



Article

New Brassinosteroid Analogs with 23,24-Dinorcholan Side Chain, and Benzoate Function at C-22. Synthesis, Assessment of Bioactivity on Plant Growth, and Molecular Docking Study

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Index	pag.
Figure S1. ^1H NMR spectrum compound 12	1
Figure S2. ^{13}C NMR spectrum compound 12	2
Figure S3. ^1H NMR spectrum compound 13	3
Figure S4. ^{13}C NMR spectrum compound 13	4
Figure S5. ^1H NMR spectrum compound 14	5
Figure S6. ^{13}C NMR spectrum compound 14	6
Figure S7. ^{13}C DEPT-135 NMR spectrum compound 14	7
Figure S8. 2D HSQC spectrum compound 14	8
Figure S9. 2D HMBC spectrum compound 14	9
Figure S10. ^1H NMR spectrum compound 15	10
Figure S11. ^{13}C NMR spectrum compound 15	11
Figure S12. ^{13}C DEPT-135 NMR spectrum compound 15	12
Figure S13. 2D HSQC ed spectrum compound 15	13
Figure S14. 2D HMBC spectrum compound 15	14
Figure S15. ^1H NMR spectrum compound 16	15
Figure S16. ^{13}C NMR spectrum compound 16	16
Figure S17. ^{13}C DEPT-135 NMR spectrum compound 16	17
Figure S18. 2D HSQC ed spectrum compound 16	18
Figure S19. 2D HMBC spectrum compound 16	19
Figure S20. ^1H NMR spectrum compound 17	20
Figure S21. ^{13}C NMR spectrum compound 17	21
Figure S22. ^{13}C DEPT-135 NMR spectrum compound 17	22
Figure S23. 2D HSQC spectrum compound 17	23
Figure S24. 2D HMBC spectrum compound 17	24
Figure S25. ^1H NMR spectrum compound 18	25
Figure S26. ^{13}C NMR spectrum compound 18	26
Figure S27. ^{13}C DEPT-135 NMR spectrum compound 18	27
Figure S28. 2D HSQC ed spectrum compound 18	28
Figure S29. 2D HMBC spectrum compound 18	29
Figure S30. ^1H NMR spectrum compound 19	30
Figure S31. ^{13}C NMR spectrum compound 19	31
Figure S32. ^{13}C DEPT-135 NMR spectrum compound 19	32
Figure S33. 2D HSQC ed spectrum compound 19	33
Figure S34. 2D HMBC spectrum compound 19	34
Figure S35. ^1H NMR spectrum compound 8	35

Figure S36. ^{13}C NMR spectrum compound 8	36
Figure S37. ^{13}C DEPT-135 NMR spectrum compound 8	37
Figure S38. 2D HSQC ed spectrum compound 8	38
Figure S39. 2D HMBC spectrum compound 8	39
Figure S40. 1D selective NOESY compound 8	40
Figure S41. ^1H NMR spectrum compound 20	41
Figure S42. ^{13}C NMR spectrum compound 20	42
Figure S43. ^{13}C DEPT-135 NMR spectrum compound 20	43
Figure S44. 2D HSQC ed spectrum compound 20	44
Figure S45. 2D HMBC spectrum compound 20	45
Figure S46. ^1H NMR spectrum compound 21	46
Figure S47. ^{13}C NMR spectrum compound 21	47
Figure S48. ^{13}C DEPT-135 NMR spectrum compound 21	48
Figure S49. 2D HSQC ed spectrum compound 21	49
Figure S50. 2D HMBC spectrum compound 21	50
Figure S51. ^1H NMR spectrum compound 22	51
Figure S52. ^{13}C NMR spectrum compound 22	52
Figure S53. ^{13}C DEPT-135 NMR spectrum compound 22	53
Figure S54. 2D HSQC ed spectrum compound 22	54
Figure S55. 2D HMBC ed spectrum compound 22	55
Figure S56. ^1H NMR spectrum compound 9	56
Figure S57. ^{13}C NMR spectrum compound 9	57
Figure S58. ^{13}C DEPT-135 NMR spectrum compound 9	58
Figure S59. 2D HSQC ed spectrum compound 9	59
Figure S60. 2D HMBC ed spectrum compound 9	60
Figure S61. ^1H NMR spectrum compound 10	61
Figure S62. ^{13}C NMR spectrum compound 10	62
Figure S63. ^{13}C DEPT-135 NMR spectrum compound 10	63
Figure S64. 2D HSQC ed spectrum compound 10	64
Figure S65. 2D HMBC ed spectrum compound 10	65
Figure S66. ^1H NMR spectrum compound 11	66
Figure S67. ^{13}C NMR spectrum compound 11	67
Figure S68. ^{13}C DEPT-135 NMR spectrum compound 11	68
Figure S69. 2D HSQC ed spectrum compound 11	69
Figure S70. 2D HMBC ed spectrum compound 11	70
Figure S71. HRSM spectra of compounds 8	71
Figure S72. HRSM spectra of compounds 9	71

Figure S73. HRSM spectra of compounds 10	72
Figure S74. HRSM spectra of compounds 11	72
Figure S75. Effect of brassinolide and BRs analogs on the Rice Lamina Inclination 1, 8-11	73
Figure S76. Predicted binding mode of compound 1, 8-11	75
Table S1. Pose analysis of docked brassinolide and synthetic analogs (8-11).....	76
Table S2. Docked ligands-heterodimer protein of 1 and BRs analogs (8-11)	77

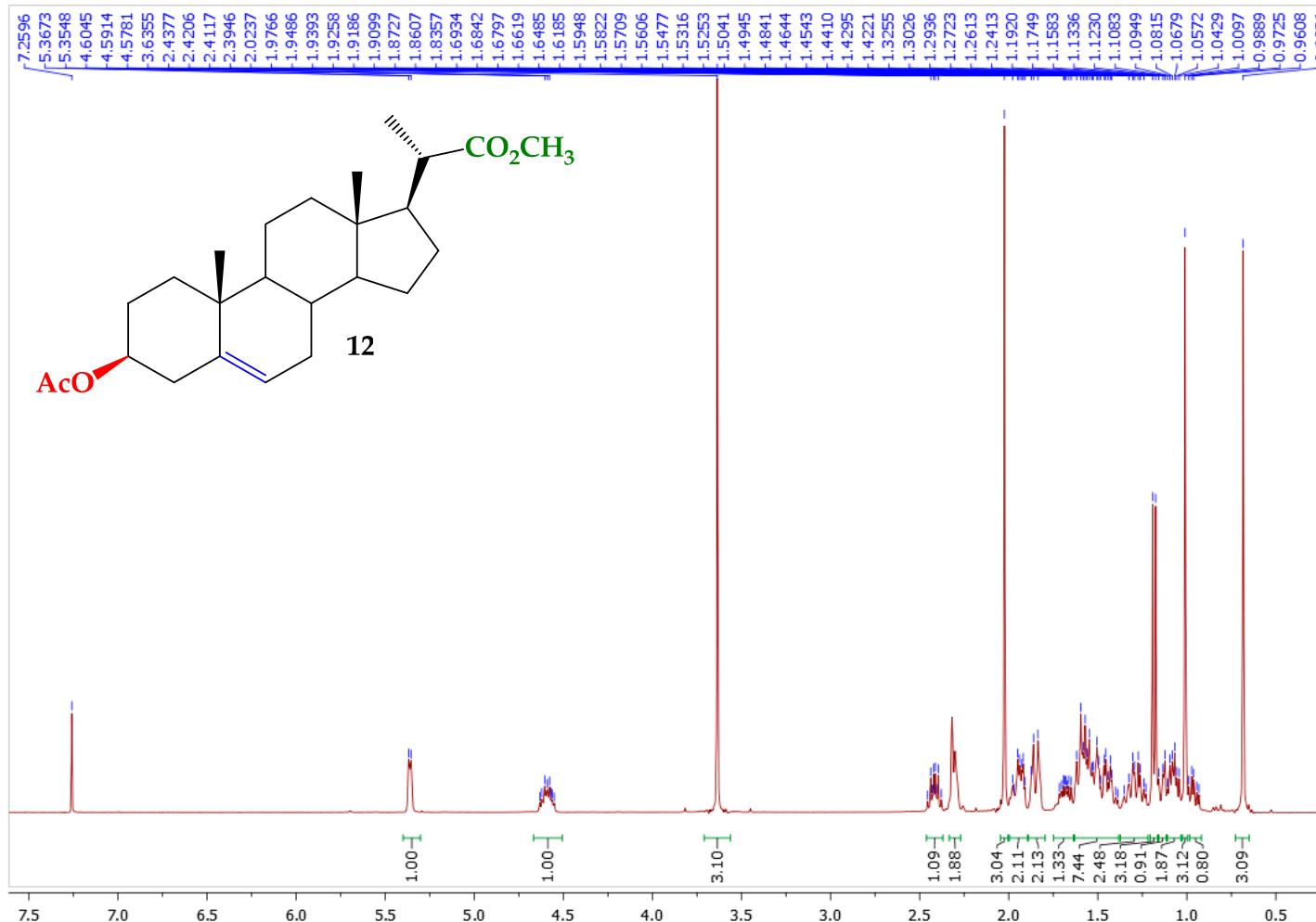


Figure S1. ¹H NMR spectrum of Methyl (20S)-3 β -Acetoxy pregn-5-ene-20-carboxylate (12)

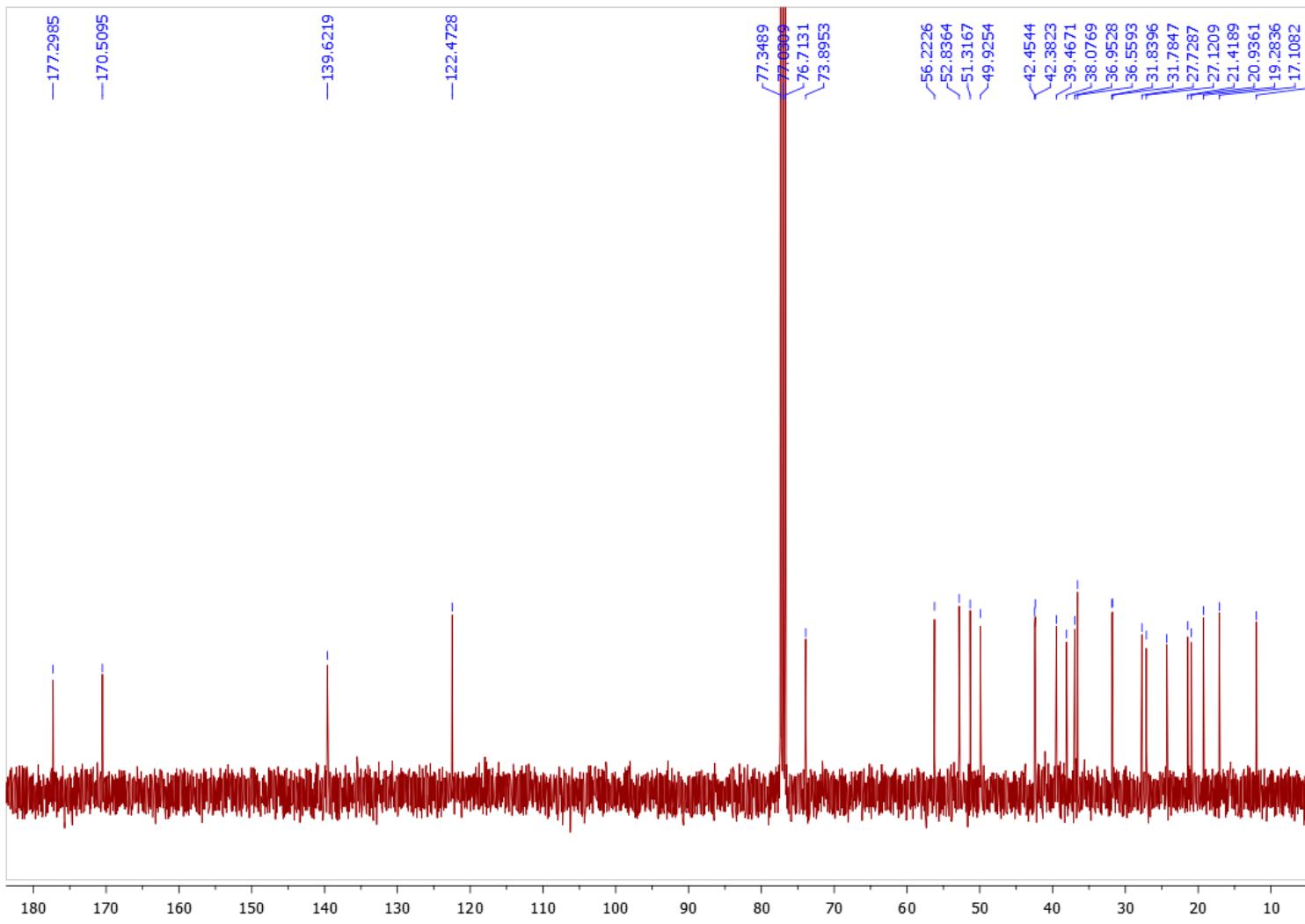


Figure S2. ¹³C NMR spectrum of Methyl (20S)-3 β -Acetoxy pregn-5-ene-20-carboxylate (**12**)

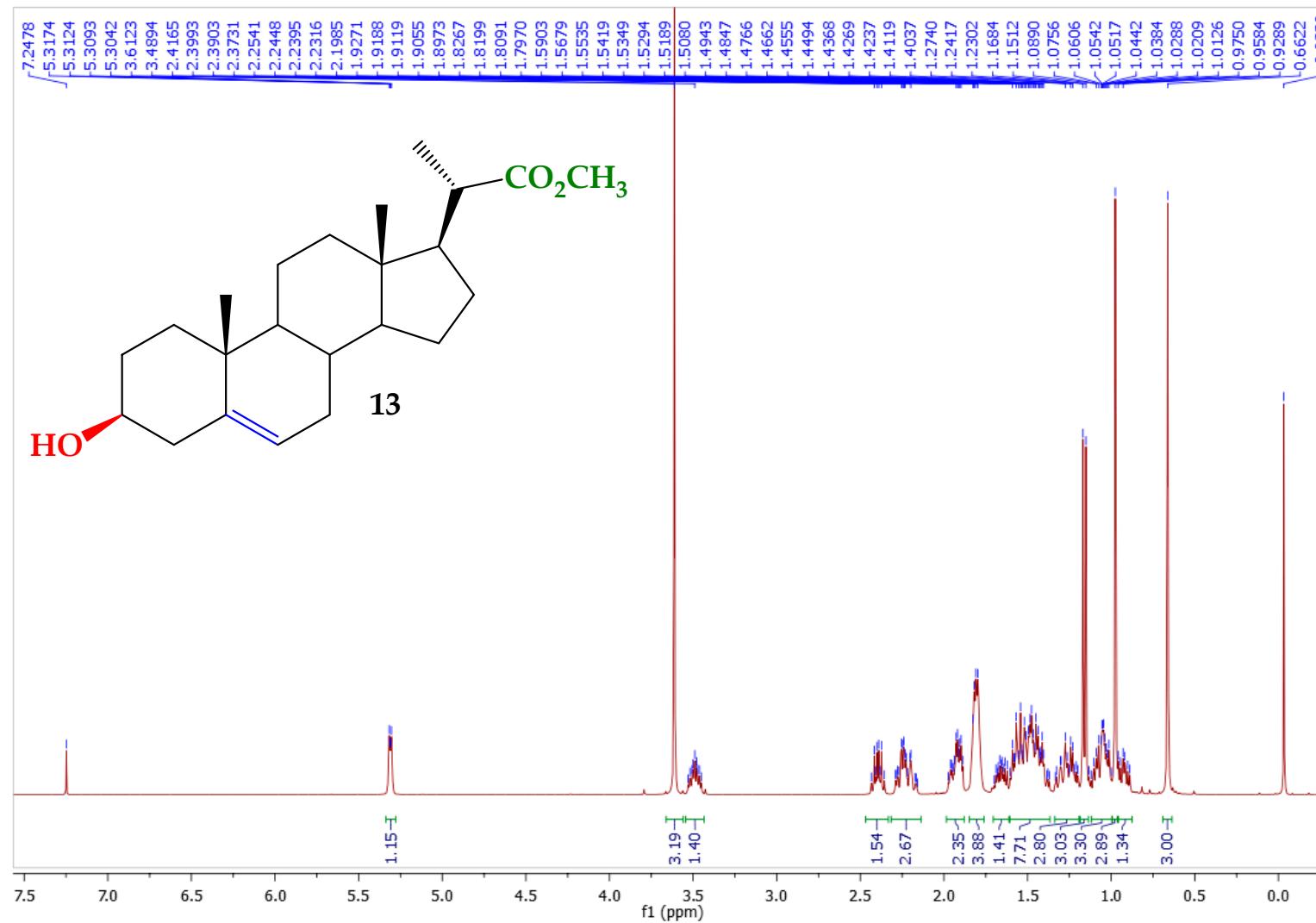


Figure S3. ¹H NMR spectrum of Methyl (20S)-3 β -hydroxy-pregn-5-ene-20-carboxylate (**13**)

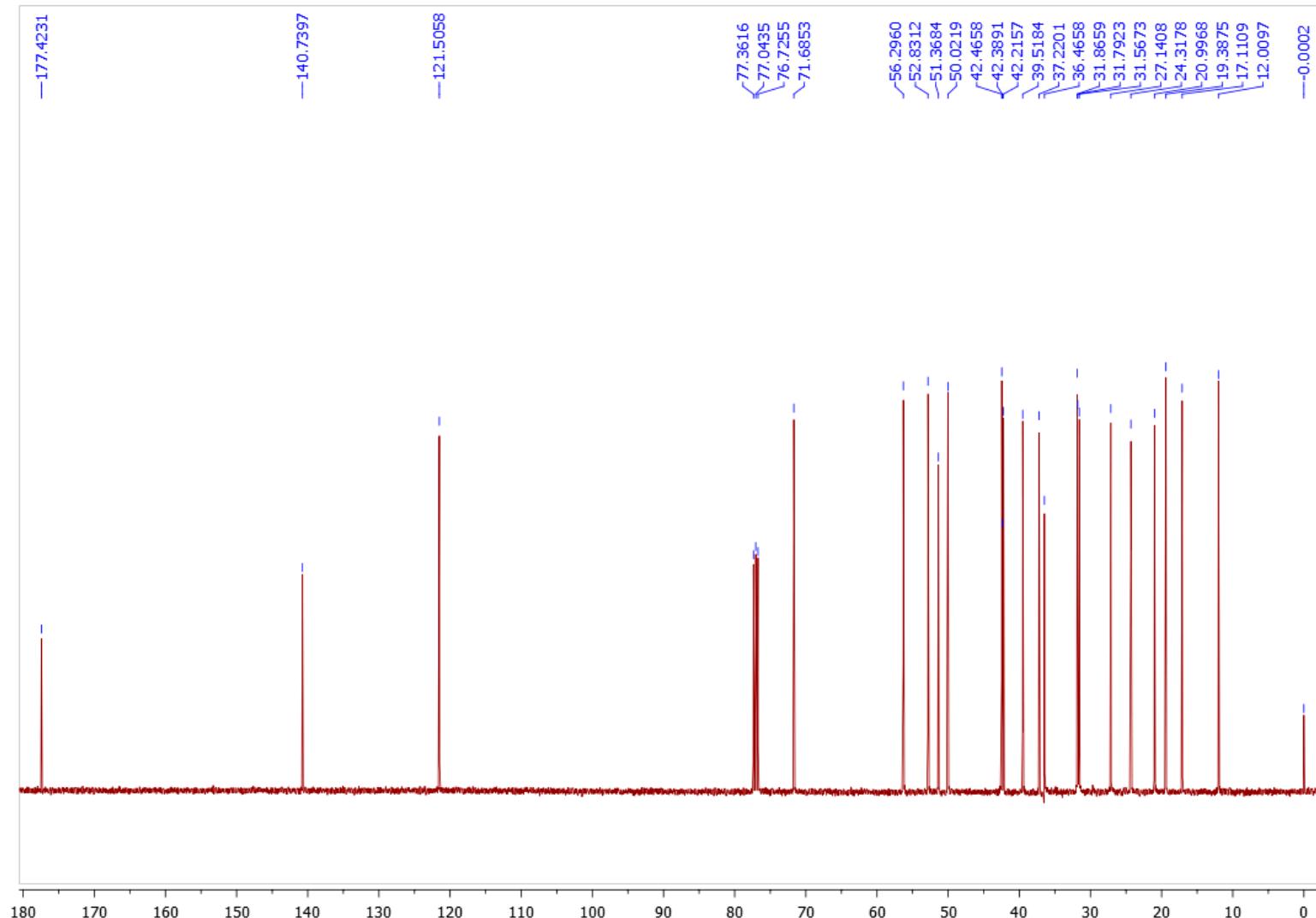


Figure S4. ^{13}C NMR spectrum of Methyl (20S)-3 β -hydroxy-pregn-5-ene-20-carboxylate (**13**)

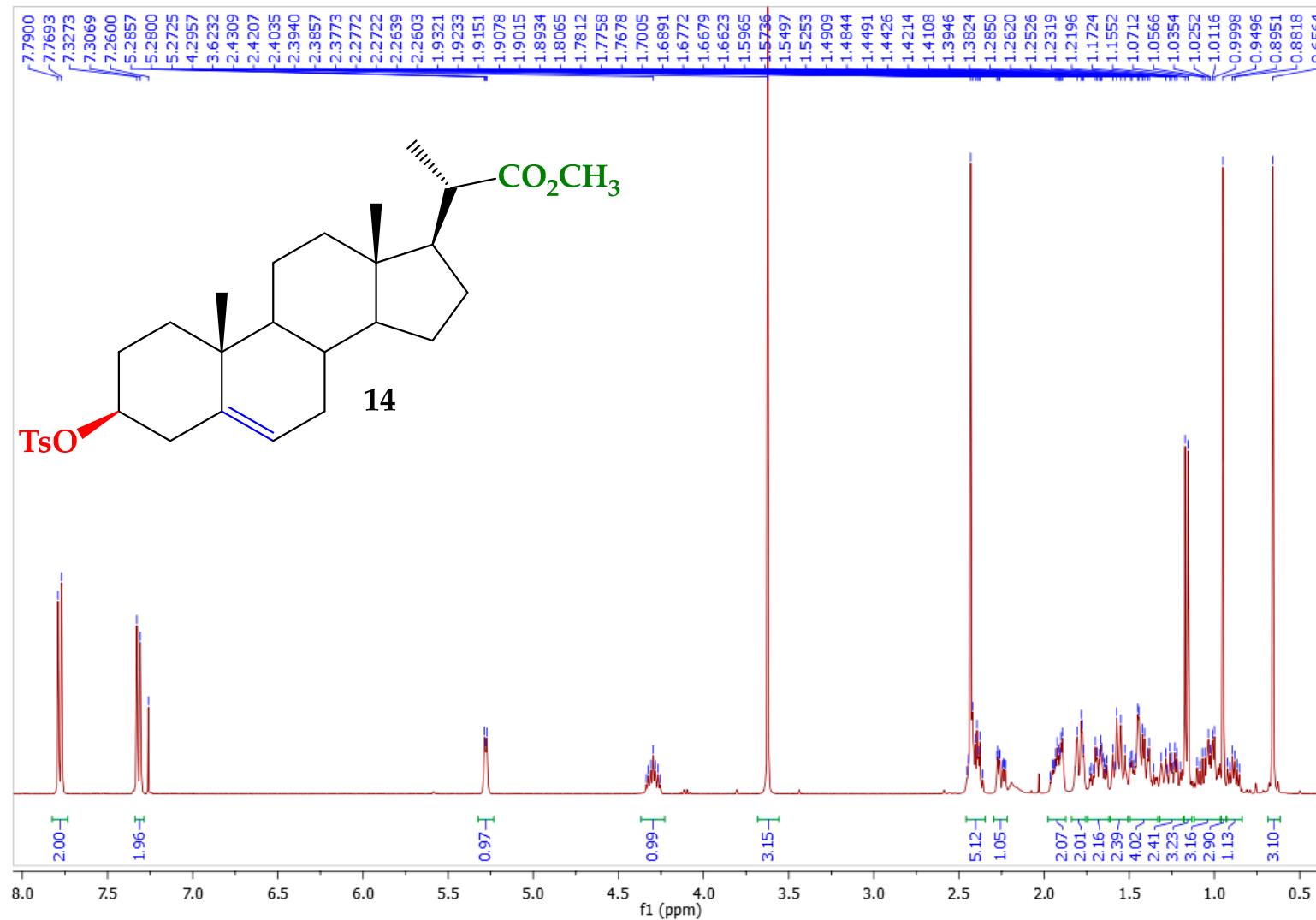


Figure S5. ¹H NMR spectrum of Methyl (20S)-3 β -(4-toluenesulfonyloxy)-pregn-5-ene-20-carboxylate (14)

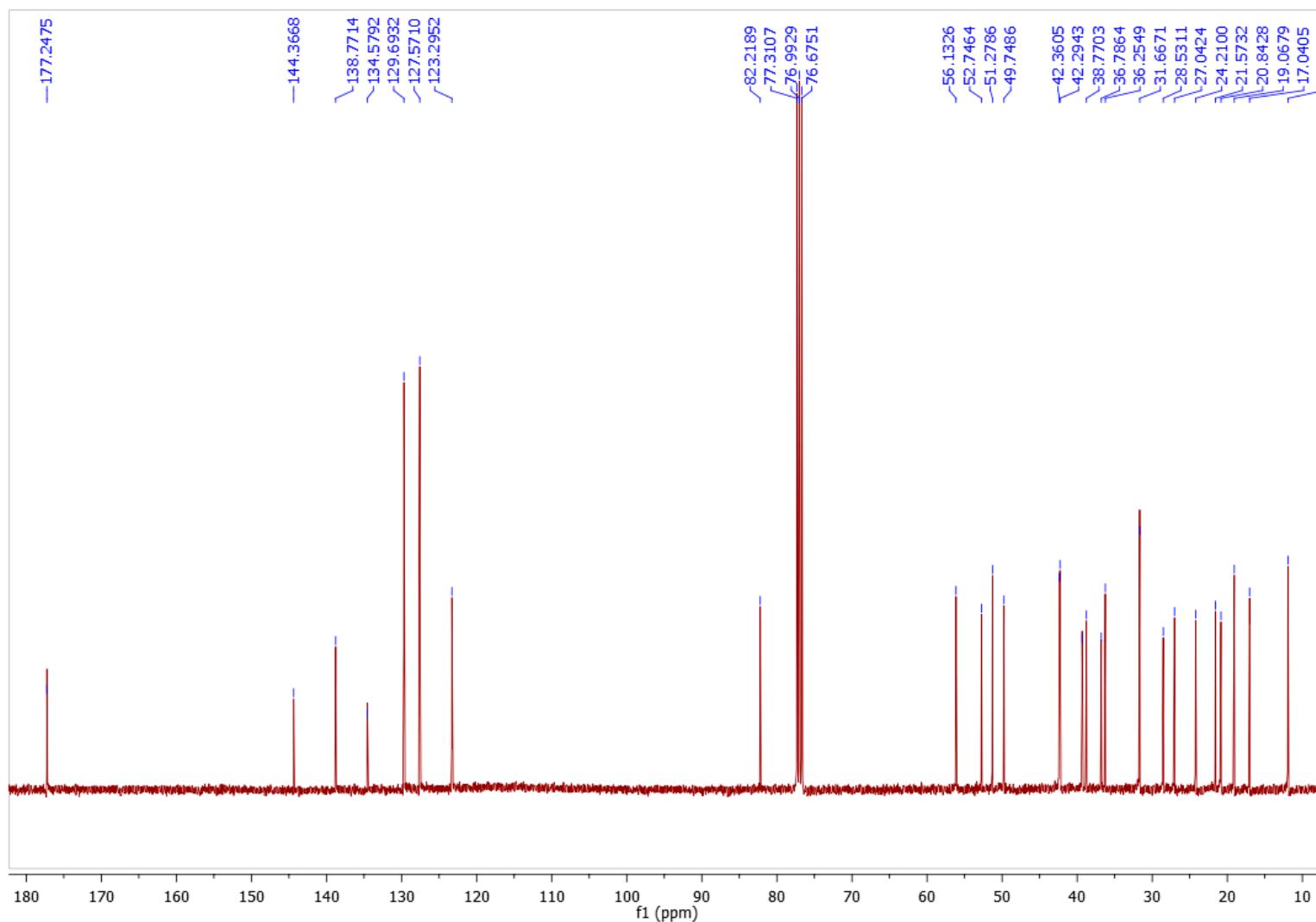


Figure S6. ^{13}C NMR spectrum of Methyl (20S)-3 β -(4-toluennsulfonyloxy)-pregn-5-ene-20-carboxylate (**14**)

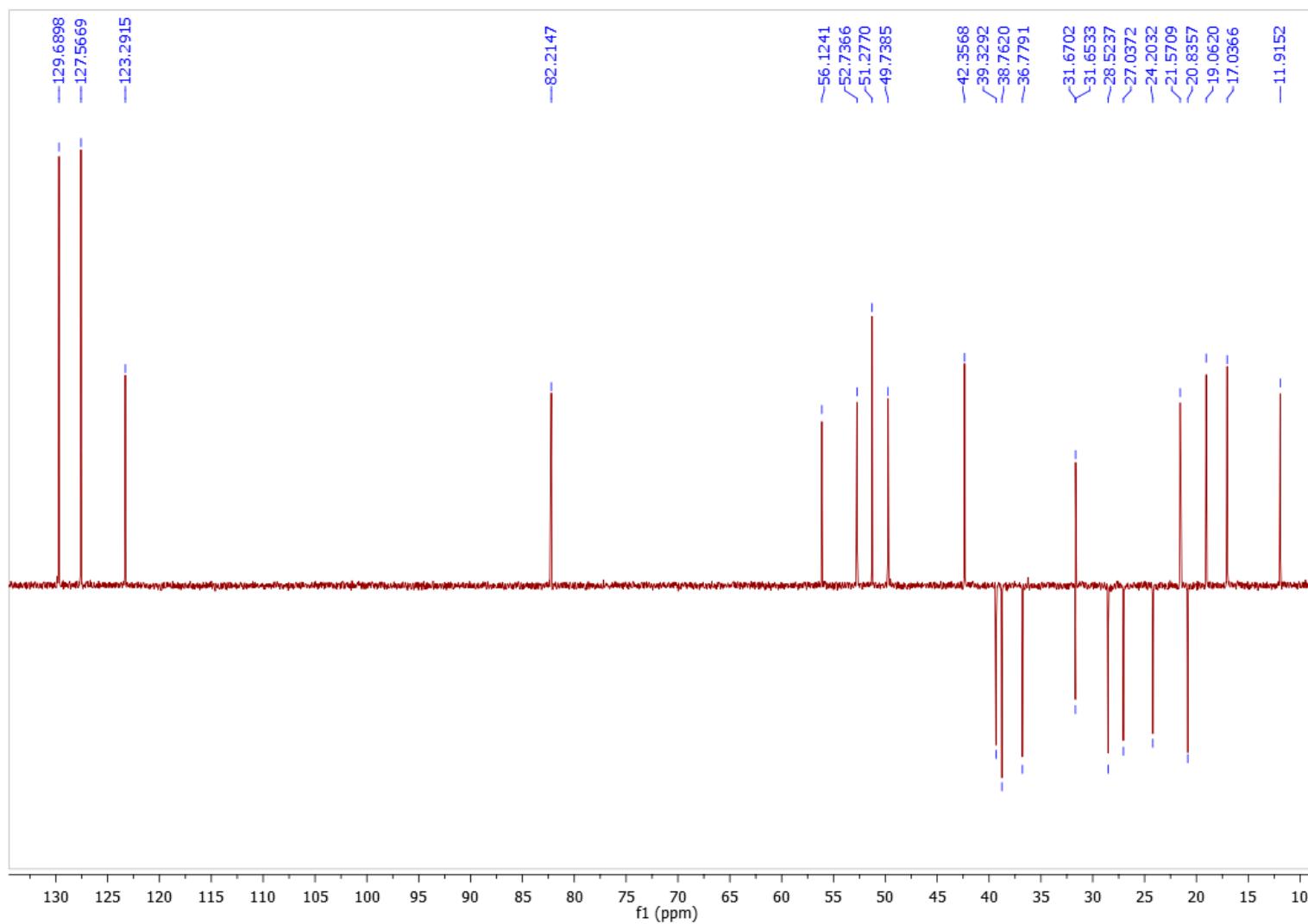


Figure S7. ¹³C DEPT-135 NMR spectrum of Methyl (20S)-3β-(4-toluennsulfonyloxy)-pregn-5-ene-20-carboxylate (**14**)

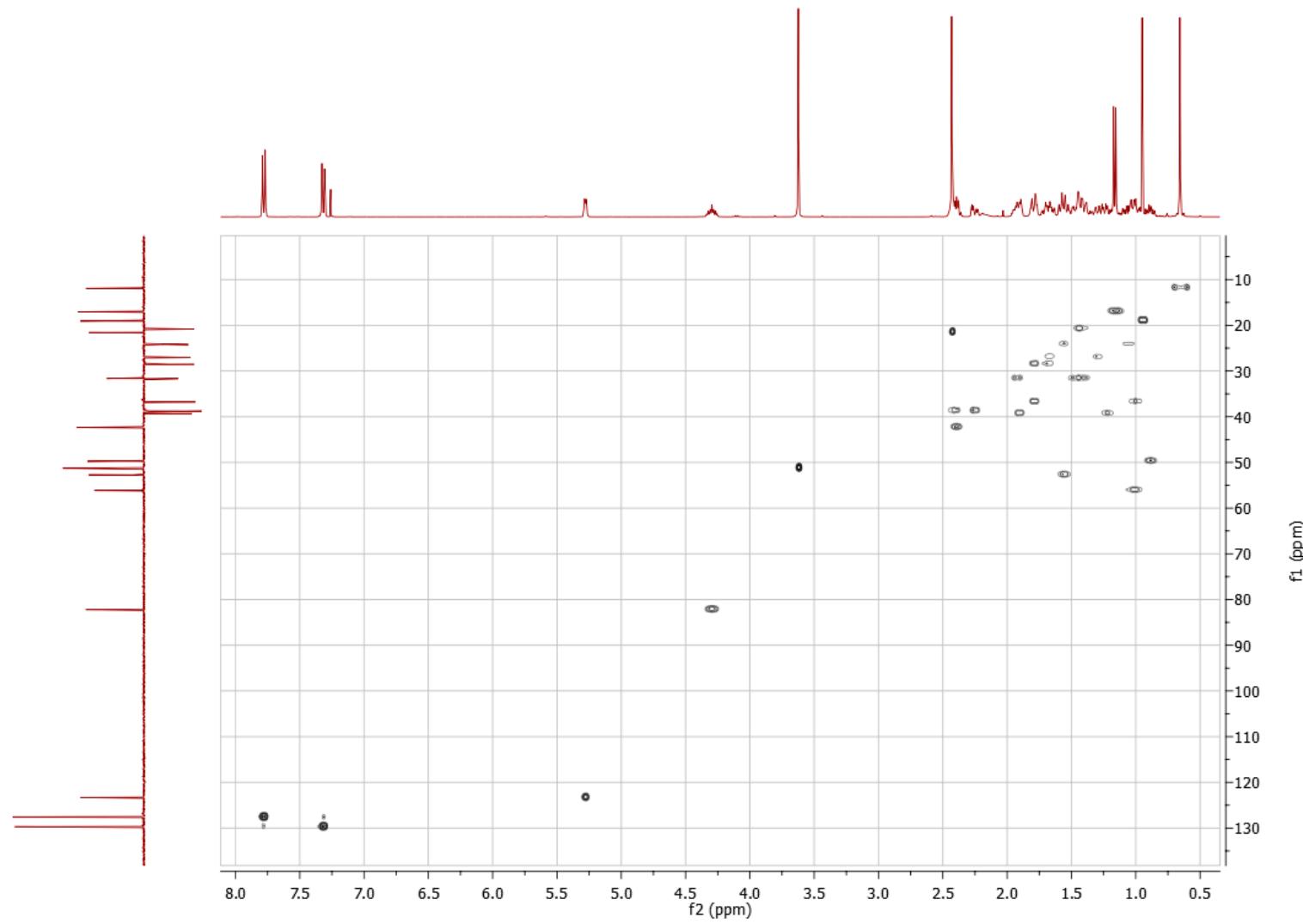


Figure S8. 2D HSQC spectrum of Methyl (20S)-3 β -(4-toluennsulfonyloxy)-pregn-5-ene-20-carboxylate (**14**)

