Synthesis

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Supporting Information

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Diastereo-Divergent Synthesis of Ring A-lactones Derived From Cholesterol and Diosgenin. A Convenient Solution for an Old Problem NMR and X-Ray Characterization

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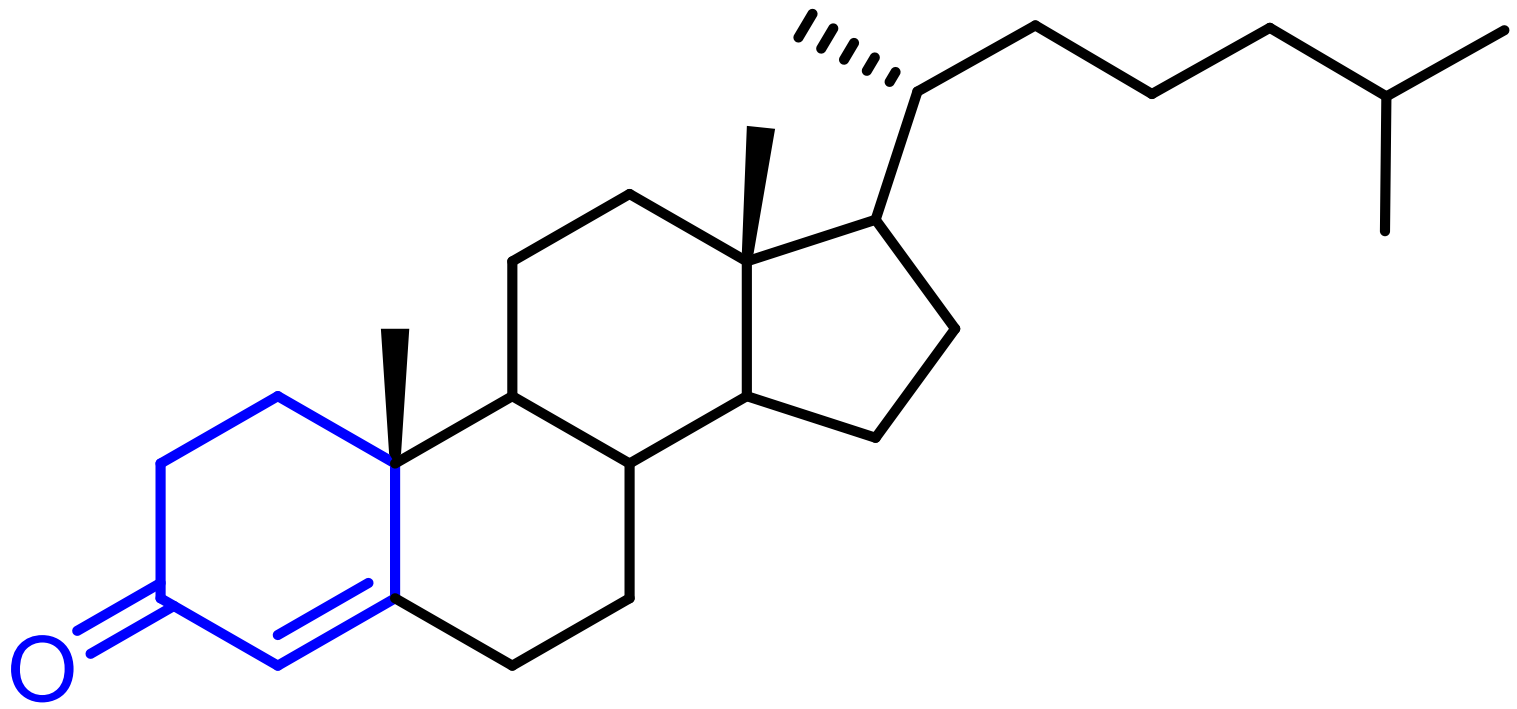

Figure S1. Cholest-4-en-3-one **(15)**

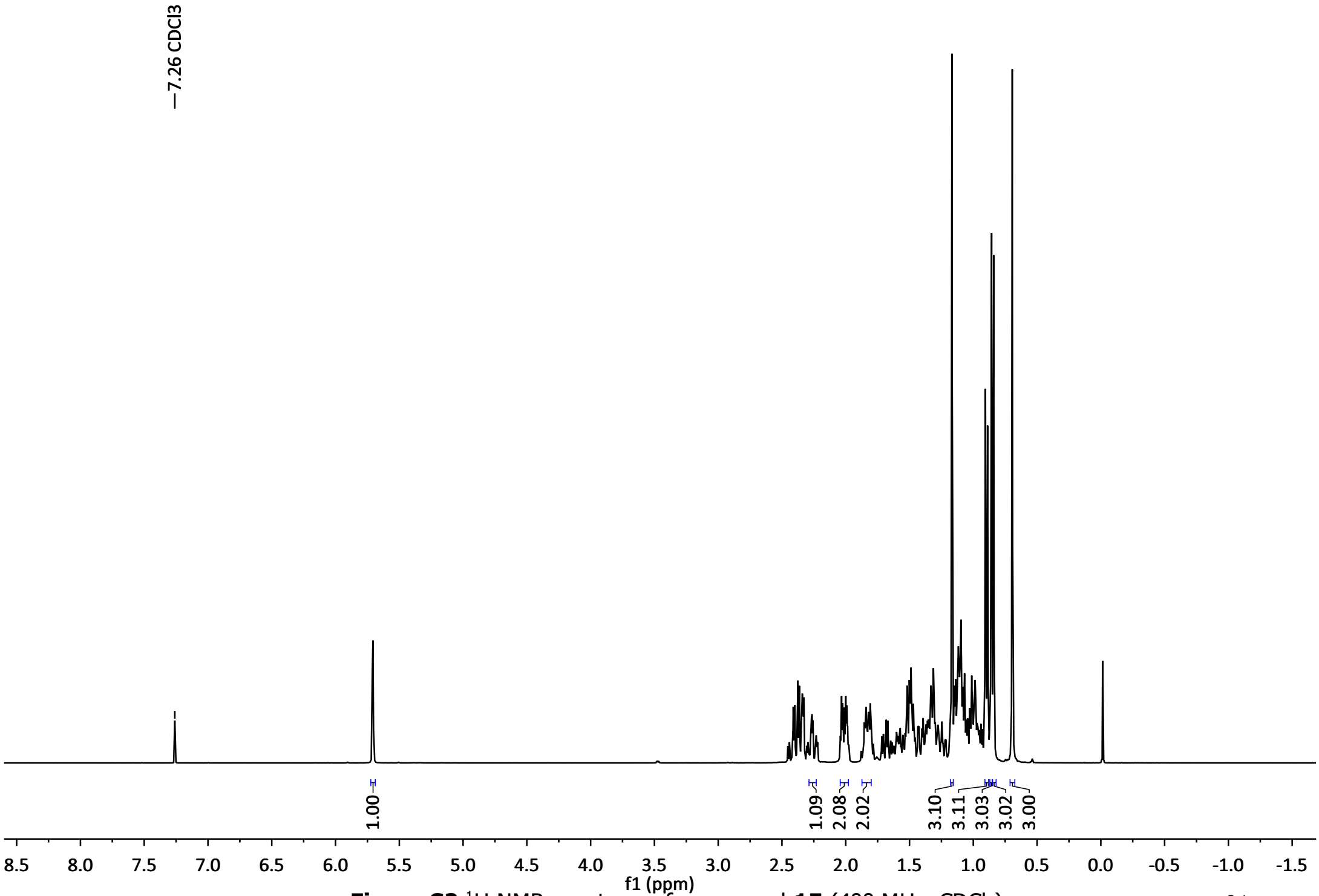

Figure S2. ^{1}H NMR spectrum of compound **15** (400 MHz, $CDCl_3$)

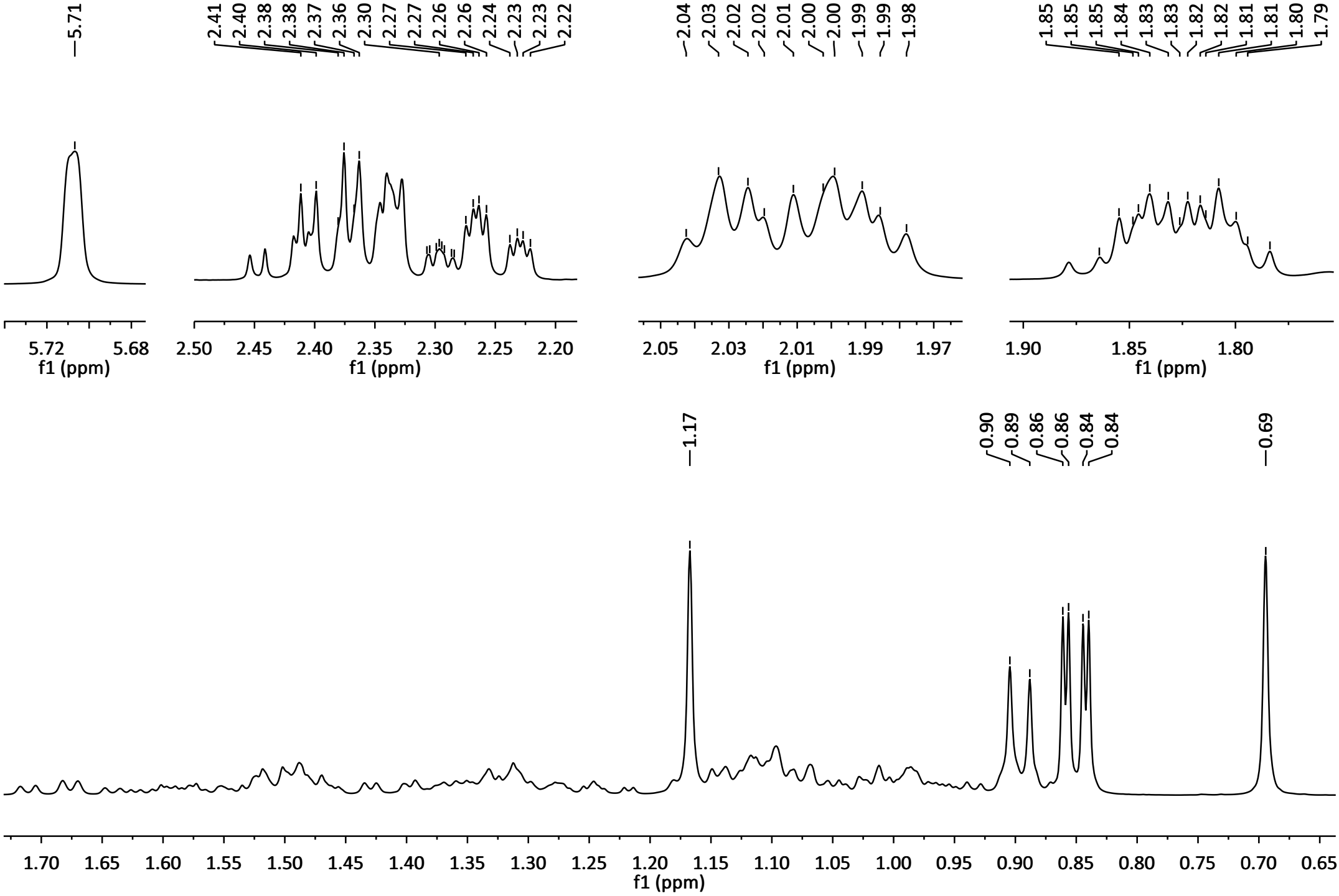

Figure S3. Sections for ^{1}H NMR spectrum of compound **15** (400 MHz, $CDCl_3$)

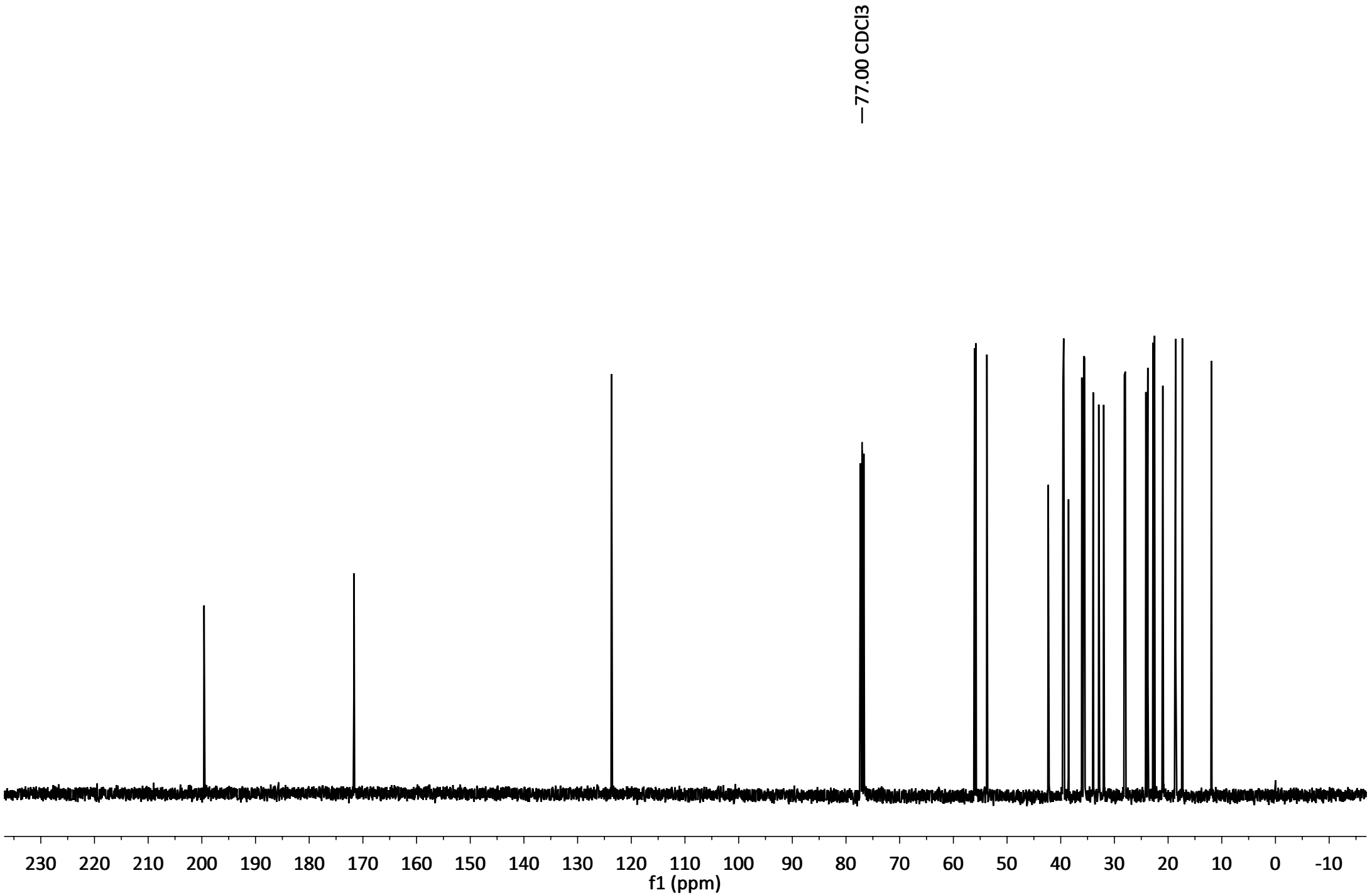

Figure S4. ^{13}C {^{1}H} NMR spectrum of compound **15** (100 MHz, $CDCl_3$)

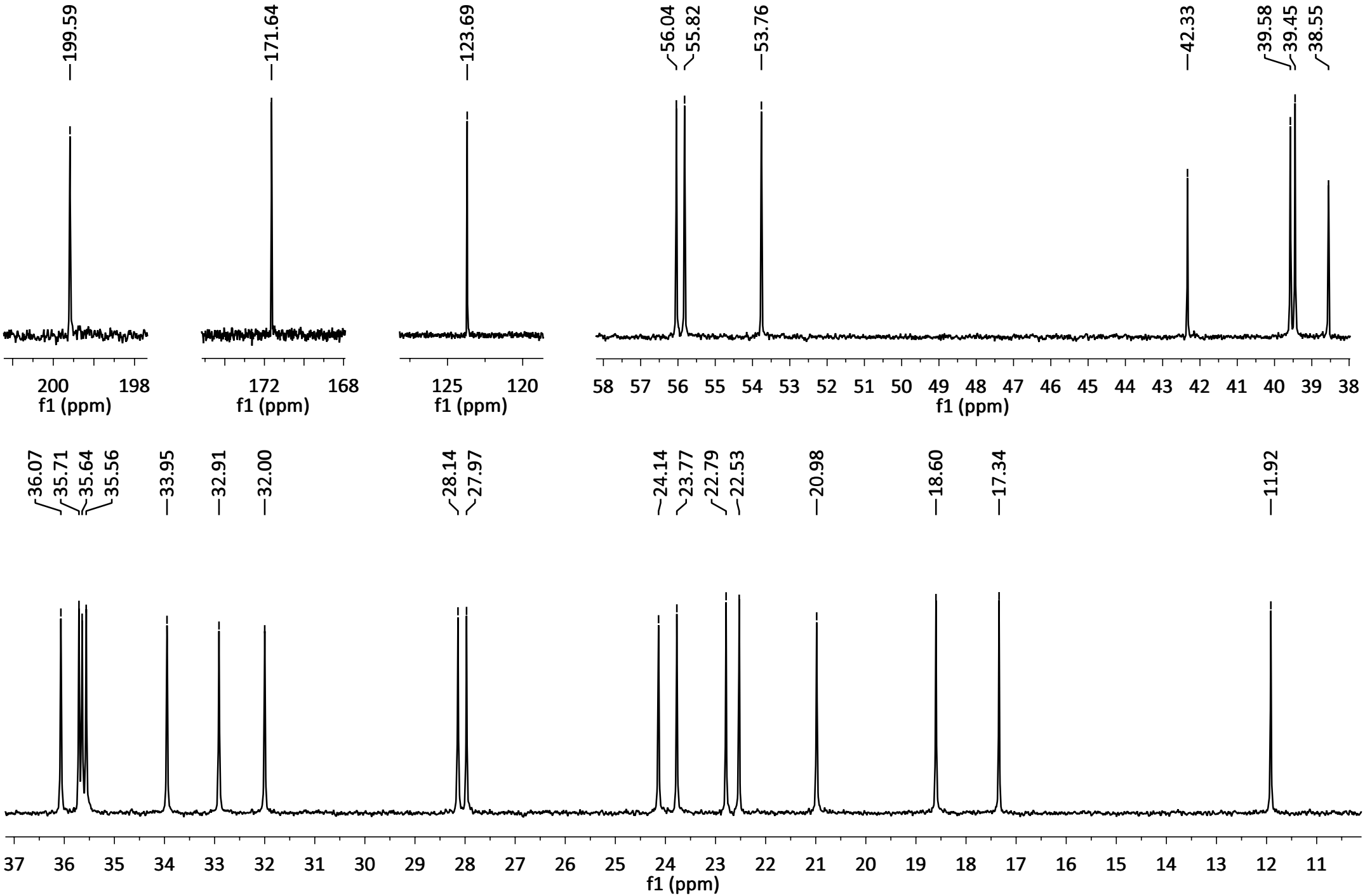

Figure S5. Sections for ^{13}C {^{1}H} NMR spectrum of compound **15** (100 MHz, $CDCl_3$)

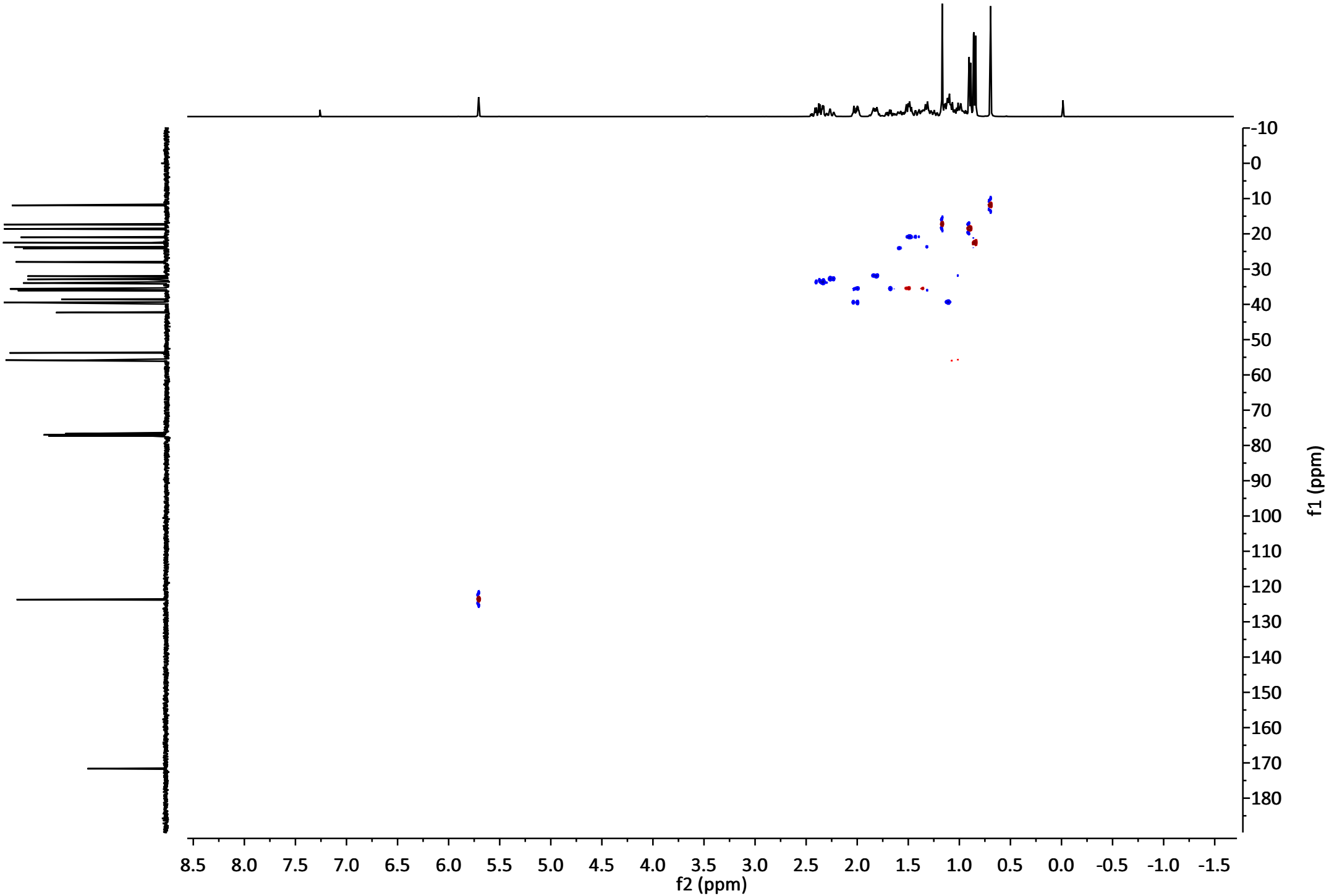

Figure S6. ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **15** (400 MHz, $CDCl_3$)

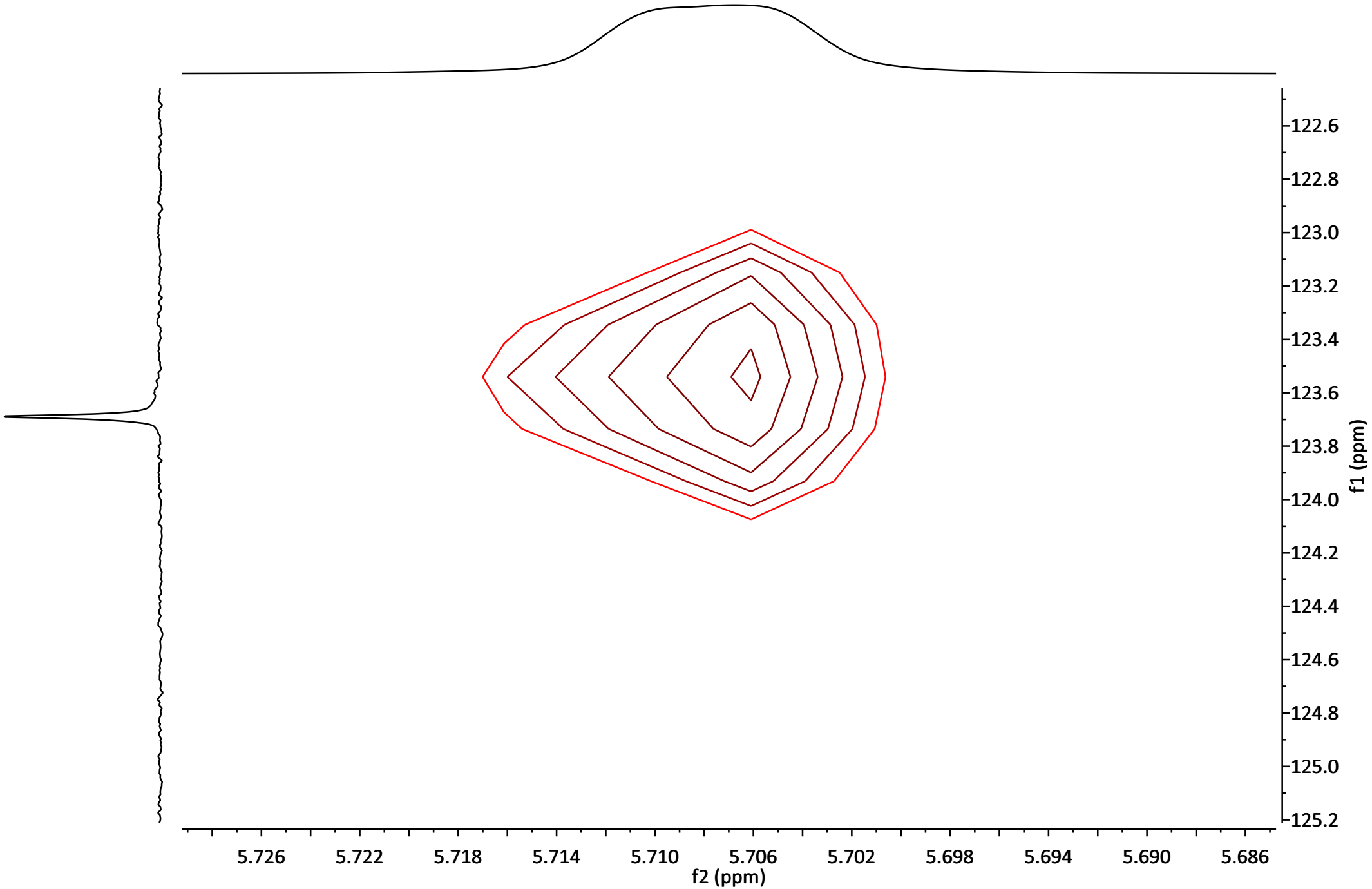

Figure S7. Section for ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **15** (400 MHz, $CDCl_3$)

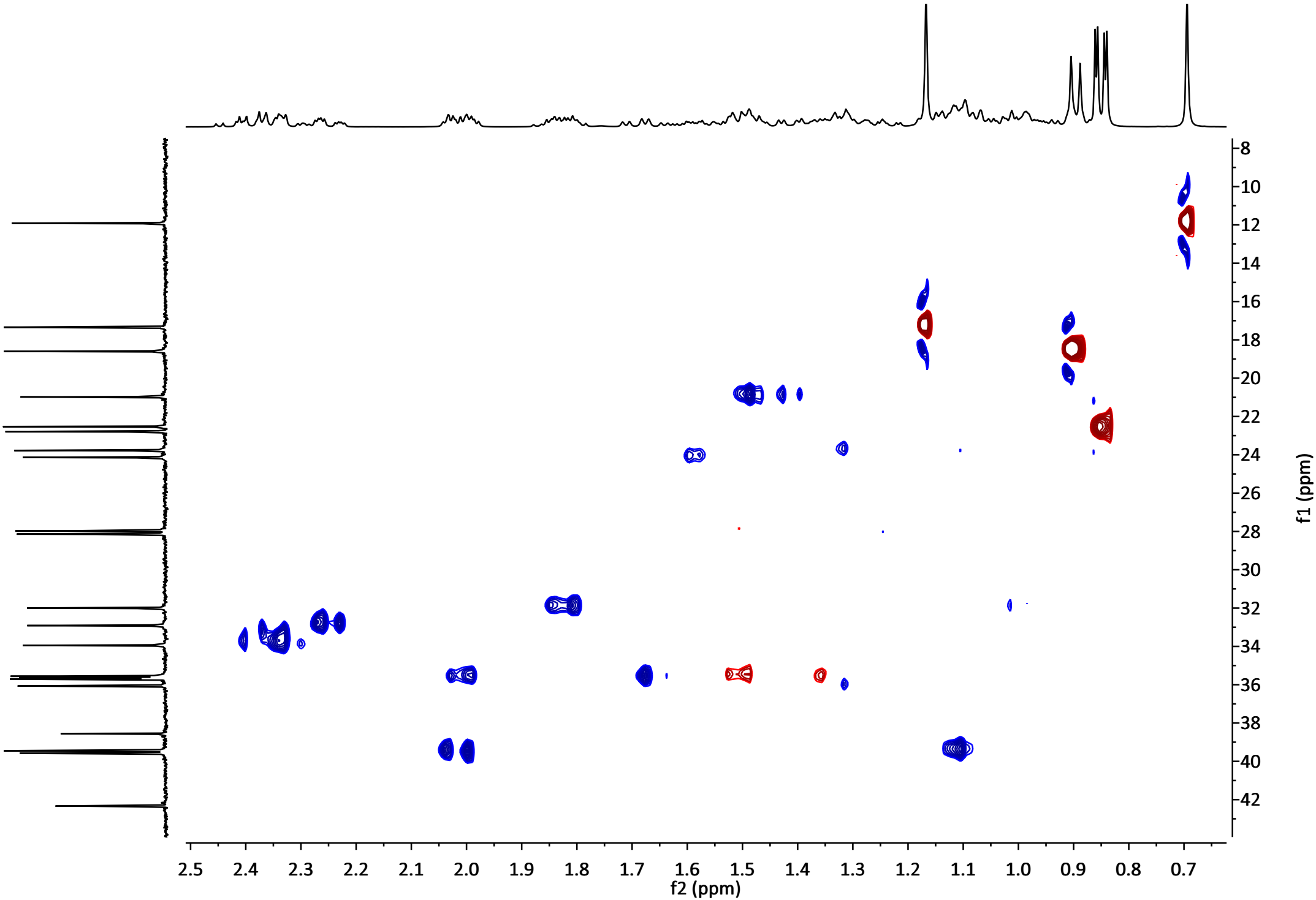

Figure S8. Section for ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **15** (400 MHz, $CDCl_3$)

