

Supplementary Materials

Cytoprotective polyketides from sponge-derived fungus *Lopadostoma pouzarii*

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Abstract: The new polyketides lopouzanones A and B as well as new 1-O-acetyl and 2-O-acetyl derivatives of dendrodochol B were isolated from sponge-derived marine fungus *Lopadostoma pouzarii* strain 168CLC-57.3. Moreover, six known polyketides gliorosein, balticolid, dendrodolide G, dihydroisocumarine, (-)-5-methylmellein and dendrodochol B were identified. Structures of isolated compounds were determined by a combination of NMR and ESIMS techniques. The absolute configurations of lopouzanones A and B were determined using the Mosher's method. The cytotoxicity of isolated compounds against human prostate cancer cells PC-3 and normal rat cardiomyocytes H9c2 were investigated. Gliorosein showed a weak DPPH radical scavenging activity and *in vitro* cardioprotective effects toward rotenone toxicity and CoCl₂-mimic hypoxia.

Keywords: marine fungi; sea sponge; secondary metabolites; polyketides; cytotoxicity; cardioprotection.

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Figure S1. ^1H NMR spectrum of lopuzanone A (**1**)

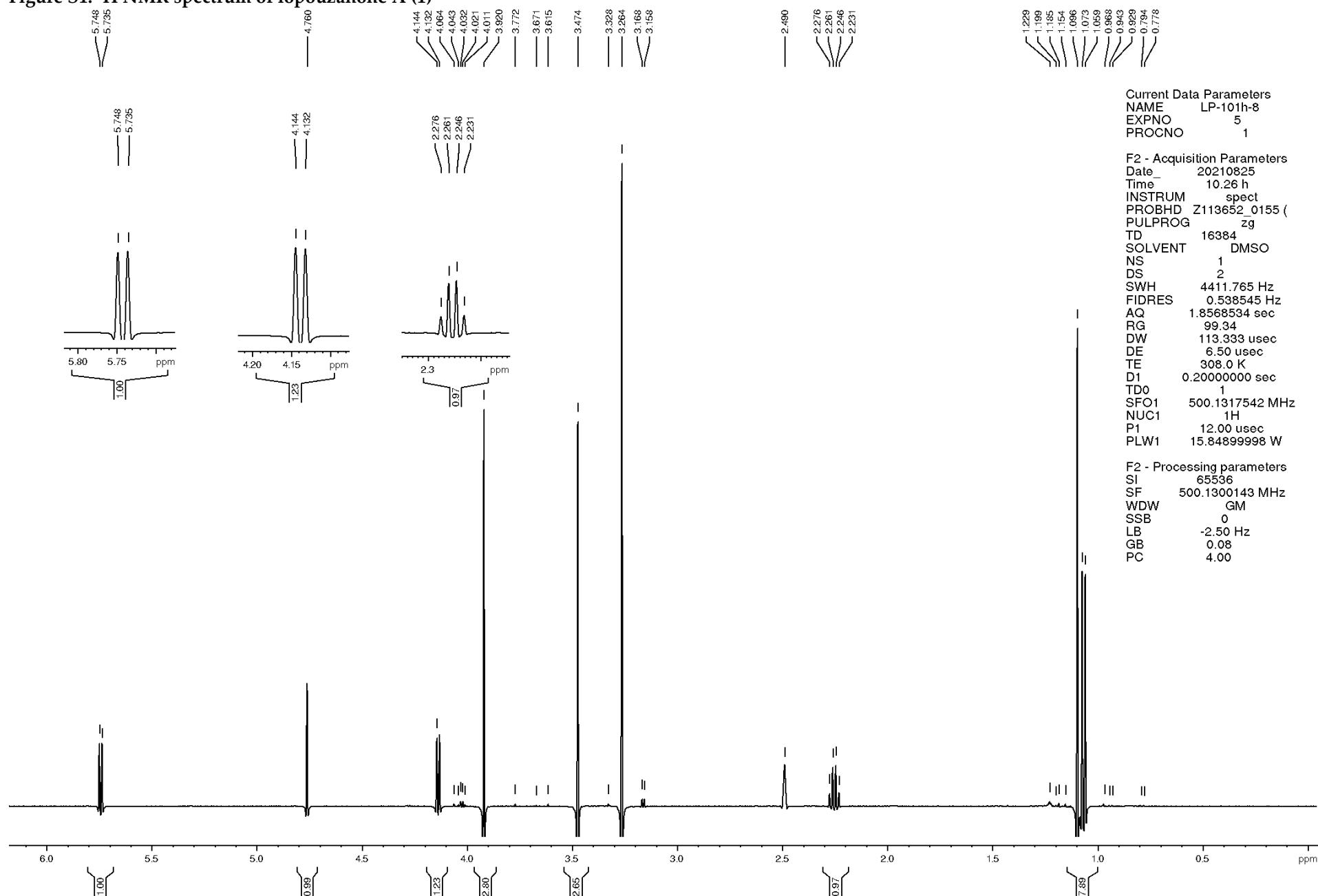


Figure S2. ^{13}C NMR spectrum of lopouzanone A (1)

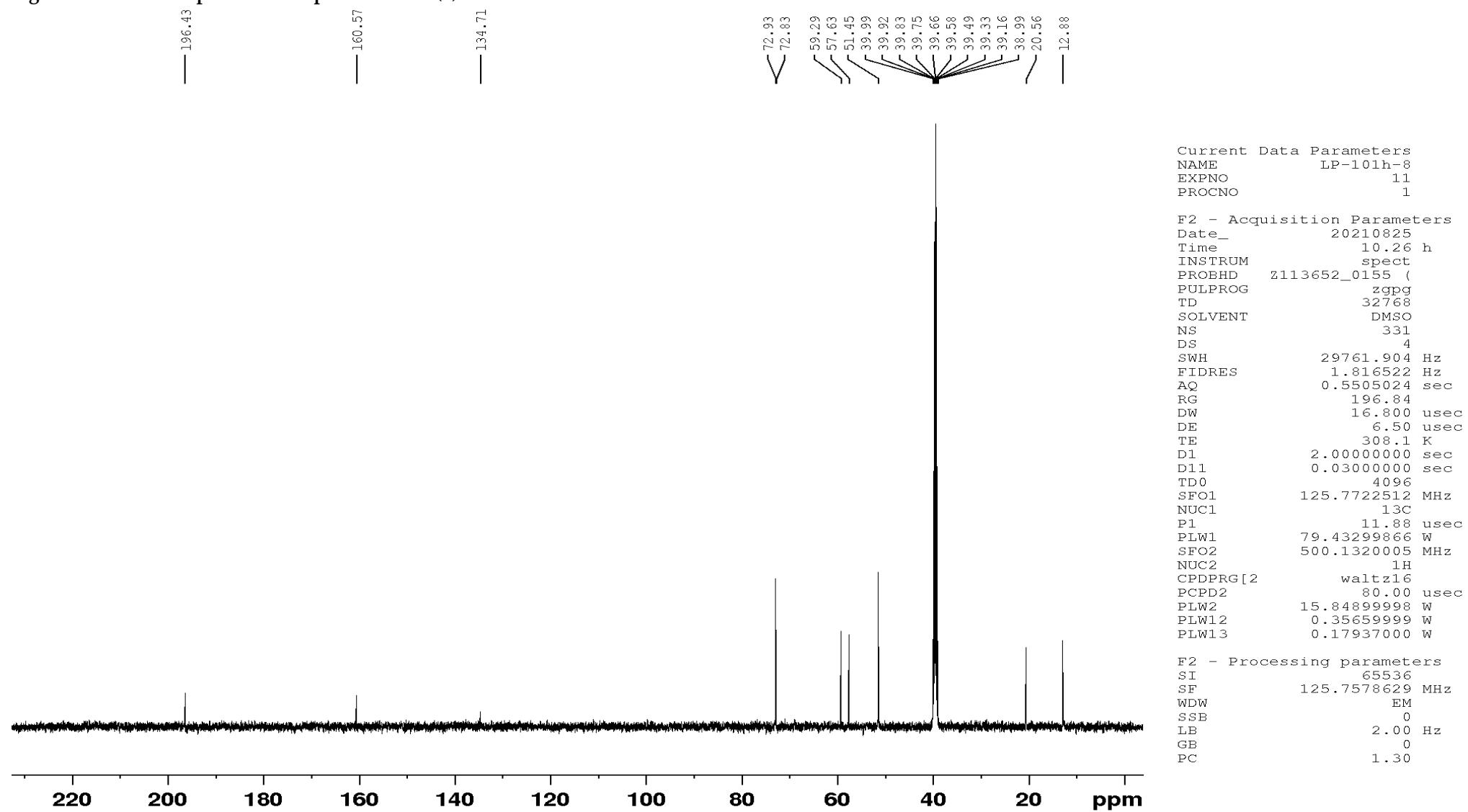


Figure S3. ^1H - ^1H COSY spectrum of lopuzanone A (1)

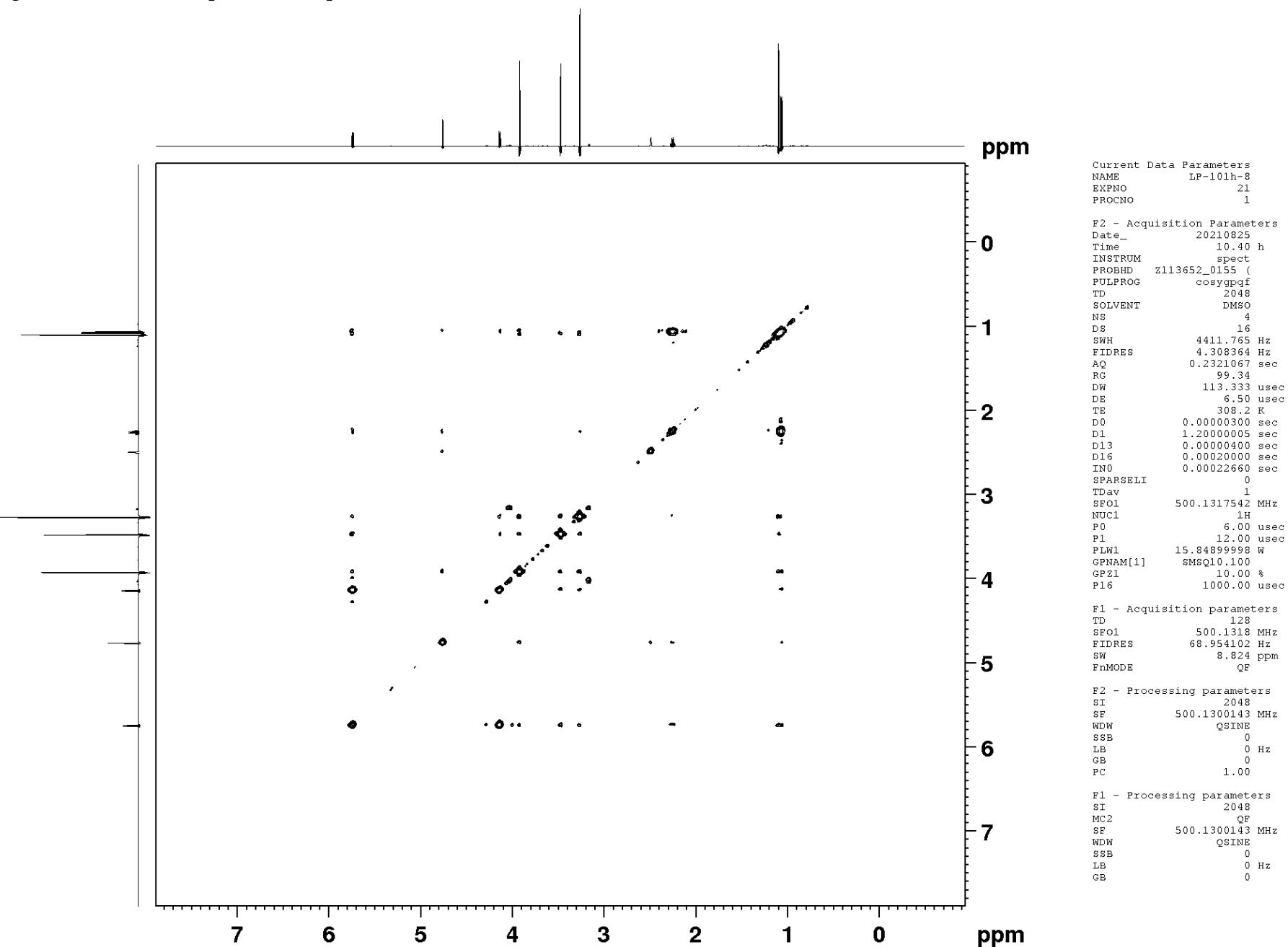


Figure S4. HMBC spectrum of lopouzanone A (1)

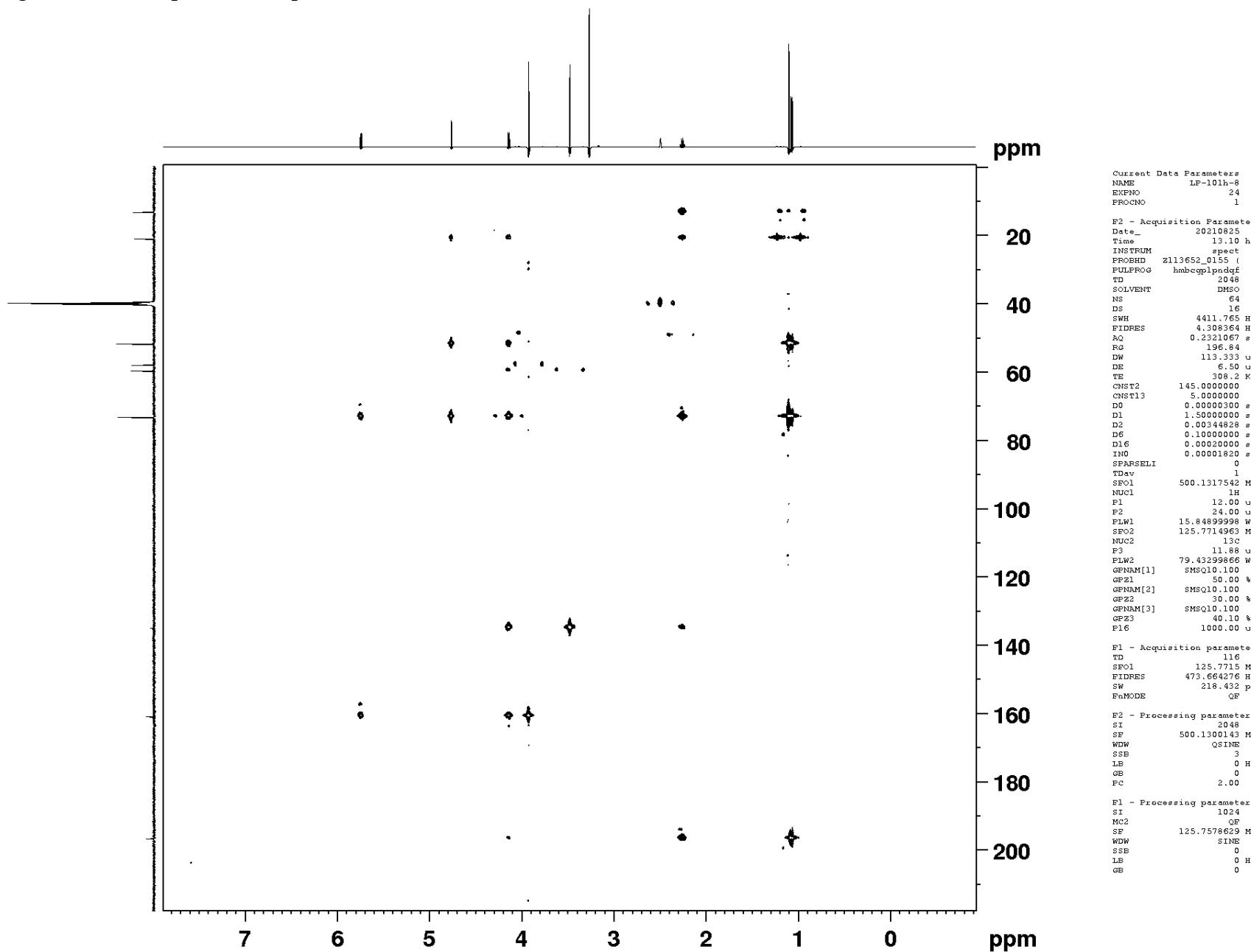
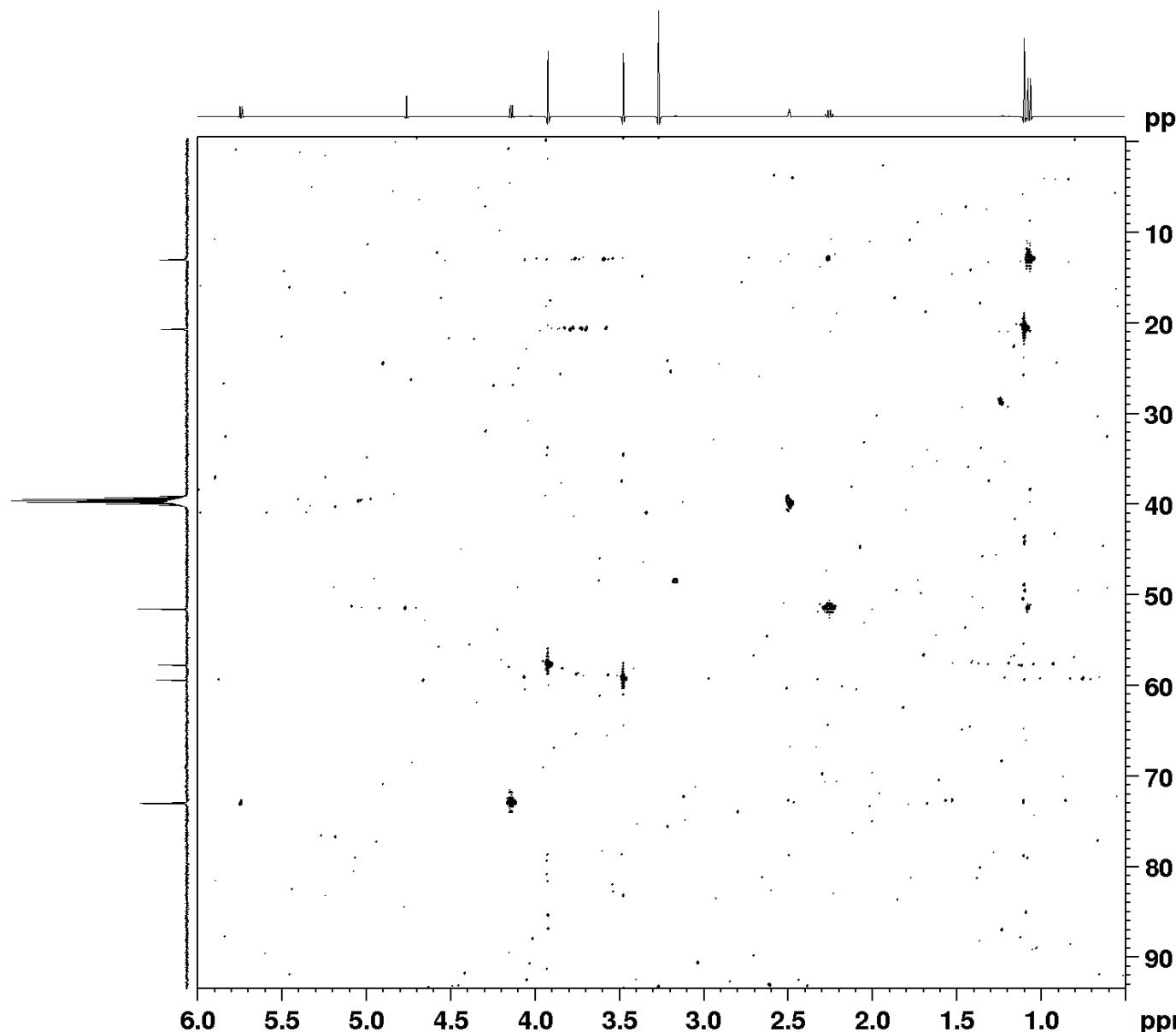


Figure S5. HSQC spectrum of lopuzanone A (1)



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CNSP17 -0.500000
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OF24 -5.00 %
P16 1000.00 usec
P19 600.00 usec

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FIDRES 184.692673 Hz
SW 93.388 ppm
PRWEDGE Echo-Antiecho

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WDW SINE
SSB 2
LB 0 Hz
OB 0
FC 1.00

P1 - Processing parameters
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WDW SINE
SSB 2
LB 0 Hz
OB 0

Figure S6. ROESY spectrum of lopouzanone A (1)

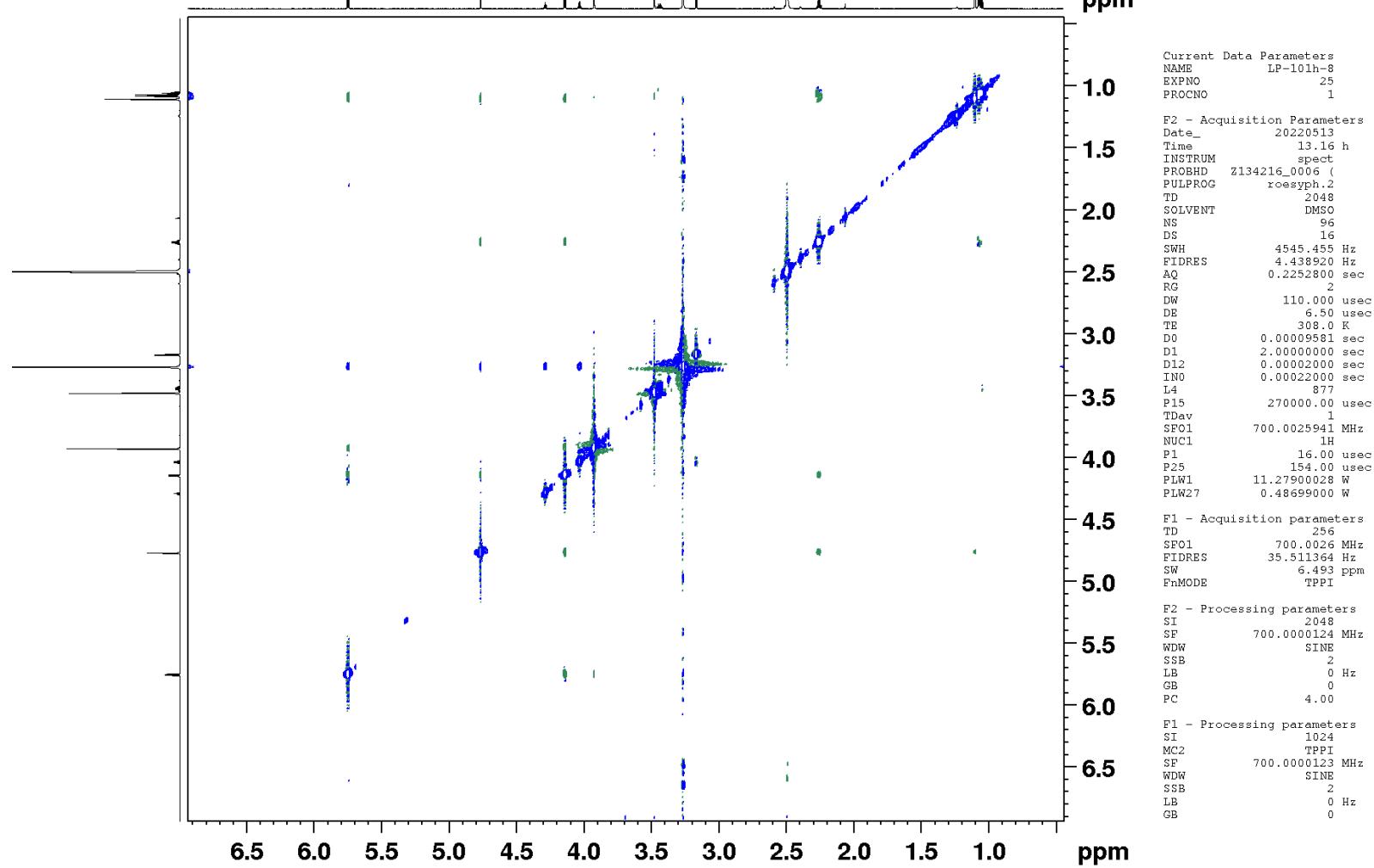


Figure S7. CD spectrum of lopouzanone A (1)

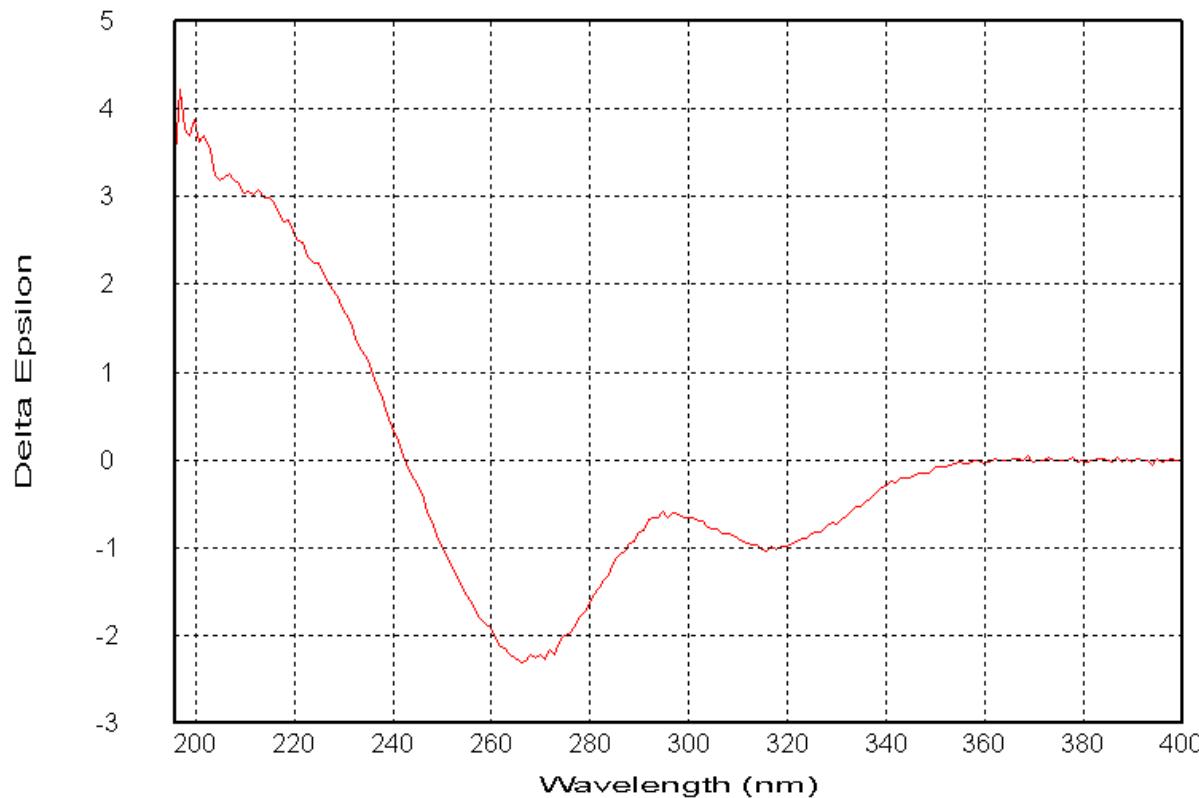


Figure S8. ^1H NMR spectrum for (R)-MTPA esters of lopouzanone A (**1**)

