

Supporting Information

Apocarotenals of phenolic carotenoids for superior antioxidant activities

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Pulse Sequence: s2pu1
Solvent: cdcl3
Ambient temperature
Sample #48, Operator: walkup2
File: SHK-1873-1_Proton_03
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, 400.0340167 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

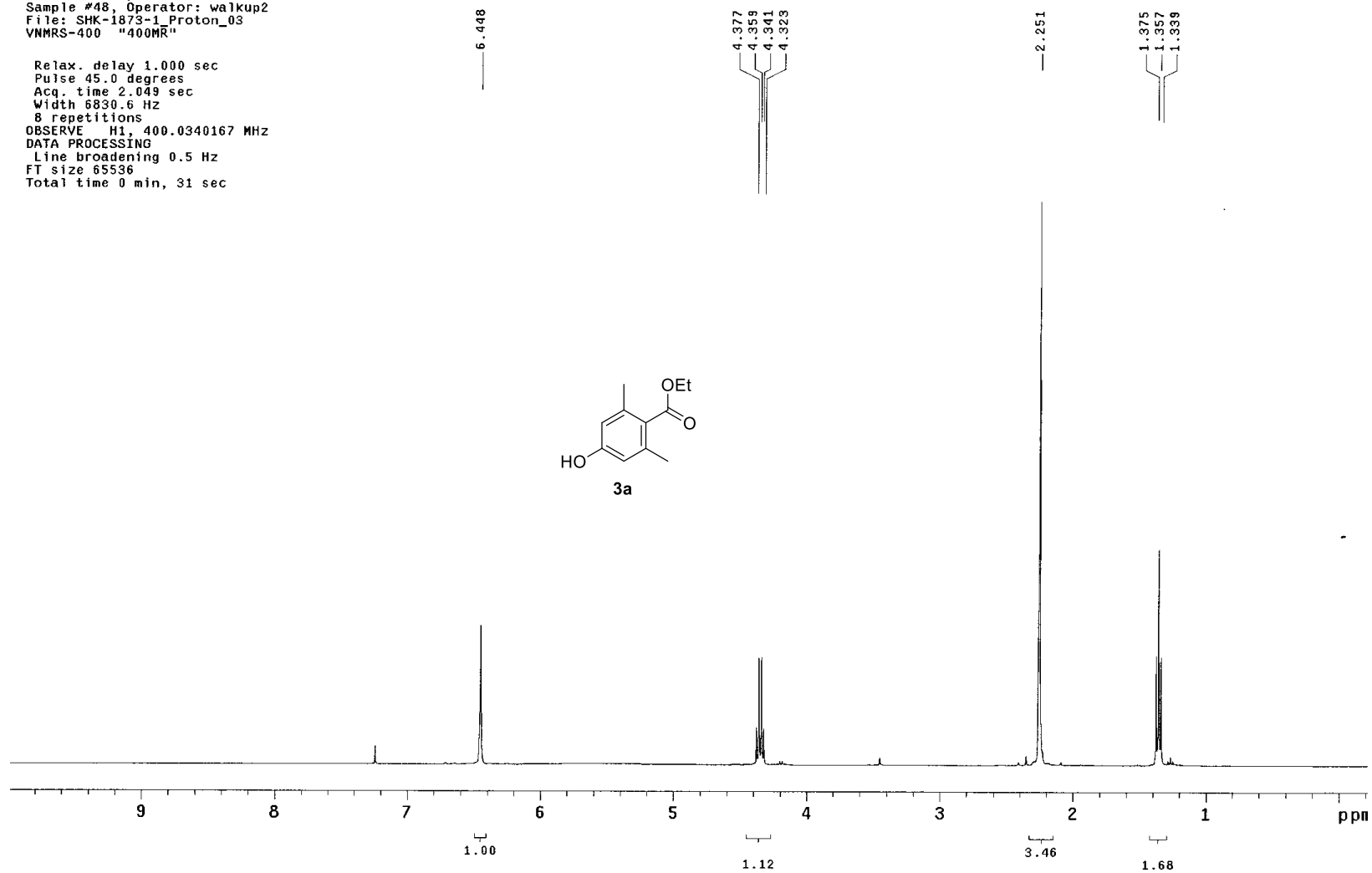


Figure S1. ¹H NMR of 3a

Sample: SHK-1873-1
Sample ID: s_45_SHK-1873-1_koo-2_20151008_01
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1873-1_Carbon_01.fid

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
Sample #45, Operator: walkup2
File: SHK-1873-1_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, 100.5886615 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

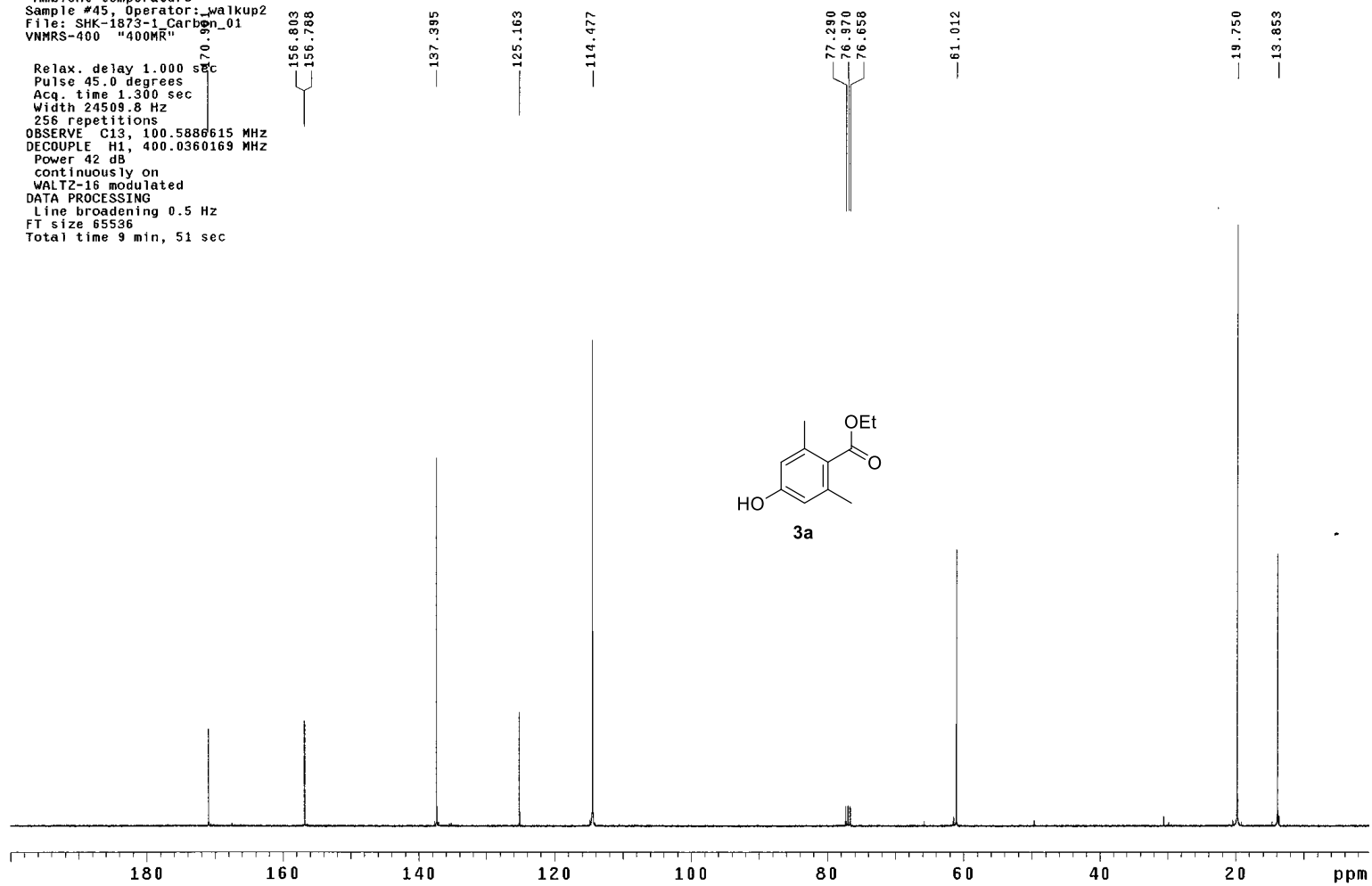


Figure S2. ^{13}C NMR of 3a

Sample: SHK-1892-1
Sample ID: s_45_SHK-1892-1_koo-2_20151020_01
File: /home/walkup2/vnmrsvs/data/koo-2/SHK-1892-1_Proton_01.fid

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #45, Operator: walkup2
File: SHK-1892-1_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, 400.0340083 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

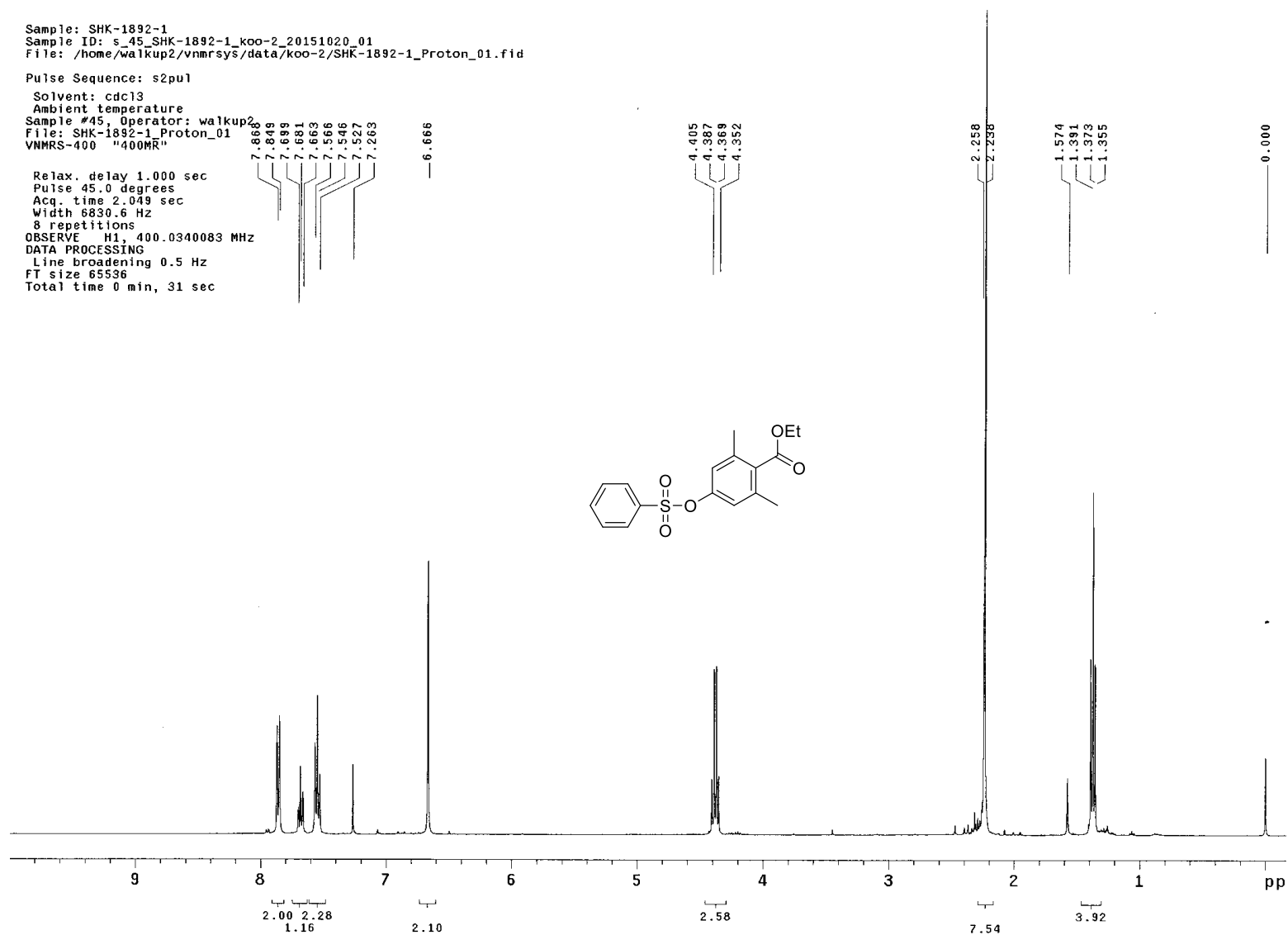


Figure S3. ¹H NMR of ethyl 2,6-dimethyl-4-((phenylsulfonyl)oxy)benzoate

Sample: SHK-1892-1
Sample ID: s_34_SHK-1892-1_koo-2_20151021_01
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1892-1_Carbon_01.fid

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Sample #34, Operator: walkup2
File: SHK-1892-1_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, 100.5886462 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

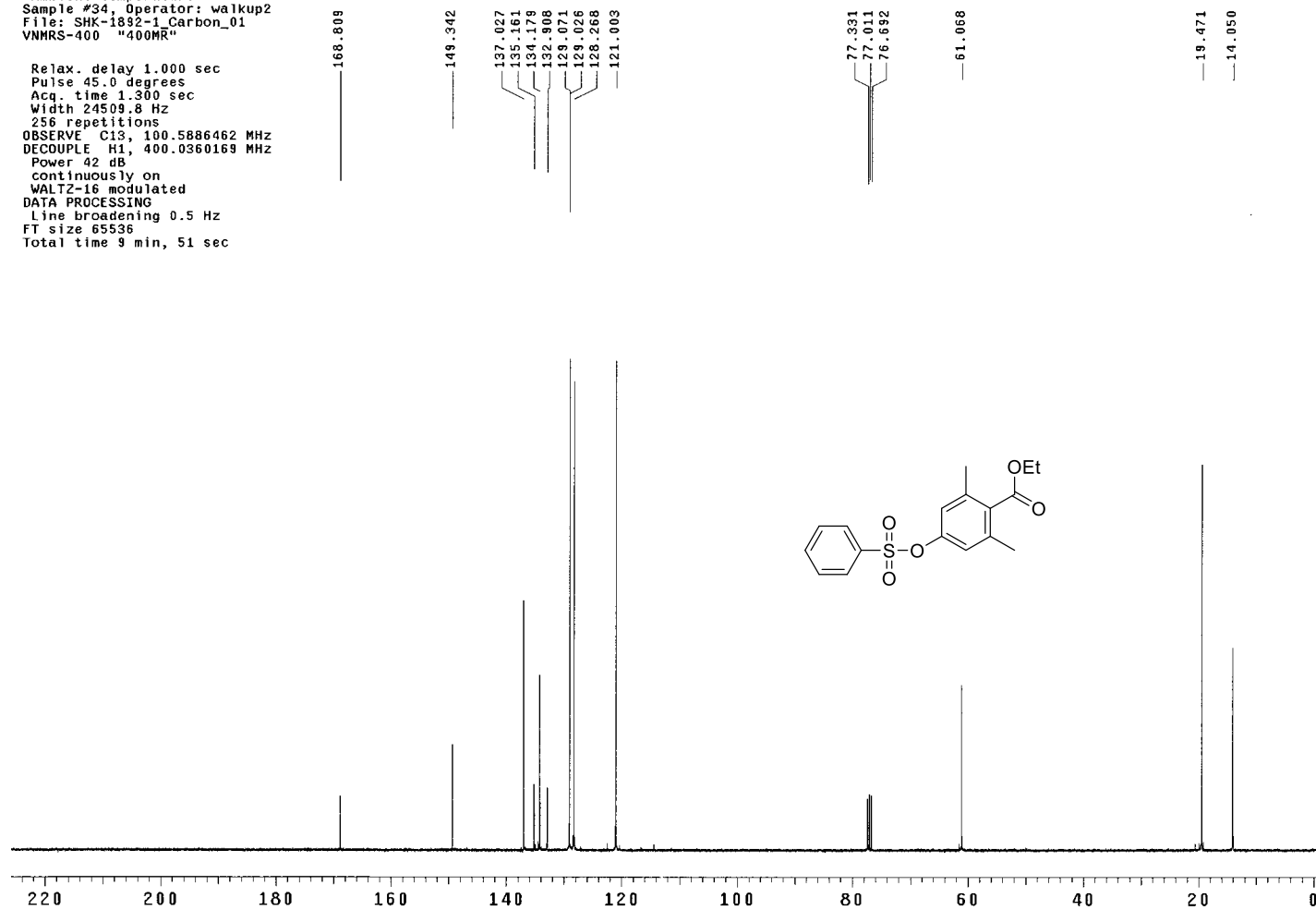


Figure S4. ^{13}C NMR of ethyl 2,6-dimethyl-4-((phenylsulfonyl)oxy)benzoate

Sample: SHK-1884-1
Sample ID: s_41_SHK-1884-1_koo-2_20151007_01
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1884-1_Proton_01.fid

Pulse Sequence: s2pu1
Solvent: cdc13
Ambient temperature
Sample #41, Operator: walkup2
File: SHK-1884-1_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, 400.0340077 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min, 31 sec

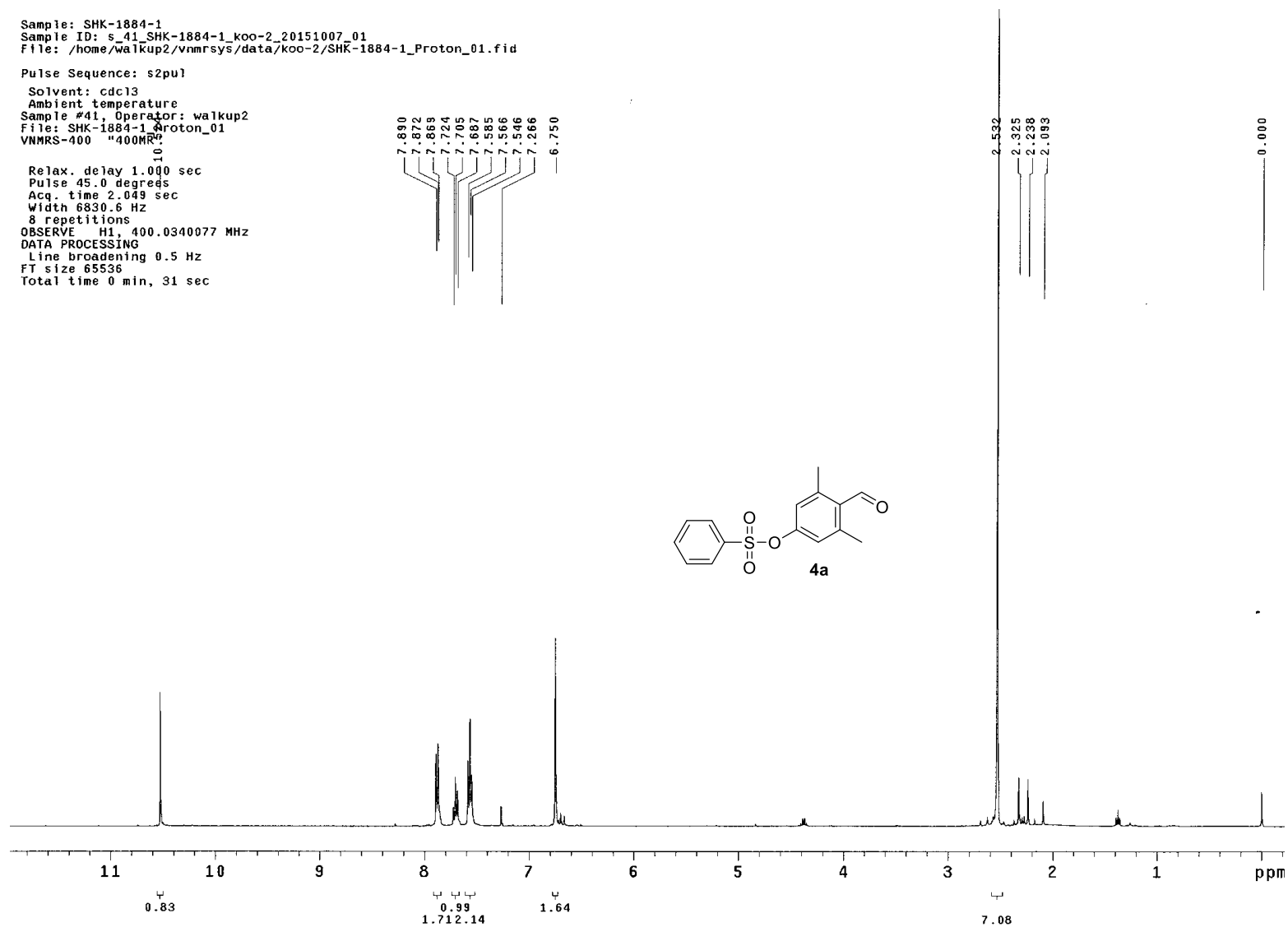


Figure S5. ¹H NMR of 4a

Sample: SHK-1886-1
Sample ID: s_50_SHK-1886-1_koo-2_20151007_01
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1886-1_Carbon_01.fid

Pulse Sequence: s2pu1
Solvent: cdc13
Ambient temperature
Sample #50, Operator: walkup2
File: SHK-1886-1_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, 100.5886442 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

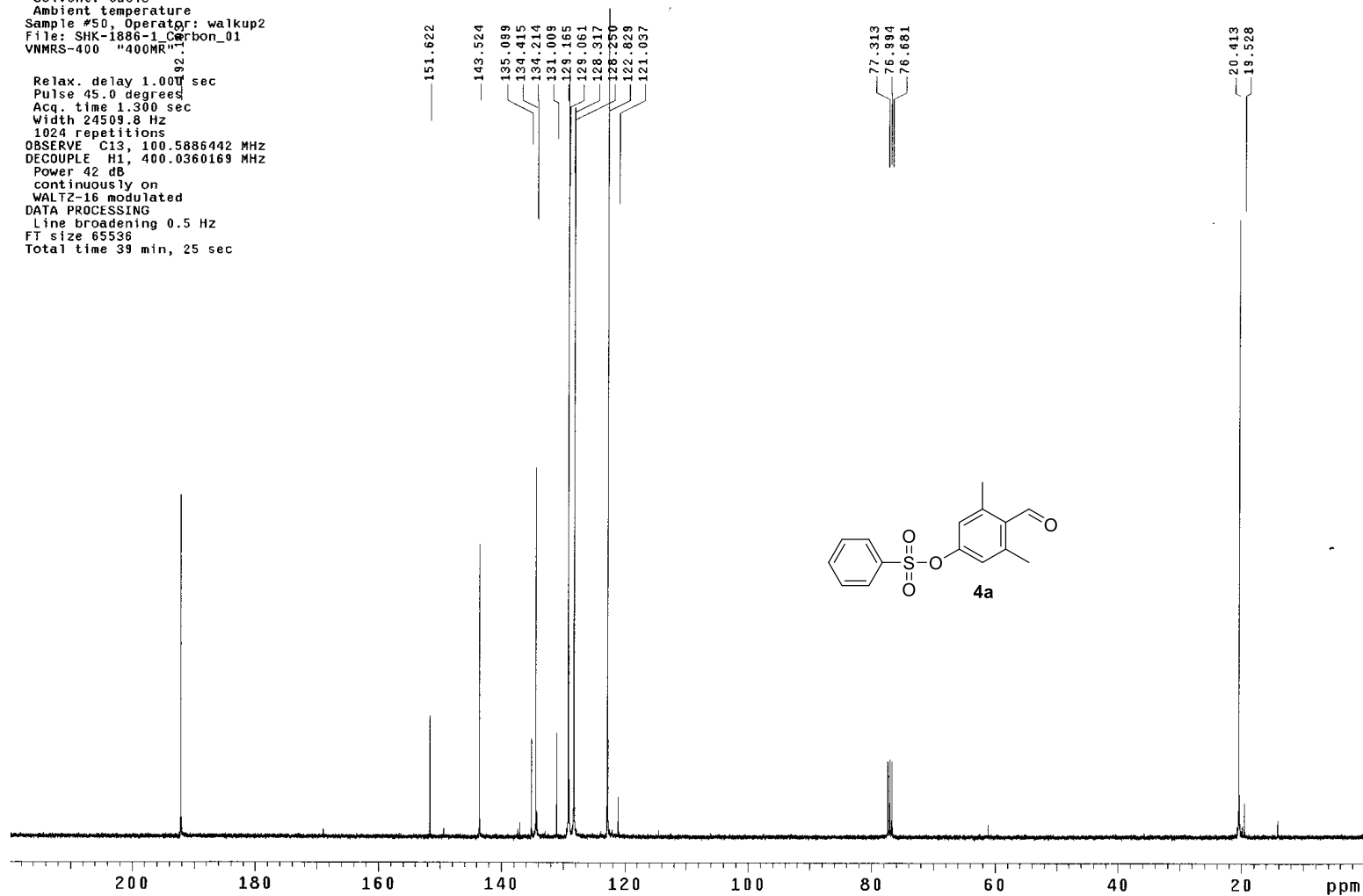


Figure S6. ^{13}C NMR of 4a

Sample: SHK-1886-1
Sample ID: s_49_SHK-1886-1_koo-2_20151007_01
File: /home/walkup2/vnmrSYS/data/koo-2/SHK-1886-1_Proton_01.fid

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

Sample #49, Operator: walkup2

File: SHK-1886-1_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, 400.0340167 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min, 31 sec

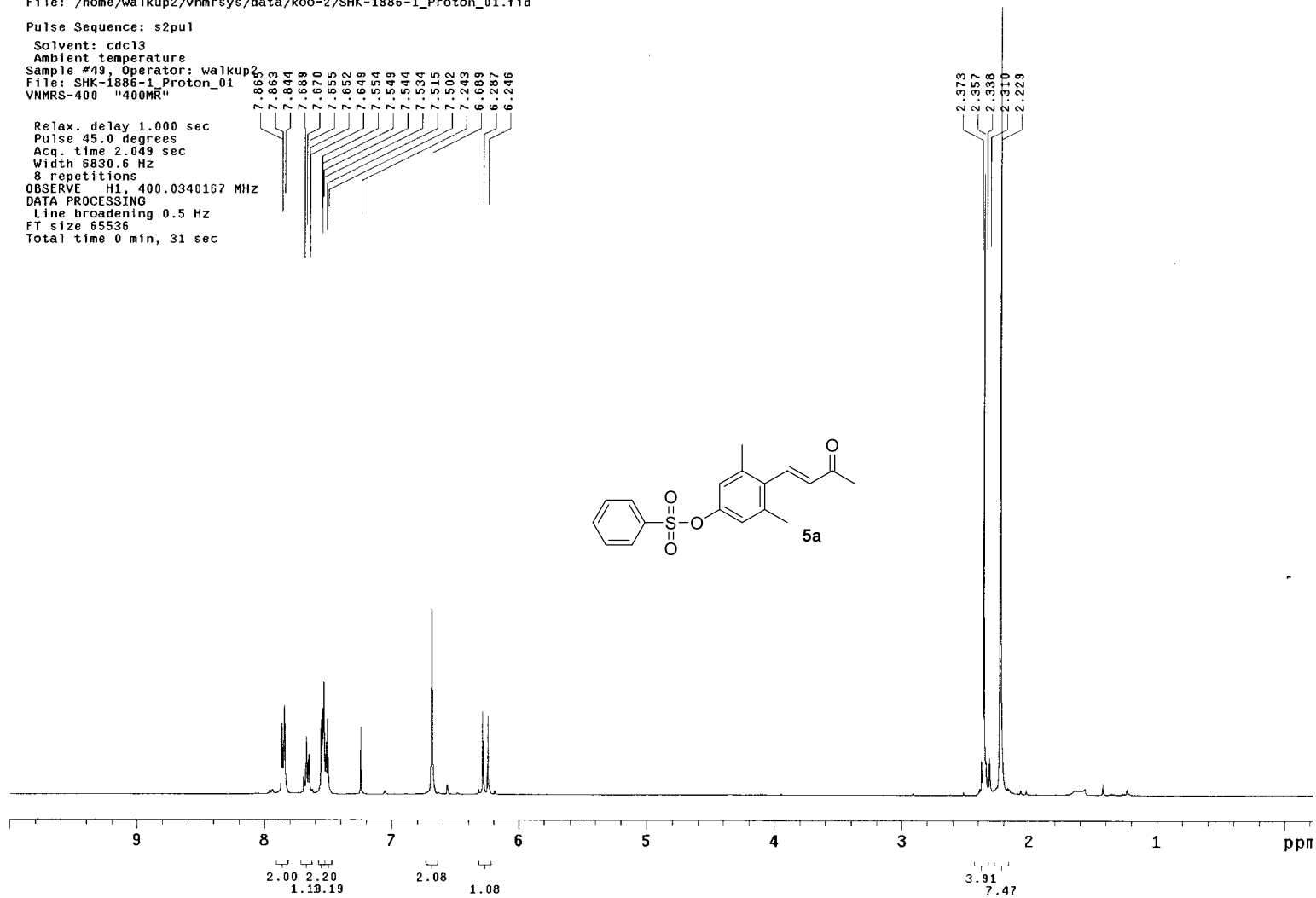


Figure S7. ¹H NMR of 5a

Sample: SHK-1886-1
Sample ID: s_44_SHK-1886-1_koo-2_20151008_01
File: /home/walkup2/vnmrsvs/data/koo-2/SHK-1886-1_Carbon_02.fid

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Sample #44, Operator: walkup2
File: SHK-1886-1_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, 100.5886635 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

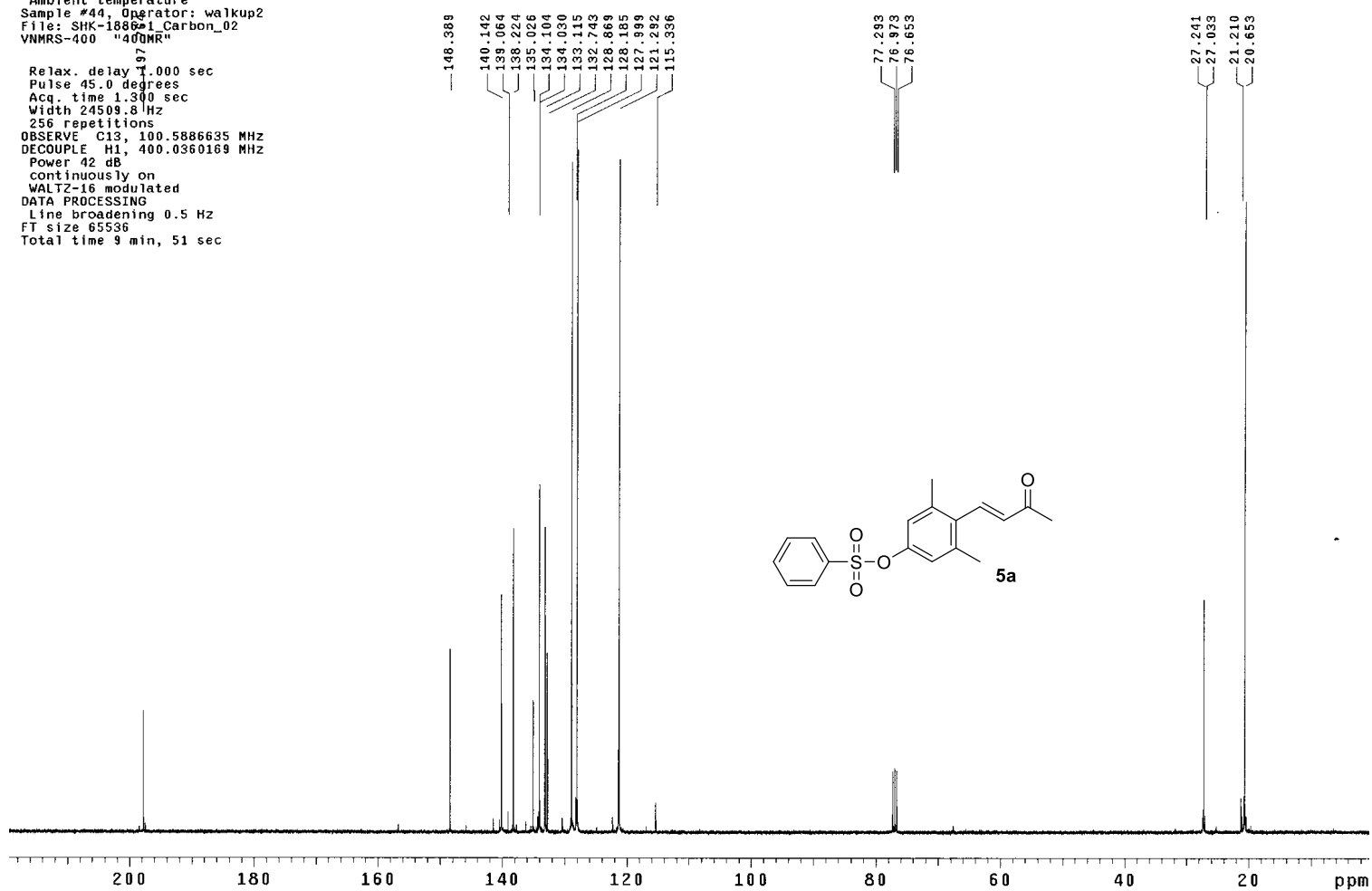


Figure S8. ^{13}C NMR of 5a

Sample Name: SHK-2276
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/1802-kcb-2
 Sample directory: SHK-2276_01
 FidFile: SHK-2276_PROTON_01
 pulse Sequence: PROTON (s2pul)
 solvent: cdcl3
 Date collected on: Mar 1 2018

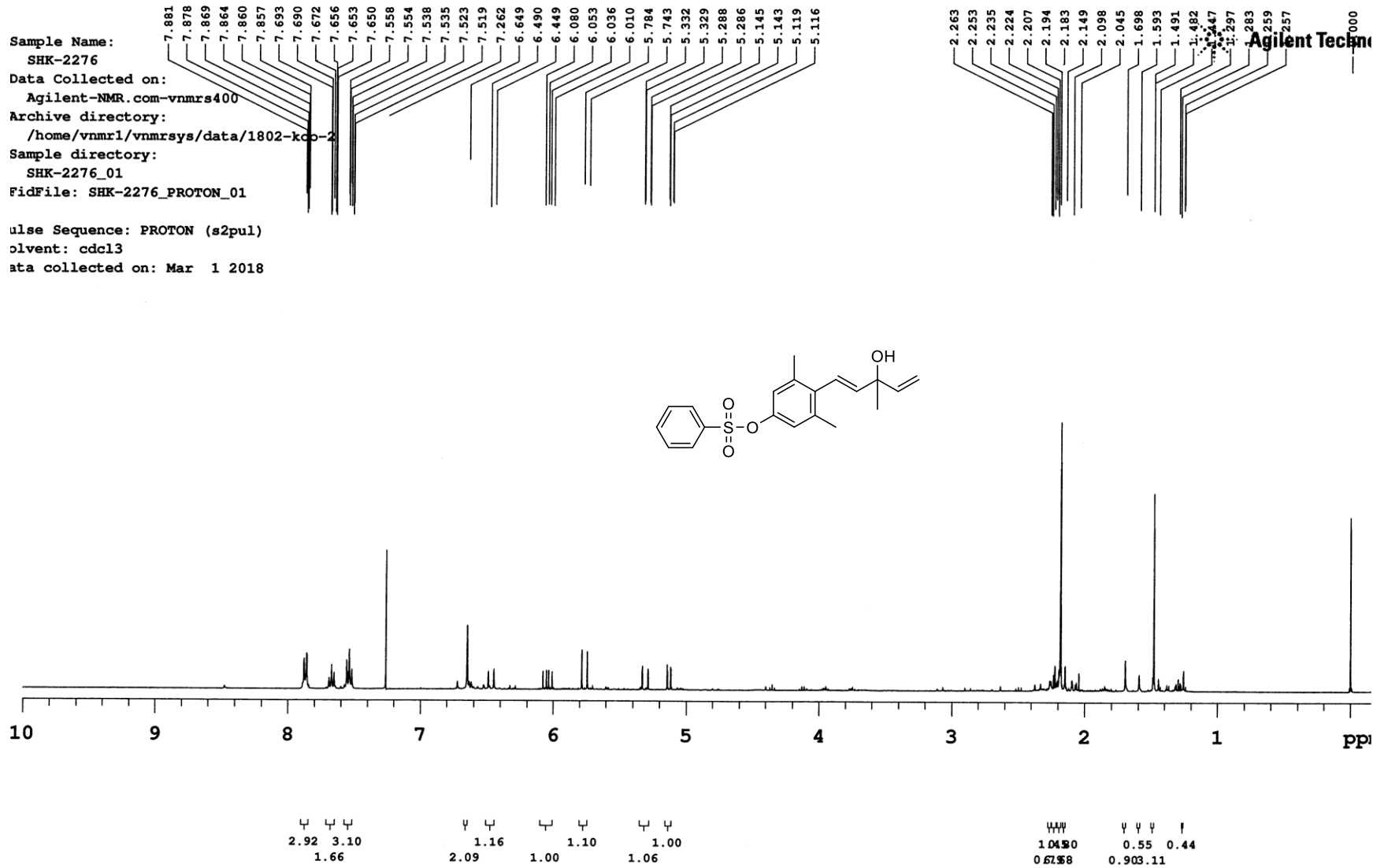


Figure S9. ¹H NMR of (E)-4-(3-hydroxy-3-methylpenta-1,4-dien-1-yl)-3,5-dimethylphenyl benzenesulfonate

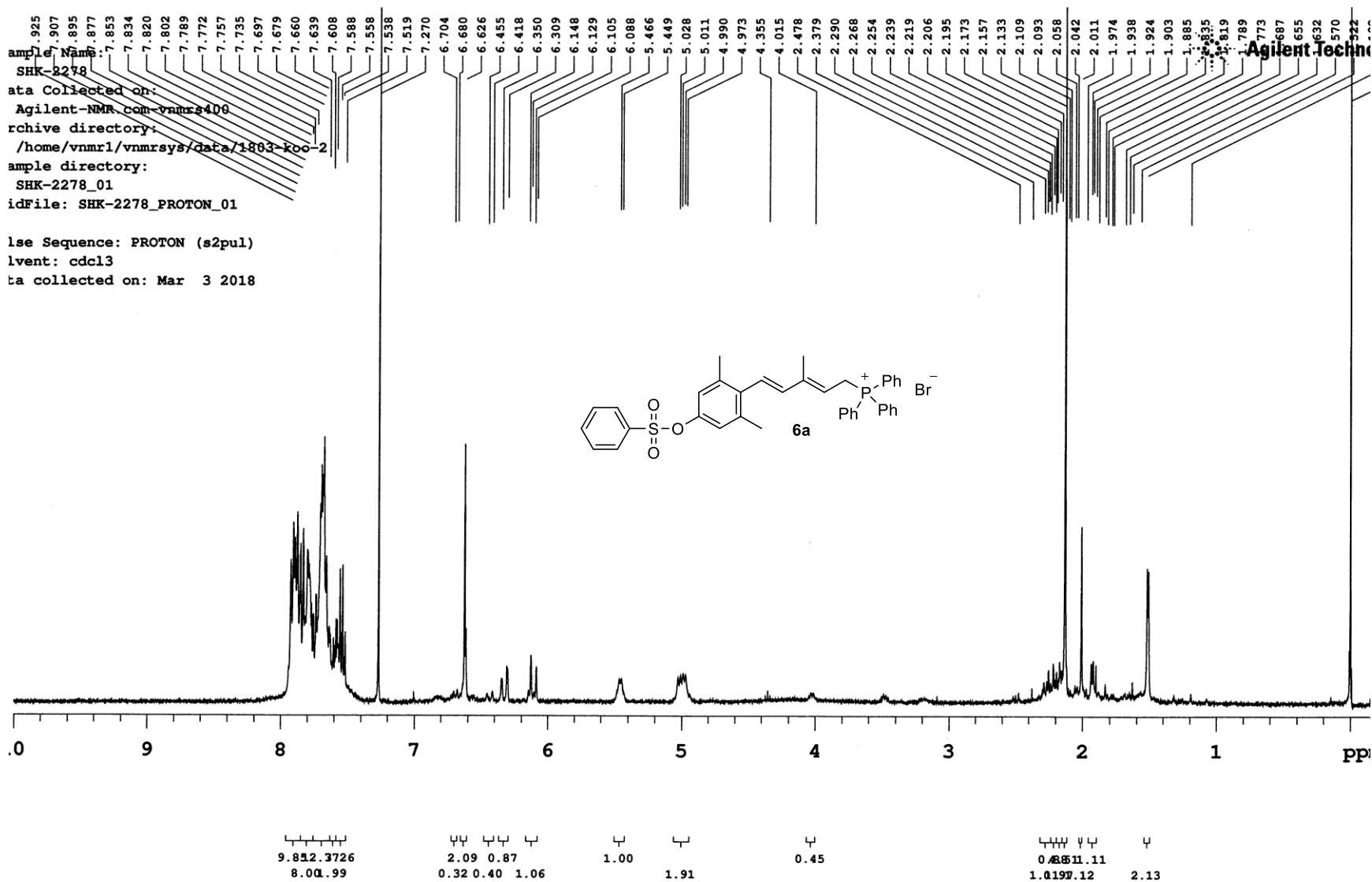


Figure S10. ¹H NMR of **6a**

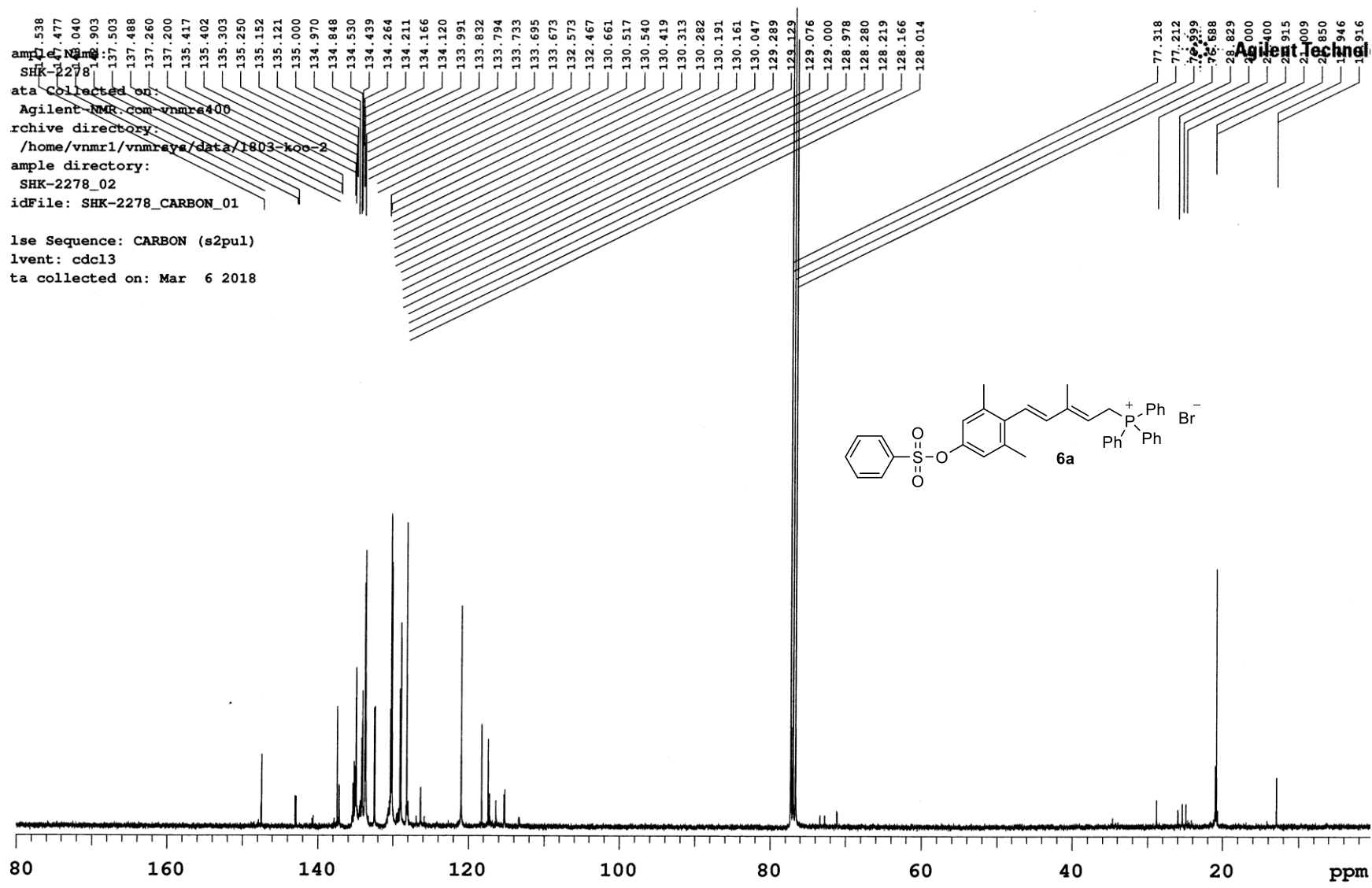


Figure S11. ¹³C NMR of **6a**

Sample: SHK-1908-2-2
 Sample ID: s_43_SHK-1908-2-2_koo-2_20151110_01
 File: /home/walkup2/vnmrsys/data/koo-2/SHK-1908-2-2_Proton_01.fid