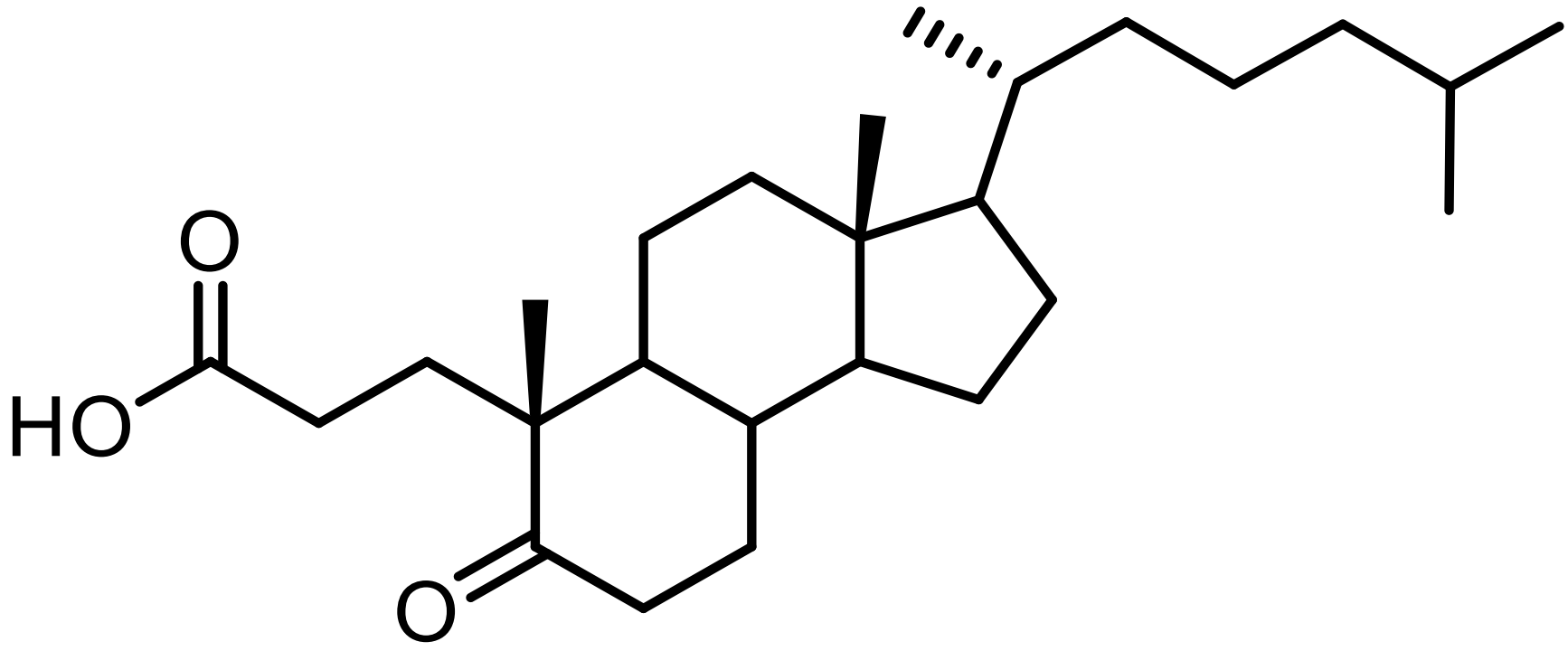

Figure S9. A-seco-4-nor-cholest-5-oxo-3-oic acid **(8)**

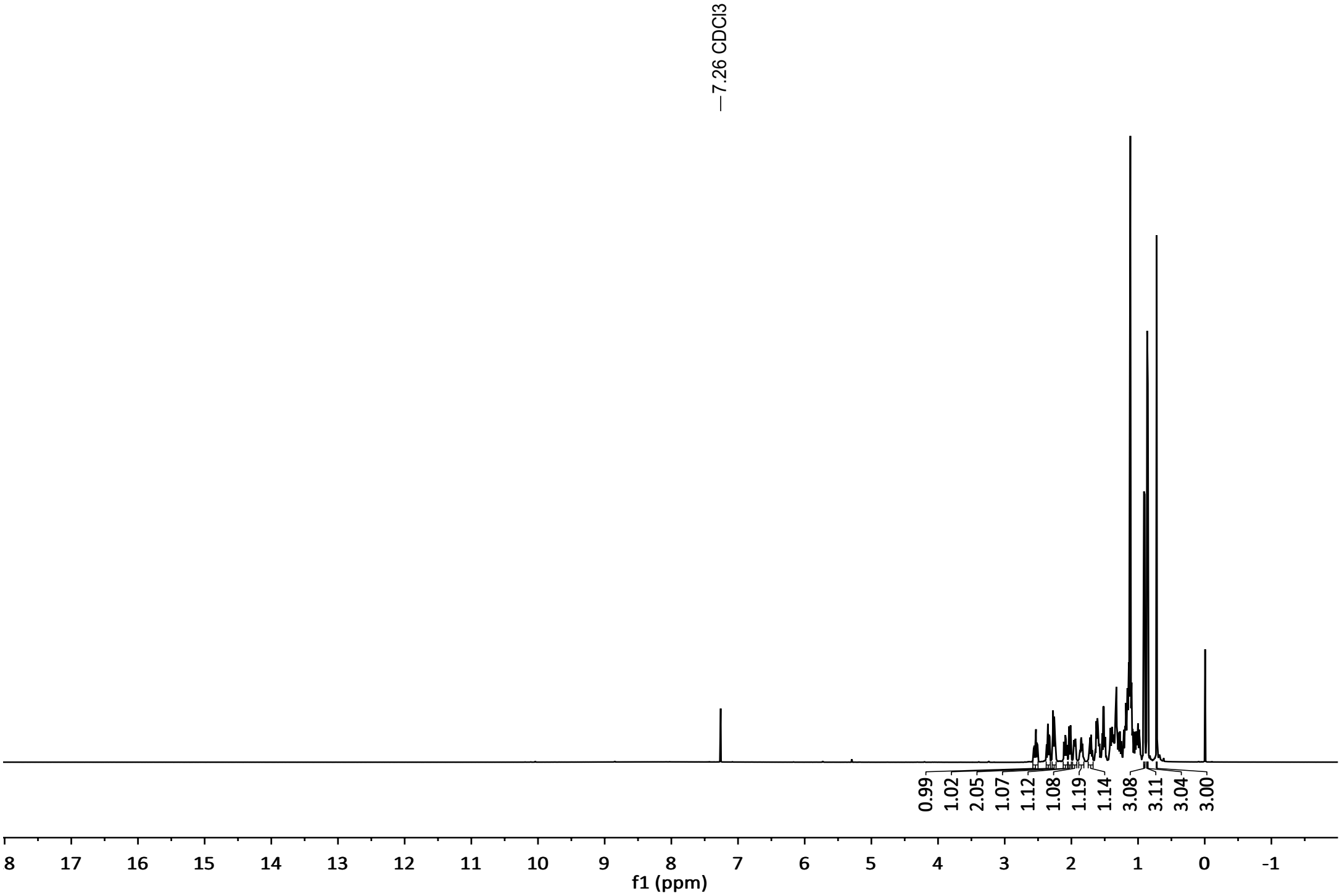

Figure S10. ^{1}H NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

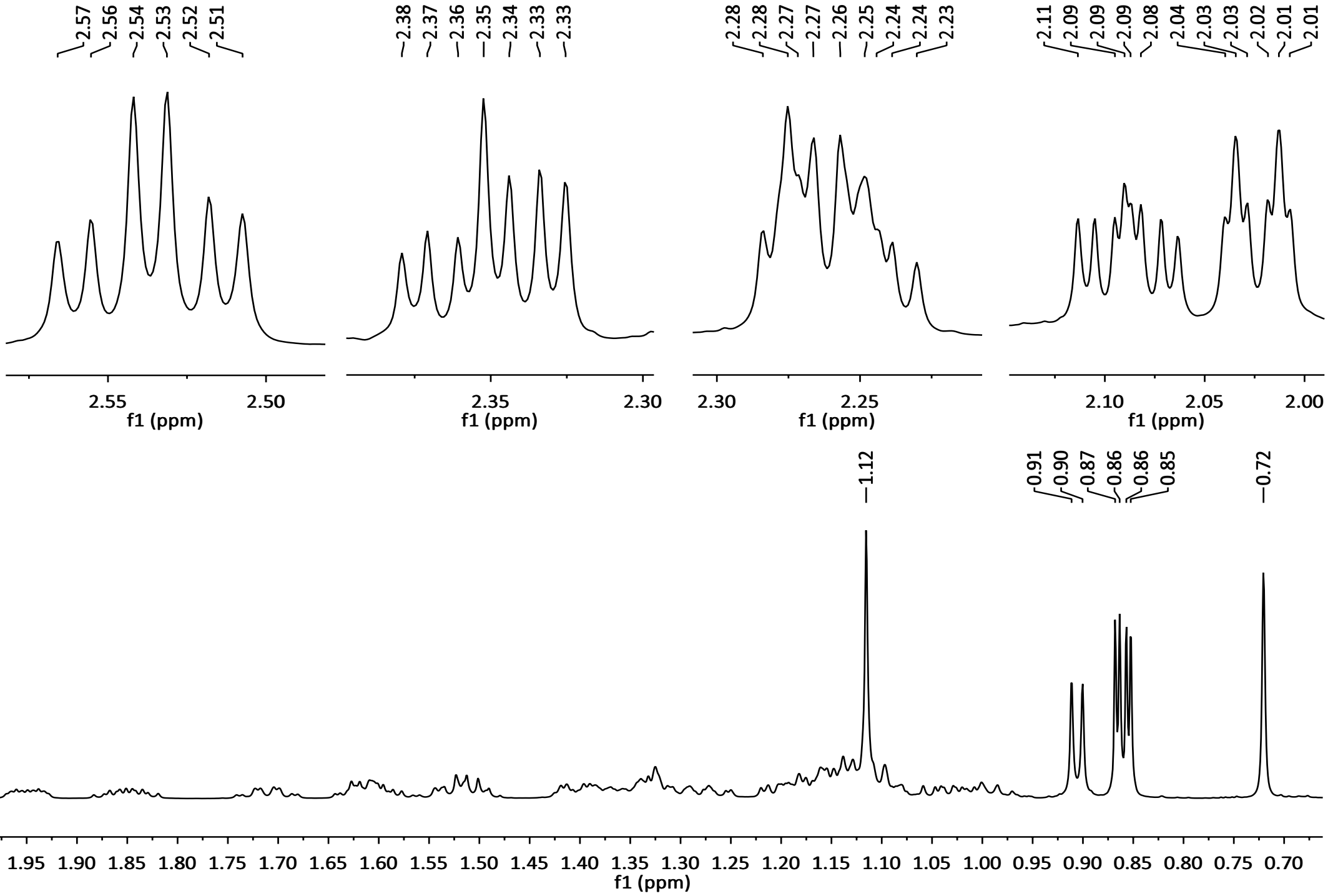

Figure S11. Sections for ^{1}H NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

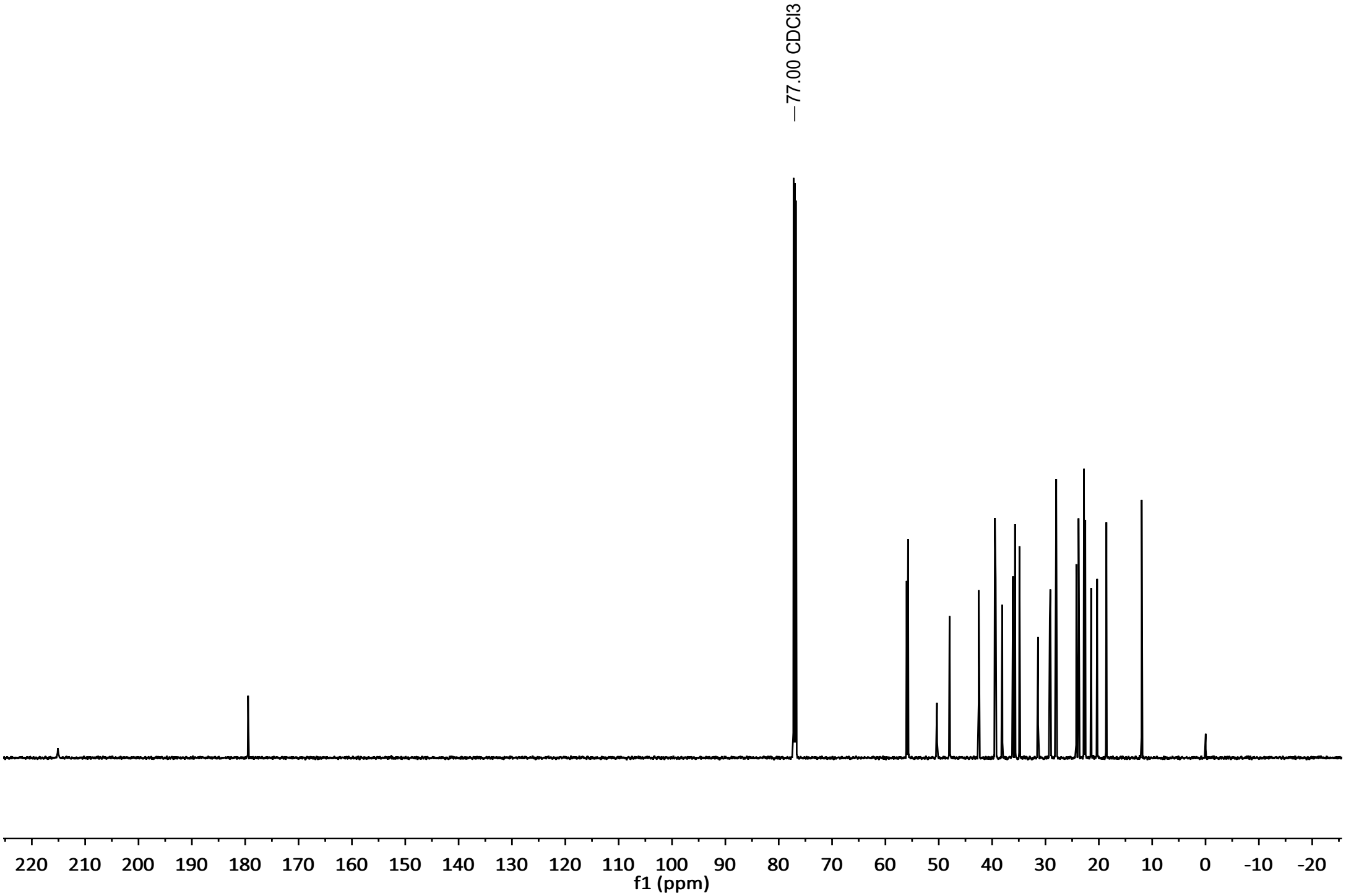

Figure S12. ^{13}C {^{1}H} NMR spectrum of compound **8** (100 MHz, $CDCl_3$)

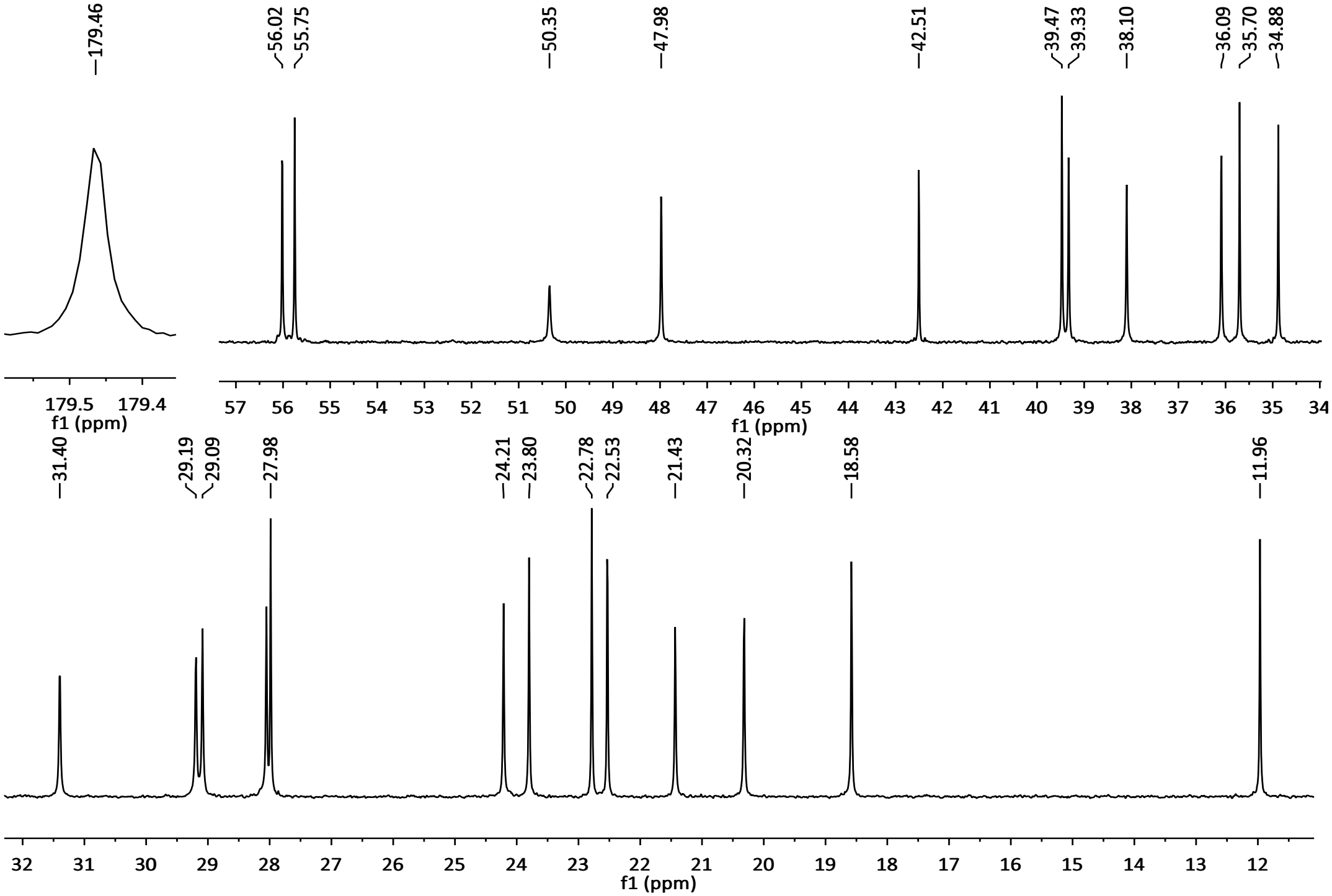

Figure S13. Sections for ^{13}C {^{1}H} NMR spectrum of compound **8** (100 MHz, $CDCl_3$)

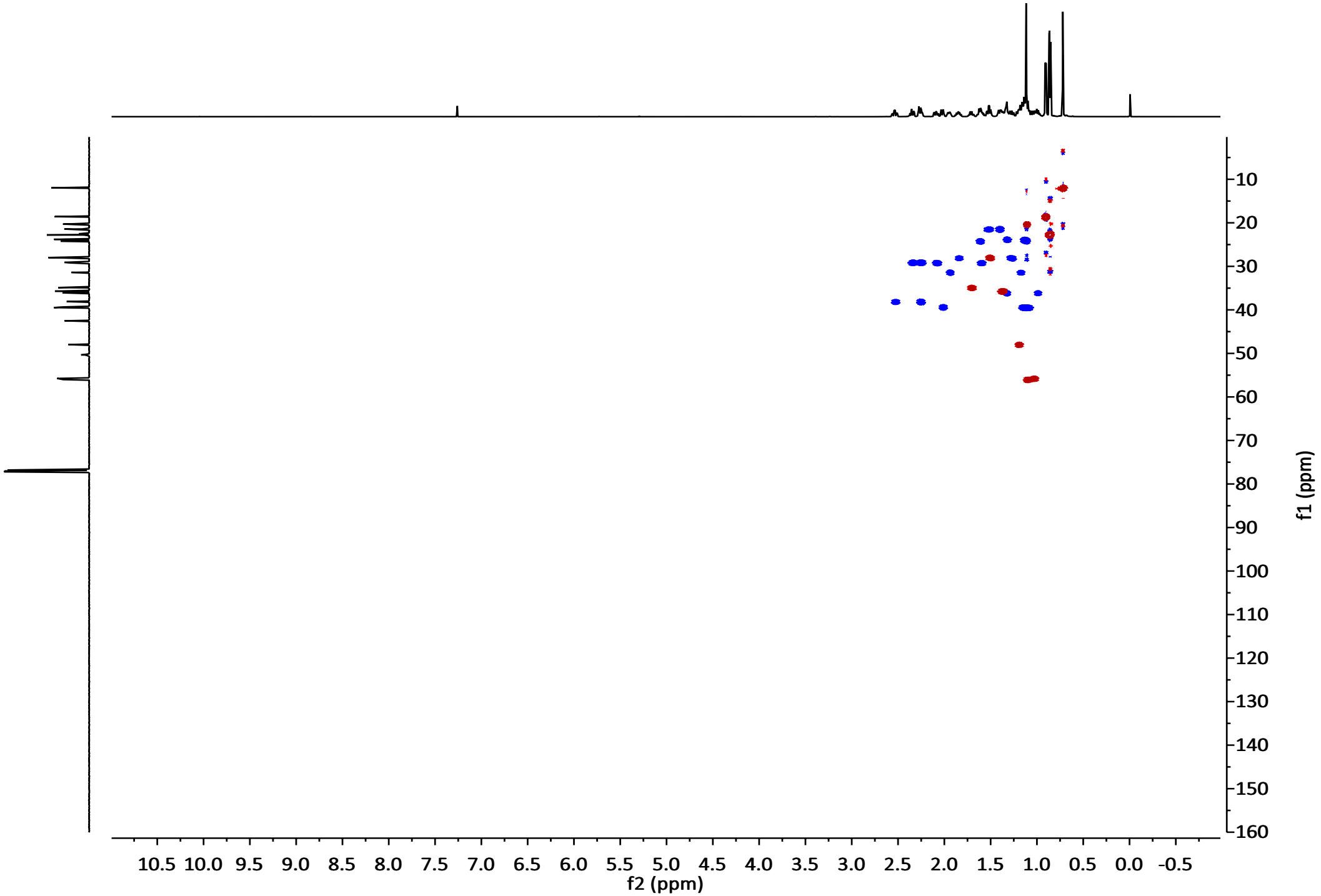

Figure S14. ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

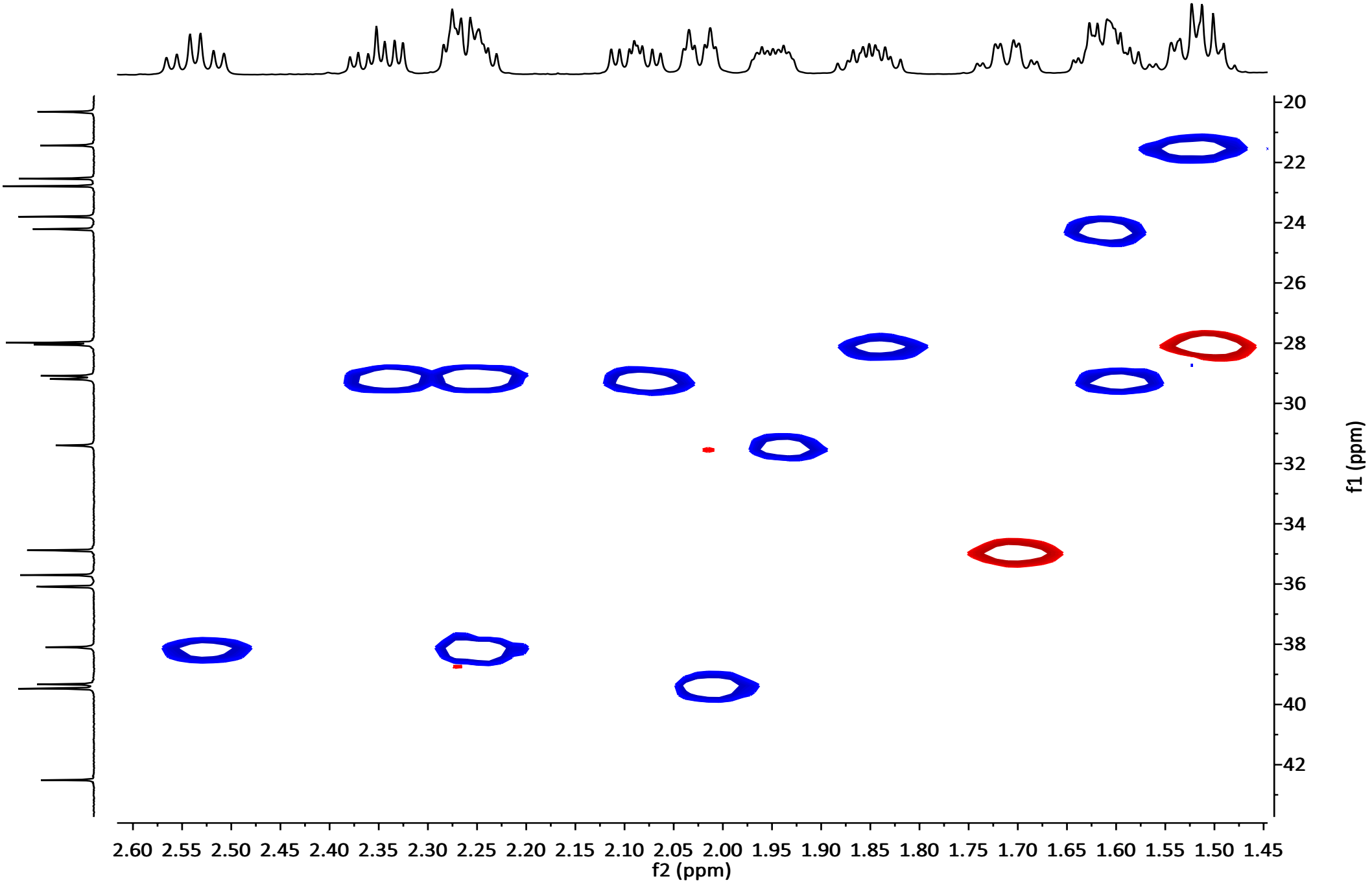

Figure S15. Section of ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

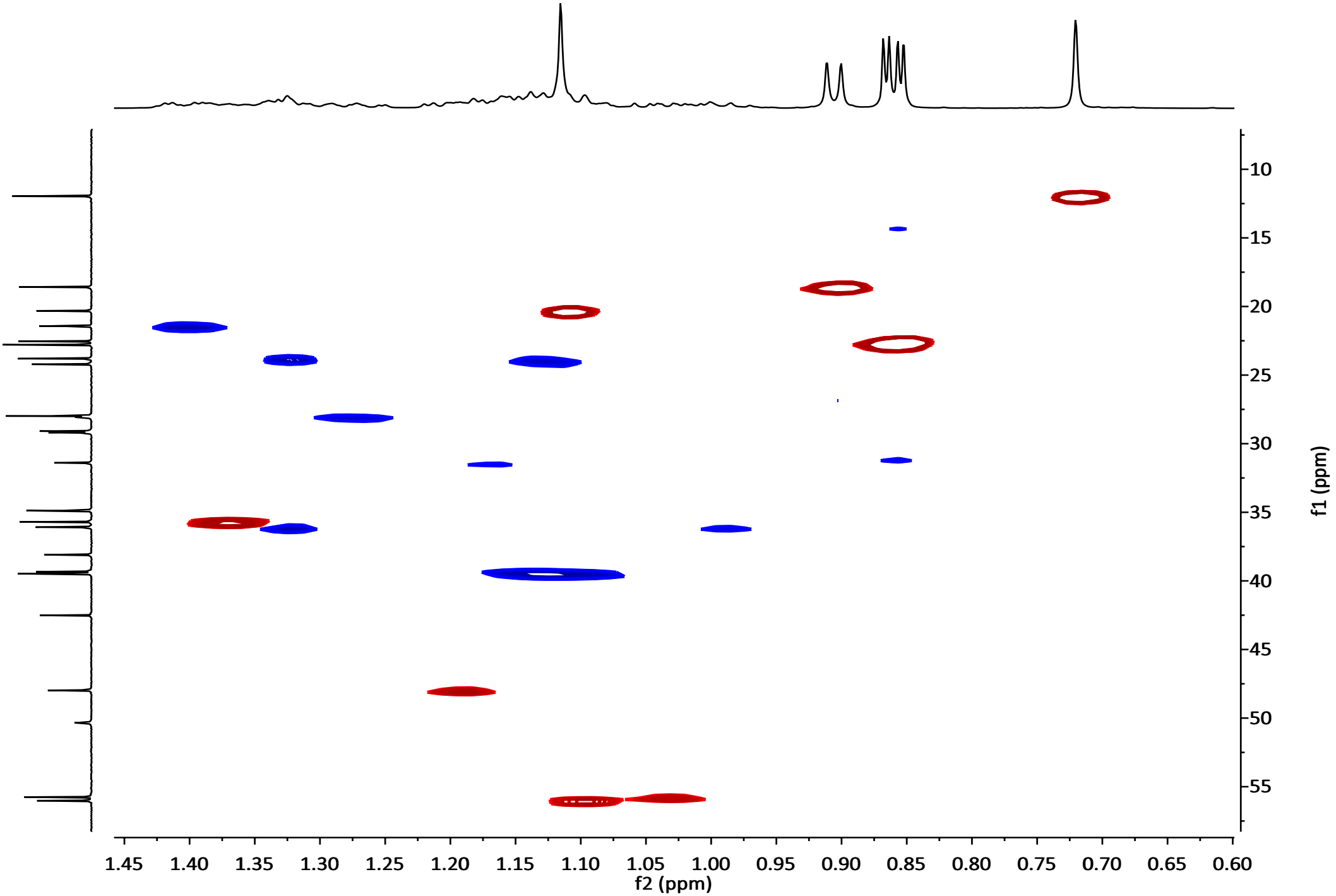

Figure S16. Section for ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

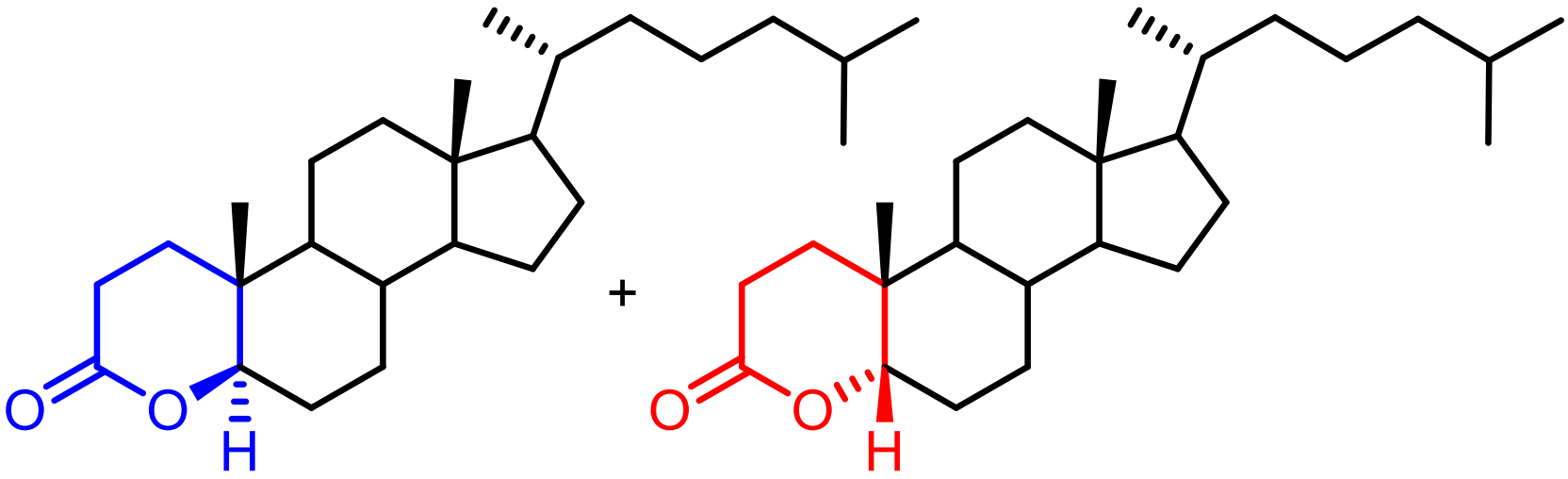

Figure S17. Diasteromeric relation of lactones **7a and 7b**

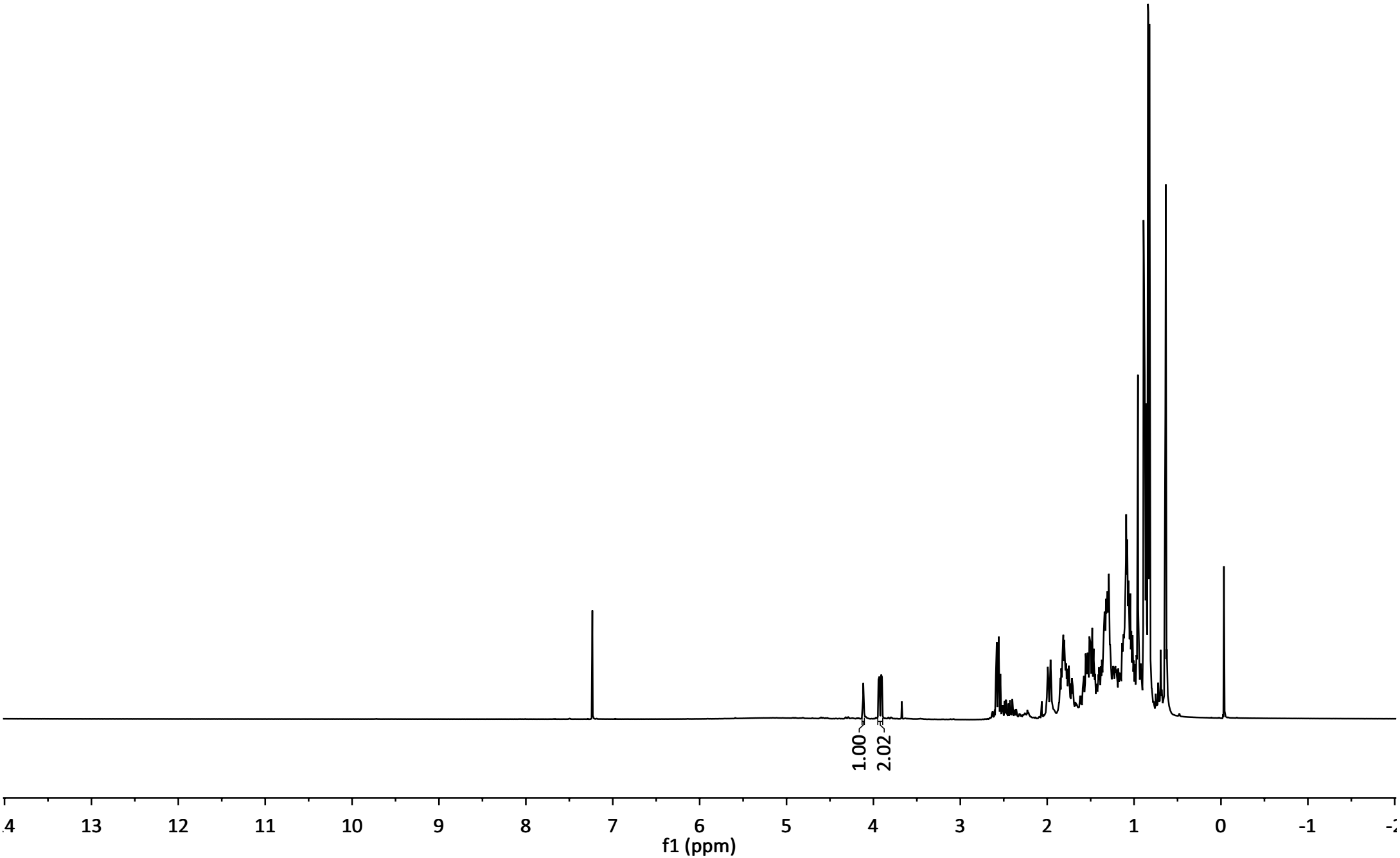

Figure S18. ^{1}H NMR spectrum of compounds mixture **7a** and **7b** (400 MHz, $CDCl_3$)

