

NMR Spectra

For

Synthesis and Energetic Properties of Homocubane Based High Energy Density Materials

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Entry	Table of Contents	Page
01	Figure S-01. ¹ H NMR Spectrum of Compound 8	6
02	Figure S-02. ¹ H NMR (Expansion) Spectrum of Compound 8	7
03	Figure S-03. ¹³ C NMR Spectrum of Compound 8	8
04	Figure S-04. ¹³ C-APT NMR Spectrum of compound 8	9
05	Figure S-05. ¹ H NMR Spectrum of Compound 9	10
06	Figure S-06. ¹ H NMR (Expansion) Spectrum of Compound 9	11
07	Figure S-07. ¹³ C NMR Spectrum of Compound 9	12
08	Figure S-08. ¹³ C-APT NMR Spectrum of Compound 9	13
09	Figure S-09. ¹ H NMR Spectrum of Compound 10	14
10	Figure S-10. ¹ H NMR (Expansion) Spectrum of Compound 10	15

11	Figure S-11. ^{13}C NMR Spectrum of Compound 10	16
12	Figure S-12. ^{13}C -APT NMR Spectrum of Compound 10	17
13	Figure S-13. ^1H NMR Spectrum of Compound 11	18
14	Figure S-14. ^{13}C NMR Spectrum of Compound 11	19
15	Figure S-15. ^{13}C -DEPT-135 NMR Spectrum of Compound 11	20
16	Figure S-16. ^1H NMR Spectrum of Compound 12	21
17	Figure S-17. ^1H NMR (Expansion) Spectrum of Compound 12	22
18	Figure S-18. ^{13}C NMR Spectrum of Compound 12	23
19	Figure S-19. ^{13}C -APT NMR Spectrum of Compound 12	24
20	Figure S-20. ^1H NMR Spectrum of Compound 13	25
21	Figure S-21. ^1H NMR (Expansion) Spectrum of Compound 13	26
22	Figure S-22. ^{13}C NMR Spectrum of Compound 13	27
23	Figure S-23. ^{13}C -DEPT-135 NMR Spectrum of Compound 13	28
24	Figure S-24. ^1H NMR Spectrum of Compound 14	29
25	Figure S-25. ^1H NMR (Expansion) Spectrum of Compound 14	30
26	Figure S-26. ^{13}C NMR Spectrum of Compound 14	31
27	Figure S-27. ^{13}C -APT NMR Spectrum of Compound 14	32
28	Figure S-28. ^1H NMR Spectrum of Compound 15	33
29	Figure S-29. ^1H NMR (Expansion) Spectrum of Compound 15	34
30	Figure S-30. ^{13}C NMR Spectrum of Compound 15	35
31	Figure S-31. ^{13}C -APT NMR Spectrum of Compound 15	36
32	Figure S-32. ^1H NMR Spectrum of Compound 16	37

33	Figure S-33. ^{13}C NMR Spectrum of Compound 16	38
34	Figure S-34. ^{13}C -APT NMR Spectrum of Compound 16	39
35	Figure S-35. ^1H NMR Spectrum of Compound 17	40
36	Figure S-36. ^1H NMR (Expansion) Spectrum of Compound 17	41
37	Figure S-37. ^{13}C NMR Spectrum of Compound 17	42
38	Figure S-38. ^1H NMR Spectrum of Compound 18	43
39	Figure S-39. ^1H NMR (Expansion) Spectrum of Compound 18	44
40	Figure S-40. ^{13}C NMR Spectrum of Compound 18	45
41	Figure S-41. ^1H NMR Spectrum of Compound 19	46
42	Figure S-42. ^1H NMR (Expansion) Spectrum of Compound 19	47
43	Figure S-43. ^{13}C NMR Spectrum of Compound 19	48
44	Figure S-44. ^{13}C -APT NMR Spectrum of Compound 19	49
45	Figure S-45. ^1H NMR Spectrum of Compound 21a	50
46	Figure S-46. ^1H NMR (Expansion) Spectrum of Compound 21a	51
47	Figure S-47. ^{13}C NMR Spectrum of Compound 21a	52
48	Figure S-48. ^{13}C -APT NMR Spectrum of Compound 21a	53
49	Figure S-49. ^1H - ^{13}C HSQC NMR Spectrum of Compound 21a	54
50	Figure S-50. ^1H NMR Spectrum of Compound 21b	55
51	Figure S-51. ^1H NMR (Expansion) Spectrum of Compound 21b	56
52	Figure S-52. ^{13}C NMR Spectrum of Compound 21b	57
53	Figure S-53. ^{13}C -APT NMR Spectrum of Compound 21b	58
54	Figure S-54. ^1H NMR Spectrum of Compound 24	59

55	Figure S-55. ^1H NMR (Expansion) Spectrum of Compound 24	60
56	Figure S-56. ^{13}C NMR Spectrum of Compound 24	61
57	Figure S-57. ^{13}C -APT NMR Spectrum of Compound 24	62
58	Figure S-58. ^1H NMR Spectrum of Compound 25	63
59	Figure S-59. ^{13}C NMR Spectrum of Compound 25	64
60	Figure S-60. ^{13}C -APT NMR Spectrum of Compound 25	65
61	Figure S-61. ^1H - ^{13}C HSQC NMR Spectrum of Compound 25	66
62	Figure S-62. ^1H NMR Spectrum of Compound 27	67
63	Figure S-63. ^{13}C NMR Spectrum of Compound 27	68
64	Figure S-64. ^{13}C -APT NMR Spectrum of Compound 27	69
65	Figure S-65. ^{15}N NMR Spectrum of Compound 27	70
66	Figure S-66. ^1H - ^{13}C HSQC NMR Spectrum of Compound 27	71
67	Figure S-67. ^1H NMR Spectrum of Compound 28	72
68	Figure S-68. ^1H NMR (Expansion) Spectrum of Compound 28	73
69	Figure S-69. ^{13}C NMR Spectrum of Compound 28	74
70	Figure S-70. ^1H NMR Spectrum of Compound 30a	75
71	Figure S-71. ^1H NMR Spectrum of Compound 30a	76
72	Figure S-72. ^{13}C NMR Spectrum of Compound 30a	77
73	Figure S-73. ^{13}C -APT NMR Spectrum of Compound 30a	78
74	Figure S-74. ^1H NMR Spectrum of Compound 30b	79
75	Figure S-75. ^1H NMR (Expansion) Spectrum of Compound 30b	80
76	Figure S-76. ^{13}C NMR Spectrum of Compound 30b	81

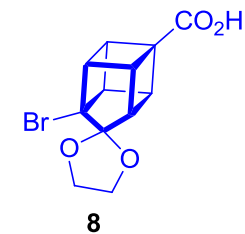
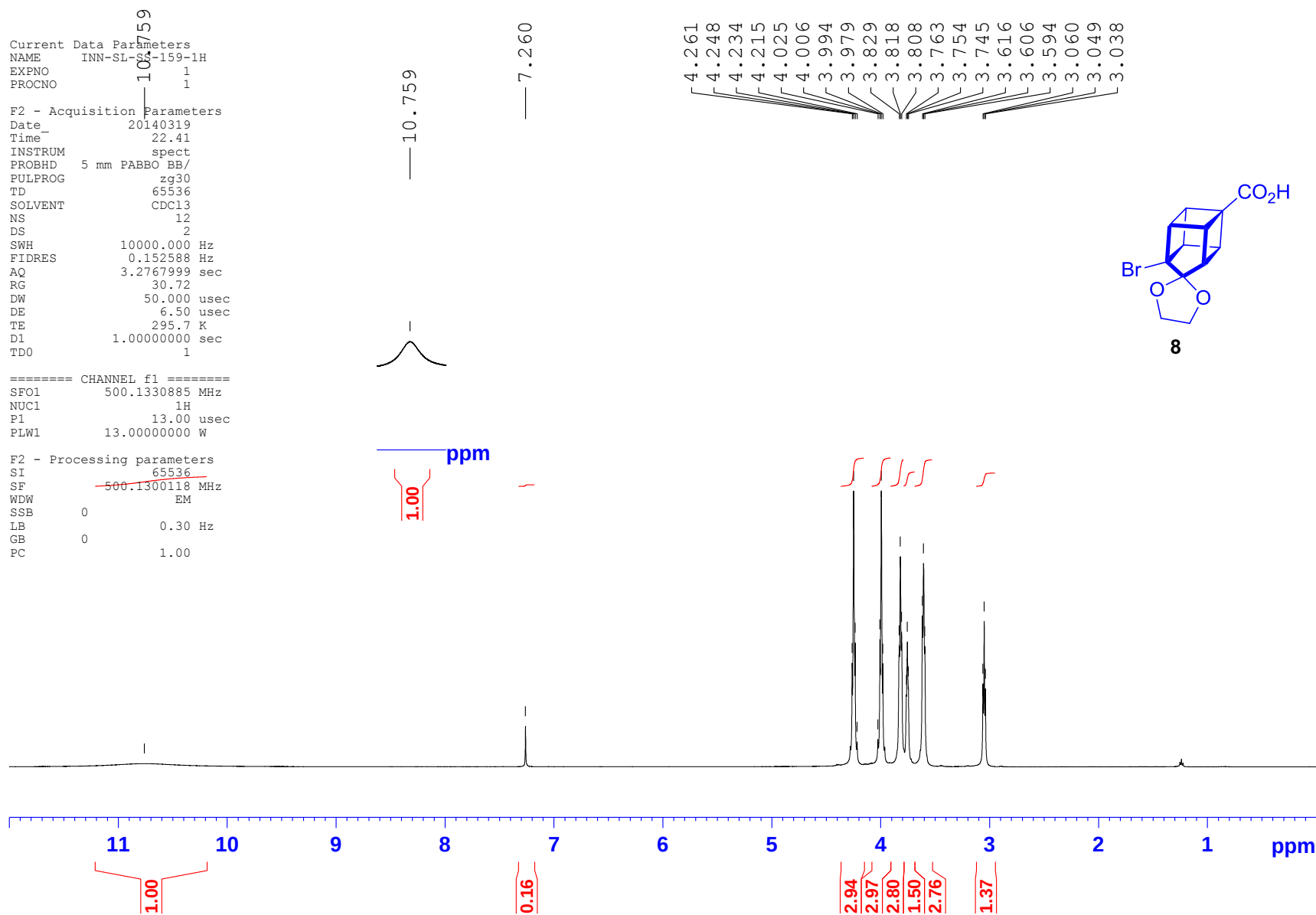
77	Figure S-77. ^{13}C -APT NMR Spectrum of Compound 30b	82
78	Figure S-78. ^1H NMR Spectrum of Compound 30c	83
79	Figure S-79. ^1H NMR (Expansion) Spectrum of Compound 30c	84
80	Figure S-80. ^{13}C NMR Spectrum of Compound 30c	85

Current Data Parameters
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PROCNO 1

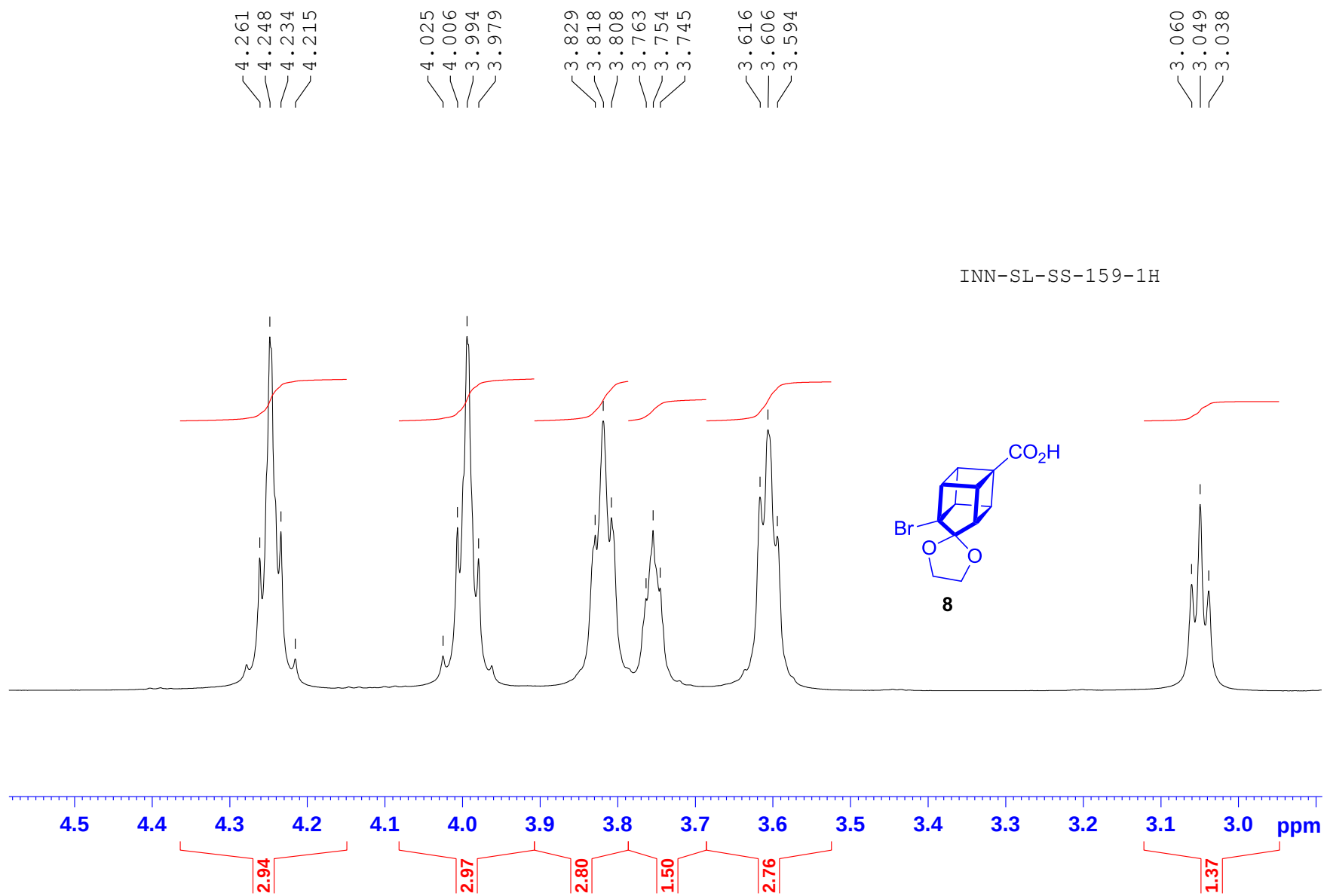
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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 12
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 30.72
DW 50.000 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 13.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
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SF 500.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S-01. ¹H NMR Spectrum of Compound 8



S-02. ^1H NMR Spectrum (Expansion) of Compound 8

Current Data Parameters
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 133
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 6.50 usec
 TE 296.3 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
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 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

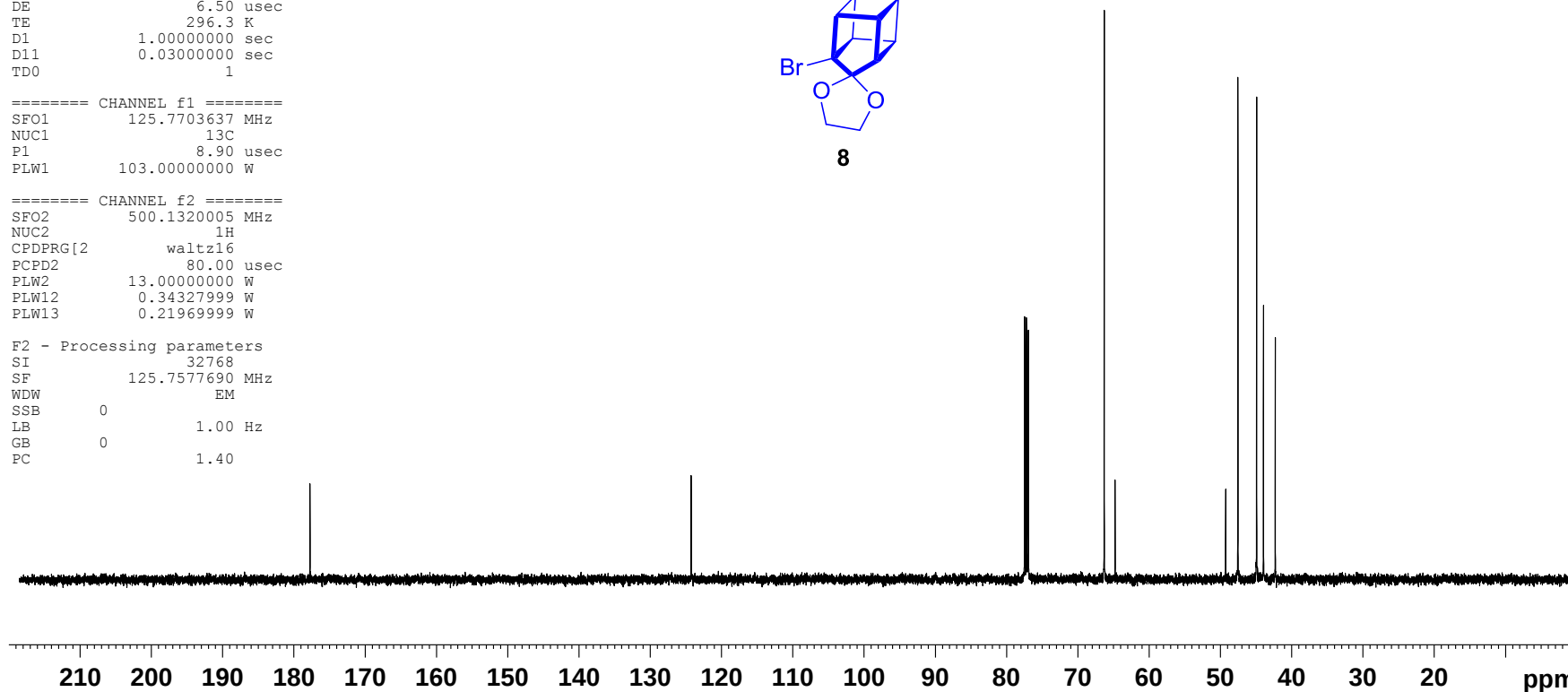
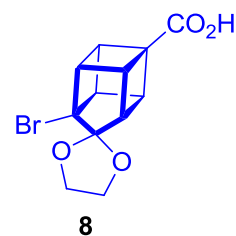
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177.75

124.26

77.45
 77.20
 76.95
 66.30
 64.78

49.25
 47.53
 44.90
 43.94
 42.29



S-03. ¹³C NMR Spectrum of Compound 8

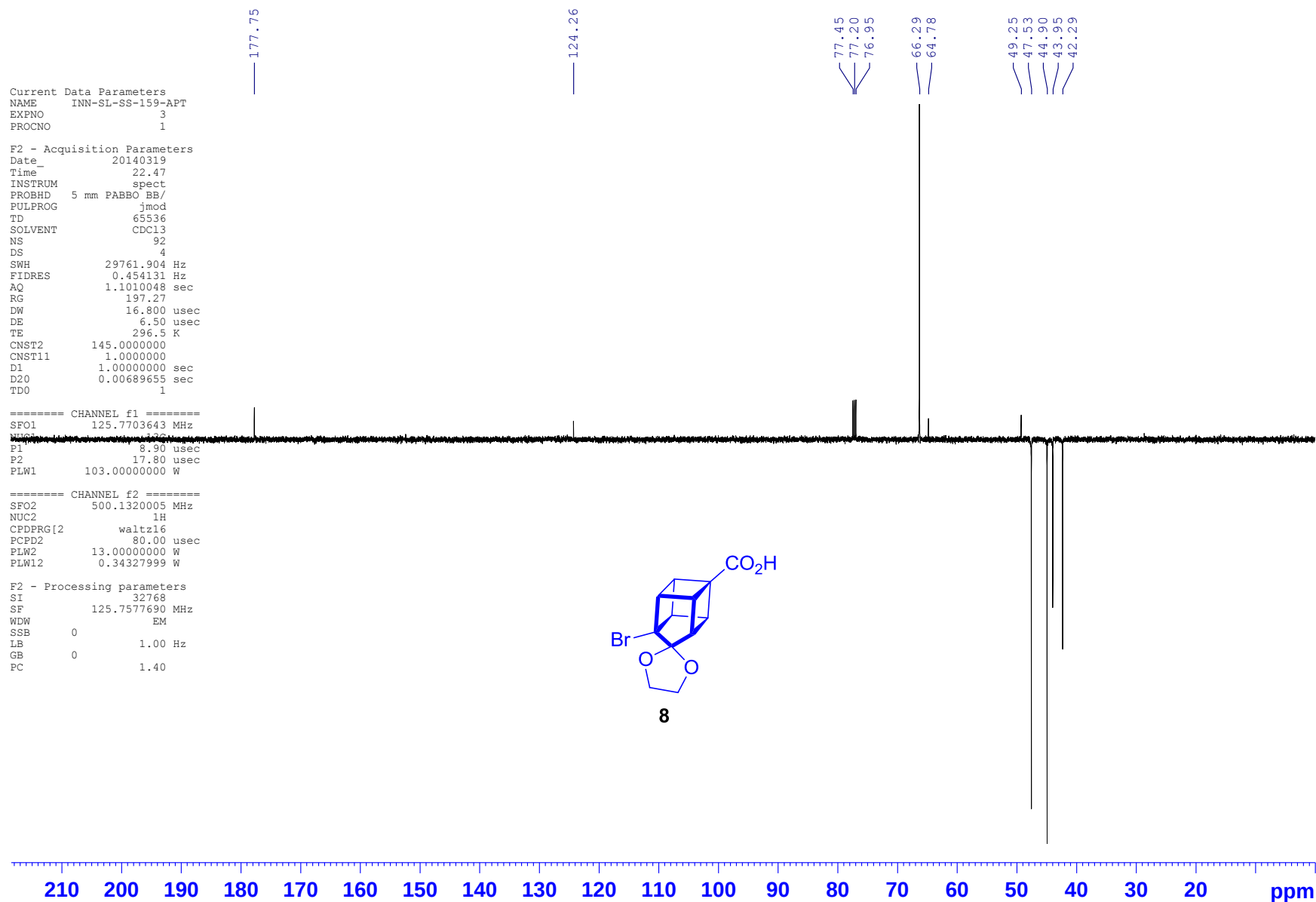
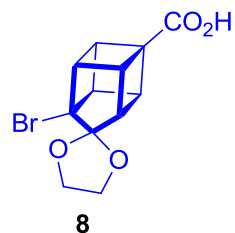
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 PROCNO 1

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 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 92
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 6.50 usec
 TE 296.5 K
 CNST2 145.000000
 CNST11 1.000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.0000000 W
 PLW12 0.34327999 W

F2 - Processing parameters
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 SF 125.7577690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



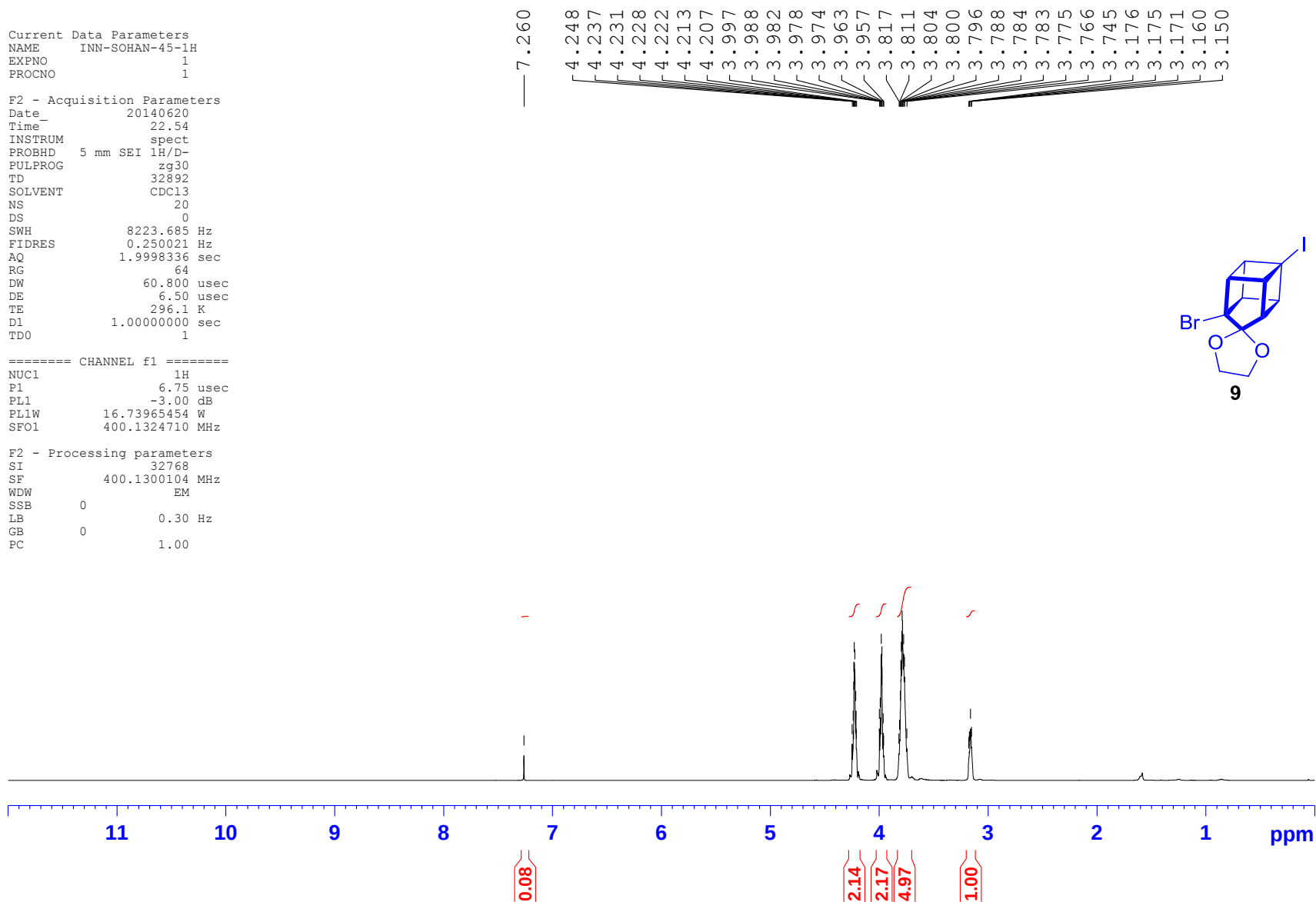
S-04. ¹³C-APT NMR Spectrum of Compound 8

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 PROCNO 1

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 PROBHD 5 mm SEI 1H/D-
 PULPROG zg30
 TD 32892
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.250021 Hz
 AQ 1.9998336 sec
 RG 64
 DW 60.800 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.75 usec
 PL1 -3.00 dB
 PL1W 16.73965454 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-05. ¹H NMR Spectrum of Compound 9

Current Data Parameters
 NAME INN-SOHA-45-13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140621
 Time_ 0.12
 INSTRUM spect
 PROBHD 5 mm SEI 1H/D-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 65
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 144
 DW 20.800 usec
 DE 6.50 usec
 TE 296.7 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.75 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.50 dB
 PL13 14.50 dB
 PL2W 10.56200695 W
 PL12W 0.29767781 W
 PL13W 0.29767781 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127550 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

124.35

77.51

77.20

76.88

66.26

64.64

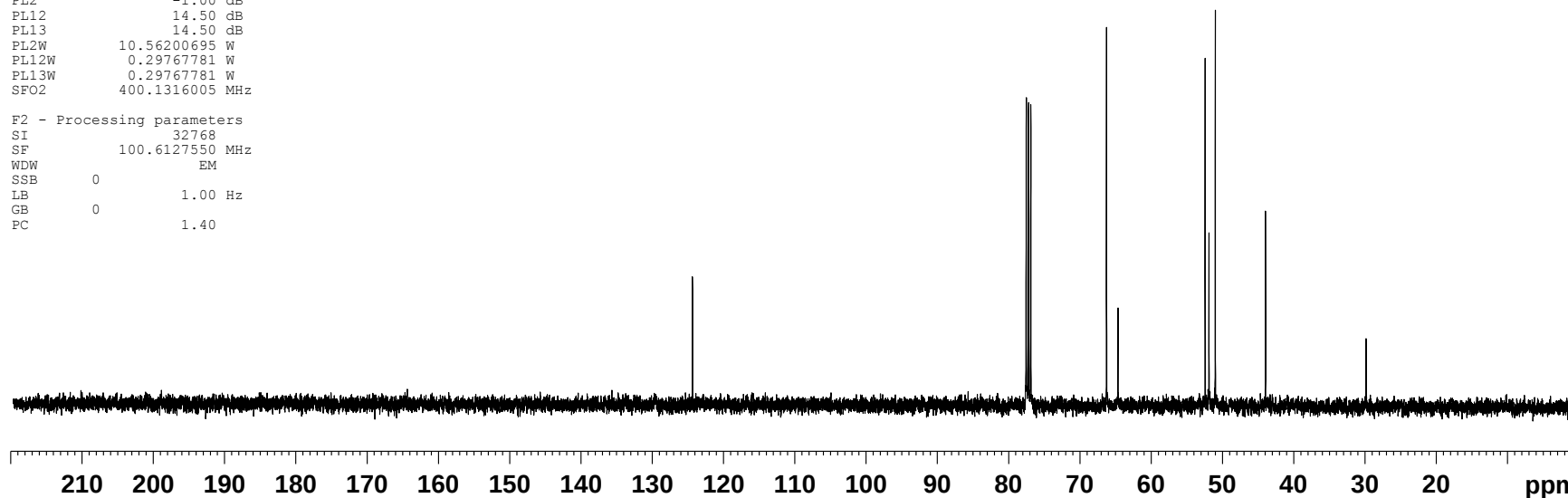
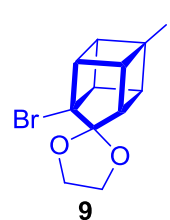
52.42

51.88

50.99

43.95

29.84



S-07. ¹³C NMR Spectrum of Compound 9

Current Data Parameters
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 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140623
 Time 23.50
 INSTRUM spect
 PROBHD 5 mm SEI 1H/D-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 295.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 13.00 usec
 P2 26.00 usec
 PL1 -3.00 dB
 PL1W 71.16858673 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 18.48 dB
 PL2W 16.73965454 W
 PL12W 0.11905462 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

124.31

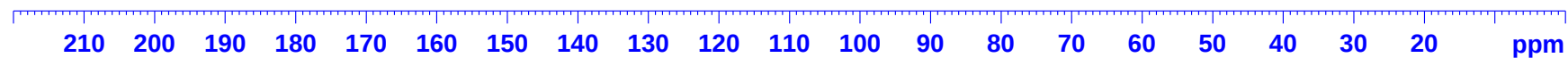
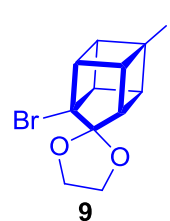
77.52
77.20
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66.23
64.61

52.37
51.84
50.95

43.91

29.82



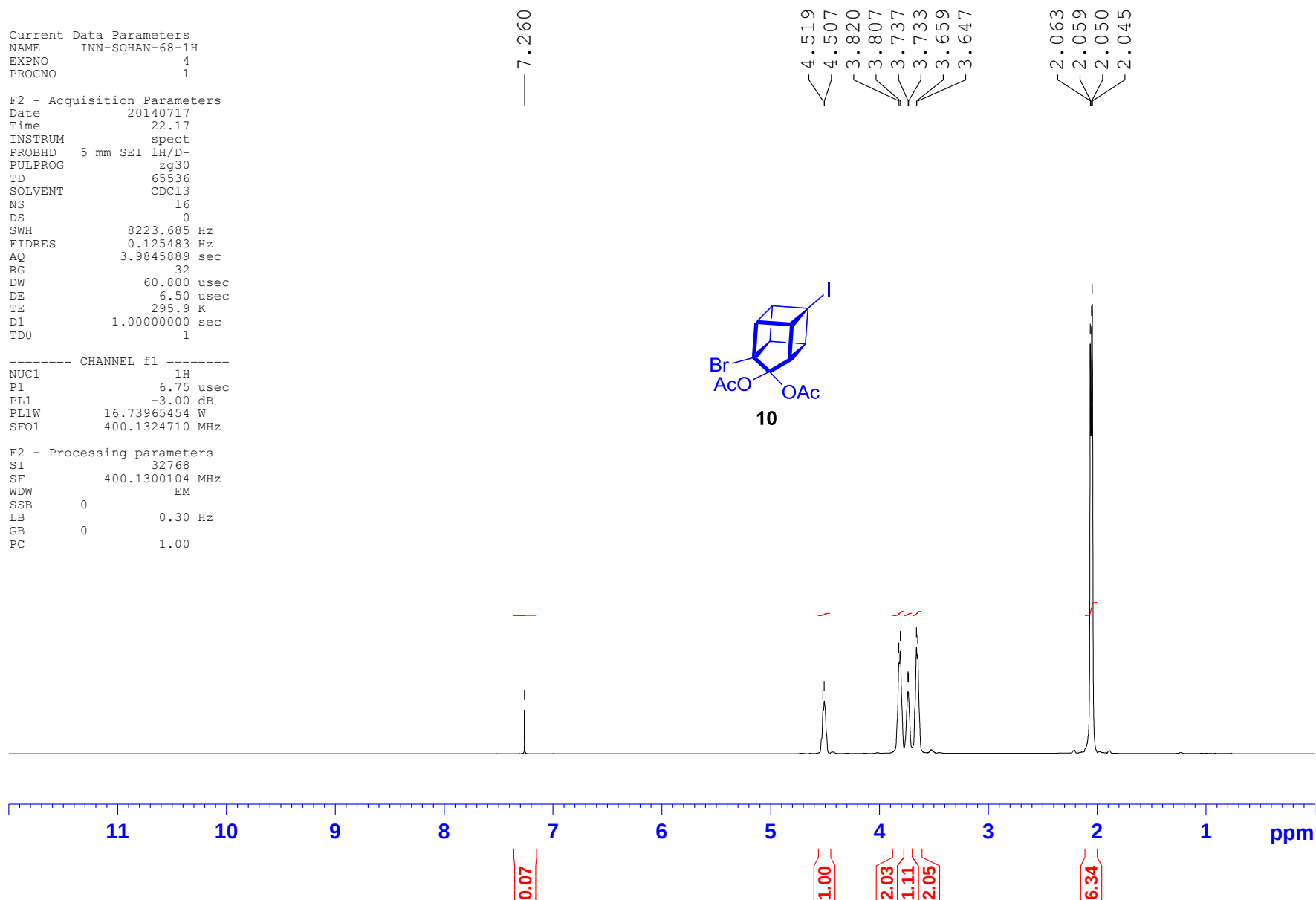
S-08. ¹³C-APT NMR Spectrum of Compound 9

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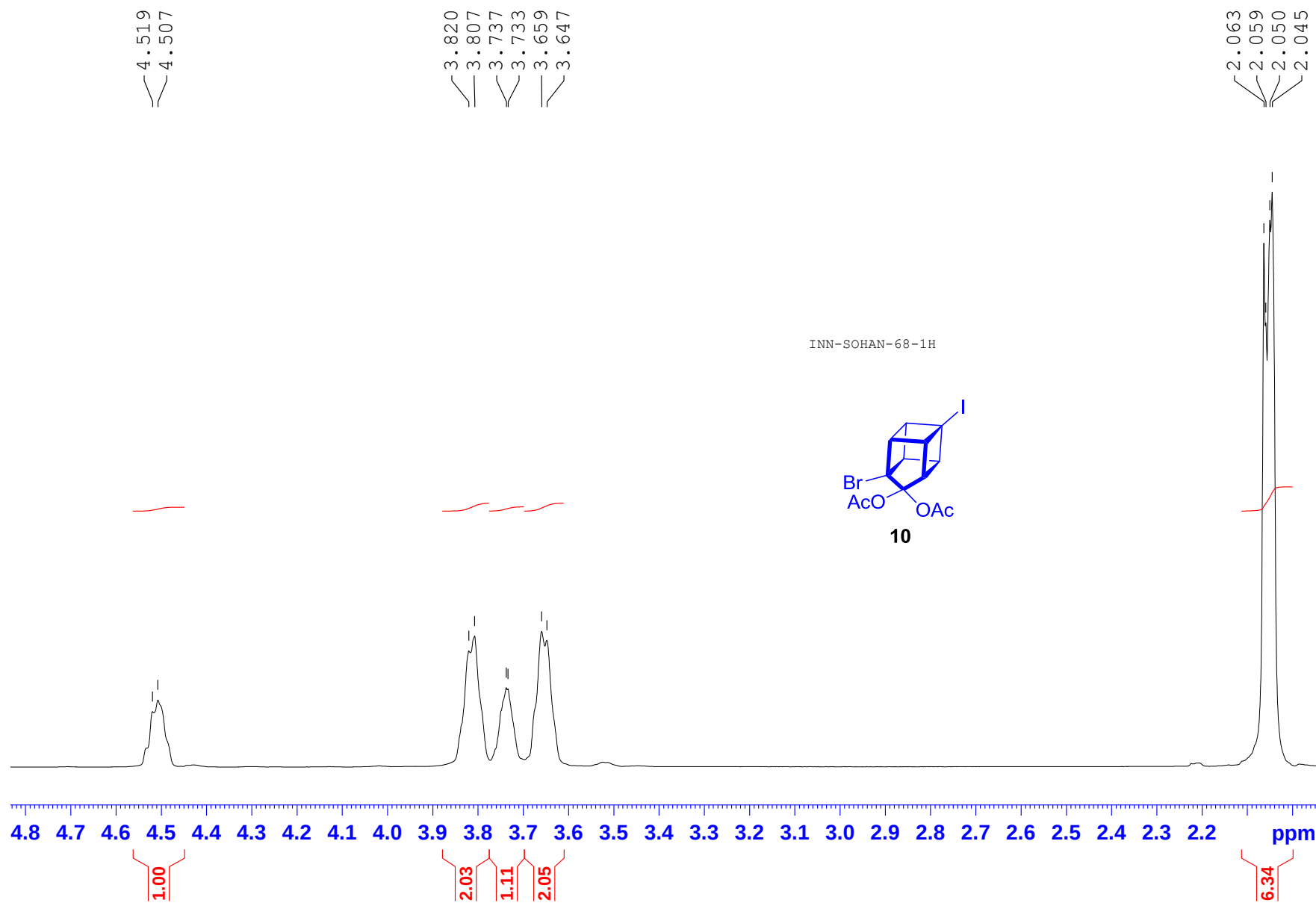
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 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.75 usec
 PL1 -3.00 dB
 PL1W 16.73965454 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-09. ¹H NMR Spectrum of Compound 10



