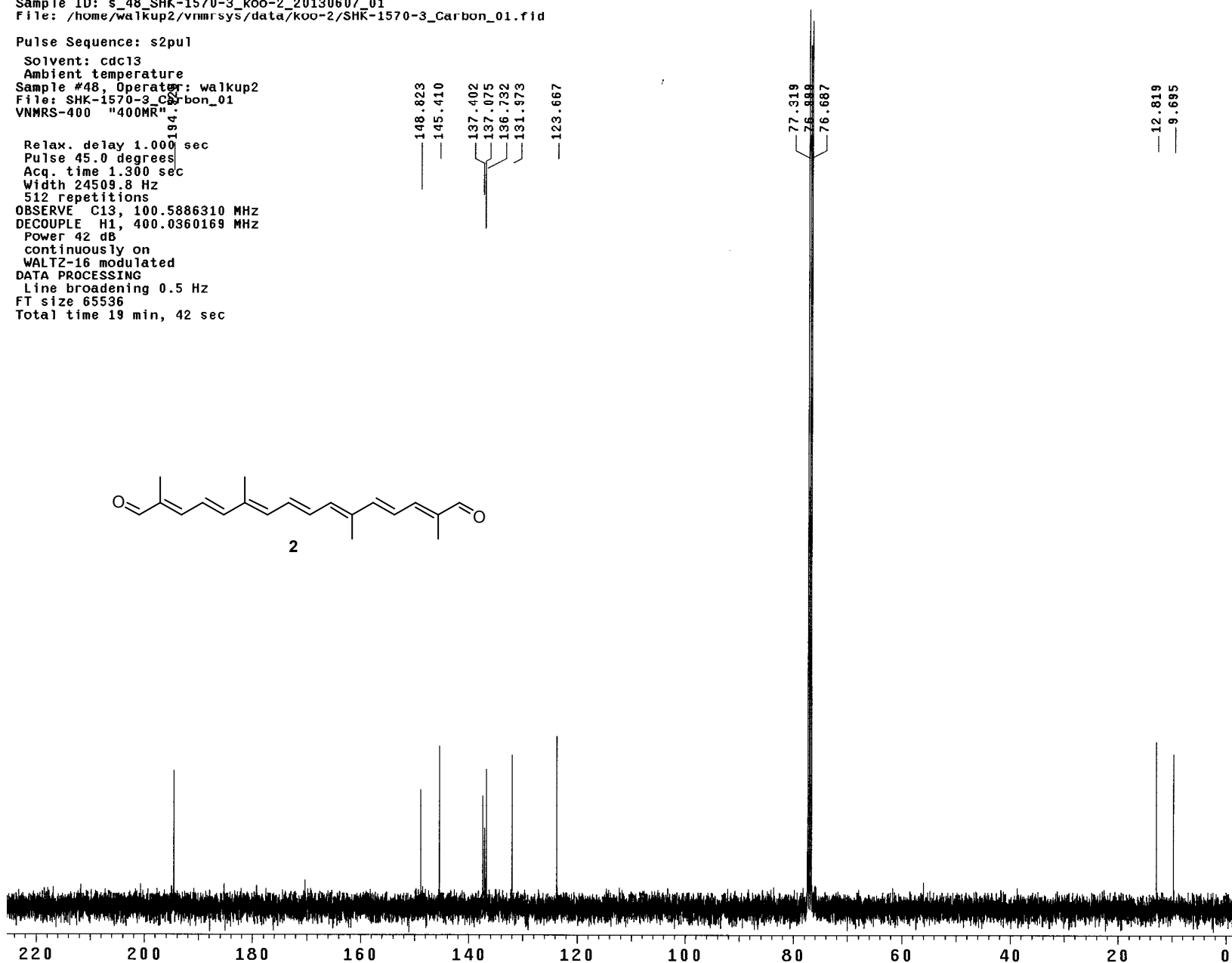


Sample: SHK-1570-3
 Sample ID: s_48_SHK-1570-3_koo-2_20130607_01
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1570-3_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: cdc13
 Ambient temperature
 Sample #48, Operator: walkup2
 File: SHK-1570-3_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, 100.5886310 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



Sample: OET-1024-2
 Sample ID: s_40_OET-1024-2_koo-3_20130530_01
 File: /home/walkup2/vnmrSYS/data/koo-3/OET-1024-2_Proton_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

Sample #40, Operator: walkup

File: OET-1024-2_Proton_01

VNMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

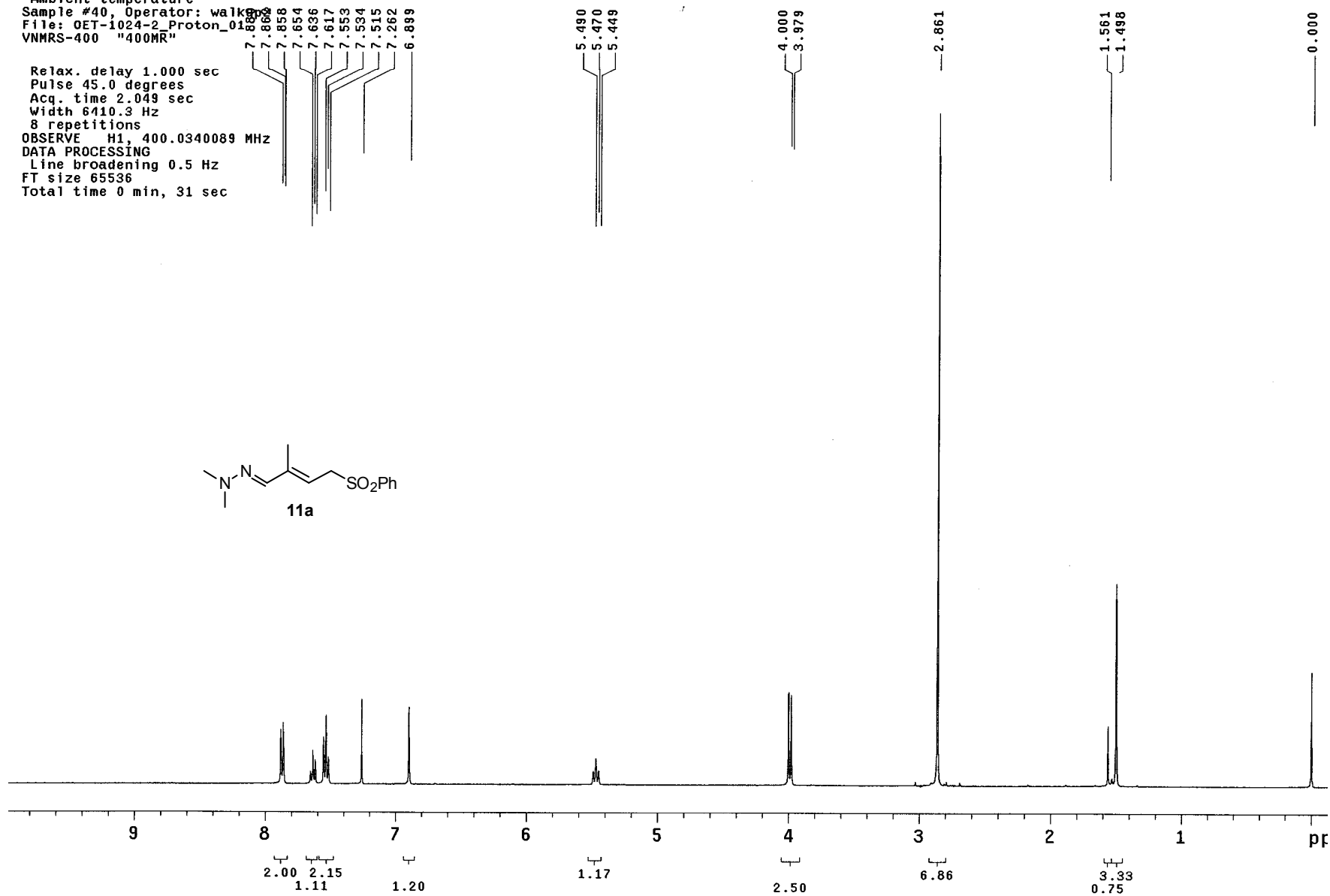
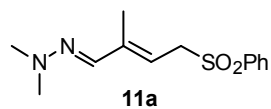
OBSERVE H1, 400.0340089 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec



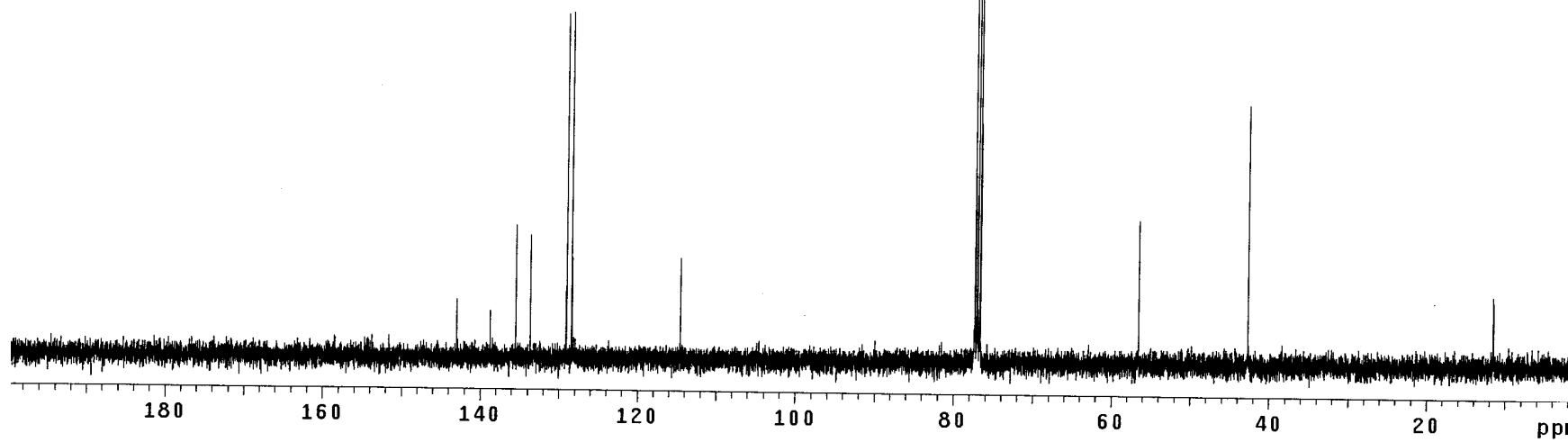
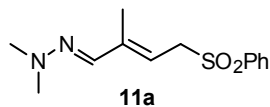
Sample: OET-1024-2-c
Sample ID: s_43_OET-1024-2-c_koo-3_20130530_01
File: /home/walkup2/vnmrSYS/data/koo-3/OET-1024-2-c_Carbon_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Sample #43, Operator: walkup2
File: OET-1024-2-c_Carbon_01
VNMRS-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
512 repetitions
OBSERVE C13, 100.5886316 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