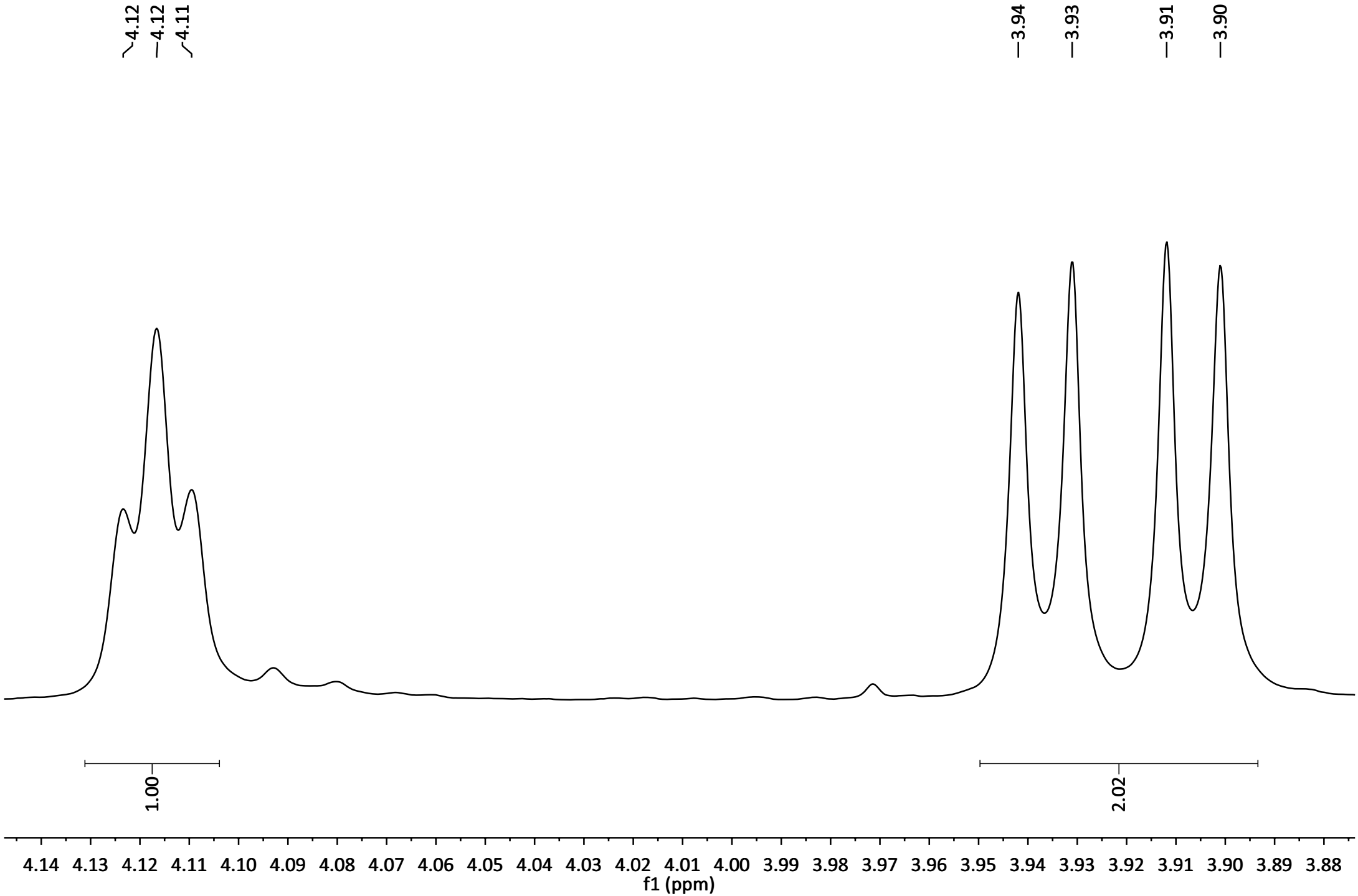

Figure S19. Section for ^{1}H NMR spectrum of compounds mixture **7a** and **7b** (400 MHz, $CDCl_3$)

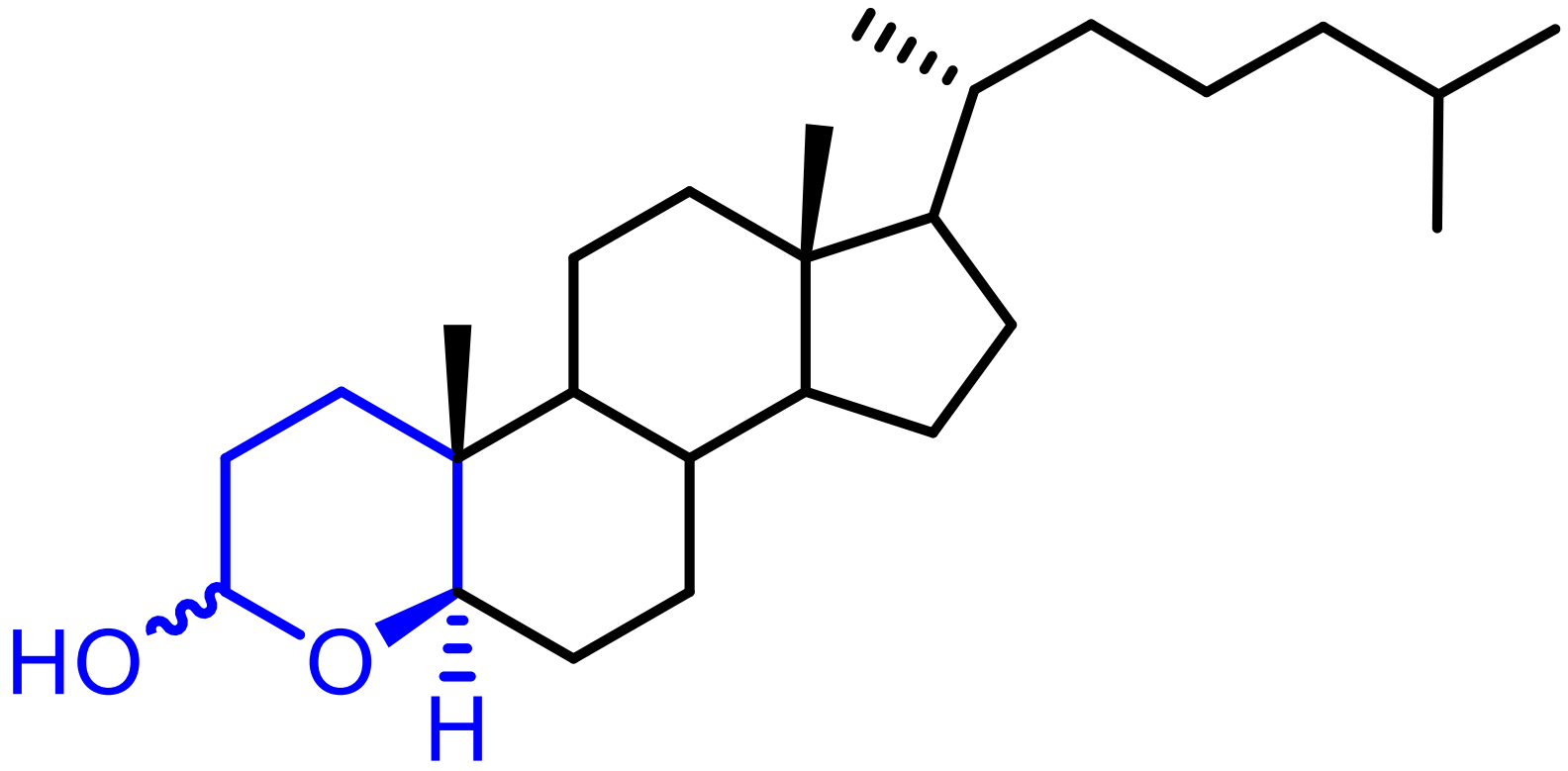

Figure S20. 4-Oxa-cholest-5-en-3-ol **(16a)**

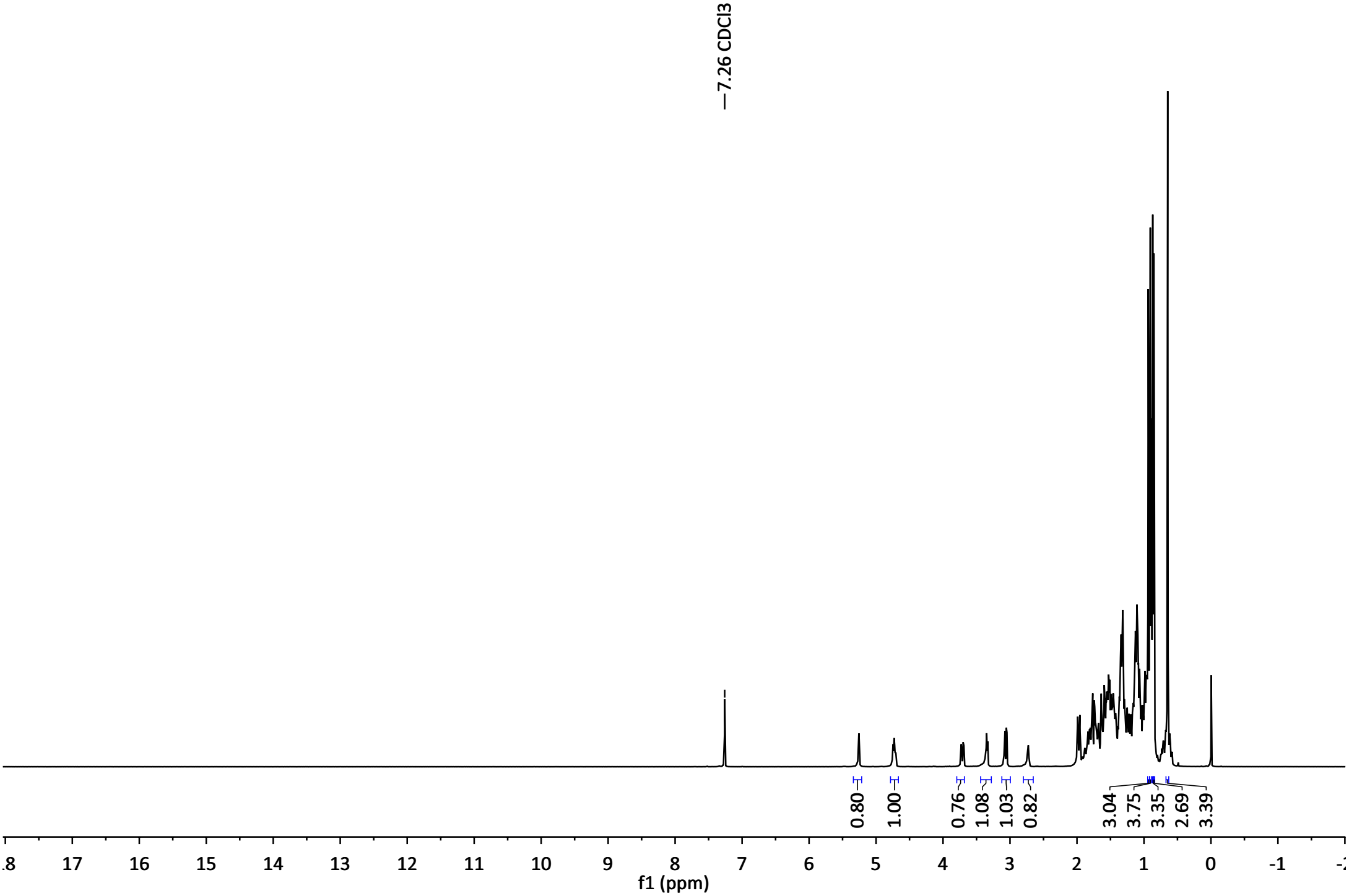

Figure S21. ^{1}H NMR spectrum of compound **16a** (400 MHz, $CDCl_3$)

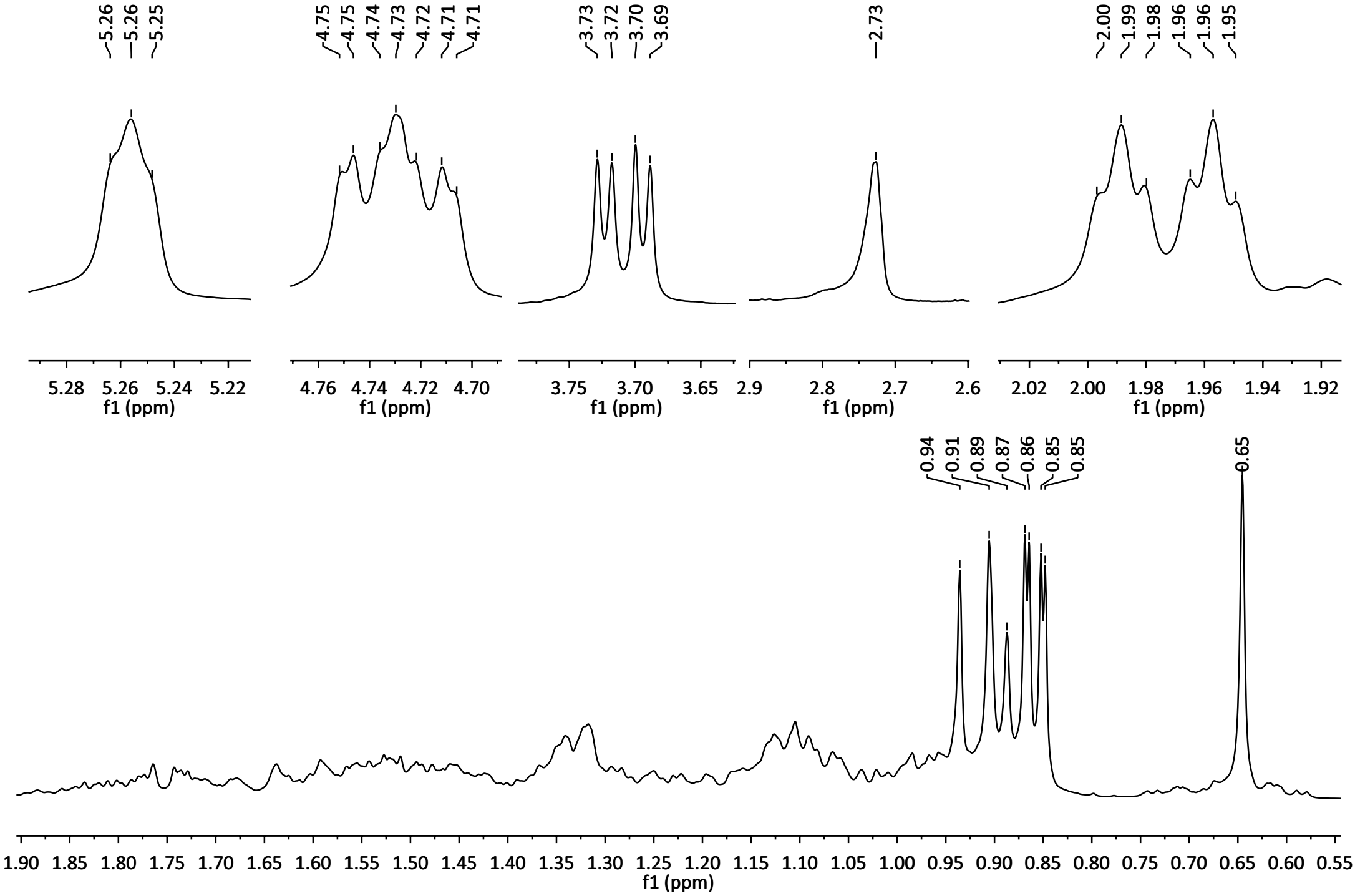

Figure S22. Sections for ^{1}H NMR spectrum of compound **16a** (400 MHz, $CDCl_3$)

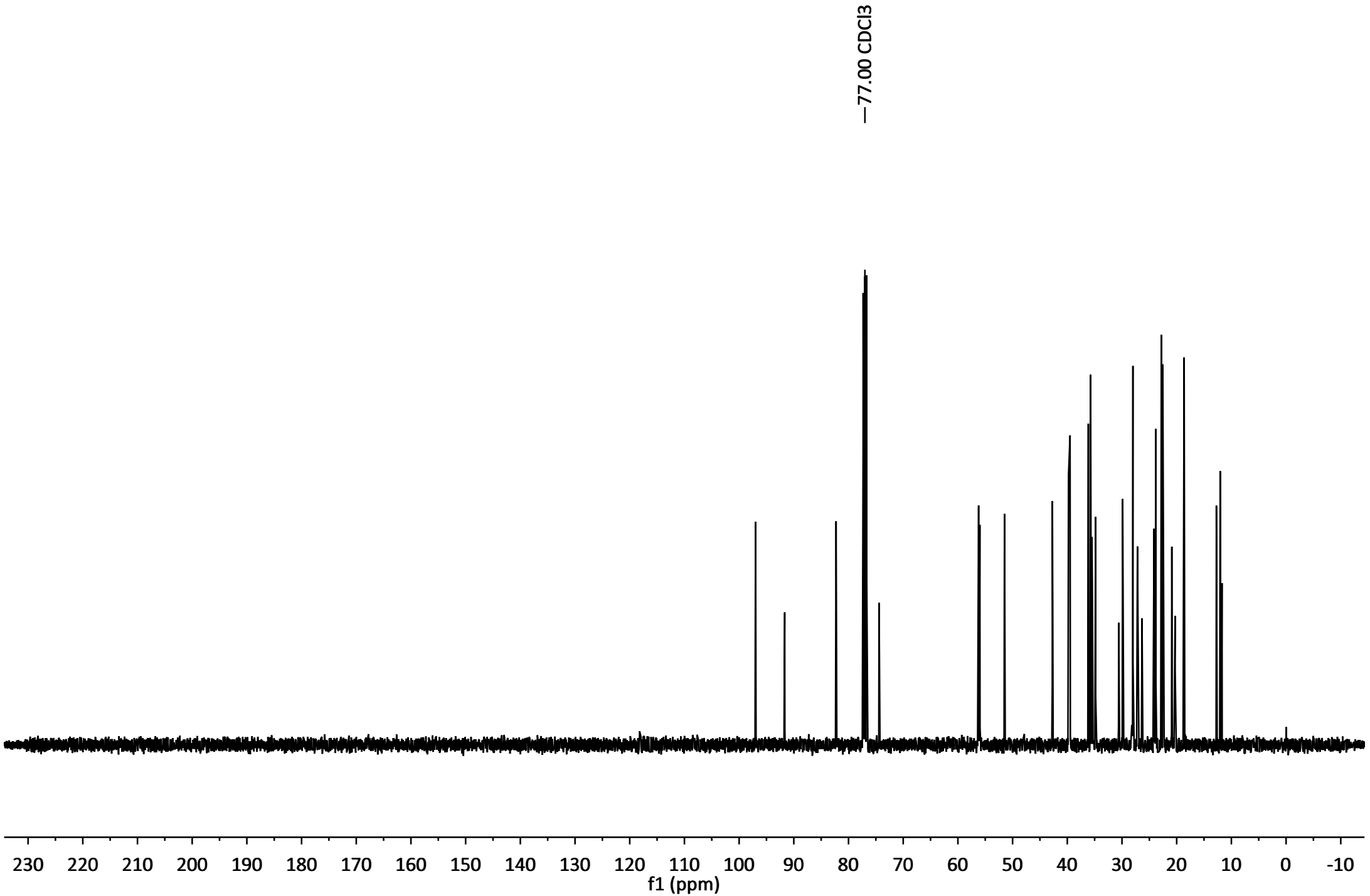

Figure S23. ^{13}C {^{1}H} NMR spectrum of compound **16a** (100 MHz, $CDCl_3$)

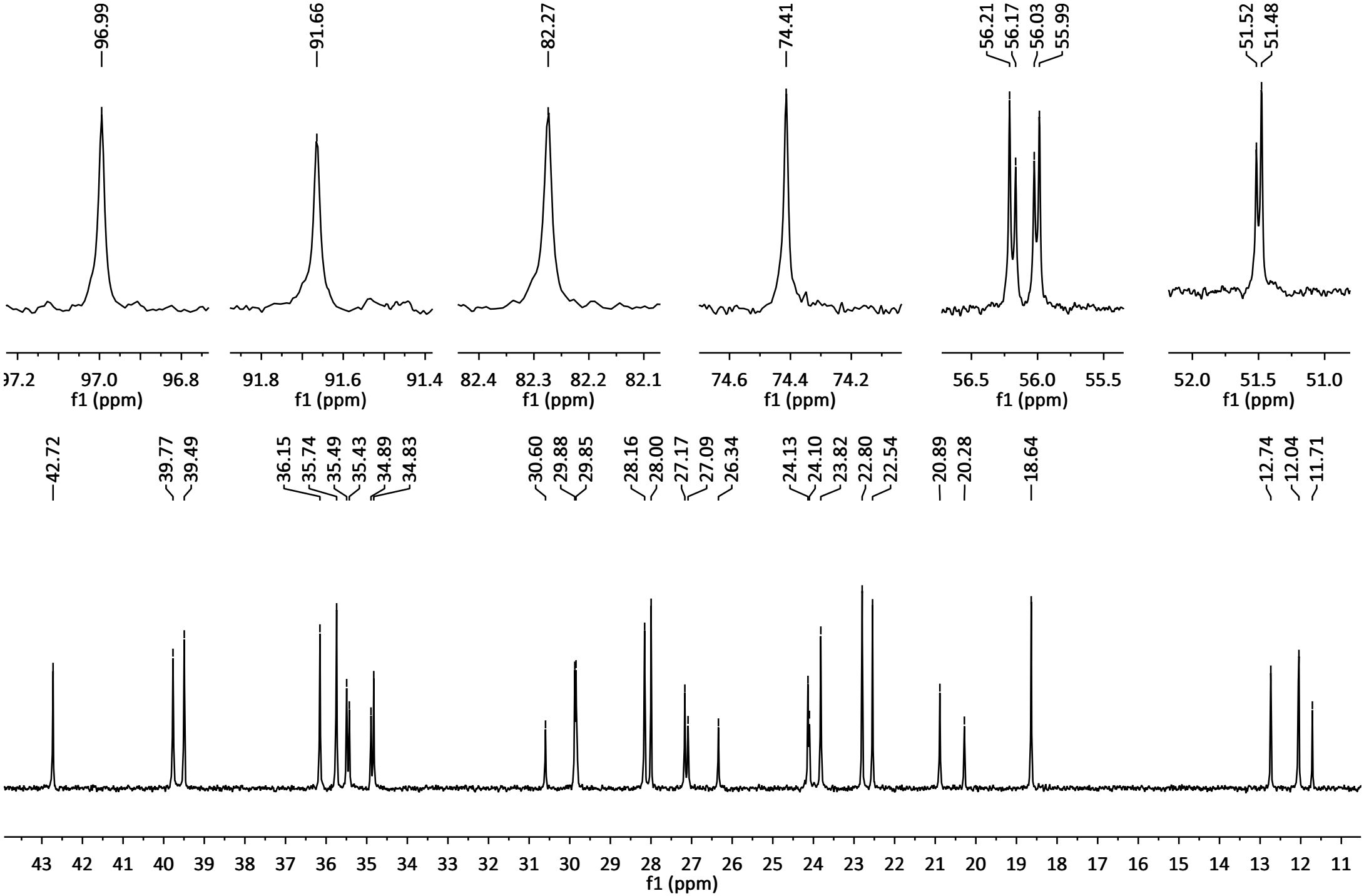

Figure S24. Sections for ^{13}C {^{1}H} NMR spectrum of compound **16a** (100 MHz, $CDCl_3$)

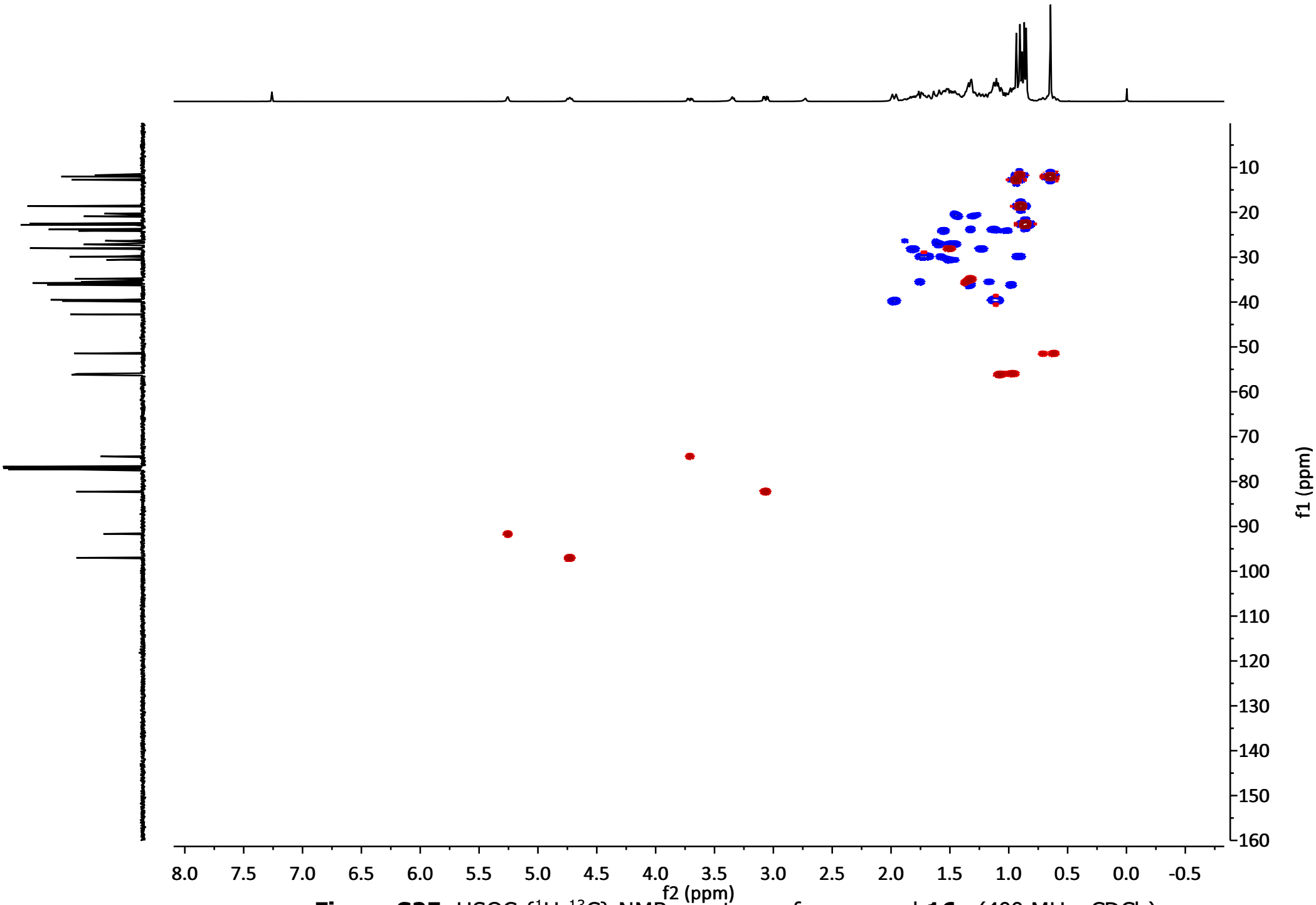

Figure S25. HSQC {^{1}H-^{13}C} NMR spectrum of compound **16a** (400 MHz, $CDCl_3$)

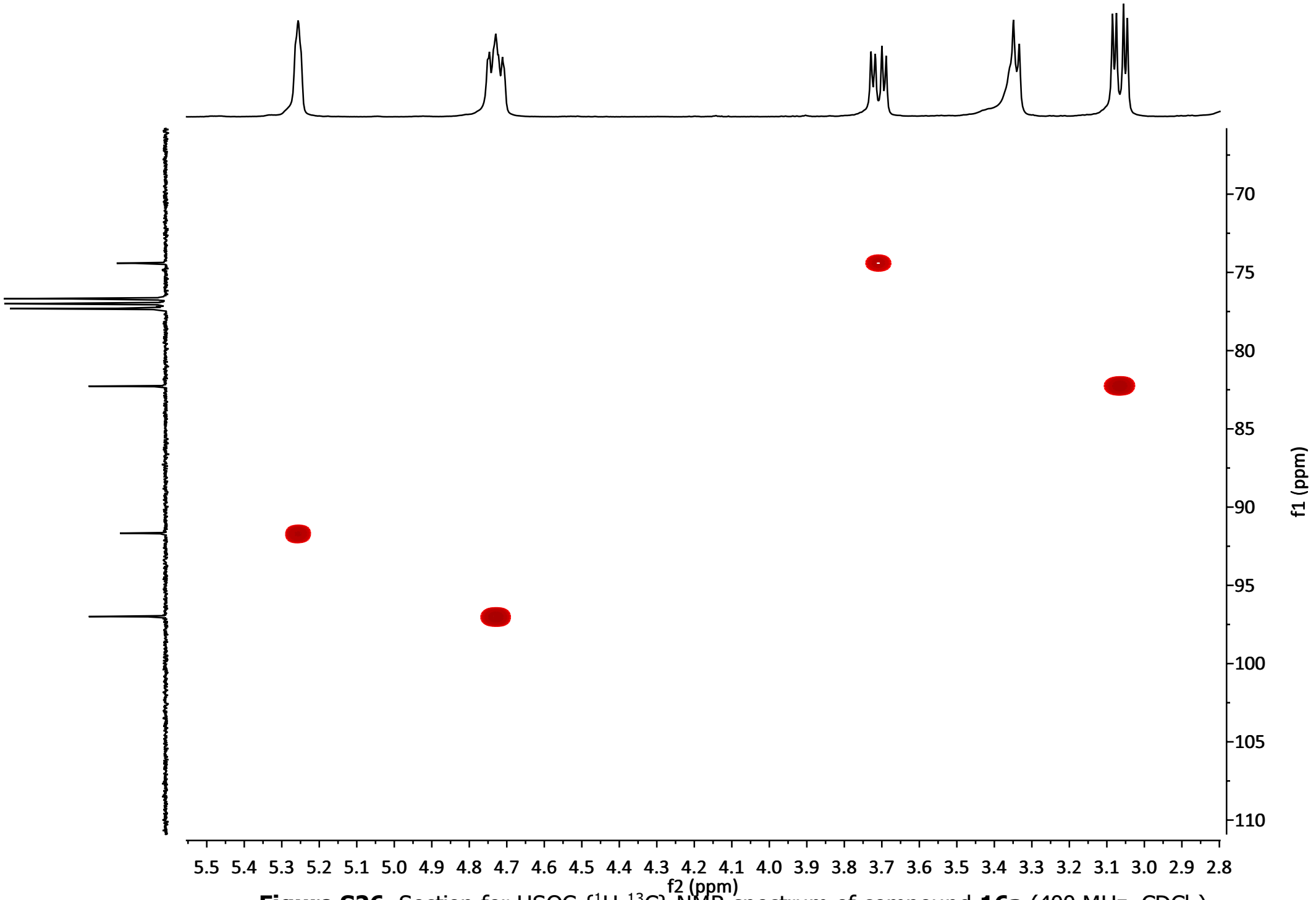

Figure S26. Section for HSQC {^{1}H-^{13}C} NMR spectrum of compound **16a** (400 MHz, $CDCl_3$)