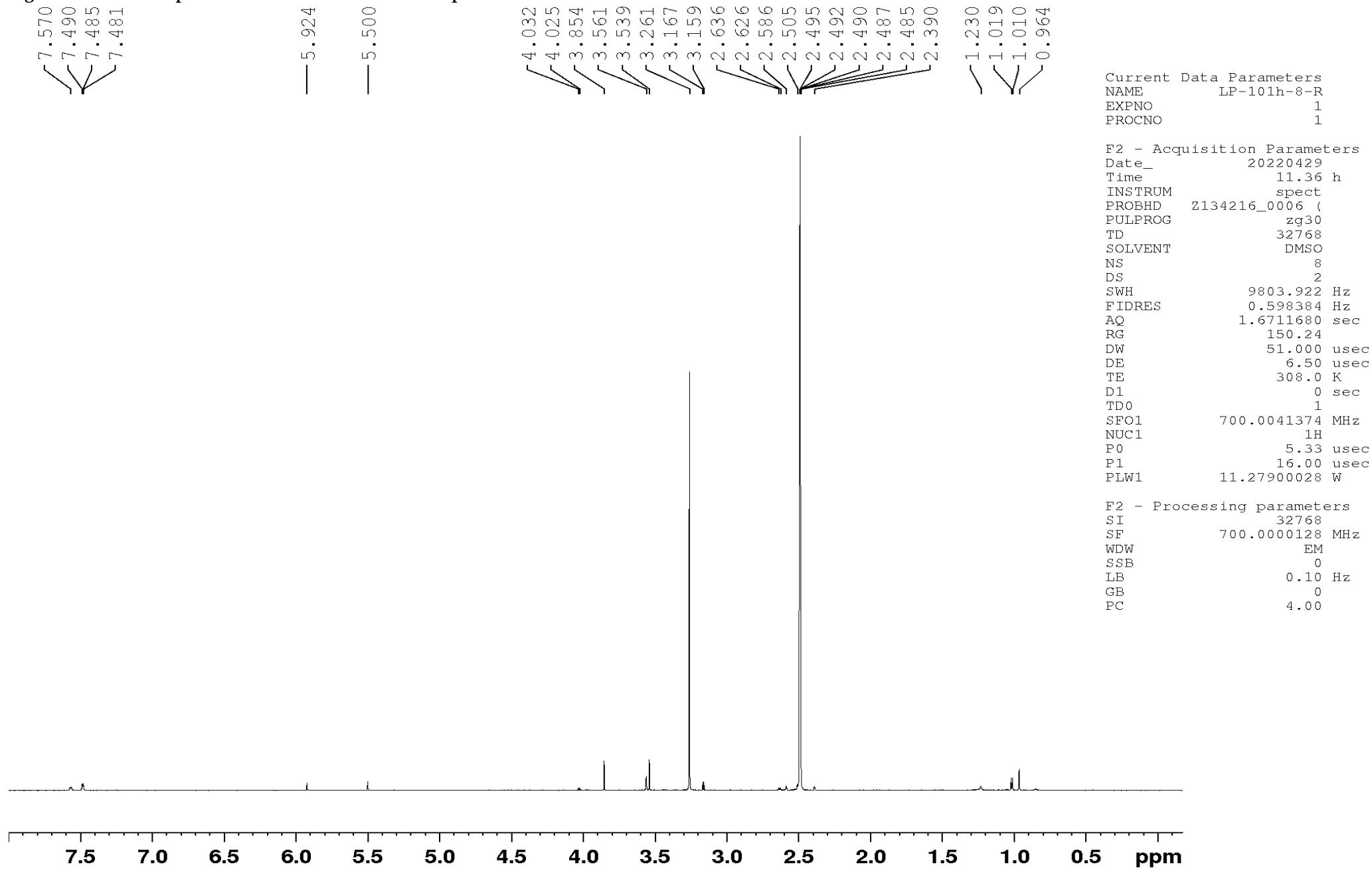


Figure S9. ^1H - ^1H COSY spectrum for (R)-MTPA esters of lopouzanone A (1)

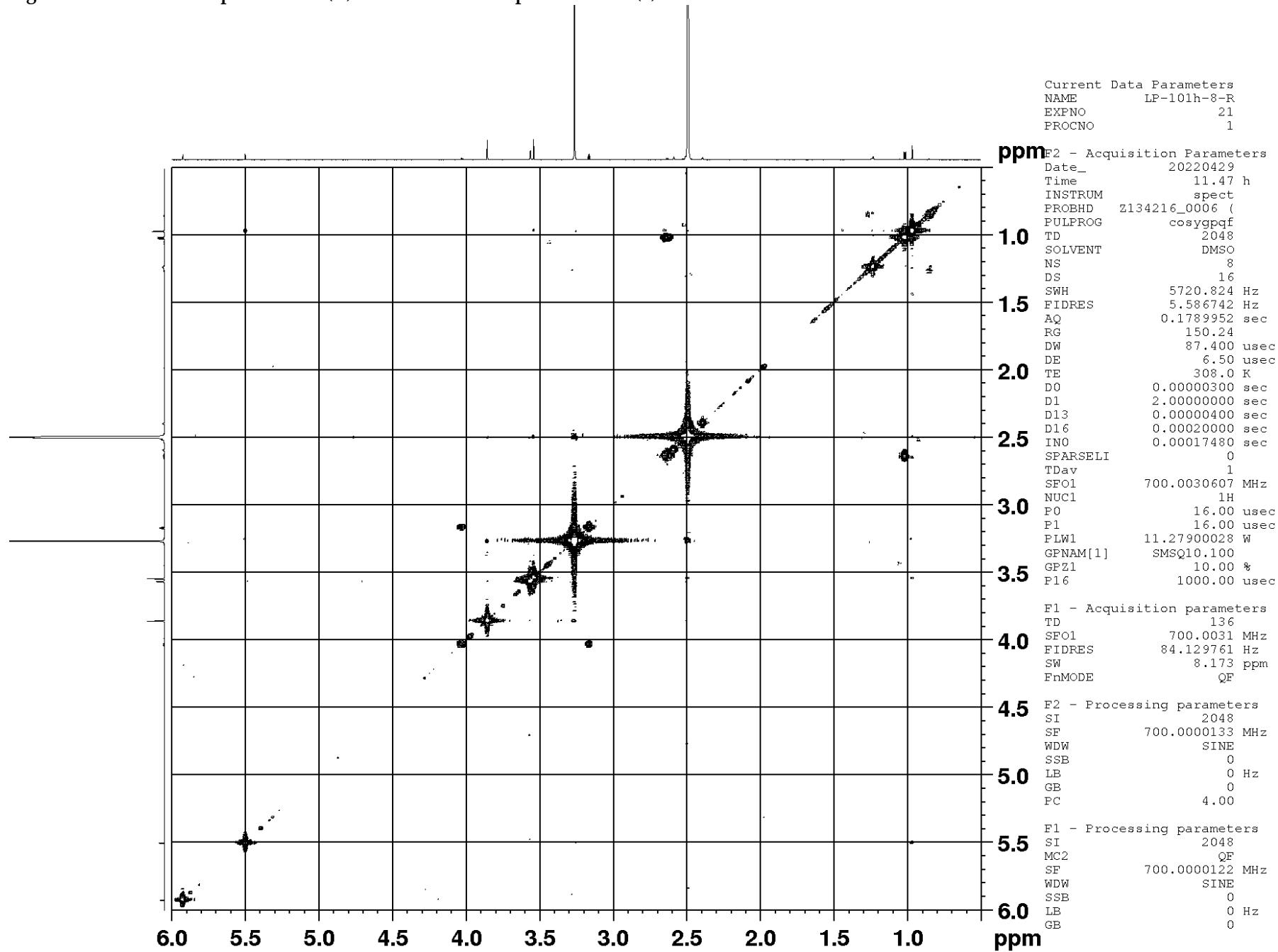


Figure S10. ^1H NMR spectrum for (S)-MTPA esters of lopouzanone A (**1**)

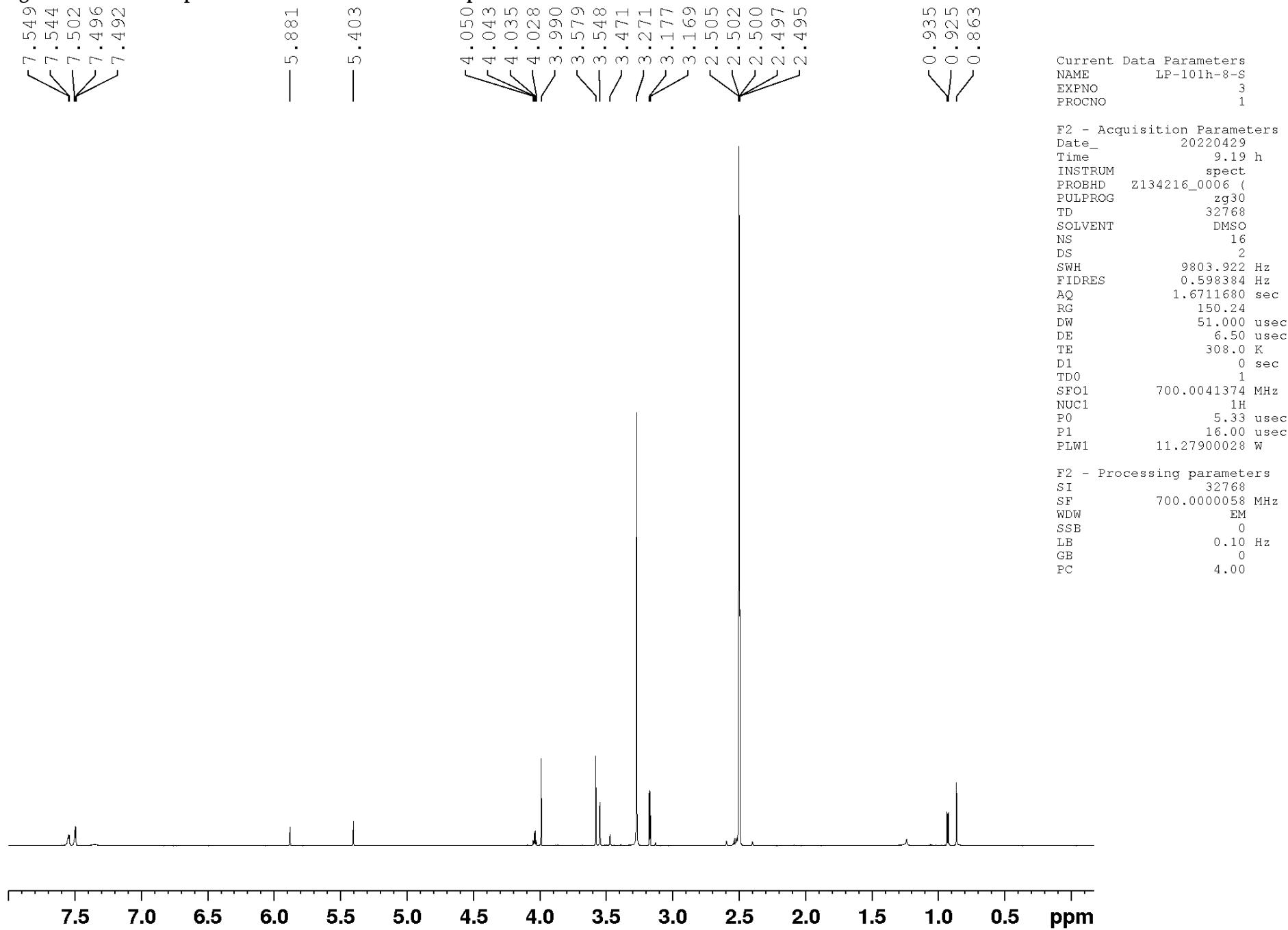


Figure S11. COSY spectrum for (S)-MTPA esters of lopouuzanone A (1)

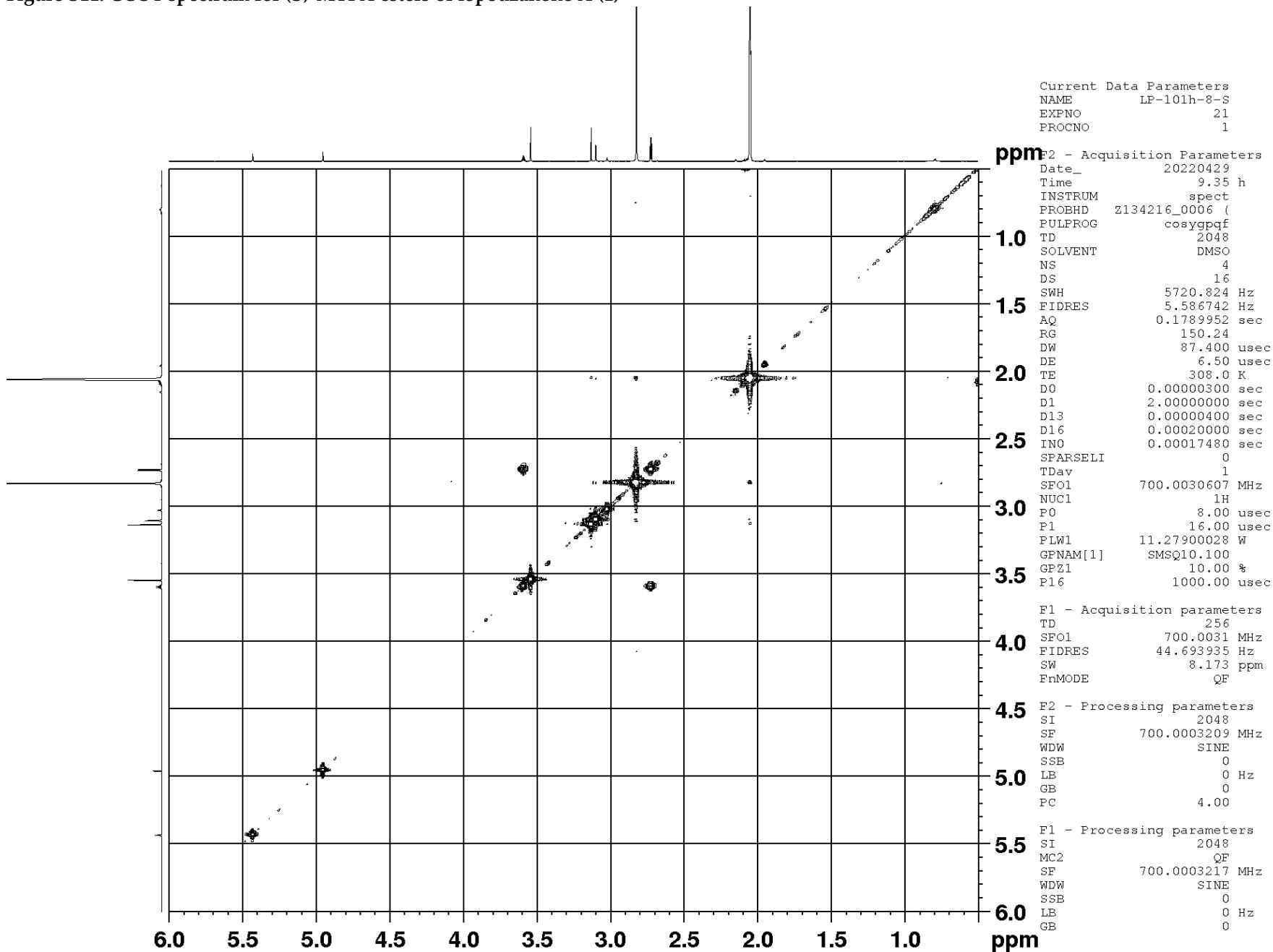


Figure S12. ^1H NMR spectrum of lopouzanone B (2)

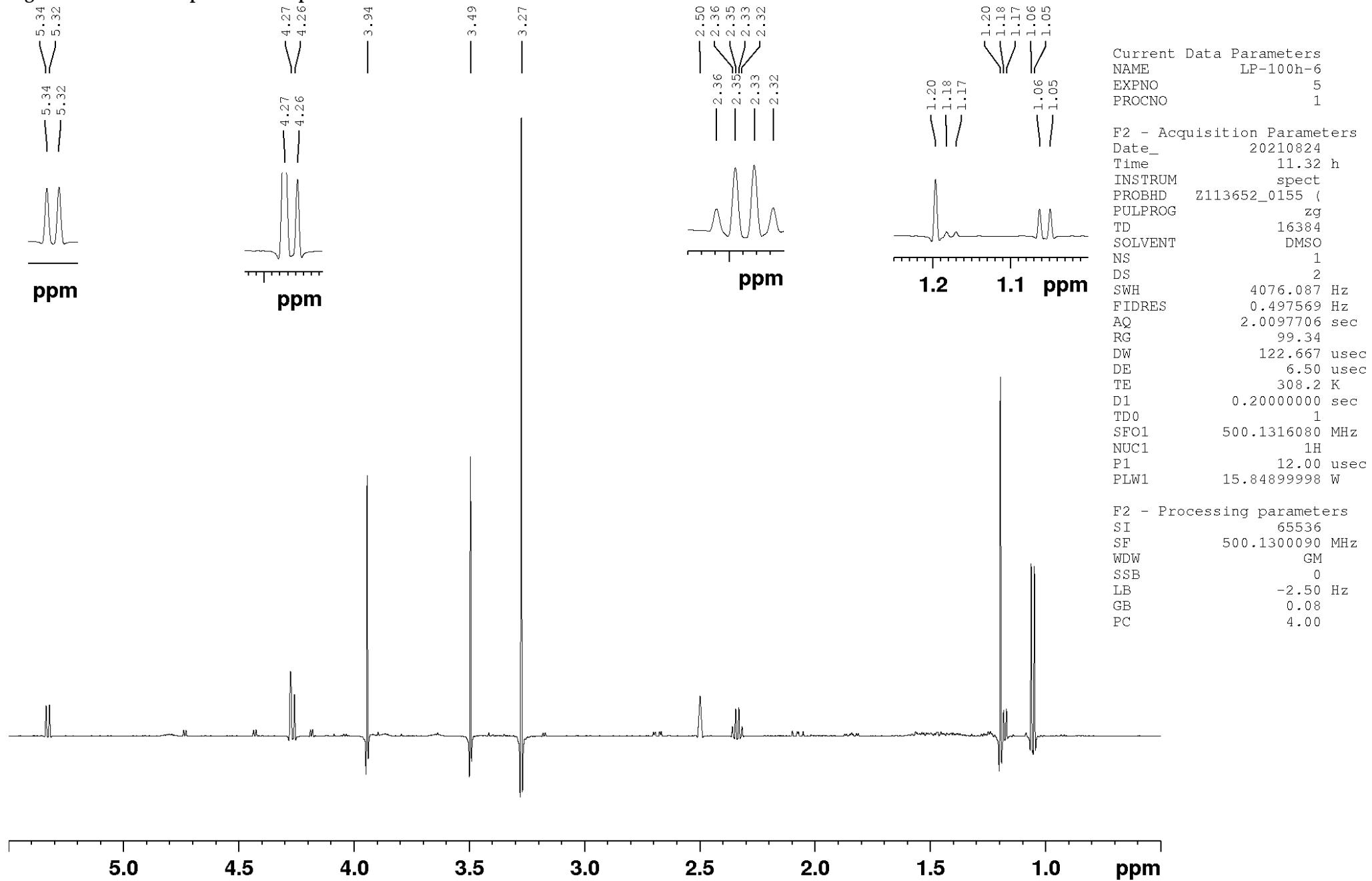


Figure S13. ^{13}C NMR spectrum of lopouzanone B (2)

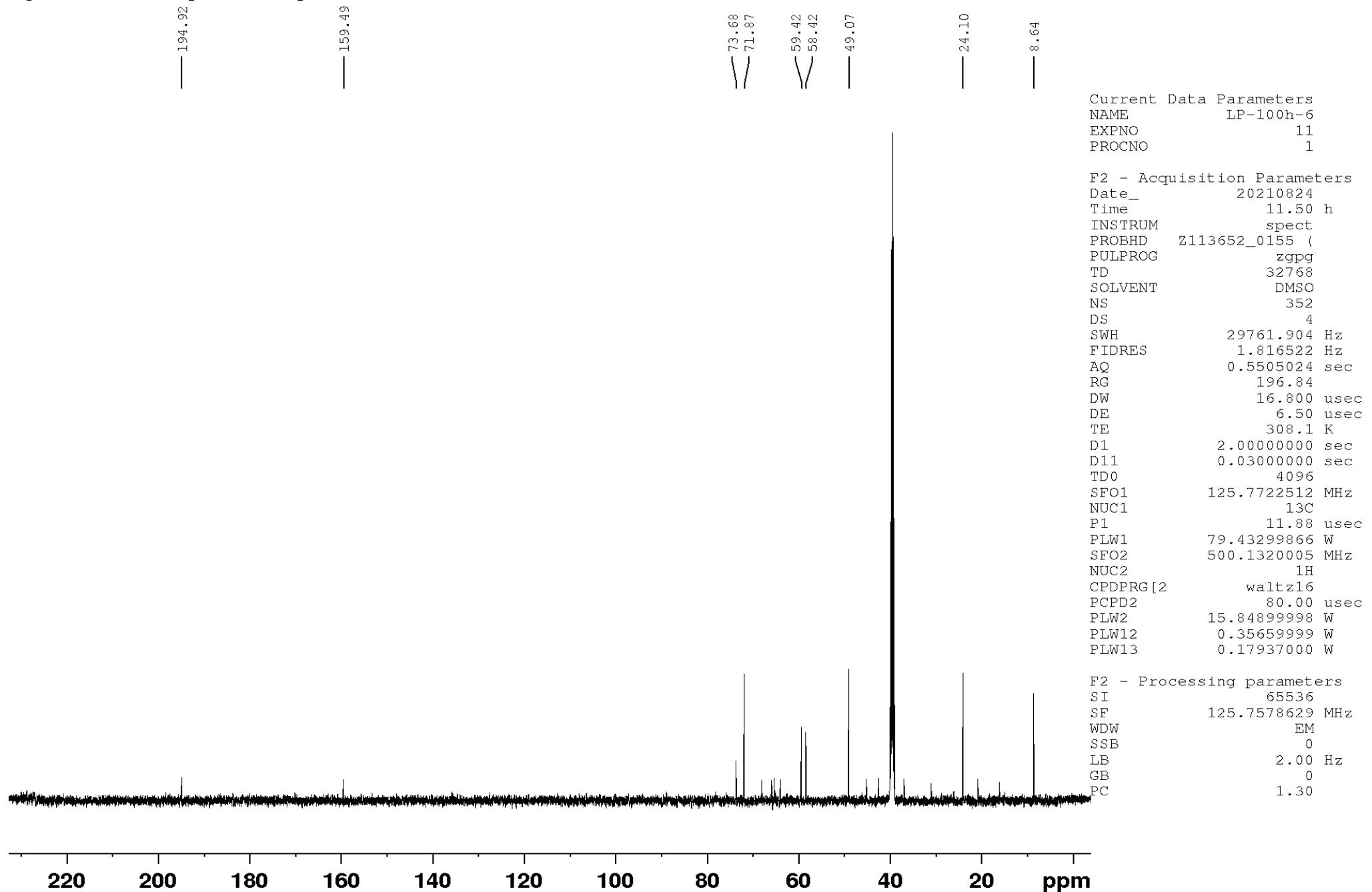


Figure S14. ^1H - ^1H COSY spectrum of lopouzanone B (2)

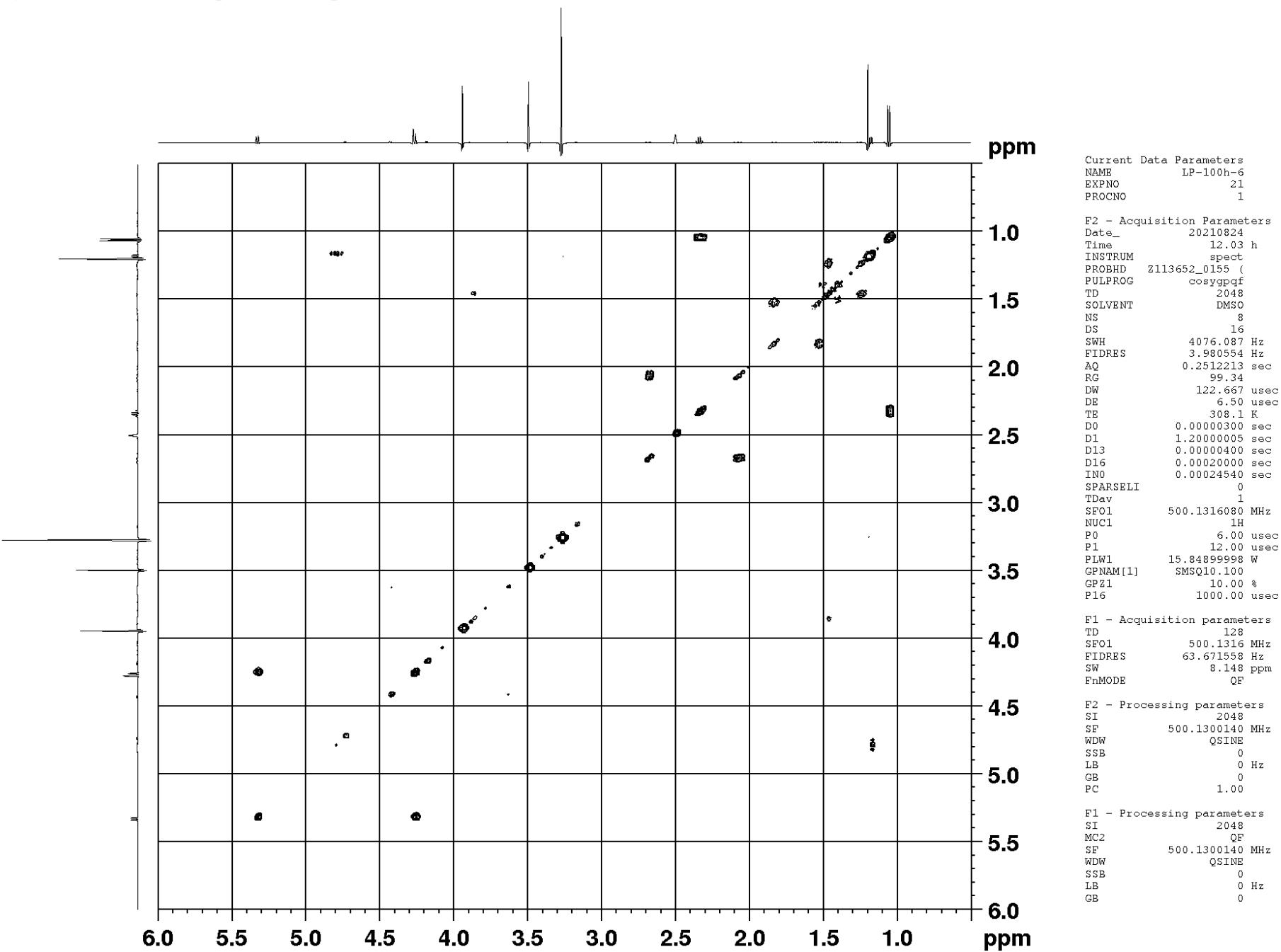


Figure S15. HMBC spectrum of lopouzanone B (2)

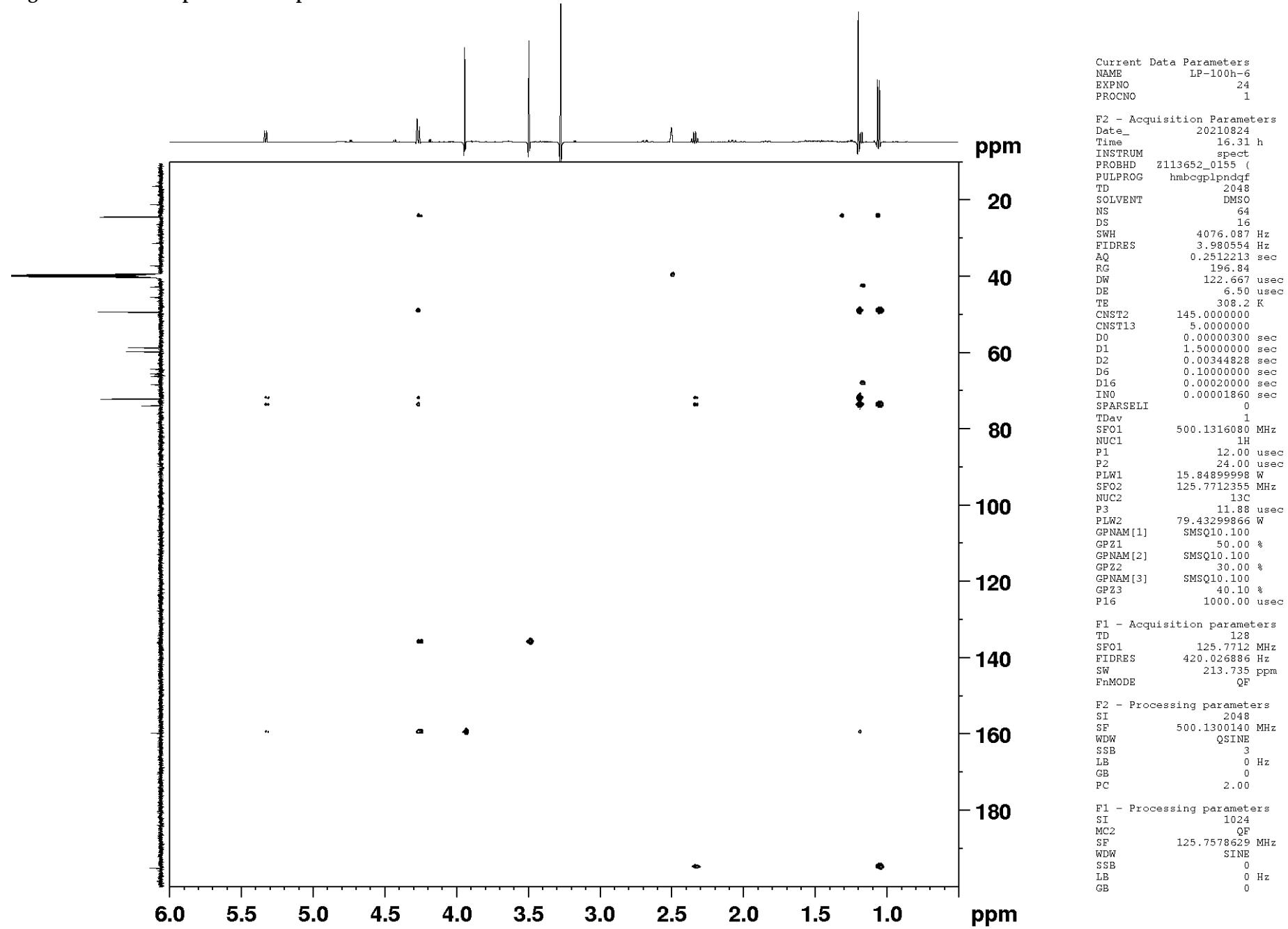


Figure S16. HSQC spectrum of lopouuzanone B (2)

