

SUPPLEMENTARY MATERIAL

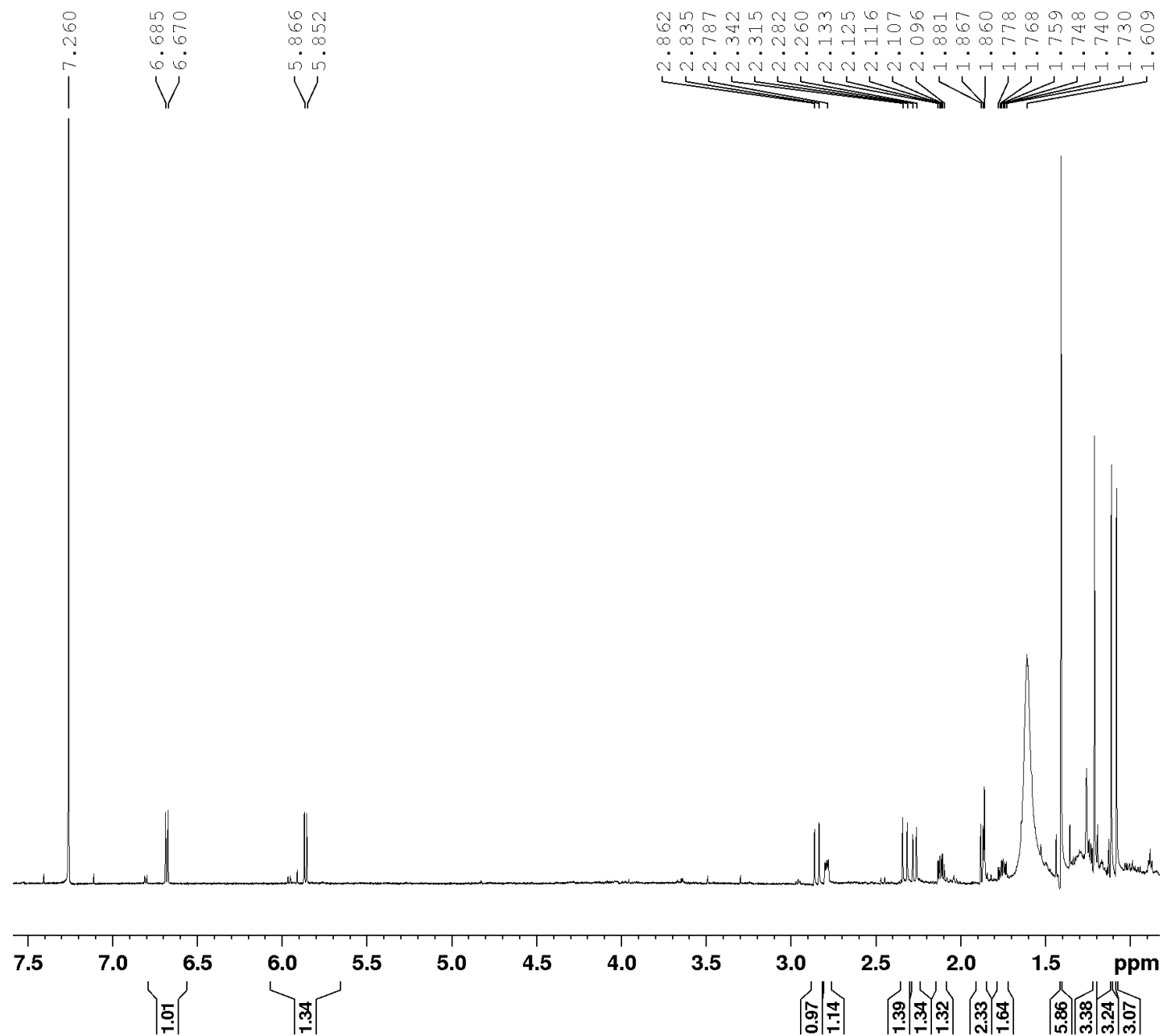
New antimicrobial cyclopiane diterpenes and polyketide derivatives from marine sediment-derived fungus *Penicillium antarcticum* KMM 4670

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Figure S1. ^1H NMR spectrum (700 MHz, CDCl_3) of **1**



Current Data Parameters

NAME CF-60ch
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20220530
Time 12.00 h
INSTRUM spect
PROBHD Z134216_0006 (
PULPROG zg30
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SOLVENT CDCl_3
NS 16
DS 2
SWH 10504.202 Hz
FIDRES 0.641126 Hz
AQ 1.5597568 sec
RG 165.68
DW 47.600 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
TD0 1
SFO1 700.0051100 MHz
NUC1 ^1H
P0 5.33 usec
P1 16.00 usec
PLW1 11.27900028 W

F2 - Processing parameters

SI 32768
SF 700.0000162 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 4.00

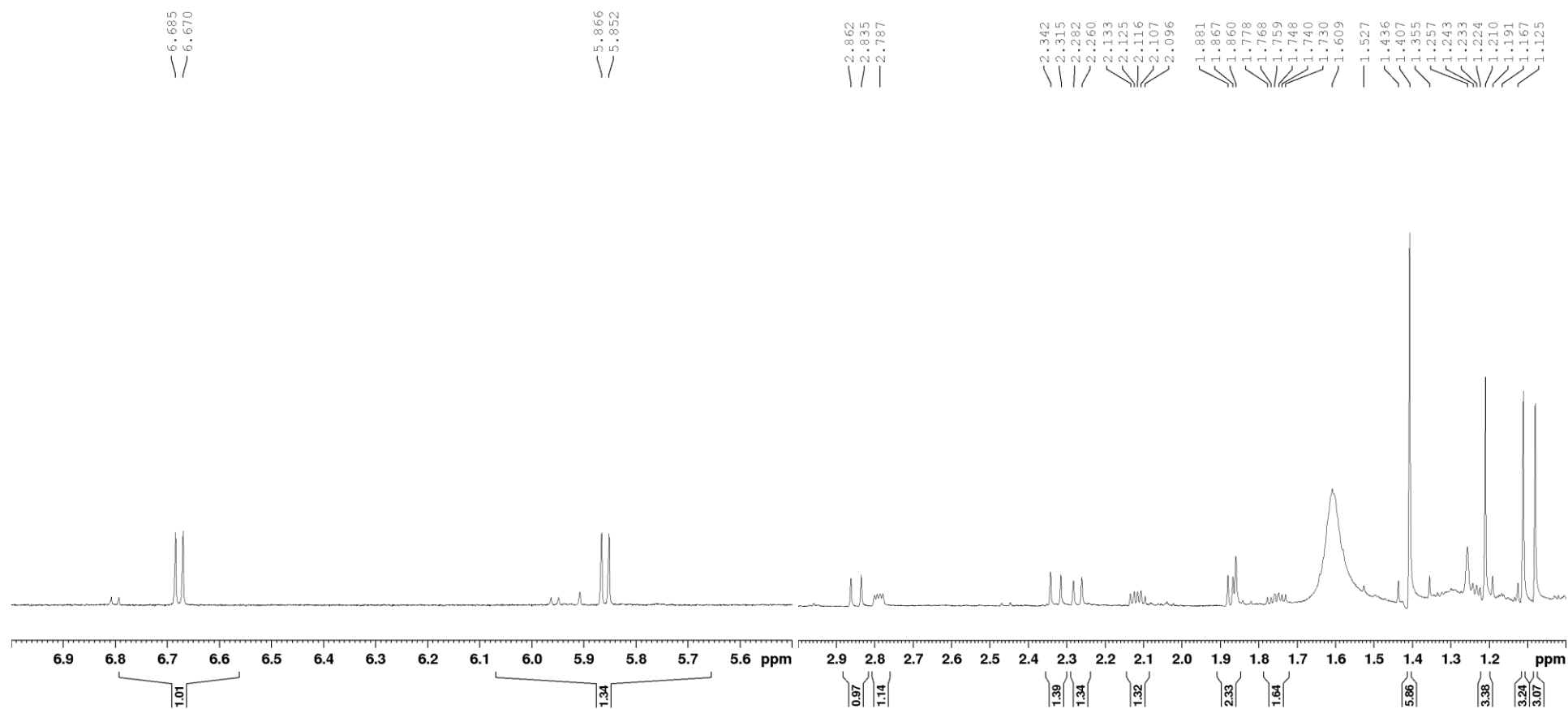
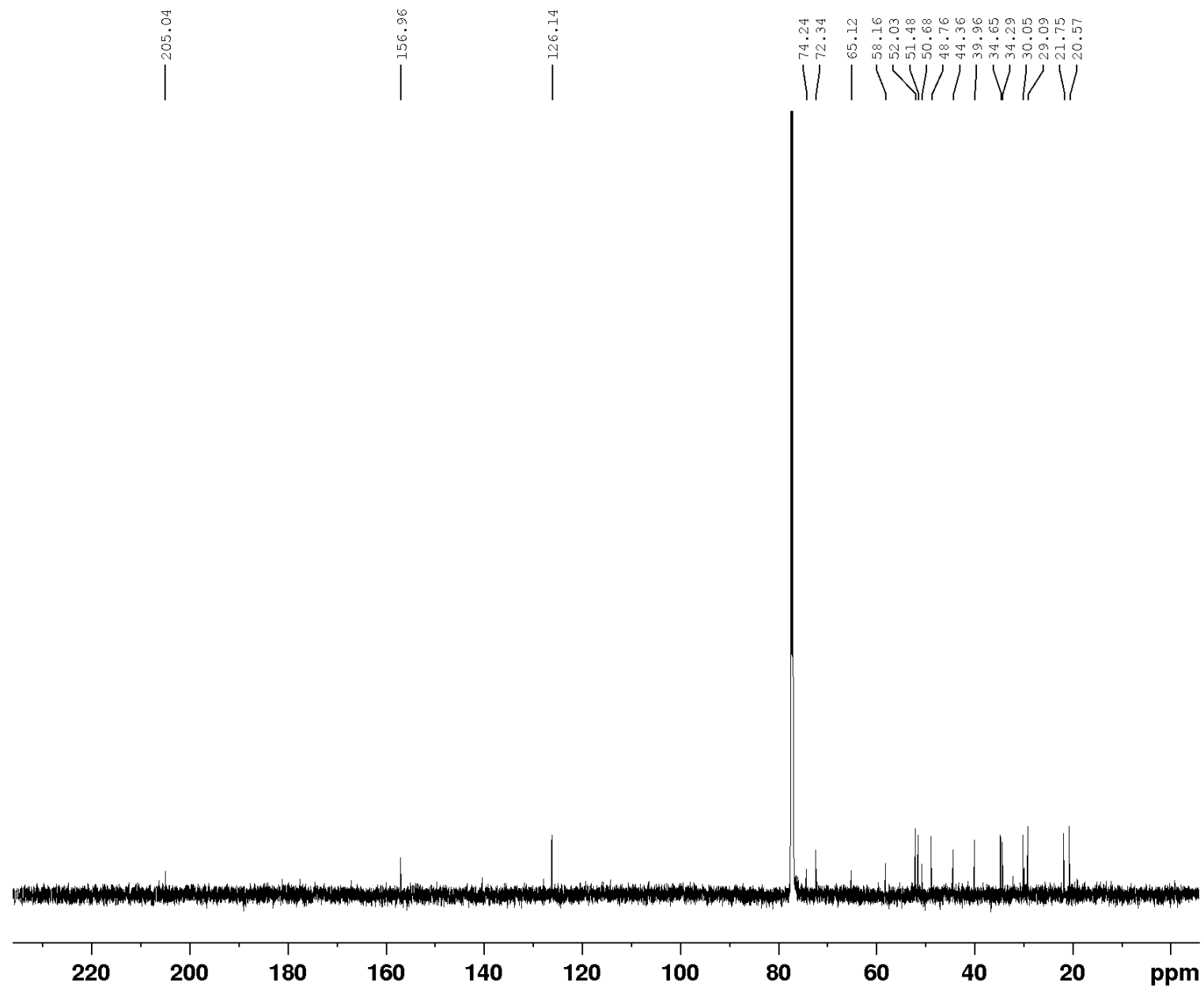


Figure S2. ^{13}C NMR spectrum (125.75 MHz, CDCl_3) of **1**



Current Data Parameters
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EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
PROBHD Z134216_0006 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl_3
NS 7592
DS 4
SWH 42613.637 Hz
FIDRES 2.600930 Hz
AQ 0.3844779 sec
RG 191.01
DW 11.733 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 4096
SFO1 176.0353837 MHz
NUC1 ^{13}C
P0 4.00 usec
P1 12.00 usec
PLW1 61.49700165 W
SFO2 700.0021000 MHz
NUC2 ^1H
CPDPRG2 waltz16
PCPD2 65.00 usec
PLW2 11.27900028 W
PLW12 0.68339998 W
PLW13 0.34412000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.20

Figure S3. DEPT NMR spectrum (700 MHz, CDCl₃) of **1**

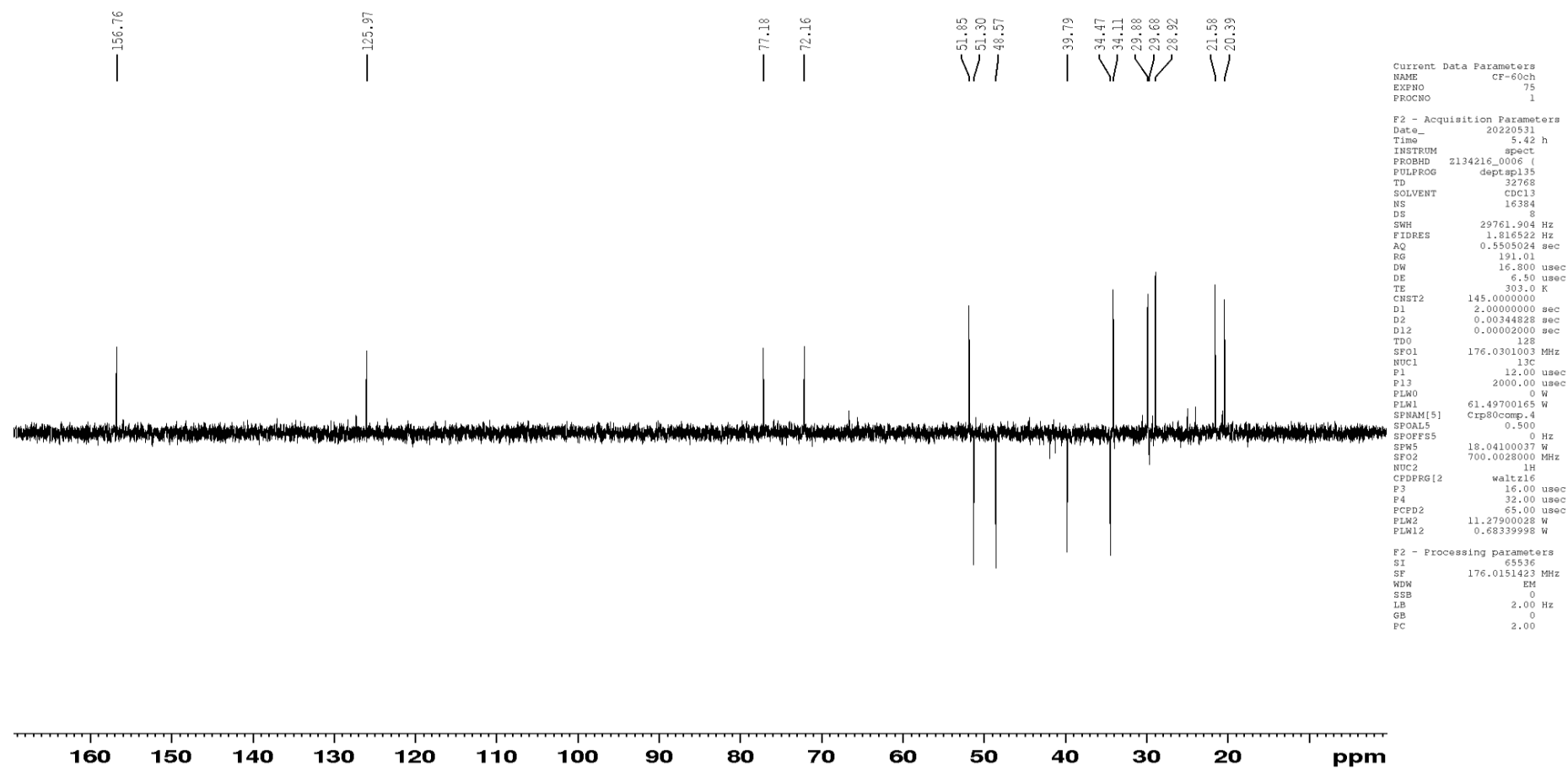


Figure S4. HSQC NMR spectrum (700 MHz, CDCl₃) of 1

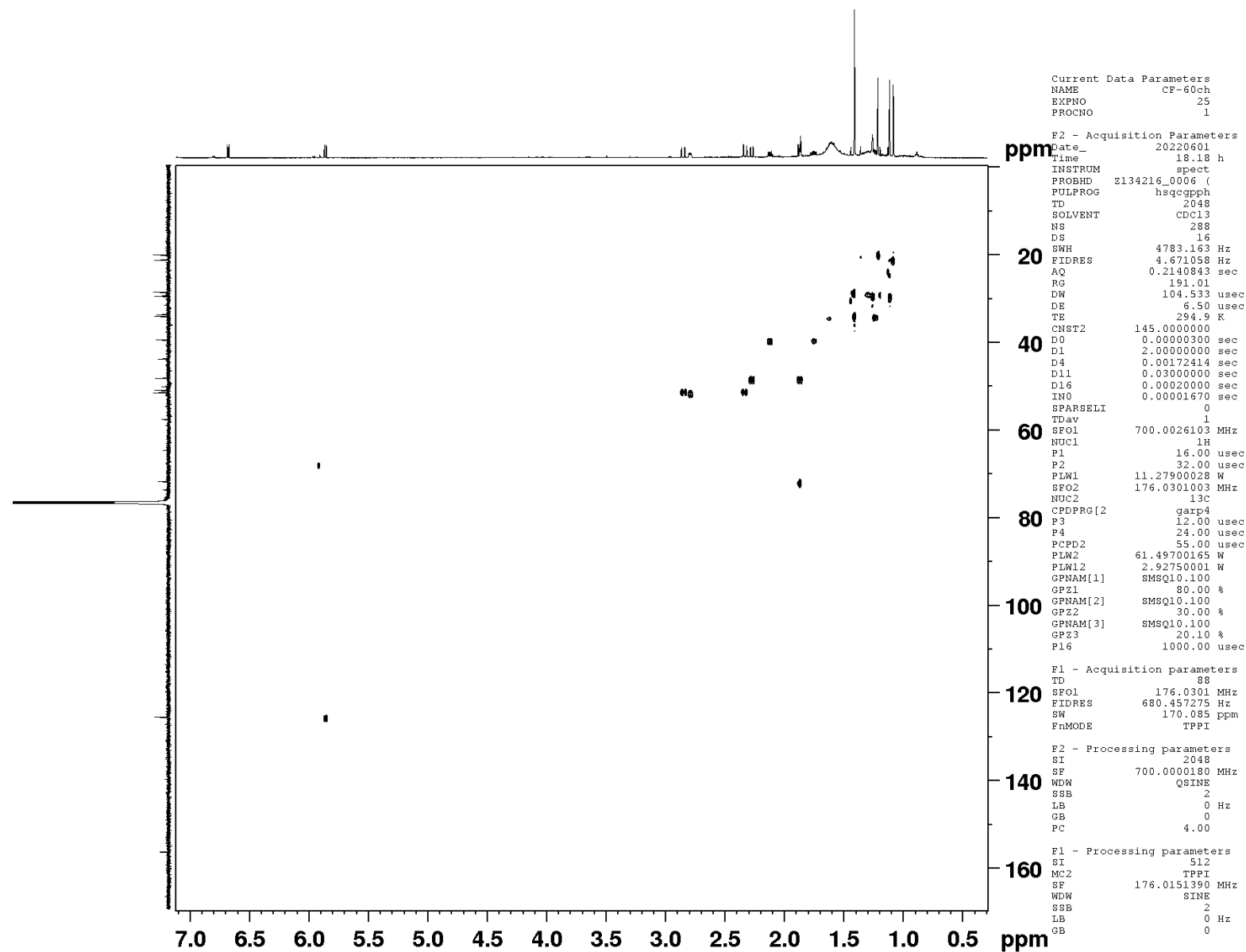
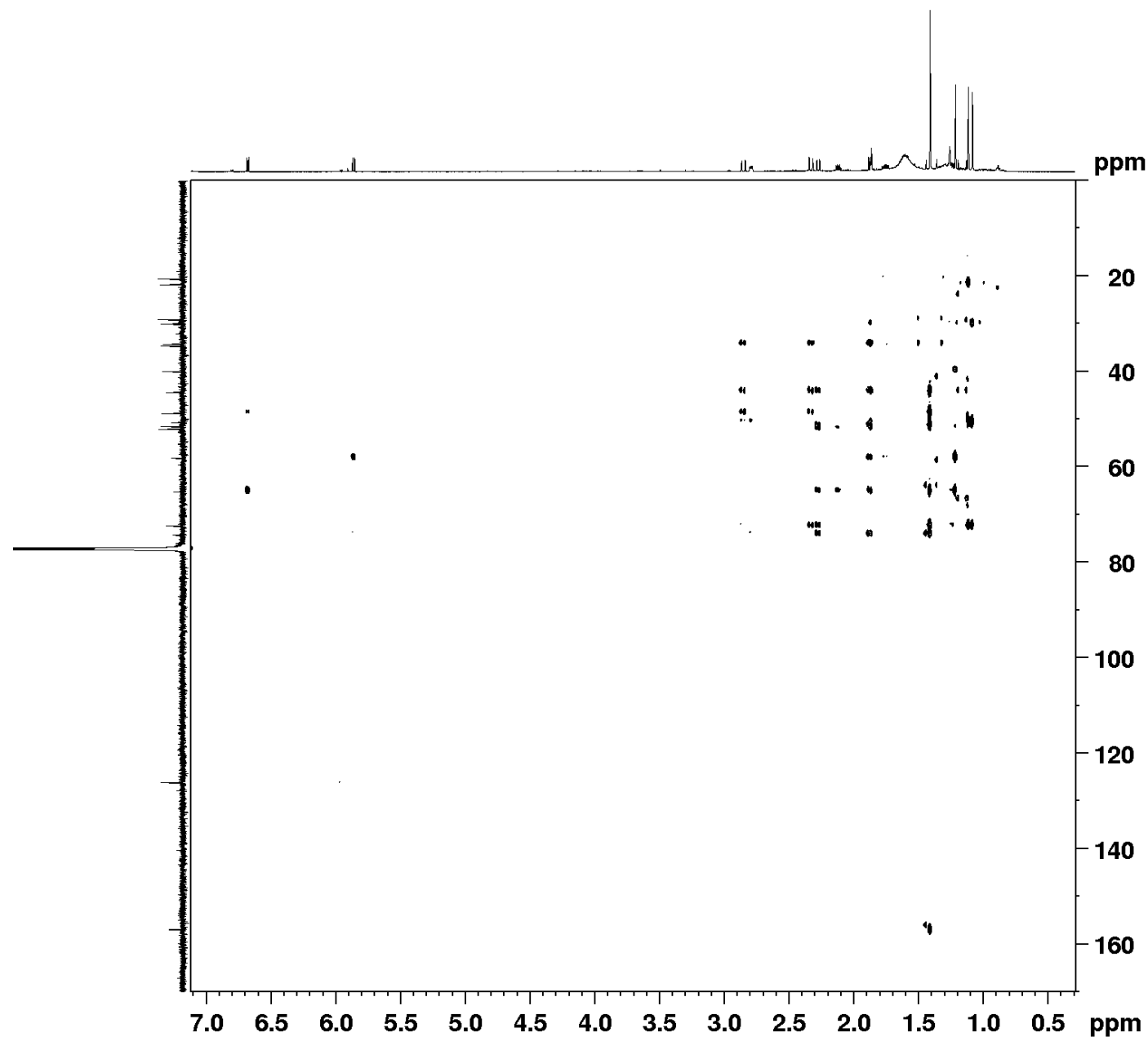