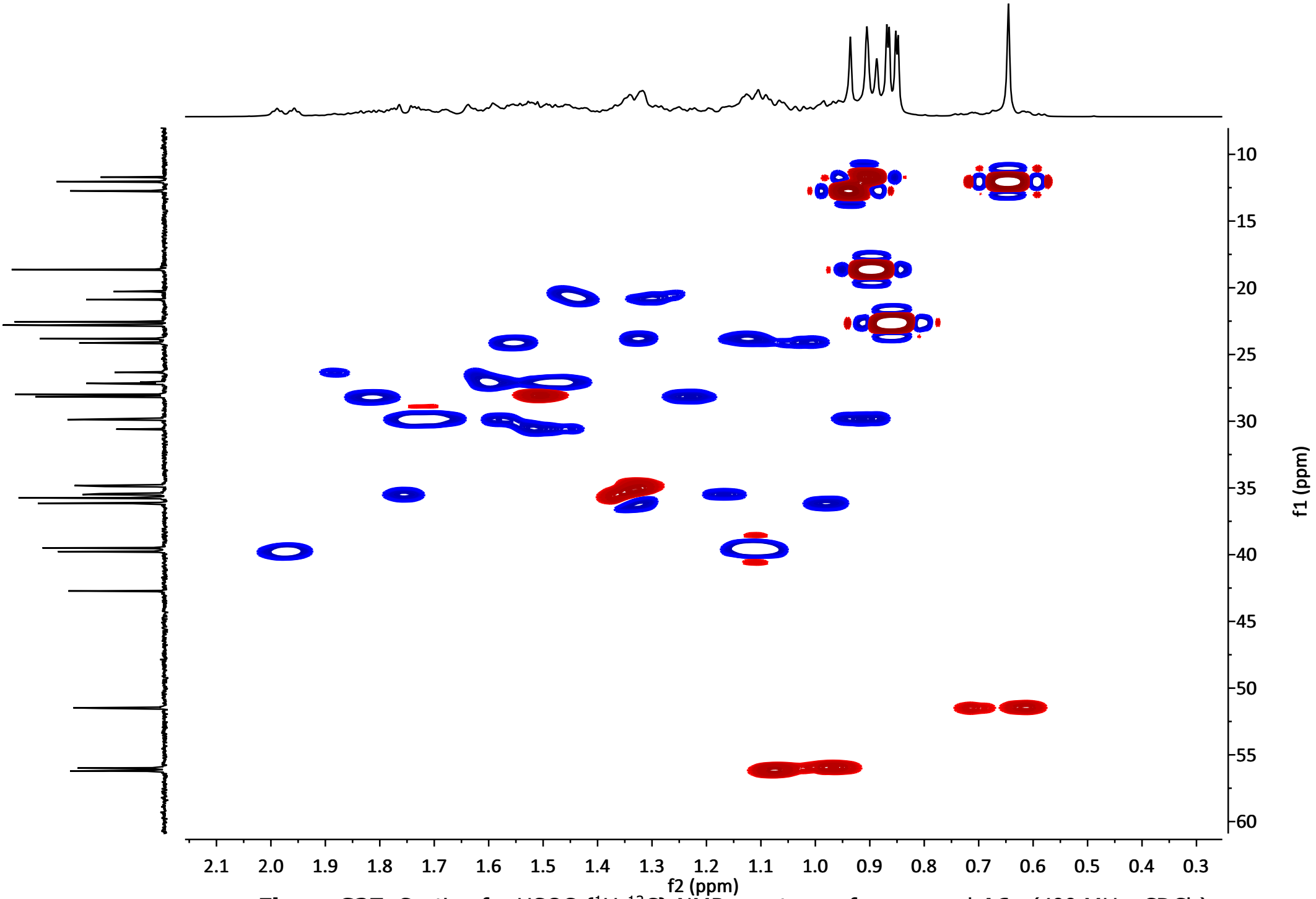

Figure S27. Section for HSQC {^{1}H-^{13}C} NMR spectrum of compound **16a** (400 MHz, $CDCl_3$)

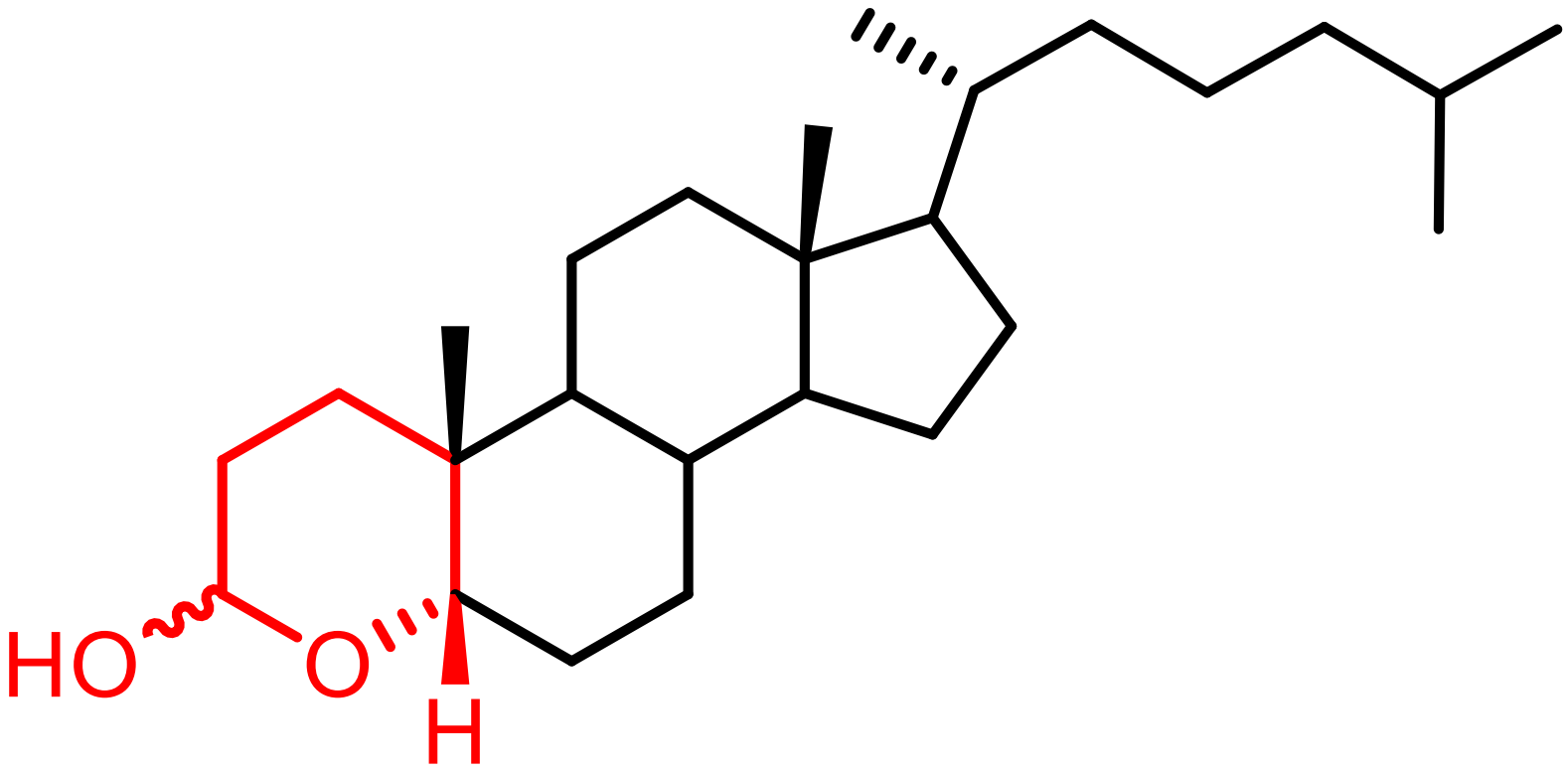

Figure S28. 4-Oxa-cholest-5-en-3-ol **(16b)**

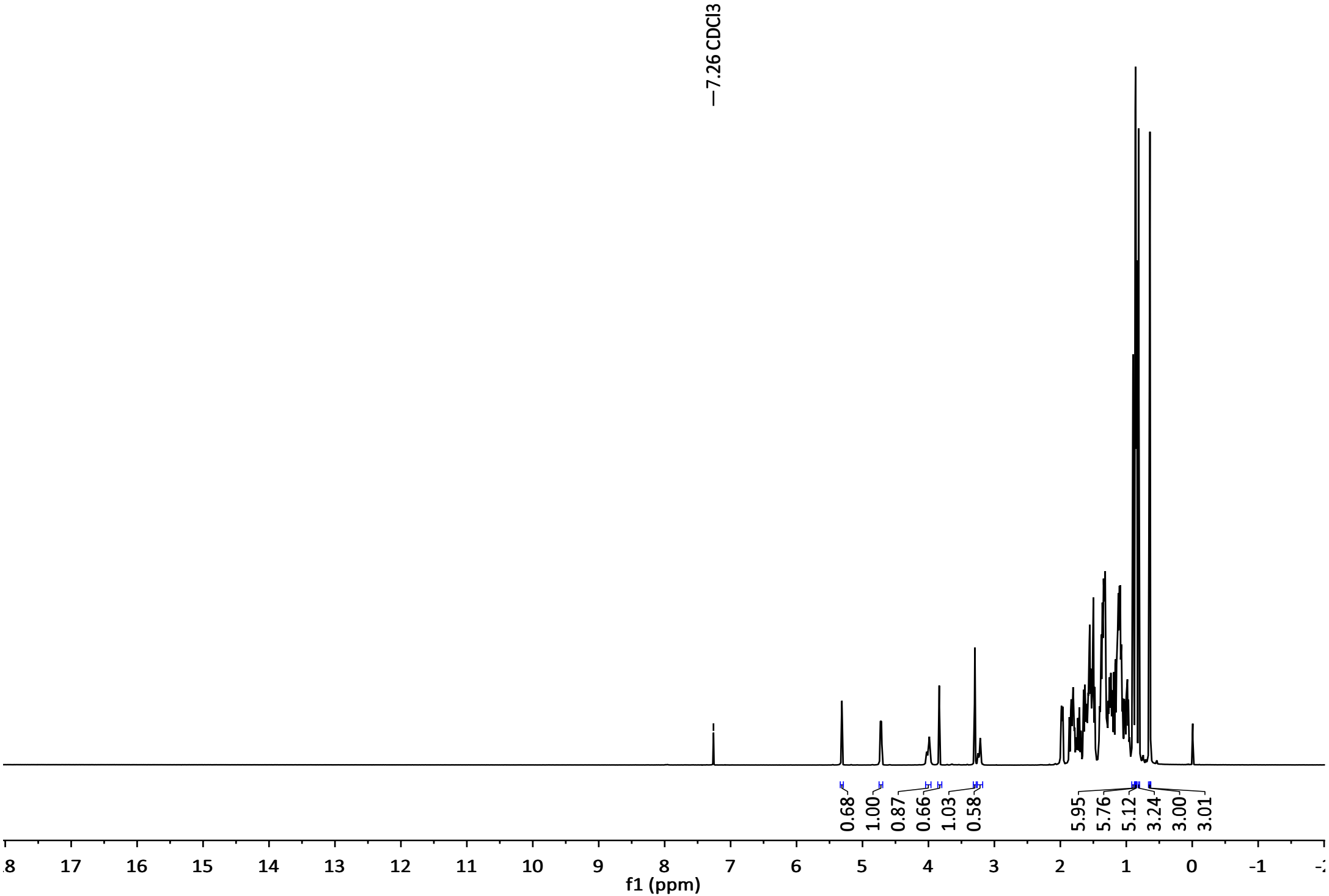

Figure S29. ^{1}H NMR spectrum of compound **16b** (400 MHz, $CDCl_3$)

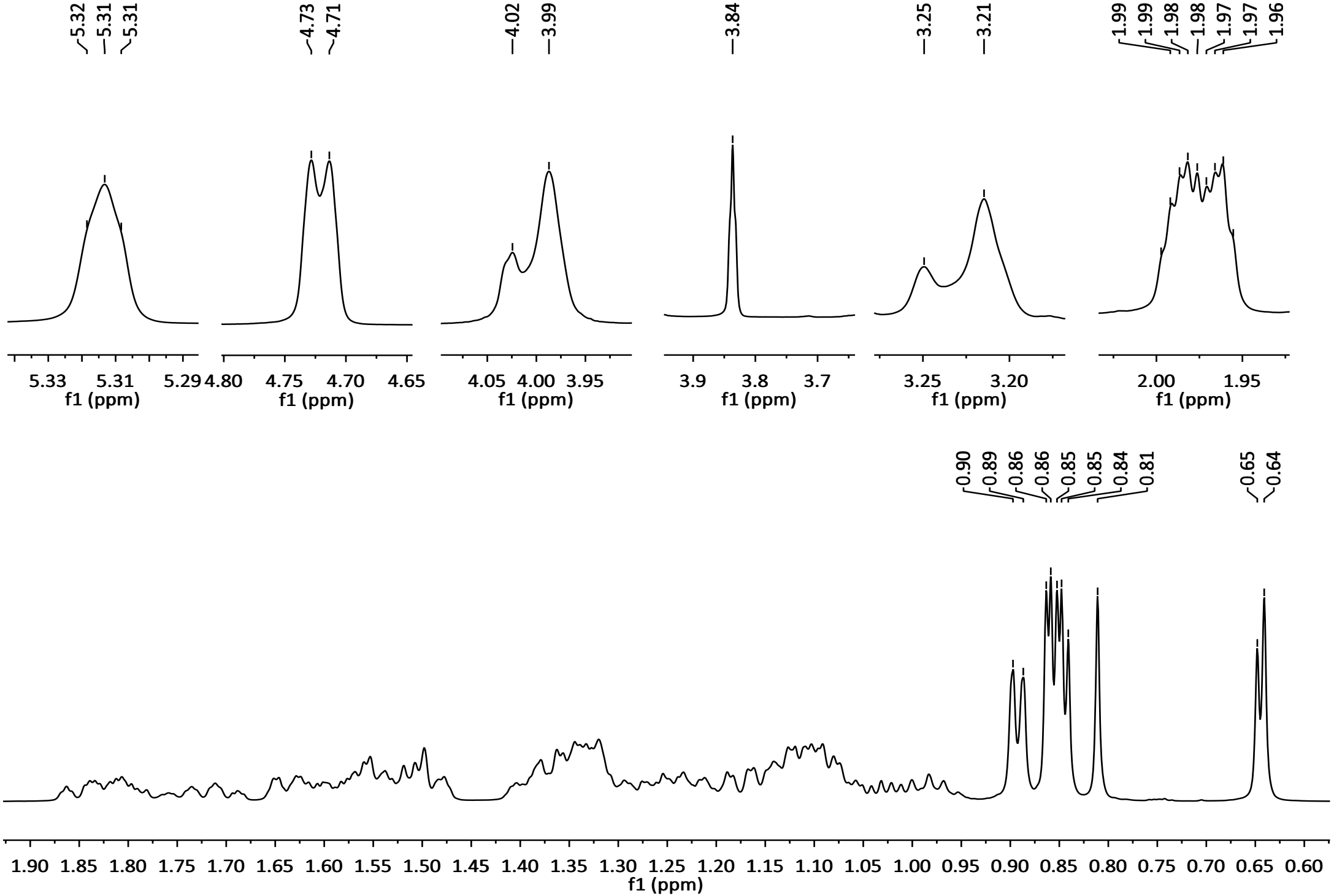

Figure S30. ^{1}H NMR spectrum of compound **16b** (400 MHz, $CDCl_3$)

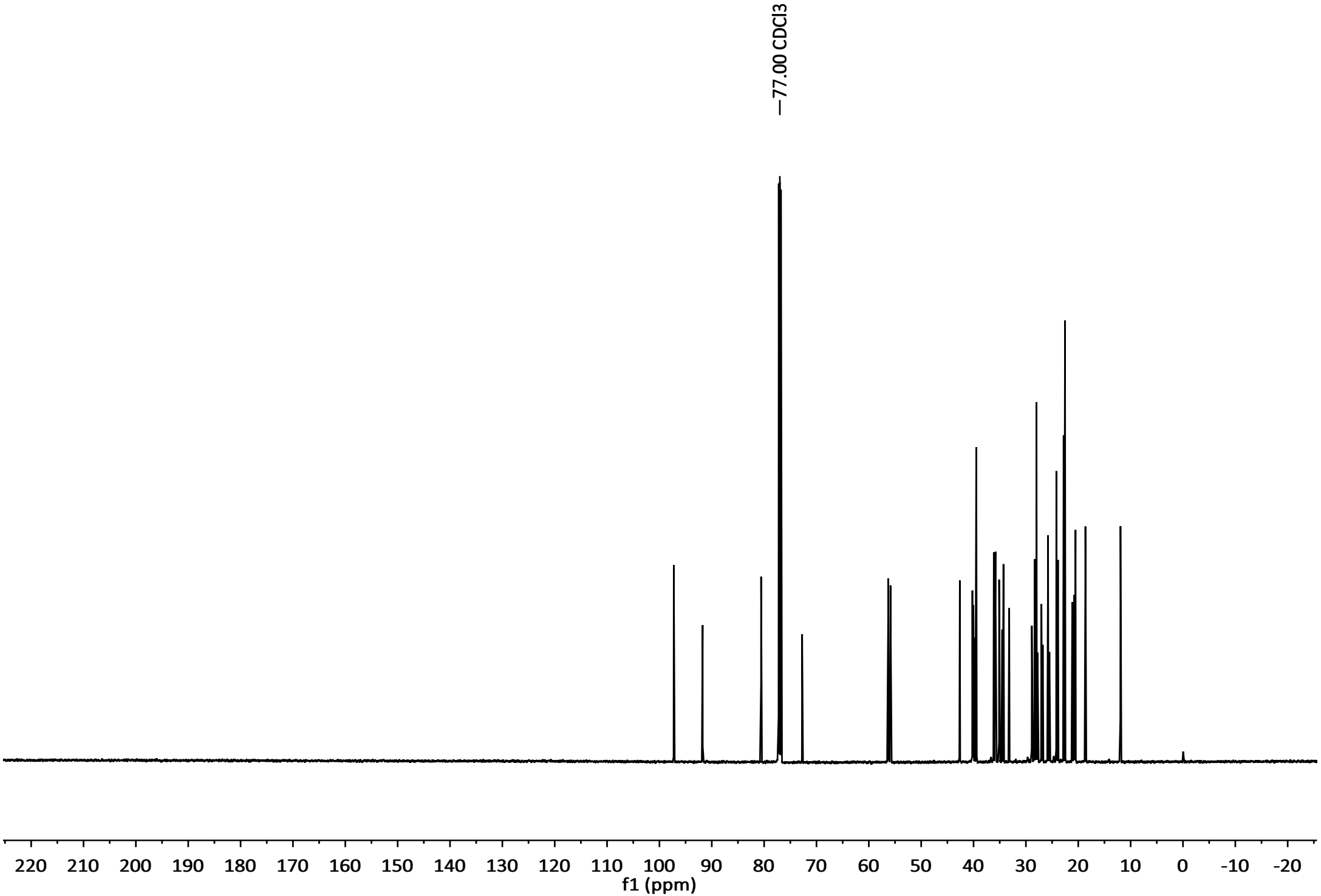

Figure S31. ^{13}C NMR spectrum of compound **16b** (100 MHz, $CDCl_3$)

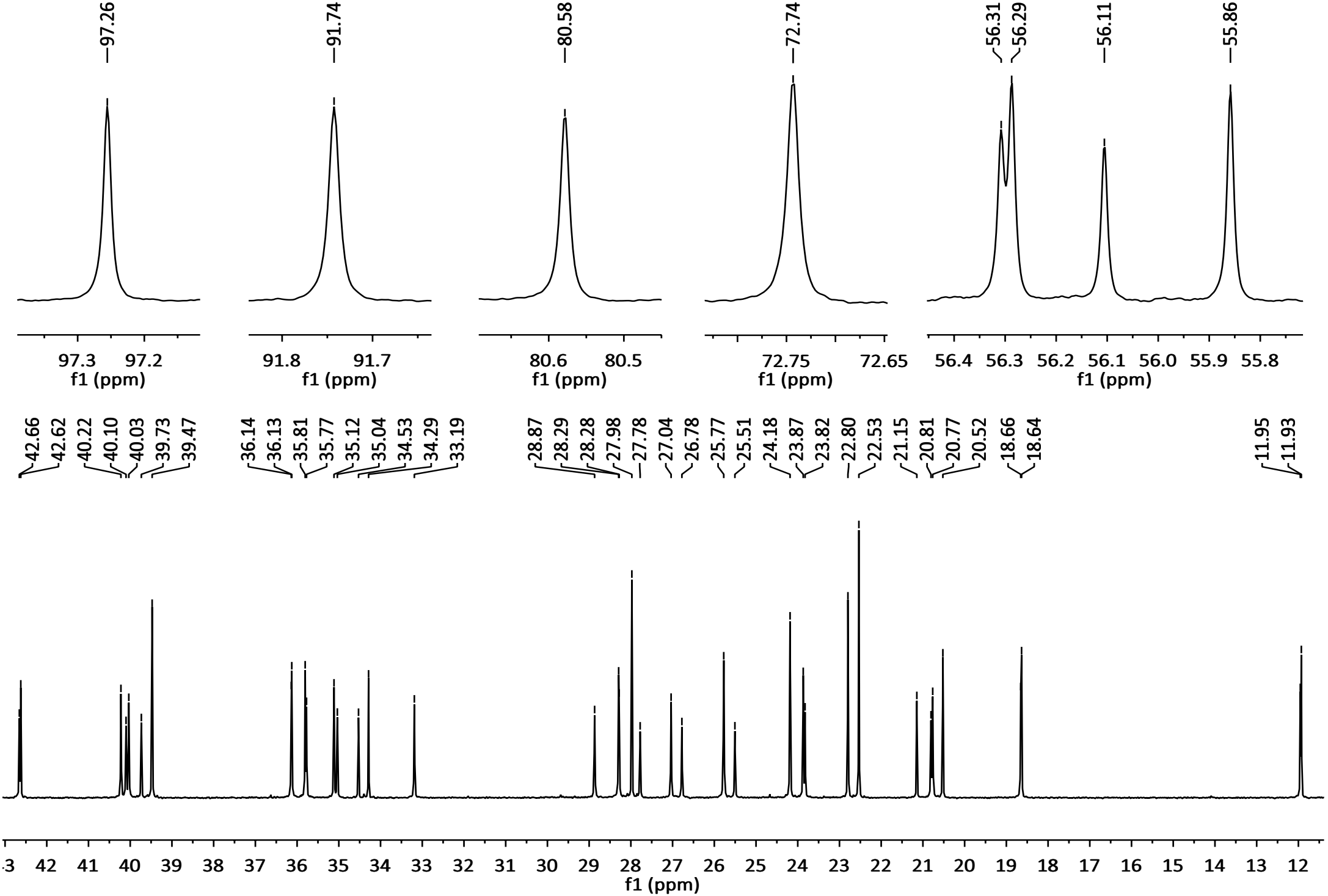

Figure S32. Sections for ^{13}C NMR spectrum of compound **16b** (100 MHz, $CDCl_3$)

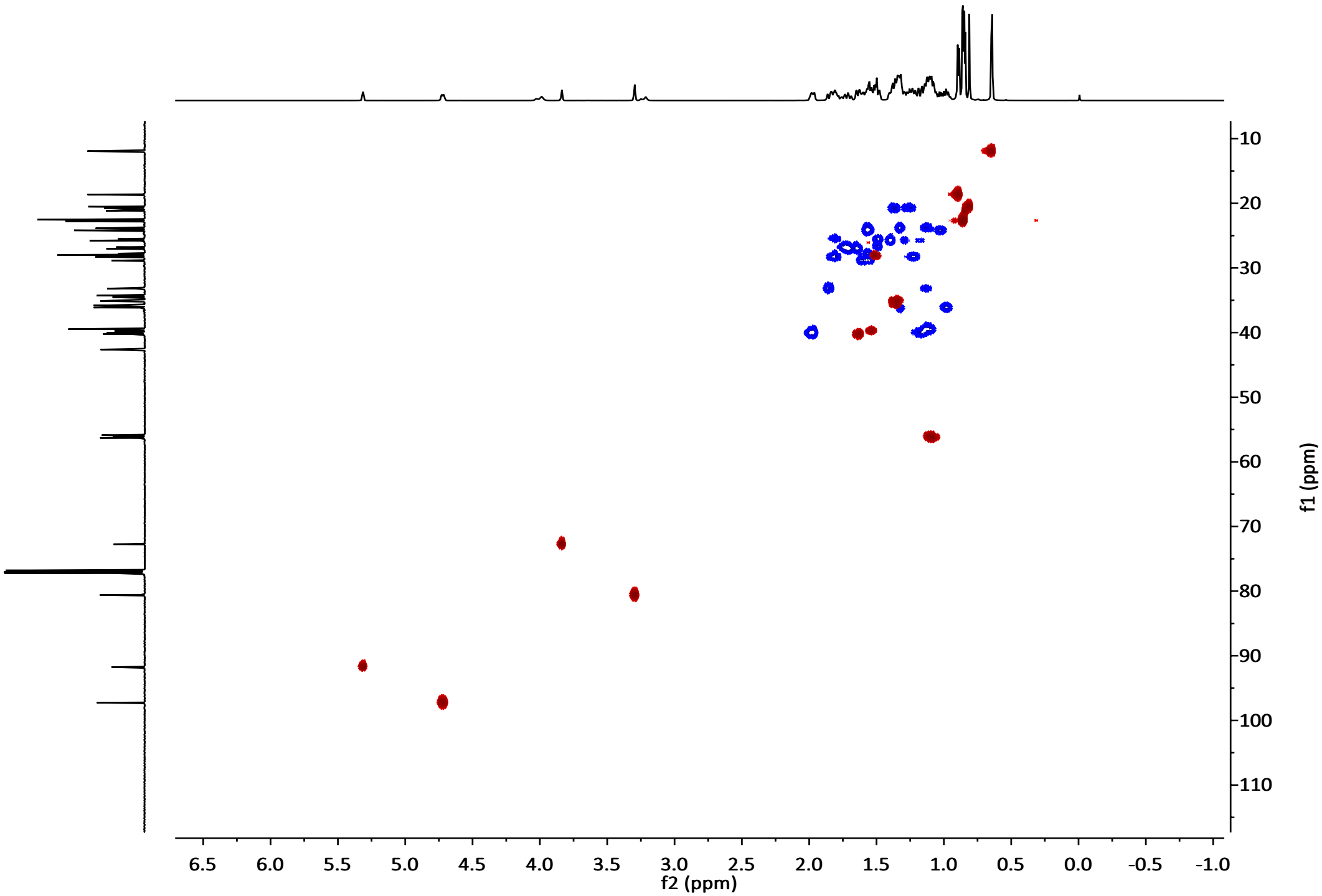

Figure S33. HSQC {^{1}H-^{13}C} NMR spectrum of compound **16b** (400 MHz, $CDCl_3$)

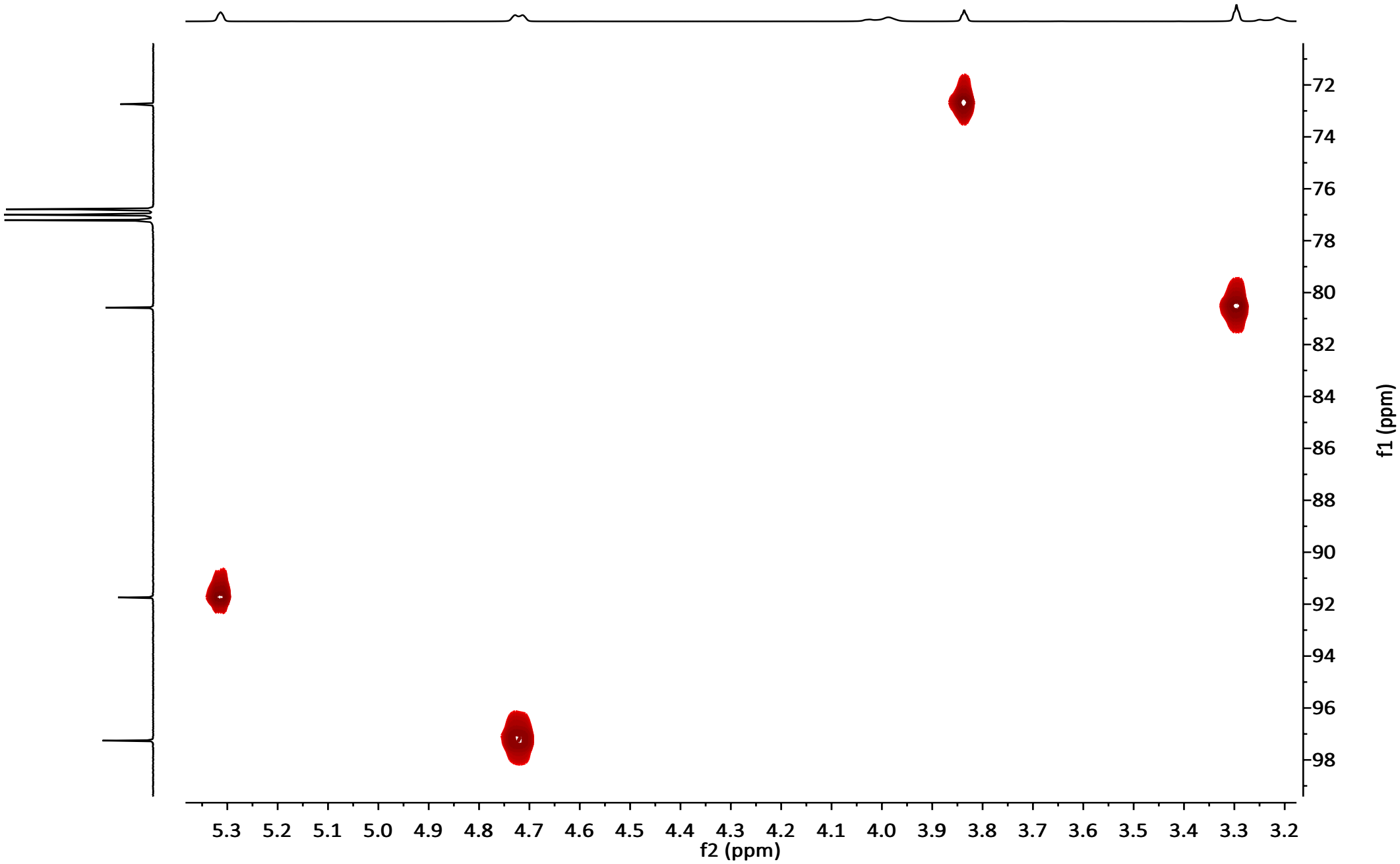

Figure S34. Section for HSQC {^{1}H-^{13}C} NMR spectrum of compound **16b** (400 MHz, $CDCl_3$)