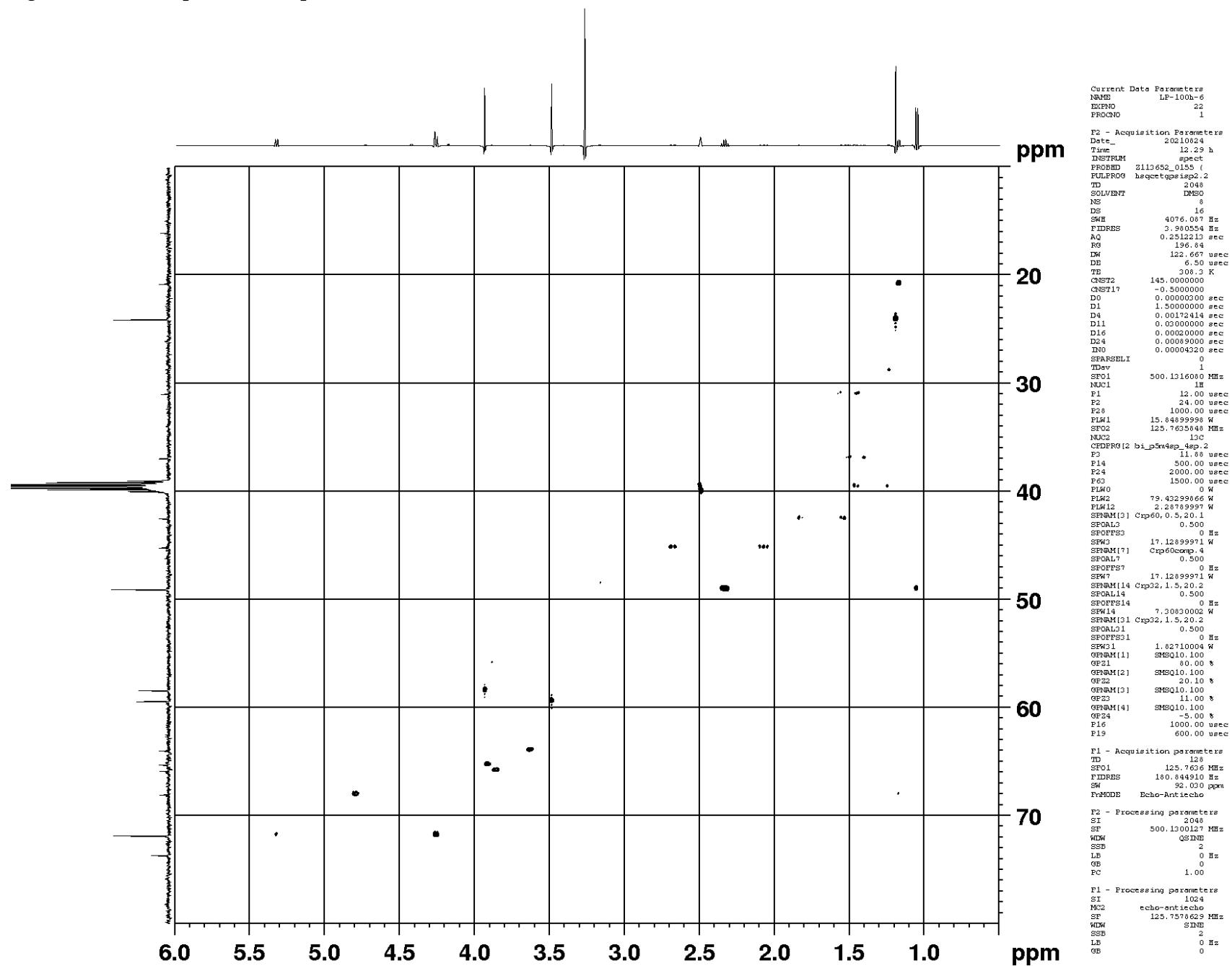


Figure S17. ROESY spectrum of lopouzanone B (2)

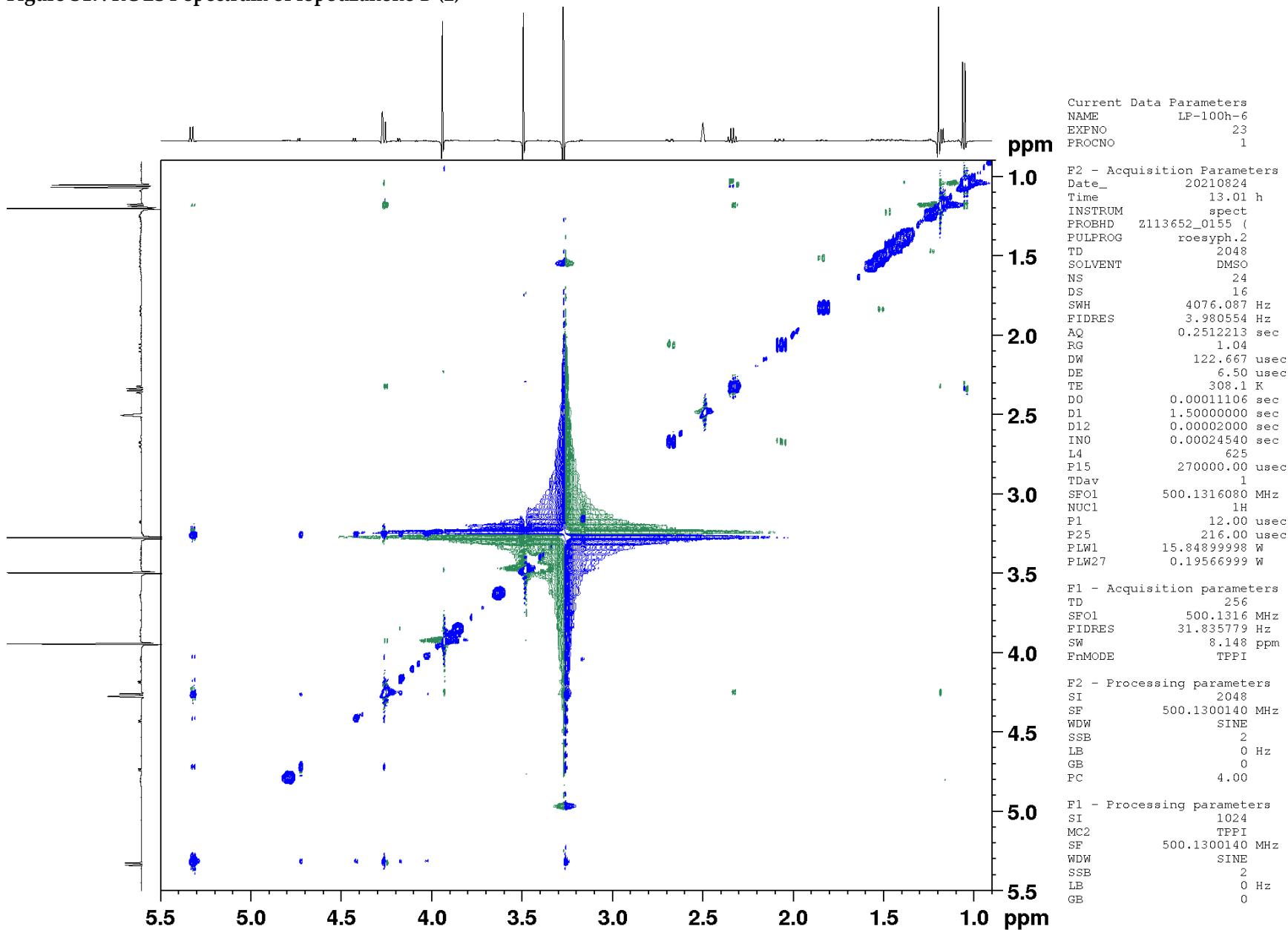


Figure S18. CD spectrum of lopouzanone B (2)

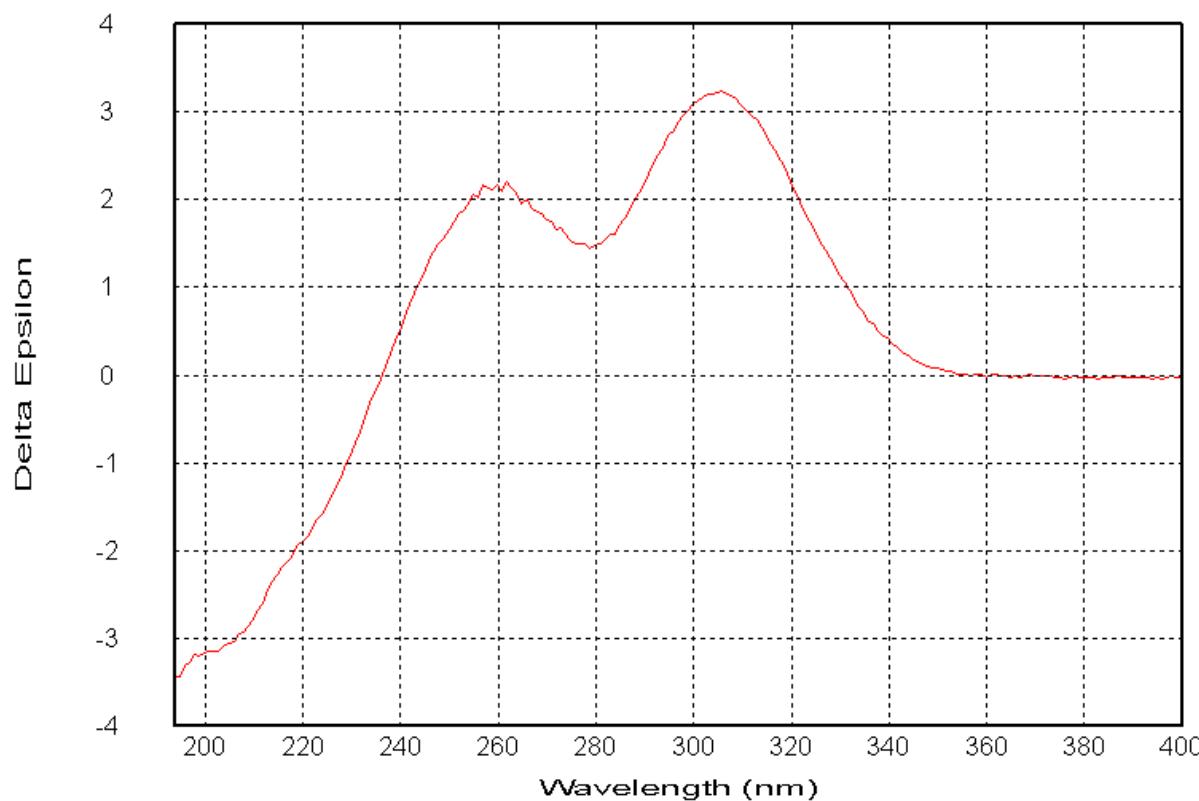


Figure S19. ^1H NMR spectrum for (R)-MTPA esters of lopouzanone B (2)

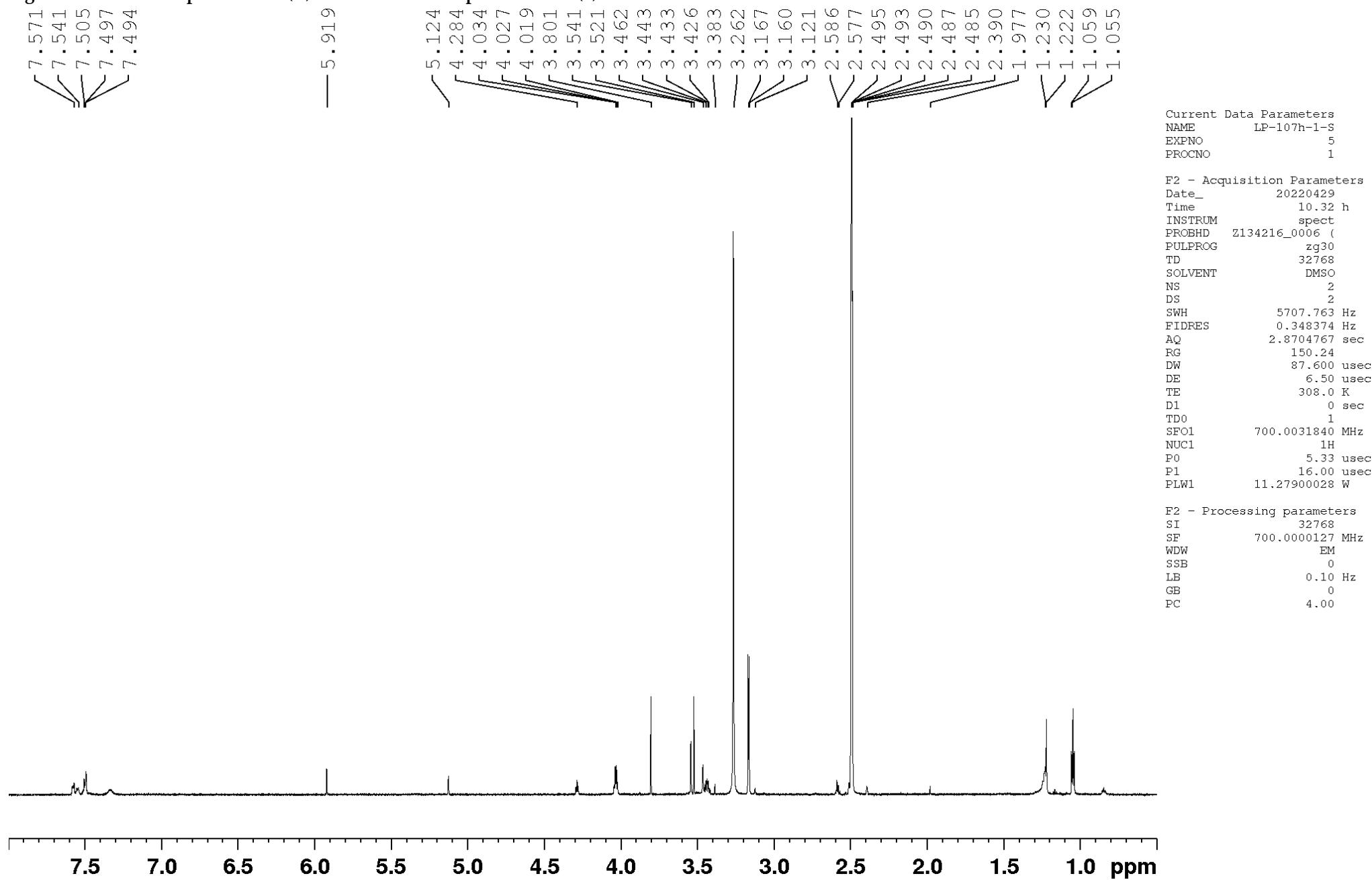


Figure S20. ^1H - ^1H COSY spectrum for (R)-MTPA esters of lopouzanone B (2)

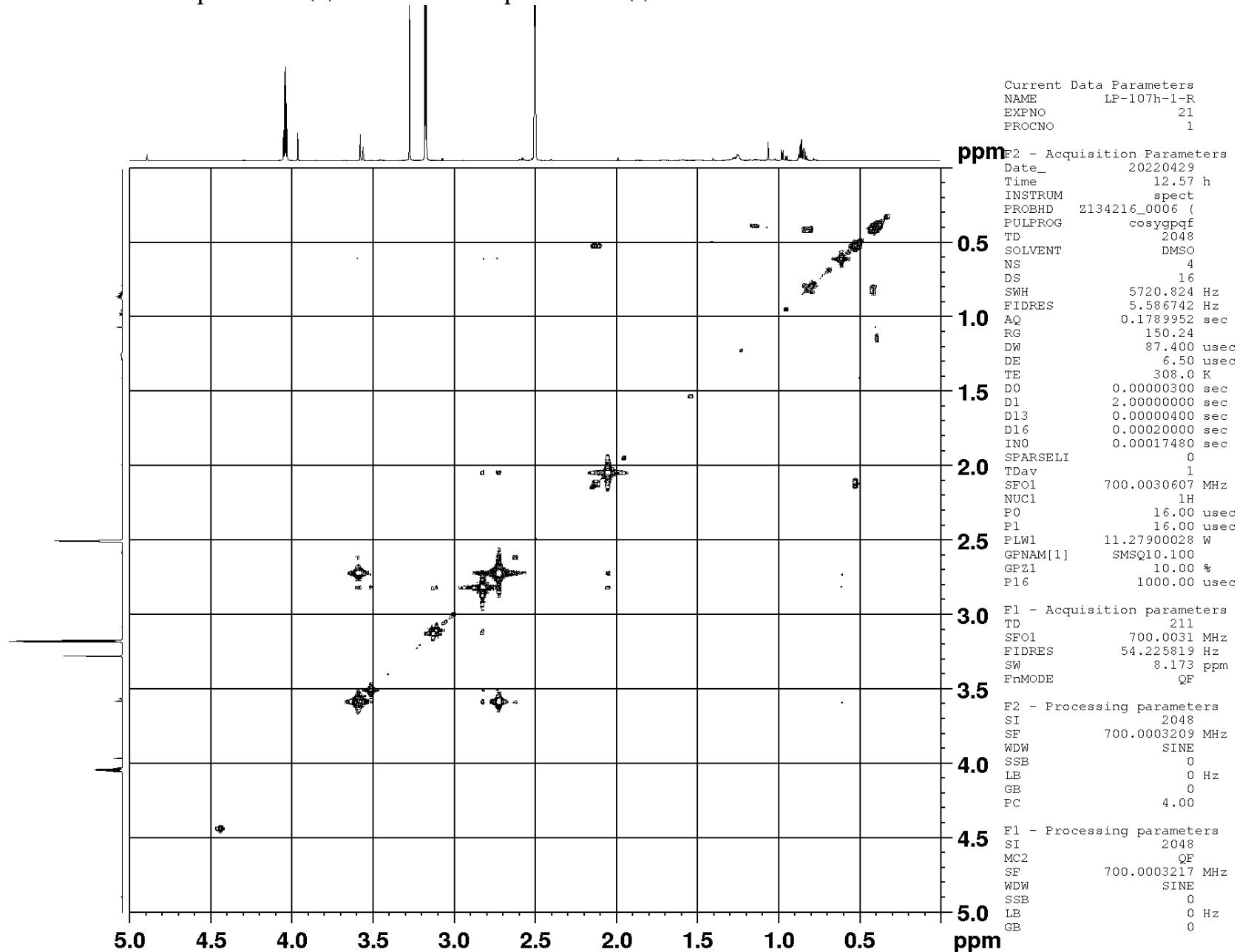


Figure S21. ^1H NMR spectrum for (S)-MTPA esters of lopouzanone B (2)

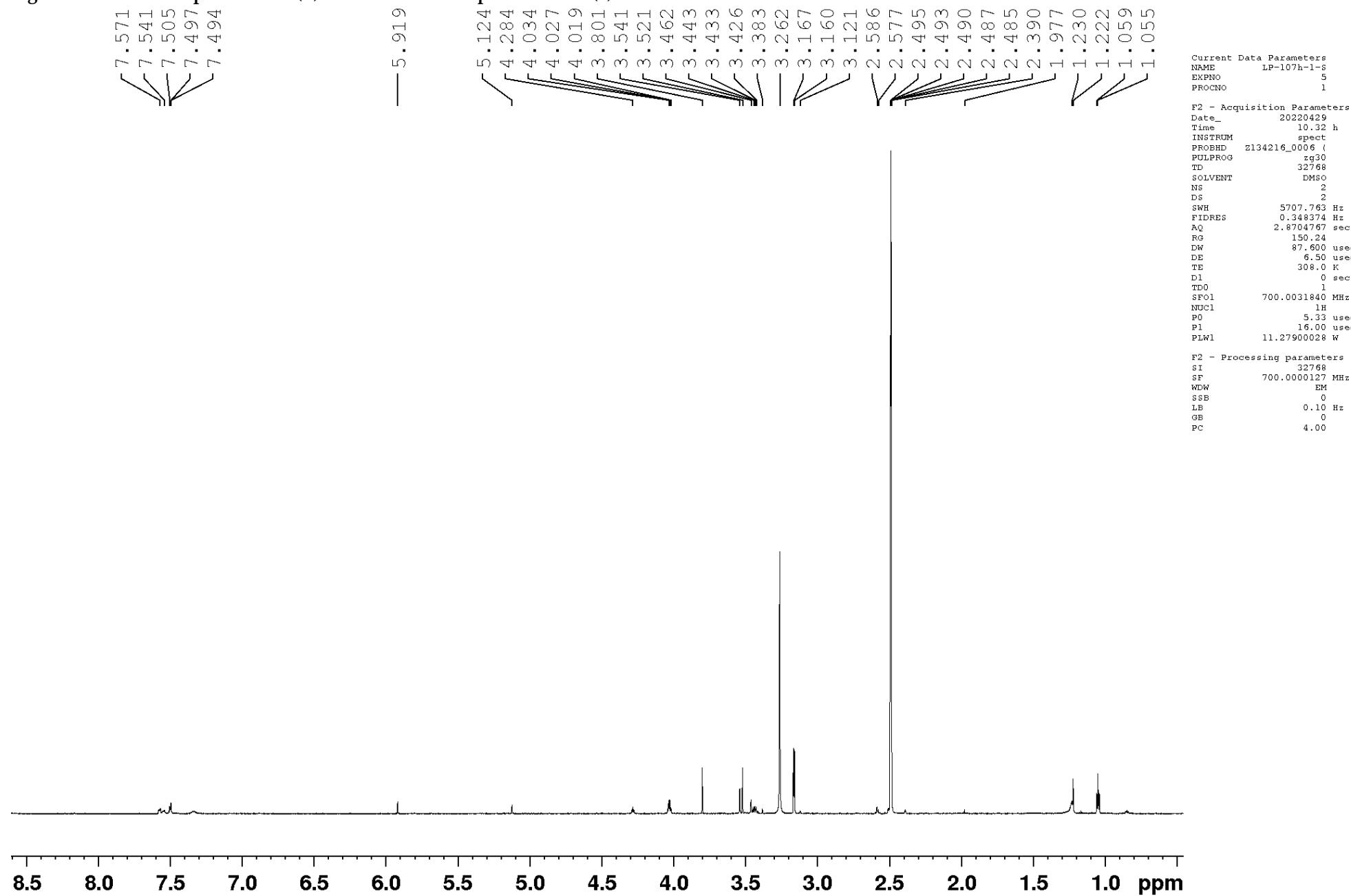


Figure S22. ^1H - ^1H COSY spectrum for (S)-MTPA esters of lopouzanone B (2)

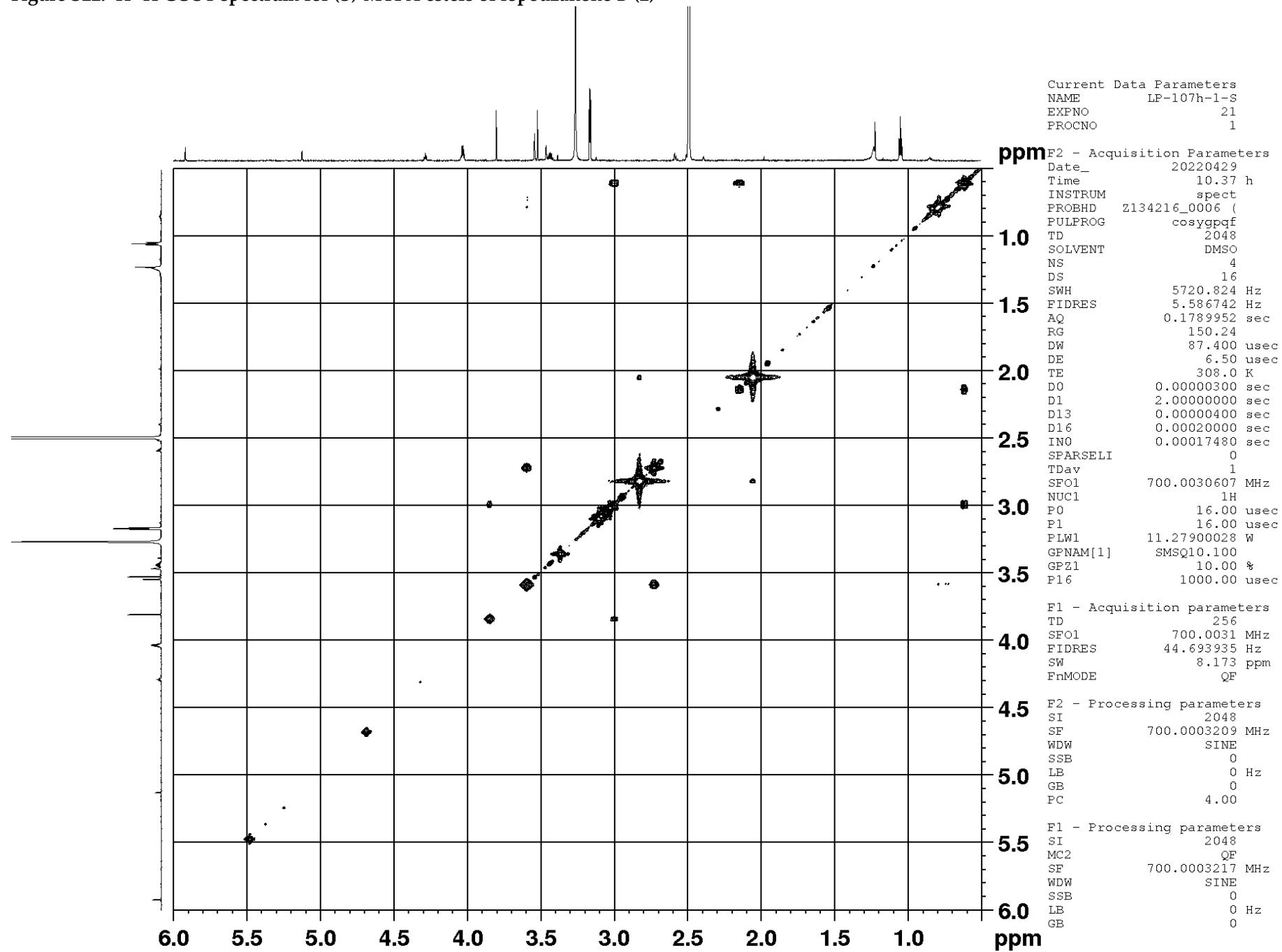


Figure S23. ^1H NMR spectrum of gliorosein (3)