Pulse Sequence: s2pu1
 Solvent: cdc13
 Ambient temperature
 Sample #43, Operator: walkup2
 File: SHK-1908-2-2_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, 400.0340089 MHz
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 0 min, 31 sec

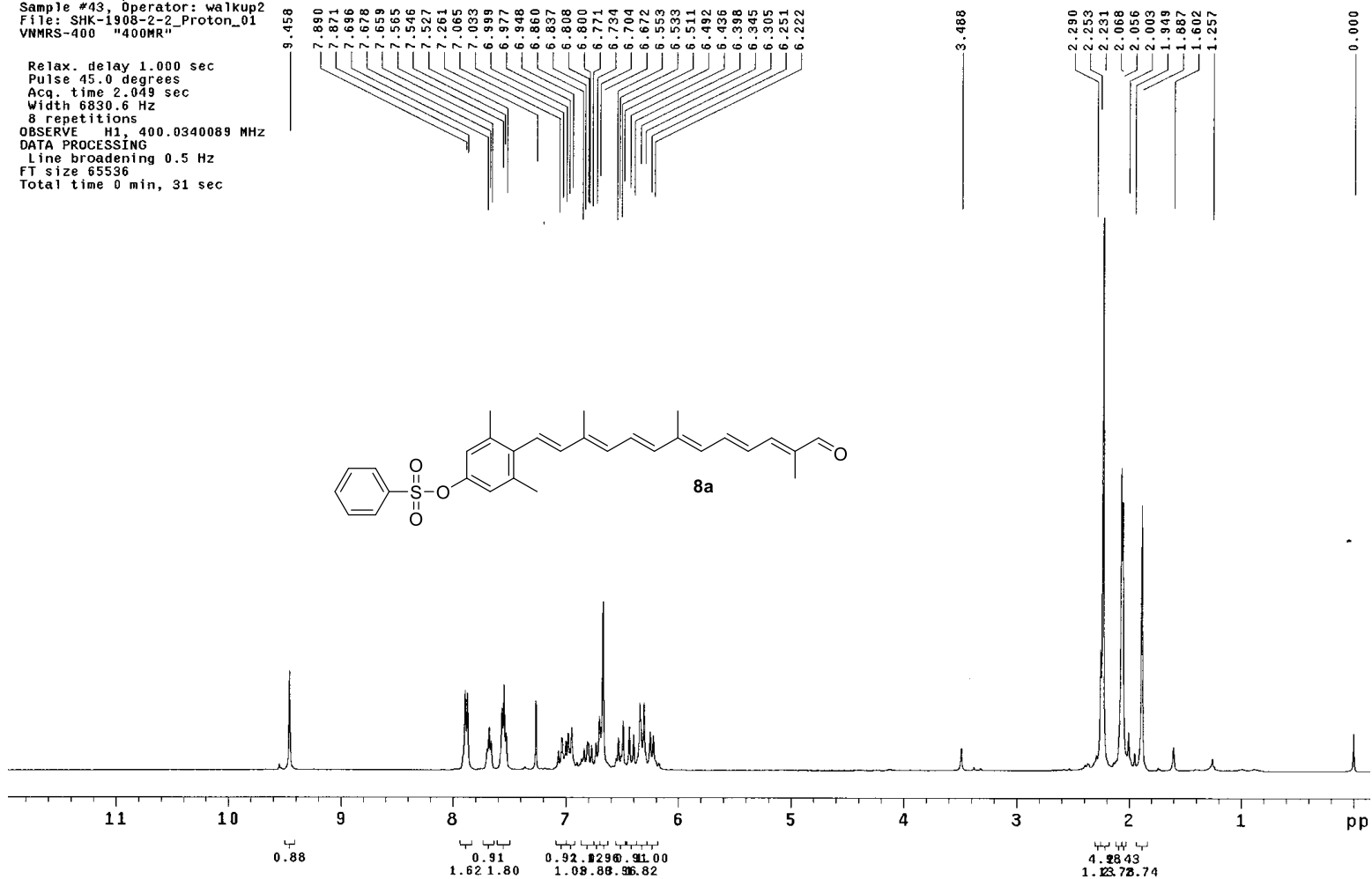


Figure S12. ¹H NMR of **8a**

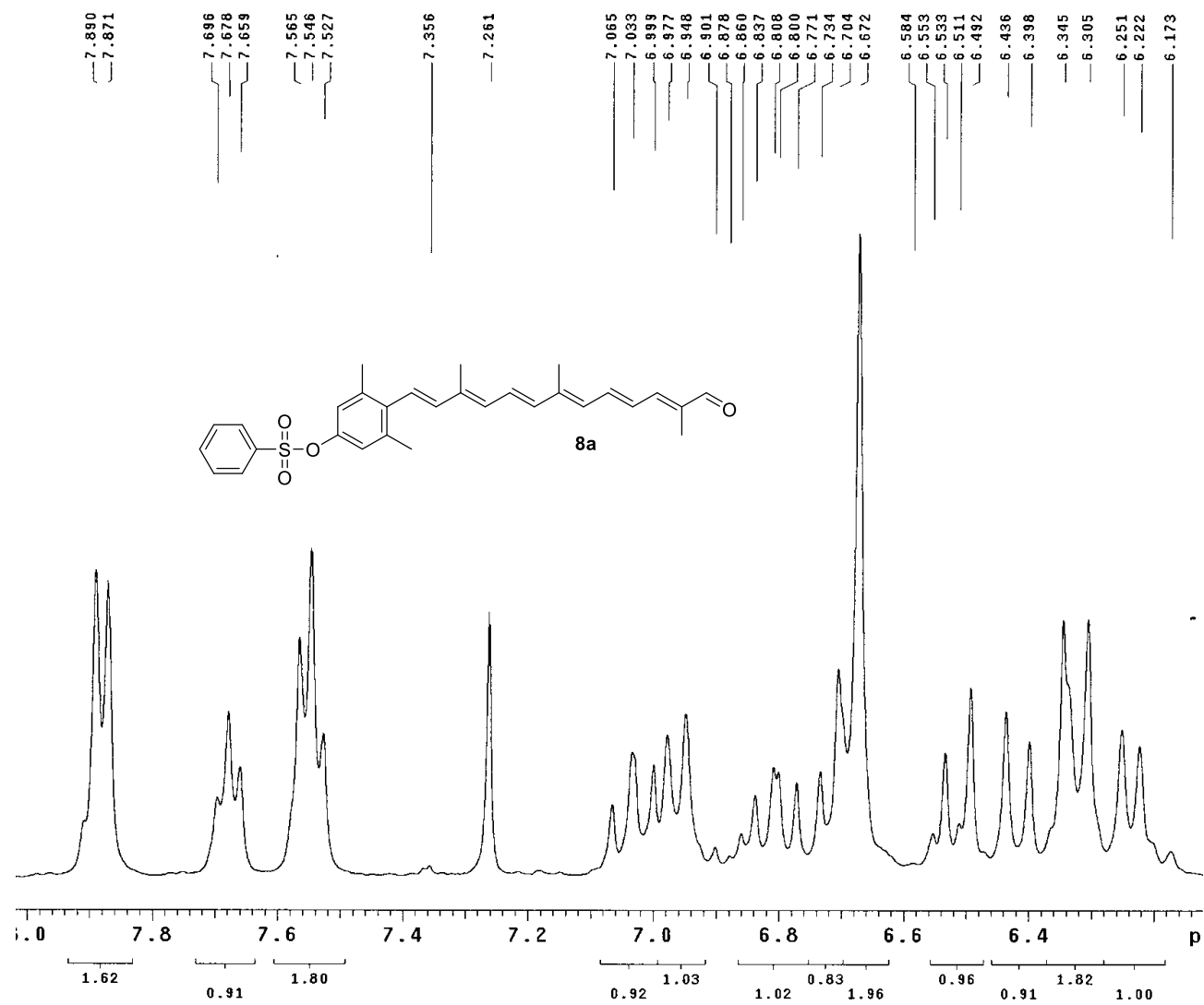


Figure S13. ¹H NMR of **8a** (expansion plot)

Sample: SHK-1908-2-2
Sample ID: s_36_SHK-1908-2-2_koo-2_20151110_01
File: /home/walkup2/vnmrsys/data/koo-2/SHK-1908-2-2_Carbon_01.fid

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #36, Operator: walkup2
File: SHK-1908-2-2_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, 100.5886386 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

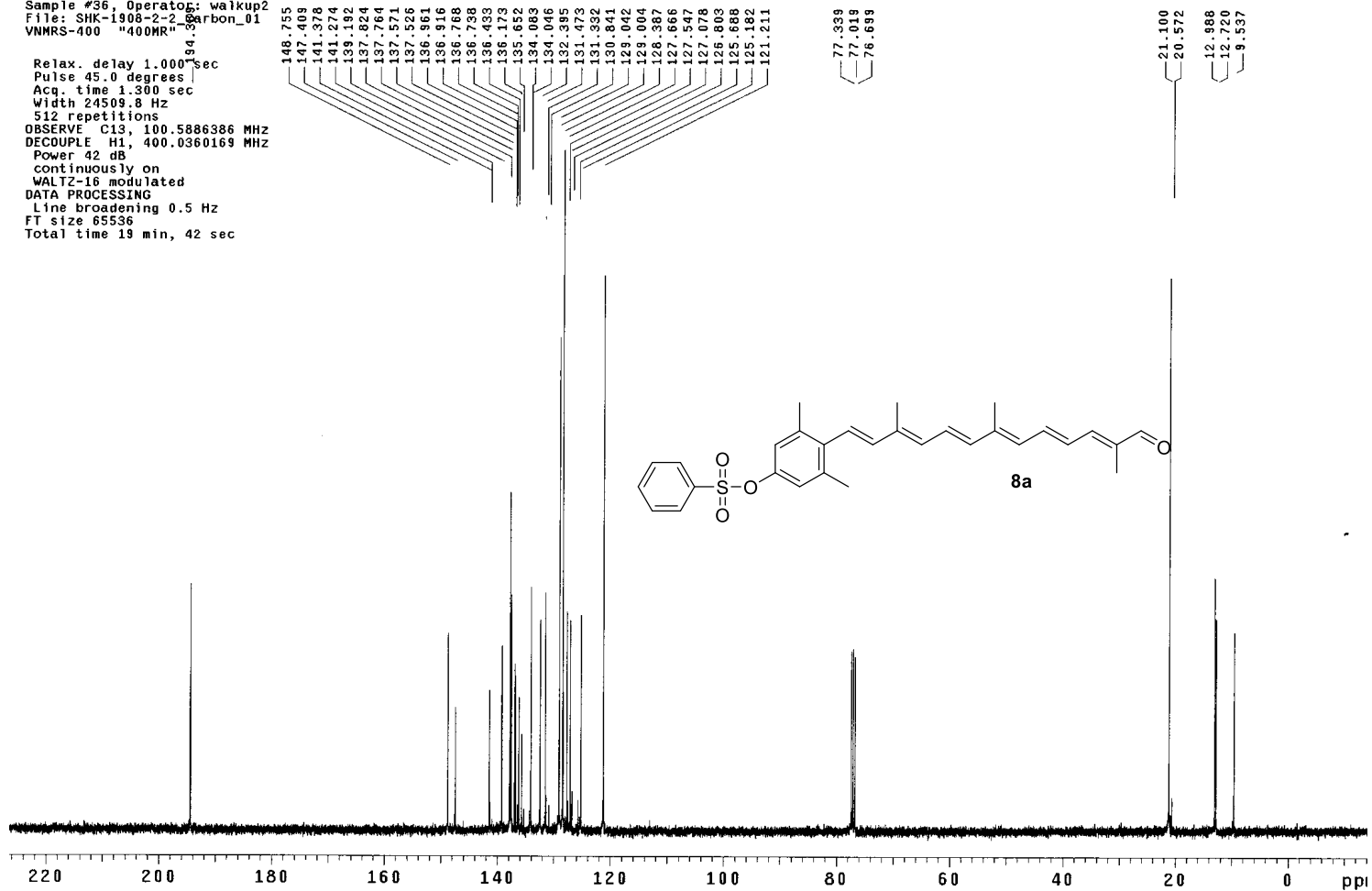


Figure S14. ¹³C NMR of 8a

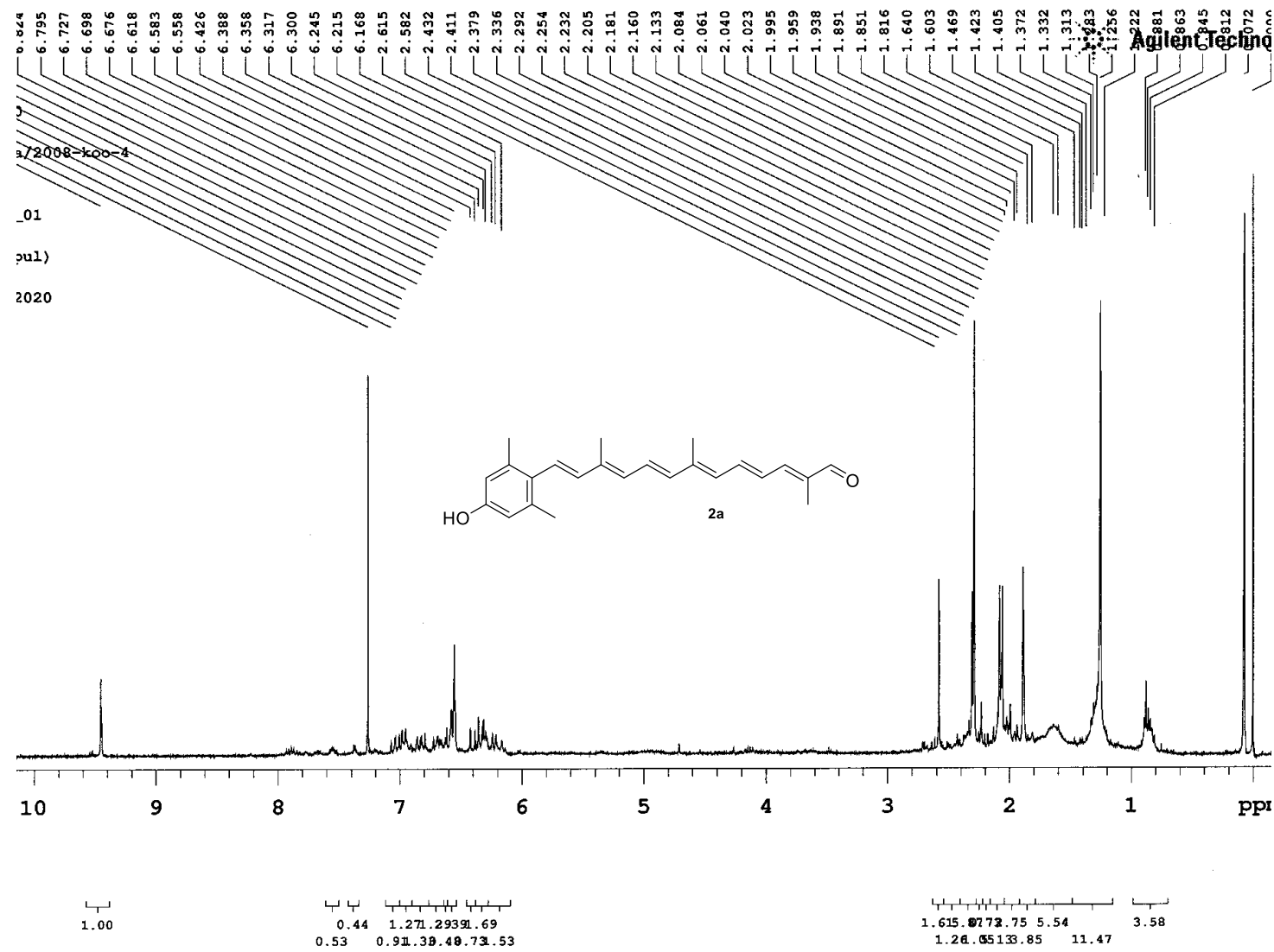


Figure S15. ¹H NMR of 2a

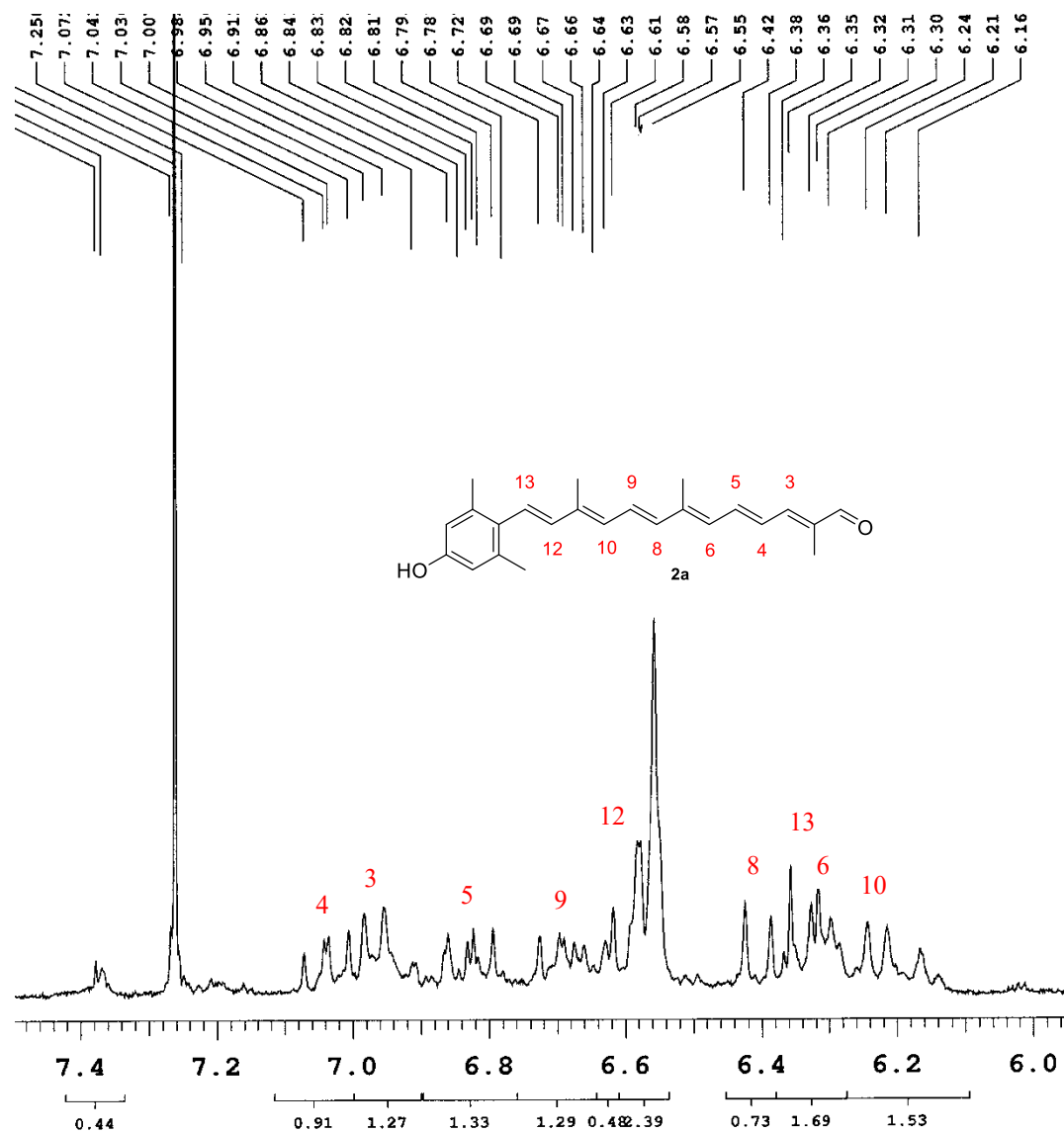


Figure S16. ¹H NMR of **2a** (expansion plot)

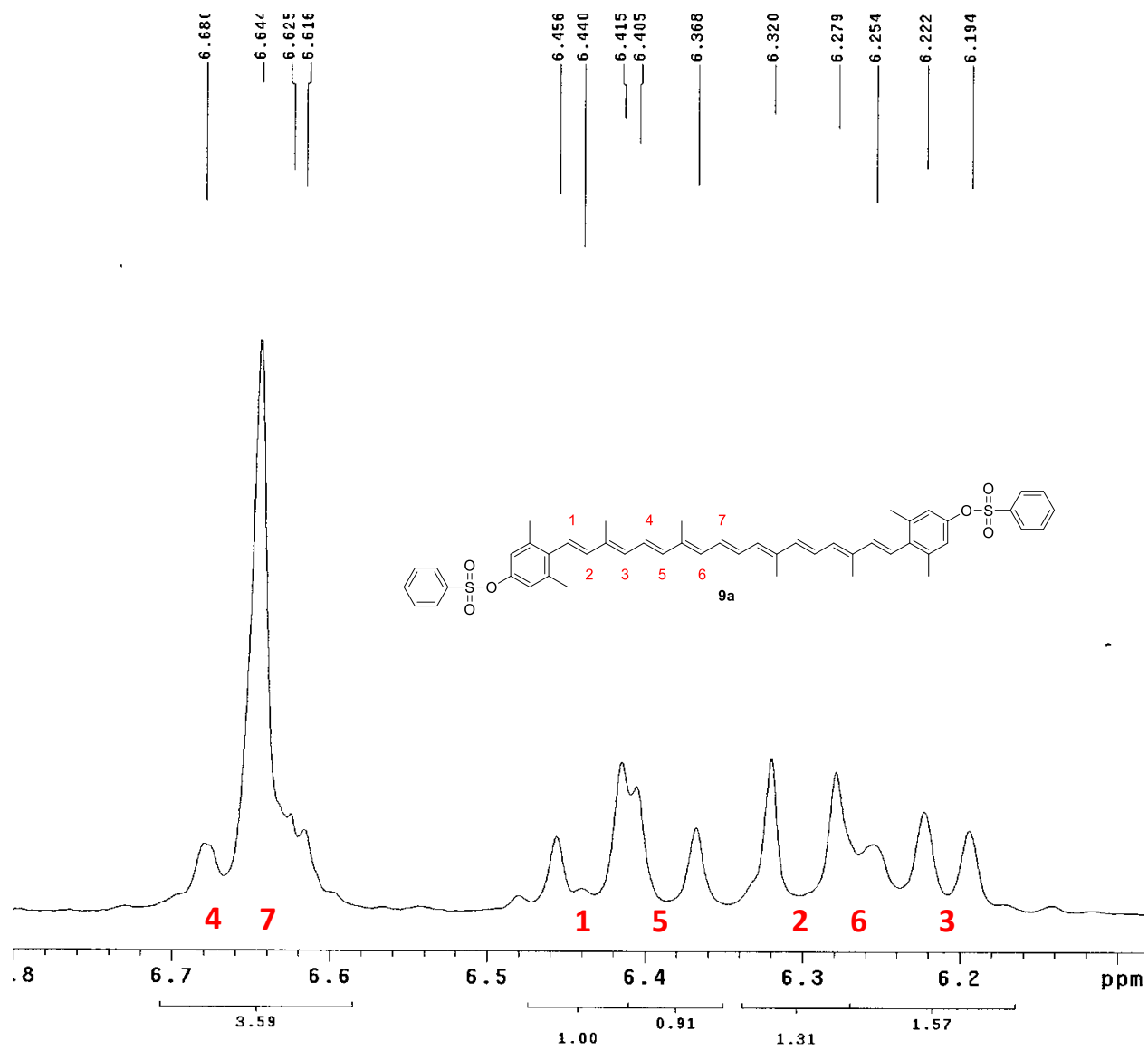


Figure S18. ¹H NMR of **9a** (expansion plot)

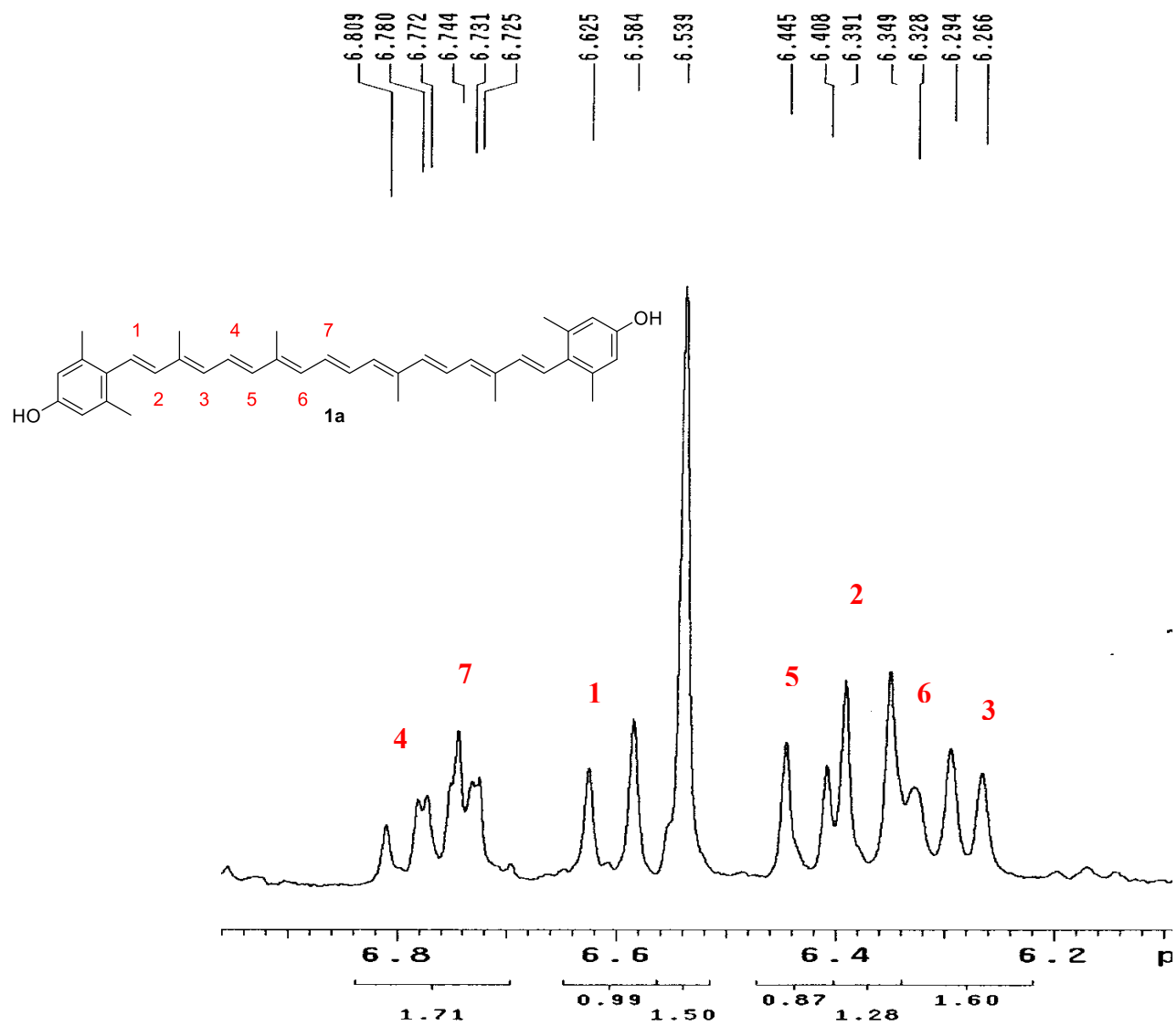


Figure S22. ^1H NMR of **1a** (expansion plot)

853
 850
 845
 836
 7.831
 7.828
 7.714
 7.711
 7.708
 7.696
 7.682
 7.687
 7.677
 7.673
 7.670
 7.568
 7.564
 7.559
 7.544
 7.539
 7.525
 7.521
 7.487
 7.480
 7.474
 7.462
 7.459
 7.452
 7.422
 7.293
 7.037
 7.030
 7.025
 7.014
 7.009
 7.002
 6.666
 6.625

Sample Name: SGS-787-1
 Data Collected on: Agilent-NMR, non-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2005-koo
 Sample directory: SGS-787-1_01
 Fidfile: SGS-787-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: May 7 2020

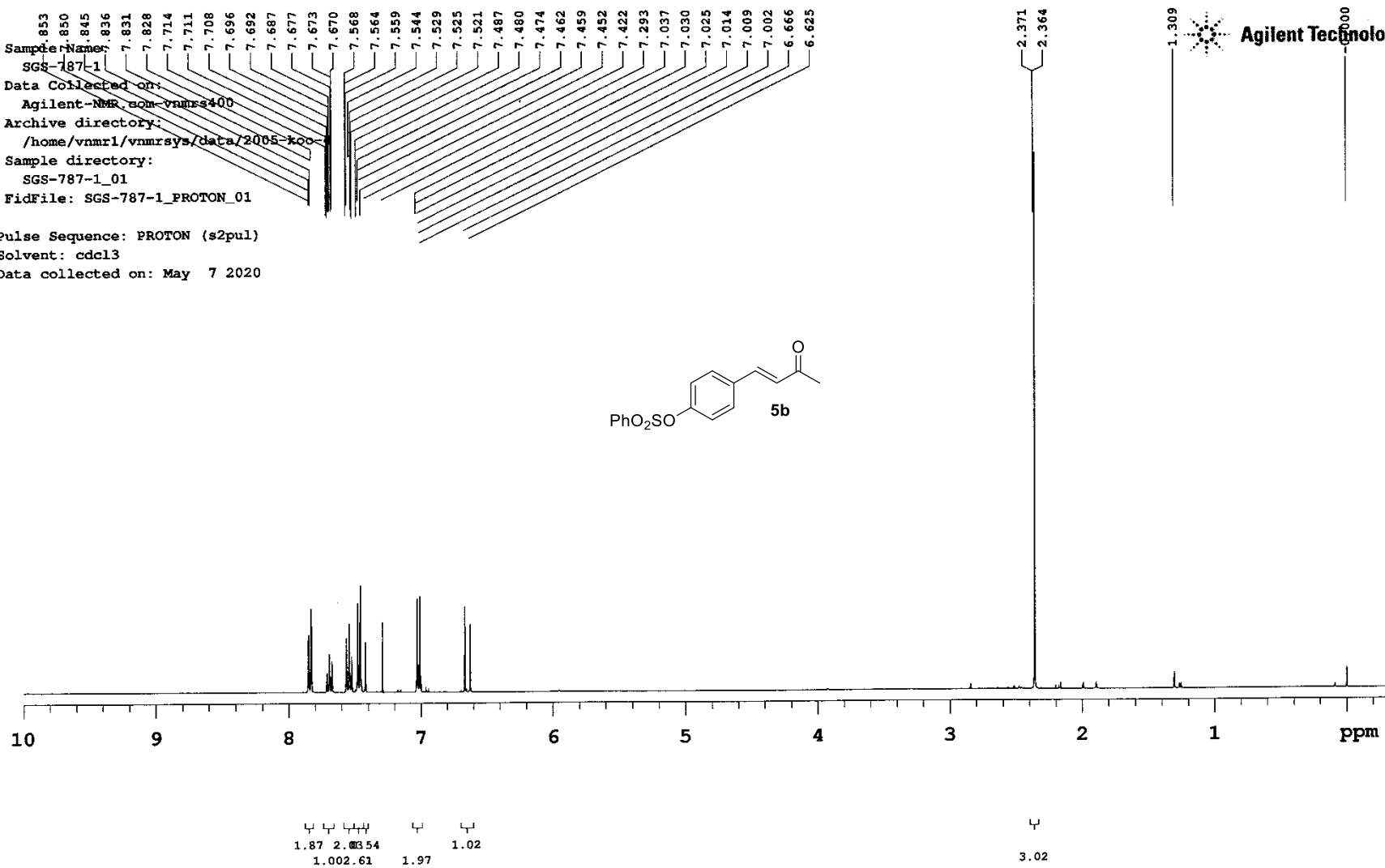


Figure S24. ¹H NMR of **5b**

Sample Name:
SGS-787-1
Data Collected on:
Agilent-NMR.com vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2005-koo-4
Sample directory:
SGS-787-1_02
FidFile: SGS-787-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 8 2020

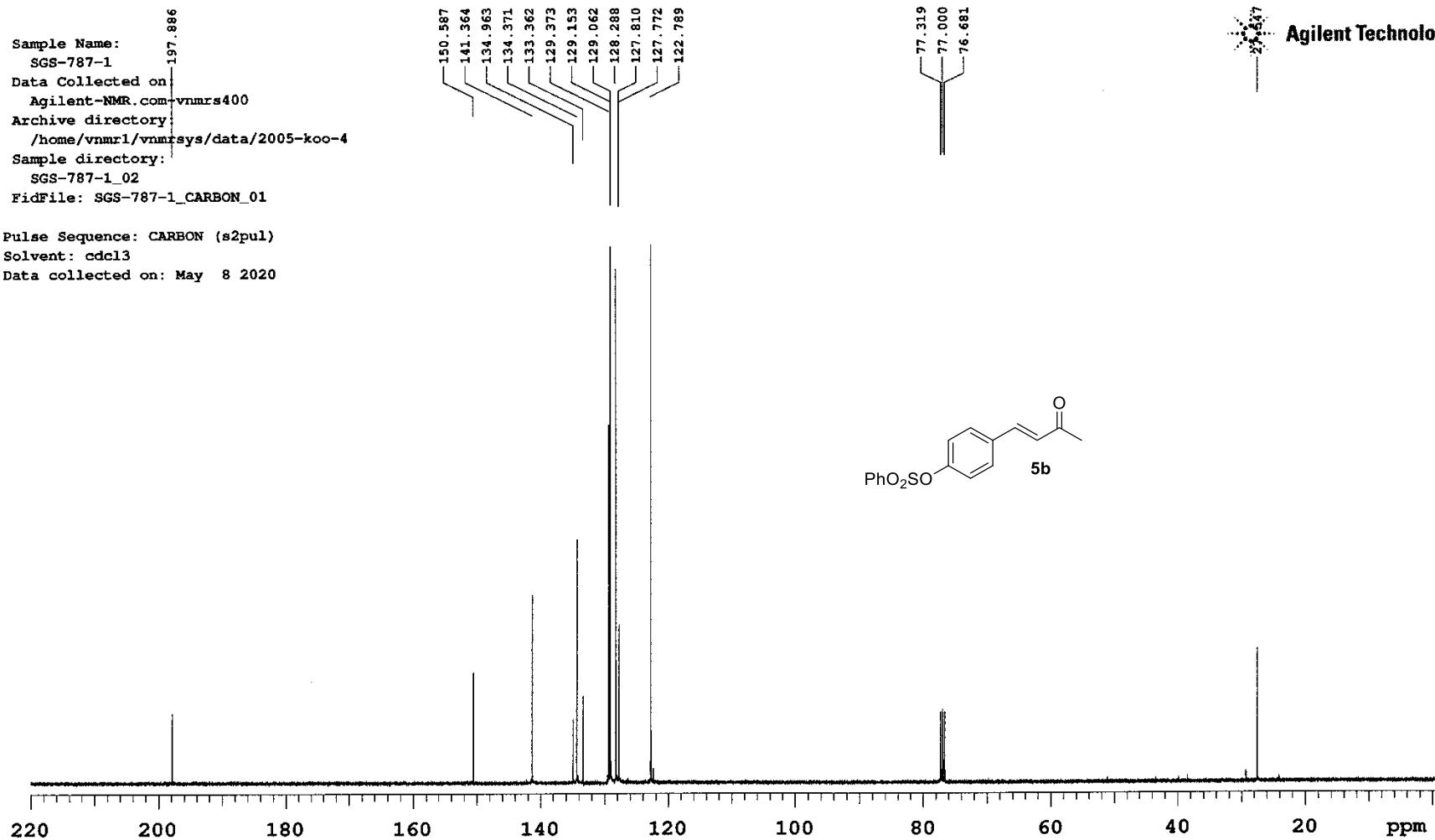


Figure S25. ^{13}C NMR of **5b**

Sample Name: SGS-791-C
 Data Collected on: Agilent-NMR.com-vmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2005-koo-4
 Sample directory: SGS-791-C_01
 FidFile: SGS-791-C_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: May 7 2020

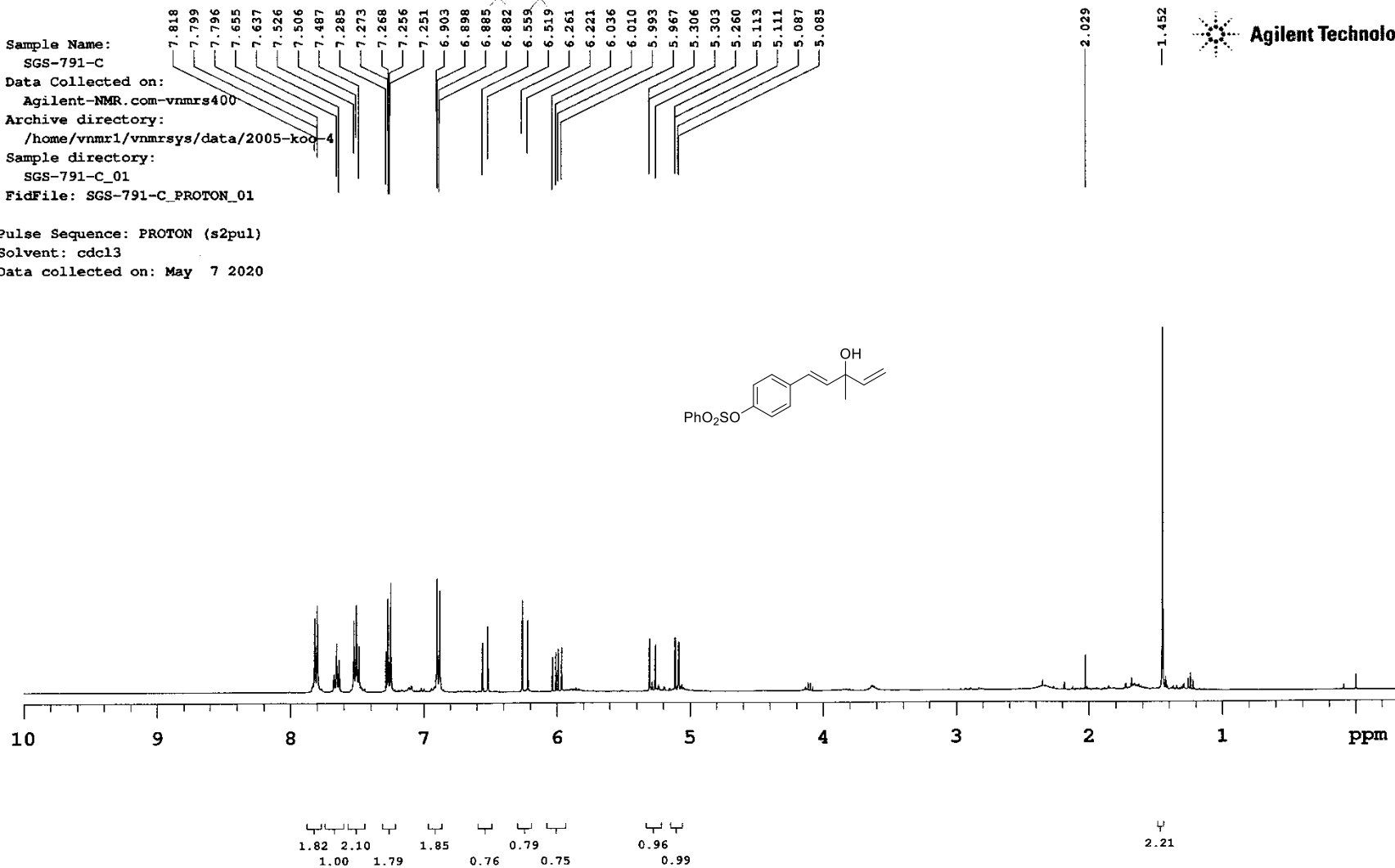


Figure S26. ¹H NMR of (E)-4-(3-hydroxy-3-methylpenta-1,4-dien-1-yl)phenyl benzenesulfonate