Figure S5. HMBC NMR spectrum (700 MHz, CDCl₃) of 1



Current Data Parameters
NAME CF-60ch
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220606
Time 15.33 h
INSTRUM spect
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PULPROG hmbcgp1ndqf
TD 4096
SOLVENT CDCl3
NS 256
DS 16
SWH 4783.163 Hz
FIDRES 2.335529 Hz
AQ 0.4281685 sec
RG 191.01
DW 104.533 usec
DE 6.50 usec
TE 303.0 K
CNST2 145.0000000
CNST13 5.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D2 0.00344828 sec
D6 0.10000000 sec
D16 0.00020000 sec
IN0 0.00001180 sec
SPARSELI 0
TDav 1
SFO1 700.0026103 MHz
NUC1 1H
P1 16.00 usec
P2 32.00 usec
PLW1 11.27900028 W
SFO2 176.0362608 MHz
NUC2 13C
P3 12.00 usec
PLW2 61.49700165 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 104
SFO1 176.0363 MHz
FIDRES 814.863098 Hz
SW 240.705 ppm
EnMODE QF

F2 - Processing parameters
SI 2048
SF 700.0000180 MHz
WDW SINE
SSB 3
LB 0 Hz
GB 0
PC 4.00

F1 - Processing parameters
SI 512
MC2 QF
SF 176.0151390 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S6. ^1H - ^1H COSY NMR spectrum (700 MHz, CDCl_3) of **1**

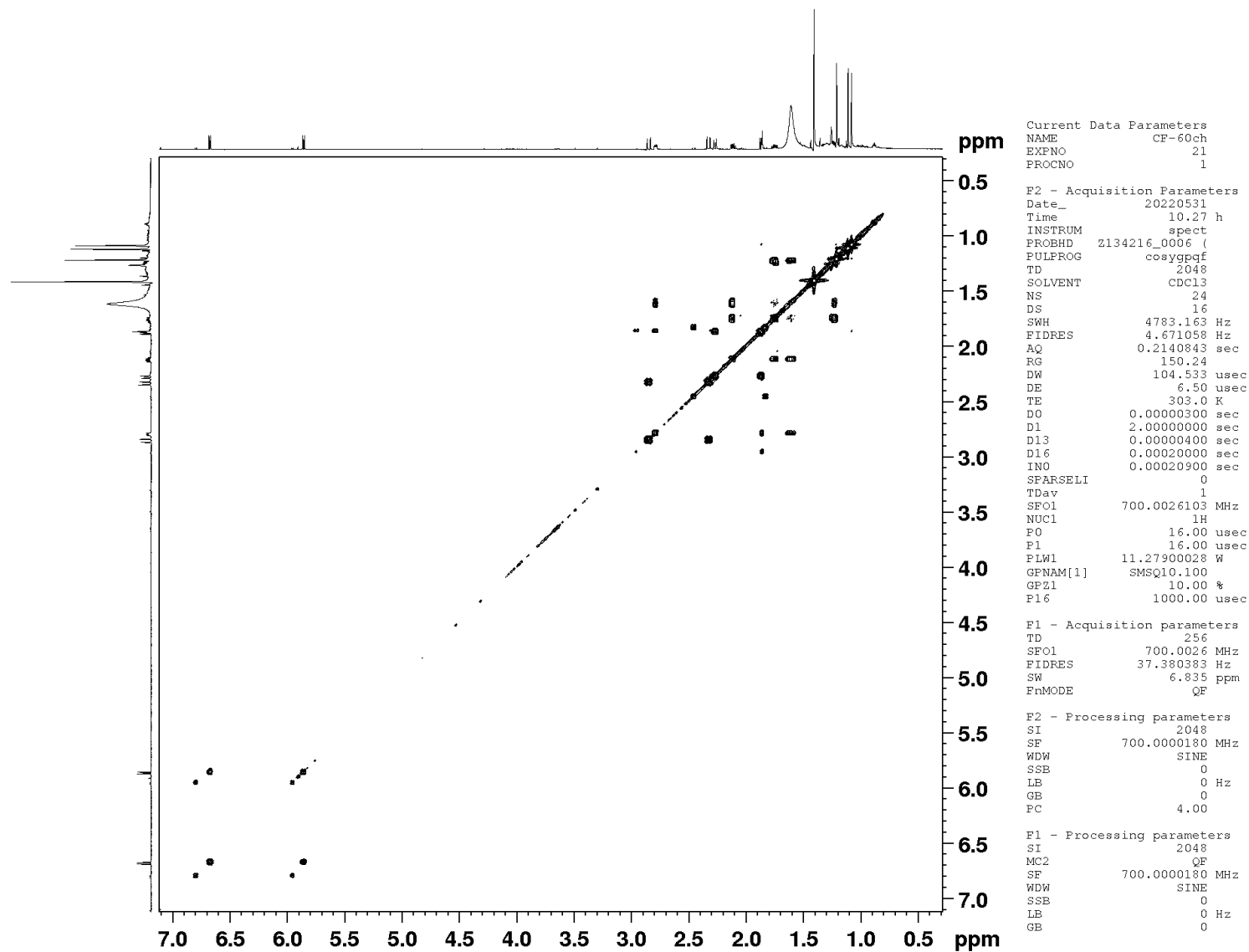


Figure S7. ROESY NMR spectrum (700 MHz, CDCl₃) of **1**

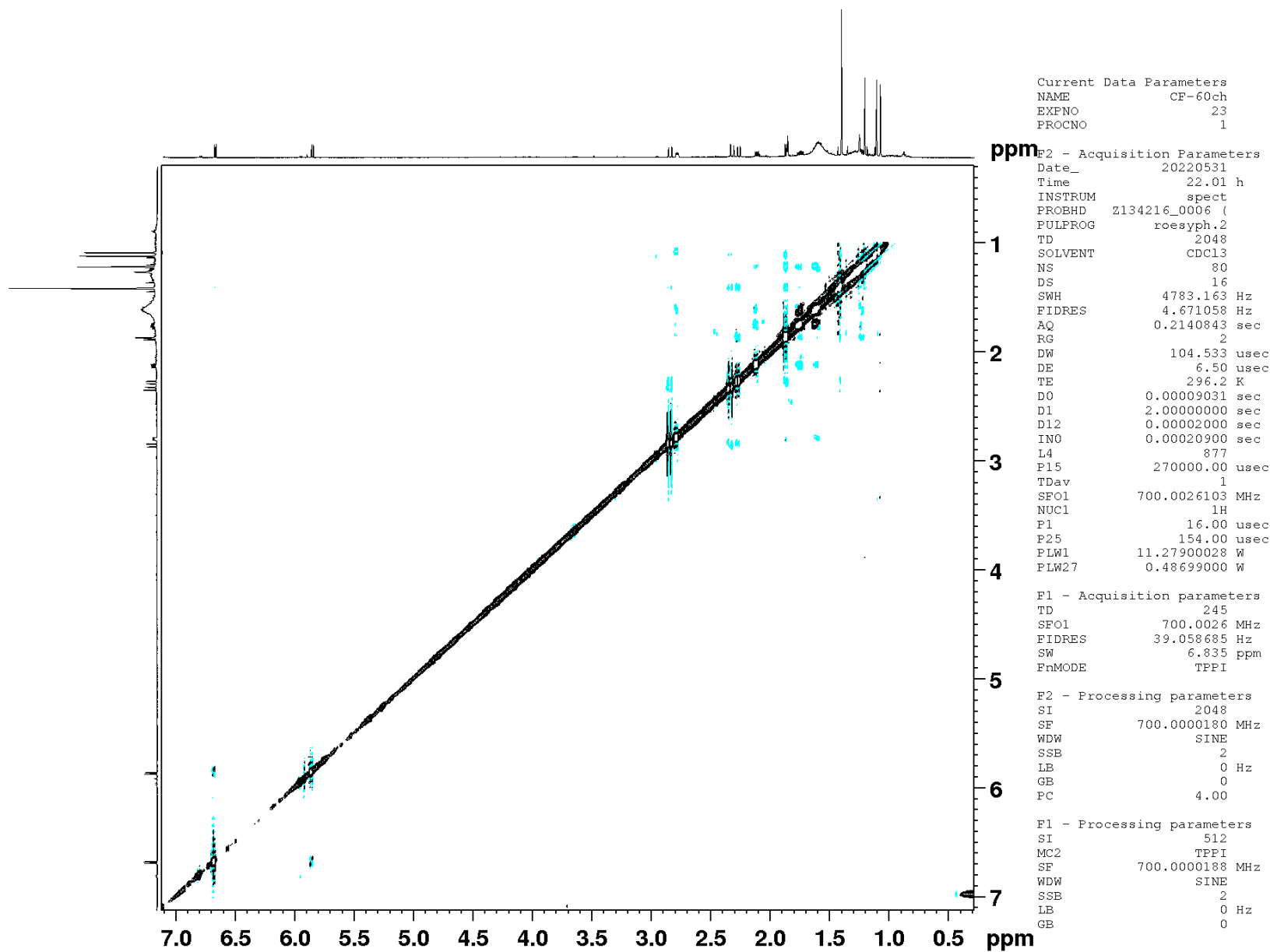
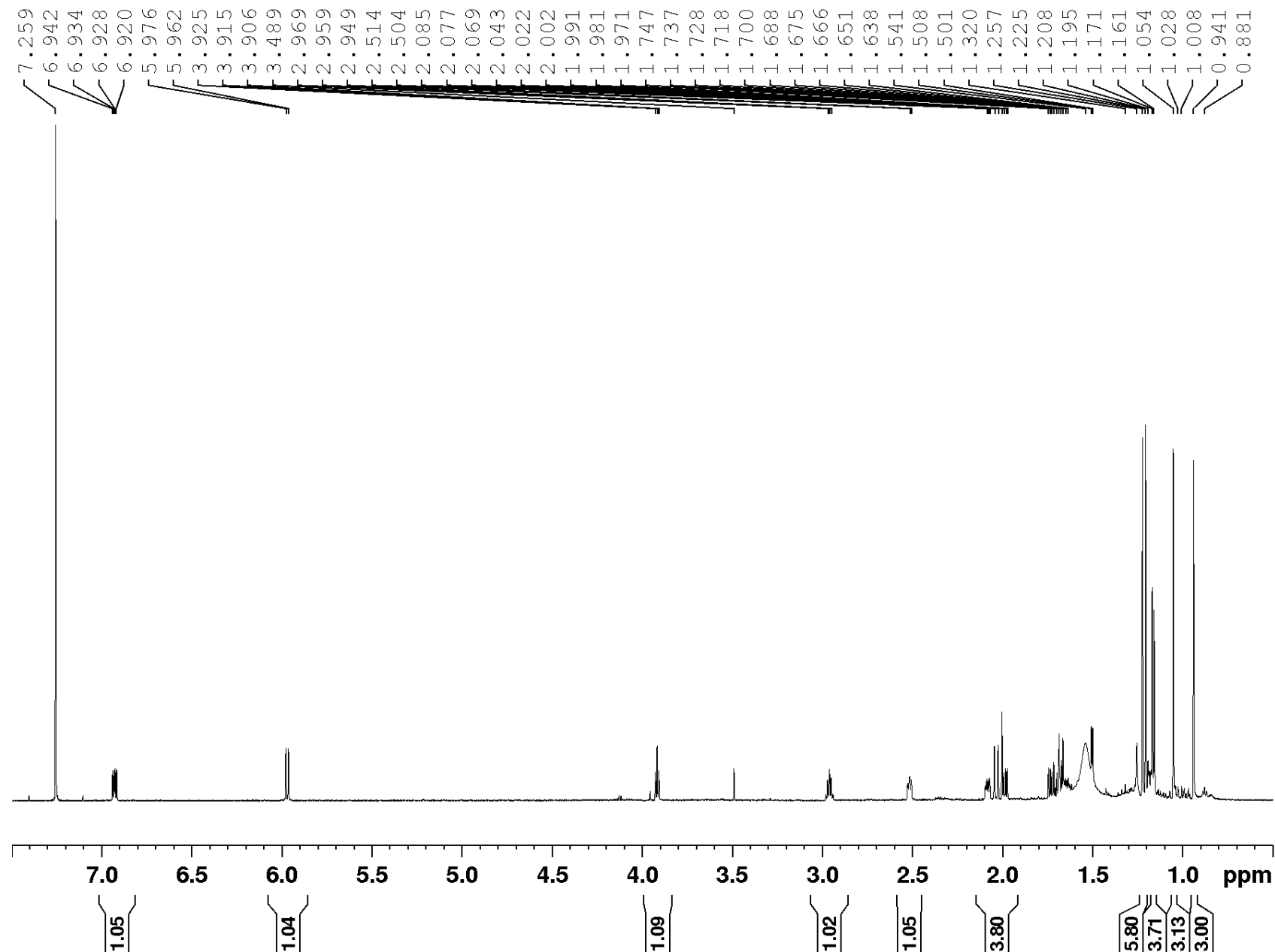


Figure S8. ^1H NMR spectrum (700 MHz, CDCl_3) of **2**



Current Data Parameters
 NAME Och-67ch
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 Time 16.33 h
 INSTRUM spect
 PROBHD Z134216_0006 (
 PULPROG zg30
 TD 32768
 SOLVENT CDCl_3
 NS 8
 DS 2
 SWH 10504.202 Hz
 FIDRES 0.641126 Hz
 AQ 1.5597568 sec
 RG 165.68
 DW 47.600 usec
 DE 6.50 usec
 TE 302.9 K
 D1 2.00000000 sec
 TD0 1
 SFO1 700.0051100 MHz
 NUC1 ^1H
 P0 5.33 usec
 P1 16.00 usec
 PLW1 11.27900028 W

F2 - Processing parameters
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 SF 700.0000178 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 4.00

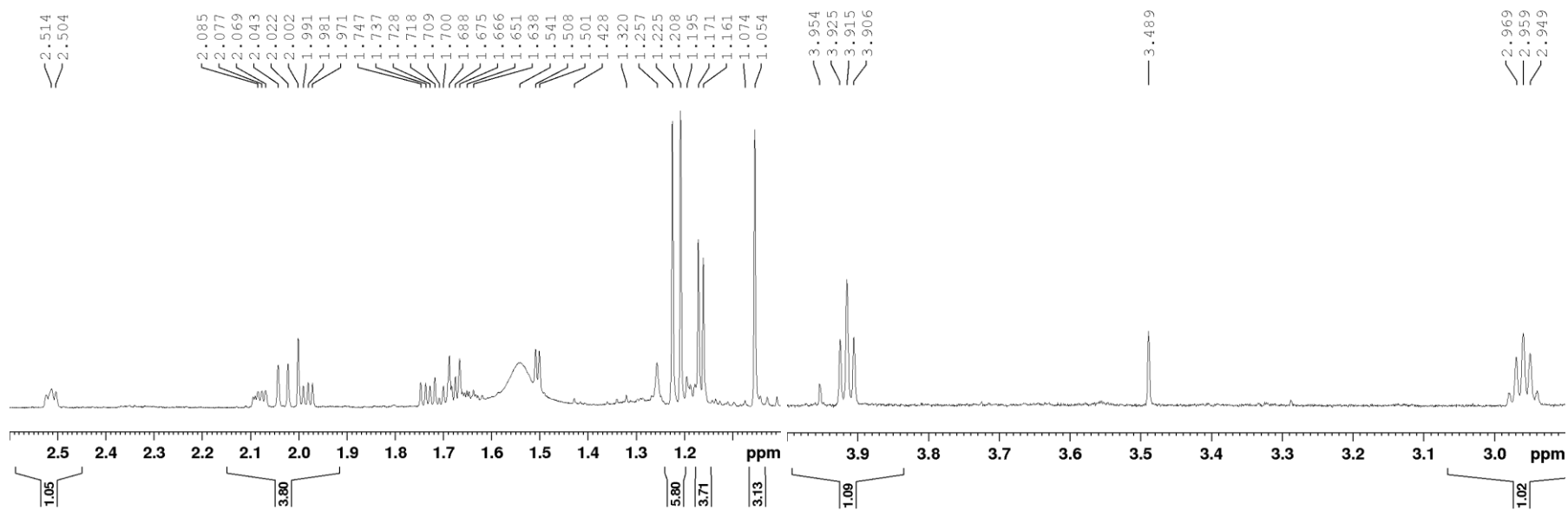
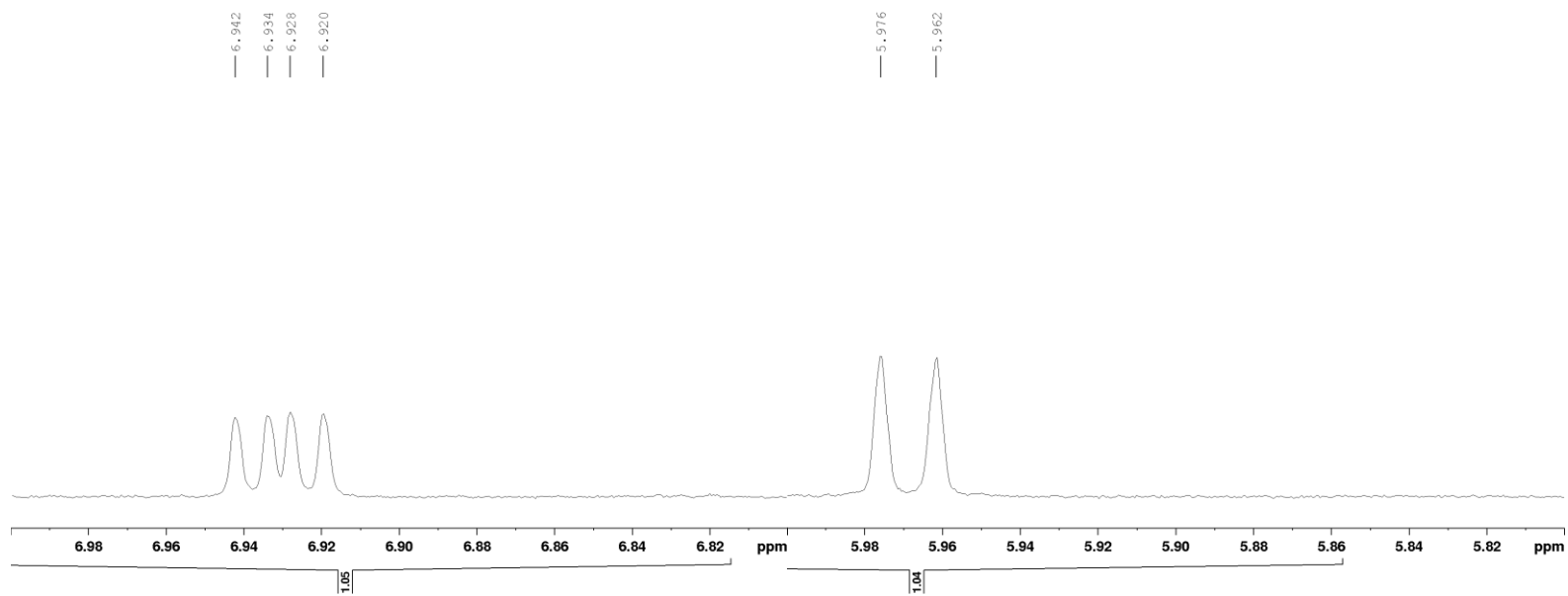