S-10. ^1H NMR Spectrum of Compound 10

Current Data Parameters
 NAME INN-SOCHAN-68R2-13C
 EXPNO 32
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190908
 Time 21.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 299
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
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 WDW EM
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 LB 1.00 Hz
 GB 0
 PC 1.40

— 168.26

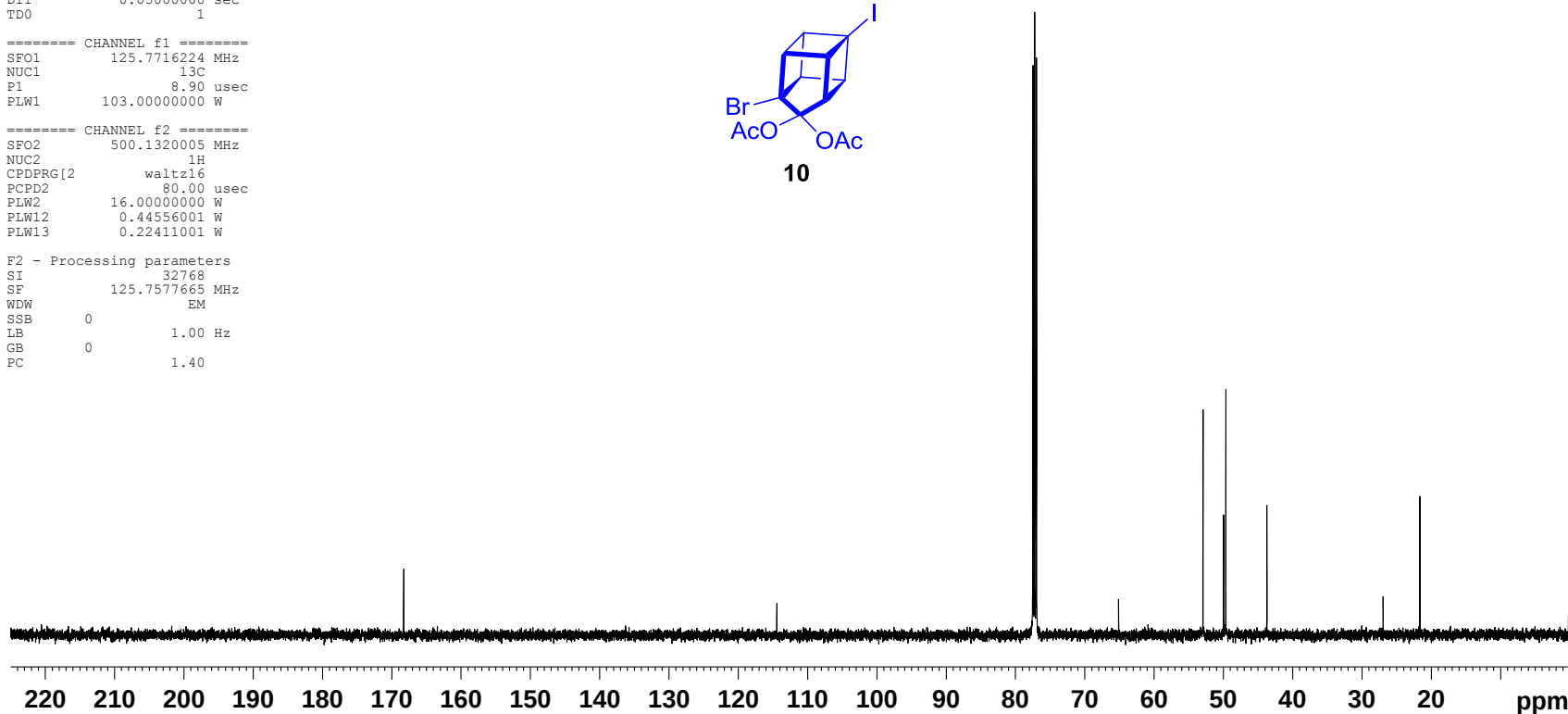
— 114.42

77.45
77.20
76.94

— 65.10

52.92
49.93
49.62
43.70

— 26.91
— 21.62



S-11. ^{13}C NMR Spectrum of Compound 10

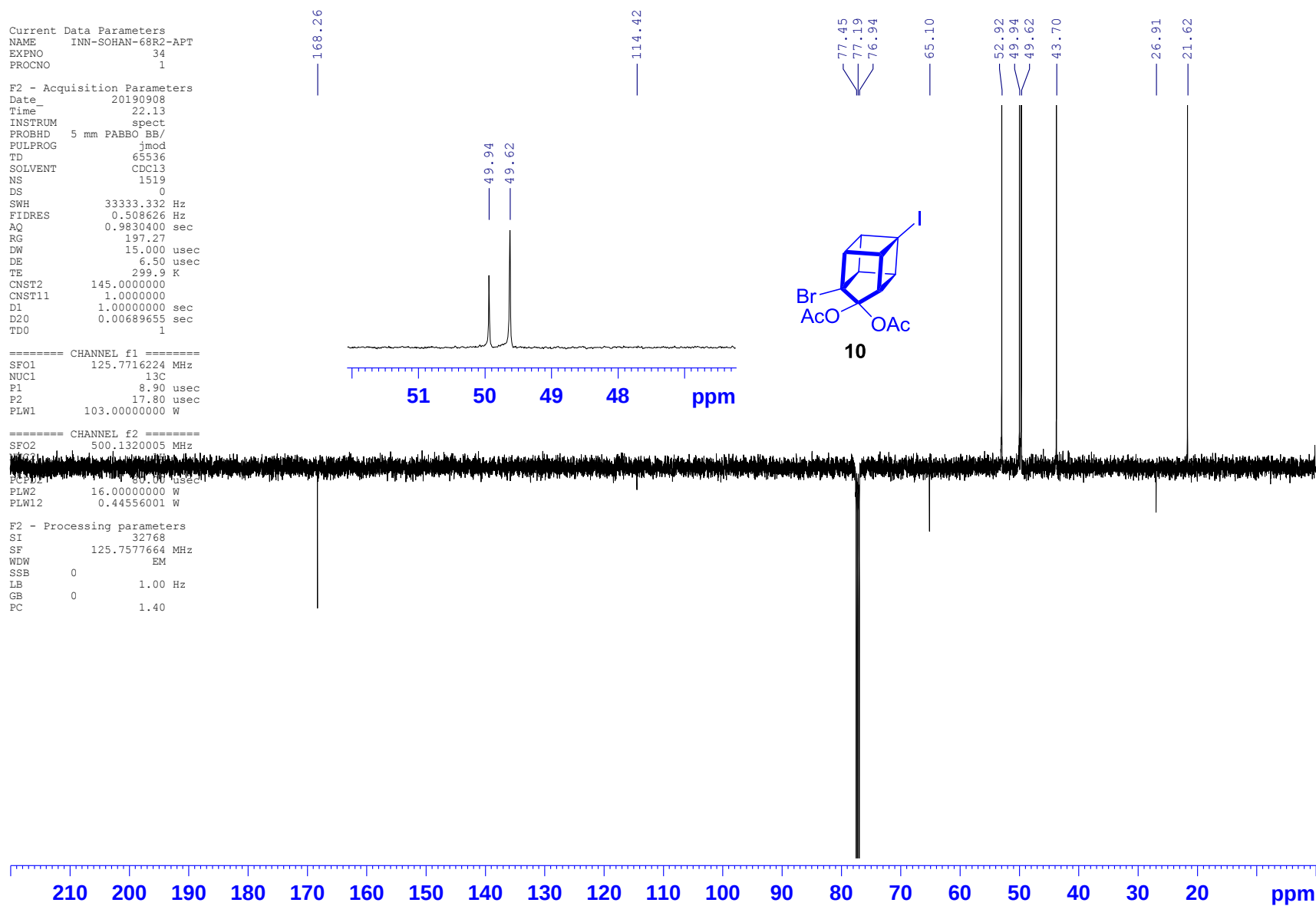
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 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1519
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 299.9 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 P1 16.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

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 LB 1.00 Hz
 GB 0
 PC 1.40



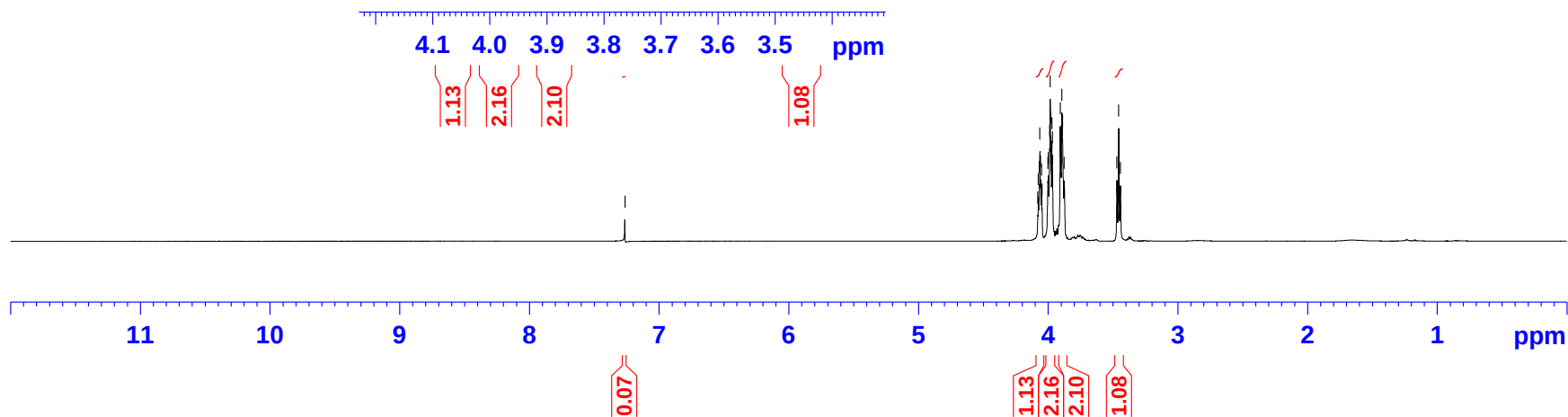
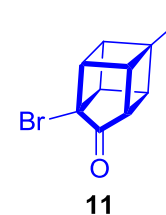
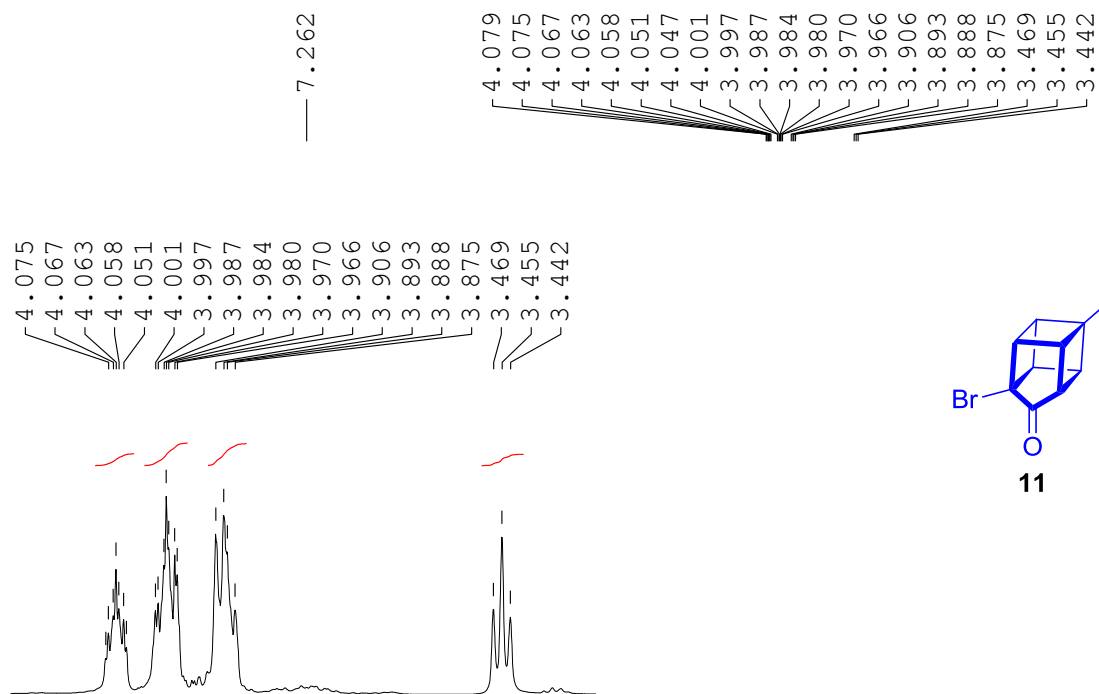
S-12. ^{13}C -APT NMR Spectrum of Compound 10

Current Data Parameters
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 PROCNO 1

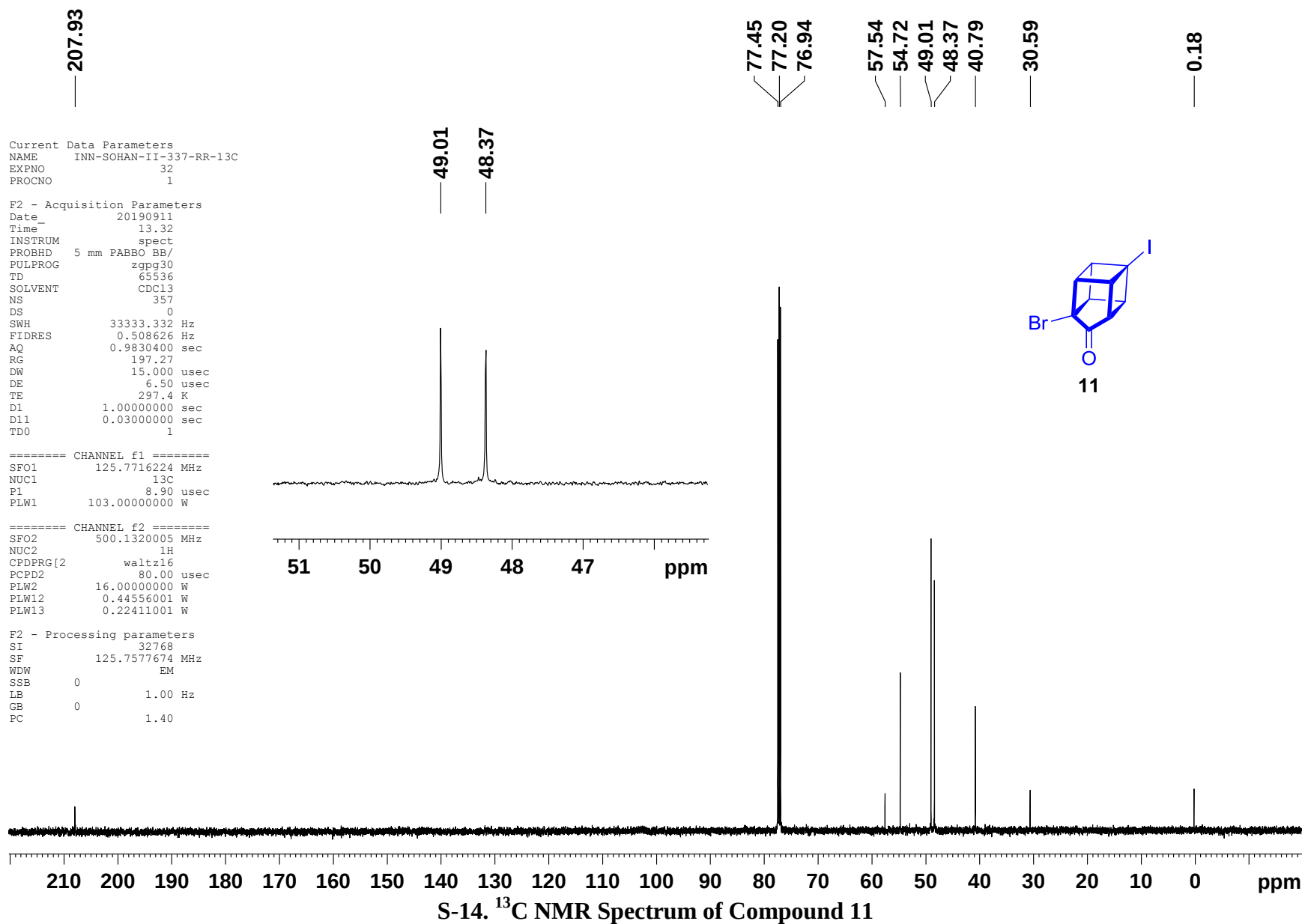
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 PULPROG zg30
 TD 54274
 SOLVENT CDC13
 NS 9
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.151522 Hz
 AQ 3.2998593 sec
 RG 101
 DW 60.800 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.75 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-13. ¹H NMR Spectrum of Compound 11



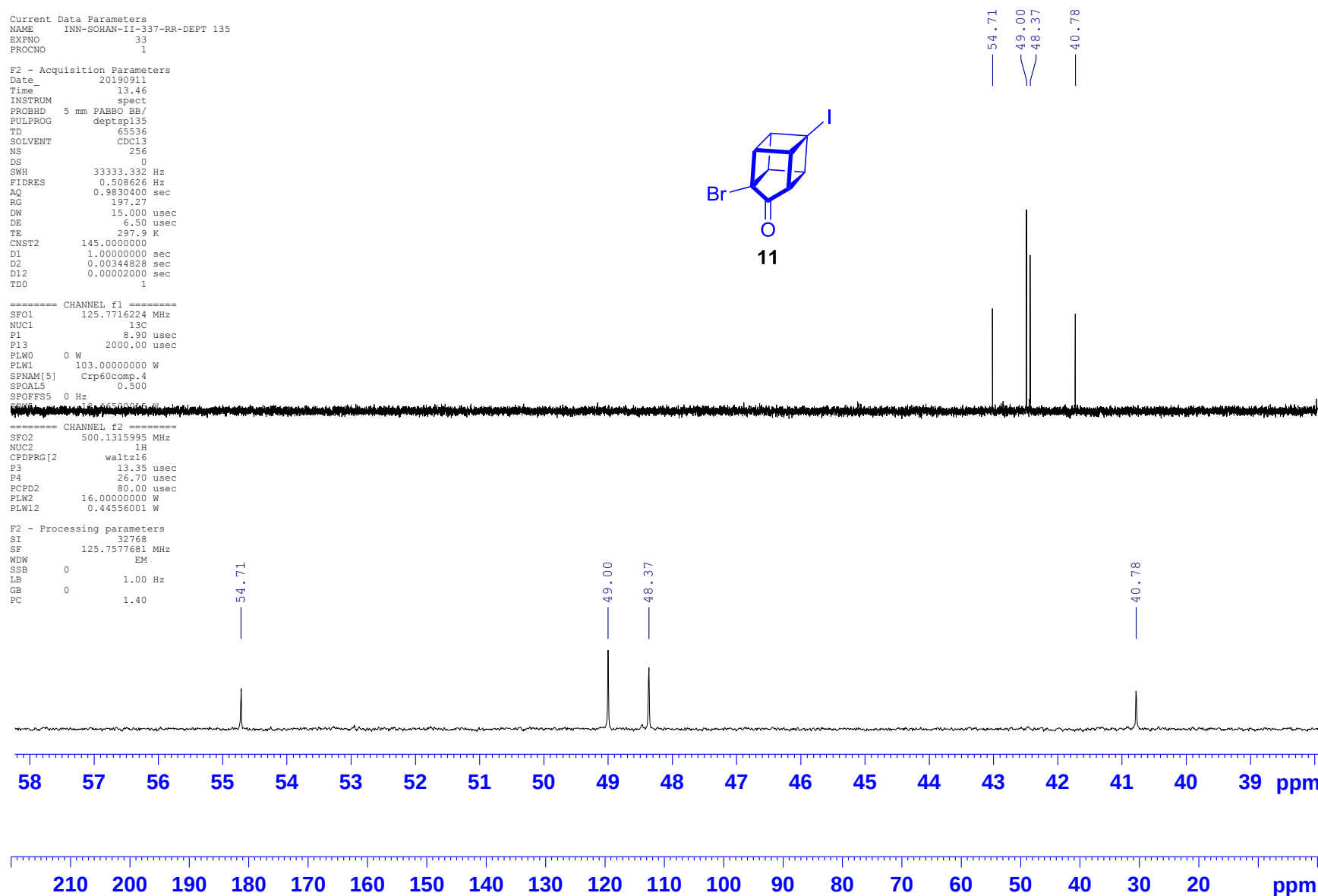
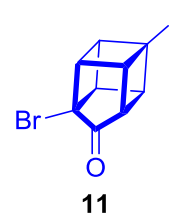
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 PULPROG deptsp135
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 SOLVENT CDCl3
 NS 256
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 297.9 K
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 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1

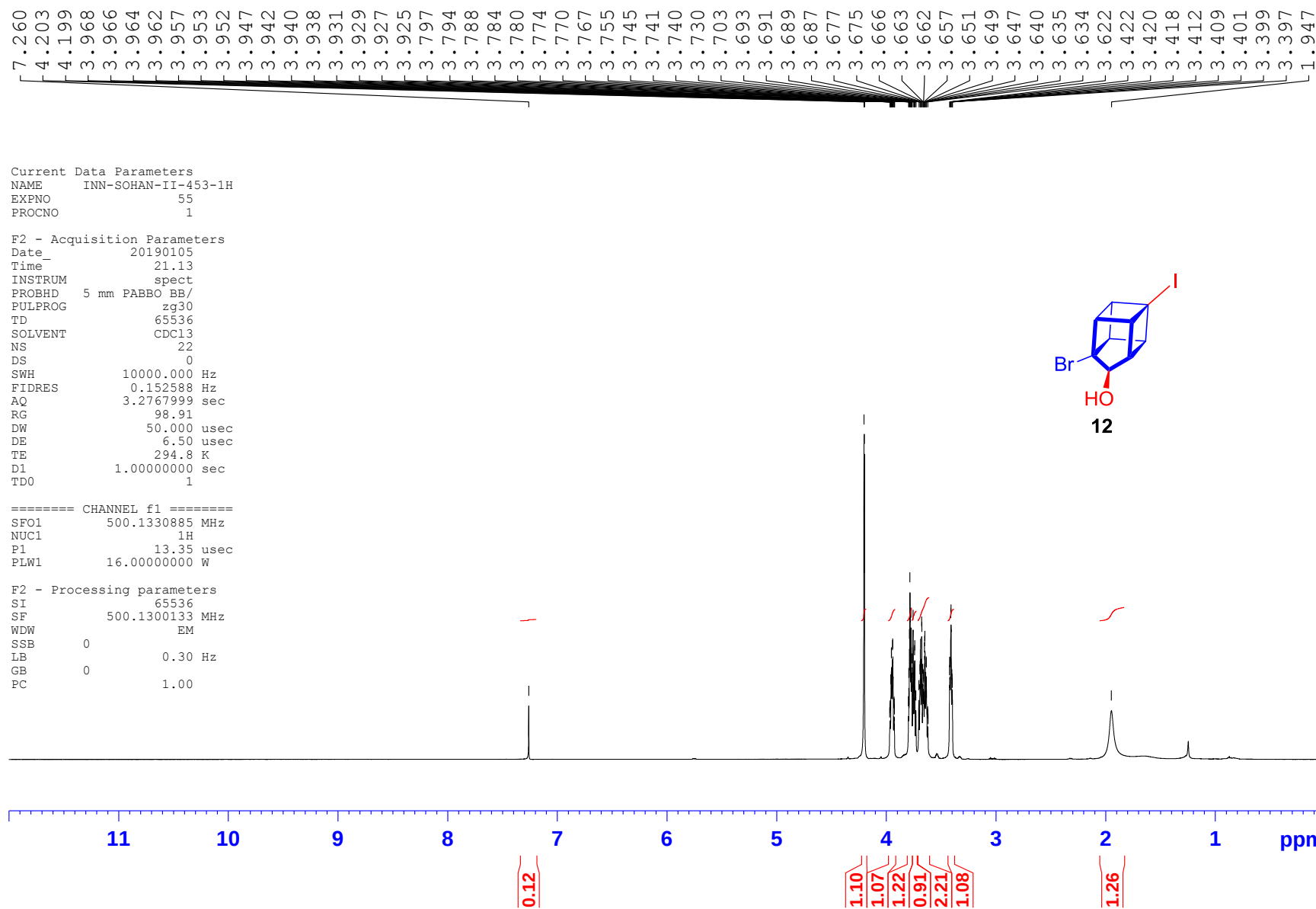
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 SFOFFS5 0 Hz
 SFOAL5 18.06500000 Hz

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz16
 P3 13.35 usec
 P4 26.70 usec
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577681 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-15. ¹³C-DEPT-135 NMR Spectrum of Compound 11



S-16. ^1H NMR Spectrum of Compound 12

Current Data Parameters
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 PROCNO 1

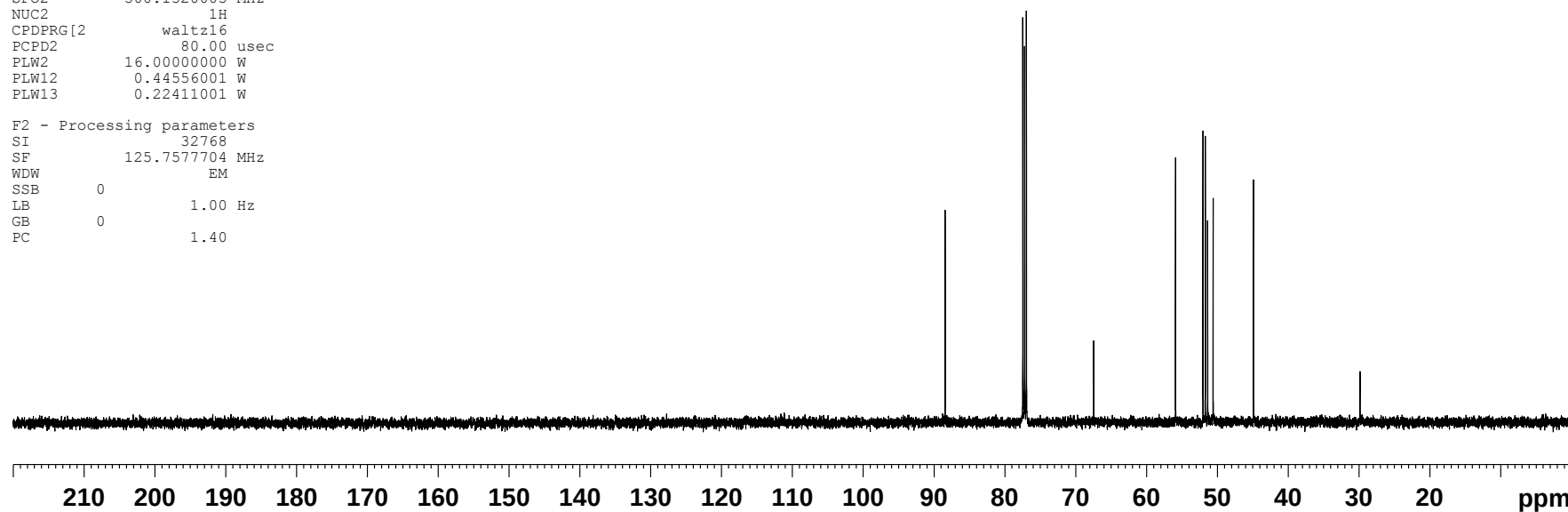
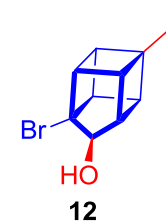
F2 - Acquisition Parameters
 Date_ 20190105
 Time_ 21.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 127
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 295.3 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577704 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

88.41
 77.45
 77.19
 76.94
 67.44
 55.90
 52.02
 51.69
 51.36
 50.59
 44.89
 29.83



S-18. ¹³C NMR Spectrum of Compound 12

Current Data Parameters
 NAME INN-SOHAN-II-453-APT
 EXPNO 57
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190105
 Time_ 21.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 130
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 295.5 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TDO 1

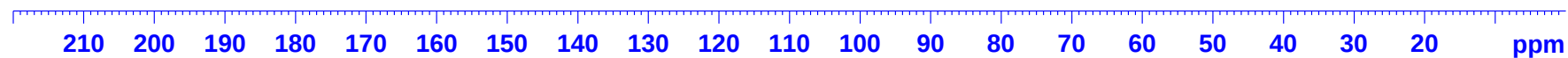
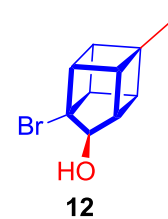
===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 F2 17.80 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters

SI 32768
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

88.42
 77.45
 77.20
 76.94
 67.45
 55.91
 52.02
 51.69
 51.37
 50.59
 44.90
 29.84



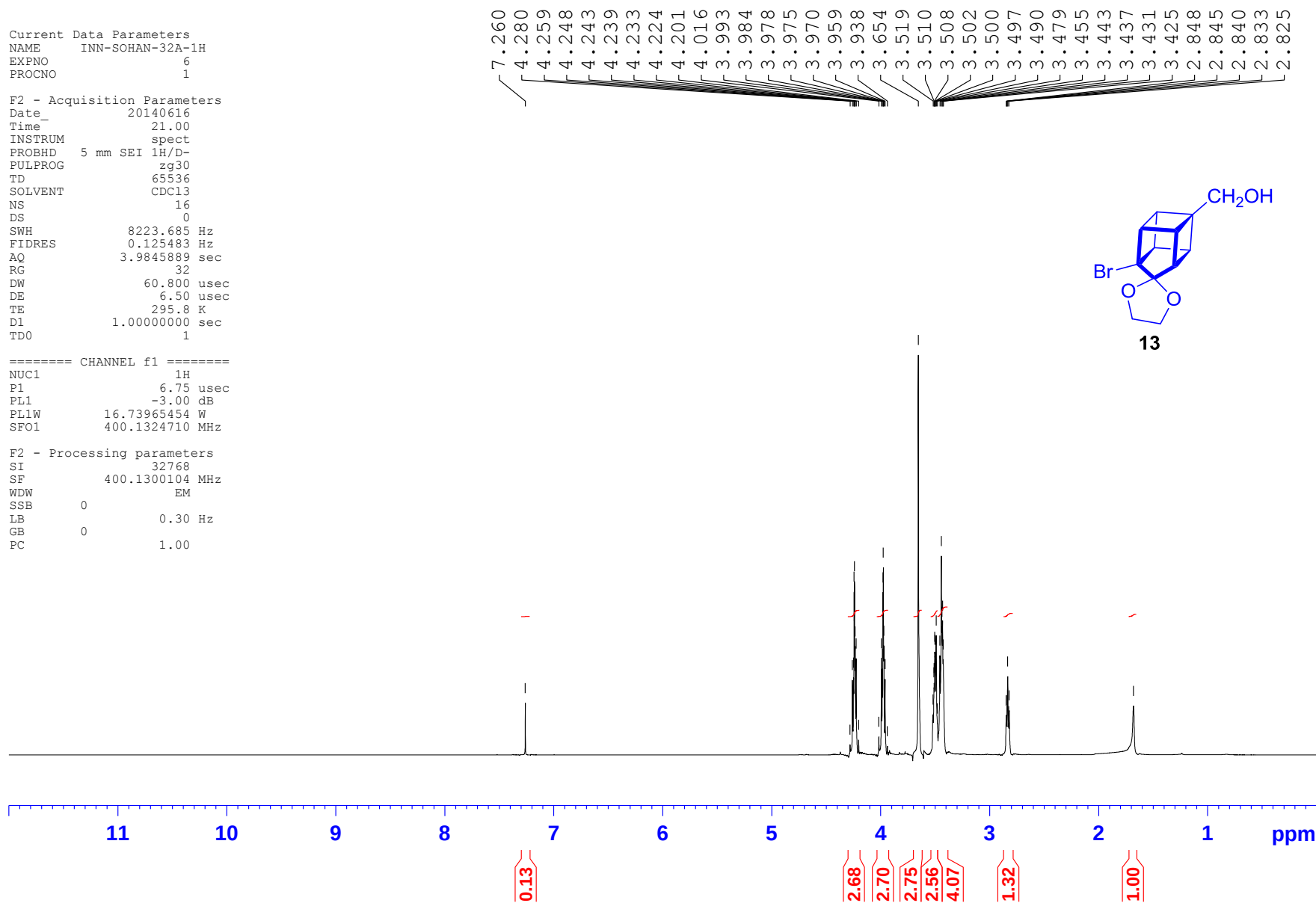
S-19. ¹³C-APT NMR Spectrum of Compound 12

Current Data Parameters
 NAME INN-SOHAN-32A-1H
 EXPNO 6
 PROCNO 1

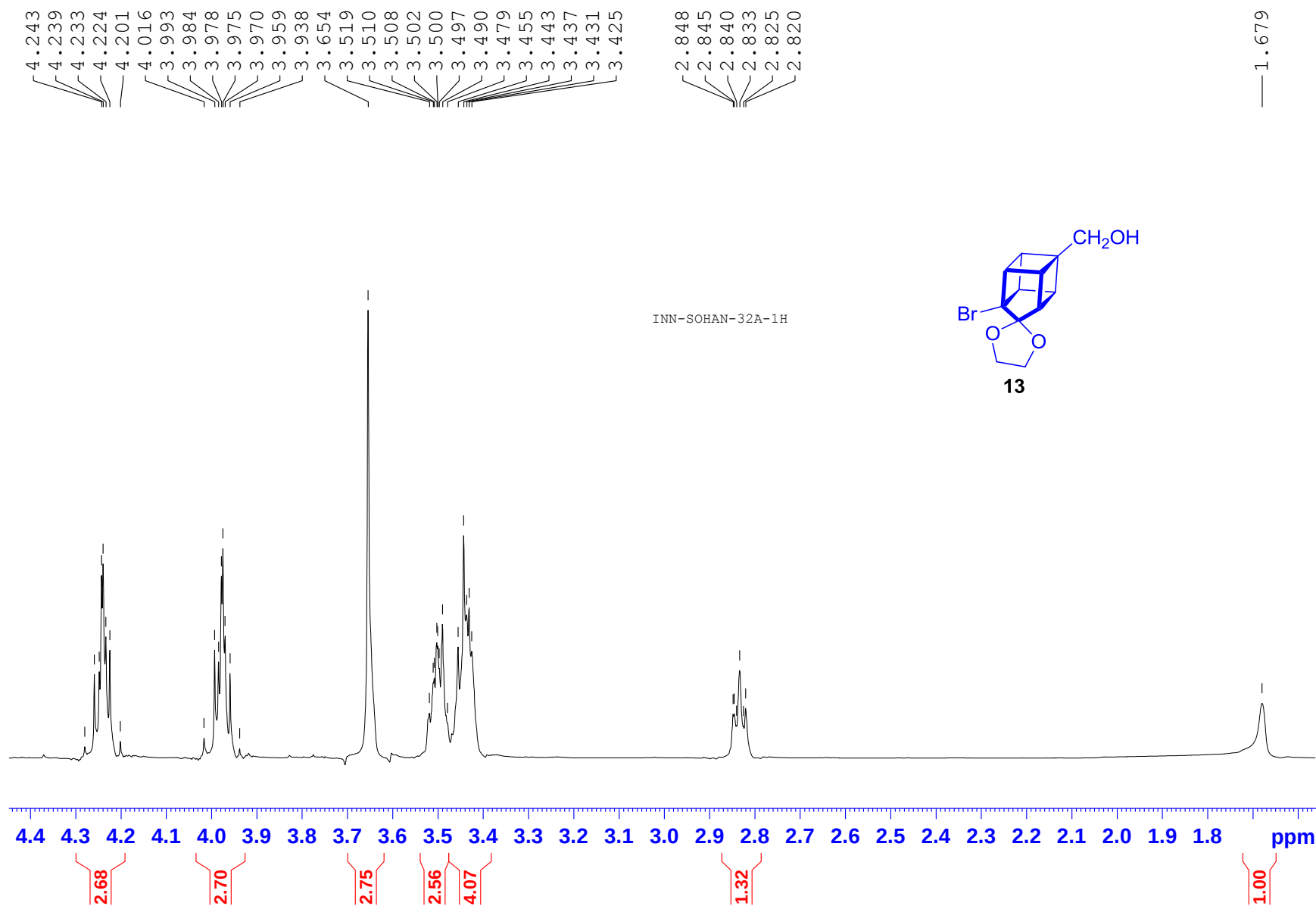
F2 - Acquisition Parameters
 Date_ 20140616
 Time_ 21.00
 INSTRUM spect
 PROBHD 5 mm SEI 1H/D-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.75 usec
 PL1 -3.00 dB
 PL1W 16.73965454 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-20. ¹H NMR Spectrum of Compound 13