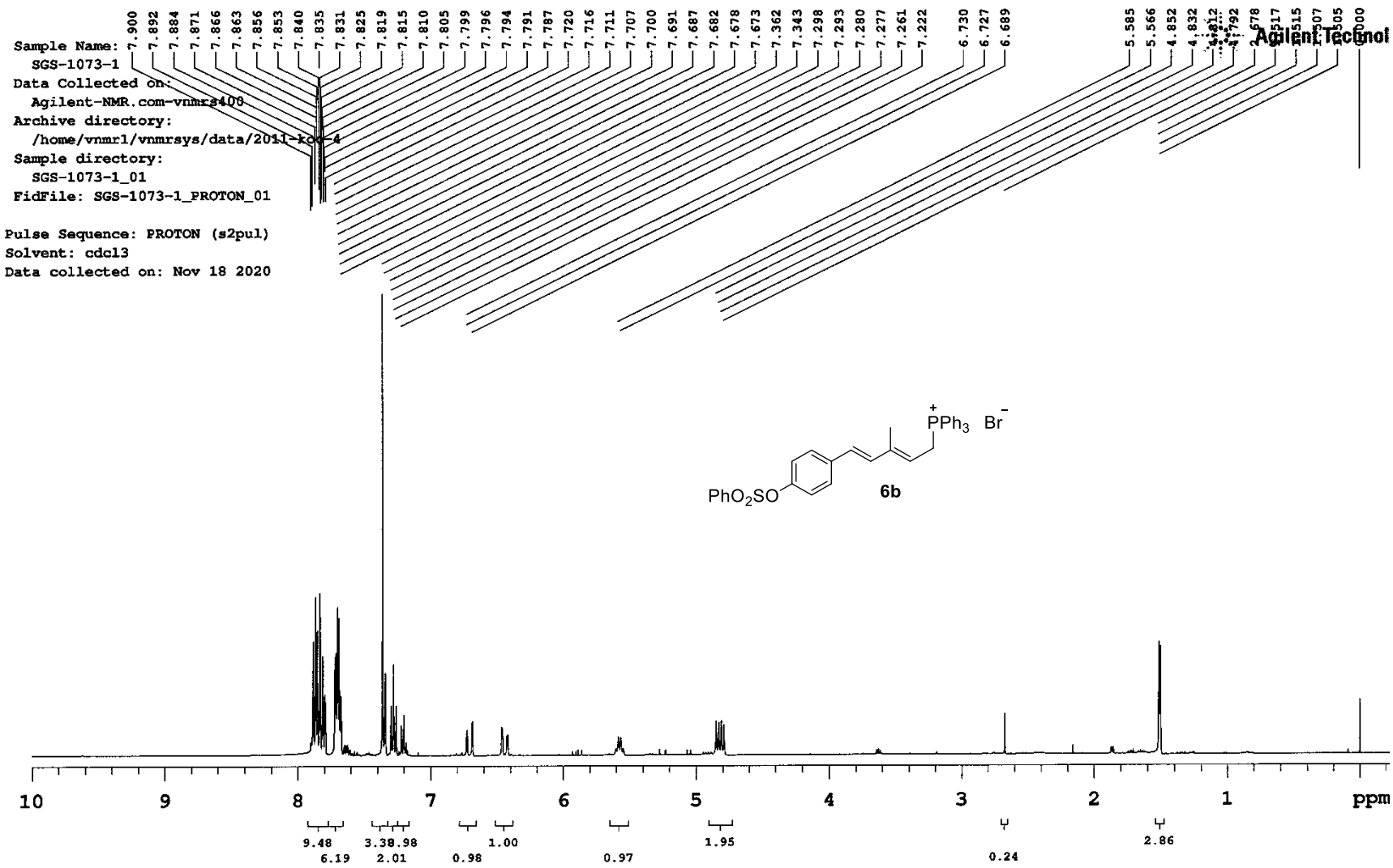


Figure S27. ¹H NMR of **6b**

854
 845
 843
 830
 7.825
 7.822
 7.685
 7.667
 7.647
 7.644
 7.543
 7.523
 7.507
 7.504
 7.333
 7.328
 7.317
 7.312
 7.266
 7.061
 7.031
 7.025
 6.995
 6.975
 6.946
 6.932
 6.927
 6.915
 6.910
 6.831
 6.822
 6.792
 6.785
 6.755
 6.733
 6.704
 6.697
 6.557
 6.517
 6.447
 6.410
 6.346
 6.316

Sample Name: SGS-820-S1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2005-kob-4
 Sample directory: SGS-820-S1_01
 FidFile: SGS-820-S1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: May 26 2020

2.044
 2.028
 1.885
 Agilent Technology
 0.000

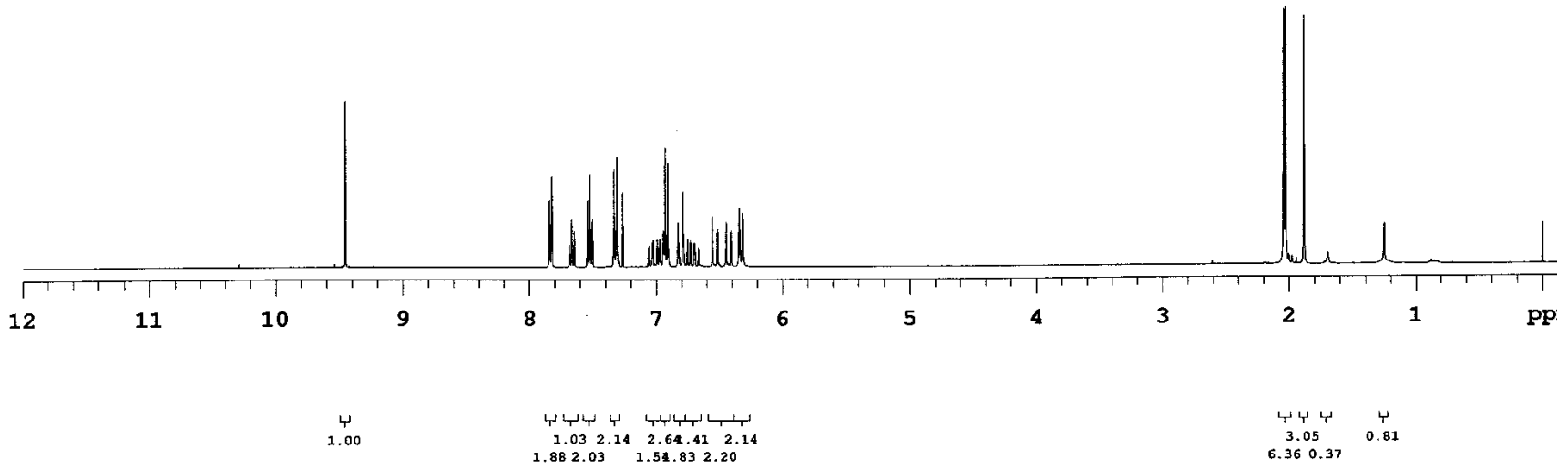
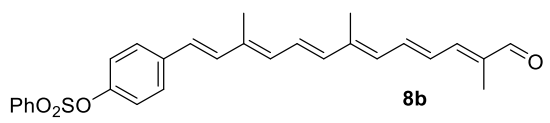


Figure S28. ¹H NMR of 8b

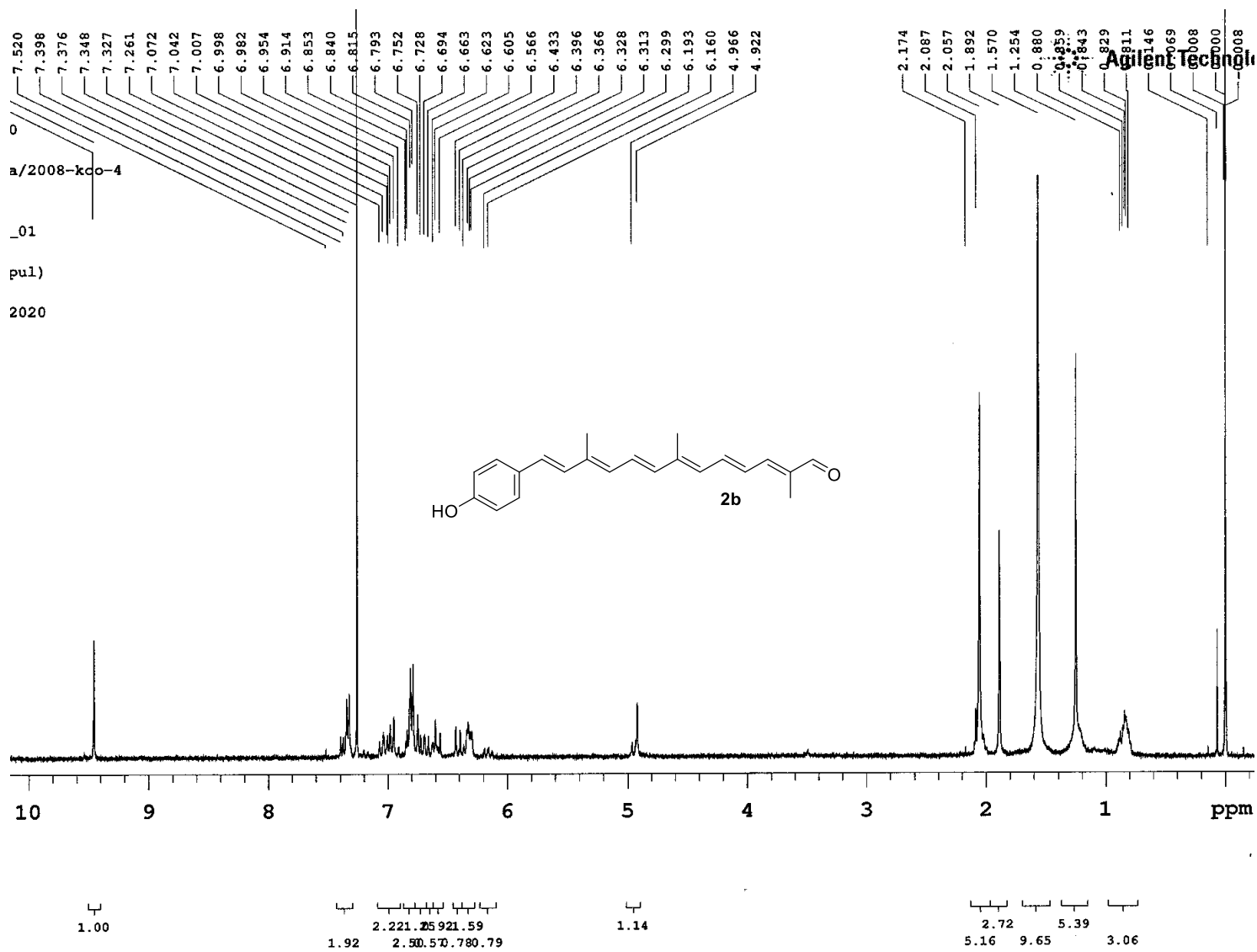


Figure S31. ^1H NMR of **2b**

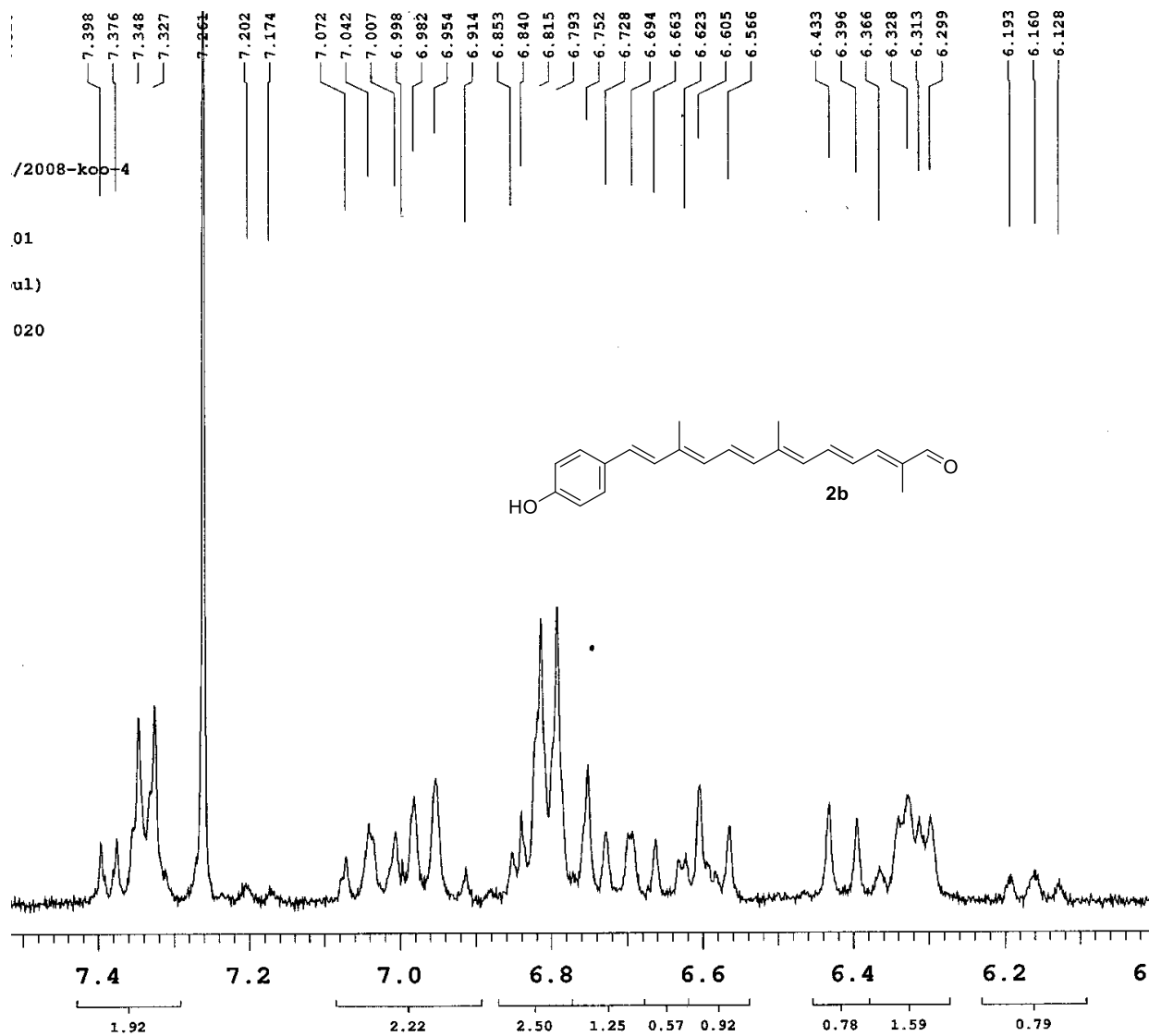


Figure S32. ^1H NMR of **2b** (expansion plot)

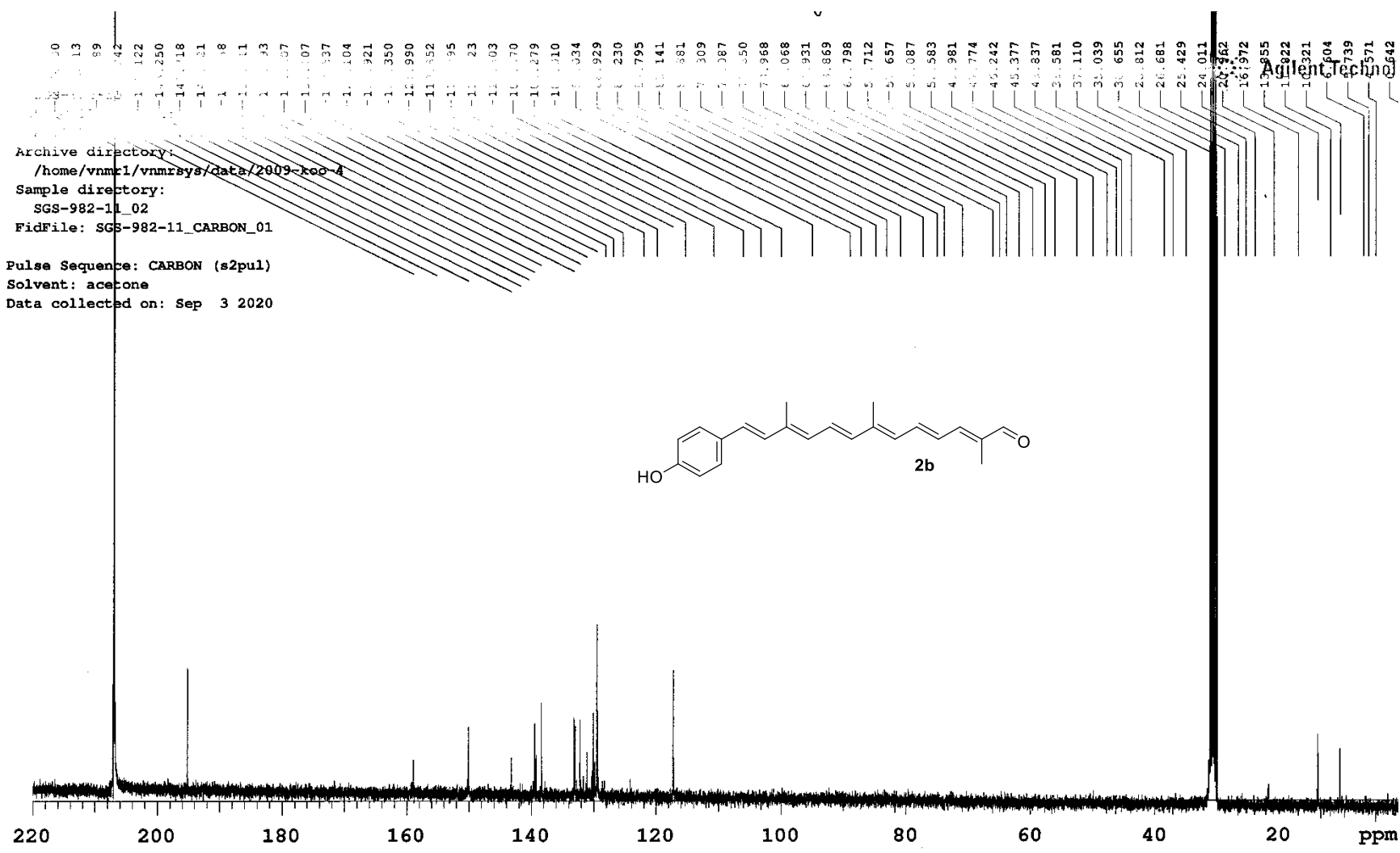


Figure S33. ¹³C NMR of **2b**

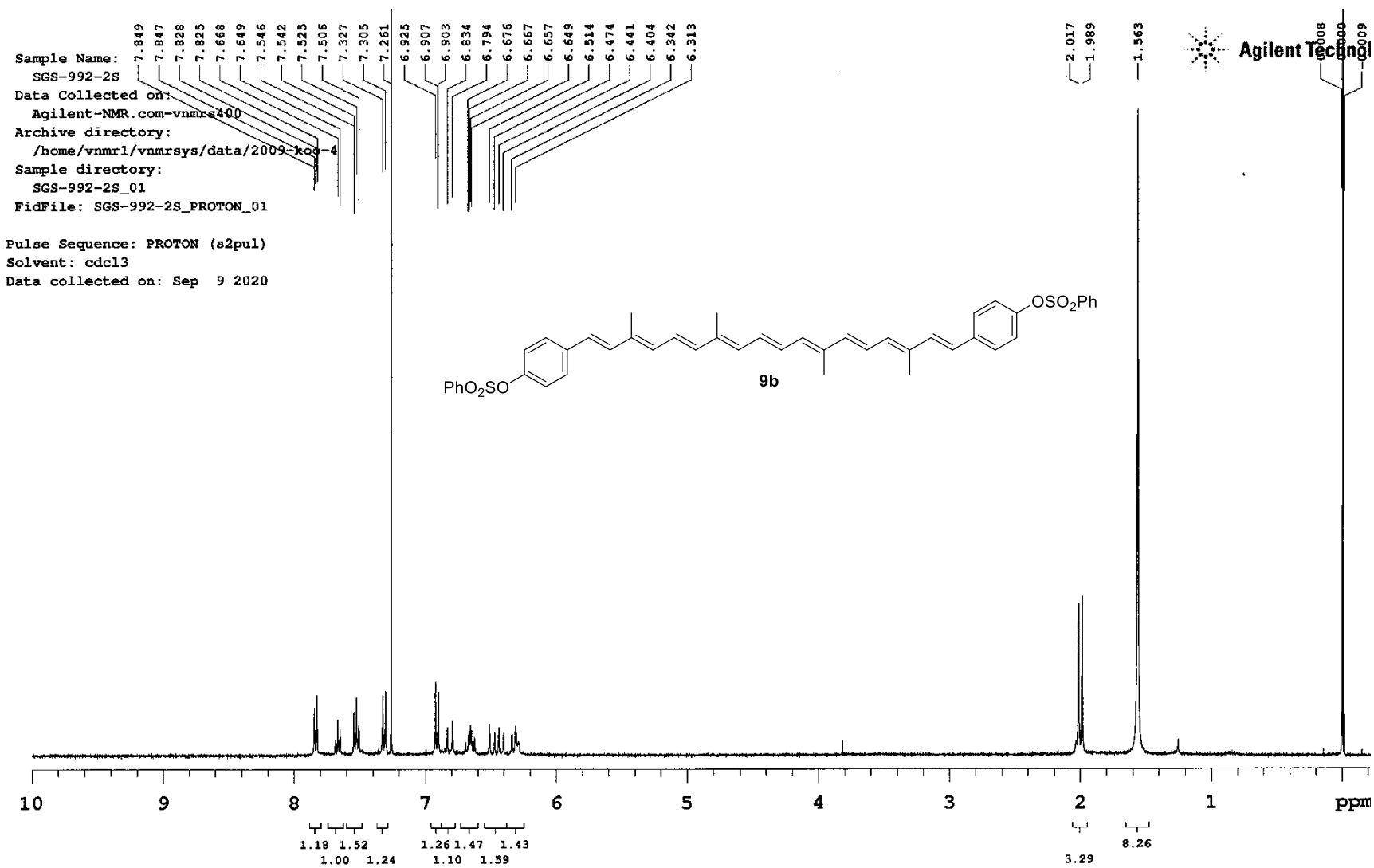


Figure S34. ^1H NMR of **9b**

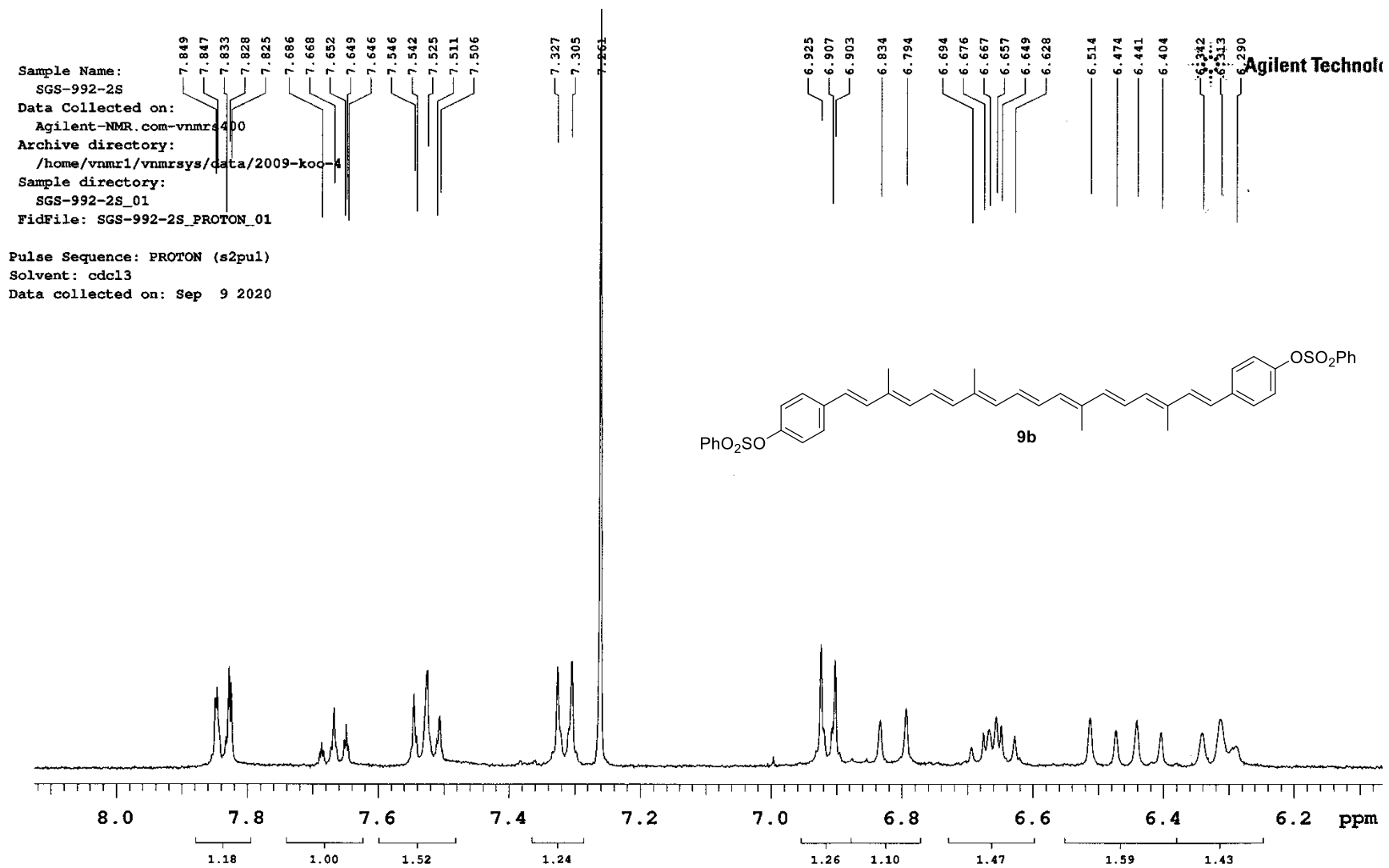


Figure S35. ^1H NMR of **9b** (expansion plot)

Sample Name:
 SGS-820-22
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:

Sample directory:

FidFile: CARBON

ulse Sequence: CARBON (s2pul)
 olvent: cdcl3
 ata collected on: Jun 12 2020

148.327
 138.717
 136.950
 136.647
 135.137
 134.675
 134.182
 133.909
 133.347
 130.427
 129.107
 128.538
 127.204
 125.709
 124.875
 122.562

77.319
 77.000
 76.682

25.854
 Agilent Technolo
 12.848
 12.810
 6.015

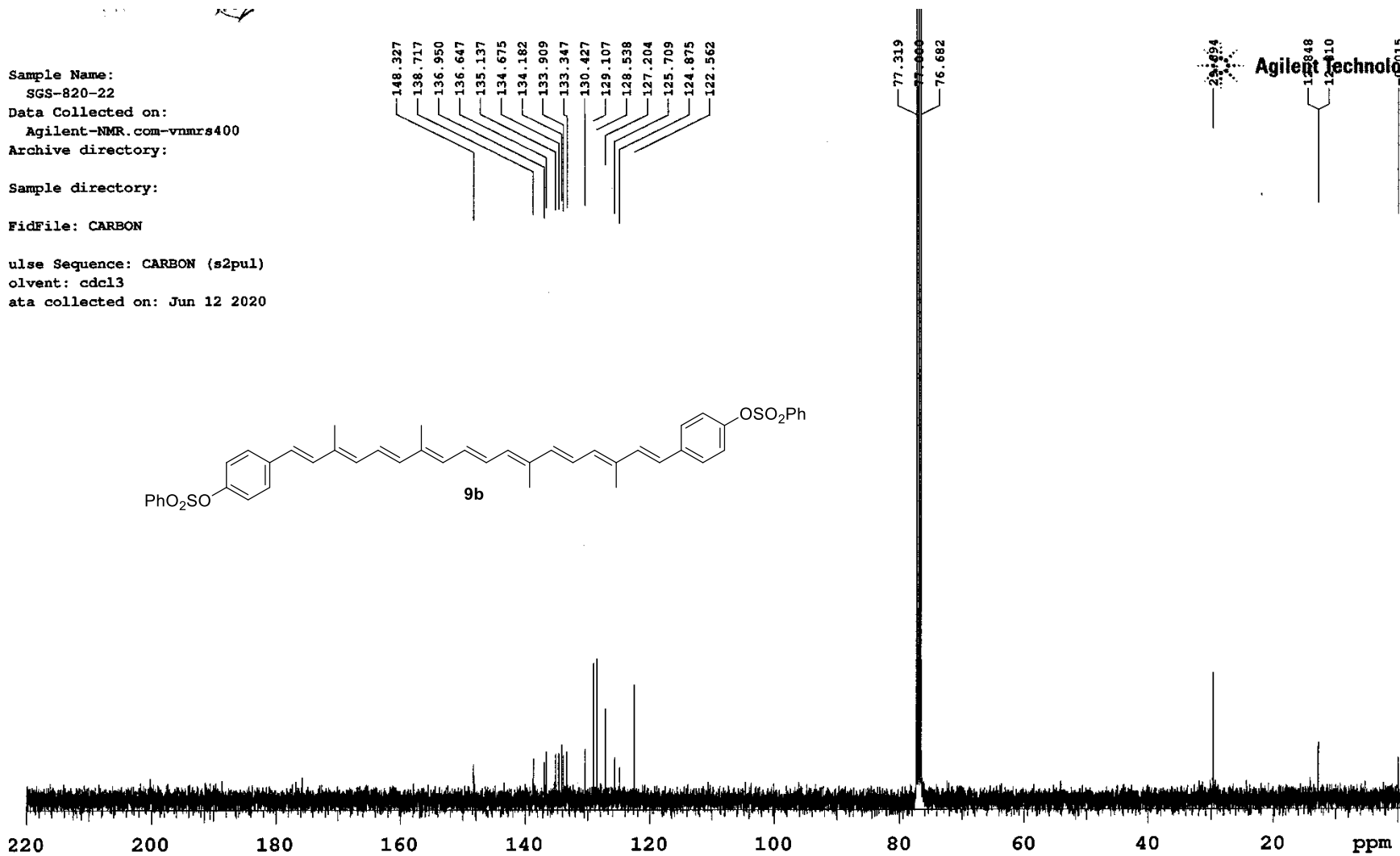
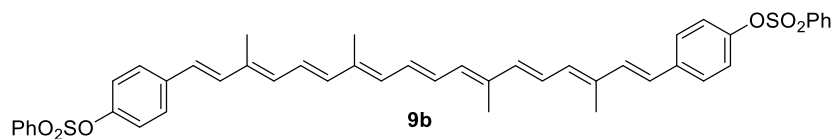


Figure S36. ¹³C NMR of **9b**

Sample Name:
 SGS-1376-2re
 Data Collected on:
 Agilent-NMR.chem.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2005-koo-4-26
 Sample directory:
 SGS-1376-2re_01
 FidFile: SGS-1376-2re_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: dms0
 Data collected on: May 26 2021

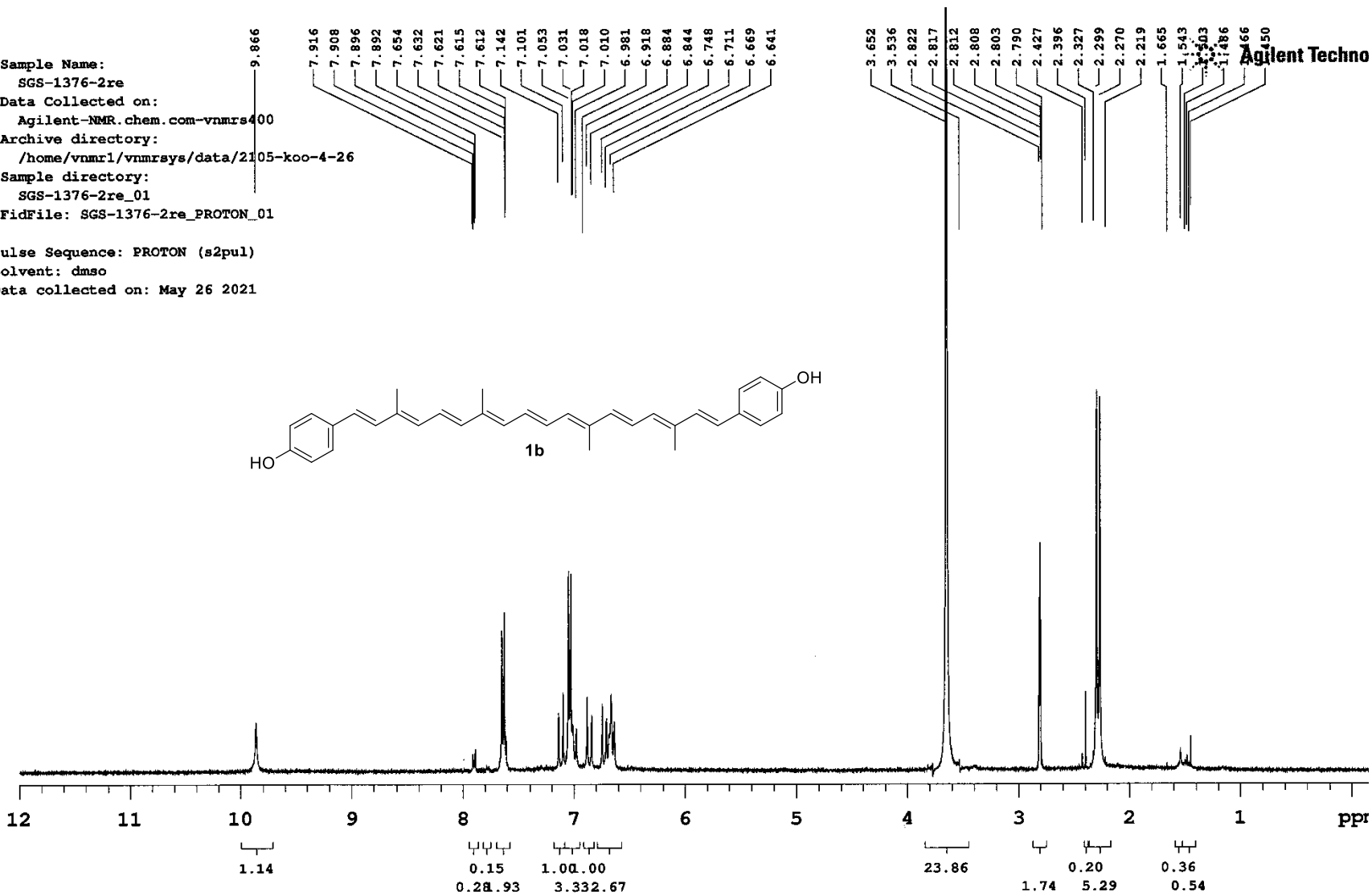


Figure S37. ¹H NMR of **1b**

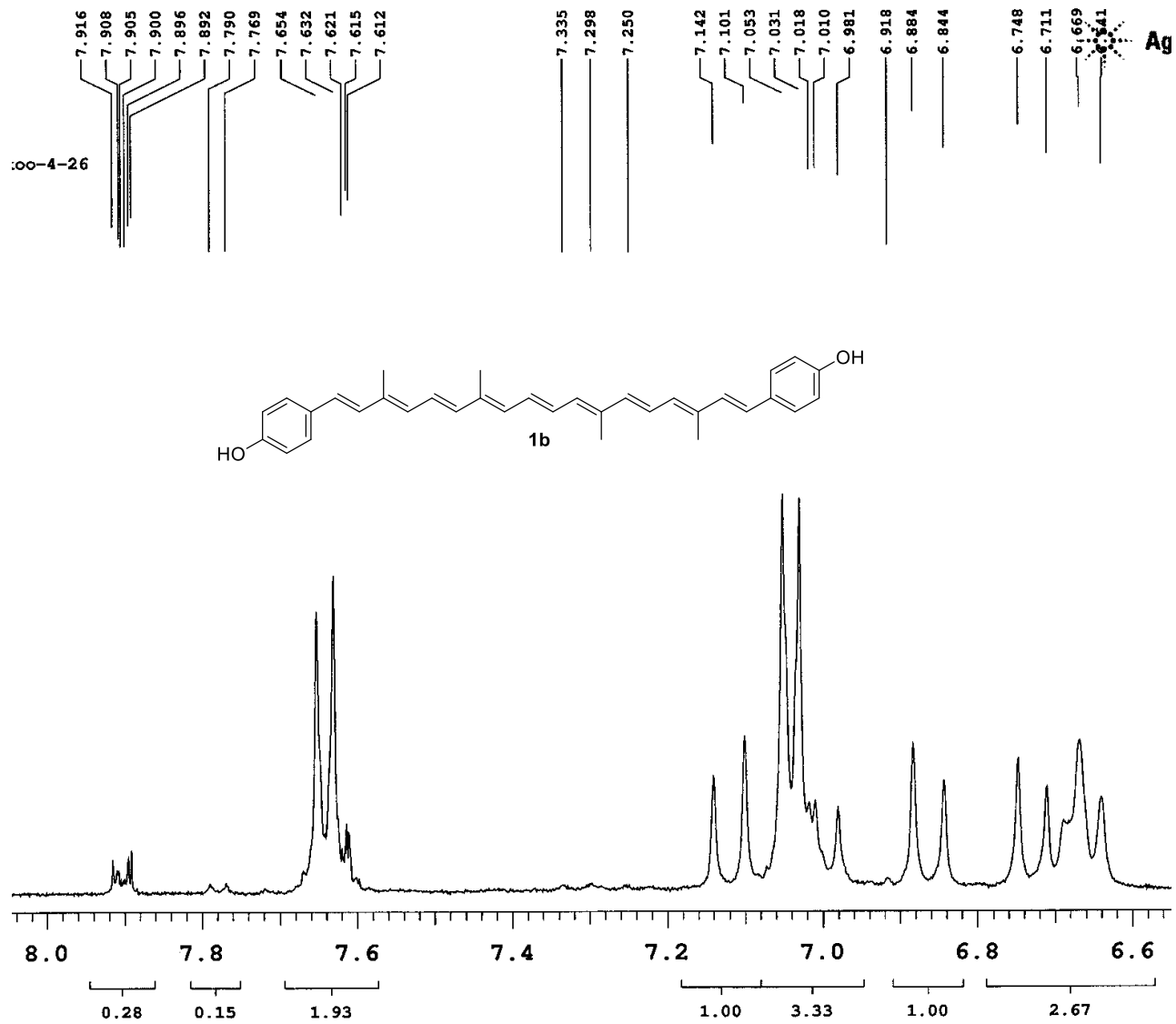


Figure S38. ¹H NMR of **1b** (expansion plot)

Sample Name:
SGS-1084-12
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2012-koo-4
Sample directory:
SGS-1084-12_02
FidFile: SGS-1084-12 CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmsd
Data collected on: Dec 2 2020

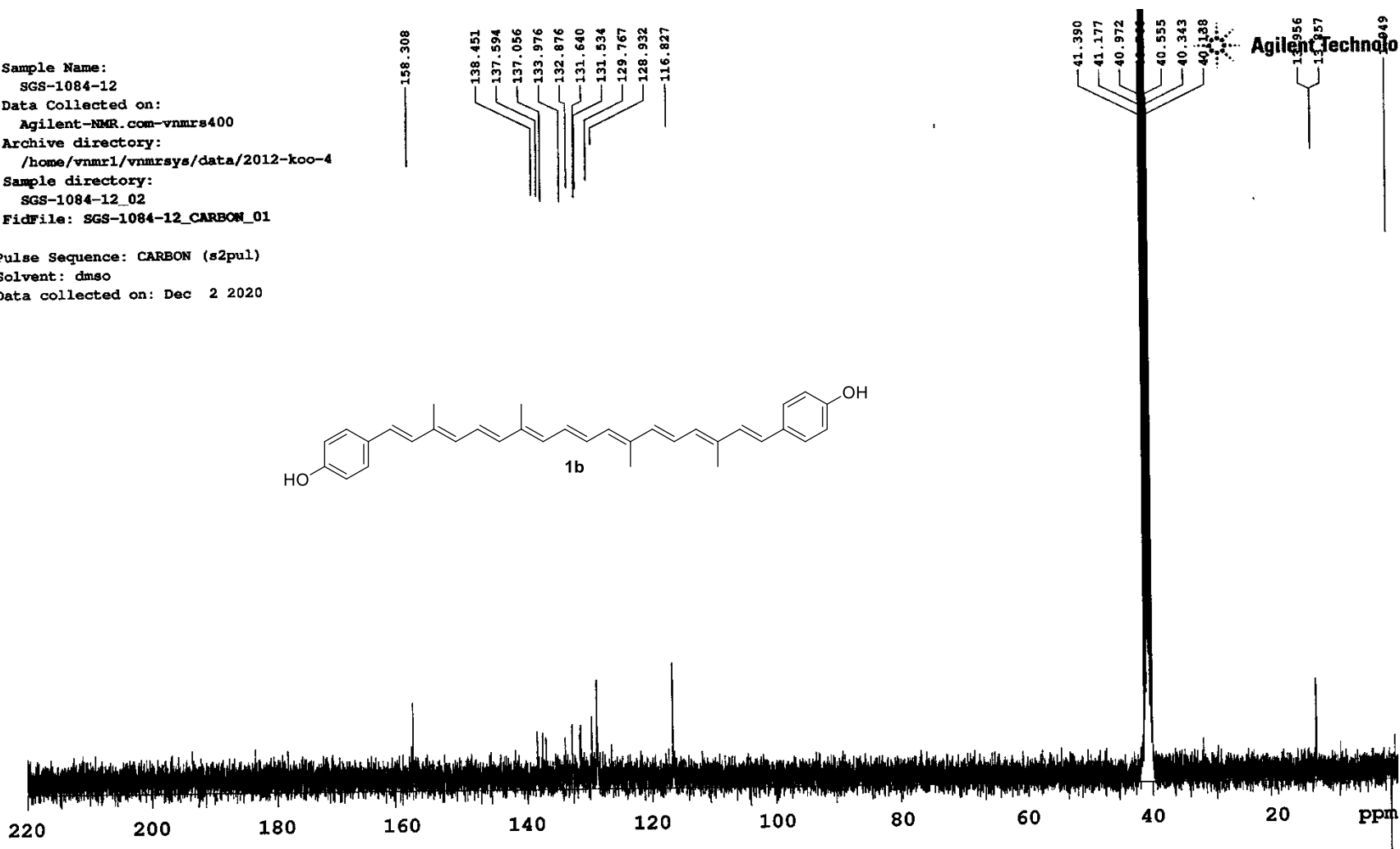


Figure S39. ¹³C NMR of **1b**

Sample Name:
LN-261-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2007-koo-4
Sample directory:
LN-261-1_01
FidFile: LN-261-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2020