Figure S9. ^{13}C NMR spectrum (125 MHz, CDCl_3) of 2

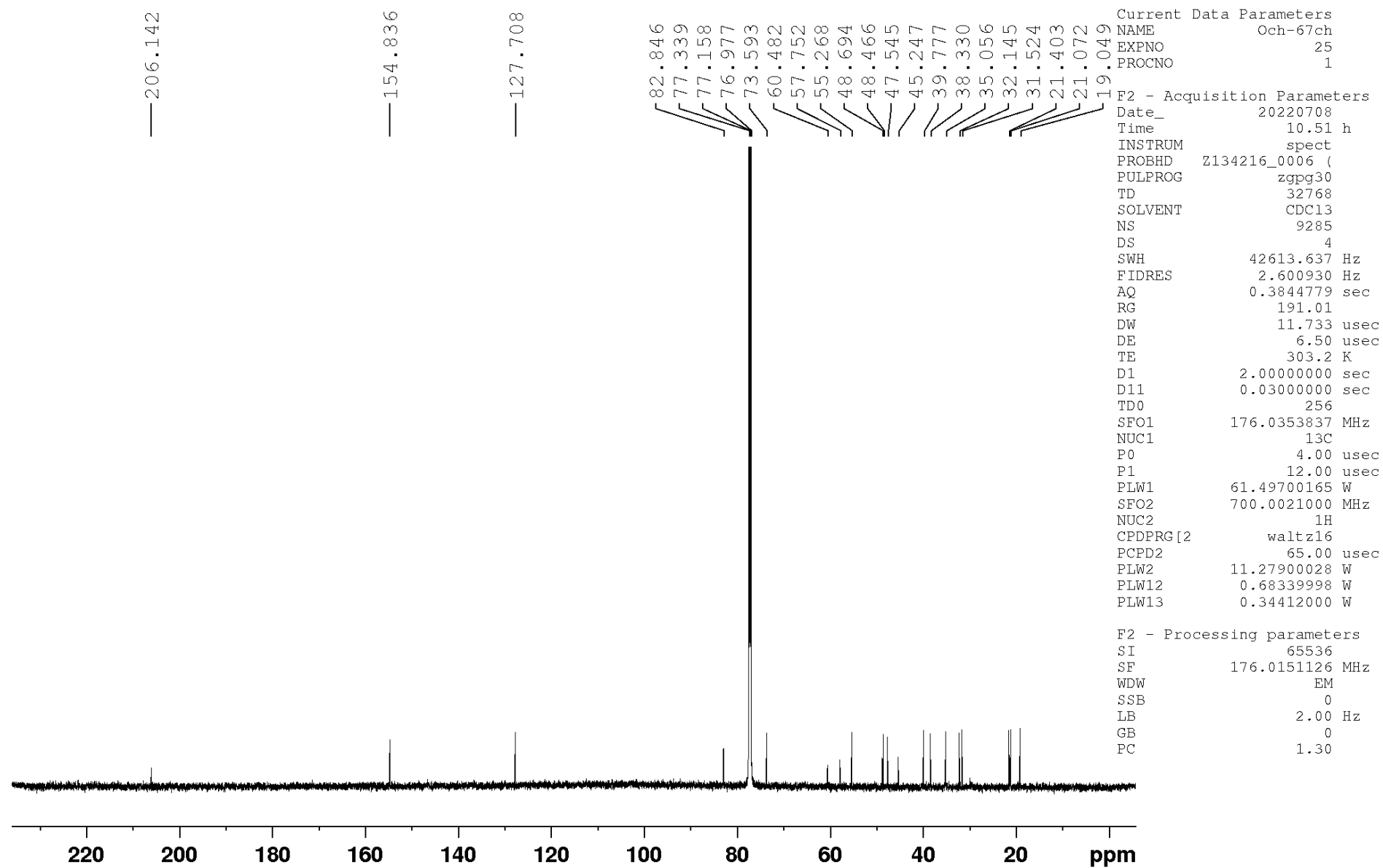


Figure S10. DEPT NMR spectrum (700 MHz, CDCl₃) of 2

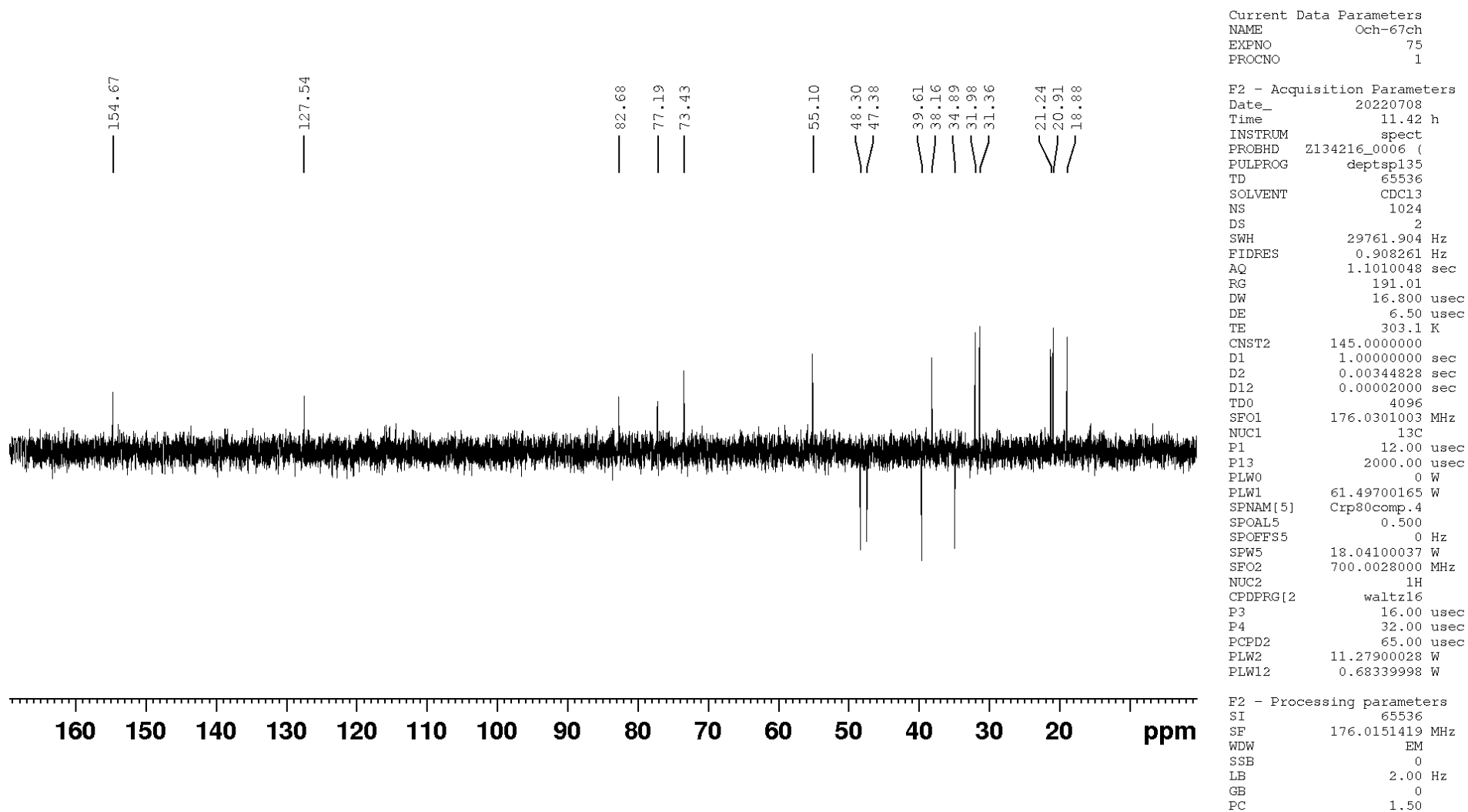


Figure S11. HSQC NMR spectrum (700 MHz, CDCl₃) of 2

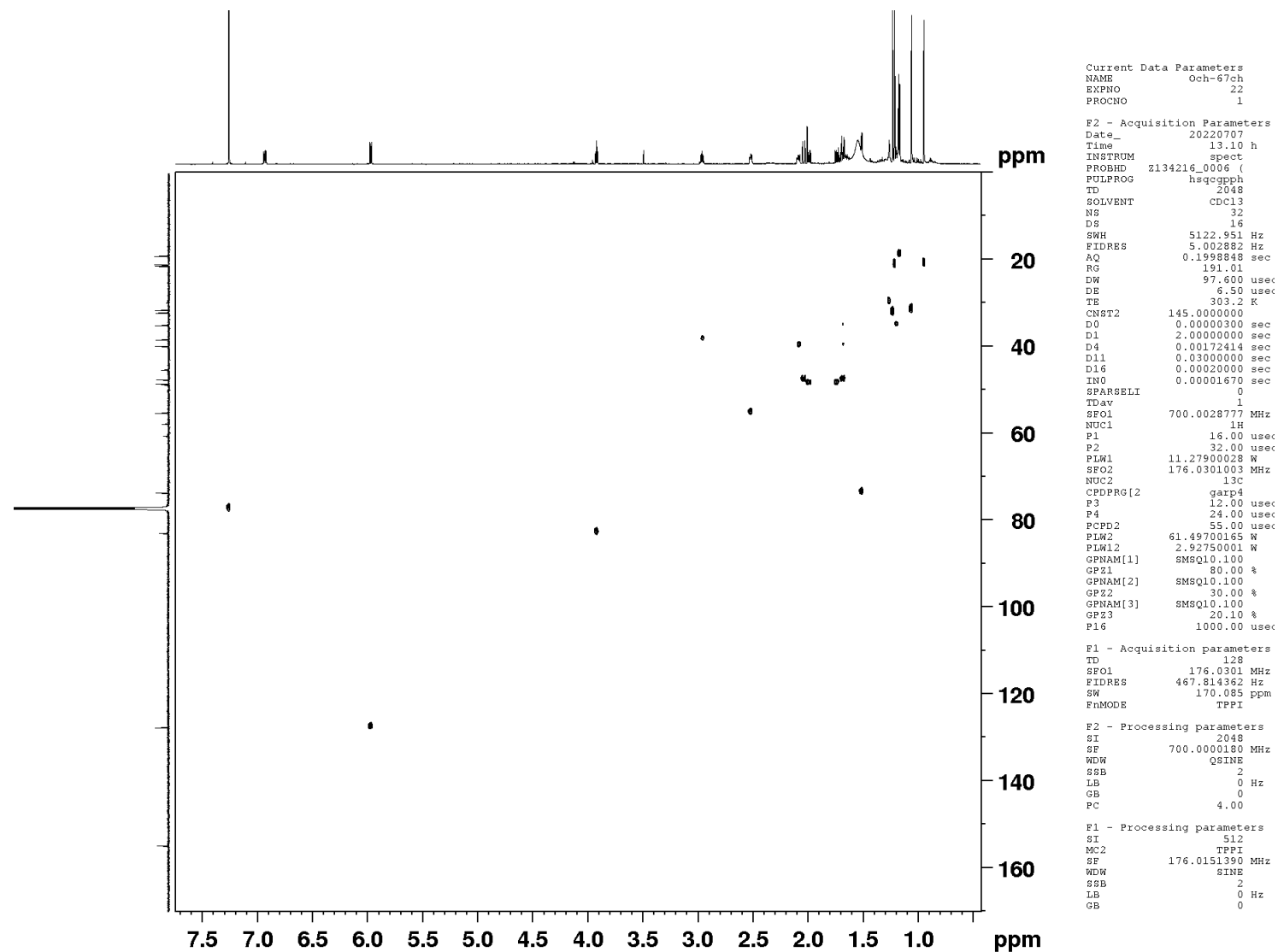
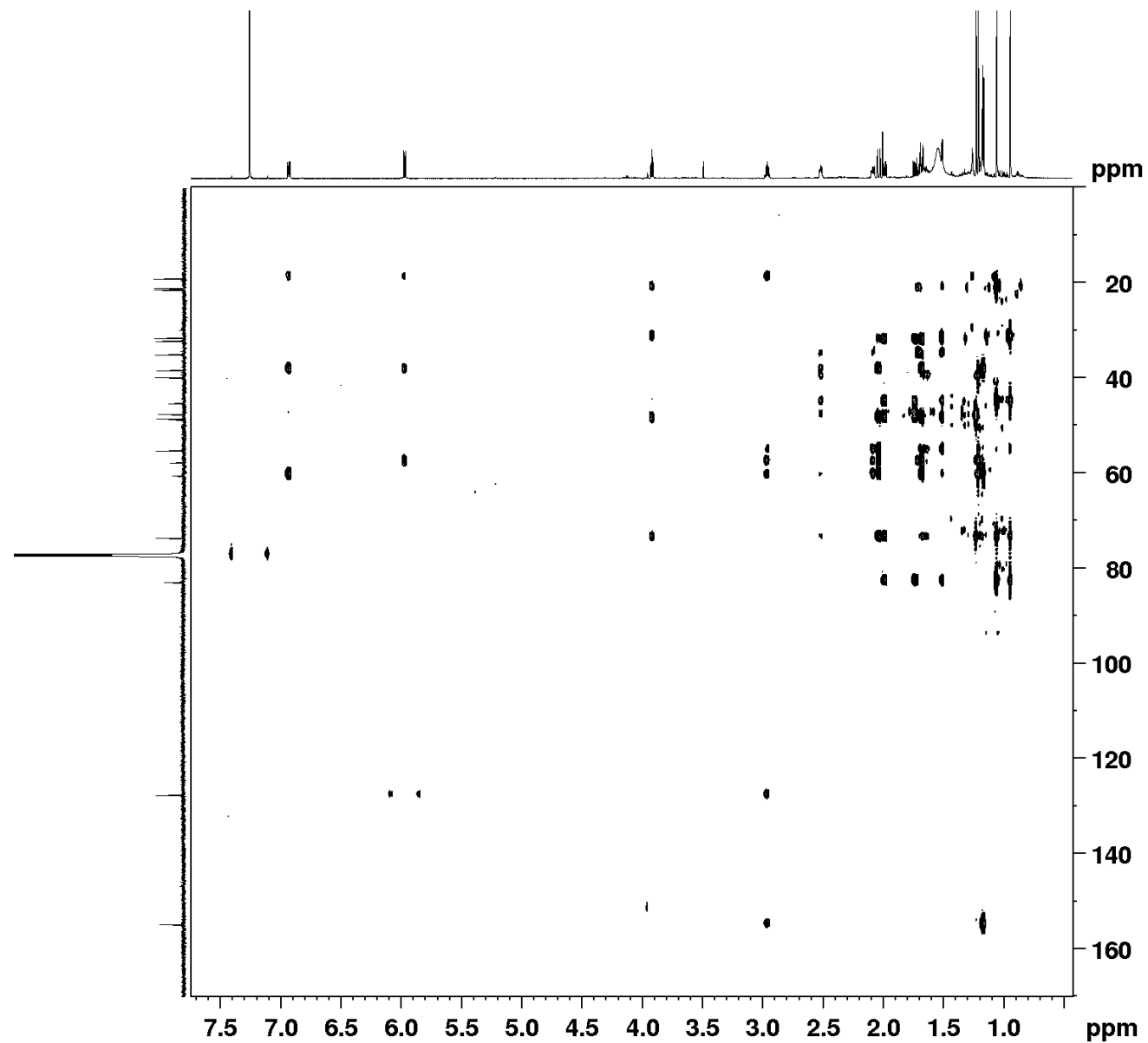


Figure S12. HMBC NMR spectrum (700 MHz, CDCl₃) of 2



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Current Data Parameters
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PROCNO    1

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Time      21.26 h
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TD         4096
SOLVENT   CDCl3
NS         80
DS         16
SWH        5122.951 Hz
FIDRES     2.501441 Hz
AQ         0.3997696 sec
RG         191.01
DW         97.600 usec
DE         6.50 usec
TE         303.0 K
CNST2     145.0000000
CNST13    5.0000000
D0         0.00000300 sec
D1         2.00000000 sec
D2         0.00344828 sec
D6         0.10000000 sec
D16        0.00020000 sec
IN0        0.00001180 sec
SPARSELI   0
TDav       1
SFO1       700.0028777 MHz
NUC1       1H
P1         16.00 usec
P2         32.00 usec
PLW1       11.27900028 W
SFO2       176.0362608 MHz
NUC2       13C
P3         12.00 usec
PLW2       61.49700165 W
GPNAM[1]   SMSQ10.100
GPZ1       50.00 %
GPNAM[2]   SMSQ10.100
GPZ2       30.00 %
GPNAM[3]   SMSQ10.100
GPZ3       40.10 %
P16        1000.00 usec

F1 - Acquisition parameters
TD         128
SFO1       176.0363 MHz
FIDRES     662.076294 Hz
SW         240.705 ppm
FnMODE     QF

F2 - Processing parameters
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SF         700.0000180 MHz
WDW        SINE
SSB        3
LB         0 Hz
GB         0
PC         4.00

F1 - Processing parameters
SI         512
MC2        QF
SF         176.0151390 MHz
WDW        SINE
SSB        0
LB         0 Hz
GB         0
    