S-21. ¹H NMR Spectrum (Expansion) of Compound 13

Current Data Parameters
 NAME INN-SOHAN-32-R1-13C
 EXPNO 42
 PROCNO 1

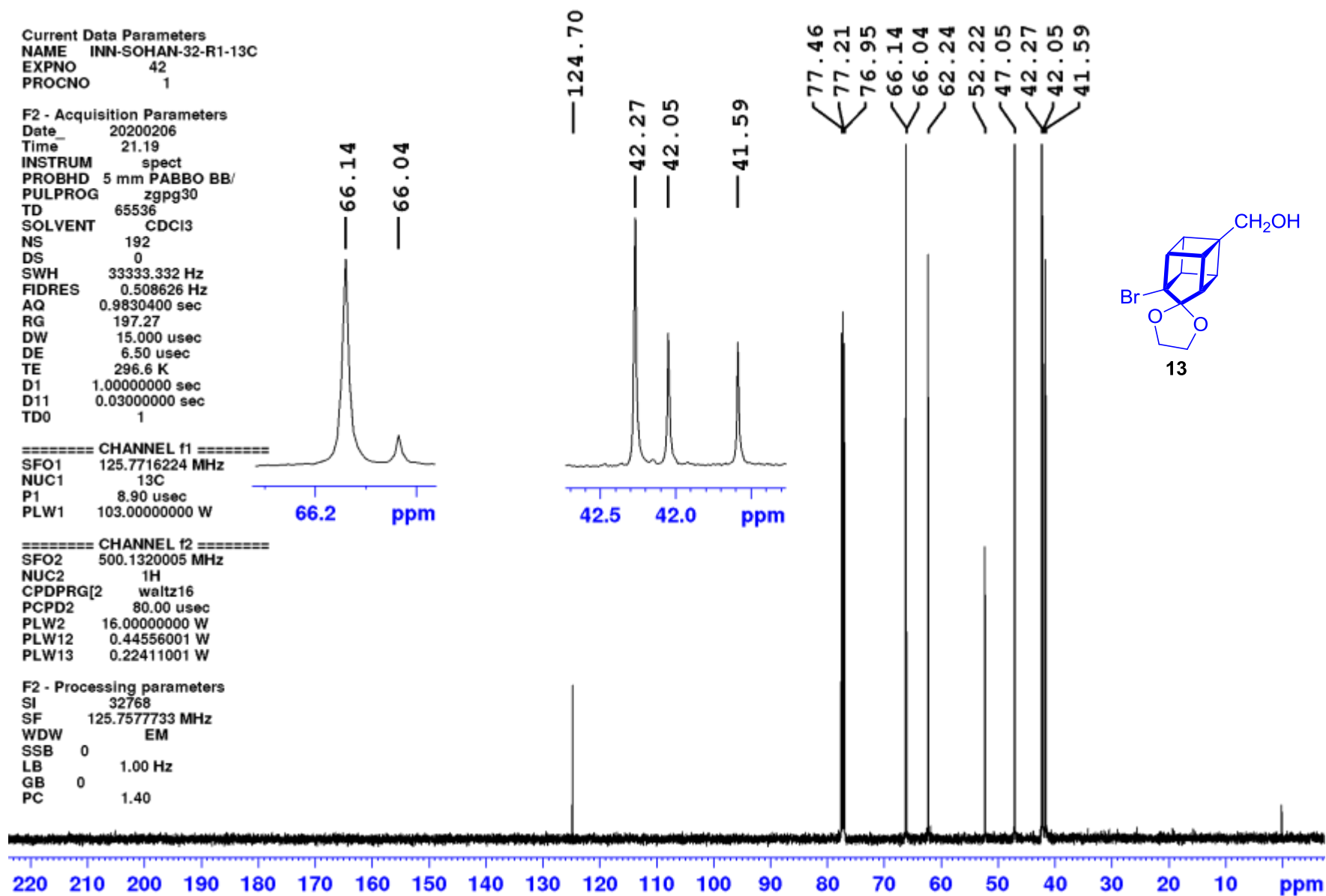
F2 - Acquisition Parameters

Date_ 20200206
 Time_ 21.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 192
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577733 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-22. ¹³C NMR Spectrum of Compound 13

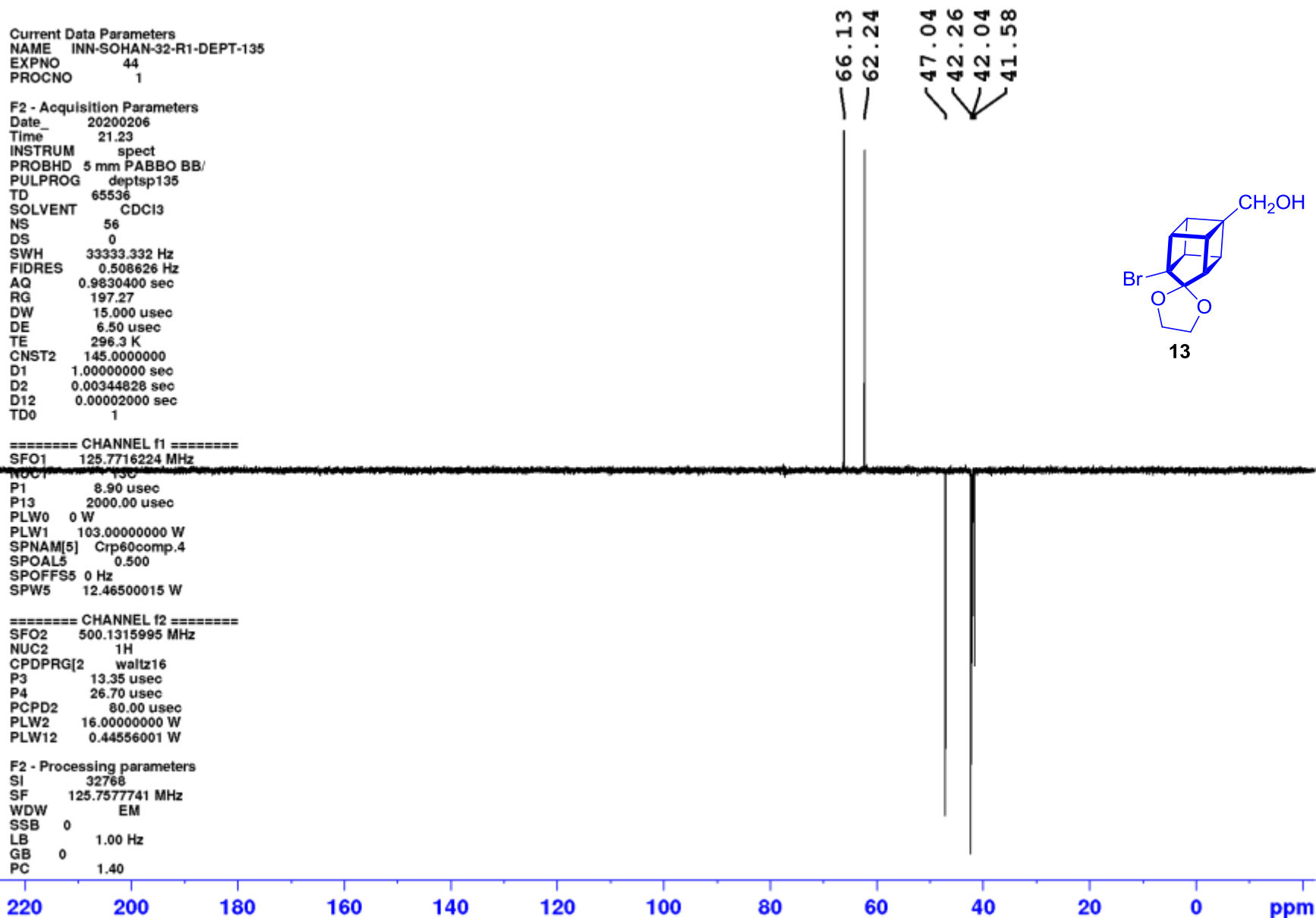
Current Data Parameters
 NAME INN-SOHAN-32-R1-DEPT-135
 EXPNO 44
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200206
 Time 21.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptsp135
 TD 65536
 SOLVENT CDCl3
 NS 56
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 296.3 K
 CNST2 145.0000000
 D1 1.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 103.00000000 W
 SPNAM[5] Crp60comp.4
 SPOAL5 0.500
 SPOFFS5 0 Hz
 SPW5 12.46500015 W

===== CHANNEL f2 =====
 SFO2 500.1315995 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P3 13.35 usec
 P4 26.70 usec
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577741 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-23. ¹³C-DEPT-135 NMR Spectrum of Compound 13

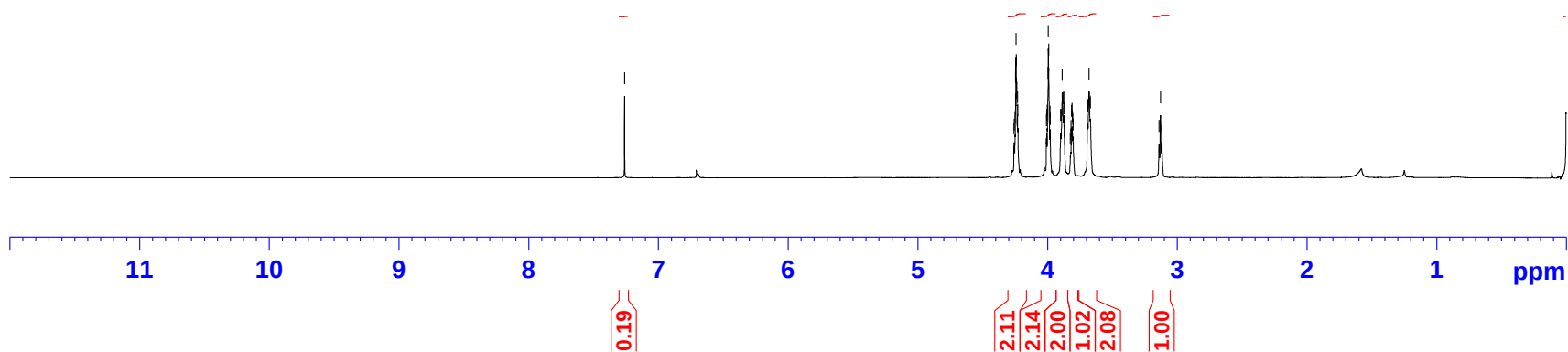
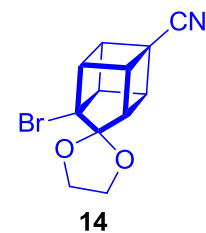
Current Data Parameters
NAME INN-SOAN-126-1H
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141003
Time_ 21.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 21
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 80.35
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

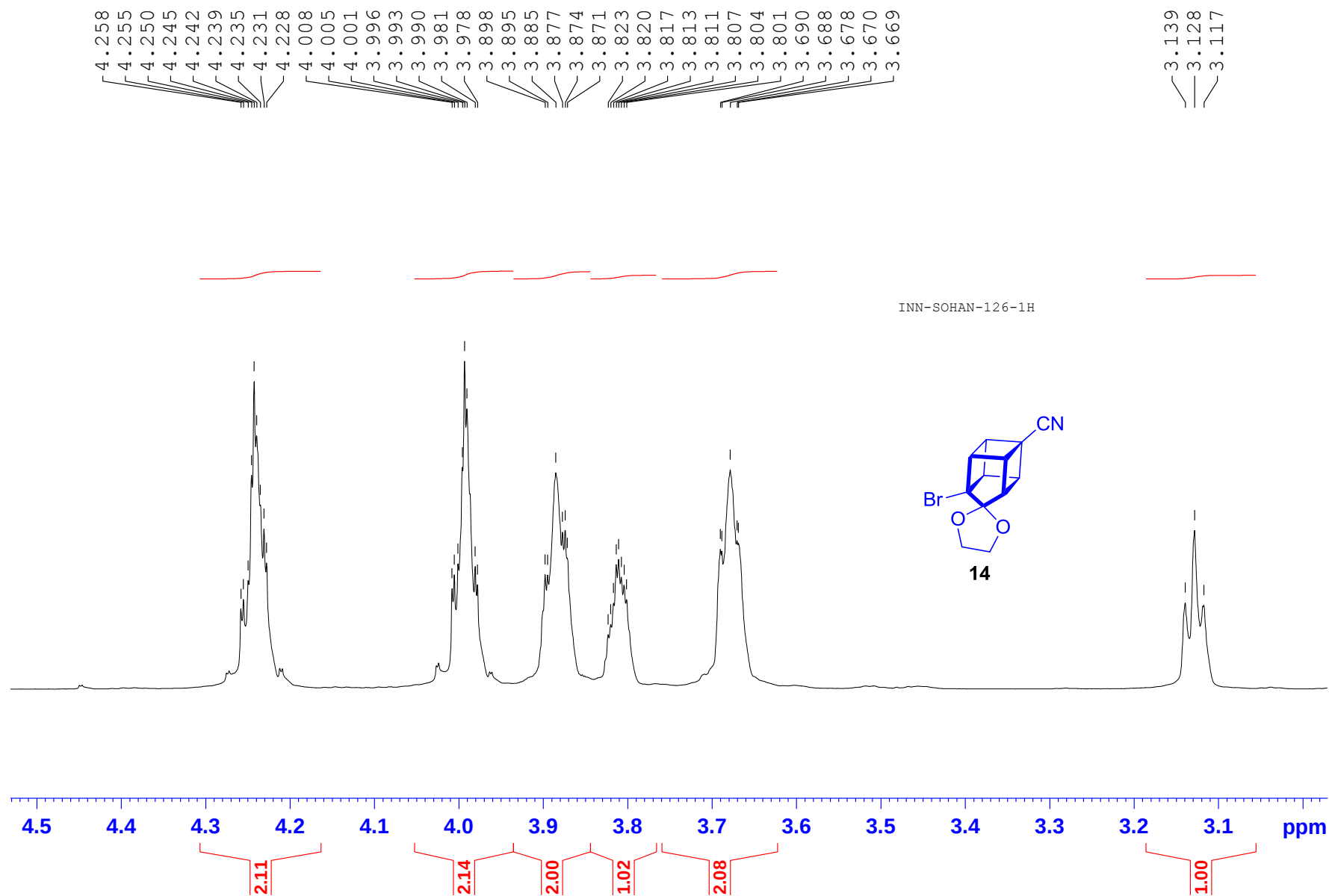
===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 13.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.260
4.258
4.255
4.250
4.245
4.242
4.239
4.235
4.231
4.228
4.008
4.005
4.001
3.996
3.993
3.990
3.981
3.978
3.898
3.895
3.885
3.877
3.874
3.871
3.823
3.820
3.817
3.813
3.811
3.807
3.804
3.801
3.690
3.688
3.678
3.670
3.669
3.139



S-24. ¹H NMR Spectrum of Compound 14



S-25. ^1H NMR Spectrum (Expansion) of Compound 14

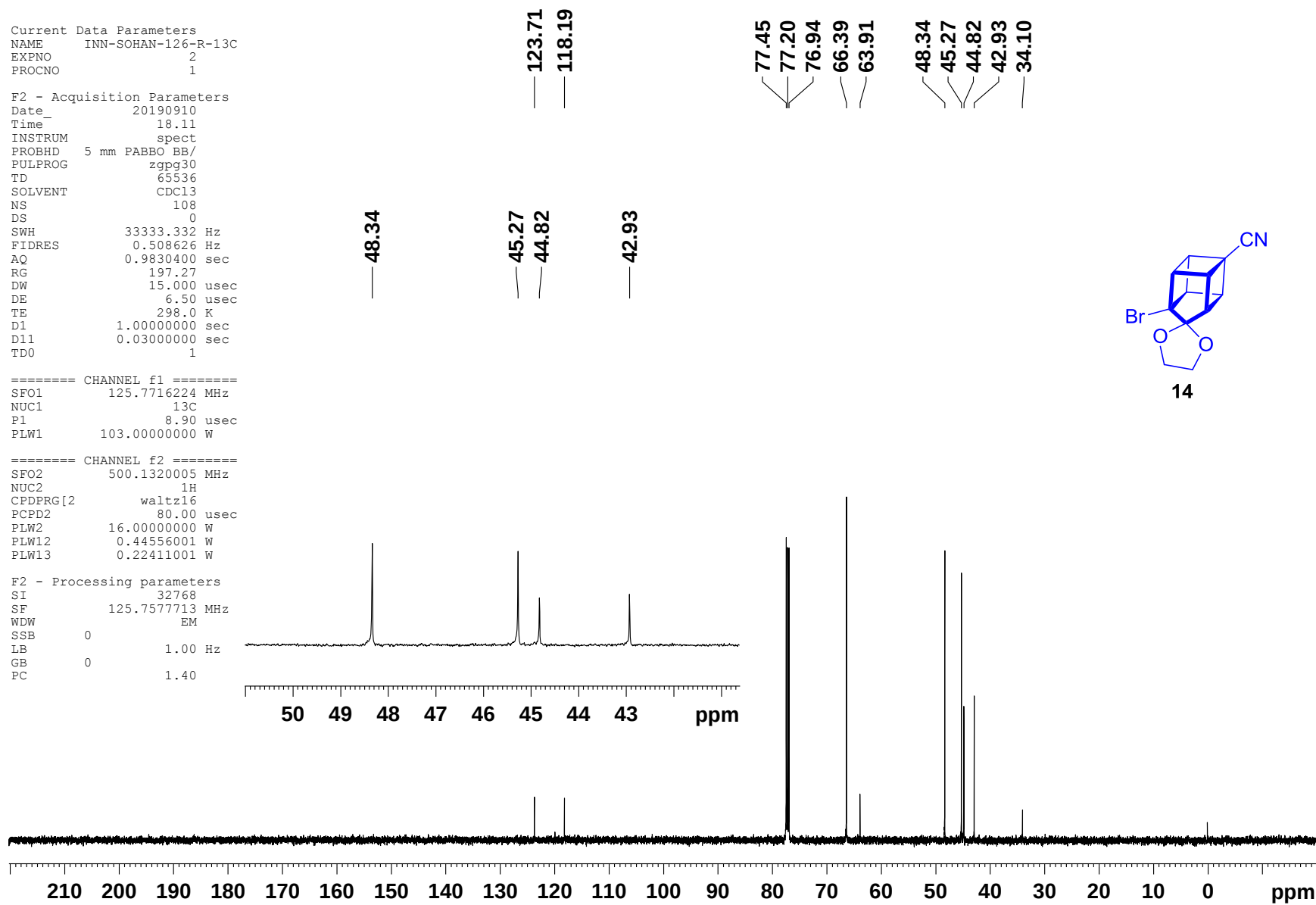
Current Data Parameters
 NAME INN-SOHAN-126-R-13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190910
 Time_ 18.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 108
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577713 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-26. ¹³C NMR Spectrum of Compound 14

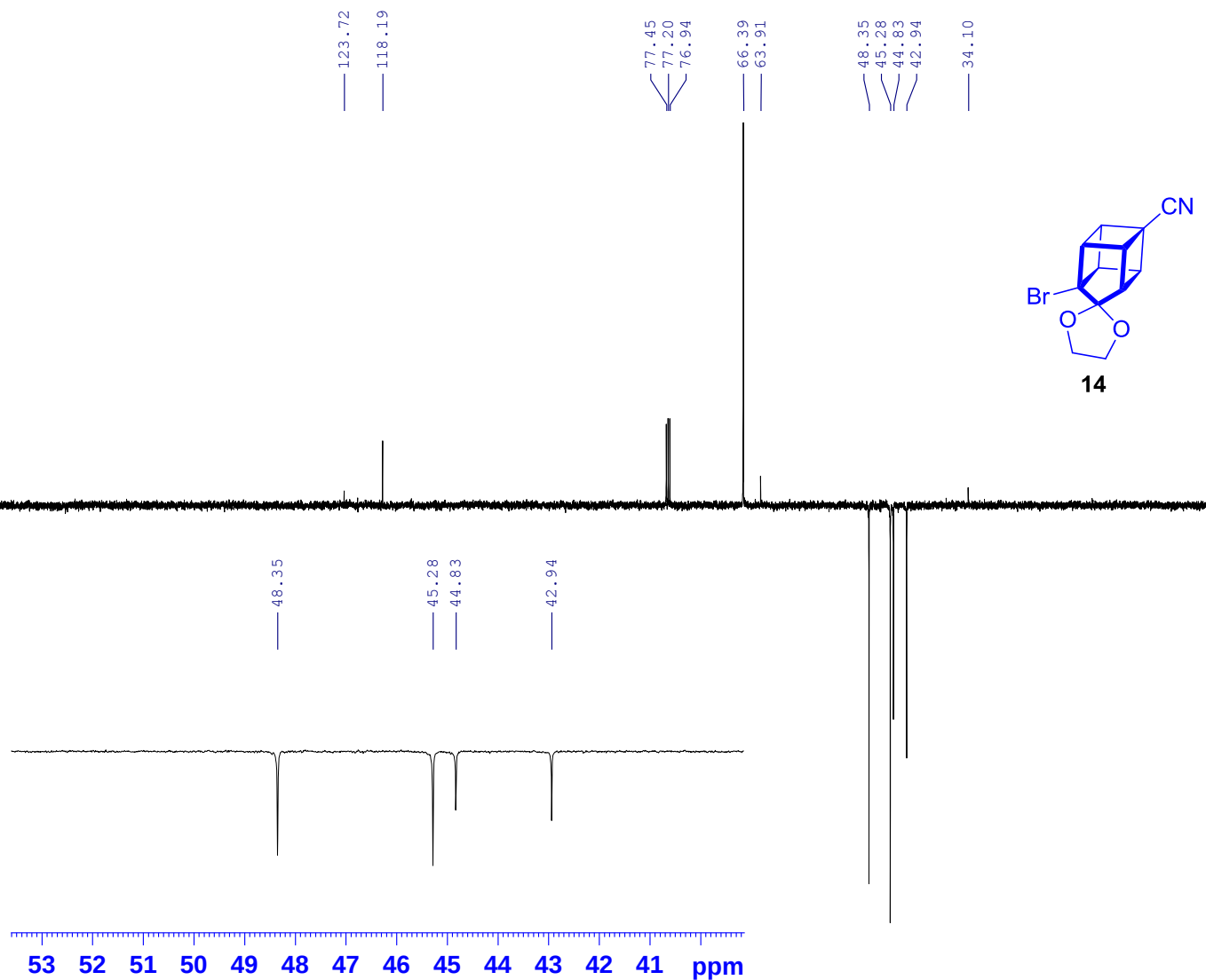
Current Data Parameters
 NAME INN-SOHN-126-R-APT
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20190910
 Time 18.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 242
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 298.5 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577708 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-27. ¹³C-APT NMR Spectrum of Compound 14

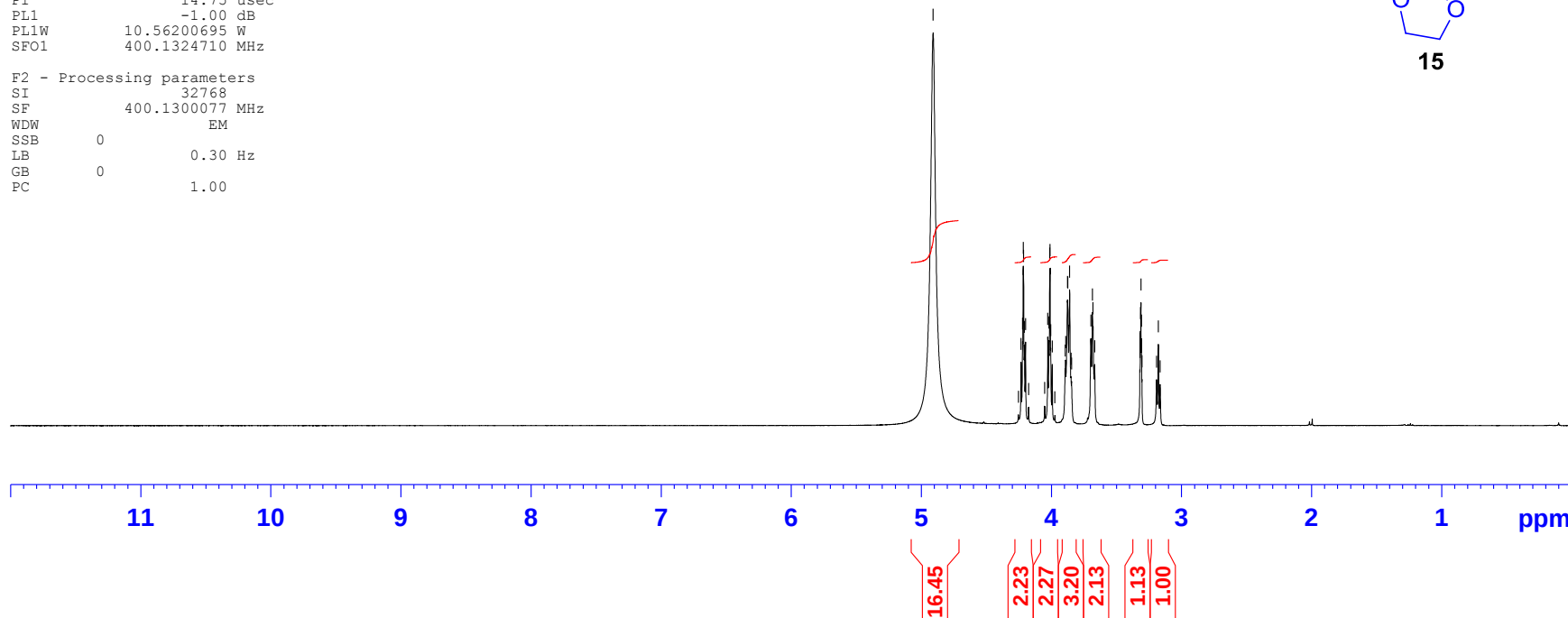
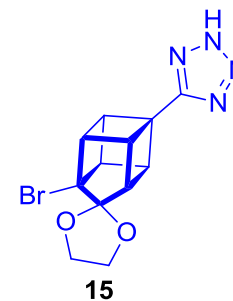
Current Data Parameters
 NAME INN-SOHAN-133-1H
 EXPNO 16
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141010
 Time_ 14.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 54274
 SOLVENT MeOD
 NS 6
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.151522 Hz
 AQ 3.2998593 sec
 RG 80.6
 DW 60.800 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

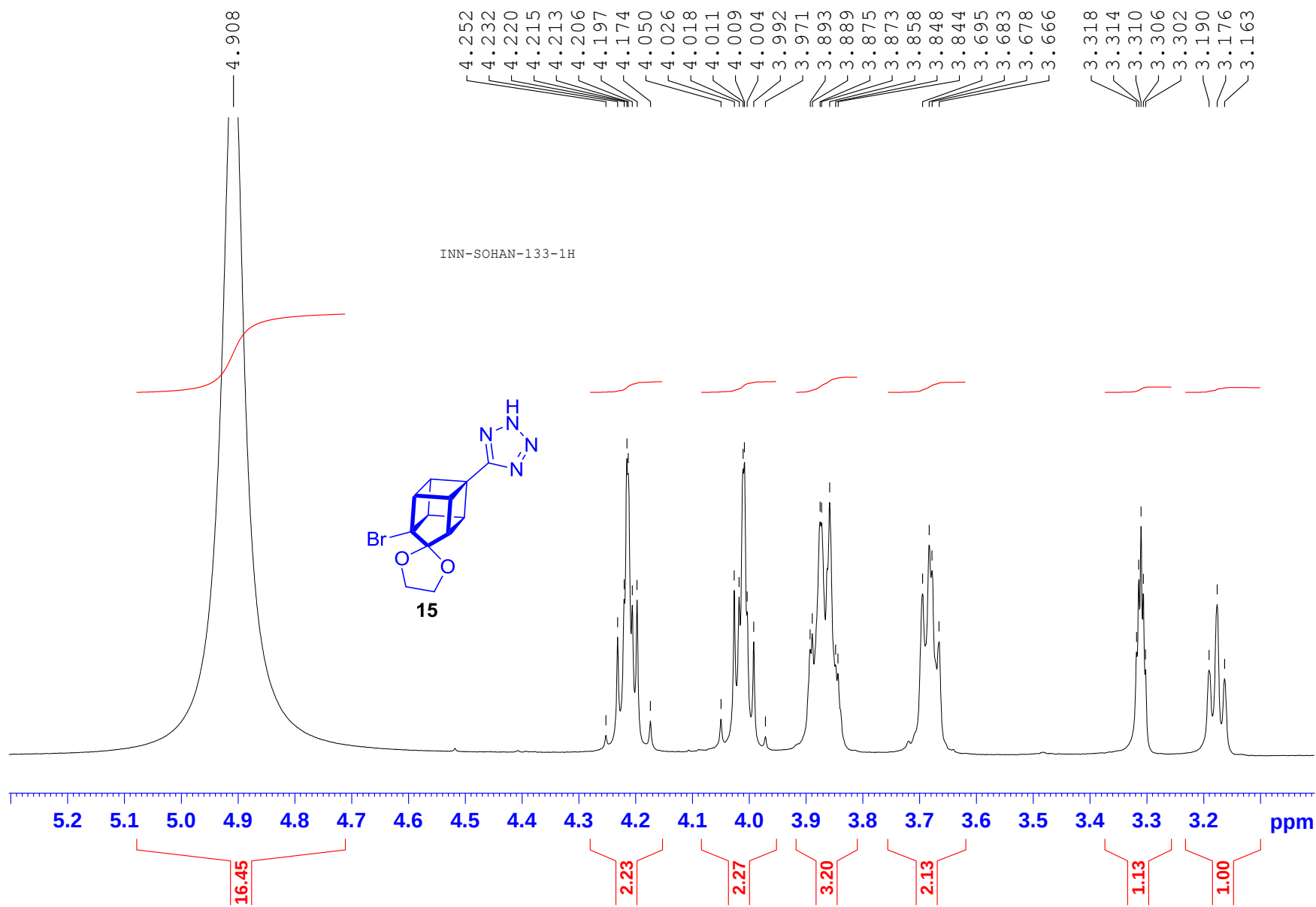
===== CHANNEL f1 =====
 NUC1 1H
 P1 14.75 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300077 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

4.908
4.252
4.232
4.220
4.215
4.213
4.206
4.197
4.174
4.050
4.026
4.018
4.011
4.009
4.004
3.992
3.971
3.893
3.889
3.875
3.873
3.858
3.848
3.844
3.695
3.683
3.678
3.666
3.318
3.314
3.310
3.306
3.302
3.190
3.176
3.163



S-28. ^1H NMR Spectrum of Compound 15



S-29. ^1H NMR Spectrum (Expansion) of compound 15

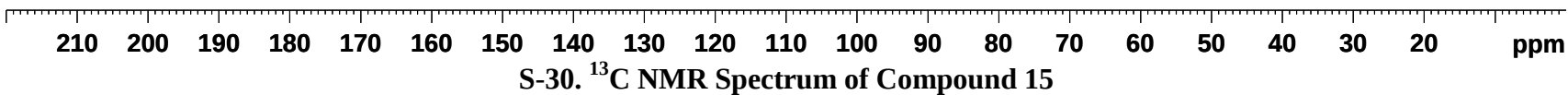
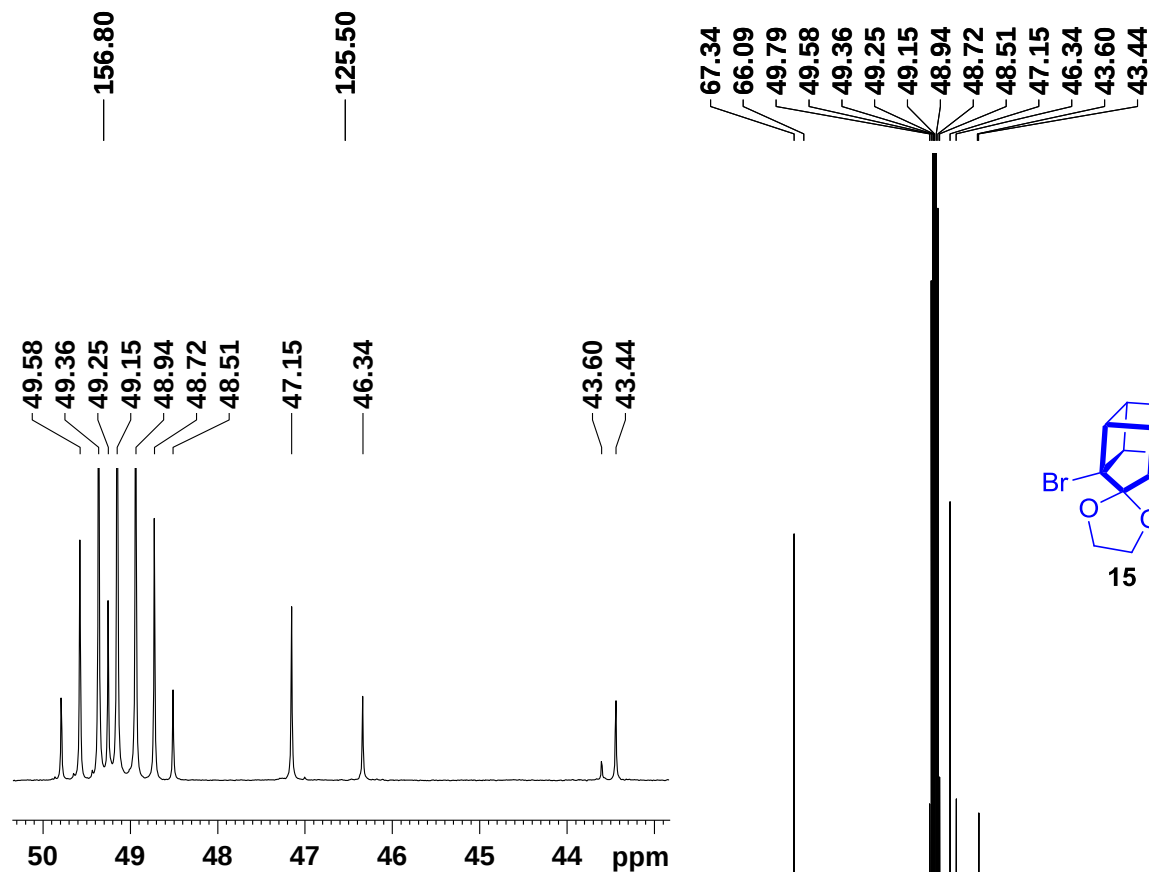
Current Data Parameters
 NAME INN-SOHA-133-1-13C
 EXPNO 19
 PROCNO 1