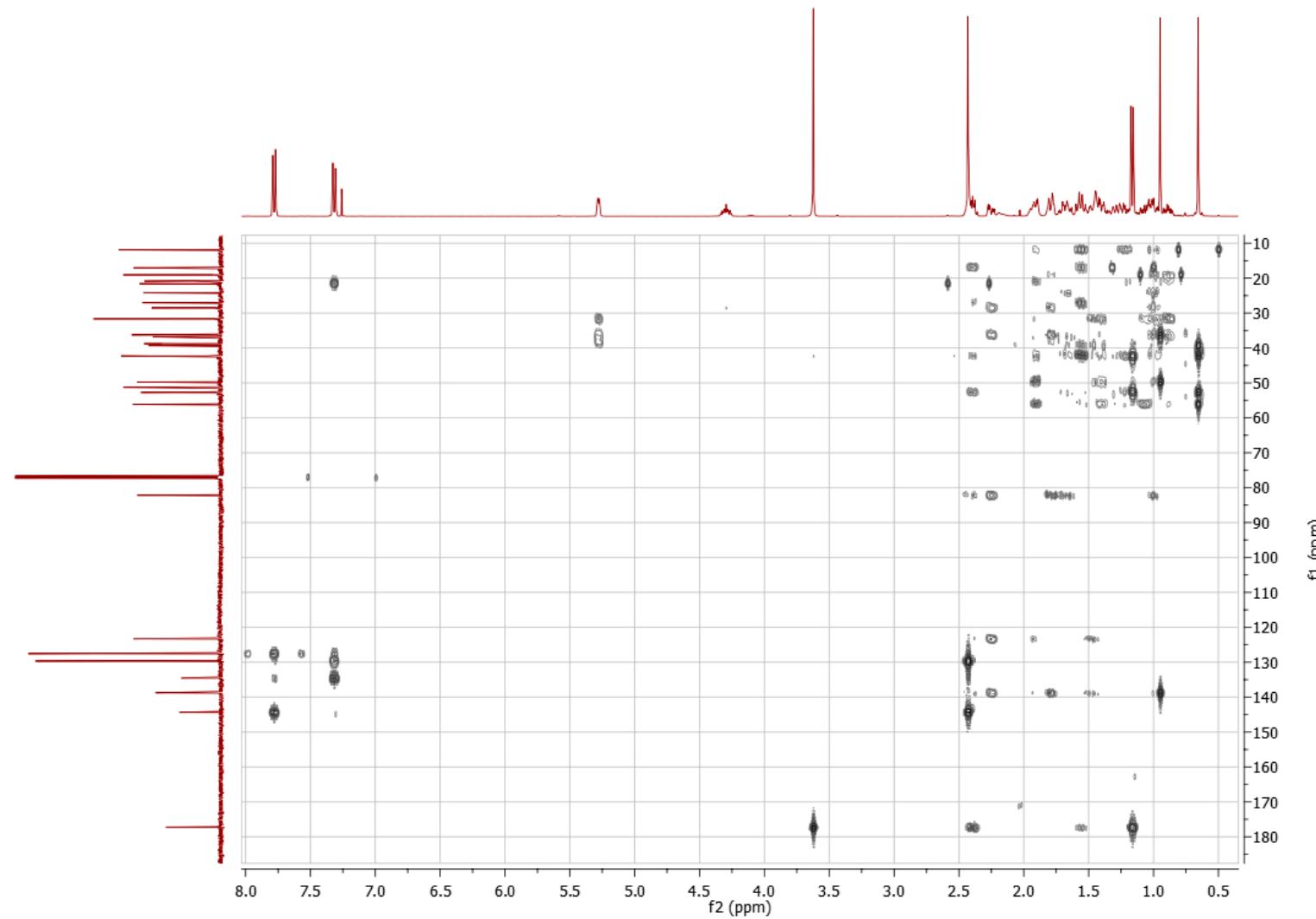


Figure S9. 2D HMBC spectrum of Methyl (20S)-3 β -(4-toluenesulfonyloxy)-pregn-5-ene-20-carboxylate (**14**)

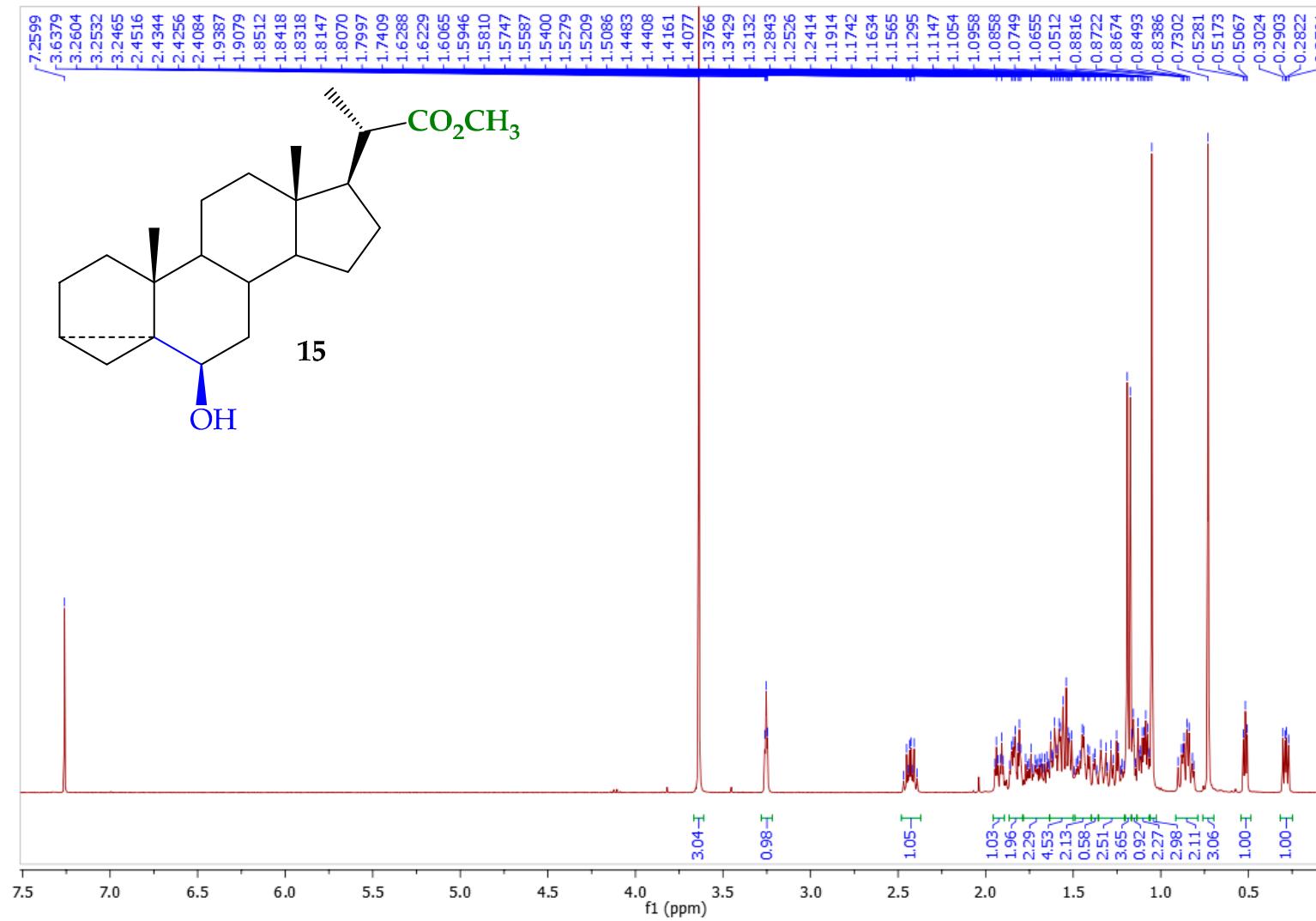


Figure S10. ¹H NMR spectrum of Methyl (20S)-6 β -hydroxy-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (15)

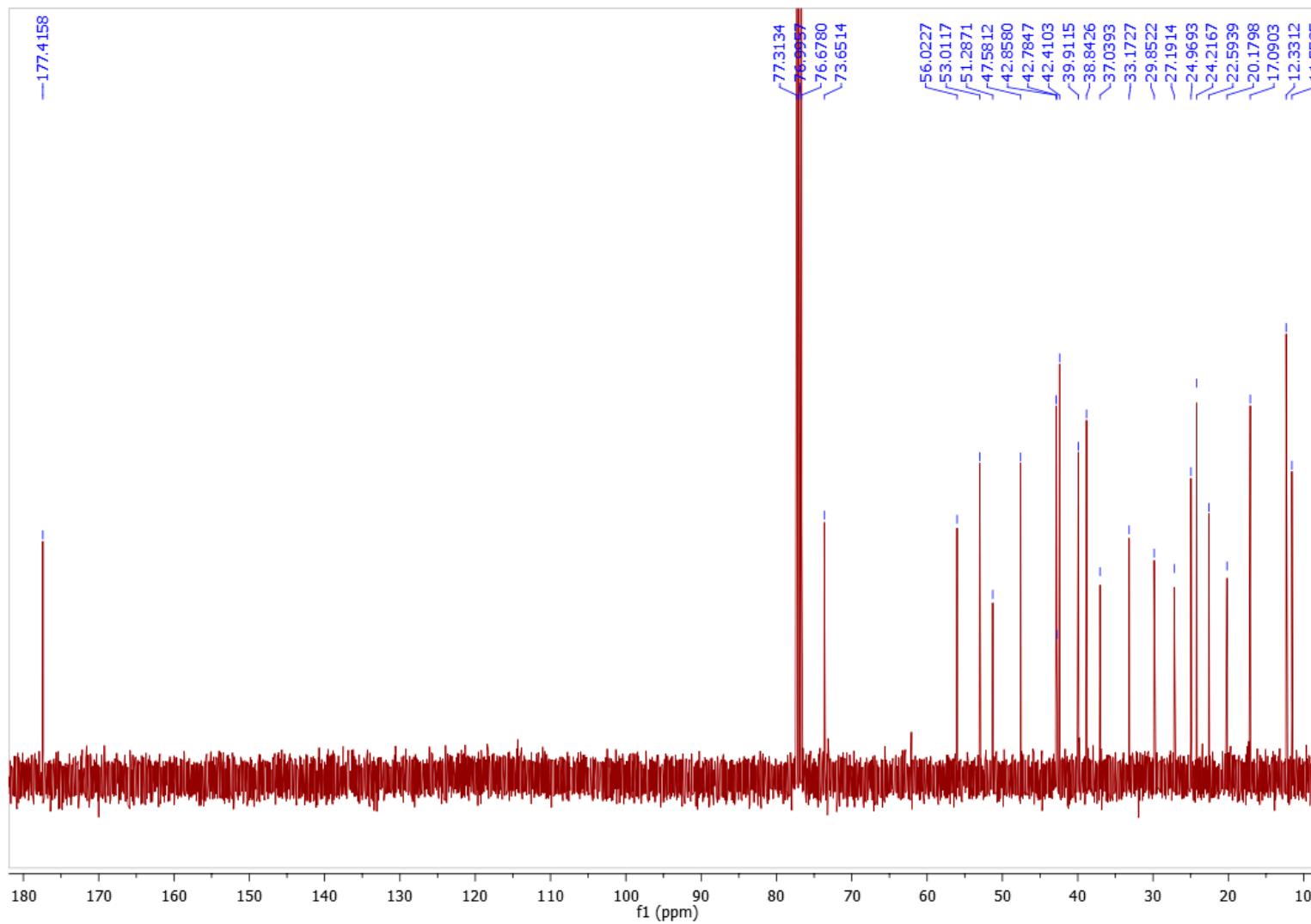


Figure S11. ¹³C NMR spectrum of Methyl (20*S*)-6 β -hydroxy-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**15**)

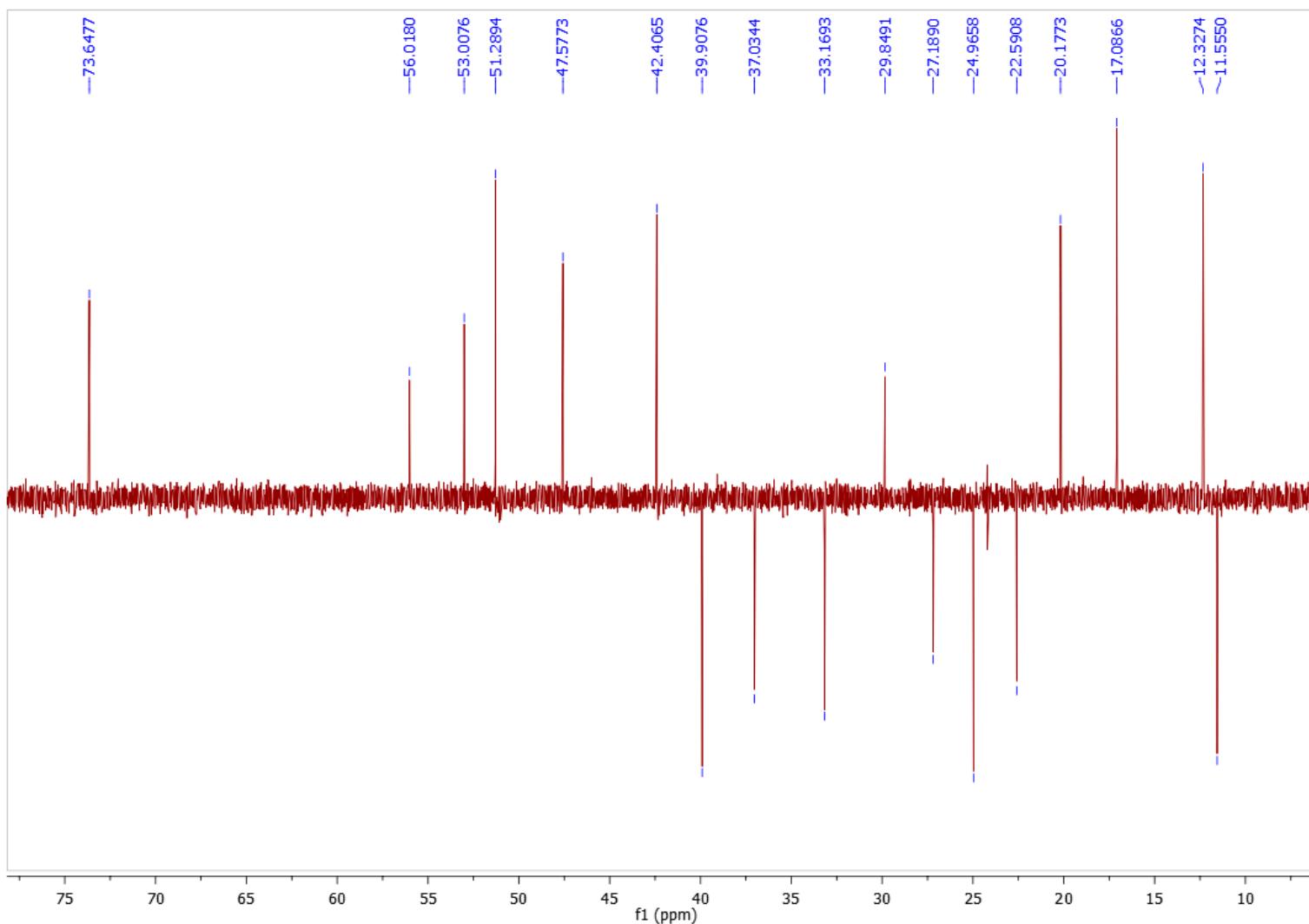


Figure S12. ¹³C DEPT-135 NMR spectrum of Methyl (20S)-6 β -hydroxy-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**15**)

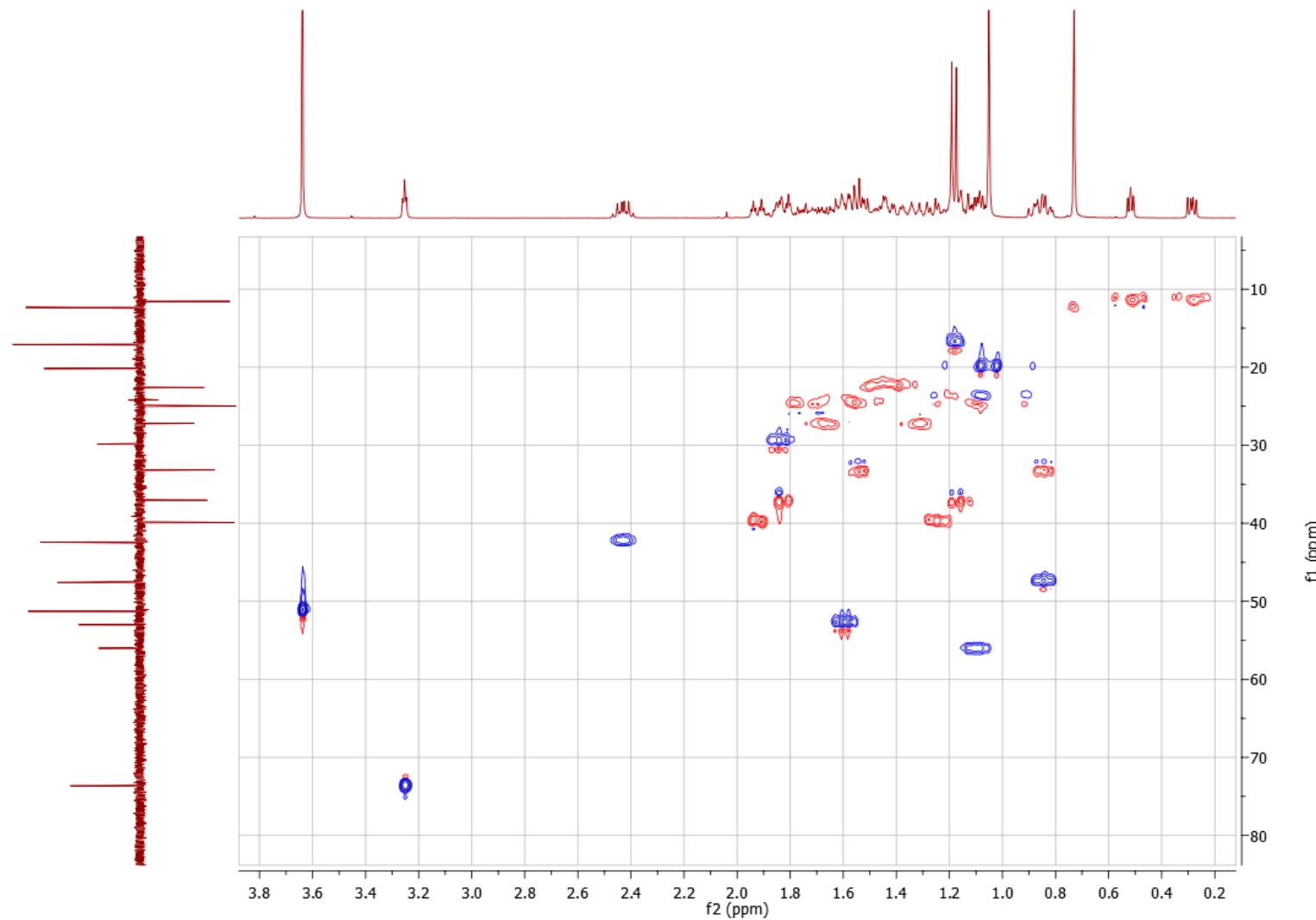


Figure S13. 2D HSQC NMR spectrum of Methyl (20S)-6 β -hydroxy-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**15**)

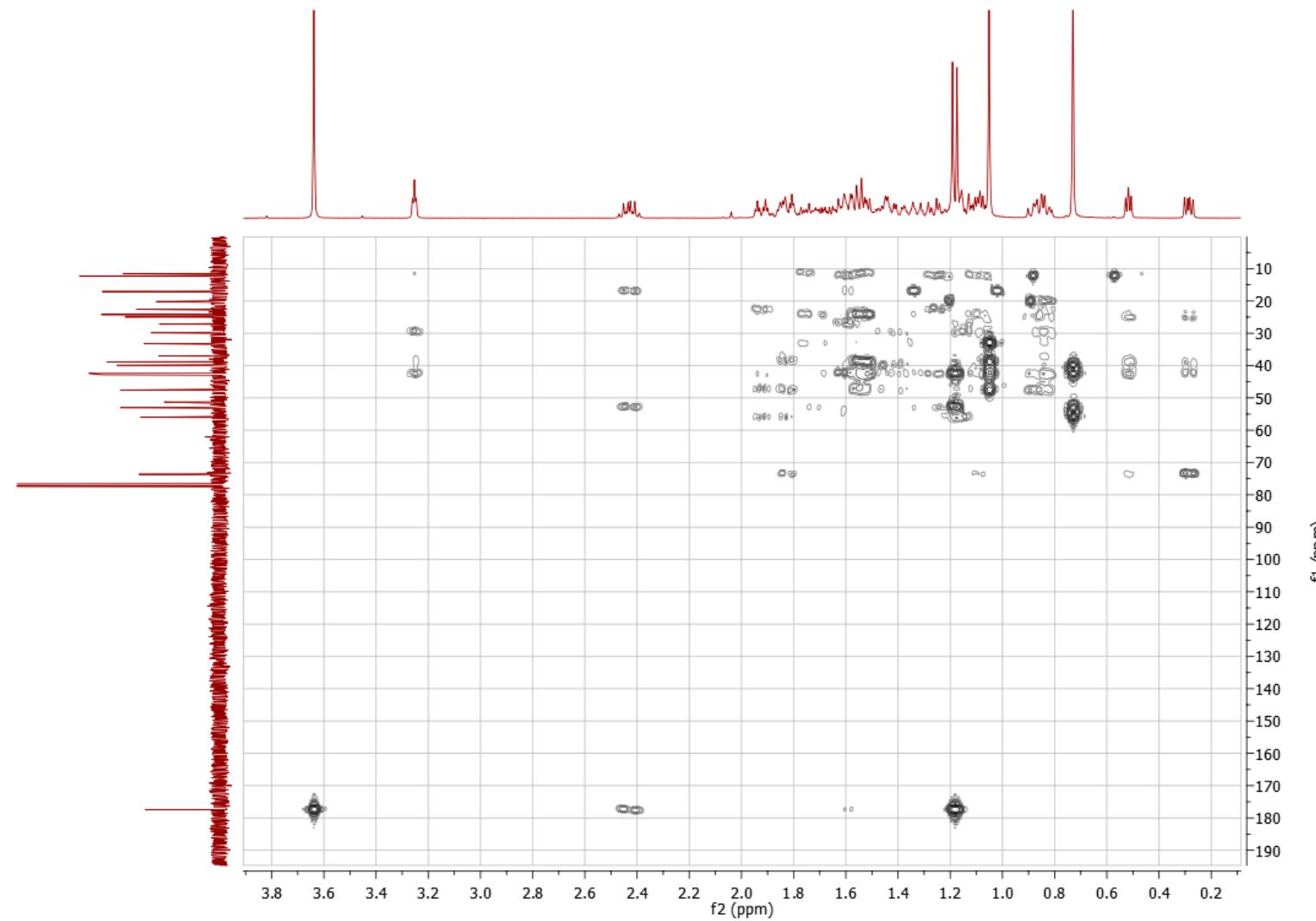


Figure S14. 2D HMBC NMR spectrum of Methyl (20S)-6 β -hydroxy-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (15)

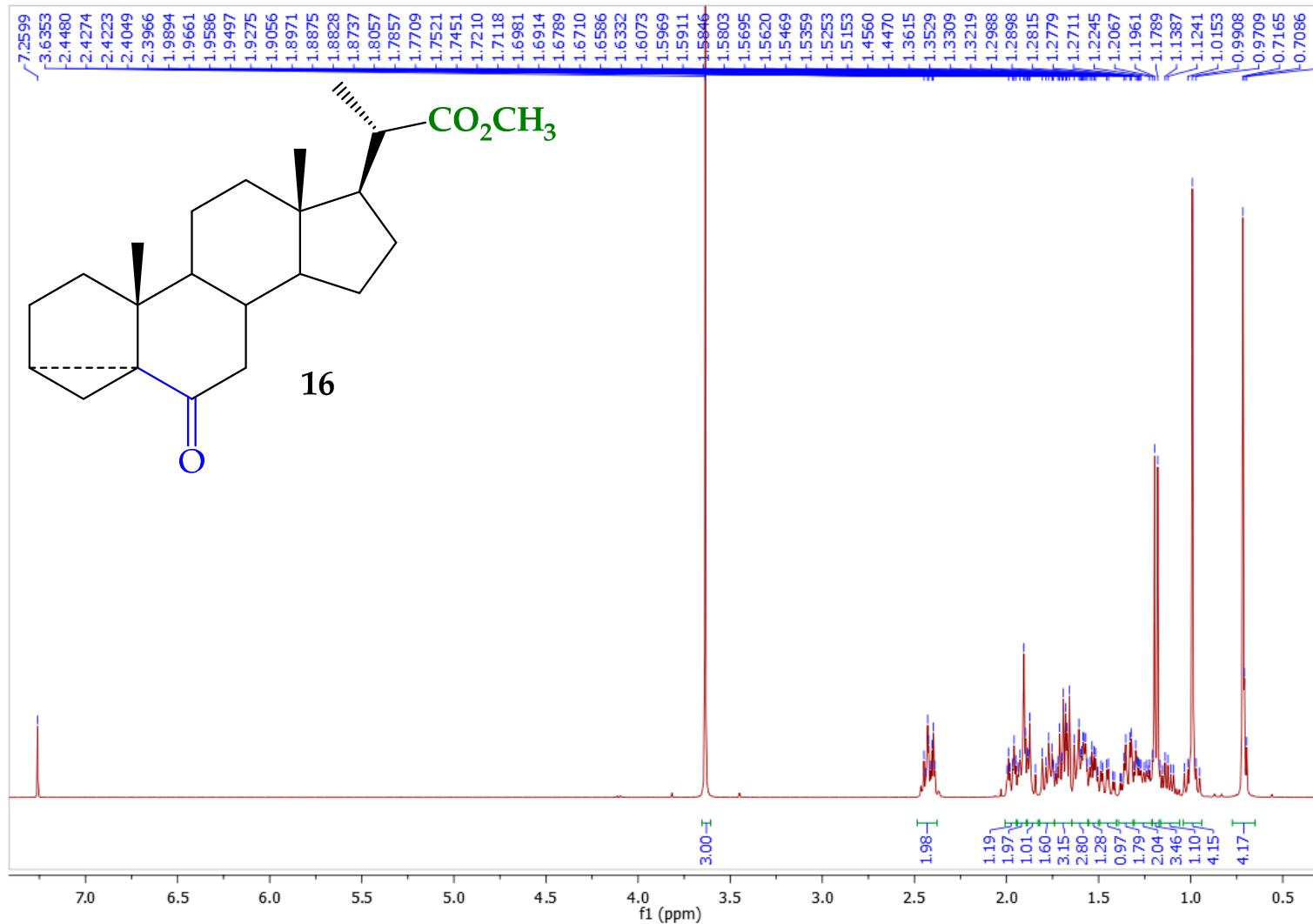


Figure S15. ¹H NMR spectrum of Methyl (20S)-6-Oxo-3 α ,5 α -pregnane-20-carboxylate (**16**)

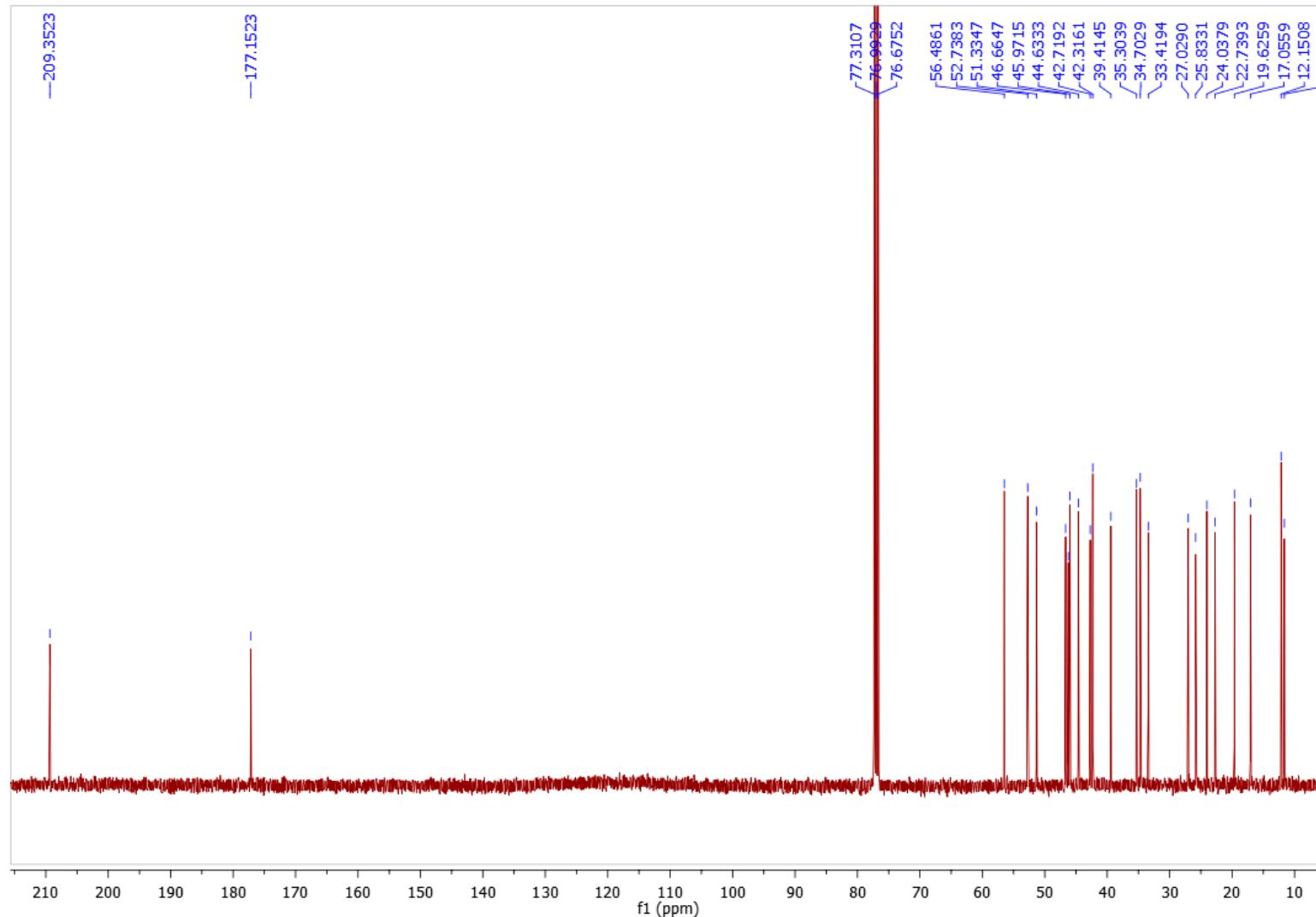


Figure S16. ¹³C NMR spectrum of Methyl (20S)-6-Oxo-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**16**)

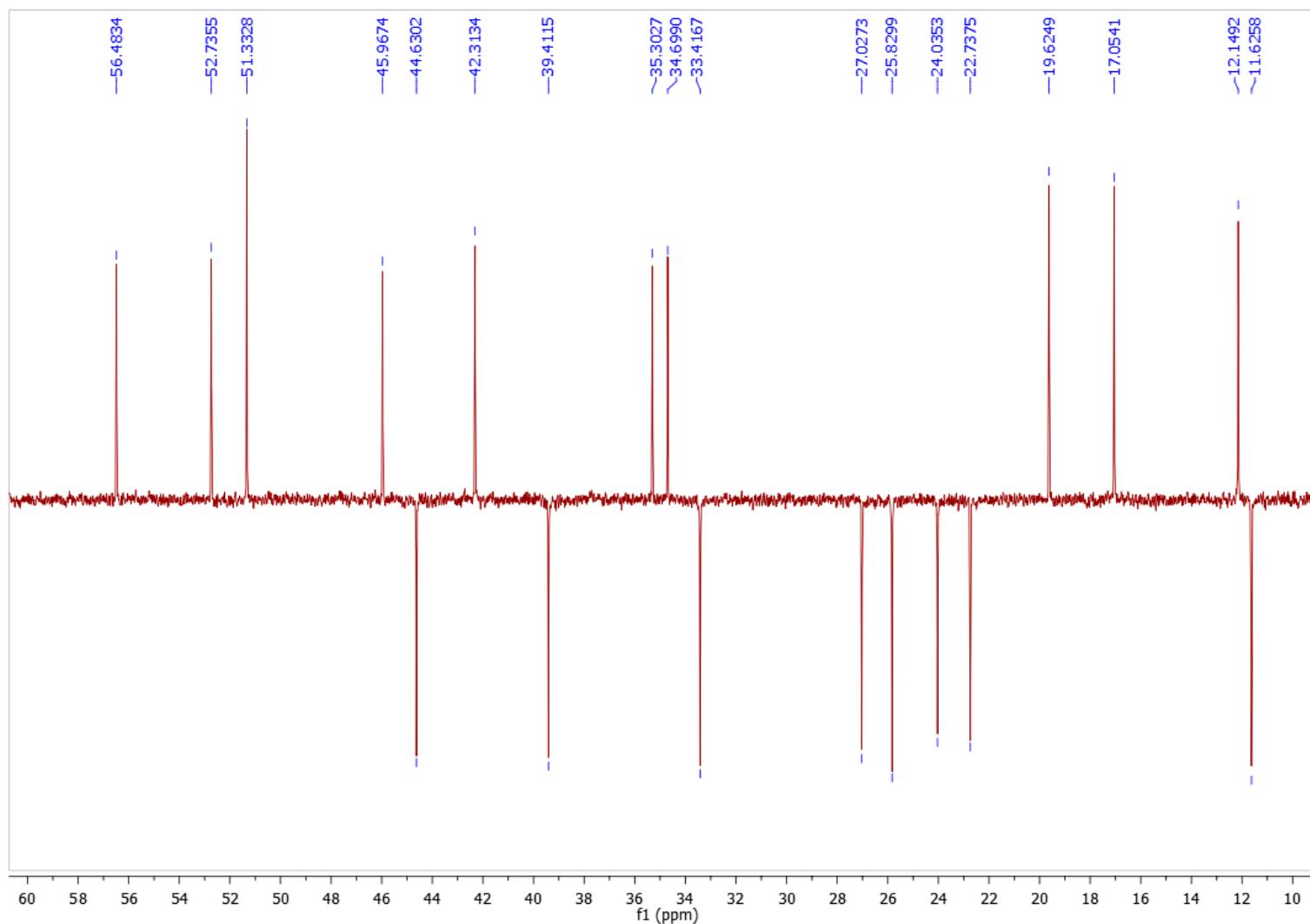


Figure S17. ¹³C DEPT-135 NMR spectrum of Methyl (20S)-6-Oxo-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**16**)