```

Figure S13. ^1H - ^1H COSY NMR spectrum (700 MHz, CDCl_3) of 2

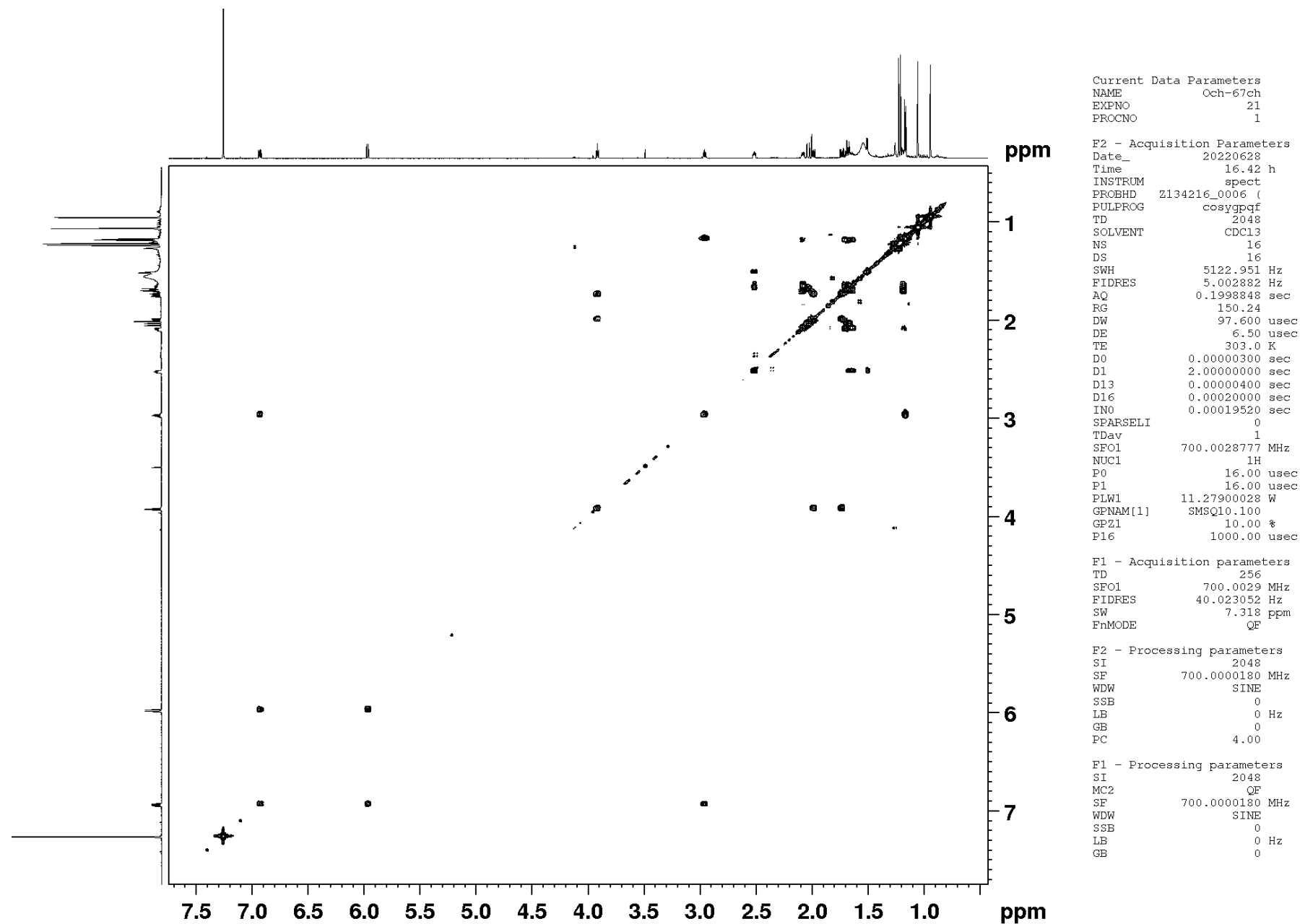


Figure S14. ROESY NMR spectrum (700 MHz, CDCl₃) of 2

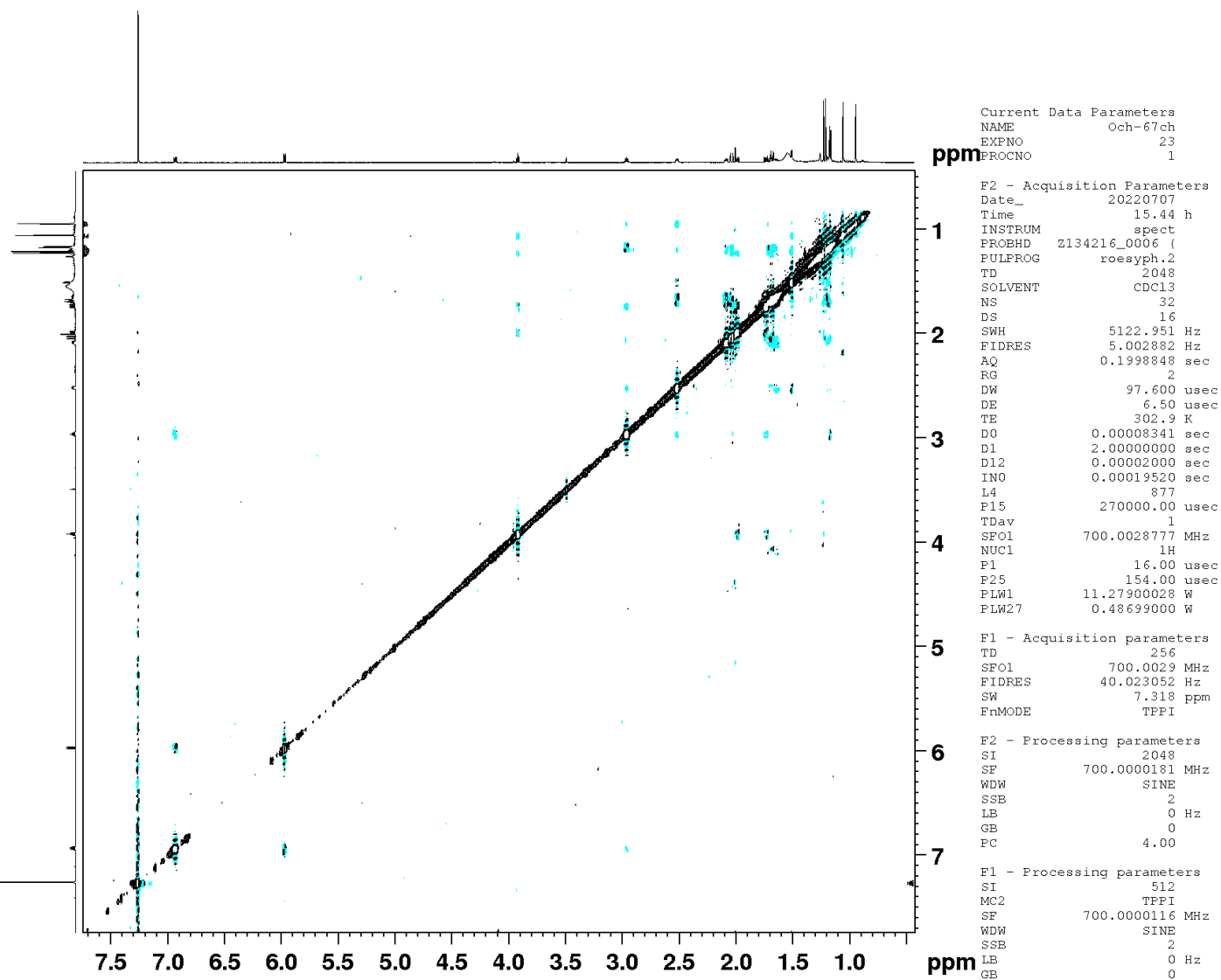
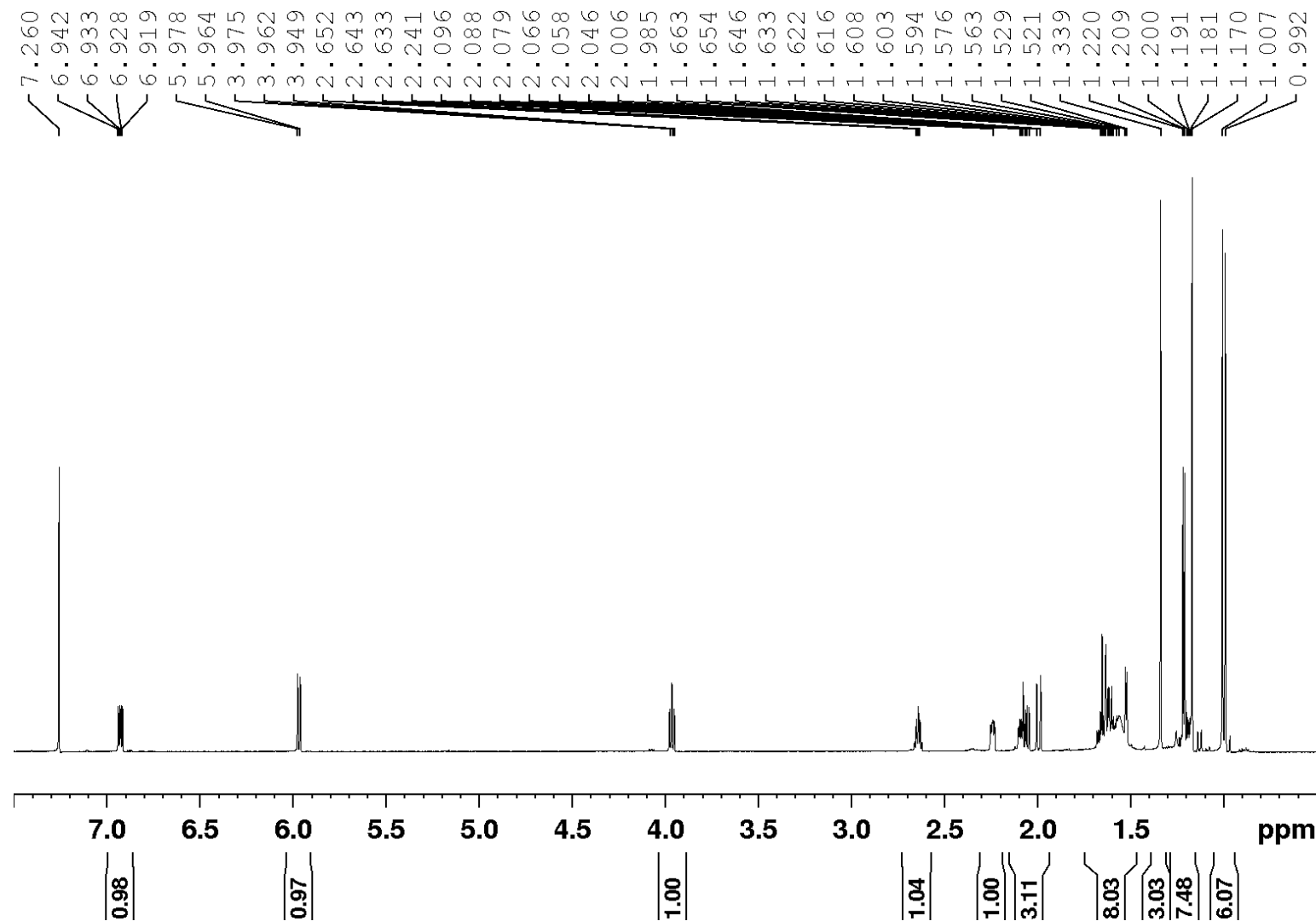


Figure S15. ¹H NMR spectrum (700 MHz, CDCl₃) of 3



Current Data Parameters

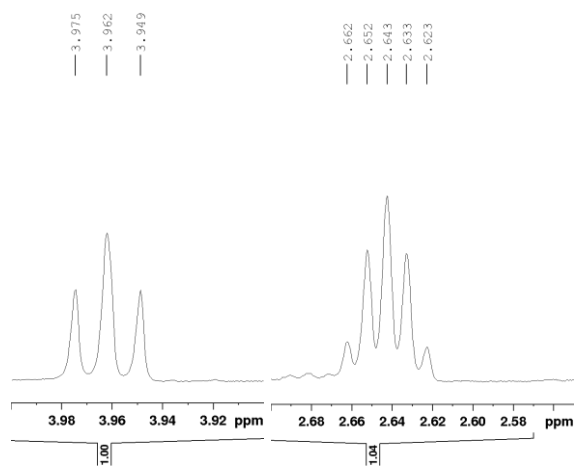
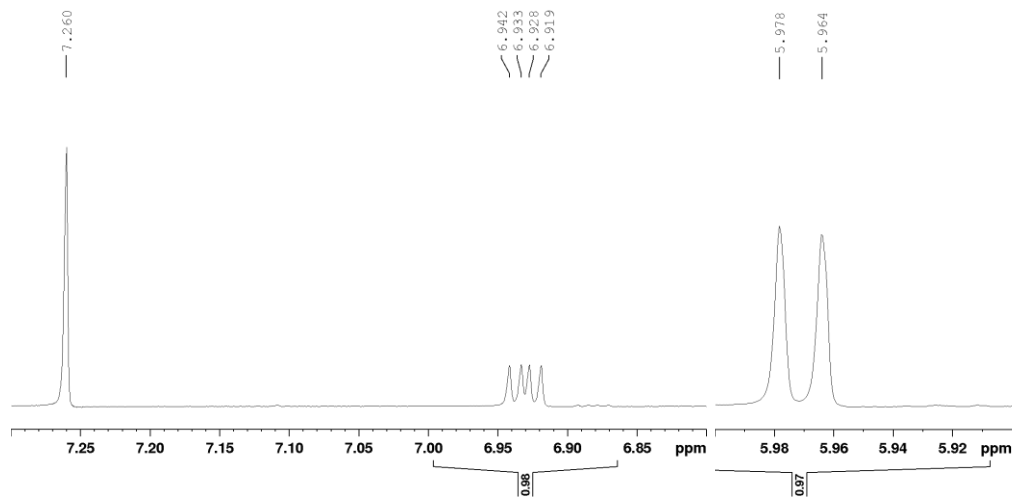
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EXPNO 2
PROCNO 1

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TD 32768
SOLVENT CDCl₃
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DS 2
SWH 10504.202 Hz
FIDRES 0.641126 Hz
AQ 1.5597568 sec
RG 165.68
DW 47.600 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
TD0 1
SFO1 700.0051100 MHz
NUC1 1H
P0 5.33 usec
P1 16.00 usec
PLW1 11.27900028 W

F2 - Processing parameters

SI 32768
SF 700.0000162 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 4.00



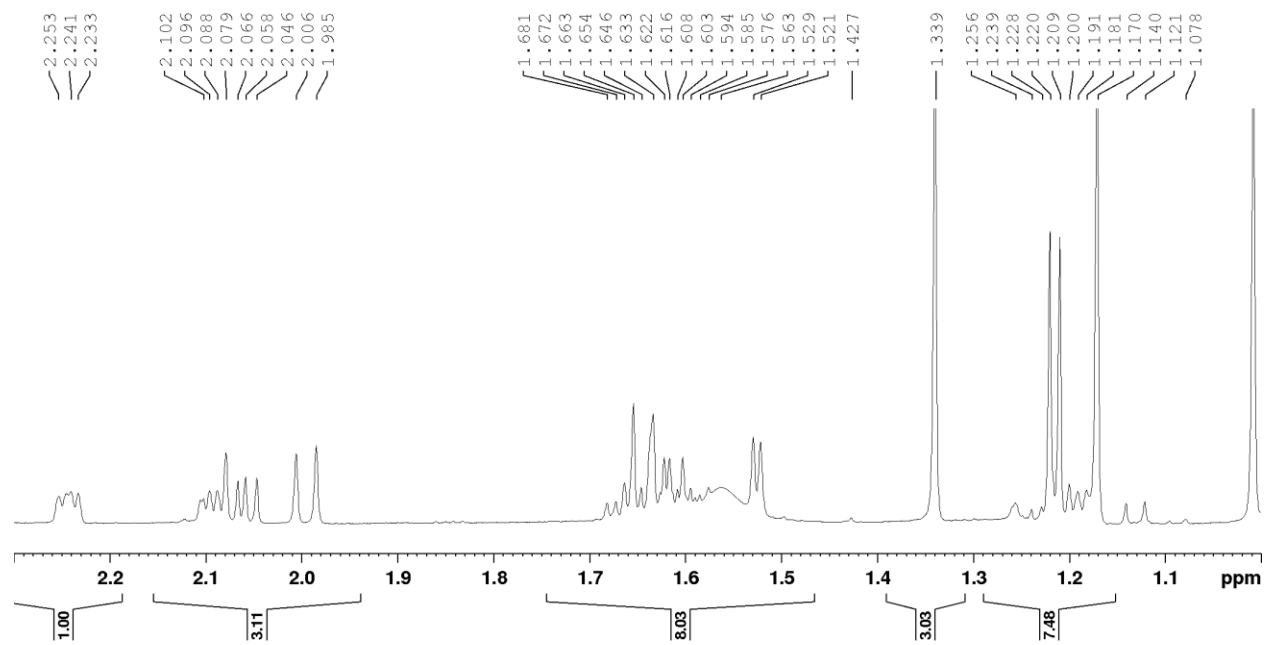


Figure S16. ^{13}C NMR spectrum (700 MHz, CDCl_3) of 3

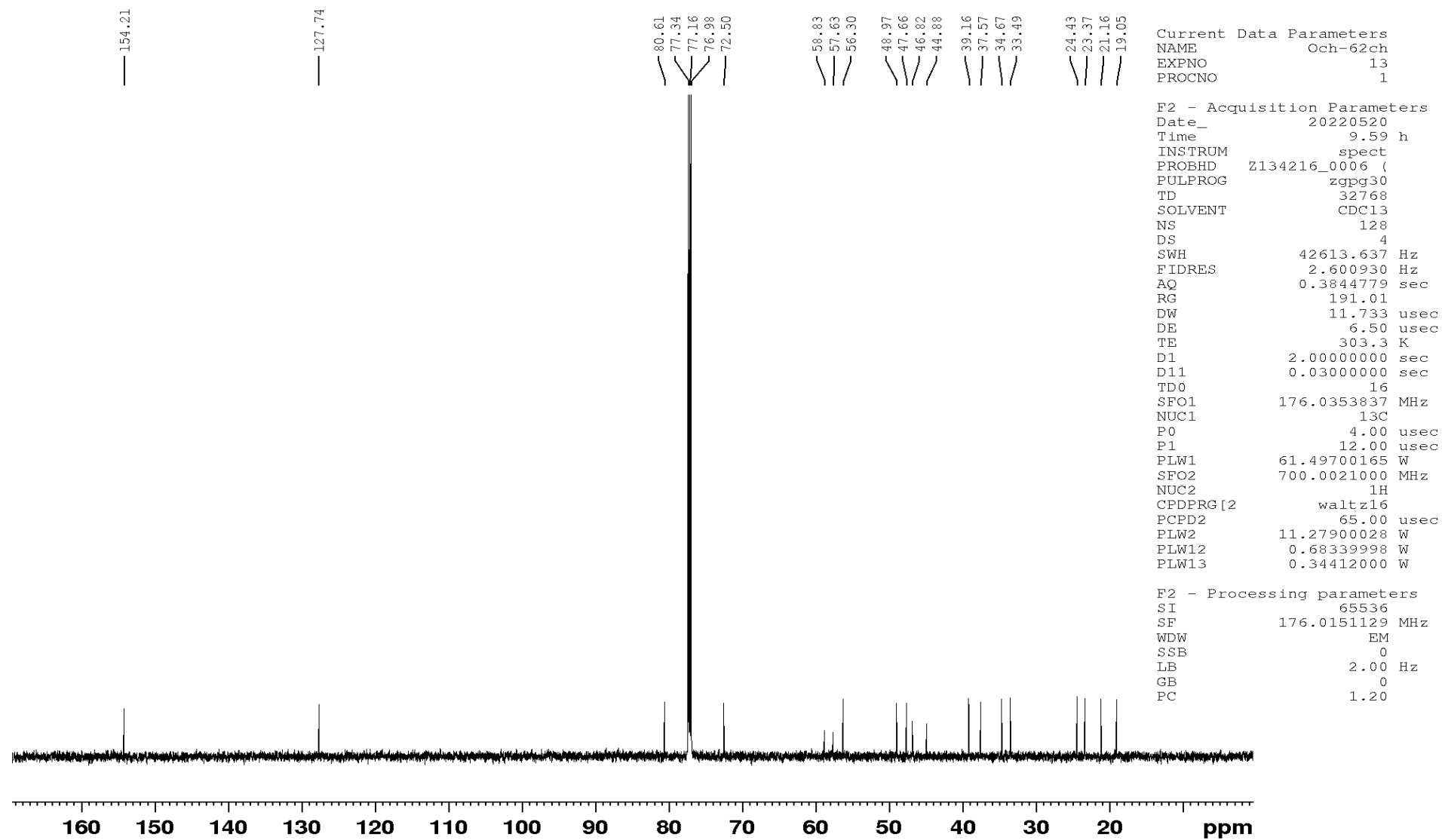
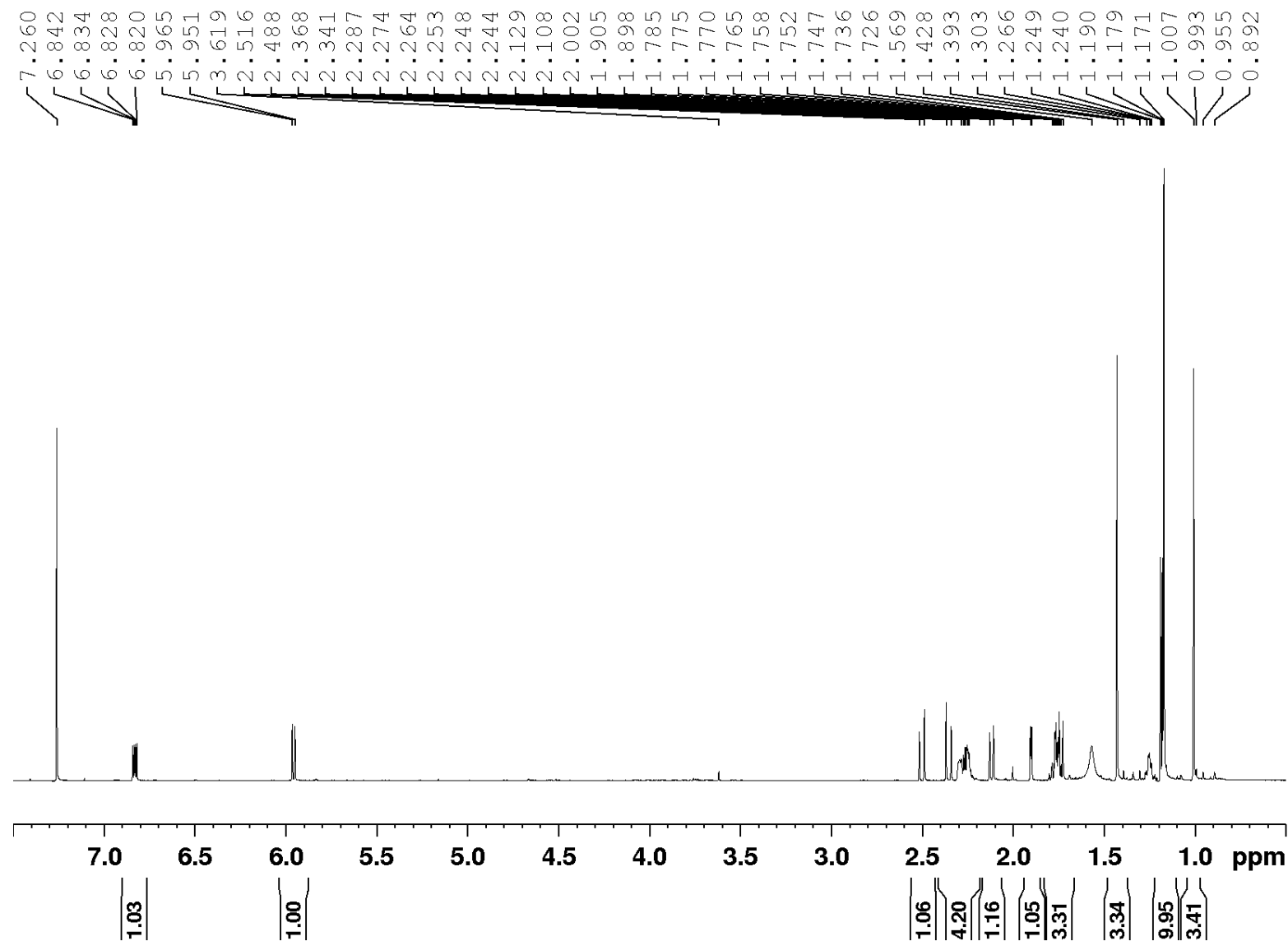