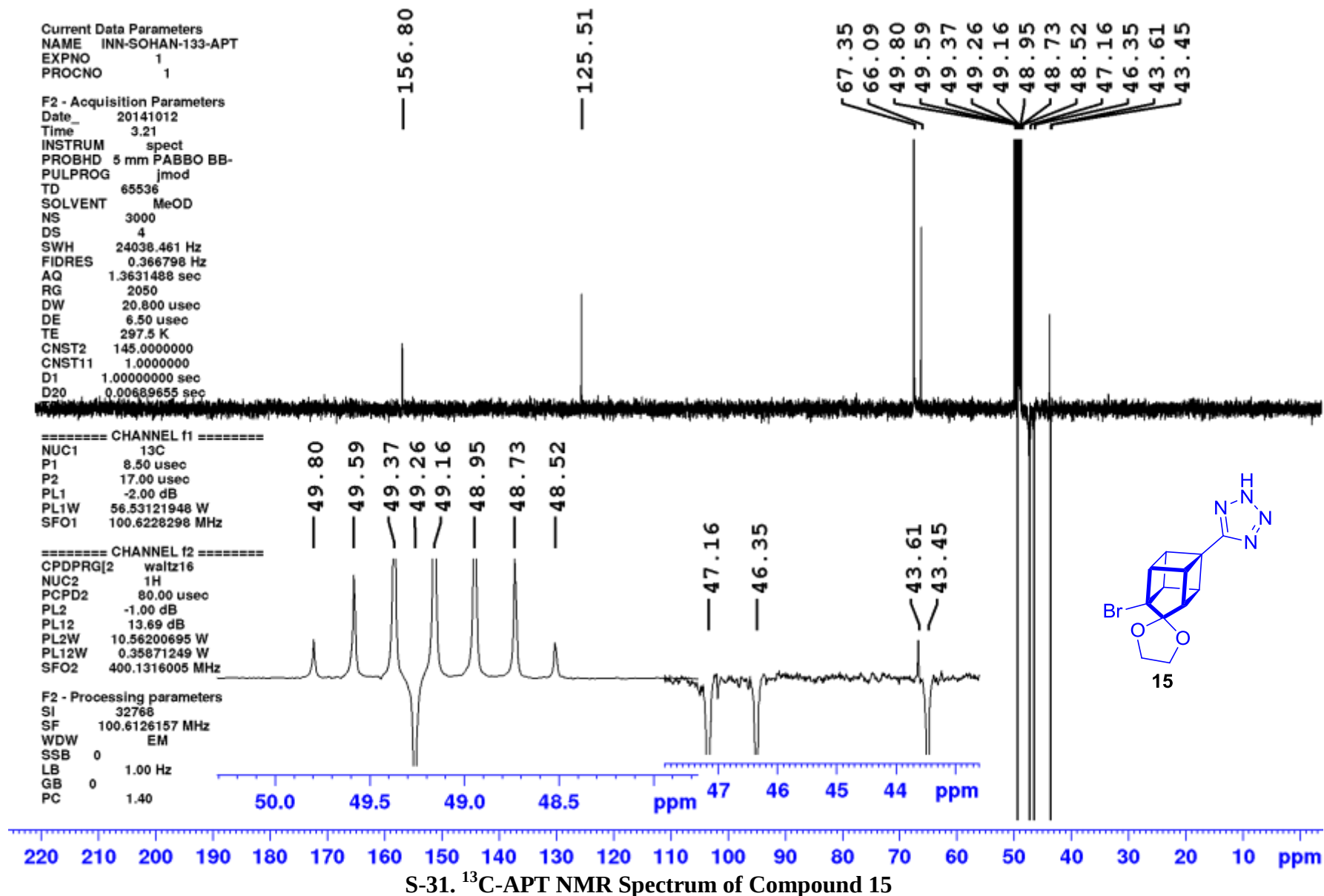
F2 - Acquisition Parameters
 Date_ 20141011
 Time_ 18.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 2912
 DS 4
 SWH 26041.666 Hz
 FIDRES 0.397364 Hz
 AQ 1.2582912 sec
 RG 2050
 DW 19.200 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 13.69 dB
 PL13 14.50 dB
 PL2W 10.56200695 W
 PL12W 0.35871249 W
 PL13W 0.29767781 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126165 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME INN-SOHAN-134-1H
 EXPNO 1
 PROCNO 1

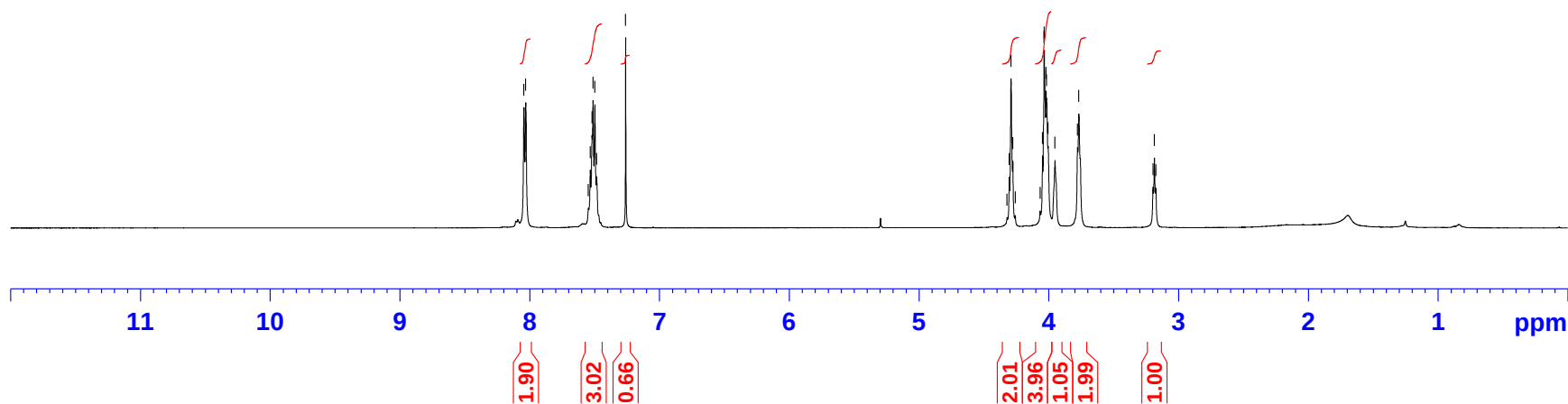
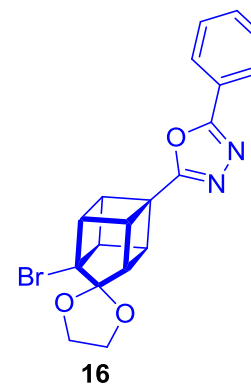
F2 - Acquisition Parameters
 Date_ 20160819
 Time_ 19.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 106.54
 DW 50.000 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 13.00000000 W

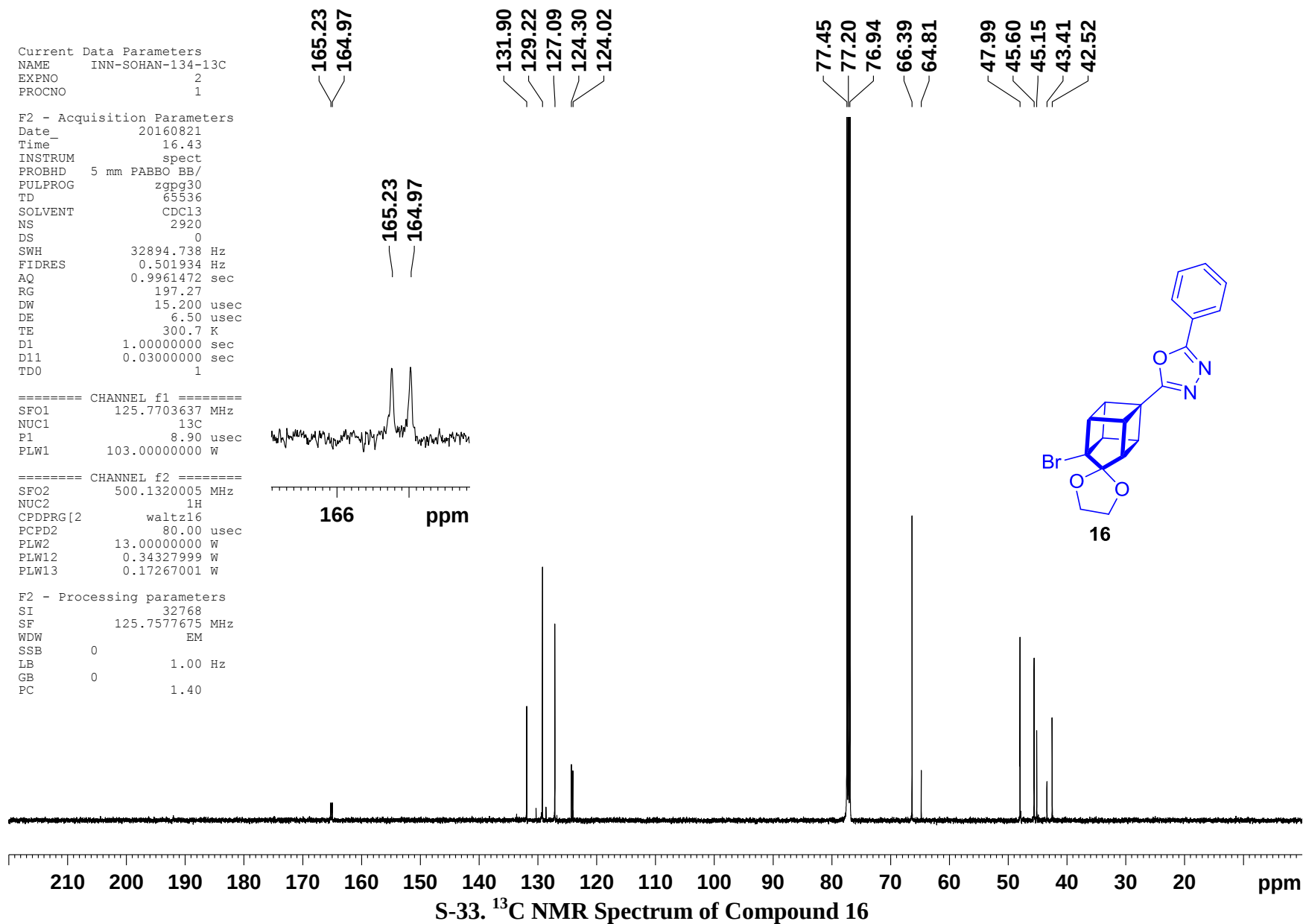
F2 - Processing parameters
 SI 65536
 SF 500.1300142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.044
8.030
7.548
7.533
7.519
7.512
7.497
7.483
7.260

4.321
4.304
4.291
4.277
4.258
4.066
4.048
4.036
4.033
4.020
4.016
4.005
3.951
3.778
3.768
3.196
3.186
3.175



S-32. ¹H NMR Spectrum of Compound 16



Current Data Parameters
 NAME INN-SOHN-134-APT
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160821
 Time 13.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 899
 DS 0
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 300.1 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577666 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

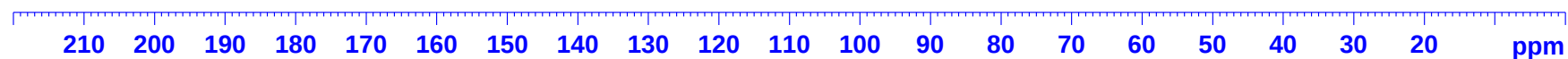
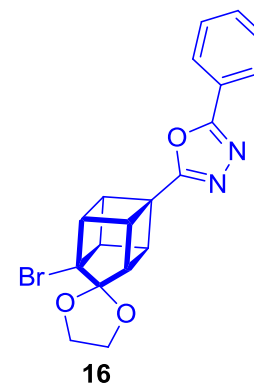
165.24
164.98

131.90
129.22
127.12
124.31
124.05

77.45
77.20
76.95

66.40
64.83

48.03
45.64
45.19
43.45
42.57



S-34. ¹³C-APT NMR Spectrum of Compound 16

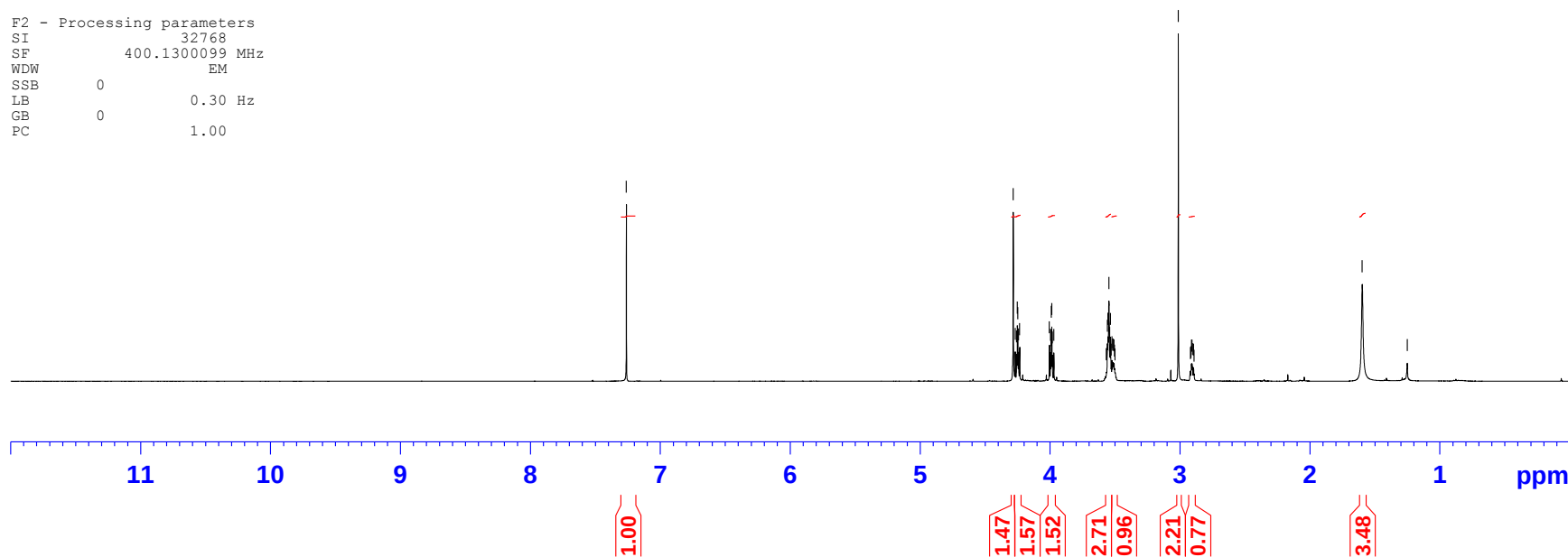
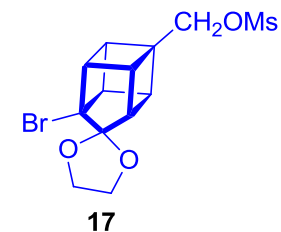
Current Data Parameters
 NAME INN-SOHAN-98-1H
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140904
 Time_ 23.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 54274
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.151522 Hz
 AQ 3.2998593 sec
 RG 181
 DW 60.800 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.00000000 sec
 TD0 1

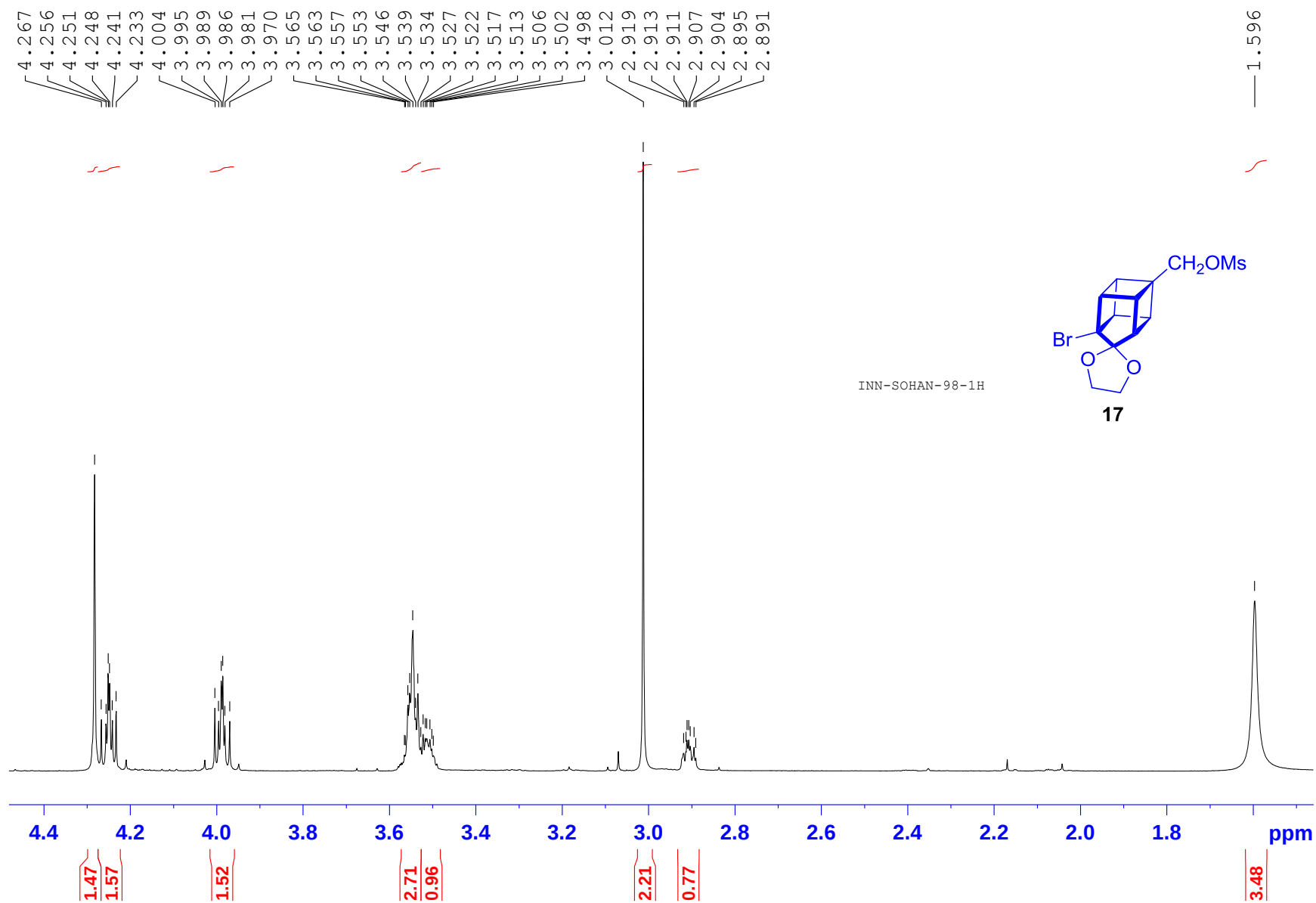
===== CHANNEL f1 =====
 NUC1 1H
 P1 14.75 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.260
4.282
4.267
4.256
4.251
4.248
4.241
4.233
4.004
3.995
3.989
3.986
3.981
3.970
3.565
3.563
3.557
3.553
3.546
3.539
3.534
3.527
3.522
3.517
3.513
3.506
3.502
3.498
3.012
2.919
2.913
2.911
2.907
2.904
2.895
2.891



S-35. ¹H NMR Spectrum of Compound 17



S-36. ¹H NMR Spectrum of Compound 17

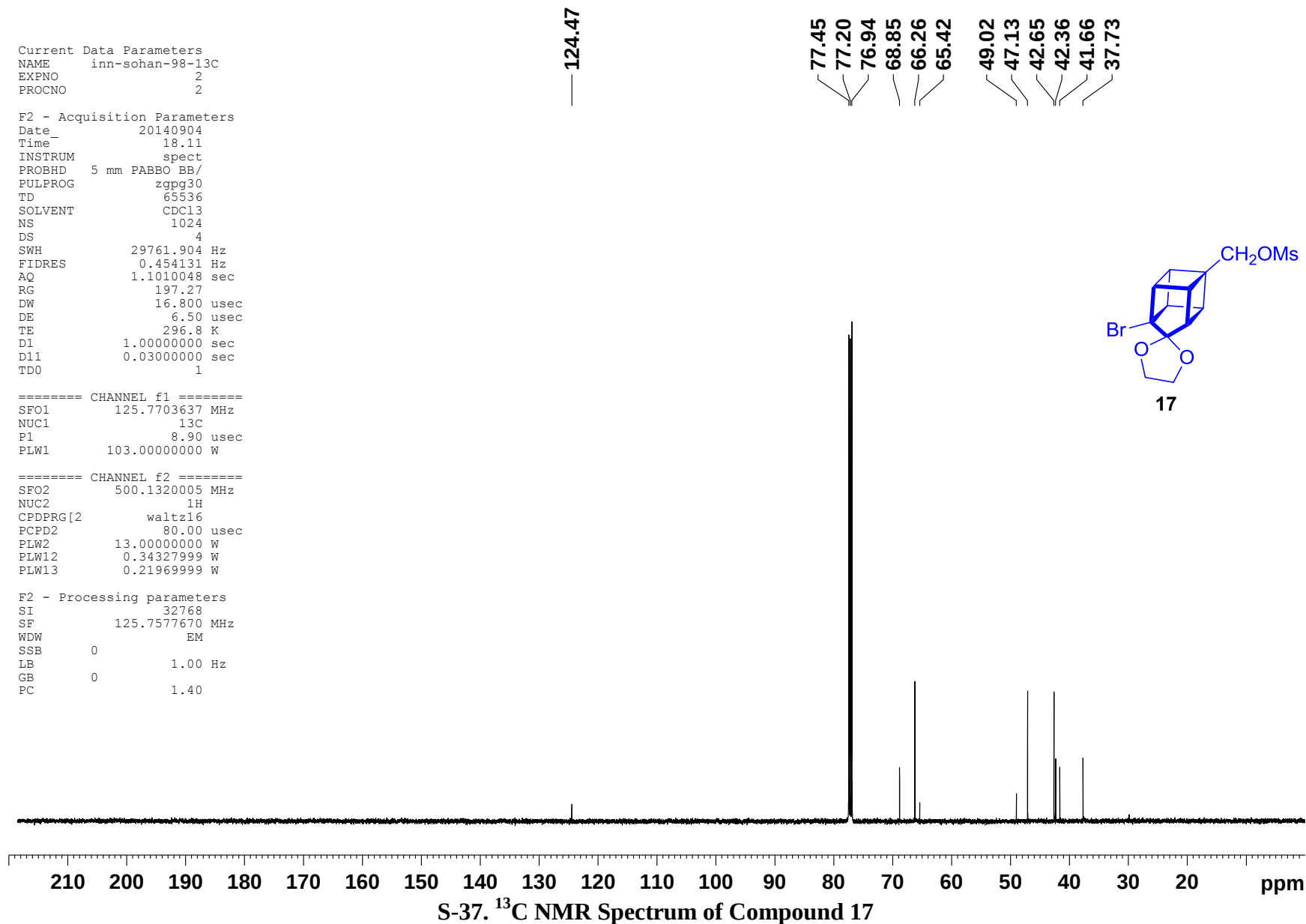
Current Data Parameters
 NAME inn-sohan-98-13C
 EXPNO 2
 PROCNO 2

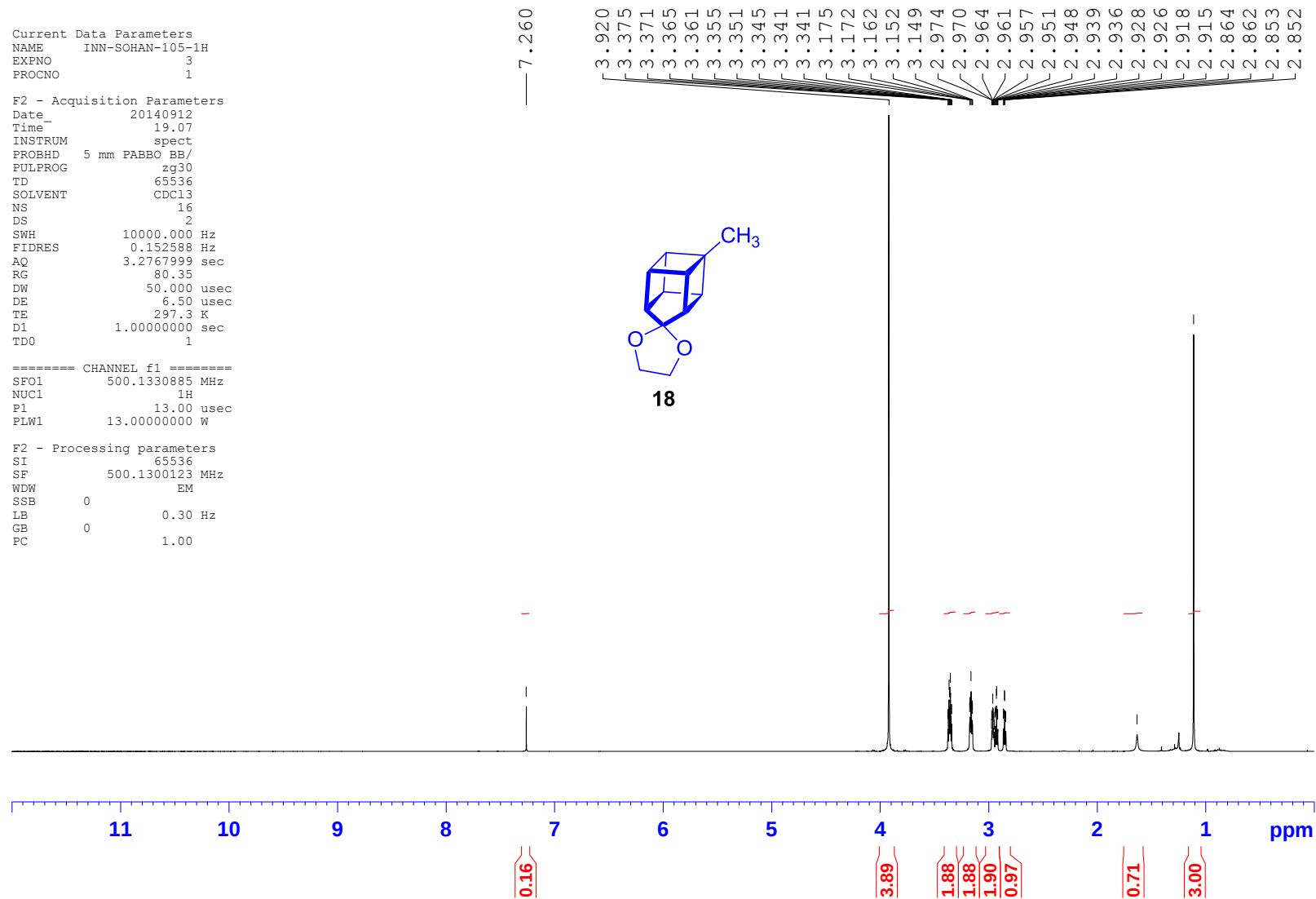
F2 - Acquisition Parameters
 Date_ 20140904
 Time_ 18.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

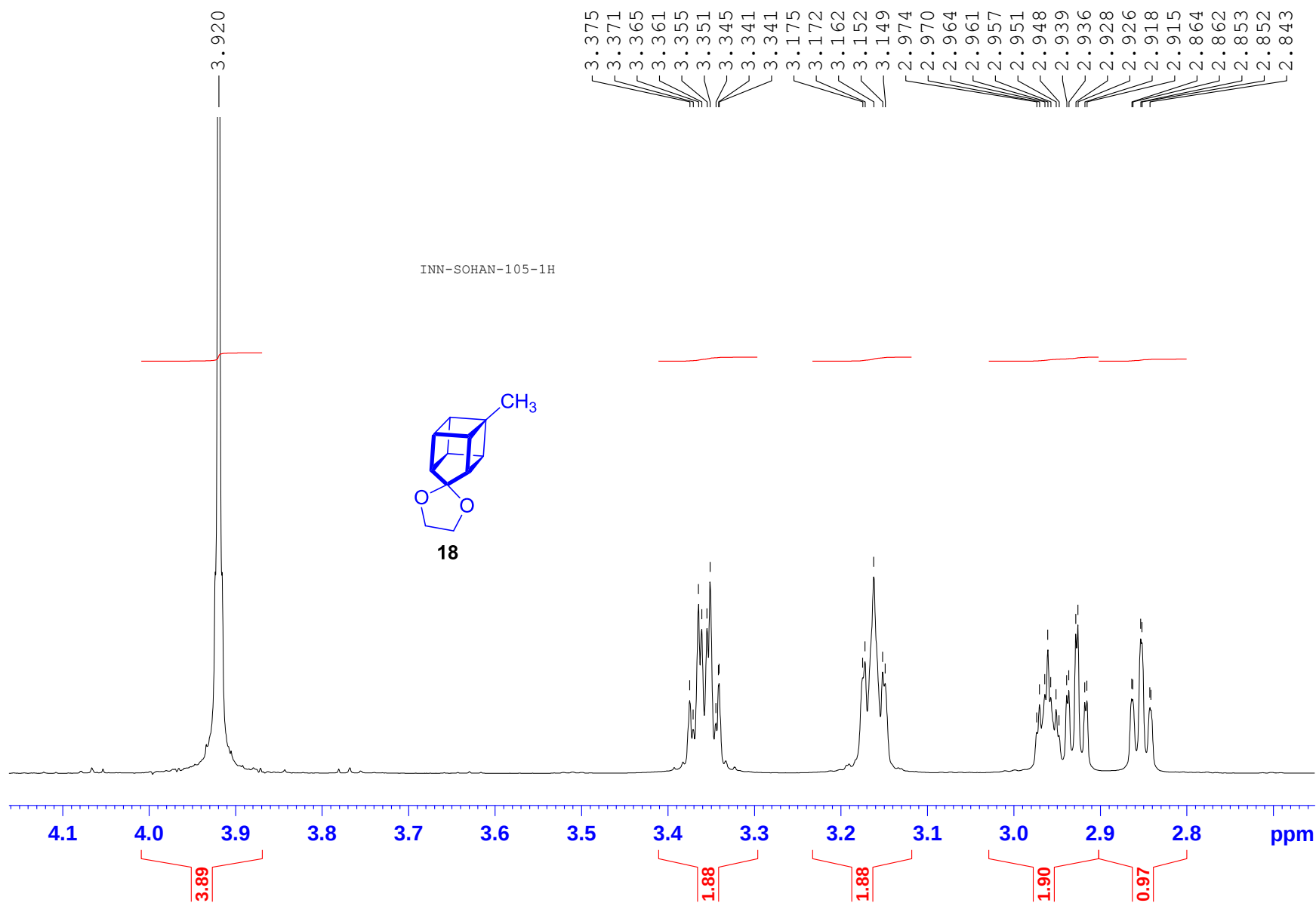
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577670 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





S-38. ^1H NMR Spectrum of Compound 18



S-39. ^1H NMR Spectrum (Expansion) of Compound 18

Current Data Parameters
 NAME INN-SOAN-105-13C
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140912
 Time_ 19.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 122
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 197.27
 DW 16.800 usec
 DE 6.50 usec
 TE 297.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577674 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

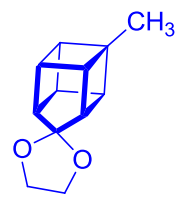
— 128.86

77.45
77.20
76.95

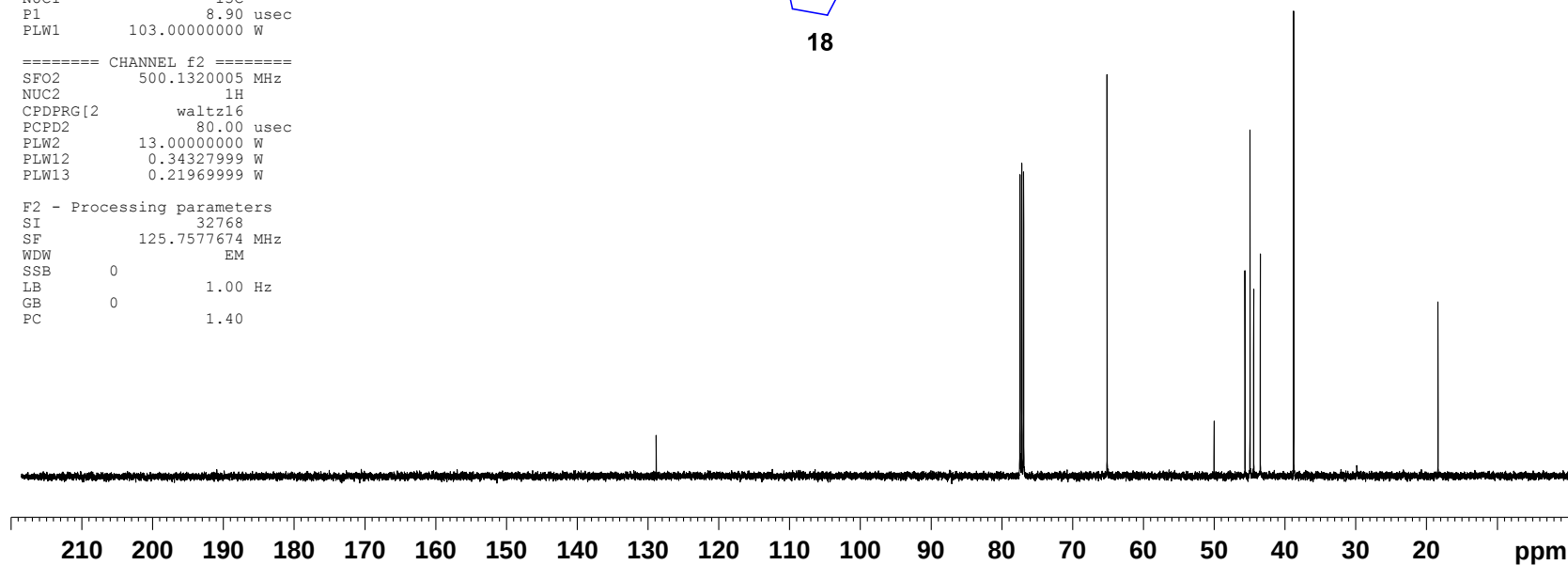
— 65.15

50.03
45.67
44.97
44.44
43.51
38.80

— 18.41



18



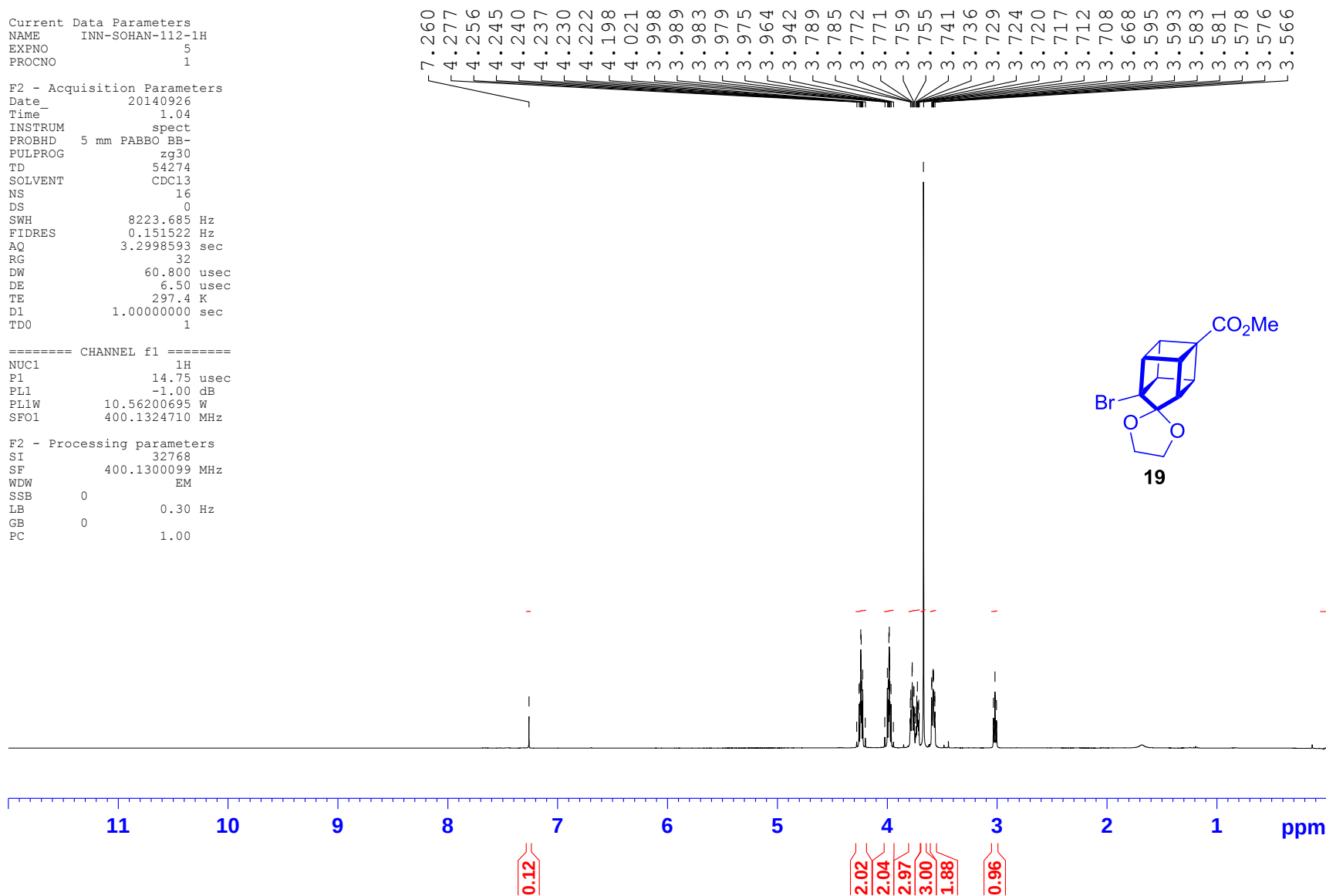
S-40. ¹³C NMR Spectrum of Compound 18

Current Data Parameters
 NAME INN-SOHN-112-1H
 EXPNO 5
 PROCNO 1

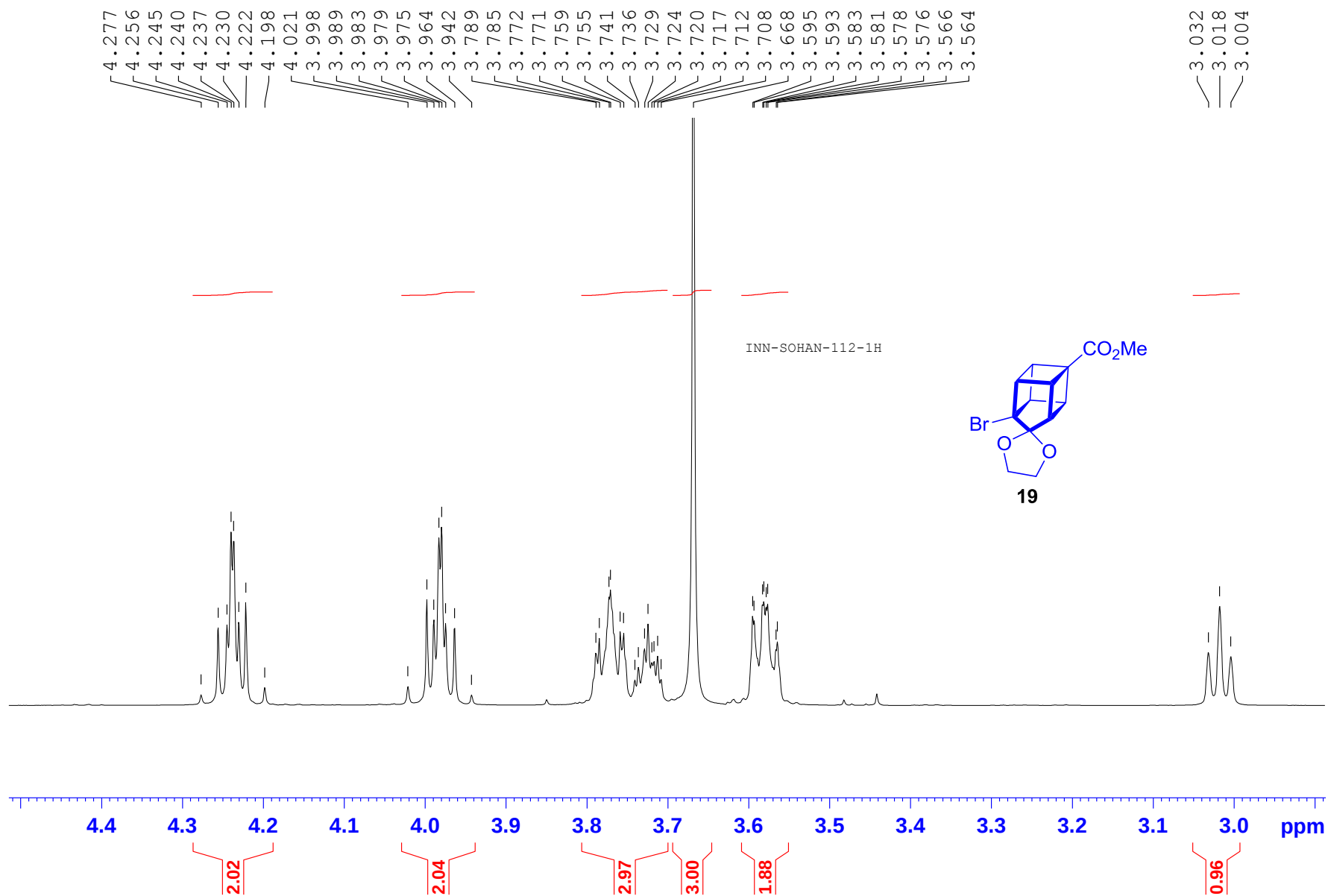
F2 - Acquisition Parameters
 Date_ 20140926
 Time_ 1.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 54274
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.151522 Hz
 AQ 3.2998593 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.75 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-41. ¹H NMR Spectrum of Compound 19