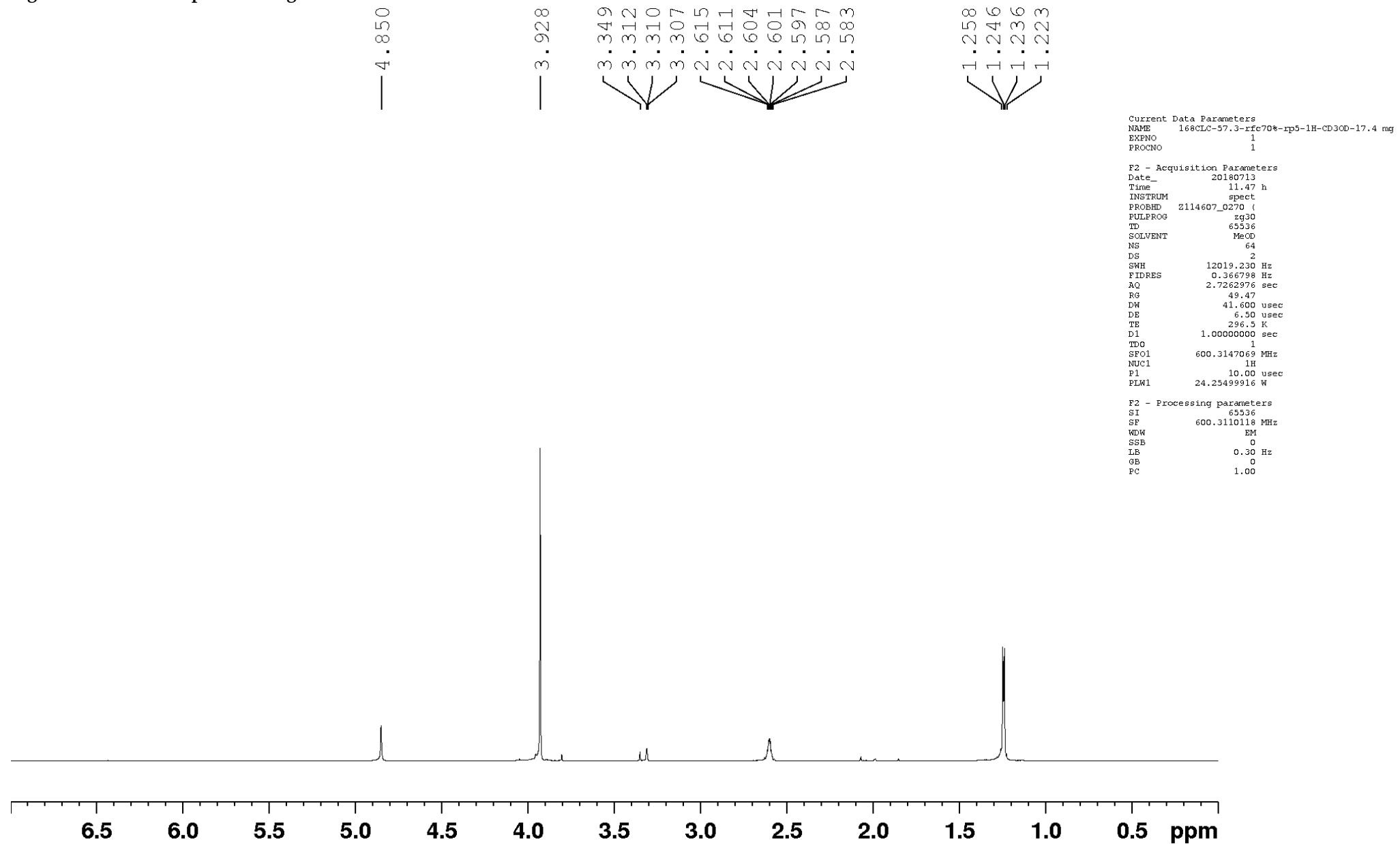


Figure S24. ^{13}C NMR spectrum of gliorosein (3)

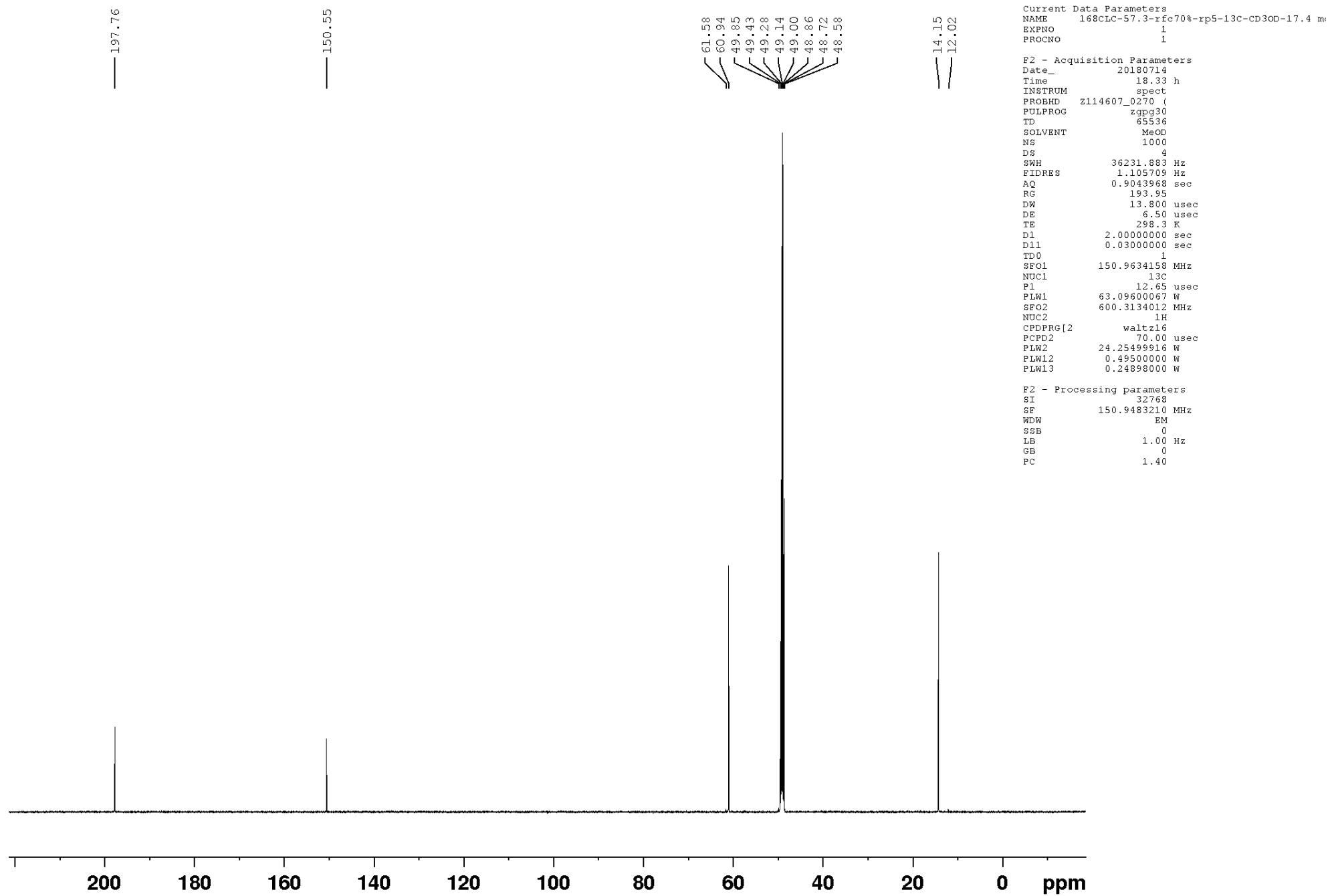


Figure S25. CD spectrum of gliorosein (3)

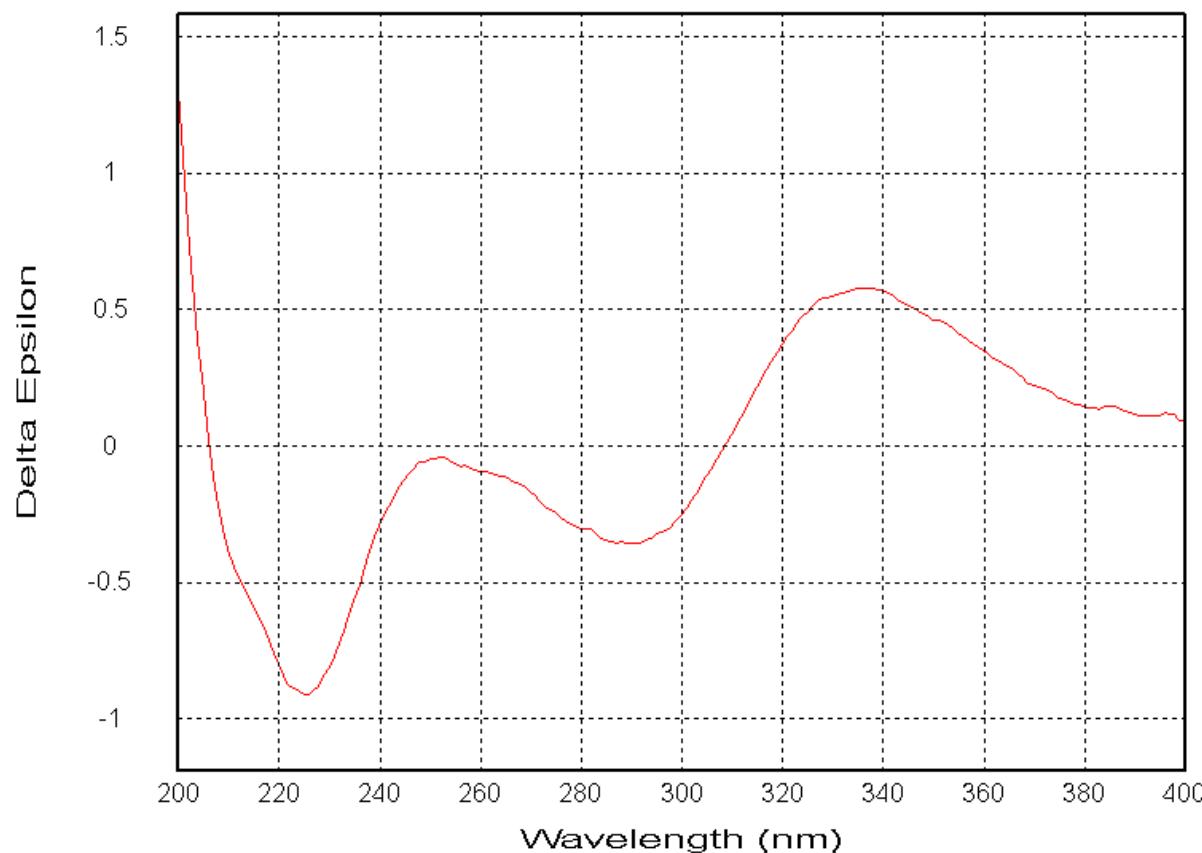


Figure S26. ^1H NMR spectrum of balticolid (4)

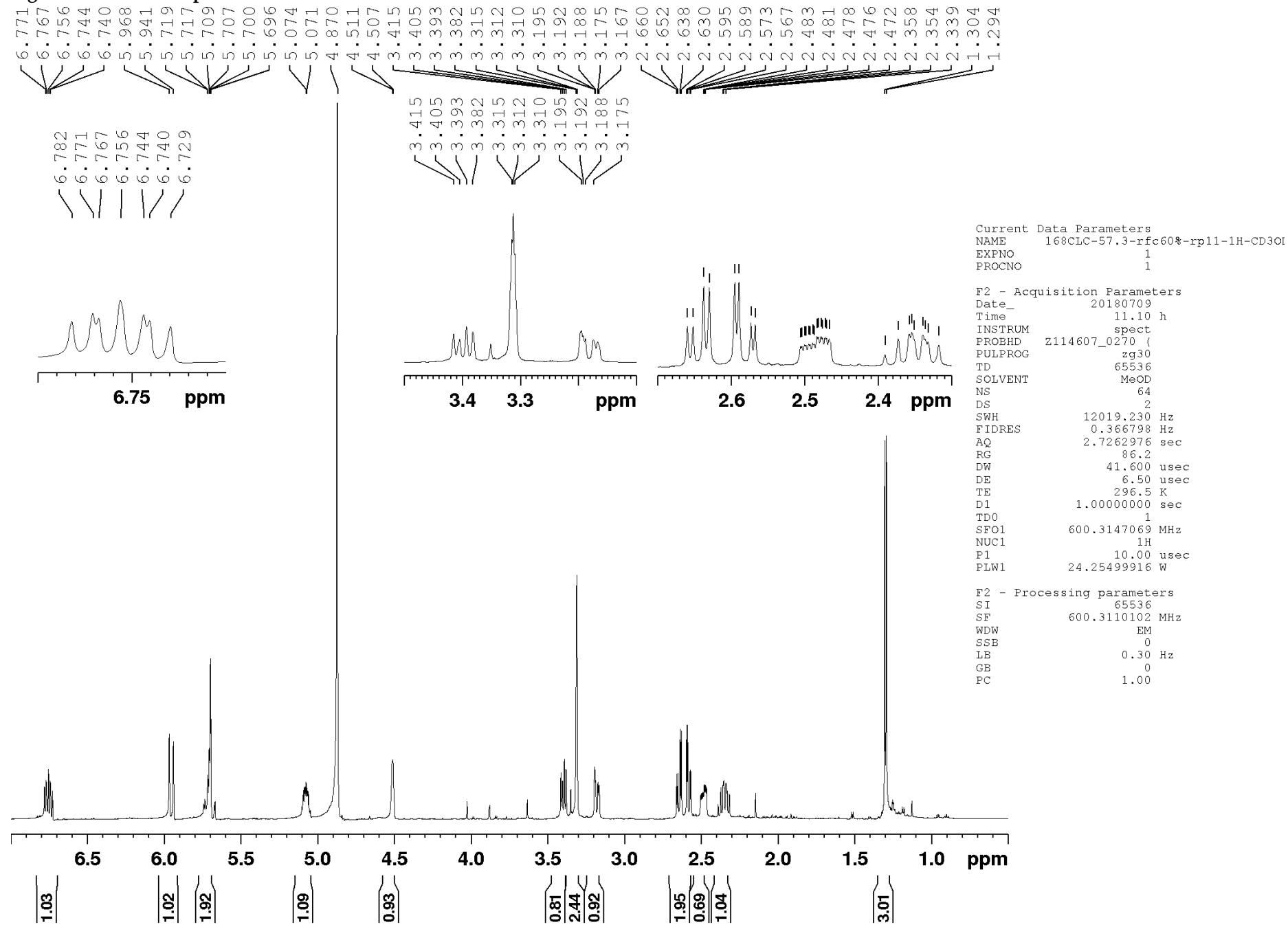


Figure S27. ^{13}C NMR spectrum of balticolid (4)

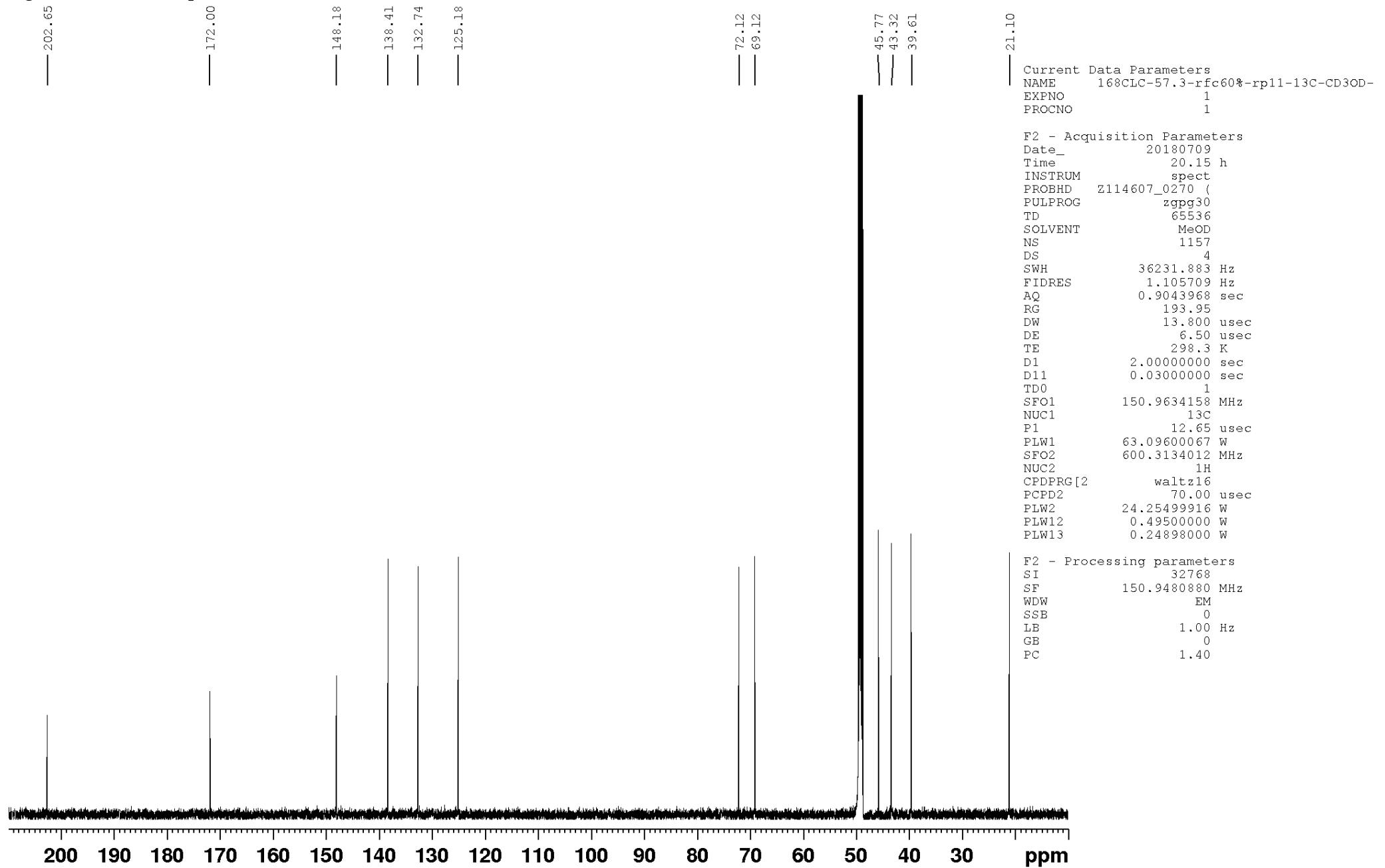


Figure S28. ^1H NMR spectrum of dendrodolide G (5)

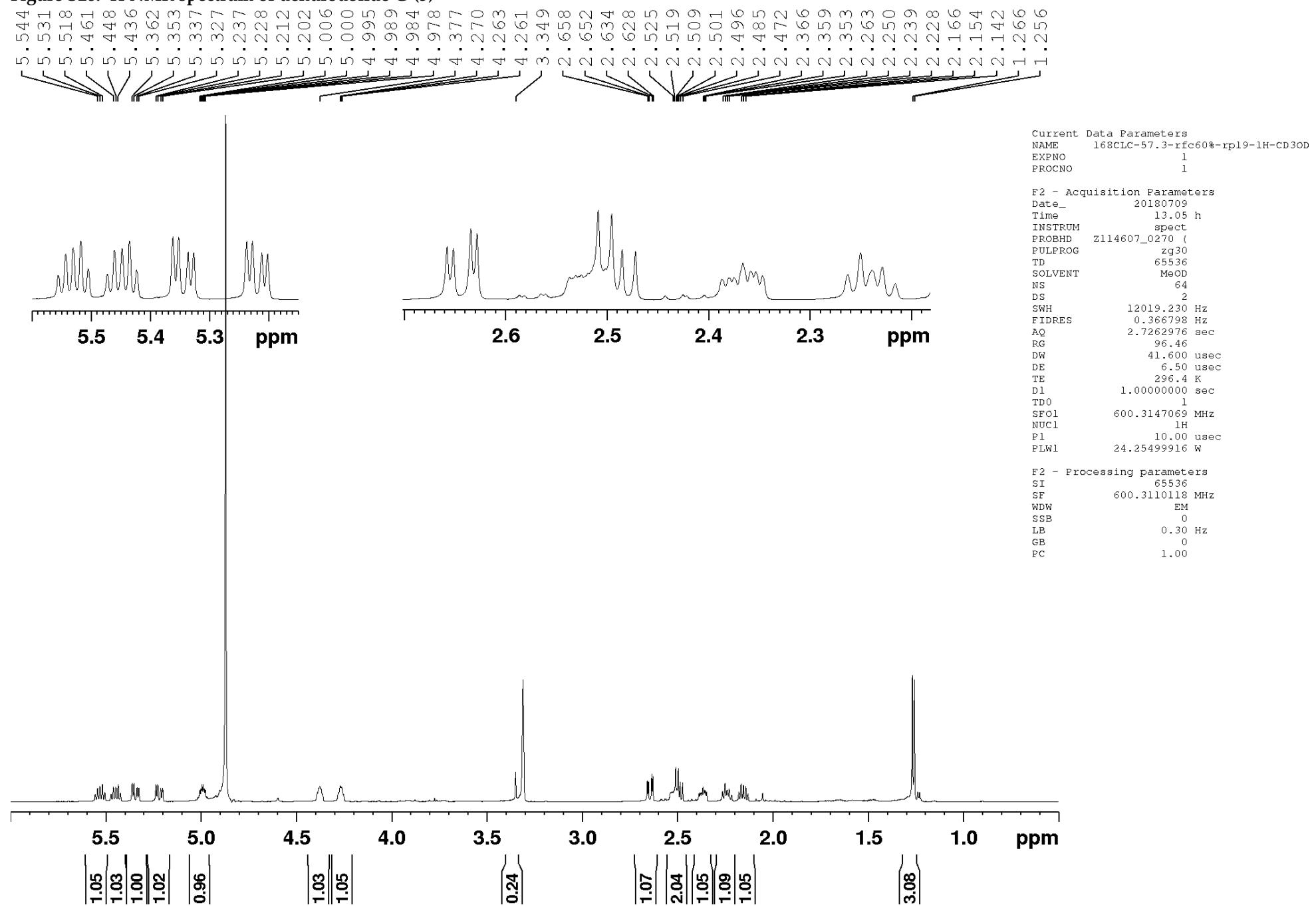


Figure S29. ^{13}C NMR spectrum of dendrodolide G (5)

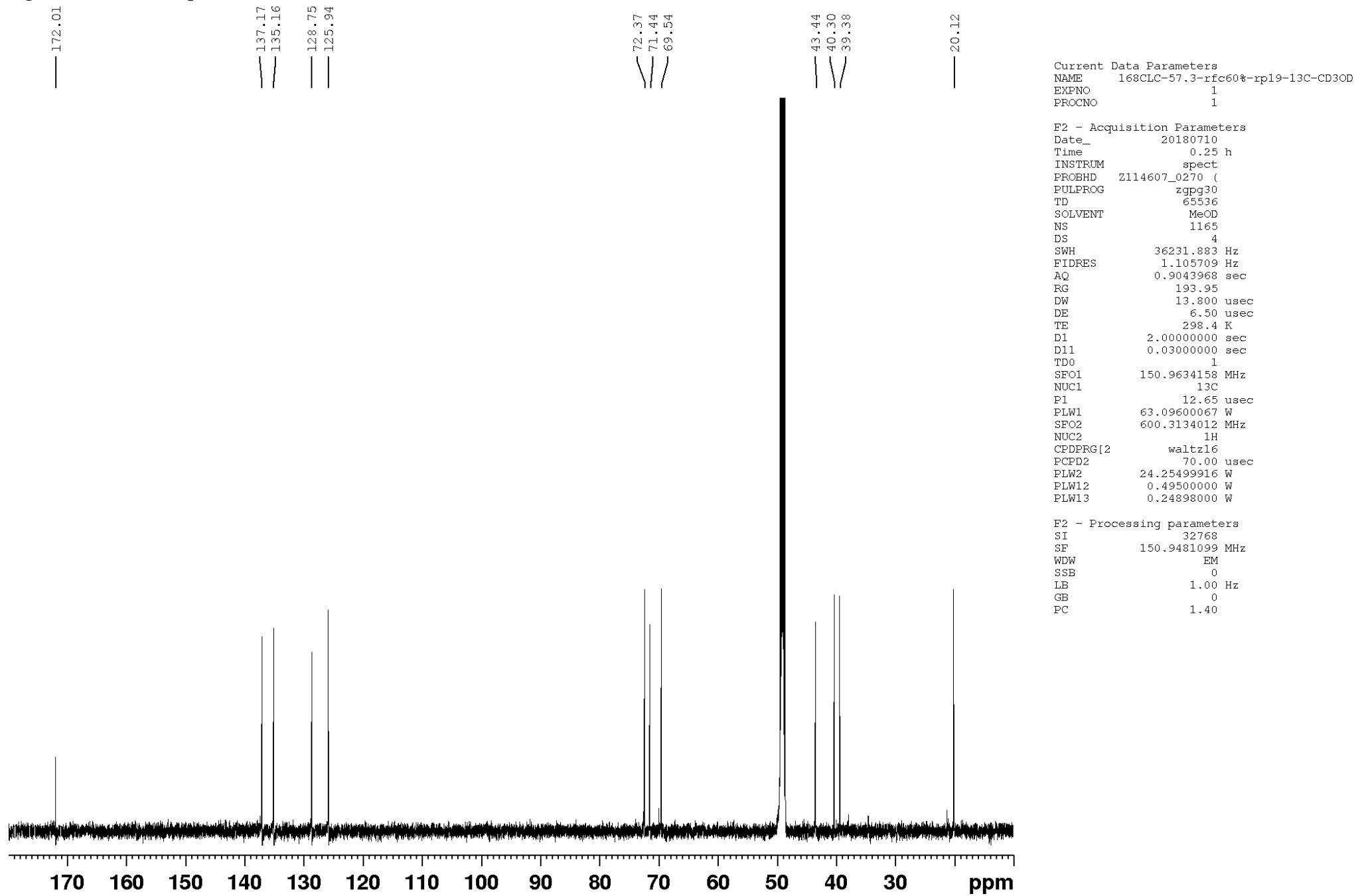


Figure S30. ^1H NMR spectrum of dihydroisocoumarine (6)

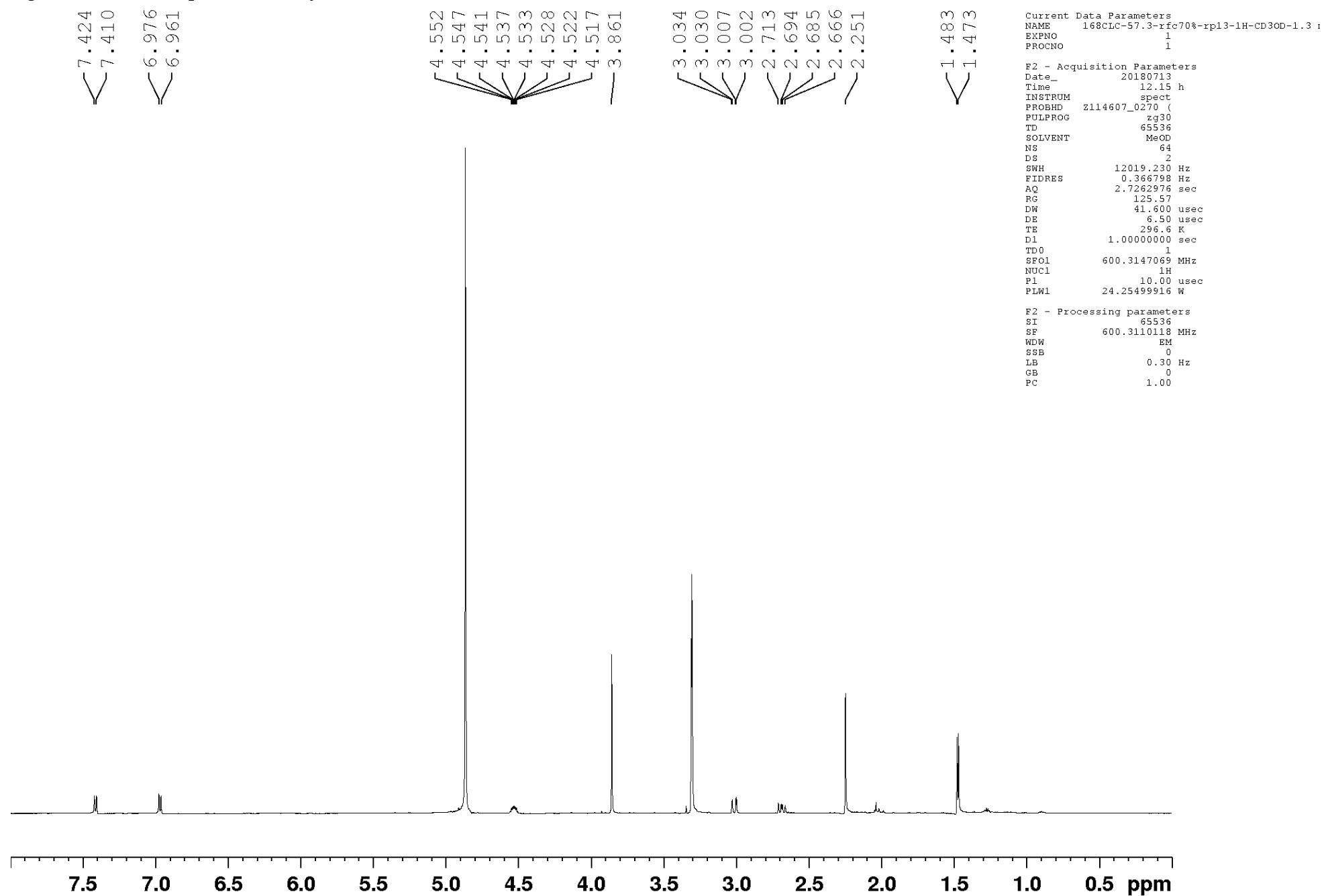


Figure S31. ^{13}C NMR spectrum of dihydroisocoumarine (6)