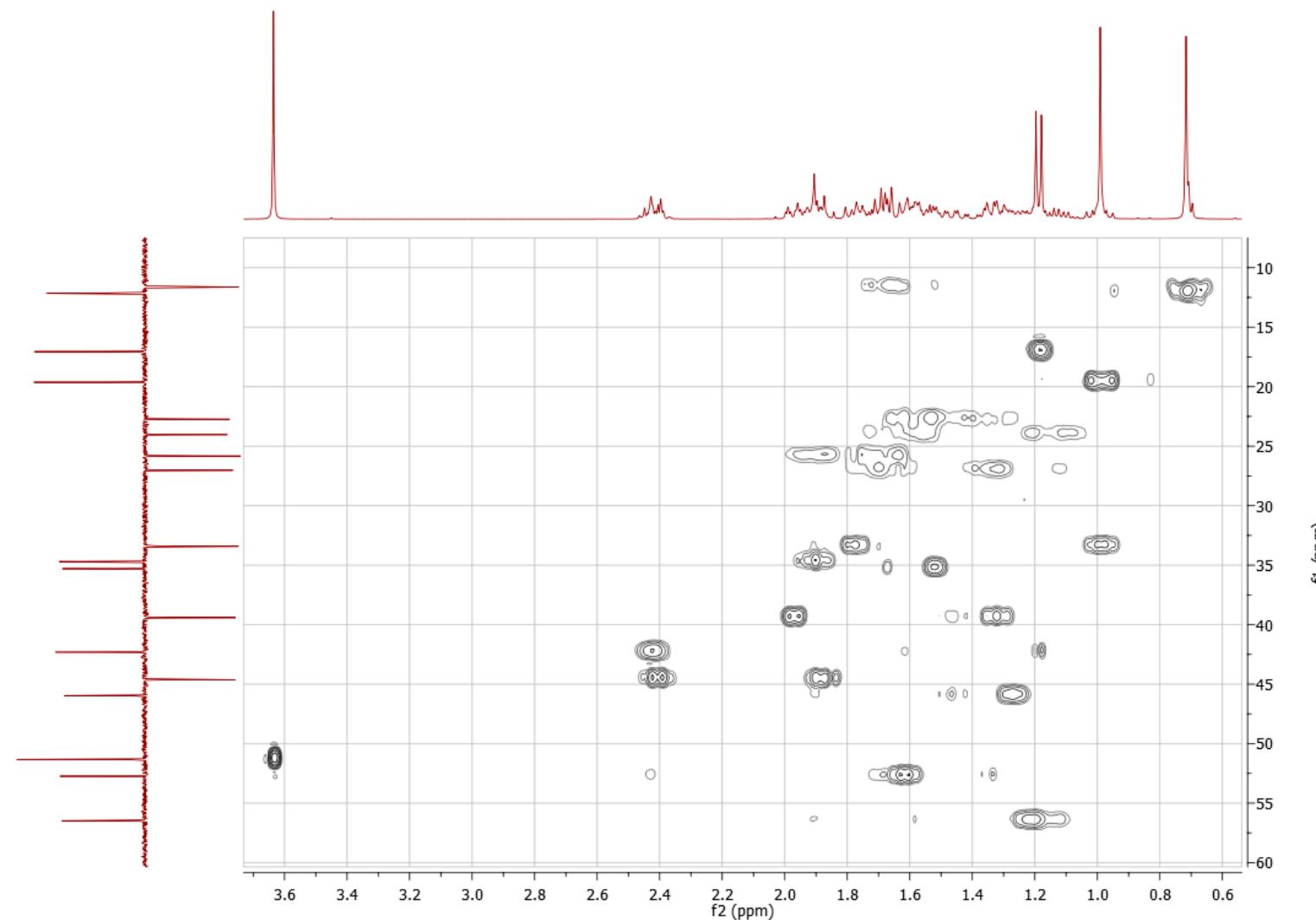


Figure S18. 2D HSQC NMR spectrum of Methyl (20S)-6-Oxo-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**16**)

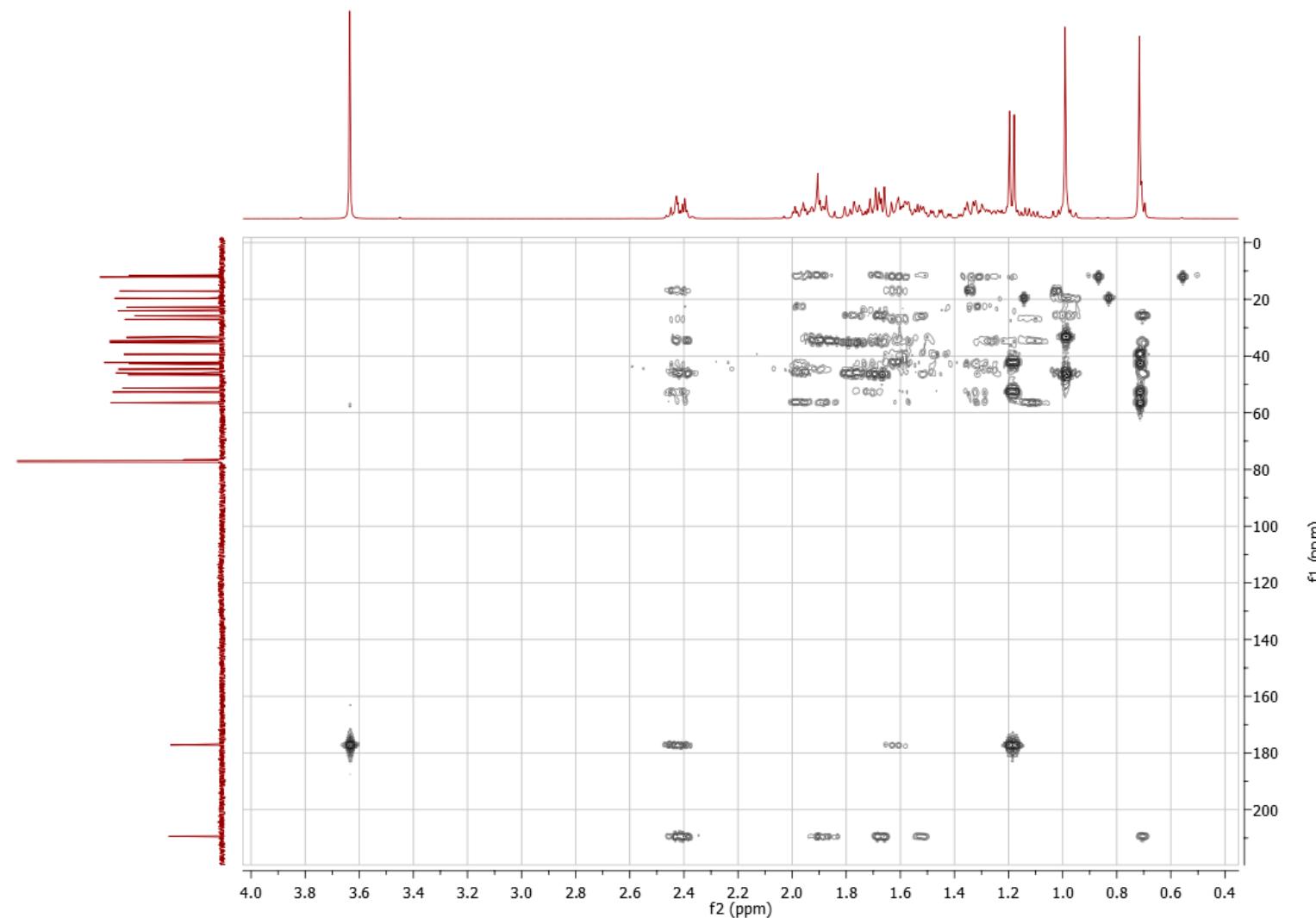


Figure S19. 2D HMBC NMR spectrum of Methyl (20S)-6-Oxo-3 α ,5 α -cyclo-5 α -pregnane-20-carboxylate (**16**)

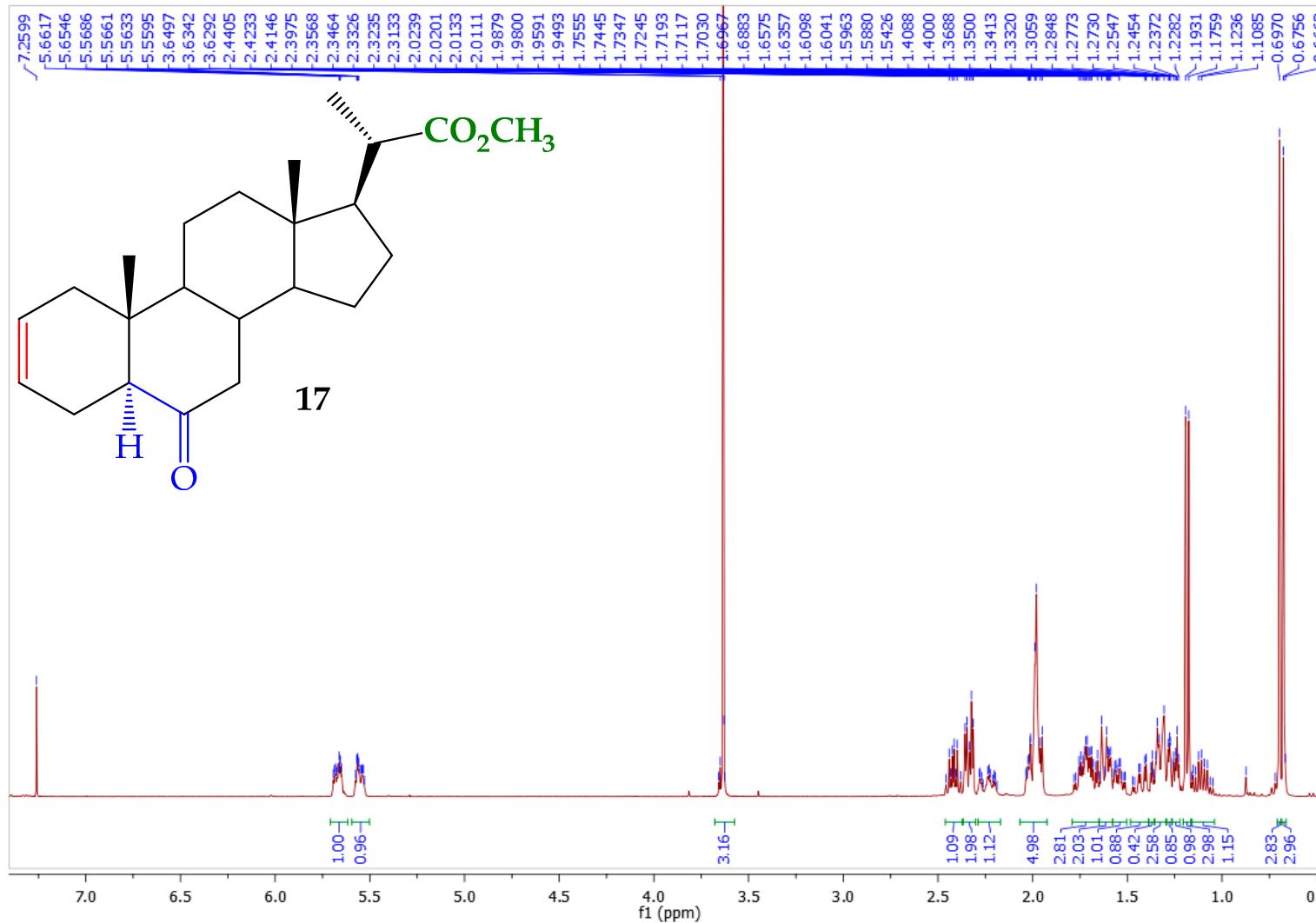


Figure S20. ¹H NMR spectrum of Methyl (20S)-6-Oxo-5 α -pregn-2-ene-20-carboxylate (17)

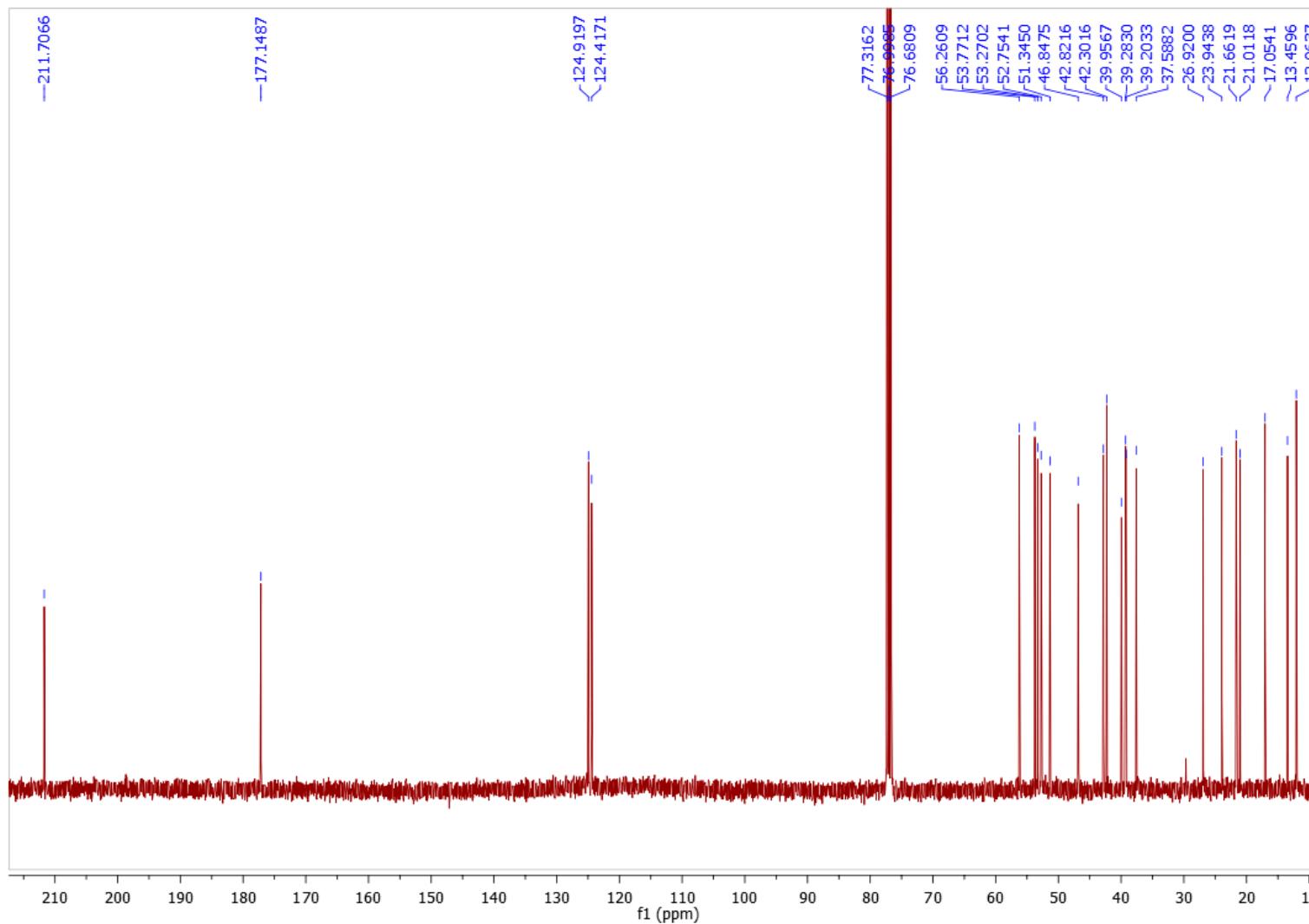


Figure S21. ^{13}C NMR spectrum of Methyl (20S)-6-Oxo-5 α -pregn-2-ene-20-carboxylate (17)

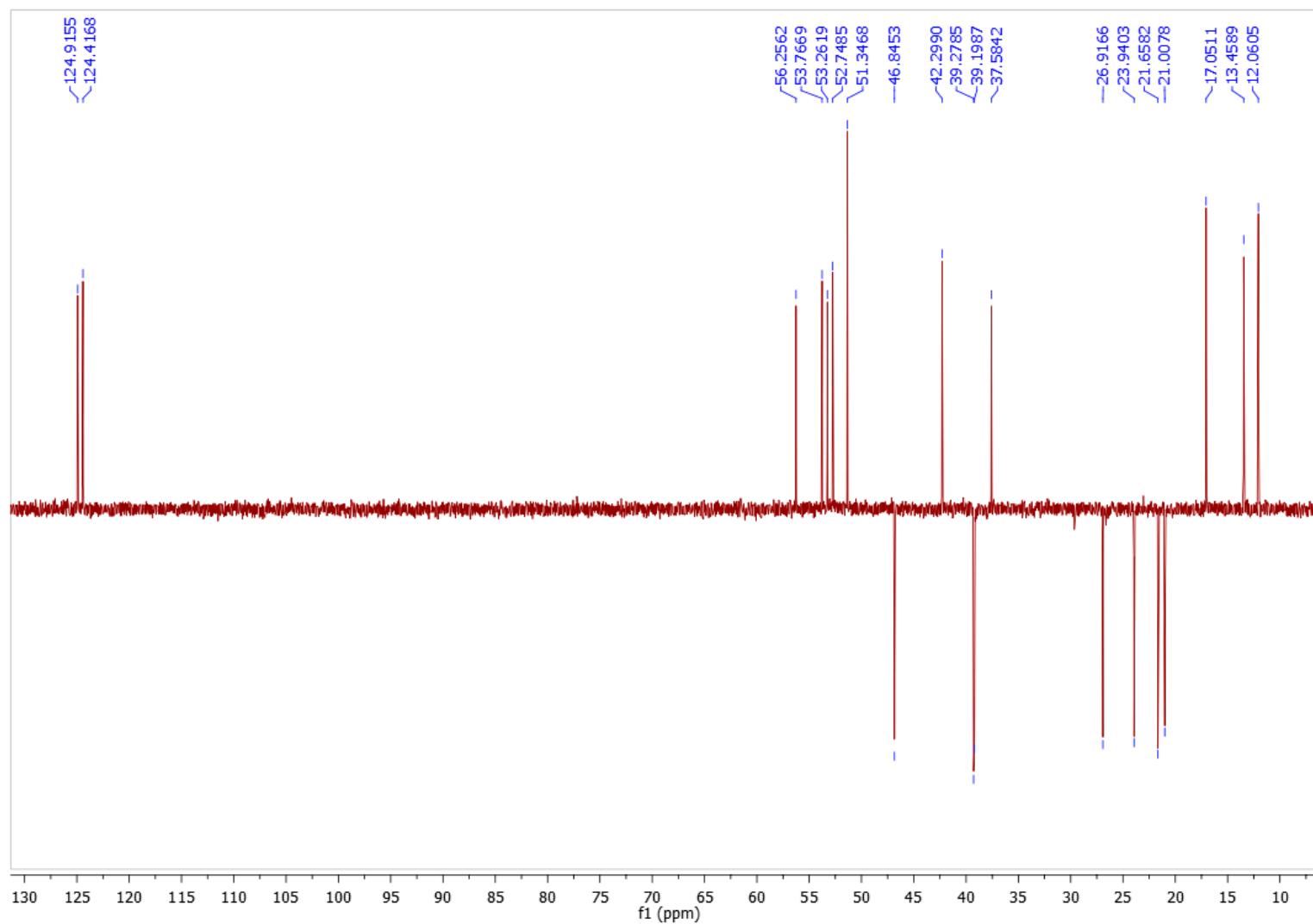


Figure S22. ^{13}C DEPT-135 NMR spectrum of Methyl (20S)-6-Oxo-5 α -pregn-2-ene-20-carboxylate (17)

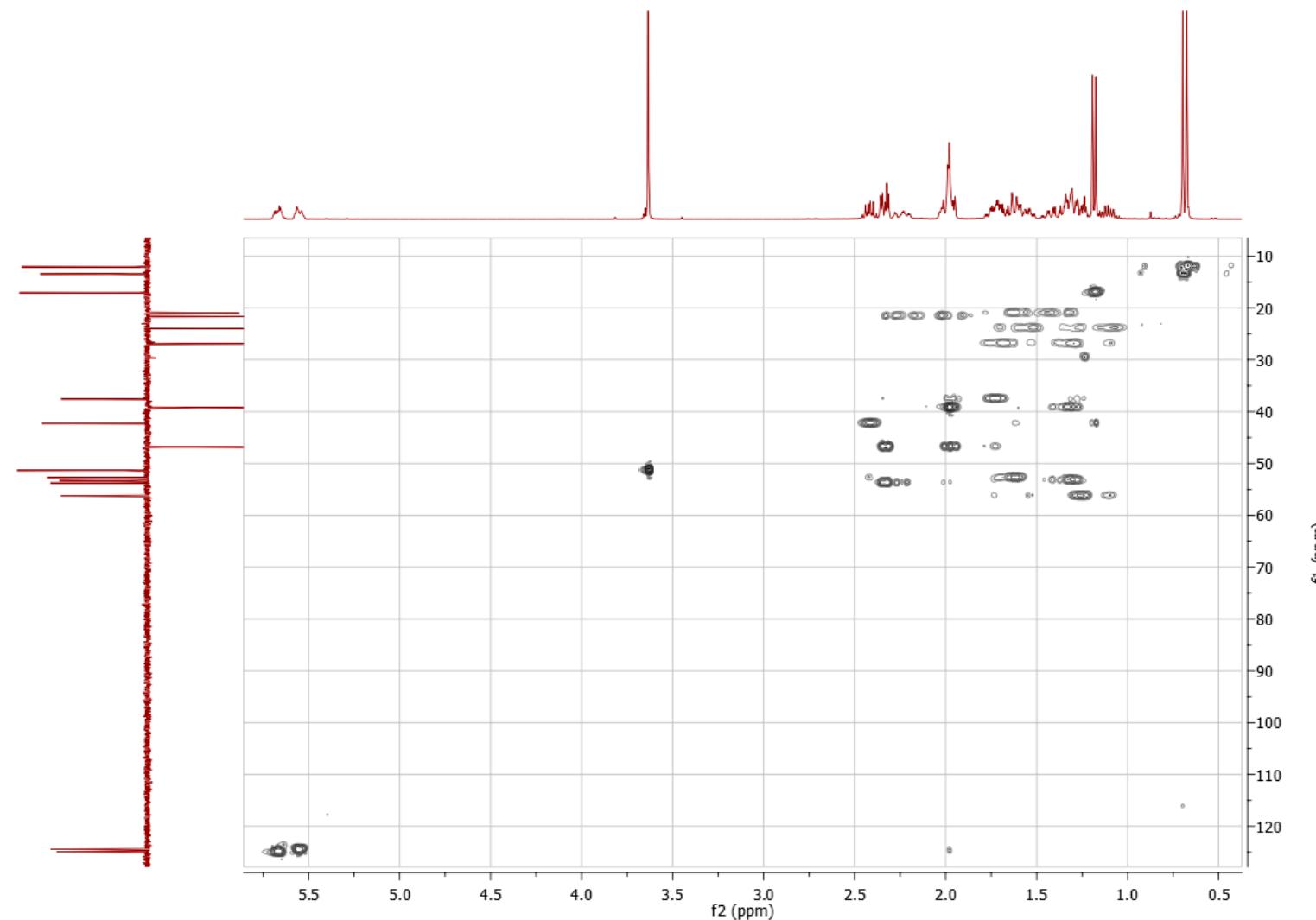


Figure S23. 2D HSQC NMR spectrum of Methyl (20S)-6-Oxo-5 α -pregn-2-ene-20-carboxylate (17)

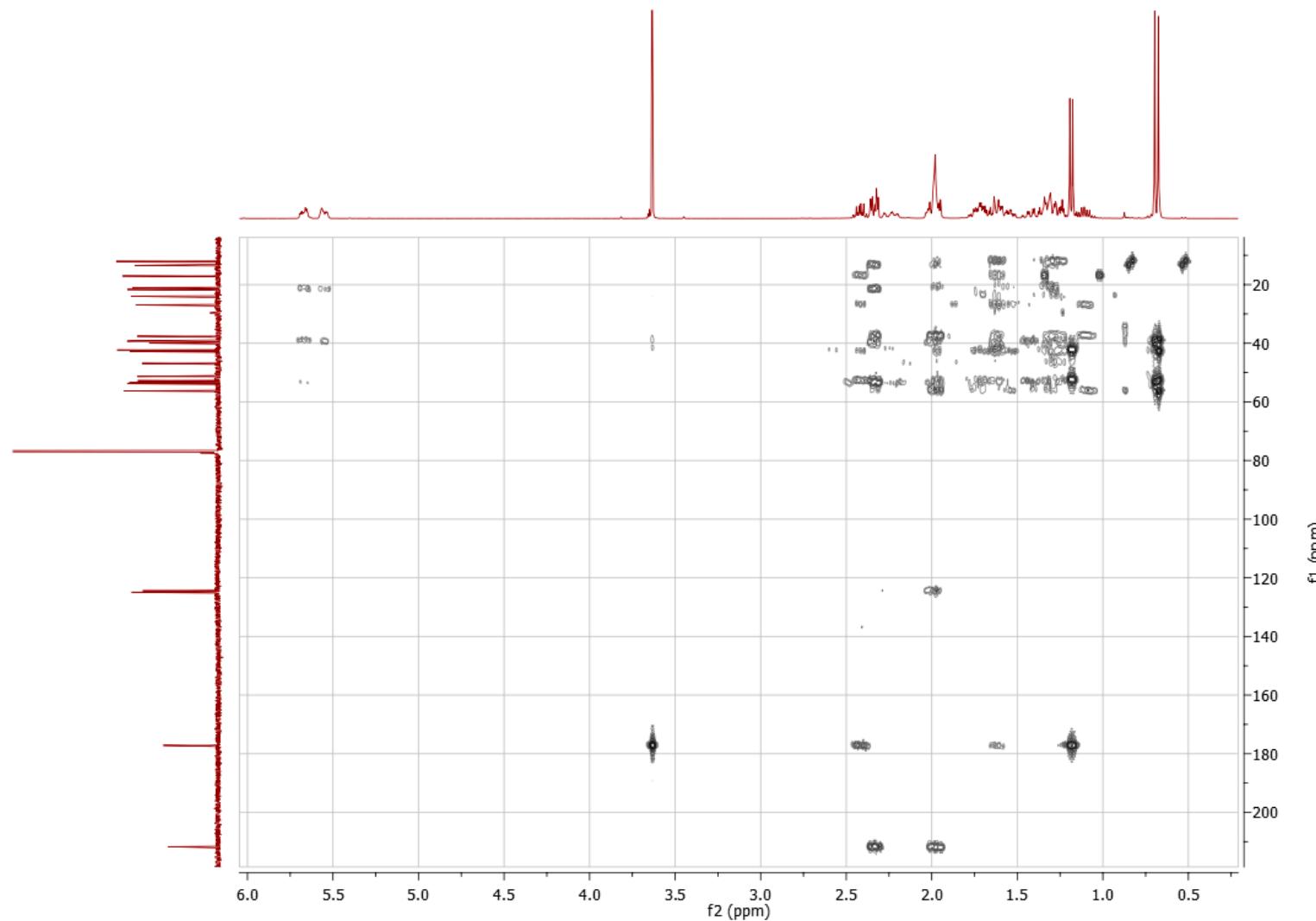


Figure S24. 2D HSQC NMR spectrum of Methyl (20S)-6-Oxo-5 α -pregn-2-ene-20-carboxylate (**17**)

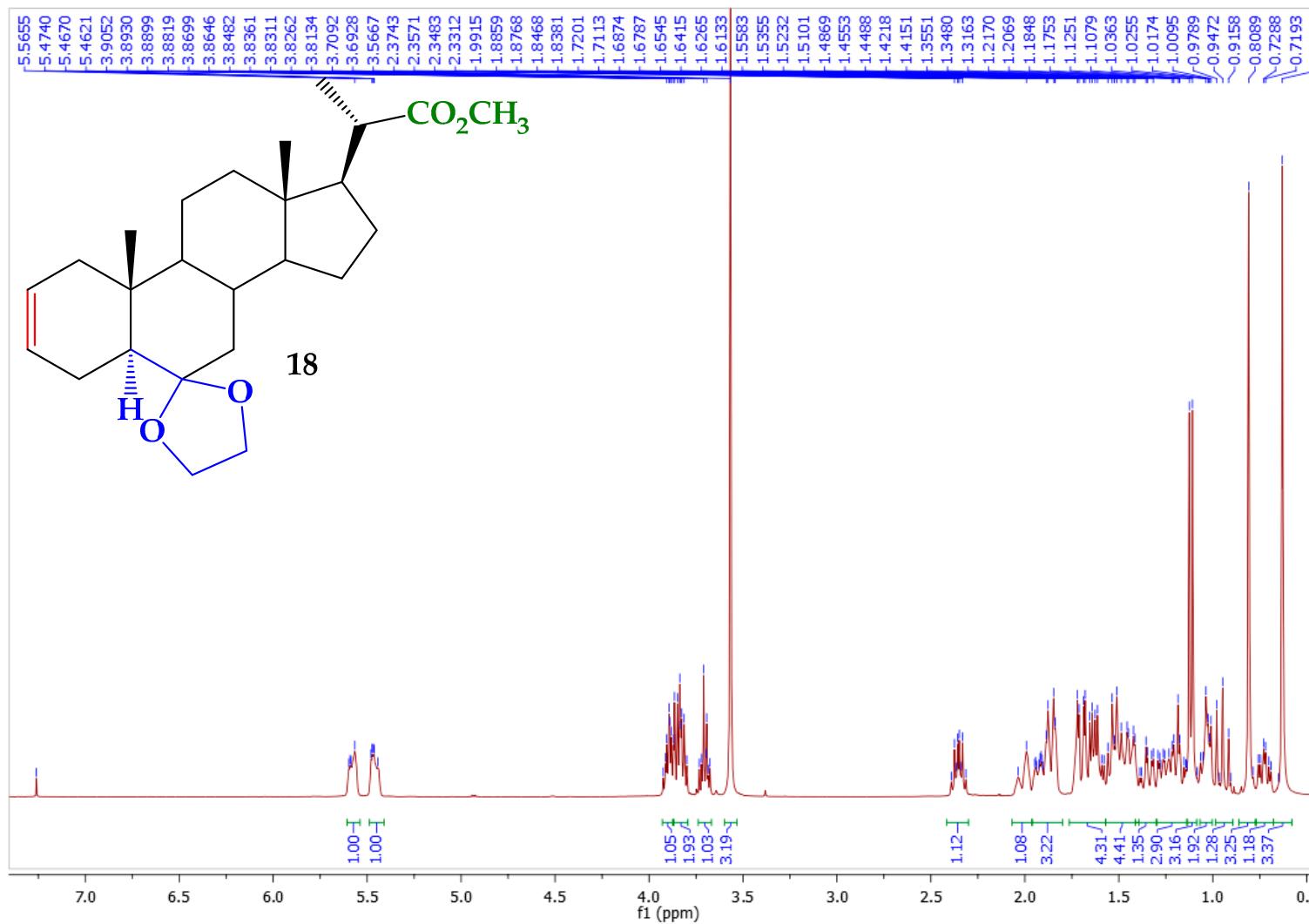


Figure S25. ^1H NMR spectrum of Methyl (20S)-6,6-ethylenedioxy-5 α -pregn-2-ene-20-carboxylate (**18**)

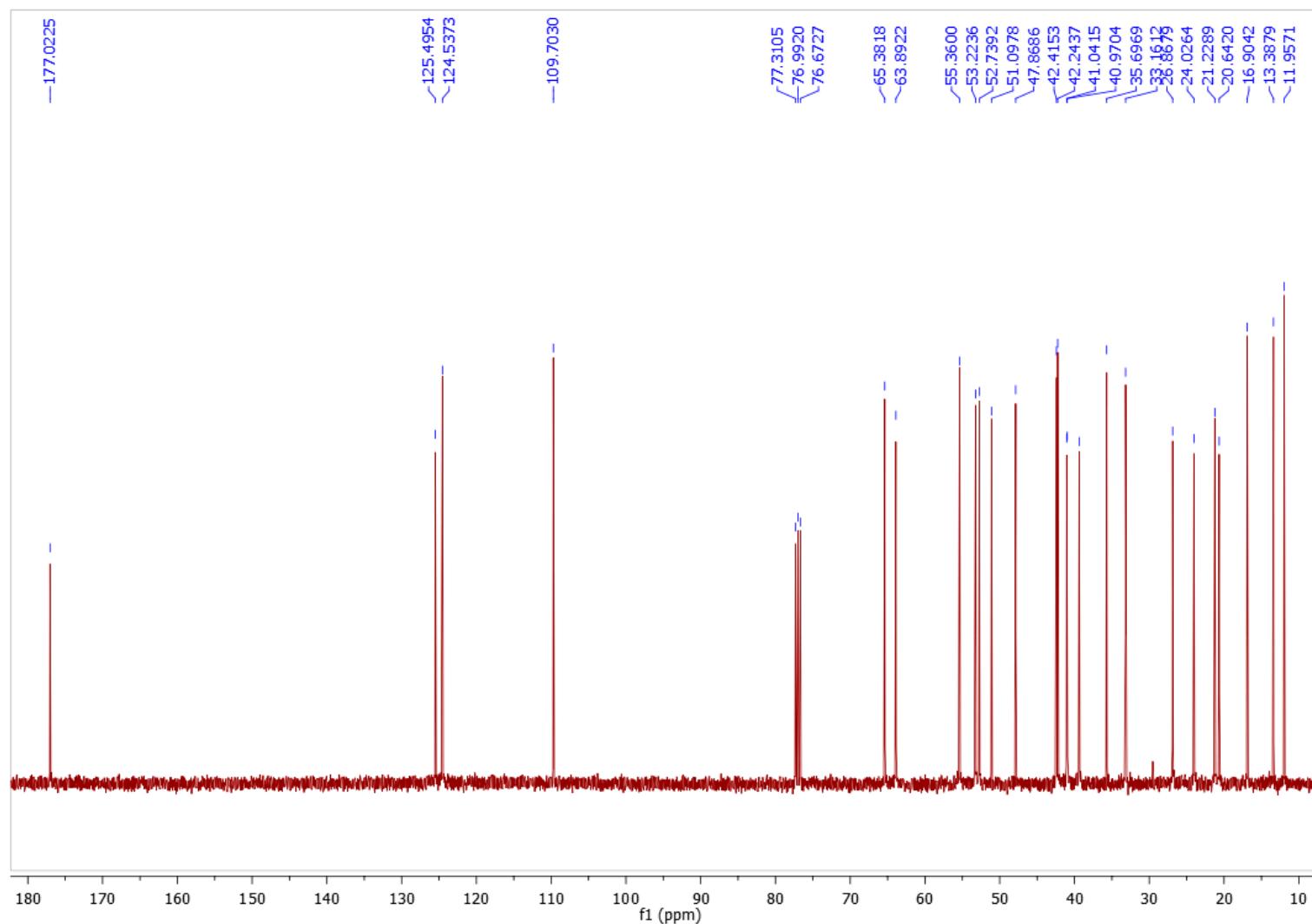


Figure S26. ${}^{13}\text{C}$ NMR spectrum of Methyl (20S)-6,6-ethylenedioxy-5 α -pregn-2-ene-20-carboxylate (18)