S-42. ^1H NMR Spectrum (Expansion) of Compound 19

Current Data Parameters
 NAME INN-SOHAN-112-13C
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140926
 Time 1.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 667
 DS 4
 SWH 26041.666 Hz
 FIDRES 0.397364 Hz
 AQ 1.2582912 sec
 RG 2050
 DW 19.200 usec
 DE 6.50 usec
 TE 298.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6238364 MHz

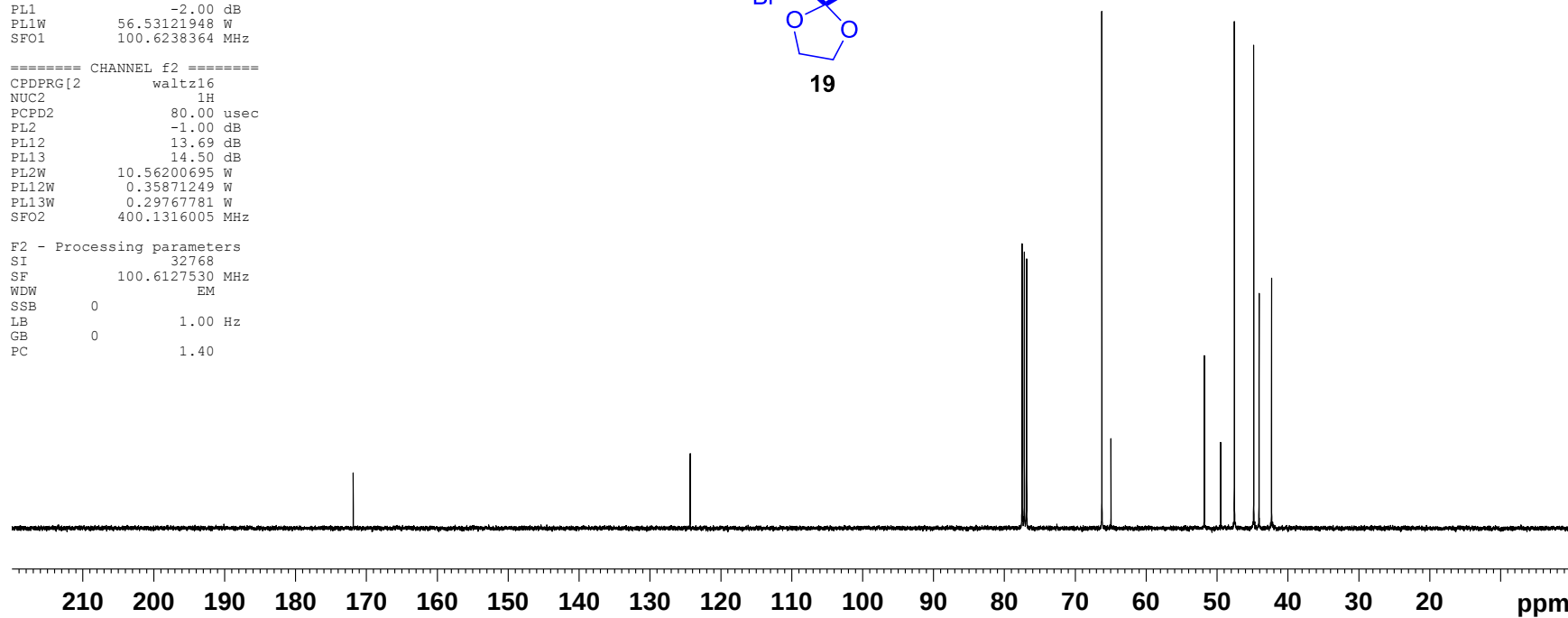
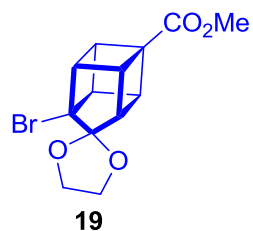
===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 13.69 dB
 PL13 14.50 dB
 PL2W 10.56200695 W
 PL12W 0.35871249 W
 PL13W 0.29767781 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127530 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 171.87

— 124.34

77.52
 77.20
 76.88
 66.25
 64.98
 51.80
 49.50
 47.56
 44.84
 44.08
 42.33



S-43. ¹³C NMR Spectrum of Compound 19

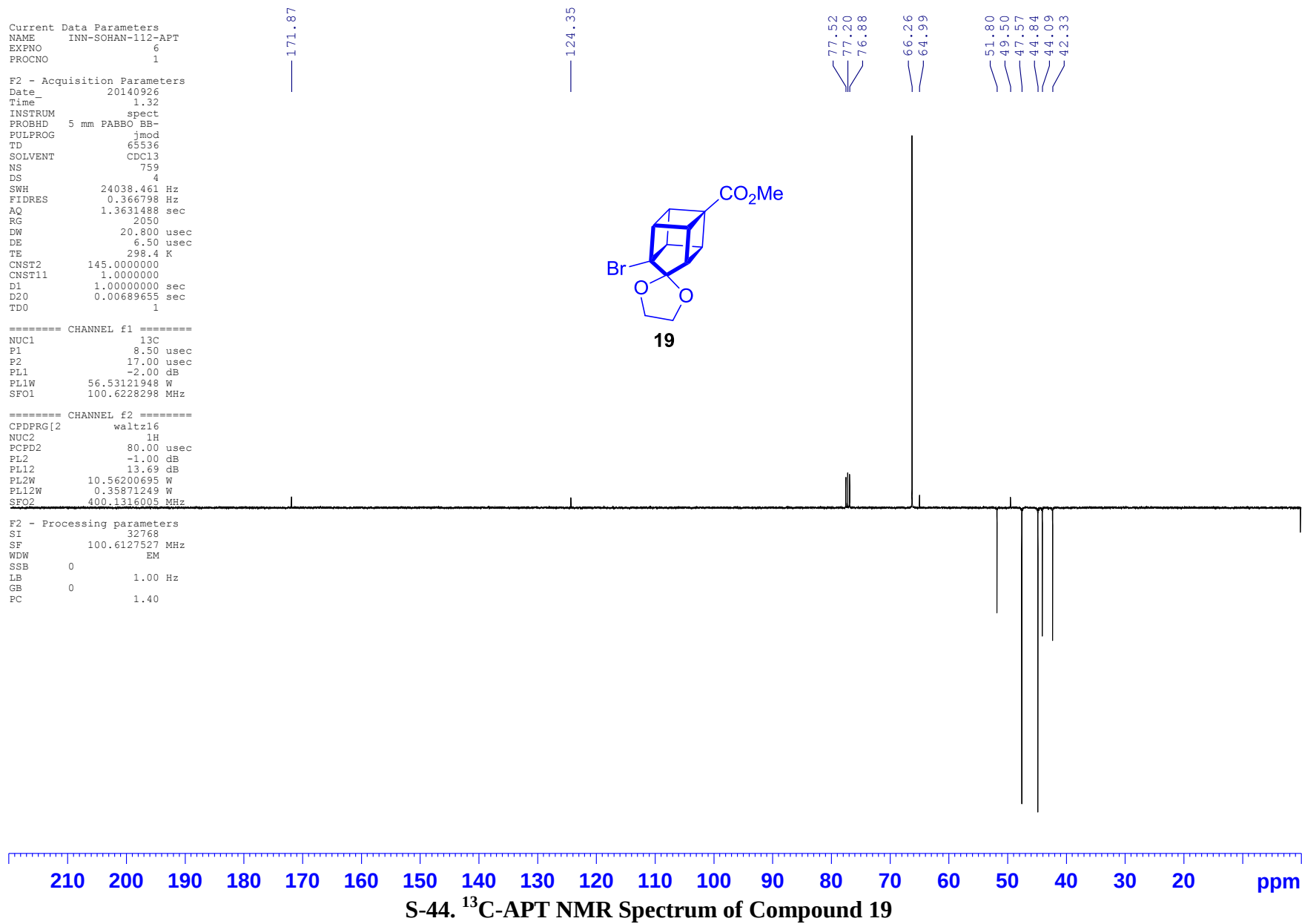
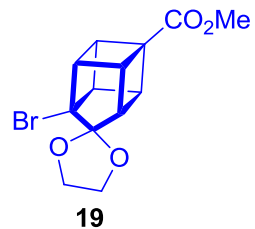
Current Data Parameters
 NAME INN-SOHA-112-APT
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140926
 Time 1.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 759
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 298.4 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 P2 17.00 usec
 PL1 -2.00 dB
 PL1W 56.53121948 W
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 13.69 dB
 PL2W 10.56200695 W
 PL12W 0.35871249 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127527 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME INN-SOHAN-II-201-A-1H
 EXPNO 31
 PROCNO 1

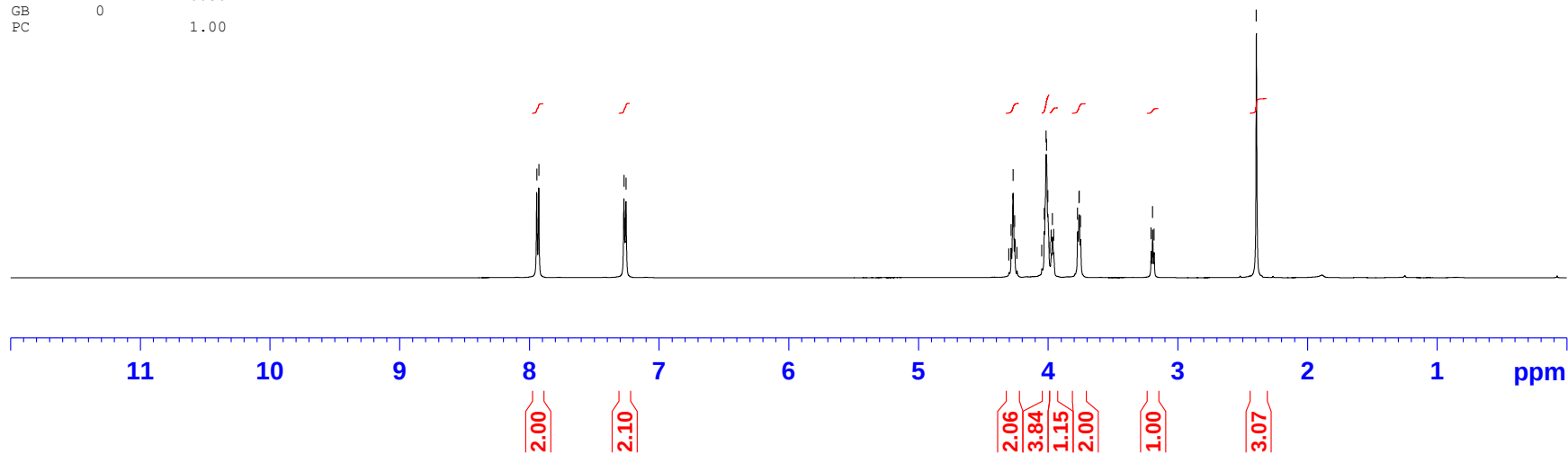
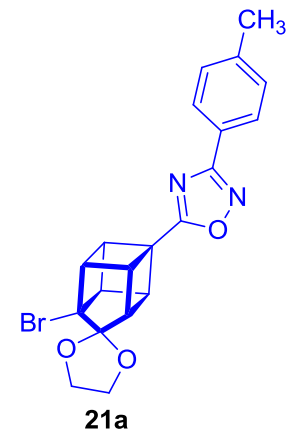
F2 - Acquisition Parameters
 Date_ 20190428
 Time_ 0.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 21
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 30.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.35 usec
 PLW1 16.00000000 W

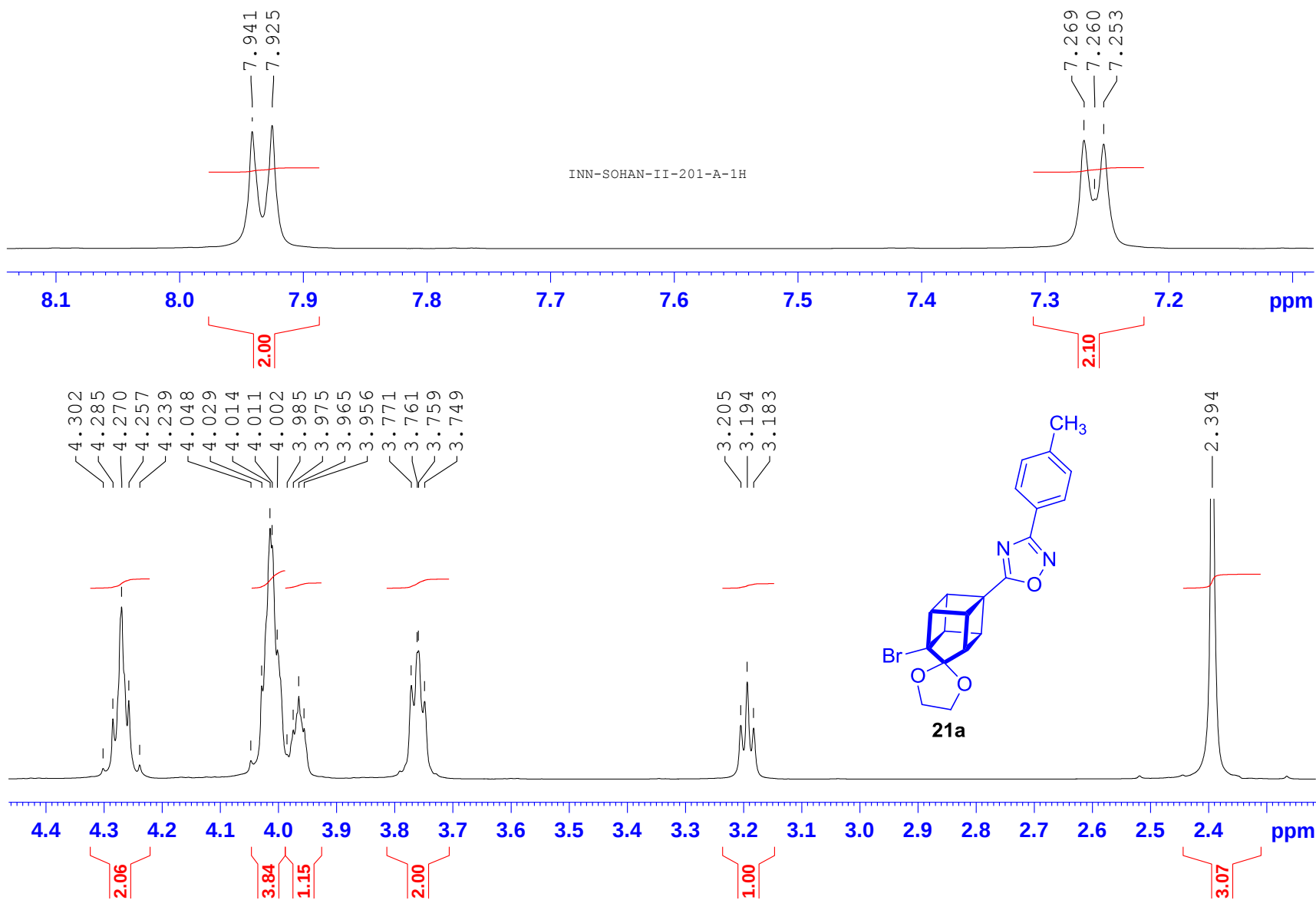
F2 - Processing parameters
 SI 65536
 SF 500.1300134 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.941
7.925
7.269
7.260
7.253

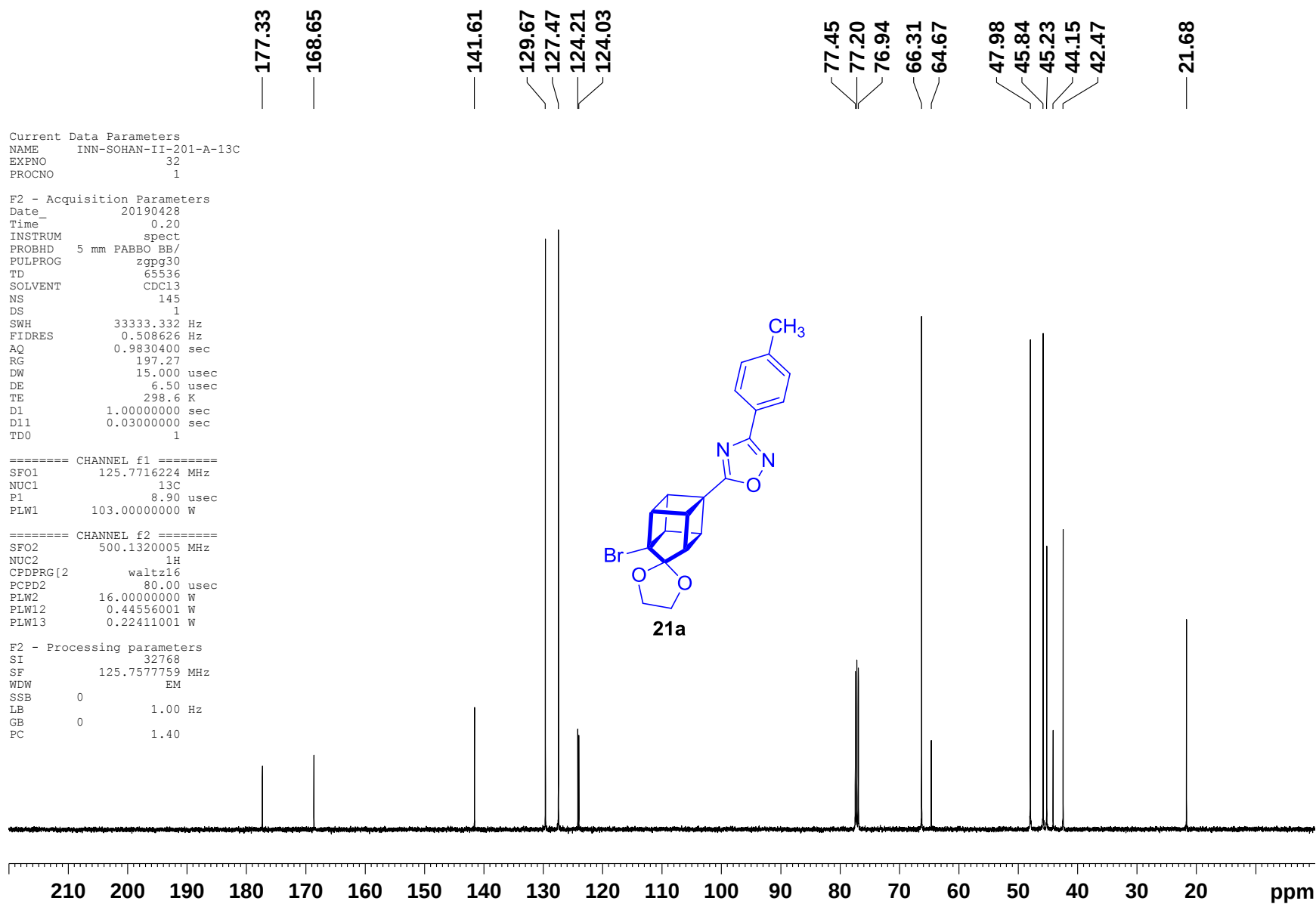
4.302
4.285
4.270
4.257
4.239
4.048
4.029
4.014
4.011
4.002
3.985
3.975
3.965
3.956
3.771
3.761
3.759
3.749
3.205
3.194
3.183
2.394



S-45. ¹H NMR Spectrum of Compound 21a



S-46. ¹H NMR Spectrum (Expansion) of Compound 21a



S-47. ¹³C NMR Spectrum of Compound 21a

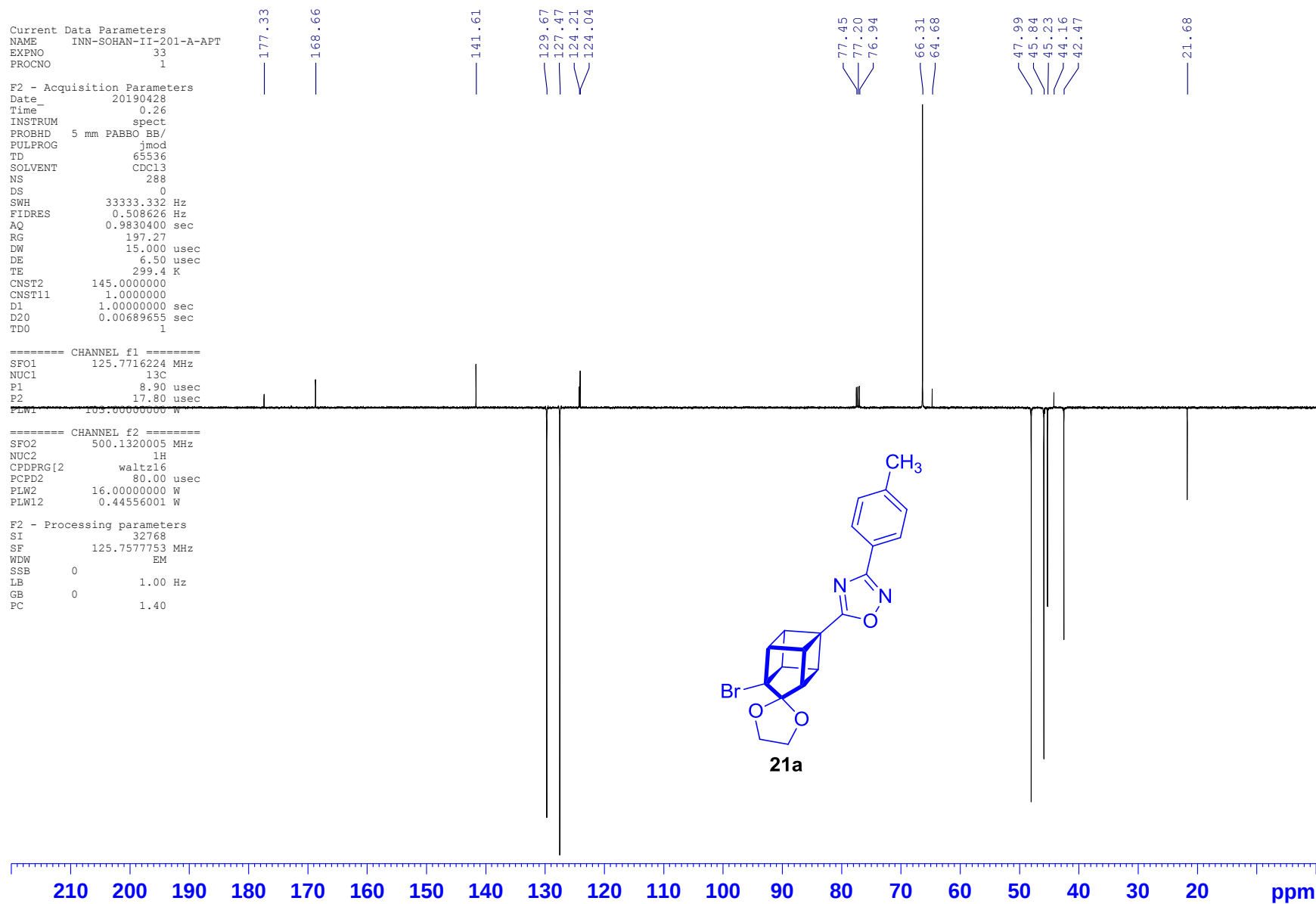
Current Data Parameters
 NAME INN-SOHN-II-201-A-APT
 EXPNO 33
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190428
 Time_ 0.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 288
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 299.4 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577753 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-48. ¹³C-APT NMR Spectrum of Compound 21a

Current Data Parameters
 NAME 100-201-A-HSQC
 EXPNO 34
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190428
 Time 0.39
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG hsqcetgpgisip2.2
 TD 1024
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4032.258 Hz
 FIDRES 3.937752 Hz
 AQ 0.1269760 sec
 RG 197.27
 DW 124.000 usec
 DE 6.50 usec
 TE 298.7 K
 CNST2 145.000000
 CNST17 -0.5000000
 D0 0.00000300 sec
 D1 1.00000000 sec
 D4 0.00172414 sec
 D11 0.01000000 sec
 D16 0.00020000 sec
 D21 0.00360000 sec
 D24 0.00089000 sec
 INO 0.00002080 sec

***** CHANNEL f1 *****
 SFO1 500.1326391 MHz
 NUC1 1H
 P1 13.35 usec
 P2 26.70 usec
 P28 2000.00 usec
 PLW1 16.00000000 W

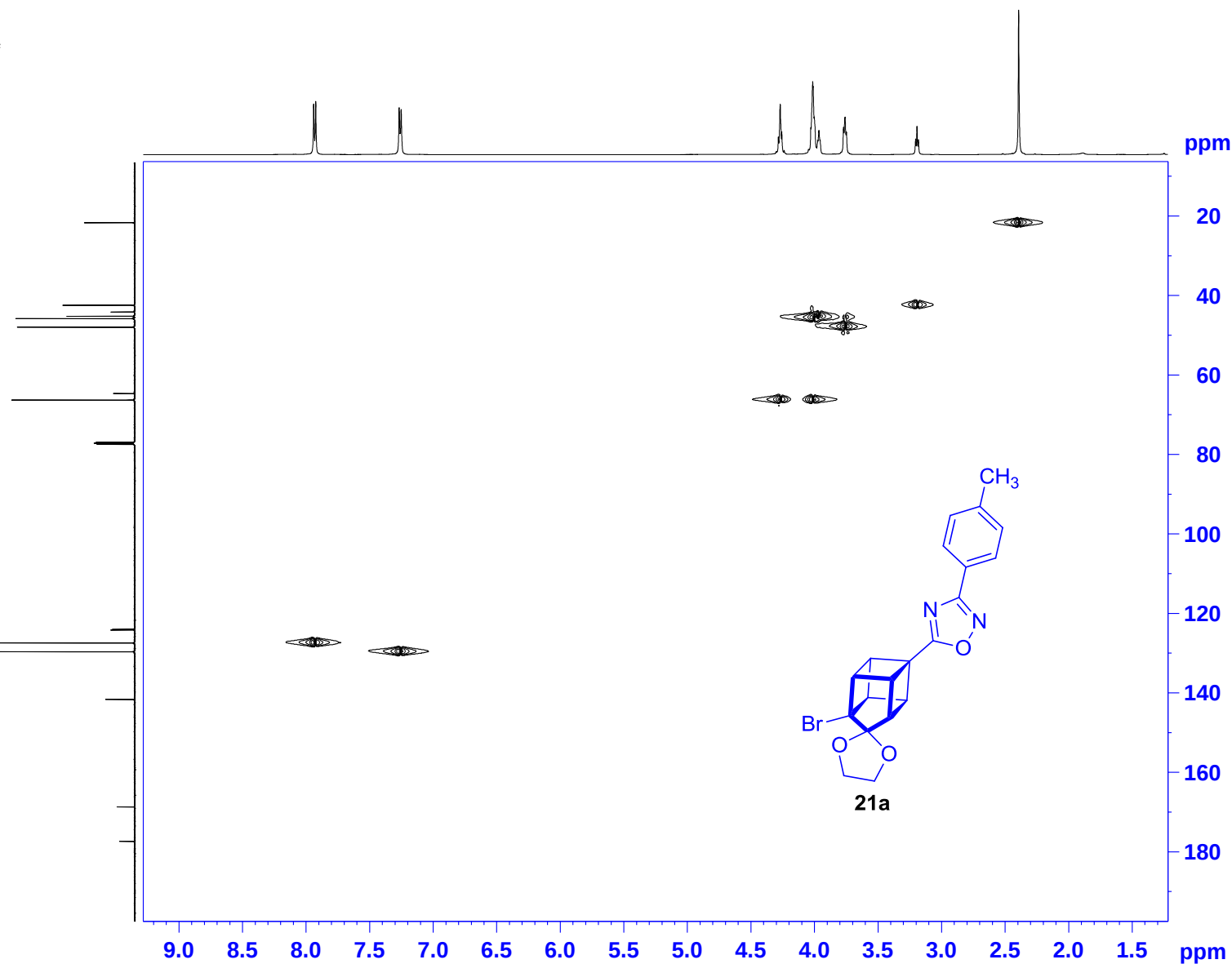
***** CHANNEL f2 *****
 SFO2 125.7705919 MHz
 NUC2 13C
 CPDPRG2 bi_psm4sp.4sp.2
 P3 8.50 usec
 P14 500.00 usec
 P24 2000.00 usec
 P63 1500.00 usec
 PLW0 0 W
 PLW2 103.00000000 W
 PLW12 1.66499996 W
 SFOFF3 0 Hz
 SFOFFS3 0 Hz
 SFW3 12.46500015 W
 SFOFF7 0 Hz
 SFOFFS7 0 Hz
 SFW7 12.46500015 W
 SFOFF14 0 Hz
 SFOFFS14 0 Hz
 SFW14 5.31860018 W
 SFOFF31 0 Hz
 SFOFFS31 0 Hz
 SFW31 1.32969999 W

***** GRADIENT CHANNEL *****
 GPM1[1] SMSQ10.100
 GPM1[2] SMSQ10.100
 GPM1[3] SMSQ10.100
 GPM1[4] SMSQ10.100
 GP21 80.00 %
 GP22 20.10 %
 GP23 11.00 %
 GP24 -5.00 %
 P16 1000.00 usec
 P19 600.00 usec

F1 - Acquisition parameters
 TD 129
 SFO1 125.7706 MHz
 FIDRES 345.877136 Hz
 SW 121.129 ppm
 F1MODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 500.1300134 MHz
 WDW QSIINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 125.7577759 MHz
 WDW QSIINE
 SSB 2
 LB 0 Hz
 GB 0



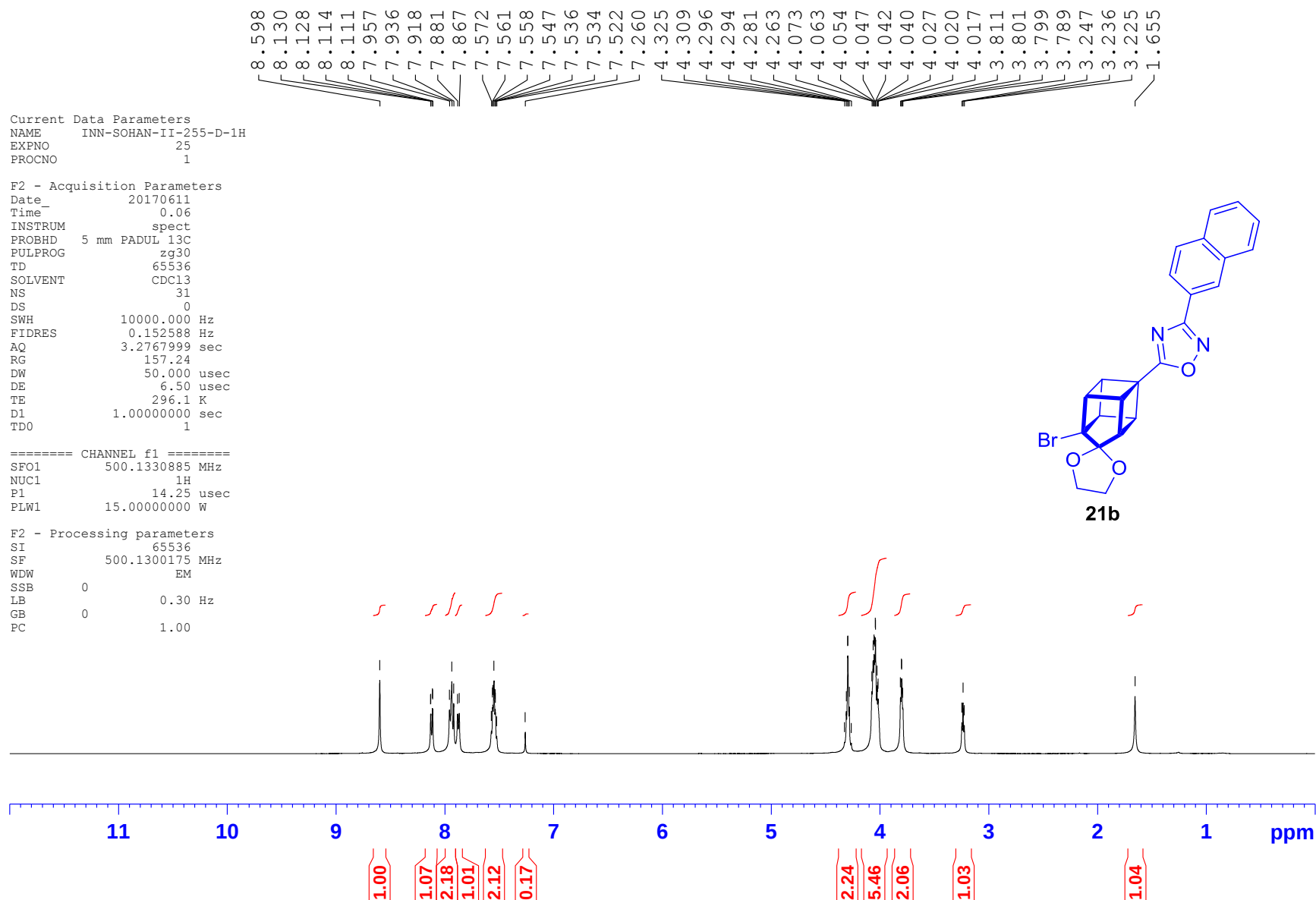
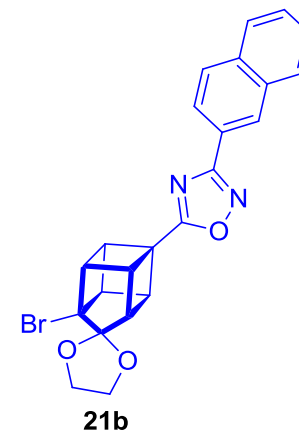
S-49. ^1H - ^{13}C HSQC NMR Spectrum of Compound 21a