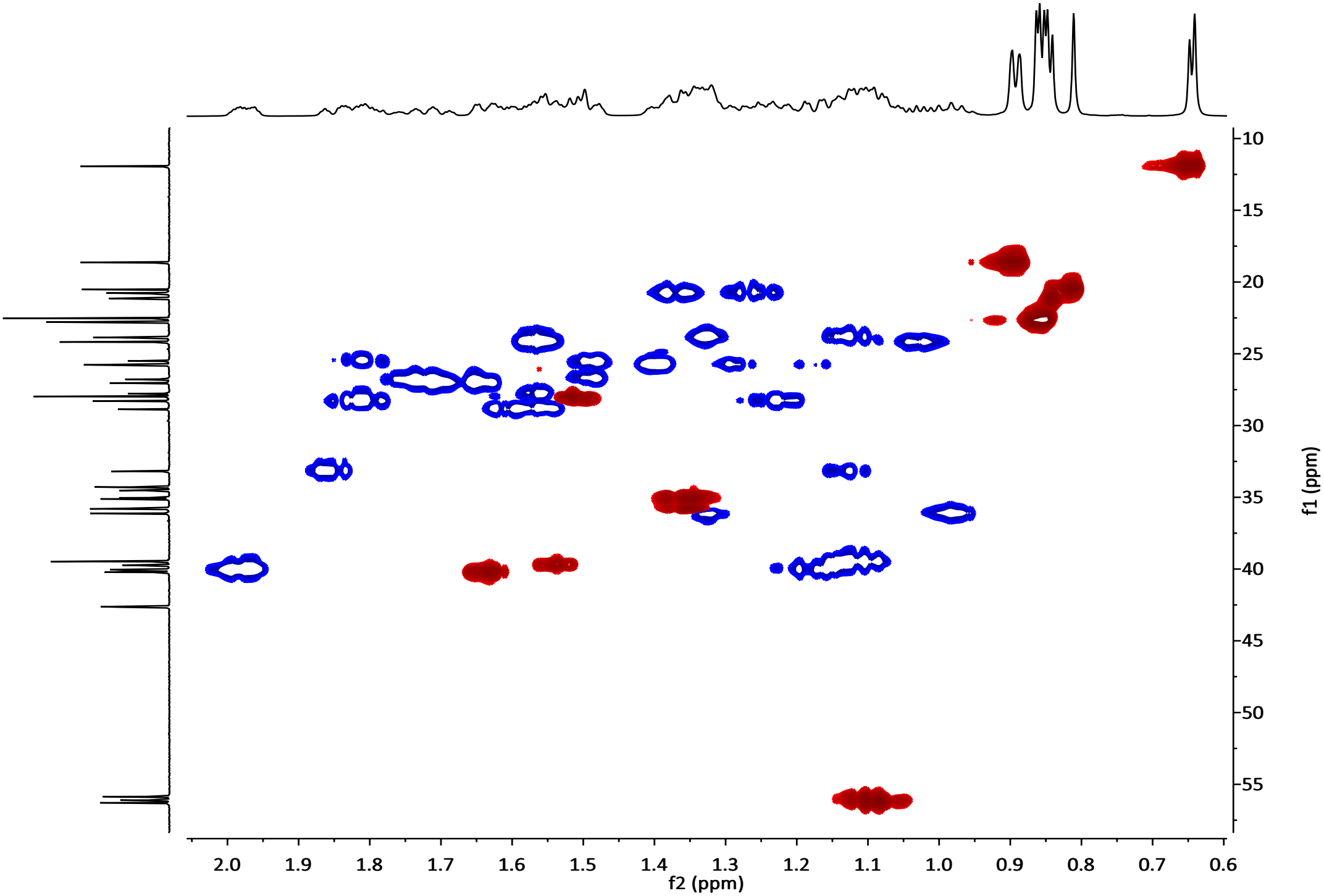

Figure S35. Section for HSQC {^{1}H-^{13}C} NMR spectrum of compound **16b** (400 MHz, $CDCl_3$)

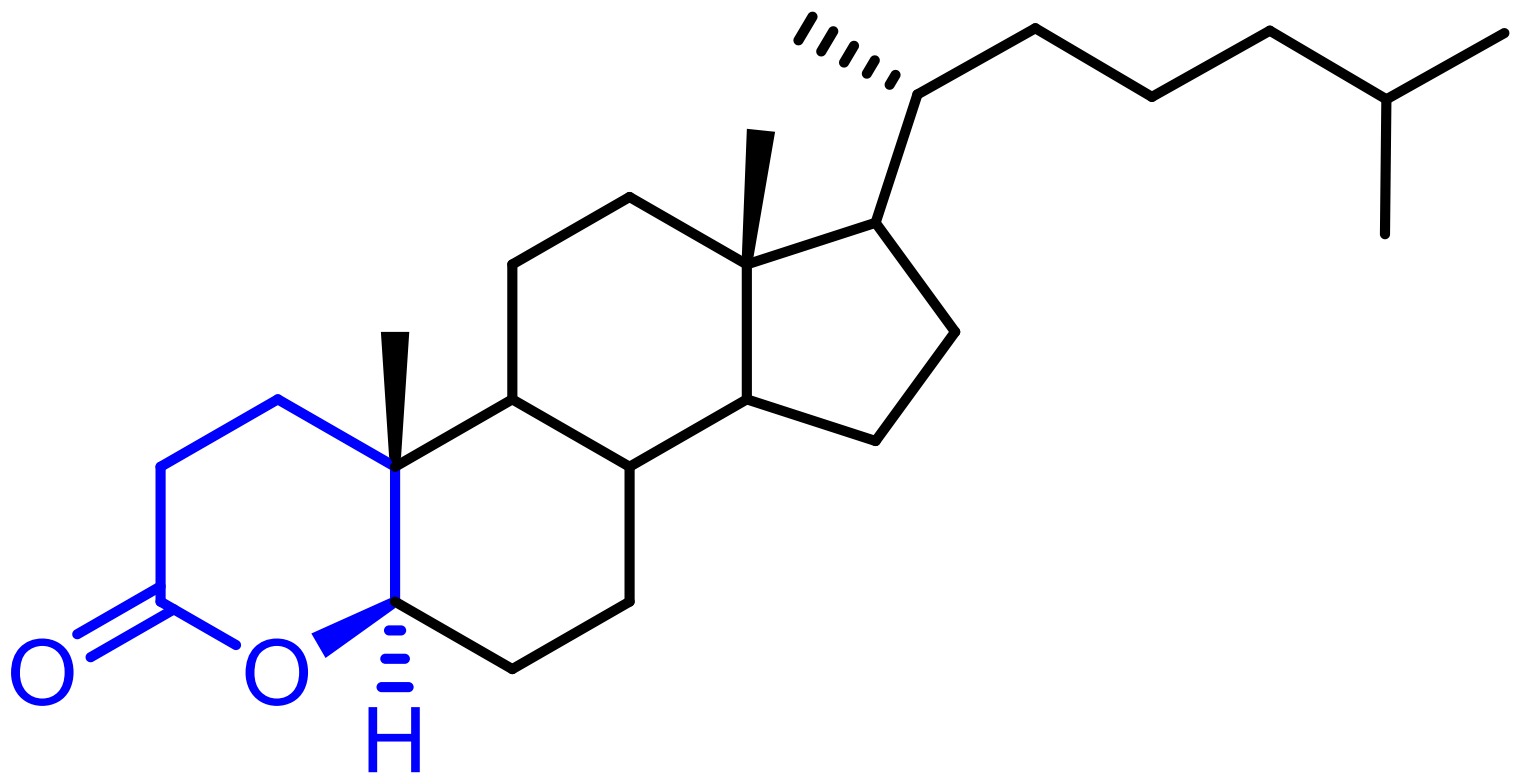

Figure S36. 4-Oxa-cholest-5-en-3-one **(7a)**

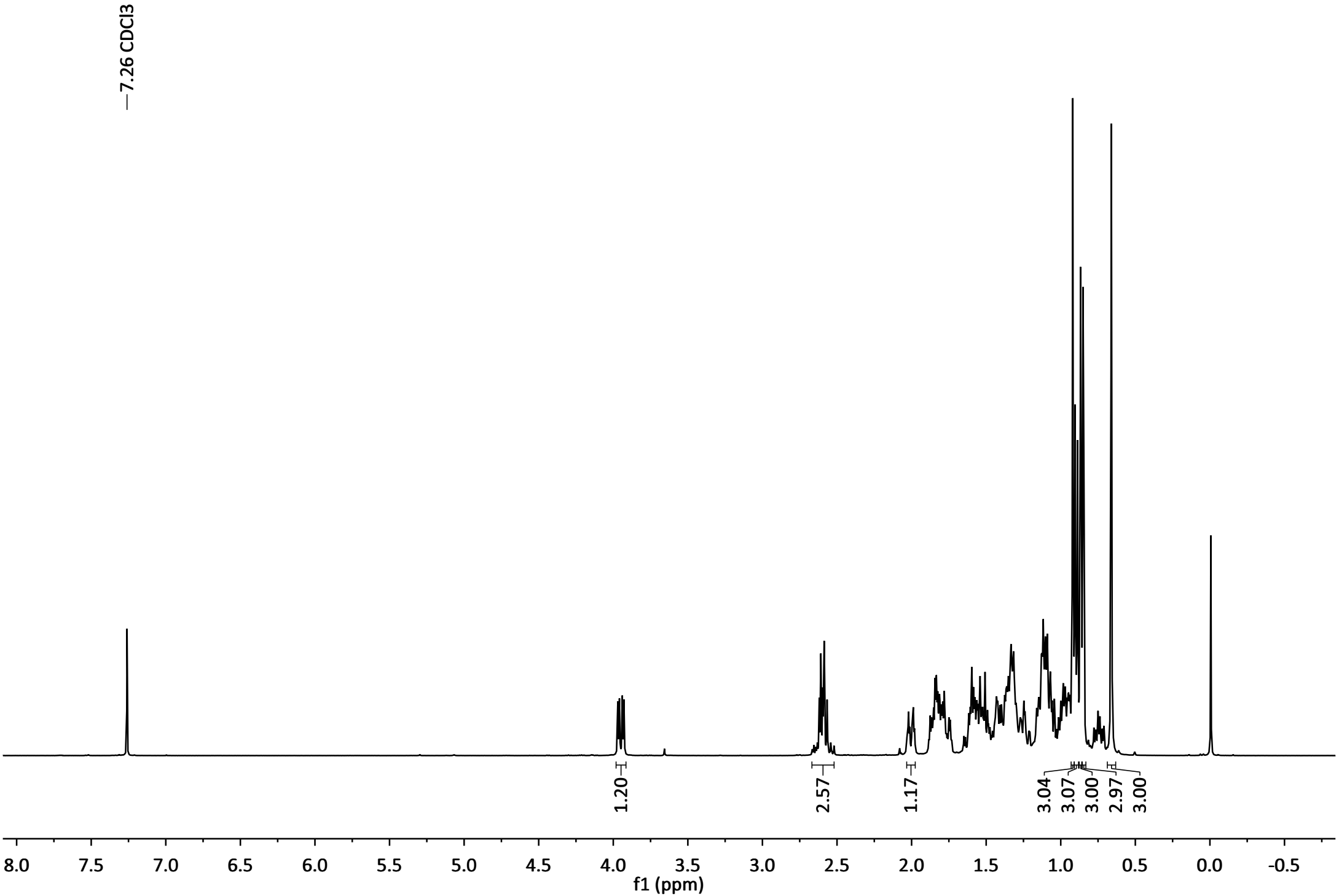

Figure S37. ^{1}H NMR spectrum of compound **7a** (400 MHz, $CDCl_3$)

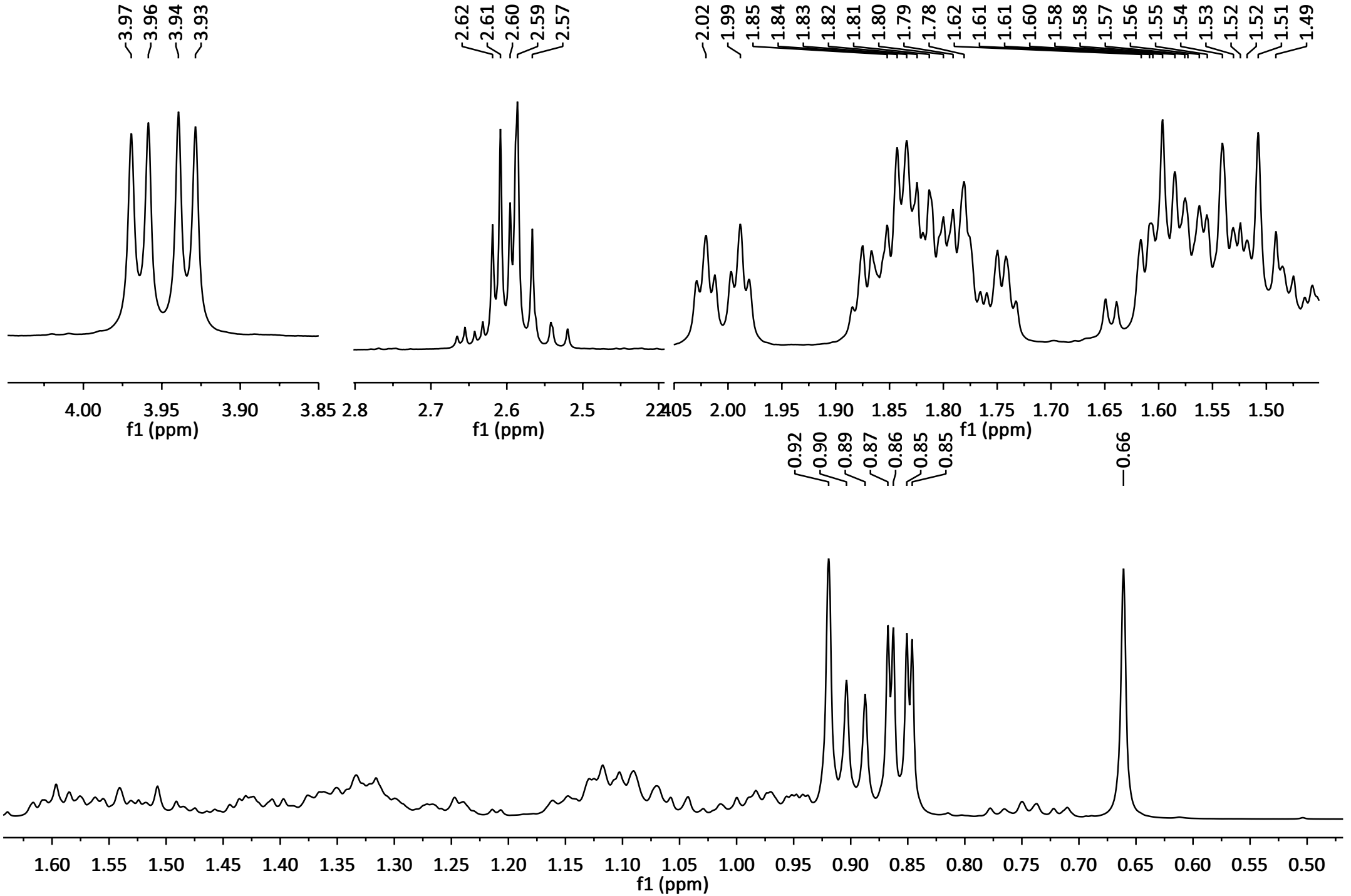

Figure S38. Sectons for ^{1}H NMR spectrum of compound **7a** (400 MHz, $CDCl_3$)

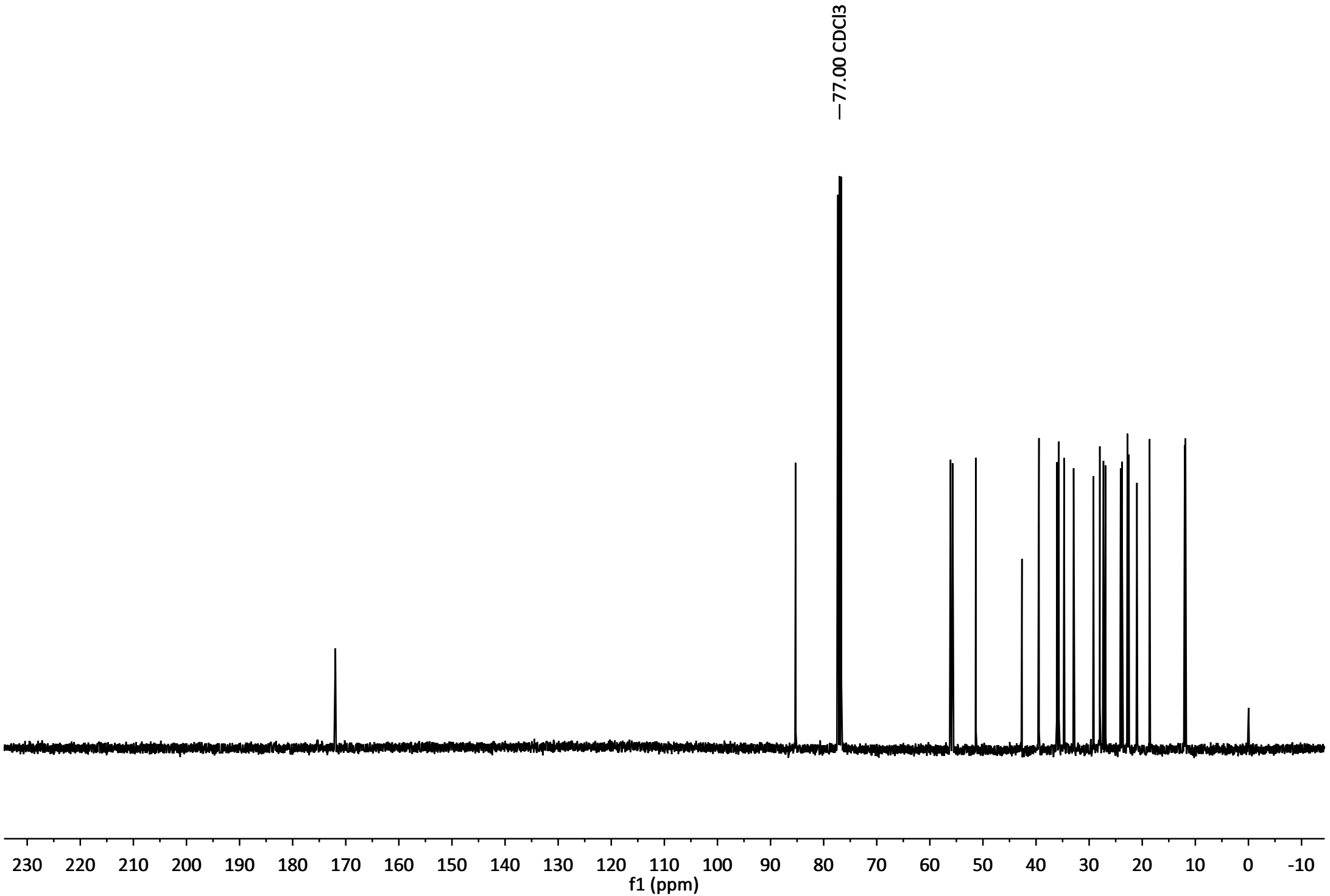

Figure S39. ^{13}C {^{1}H} NMR spectrum of compound **7a** (100 MHz, $CDCl_3$)

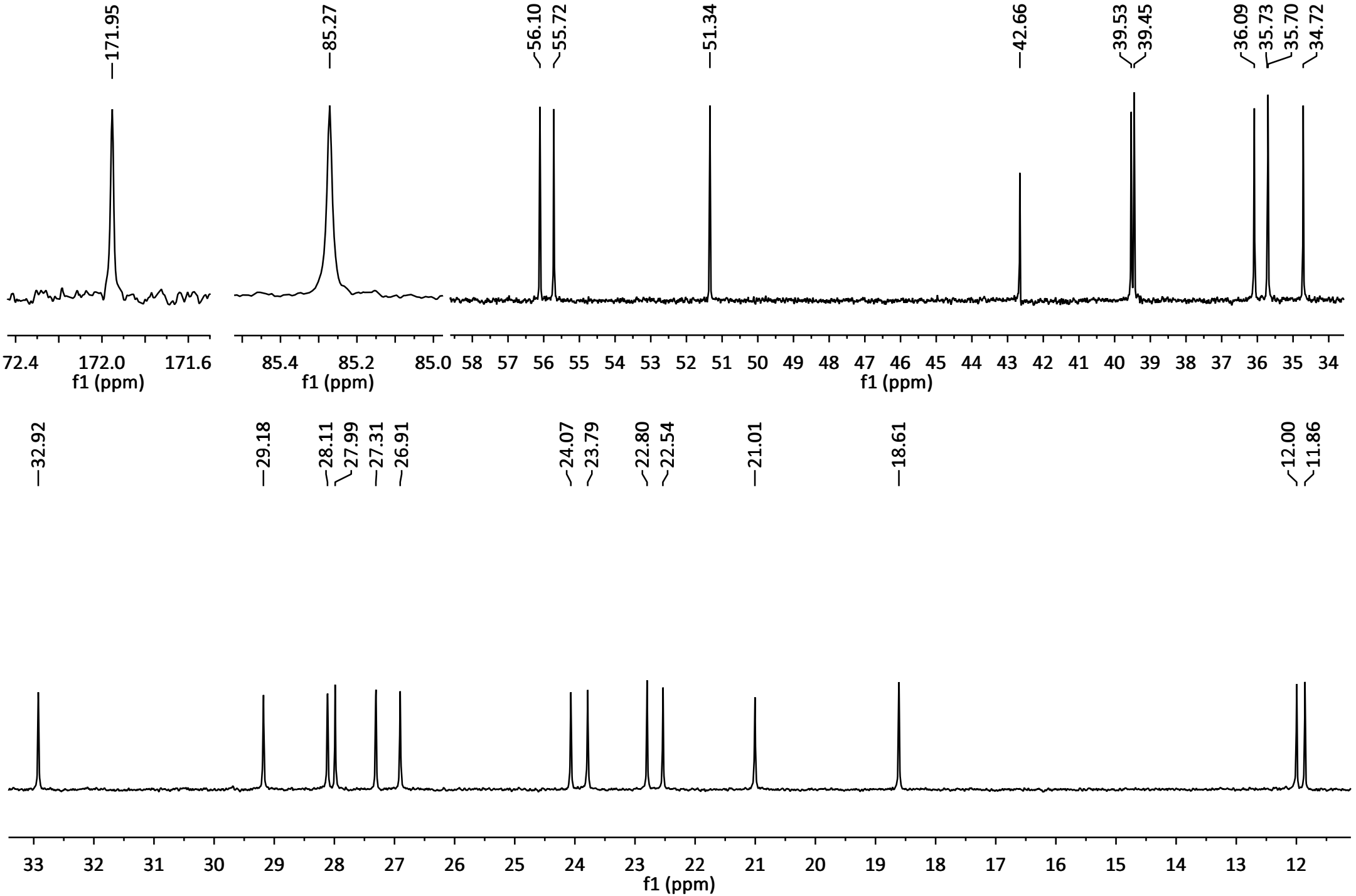

Figure S40. Sections for $^{13}C\{^{1}H\}$ NMR spectrum of compound **7a** (100 MHz, $CDCl_3$)

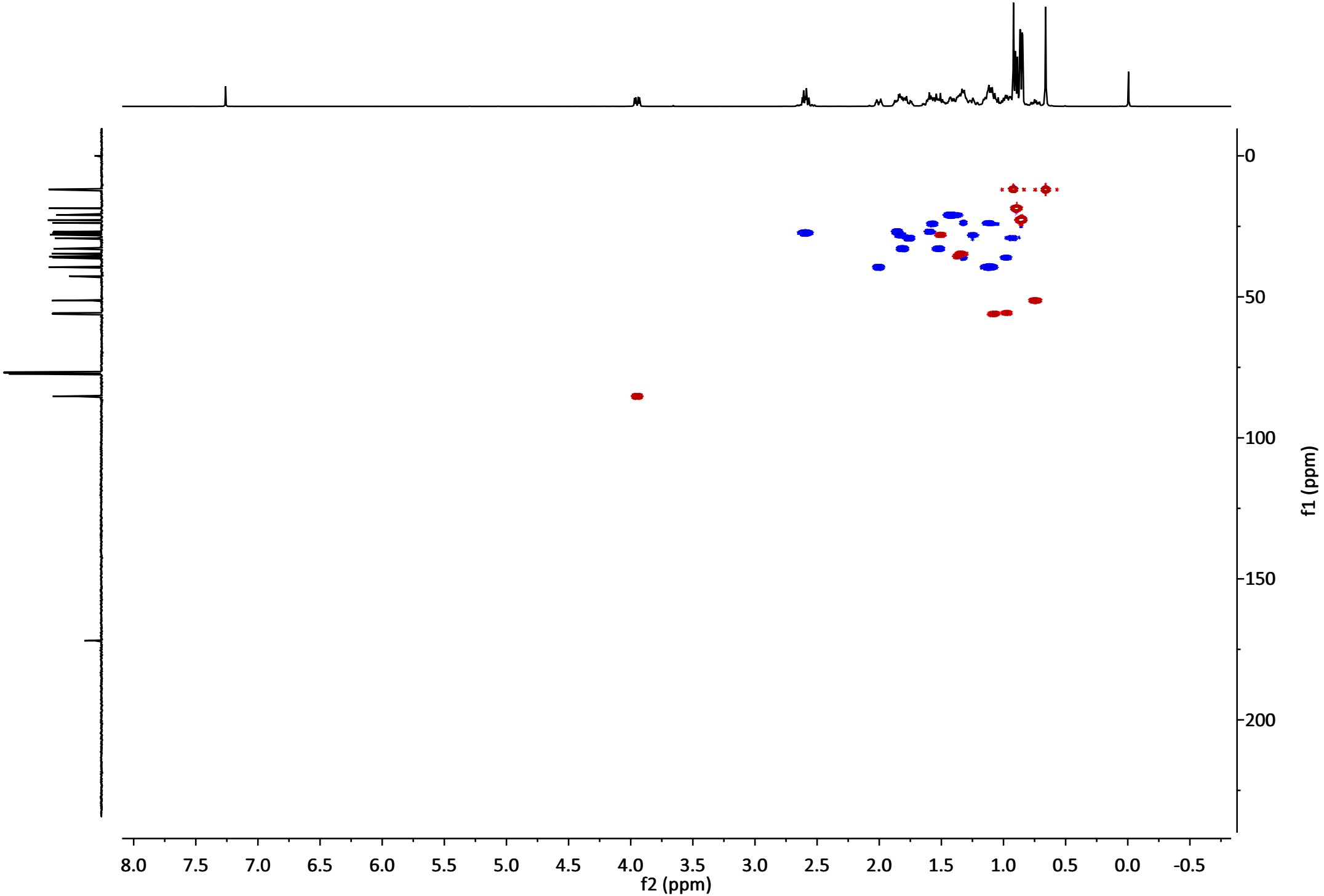

Figure S41. ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **7a** (400 MHz, $CDCl_3$)

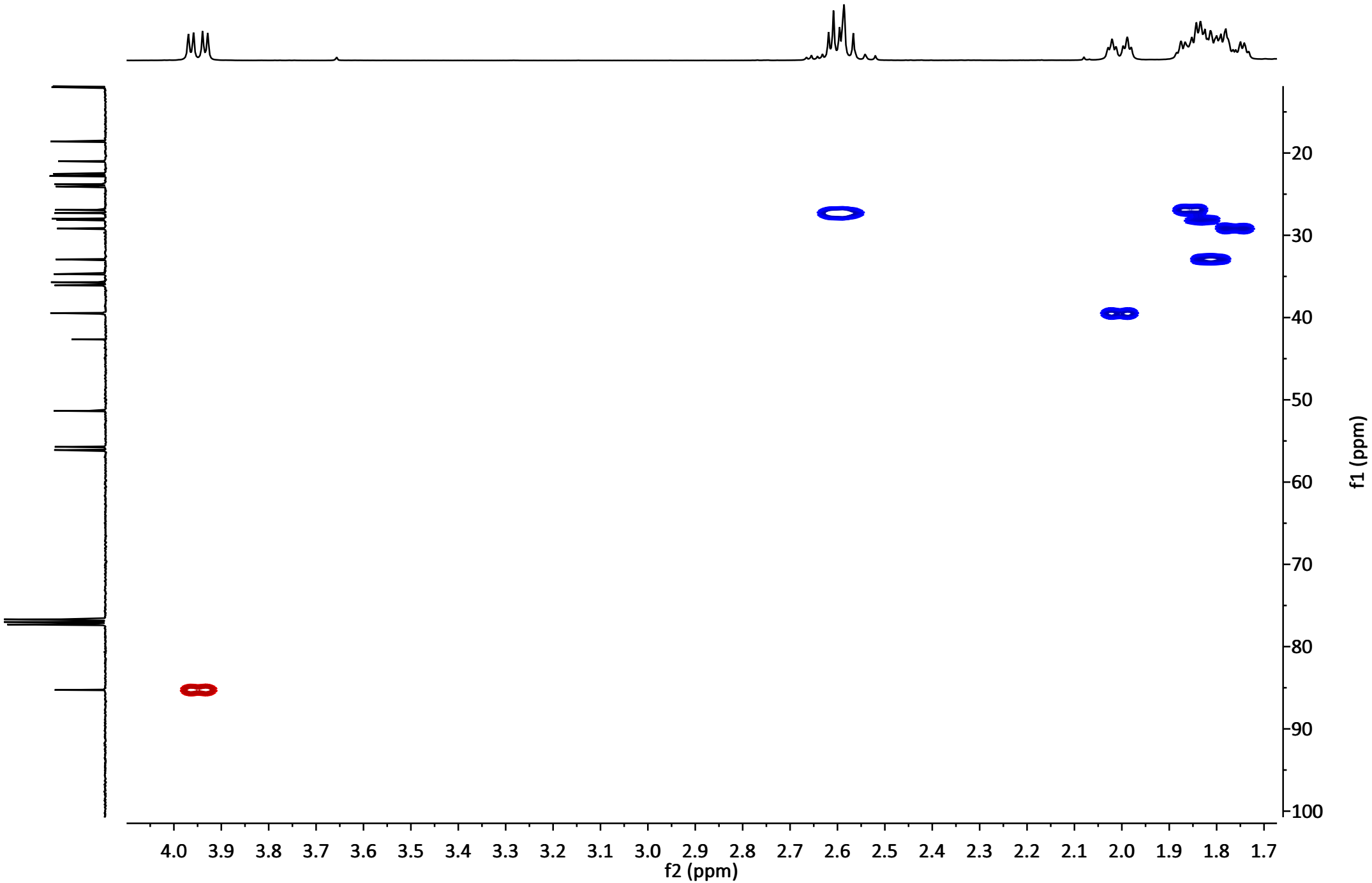

Figure S42. Section for ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **7a** (400 MHz, $CDCl_3$)