143.024
138.778
135.521
133.640
129.089
128.390
114.567
77.320
77.000
76.688
56.536
42.646
11.511



Sample: SHK-1501-1
 Sample ID: s_40_SHK-1501-1_koo-2_20130326_01
 File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1501-1_Proton_01.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Sample #40, Operator: walkup2

File: SHK-1501-1_Proton_01

VNMR-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

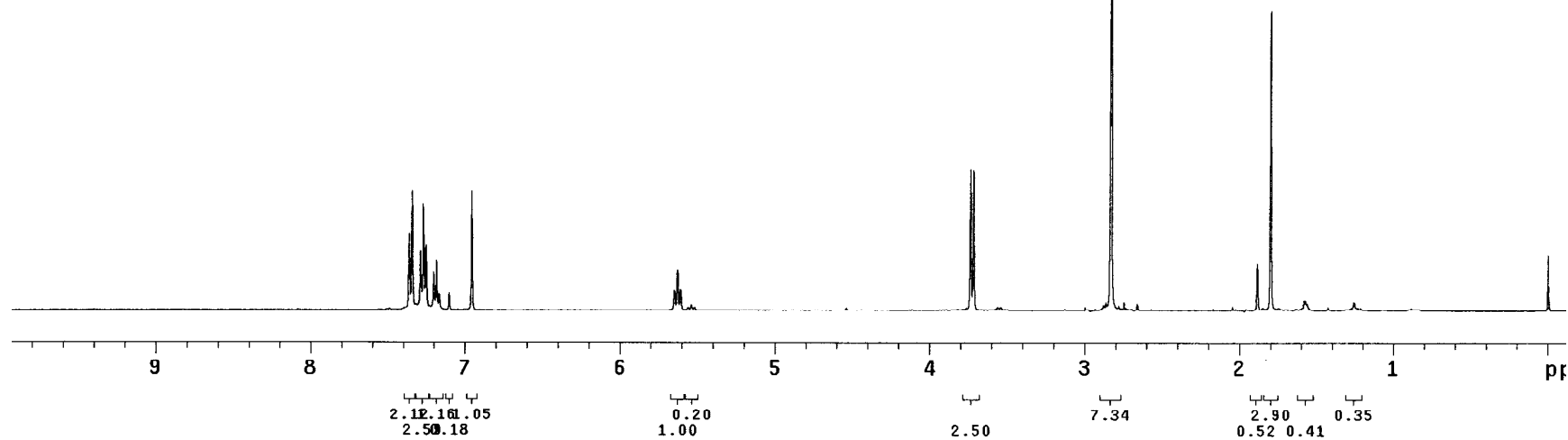
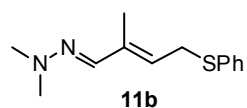
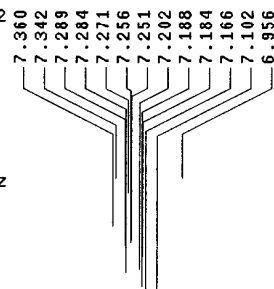
OBSERVE H1, 400.0340111 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec

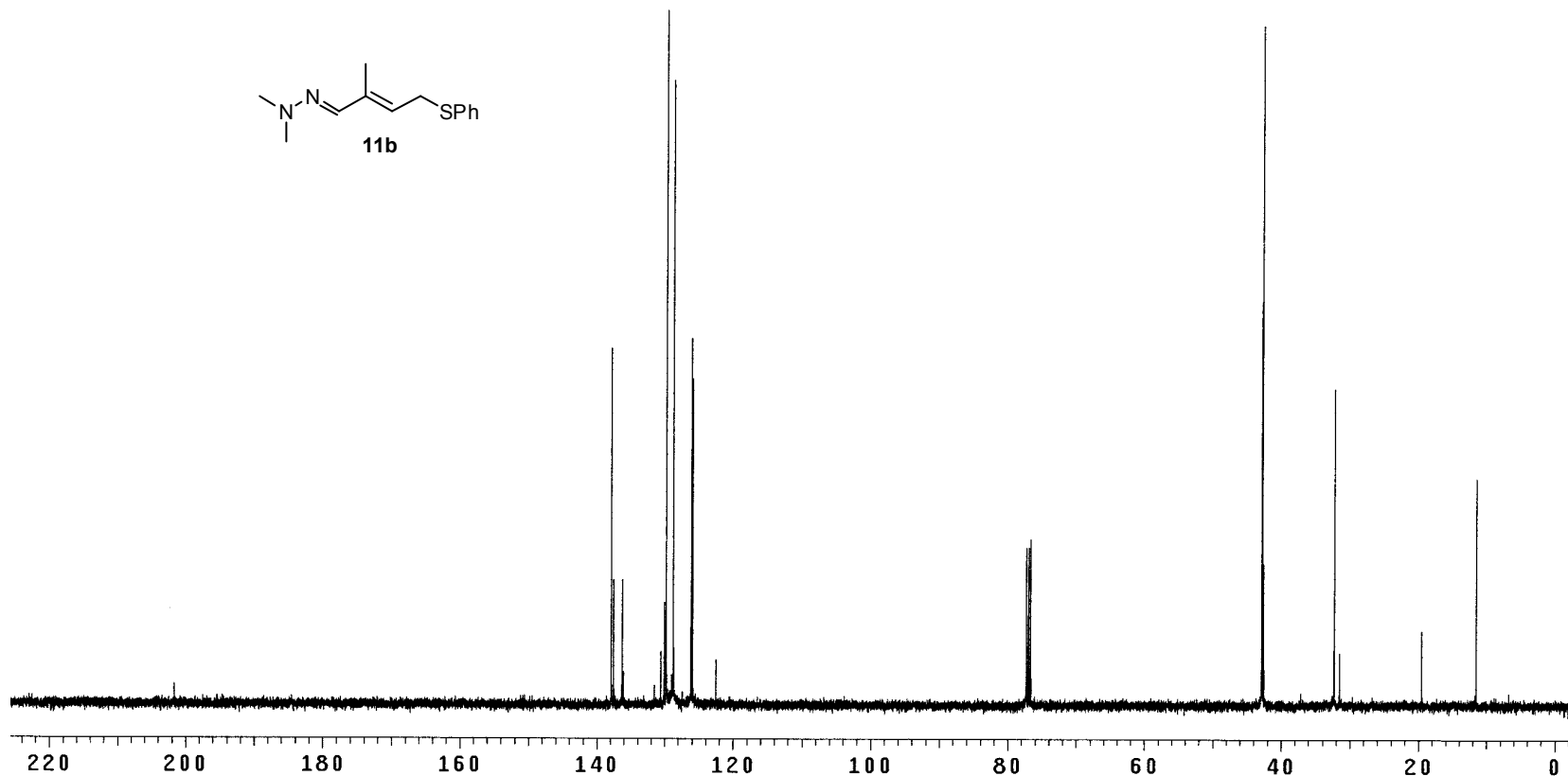
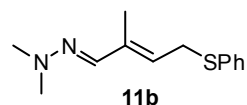
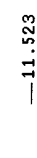
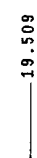
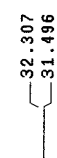
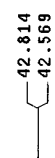
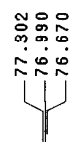
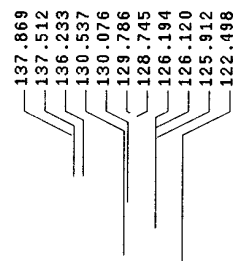


Sample: SHK-1501-1
 Sample ID: s_46_SHK-1501-1_koo-2_20130403_01
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1501-1_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: cdc13
 Ambient temperature
 Sample #46, Operator: walkup2
 File: SHK-1501-1_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, 100.5886416 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

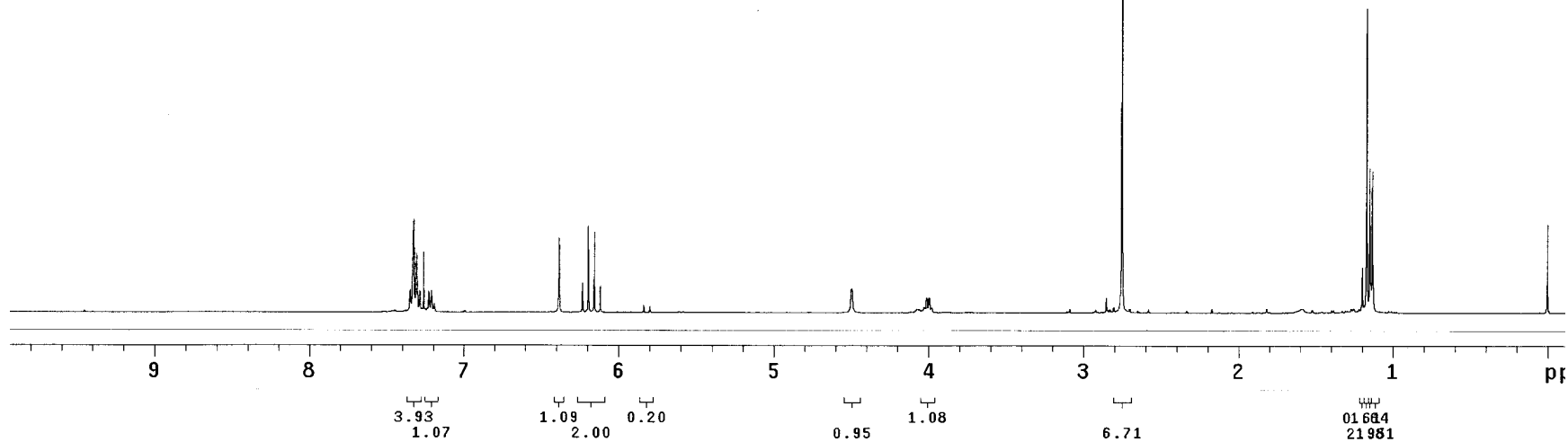
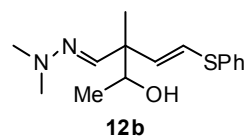
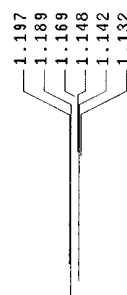
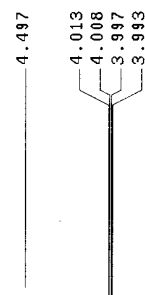
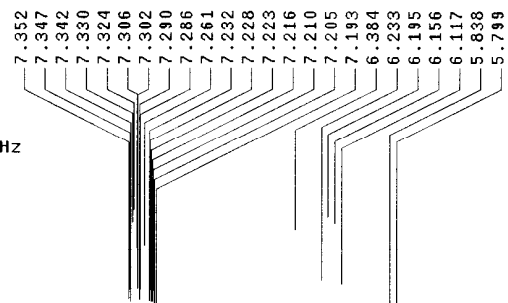