Current Data Parameters
NAME INN-SOHAN-II-255-D-1H
EXPNO 25
PROCNO 1

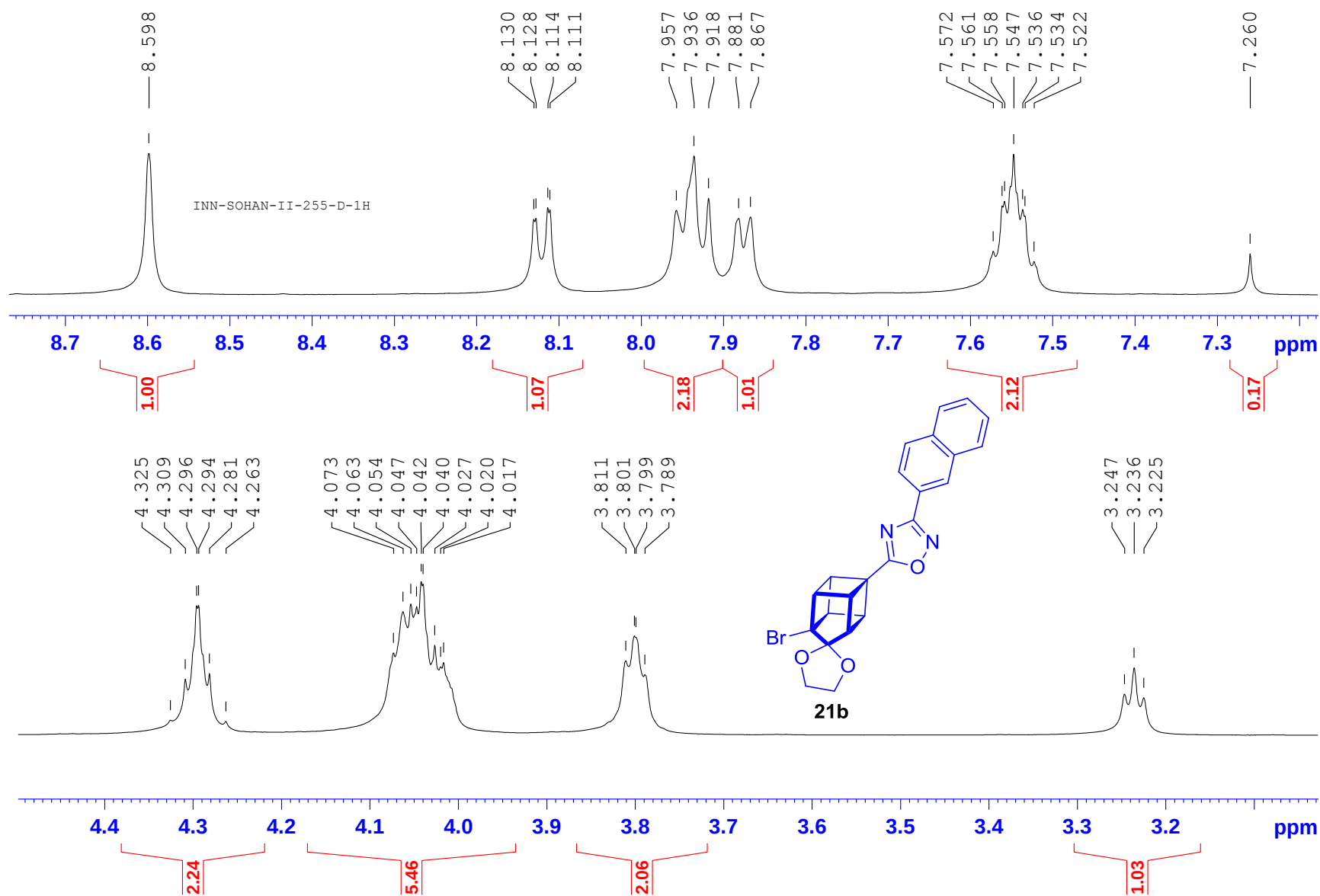
F2 - Acquisition Parameters
Date_ 20170611
Time_ 0.06
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 31
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 157.24
DW 50.000 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 14.25 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300175 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S-50. ¹H NMR Spectrum of Compound 21b



S-51. ^1H NMR Spectrum (Expansion) of Compound 21b

Current Data Parameters
 NAME INN-SOHAN-II-255-D-13C
 EXPNO 26
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170611
 Time_ 0.09
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 367
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 296.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716219 MHz
 NUC1 13C
 P1 8.00 usec
 PLW1 60.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 15.00000000 W
 PLW12 0.47593001 W
 PLW13 0.23939000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577720 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

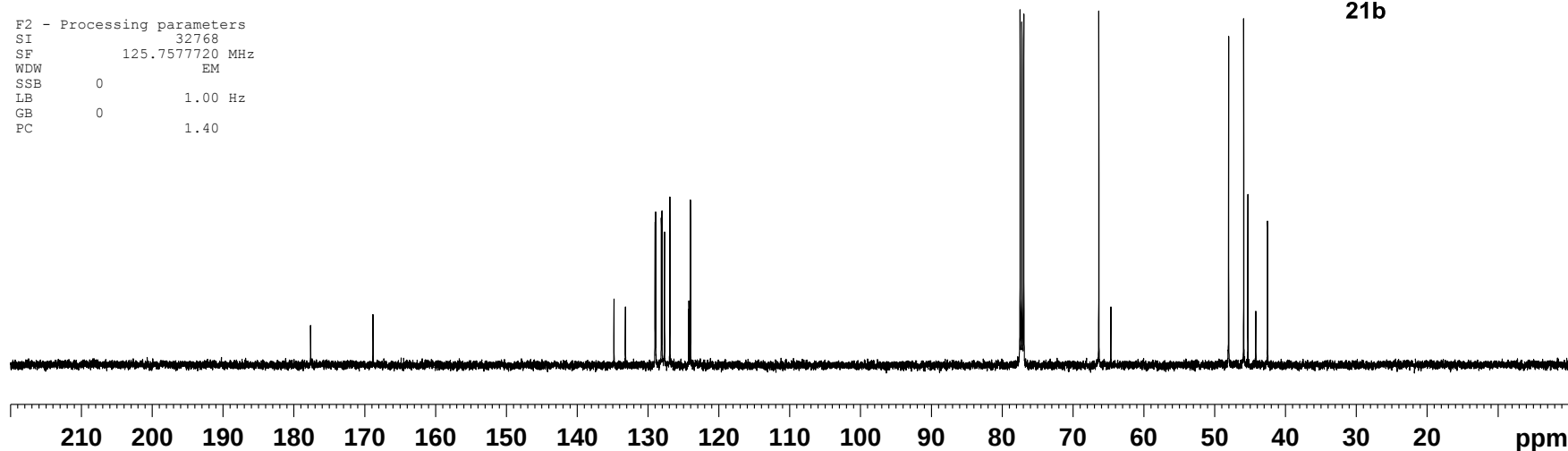
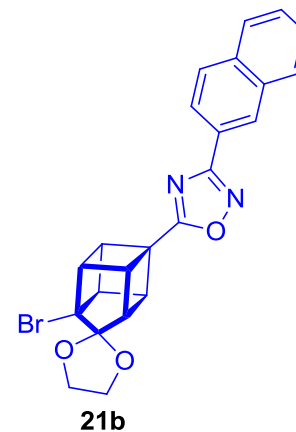
177.63

168.82

134.80
 133.18
 128.99
 128.91
 128.11
 128.03
 127.67
 126.90
 124.26
 124.20
 123.99

77.45
 77.19
 76.94
 66.38
 64.68

48.05
 45.92
 45.33
 44.22
 42.55



S-52. ¹³C NMR Spectrum of Compound 21b

Current Data Parameters
 NAME INN-SOHAN-II-255-D-APT
 EXPNO 27
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170611
 Time 14.43
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 675
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 295.8 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PLW1 60.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 15.00000000 W
 PLW12 0.47593001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577715 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

177.64

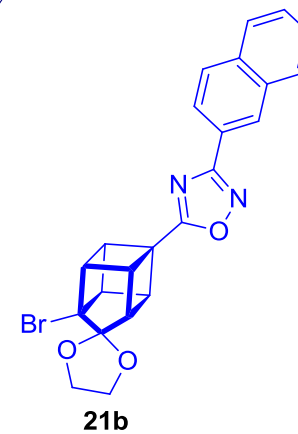
168.82

134.80
 133.19
 129.00
 128.91
 128.11
 128.03
 127.67
 126.91
 124.26
 124.21
 124.00

77.45
 77.20
 76.95

66.39
 64.69

48.06
 45.93
 45.33
 44.22
 42.55



S-53. ¹³C-APT NMR Spectrum of Compound 21b

Current Data Parameters
 NAME INN-SOHA-II-123-R-1H
 EXPNO 1
 PROCNO 1

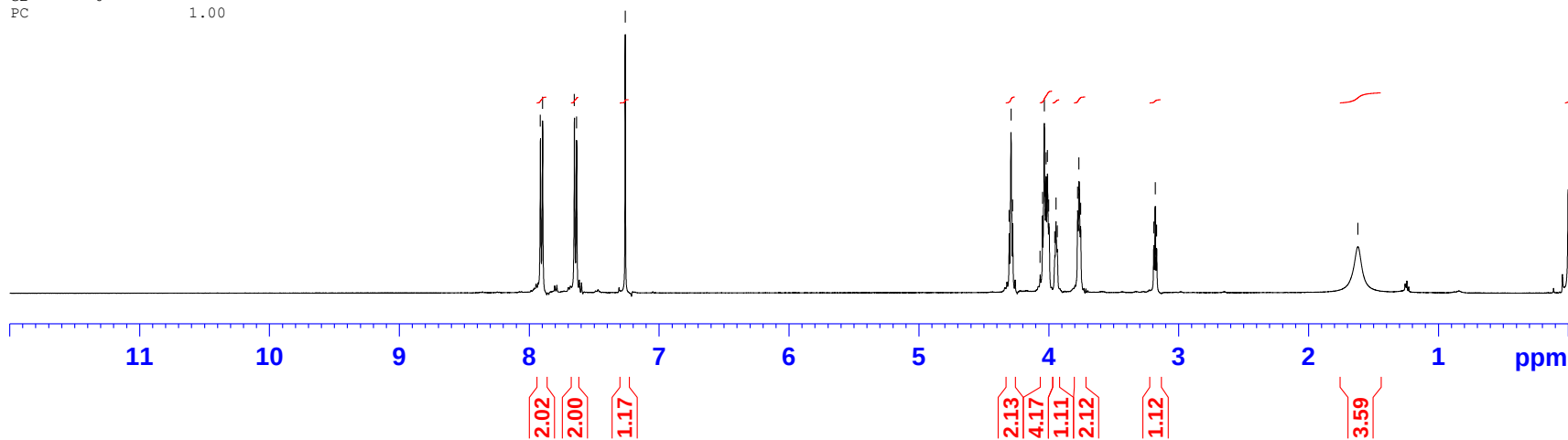
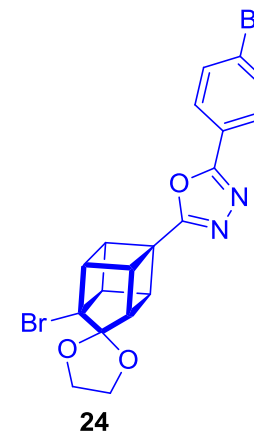
F2 - Acquisition Parameters
 Date_ 20191011
 Time_ 16.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 157.24
 DW 50.000 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.35 usec
 PLW1 16.00000000 W

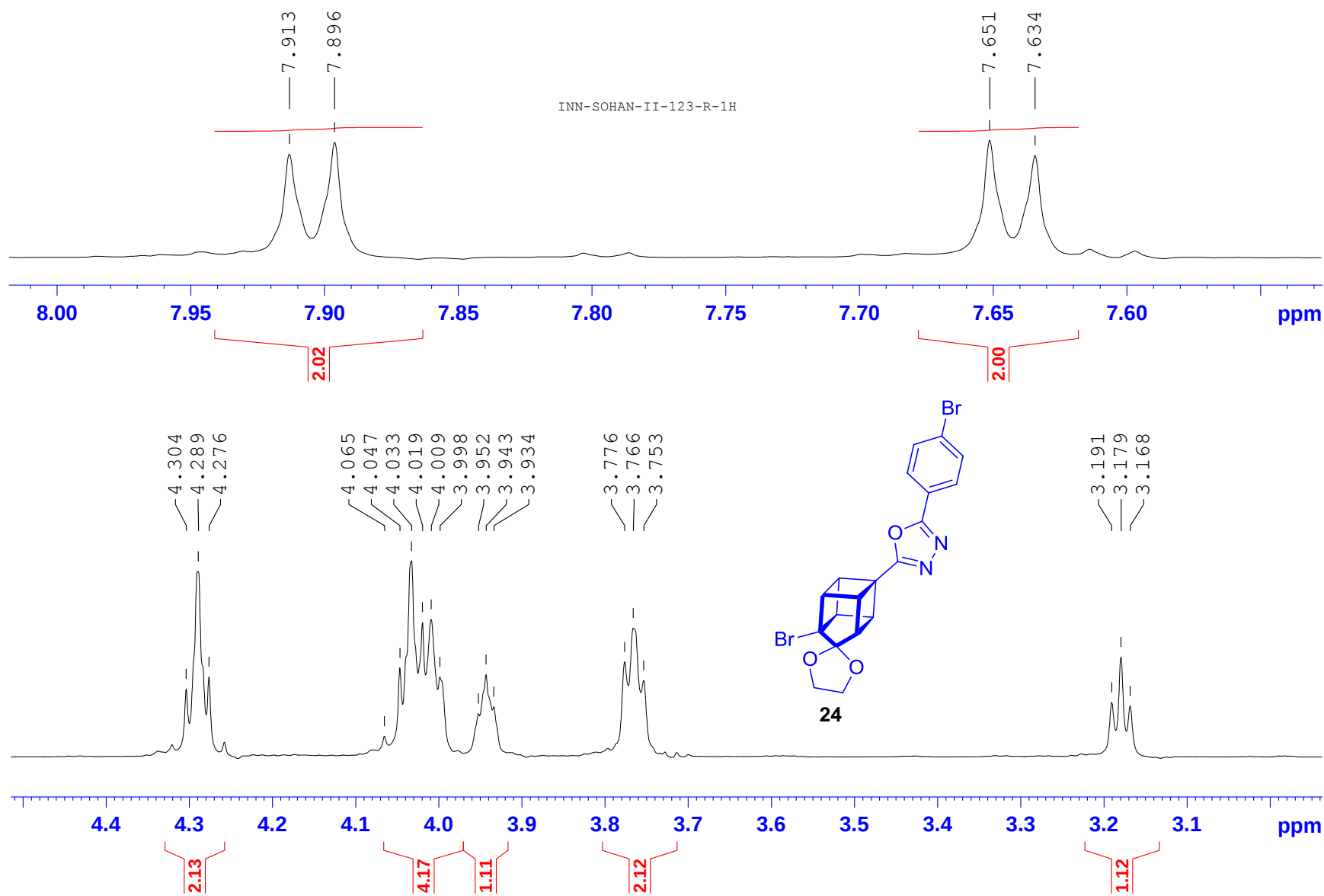
F2 - Processing parameters
 SI 65536
 SF 500.1300138 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.913
7.896
7.651
7.634
7.260

4.304
4.289
4.276
4.065
4.047
4.033
4.019
4.009
3.998
3.952
3.943
3.934
3.776
3.766
3.753
3.191
3.179
3.168



S-54. ¹H NMR Spectrum of Compound 24



S-55. ^1H NMR Spectrum (Expansion) of Compound 24

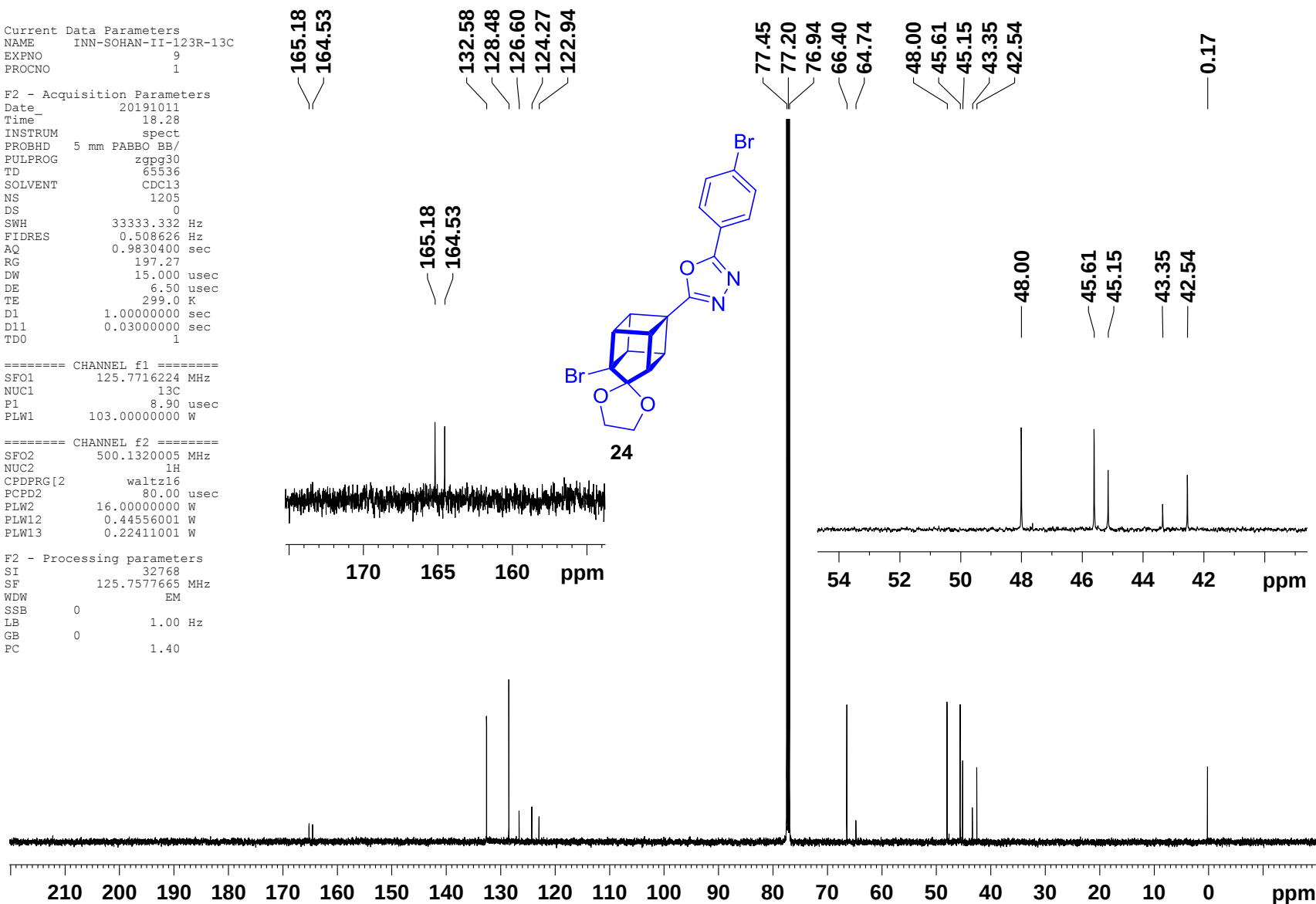
Current Data Parameters
 NAME INN-SOHAN-II-123R-13C
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191011
 Time_ 18.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1205
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577665 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



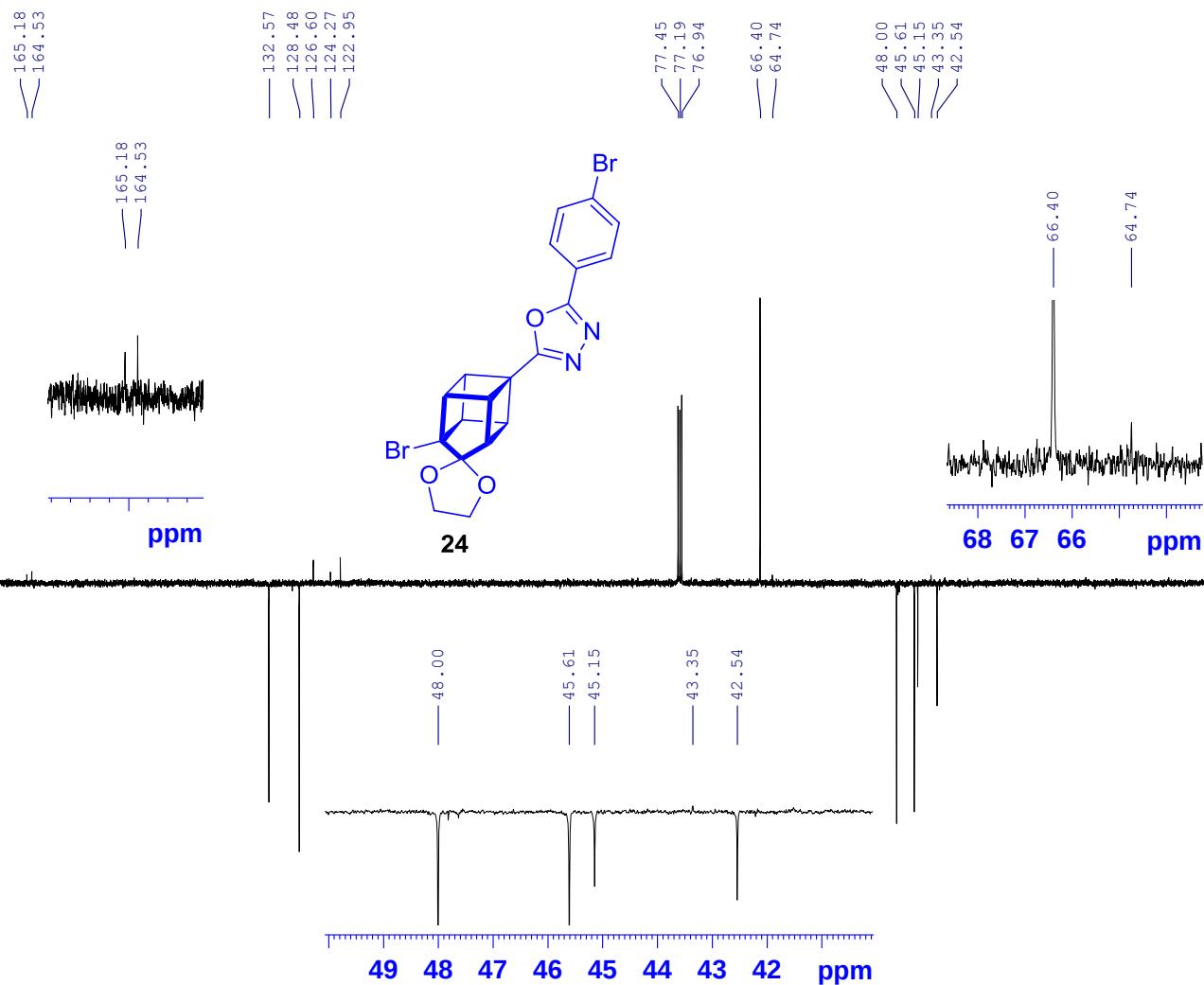
Current Data Parameters
 NAME INN-SOHN-II-123R-APT
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date 20191011
 Time 21.46
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1295
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 299.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577665 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-57. ¹³C-APT NMR Spectrum of Compound 24

Current Data Parameters
 NAME INN-SOHAN-II-286-A-1H
 EXPNO 14
 PROCNO 1

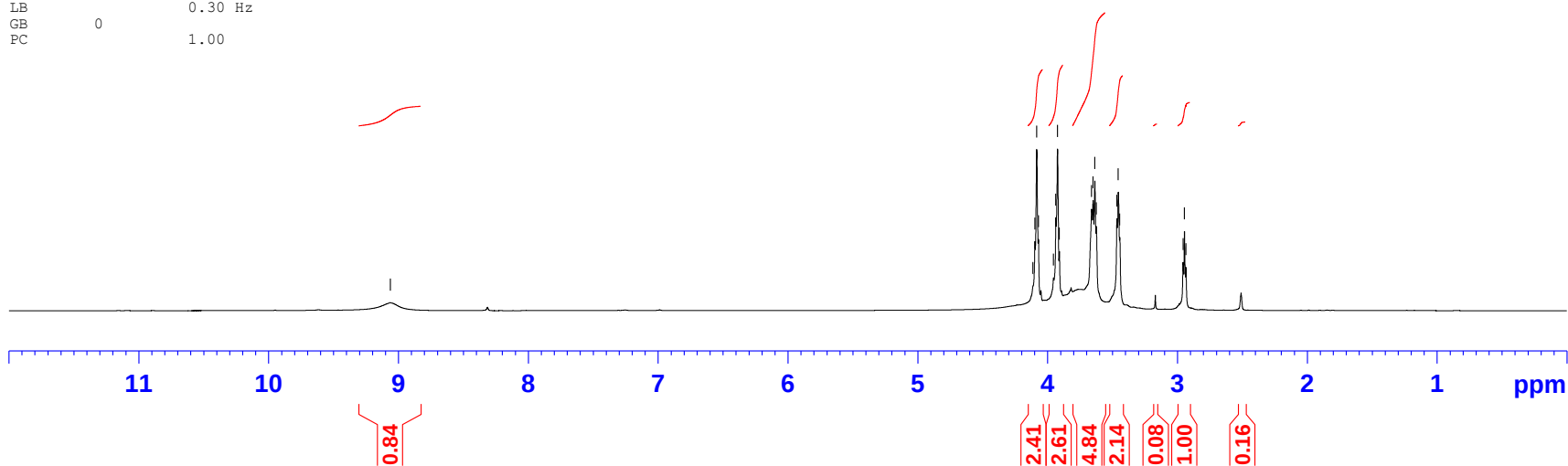
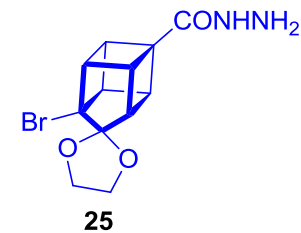
F2 - Acquisition Parameters
 Date_ 20170726
 Time_ 14.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 100
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 24.72
 DW 50.000 usec
 DE 6.50 usec
 TE 297.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300006 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 9.062

4.113
 4.097
 4.084
 4.070
 3.954
 3.936
 3.923
 3.908
 3.661
 3.649
 3.635
 3.624
 3.465
 3.455
 3.444
 2.956
 2.945
 2.935



S-58. ¹H NMR Spectrum of compound 25

Current Data Parameters
 NAME INN-SOHN-II-286-N-13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191008
 Time_ 1.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 621
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

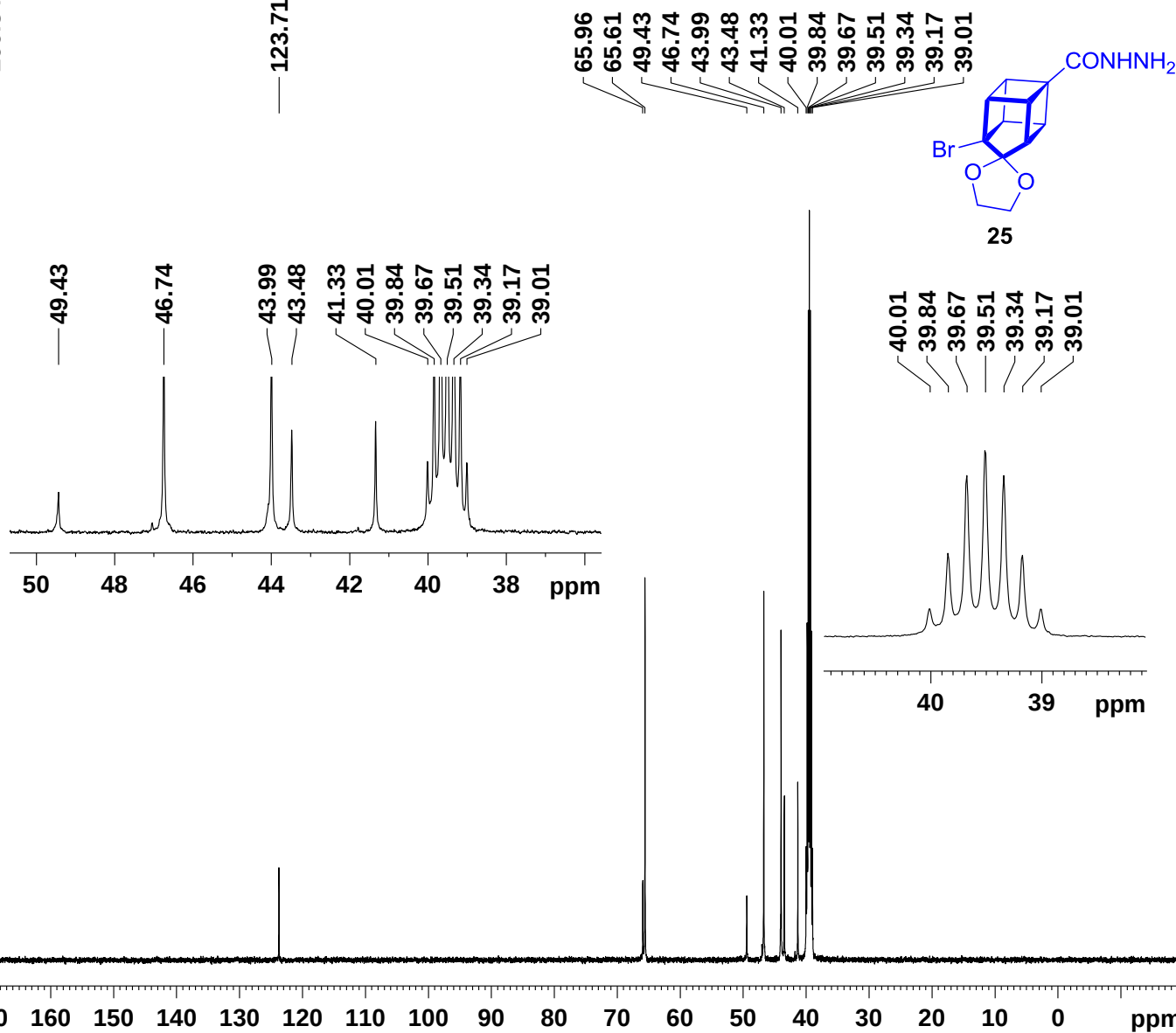
===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578292 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

169.34

123.71



S-59. ¹³C NMR Spectrum of Compound 25

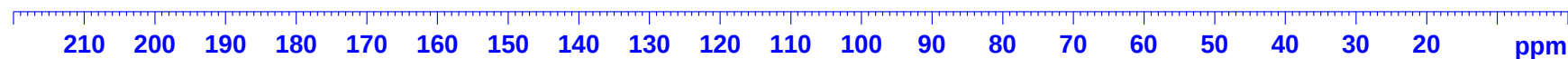
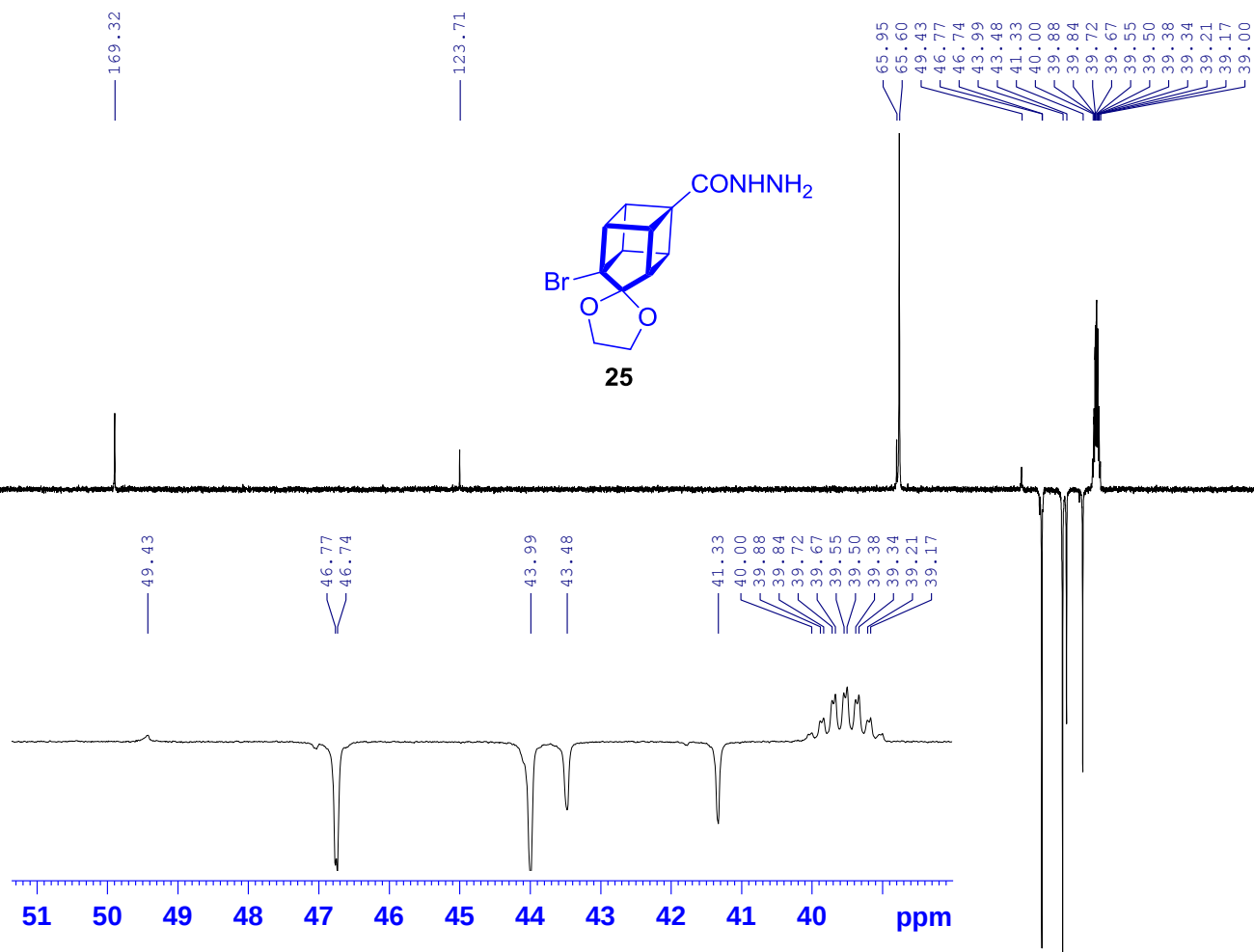
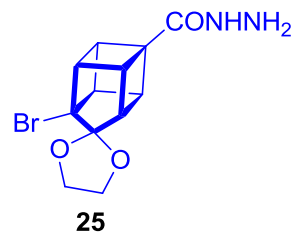
Current Data Parameters
 NAME INN-SOHAN-II-286-N-APT
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20191008
 Time 1.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 298.1 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 PL1 8.90 usec
 F2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578307 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-60. ¹³C-APT NMR Spectrum of Compound 25