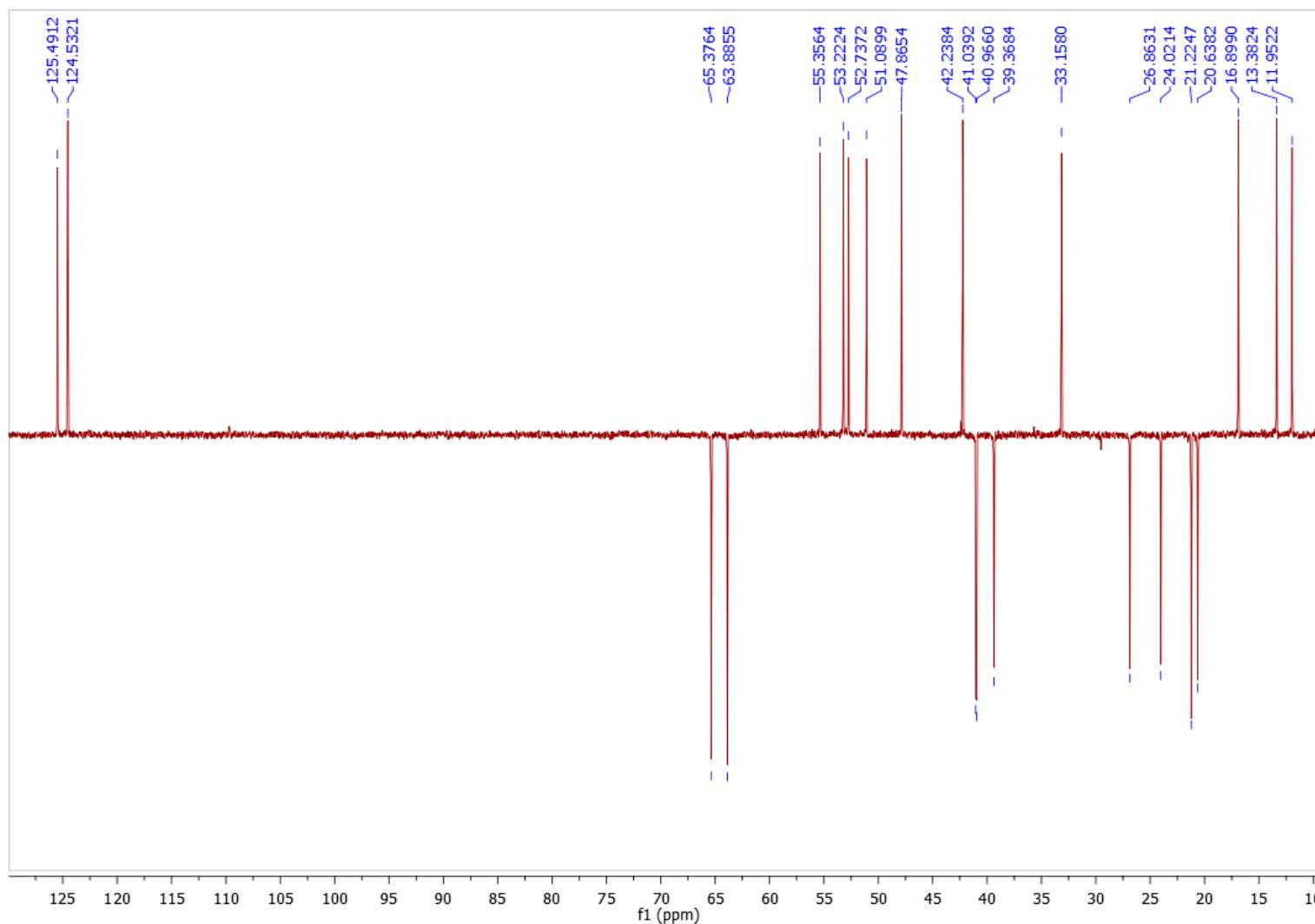


Figure S27. ¹³C DEPT-135 NMR spectrum of Methyl (20S)-6,6-ethylenedioxy-5 α -pregn-2-ene-20-carboxylate (**18**)

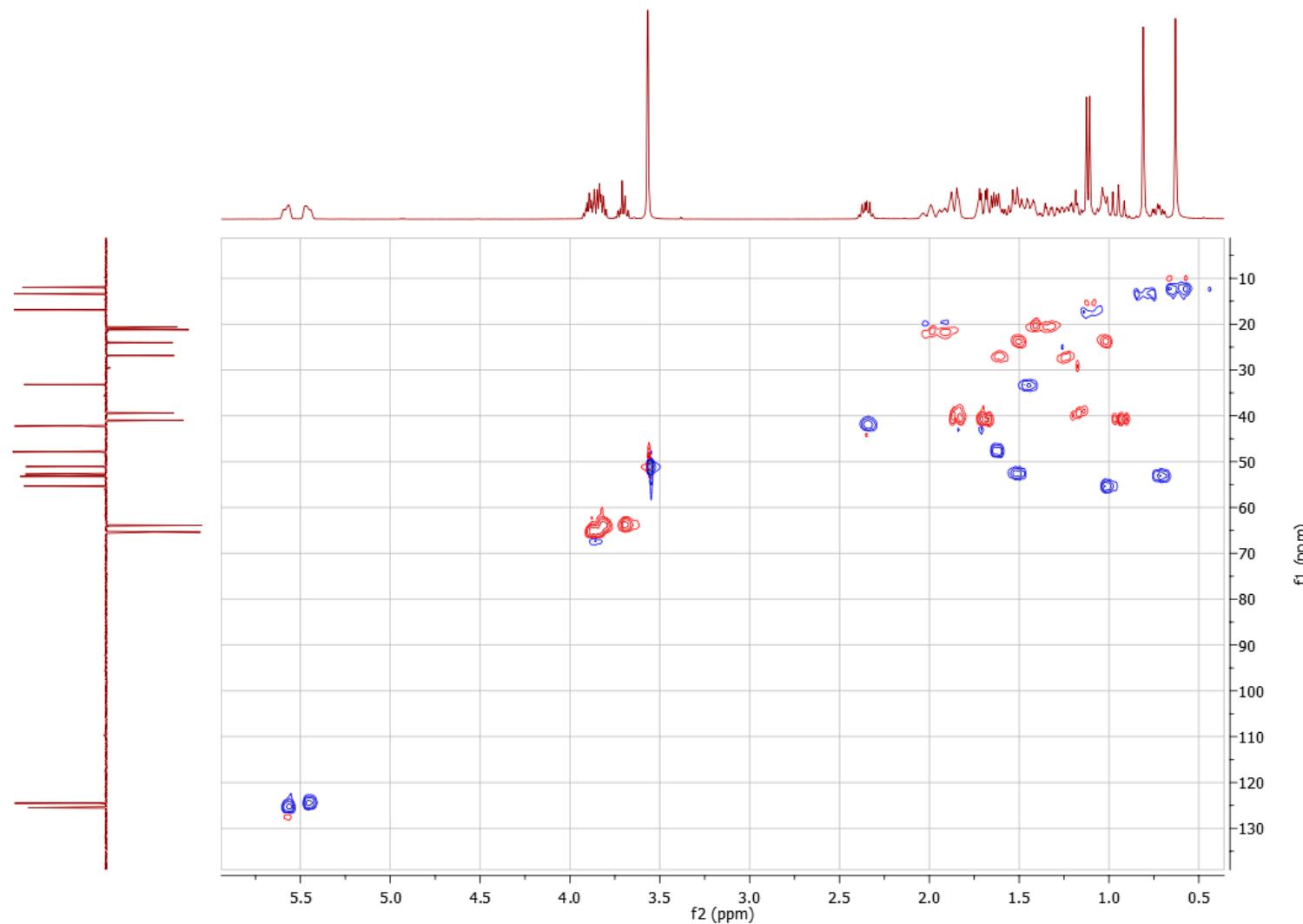


Figure S28. 2D HSQC NMR spectrum of Methyl (20S)-6,6-ethylenedioxy-5 α -pregn-2-ene-20-carboxylate (18)

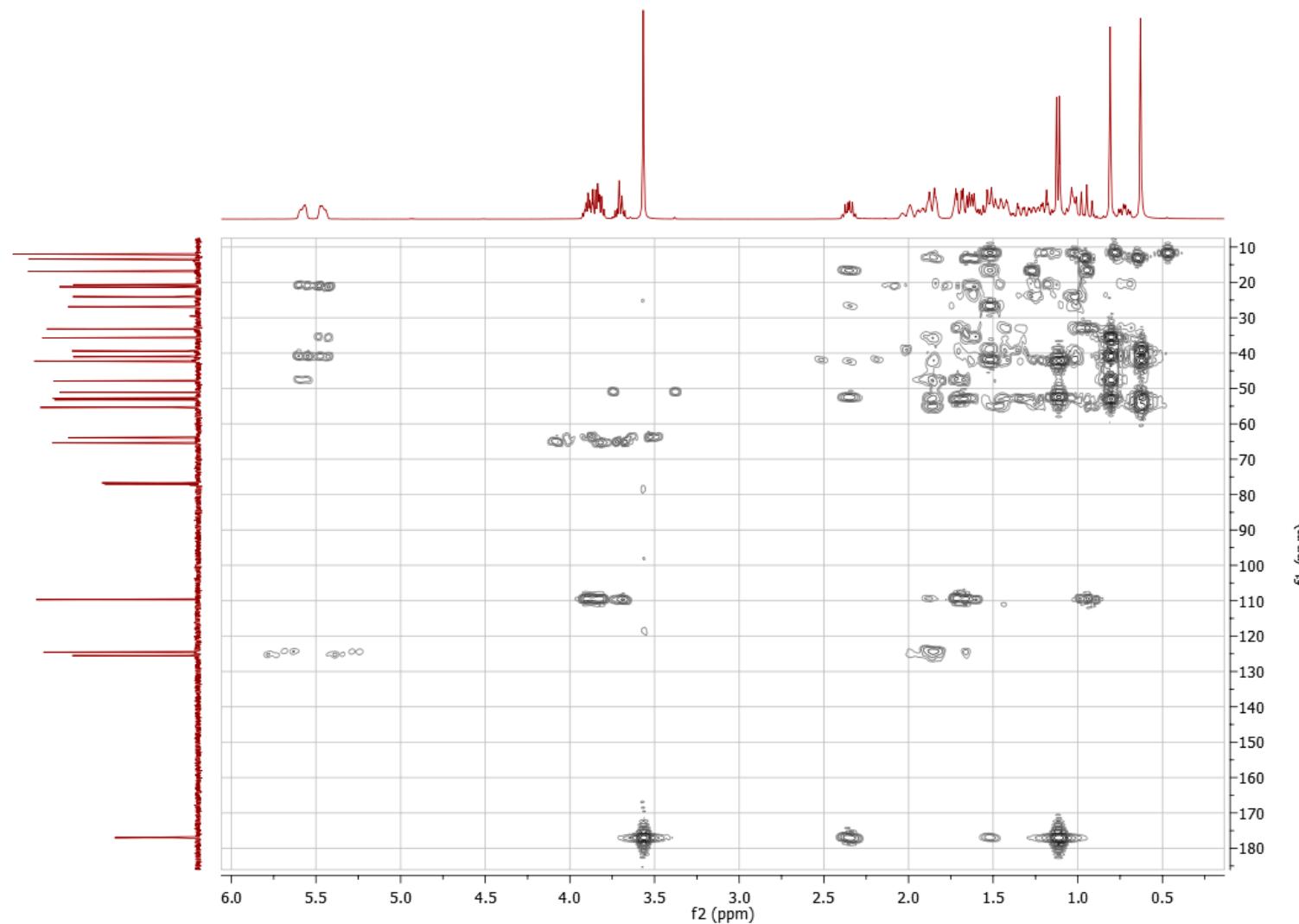


Figure S29. 2D HMBC NMR spectrum of Methyl (20S)-6,6-ethylenedioxy-5 α -pregn-2-ene-20-carboxylate (**18**)

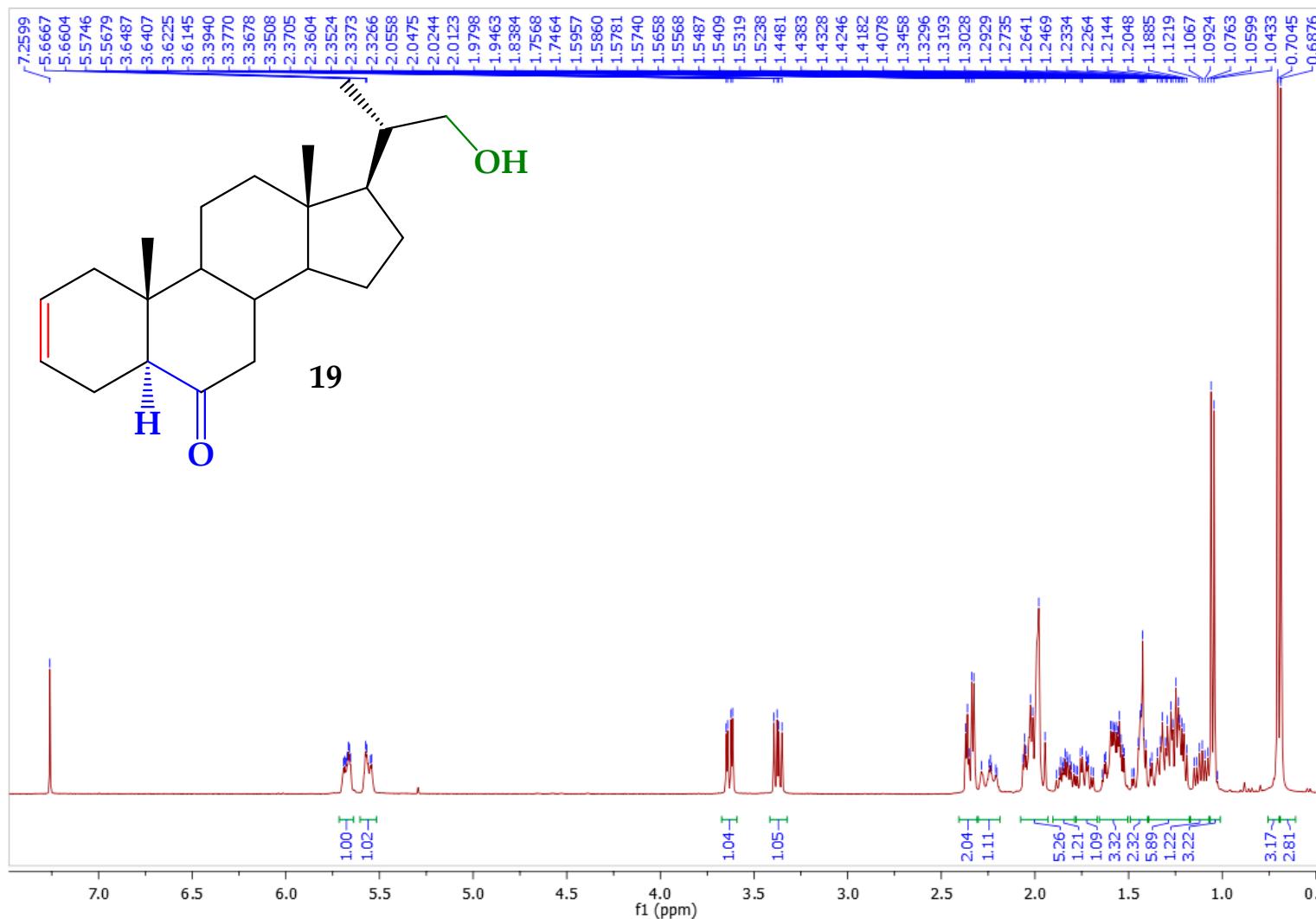


Figure S30. ¹H NMR spectrum of 22-hydroxy-5 α -cholan-2-ene-23,24-dinor-6-one (**19**)

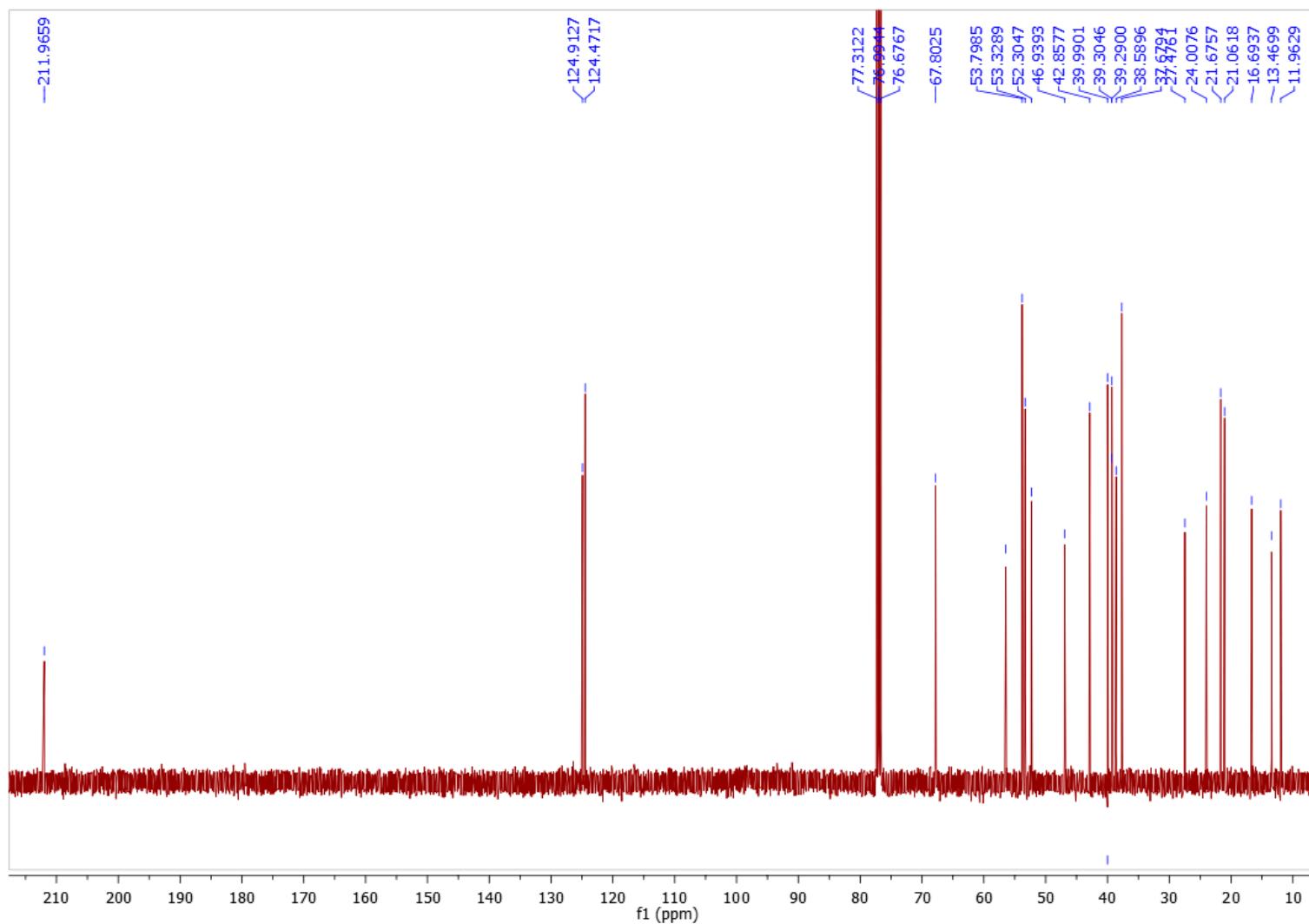


Figure S31. ¹³C NMR spectrum of 22-hydroxy-5 α -cholan-2-ene-23,24-dinor-6-one (19)

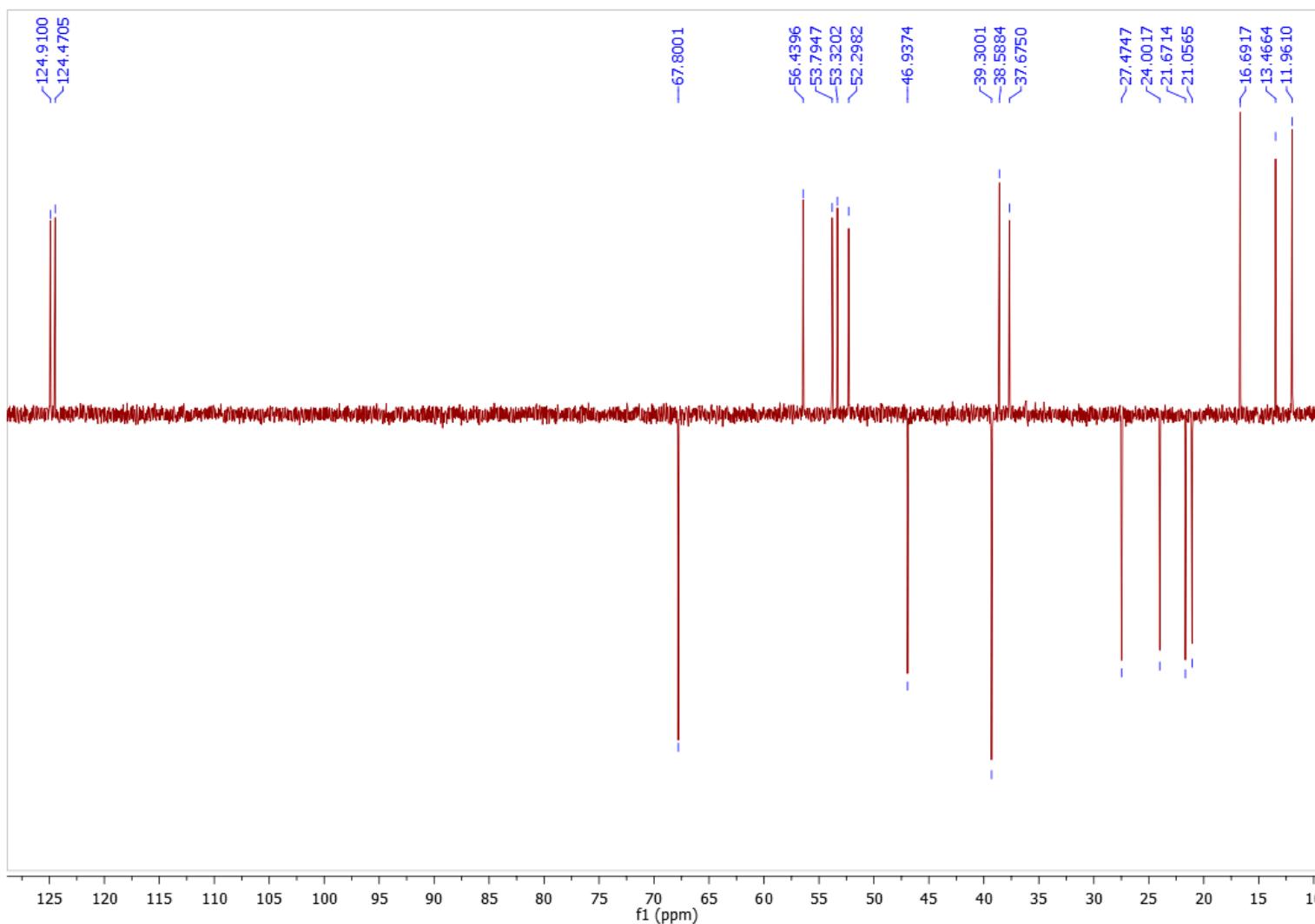


Figure S32. ^{13}C DEPT-135 NMR spectrum of 22-hydroxy-5 α -cholan-2-ene-23,24-dinor-6-one (19)

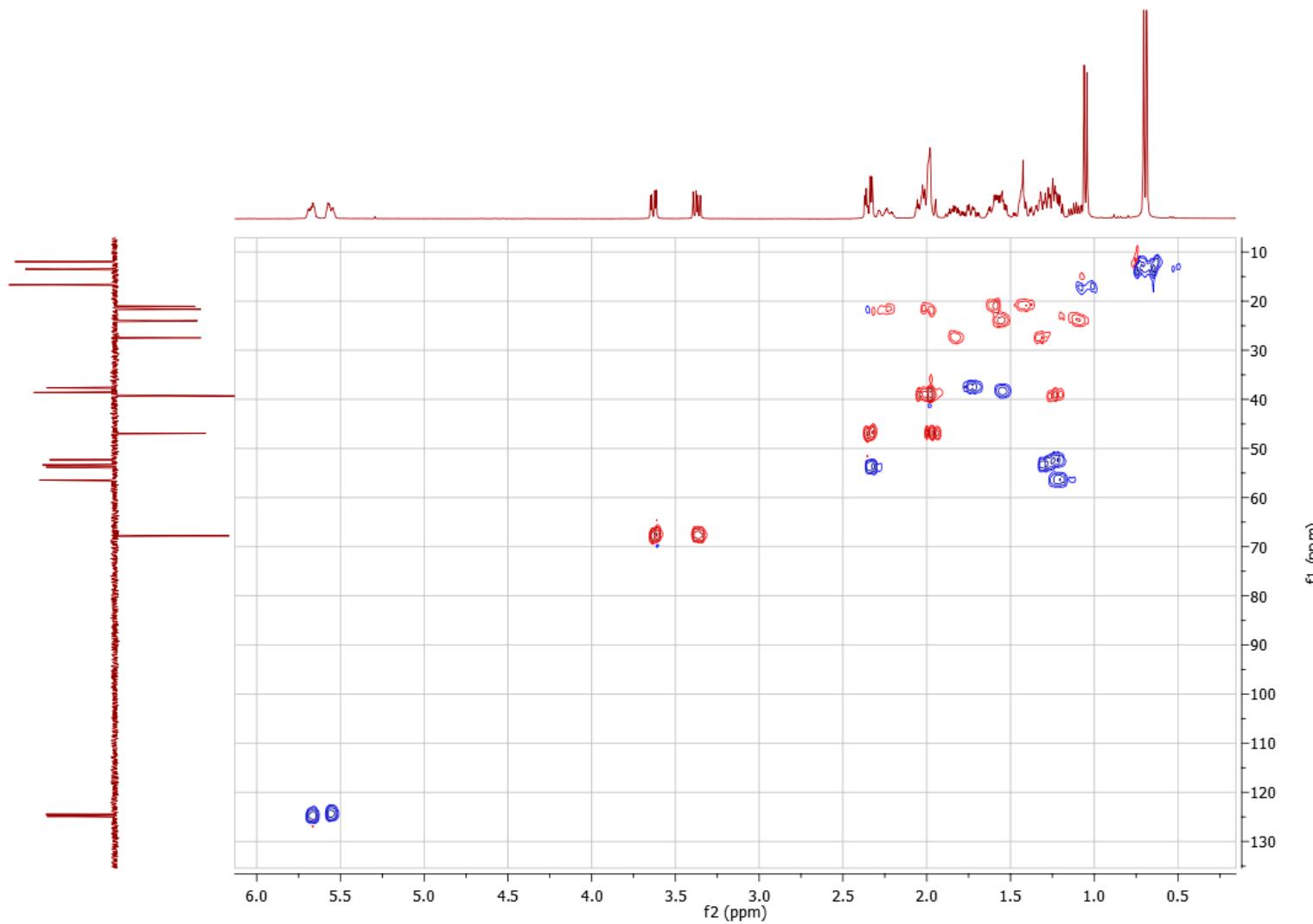


Figure S33. 2D HSQC NMR spectrum of 22-hydroxy-5 α -cholan-2-ene-23,24-dinor-6-one (**19**)

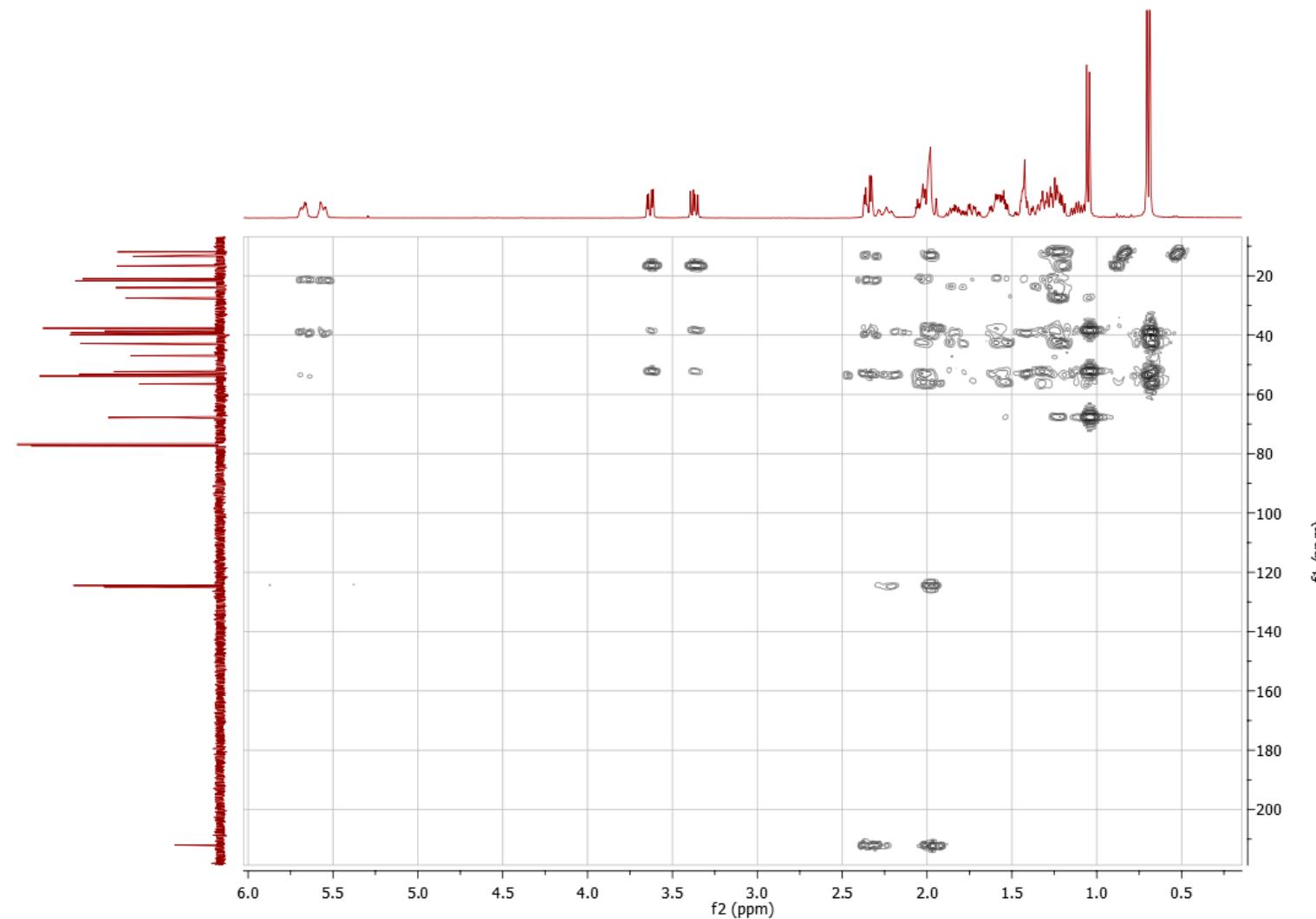


Figure S34. 2D HMBC NMR spectrum of 22-hydroxy-5 α -cholan-2-ene-23,24-dinor-6-one (**19**)

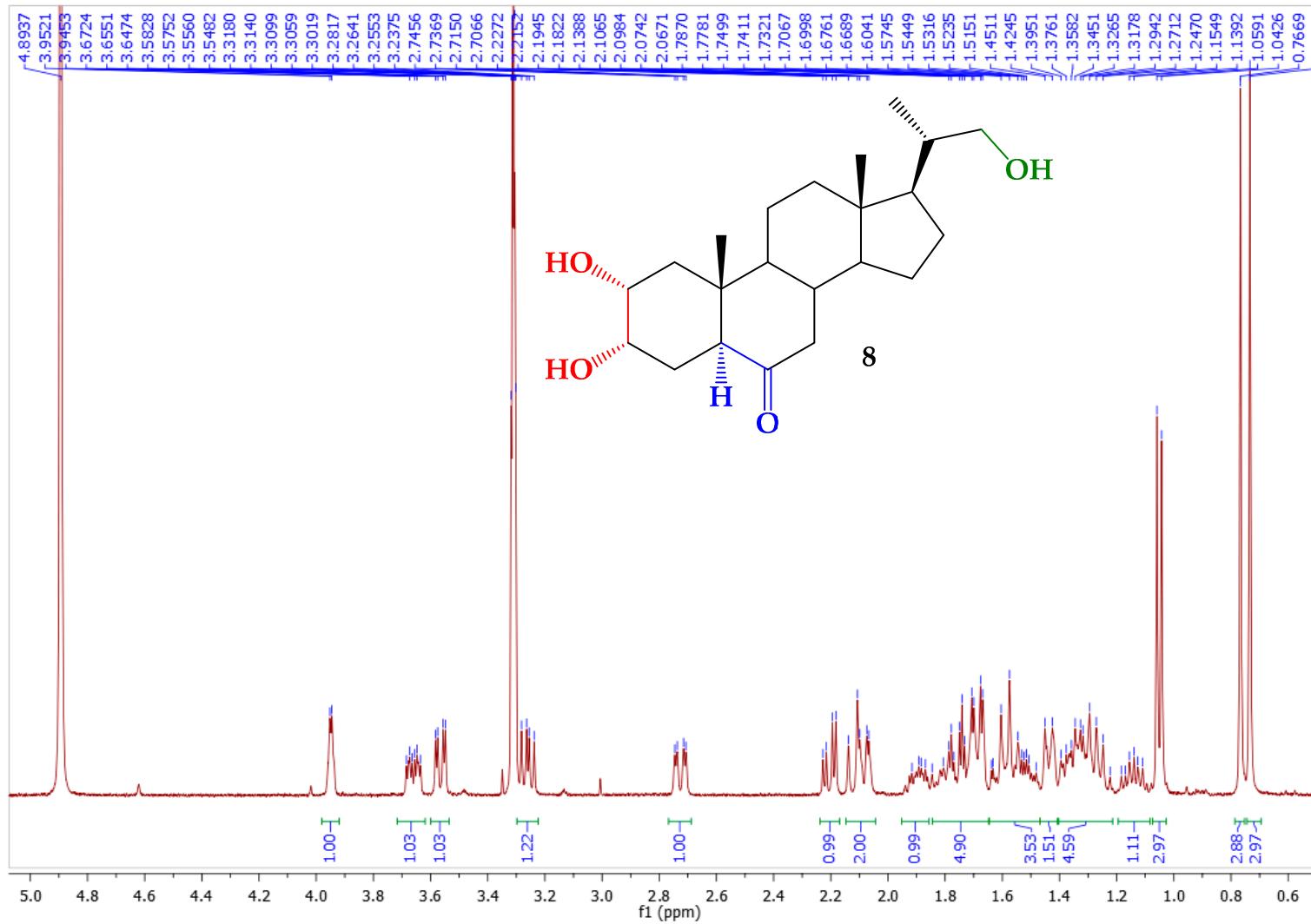


Figure S35. ¹H NMR spectrum of 2 α ,3 α ,22-trihydroxy-5 α -cholan-23,24-dinor-6-one (8)