Figure S17. ¹H NMR spectrum (700 MHz, CDCl₃) of 4



Current Data Parameters
NAME Och-83ch
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 10504.202 Hz
FIDRES 0.641126 Hz
AQ 1.5597568 sec
RG 165.68
DW 47.600 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
TD0 1
SFO1 700.0051100 MHz
NUC1 1H
P0 5.33 usec
P1 16.00 usec
PLW1 11.27900028 W

F2 - Processing parameters
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SF 700.0000162 MHz
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SSB 0
LB 0.10 Hz
GB 0
PC 4.00

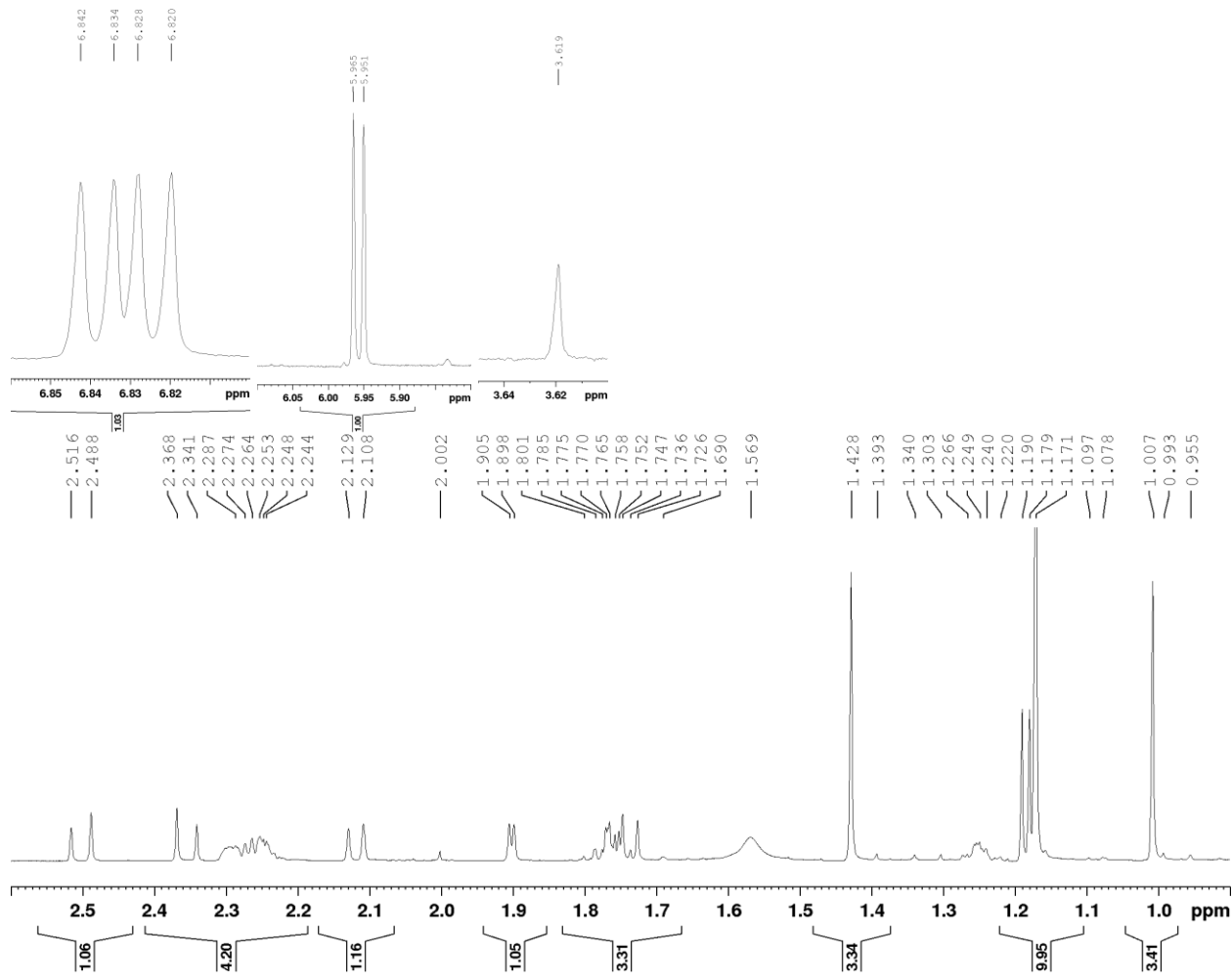


Figure S18. ^{13}C NMR spectrum (700 MHz, CDCl_3) of 4

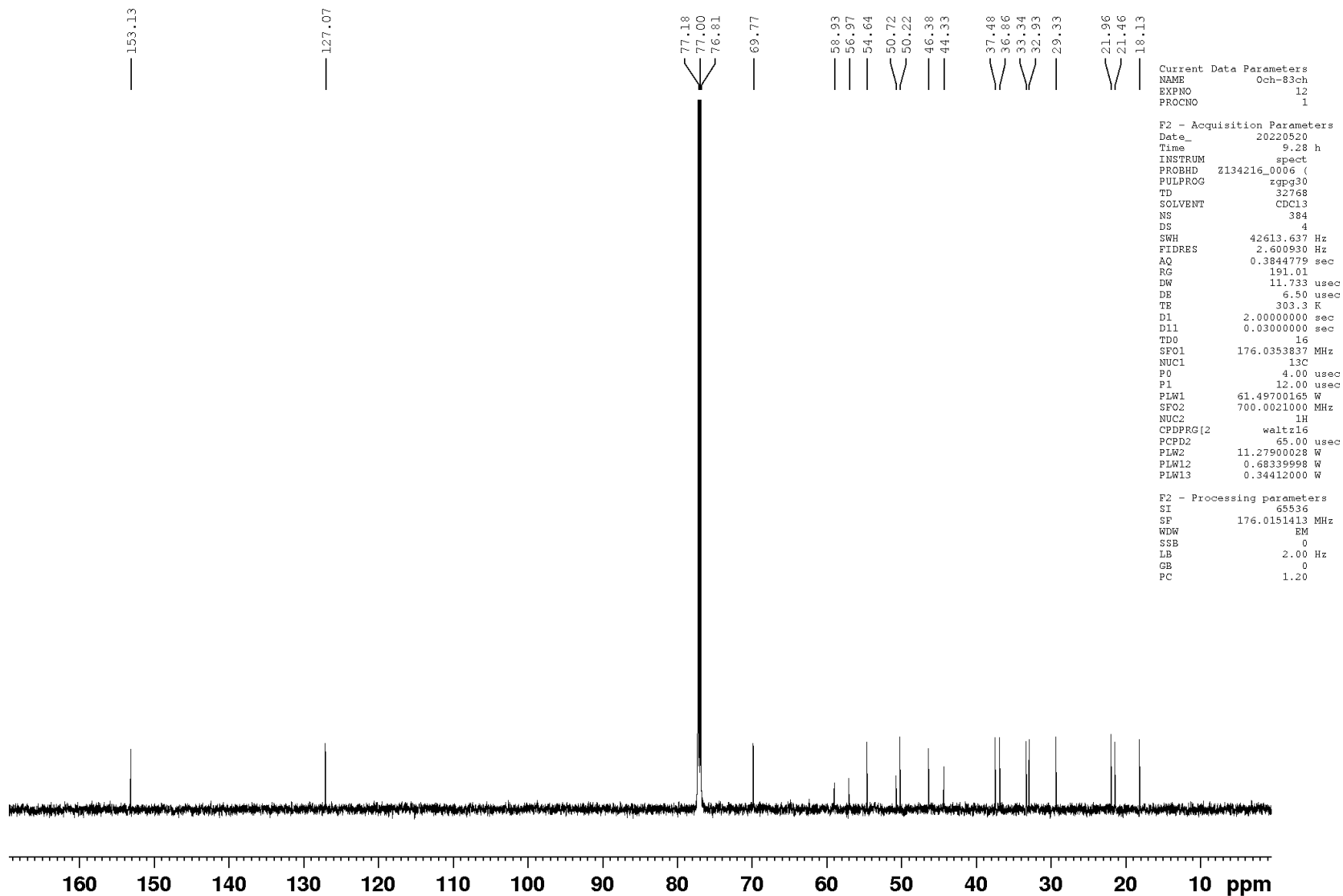


Figure S19. ^1H NMR spectrum (500 MHz, CDCl_3) of **5**

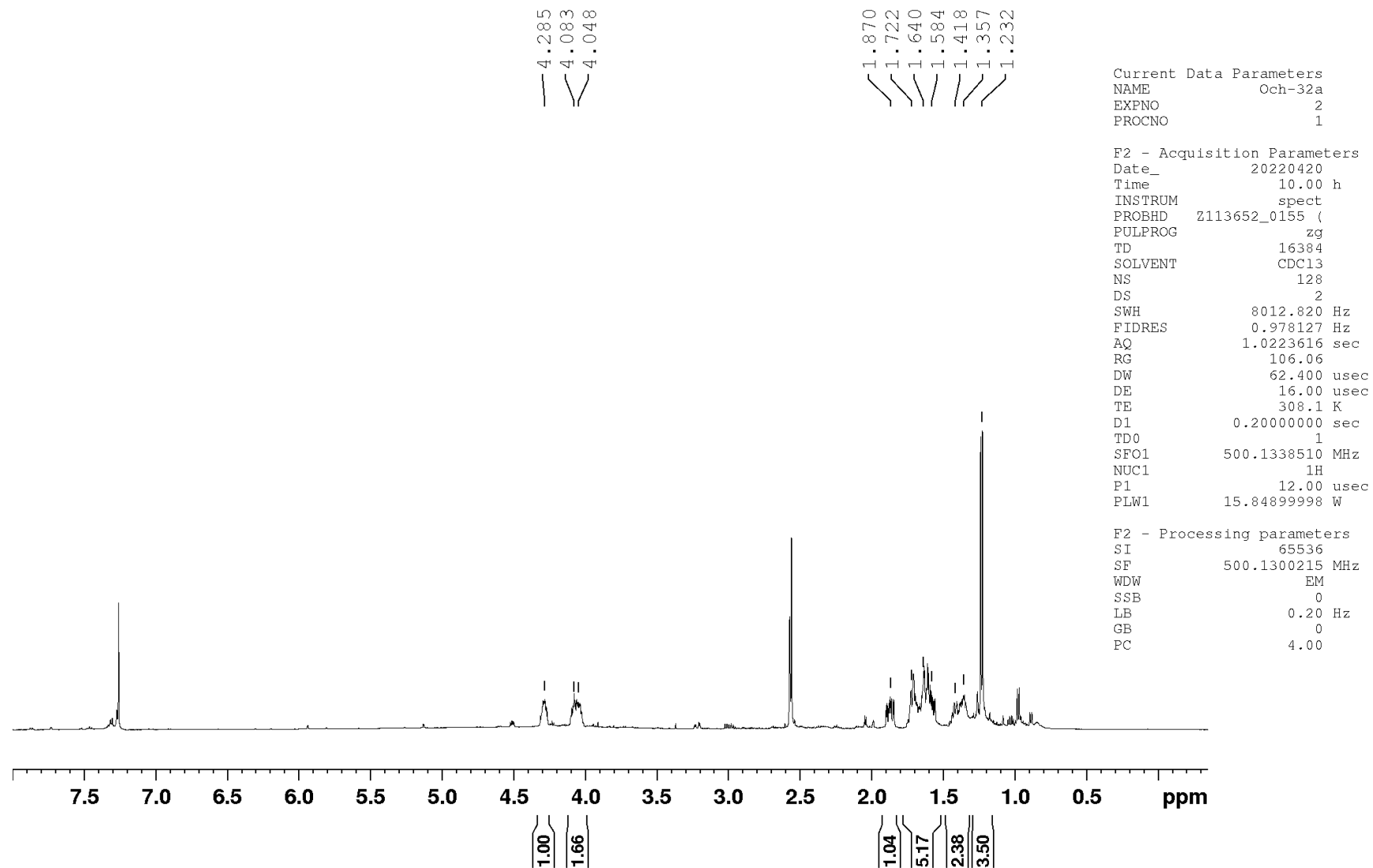


Figure S20. ^{13}C NMR spectrum (500 MHz, CDCl_3) of 5

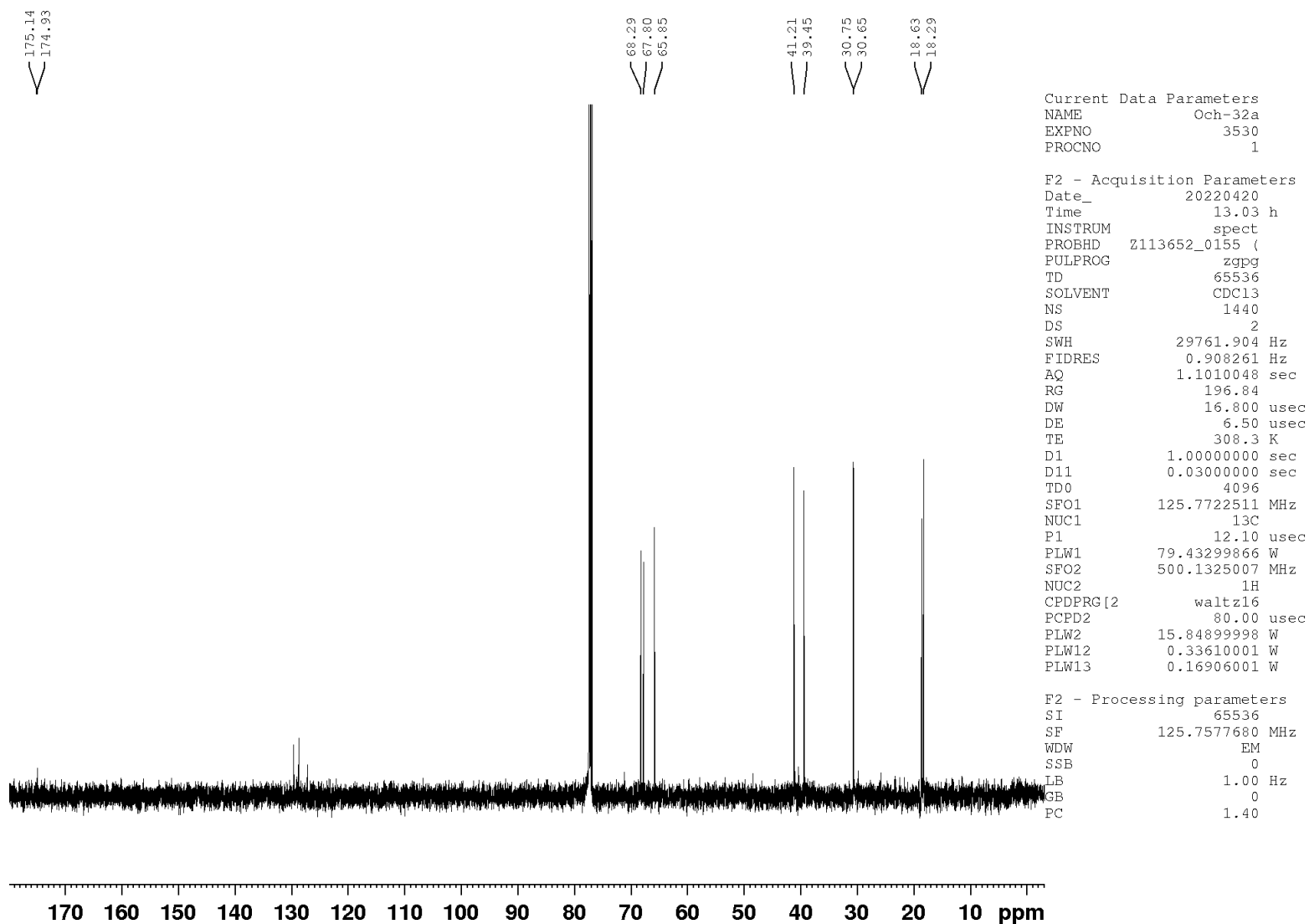


Figure S21. DEPT NMR spectrum (500 MHz, CDCl₃) of 5

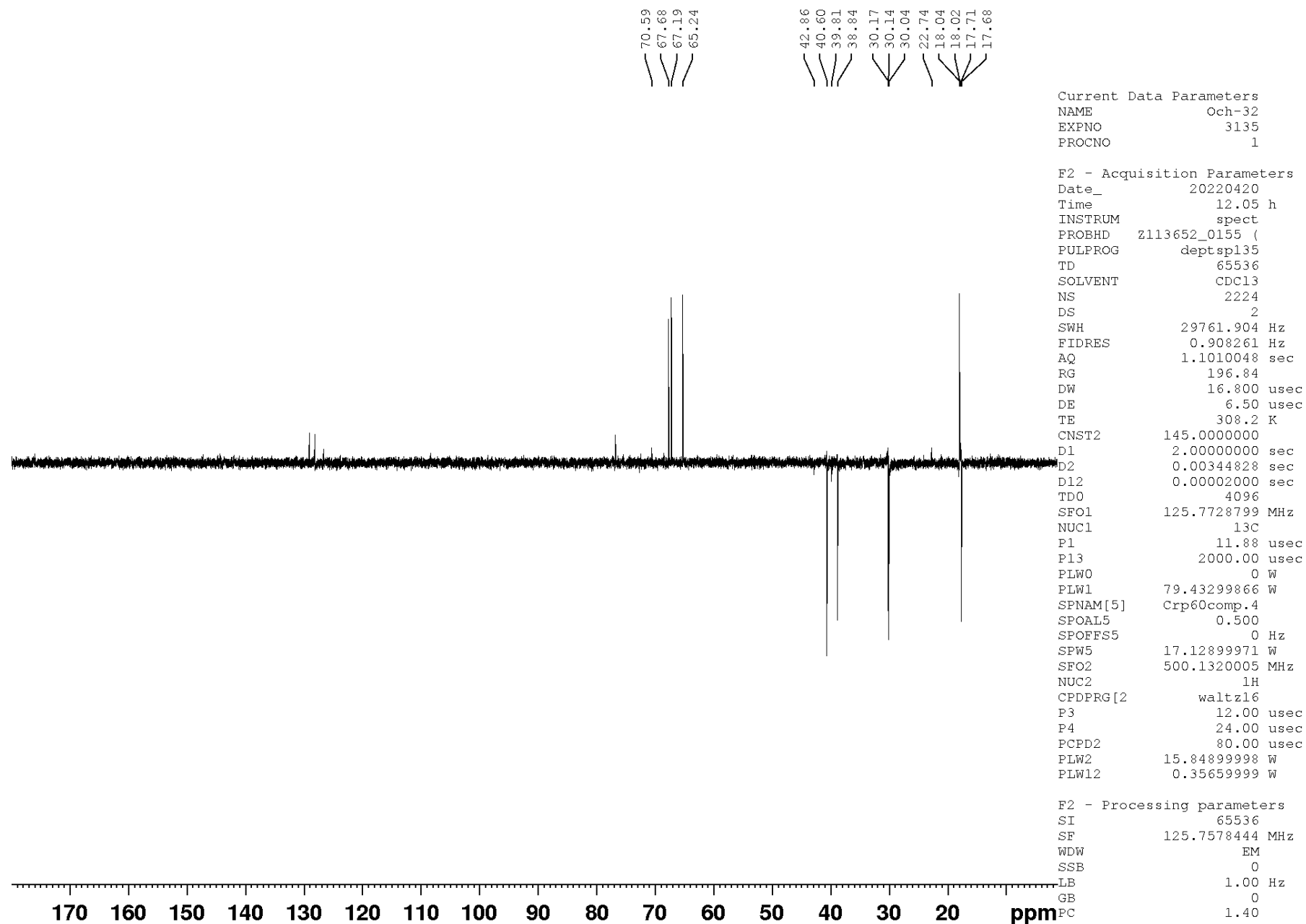


Figure S22. HSQC NMR spectrum (500 MHz, CDCl₃) of 5

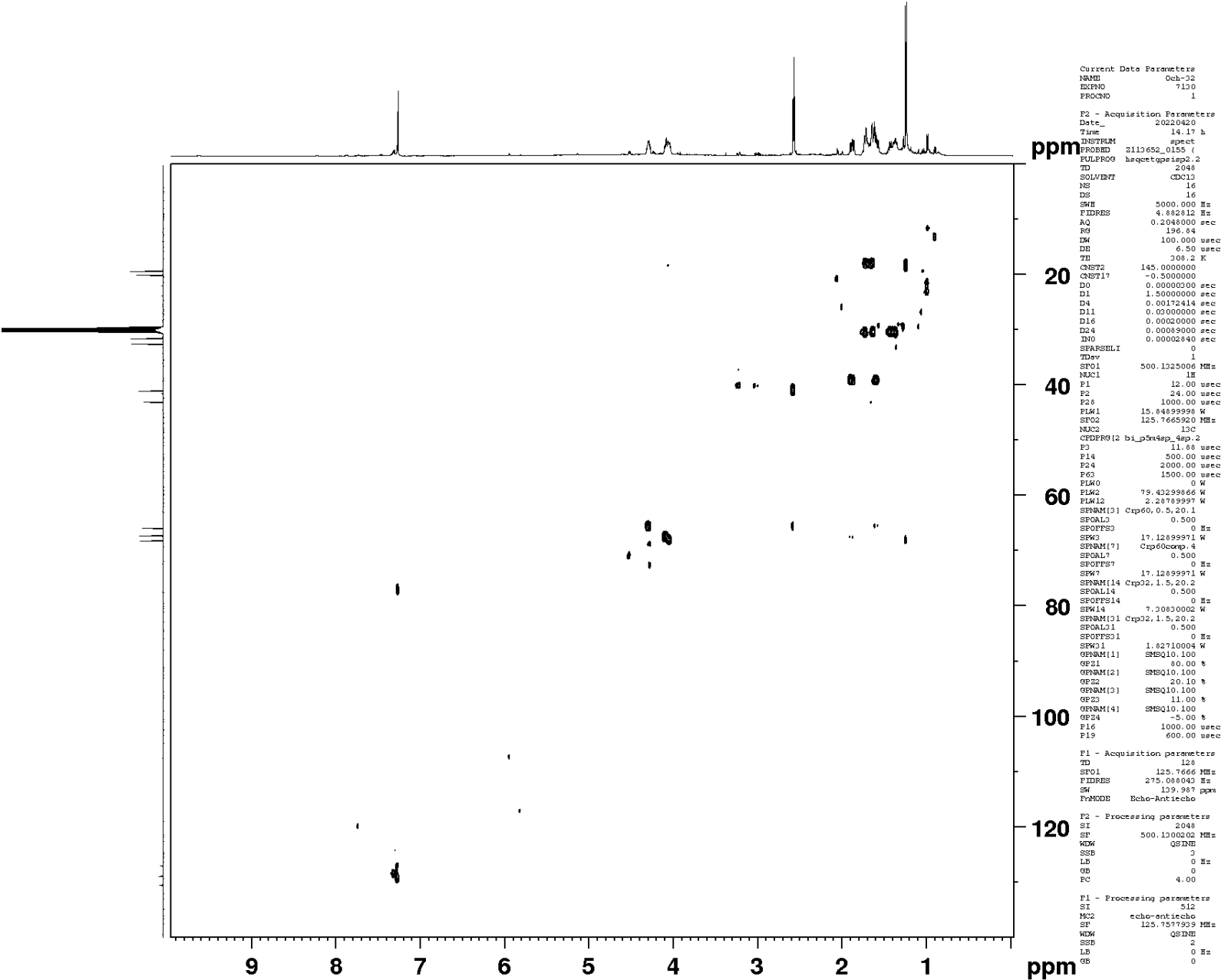