Sample: KYH-699-2
File: exp

Pulse Sequence: s2pu1

Solvent: cdcl3
Ambient temperature
Operator: walkup2
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: KYH-699-2-C
File: /home/walkup2/vnmrsys/data/koo-1/KYH-699-2-C_C.fid

Pulse Sequence: s2pul1

Solvent: cdc13
Ambient temperature
Operator: walkup2
File: KYH-699-2-C_C
VNMR-400 "400MR"

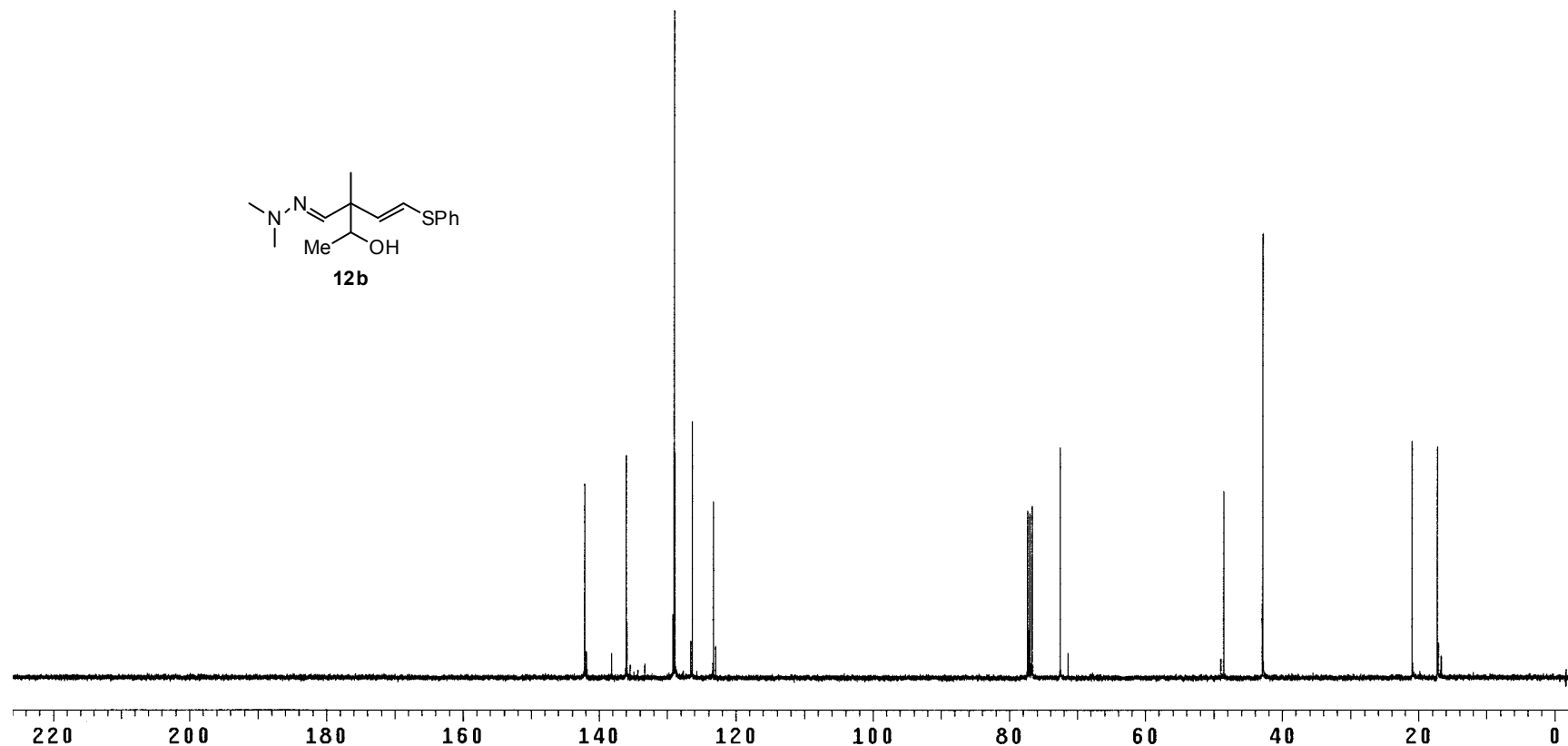
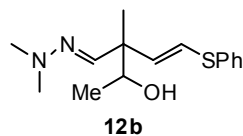
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
512 repetitions
OBSERVE C13, 100.5886417 MHz
DECOUPLE H1, 400.0360169 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min, 42 sec

142.077
135.994
128.930
126.312
123.278

77.294
76.982
76.662
72.535

48.568
42.858

20.959
17.270

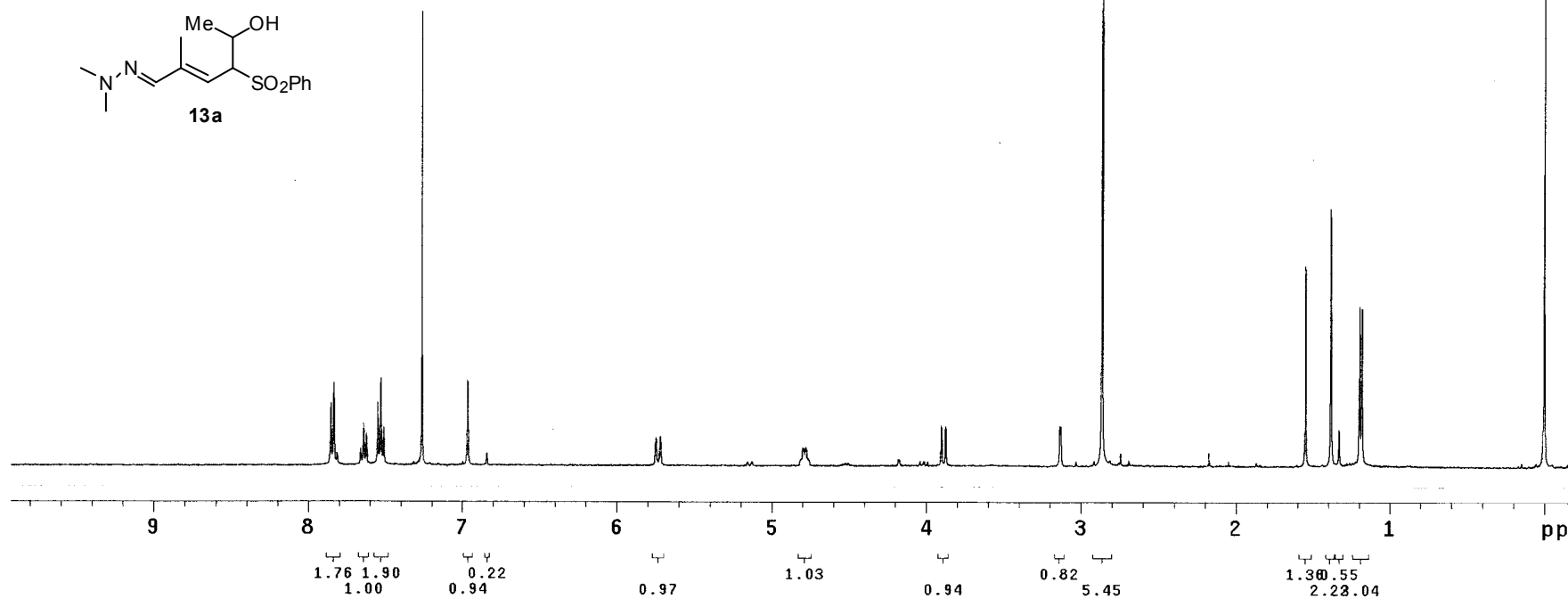
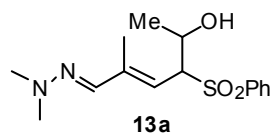
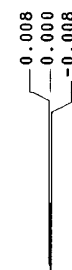
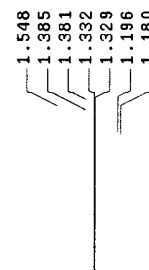
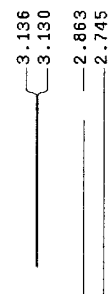
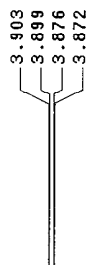
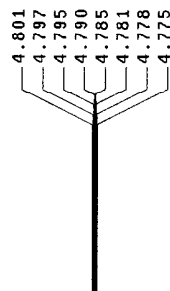
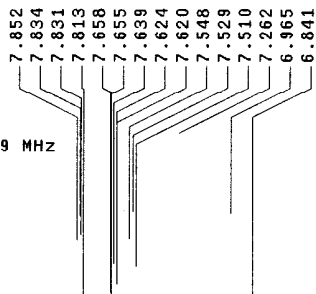