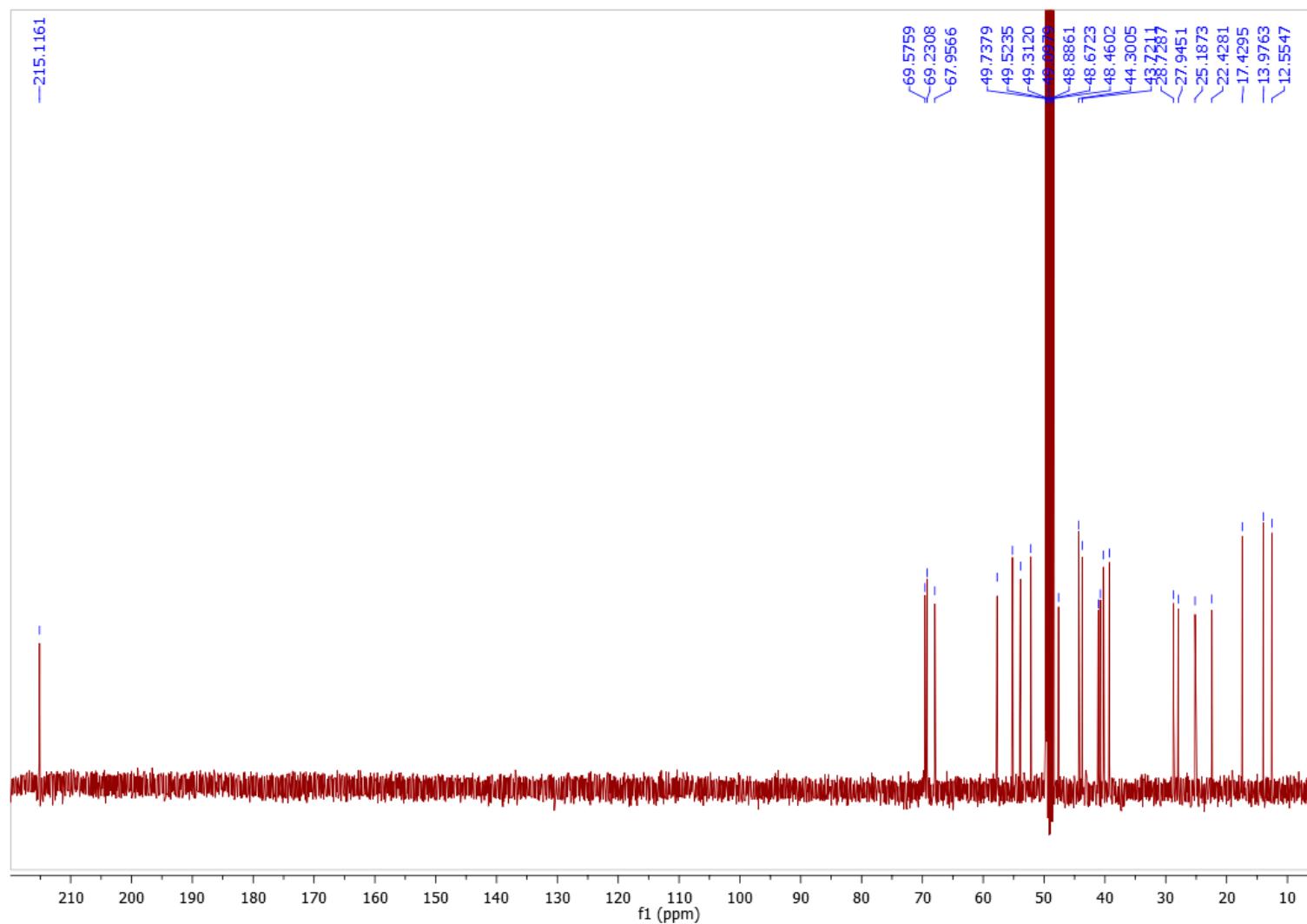


Figure S36. ¹³C NMR spectrum of 2 α ,3 α ,22-trihydroxy-5 α -cholan-23,24-dinor-6-one (8)

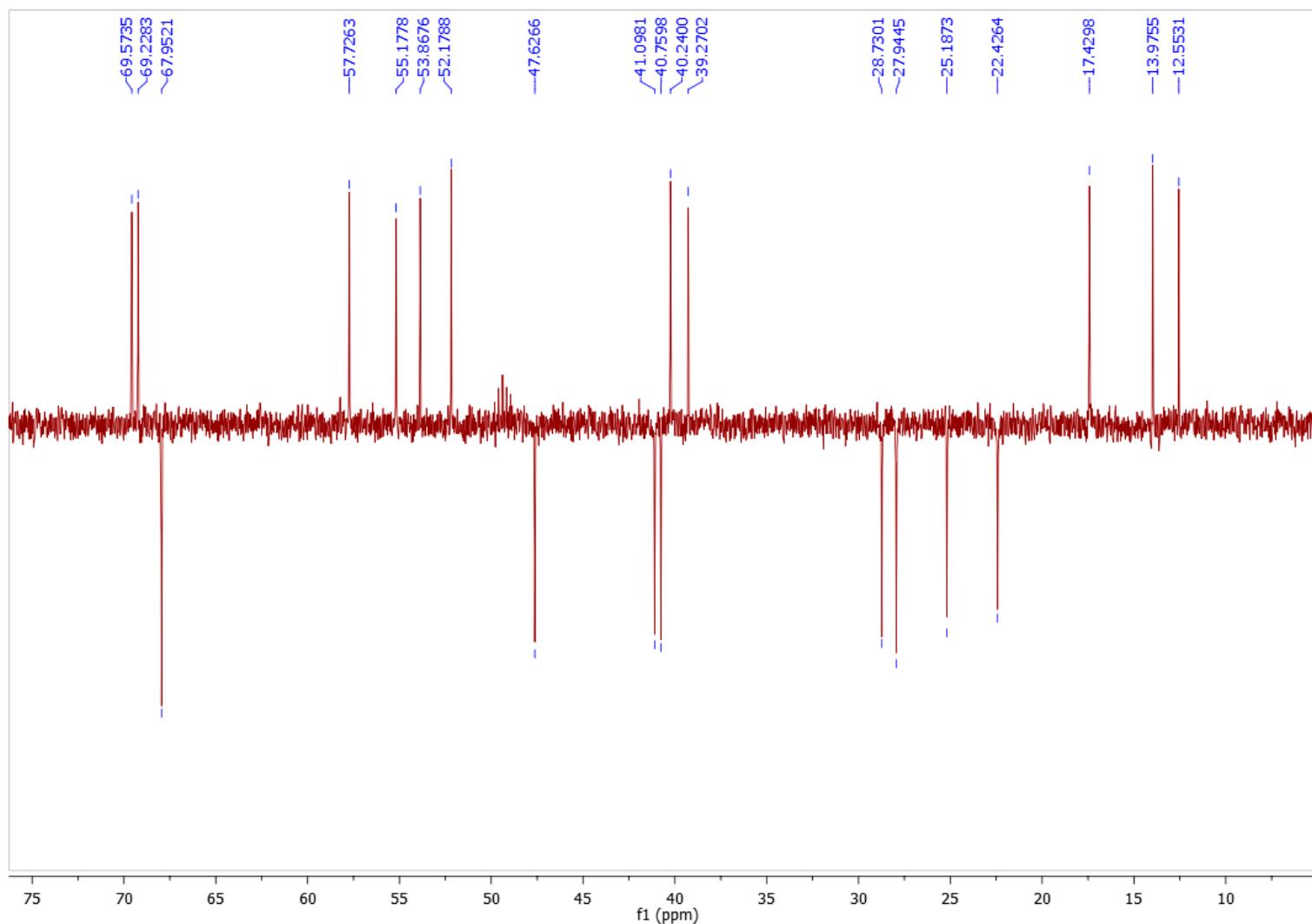


Figure S37. ^{13}C DEPT-135 NMR spectrum of $2\alpha,3\alpha,22$ -thrihydroxy- 5α -cholan- $23,24$ -dinor-6-one (8)

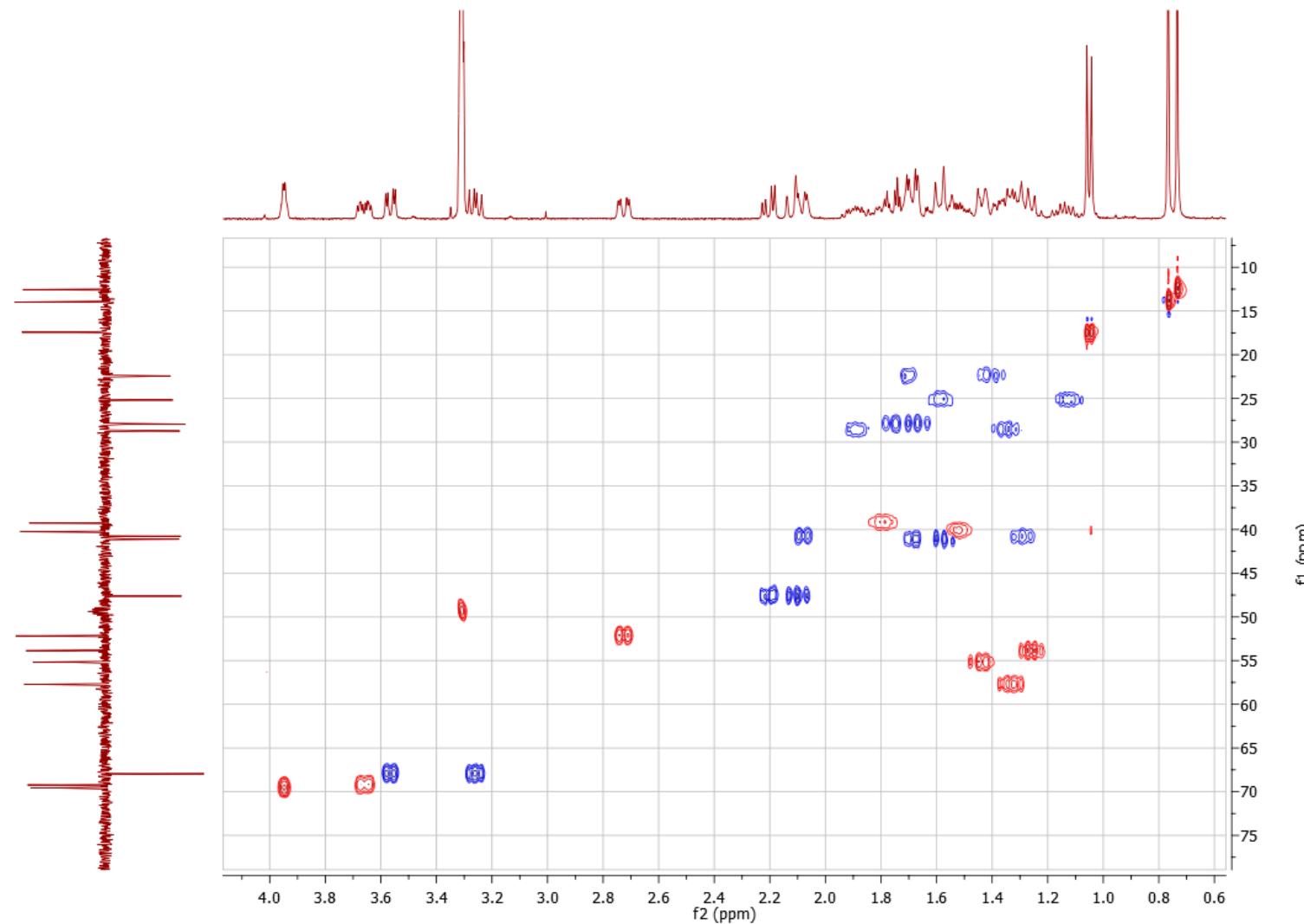


Figure S38. 2D HSQC NMR spectrum of $2\alpha,3\alpha,22$ -thrihydroxy- 5α -cholan- $23,24$ -dinor-6-one (8)

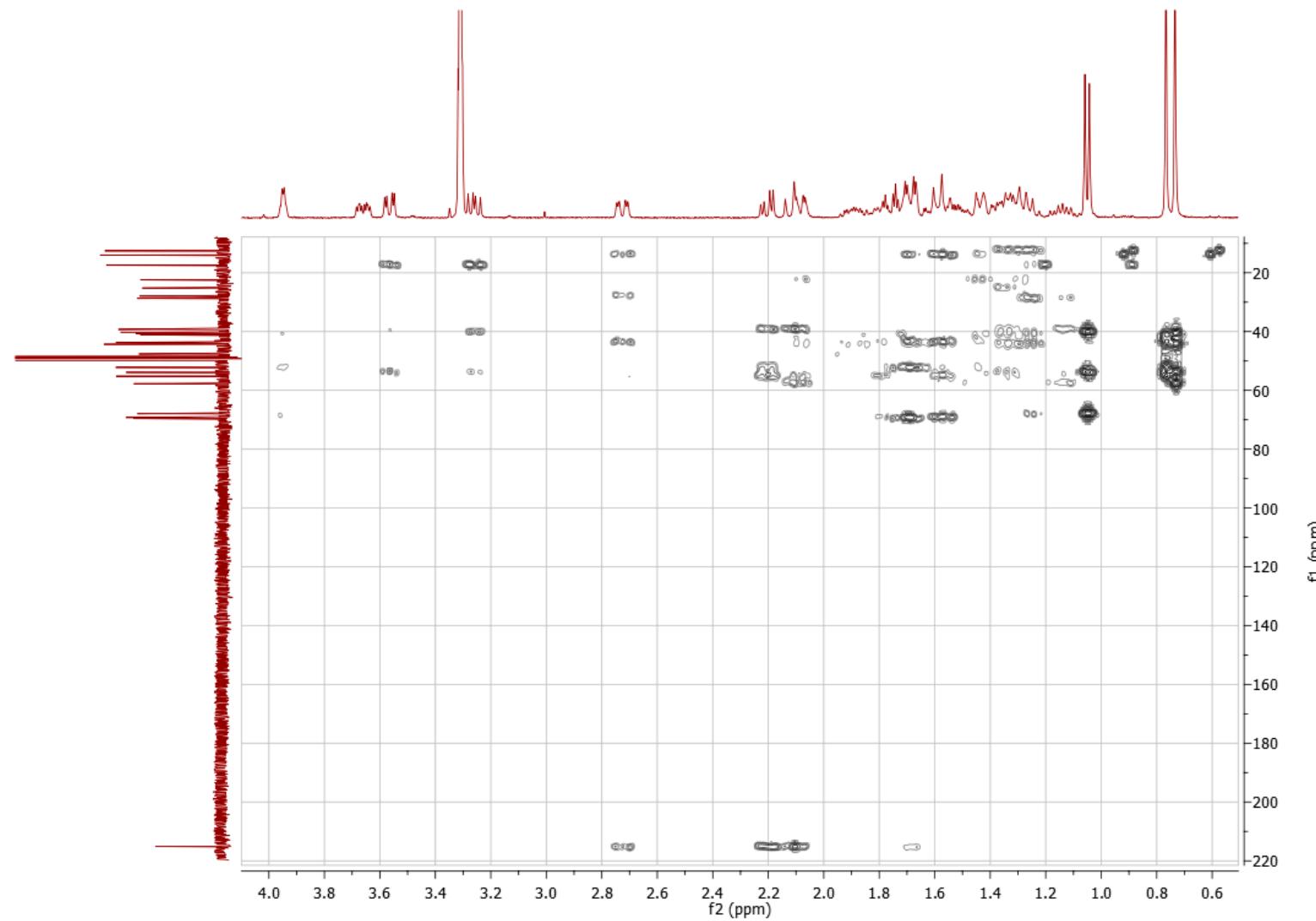


Figure S39. 2D HMBC NMR spectrum of $2\alpha,3\alpha,22$ -trihydroxy- 5α -cholan-23,24-dinor-6-one (8)

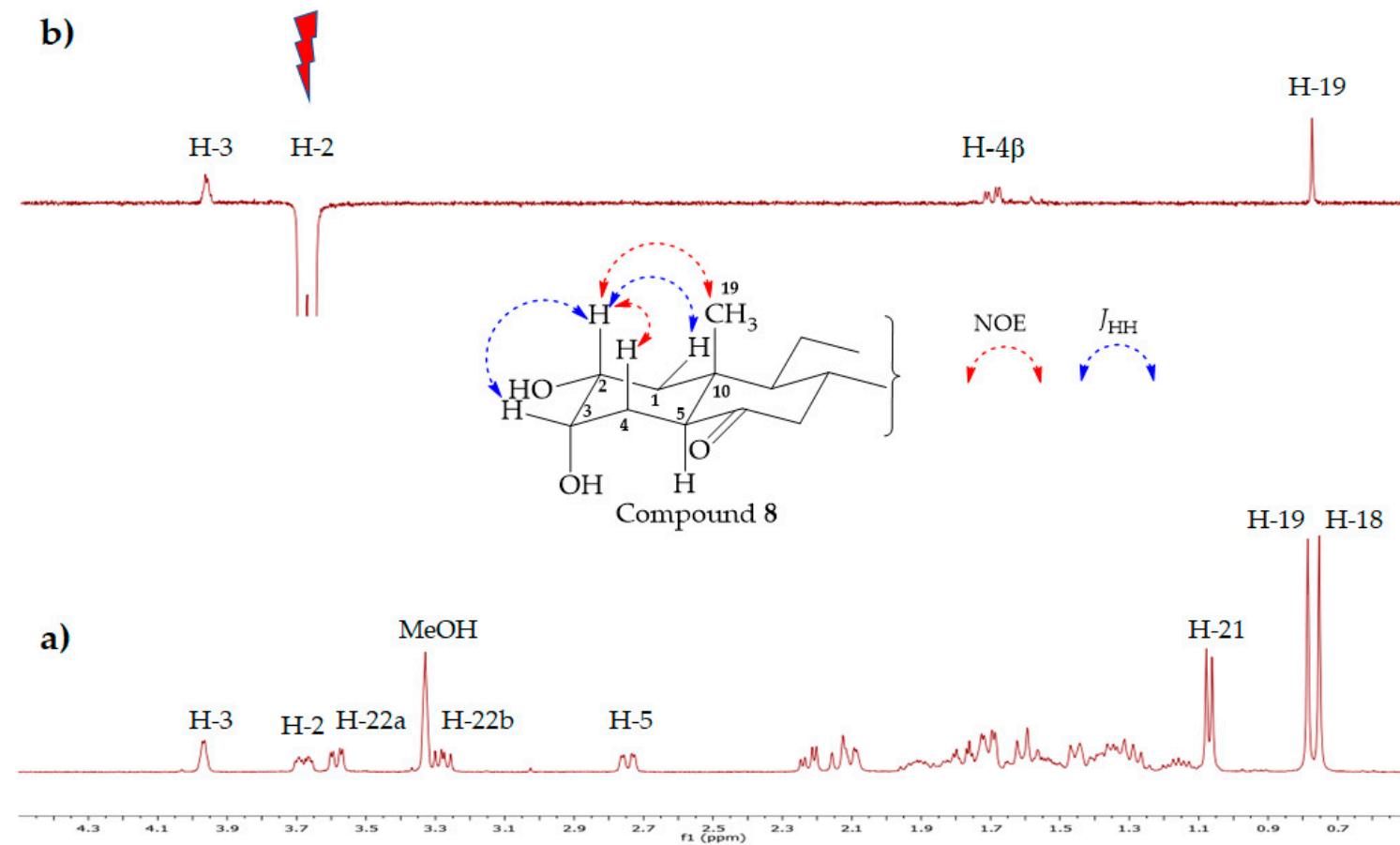


Figure S40. 1D selective NOESY NMR spectrum of $2\alpha,3\alpha,22$ -trihydroxy- 5α -cholan-23,24-dinor-6-one (8)

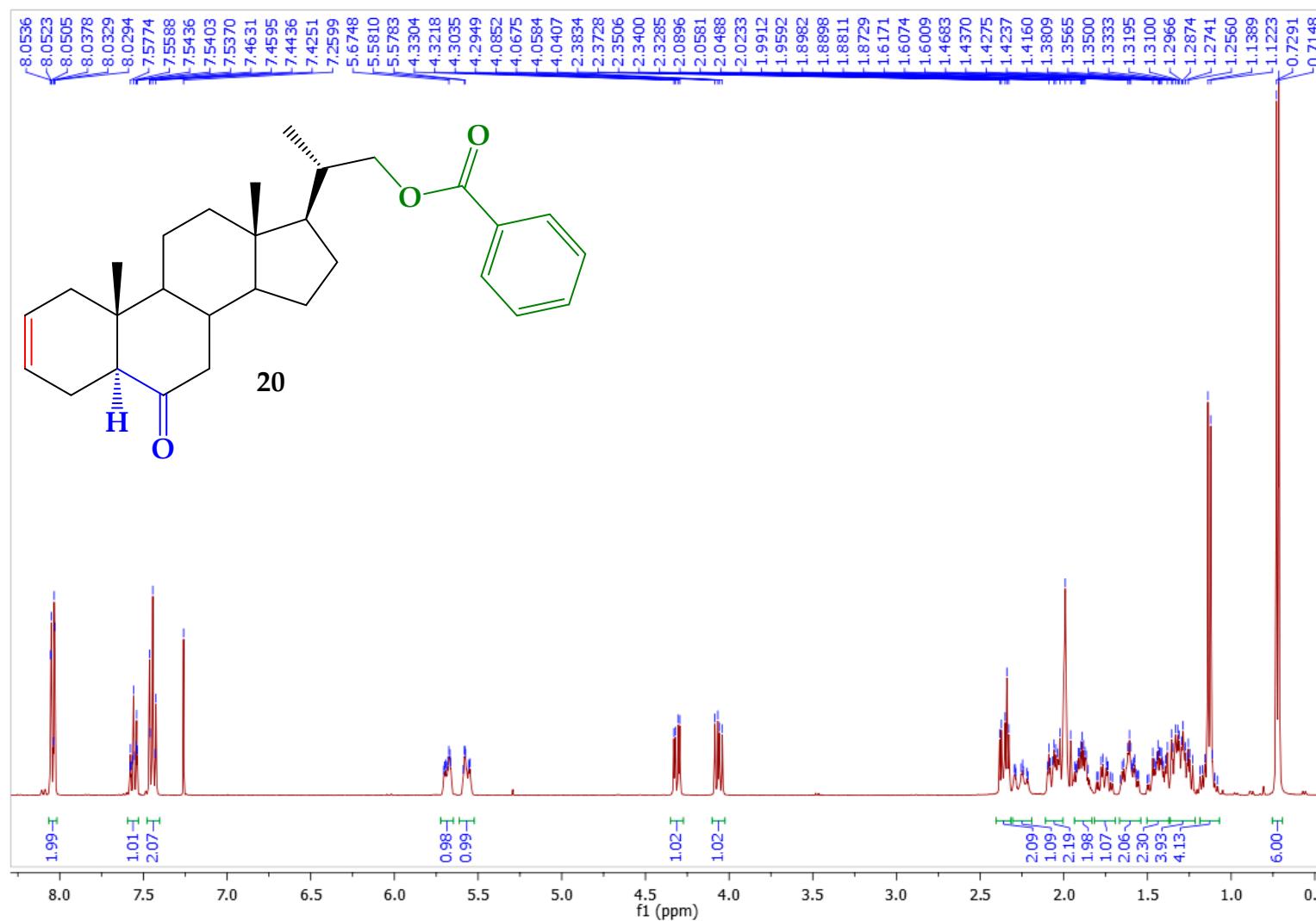


Figure S41. ¹H NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-benzoate-22-yl (20)

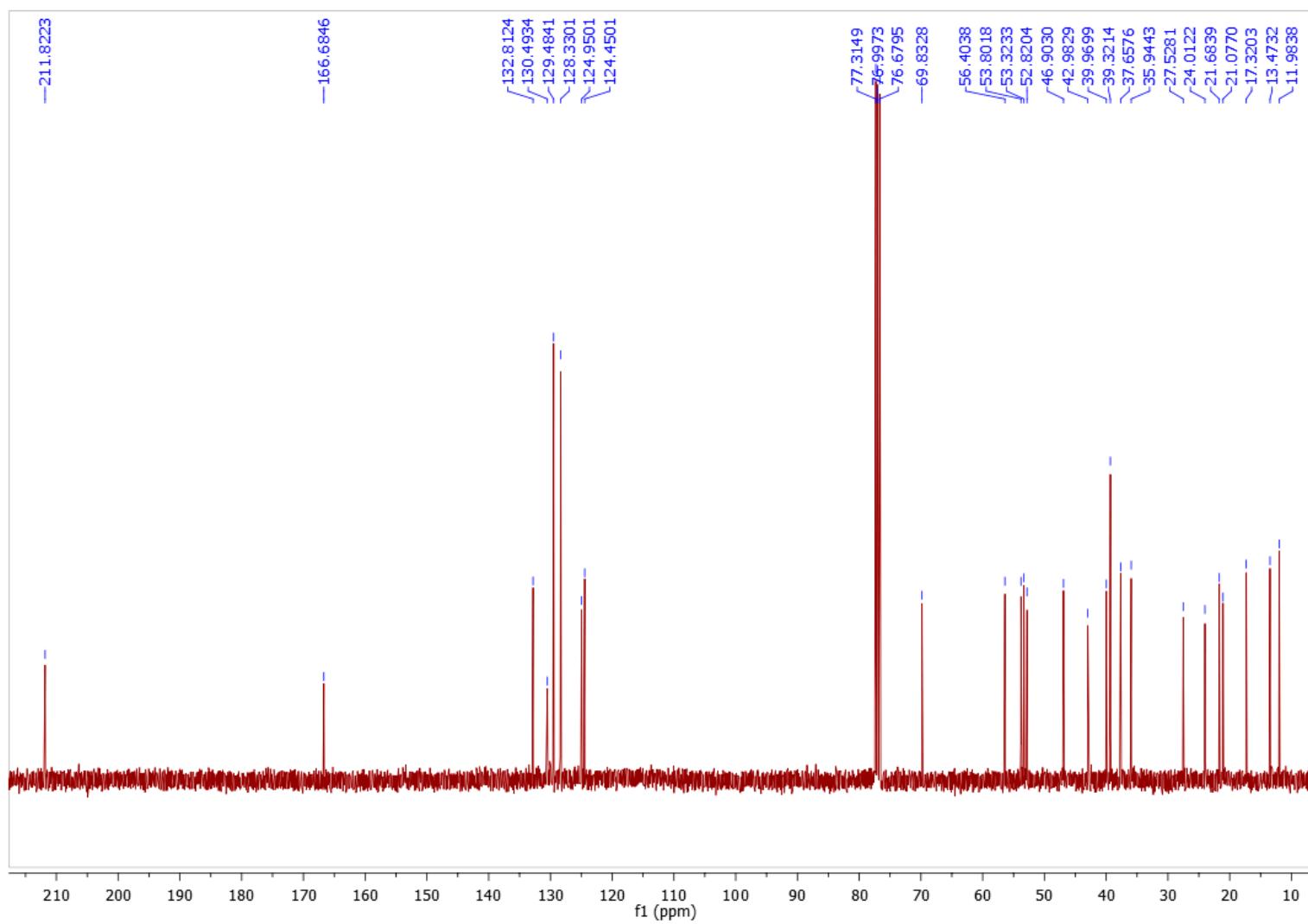


Figure S42. ^{13}C NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-benzoate-22-yl (20)

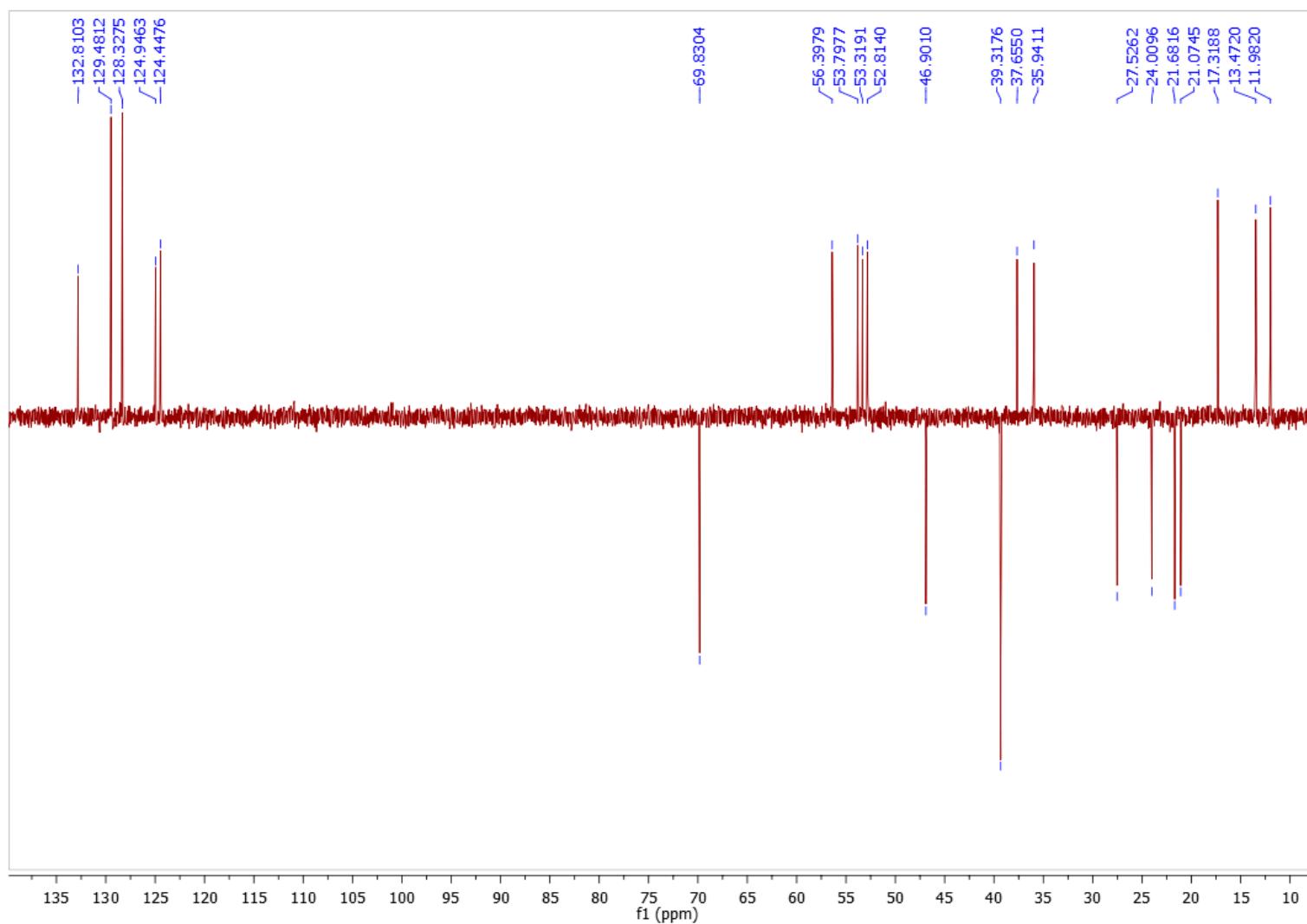


Figure S43. ^{13}C DEPT-135 NMR spectrum of 5α -cholan-6-oxo-2-ene-23,24-dinor-22-benzoate-22-yl (20)

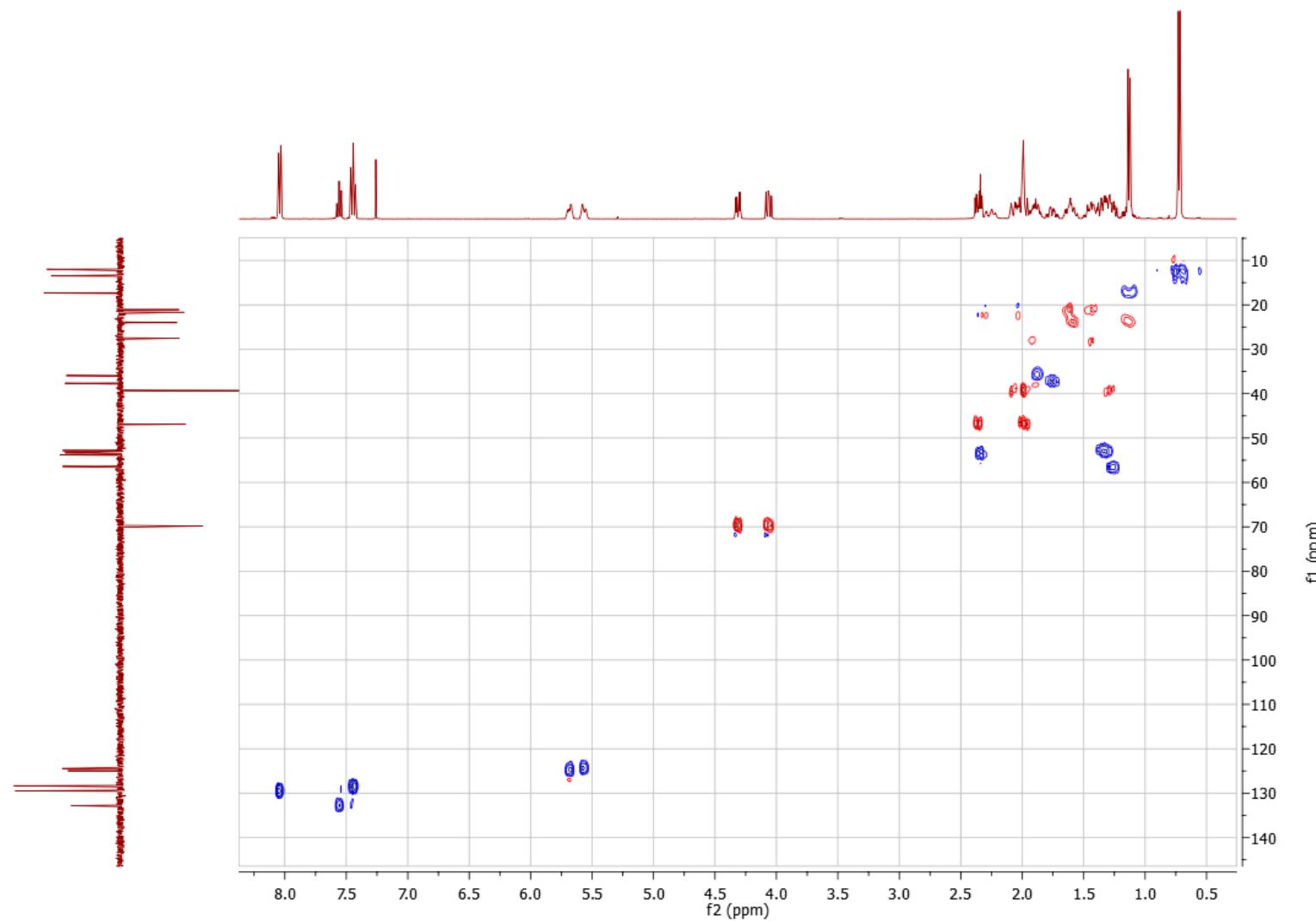


Figure S44. 2D HSQC NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-benzoate-22-yl (**20**)

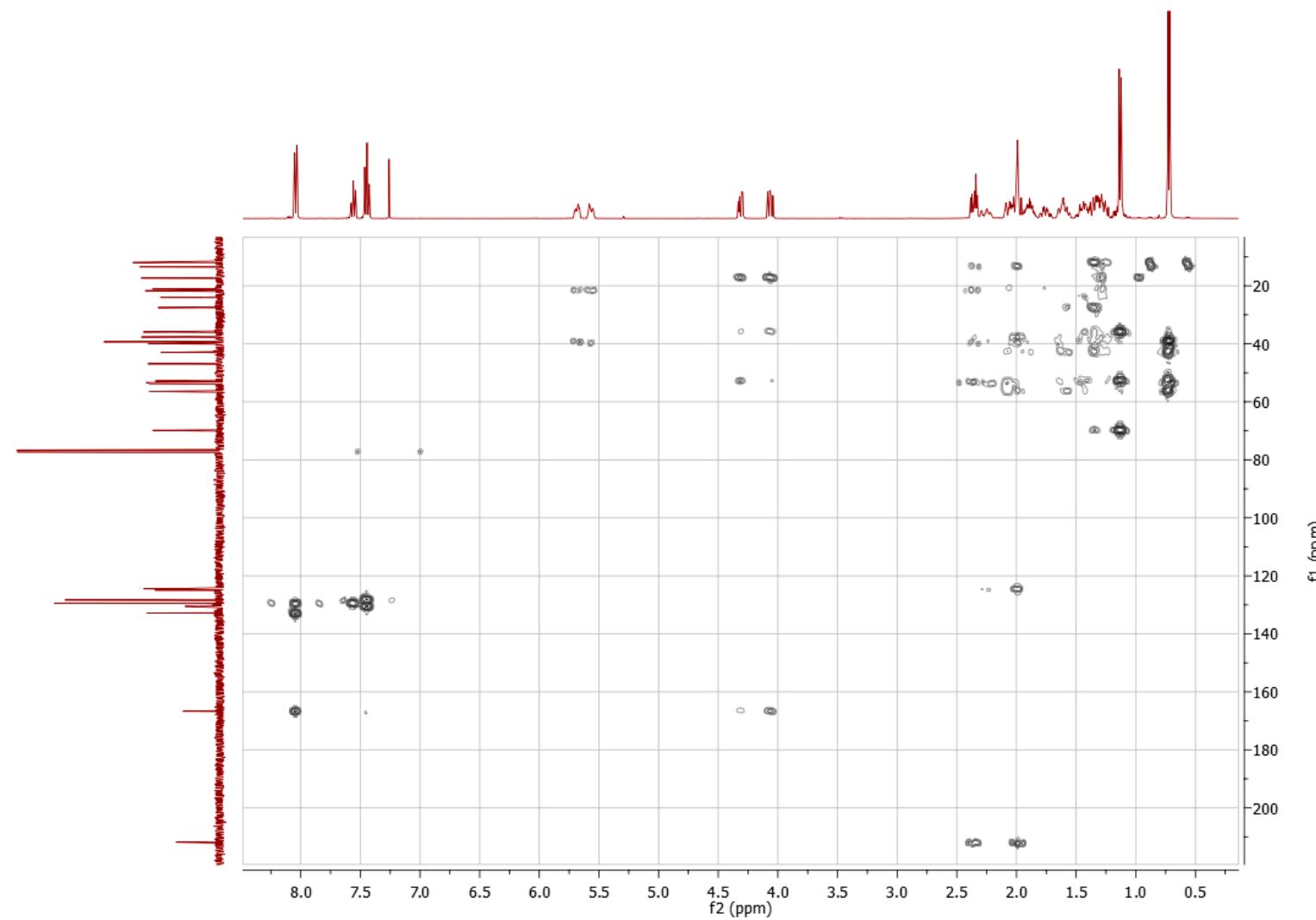


Figure S44. 2D HMBC NMR spectrum of 5α -cholan-6-oxo-2-ene-23,24-dinor-22-benzoate-22-yl (20)