Figure S23. HMBC NMR spectrum (500 MHz, CDCl₃) of 5

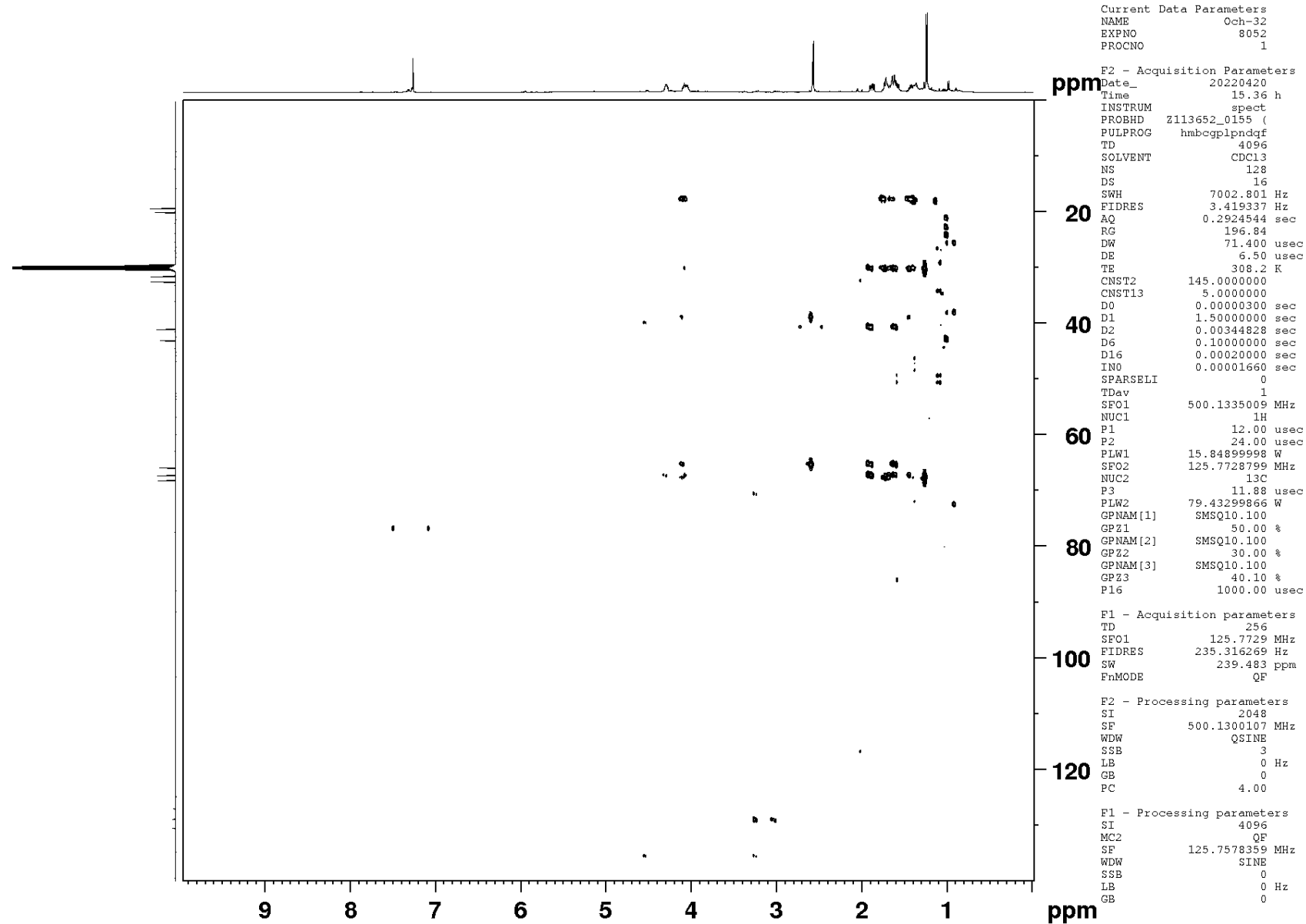


Figure S24. ^1H - ^1H COSY NMR spectrum (500 MHz, CDCl_3) of **5**

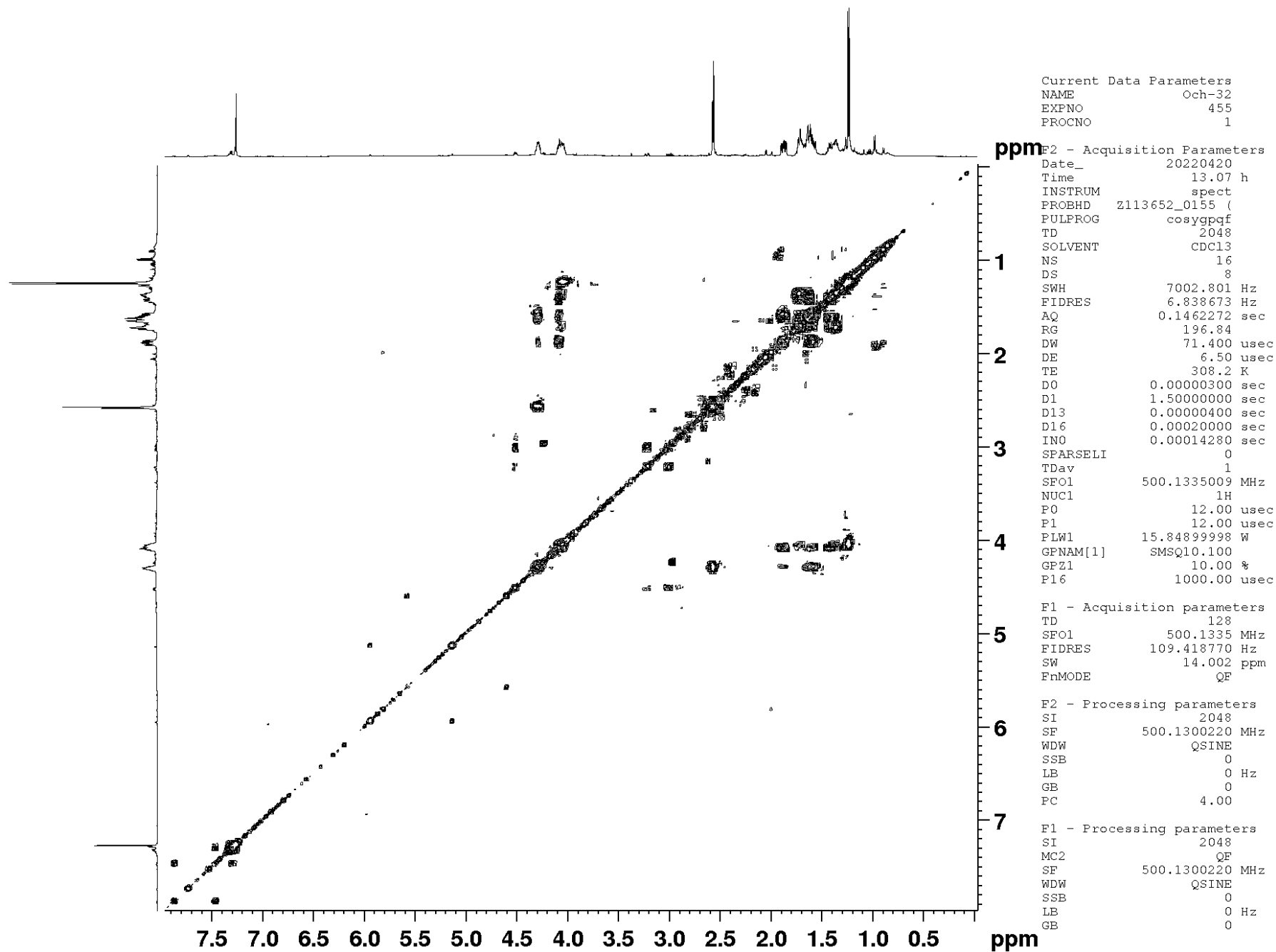


Figure S25. NOESY NMR spectrum (500 MHz, CDCl₃) of 5

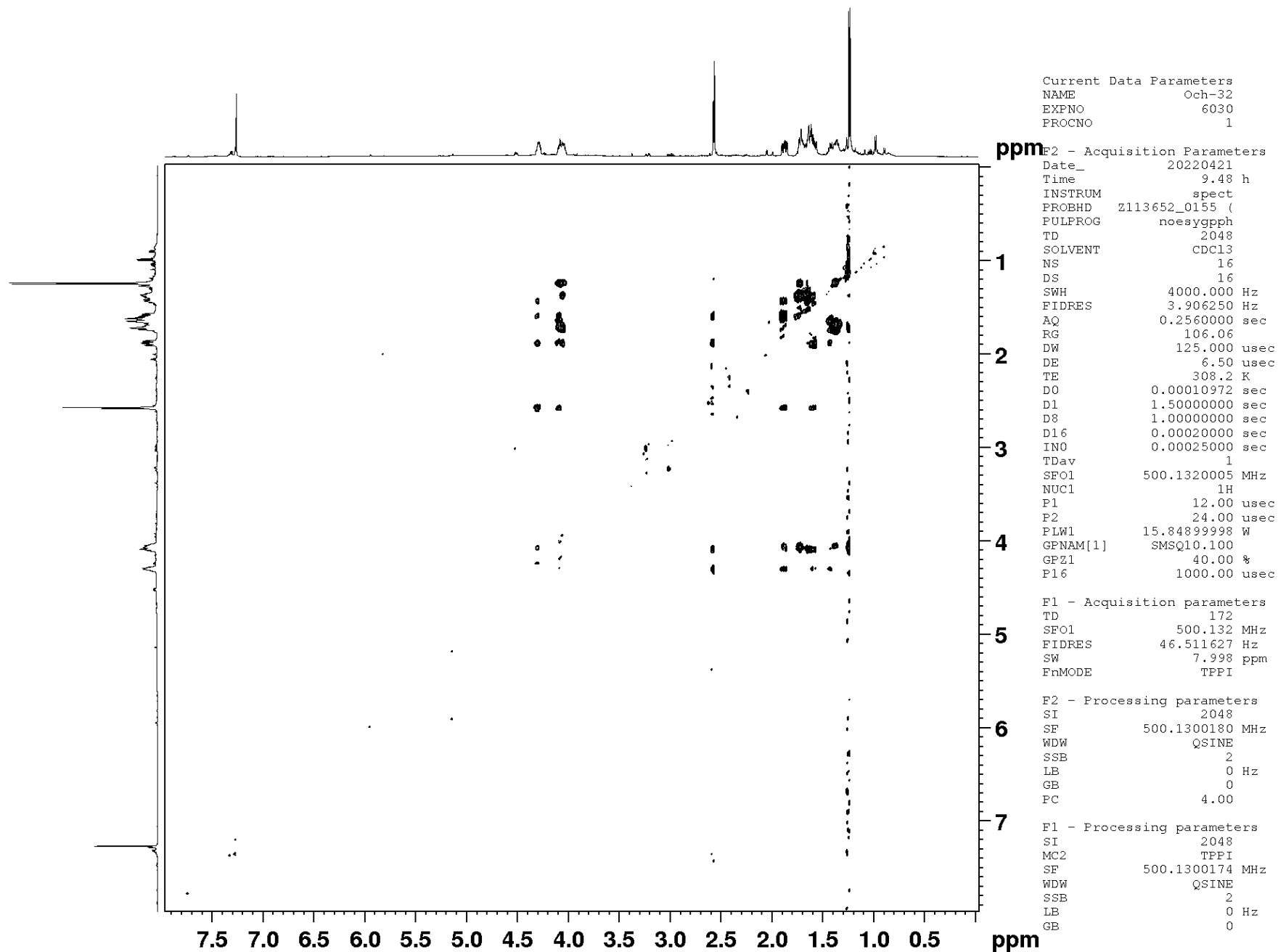
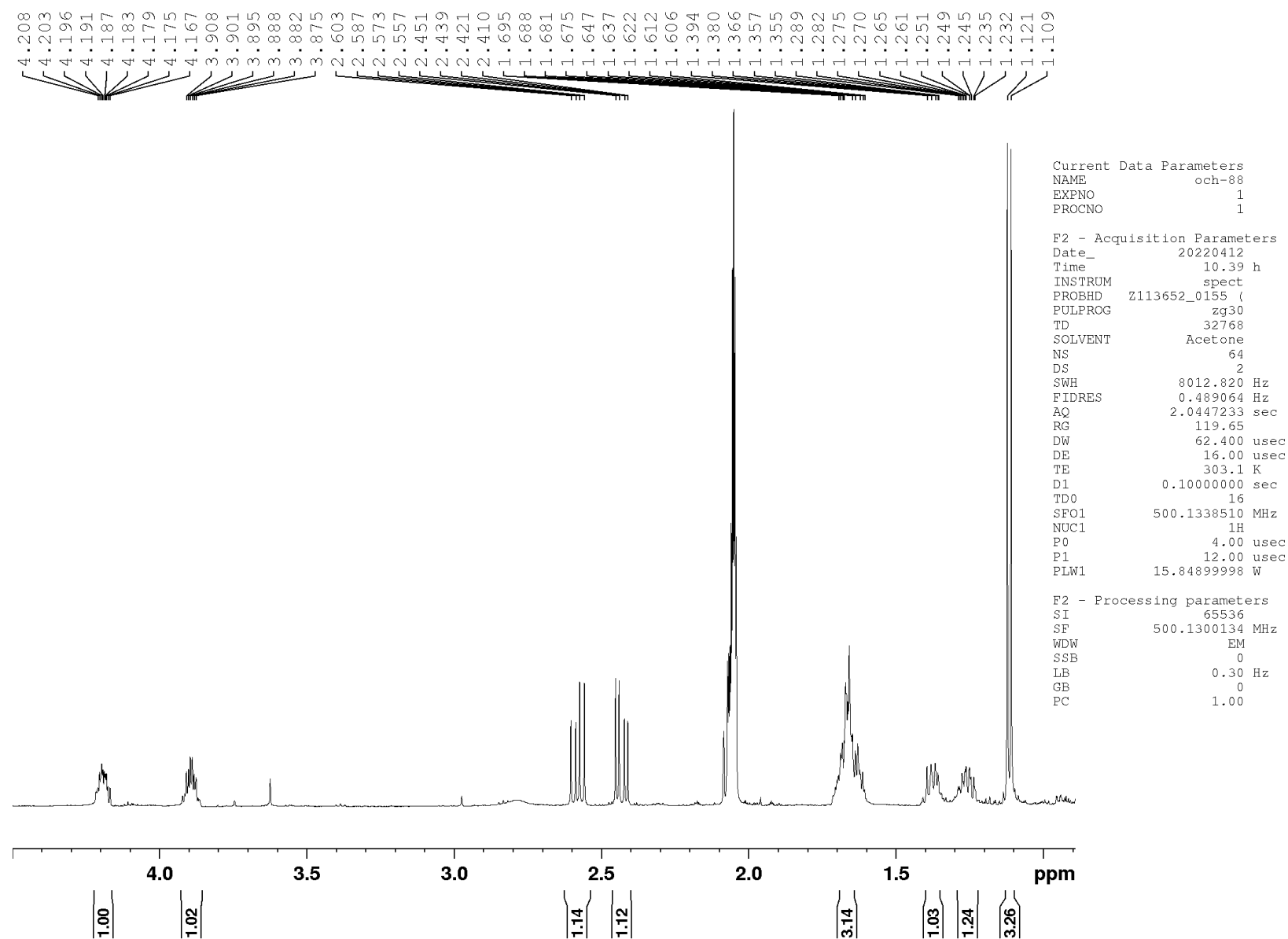


Figure S26. ¹H NMR spectrum (500 MHz, acetone-d₆) of 6



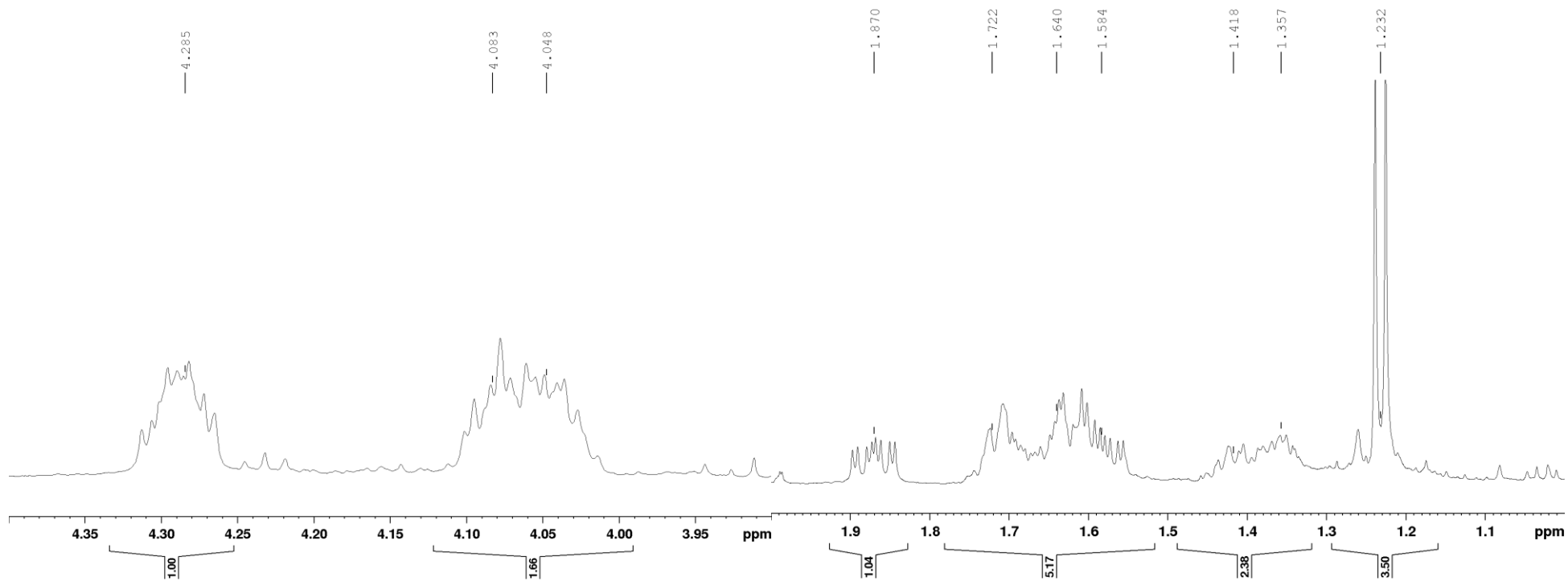
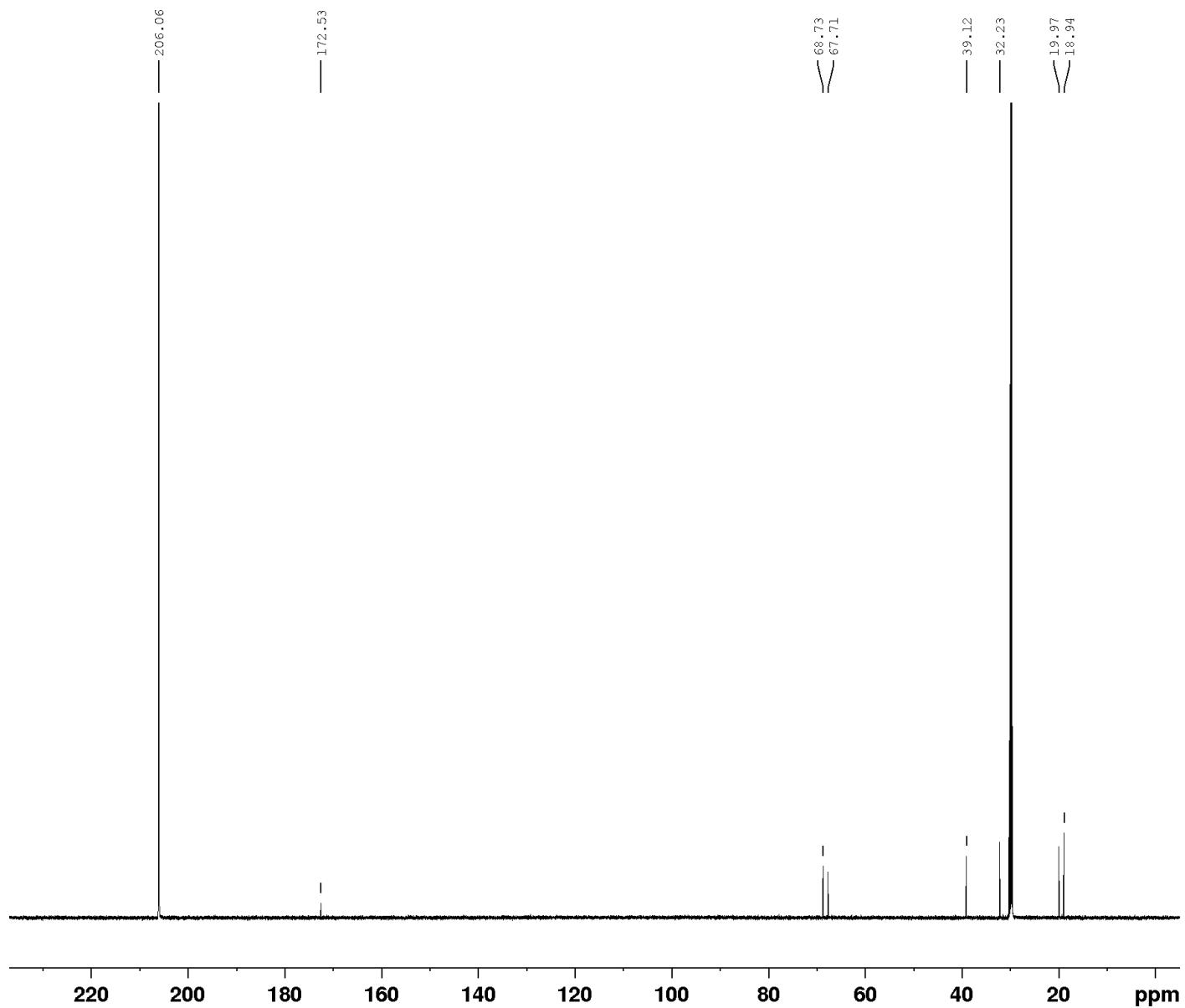


Figure S27. ^{13}C NMR spectrum (500 MHz, acetone- d_6) of 6



Current Data Parameters
NAME och-88
EXPNO 3730
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220410
Time 14.06 h
INSTRUM spect
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PULPROG zgpgg
TD 65536
SOLVENT Acetone
NS 400
DS 2
SWH 42613.637 Hz
FIDRES 1.300465 Hz
AQ 0.7689557 sec
RG 191.01
DW 11.733 usec
DE 6.50 usec
TE 308.3 K
D1 4.00000000 sec
D11 0.03000000 sec
TD0 4096
SFO1 176.0353807 MHz
NUC1 13C
P1 12.00 usec
PLW1 61.49700165 W
SFO2 700.0035000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 65.00 usec
PLW2 11.27900028 W
PLW12 0.68339998 W