Sample: KYH-696-1R
File: exp

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Operator: walkup2
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, 400.0340089 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec



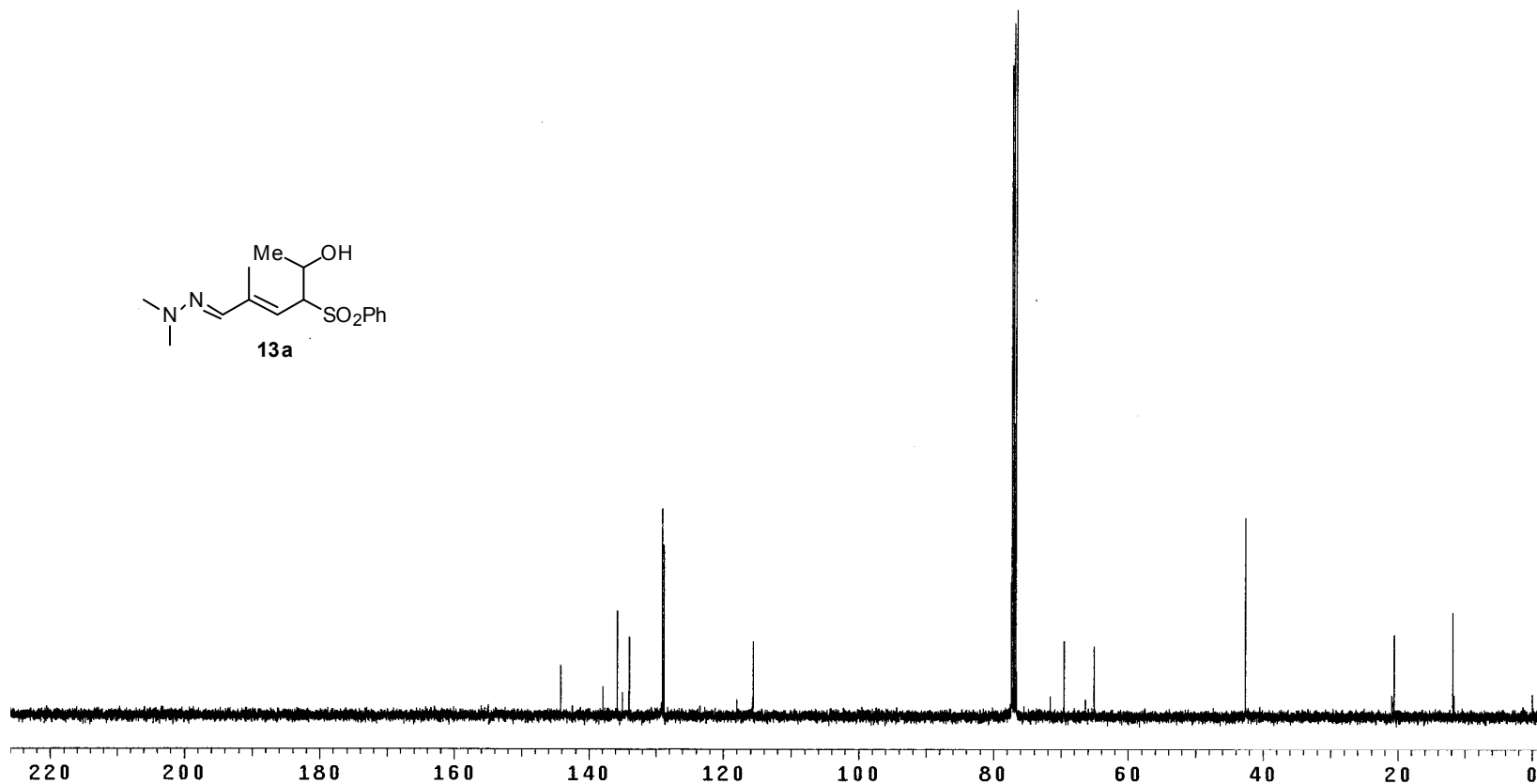
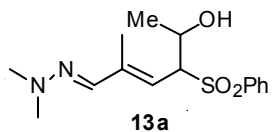
Sample: KYH-627-1-c
 Sample ID: s_41_KYH-627-1-c_koo-1_20131217_01
 File: /home/walkup2/vnmrsys/data/koo-1/KYH-627-1-c_Carbon_01.fid

Pulse Sequence: s2pu1

Solvent: cdcl3
 Ambient temperature
 Sample #41, Operator: walkup2
 File: KYH-627-1-c_Carbon_01
 VNMRs-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 1024 repetitions
 OBSERVE C13, 100.5886340 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

144.175
 135.713
 133.914
 129.021
 128.894
 128.746
 115.614
 77.303
 76.991
 76.871
 69.555
 65.049
 42.622
 42.584
 20.596
 11.747

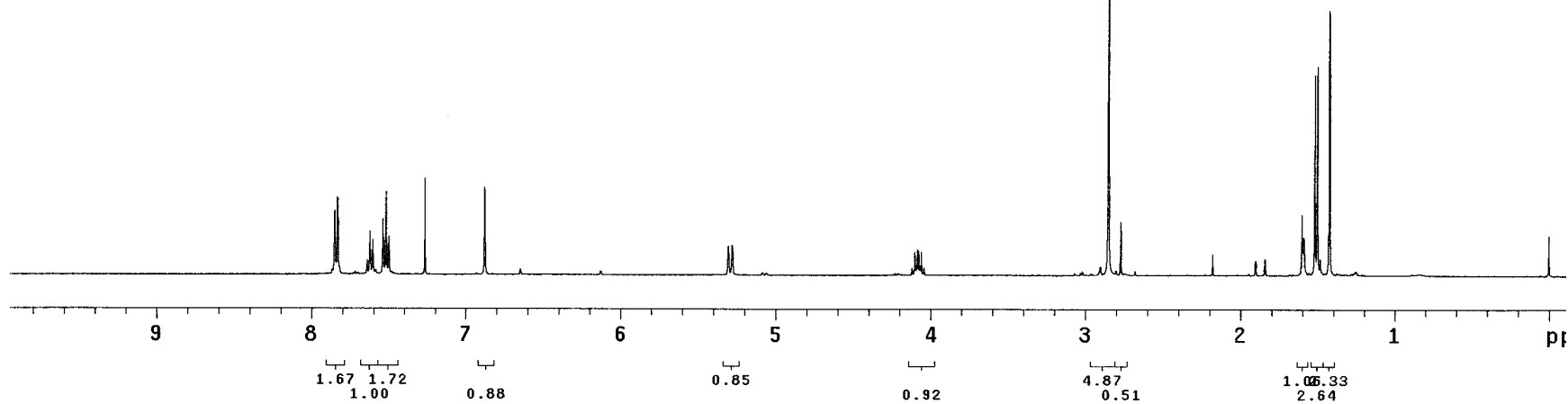
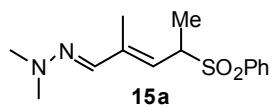
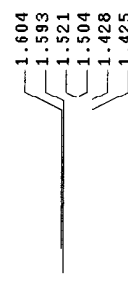
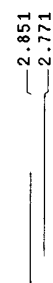
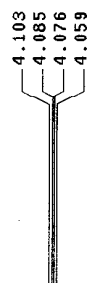
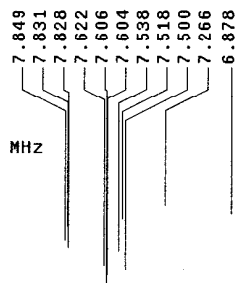


Sample: NDA-249
File: exp

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Operator: walkup2
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, 400.0340081 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

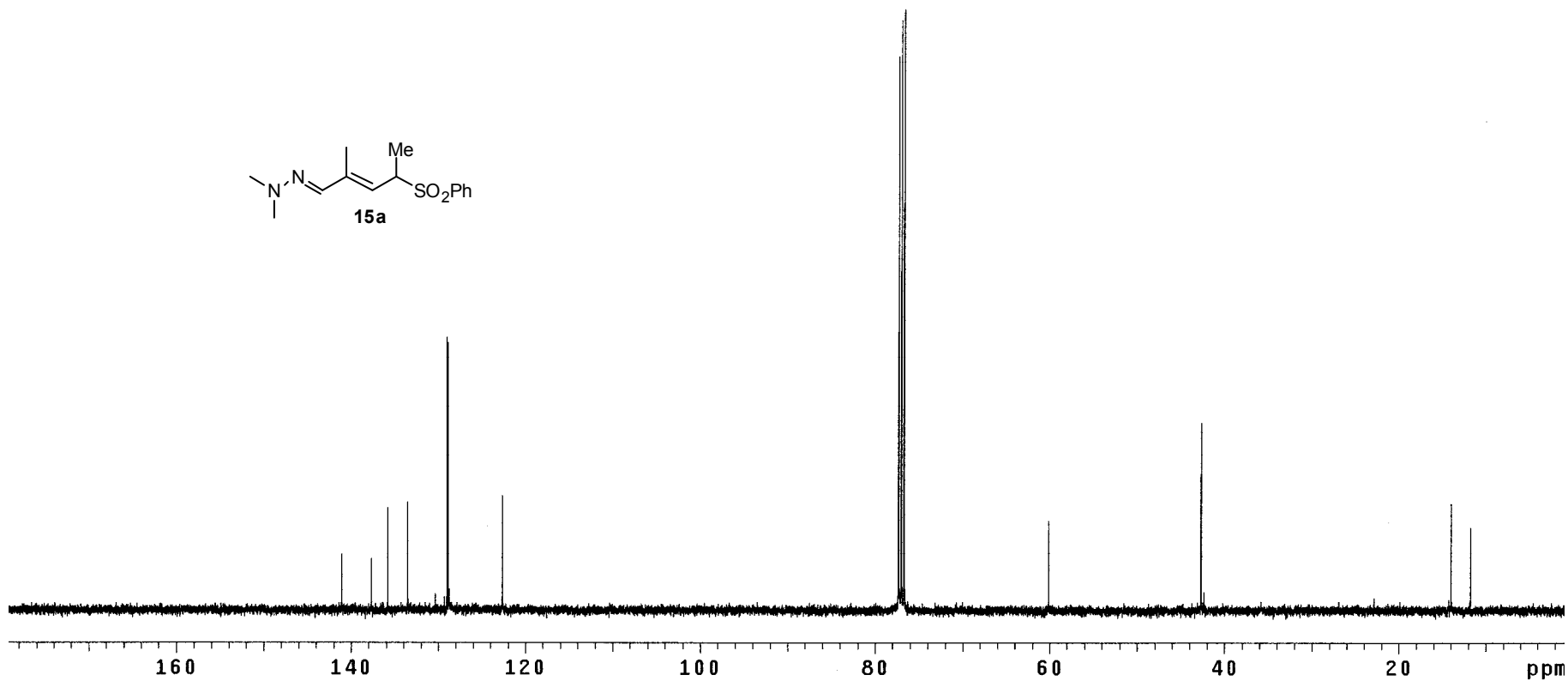
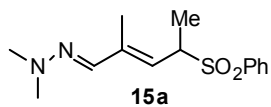
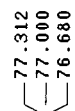
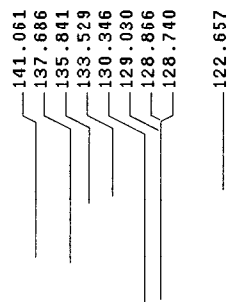