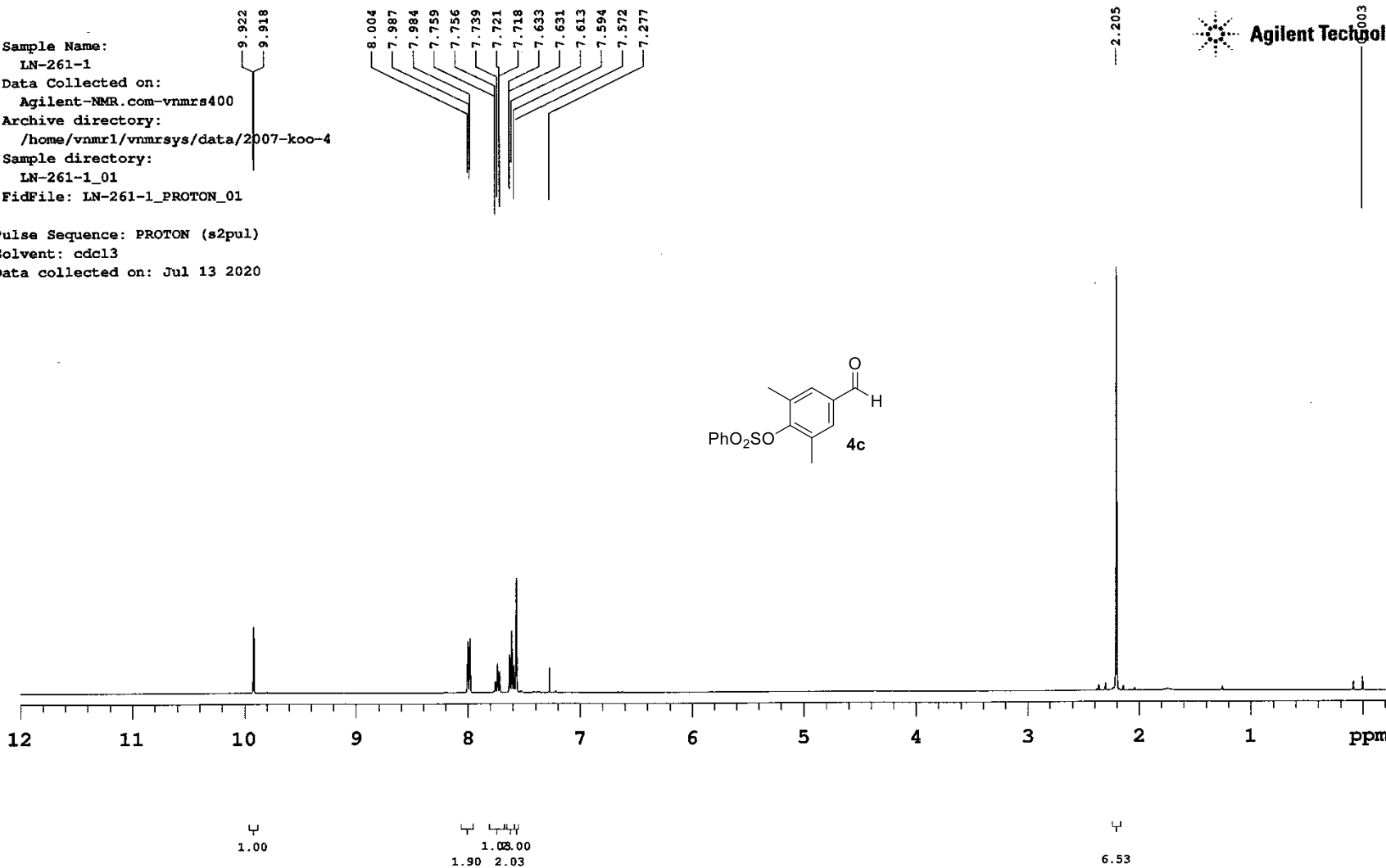


Figure S40. ¹H NMR of **4c**

Sample Name:
LN-261-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2007-koo-4
Sample directory:
LN-261-1_02
FidFile: LN-261-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2020

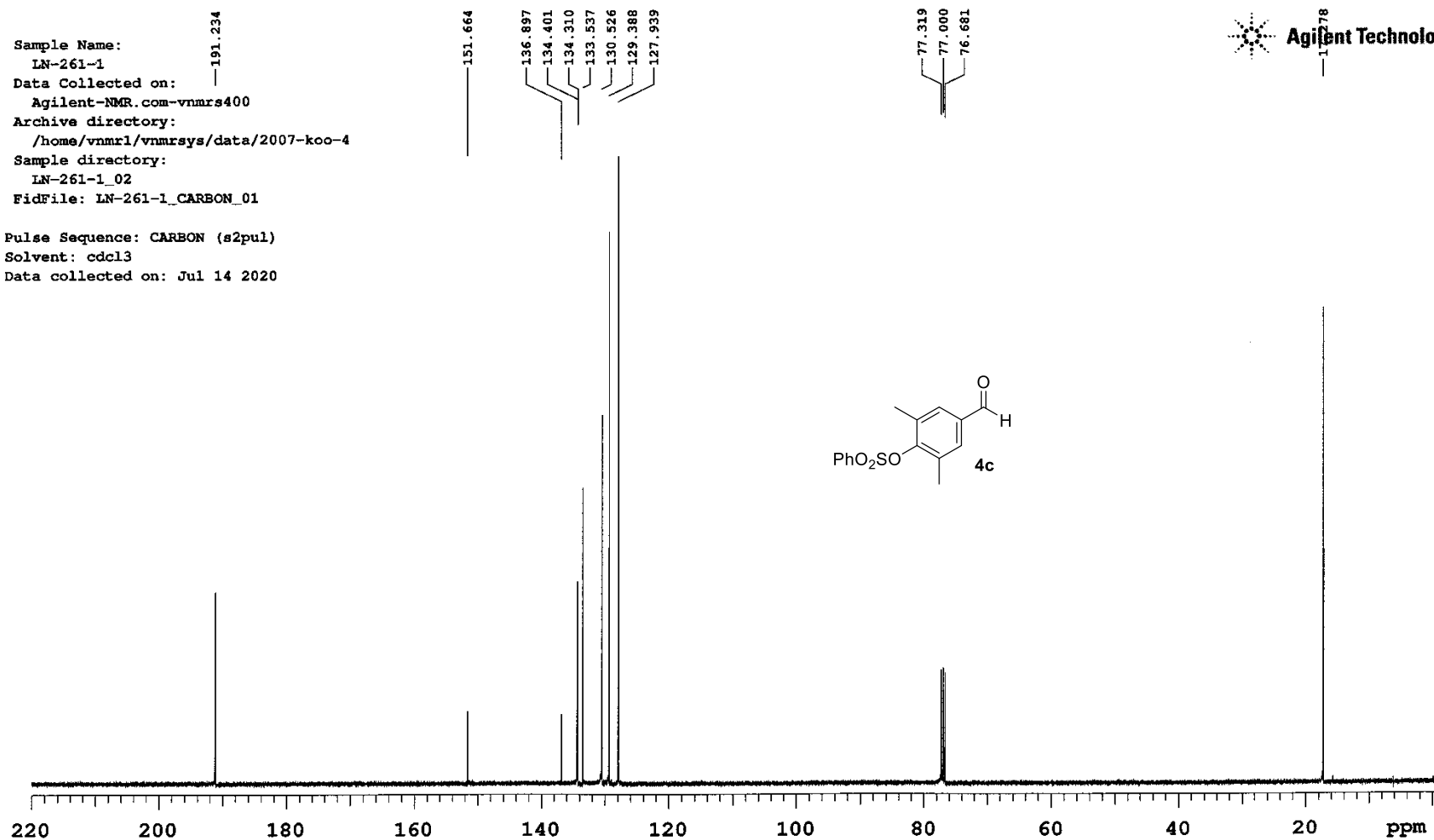


Figure S41. ^{13}C NMR of **4c**

Sample Name:
SGS-918-A1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2007-koo-
Sample directory:
SGS-918-A1_01
FidFile: SGS-918-A1_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2020

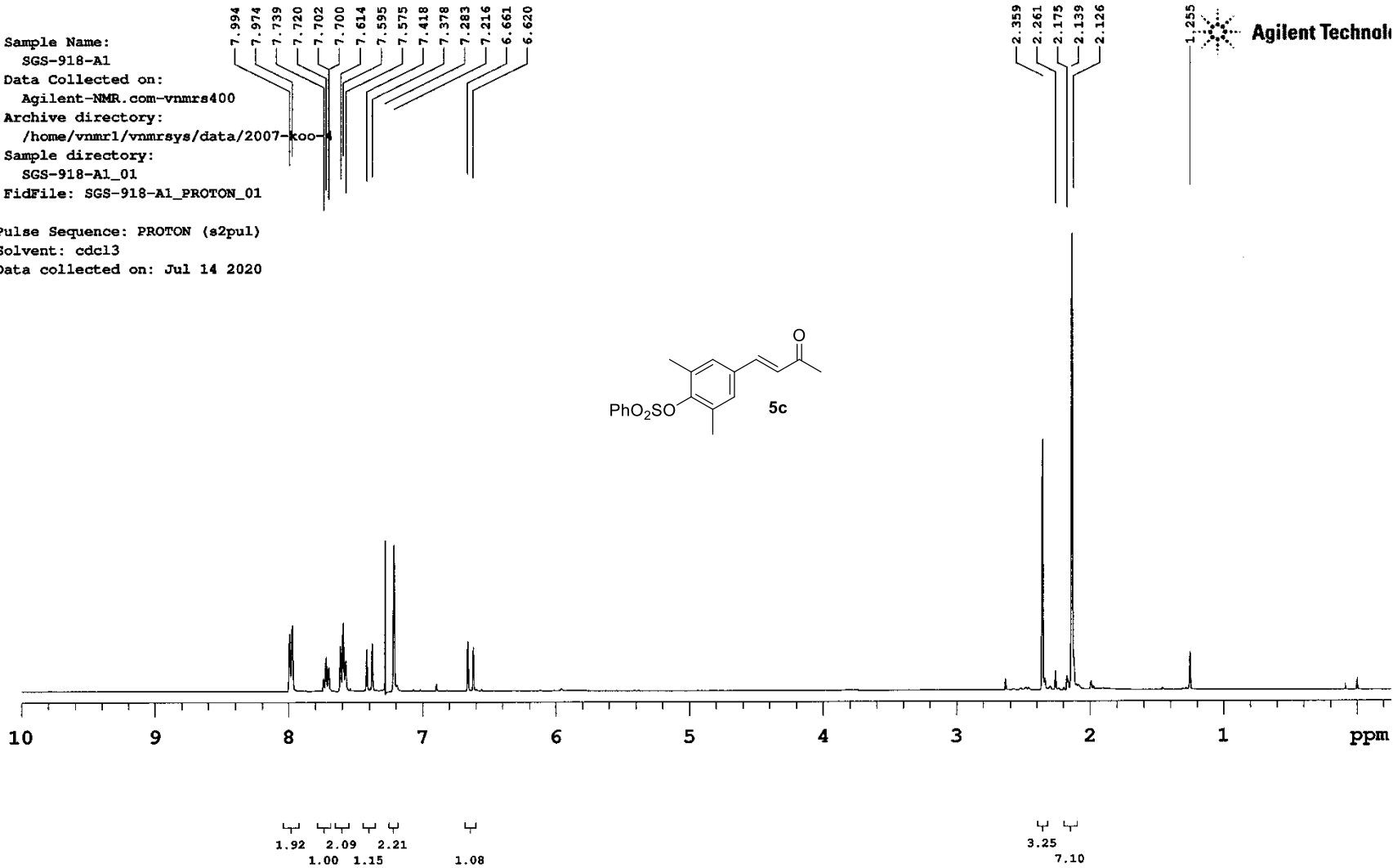


Figure S42. ¹H NMR of 5c

Sample Name: SGS-918-A1
Data Collected on: Agilent-NMR.com-vnmrs400
Archive directory: /home/vnmr1/vnmr/sys/data/2007-koo-4
Sample directory: SGS-918-A1_02
FidFile: SGS-918-A1_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2020

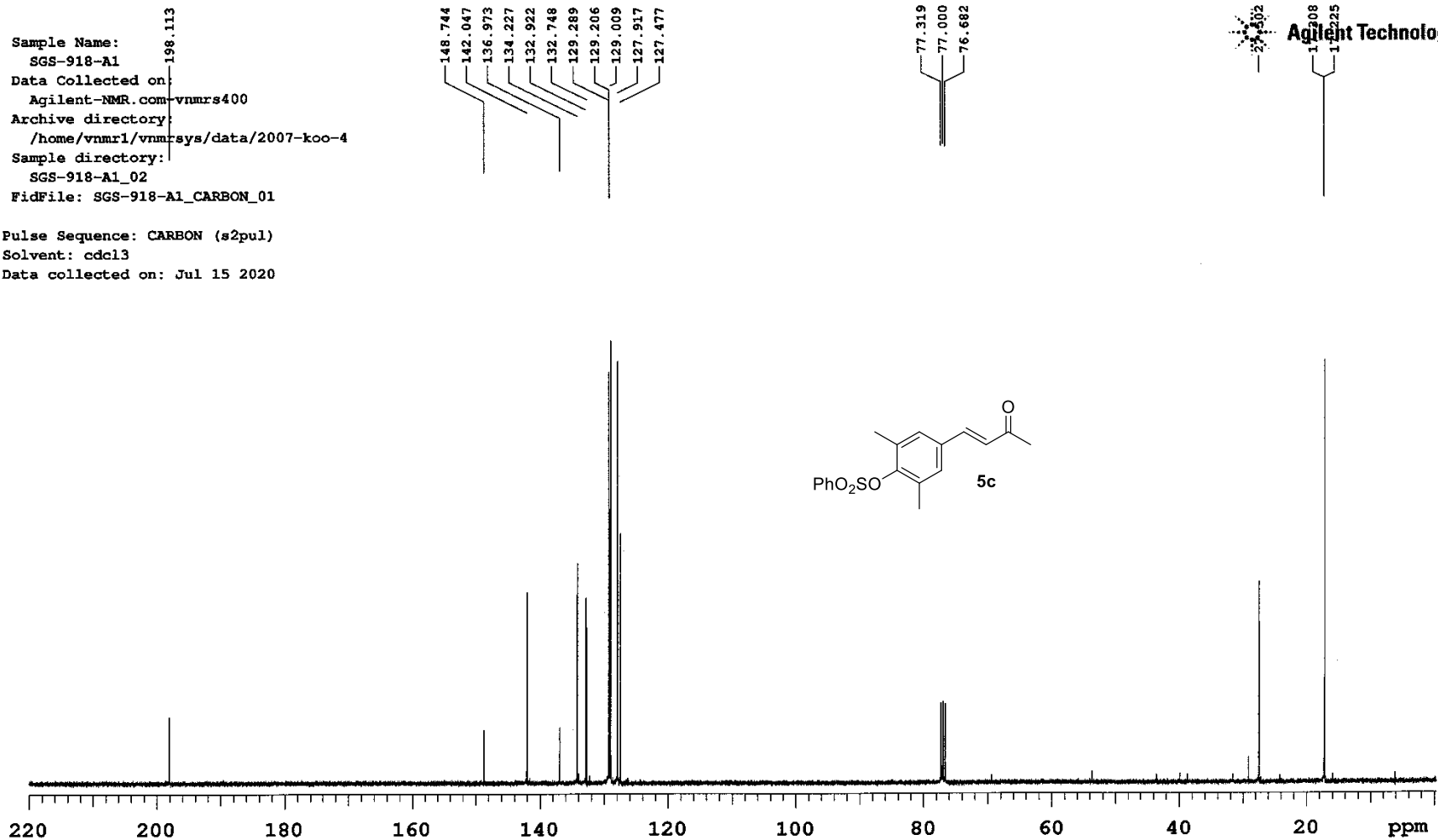


Figure S43. ¹³C NMR of 5c

955
 935
 912
 891
 870
 860
 839
 824
 817
 806
 787
 7731
 7713
 7702
 7691
 7683
 7673
 7664
 7642
 7634
 7623
 7600
 7579
 7560
 7324
 7305
 7157
 7040
 7026
 6914
 6875
 6661
 6621
 6348
 6333
 6307
 6293
 5618
 5599
 5582
 5562
 5287
 5269
 4980
 4961
 4941
 4921
 4877
 4856
 4836
 4817
 2141
 2119
 2085
 2069
 2001
 1940
 1843
 1829
 1481
 1471
 1259
 1008
 1000
 1009

Sample Name: SGS-925-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2007-k04
 Sample directory: SGS-925-1_01
 FidFile: SGS-925-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 16 2020

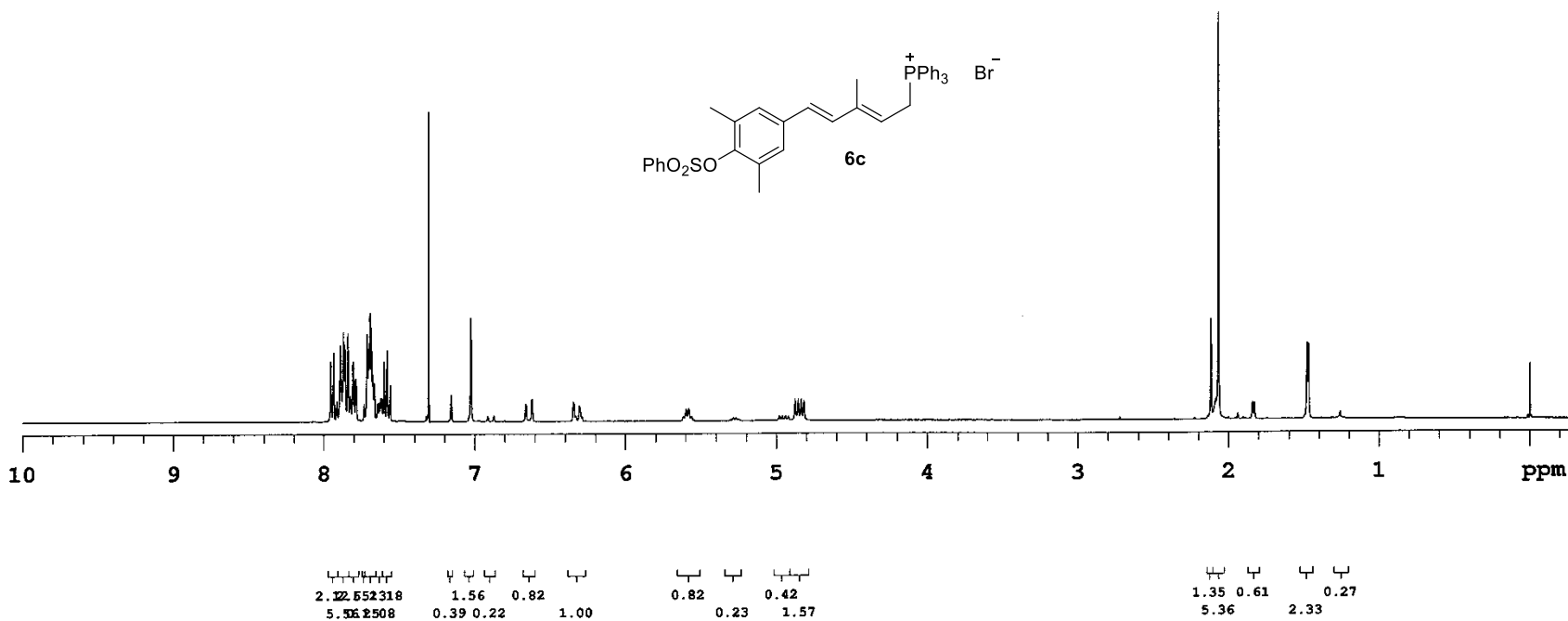
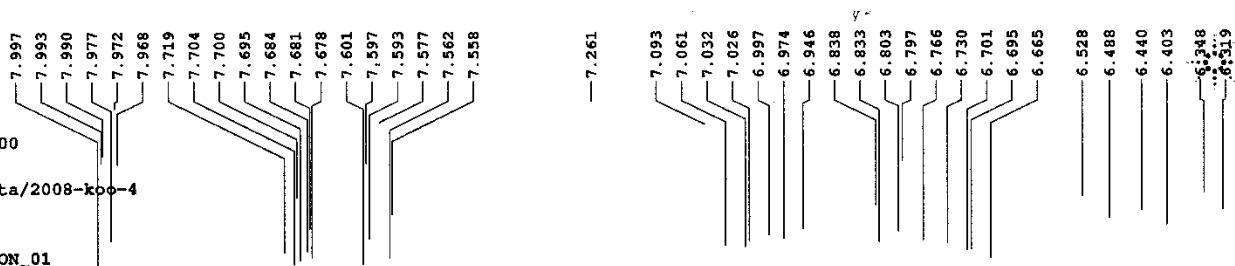


Figure S45. ¹H NMR of **6c**

Sample Name:
SGS-940-ly
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2008-koo-4
Sample directory:
SGS-940-ly_01
FidFile: SGS-940-ly_PROTON_01



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 12 2020

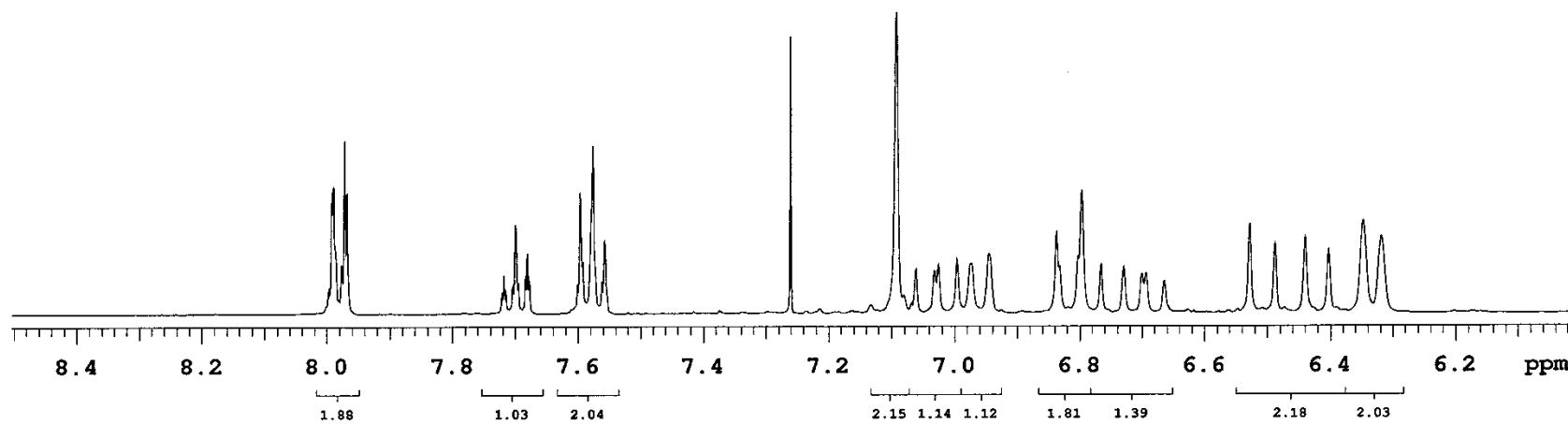
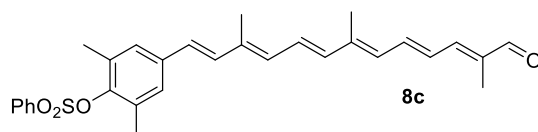


Figure S47. ^1H NMR of **8c** (expansion plot)

Sample Name:
SGS-940-ly
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2008-koo-4
Sample directory:
SGS-940-ly_02
FidFile: SGS-940-ly_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2020

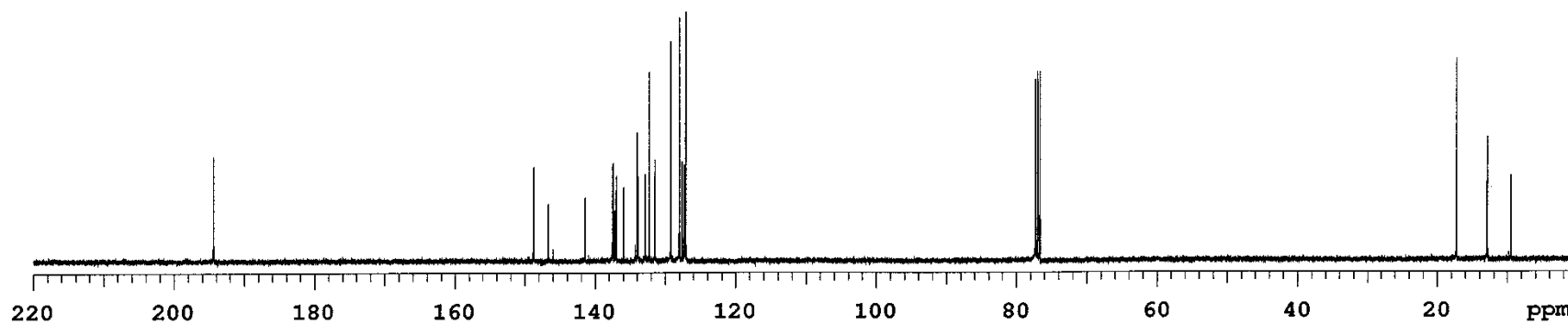
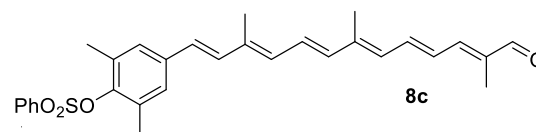
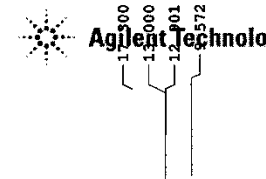
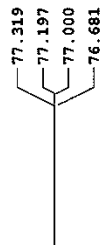
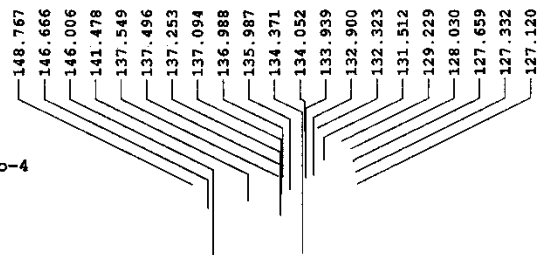


Figure S48. ¹³C NMR of 8c

Sample Name: SGS-965-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2008-koo-4
 Sample directory: SGS-965-i_01
 FidFile: SGS-965-1_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 13 2020

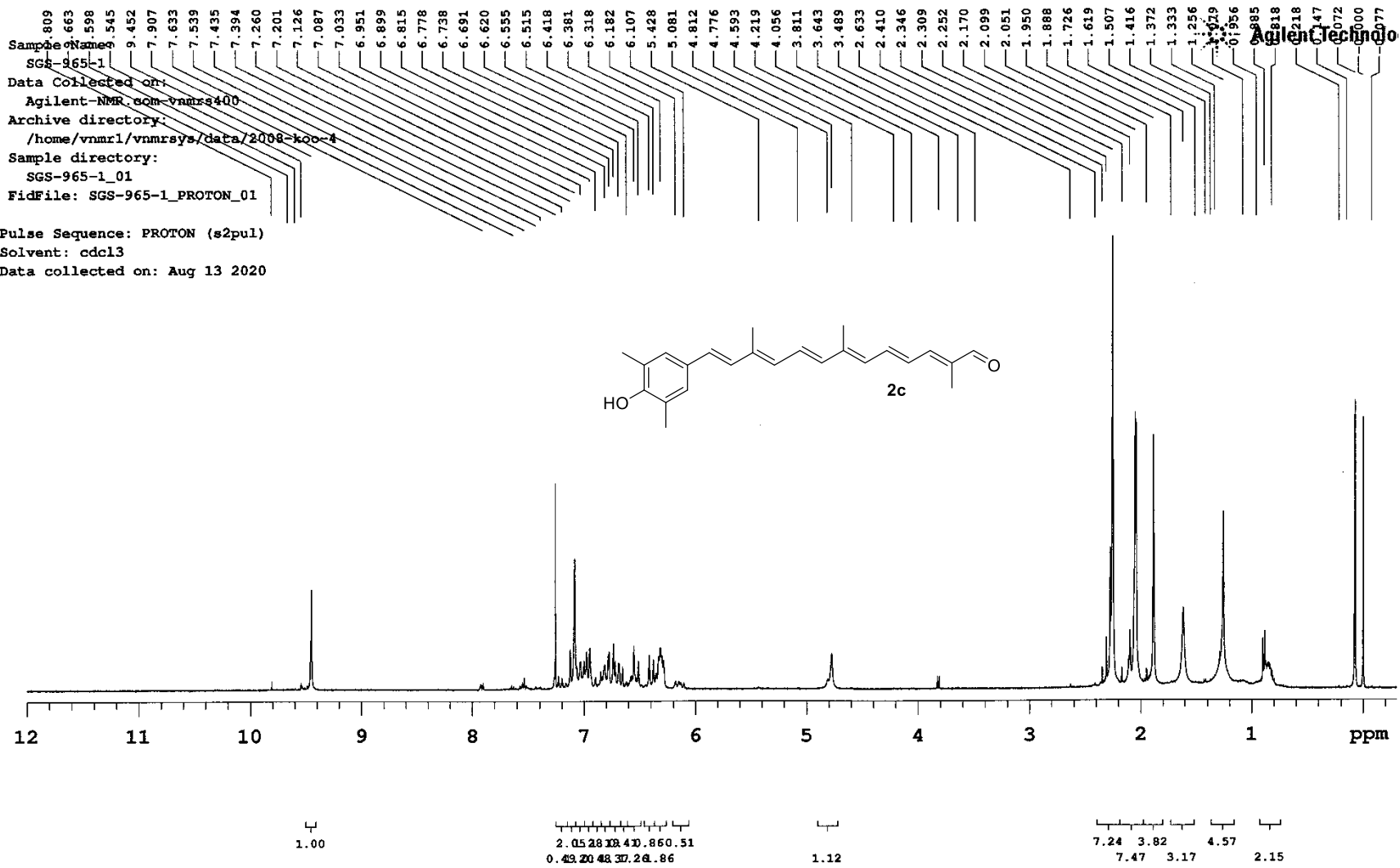


Figure S49. ¹H NMR of 2c

Sample Name: SGS-965-1
Data Collected on: Agilent-NMR.com-vnmrs400
Archive directory: /home/vnmr1/vnmrsys/data/2008-koc-4
Sample directory: SGS-965-1_01
FidFile: SGS-965-1_PROTON_Q1

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 13 2020

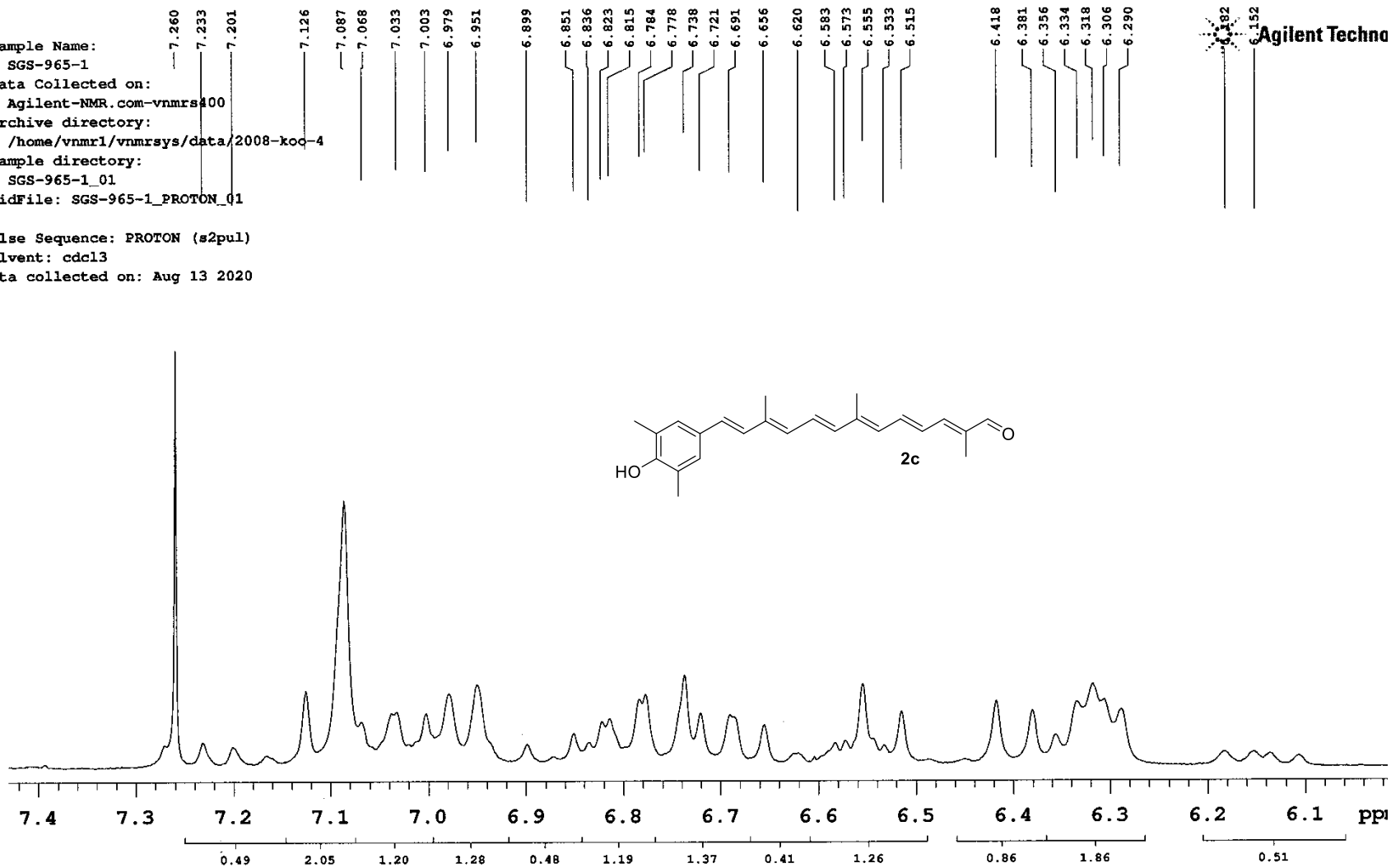


Figure S50. ¹H NMR of 2c (expansion plot)

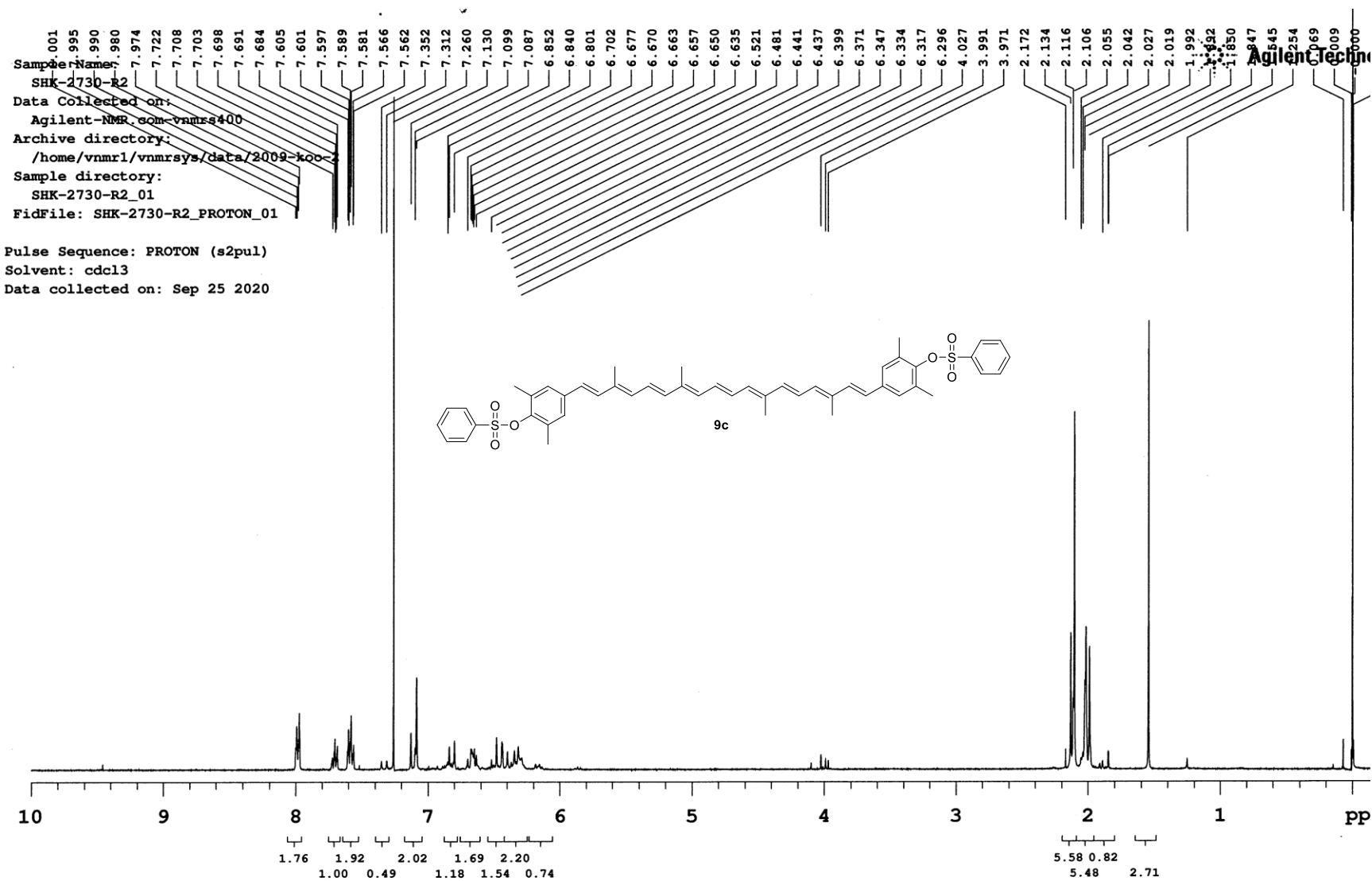


Figure S51. ¹H NMR of **9c**

Sample Name:
 SHK-2735-1
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2009-koo-2
 Sample directory:
 SHK-2735-1_01
 FidFile: SHK-2735-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: acetone
 Data collected on: Sep 25 2020

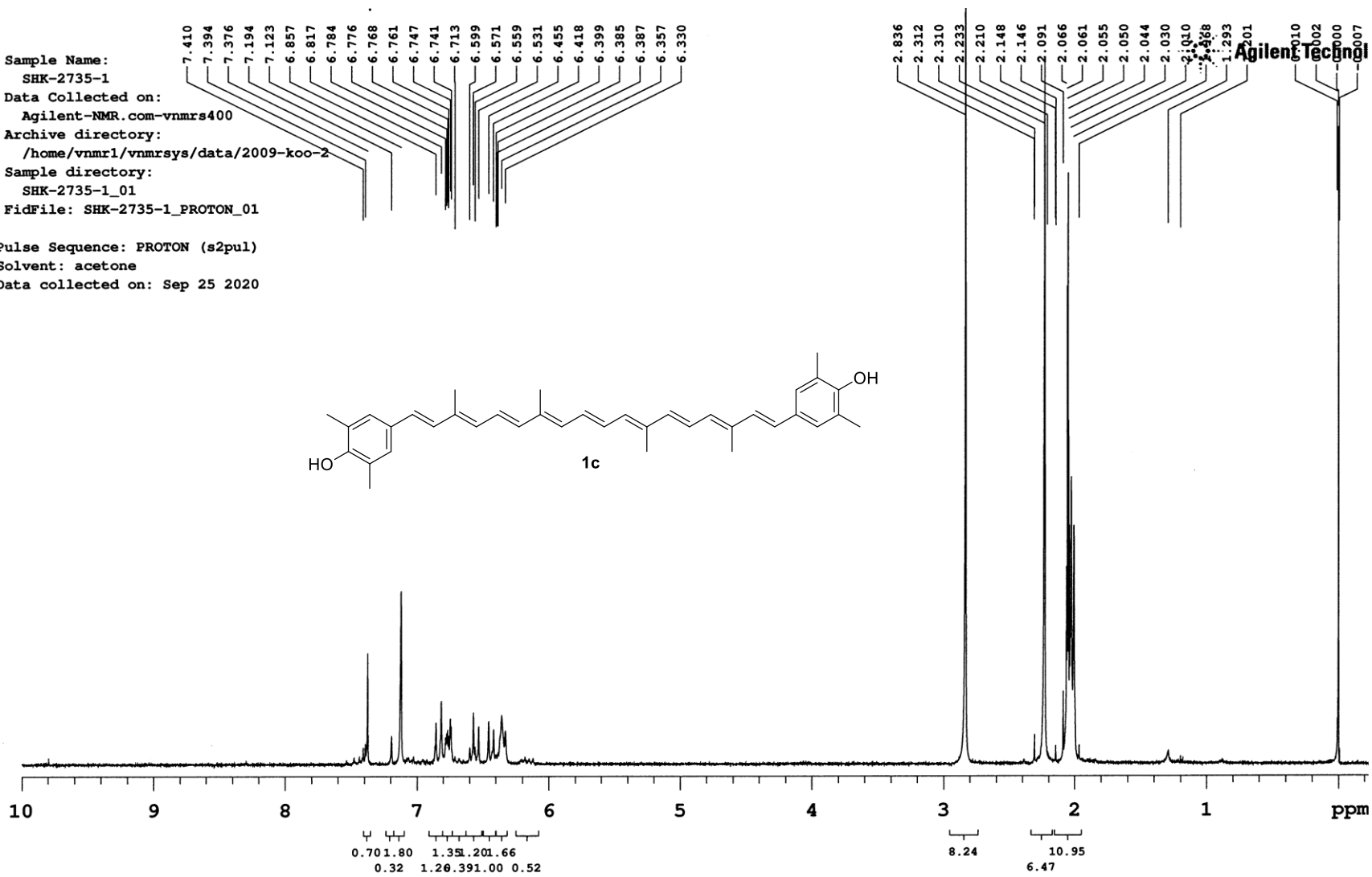


Figure S53. ^1H NMR of **1c**

Sample Name: SHK-2735-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2009-koo-2
 Sample directory: SHK-2735-1_01
 FidFile: SHK-2735-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: acetone
 Data collected on: Sep 25 2020