PLW13 0.34412000 W

F2 - Processing parameters
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SF 176.0149724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S28. UV spectrum of 1

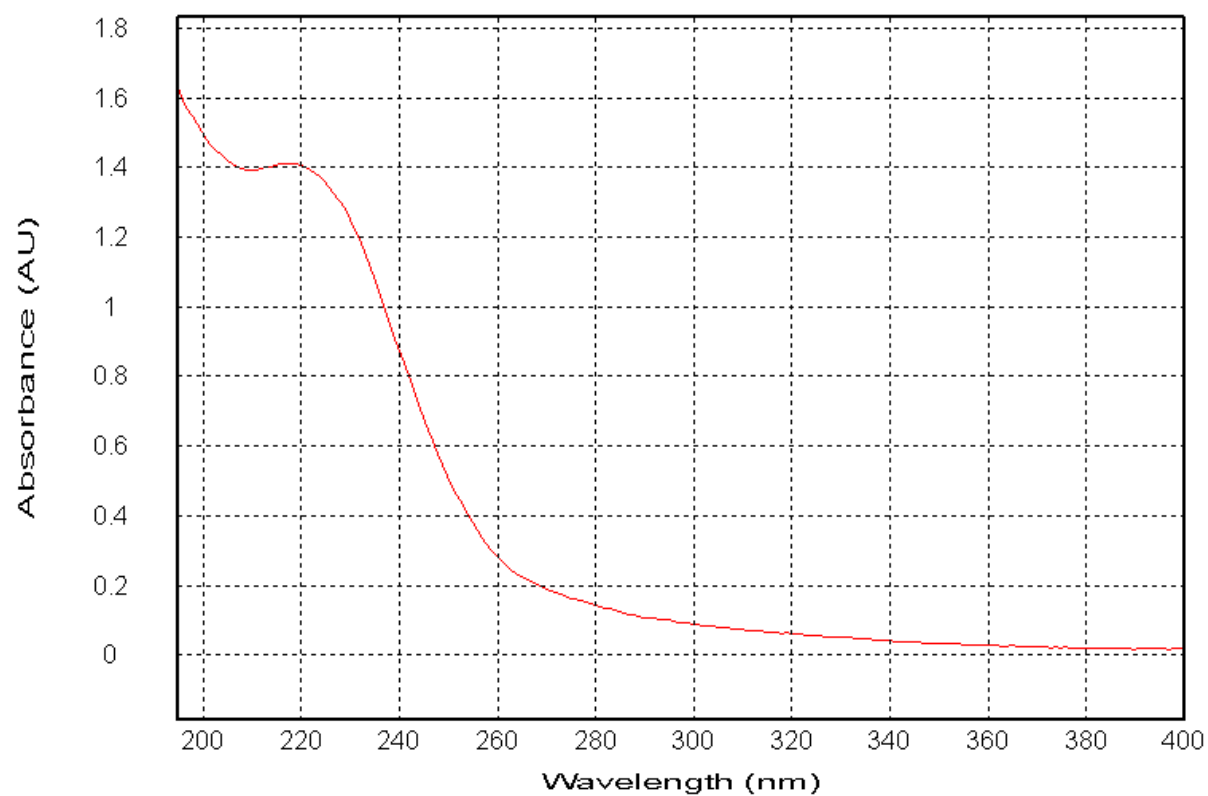


Figure S29. CD spectrum of 1

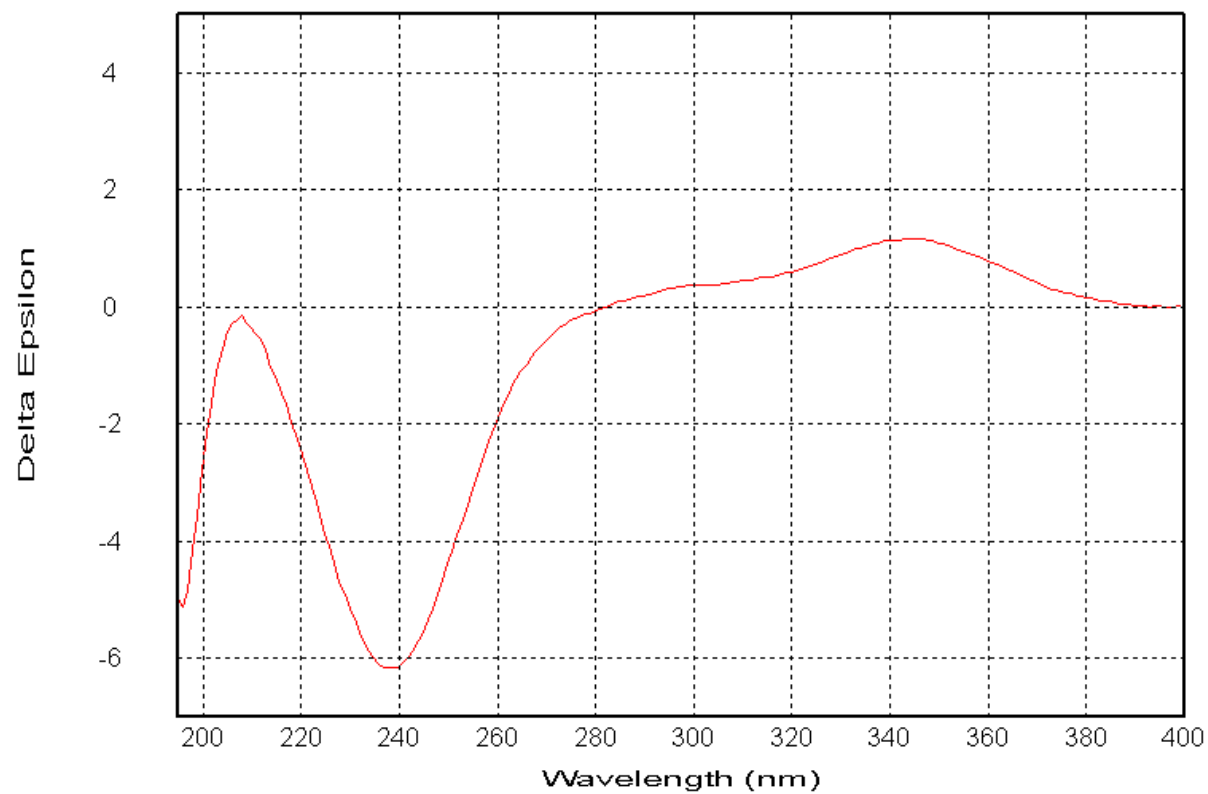


Figure S30. UV spectrum of 2

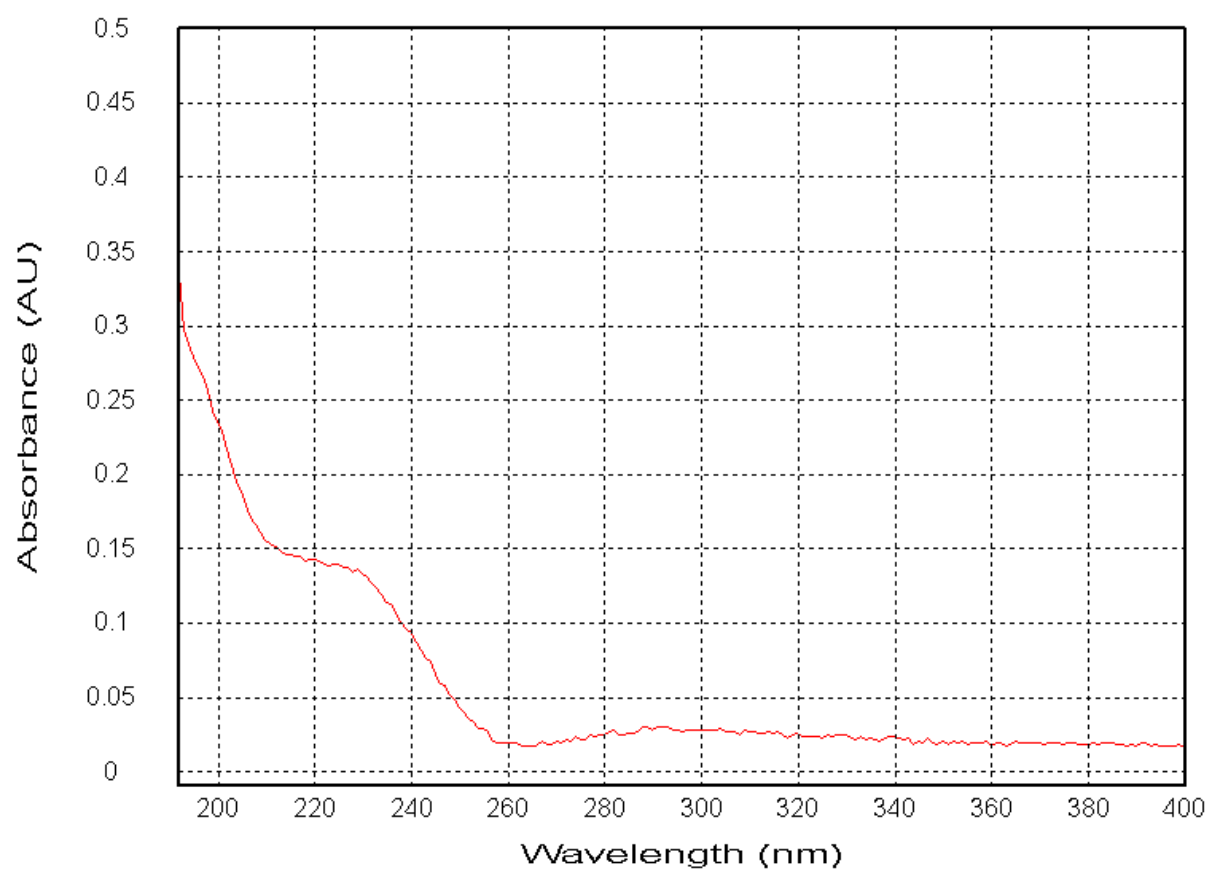


Figure S31. CD spectrum of 2

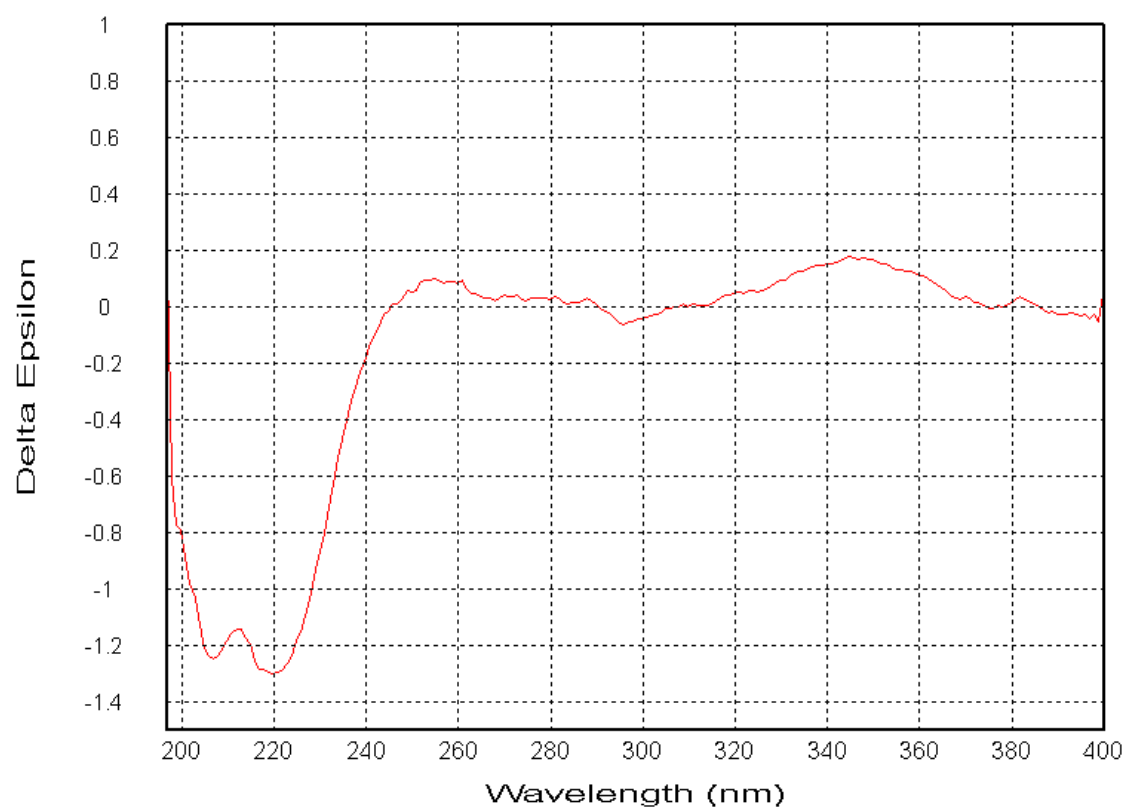


Figure S32. UV spectrum of 3

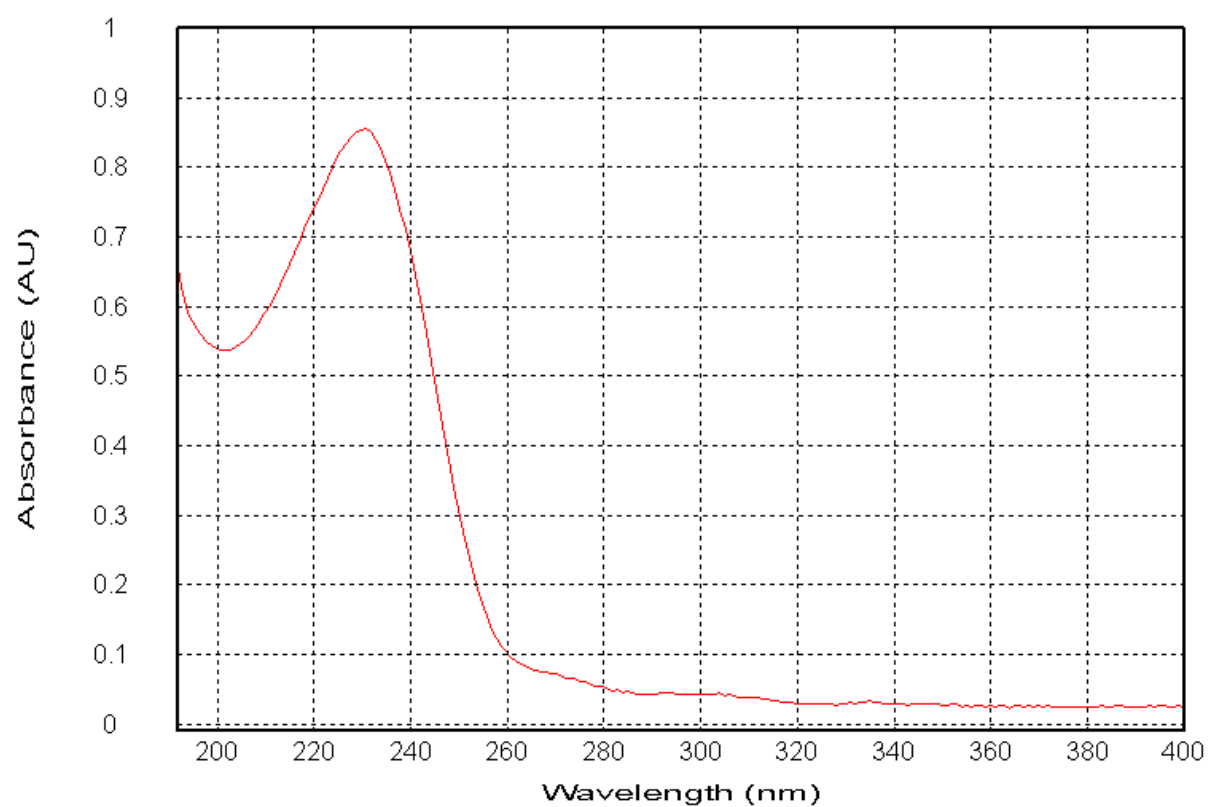


Figure S33. CD spectrum of 3

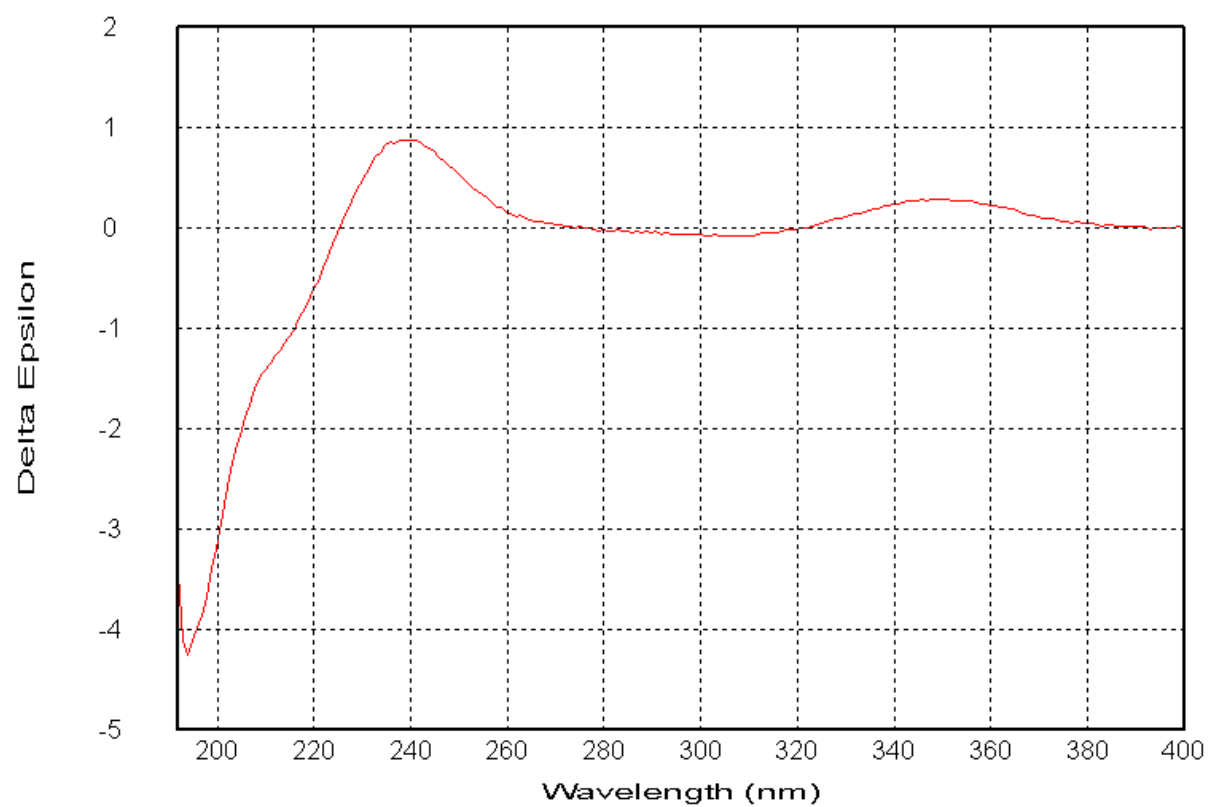


Figure S34. UV spectrum of 4

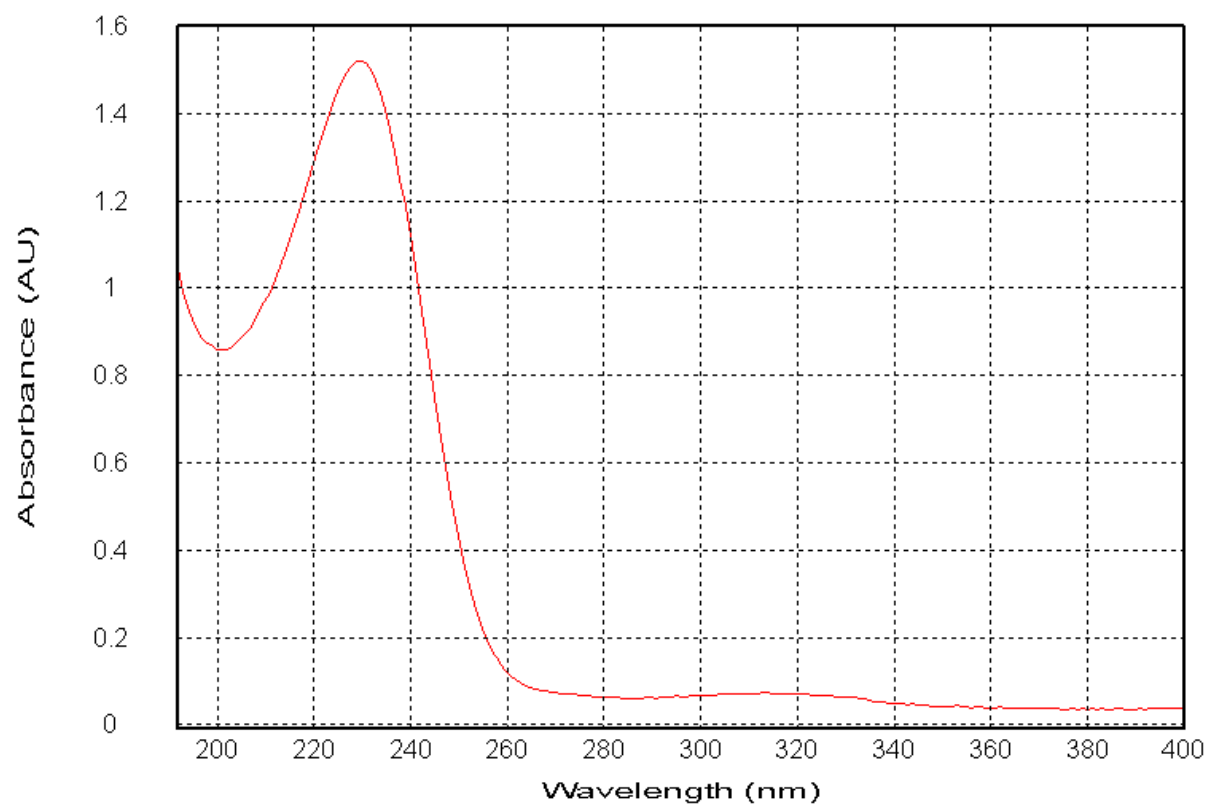


Figure S35. The experimental and calculated ECD spectra of 4

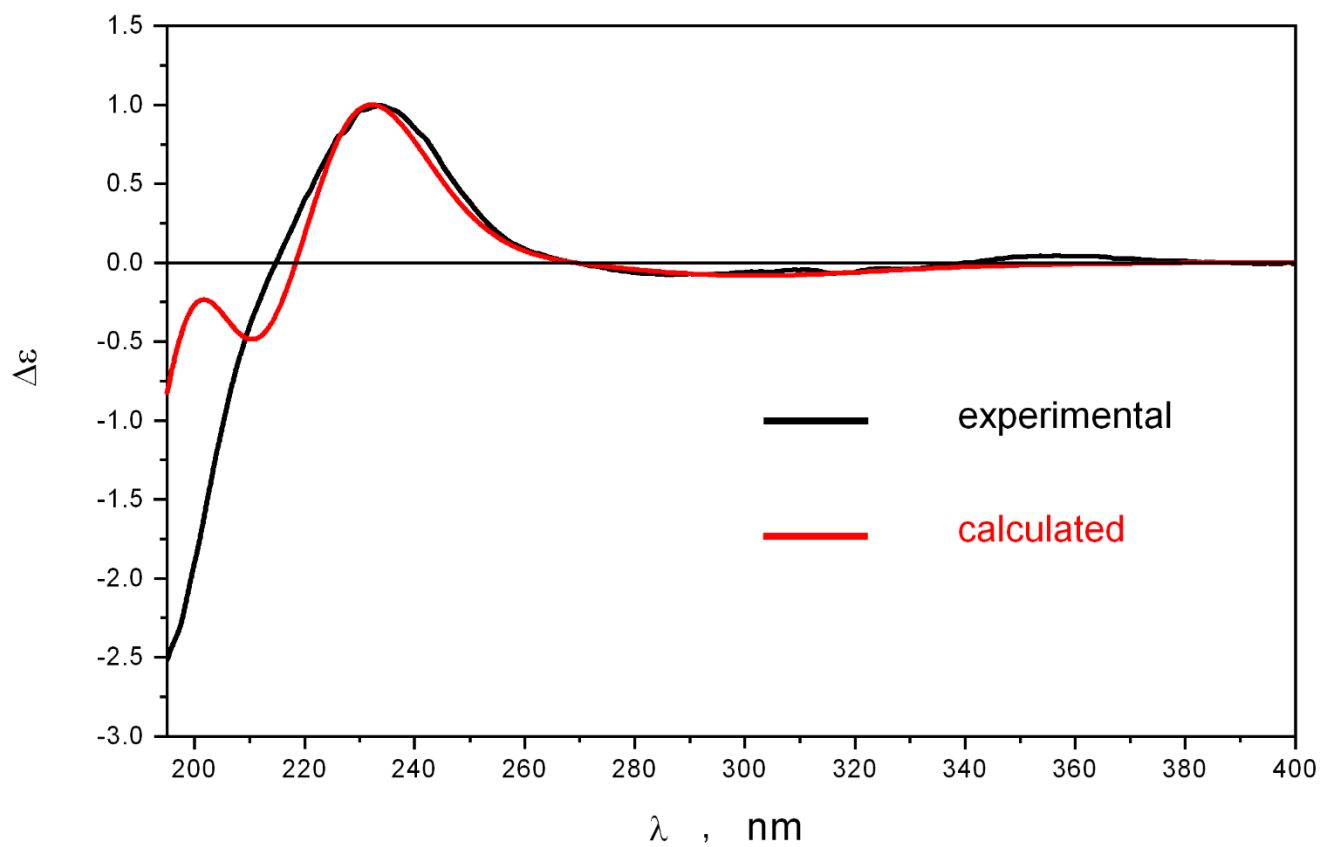


Figure S36. UV spectrum of 5

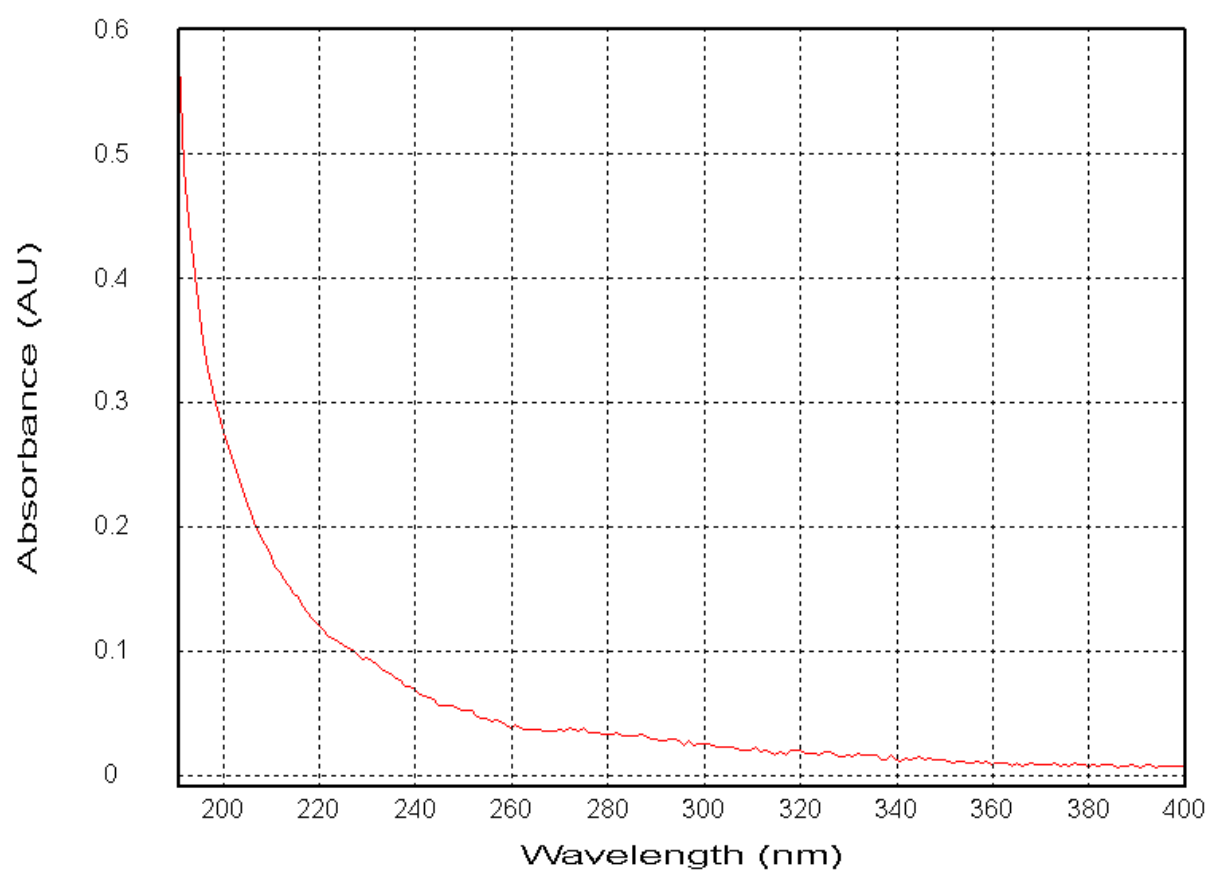


Figure S37. CD spectrum of 5

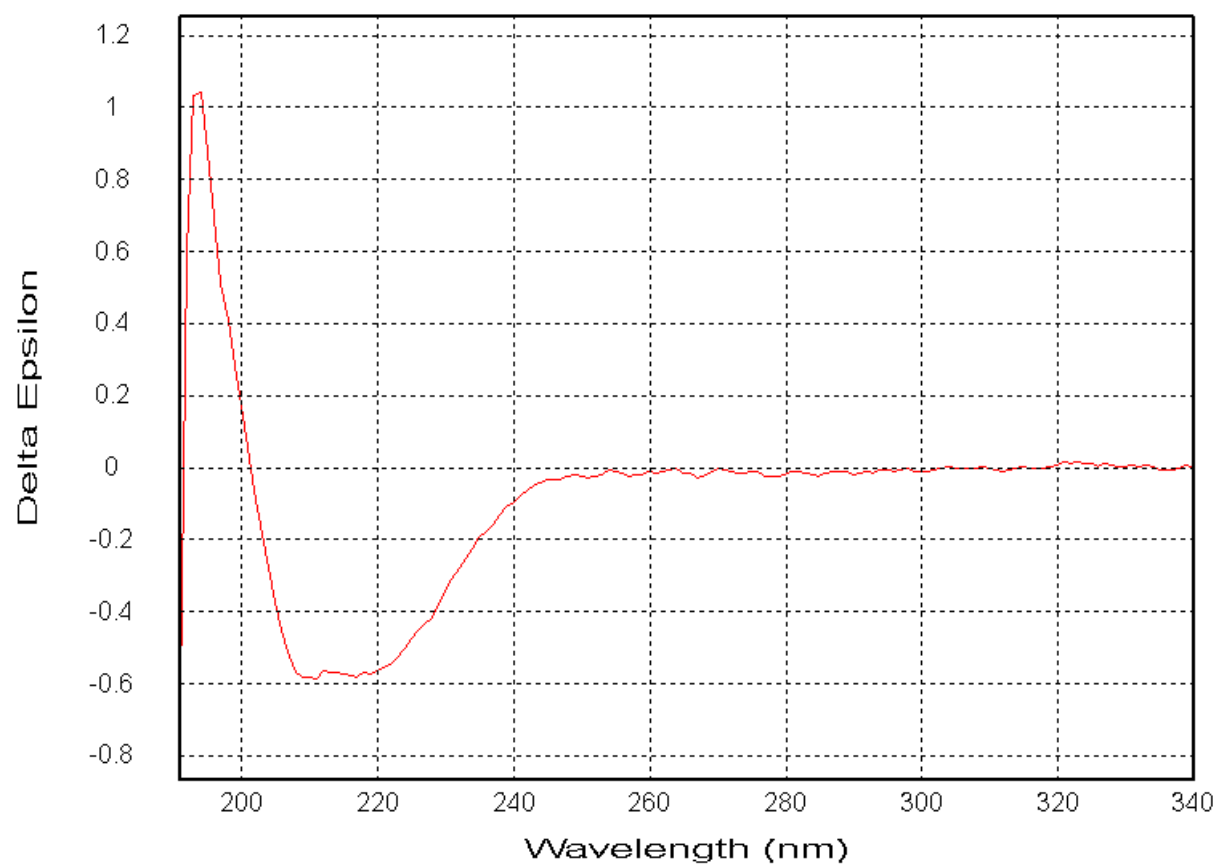


Figure S38. HR (+)ESI MS spectrum of 1

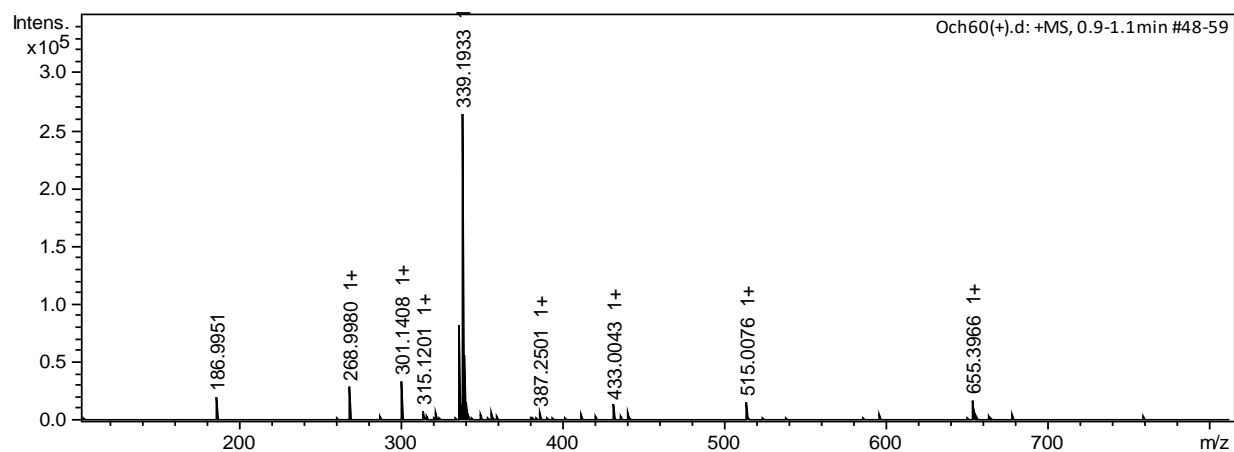


Figure S39. HR (+)ESI MS spectrum of 2

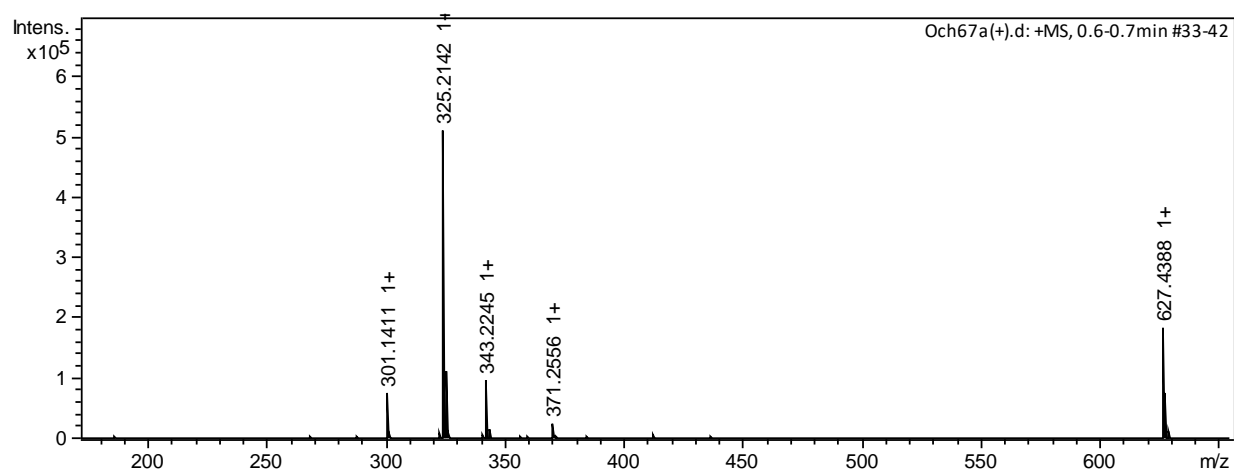