Sample: KYH-692-1-C
File: exp

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Operator: walkup2
VNMR-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
1500 repetitions
OBSERVE C13, 100.5886346 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 57 min, 44 sec



Sample: KYH-706

File: /home/walkup2/vnmrsys/data/koo-1/KYH-706_proton.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

Operator: walkup2

File: KYH-706_proton

VNMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6830.6 Hz

16 repetitions

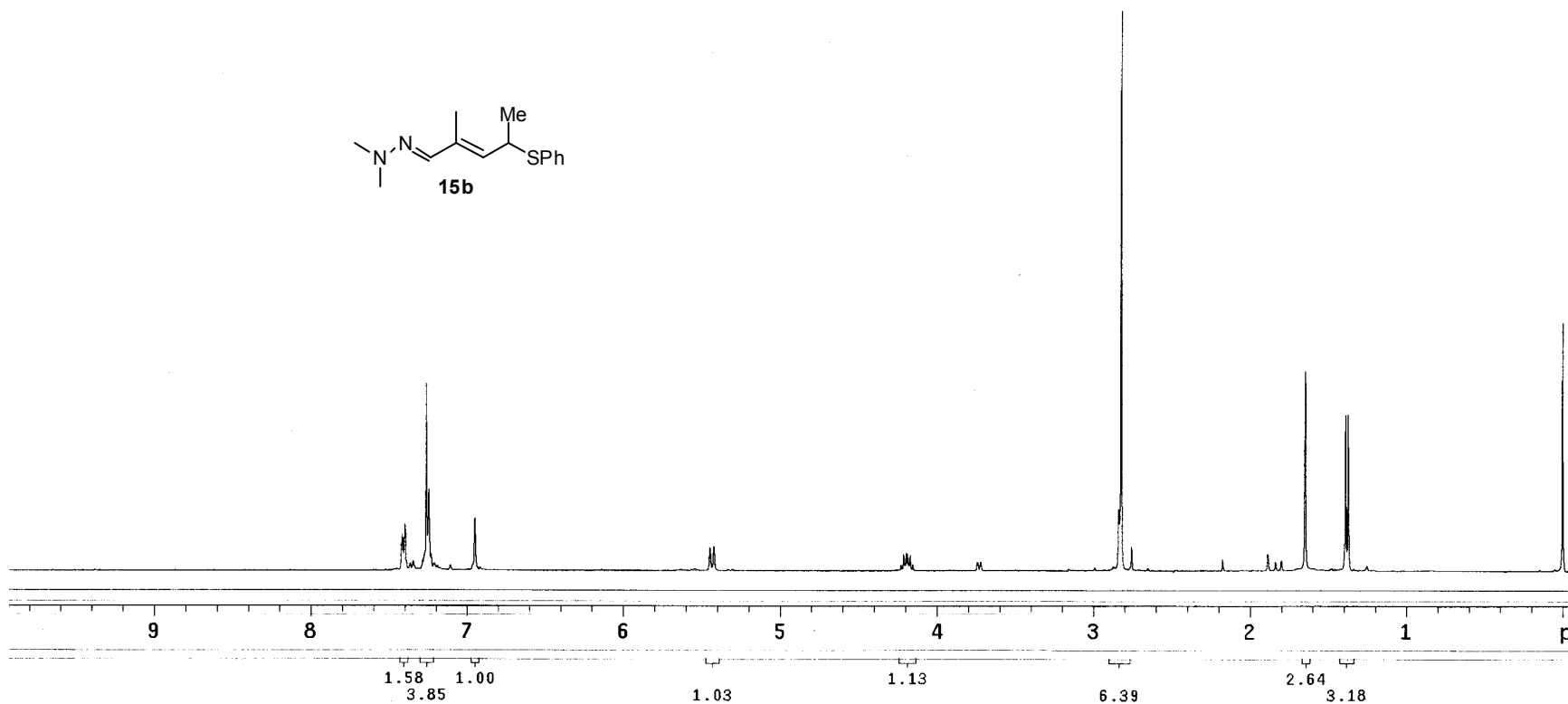
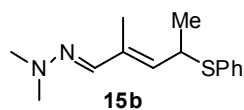
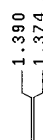
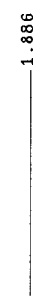
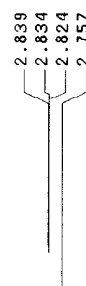
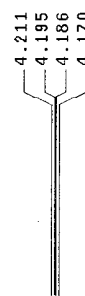
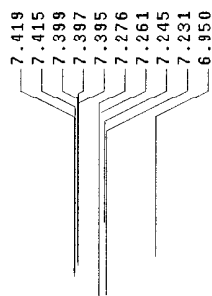
OBSERVE H1, 400.0340094 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FI size 65536

Total time 0 min, 55 sec



Sample: KYH-706-c
File: /home/walkup2/vnmrsys/data/koo-1/KYH-706-c_C.fid

Pulse Sequence: s2pu1

Solvent: cdcl3
Ambient temperature
Operator: walkup2
File: KYH-706-c_C
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, 100.5886346 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

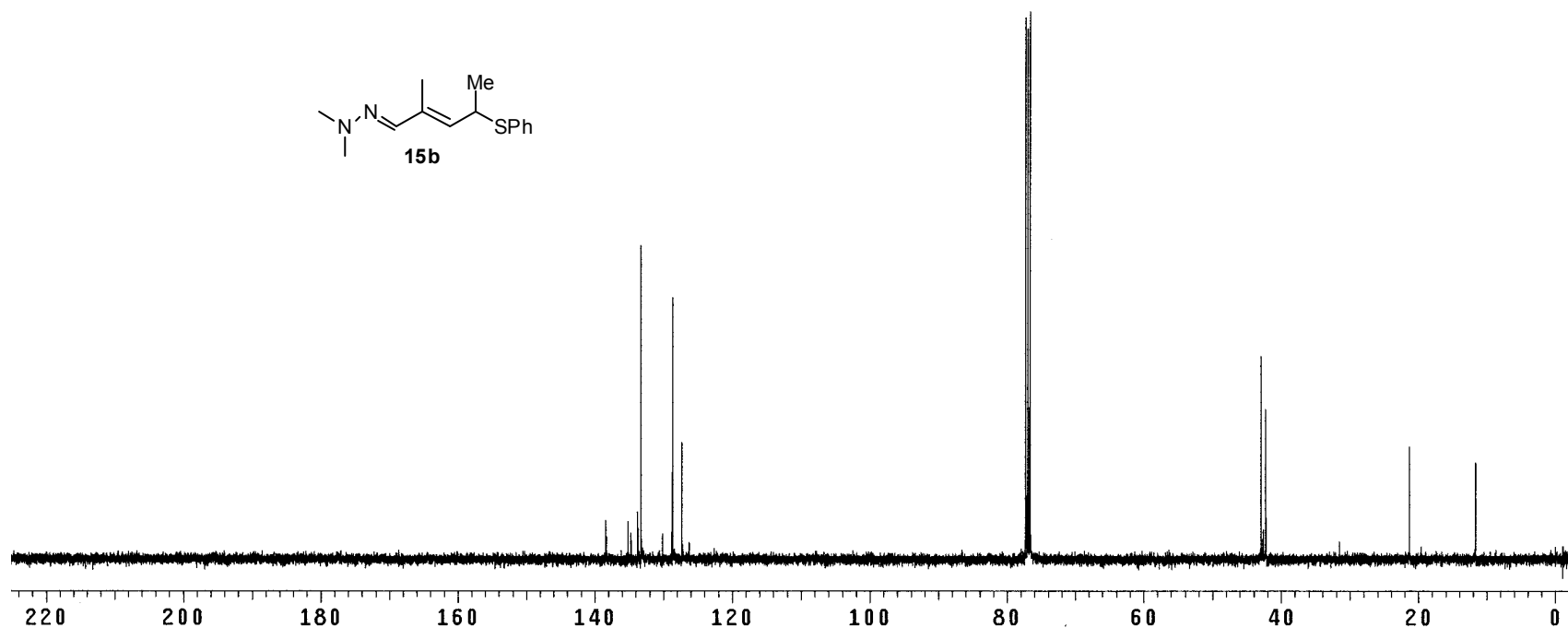
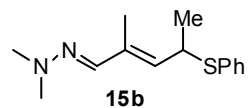
133.224
128.658
127.282

77.305
76.992
76.673

42.935
42.236

21.282

11.645



Sample: OET-1017
 Sample ID: s_46_OET-1017_koo-3_20130521_01
 File: /home/walkup2/vnmrsys/data/koo-3/OET-1017_Proton_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