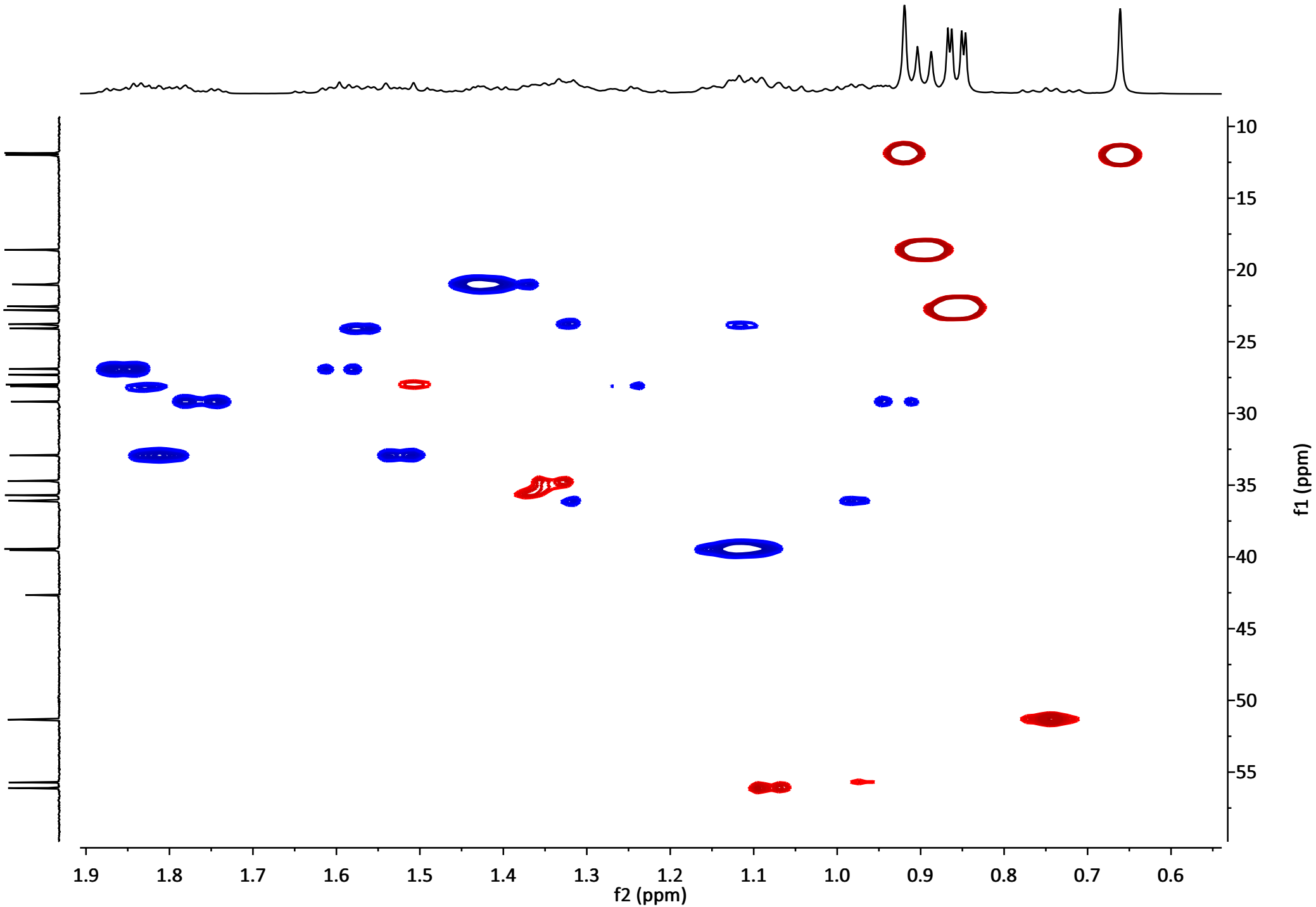

Figure S43. ^{1}H-^{13}C {^{1}H} HSQC NMR spectrum of compound **7a** (400 MHz, $CDCl_3$)

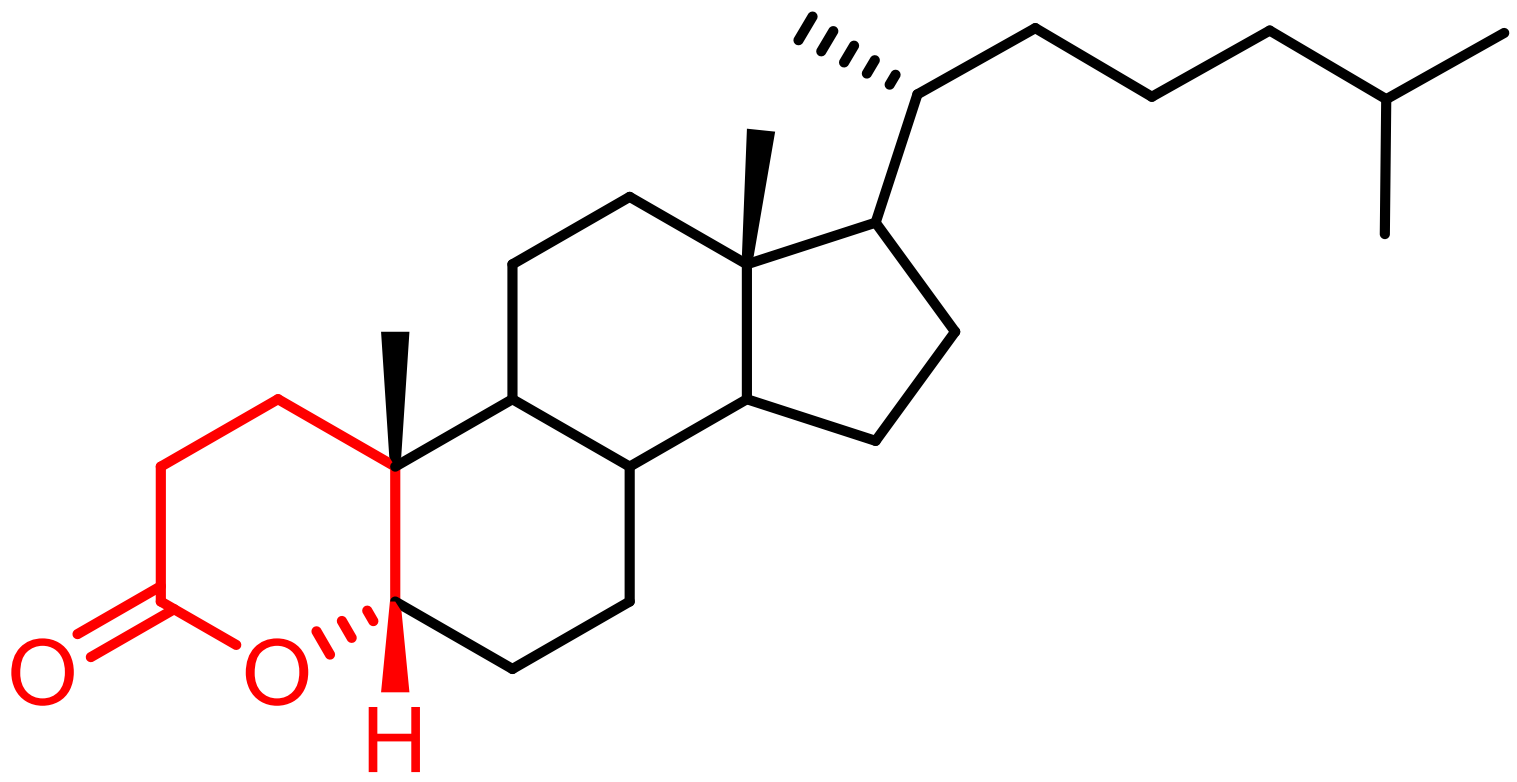

Figure S44. 4-Oxa-cholest-5-en-3-one **(7b)**

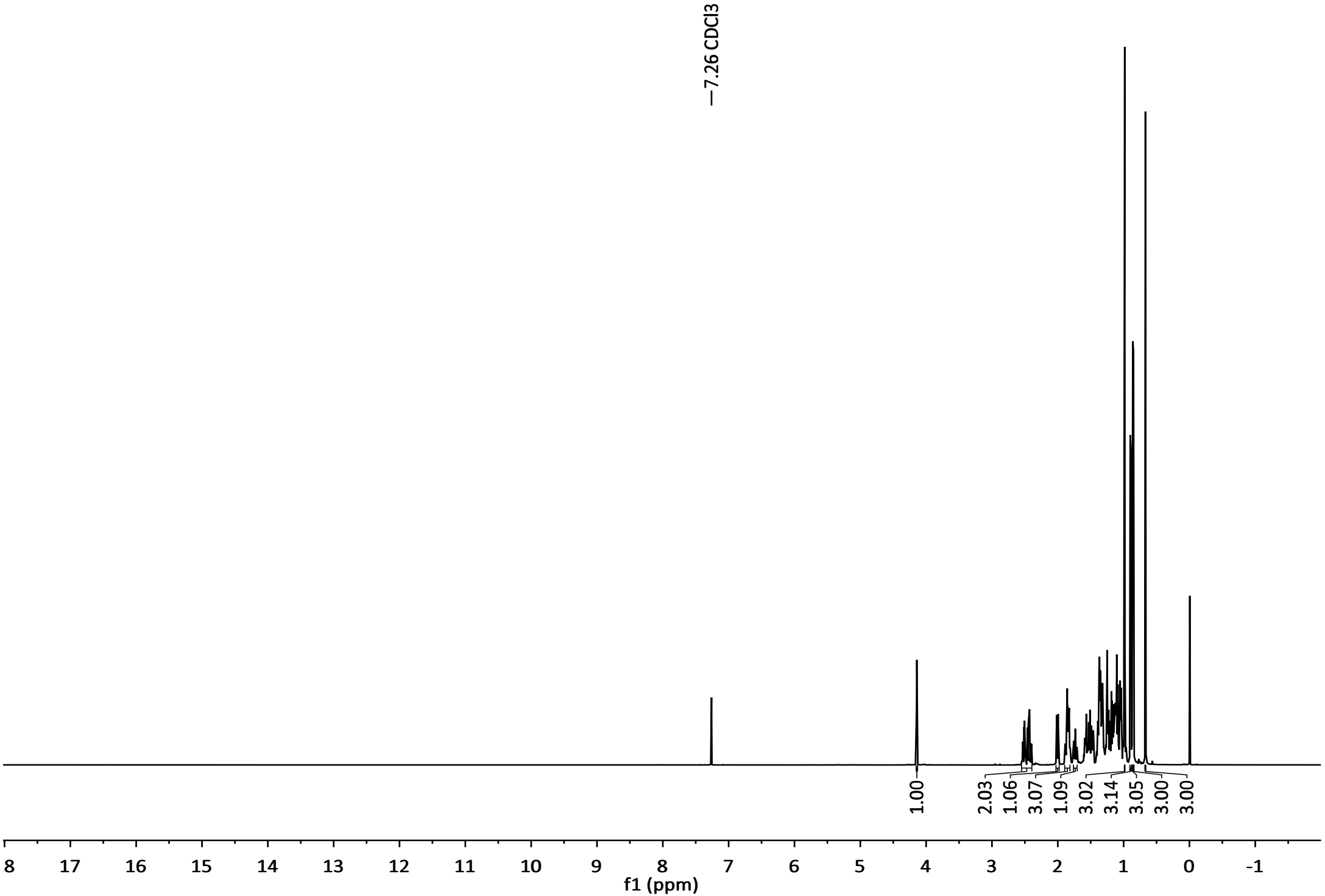

Figure S45. ^{1}H NMR spectrum of compound **7b** (400 MHz, $CDCl_3$)

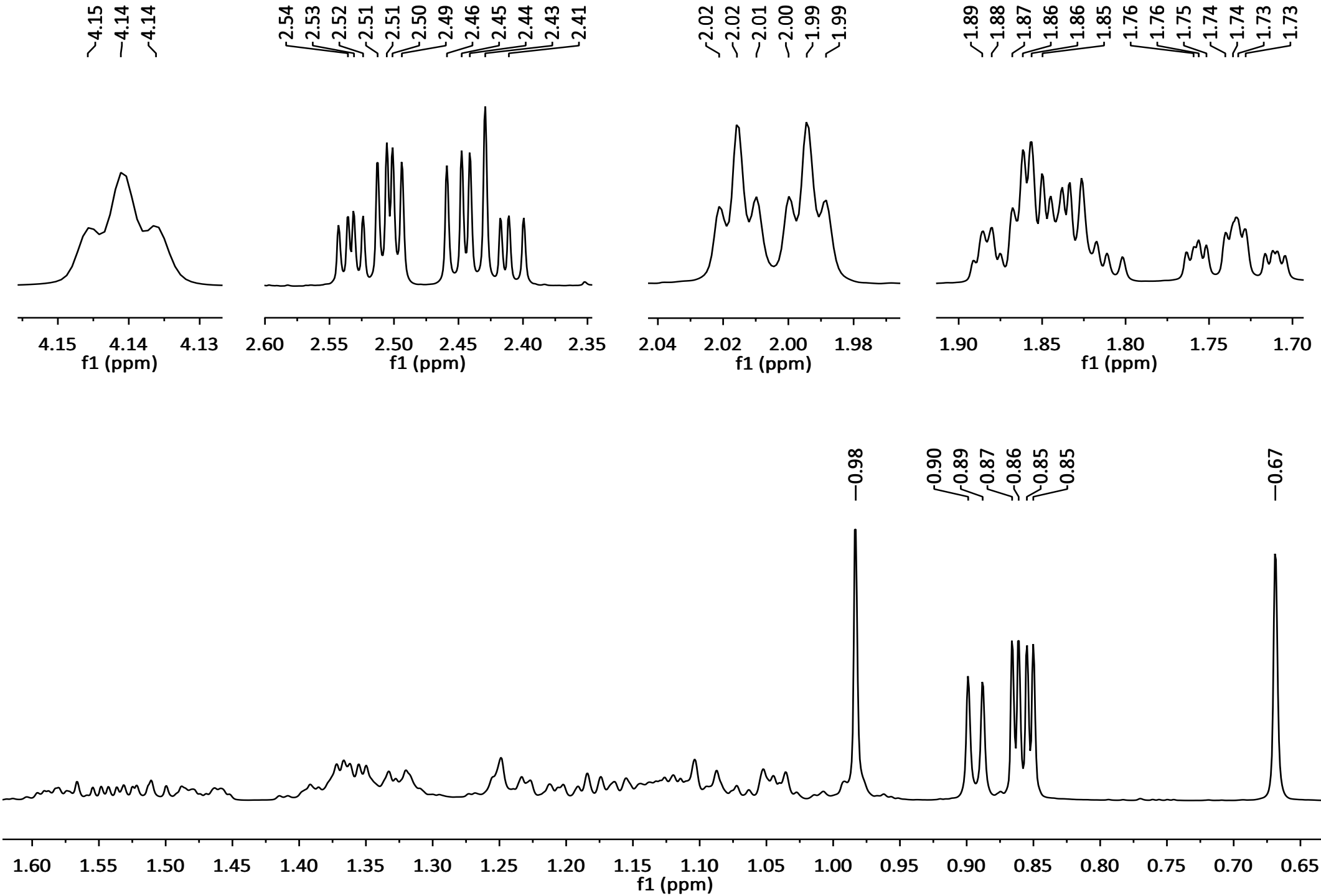

Figure S46. Sections for ^{1}H NMR spectrum of compound **7b** (400 MHz, $CDCl_3$)

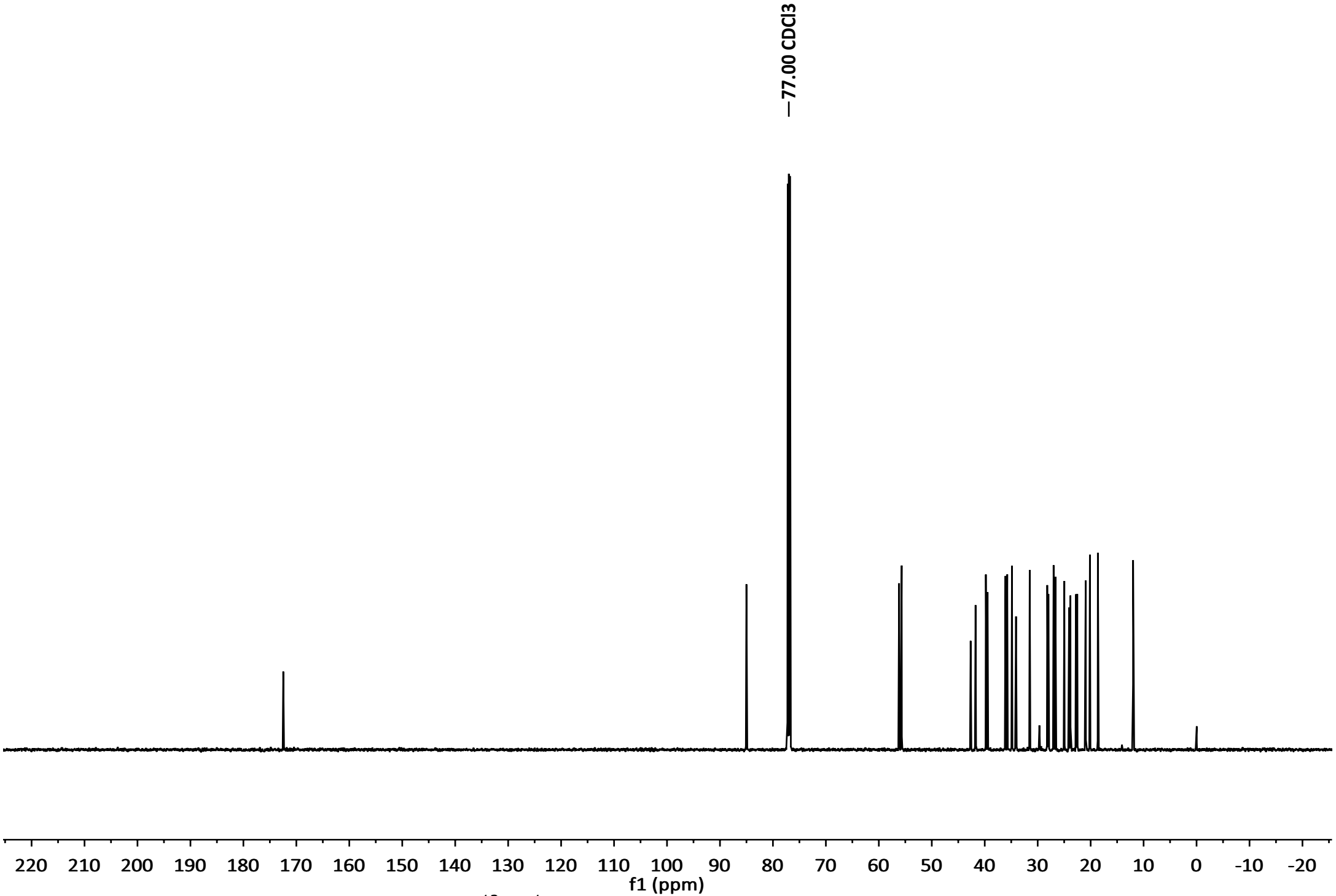

Figure S47. ^{13}C {^{1}H} NMR spectrum of compound **7b** (100 MHz, $CDCl_3$)

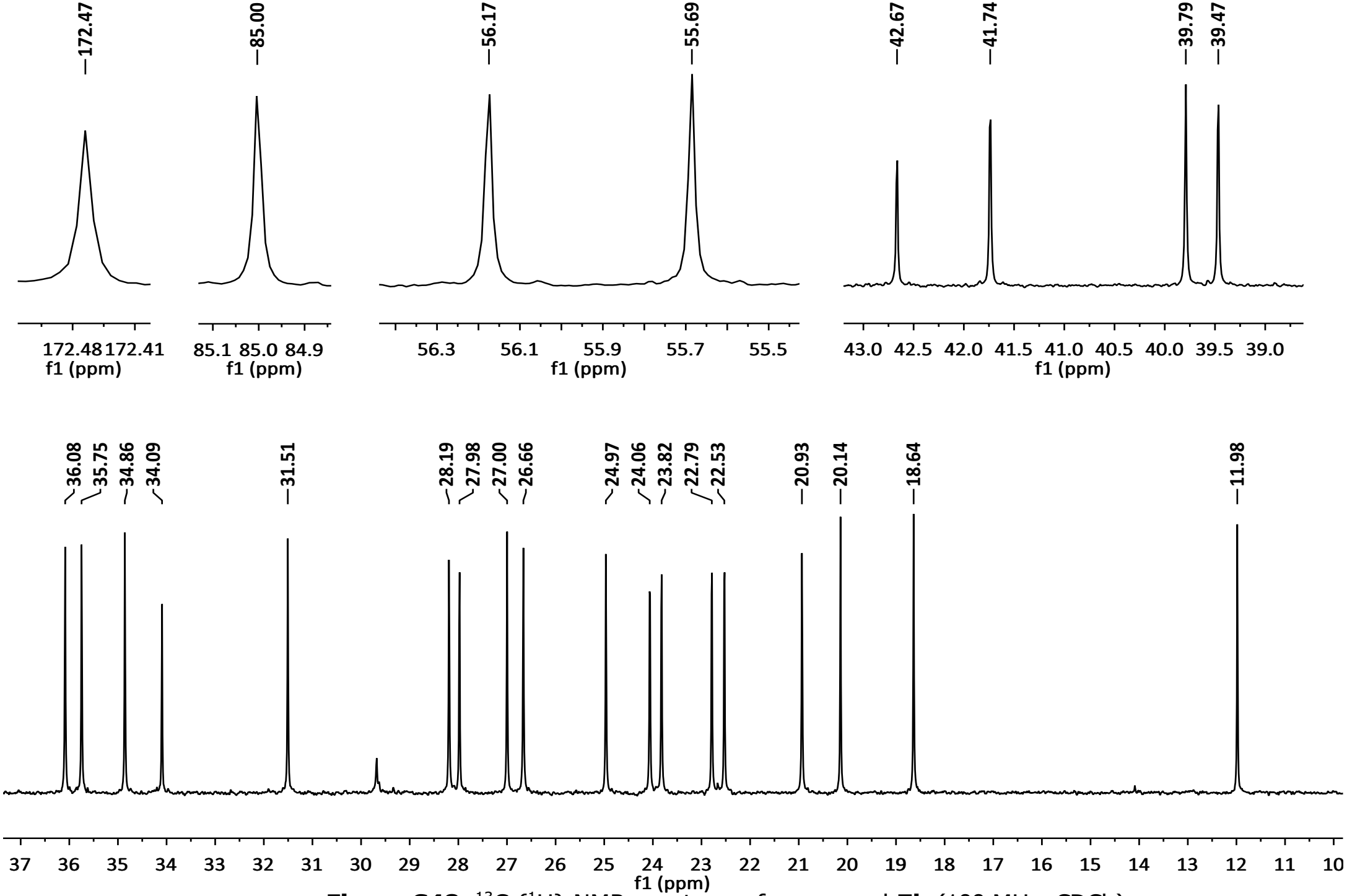

Figure S48. ^{13}C {^{1}H} NMR spectrum of compound **7b** (100 MHz, $CDCl_3$)

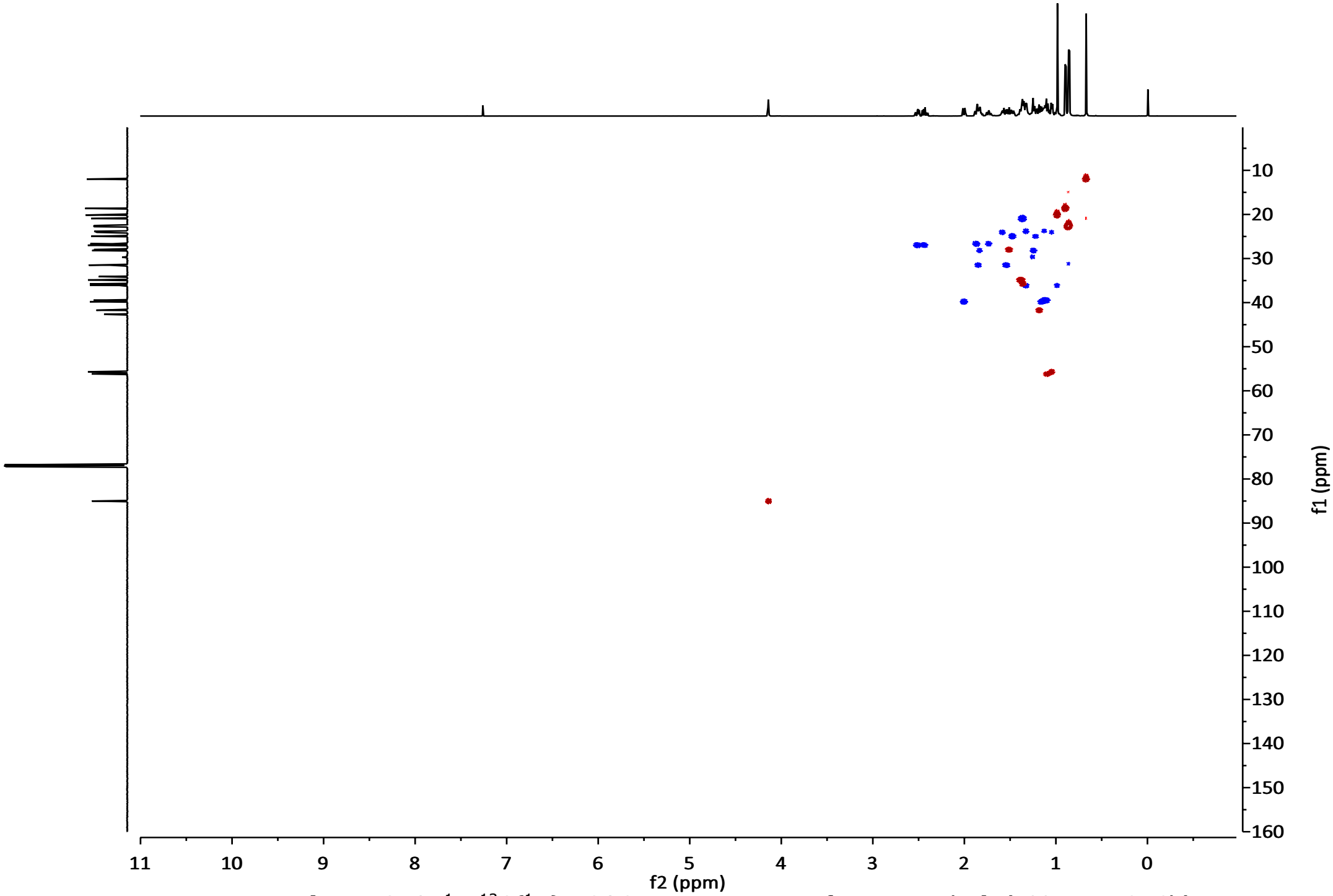

Figure S49. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **7b** (400 MHz, $CDCl_3$)

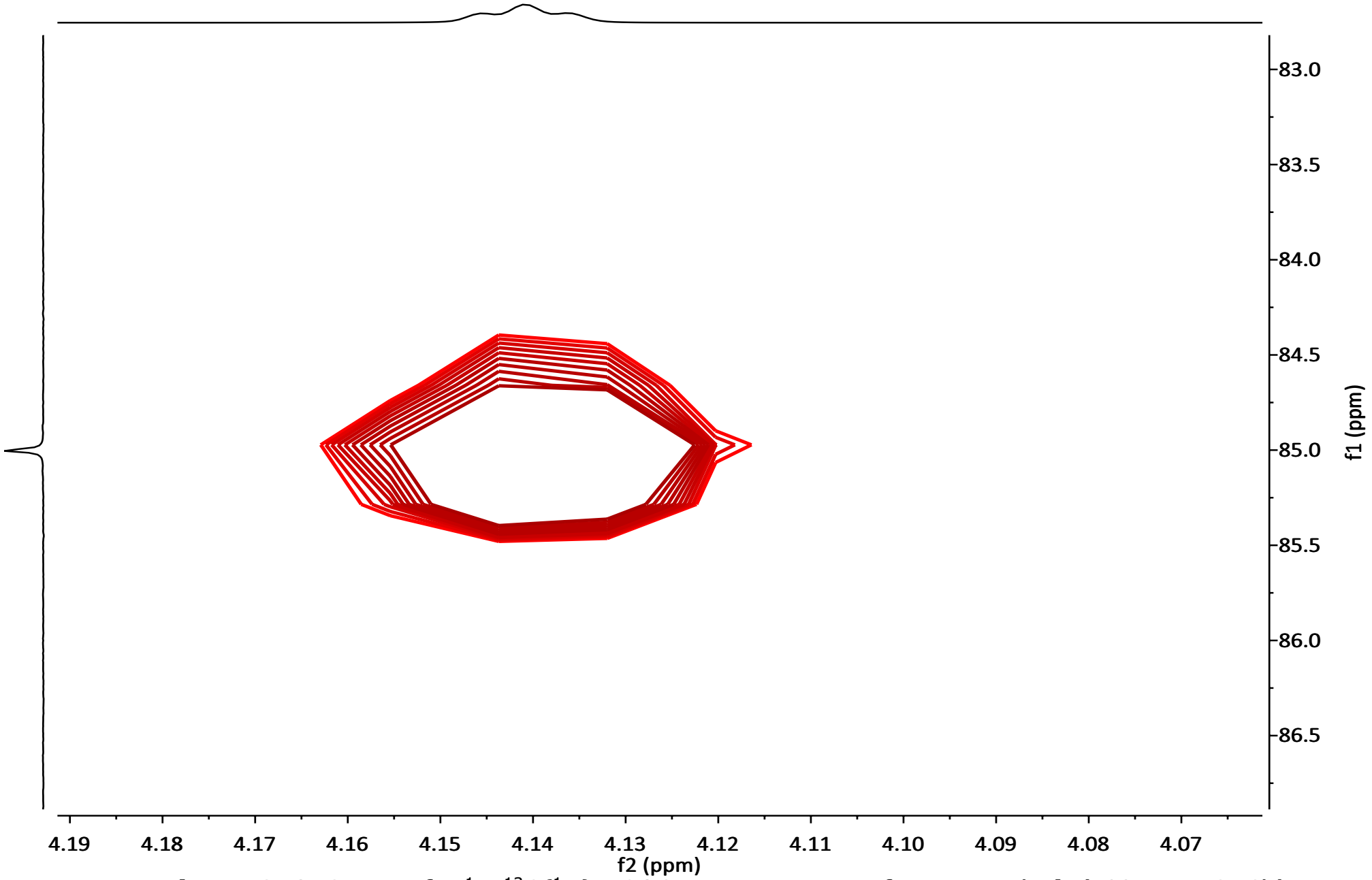

Figure S50. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **7b** (400 MHz, $CDCl_3$)

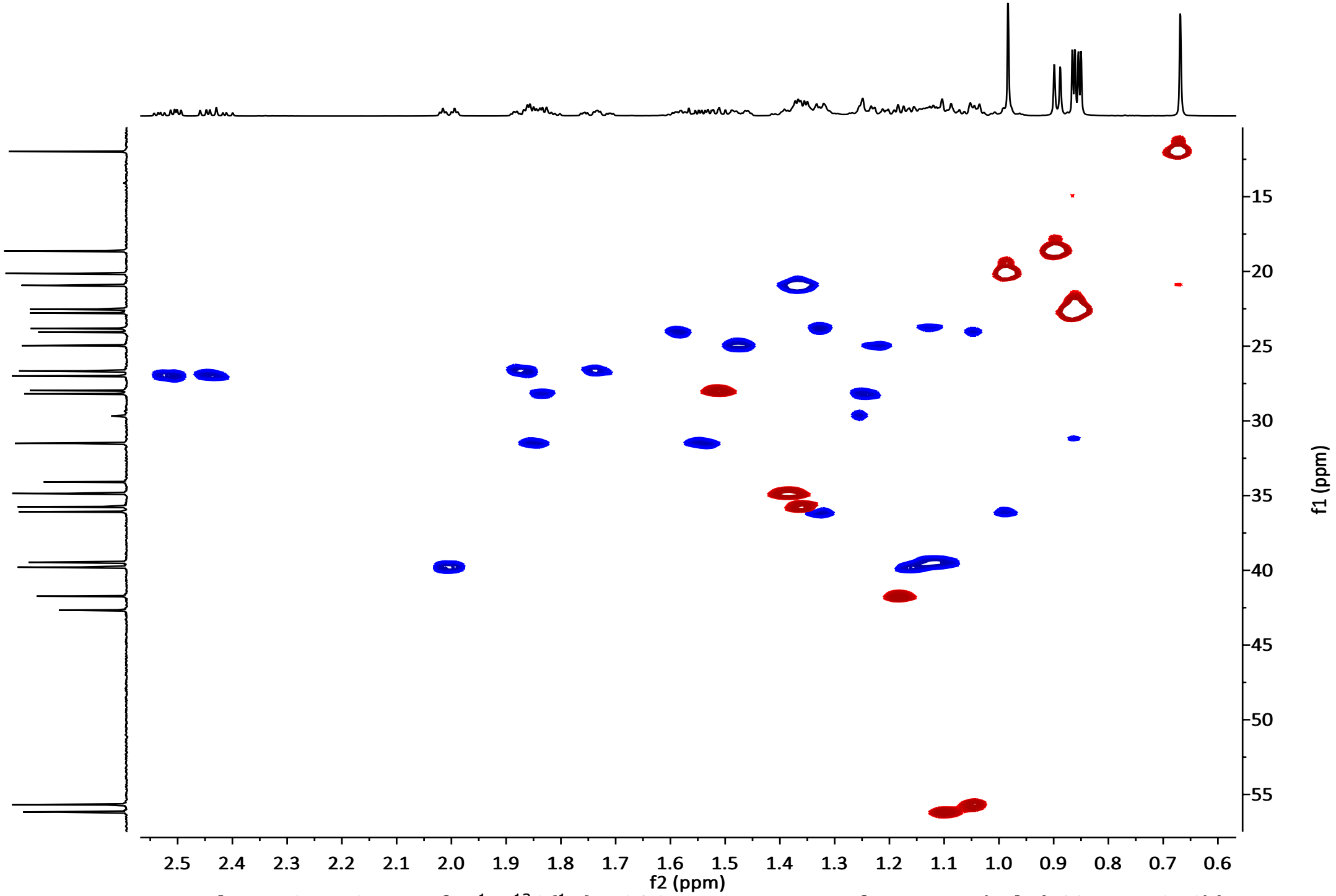

Figure S51. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **7b** (400 MHz, $CDCl_3$)