Current Data Parameters
 NAME INH-SORAN-11-286-N-HSQC
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date 20191008
 Time 2.19
 INSTRUM spect
 PROBRND 5 mm PARBO BB/
 PULPROG hsqcetdcpzg2.2
 TD 1024
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 4783.163 Hz
 FIDRES 4.671058 Hz
 AQ 0.1070421 sec
 RG 197.27
 DW 104.533 usec
 DE 6.50 usec
 TE 298.9 K
 CREST2 145.000000
 CREST17 -0.500000
 D0 0.0000300 sec
 D1 1.0000000 sec
 D4 0.00172414 usec
 D11 0.0300000 usec
 D16 0.00020000 sec
 D11 0.00360000 sec
 D24 0.00089000 sec
 INO 0.00002320 sec

===== CHANNEL f1 =====
 SFO1 500.1331599 MHz
 NUC1 1H
 F1 13.35 usec
 F2 26.70 usec
 F28 2000.00 usec
 F1X1 16.0000000 W

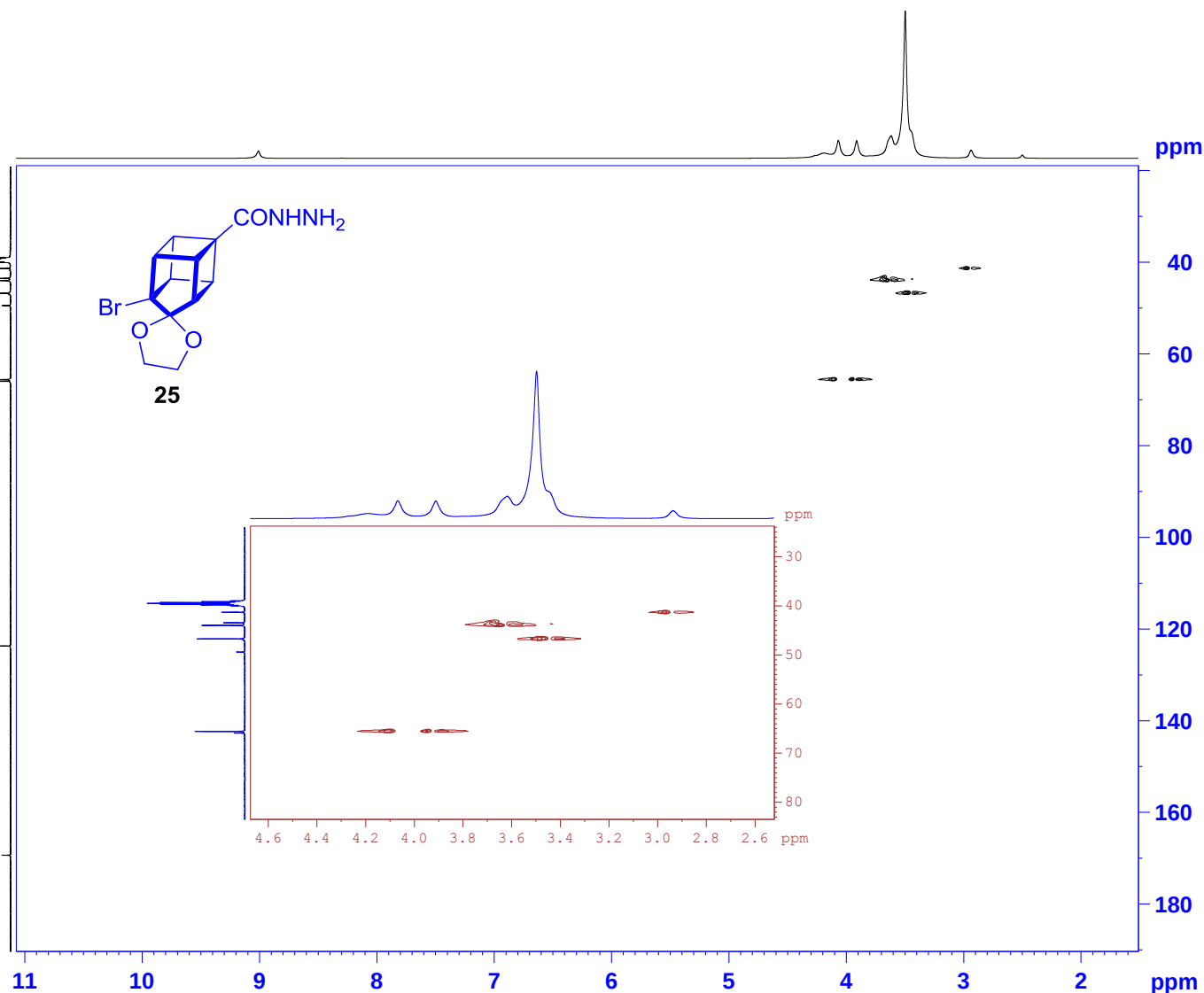
===== CHANNEL f2 =====
 SFO2 125.7709875 MHz
 NUC2 13C
 CPOPRG2 bi_p5m4sp_4sp.2
 F3 8.50 usec
 F14 500.00 usec
 F24 2000.00 usec
 F1X1 1500.00 usec
 F1X2 0 W
 F1X2 103.00000000 W
 F1X2 1.66489896 W
 SFOAL3 Crp60,0.5,20.1
 SFOAL3 0.500
 SPOFFS3 0 Hz
 SFW3 12.46500015 W
 SFOAL7 Crp60comp.4
 SFOAL7 0.500
 SPOFFS7 0 Hz
 SFW7 12.46500015 W
 SFOAL14 Crp32,1.5,20.2
 SFOAL14 0.500
 SPOFFS14 0 Hz
 SFW14 5.31860018 W
 SFOAL31 Crp32,1.5,20.2
 SFOAL31 0.500
 SPOFFS31 0 Hz
 SFW31 1.32969999 W

===== GRADIENT CHANNEL =====
 GPRAM[1] SMSQ10.100
 GPRAM[2] SMSQ10.100
 GPRAM[3] SMSQ10.100
 GPRAM[4] SMSQ10.100
 GP21 80.00 %
 GP22 20.10 %
 GP23 11.00 %
 GP24 -5.00 %
 F16 1000.00 usec
 F19 600.00 usec

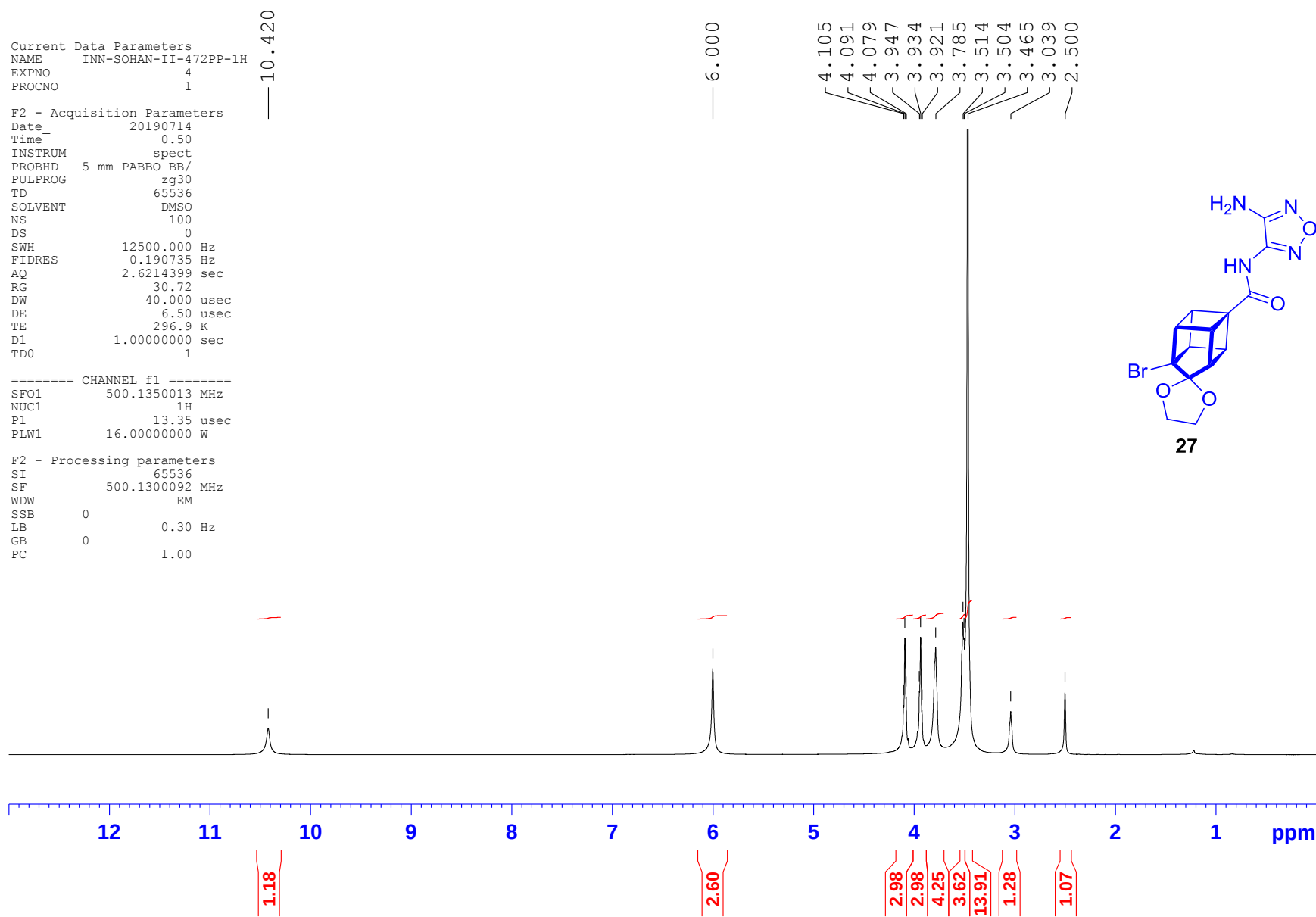
F1 - Acquisition parameters
 TD 352
 SFO1 125.771 MHz
 FIDRES 122.452980 Hz
 SW 171.357 ppm
 F2MODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 500.1300132 MHz
 WCN 2
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 ME2 echo-antiecho
 SF 125.7578292 MHz
 WCN 2
 SSB 2
 LB 0 Hz
 GB 0



S-61. ^1H - ^{13}C HSQC NMR Spectrum of Compound 25



S-62. ¹H NMR Spectrum of Compound 27

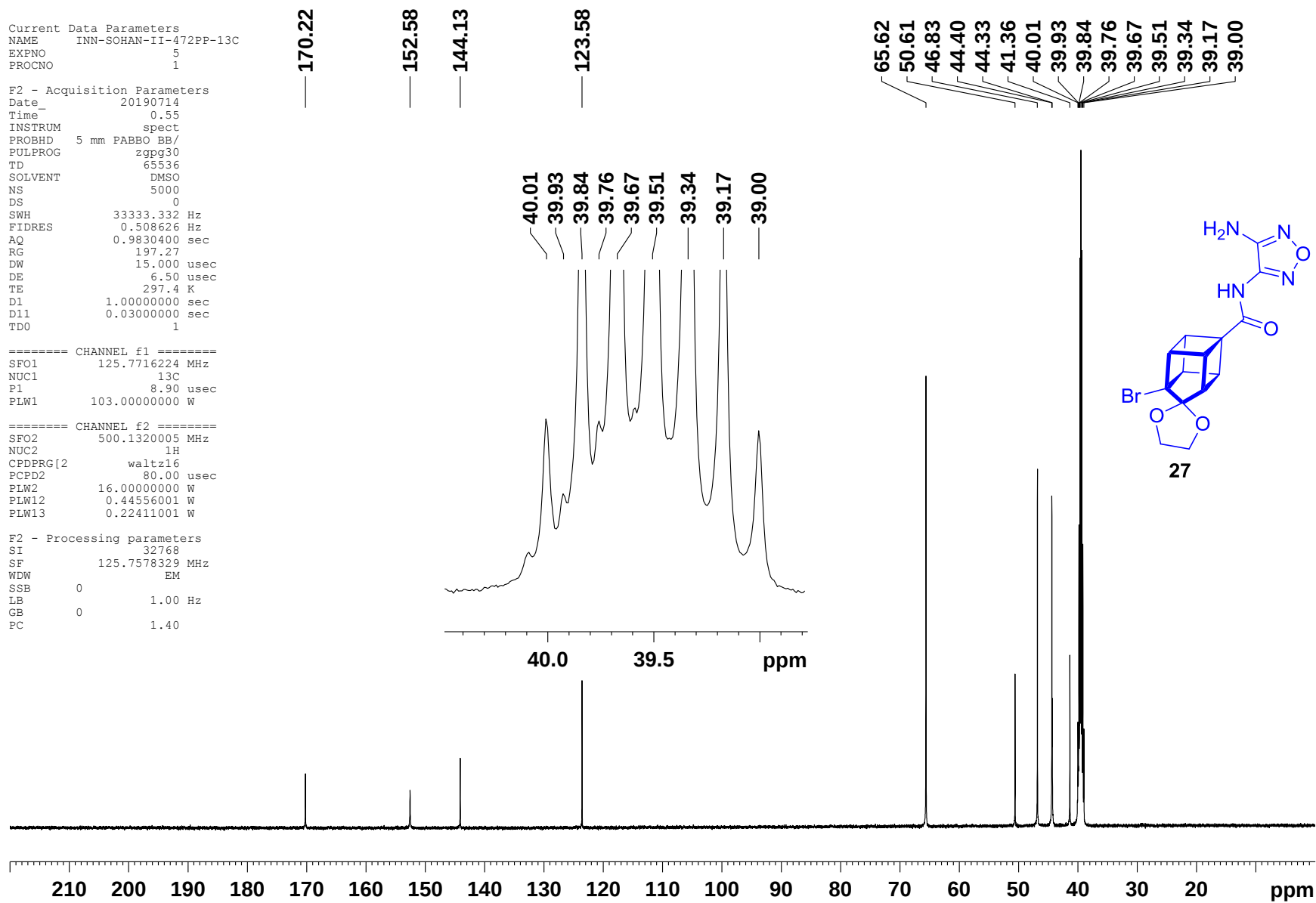
Current Data Parameters
 NAME INN-SOHN-II-472PP-13C
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190714
 Time_ 0.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 5000
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.00000000 W
 PLW12 0.44556001 W
 PLW13 0.22411001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578329 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



S-63. ¹³C NMR Spectrum of Compound 27

Current Data Parameters
 NAME INN-SOHAN-II-472PP-APT
 EXPNO 6
 PROCNO 1

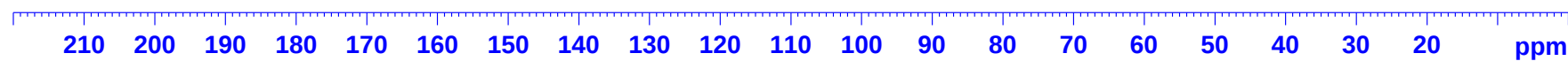
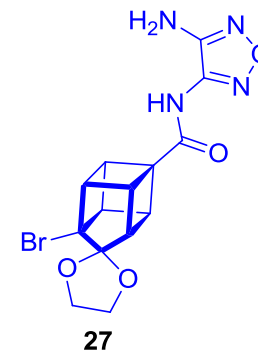
F2 - Acquisition Parameters
 Date_ 20190714
 Time_ 5.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT DMSO
 NS 3072
 DS 0
 SWH 33333.332 Hz
 FIDRES 0.508626 Hz
 AQ 0.9830400 sec
 RG 197.27
 DW 15.000 usec
 DE 6.50 usec
 TE 298.6 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7716224 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

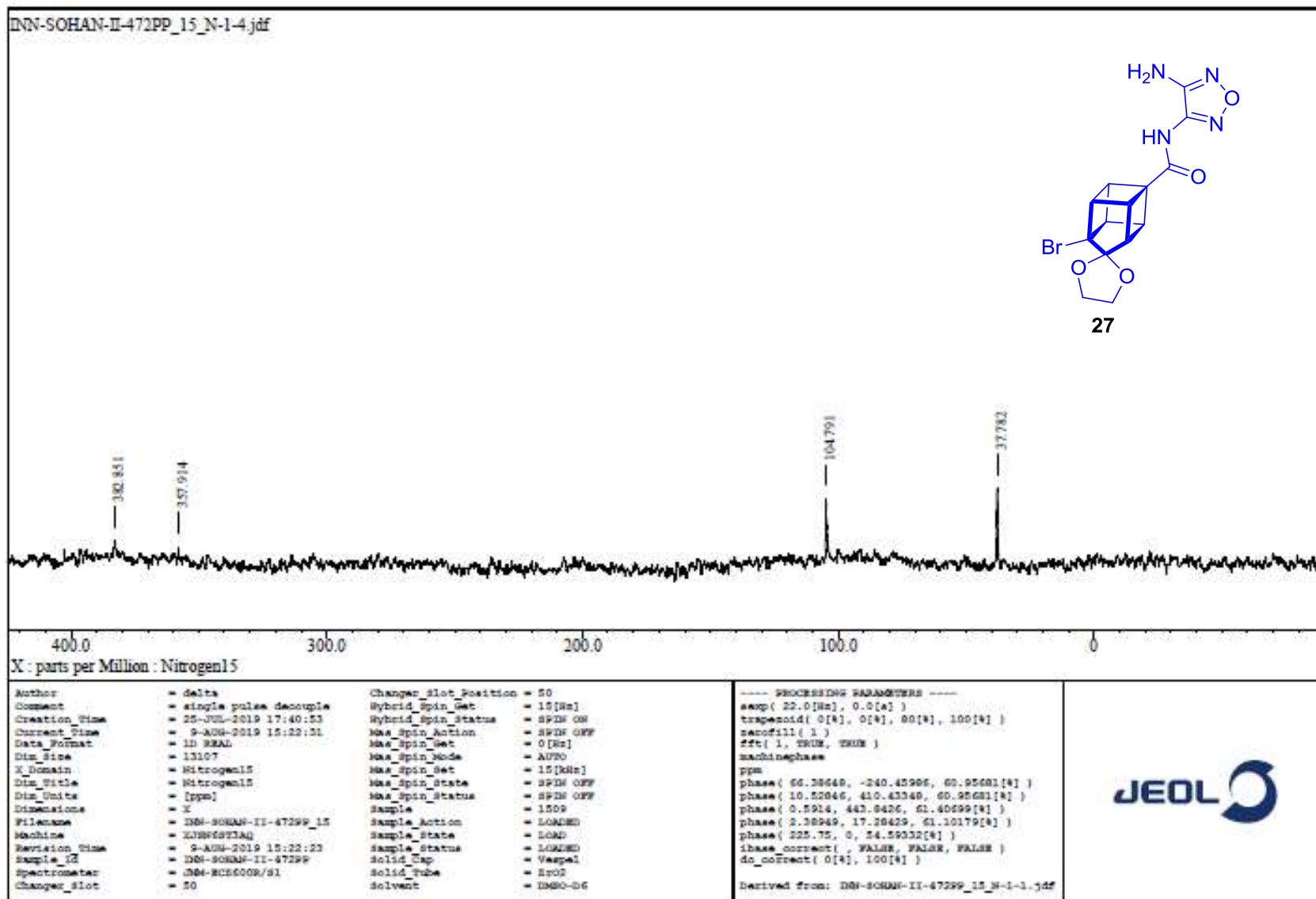
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 16.0000000 W
 PLW12 0.44556001 W

F2 - Processing parameters
 SI 32768
 SF 125.7578403 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

170.16
 152.49
 144.08
 123.53
 65.56
 50.57
 47.38
 44.36
 44.28
 41.32
 40.01
 39.93
 39.84
 39.76
 39.68
 39.51
 39.34
 39.17
 39.01



S-64. ¹³C-APT NMR Spectrum of Compound 27



S-65. ^1H - ^{15}N NMR Spectrum of Compound 27

Current Date Parameters
 NAME INN-SORAN-II-472PP-HSQC
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190714
 Time 5.30
 INSTRUM spect
 PROBRD 5 mm PABBO BB/
 PULPROG hsqcetgpgp2.2
 TD 1024
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 6167.763 Hz
 FIDRES 6.023206 Hz
 AQ 0.0830123 sec
 RG 197.27
 DW 81.067 usec
 DE 6.50 usec
 TE 298.2 K
 CNET2 145.000000
 CNST17 -0.500000
 DO 0.0000300 sec
 D1 1.0000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 D21 0.00360000 sec
 D24 0.00089000 sec
 INO 0.00002320 sec

===== CHANNEL f1 =====
 SFO1 500.1335257 MHz
 NUC1 1H
 P1 13.35 usec
 P2 26.70 usec
 P28 2000.00 usec
 PLW1 16.00000000 W

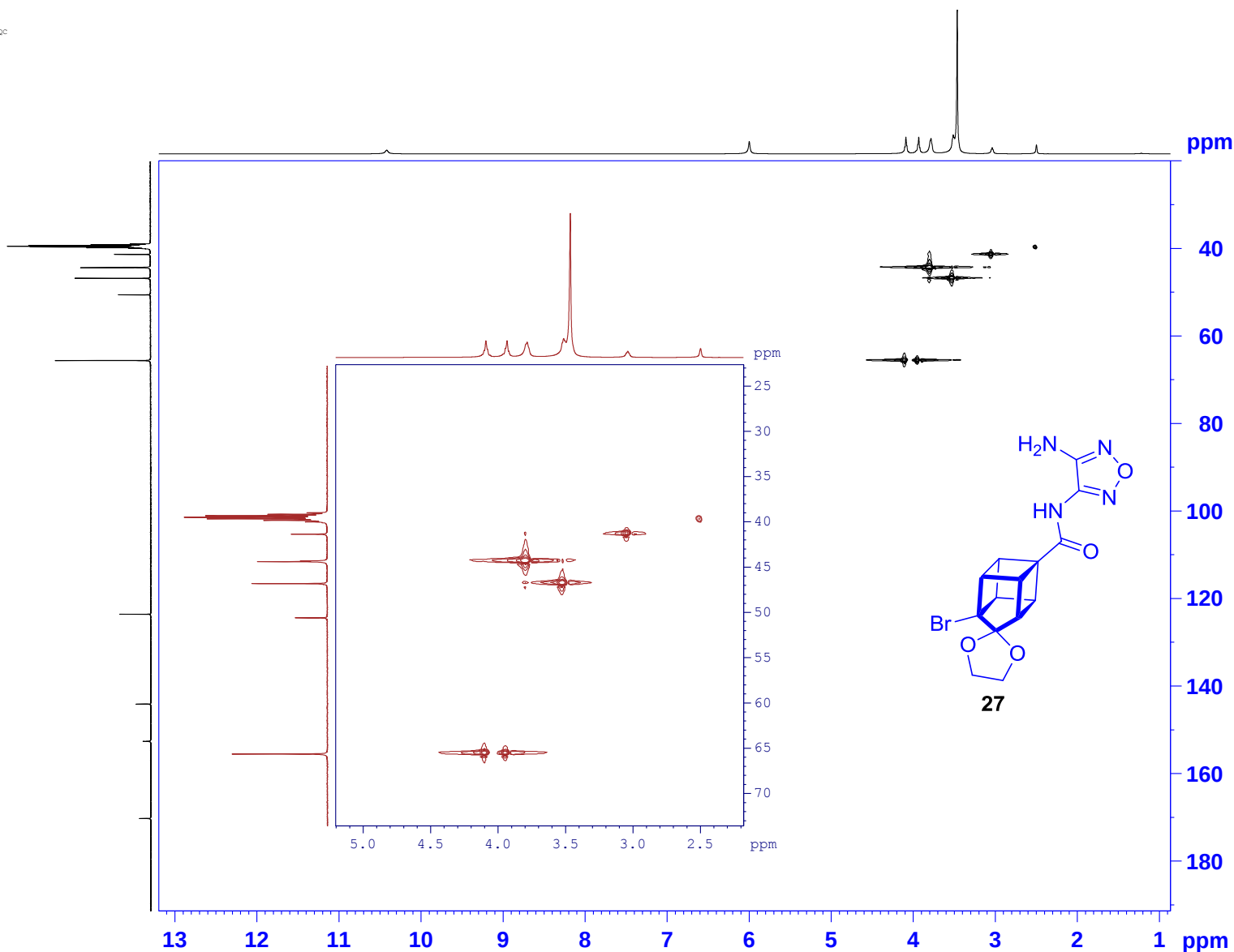
===== CHANNEL f2 =====
 SFO2 125.7711224 MHz
 NUC2 13C
 CPDPRG2 bi_psm4ep_4sp.2
 P3 8.90 usec
 P14 500.00 usec
 P24 2000.00 usec
 P63 1500.00 usec
 PLW0 0 W
 PLW2 103.00000000 W
 PLW12 1.66499996 W
 SPWAM[3] Crp60,0.5,20.1
 SPWAL3 0.500
 SPOFFS3 0 Hz
 SPW3 12.46500015 W
 SPWAM[7] Crp60comp.4
 SPWAL7 0.500
 SPOFFS7 0 Hz
 SPW7 12.46500015 W
 SPWAM[14] Crp32,1.5,20.2
 SPWAL14 0.500
 SPOFFS14 0 Hz
 SPW14 5.31860018 W
 SPWAM[31] Crp32,1.5,20.2
 SPWAL31 0.500
 SPOFFS31 0 Hz
 SPW31 1.32969999 W

===== GRADIENT CHANNEL =====
 GPRAM[1] SMSQ10.100
 GPRAM[2] SMSQ10.100
 GPRAM[3] SMSQ10.100
 GPRAM[4] SMSQ10.100
 GP21 80.00 %
 GP22 20.10 %
 GP23 11.00 %
 GP24 -5.00 %
 P16 1000.00 usec
 P19 600.00 usec

F1 - Acquisition parameters
 TD 512
 SFO1 125.7711 MHz
 FIDRES 84.186424 Hz
 SW 171.357 ppm
 F1MODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 500.1300993 MHz
 WDW QSI
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 125.7578319 MHz
 WDW QSI
 SSB 2
 LB 0 Hz
 GB 0



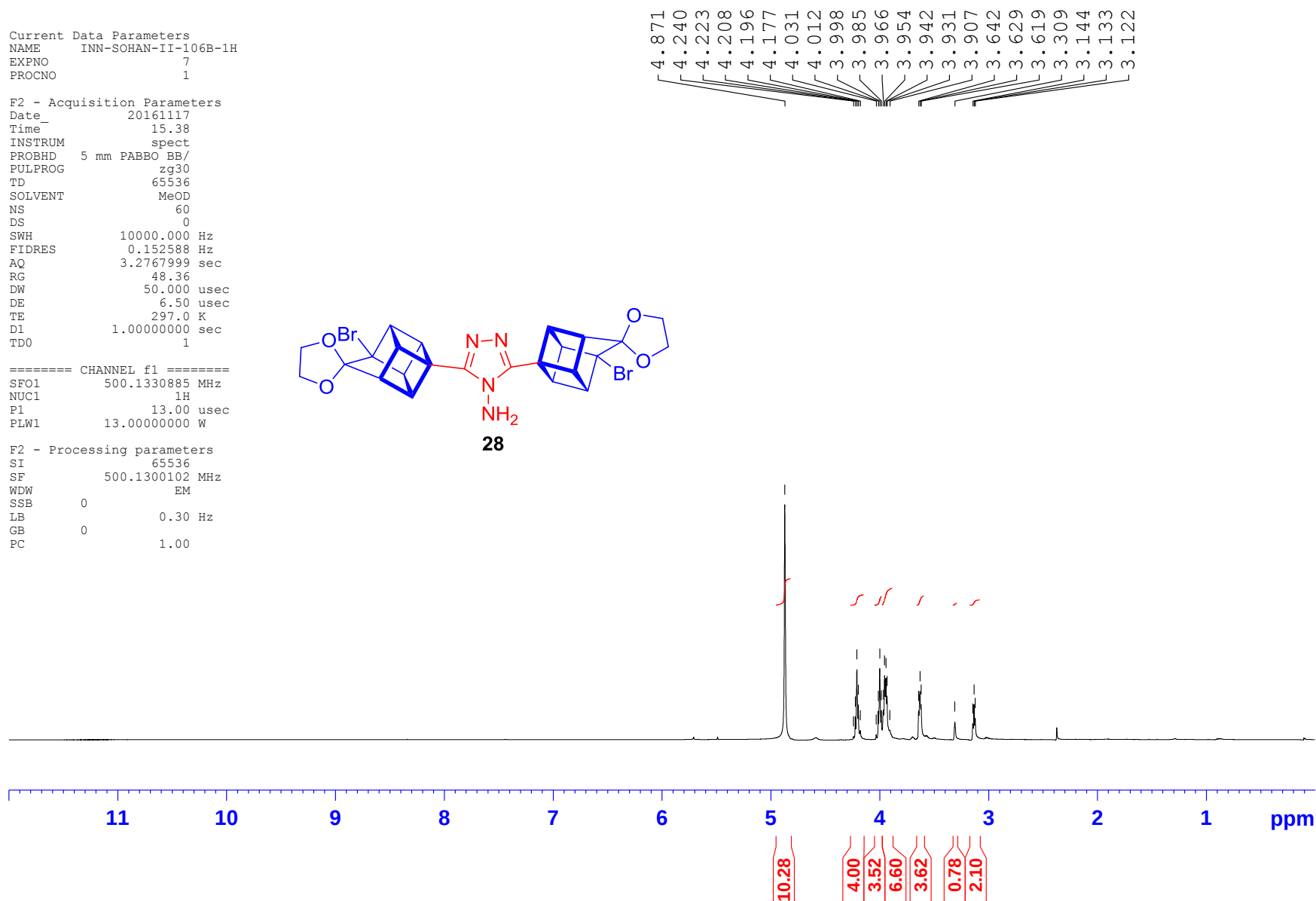
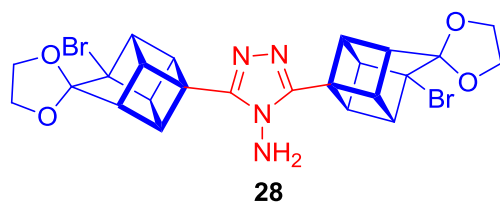
S-66. ^1H - ^{13}C HSQC NMR Spectrum of Compound 27

Current Data Parameters
 NAME INN-SOHAN-II-106B-1H
 EXPNO 7
 PROCNO 1

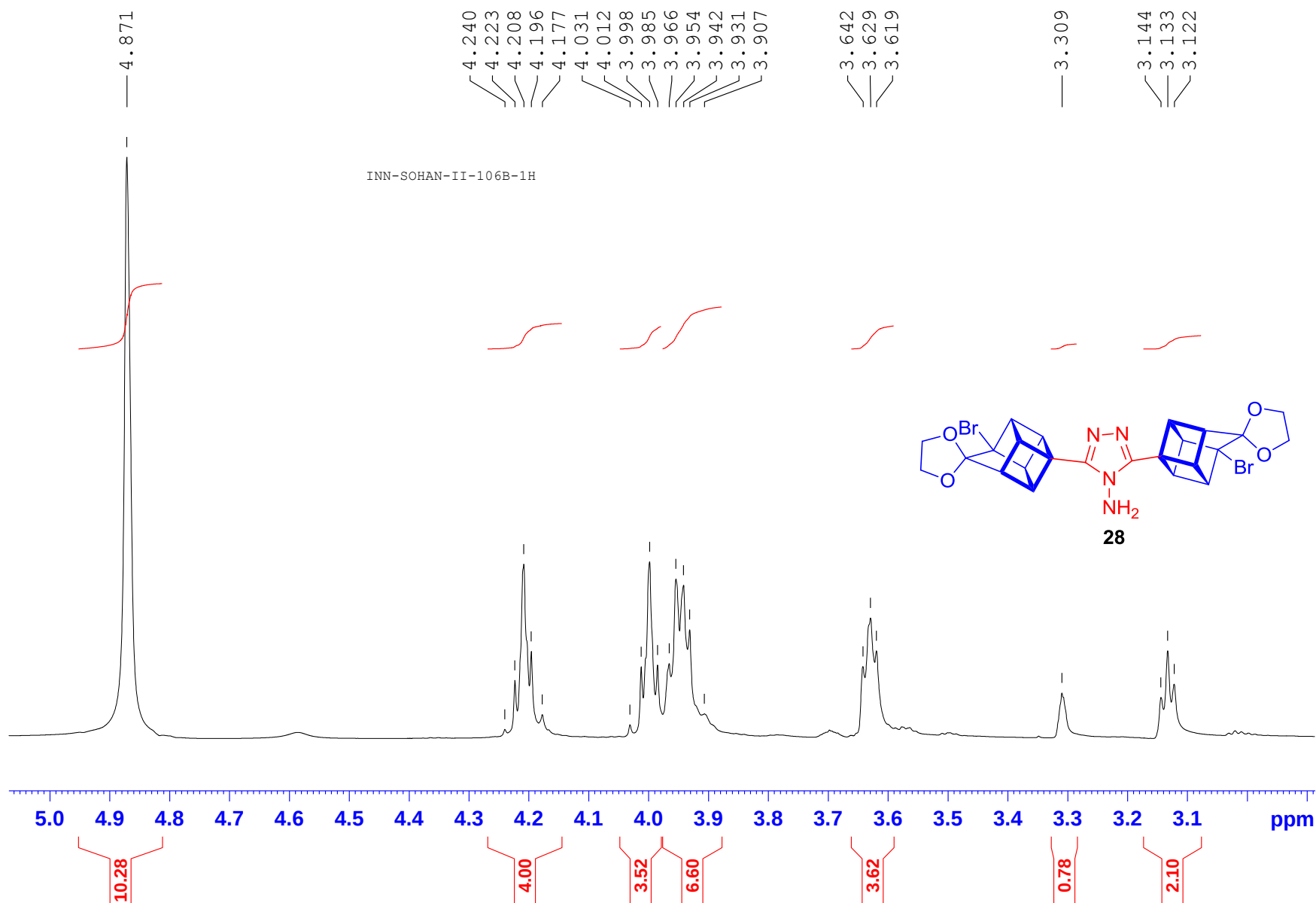
F2 - Acquisition Parameters
 Date_ 20161117
 Time_ 15.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 60
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 48.36
 DW 50.000 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S-67. 1H NMR Spectrum of Compound 28



S-68. ^1H NMR Spectrum (Expansion) of Compound 28

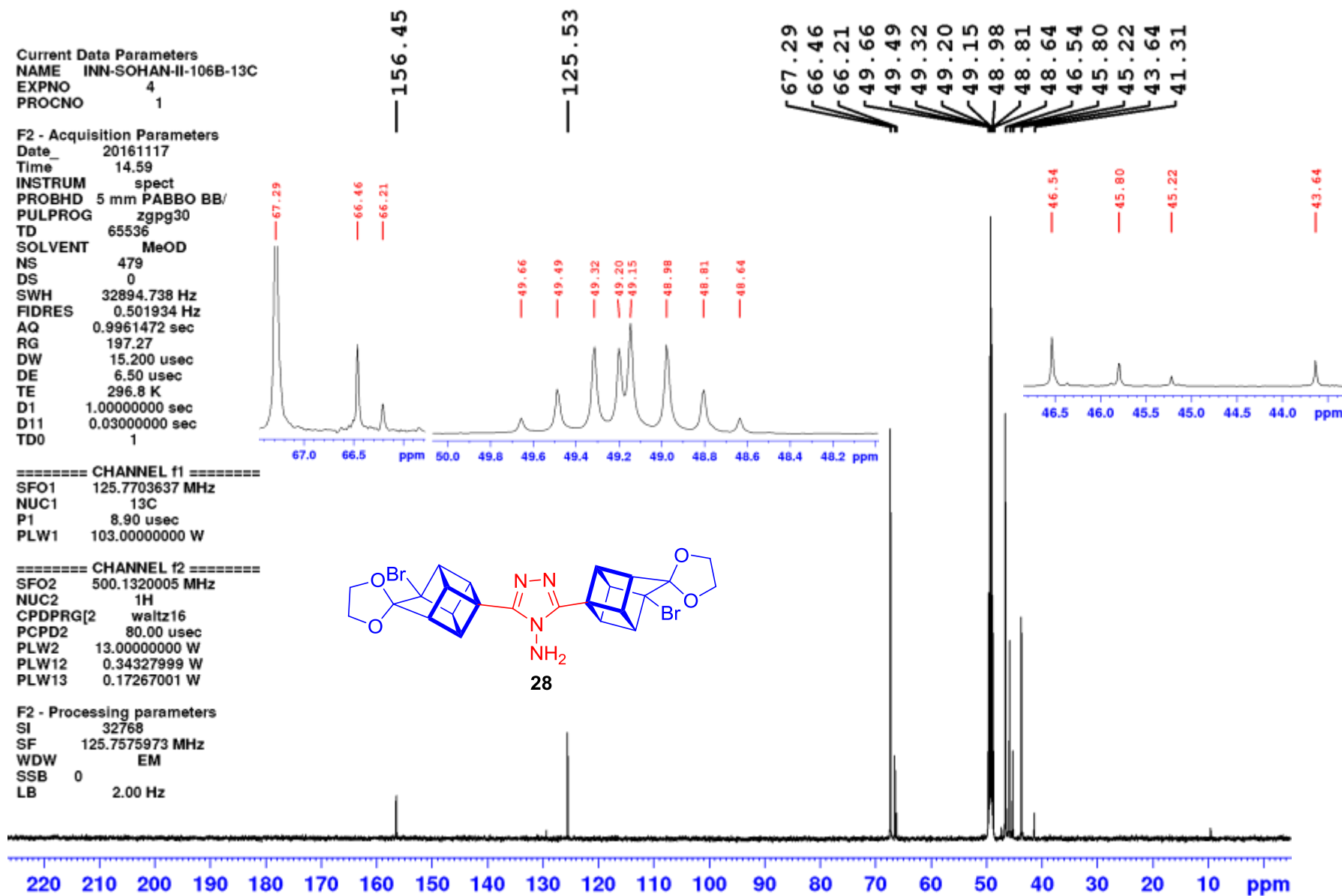
Current Data Parameters
 NAME INN-SOHAN-II-106B-13C
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161117
 Time 14.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 479
 DS 0
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