Sample #46, Operator: walkup

File: OET-1017_Proton_01

VNMR-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

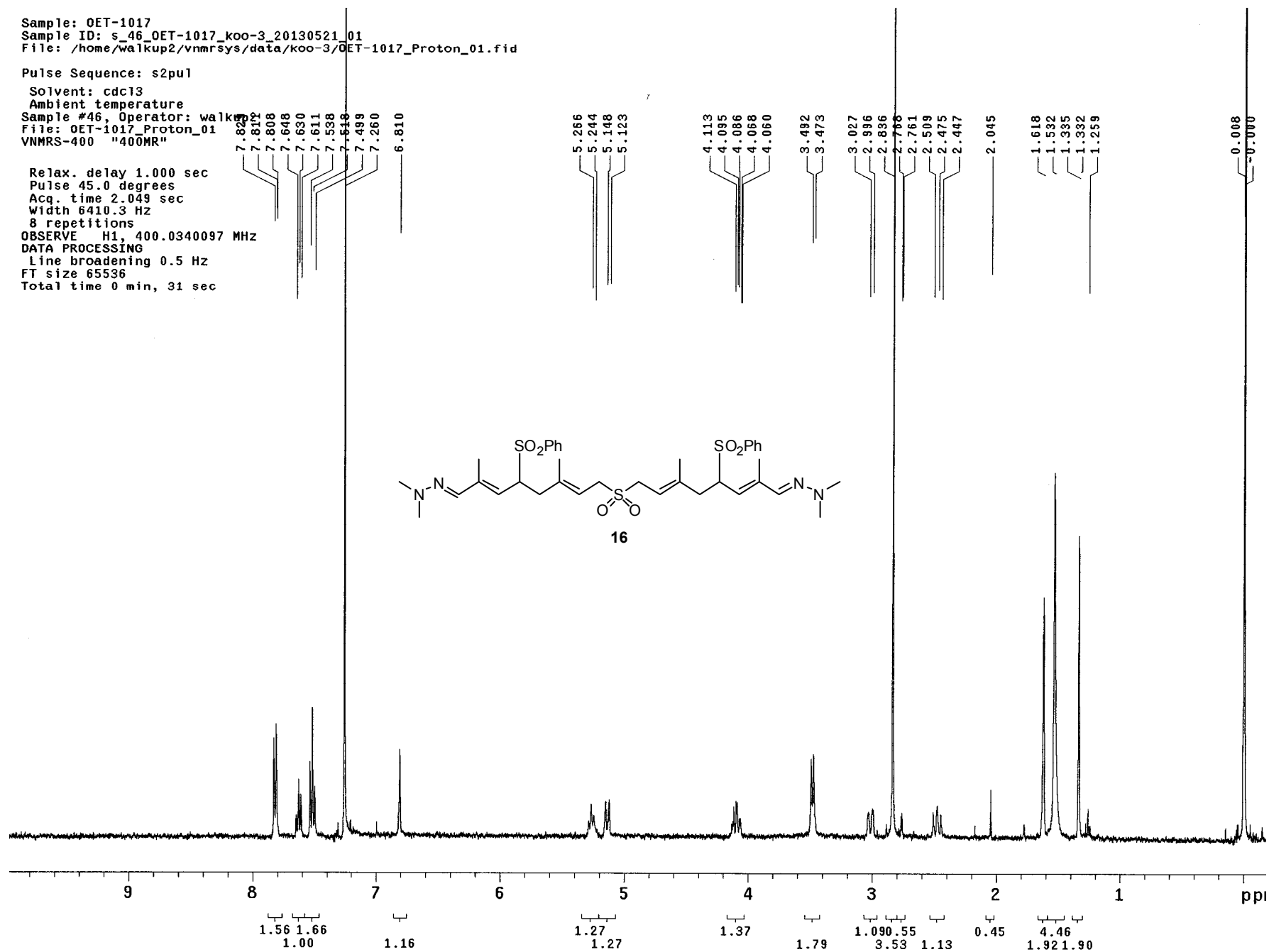
OBSERVE H1, 400.0340097 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec

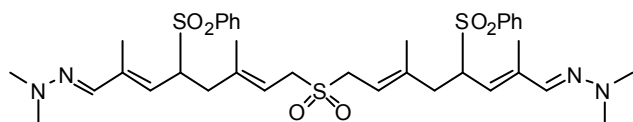


Sample: OET-1069-cou
 Sample ID: s_43_OET-1069-cou_koo-3_20130723_02
 File: /home/walkup2/vnmr/sys/data/koo-3/OET-1069-cou_Carbon_01.fid

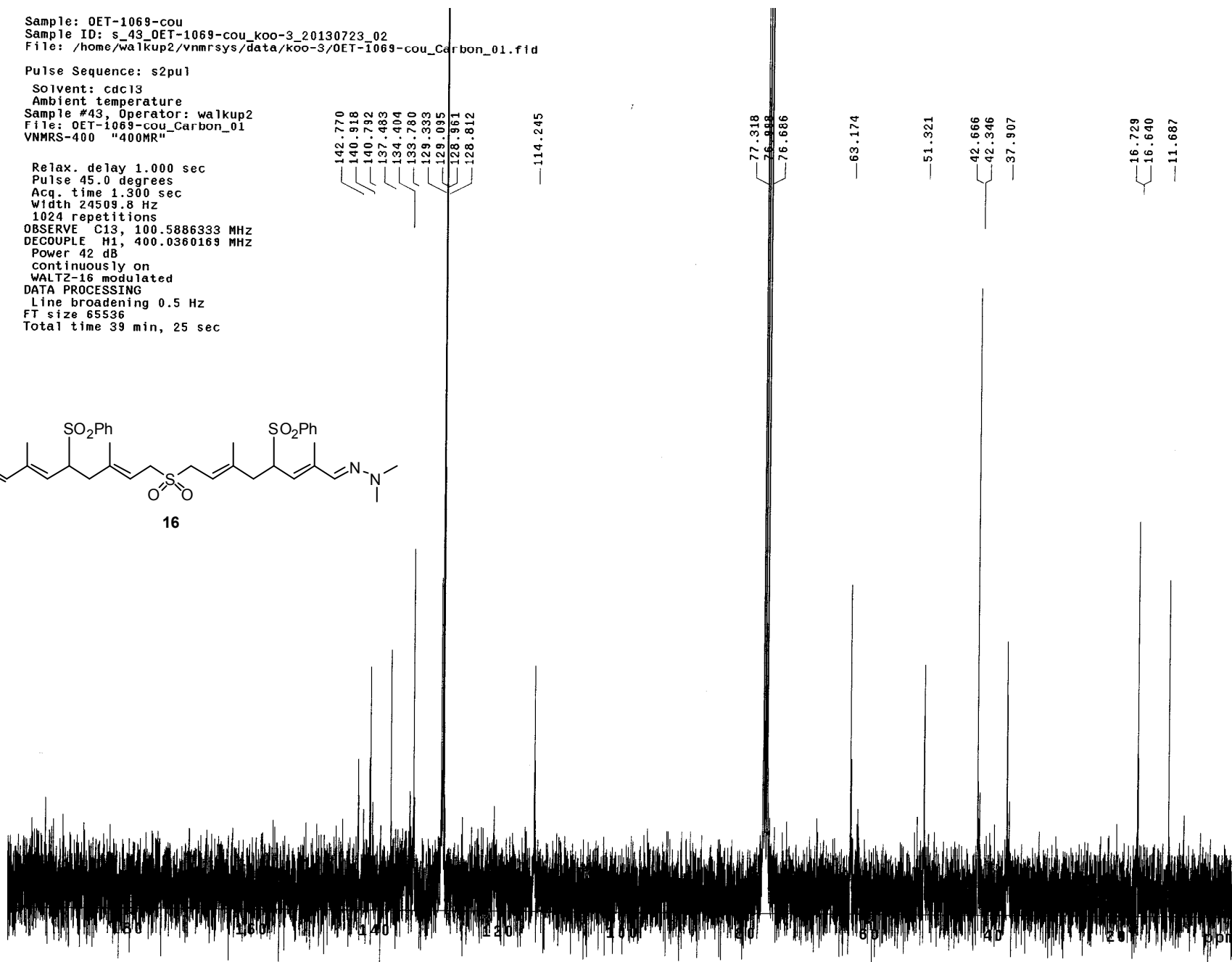
Pulse Sequence: s2pu1

Solvent: cdc13
 Ambient temperature
 Sample #43, Operator: walkup2
 File: OET-1069-cou_Carbon_01
 VNMR5-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 24509.8 Hz
 1024 repetitions
 OBSERVE C13, 100.5886333 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



16



Sample: OET-1023-3
 Sample ID: s_44_OET-1023-3_koo-3_20130527_01
 File: /home/waikup2/vnmrSYS/data/koo-3/OET-1023-3_Proton_01.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