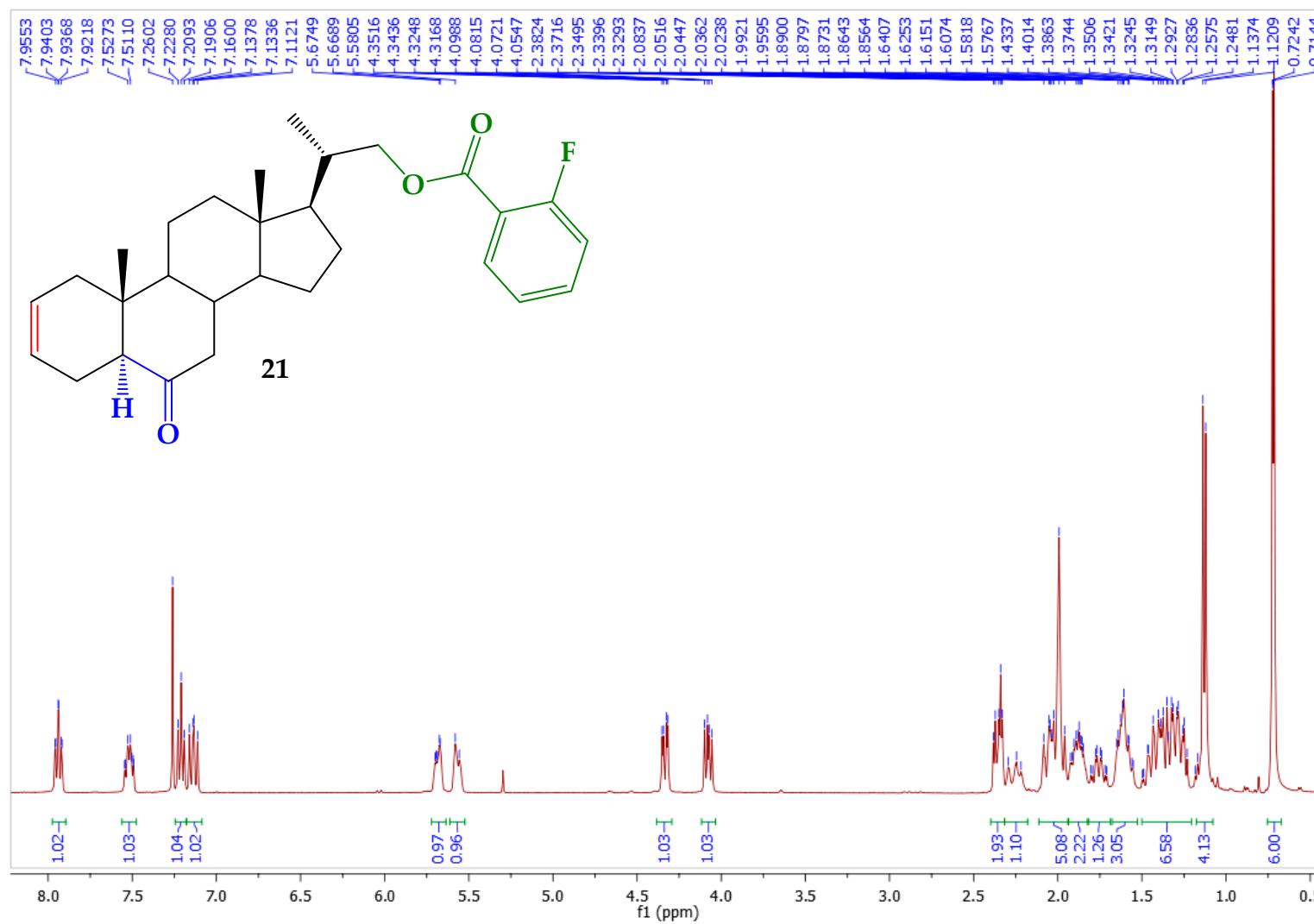


Figure S46. ¹H NMR spectrum of *5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(2-Fluoro) benzoate-22-yl* (**21**)

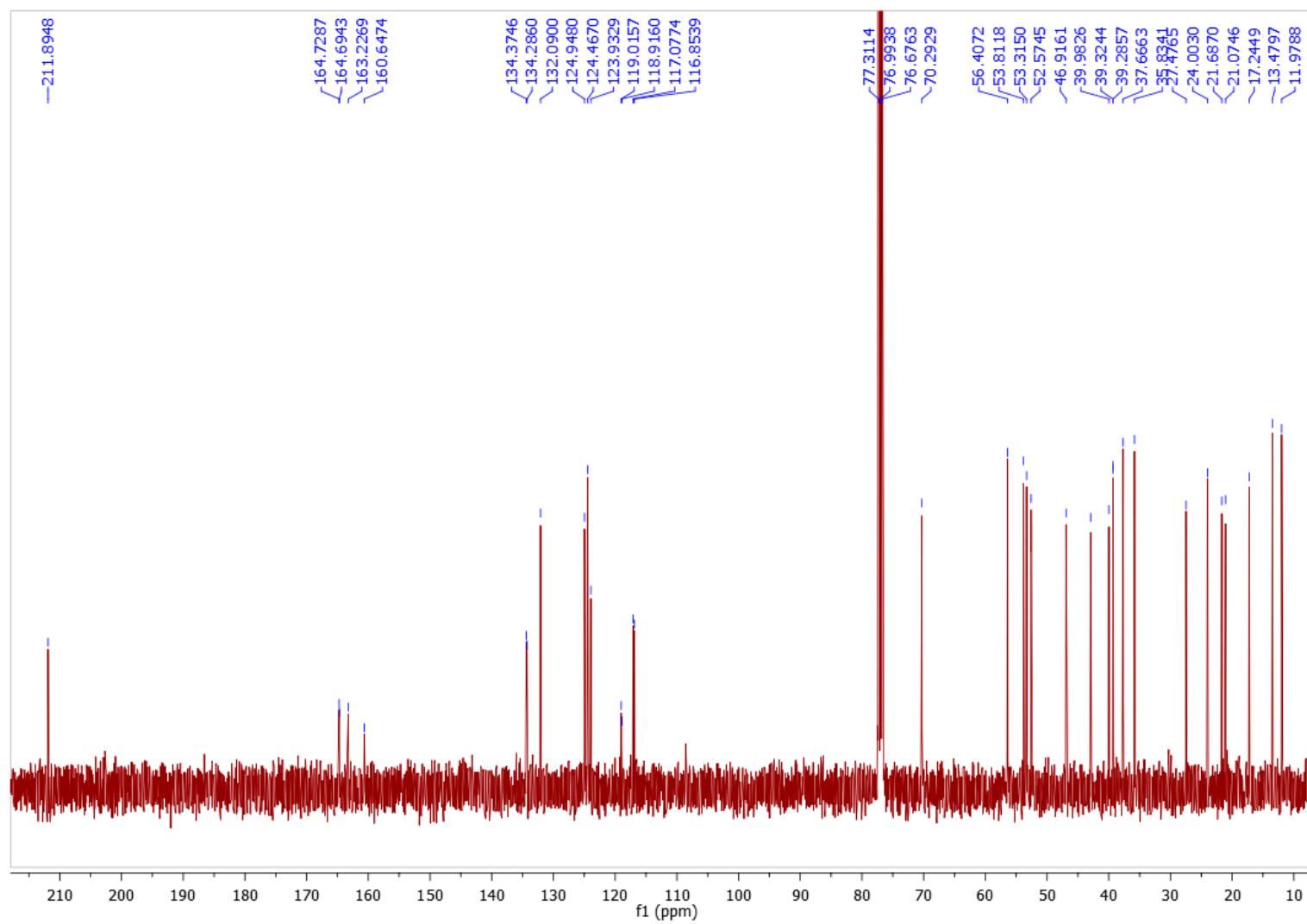


Figure S47. ¹³C NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(2-Fluoro) benzoate-22-yl (21)

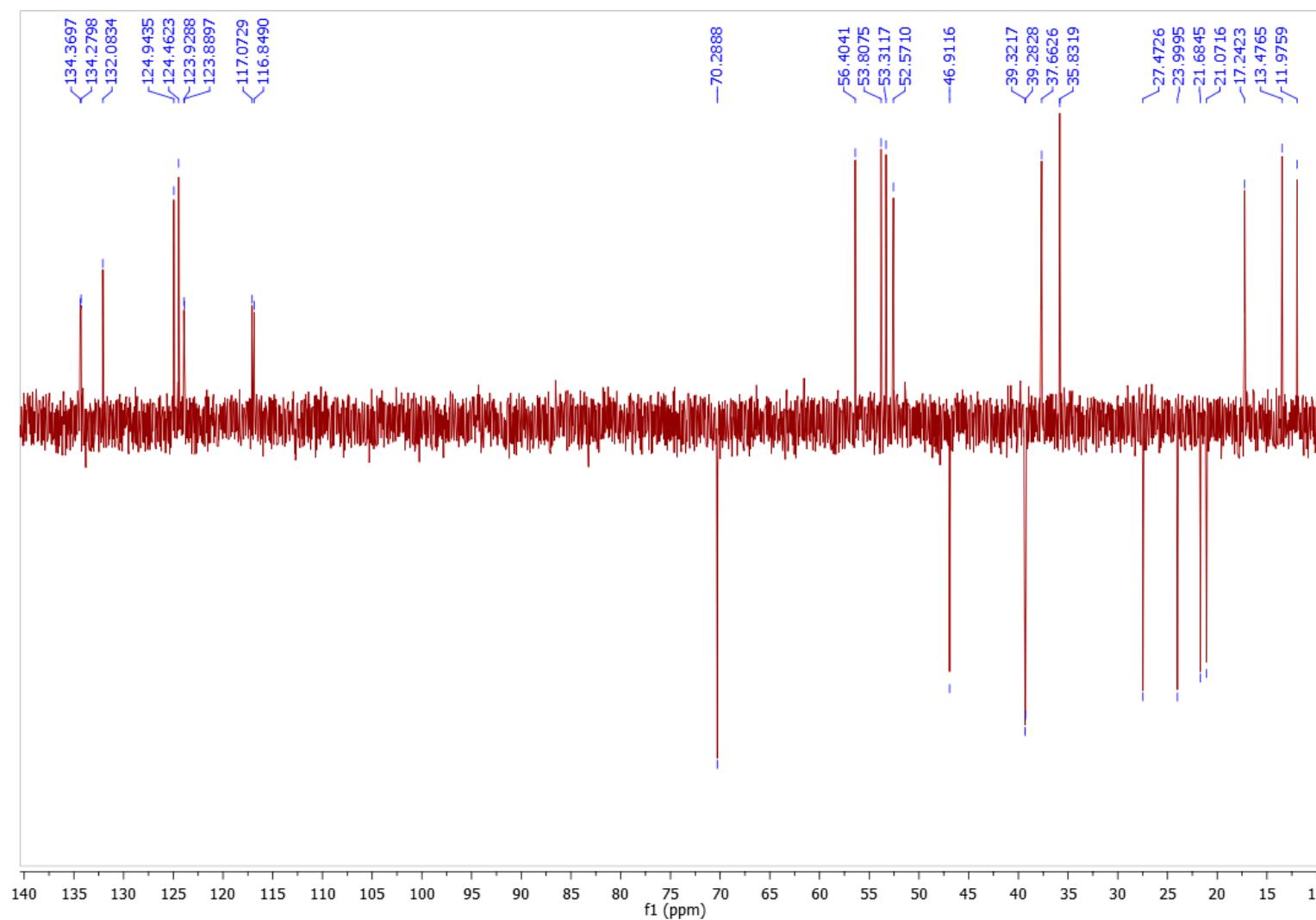


Figure S48. ^{13}C DEPT-135 NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(2-Fluoro) benzoate-22-yl (21)

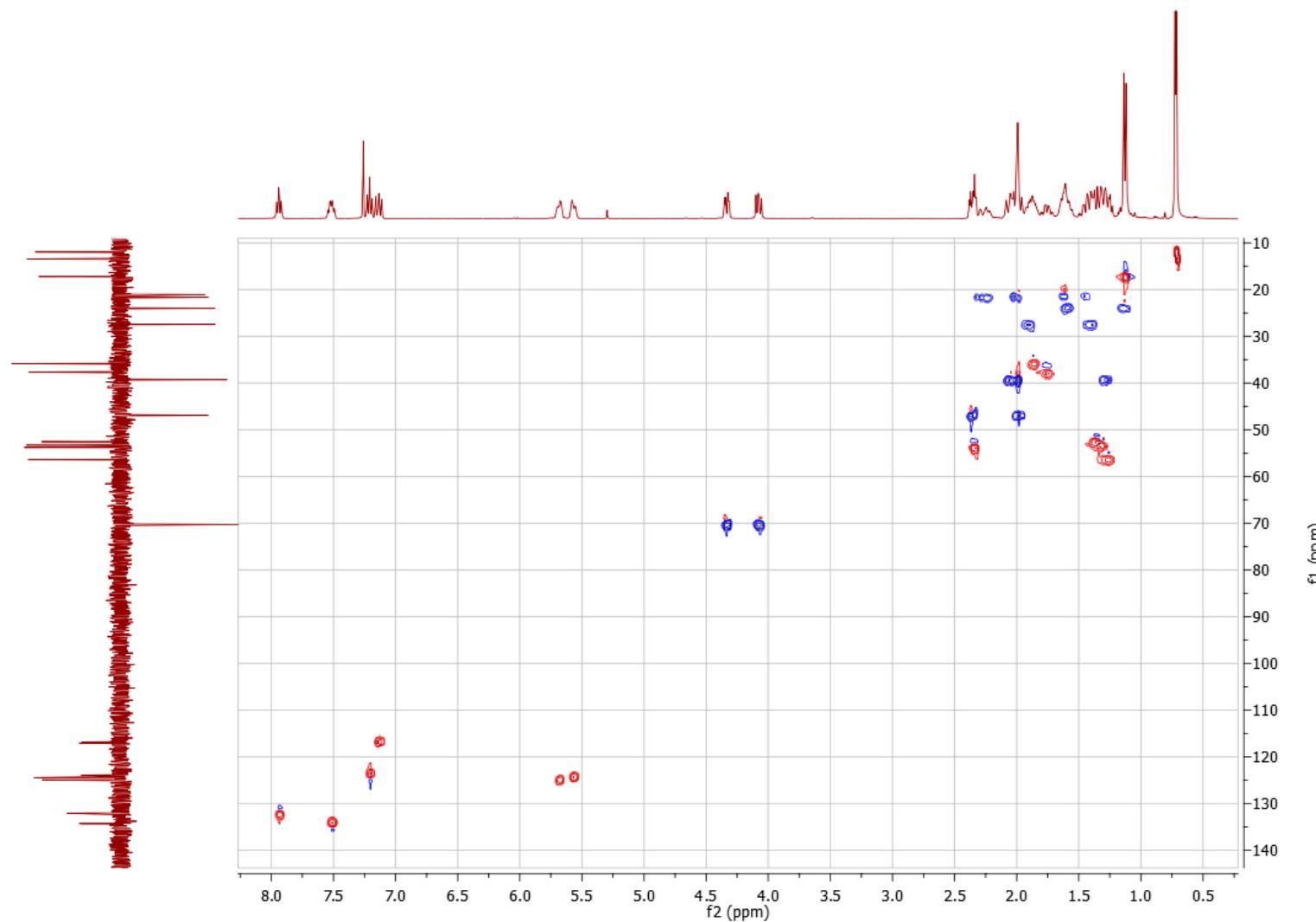


Figure S49. 2D HSQC NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(2-Fluoro) benzoate-22-yl (**21**)

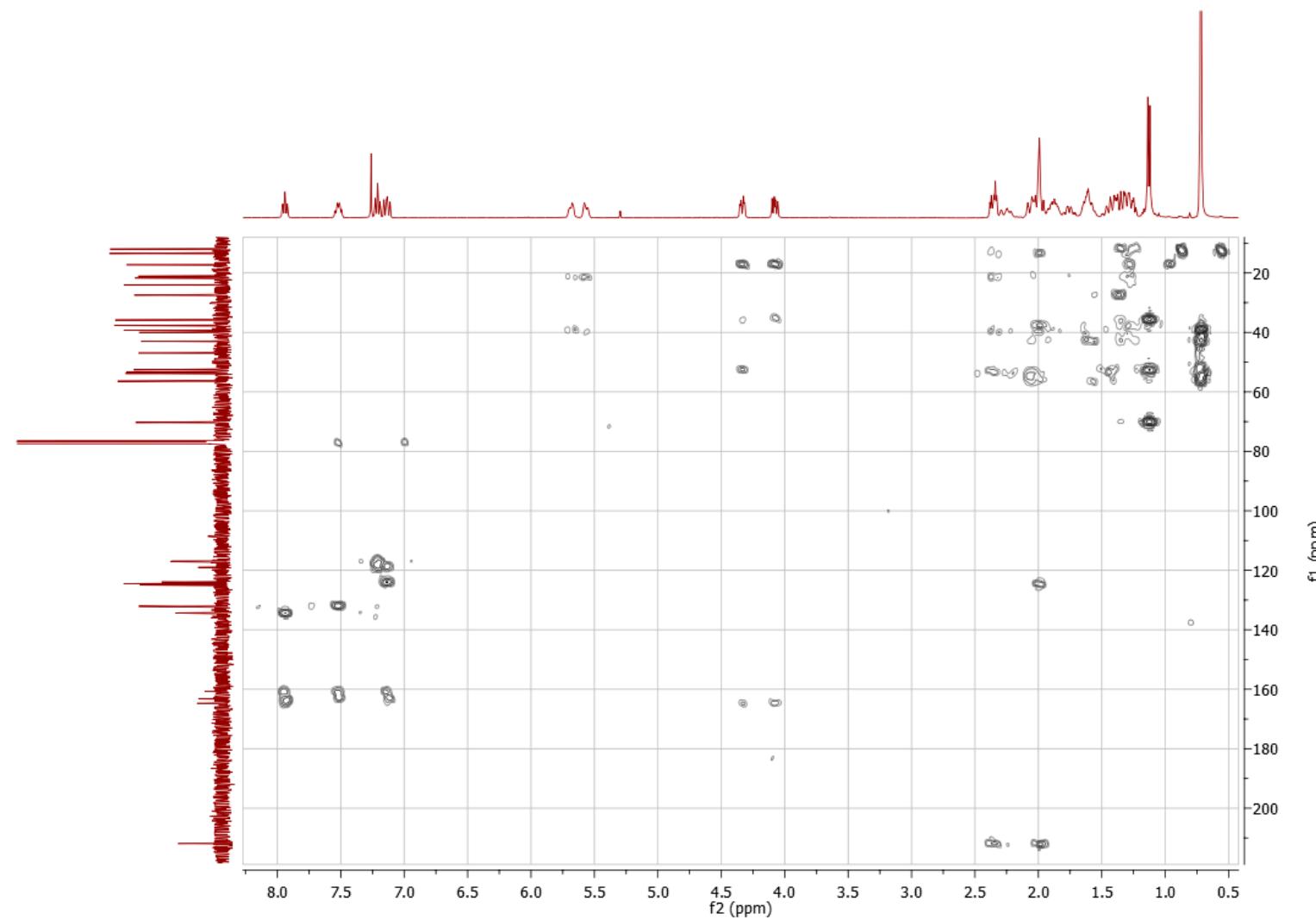


Figure S50. 2D HMBC NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(2-Fluoro) benzoate-22-yl (21)

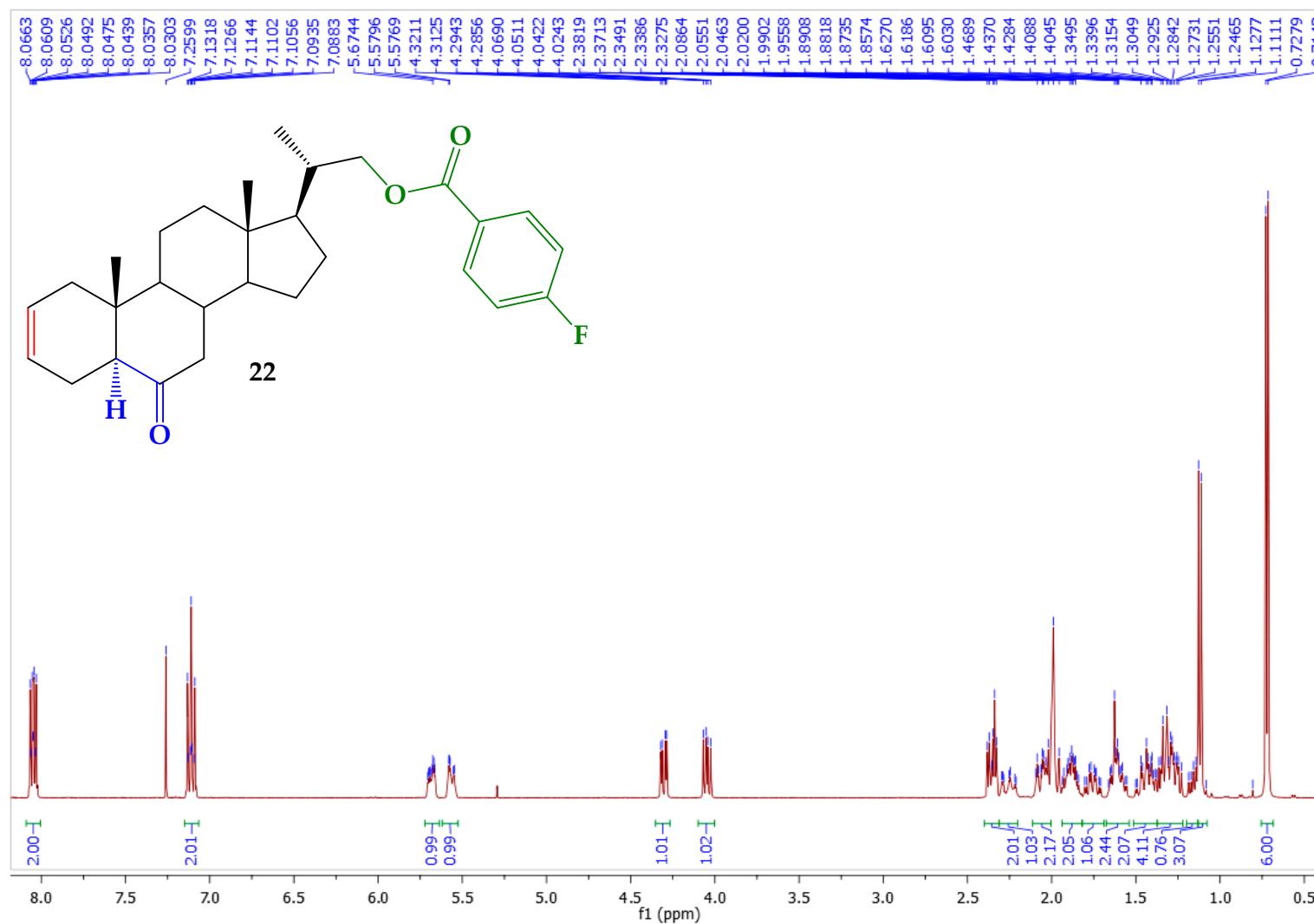


Figure S51. ¹H NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (22)

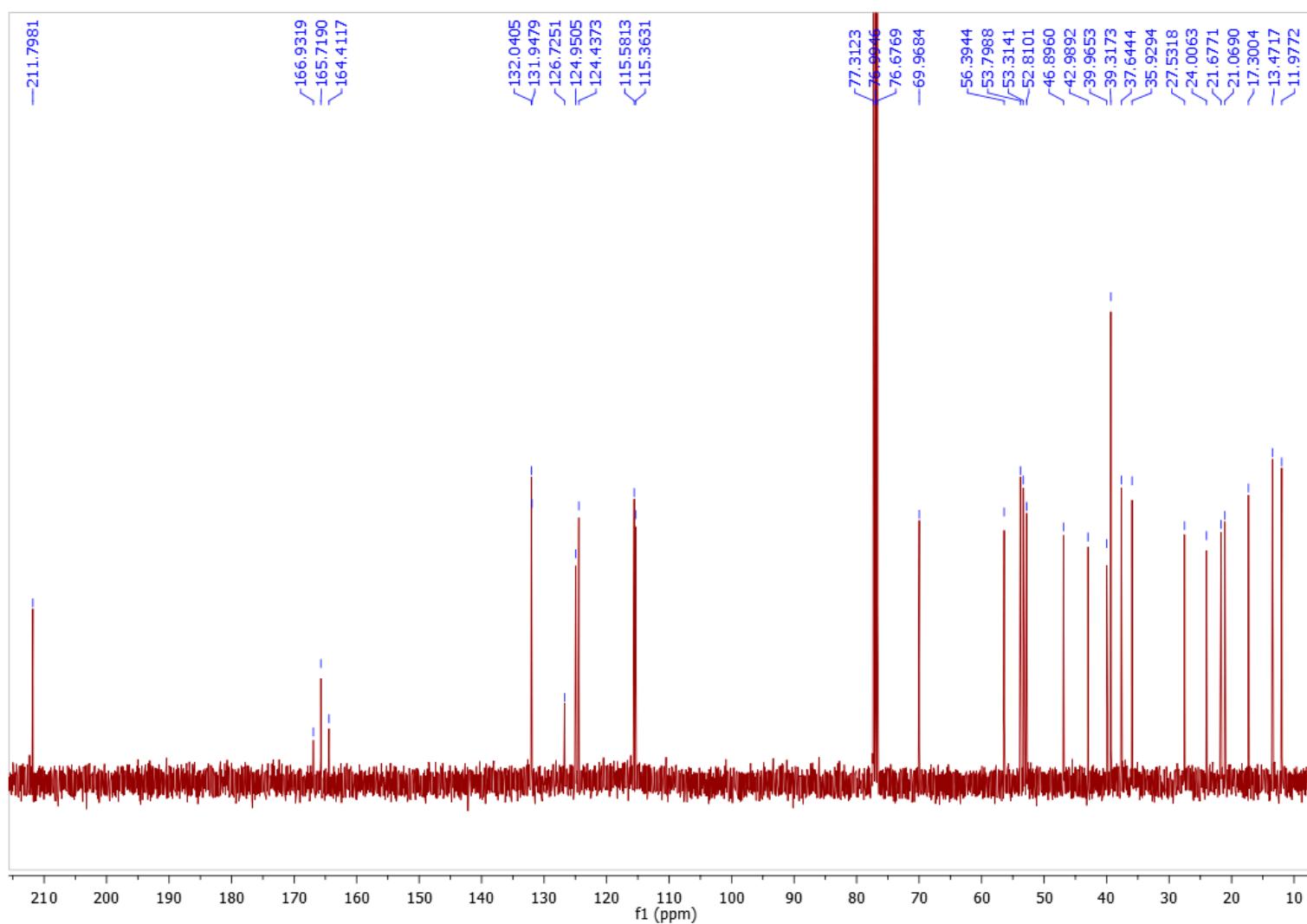


Figure S52. ¹³C NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (22)

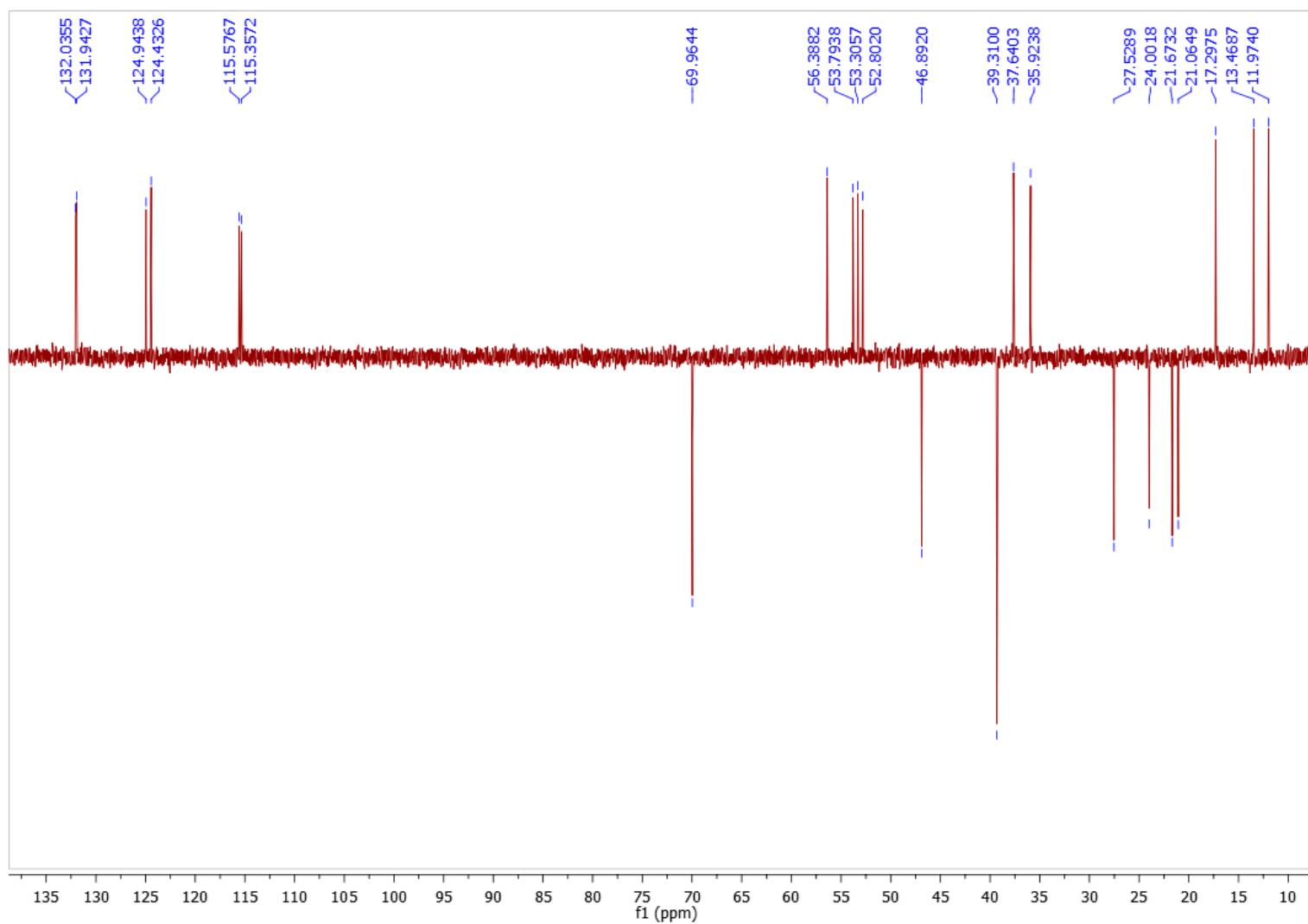


Figure S53. ¹³C DEPT-135 NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (22)

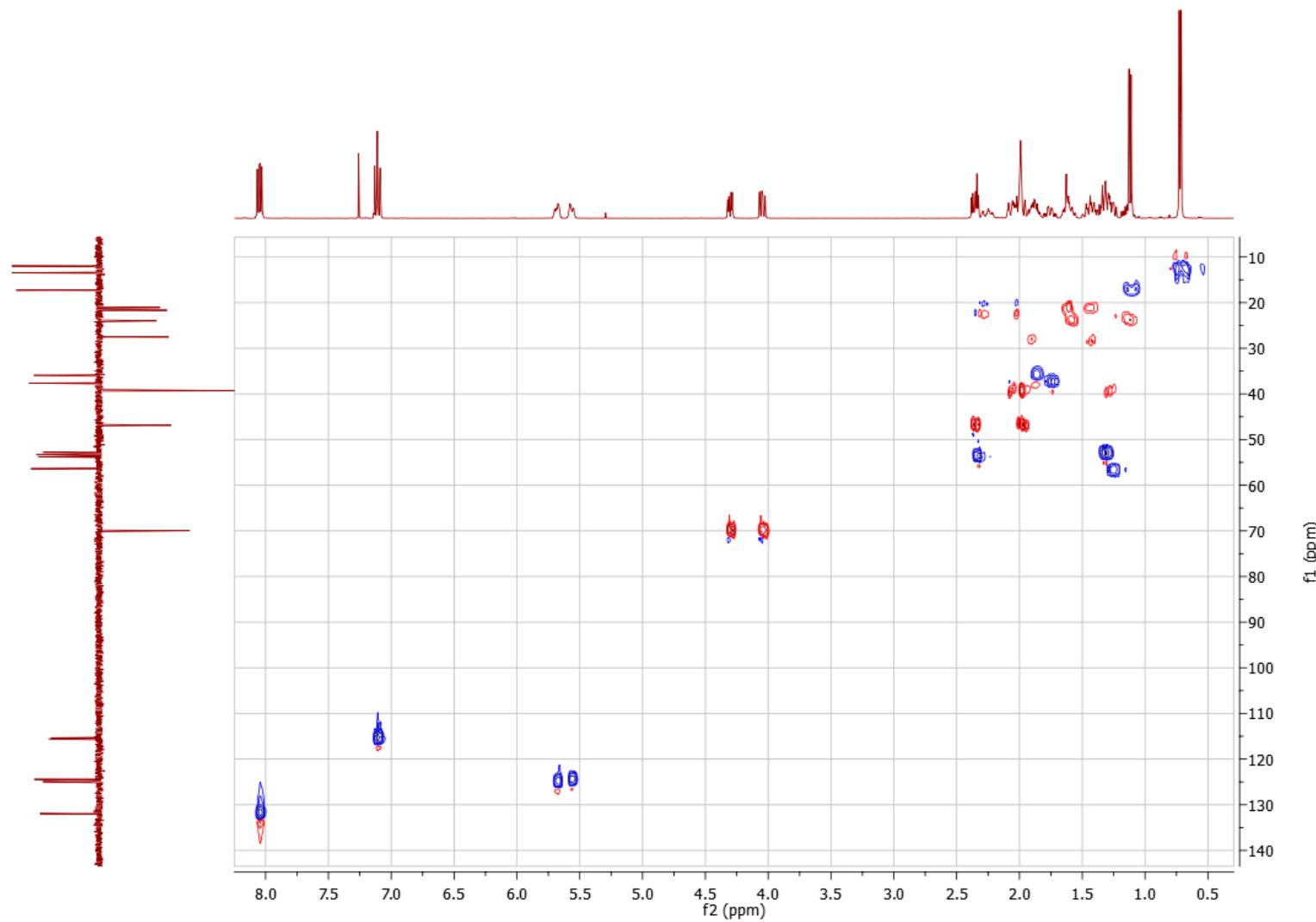


Figure S54. 2D HSQC NMR spectrum of 5 α -cholan-6-oxo-2-ene-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (**22**)