Figure S40. HR (+)ESI MS spectrum of 3

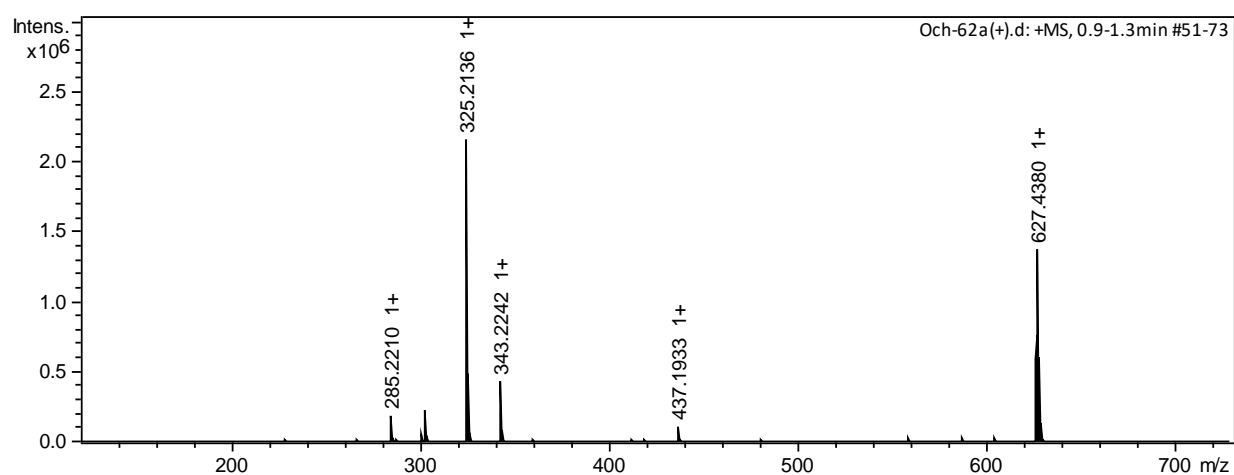


Figure S41. HR (+)ESI MS spectrum of 4

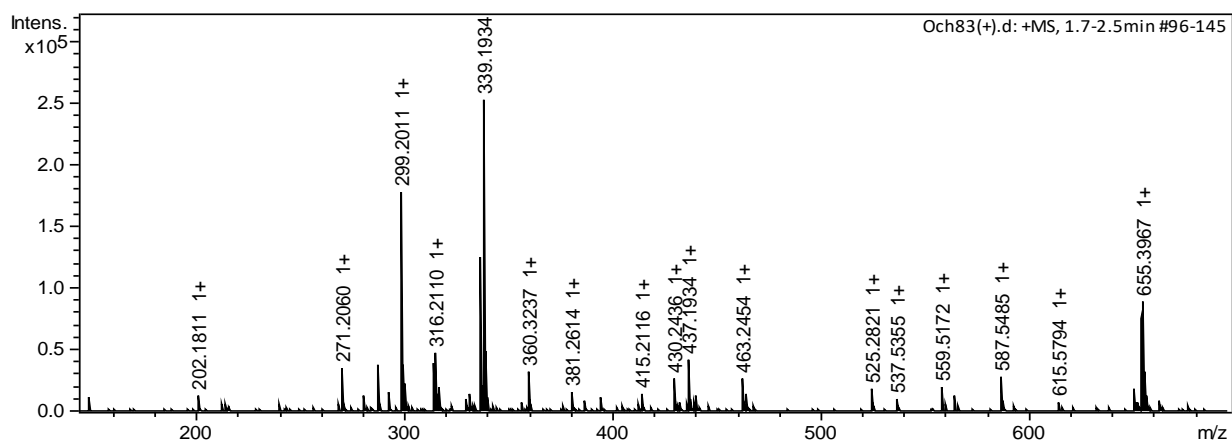


Figure S42. HR (+)ESI MS spectrum of 5

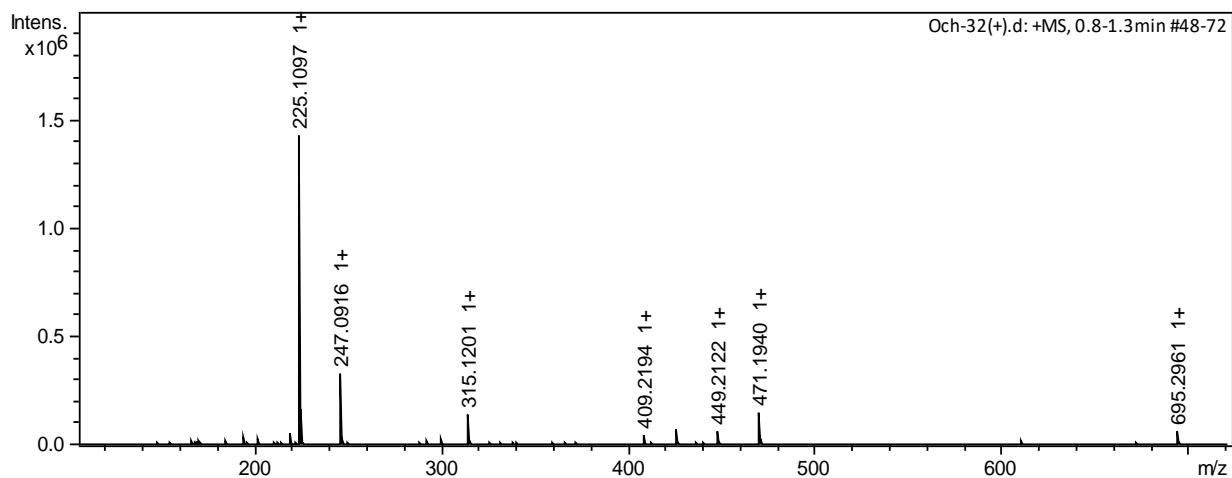


Figure S43. HR (+)ESI MS spectrum of 6

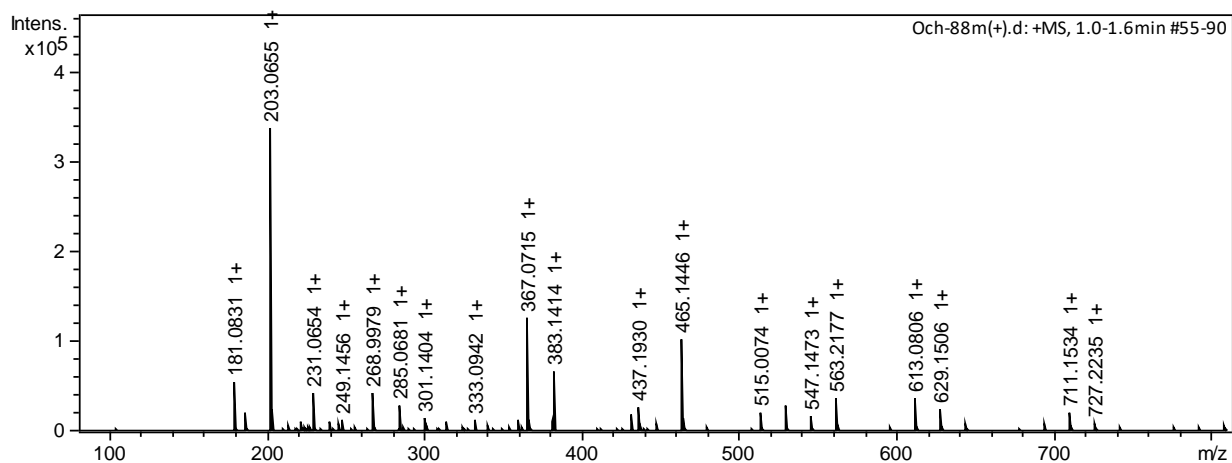


Figure S44. ¹H NMR spectrum for (*R*)-MTPA esters (500 MHz, CDCl₃) of (3b)

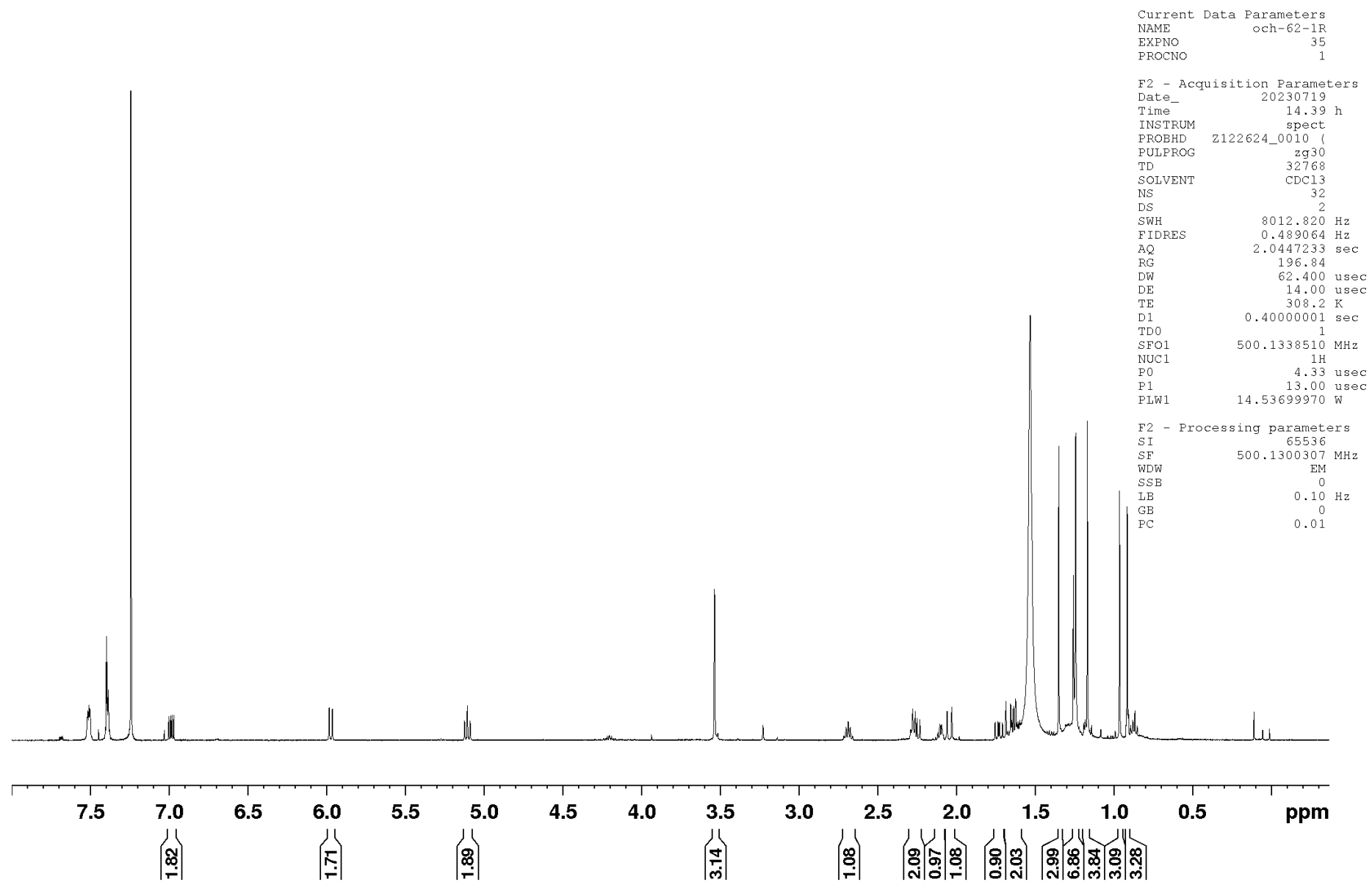


Figure S45. ^1H - ^1H COSY NMR spectrum for (R)-MTPA esters (500 MHz, CDCl_3) of (3b)

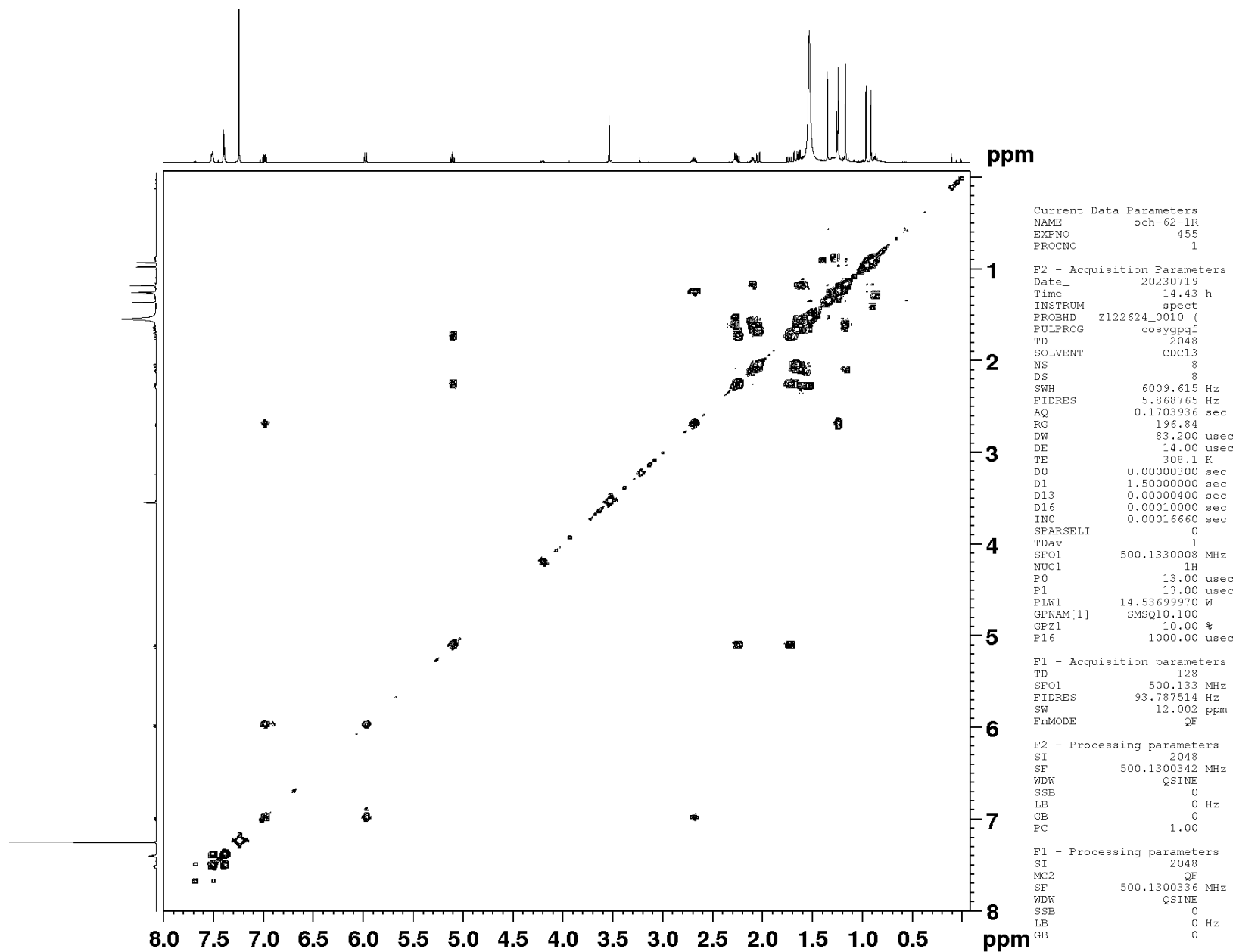


Figure S46. HR (+)ESI MS spectrum of for (R)-MTPA esters of (3b)

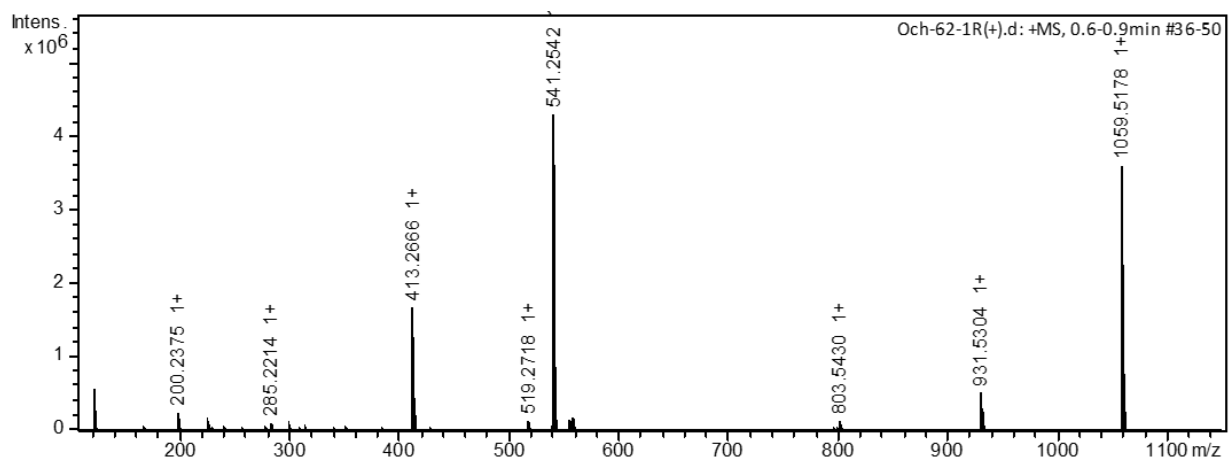


Figure S47. ¹H NMR spectrum for (S)-MTPA esters (500 MHz, CDCl₃) of (3a)

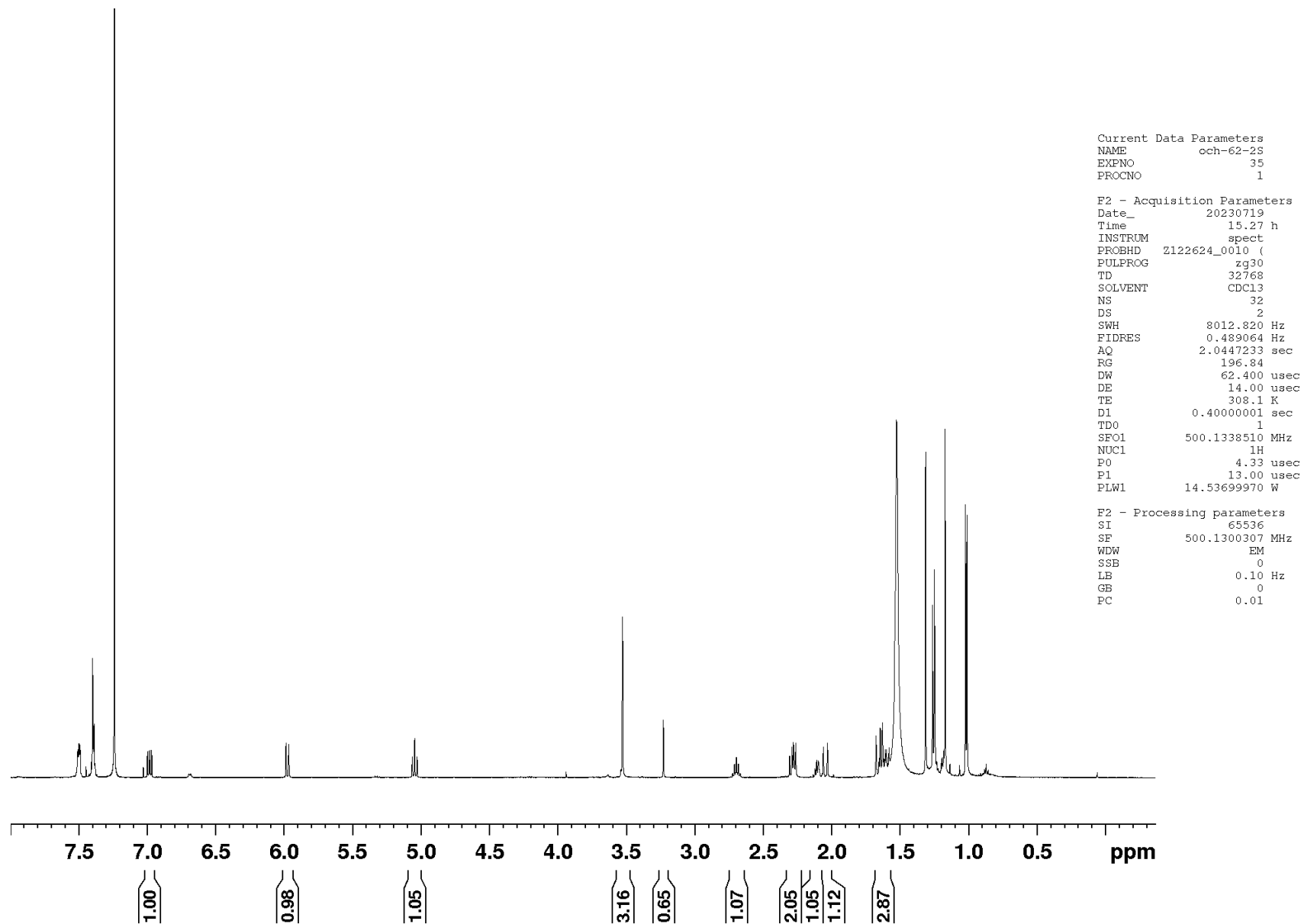


Figure S48. ^1H - ^1H COSY NMR spectrum for (S)-MTPA esters (500 MHz, CDCl_3) of (3a)

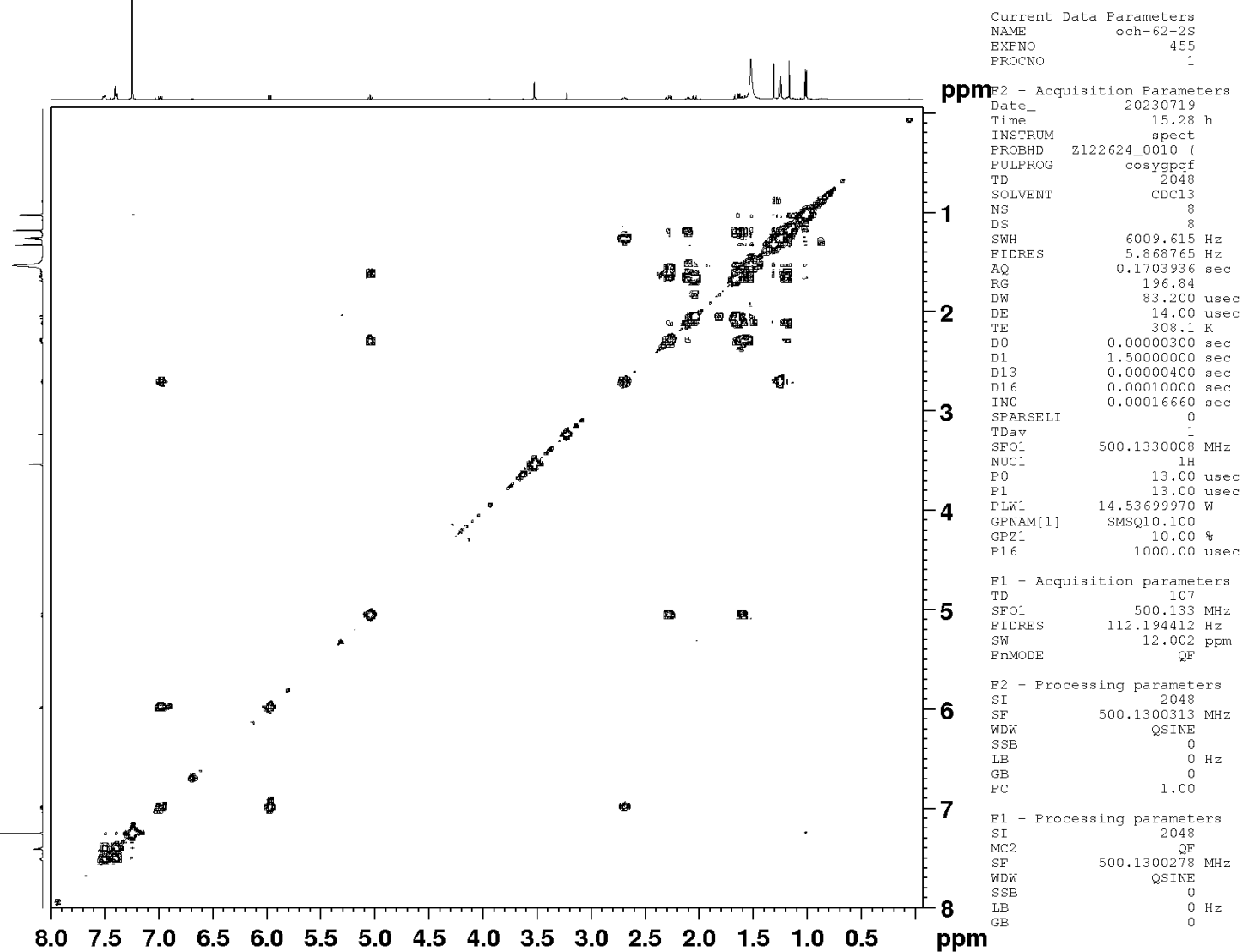


Figure S49. HR (+)ESI MS spectrum of for (S)-MTPA esters of (3a)

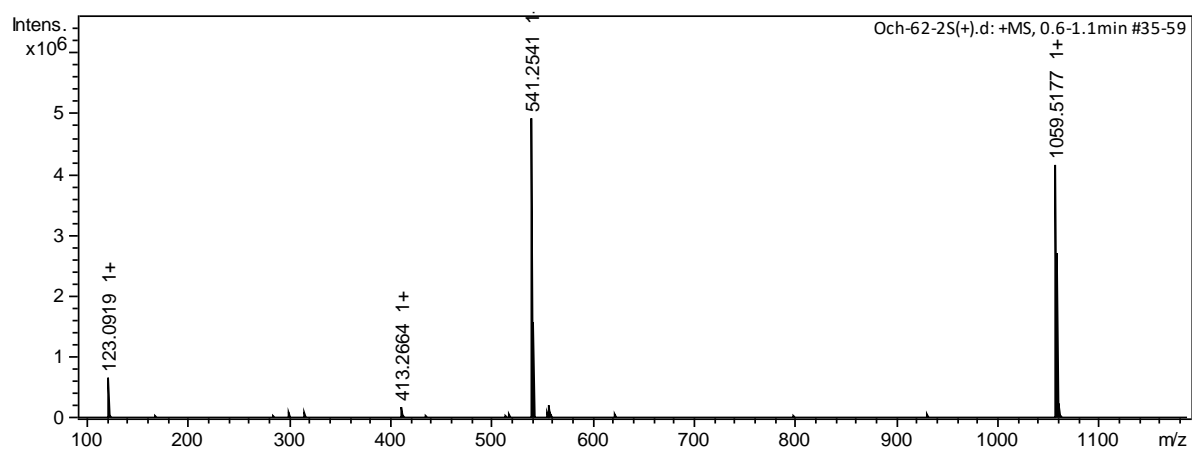


Figure S50. Comparison of the experimental ECD spectra of compounds 1–4