Sample # 4

File: OET-1023-3_koo-3_20130527_01

VNMRS-400

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

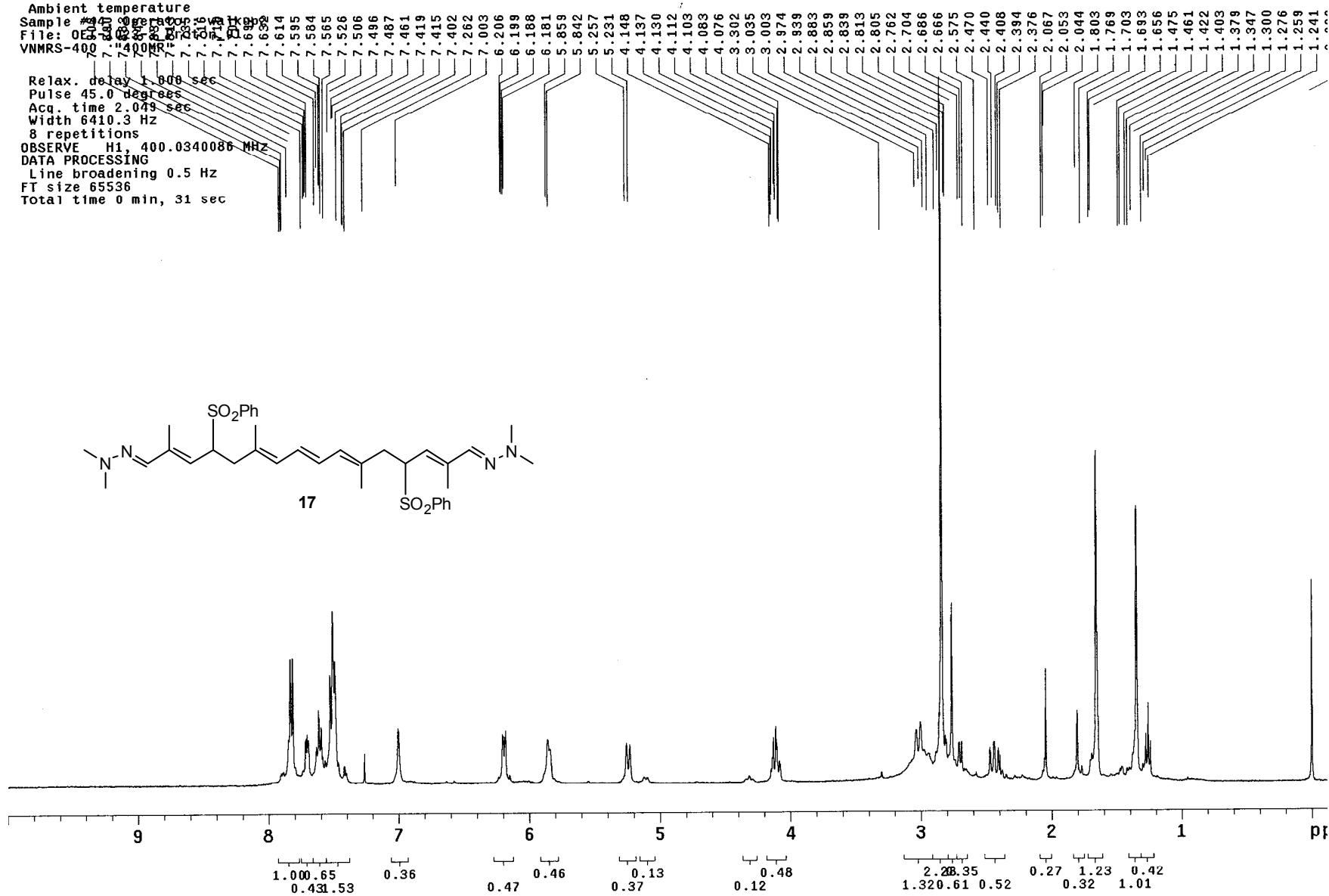
OBSERVE H1, 400.0340086 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec



Sample: OET-1213-C
File: /home/walkup2/vnmrsys/data/koo-3/OET-1213-C_C.fid

Pulse Sequence: s2pul

Solvent: cdc13
Ambient temperature
Operator: walkup2
File: OET-1213-C_C
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, 100.5886354 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

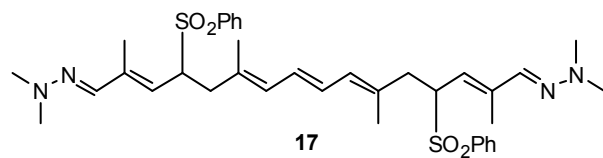
142.354
142.339
137.766
137.394
135.654
133.565
133.476
133.074
133.007
129.282
129.044
128.850
128.709
128.471
128.367
128.263
127.802
121.333

77.311
77.200
76.992
76.679

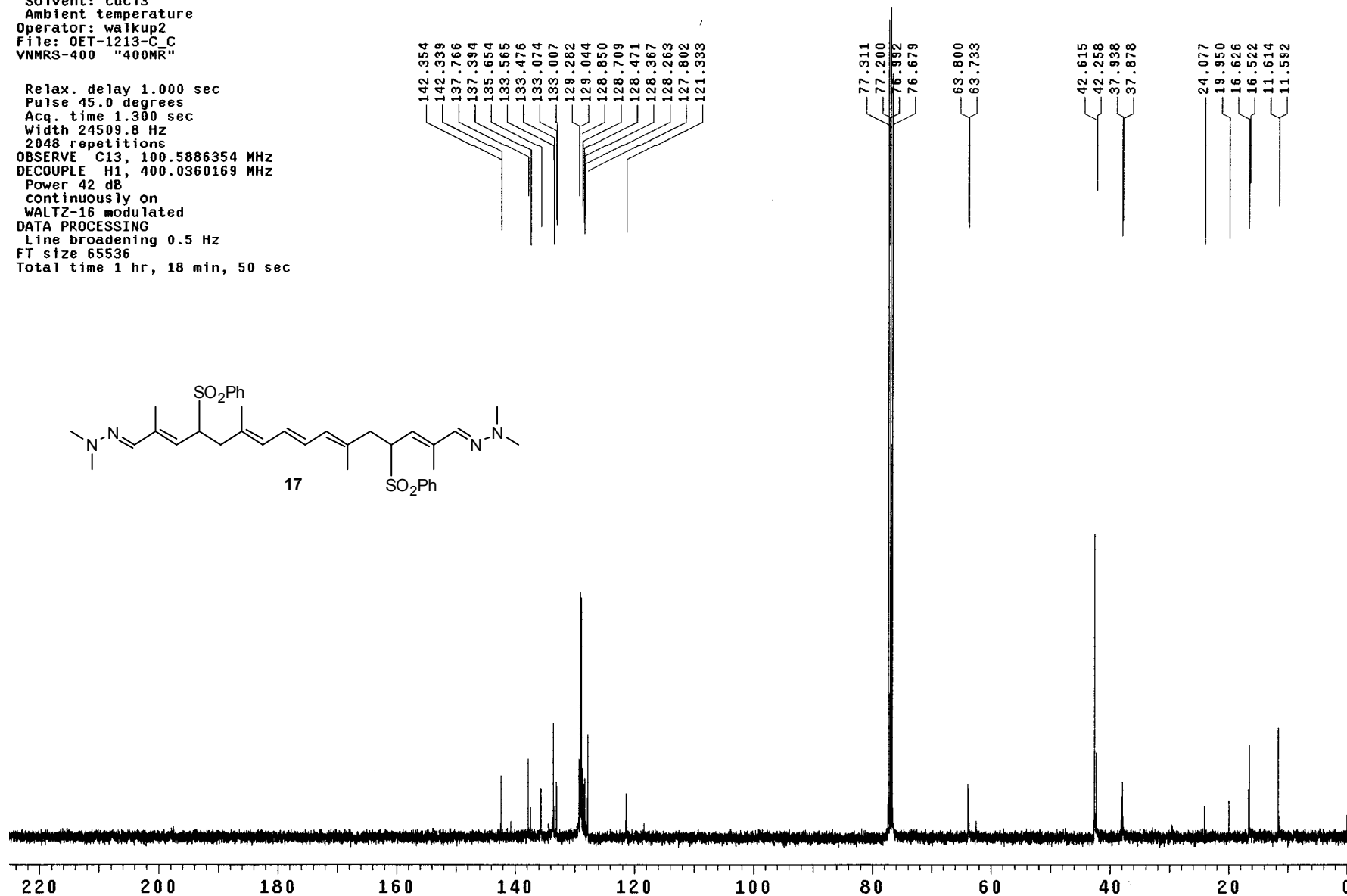
63.800
63.733

42.615
42.258
37.938
37.878

24.077
19.950
16.626
16.522
11.614
11.592



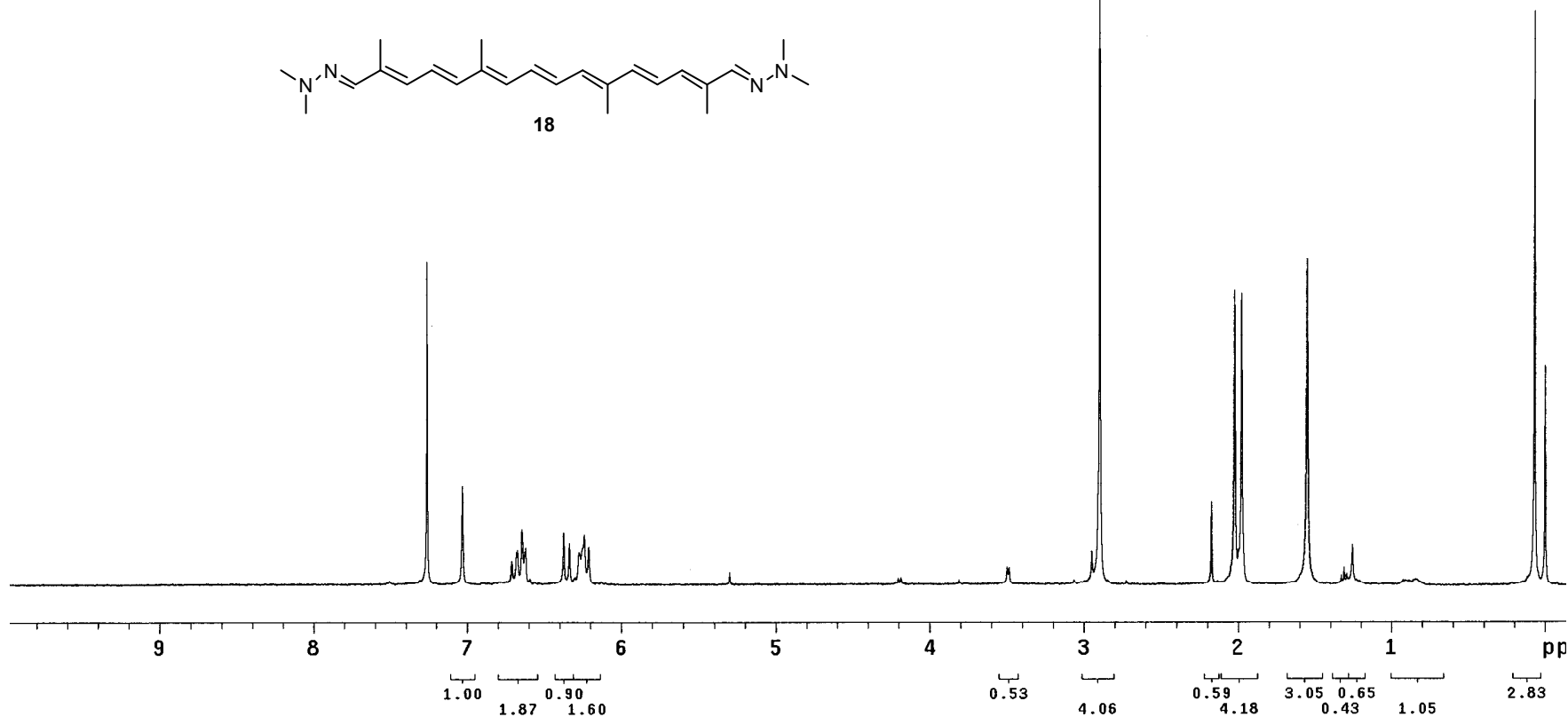
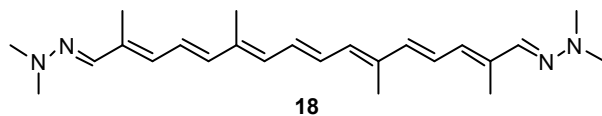
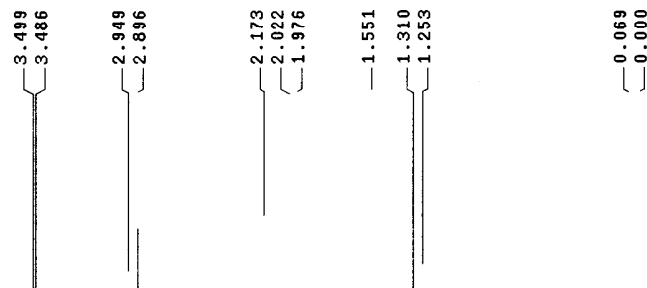
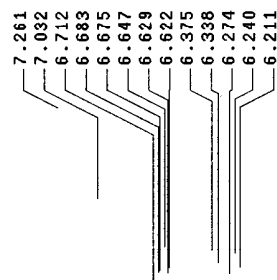
17