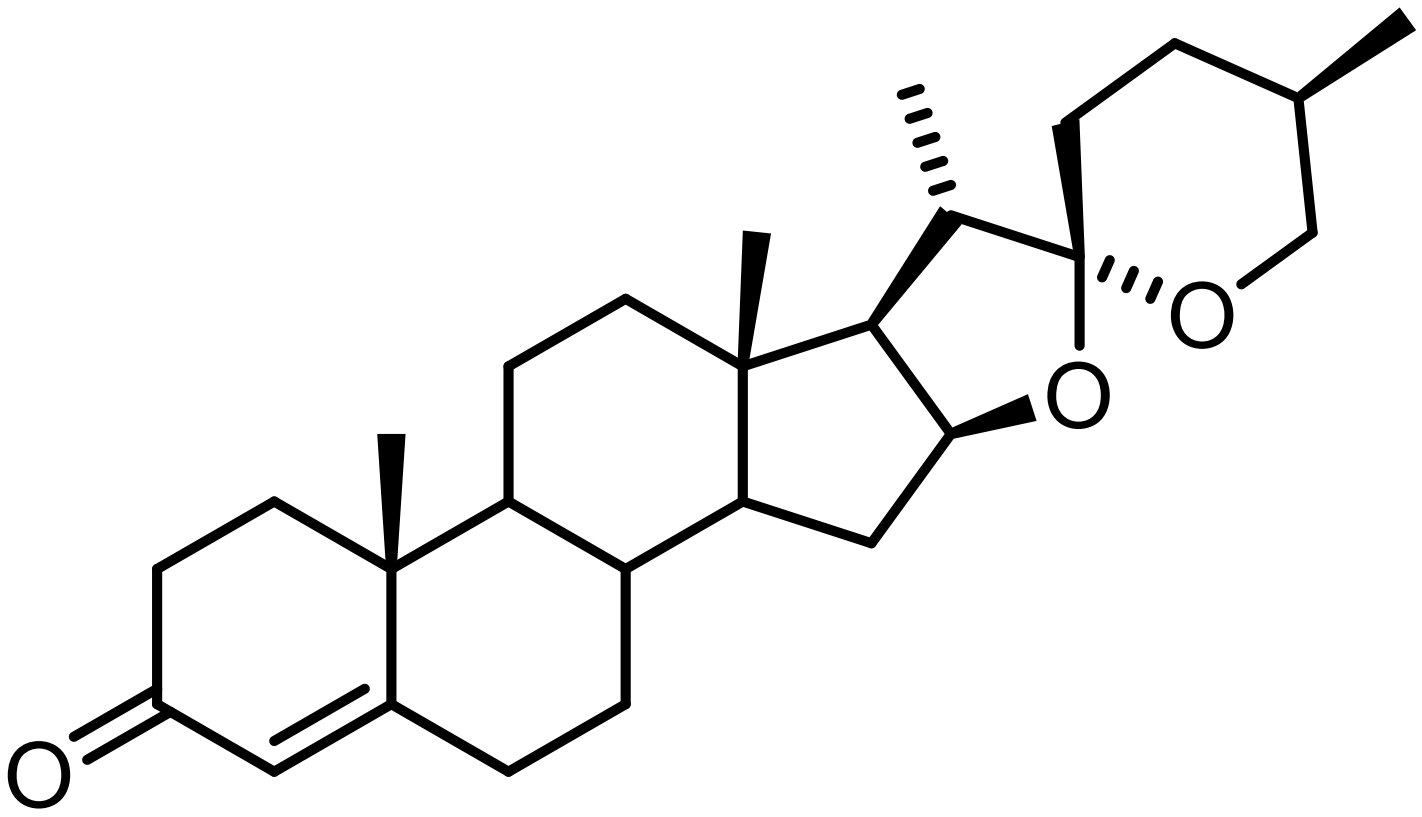

Figure S52. (25R)-Spirost-4-en-3-one **(18)**

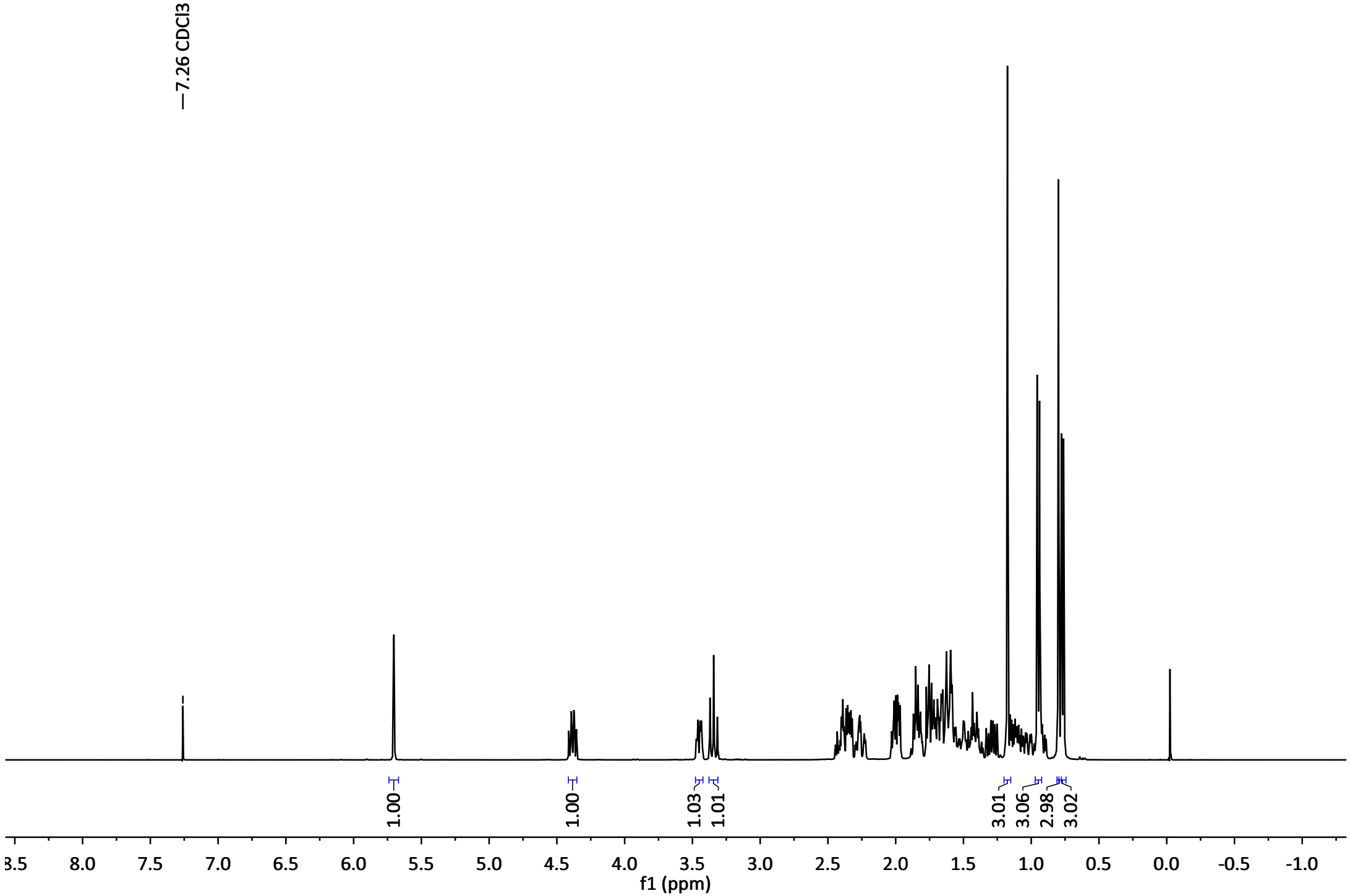

Figure S53. ^{1}H NMR spectrum of compound **18** (400 MHz, $CDCl_3$)

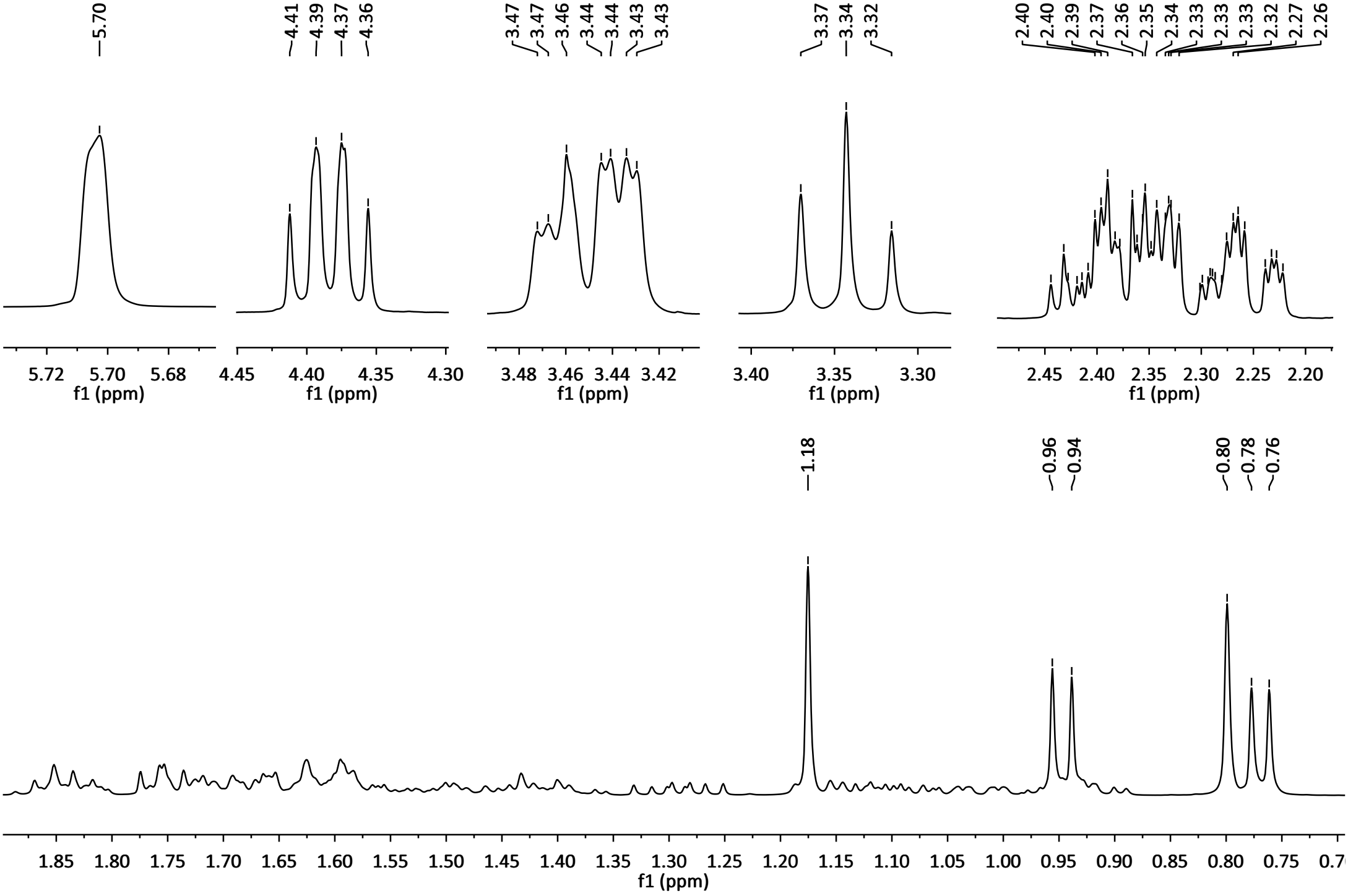

Figure S54. ^{1}H NMR spectrum of compound **18** (400 MHz, $CDCl_3$)

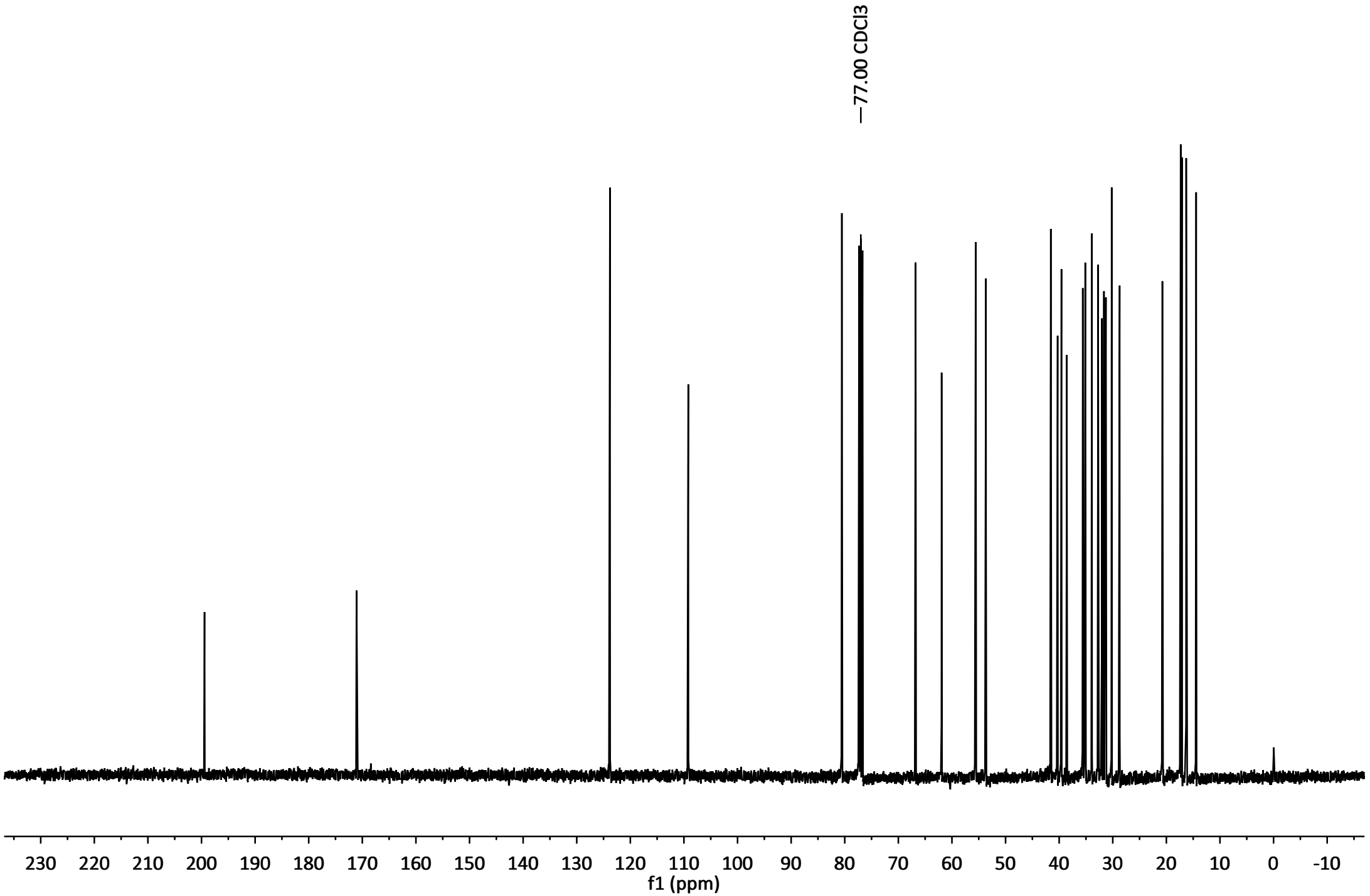

Figure S55. ^{13}C NMR spectrum of compound **18** (100 MHz, $CDCl_3$)

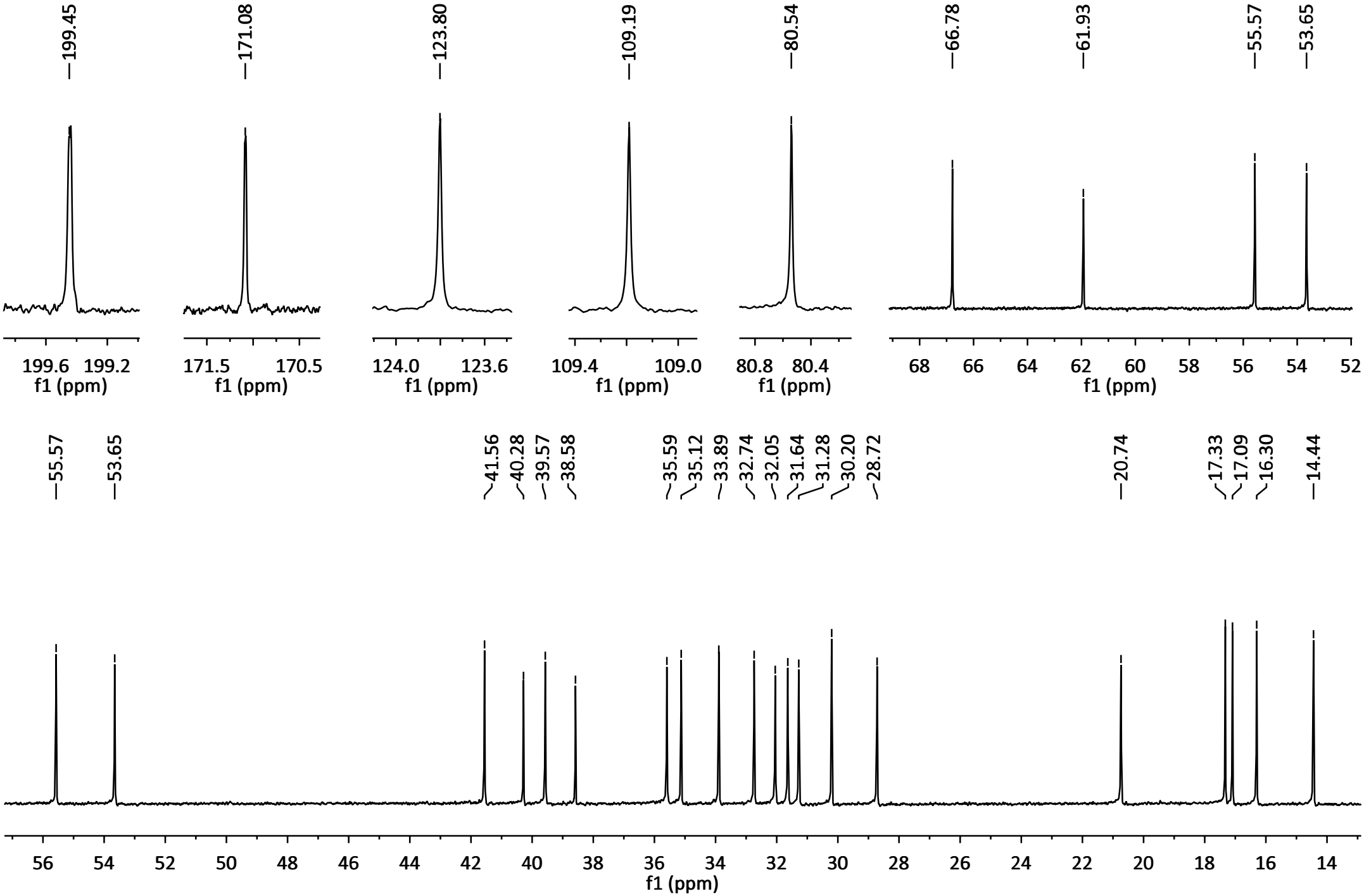

Figure S56. ^{13}C NMR spectrum of compound **18** (100 MHz, $CDCl_3$)

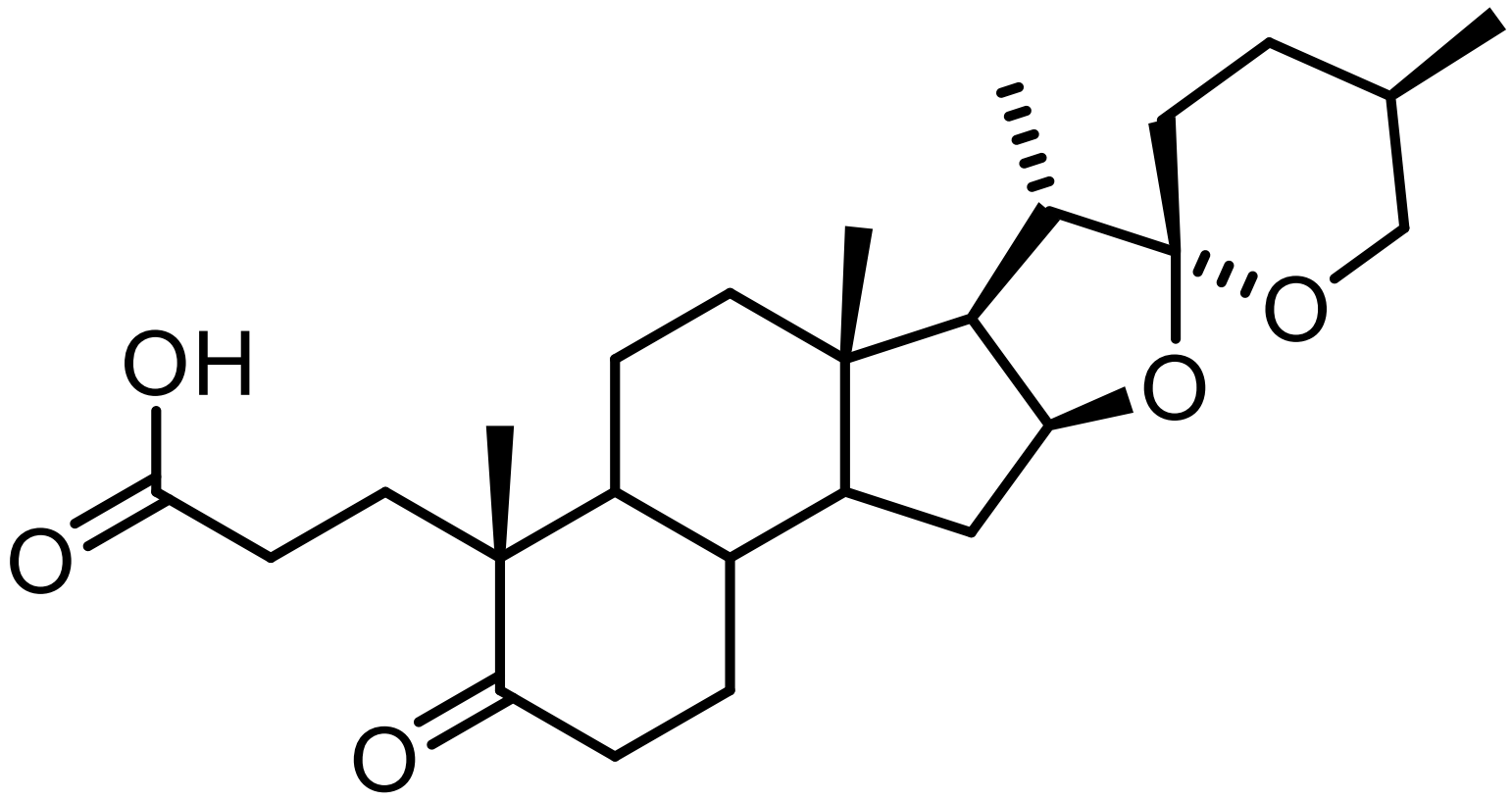

Figure S57. (25R)-A-seco-4-nor-spirost-5-oxo-3-oic acid **(19)**

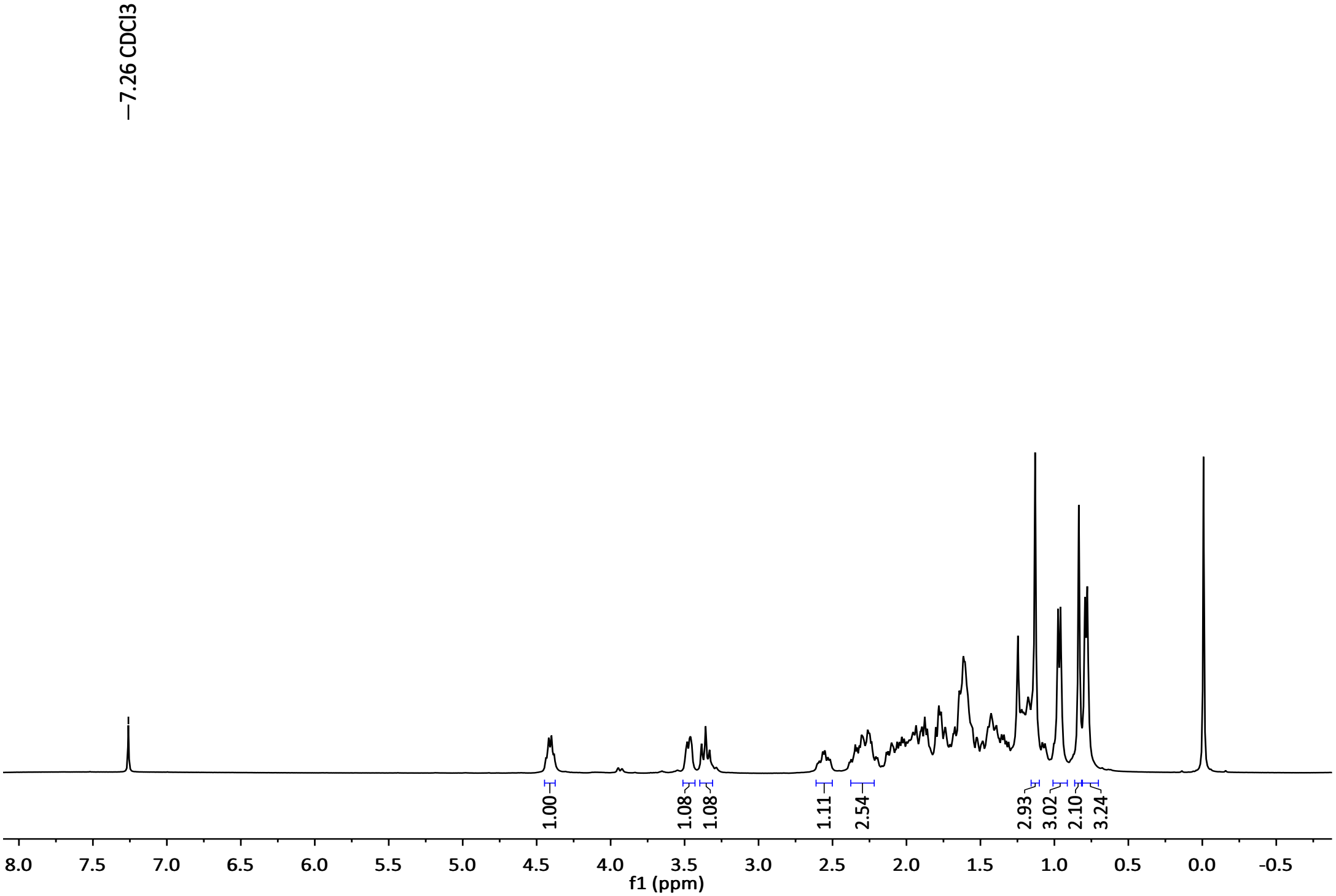

Figure S58. ^{1}H NMR spectrum of compound **19** (400 MHz, $CDCl_3$)

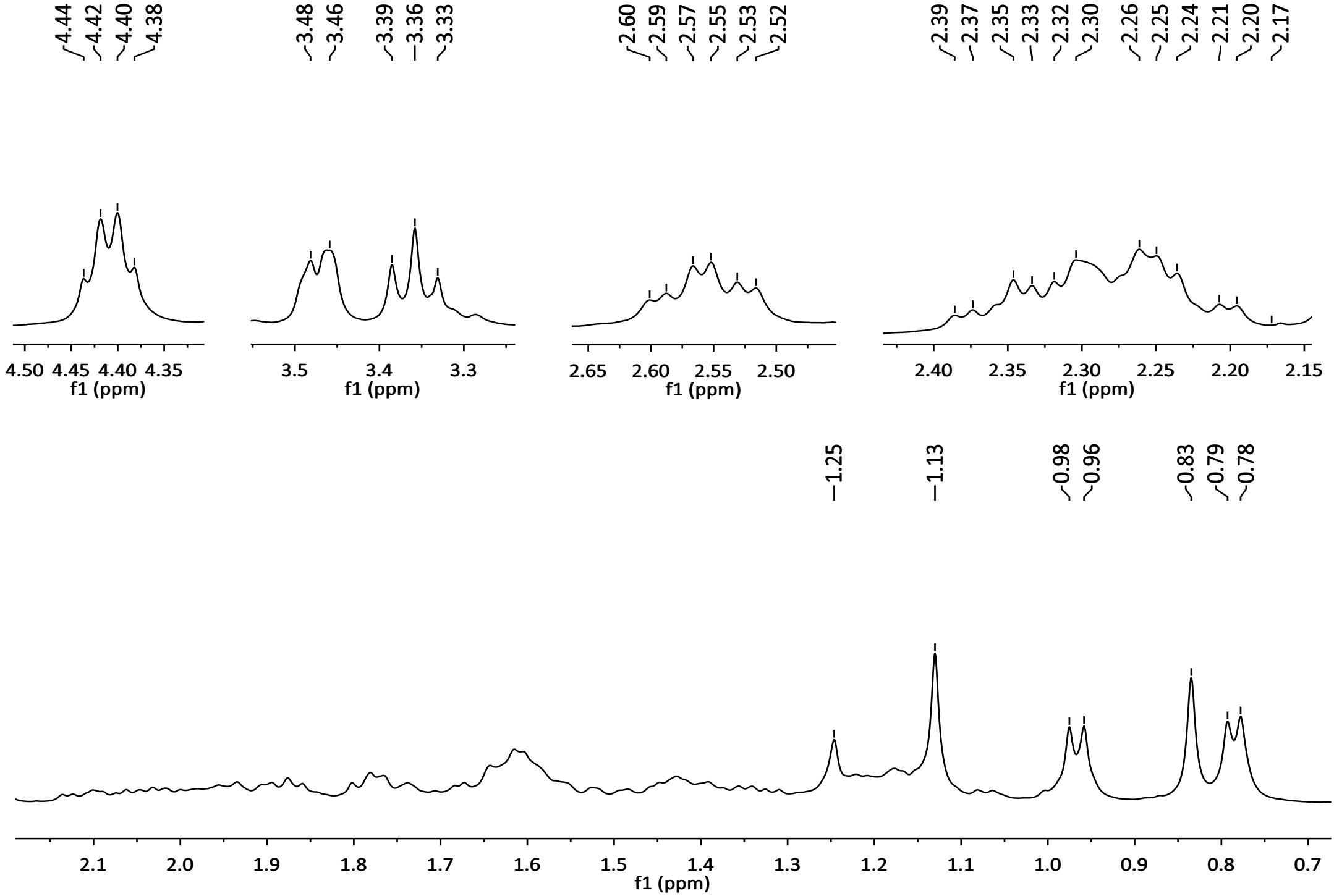

Figure S59. Sections for ^{1}H NMR spectrum of compound **19** (400 MHz, $CDCl_3$)