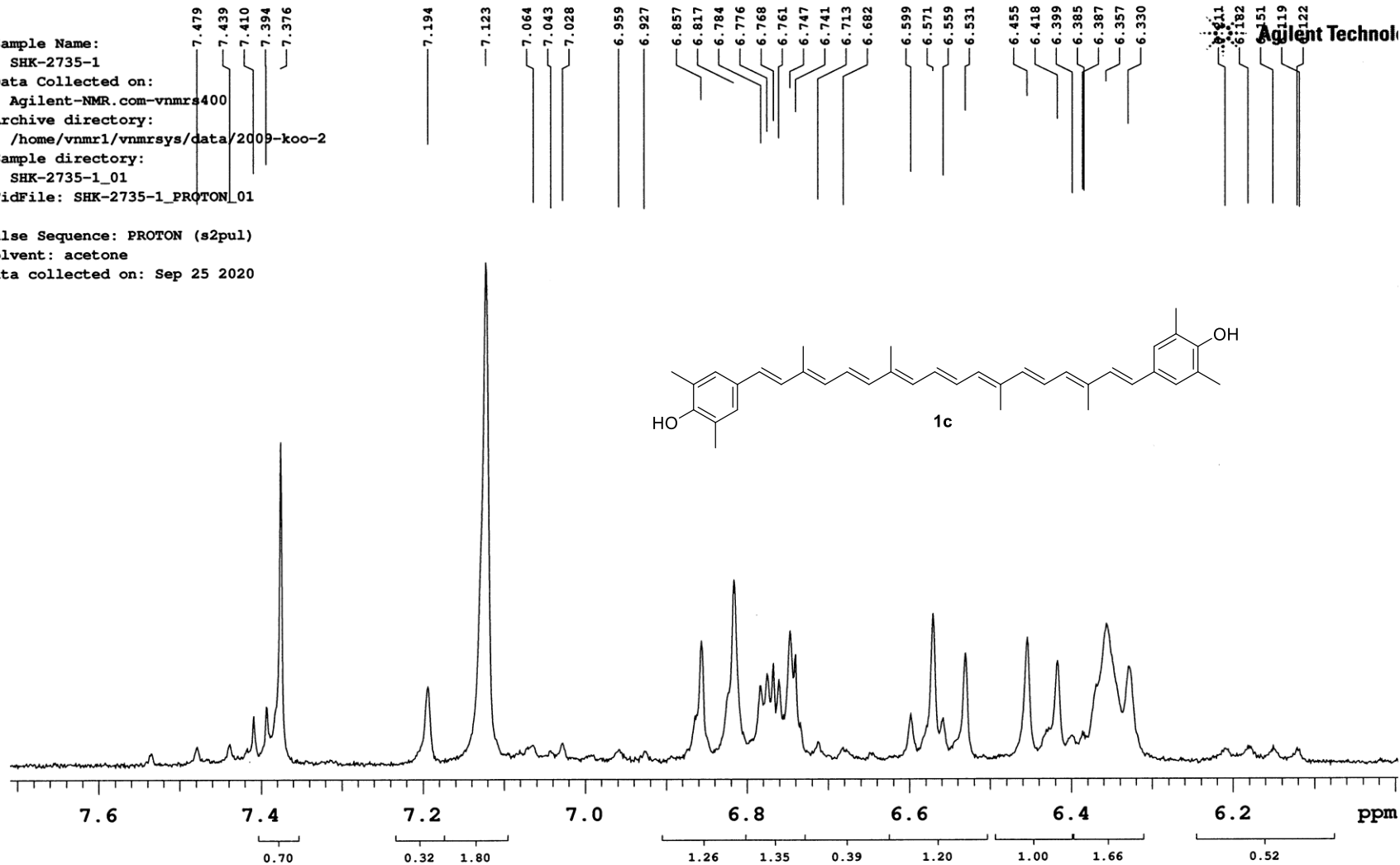


Figure S54. ¹H NMR of **1c** (expansion plot)

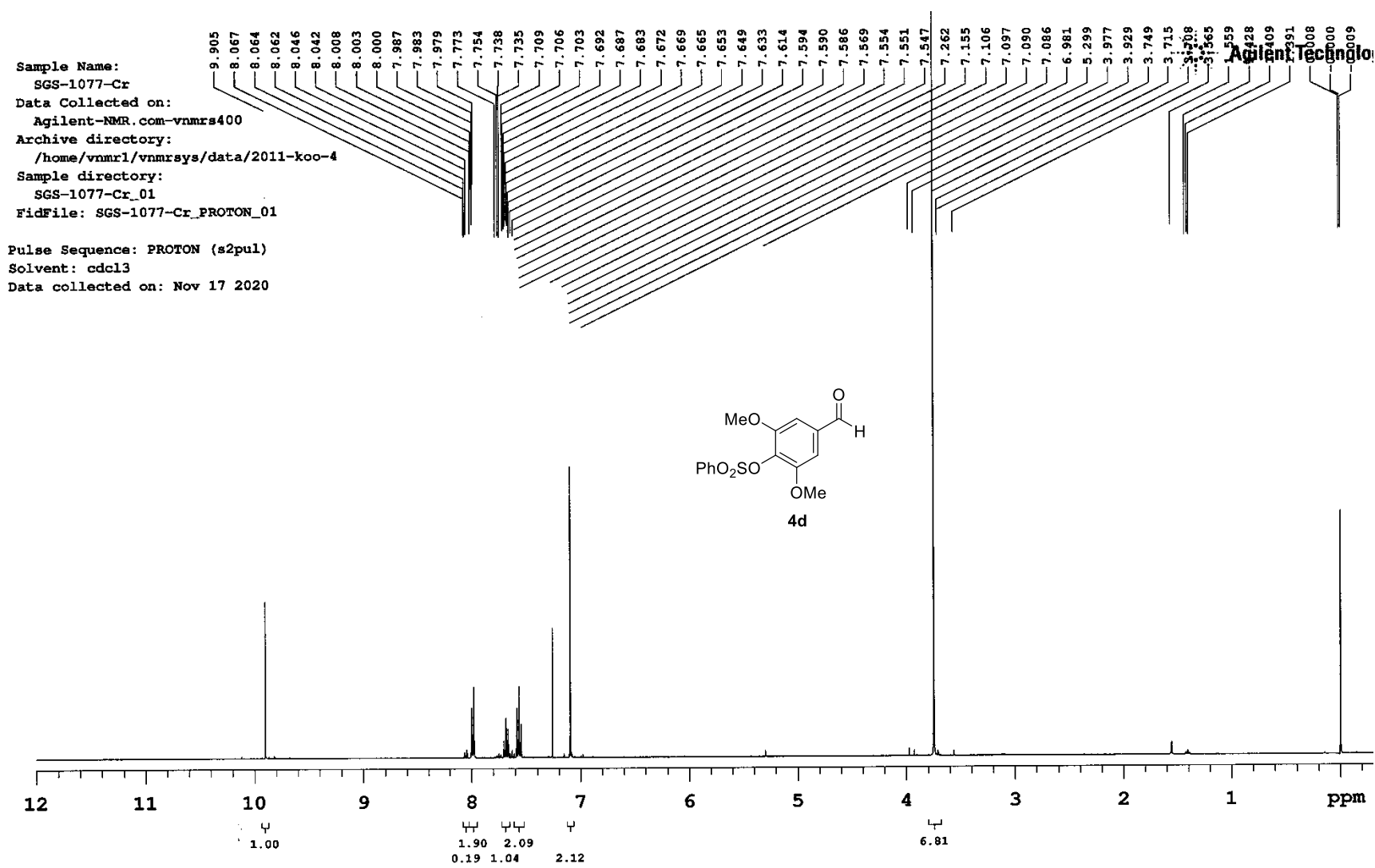


Figure S55. ¹H NMR of 4d

Sample Name:
SGS-1100-1
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2101-koo-4
Sample directory:
SGS-1100-1_03
FidFile: SGS-1100-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 6 2021

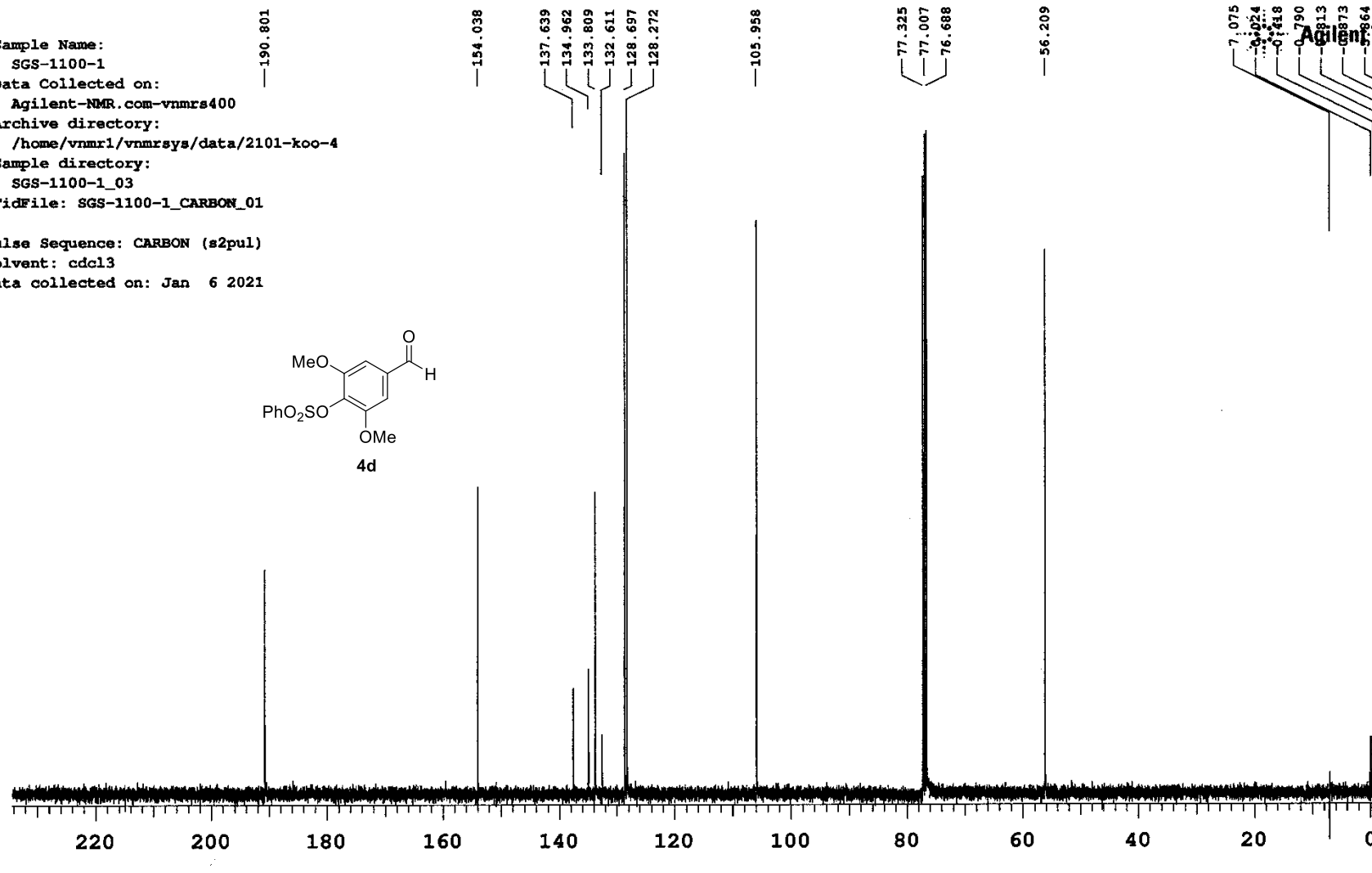
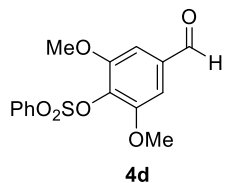


Figure S56. ^{13}C NMR of 4d

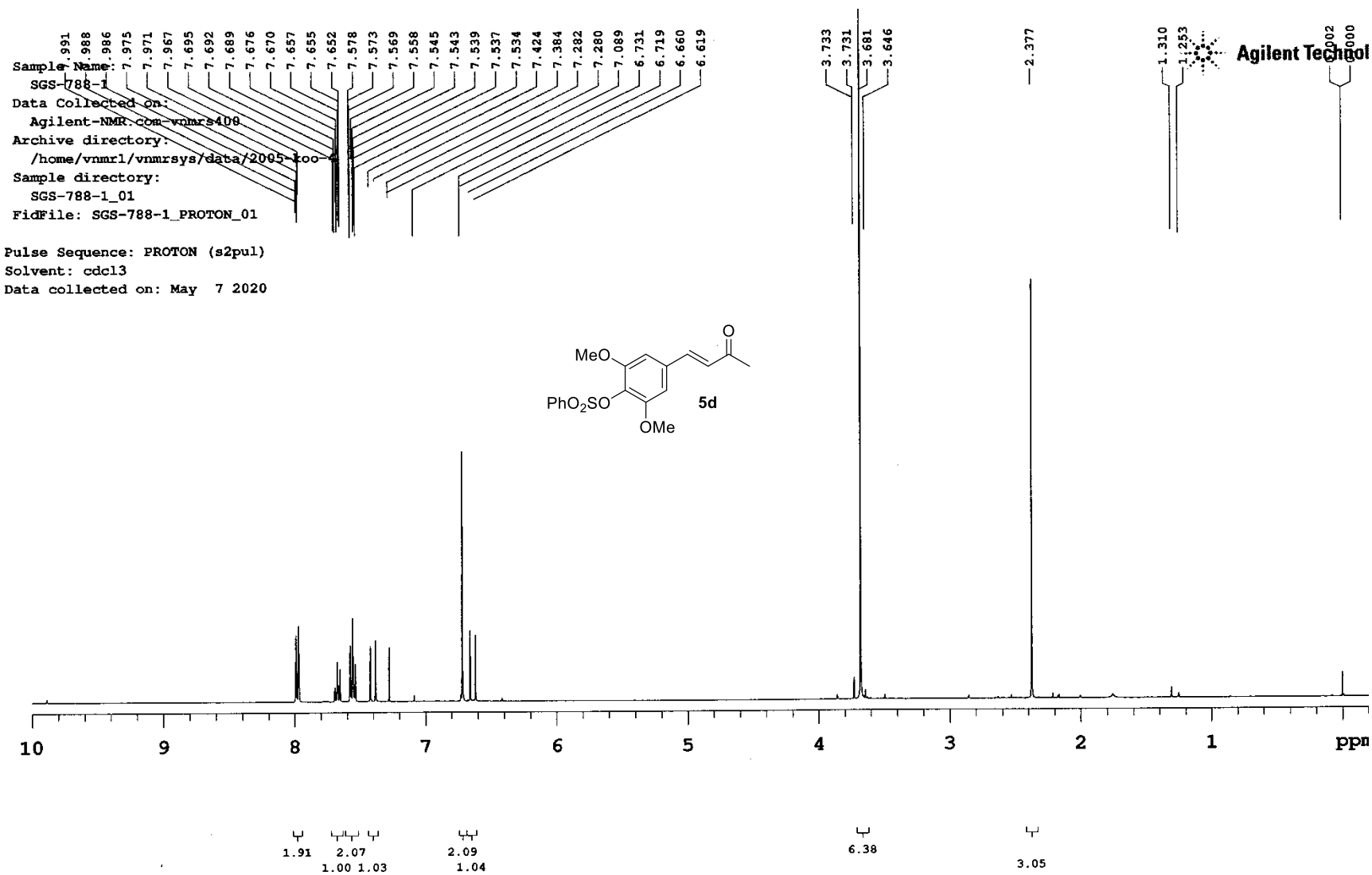


Figure S57. ¹H NMR of **5d**

Sample Name: SGS-788-1
Data Collected on: Agilent-NMR.com-vnmrs400
Archive directory: /home/vnmr1/vnmrsys/data/2005-koo-4
Sample directory: SGS-788-1_02
FidFile: SGS-788-1_CARBON_01
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 8 2020

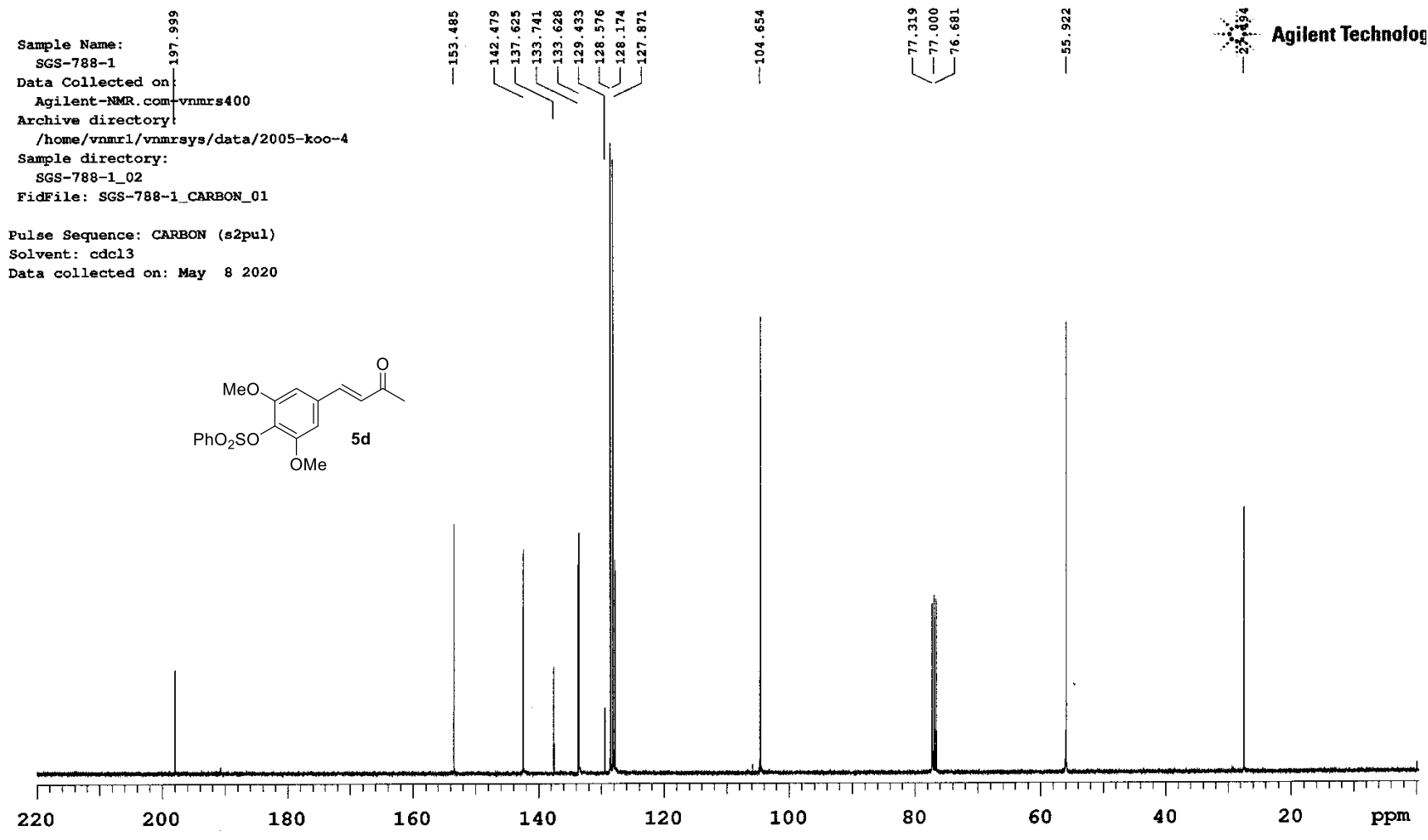
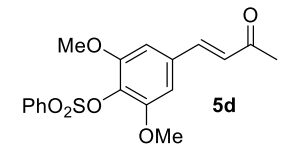


Figure S58. ¹³C NMR of 5d

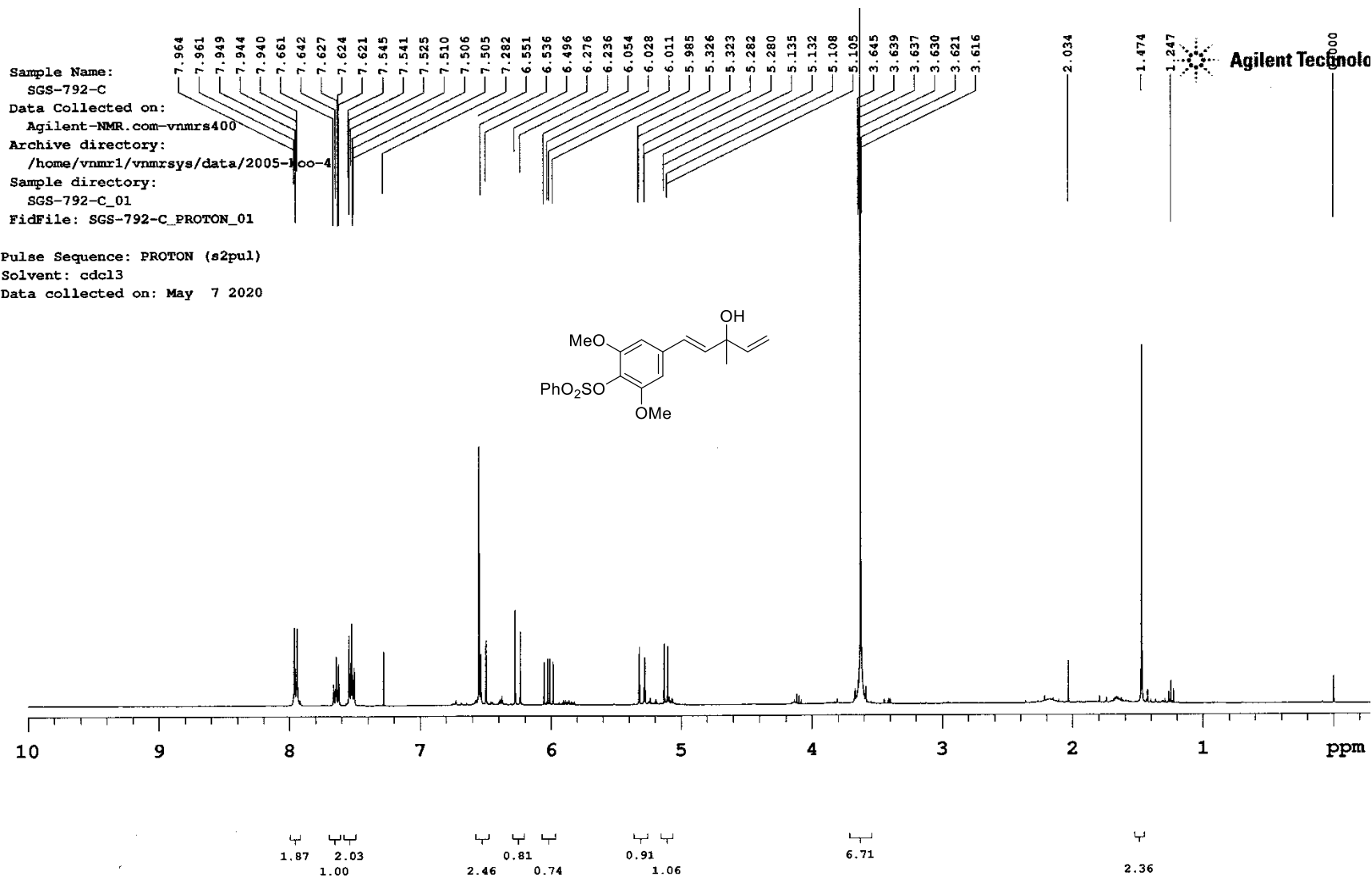


Figure S59. ¹H NMR of (*E*)-4-(3-hydroxy-3-methylpenta-1,4-dien-1-yl)-2,6-dimethoxyphenyl benzenesulfonate

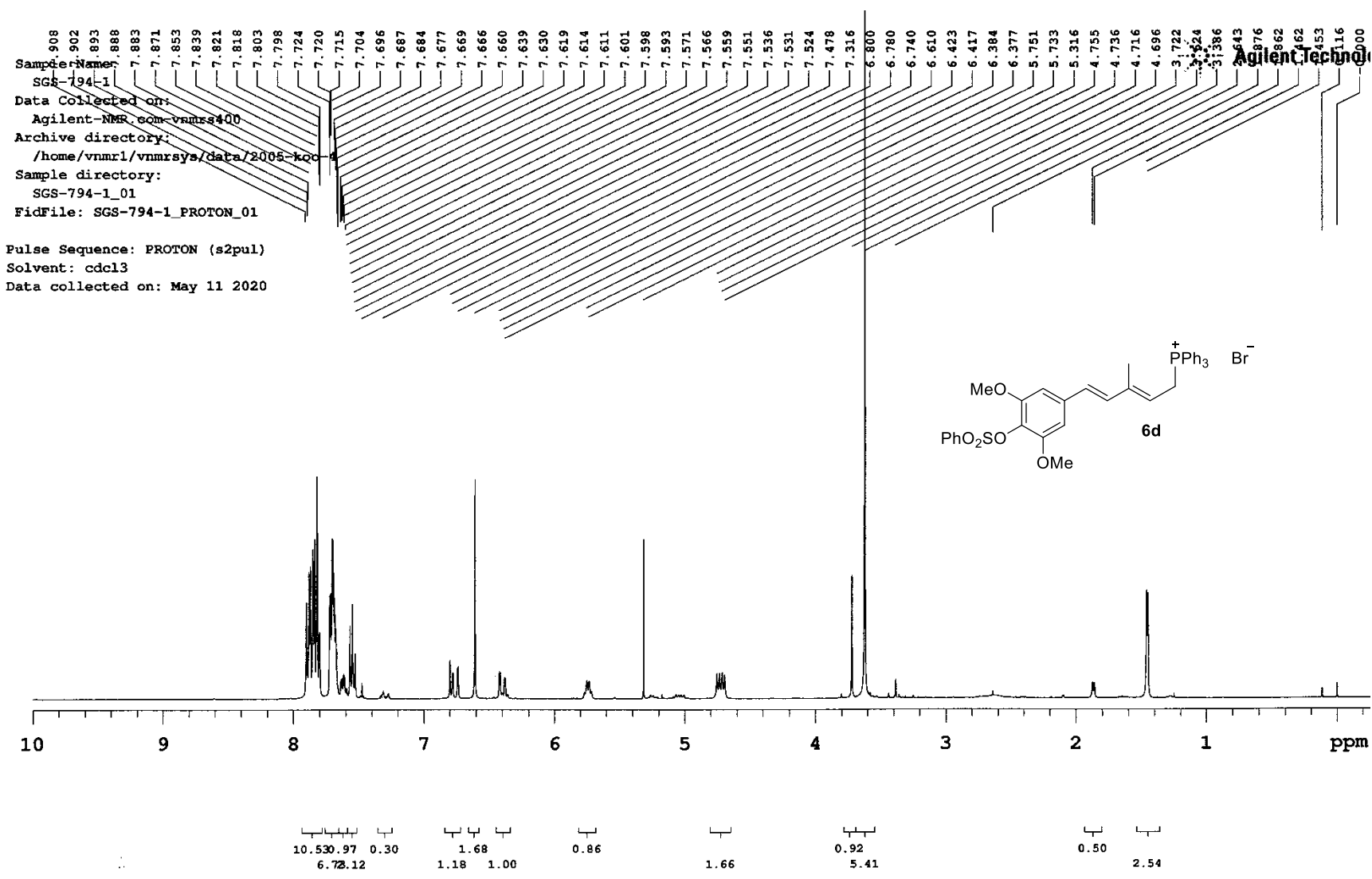


Figure S60. ¹H NMR of **6d**

Sample Name: 446
 SGS-808-S
 Data Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2005-ko0-4
 Sample directory:
 SGS-808-s_01
 FidFile: SGS-808-S_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: May 26 2020

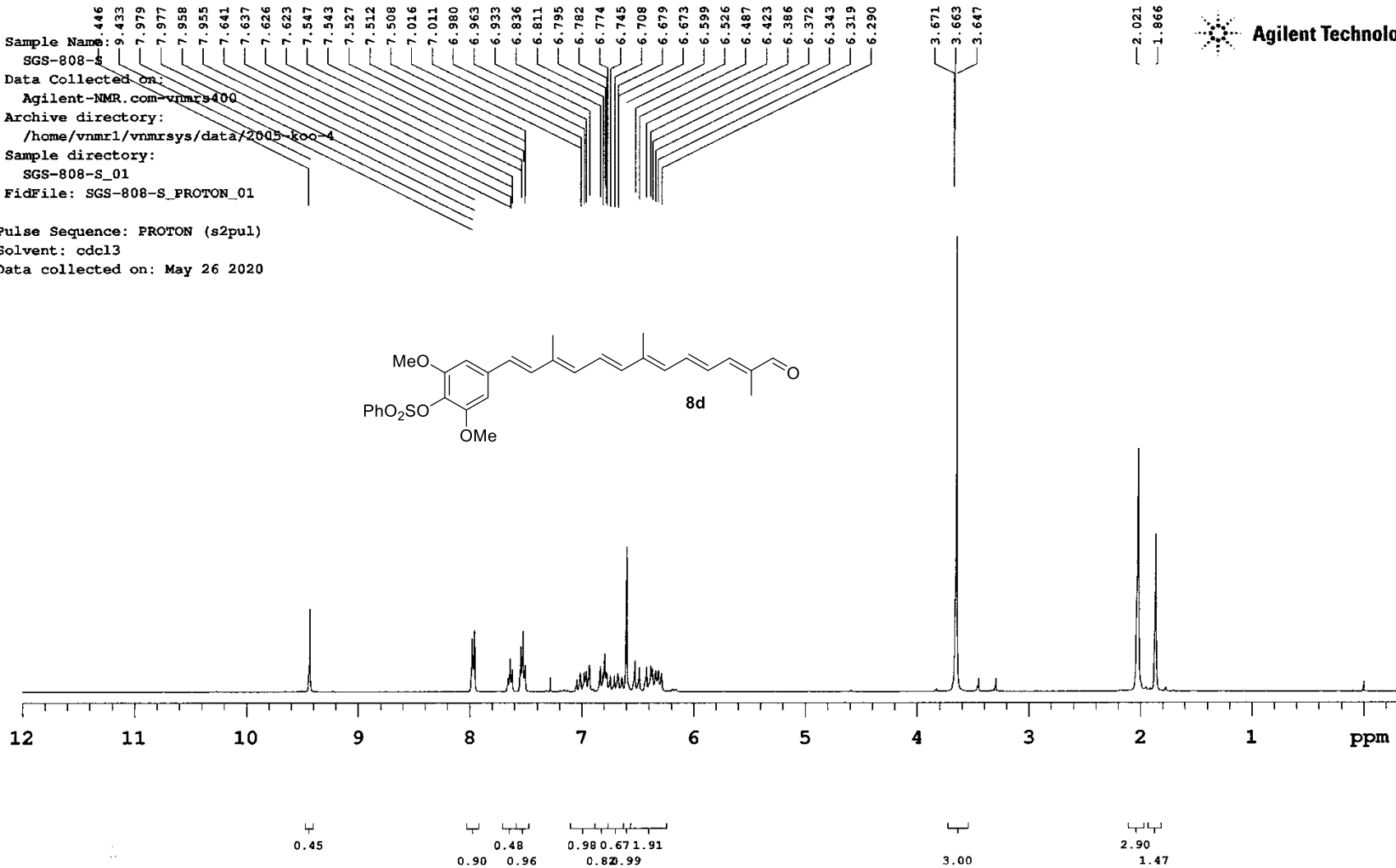


Figure S61. ¹H NMR of **8d**

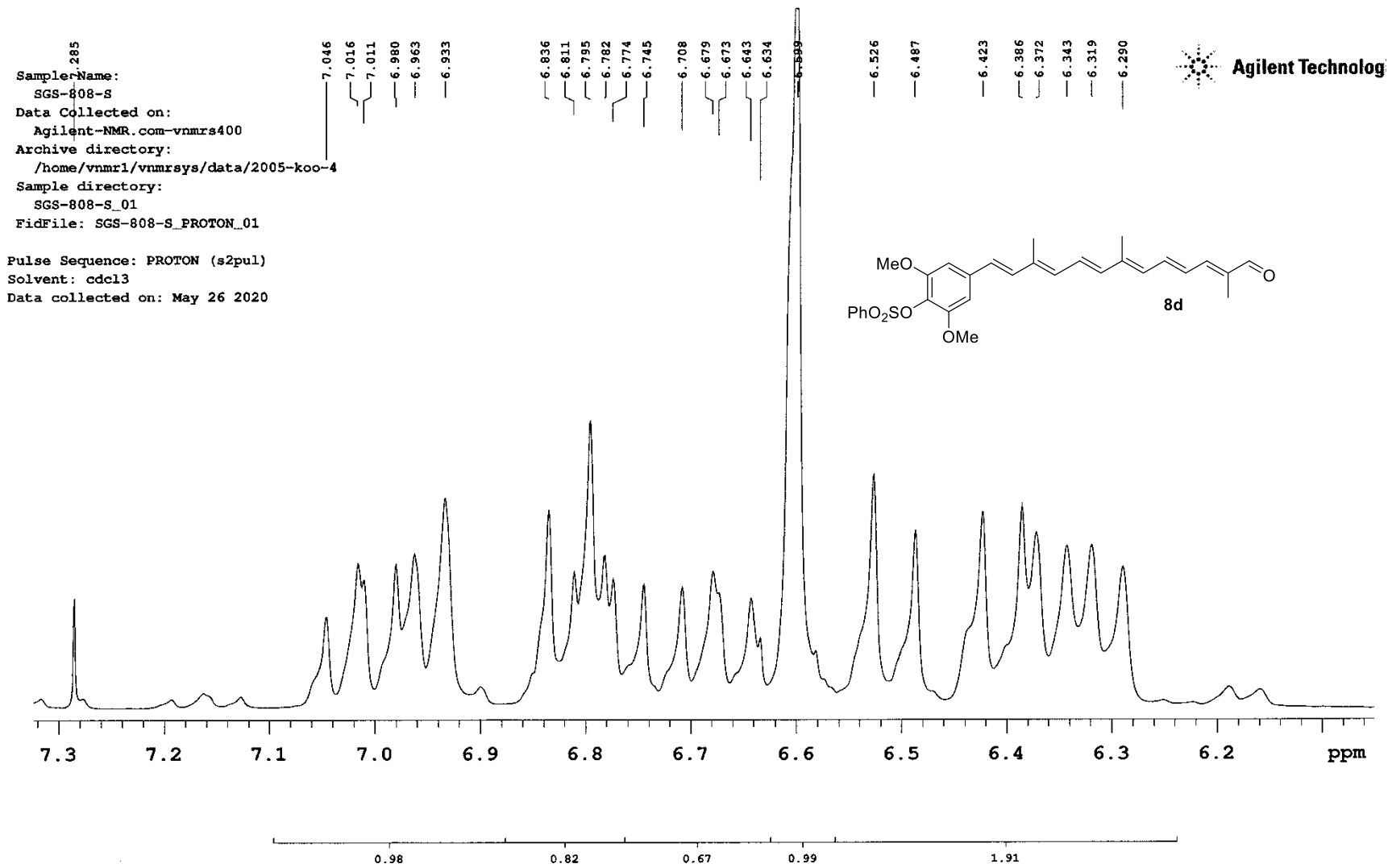


Figure S62. ¹H NMR of **8d** (expansion plot)

Sample Name: SGS-808-s
Data Collected on: Agilent-NMR.com-vnmrs400
Archive directory: /home/vnmr1/vnmrsys/data/2005-koo-4
Sample directory: SGS-808-s_01
FidFile: SGS-808-s_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 28 2020

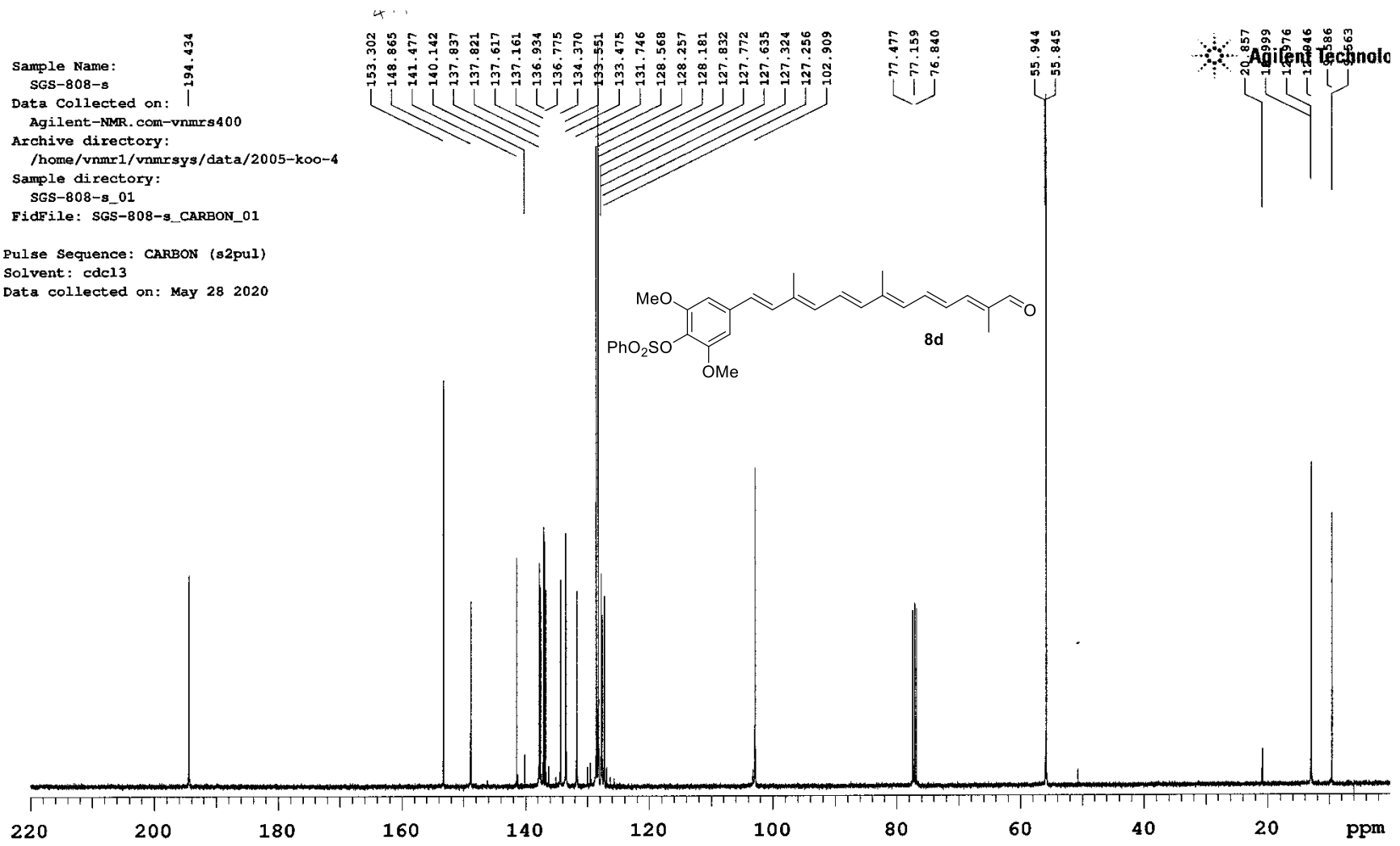


Figure S63. ¹³C NMR of 8d

Sample Name: SGS-846-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2006-koo-4
 Sample directory: SGS-846-1_01
 FidFile: SGS-846-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 9 2020

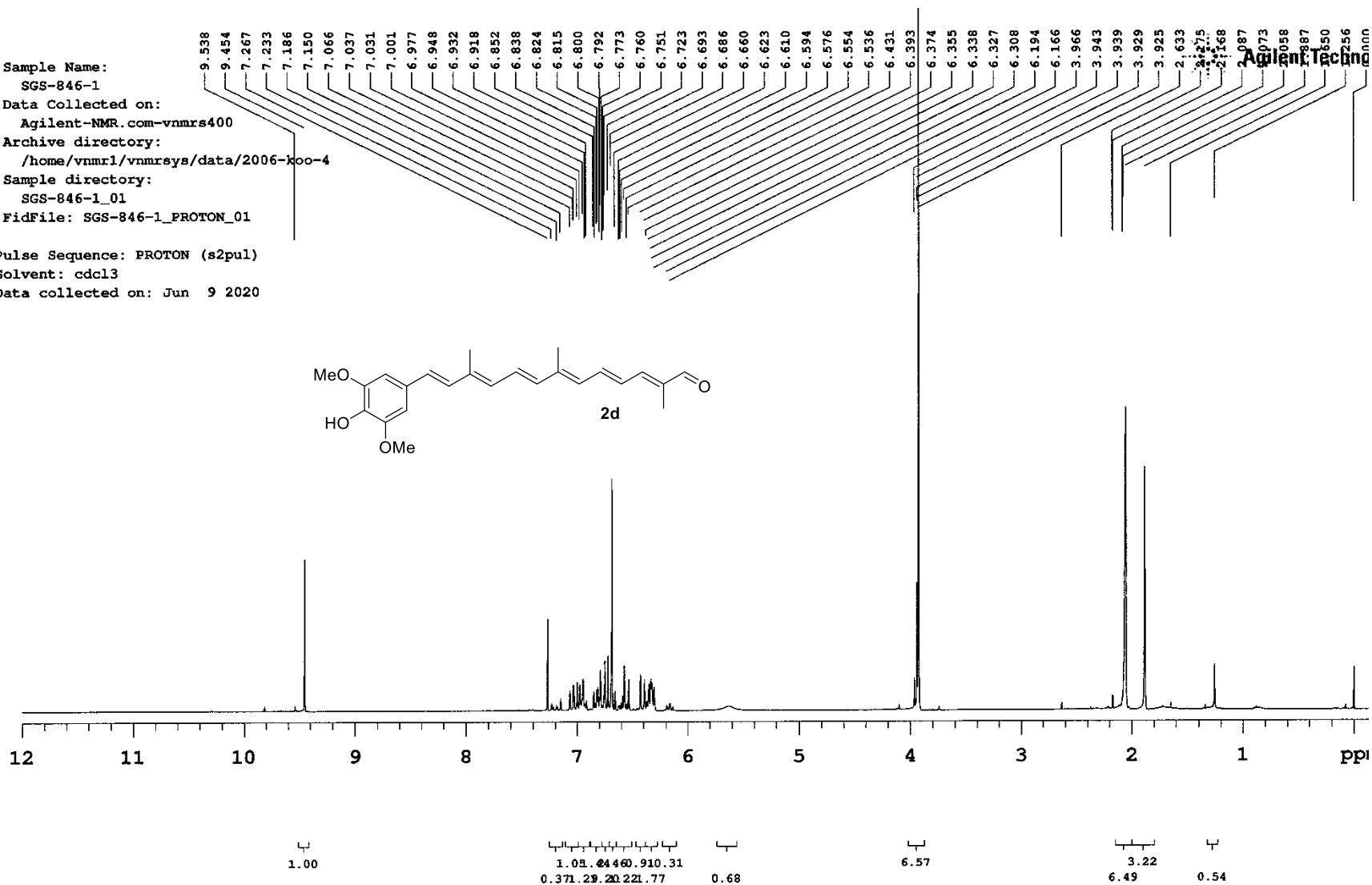


Figure S64. ¹H NMR of **2d**

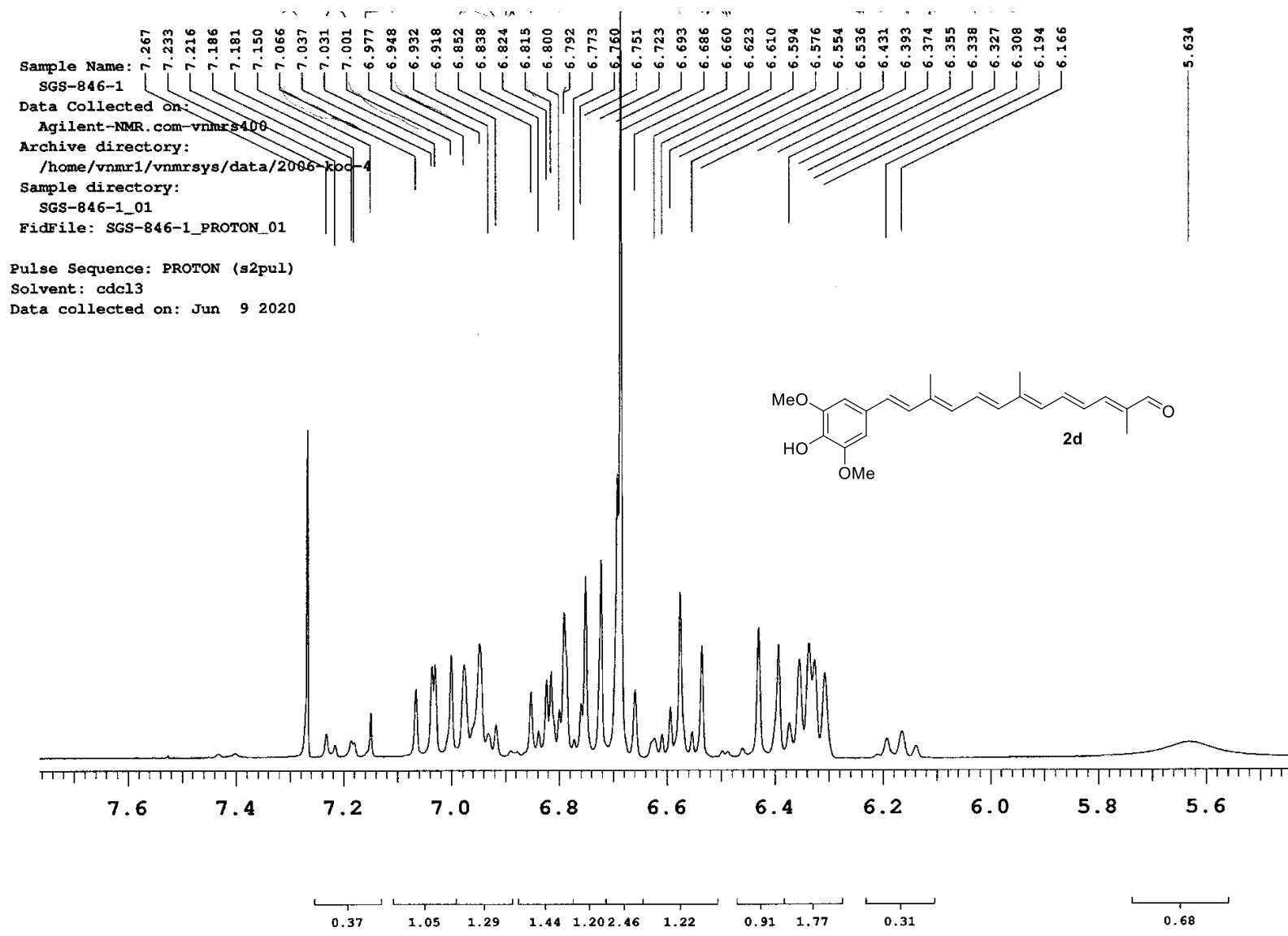


Figure S65. ¹H NMR of **2d** (expansion plot)