Sample: OET-1184
 Sample ID: s_43_OET-1184_koo-3_20131031_01
 File: /home/walkup2/vnmr5sys/data/koo-3/OET-1184_Proton_01.f1d

Pulse Sequence: s2pu1
 Solvent: cdc13
 Ambient temperature
 Sample #43, Operator: walkup2
 File: OET-1184_Proton_01
 VNMR5-400 "400MR"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions
 OBSERVE H1, 400.0340093 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec

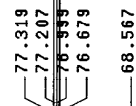
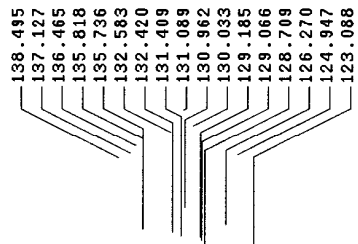


Sample: OET-1179-1
Sample ID: s_33_OET-1179-1_koo-3_20131025_01
File: /home/walkup2/vnmrSYS/data/koo-3/OET-1179-1_Carbon_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Sample #33, Operator: walkup2
File: OET-1179-1_Carbon_01
VNMR-400 "400MR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
2056 repetitions
OBSERVE C13, 100.5886324 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, 19 min, 8 sec

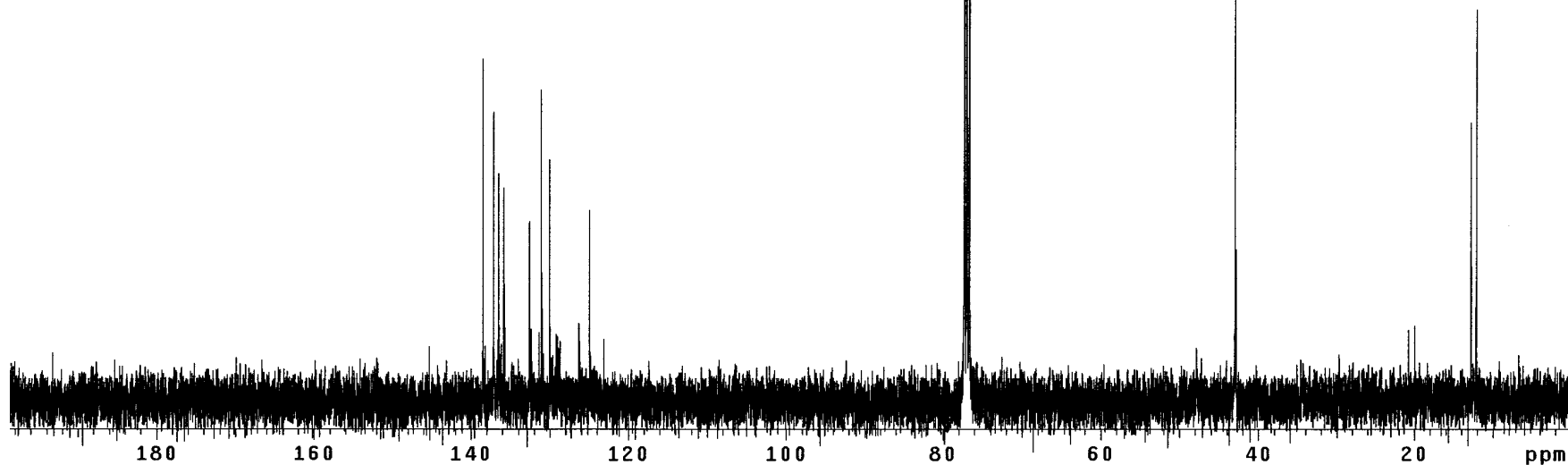
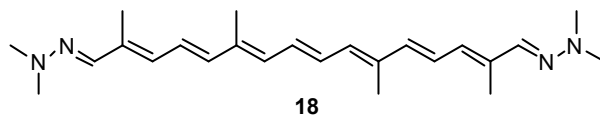


68.567

42.972
42.823

20.708
19.935

12.789
12.112



Pulse Sequence: s2pu1

Ambient temperature

File: 0ET-1181-1_Proton_01

VNMRS-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

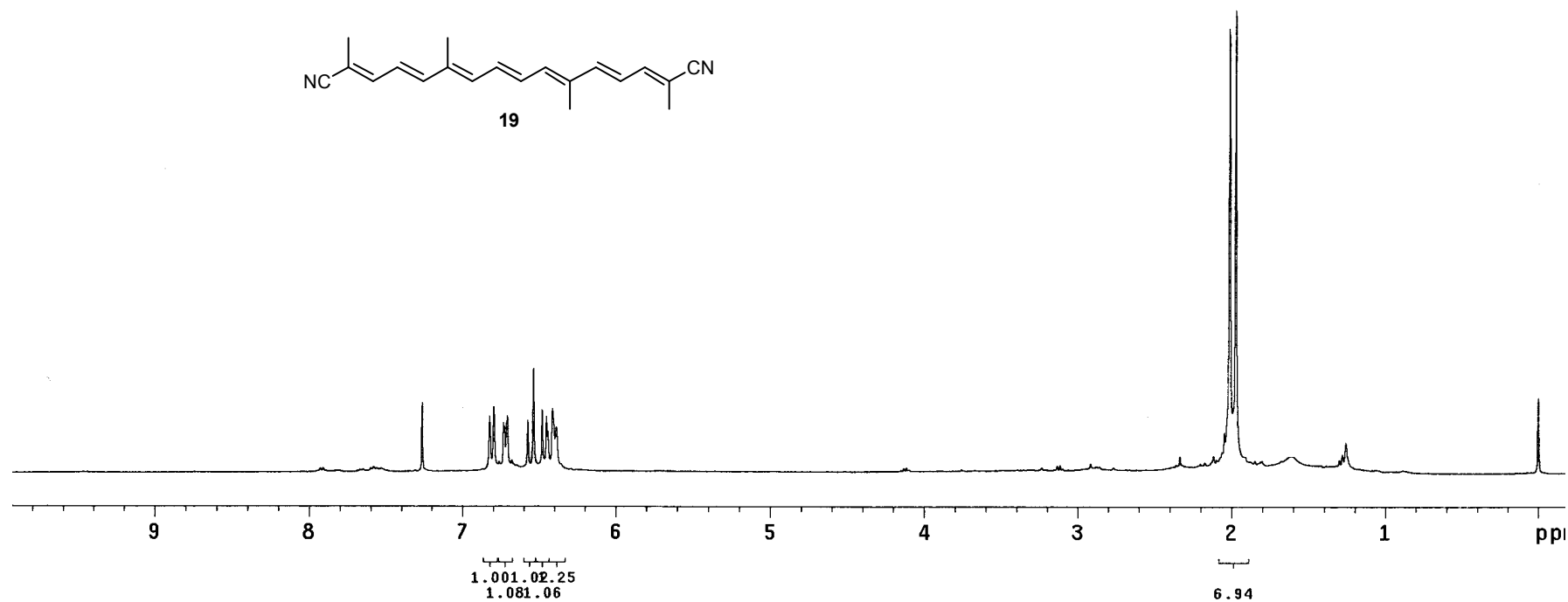
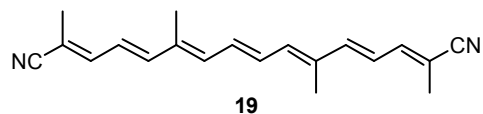
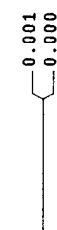
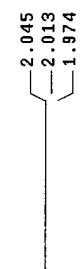
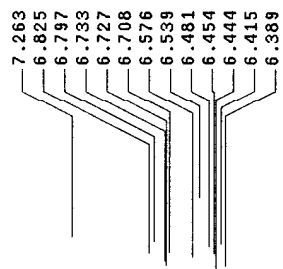
OBSERVE H1, 400.0340082 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec



Sample: OET-1196
 Sample ID: s_50_OET-1196_koo-3_20131119_01
 File: /home/walkup2/vnmr5ys/data/koo-3/OET-1196_Carbon_01.fid

Pulse Sequence: s2pul1

Solvent: cdc13

Ambient temperature

Sample #50, Operator: walkup2

File: OET-1196_Carbon_01

VNMR5-400 "400MR"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24509.8 Hz

2000 repetitions

OBSERVE C13, 100.5886333 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, 16 min, 59 sec