 ===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.17267001 W

F2 - Processing parameters
 SI 32768
 SF 125.7575973 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz



S-69. ¹³C NMR Spectrum of Compound 28

Current Data Parameters
 NAME INN-SOHAN-II-77-1H
 EXPNO 4
 PROCNO 1

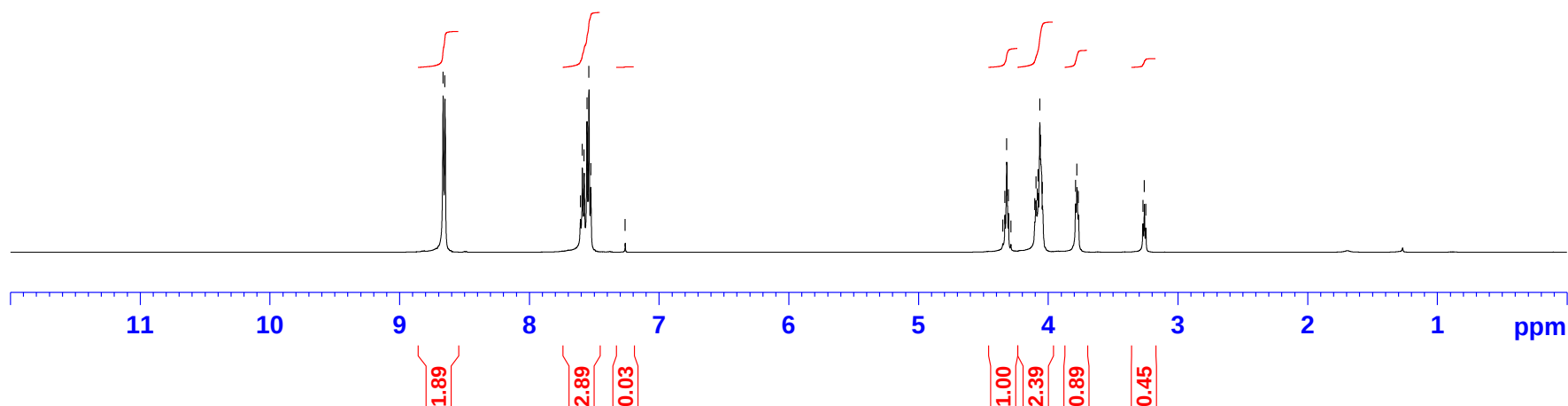
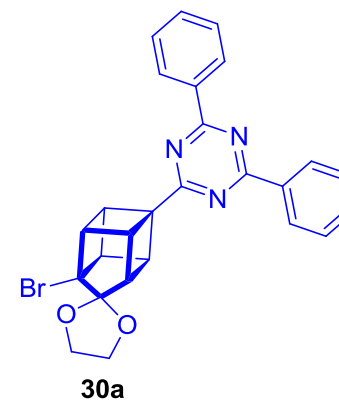
F2 - Acquisition Parameters
 Date_ 20160413
 Time 19.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 30.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 13.00000000 W

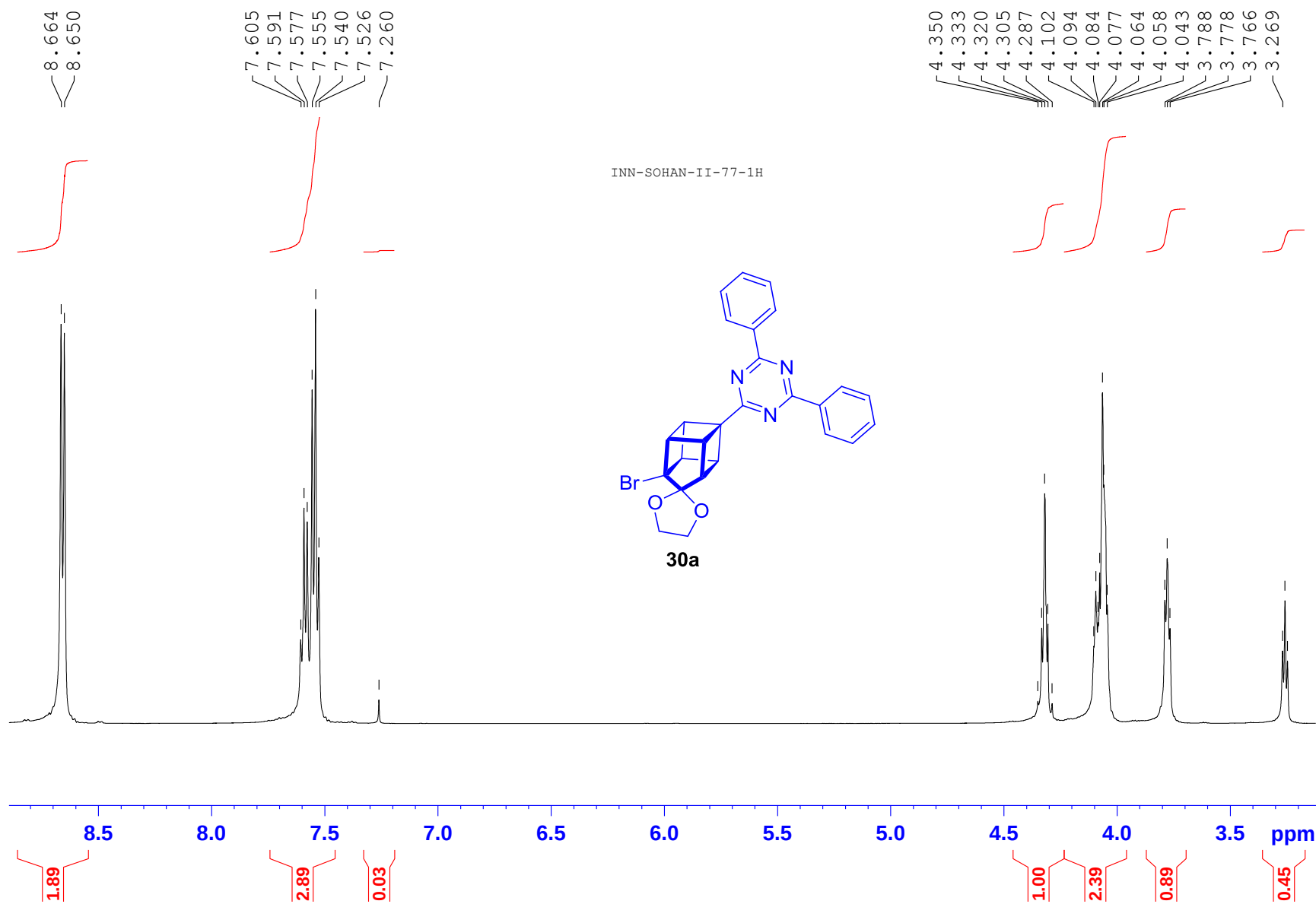
F2 - Processing parameters
 SI 65536
 SF 500.1300122 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.664
8.650
7.605
7.591
7.577
7.555
7.540
7.526
7.260

4.350
4.333
4.320
4.305
4.287
4.102
4.094
4.084
4.077
4.064
4.058
4.043
3.788
3.778
3.766
3.269
3.258
3.247



S-70. ¹H NMR Spectrum of Compound 30a



S-71. ^1H NMR Spectrum (Expansion) of Compound **30a**

Current Data Parameters
 NAME INN-SOHAN-II-77-13C
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160413
 Time_ 20.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 147
 DS 4
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 298.6 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.21969999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577738 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

177.53

171.38

136.12

132.66

129.04

128.75

124.60

77.45

77.20

76.94

66.29

65.74

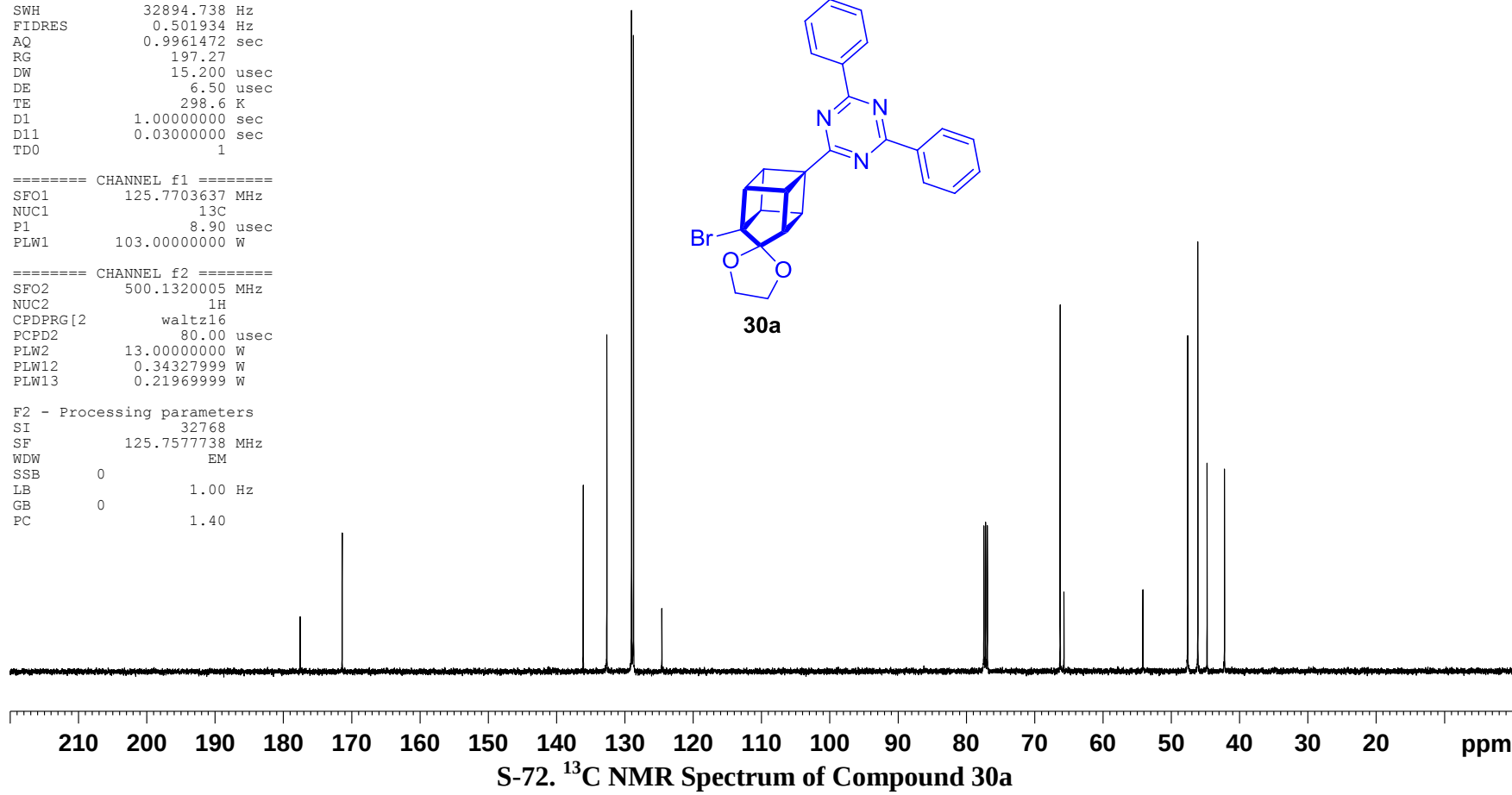
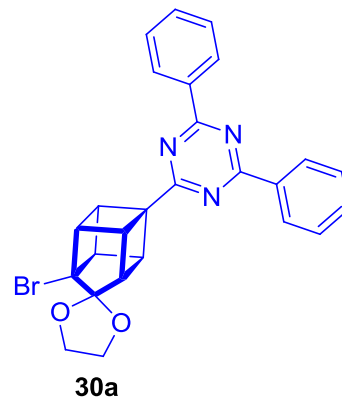
54.18

47.61

46.13

44.78

42.23



Current Data Parameters
 NAME INN-SOHN-II-77-APT
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160413
 Time 20.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 166
 DS 4
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 299.0 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.0000000 W
 PLW2 0.54321955 W

F2 - Processing parameters
 SI 32768
 SF 125.7577733 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 177.53

— 171.39

— 136.13

— 132.66

— 129.05

— 128.76

— 124.61

— 77.46

— 77.20

— 76.95

— 66.29

— 65.74

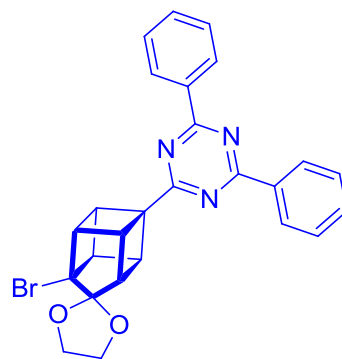
— 54.18

— 47.62

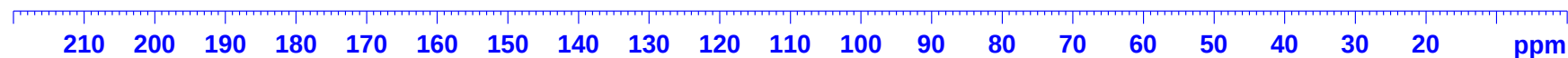
— 46.14

— 44.79

— 42.23



30a



S-73. ¹³C-APT NMR Spectrum of Compound 30a

Current Data Parameters
 NAME INN-SOHAN-II-112-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160812
 Time_ 13.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 48
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 80.35
 DW 50.000 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 13.00 usec
 PLW1 13.00000000 W

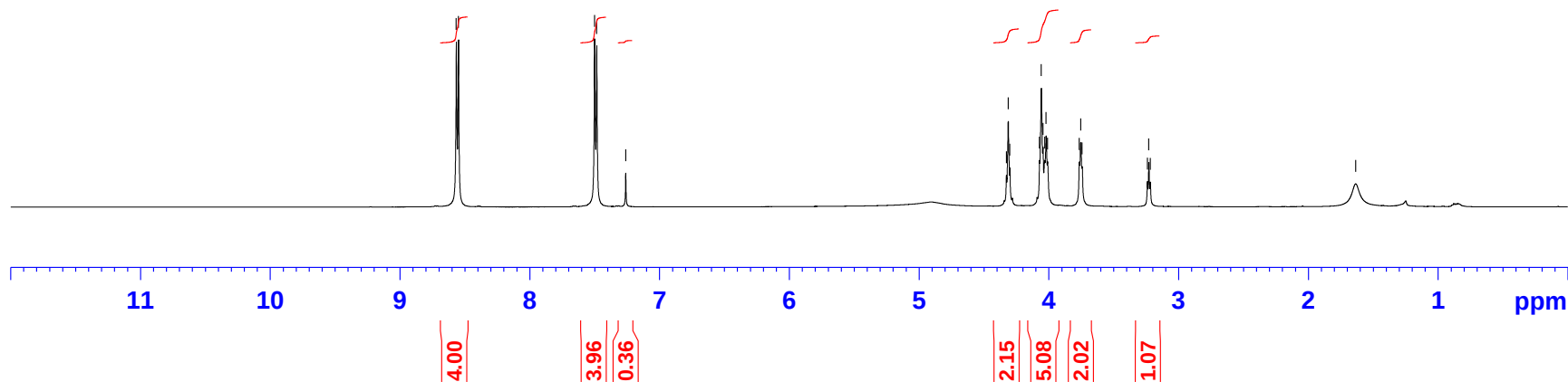
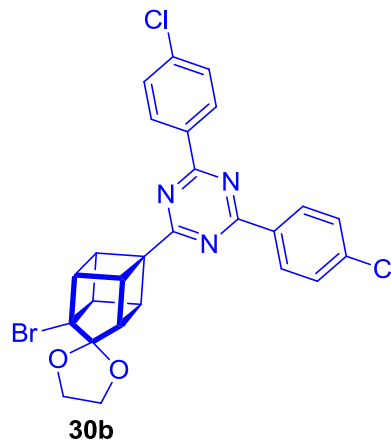
F2 - Processing parameters
 SI 65536
 SF 500.1300140 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.566
8.549

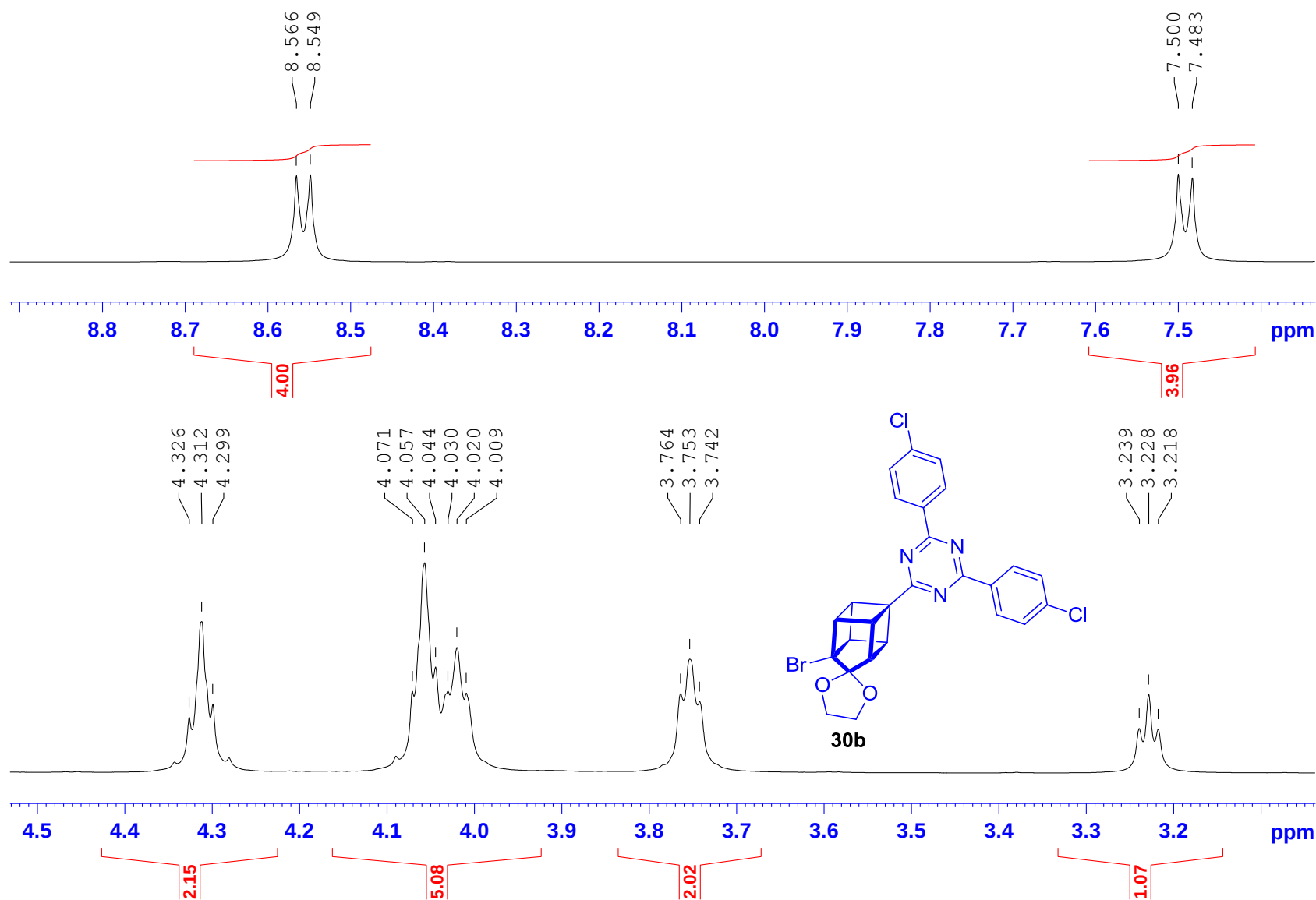
7.500
7.483
7.260

4.326
4.312
4.299
4.071
4.057
4.044
4.030
4.020
4.009
3.764
3.753
3.742
3.239
3.228
3.218

1.635



S-74. ¹H NMR Spectrum of Compound 30b



S-75. ^1H NMR Spectrum (Expansion) of Compound 30b

Current Data Parameters
 NAME INN-SOHAN-II-112-13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160812
 Time 13.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 0
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 296.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 FCPD2 80.00 usec
 PLW2 13.00000000 W
 PLW12 0.34327999 W
 PLW13 0.17267001 W

F2 - Processing parameters
 SI 32768
 SF 125.7577691 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

177.82

170.58

139.16

134.44

130.40

129.11

124.57

77.45

77.20

76.94

66.34

65.59

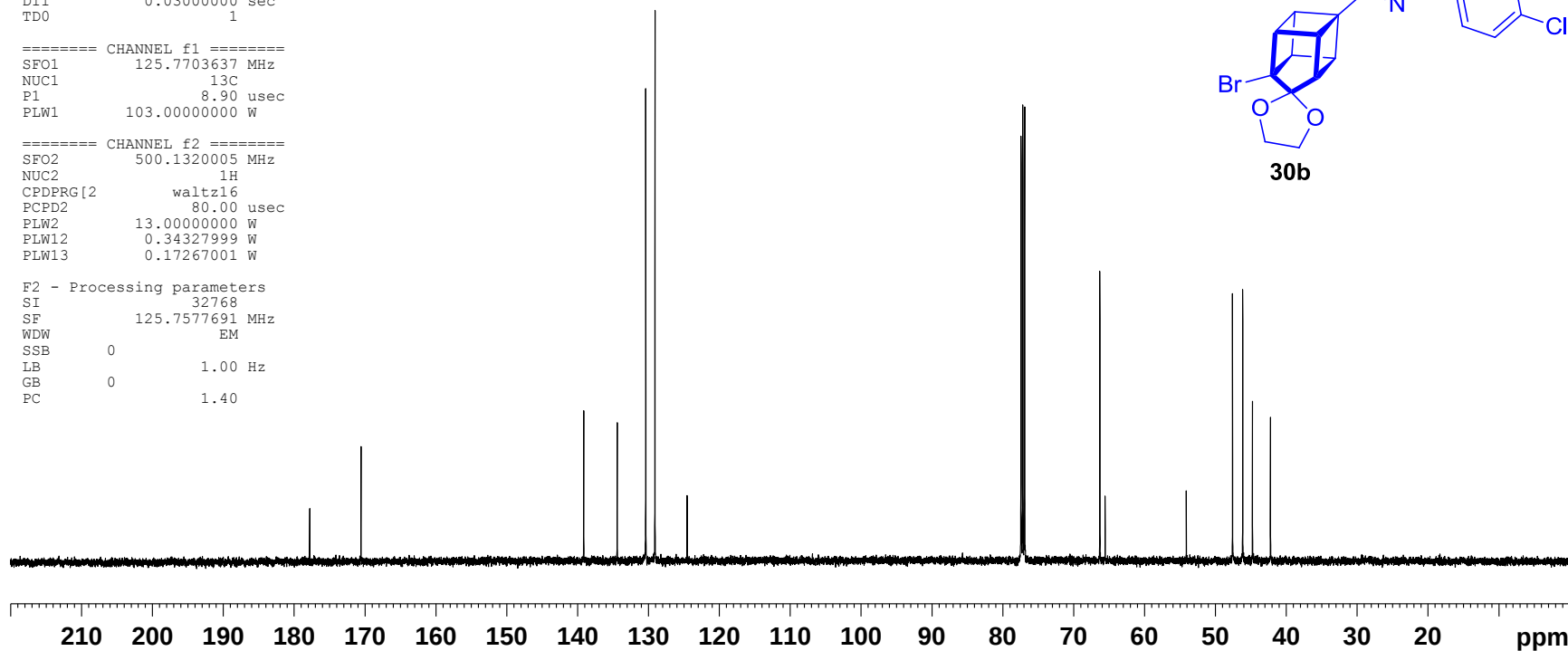
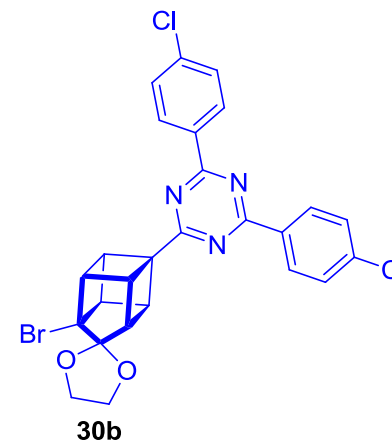
54.13

47.61

46.17

44.79

42.25



S-76. ¹³C NMR Spectrum of Compound 30b

Current Data Parameters
 NAME INN-SOHN-II-112-APT
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date 20160812
 Time 14.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1446
 DS 0
 SWH 32894.738 Hz
 FIDRES 0.501934 Hz
 AQ 0.9961472 sec
 RG 197.27
 DW 15.200 usec
 DE 6.50 usec
 TE 296.5 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 1.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 8.90 usec
 P2 17.80 usec
 PLW1 103.0000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.0000000 W
 PLW12 0.34327999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577703 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

177.81

170.58

139.15

134.43

130.39

129.09

124.57

77.44
77.18
76.93

66.33
65.58

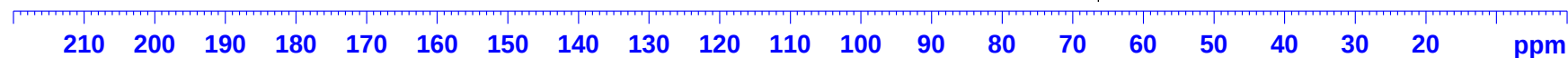
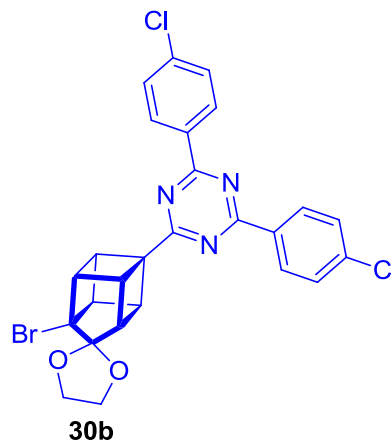
54.13

47.60

46.16

44.78

42.24



S-77. ¹³C-APT NMR Spectrum of Compound 30b

Current Data Parameters
 NAME INN-SOHAN-II-429-1H
 EXPNO 77
 PROCNO 1

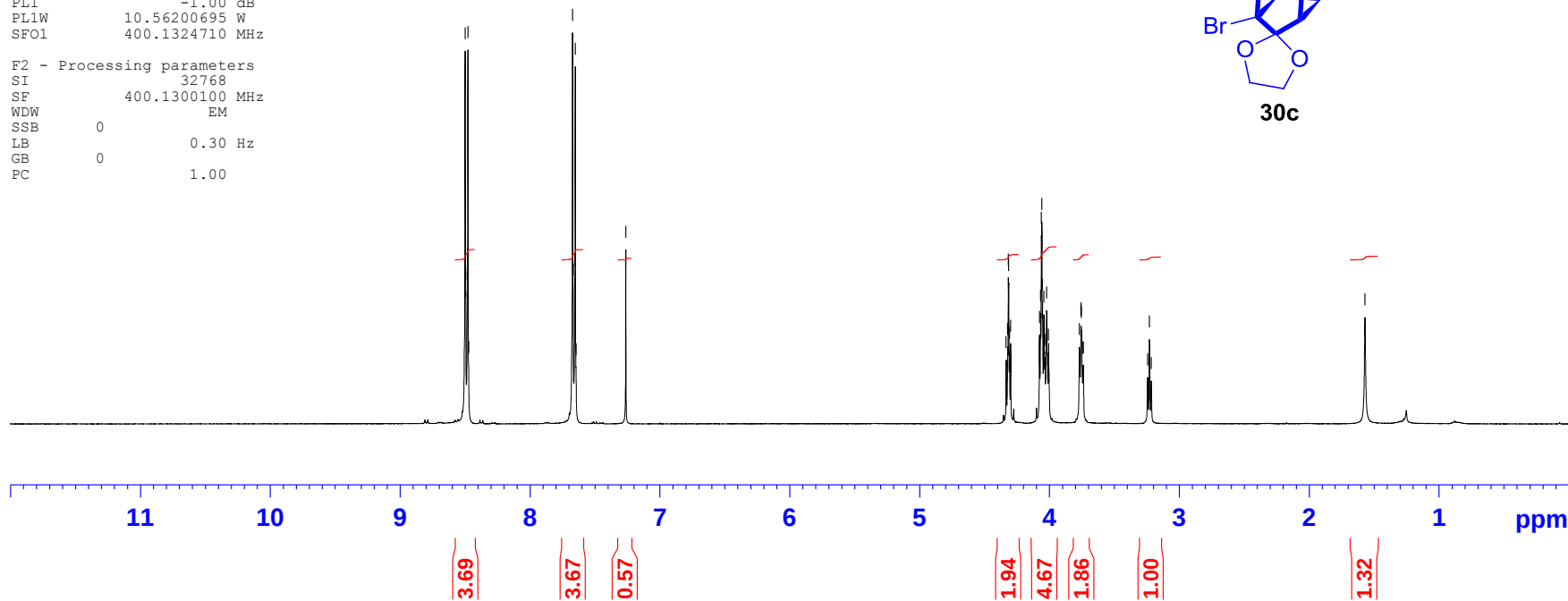
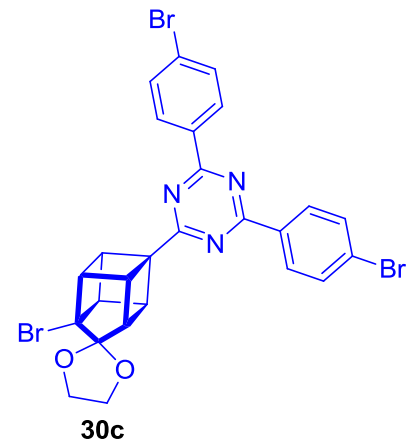
F2 - Acquisition Parameters
 Date_ 20190106
 Time_ 23.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 54274
 SOLVENT CDC13
 NS 25
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.151522 Hz
 AQ 3.2998593 sec
 RG 161
 DW 60.800 usec
 DE 6.50 usec
 TE 294.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.75 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz

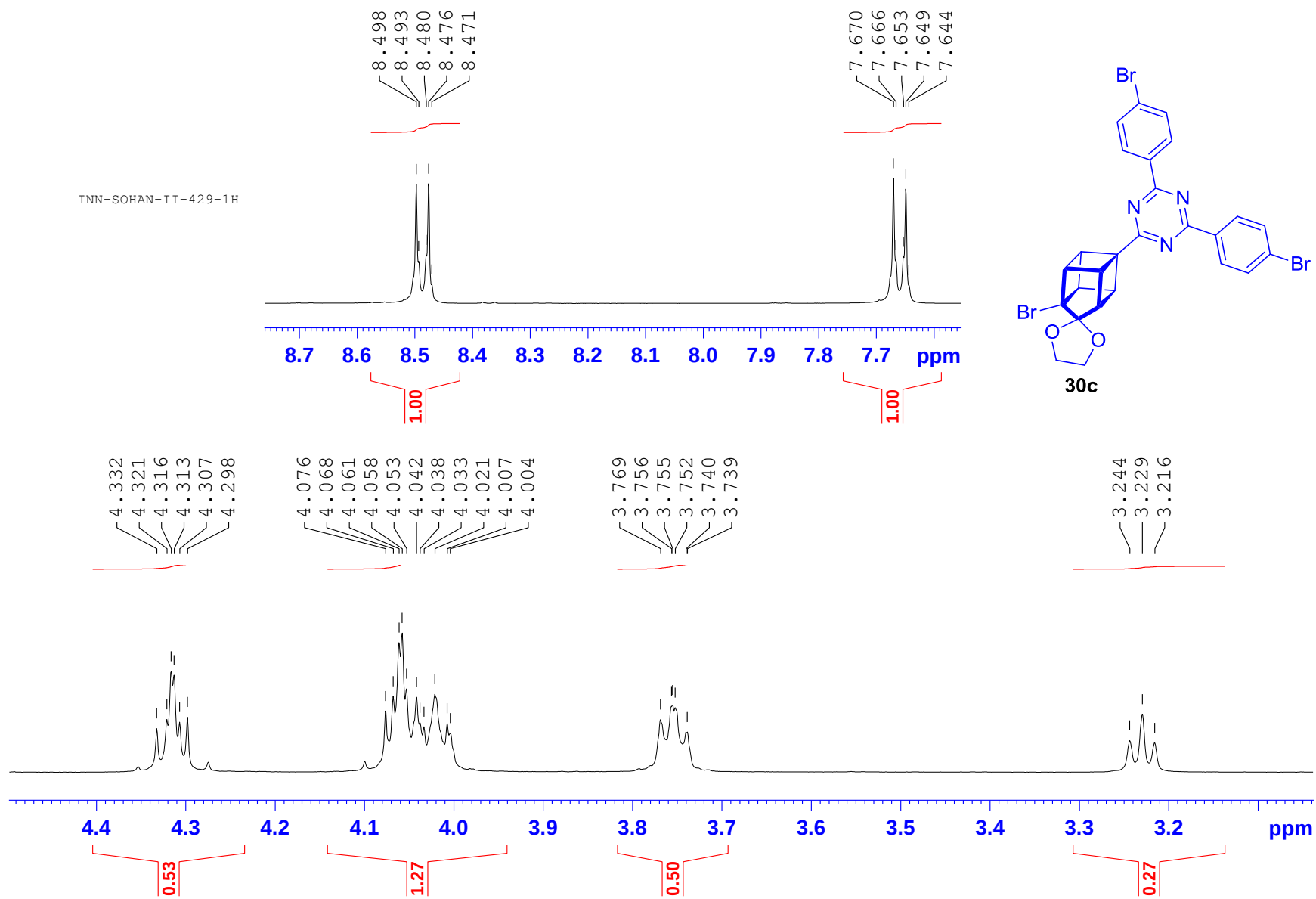
F2 - Processing parameters
 SI 32768
 SF 400.1300100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.498
8.493
8.480
8.476
8.471
7.670
7.666
7.653
7.649
7.644
7.260

4.332
4.321
4.316
4.313
4.307
4.298
4.076
4.068
4.061
4.058
4.053
4.042
4.038
4.033
4.021
4.007
4.004
3.769
3.756
3.755
3.752
3.740
3.739
3.244
3.229
3.216
1.570



S-78. ¹H NMR Spectrum of Compound 30c



S-79. ¹H NMR Spectrum (Expansion) of Compound 30c

Current Data Parameters
NAME INN-SOHAN-II-429-13C
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190106
Time_ 23.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 556
DS 0
SWH 26785.715 Hz
FIDRES 0.408718 Hz
AQ 1.2233387 sec
RG 1030
DW 18.667 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 56.53121948 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 13.69 dB
PL13 14.50 dB
PL2W 10.56200695 W
PL12W 0.35871249 W
PL13W 0.29767781 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127515 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

177.89

170.75

134.90

132.11

130.60

127.87

124.58

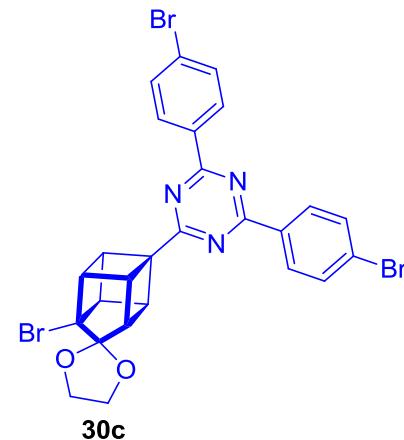
77.52

77.20

76.88

66.35

65.59



54.15

47.62

46.20

44.81

42.27

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

S-80. ¹³C NMR Spectrum of Compound 30c