Sample Name: SGS-846-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2006-koo-4
 Sample directory: SGS-846-1_02
 FidFile: SGS-846-1_CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 10 2020

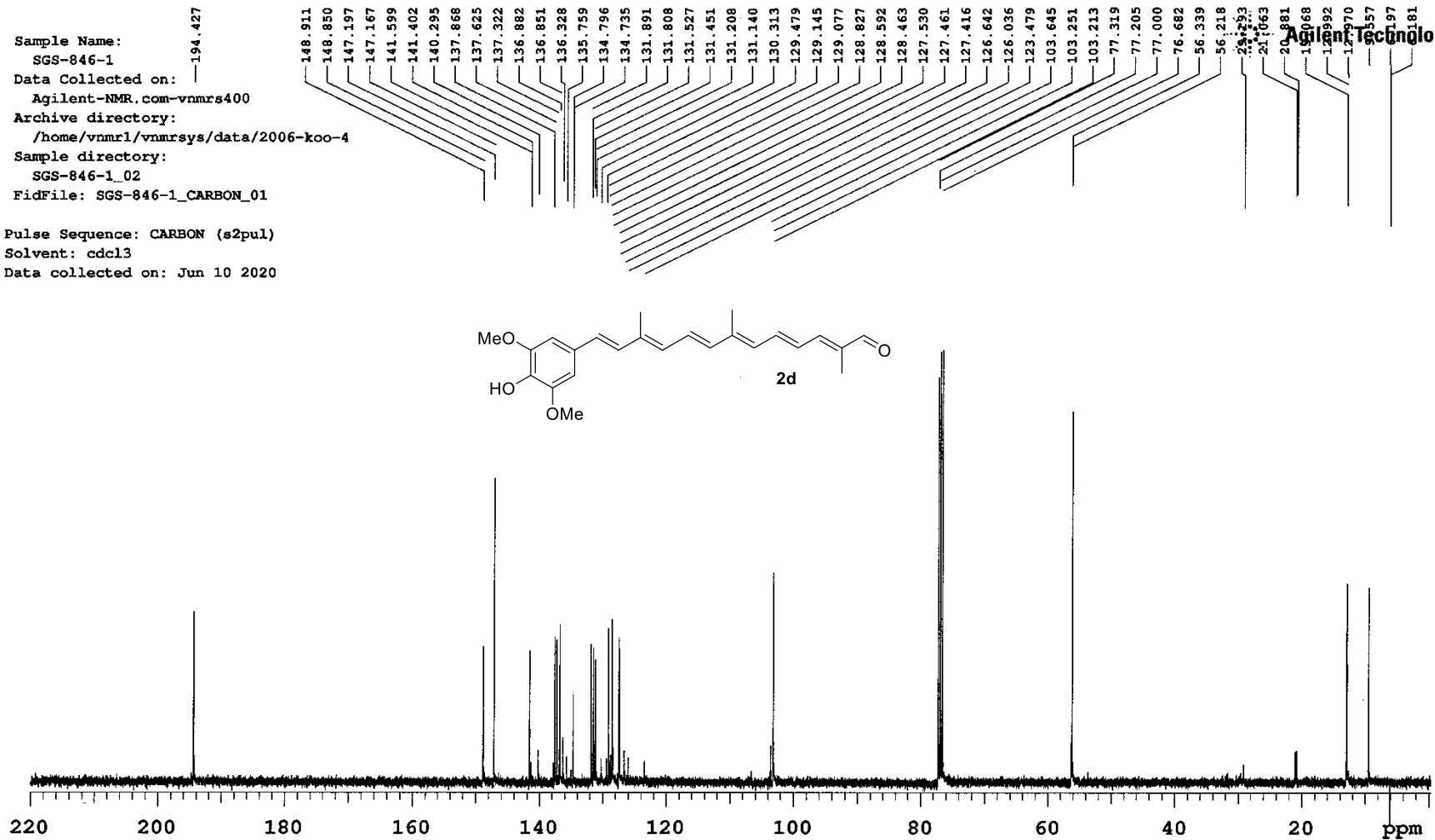


Figure S66. ¹³C NMR of 2d

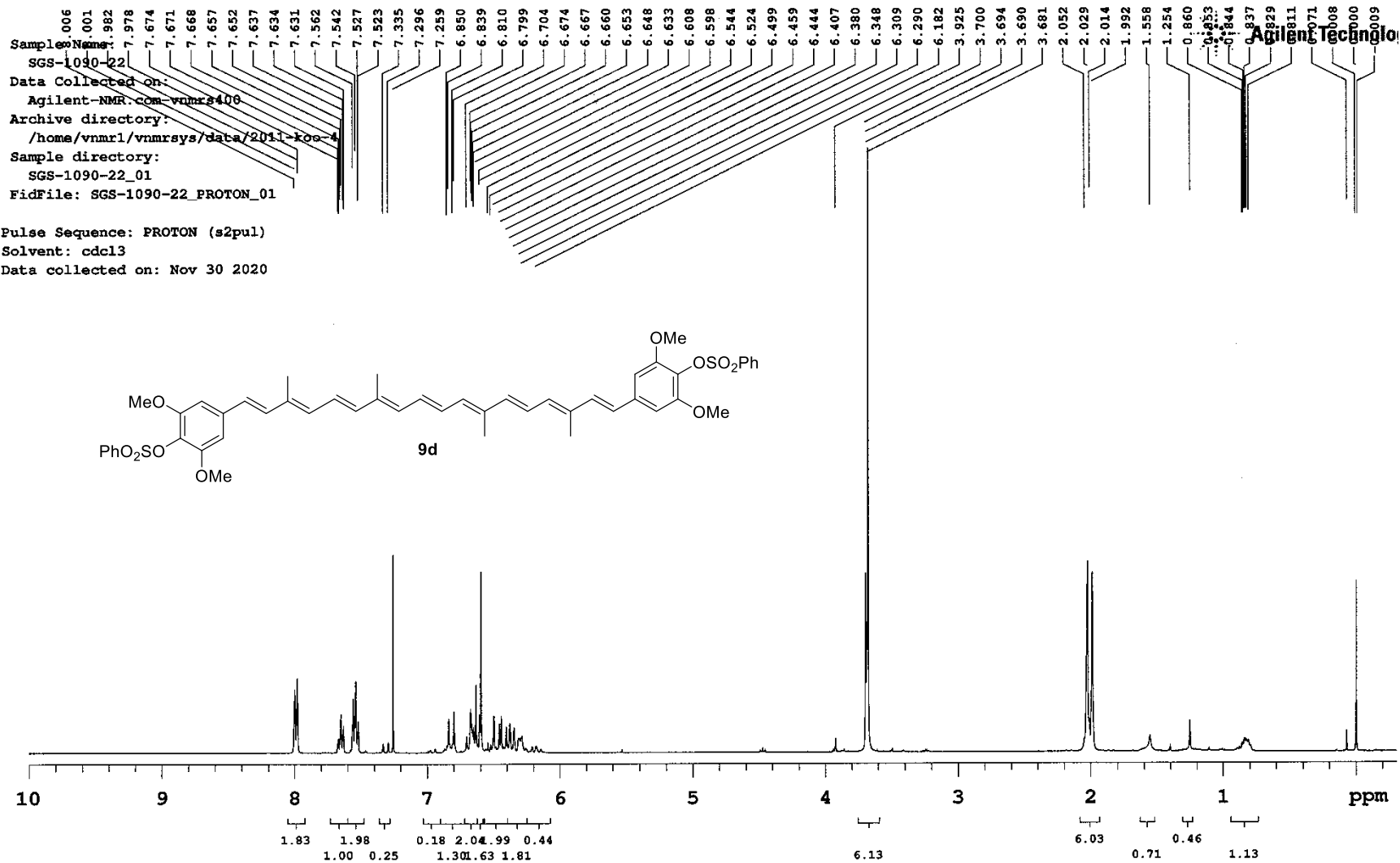
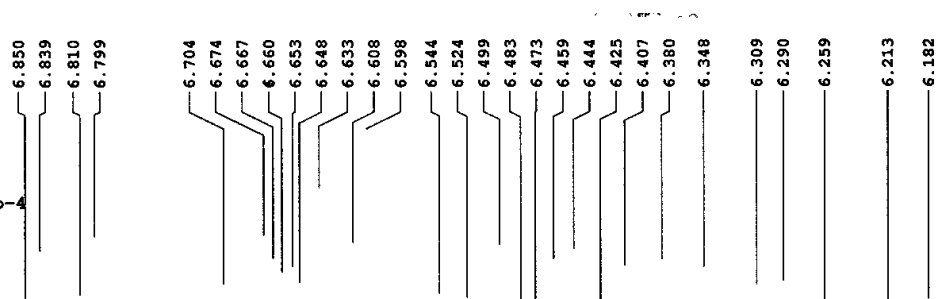


Figure S67. ¹H NMR of **9d**

Sample Name:
 SGS-1090-22
 Data Collected on:
 Agilent-NMR.com-vmnrs400
 Archive directory:
 /home/vnmr1/vnmrsys/data/2011-koo-4
 Sample directory:
 SGS-1090-22_01
 Fidfile: SGS-1090-22_PROTON_01



Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Nov 30 2020

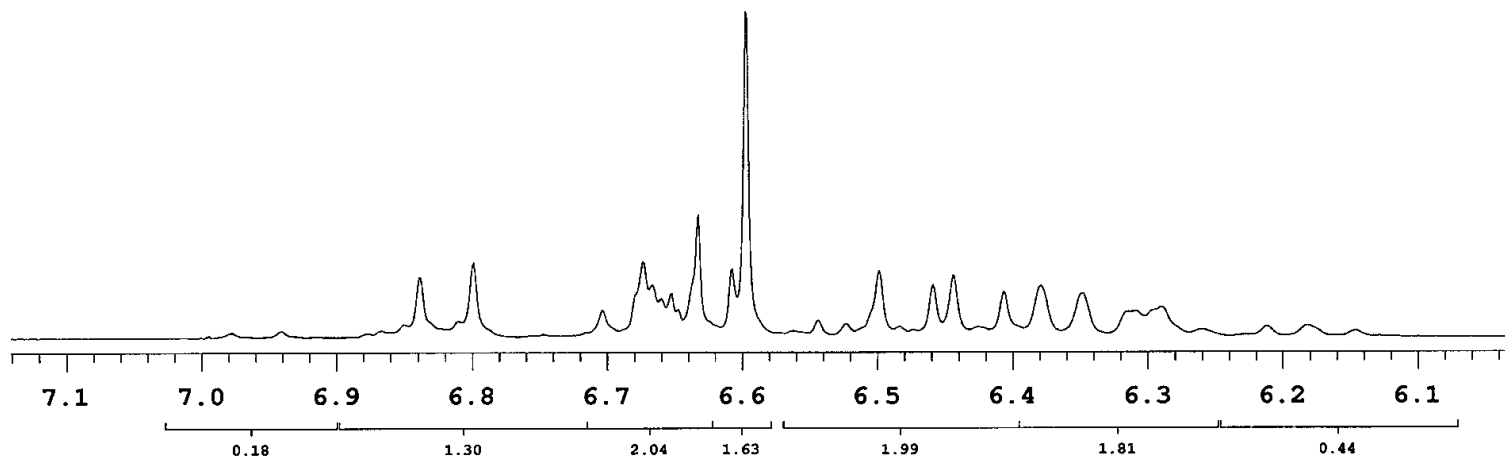
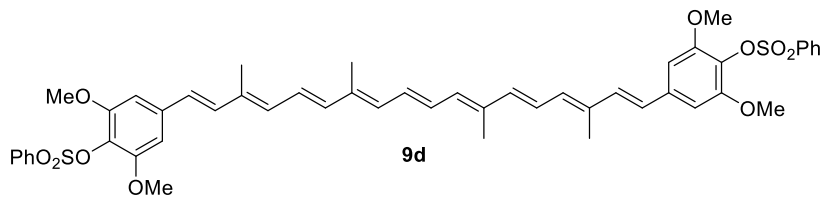


Figure S68. ¹H NMR of **9d** (expansion plot)

Sample Name:
SGS-1090-22
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2012-koo-4
Sample directory:
SGS-1090-22_01
FidFile: SGS-1090-22_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 2 2020

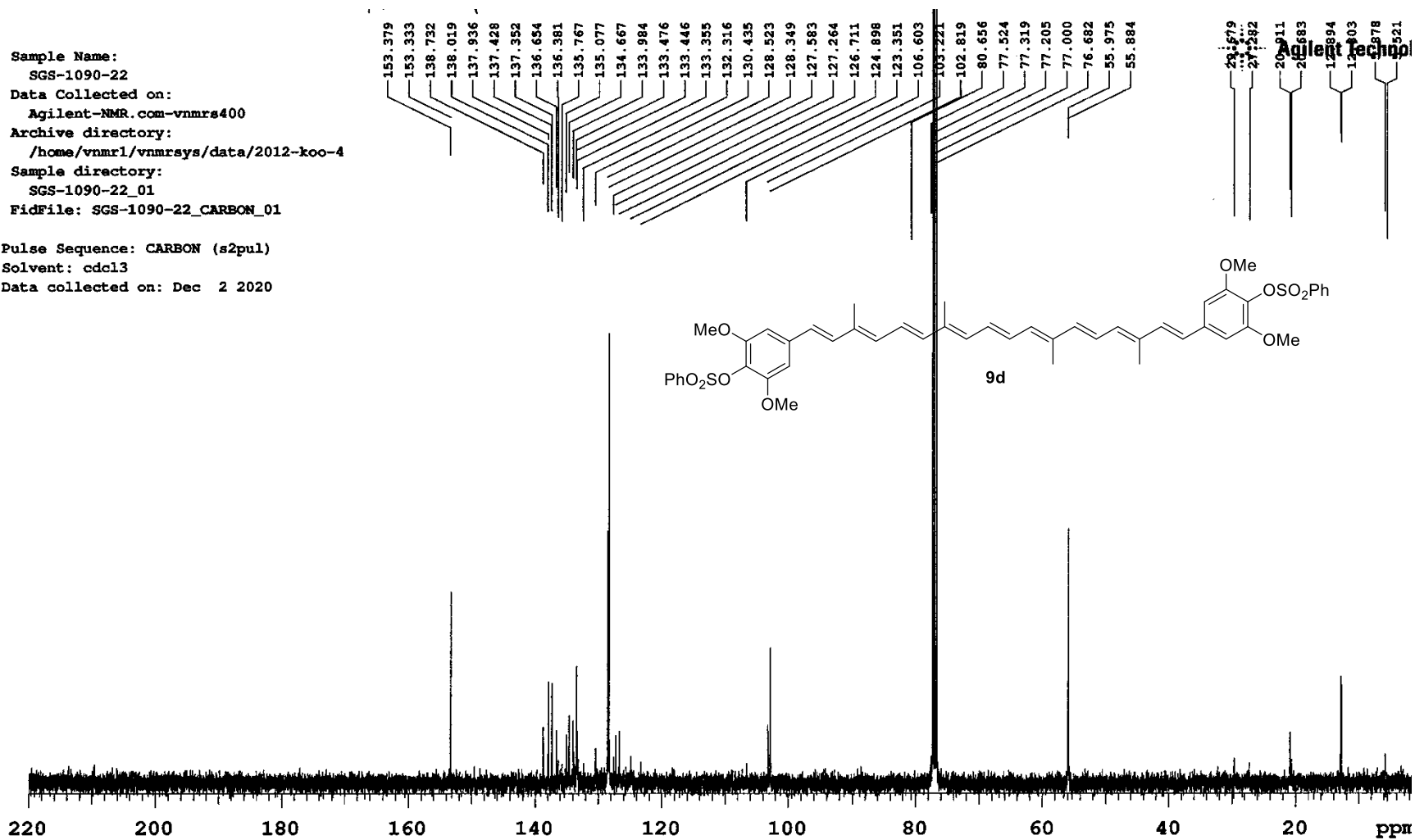


Figure S69. ¹³C NMR of 9d

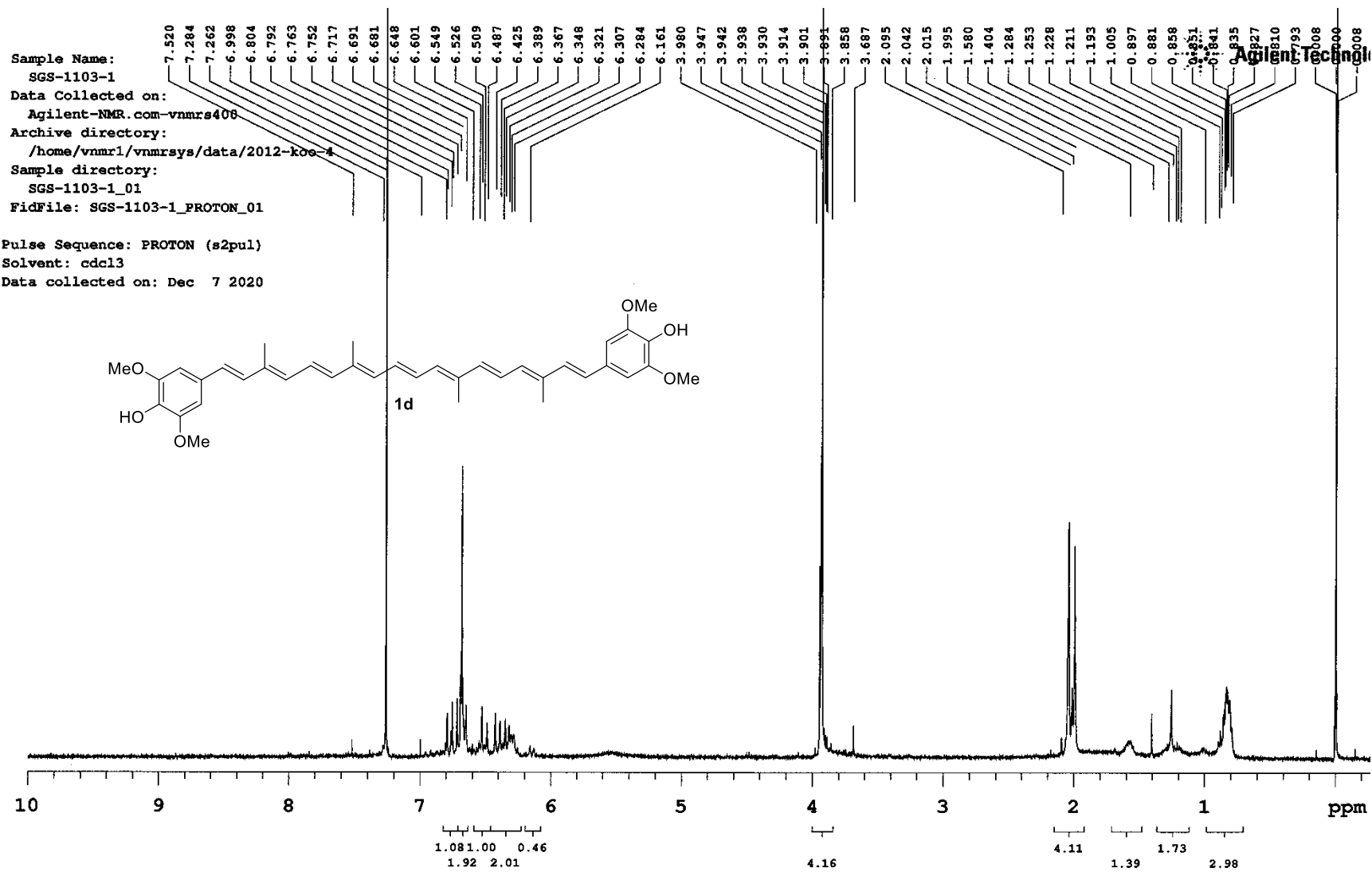


Figure S70. ¹H NMR of 1d

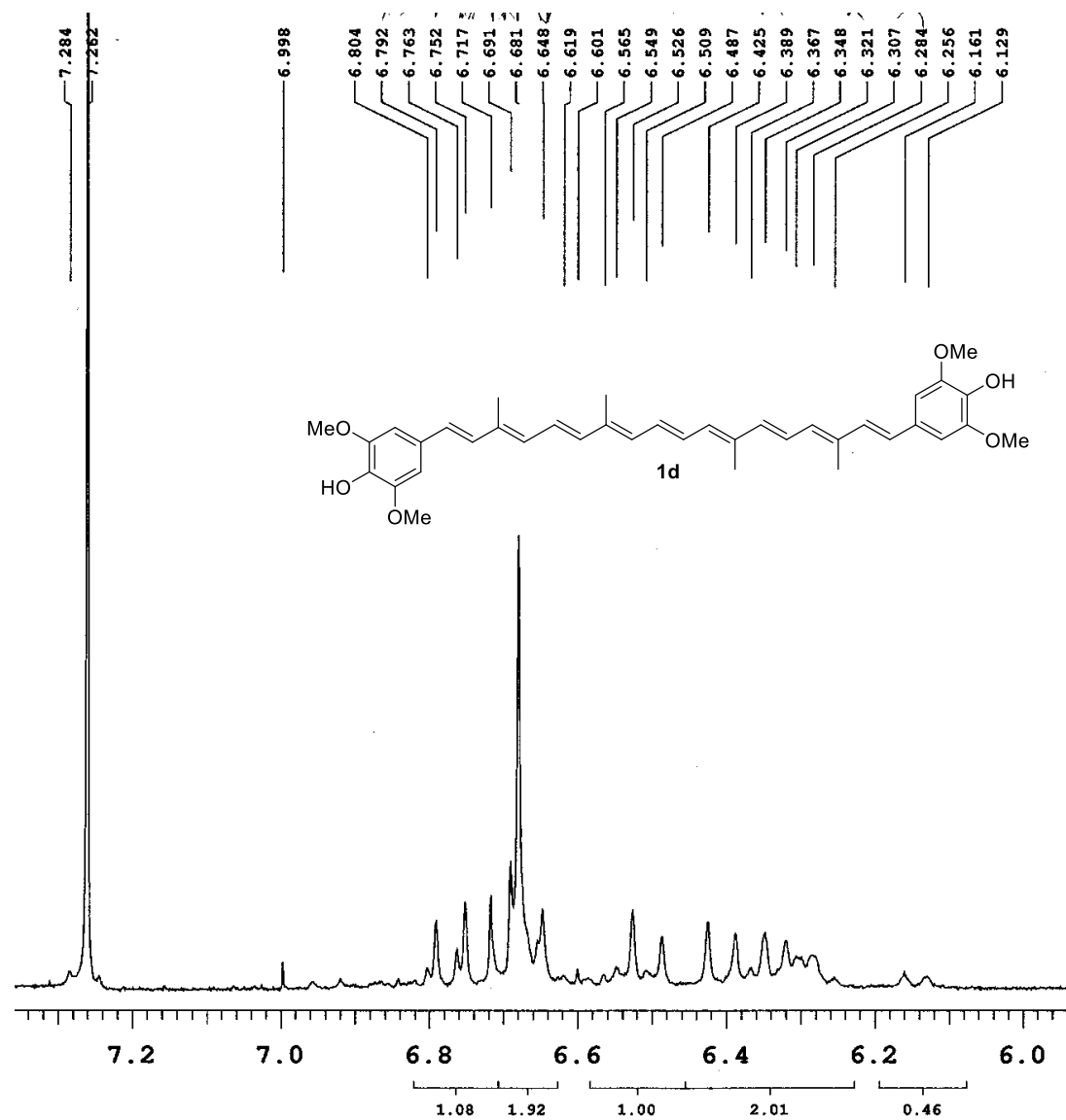


Figure S71. ^1H NMR of **1d** (expansion plot)

Sample Name:
SGS-456-11
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2006-koo-4
Sample directory:
SGS-456-11_01
FidFile: SGS-456-11_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2020

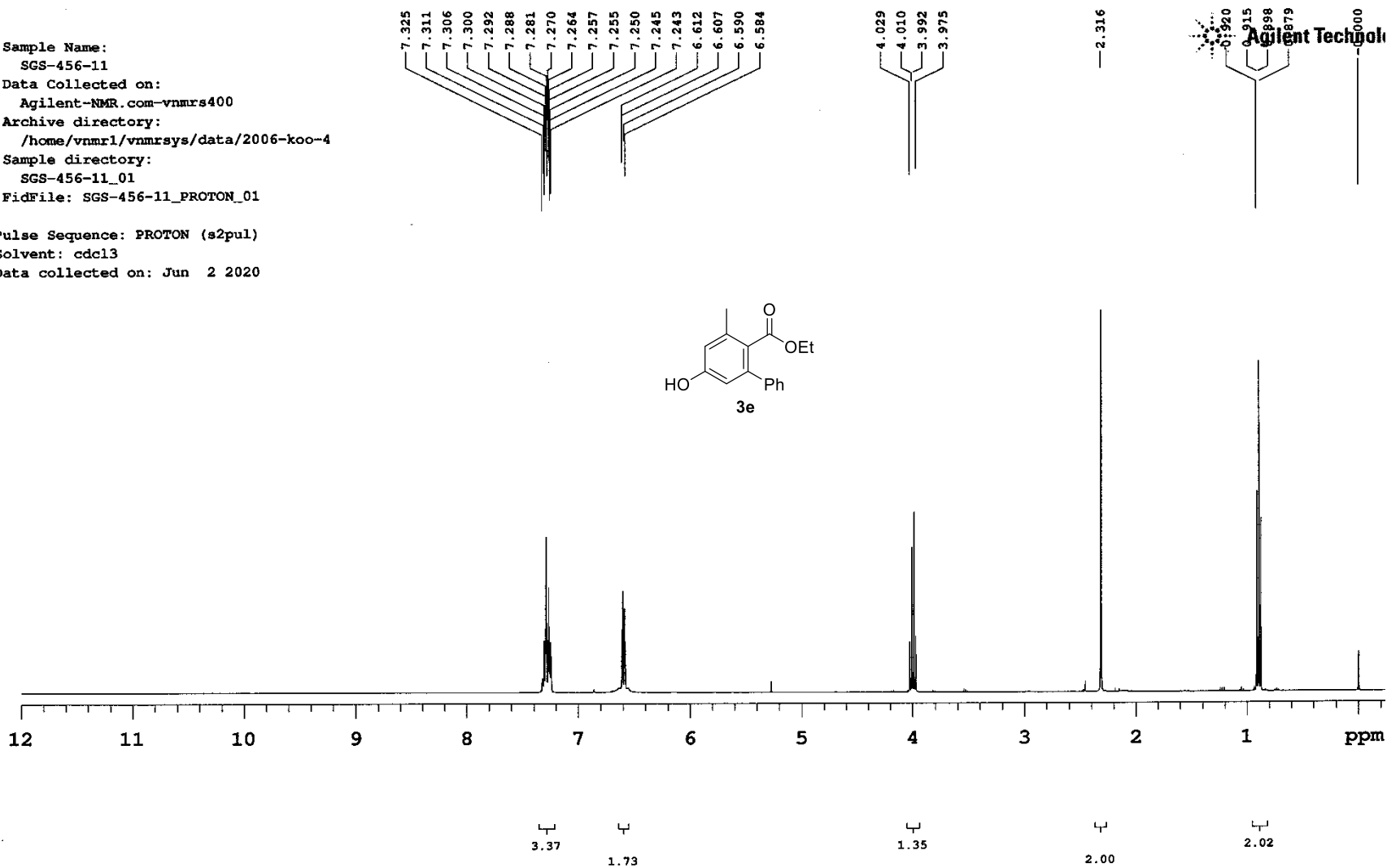


Figure S72. ^1H NMR of **3e**

Sample Name:
SGS-465-11
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2006-koo-4
Sample directory:
SGS-465-11_01
FidFile: SGS-465-11_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 5 2020

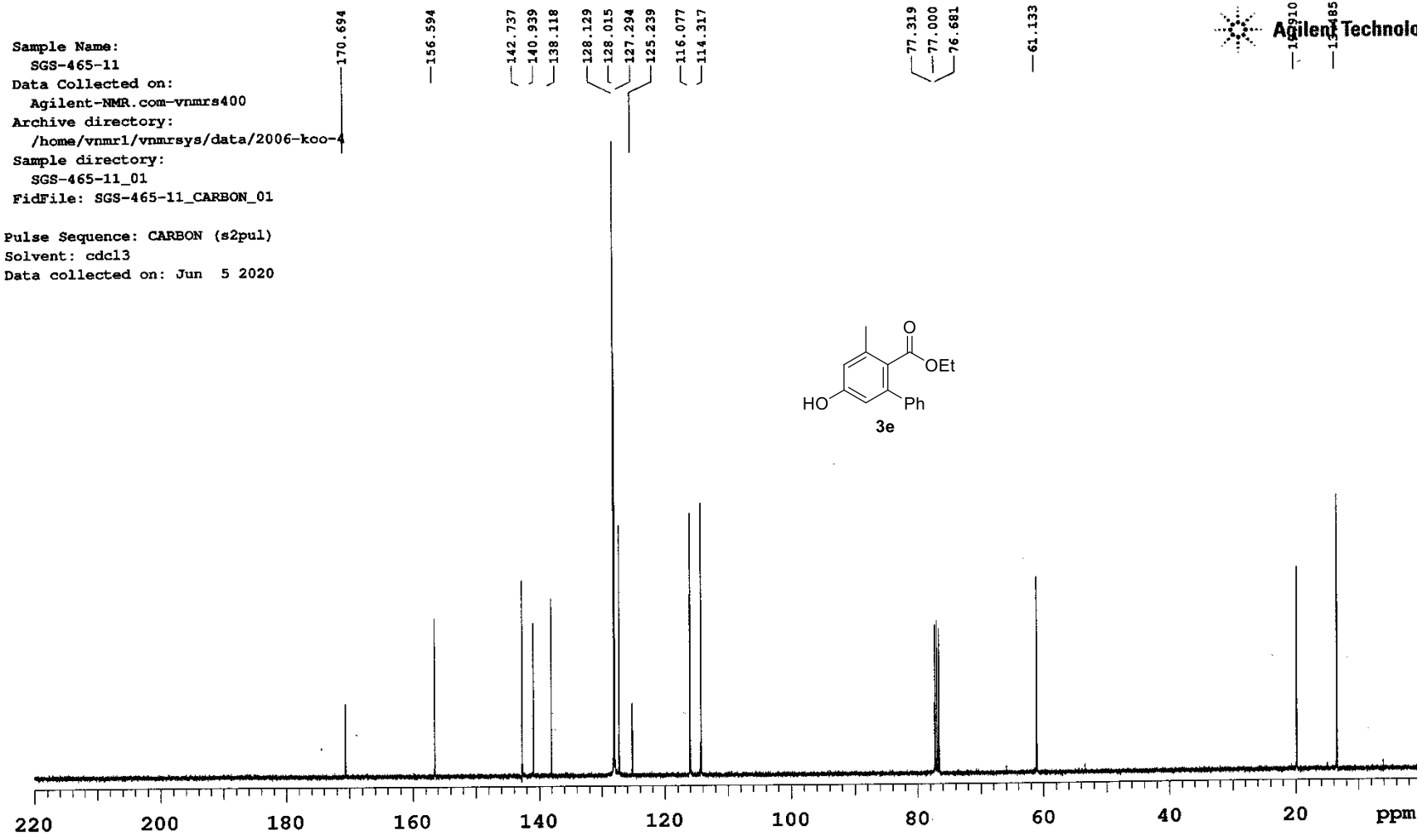
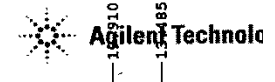


Figure S73. ¹³C NMR of 3e

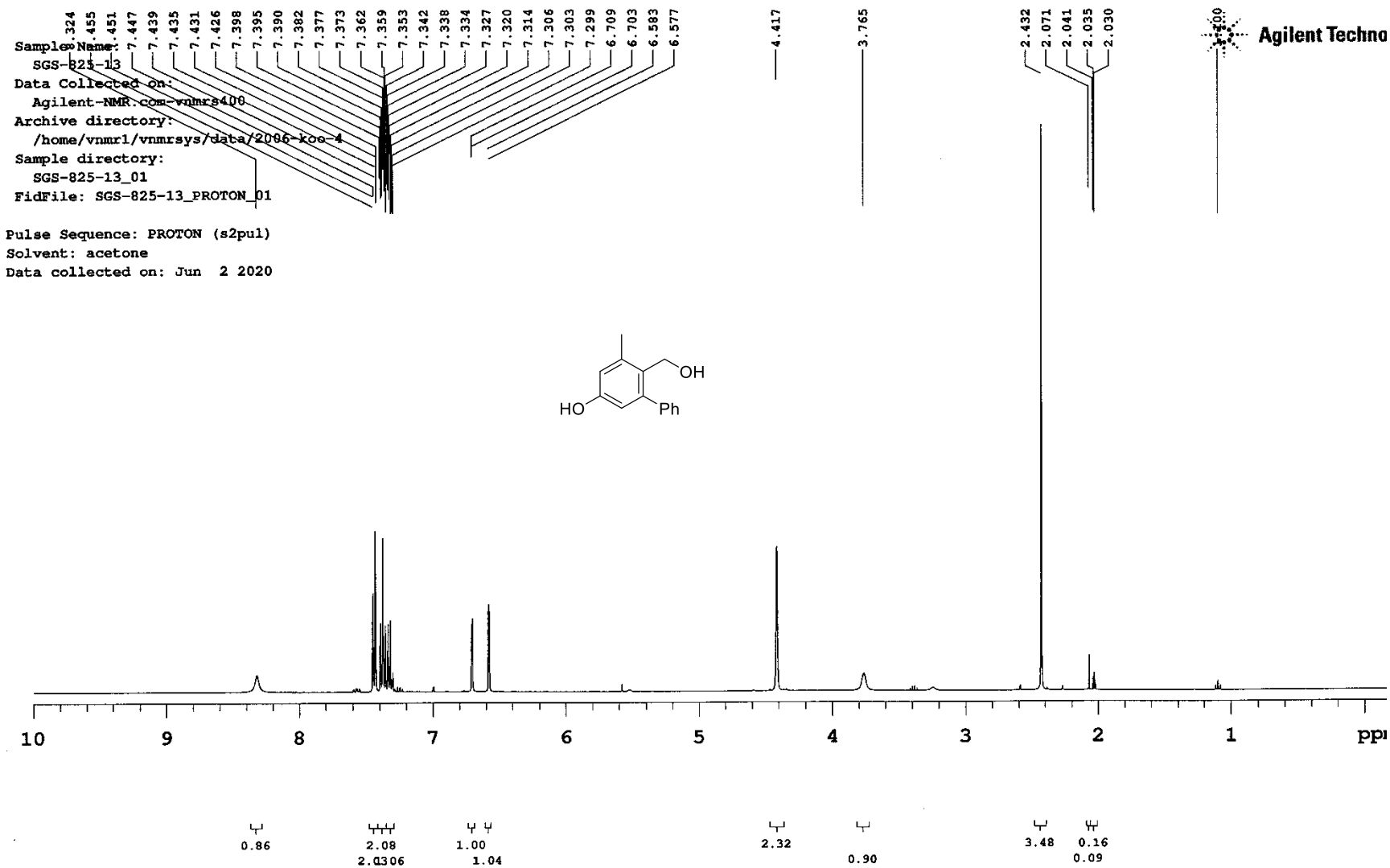


Figure S74. ^1H NMR of 6-(hydroxymethyl)-5-methyl-[1,1'-biphenyl]-3-ol

Sample Name: 2006-koo-4
SGS-825-13
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2006-koo-4
Sample directory:
SGS-825-13_02
FidFile: SGS-825-13_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: acetone
Data collected on: Jun 5 2020

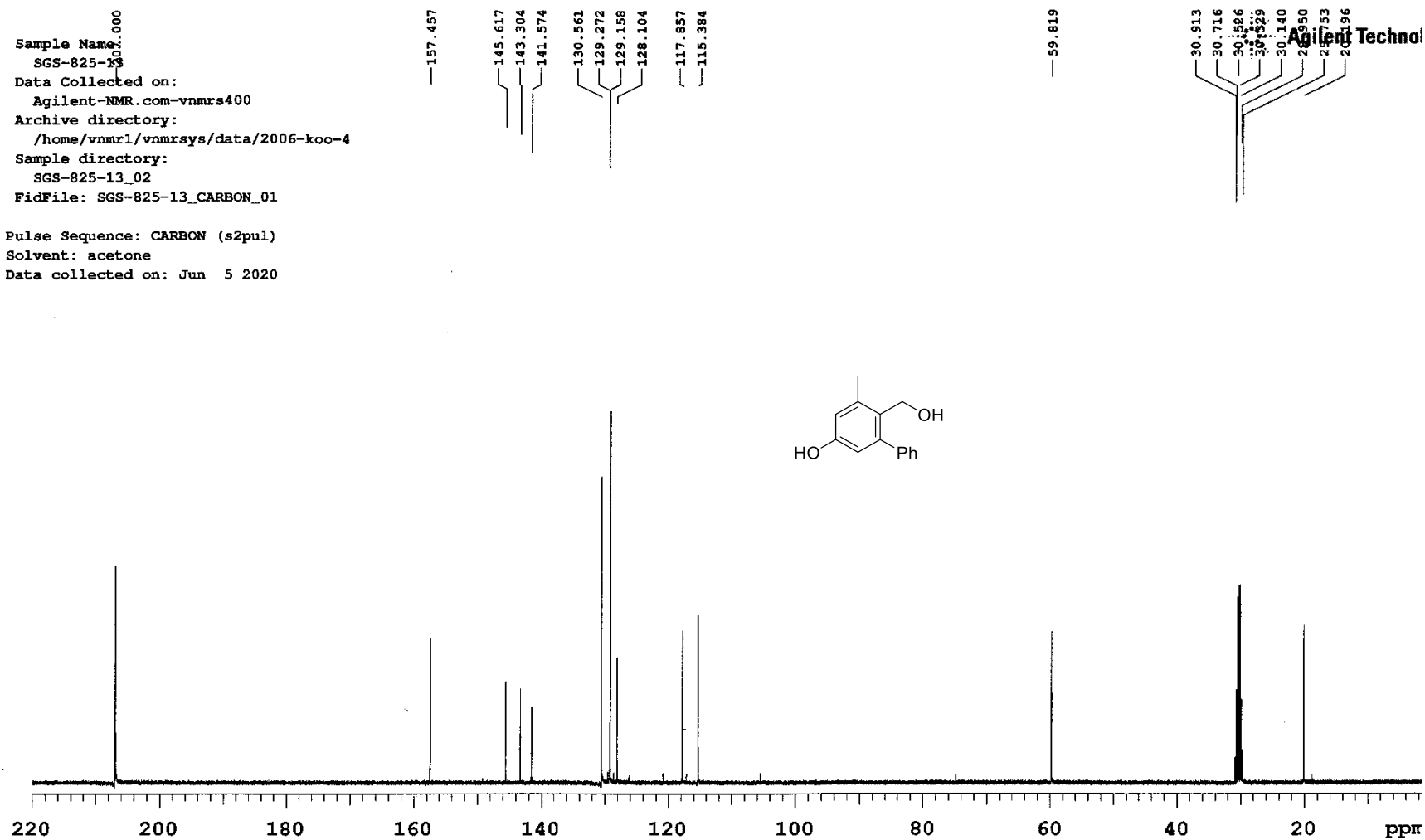


Figure S75. ^{13}C NMR of 6-(hydroxymethyl)-5-methyl-[1,1'-biphenyl]-3-ol

Sample Name: SGS-477-P
Data Collected on: Agilent-NMR.com-vnmrs400
Archive directory: /home/vnmr1/vnmrsys/data/2006-koo-4
Sample directory: SGS-477-P_01
FidFile: SGS-477-P_PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 1 2020