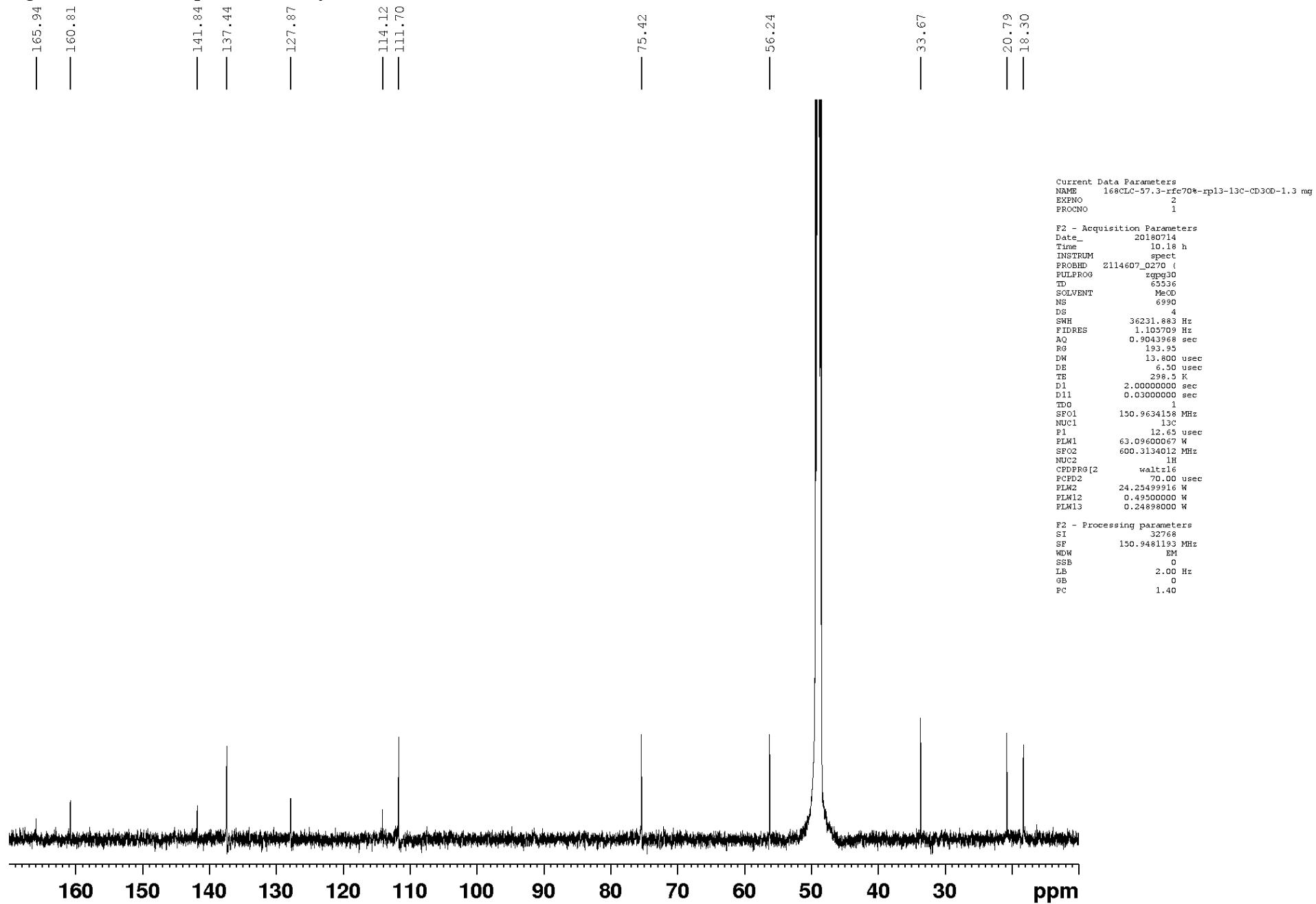


Figure S32. ^1H NMR spectrum of ($-$)-5-methylmellein (7)

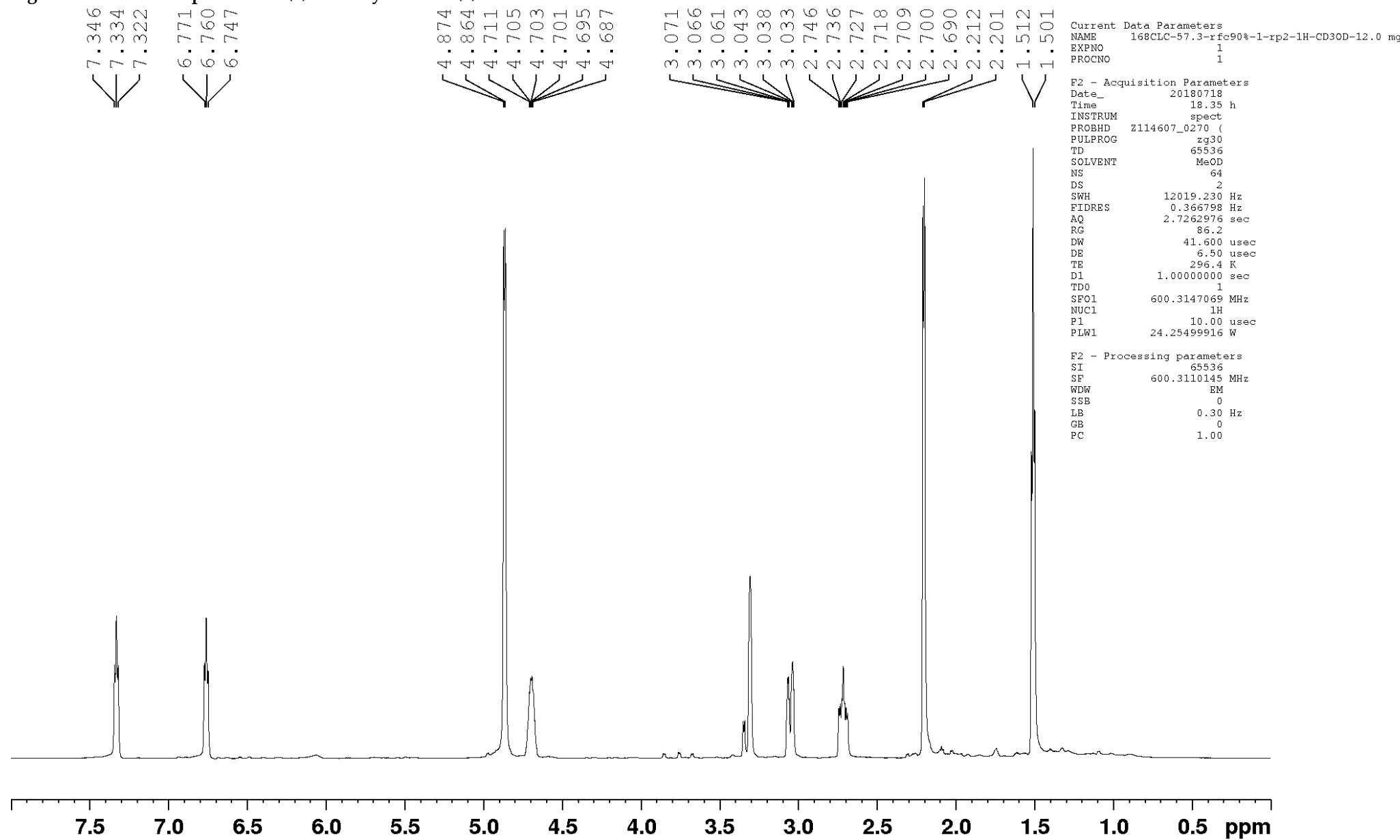


Figure S33. ^{13}C NMR spectrum of (-)-5-methylmellein (7)

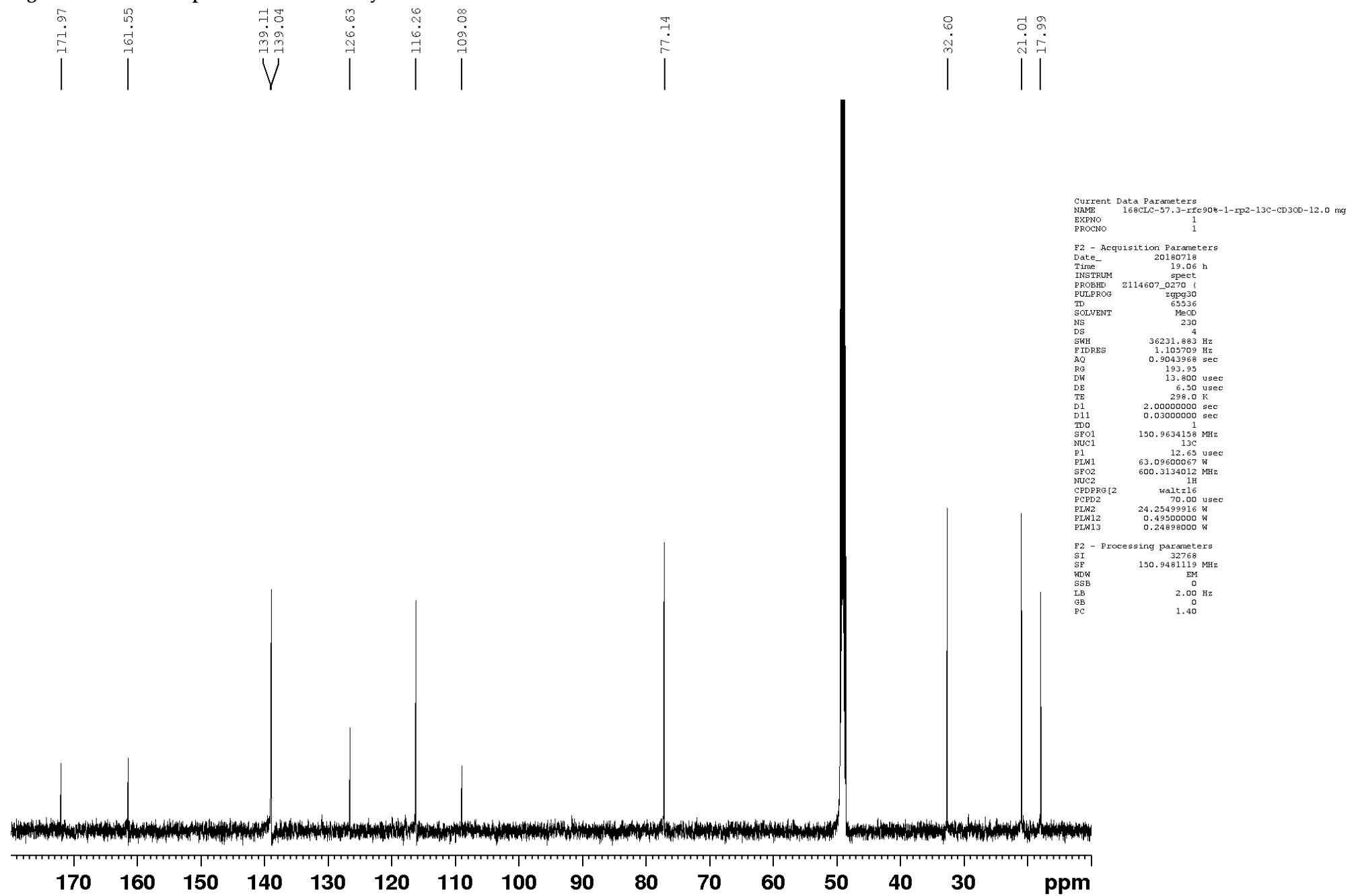


Figure S34. ^1H NMR spectrum of dendrodochol B (8)

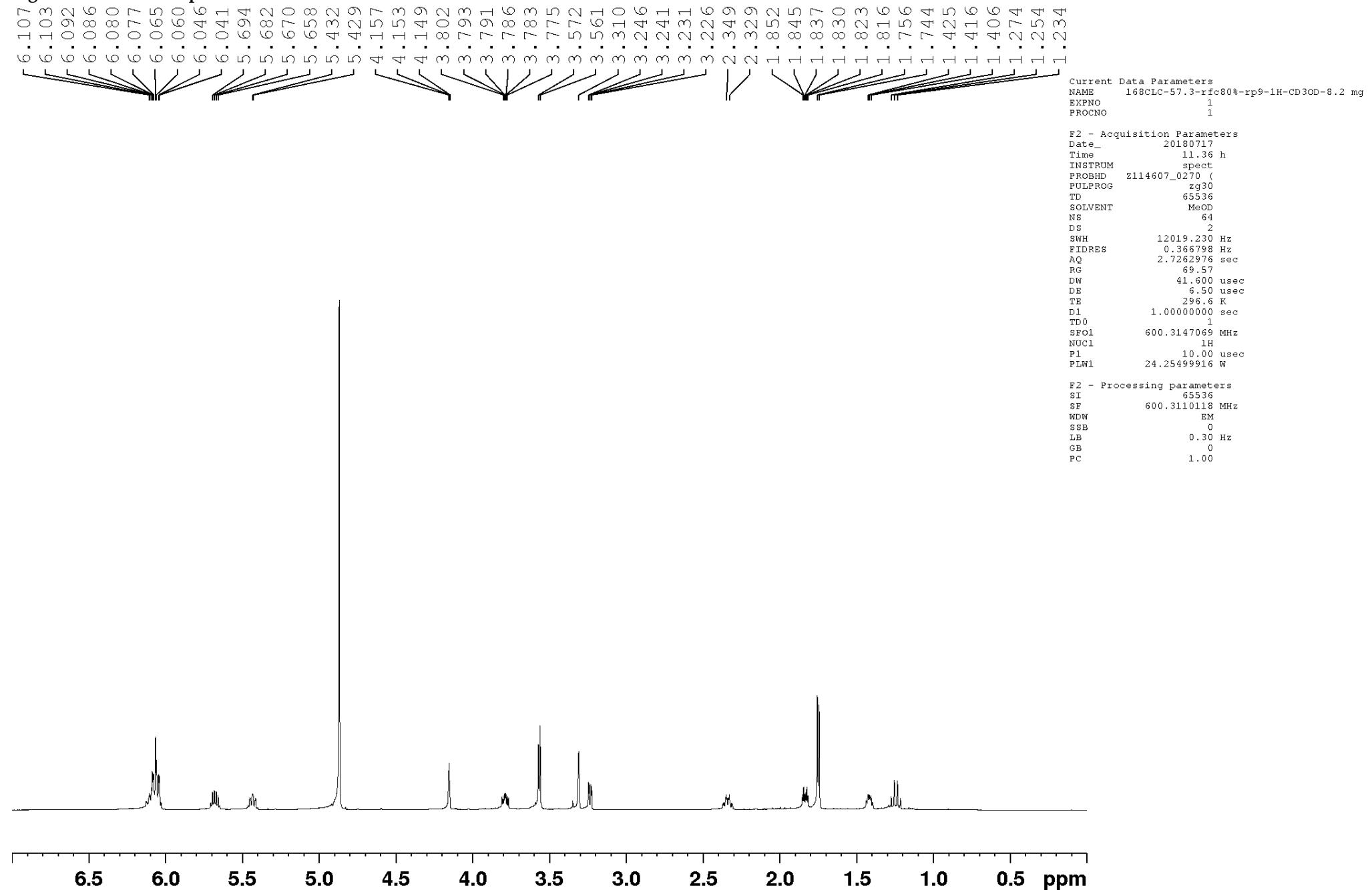


Figure S35. ^{13}C NMR spectrum of dendrodochol B (8)

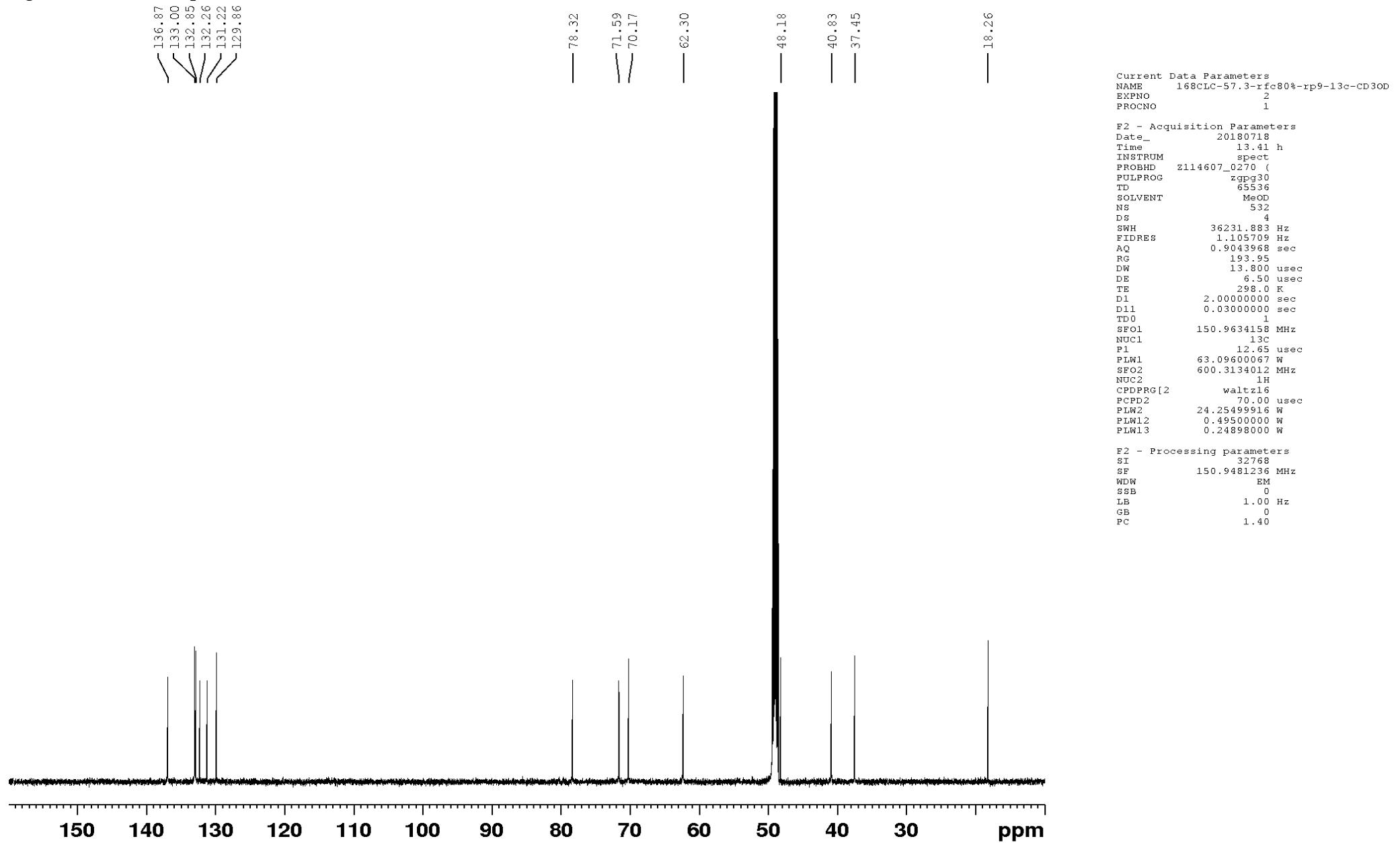
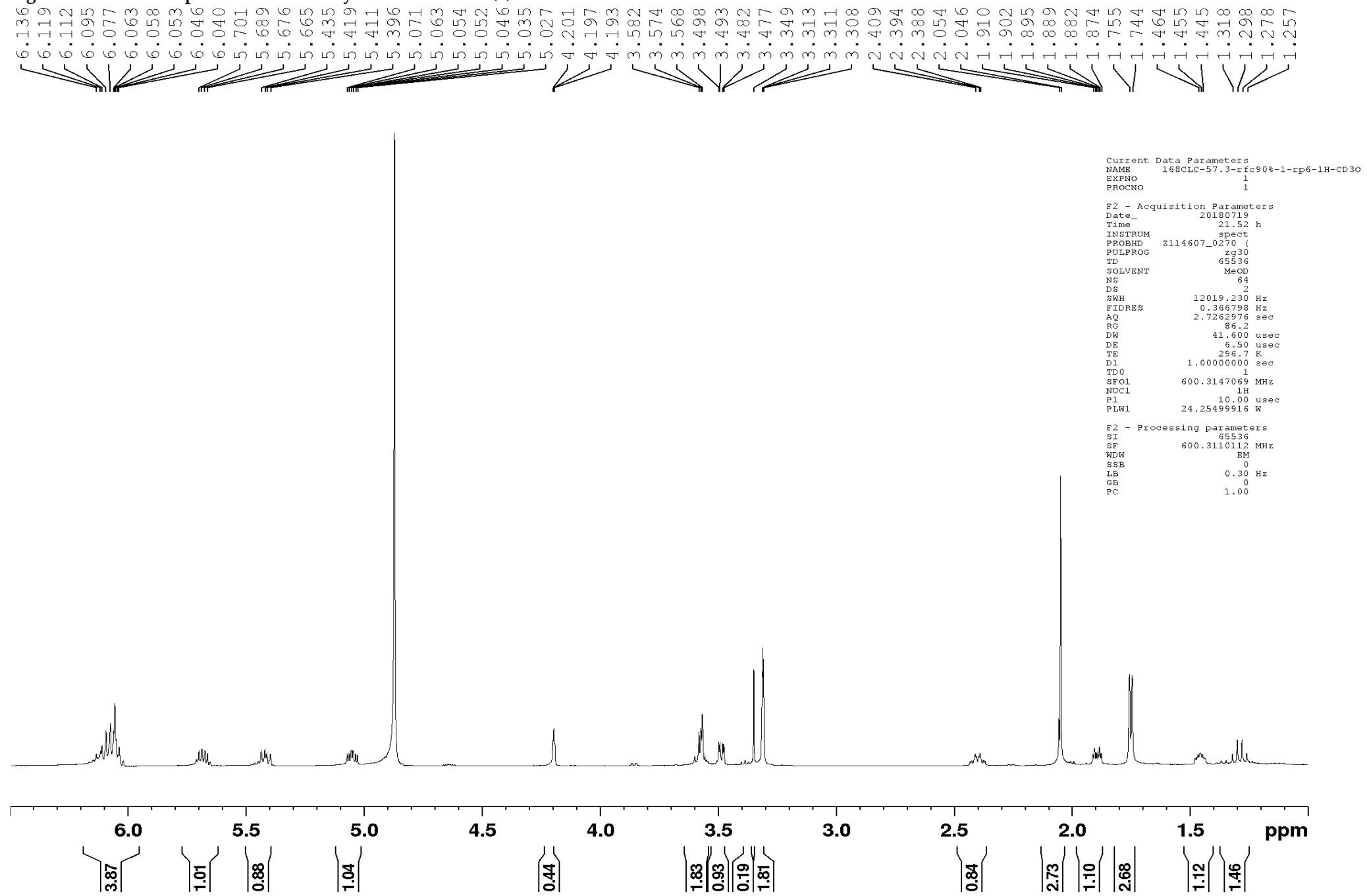
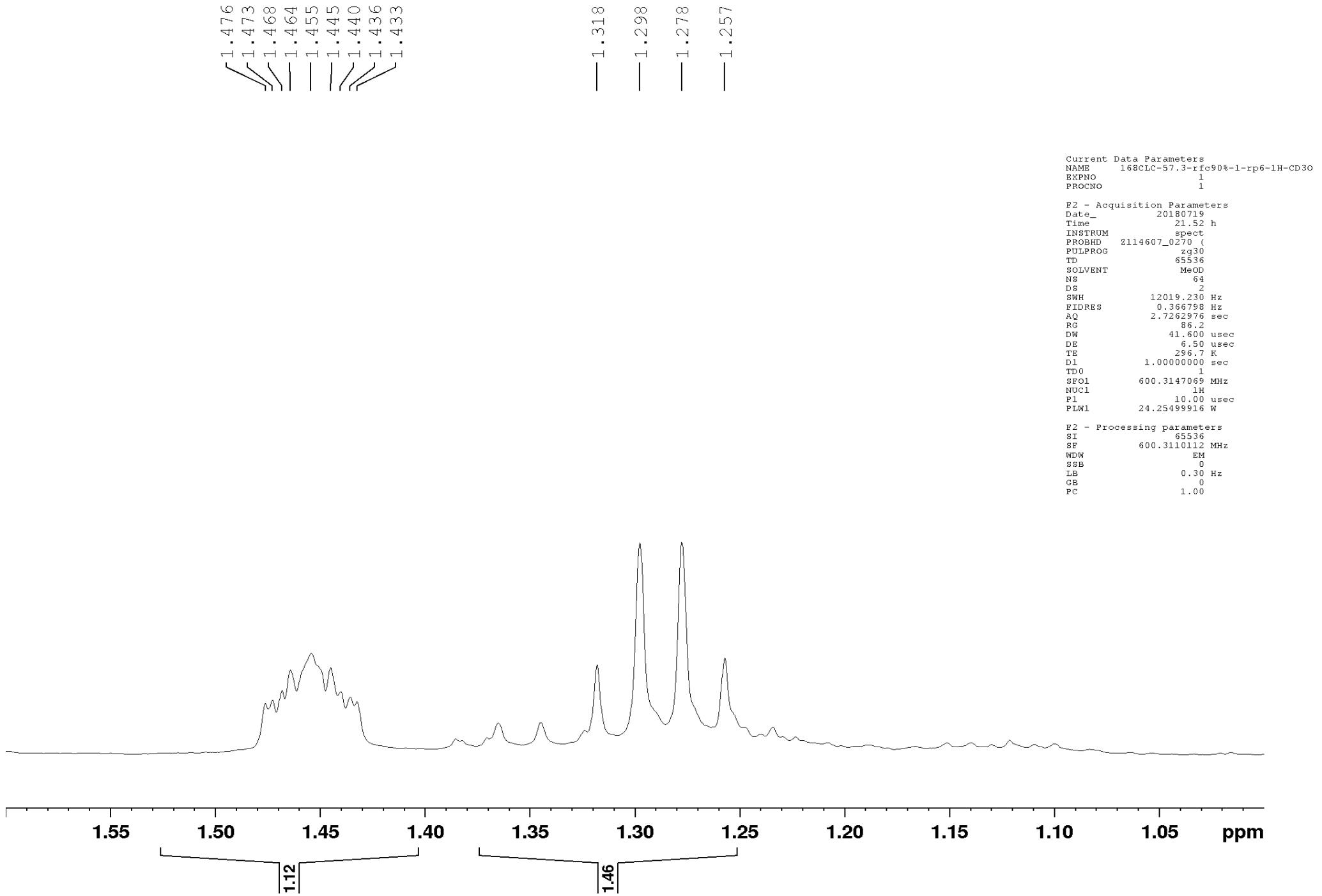
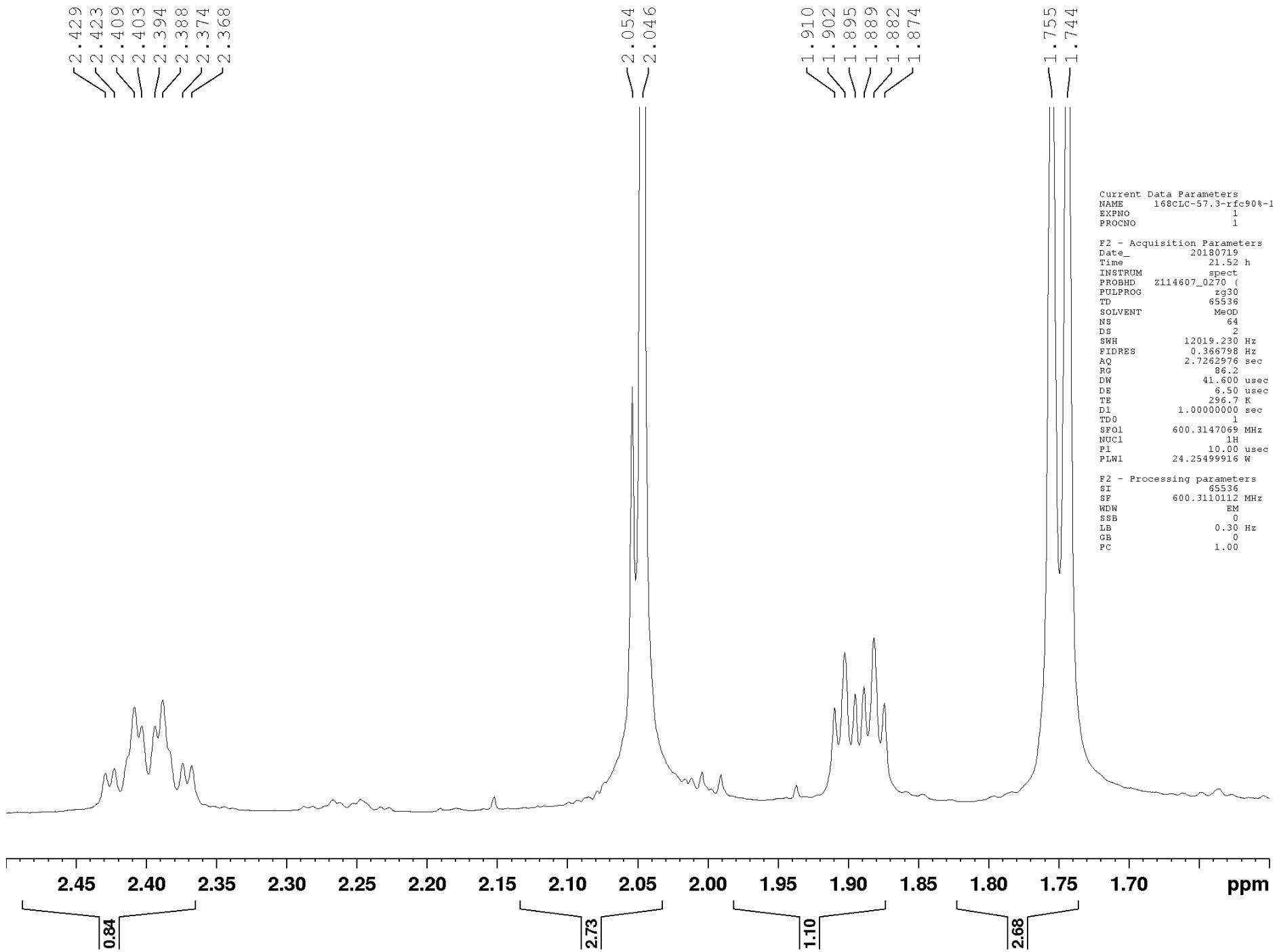