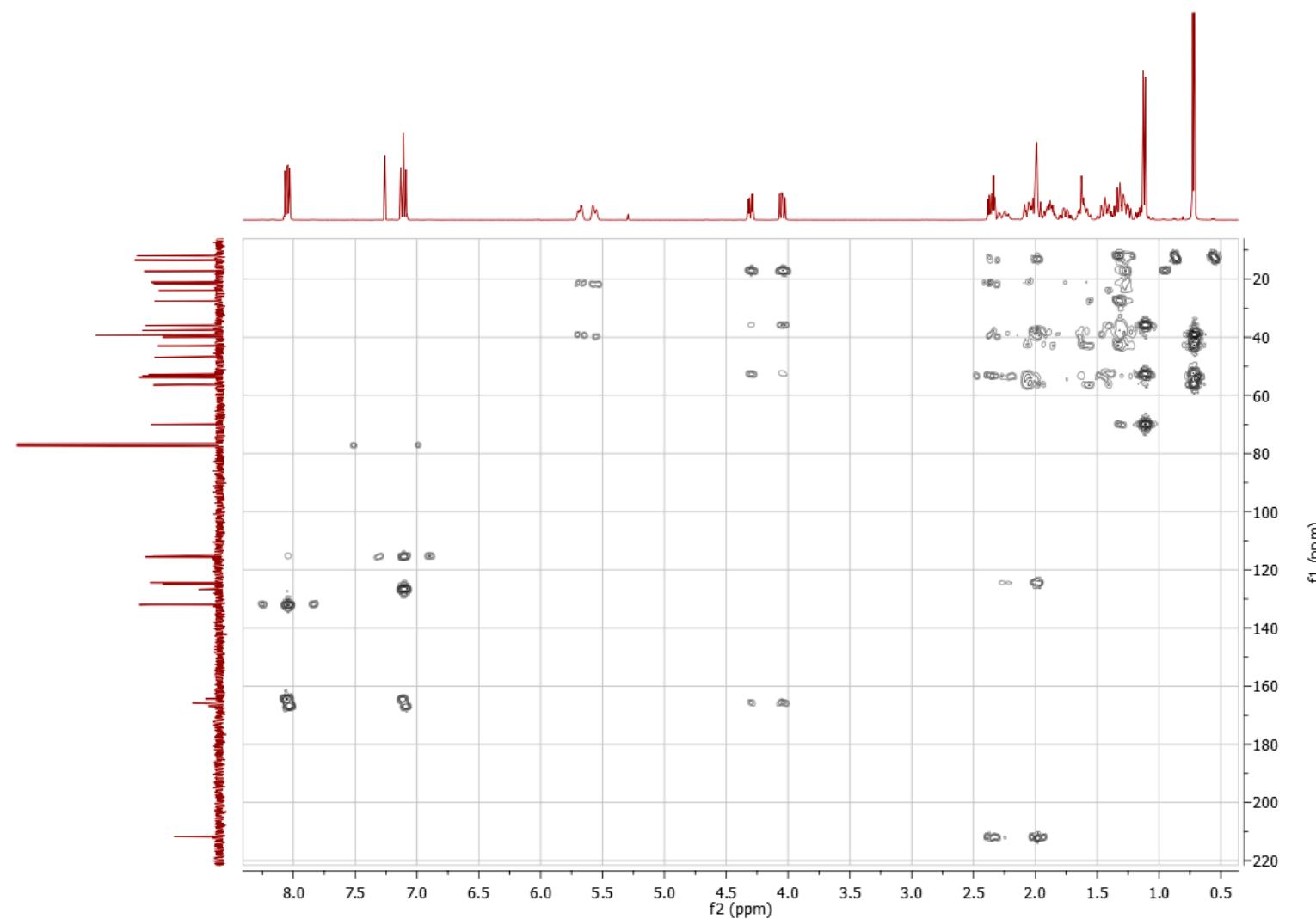


Figure S55. 2D HMBC NMR spectrum of 5α -cholan-6-oxo-2-ene-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (22)

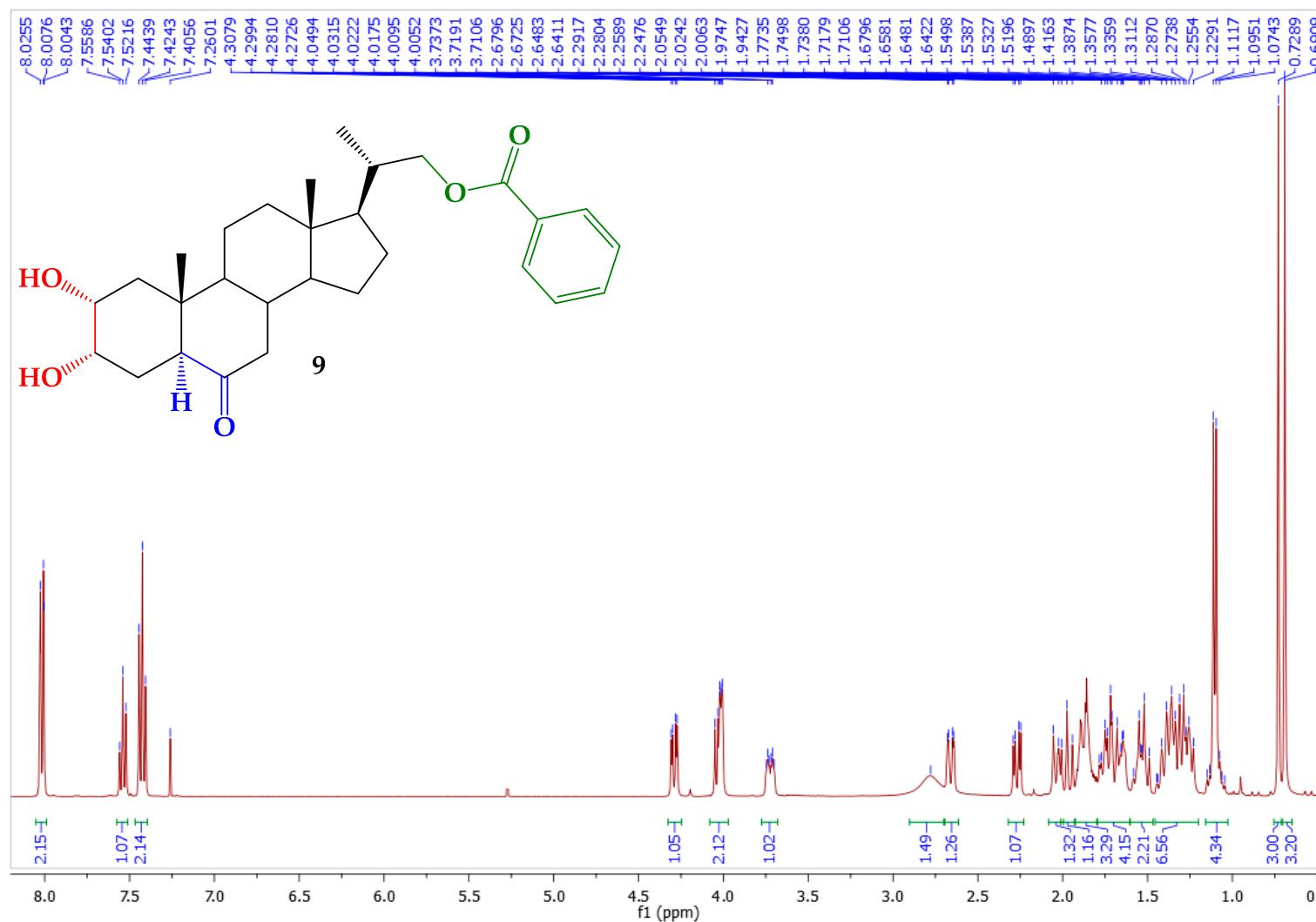


Figure S56. ¹H NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-benzoate-22-yl (9)

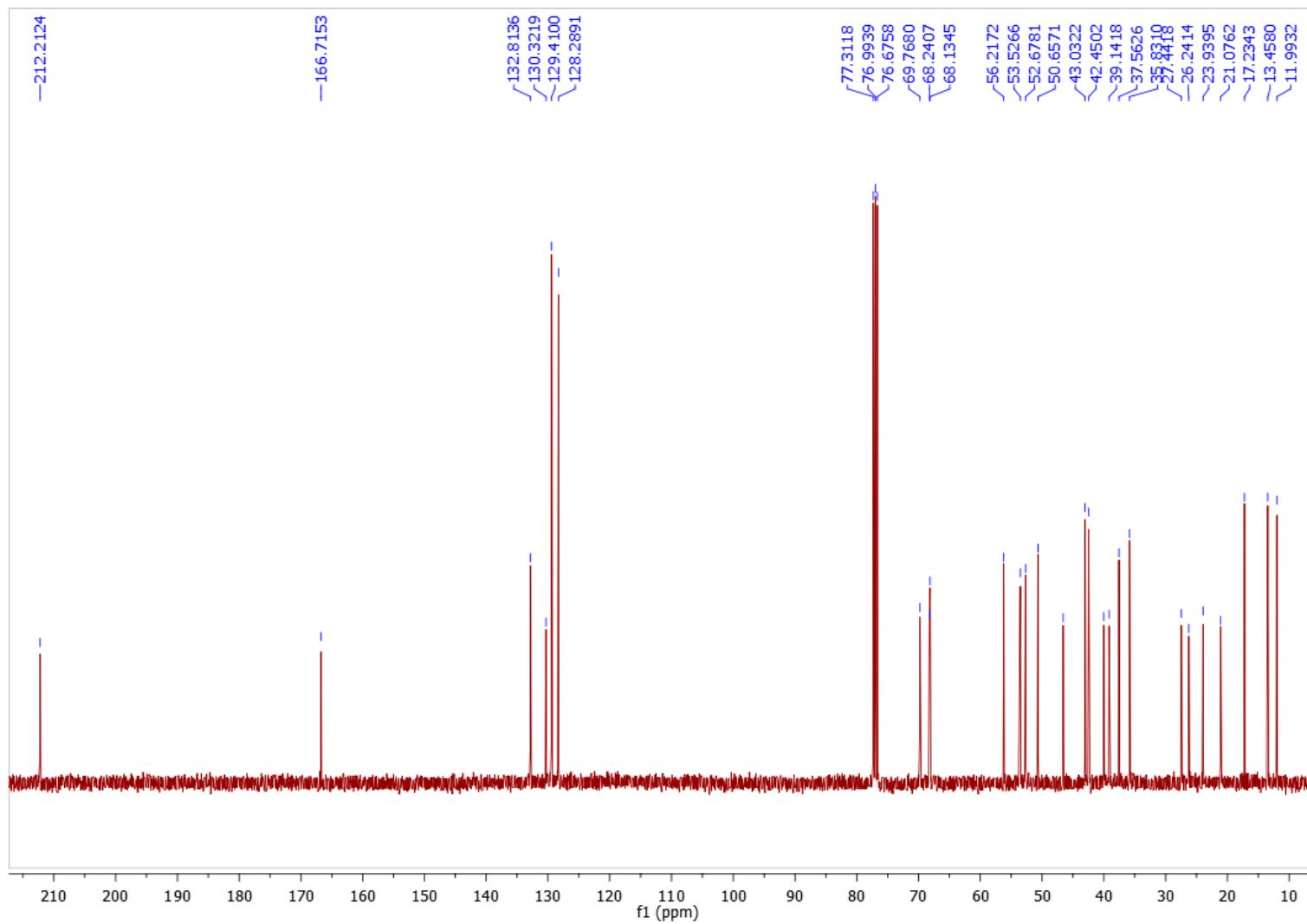


Figure S57. ¹³C NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-benzoate-22-yl (9)

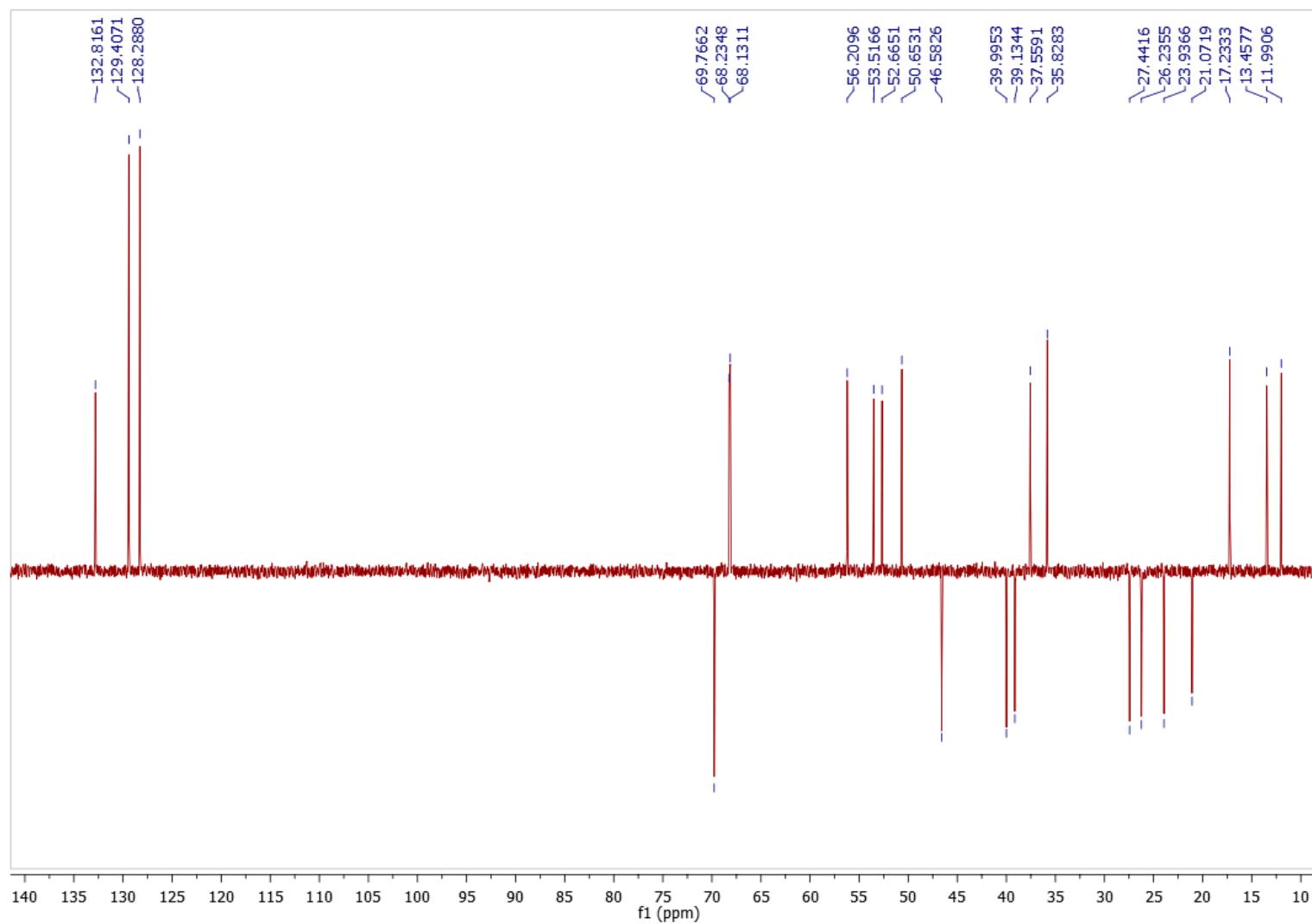


Figure S58. ^{13}C DEPT-135 NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-benzoate-22-yl (9)



Figure S59. 2D HSQC NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-benzoate-22-yl (**9**)

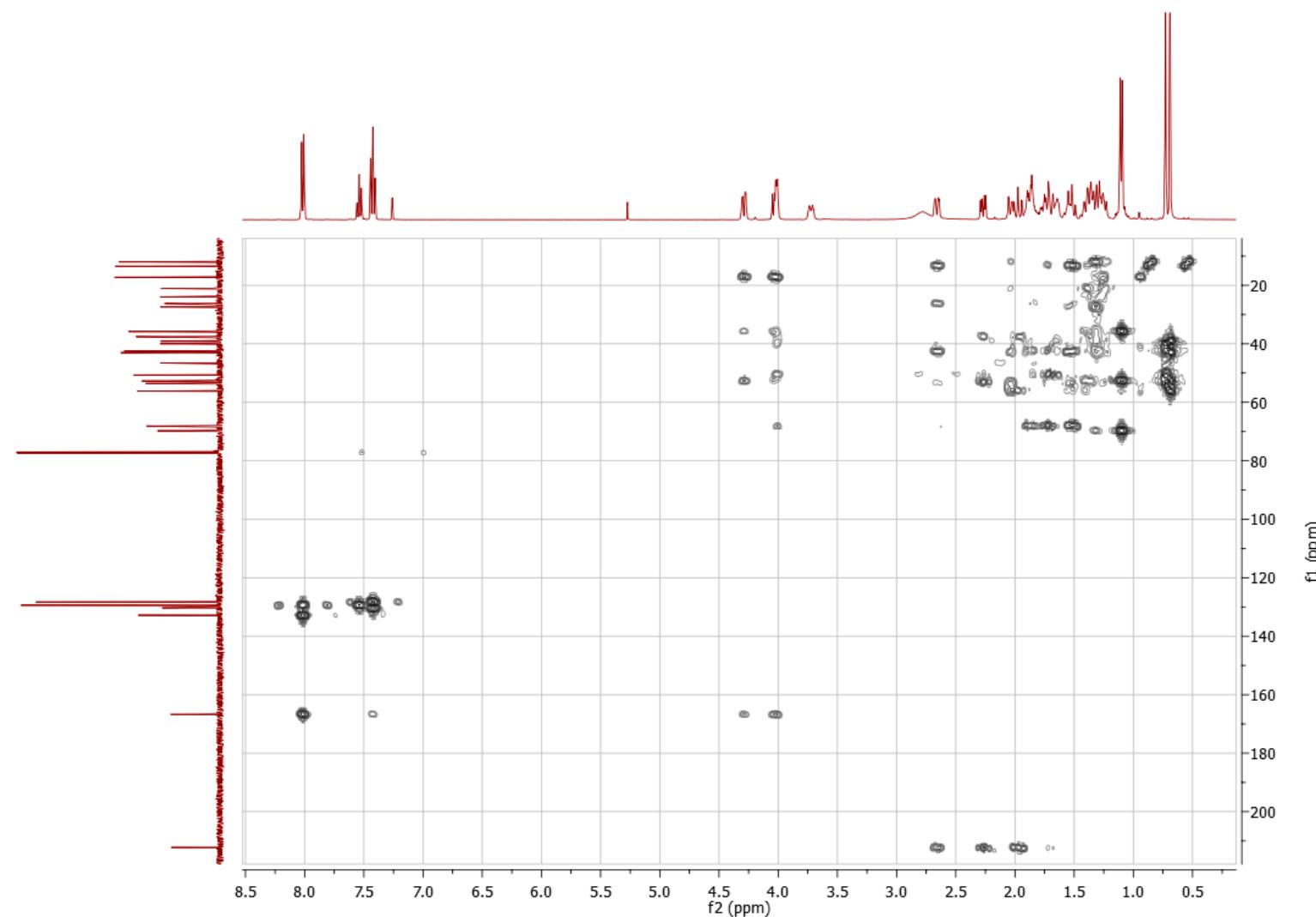


Figure S60. 2D HMBC NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-benzoate-22-yl (9)

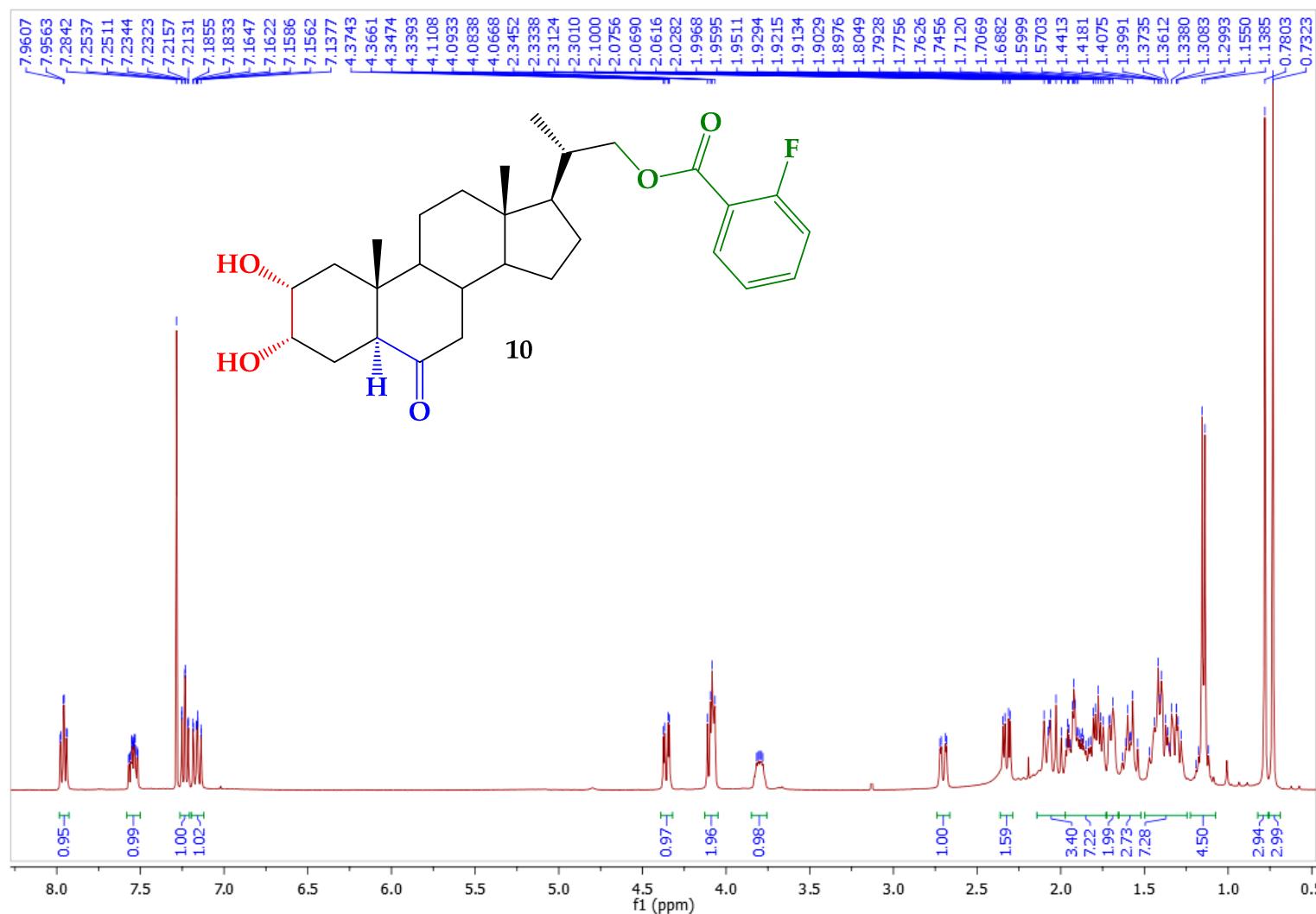


Figure S61. ¹H NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (10)

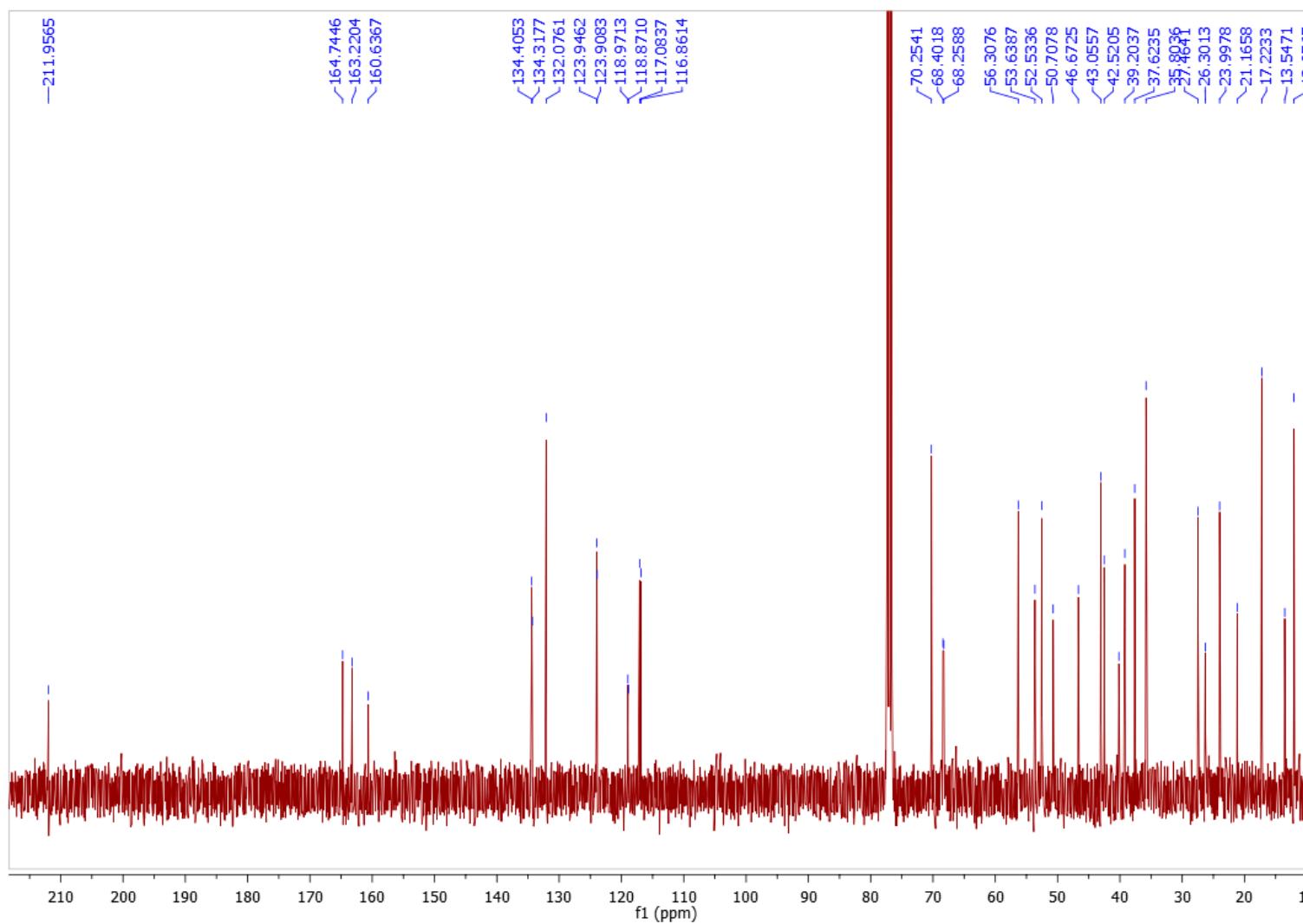


Figure S62. ¹³C NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (**10**)

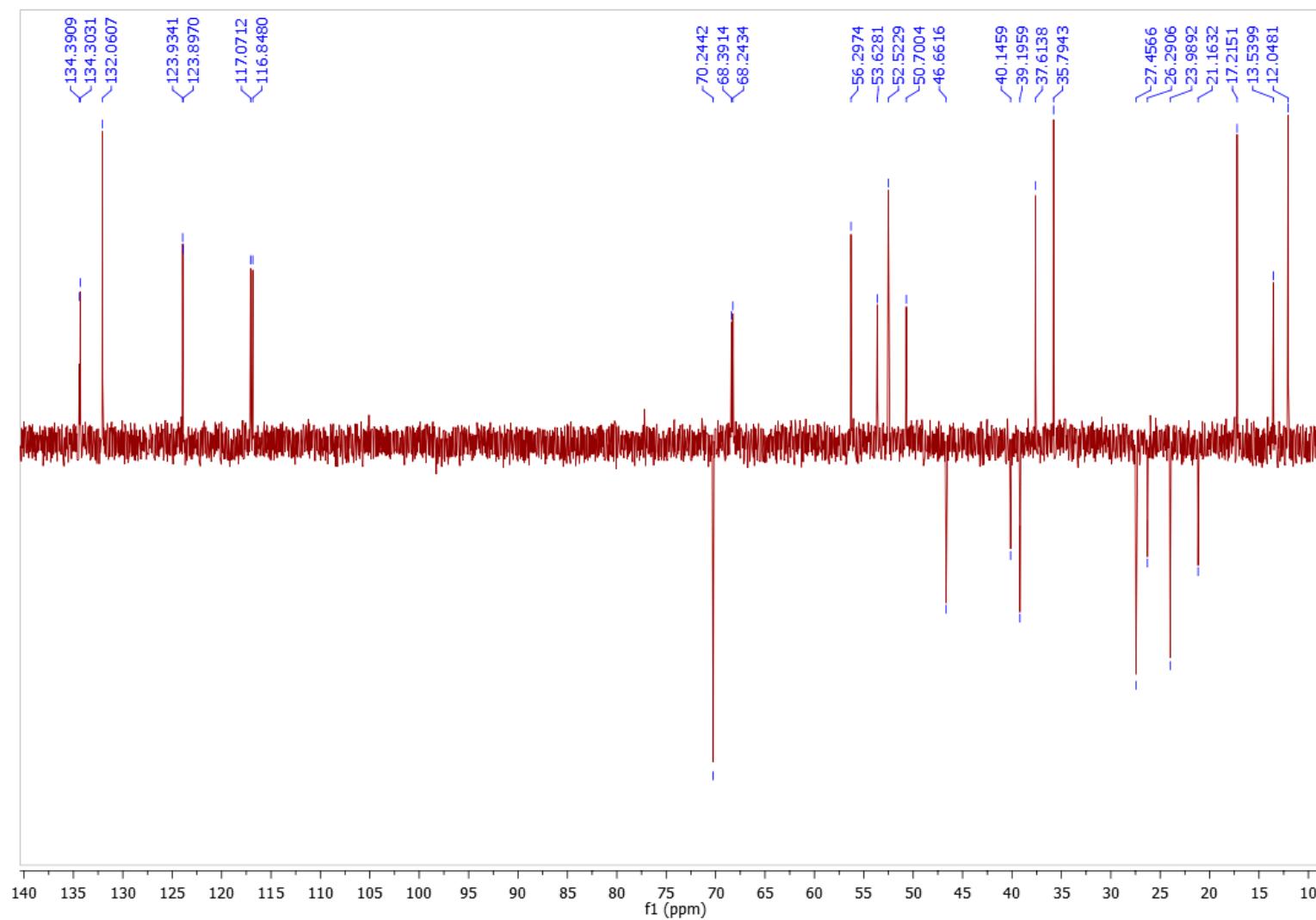


Figure S63. ^{13}C DEPT-135 NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (10)

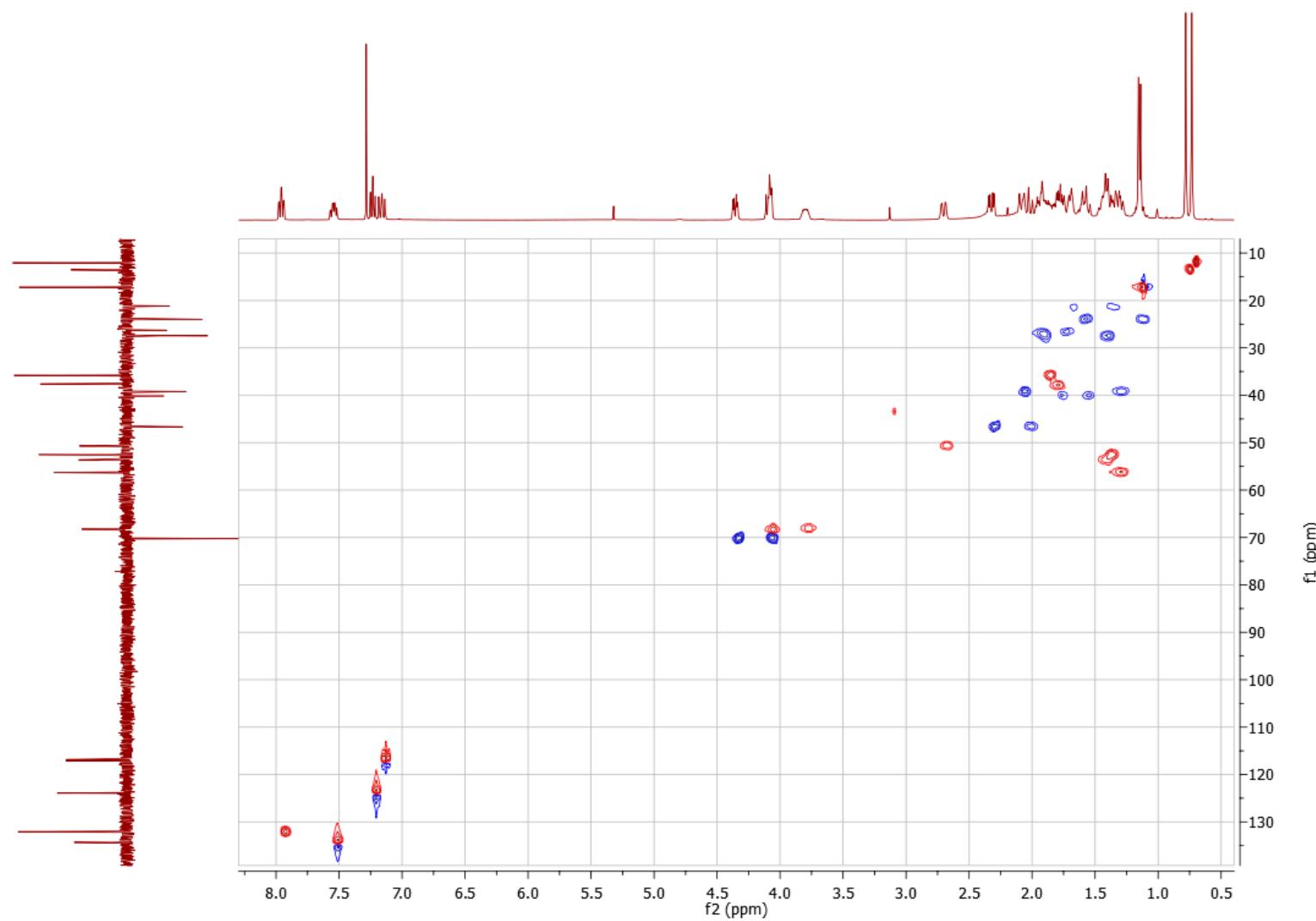


Figure S64. 2D HSQC NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (**10**)