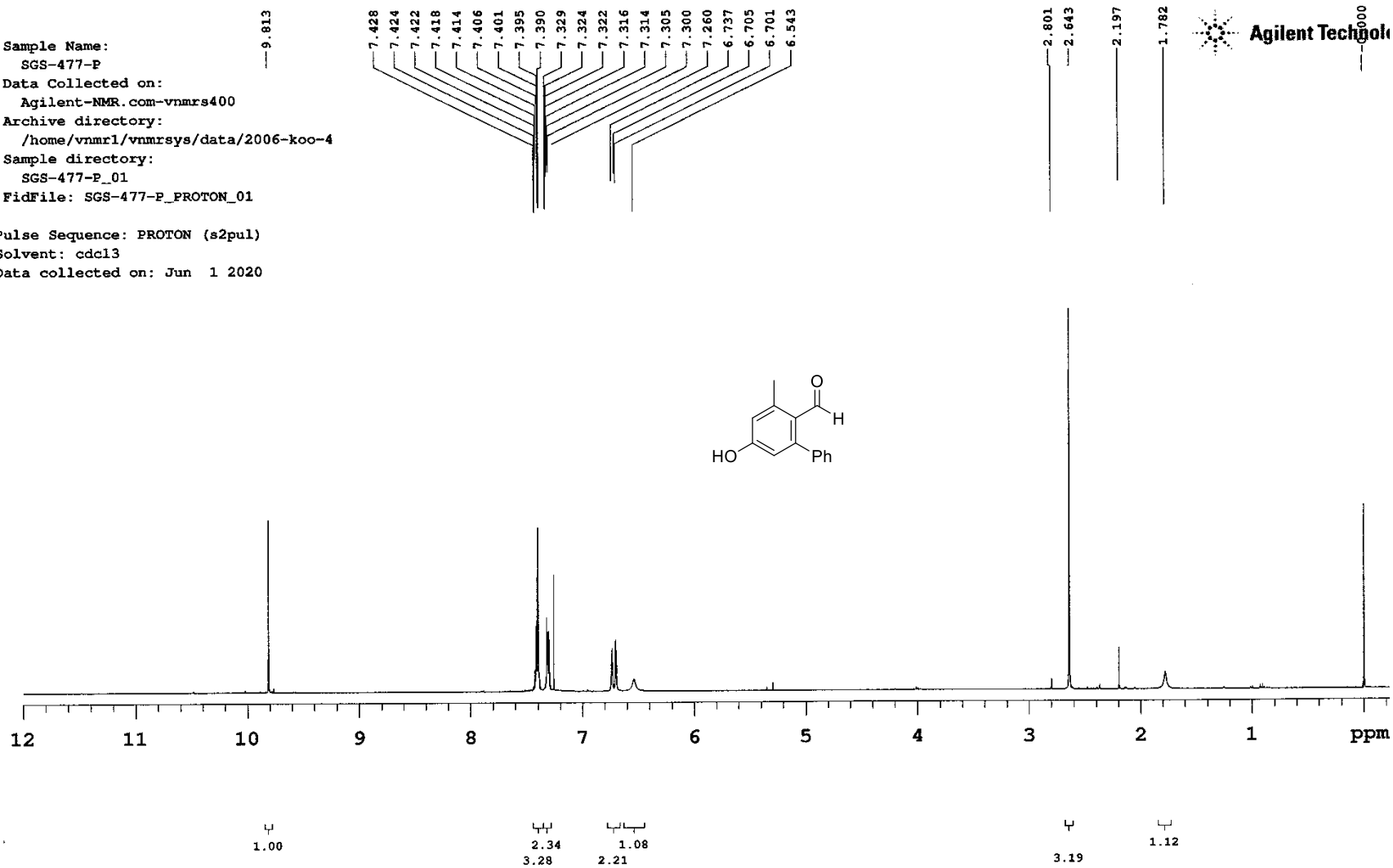


Figure S76. ¹H NMR of 5-hydroxy-3-methyl-[1,1'-biphenyl]-2-carbaldehyde

Sample Name:
SGS-477-P
Data Collected on:
Agilent-NMR.com-vnmrs400
Archive directory:
/home/vnmr1/vnmrsys/data/2006-koo-4
Sample directory:
SGS-477-P_02
FidFile: SGS-477-P_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2020

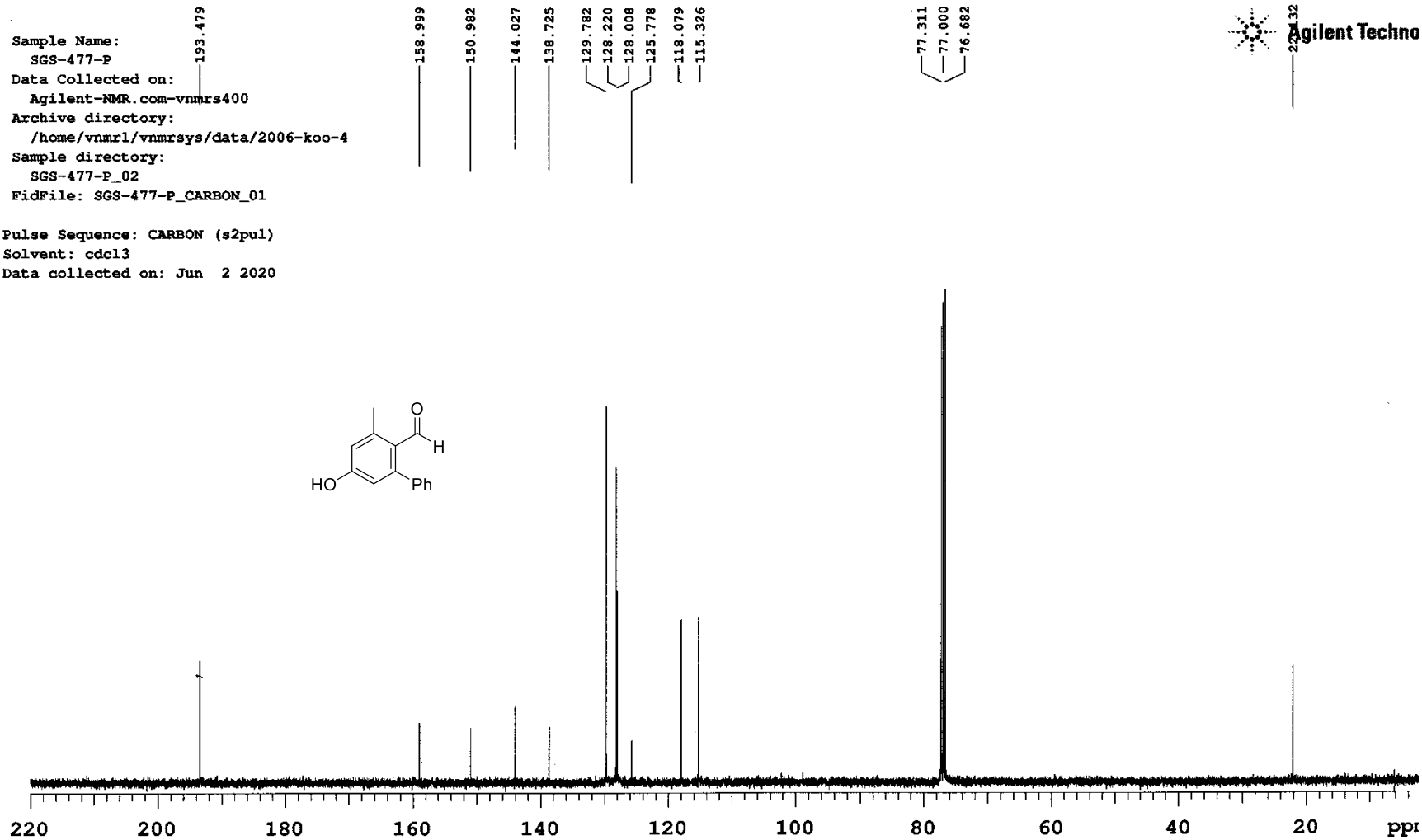


Figure S77. ^{13}C NMR of 5-hydroxy-3-methyl-[1,1'-biphenyl]-2-carbaldehyde

Sample Name: SGS-852-p1
 Data Collected on: Agilent-NMR.chem.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2105-K00-4-06
 Sample directory: SGS-852-p1_01
 FidFile: SGS-852-p1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: May 6 2021

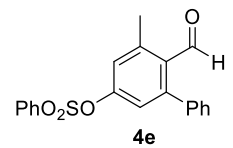
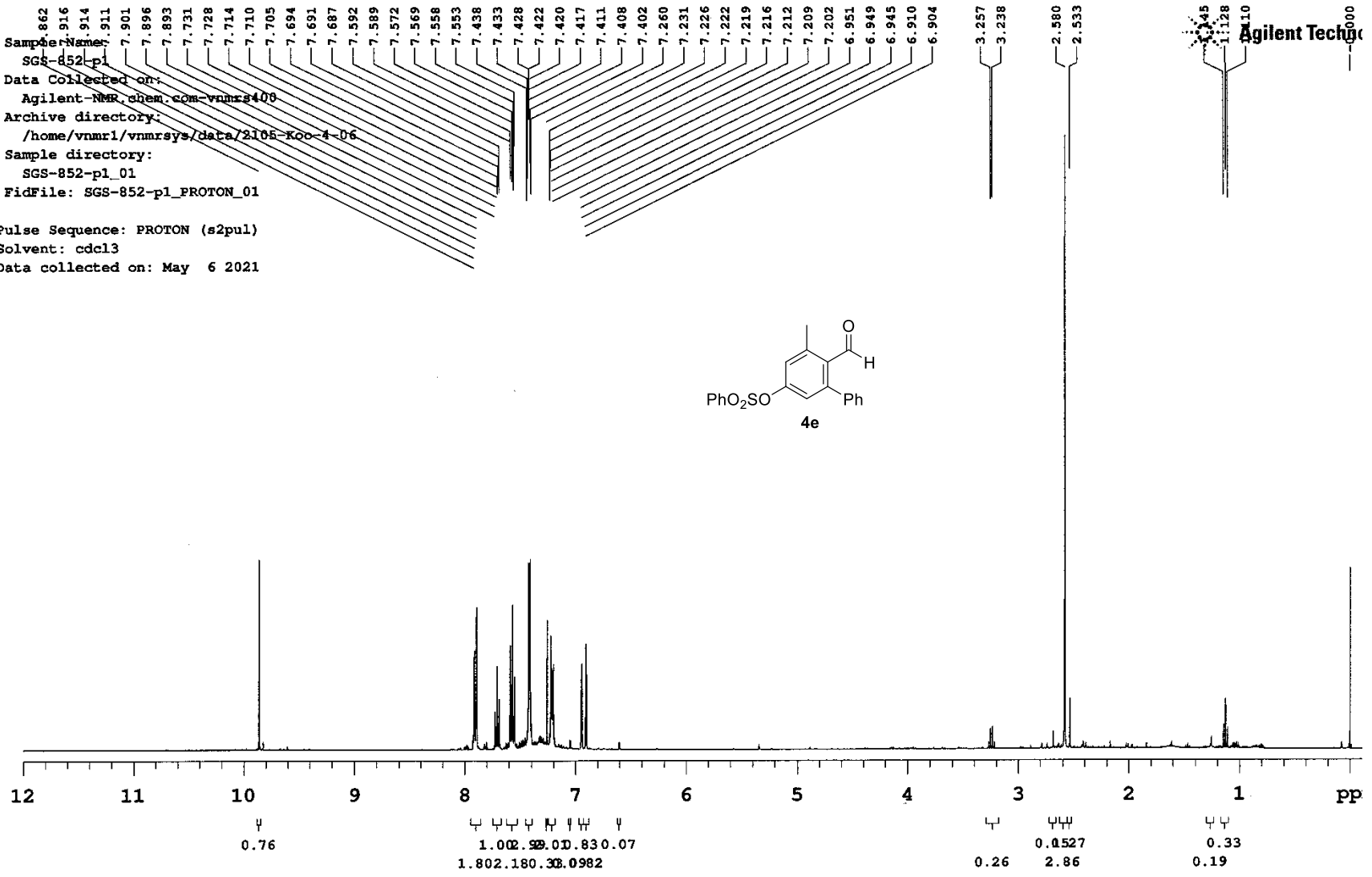


Figure S78. ¹H NMR of 4e

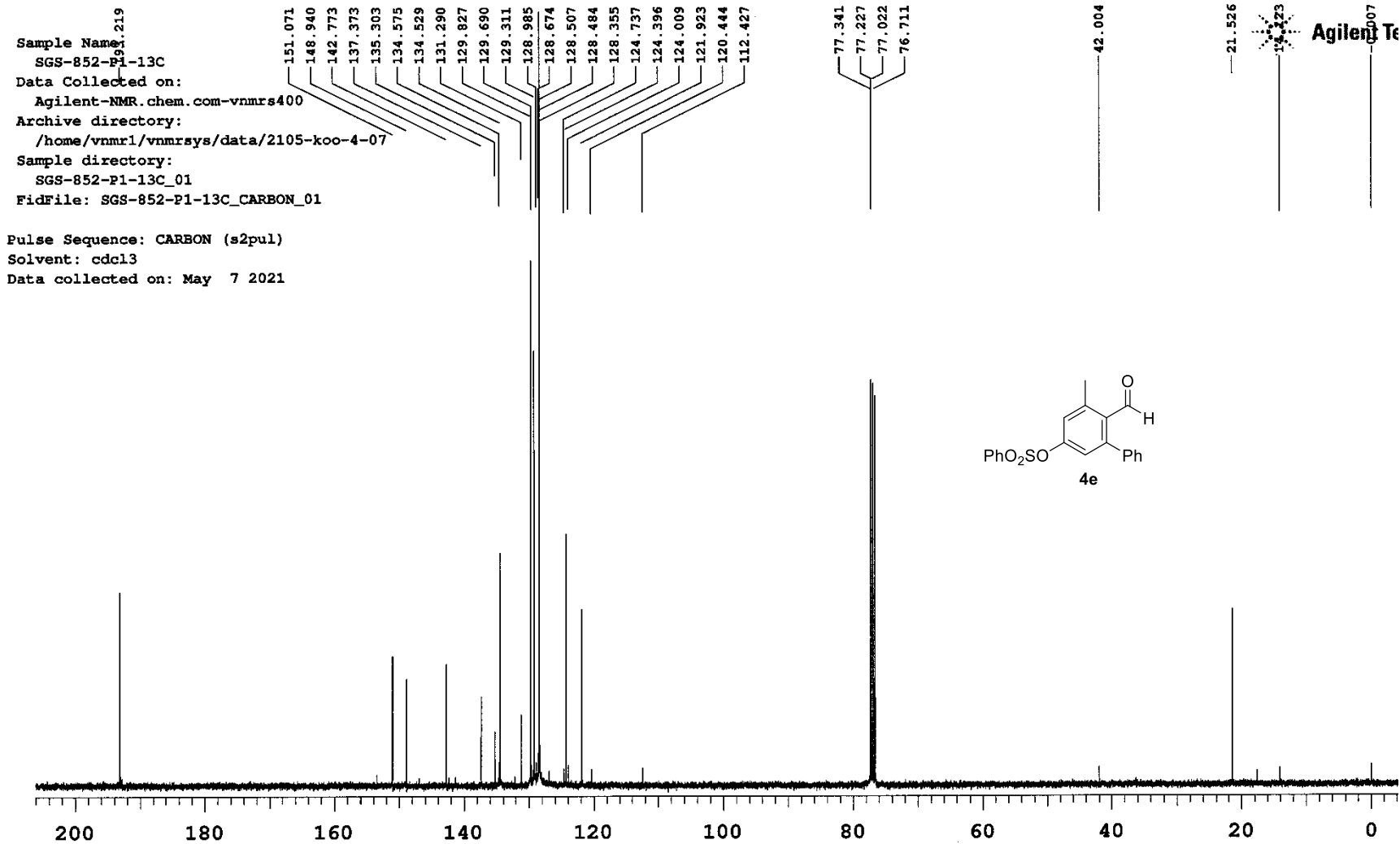


Figure S79. ¹³C NMR of **4e**

Sample Name: LN-220-1
 Data Collected on: Agilent-NMR.com-vnmr400
 Archive directory: /home/vnmr1/vnmrsys/Data/2006-koo-4
 Sample directory: LN-220-1_01
 FidFile: LN-220-1_PROTON_01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 29 2020

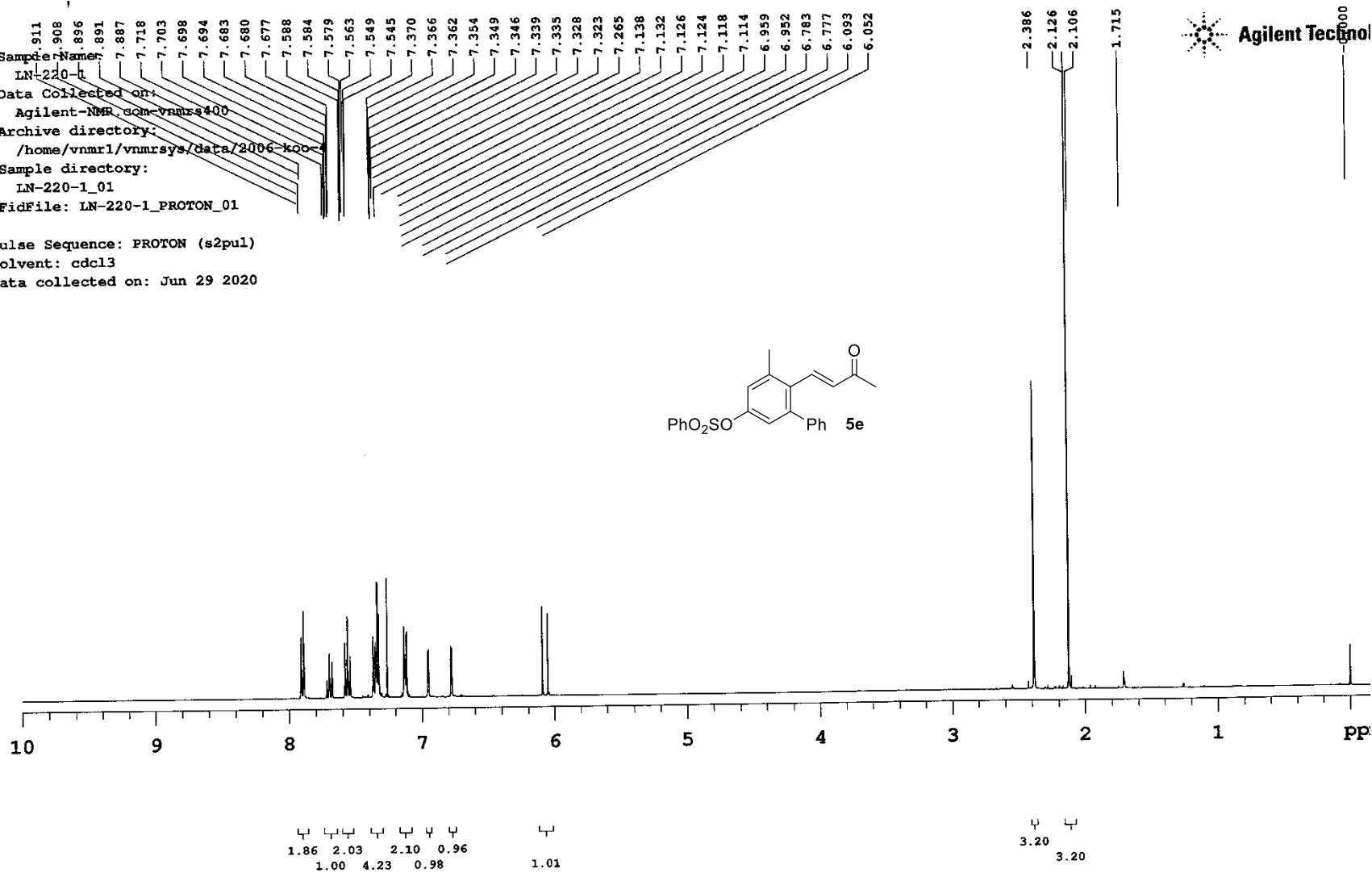
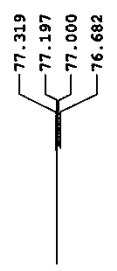
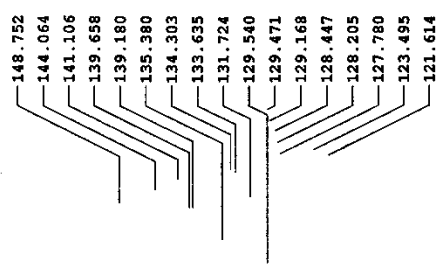


Figure S80. ¹H NMR of 5e

Sample Name: LN-220-1
 Data Collected on: 198.068
 Agilent-NMR.com vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2006-koo-4
 Sample directory: LN-220-1_02
 FidFile: LN-220-1 CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 30 2020



Agilent Technol

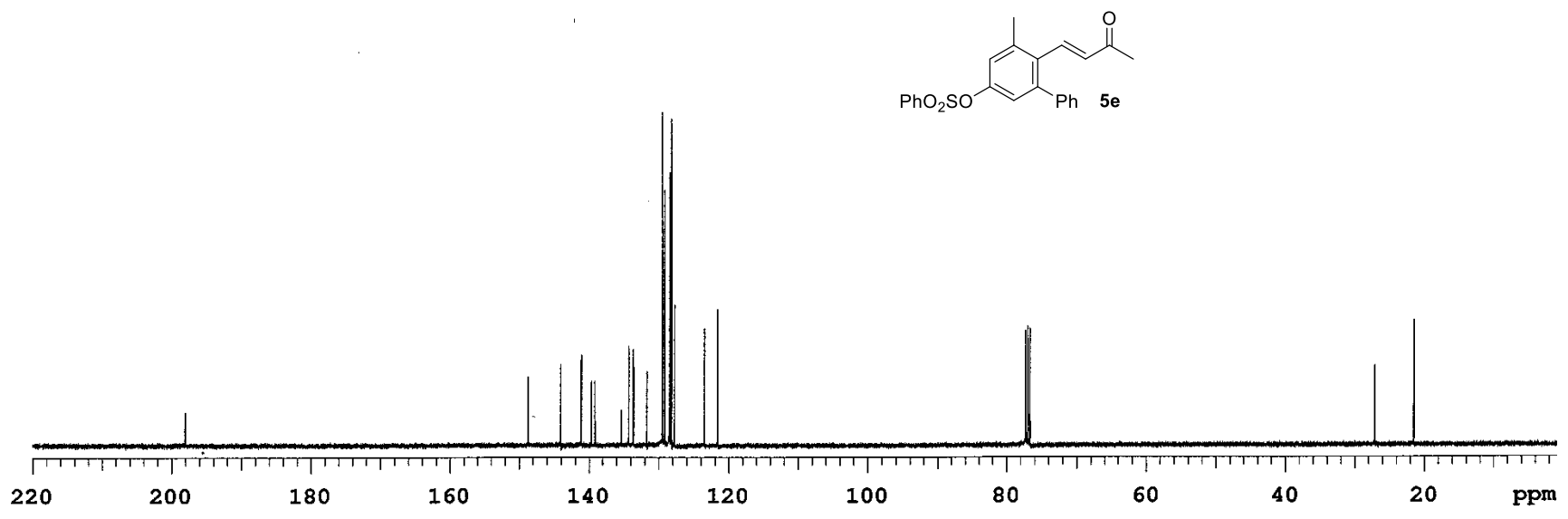


Figure S81. ¹³C NMR of 5e

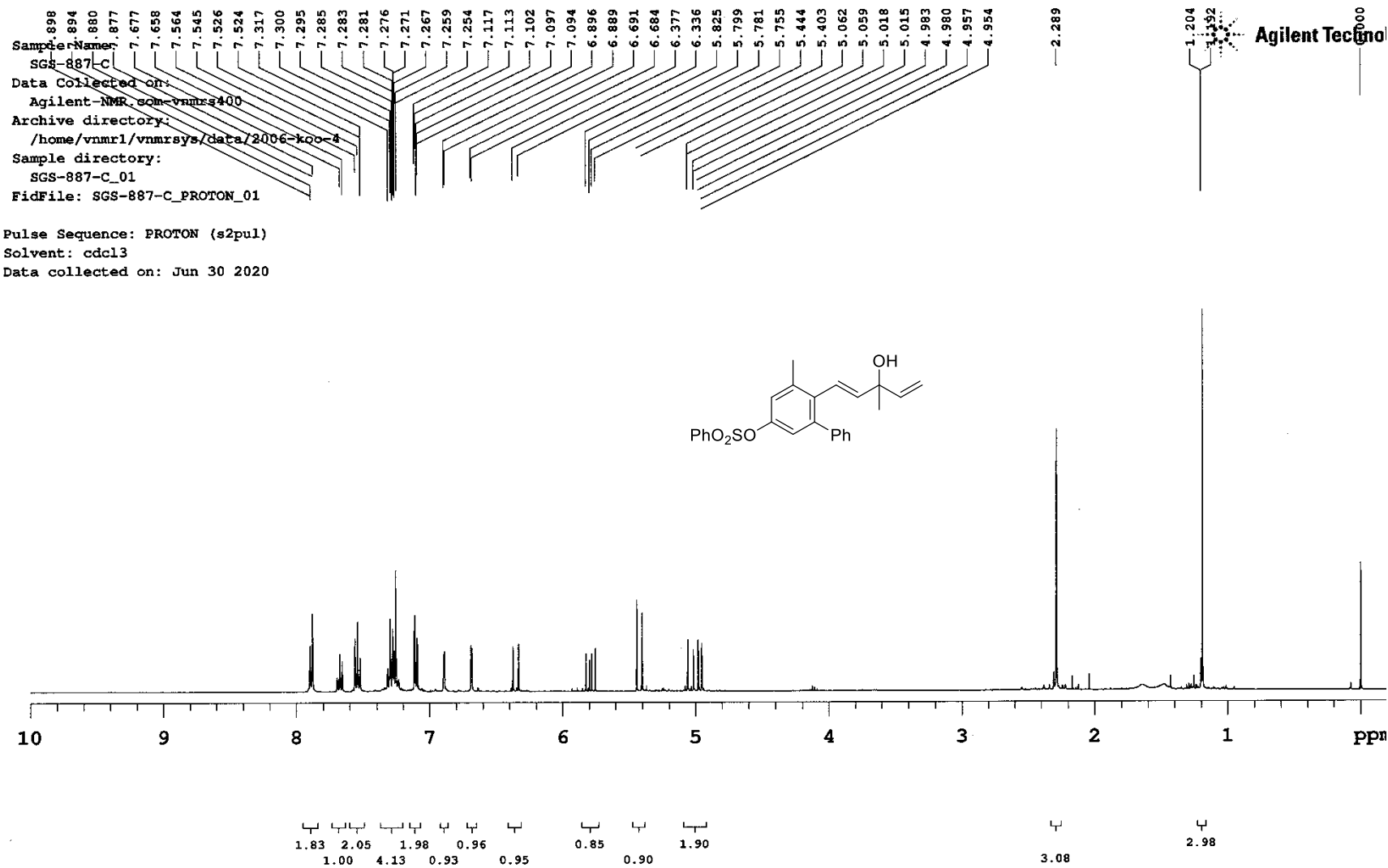


Figure S82. ¹H NMR of (*E*)-6-(3-hydroxy-3-methylpenta-1,4-dien-1-yl)-5-methyl-[1,1'-biphenyl]-3-yl benzenesulfonate

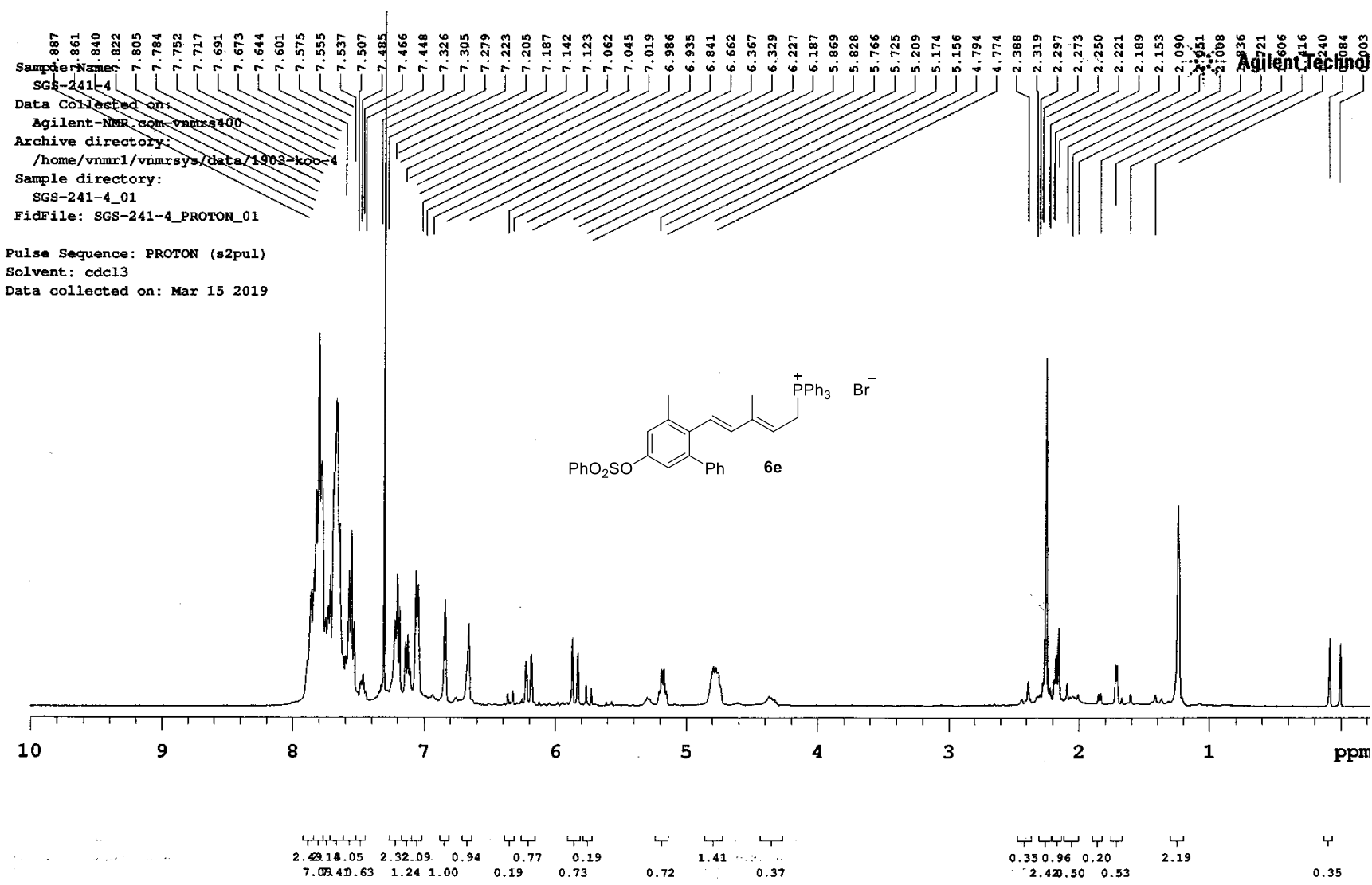


Figure S83. ^1H NMR of **6e**

Sample Name: SGS-931-ly
 Data Collected on: Agilent-NMR-cdm-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2008-kqo-4
 Sample directory: SGS-931-ly_01
 FidFile: SGS-931-ly_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 12 2020

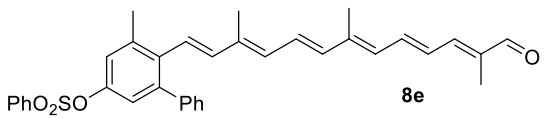
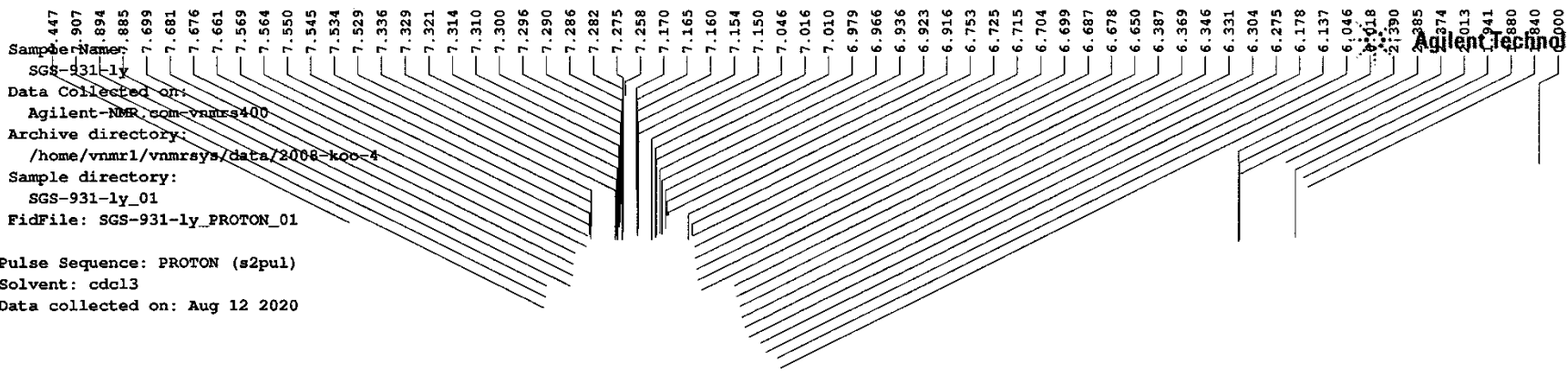


Figure S84. ¹H NMR of **8e**

914
 907
 894
 889
 885
 7.699
 7.684
 7.681
 7.676
 7.665
 7.661
 7.573
 7.569
 7.564
 7.550
 7.545
 7.534
 7.529
 7.525
 7.336
 7.329
 7.326
 7.321
 7.314
 7.310
 7.300
 7.296
 7.290
 7.286
 7.282
 7.275
 7.263
 7.258
 7.170
 7.165
 7.160
 7.154
 7.150
 7.147
 7.046
 7.016
 7.010
 6.979
 6.966
 6.936
 6.923
 6.916
 6.753
 6.725
 6.715
 6.704
 6.699
 6.687
 6.678
 6.650
 6.387
 6.369
 6.346
 6.331
 6.304
 6.275
 6.178
 6.137
 6.046
 6.018

Sample Name: SGS-931-1y
 Date Collected on:
 Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2008-koor-4
 Sample directory: SGS-931-1y_01
 File: SGS-931-1y_PROTON_01

 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Date collected on: Aug 12 2020

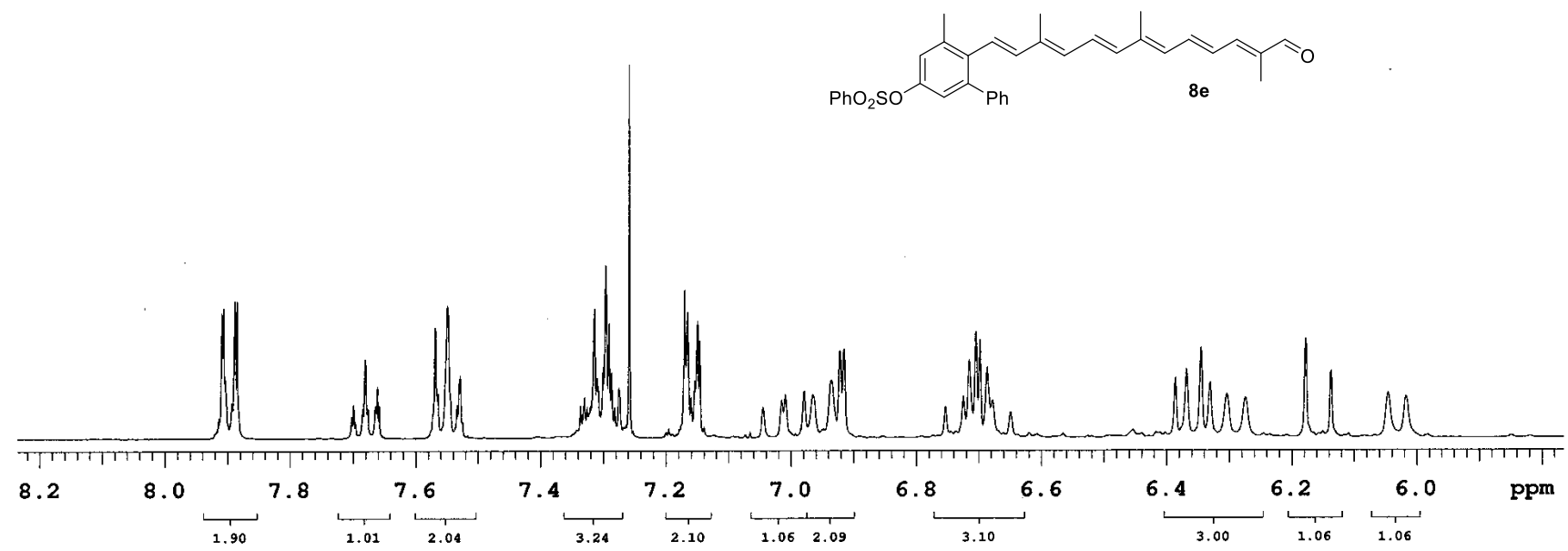


Figure S85. ¹H NMR of **8e** (expansion plot)

Sample Name: SGS-931-ly
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2008-koo-4
 Sample directory: SGS-931-ly_02
 FidFile: SGS-931-ly CARBON_01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 13 2020

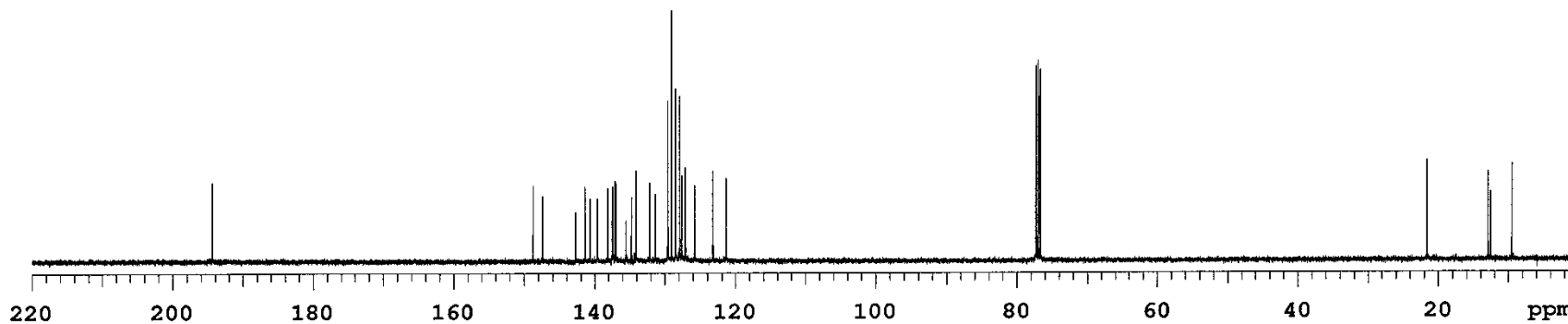
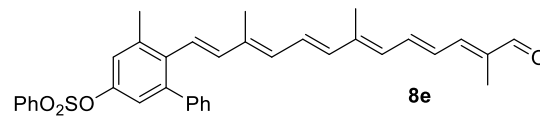
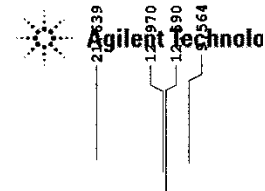
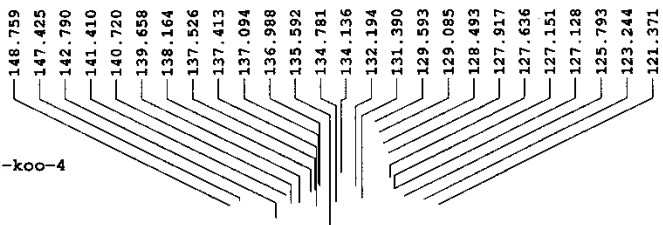


Figure S86. ¹³C NMR of **8e**

Sample Name: SGS-964-1
 Data Collected on: Agilent-NMR.com-vnmrs400
 Archive directory: /home/vnmr1/vnmrsys/data/2008-koo-4
 Sample directory: SGS-964-1_01
 FidFile: SGS-964-1_PROTON_01
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 13 2020

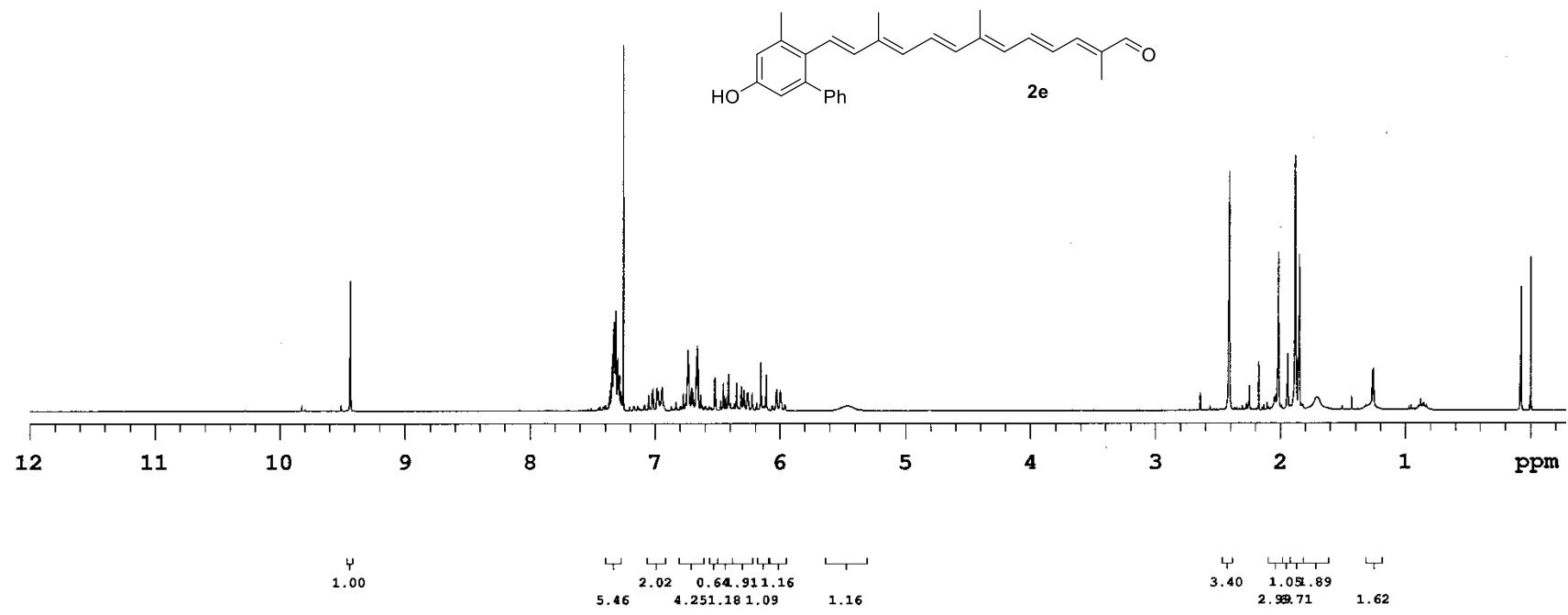
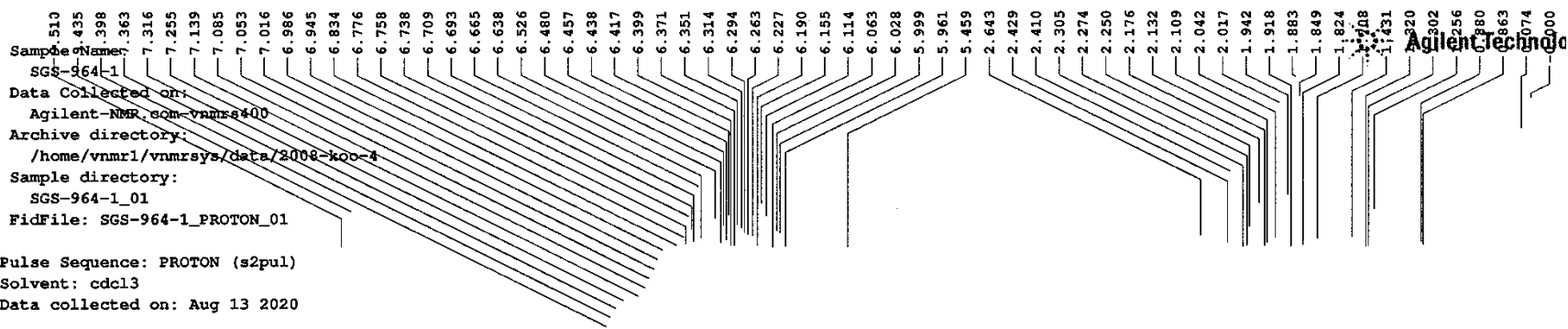