Figure S36. ^1H NMR spectrum of 1-O-acetylidendrocholesterol B (9)





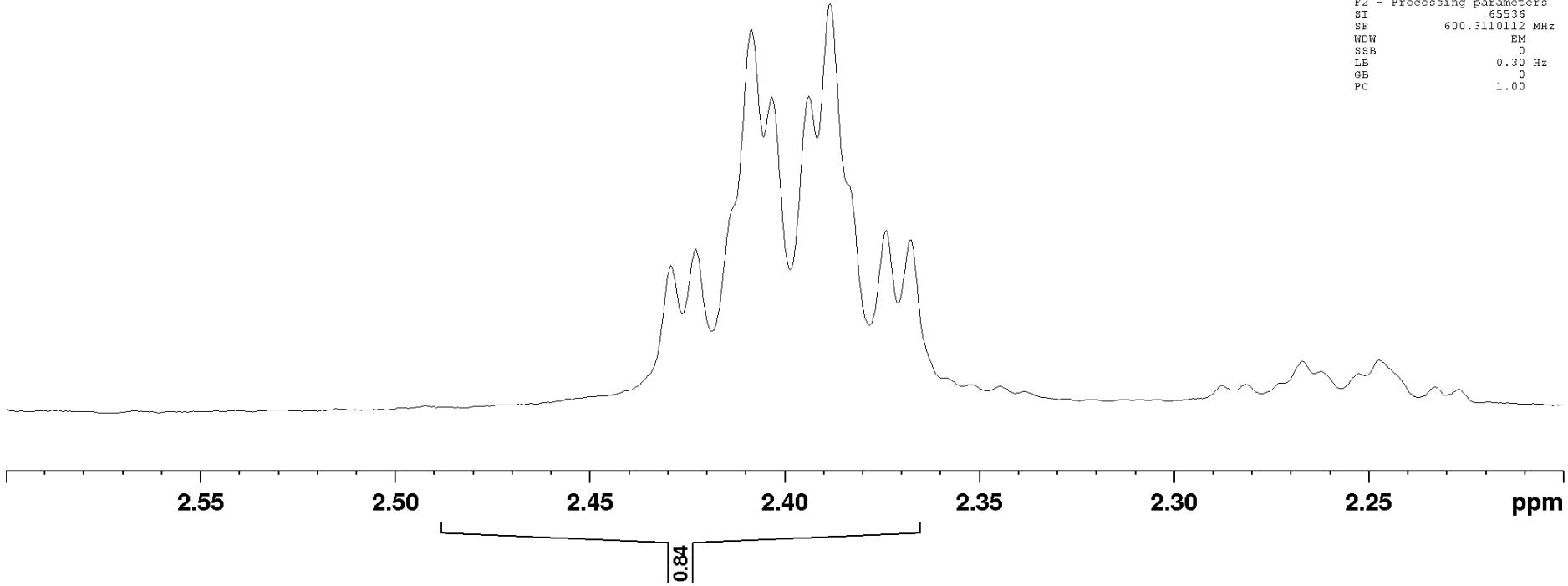


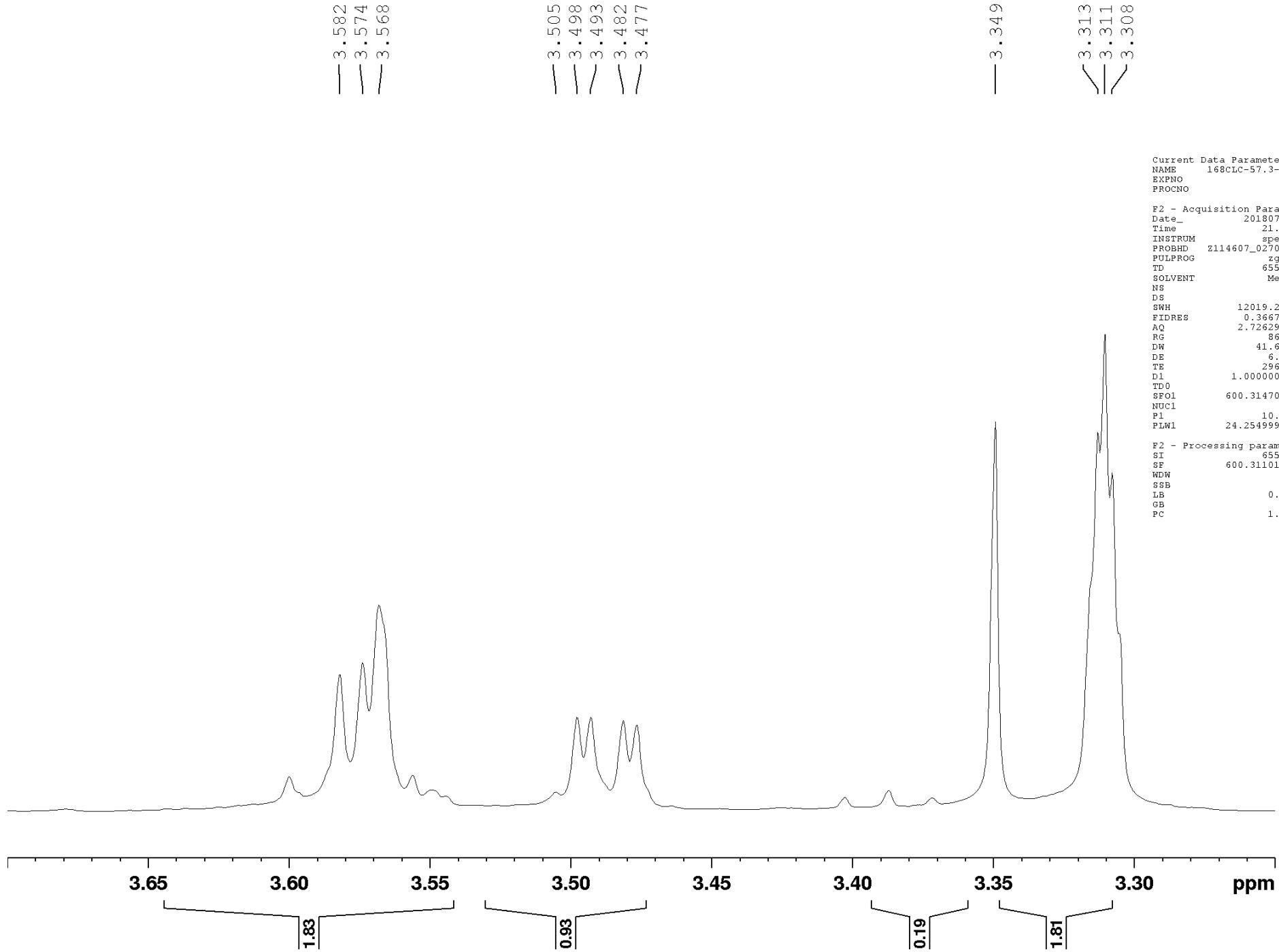
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PROCNO 1

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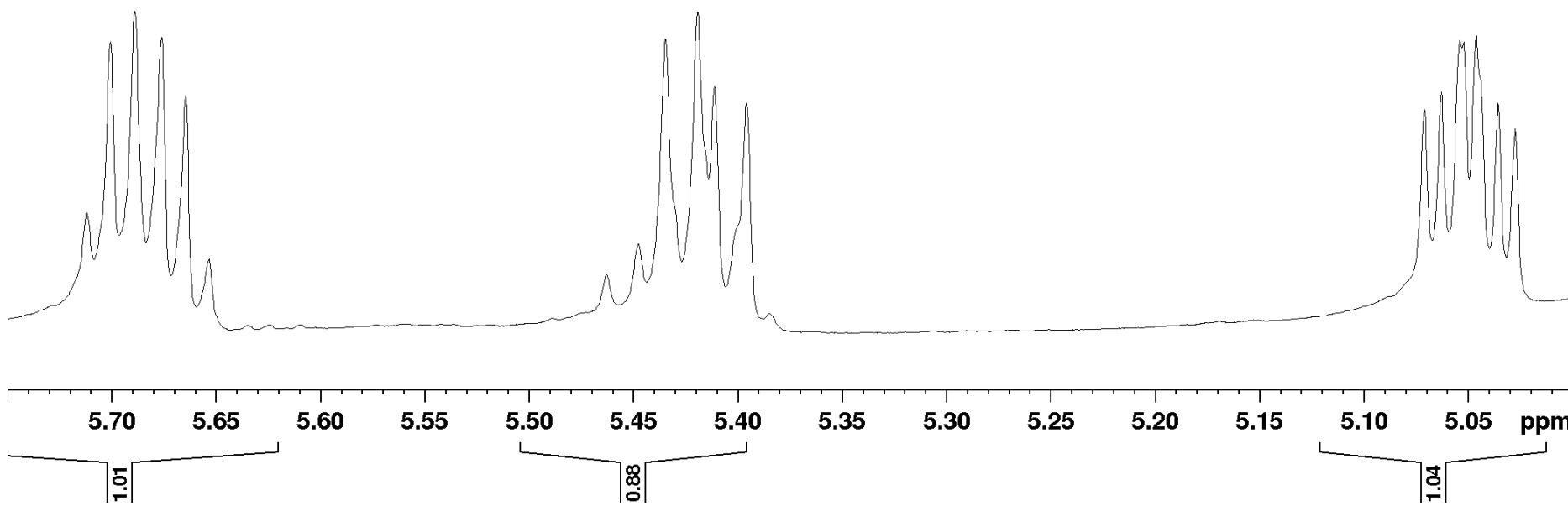
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PROCNO 1

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DE 6.50 usec
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TD0 1
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NUC1 1H
P1 10.00 usec
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E2 - Processing parameters
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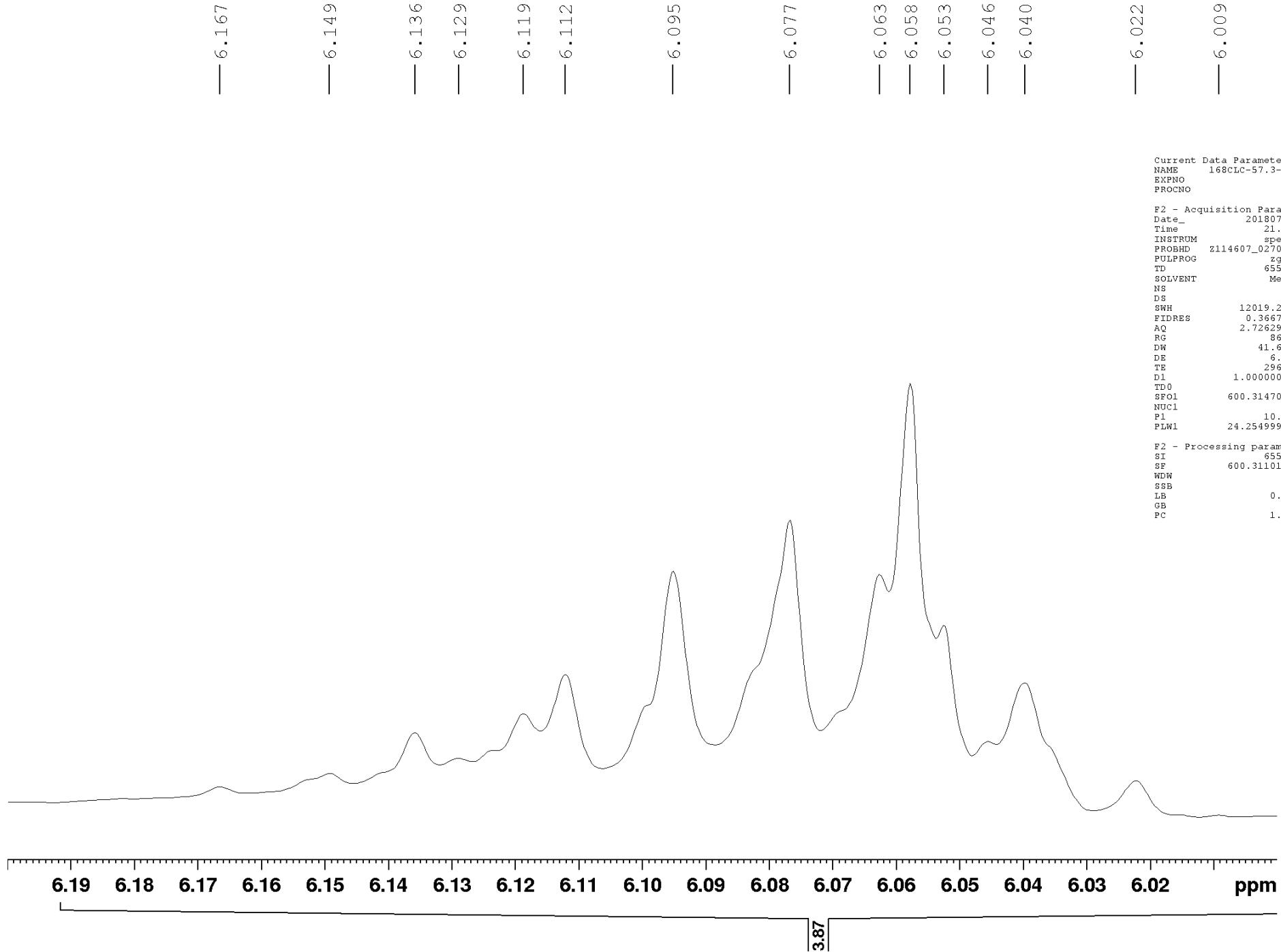


Figure S37. ^{13}C NMR spectrum of 1-O-acetylidendrodochol B (9)

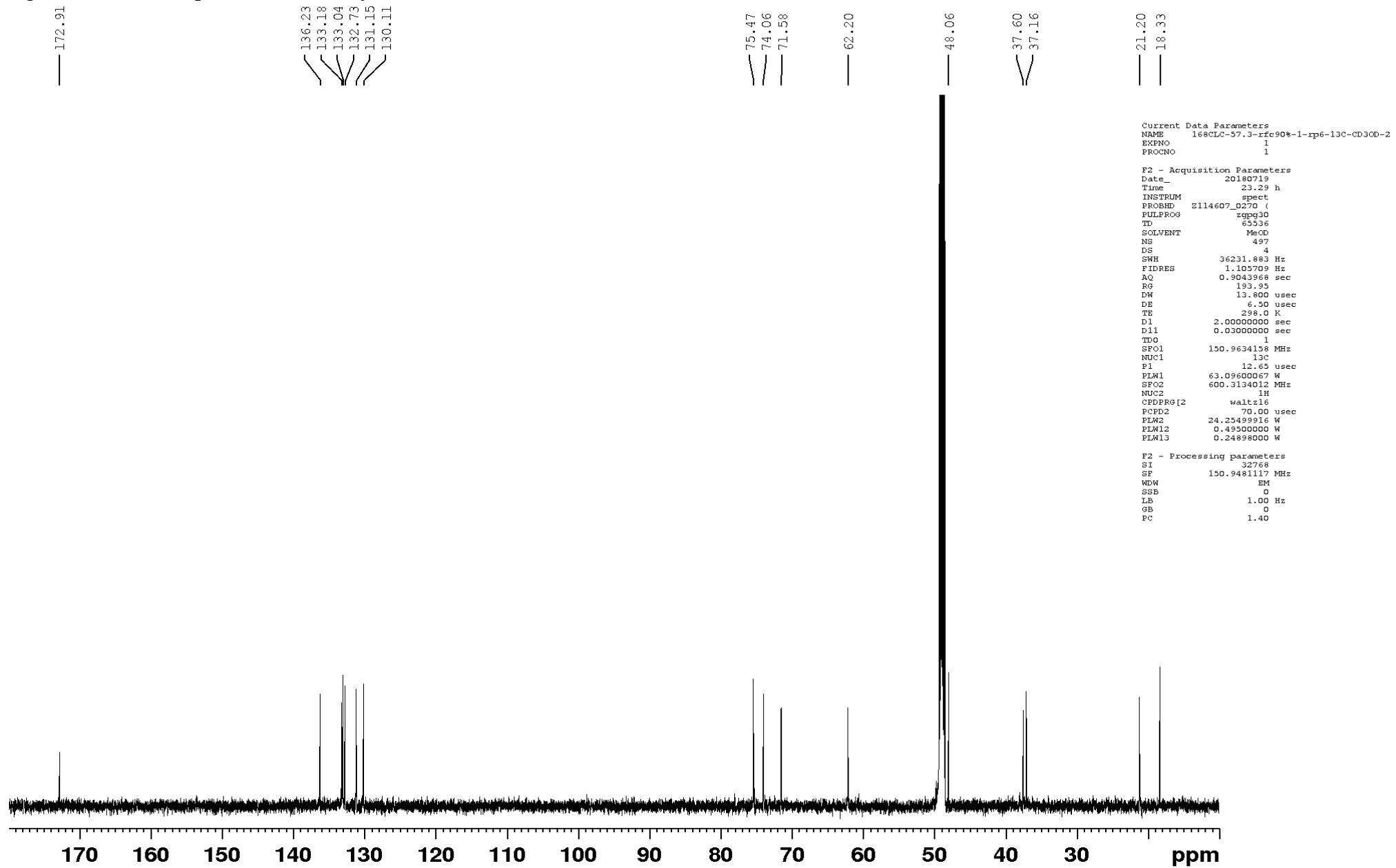


Figure S38. ^1H - ^1H spectrum of 1-O-acetylidendrochol B (9)

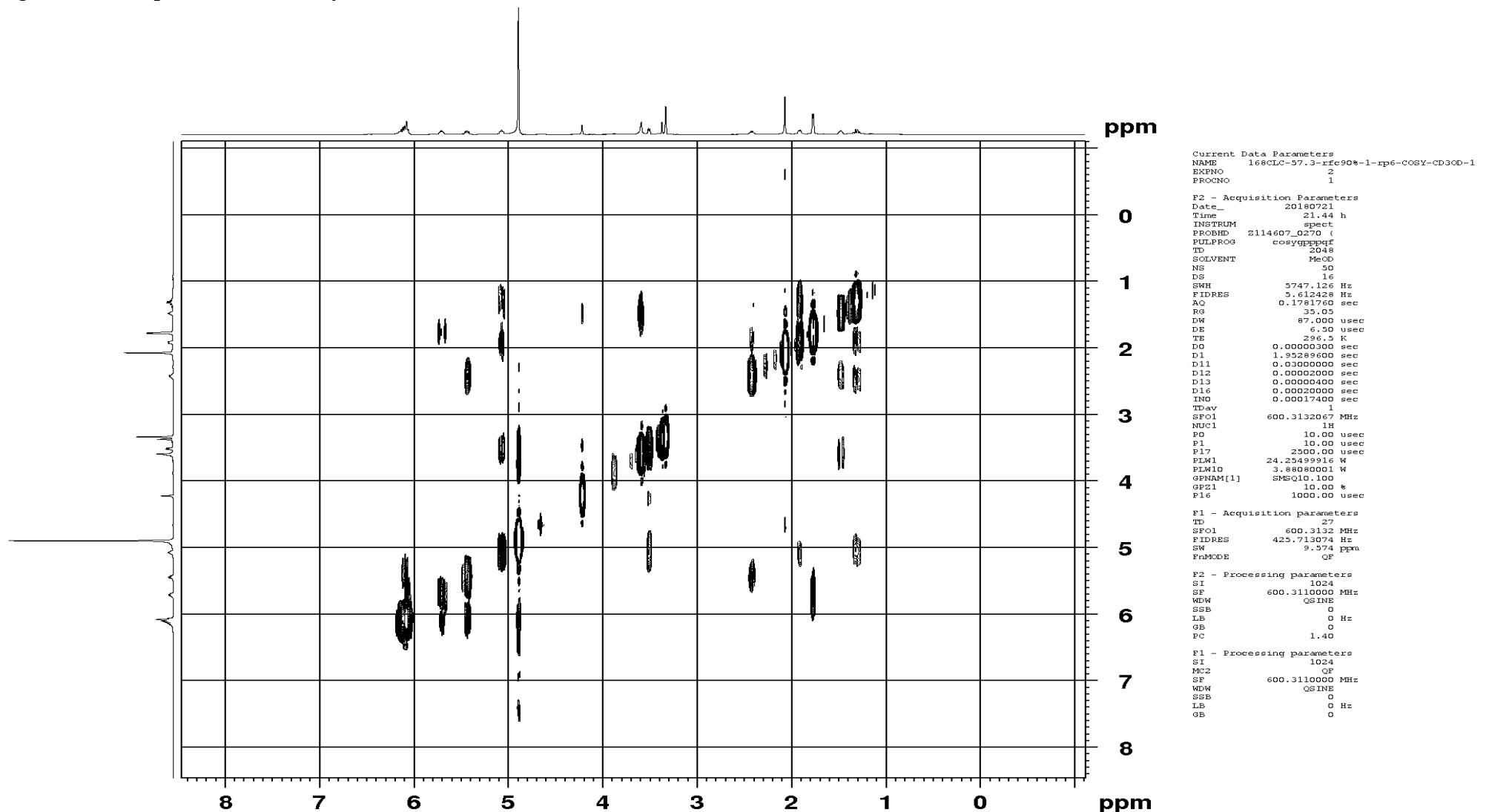


Figure S39. HMBC spectrum of 1-O-acetylidendrochole B (9)

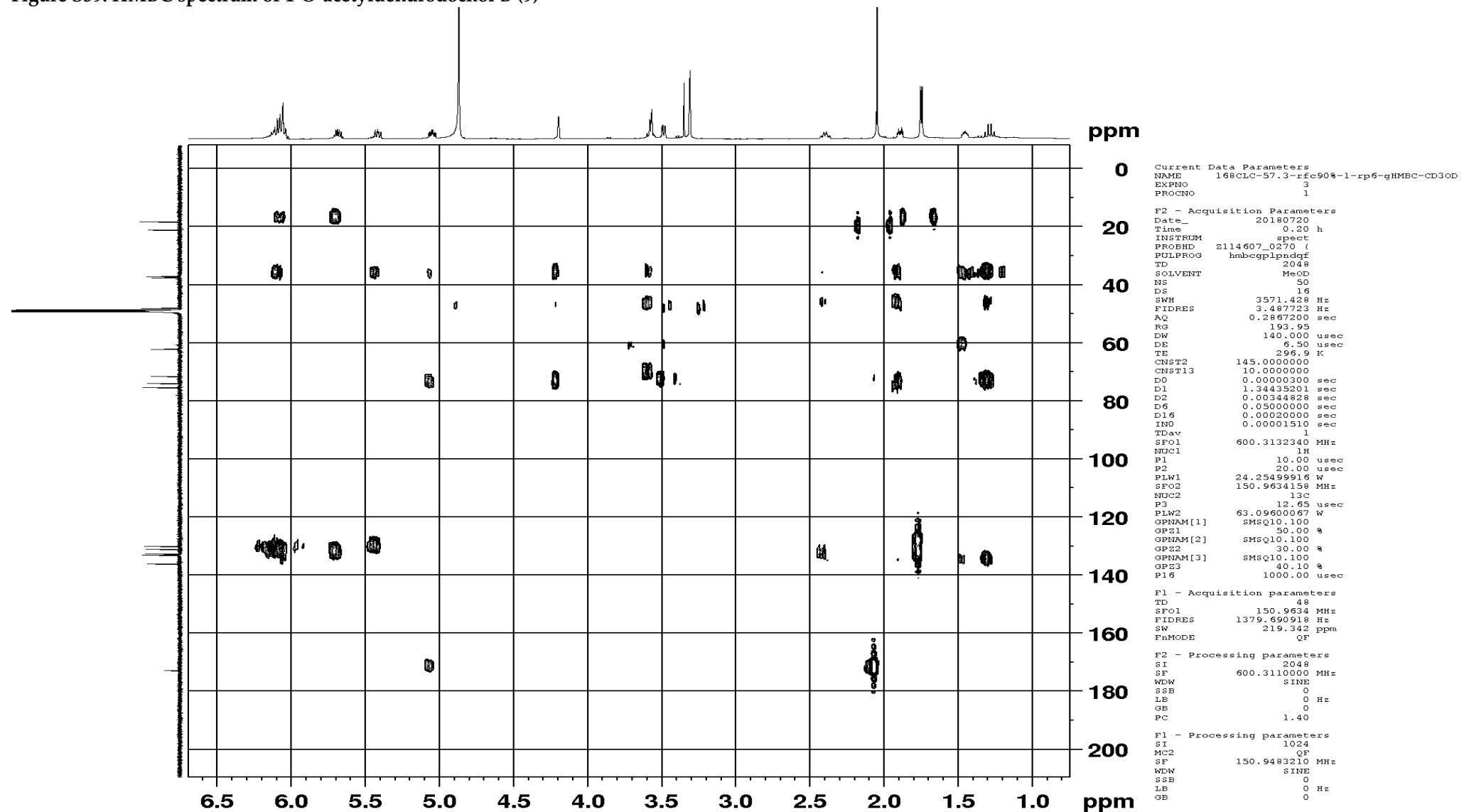


Figure S40. HSQC spectrum of 1-O-acetylidendrochol B (9)