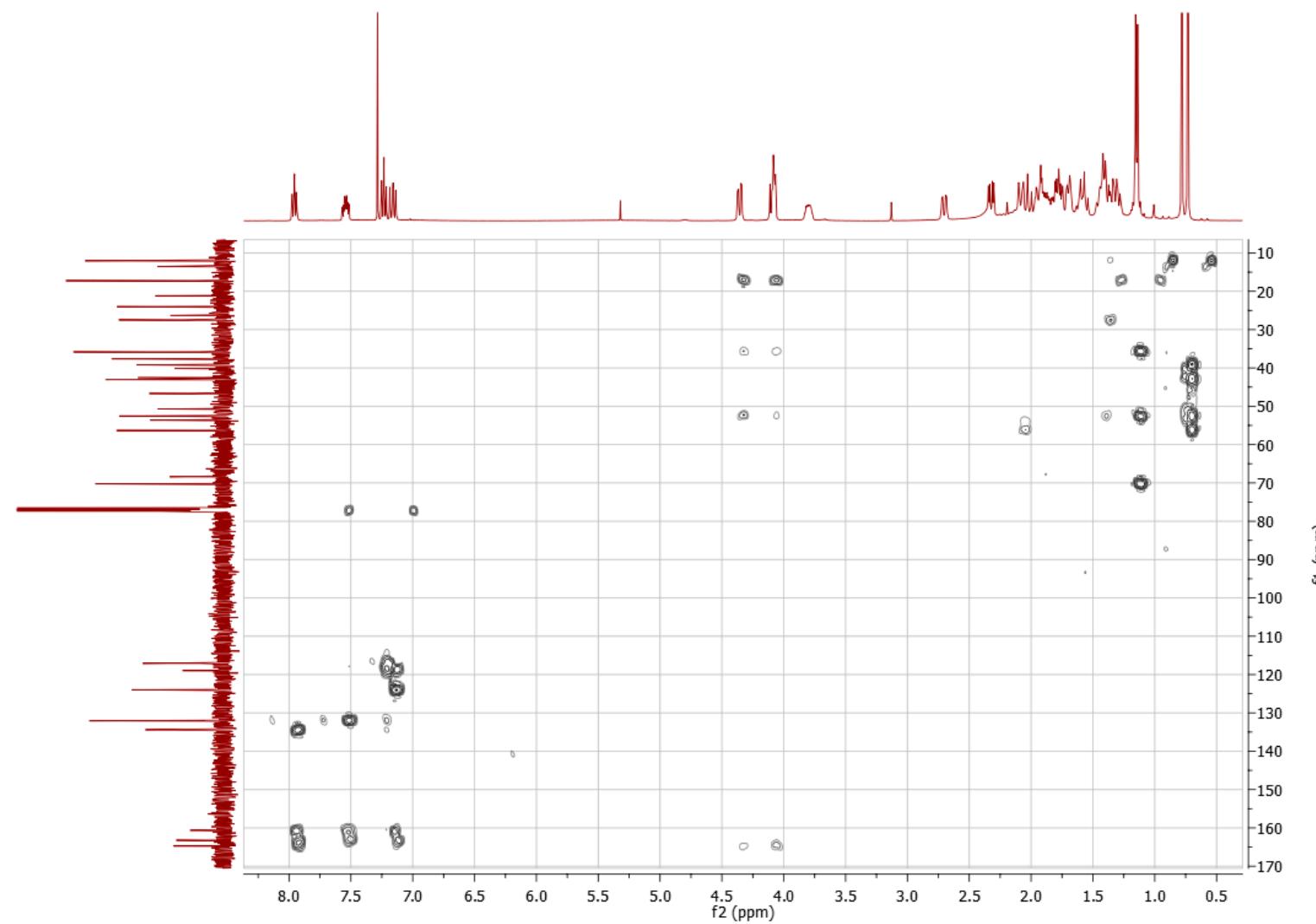


Figure S65. 2D HMBC NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (10)

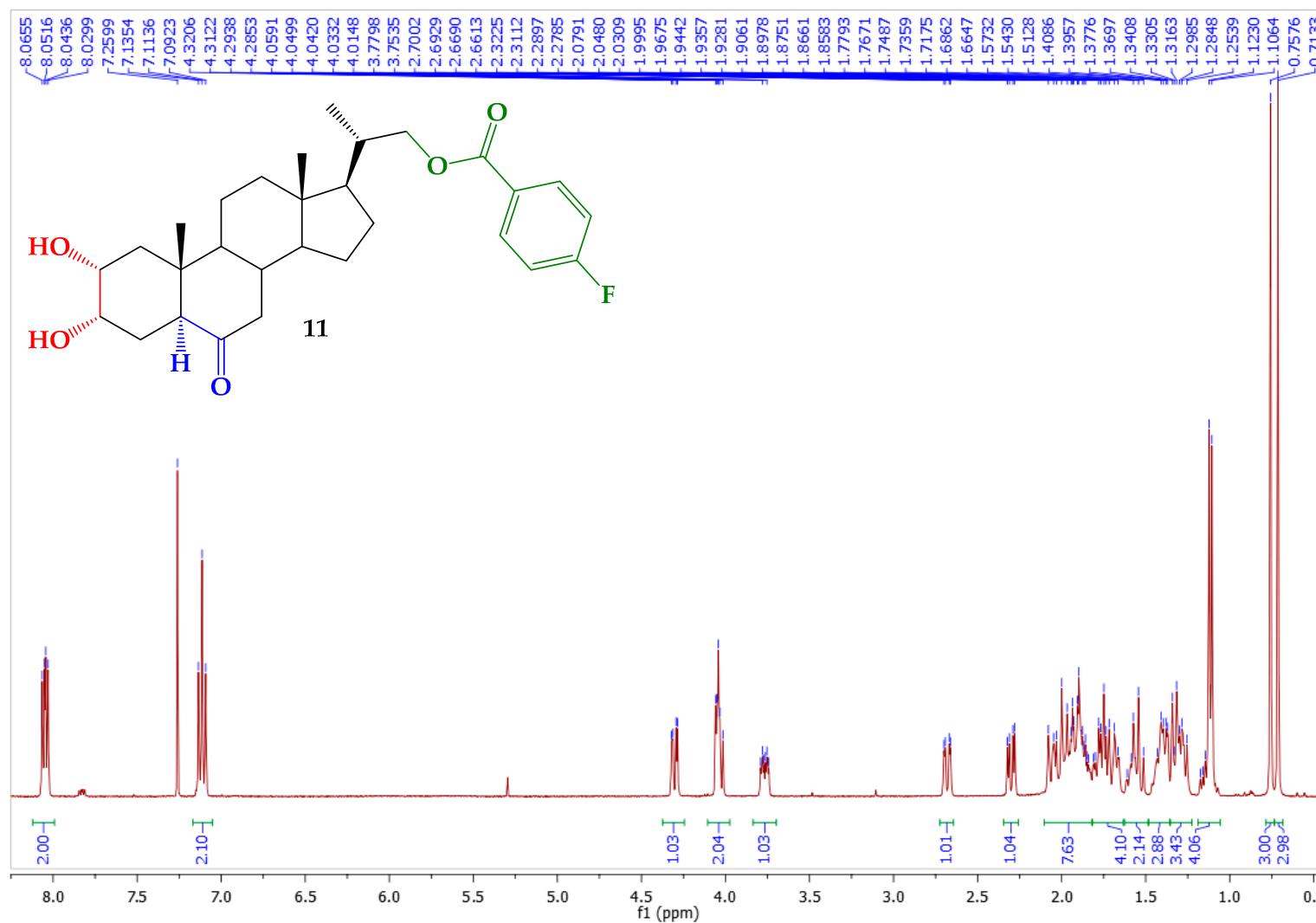


Figure S66. ¹H NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (11)

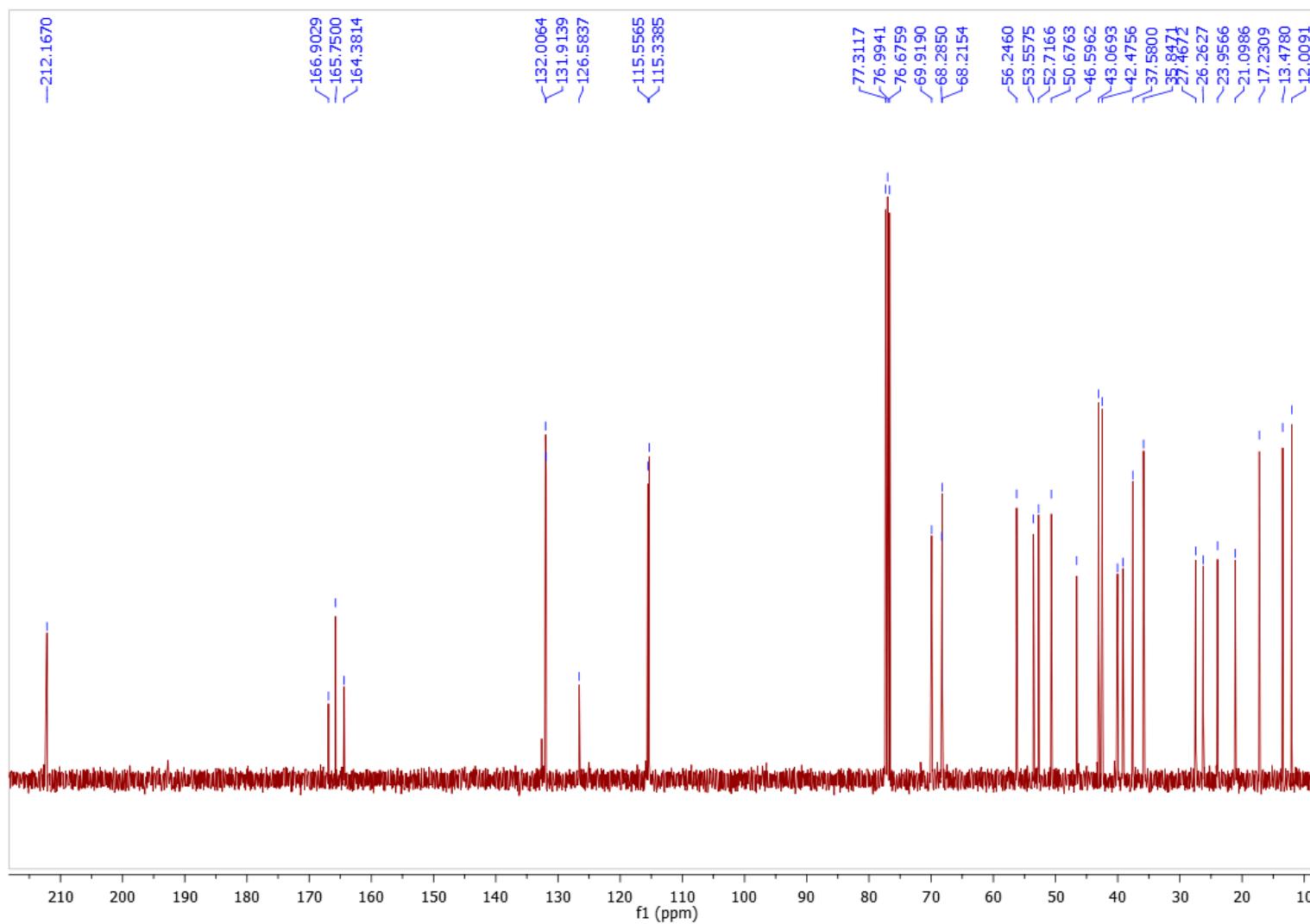


Figure S67. ¹³C NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (**11**)

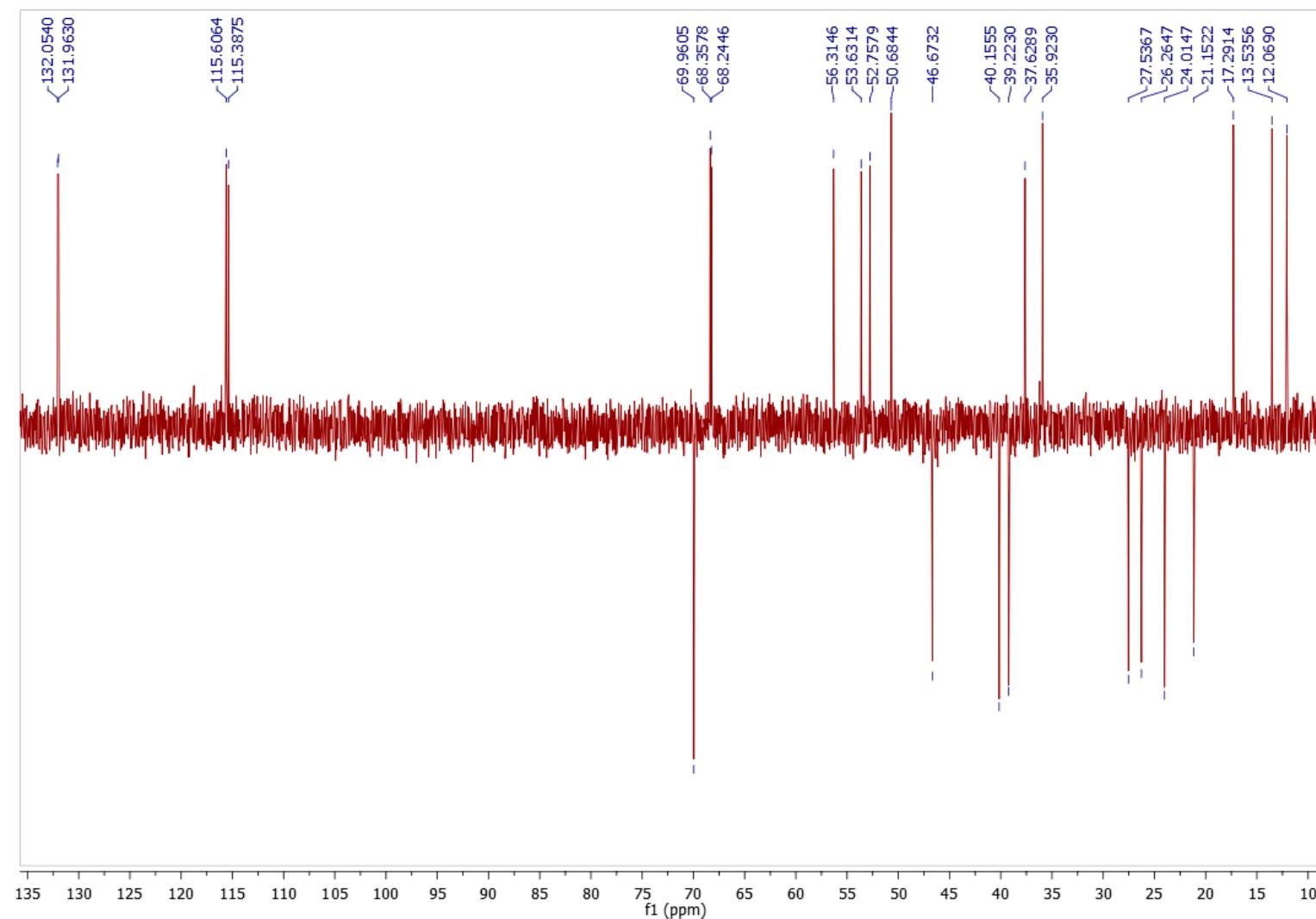


Figure S68. ^{13}C DEPT-135 NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (11)



Figure S69. 2D HSQC NMR spectrum of 2 α ,3 α -dihydroxy-5 α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (**11**)

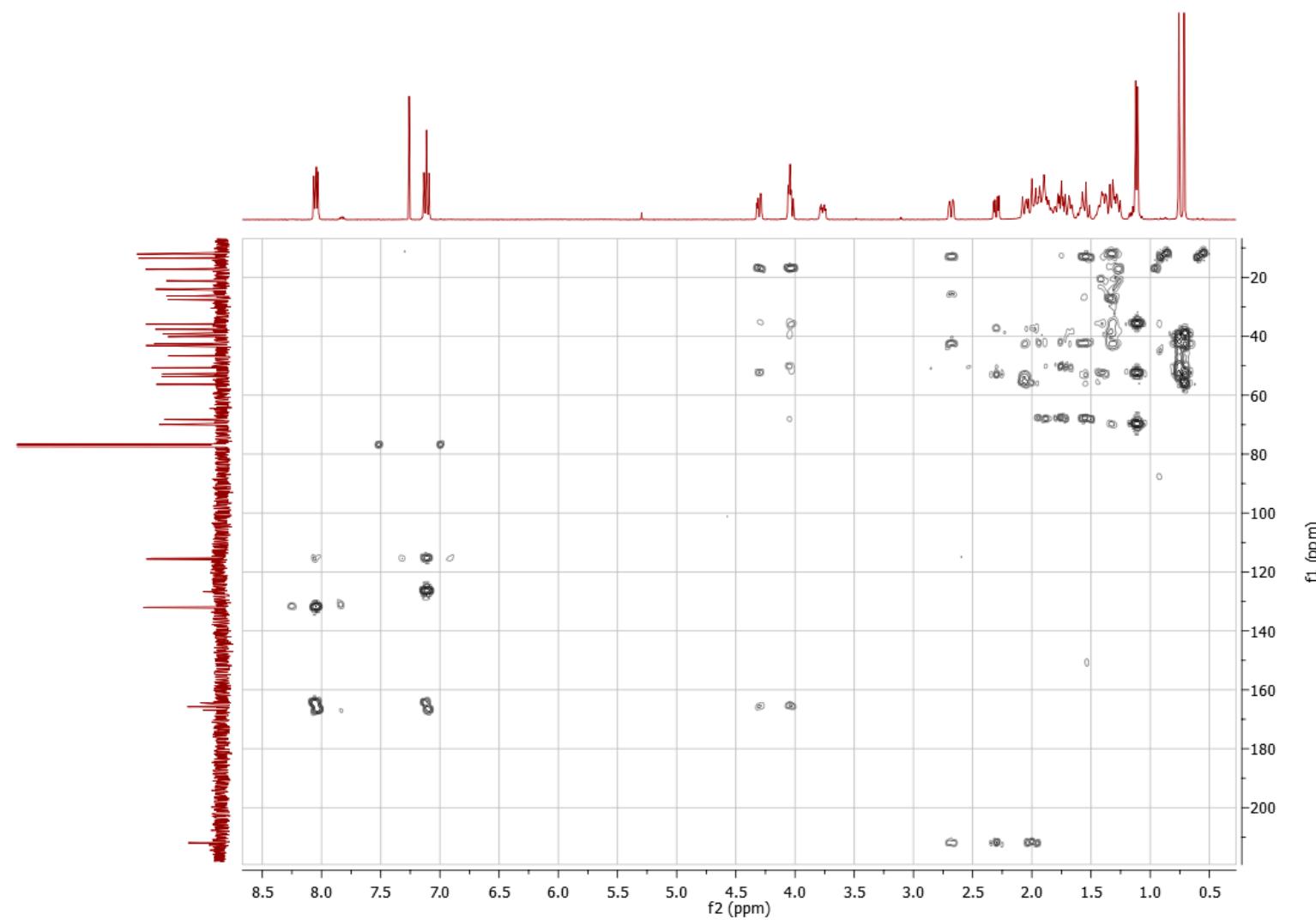


Figure S70. 2D HMBC NMR spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (11)

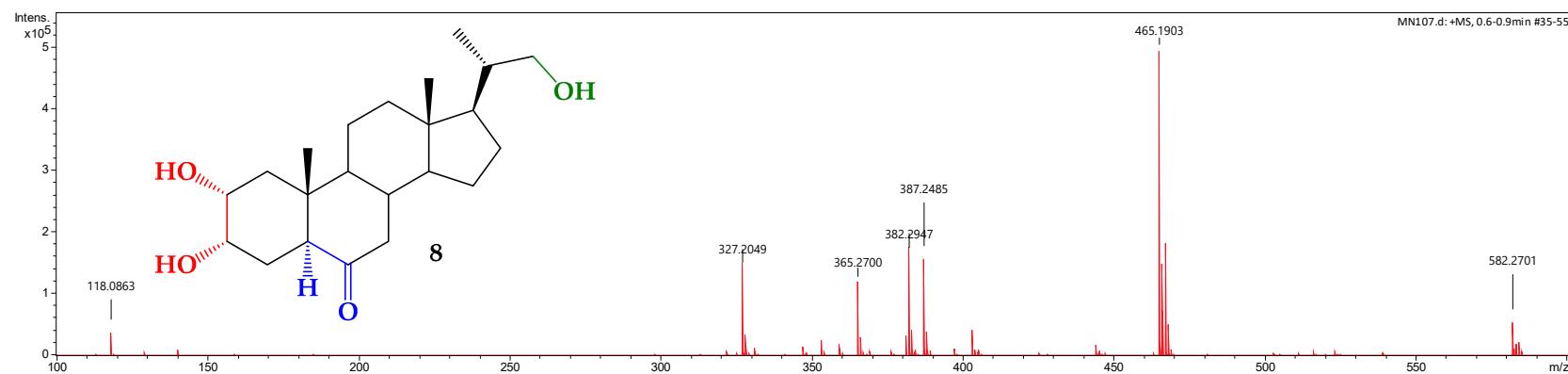


Figure S71. HRSM spectrum of $2\alpha,3\alpha,22$ -trihydroxy- 5α -cholan- $23,24$ -dinor-6-one (8)

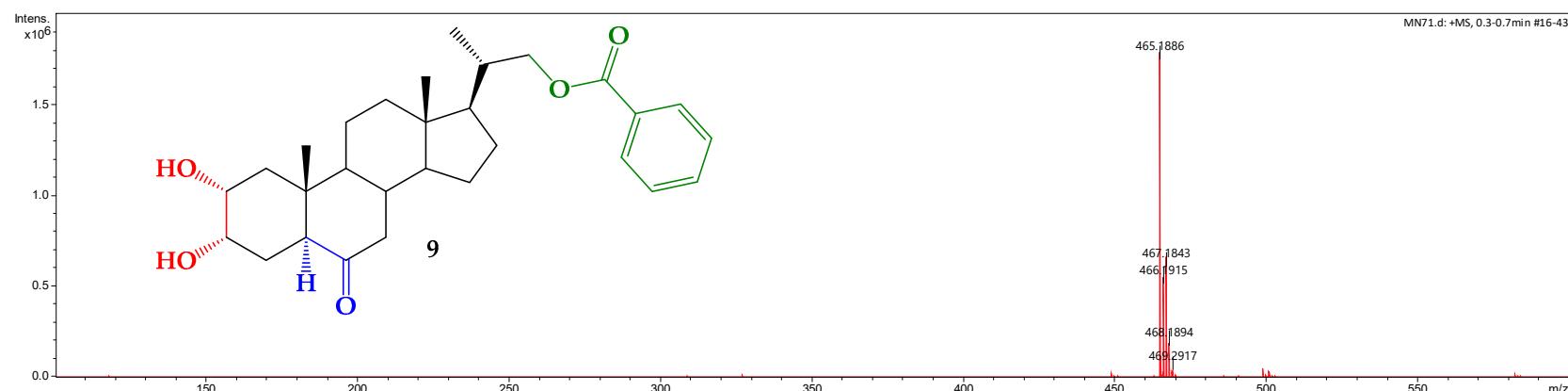


Figure S72. HRSM spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo- $23,24$ -dinor- 22 -benzoate- 22 -yl (9)

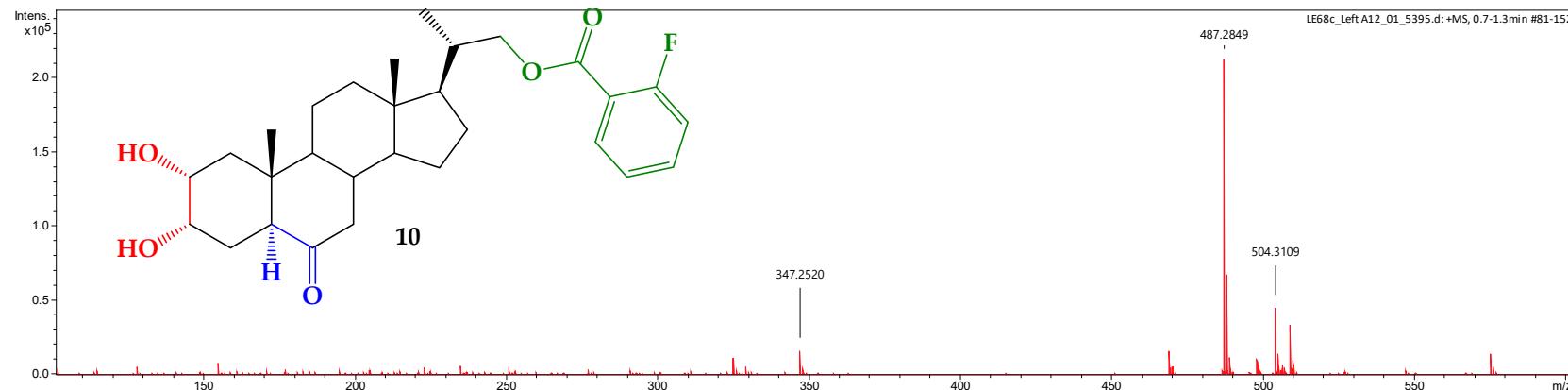


Figure S73. HRMS spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(2-Fluoro)-benzoate-22-yl (**10**)

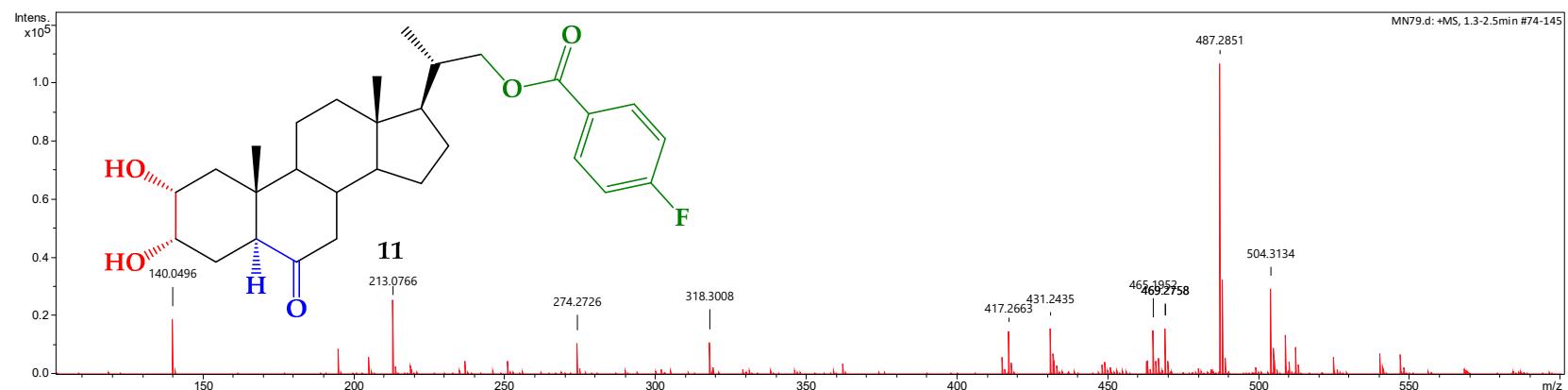


Figure S74. HRMS spectrum of $2\alpha,3\alpha$ -dihydroxy- 5α -cholan-6-oxo-23,24-dinor-22-(4-Fluoro)-benzoate-22-yl (**11**)

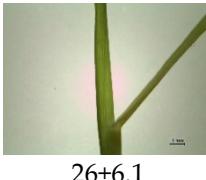
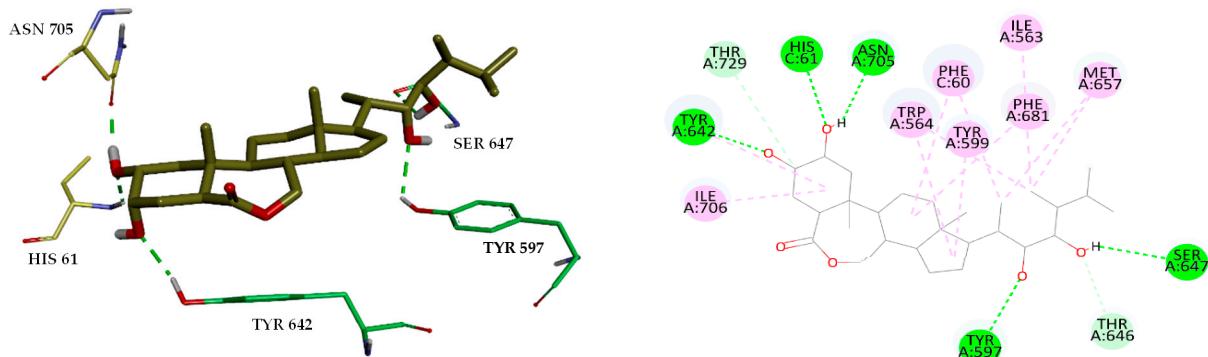
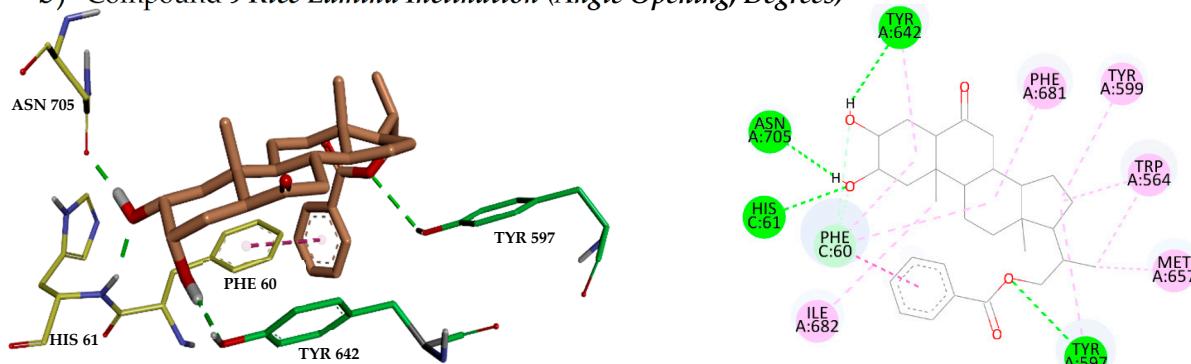
Compound	RLIT (Angle Opening, Degrees)	
	1×10^{-7} M	1×10^{-6} M
		
	46 ± 8.0	89 ± 4.9
		
	26 ± 6.1	16 ± 4.1
		
	21 ± 2.1	10 ± 2.6
		
	42 ± 0.0	24 ± 2.7
		
	33 ± 2.0	36 ± 2.0
Negative control (H_2O)		3 ± 2.6

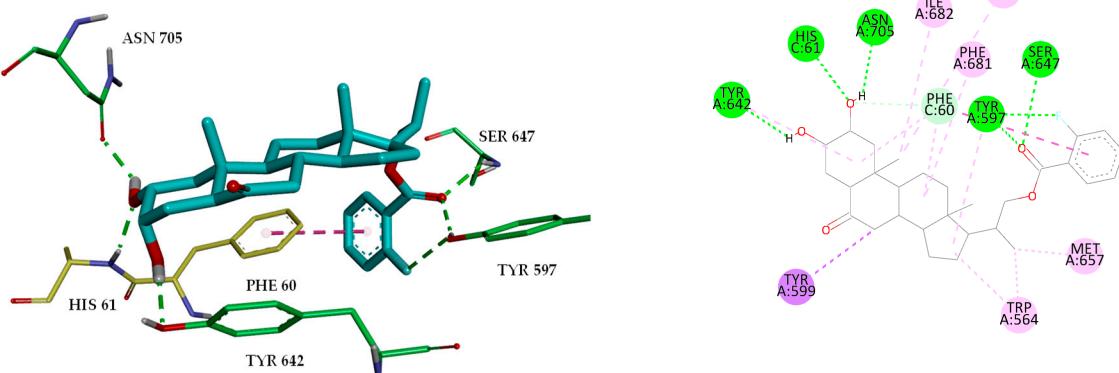
Figure S75. Rice-lamina assays using the second leaf lamina joints (Angle Opening, Degrees) of excised leaf segments treated with BRs analogs (**8–10** and **19**) at different concentrations: 1×10^{-7} and 1×10^{-6} M. Brassinolide was used as positive control at the same concentrations.

a) Brassinolide (**1**)

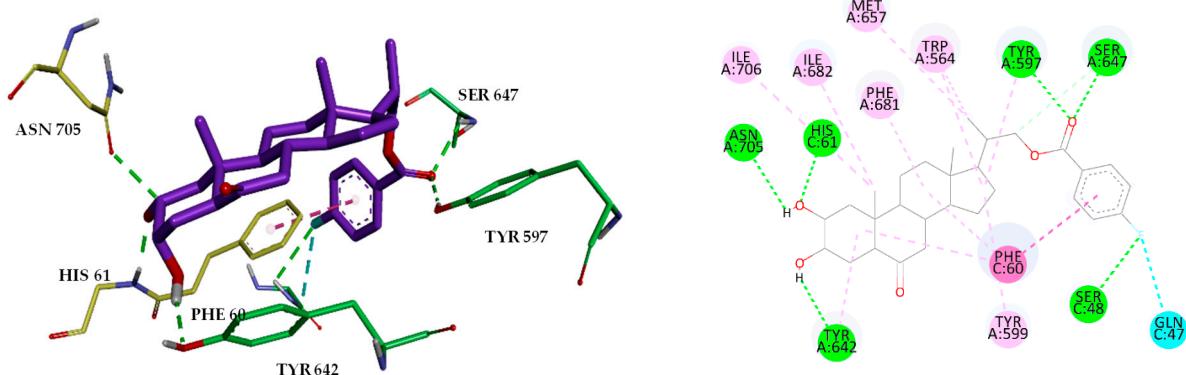
b) Compound 9 Rice Lamina Inclination (Angle Opening, Degrees)



c) Compound 10



d) Compound 11



e) Compound 8

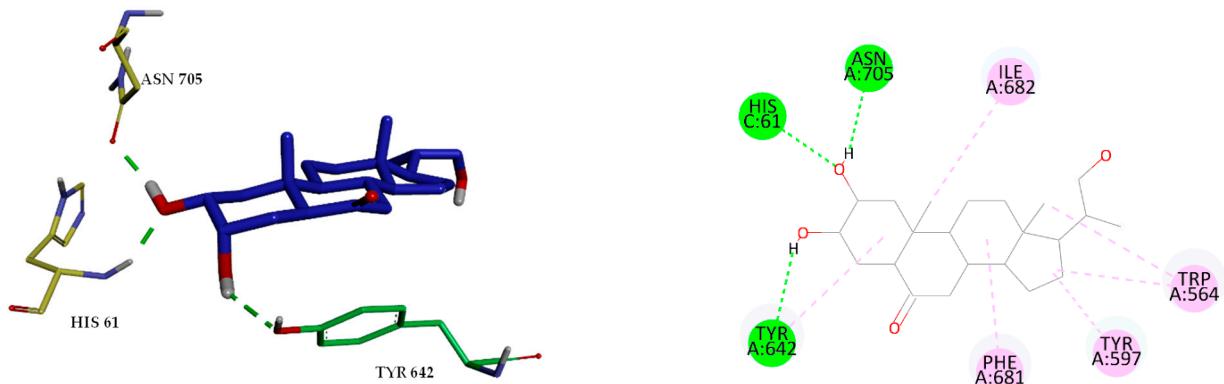


Figure S76. Protein-ligand interactions with a) brassinolide (**1**); b) Compound **8**; c) Compound **9**; d) Compound **10**, and e) Compound **19**. Hydrogen bonds are represented in green segmented lines. $\pi-\pi$ stacking are represented in dark pink segmented lines. Hydrophobic interactions are represented in pink segmented lines. Visualization of the docked poses was performed using Discovery Studio Visualizer (BIOVIA, San Diego, CA, USA).

Table S1. Pose analysis of docked brassinolide (**1**) and synthetic analogs (**8–10** and **19**). ΔE_b : Binding Energy in kcal/mol.

Code	ΔE_b	Structure
1	-12.6	
8	-11.9	
9	-12.9	
10	-13.2	
11	-13.1	

Table S2. Docked compounds-heterodimer protein contacts of brassinolide (**1**) and synthetic analogs (**8-10** and **19**).

Compound	Protein Contacts	
	Hydrogen bonds	Non-polar interactions
1	Tyr642 Asn705 His61 Tyr597 Ser647	Ile706, Tyr599, Phe681, Met657, Thr646, Trp564, Ile563, Phe60, Tyr642, Thr729
8	Tyr642 Asn705 His61	Tyr642, Trp564, Tyr597, Phe681, Ile682
9	Tyr642 Asn705 His61 Tyr597	Tyr642, Tyr599, Trp564, Tyr597, Met657, Phe681, Ile682, Phe60
10	Tyr642 Asn705 His61 Tyr597 Ser647	Tyr642, Tyr599, Trp564, Tyr597, Met657, Phe681, Ile682, Phe60, Ile706
11	Tyr642 Asn705 His61 Tyr597 Ser647 Ser48	Tyr642, Tyr599, Trp564, Tyr597, Met657, Phe681, Ile682, Phe60, Ile706, Ser48, Gln47