Figure S87. ¹H NMR of 2e

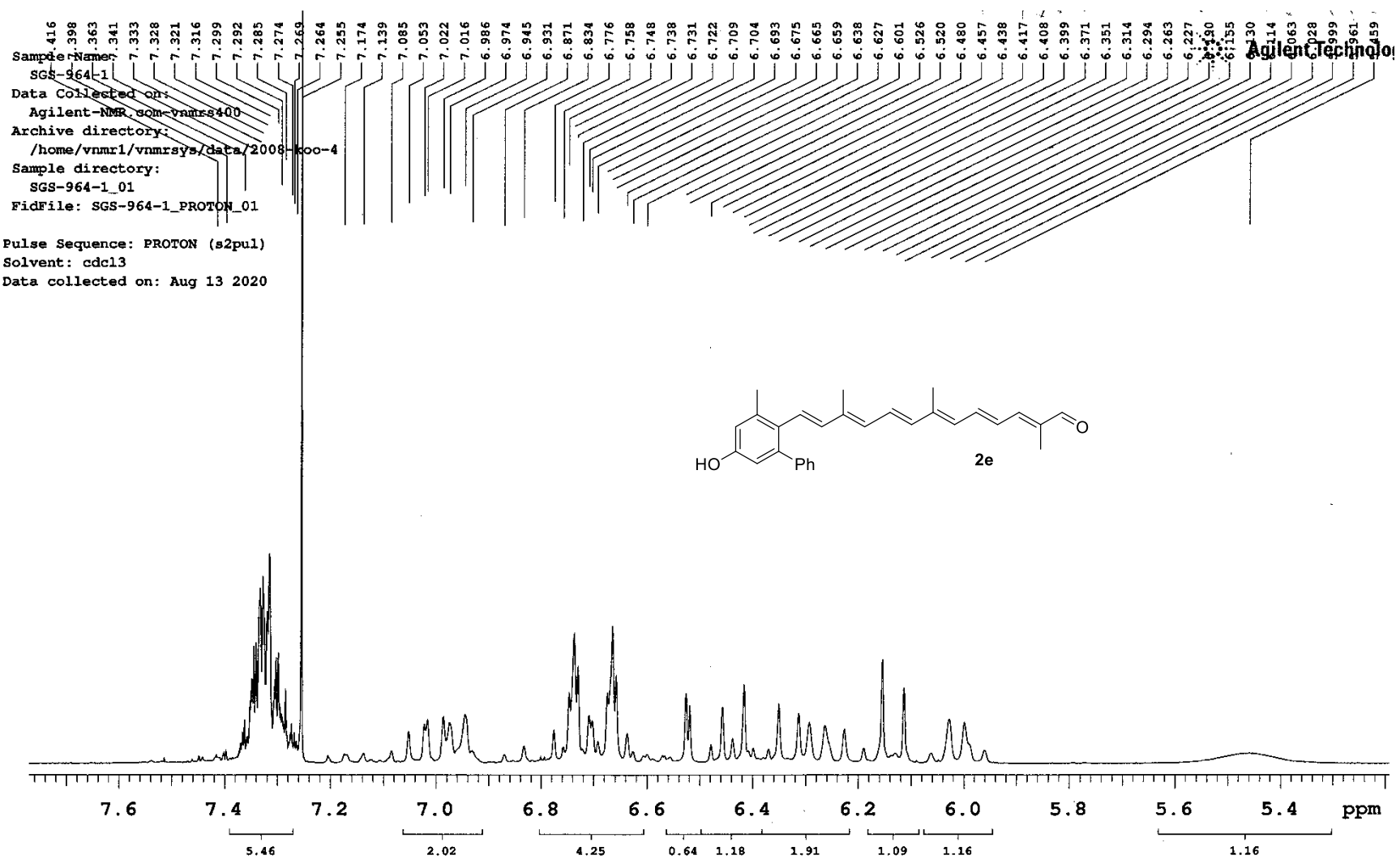
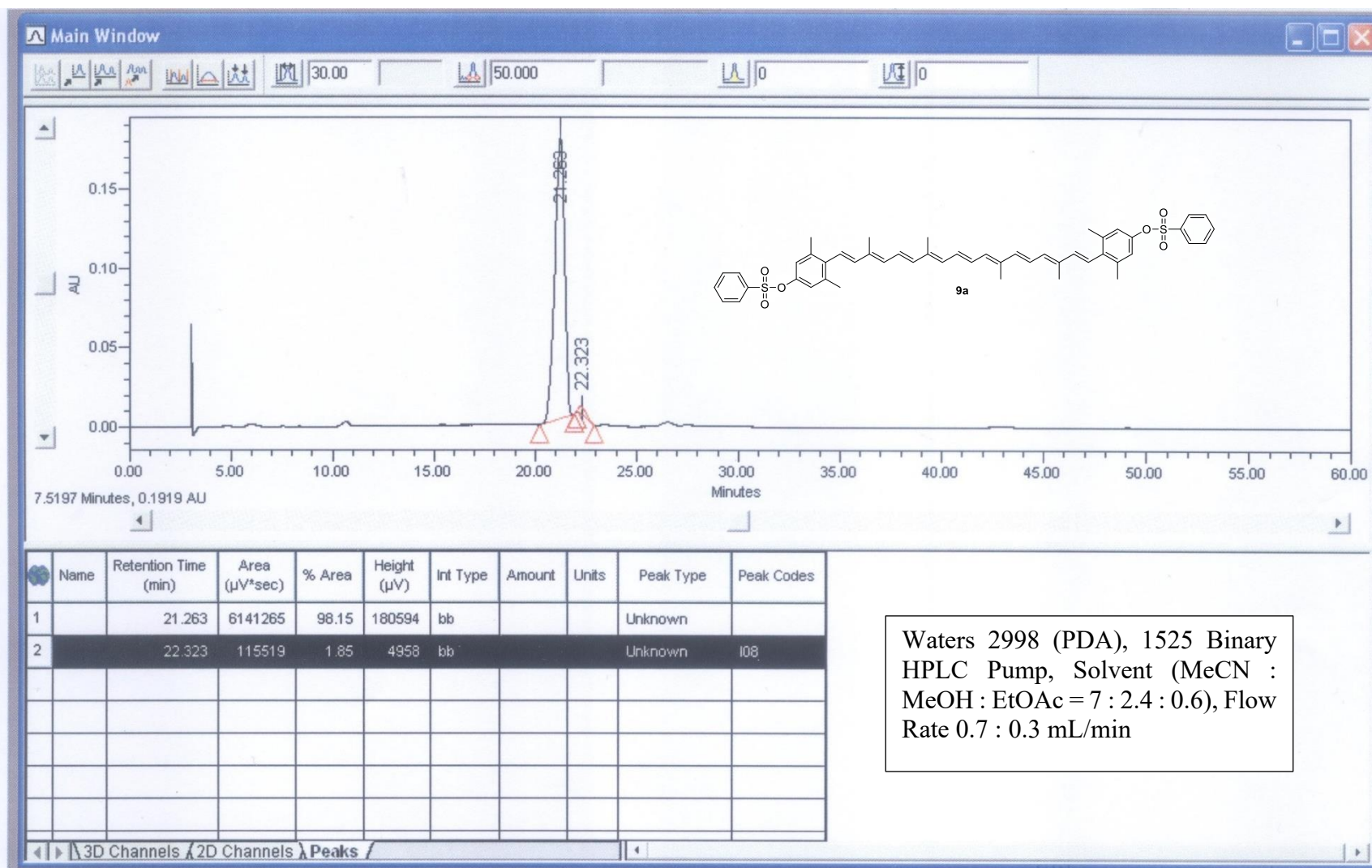
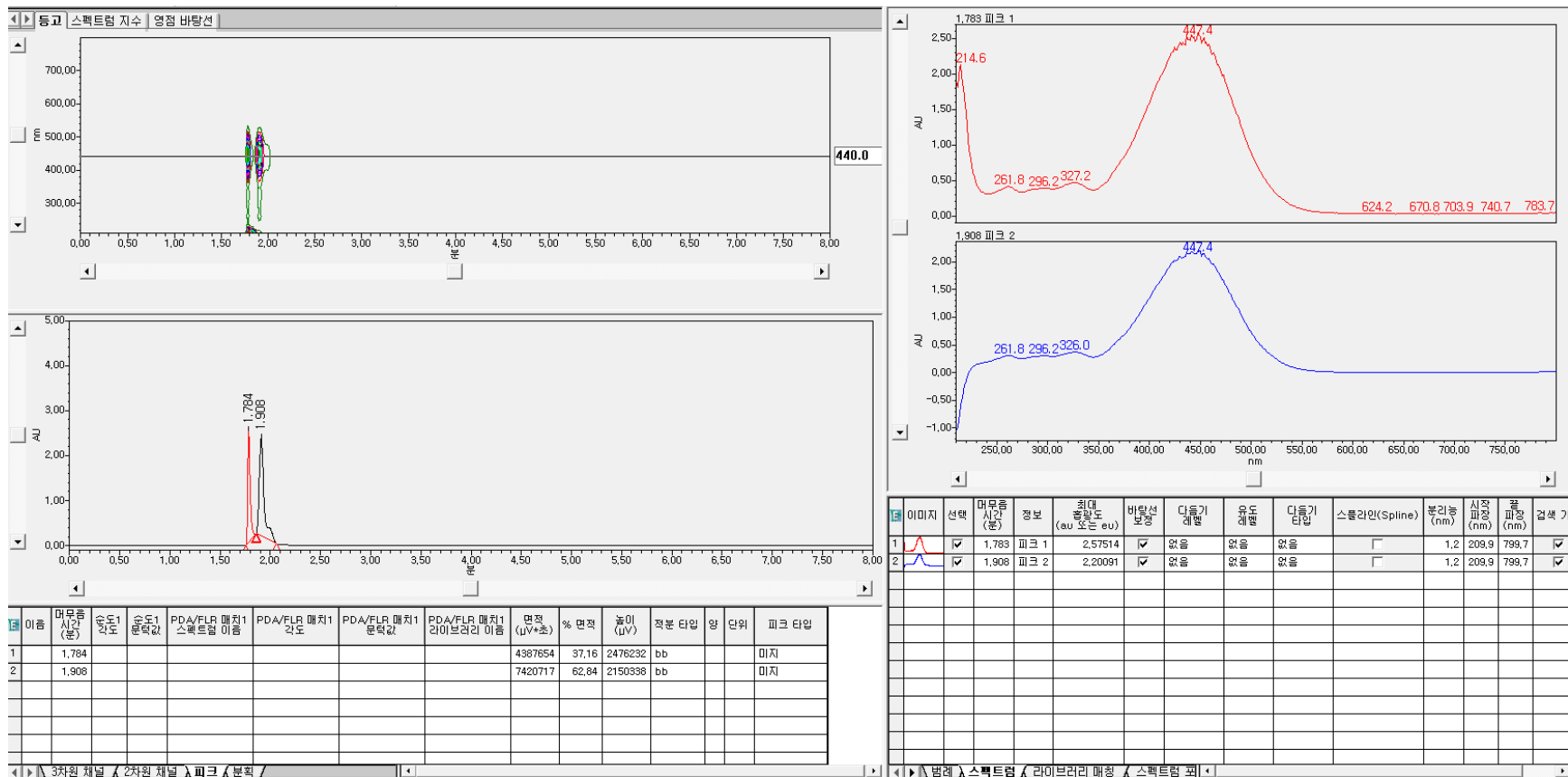
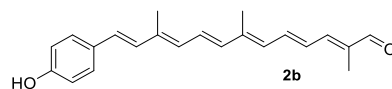


Figure S88. ¹H NMR of **2e** (expansion plot)



Waters 2998 (PDA), 1525 Binary HPLC Pump, Solvent (MeCN : MeOH : EtOAc = 7 : 2.4 : 0.6), Flow Rate 0.7 : 0.3 mL/min

Figure S90. HPLC analysis of carotene **9a** (98% purity all-*E* form)

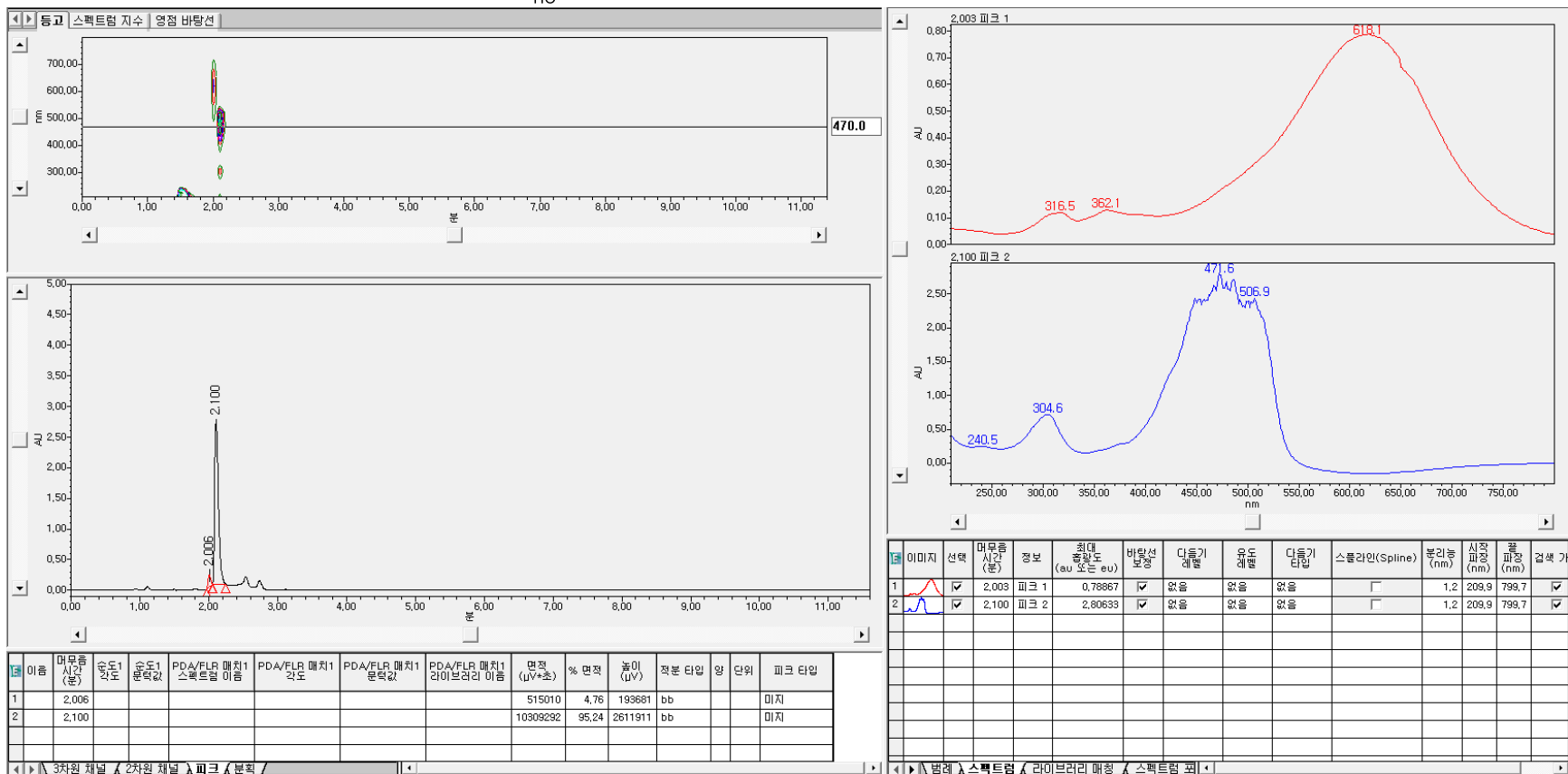
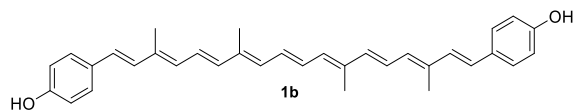


Column: Angilent proposhell 120 EC-C18, 4 μm, 4.6 × 150 mm

Pump A: 31% MeOH, 64% TBME, 4% H₂O; Pump B: MeCN

Flow rate: A = 0.5 mL/min, B = 0.5 mL/min.

Figure S91. HPLC analysis of apocarotenal **2b** (all-*E/Z* = 63:37 purity)

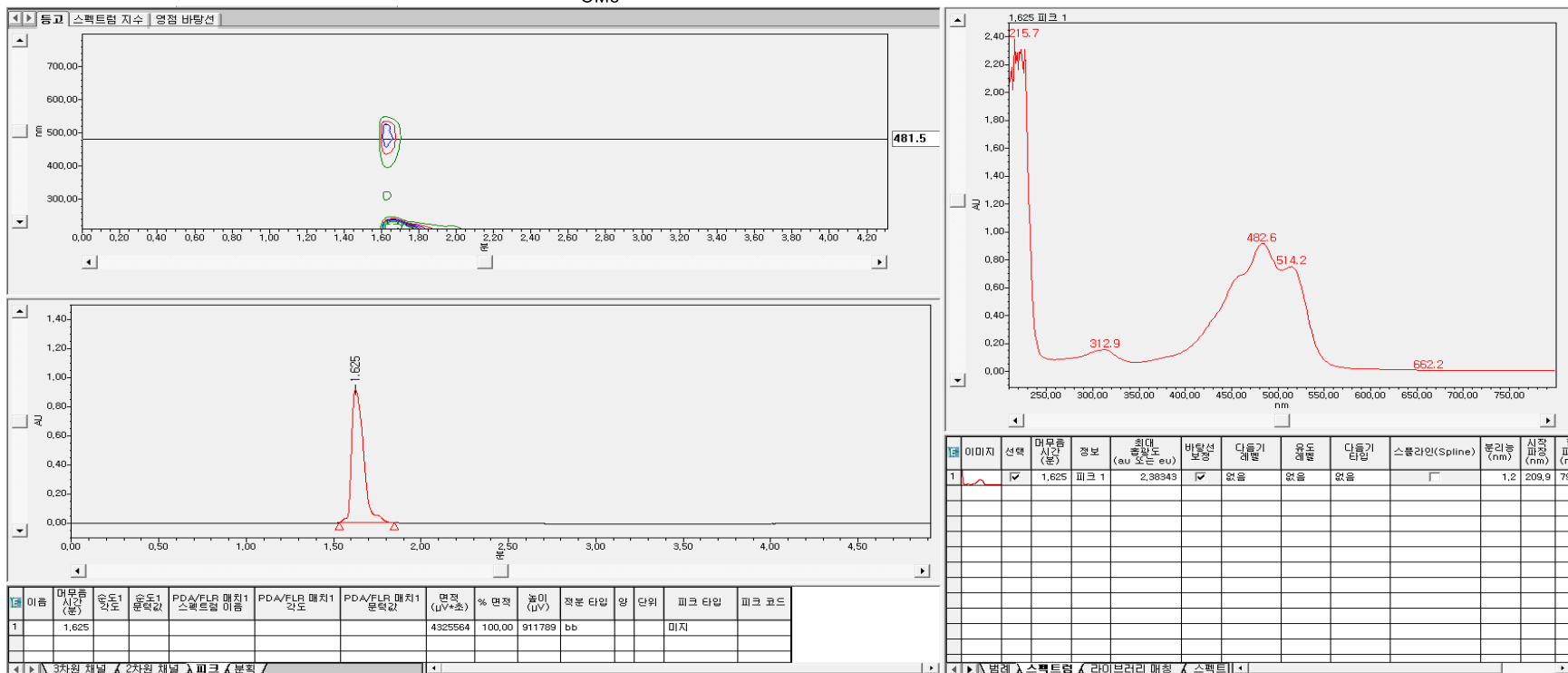
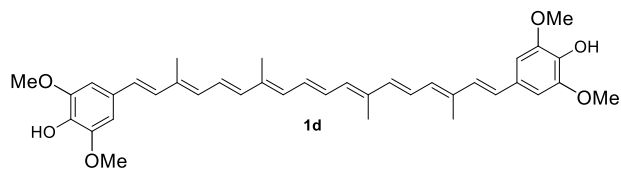


Column: Angilent proposhell 120 EC-C18, 4 μm, 4.6 × 150 mm

Pump A: 31% MeOH, 64% TBME, 4% H₂O; Pump B: MeCN

Flow rate: A = 0.5 mL/min, B = 0.5 mL/min.

Figure S92. HPLC analysis of carotene**1b** (95% purity with 5% oxidized quinone form)



Column: Angilent proposhell 120 EC-C18, 4 μ m, 4.6 \times 150mm

Pump A: 81% MeOH, 15% TBME, 4% H₂O; Pump B: 31% MeOH, 64% TBME, 4% H₂O,

Flow rate: A = 0.425 mL/min, B = 0.825 mL/min.

Purity: 100%

Figure S93. HPLC analysis of carotene **1d** (100% purity all-*E*)

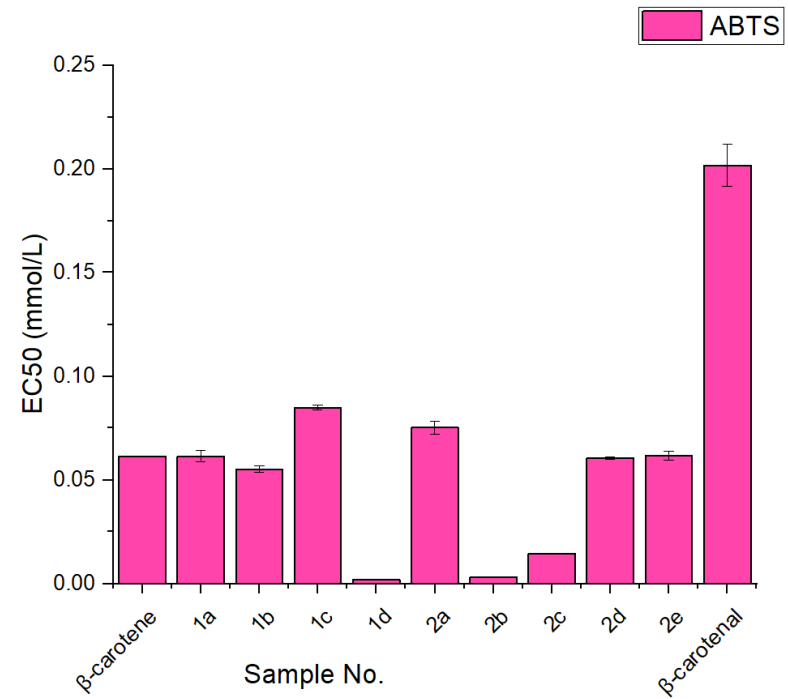
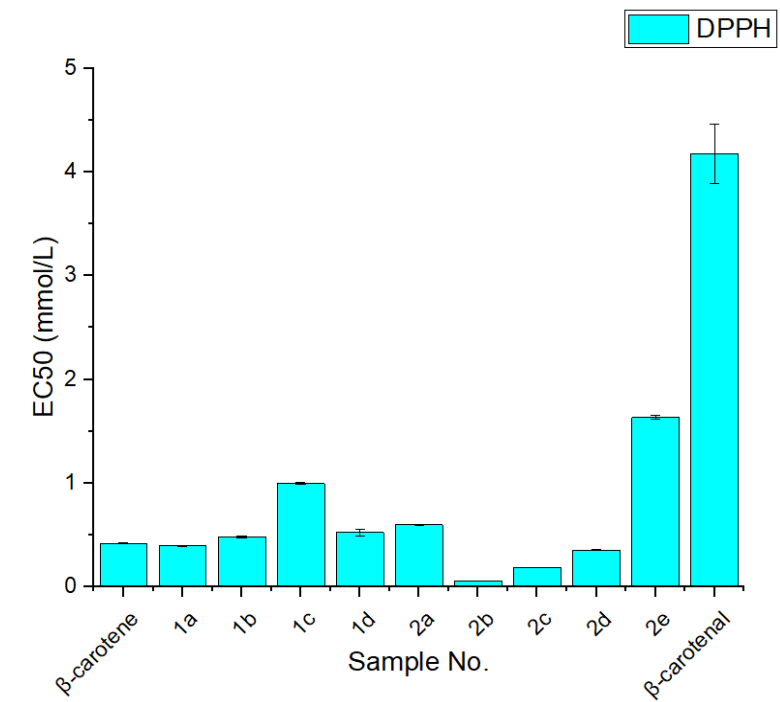


Figure S94. EC₅₀ of carotenoids for DPPH and ABTS assays

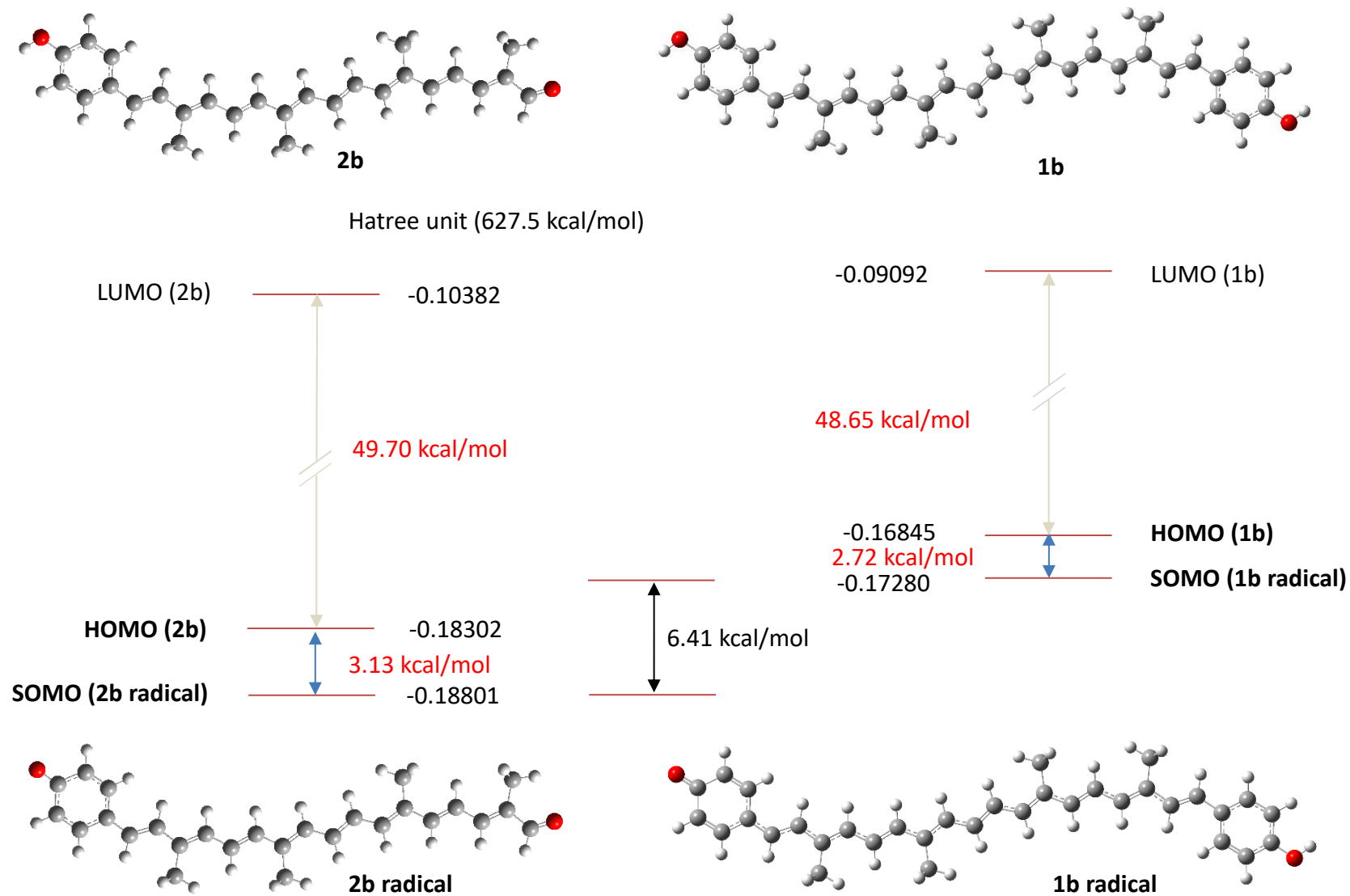


Figure S95. DFT calculation of the energy levels for **2b** and **1b** using basic function set RB3LYP/6-311G(d,p).

Table S1. Cartesian coordinates for optimized geometry cartesian coordinates (Å) of the optimized structure of carotene **2b**, calculated at the B3LYP/6-311G(d,p) level of theory.

Atom	X	Y	Z
C	4.919124	1.250484	-0.000069
C	3.674156	0.683545	0.000041
H	3.634163	-0.404296	0.000042
C	2.403572	1.341874	0.000175
H	2.388641	2.425991	0.000375
C	1.217331	0.671447	0.000046
H	1.251718	-0.416333	-0.000171
C	-0.098899	1.256545	0.000124
C	-1.184059	0.417031	0.000028
H	-0.972693	-0.650659	-0.000037
C	-2.565892	0.767816	-0.000011
H	-2.836645	1.819838	-0.00019
C	-3.581464	-0.145878	0.000193
H	-3.316828	-1.199115	0.00043
C	-4.960681	0.217094	0.000122
H	-5.160083	1.287358	0.000026
C	-6.055792	-0.608181	0.000147
C	-7.360731	0.001105	0.000008
H	-7.374176	1.089671	-0.000125
C	-8.561012	-0.641782	0.000015
H	-8.588561	-1.726114	0.000158
C	5.146957	2.741097	-0.000173
H	5.722145	3.045616	-0.880528
H	4.217458	3.307041	-0.000333

H	5.722	3.045814	0.880201
C	-0.2211	2.760208	0.000365
H	-1.255706	3.097258	0.00077
H	0.26837	3.188379	0.880867
H	0.267804	3.188659	-0.88031
C	-5.960612	-2.113097	0.000356
H	-6.457078	-2.533739	0.880775
H	-6.456961	-2.534005	-0.879993
H	-4.931332	-2.466614	0.000485
C	6.071983	0.374465	-0.00011
H	5.840858	-0.687568	-0.000118
C	7.368279	0.762549	-0.000099
H	7.588337	1.826429	-0.000054
C	8.548726	-0.094966	-0.000096
C	8.495809	-1.503818	-0.000163
C	9.823088	0.496087	0.000005
C	9.645269	-2.273619	-0.000138
H	7.53716	-2.008517	-0.000248
C	10.985216	-0.265785	0.000026
H	9.903081	1.578175	0.000062
C	10.902392	-1.658576	-0.000049
H	9.596163	-3.355782	-0.000189
H	11.955823	0.221934	0.000102
O	11.999026	-2.469297	-0.000001
H	12.795589	-1.928326	-0.000084
C	-9.813629	0.053931	-0.000163
H	-9.760227	1.142394	-0.000331

C	-11.052215	-0.507237	-0.000144
C	-12.200425	0.409504	-0.000302
H	-11.924781	1.487026	-0.000363
C	-11.33174	-1.985319	0.000093
H	-12.409922	-2.146142	-0.000741
H	-10.909356	-2.476102	-0.882295
H	-10.910914	-2.475482	0.883584
O	-13.367269	0.071556	-0.000391

total energy = -1197.622658 a.u.

the number of imaginary frequencies = 0

Table S2. Cartesian coordinates for optimized geometry cartesian coordinates (Å) of the optimized structure of carotene **2b** radical, calculated at the B3LYP/6-311G(d,p) level of theory.

Atom	X	Y	Z
C	5.009028	1.227398	0.000733
C	3.727355	0.67042	0.000913
H	3.680429	-0.416873	0.001232
C	2.491664	1.338391	0.000569
H	2.485158	2.422307	0.000023
C	1.27854	0.67386	0.000771
H	1.307169	-0.413762	0.001225
C	-0.011039	1.26882	0.000428
C	-1.116238	0.430469	0.000735
H	-0.908965	-0.637924	0.001343
C	-2.482396	0.790019	0.000336
H	-2.749859	1.842618	-0.000406
C	-3.509412	-0.125841	0.000852

H	-3.2451	-1.179058	0.001628
C	-4.879447	0.238717	0.000429
H	-5.080694	1.308435	-0.000161
C	-5.979298	-0.590862	0.000634
C	-7.28052	0.017146	0.000006
H	-7.296247	1.105466	-0.000478
C	-8.481561	-0.629373	-0.000023
H	-8.505946	-1.713755	0.000524
C	5.237852	2.72062	0.000224
H	5.805655	3.028043	-0.88294
H	4.307287	3.284356	0.003808
H	5.812062	3.02775	0.87927
C	-0.130489	2.774168	-0.000384
H	-1.164998	3.111208	-0.000465
H	0.356386	3.203646	0.880524
H	0.356235	3.202722	-0.881819
C	-5.879321	-2.095145	0.001476
H	-6.374607	-2.516402	0.882027
H	-6.374176	-2.517397	-0.87883
H	-4.849425	-2.446434	0.001929
C	6.111023	0.347323	0.000757
H	5.872175	-0.71162	0.001084
C	7.450554	0.722047	0.00012
H	7.673264	1.785096	-0.000361
C	8.572383	-0.126045	-0.000174
C	8.489562	-1.563672	0.000233
C	9.887044	0.457572	-0.000937

C	9.601945	-2.339169	-0.00007
H	7.513702	-2.035502	0.000796
C	11.013653	-0.299544	-0.001253
H	9.959849	1.54127	-0.001254
C	10.951016	-1.762538	-0.00085
H	9.542513	-3.421585	0.000241
H	12.002575	0.144033	-0.001823
O	11.964565	-2.467231	-0.001153
C	-9.735097	0.061861	-0.000663
H	-9.686685	1.150394	-0.001107
C	-10.971249	-0.506351	-0.000735
C	-12.12515	0.405996	-0.001243
H	-11.856144	1.484807	-0.001345
C	-11.244516	-1.985087	-0.000098
H	-12.32185	-2.150749	-0.004276
H	-10.816916	-2.474605	-0.880552
H	-10.824635	-2.472137	0.885489
O	-13.288756	0.059537	-0.001602

total energy = -1197.991186 a.u.

the number of imaginary frequencies = 0

Table S3. Cartesian coordinates for optimized geometry cartesian coordinates (Å) of the optimized structure of carotene **1b**, calculated at the B3LYP/6-311G(d,p) level of theory.

Atom	X	Y	Z
C	7.937208	1.338414	0.000023
C	6.719502	0.715869	-0.000029
H	6.730016	-0.372863	-0.000027

C	5.418384	1.312999	-0.000091
H	5.350956	2.395155	-0.000112
C	4.266282	0.585445	-0.000132
H	4.355259	-0.499482	-0.000113
C	2.921804	1.102244	-0.000189
C	1.880595	0.209343	-0.000219
H	2.147596	-0.84613	-0.000218
C	0.481243	0.484797	-0.00023
H	0.152918	1.520331	-0.000199
C	-0.481241	-0.484774	-0.000264
H	-0.152917	-1.520308	-0.000283
C	-1.880592	-0.209319	-0.000256
H	-2.147593	0.846154	-0.000289
C	-2.921799	-1.102222	-0.000204
C	-4.26628	-0.585428	-0.000175
H	-4.355261	0.499499	-0.000209
C	-5.418381	-1.312985	-0.000106
H	-5.350949	-2.395141	-0.000072
C	8.09701	2.837931	0.000028
H	8.657483	3.16917	-0.880394
H	7.142164	3.360169	0.000153
H	8.657688	3.169144	0.880325
C	2.723656	2.597946	-0.000164
H	1.672822	2.881018	-0.000172
H	3.190161	3.051543	0.880376
H	3.190179	3.051563	-0.880685
C	-2.723644	-2.597922	-0.000156

H	-3.190073	-3.051496	0.880437
H	-3.190237	-3.051567	-0.880625
H	-1.672807	-2.880988	-0.000246
C	9.129315	0.516326	0.00006
H	8.946288	-0.555212	0.000045
C	10.407053	0.961355	0.000081
H	10.580277	2.033883	0.000059
C	11.624392	0.155852	0.000107
C	11.633622	-1.25389	0.000214
C	12.87209	0.801172	0.000036
C	12.815799	-1.973137	0.000227
H	10.697897	-1.799966	0.000298
C	14.066508	0.090394	0.00005
H	12.905087	1.885748	-0.000035
C	14.044798	-1.304421	0.000141
H	12.813411	-3.056473	0.000312
H	15.014955	0.620138	-0.000008
O	15.177034	-2.066735	0.000168
H	15.948005	-1.490021	0.000111
C	-6.7195	-0.71586	-0.000078
H	-6.730017	0.372872	-0.00011
C	-7.937204	-1.338408	-0.000011
C	-9.129315	-0.516325	0.000021
H	-8.946292	0.555214	-0.000027
C	-8.097001	-2.837926	0.000047
H	-8.657534	-3.169125	0.880444
H	-8.657617	-3.169181	-0.880276

H	-7.142153	-3.360161	0.000016
C	-10.407051	-0.961359	0.000084
H	-10.580272	-2.033887	0.000094
C	-11.624392	-0.155859	0.000116
C	-11.633633	1.253879	0.00021
C	-12.872088	-0.801191	0.000062
C	-12.815817	1.97312	0.000231
H	-10.697914	1.799964	0.000292
C	-14.066507	-0.090423	0.000073
H	-12.90507	-1.885767	-0.000001
C	-14.04481	1.304397	0.000157
H	-12.813431	3.056456	0.000311
H	-15.014953	-0.620169	0.000021
O	-15.177046	2.0667	0.000172
H	-15.948016	1.489985	0.000104

total energy = -1468.044815 a.u.

the number of imaginary frequencies = 0

Table S4. Cartesian coordinates for optimized geometry cartesian coordinates (Å) of the optimized structure of carotene **1b** radical, calculated at the B3LYP/6-311G(d,p) level of theory.

Atom	X	Y	Z
C	7.864796	1.329614	-0.000004
C	6.642934	0.706692	0.000055
H	6.653002	-0.381887	0.000131
C	5.348774	1.30578	0.000045
H	5.283335	2.387966	0.000075
C	4.188954	0.579506	-0.000011

H	4.275713	-0.505386	-0.000036
C	2.855633	1.101107	-0.000035
C	1.80252	0.206538	-0.000123
H	2.06805	-0.849155	-0.000182
C	0.417652	0.489212	-0.000133
H	0.092048	1.525428	-0.000088
C	-0.561616	-0.482843	-0.000207
H	-0.237138	-1.51937	-0.000236
C	-1.941258	-0.196711	-0.000243
H	-2.204851	0.859457	-0.000174
C	-3.005858	-1.091132	-0.000317
C	-4.320811	-0.564748	-0.000243
H	-4.406012	0.520056	-0.000206
C	-5.501541	-1.290581	-0.000185
H	-5.438977	-2.372805	-0.000195
C	8.023976	2.828981	-0.000041
H	8.584319	3.159894	-0.880442
H	7.069428	3.351537	-0.000039
H	8.584328	3.159931	0.880344
C	2.657094	2.596726	0.000062
H	1.606479	2.88011	-0.00005
H	3.122769	3.050188	0.880826
H	3.12298	3.050326	-0.880518
C	-2.806989	-2.588517	-0.000352
H	-3.269455	-3.043517	0.881059
H	-3.270368	-3.043597	-0.881233
H	-1.75573	-2.86946	-0.000899

C	9.05283	0.506534	0.000042
H	8.869445	-0.564754	0.000068
C	10.332255	0.951689	0.000047
H	10.505028	2.024238	0.000019
C	11.548222	0.147114	0.000074
C	11.557021	-1.262991	0.000124
C	12.795856	0.793458	0.00004
C	12.738977	-1.981609	0.000143
H	10.621416	-1.809186	0.000155
C	13.98996	0.0832	0.000055
H	12.828382	1.877992	0
C	13.968067	-1.312054	0.000106
H	12.737393	-3.064873	0.000187
H	14.938344	0.612801	0.00003
O	15.098826	-2.073946	0.000121
H	15.871237	-1.498978	0.000067
C	-6.767421	-0.687658	-0.000115
H	-6.77642	0.400743	-0.000116
C	-8.021774	-1.308383	-0.000038
C	-9.165926	-0.48742	-0.00002
H	-8.982162	0.582538	-0.000125
C	-8.172688	-2.811774	0.000088
H	-8.72675	-3.148624	0.881297
H	-8.727075	-3.148759	-0.880861
H	-7.213779	-3.325918	-0.00004
C	-10.485883	-0.930048	0.00012
H	-10.653159	-2.003366	0.000241

C	-11.649644	-0.142432	0.000116
C	-11.643114	1.297546	-0.000189
C	-12.932859	-0.79241	0.000432
C	-12.794591	2.01402	-0.000178
H	-10.693172	1.819831	-0.000433
C	-14.097376	-0.094839	0.000449
H	-12.94966	-1.878571	0.000662
C	-14.112173	1.369161	0.000139
H	-12.791023	3.098154	-0.000403
H	-15.061689	-0.589841	0.000689
O	-15.161361	2.020507	0.000153

total energy = -1467.415215 a.u.

the number of imaginary frequencies = 0