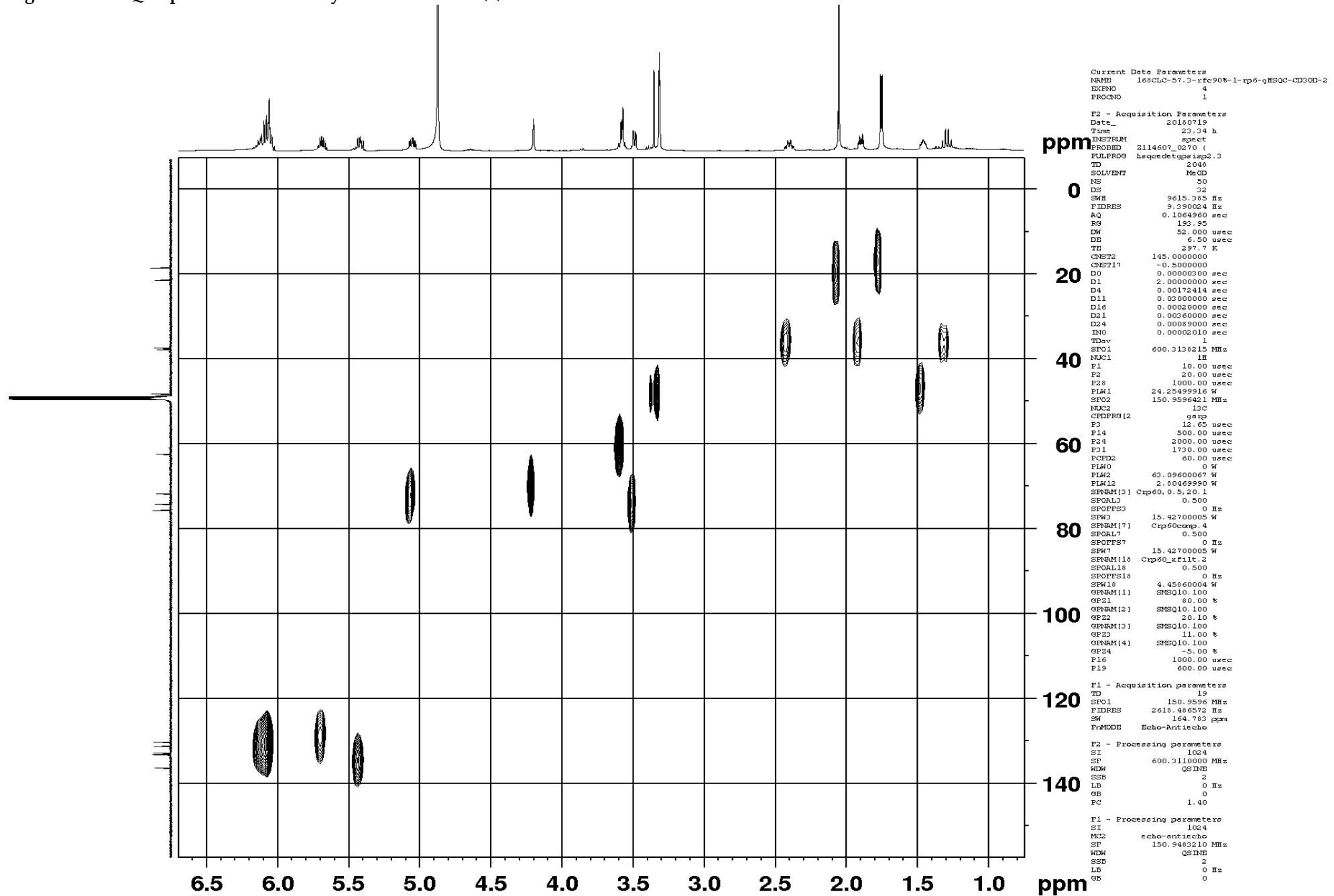


Figure S41. CD spectrum of 1-O-acetylidendrochol B (9)

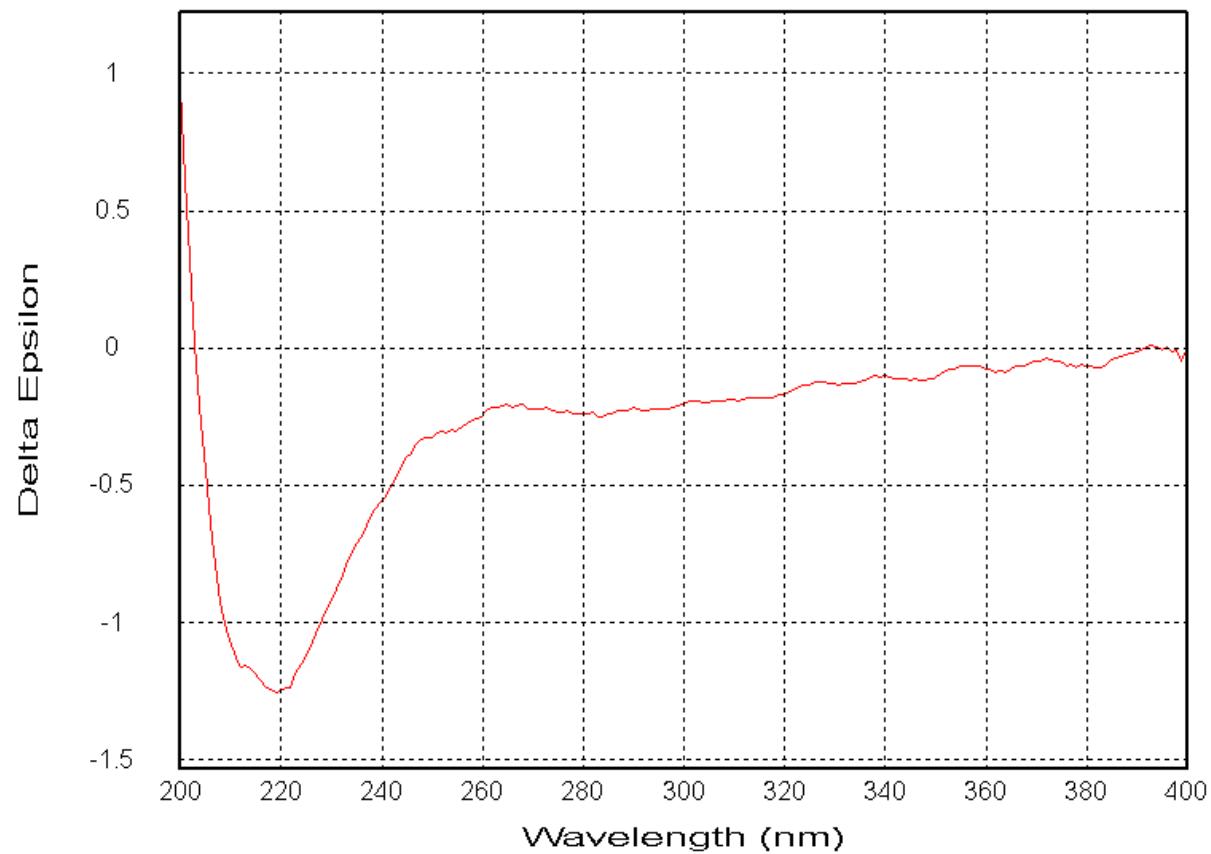
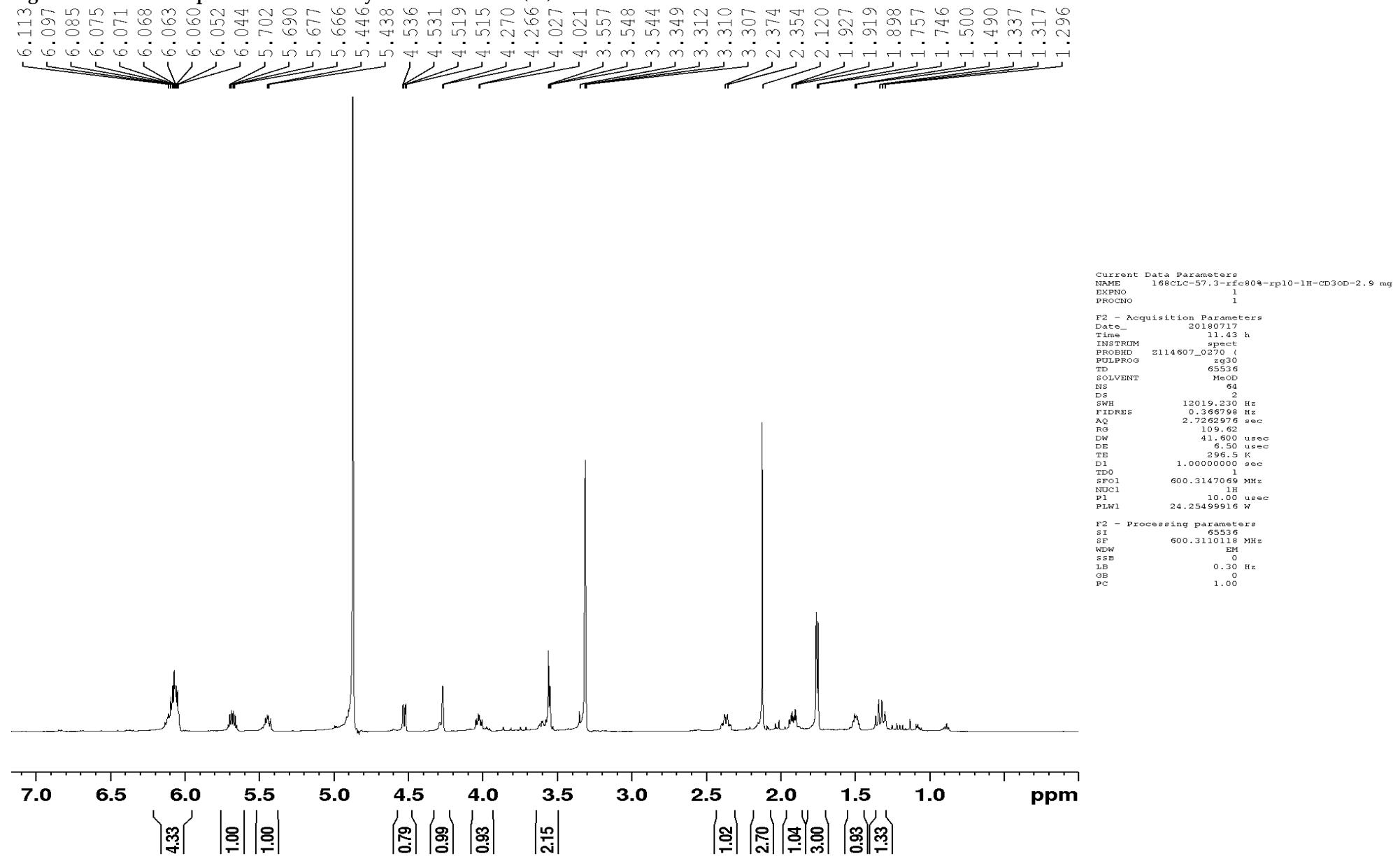
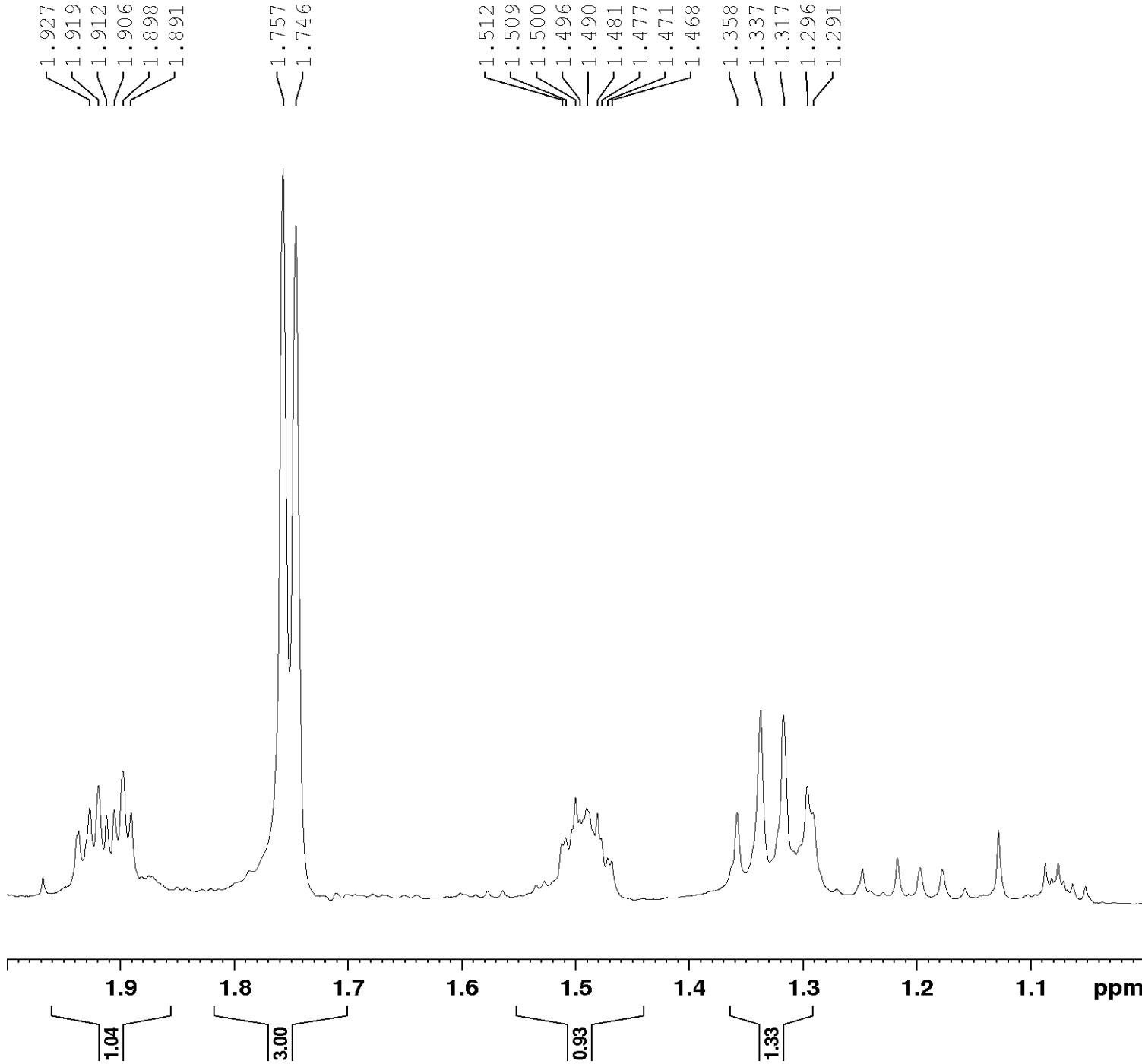


Figure S42. ^1H NMR spectrum of 2-O-acetylidendrodochol B (10)

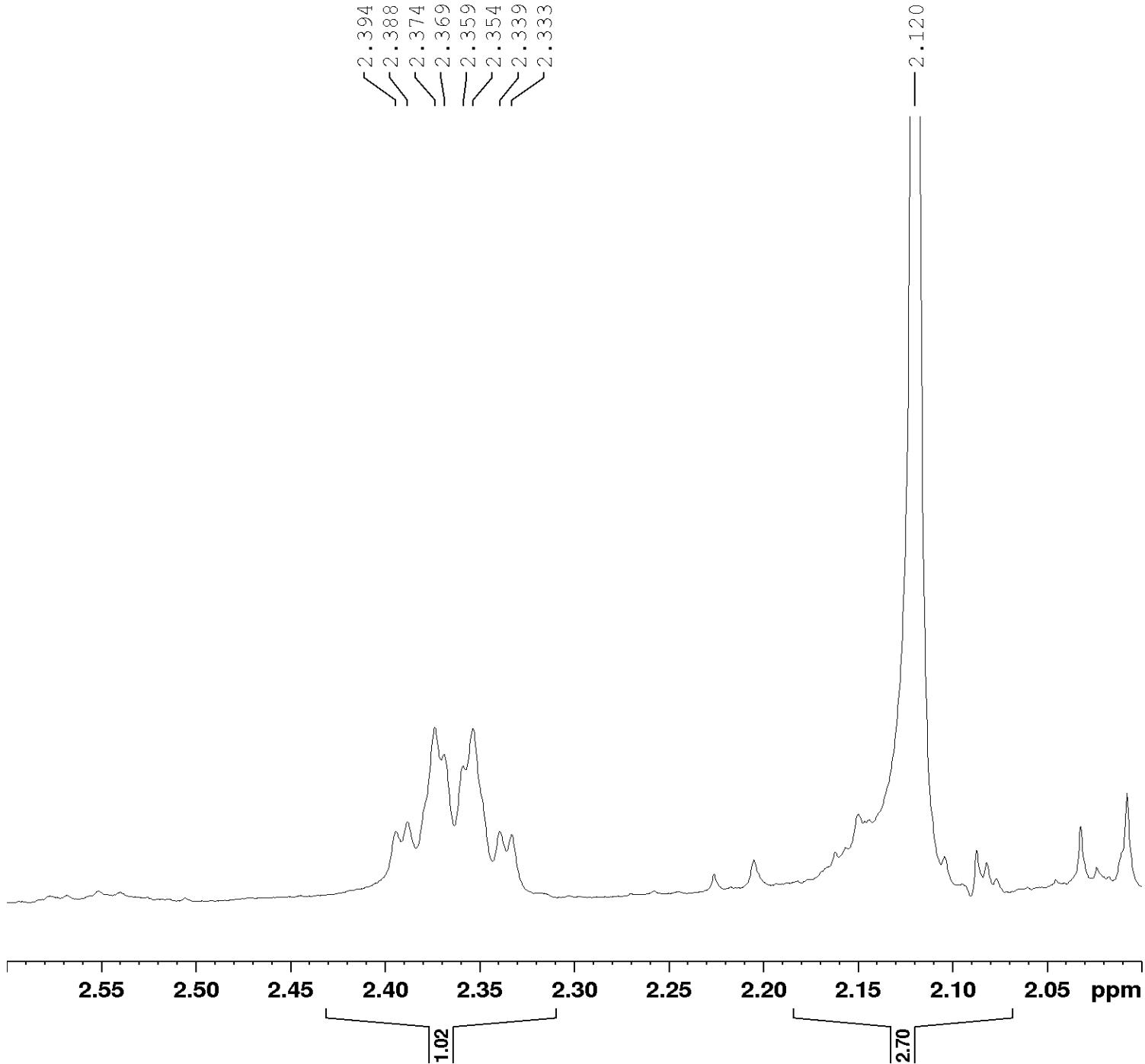




Current Data Parameters
 NAME 168CLC-57.3-rfc80%-rp10-1H-CD3OD-2.9 mg
 EXPNO 1
 PROCN0 1

F2 - Acquisition Parameters
 Date_ 20180717
 Time 11.43 h
 INSTRUM spect
 PROBHD Z114607_0270 (
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 64
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 2.7262976 sec
 RG 109.62
 DW 41.600 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.0000000 sec
 TD0 1
 SFO1 600.3147069 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 24.25499916 W

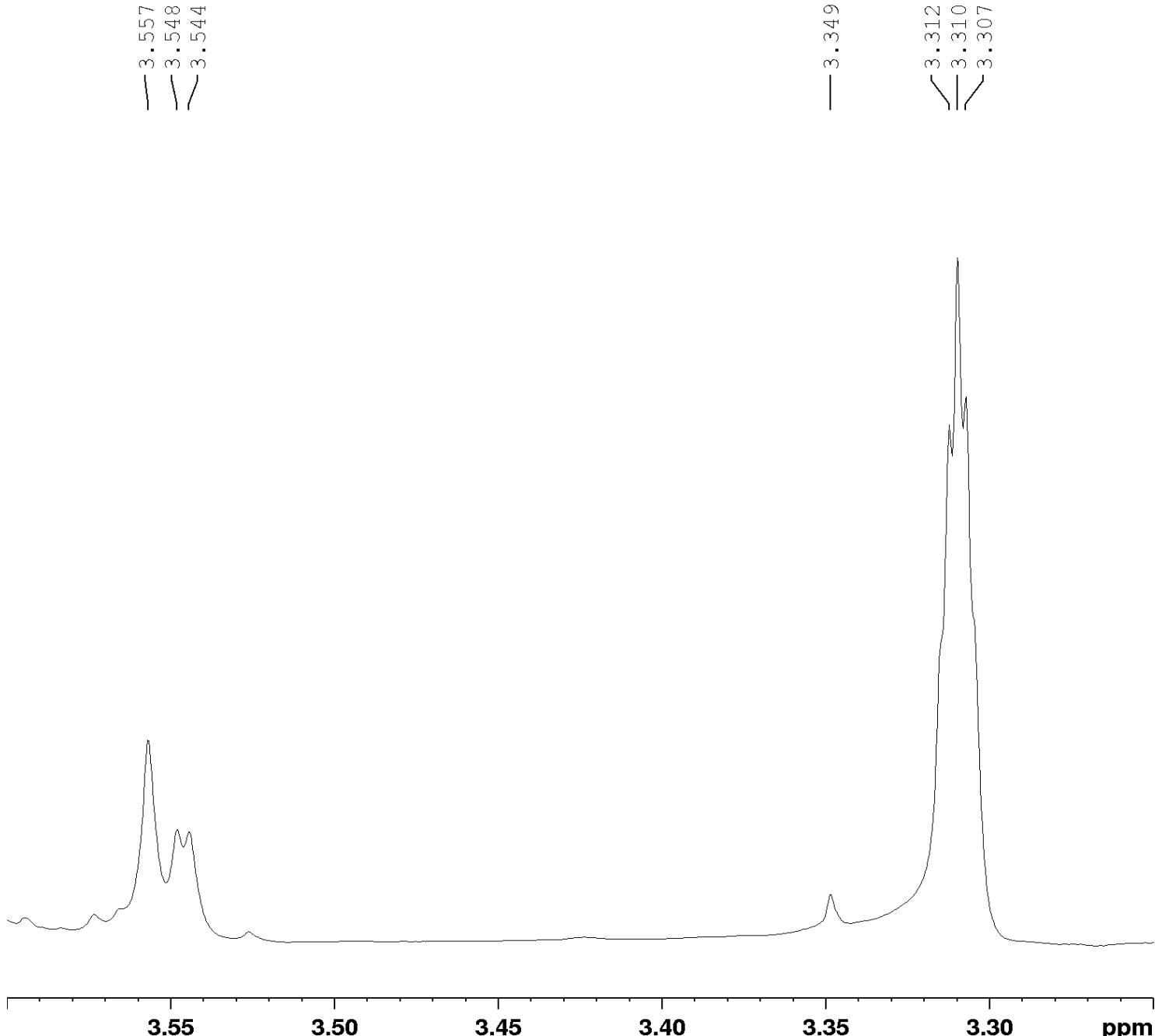
F2 - Processing parameters
 SI 65536
 SF 600.3110118 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 168CLC-57.3-rfc80%-rp10-1H-CD3OD-2.9 mg
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180717
Time 11.43 h
INSTRUM spect
PROBHD Z114607_0270 (
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 109.62
DW 41.600 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 600.3147069 MHz
NUC1 1H
P1 10.00 usec
PLW1 24.25499916 W

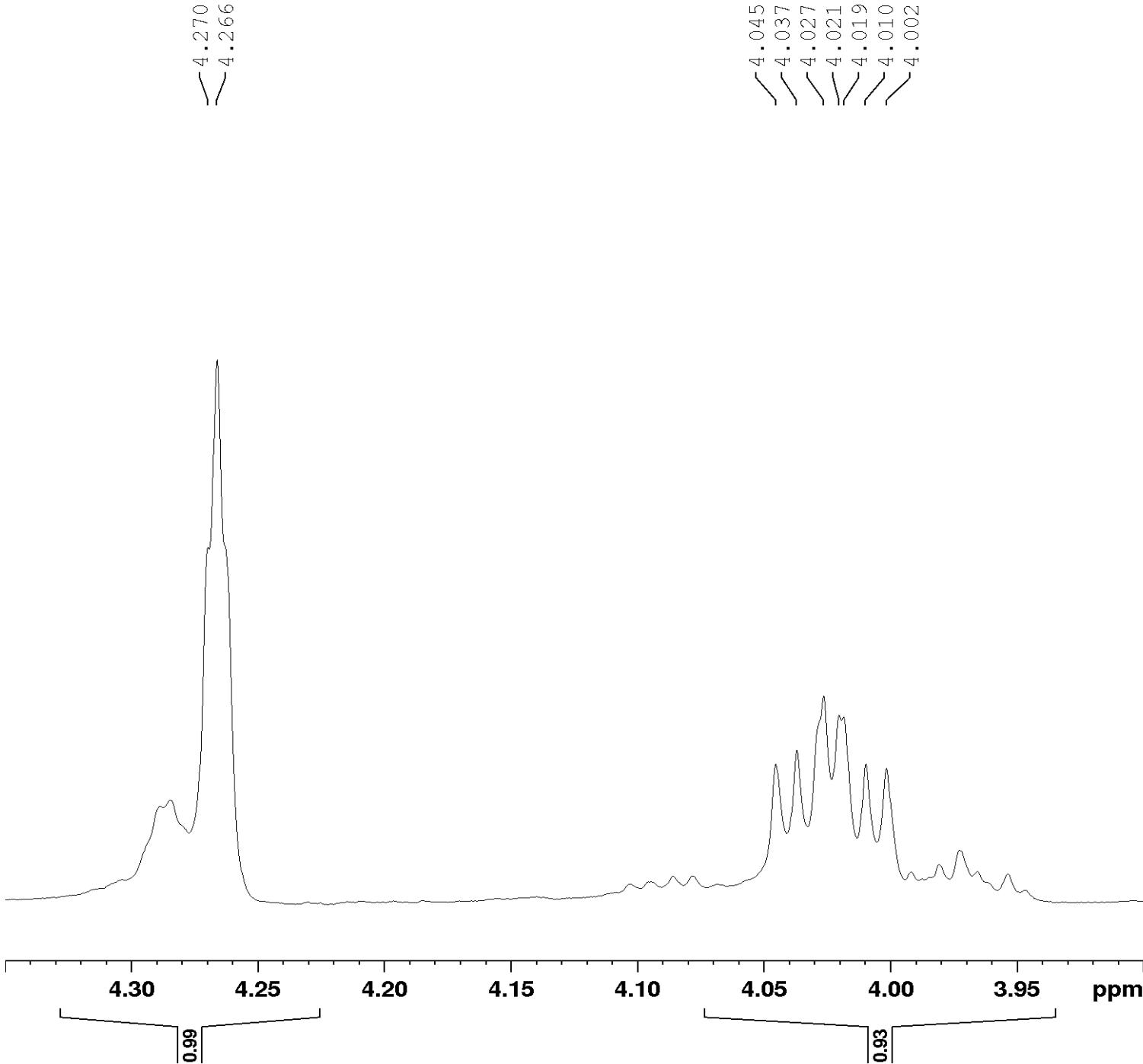
F2 - Processing parameters
SI 65536
SF 600.3110118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

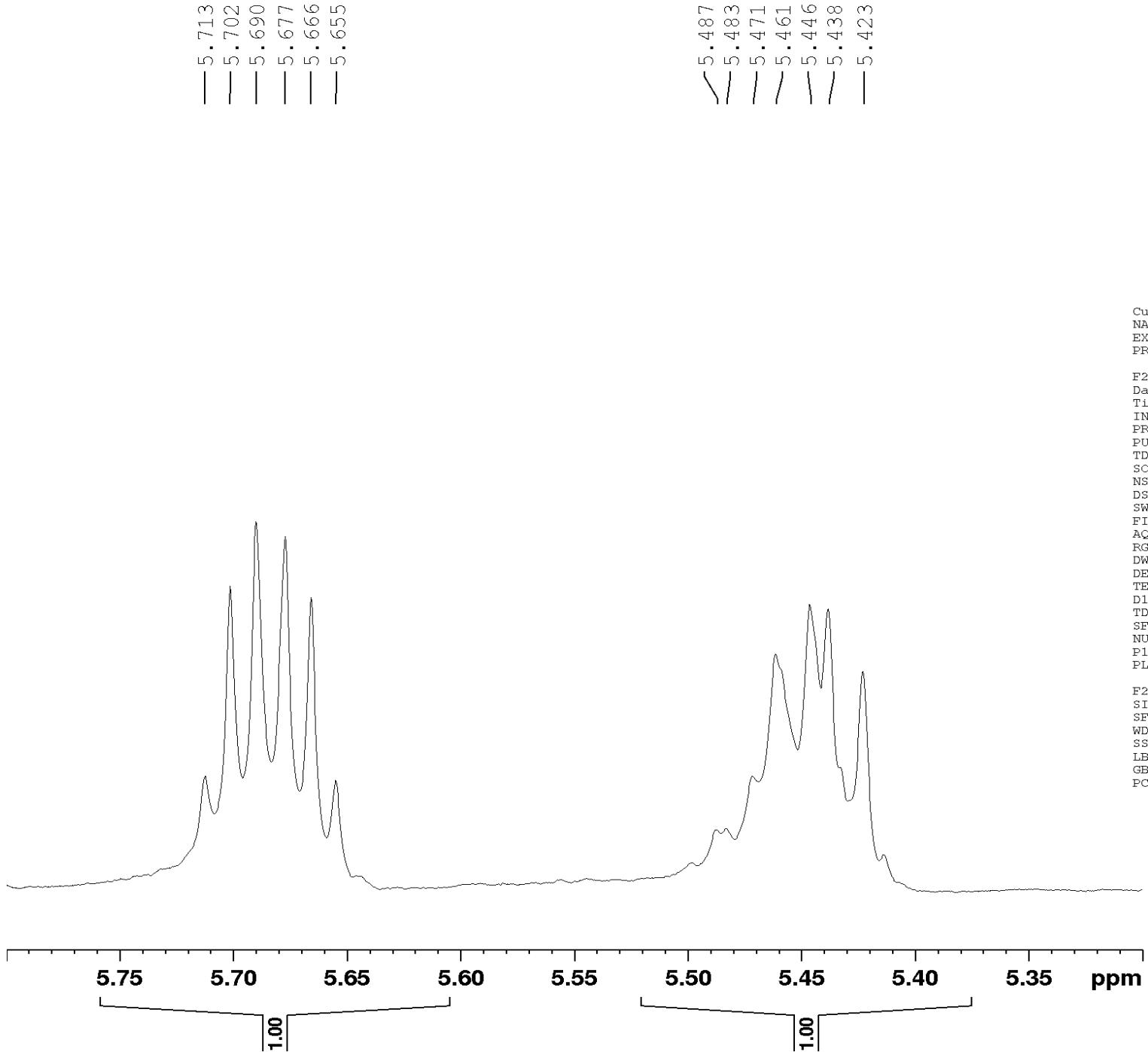


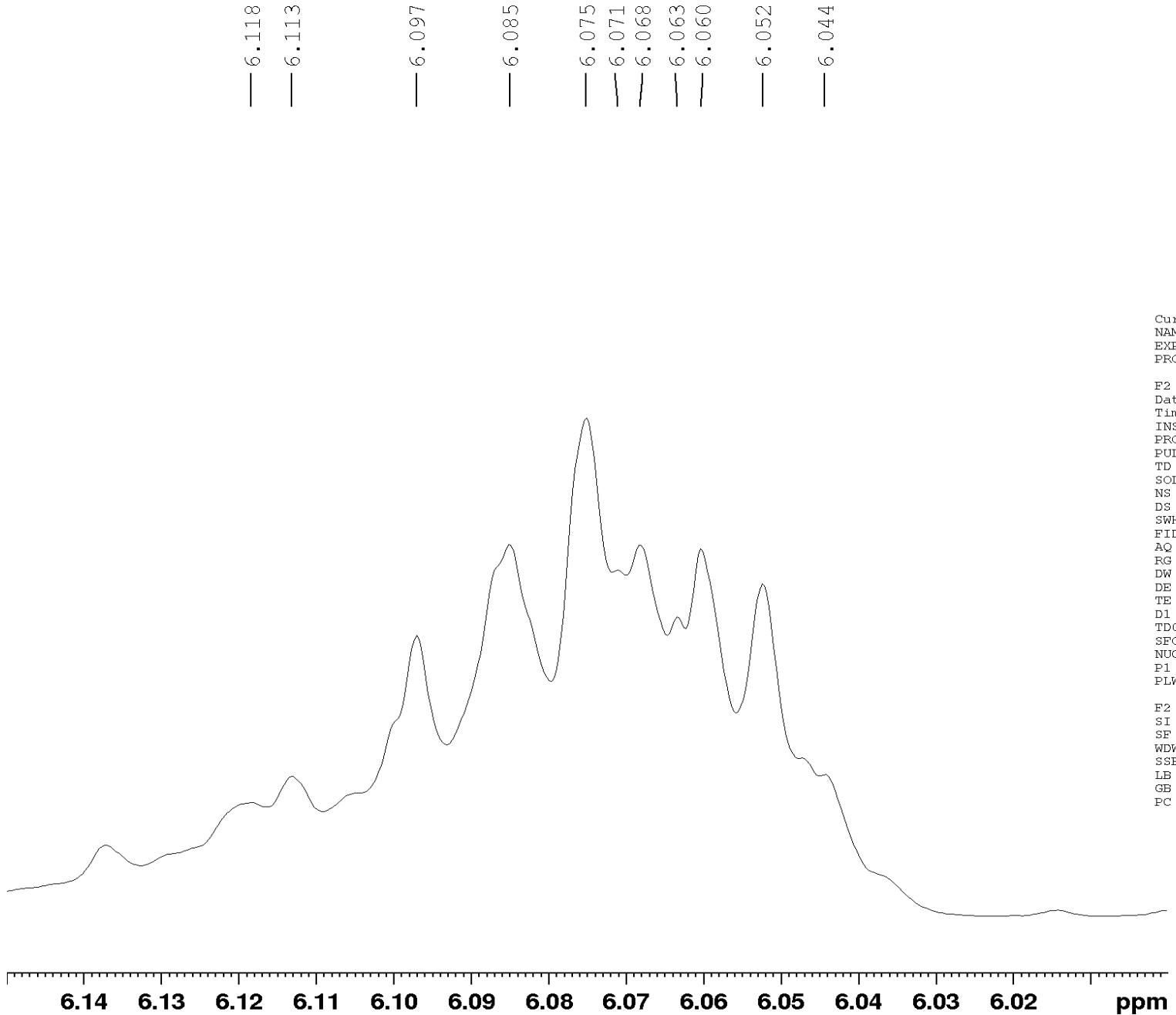
Current Data Parameters
NAME 168CLC-57.3-rfc80%-rp10-1H-CD3OD-2.9 mg
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180717
Time 11.43 h
INSTRUM spect
PROBHD Z114607_0270 (
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 109.62
DW 41.600 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 600.3147069 MHz
NUC1 1H
P1 10.00 usec
PLW1 24.25499916 W

F2 - Processing parameters
SI 65536
SF 600.3110118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







Current Data Parameters
NAME 168CLC-57.3-rfc80*-rp10-1H-CD3OD-2.9 mg
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180717
Time 11.43 h
INSTRUM spect
PROBHD Z114607_0270 (zg30
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 109.62
DW 41.600 usec
DE 6.50 usec
TE 296.5 K
D1 1.0000000 sec
TD0 1
SF01 600.3147069 MHz
NUC1 1H
P1 10.00 usec
PLW1 24.25499916 W

F2 - Processing parameters
SI 65536
SF 600.3110118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S43. ^{13}C NMR spectrum of 2-O-acetylidendrodochol B (10)

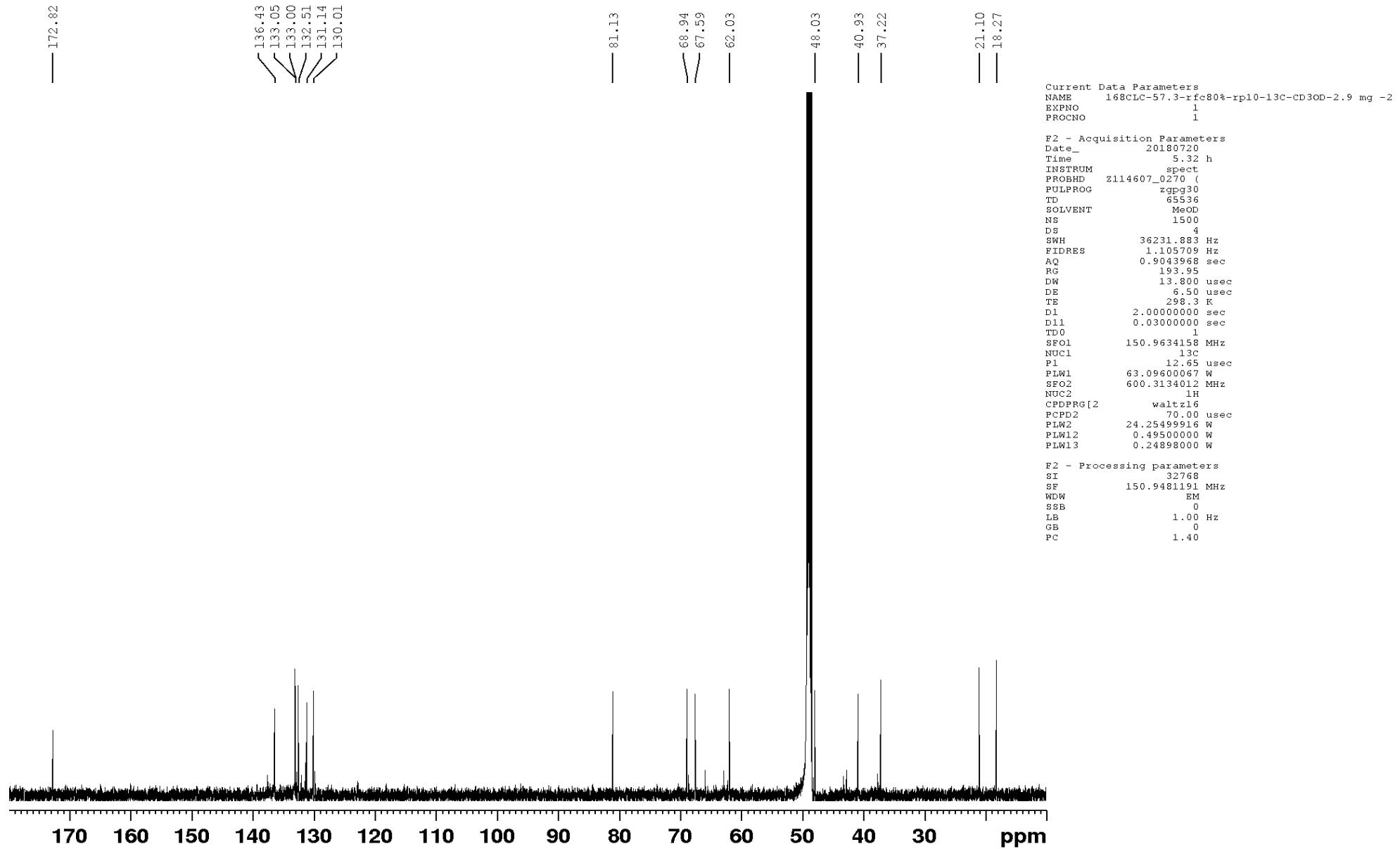


Figure S44. HMBC spectrum of 2-O-acetylidendrochol B (10)

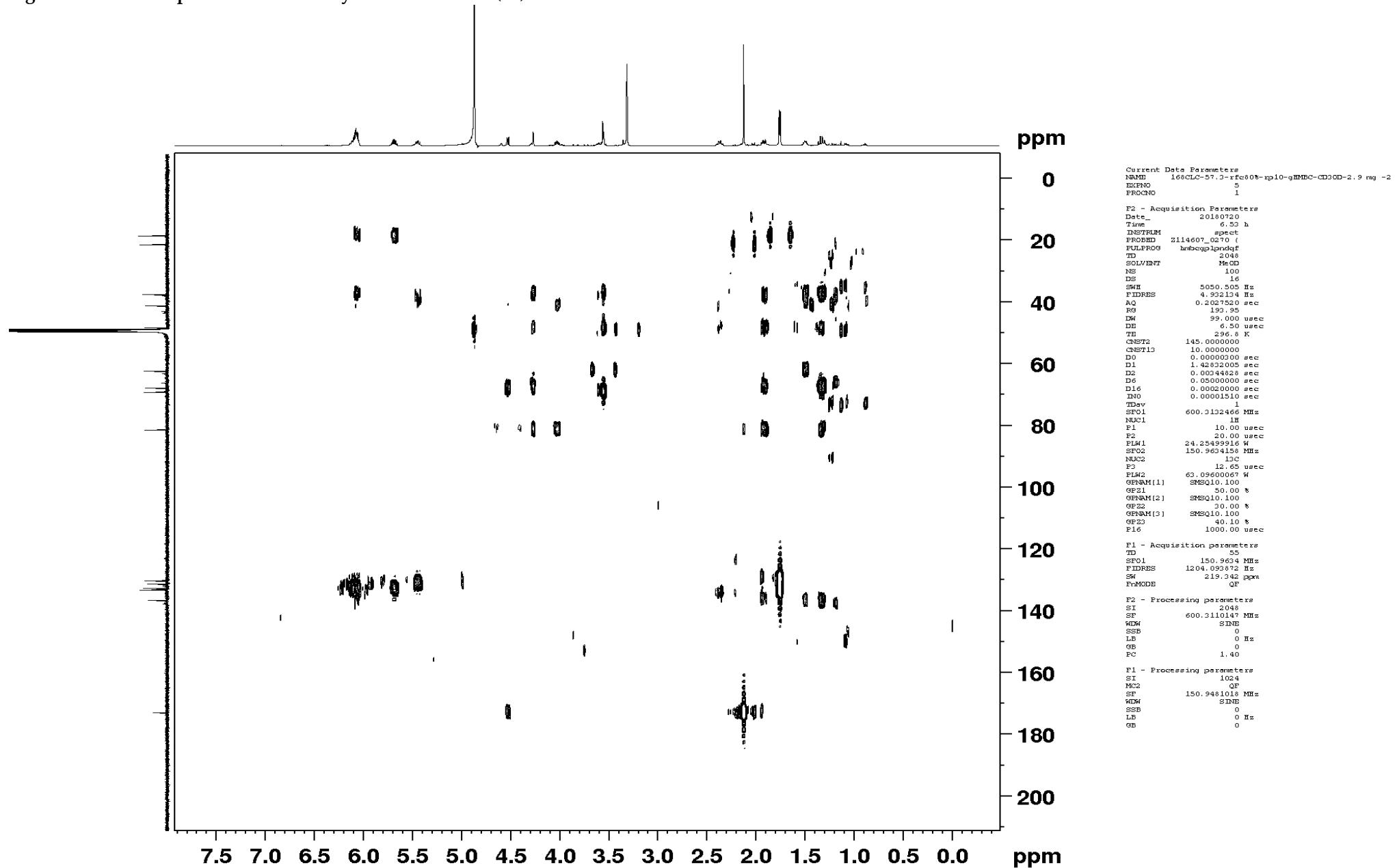


Figure S45. HSQC spectrum of 2-O-acetylidendrochol B (10)

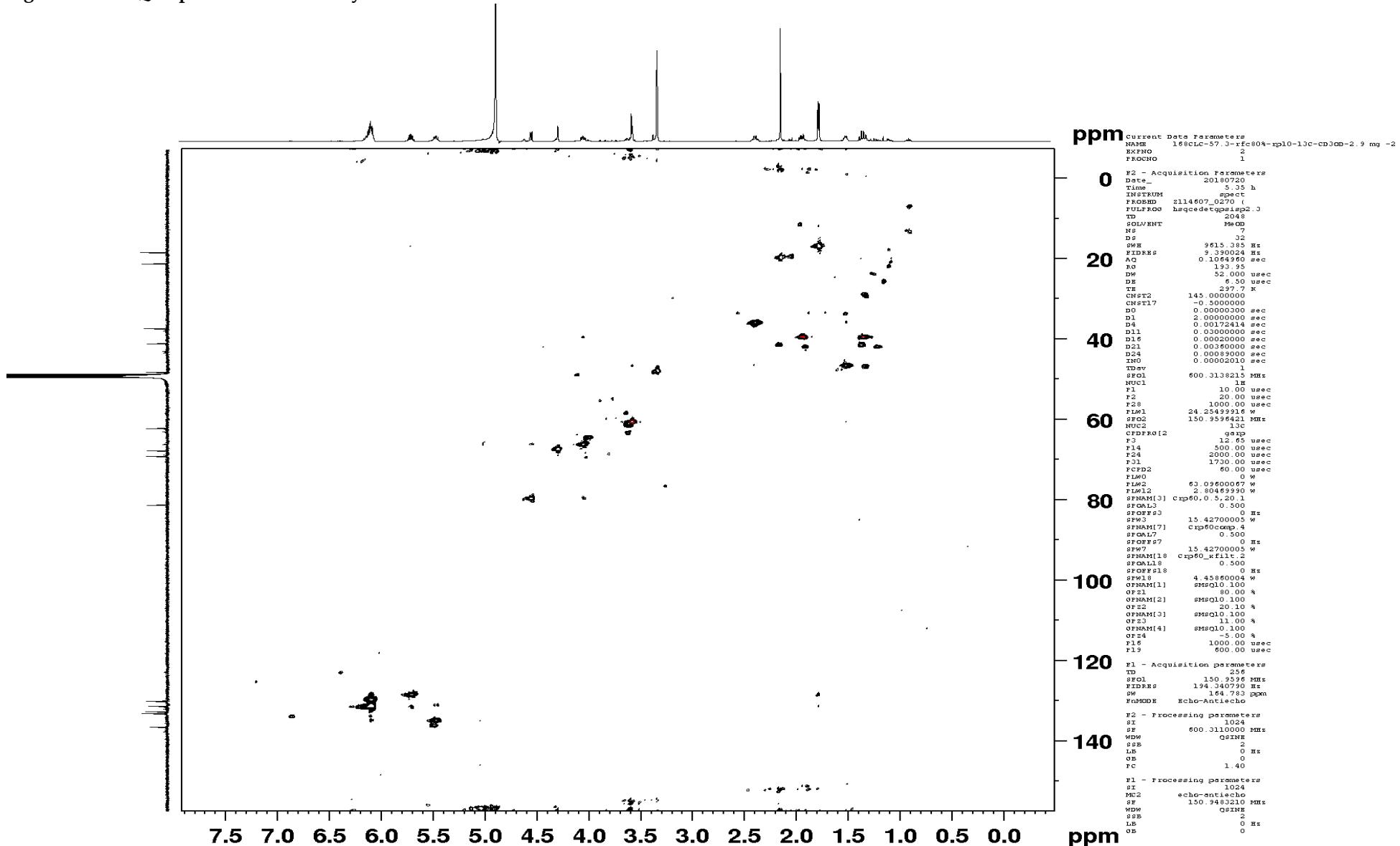


Figure S46. HR (+)ESI MS spectrum of lopouzanone A (1)

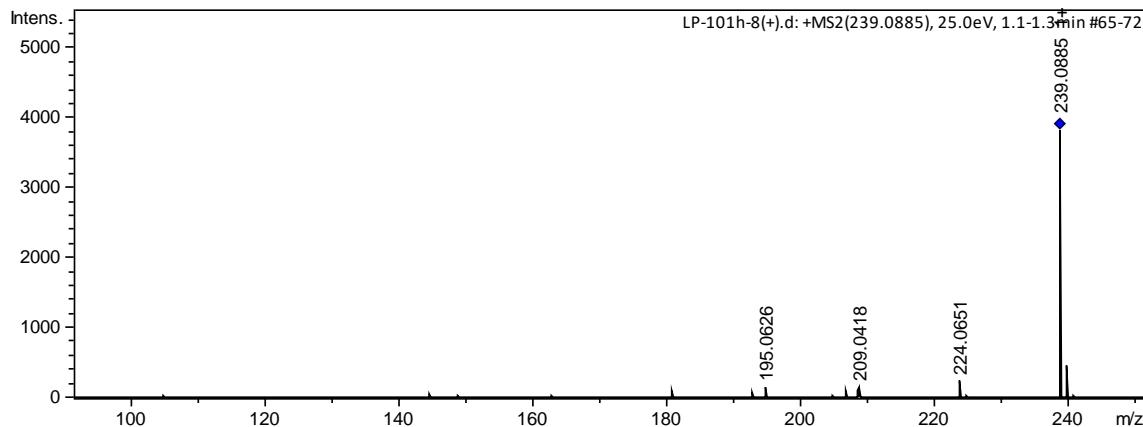
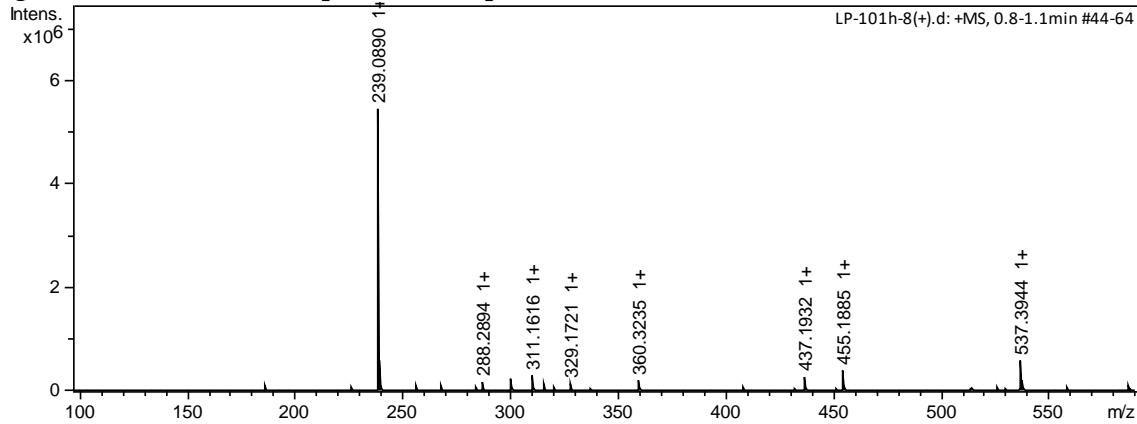


Figure S47. HR (+)ESI MS spectrum of lopouzanone B (2)

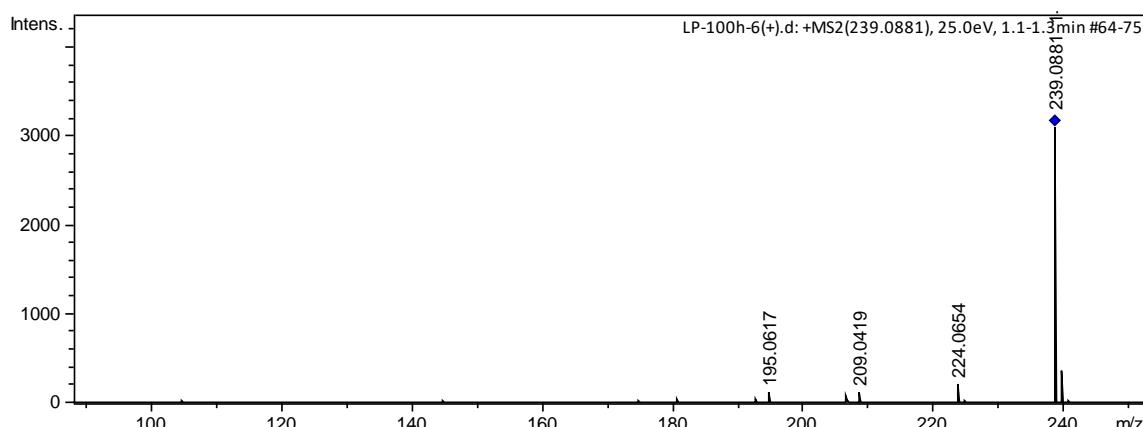
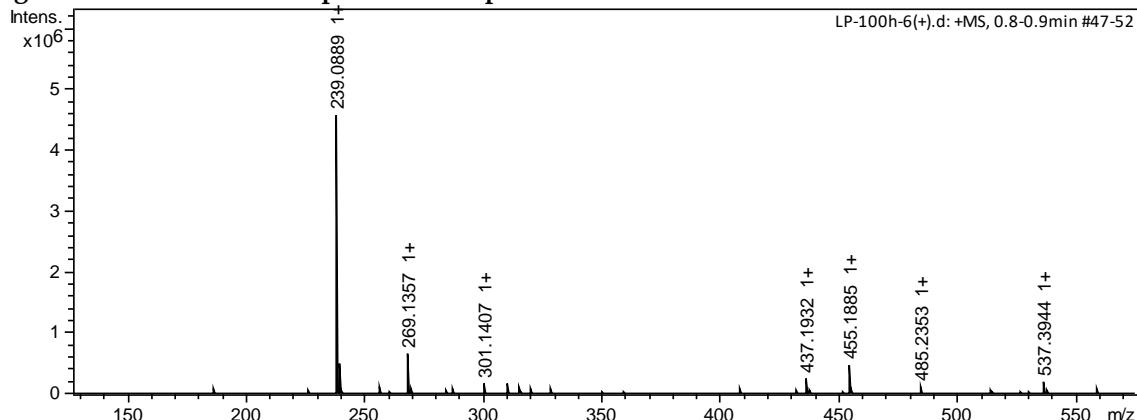


Figure S48. HR (+)ESI MS spectrum of dendrodochol B (8)

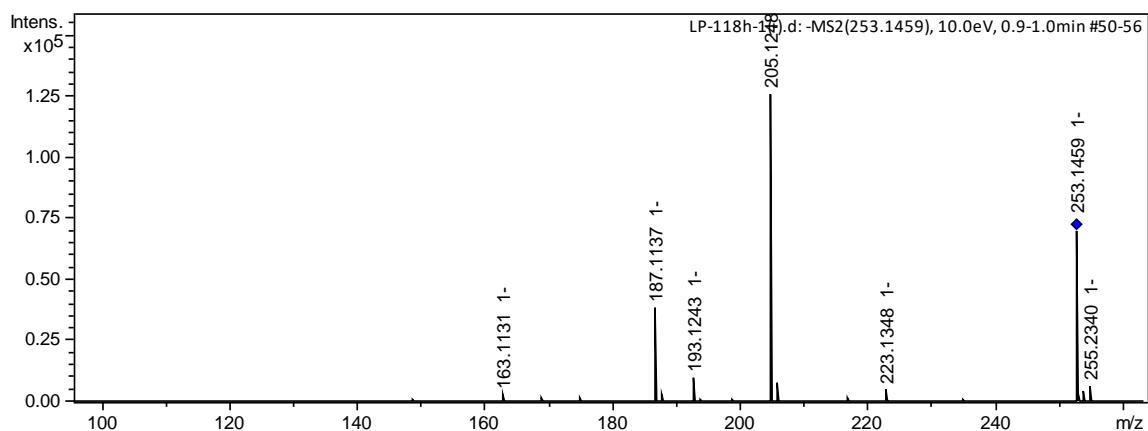


Figure S49. HR (+)ESI MS spectrum of 1-O-acetylidendrodochol B (9)

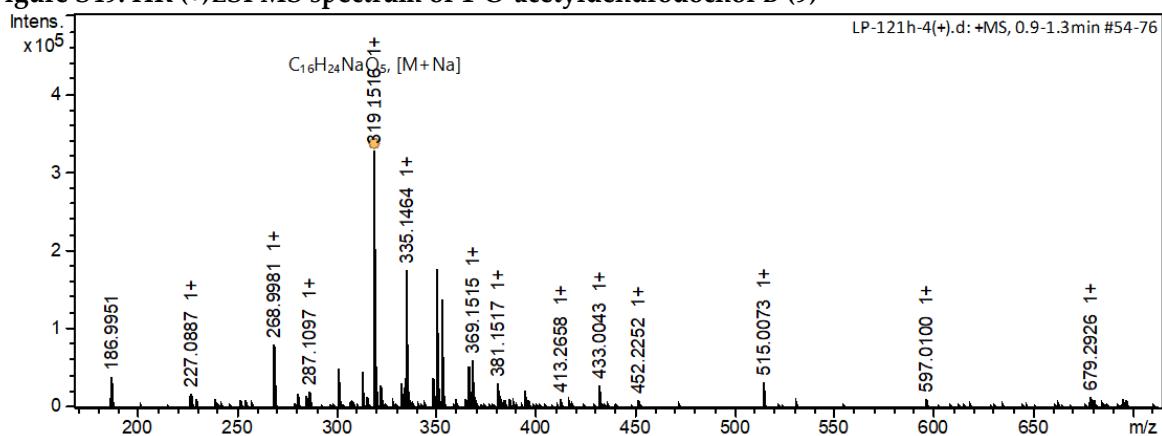


Figure S50. HR (+)ESI MS spectrum of 2-O-acetylidendrodochol B (10)