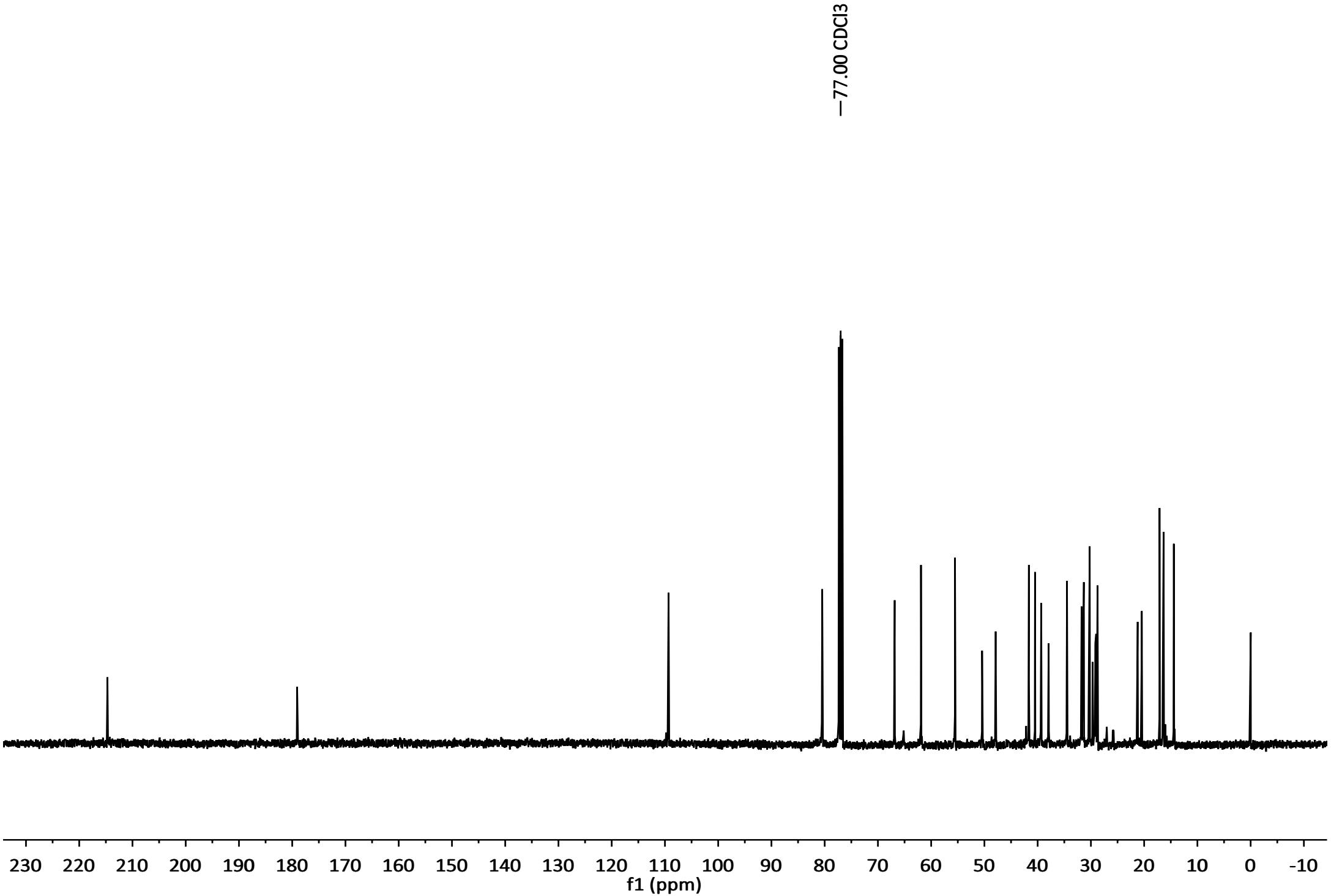

Figure S60. ^{13}C NMR spectrum of compound **19** (100 MHz, $CDCl_3$)

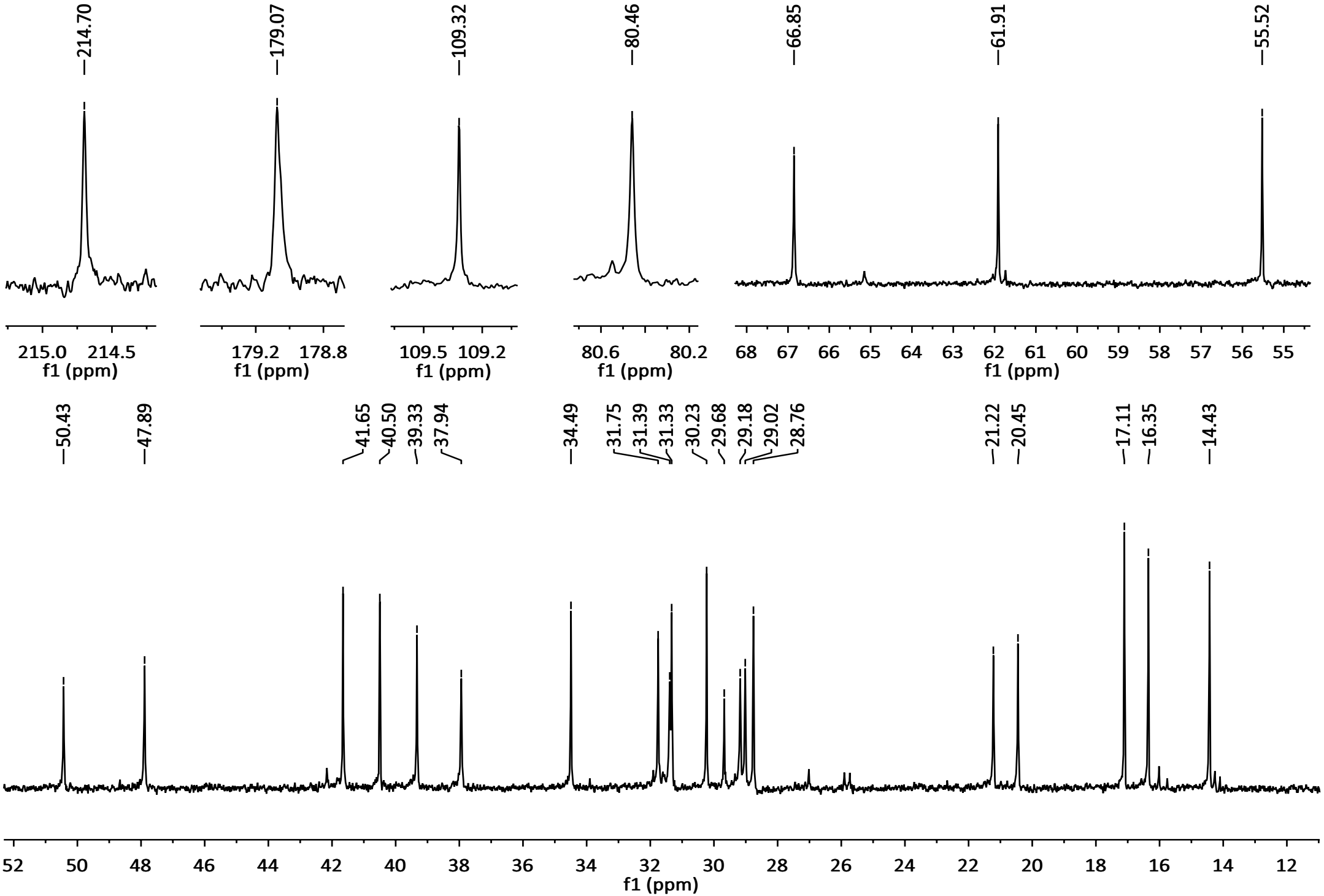

Figure S61. Sections for ^{13}C NMR spectrum of compound **19** (100 MHz, $CDCl_3$)

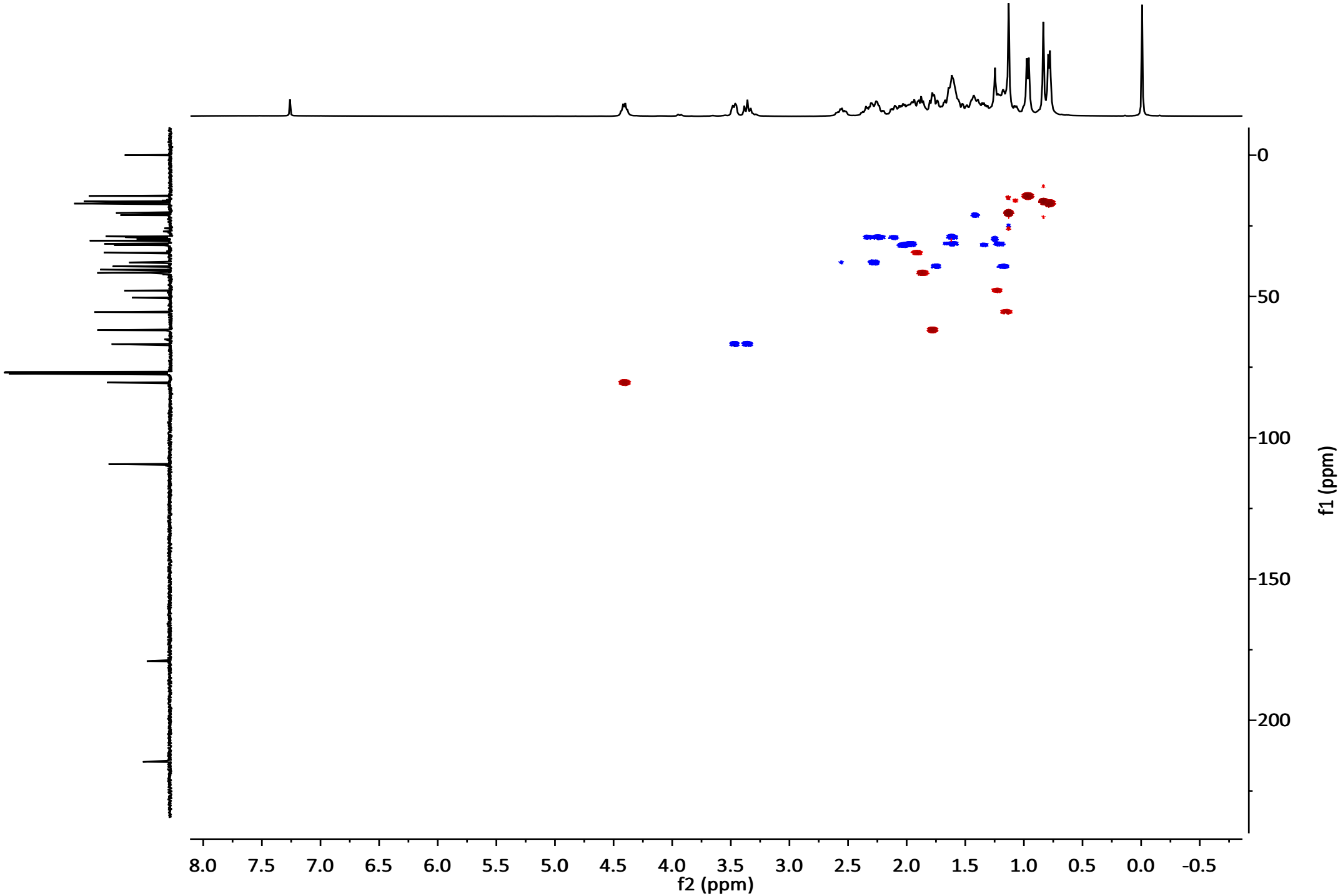

Figure S62. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **19** (400 MHz, $CDCl_3$)

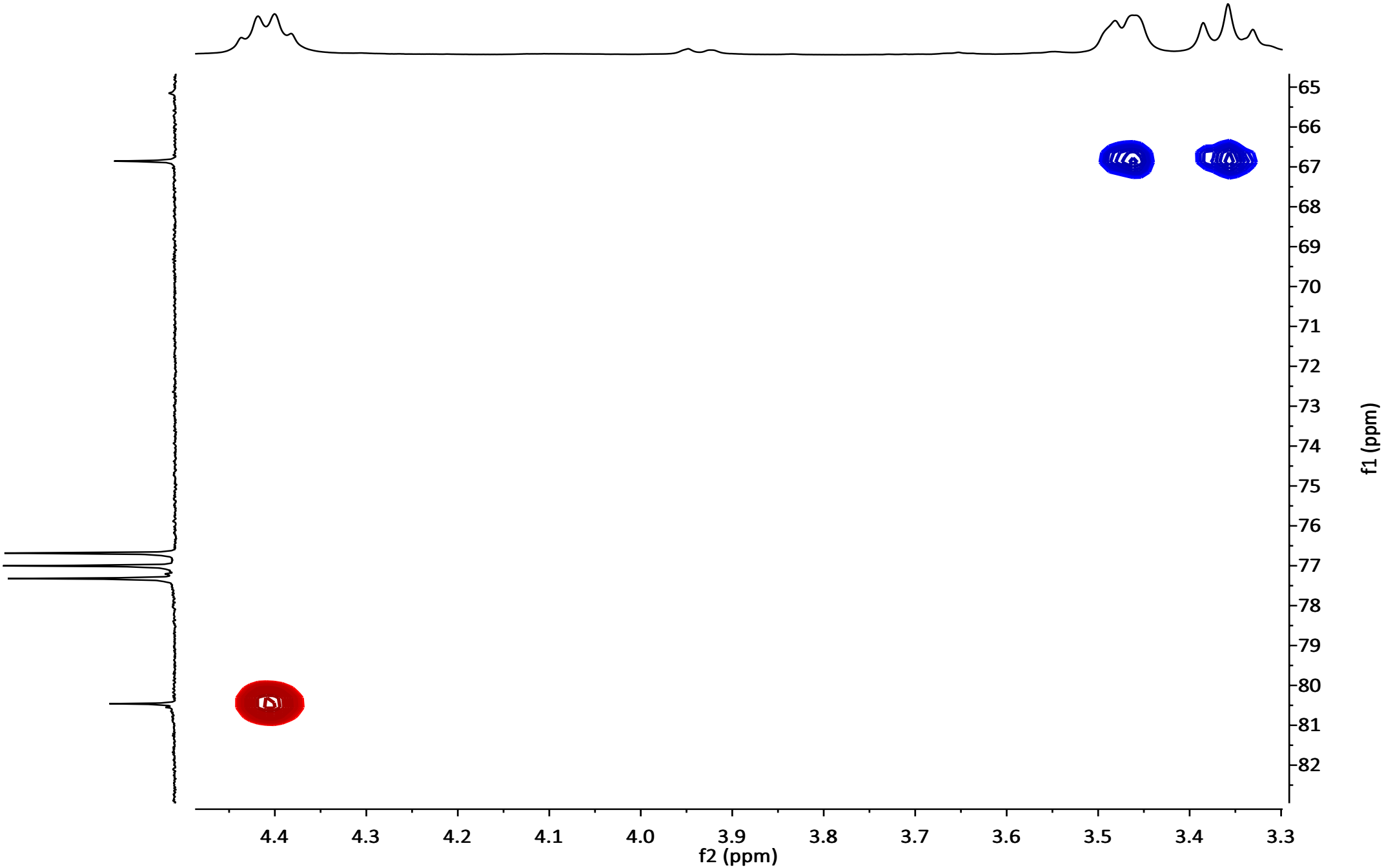

Figure S63. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **19** (400 MHz, $CDCl_3$)

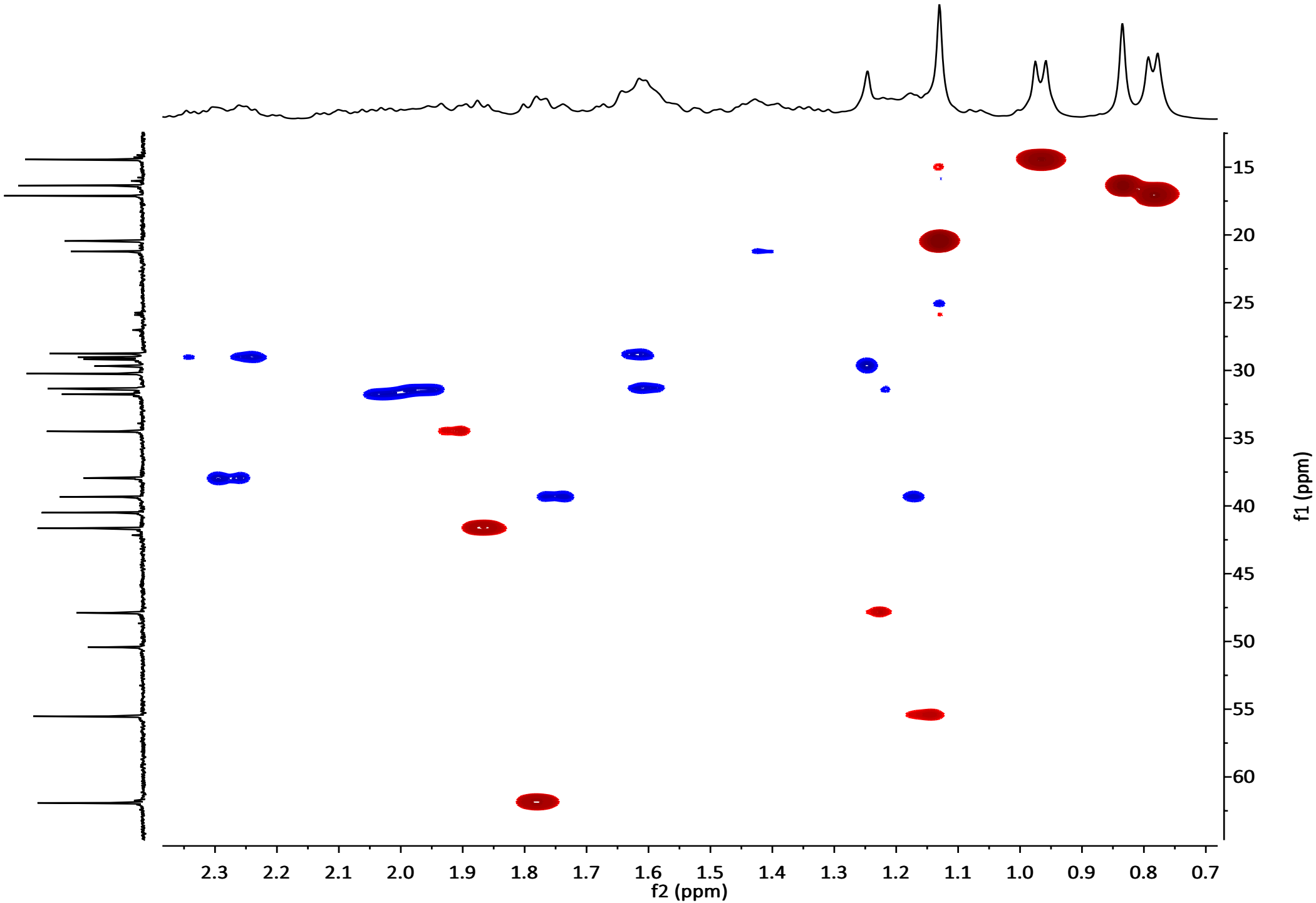

Figure S64. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **19** (400 MHz, $CDCl_3$)

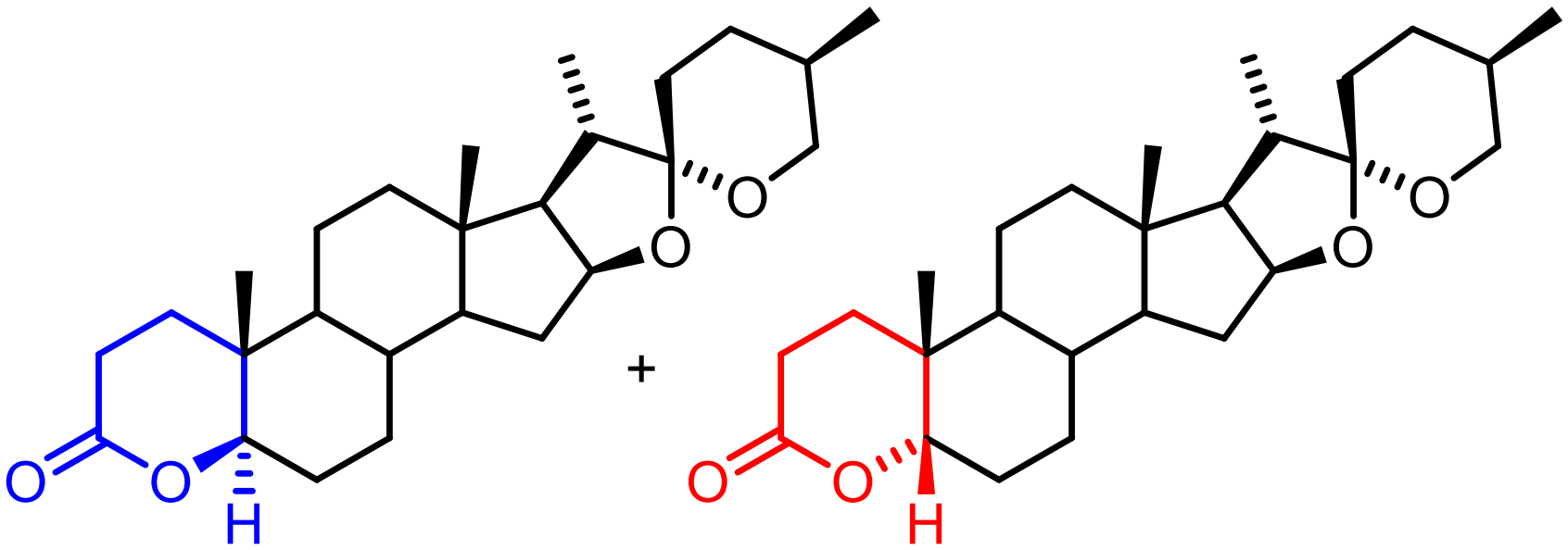

Figure S65. Diasteromeric relation of lactones **20a** and **20b**

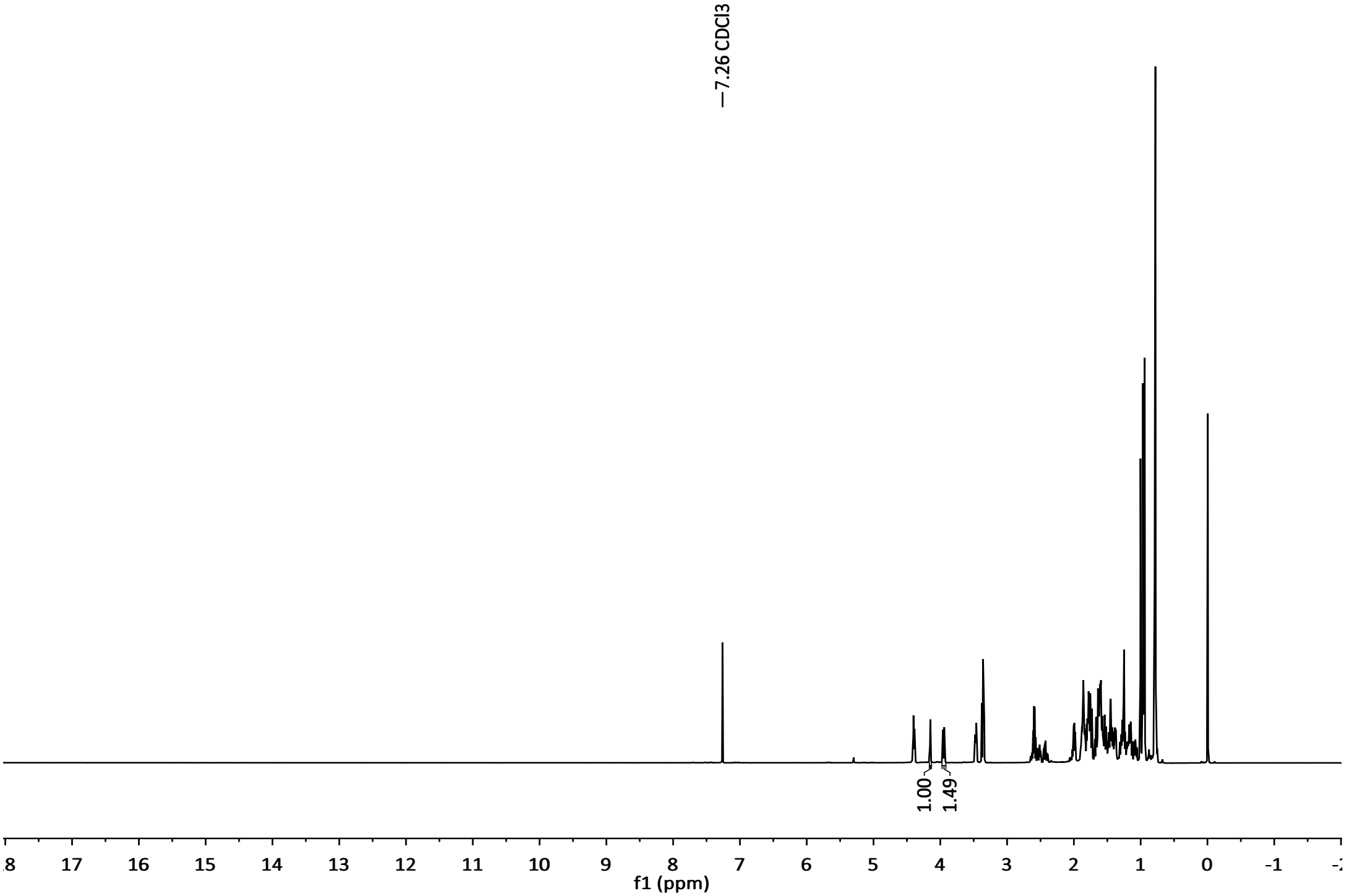

Figure S66. ^{1}H NMR spectrum of compound **20ab** (600 MHz, $CDCl_3$)

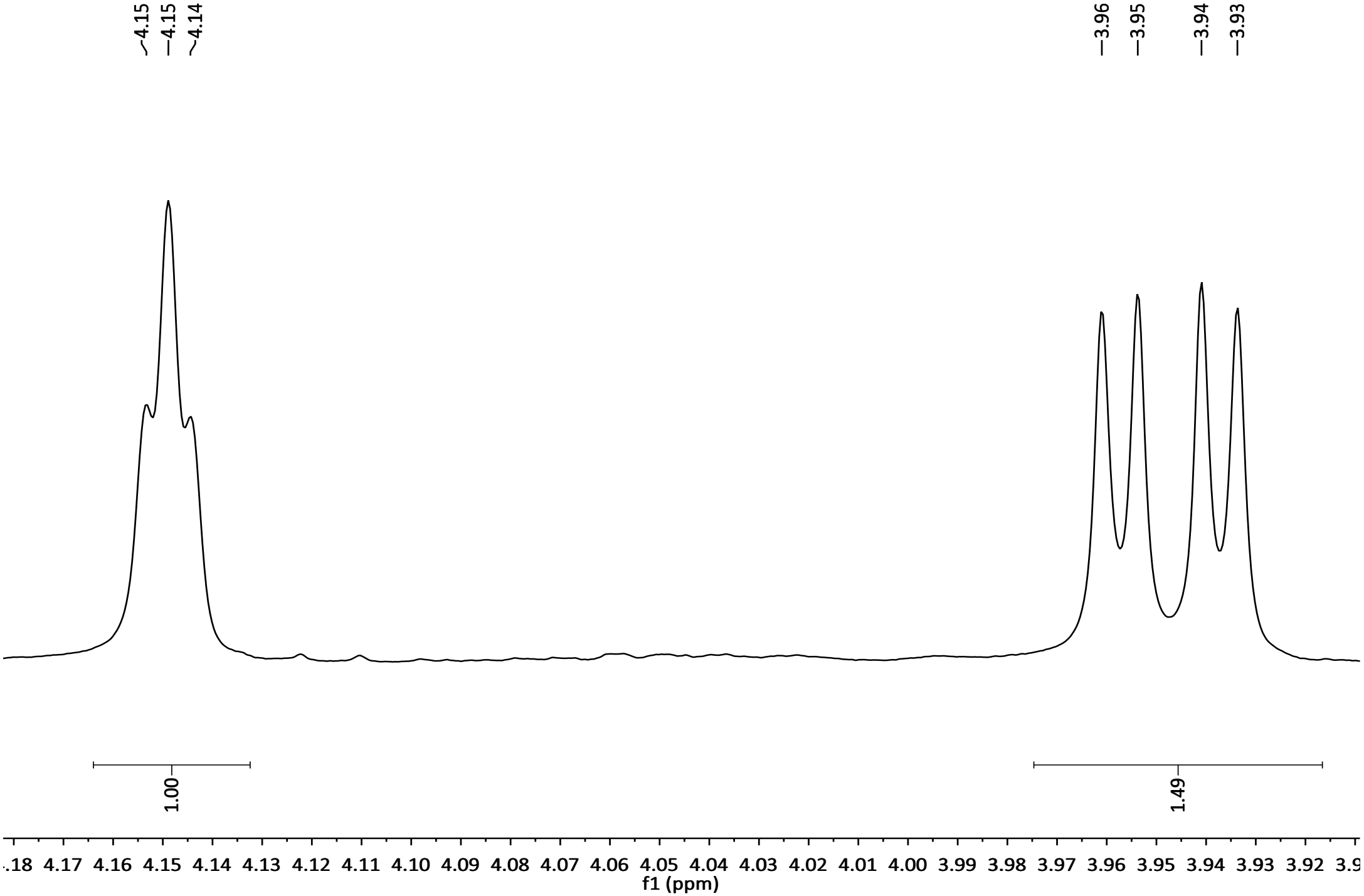

Figure S67. Section for ^{1}H NMR spectrum of compound **20ab** (600 MHz, $CDCl_3$)

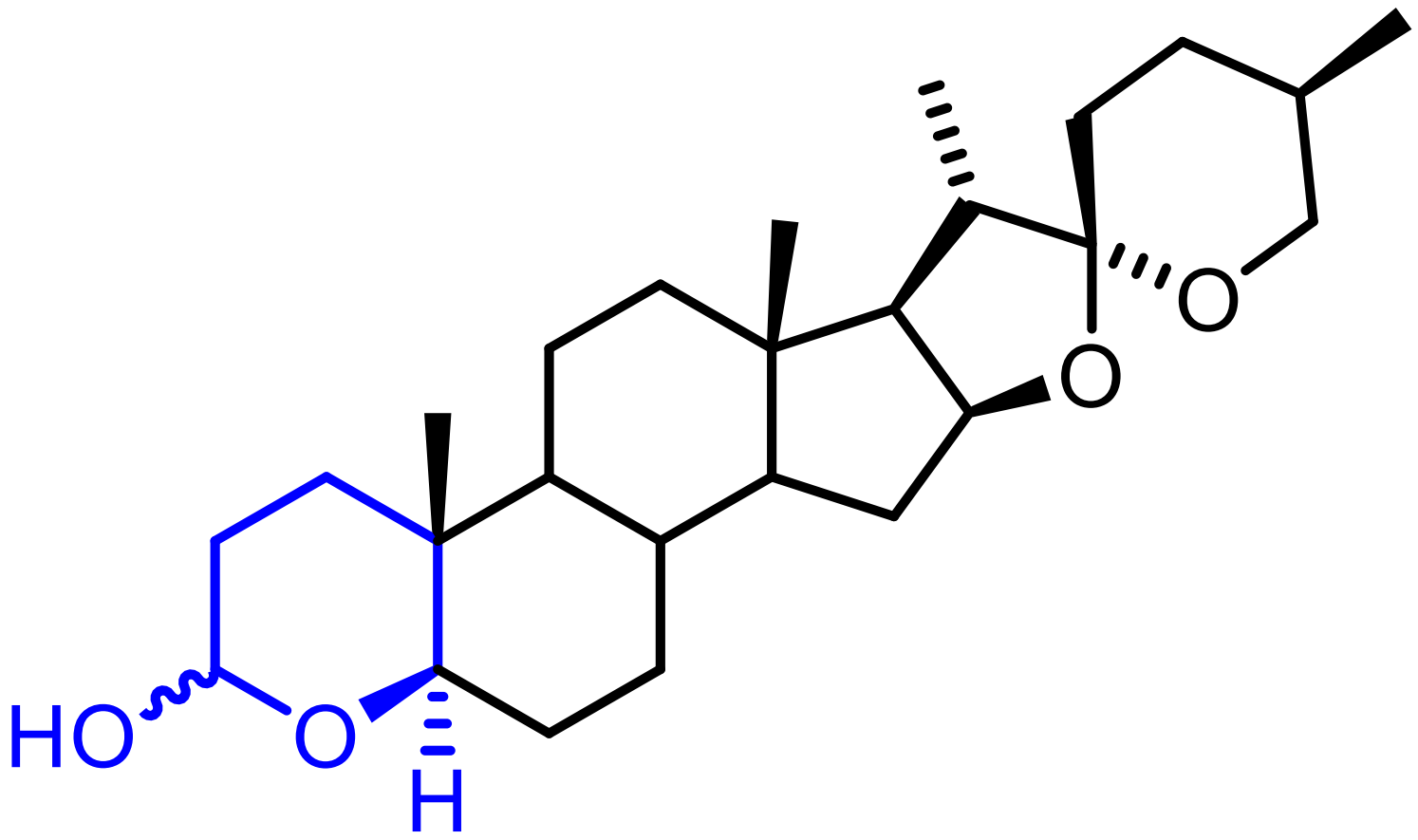

Figure S68. (25R)-4-oxa-5α-spirostan-3ε-ol **(21a)**

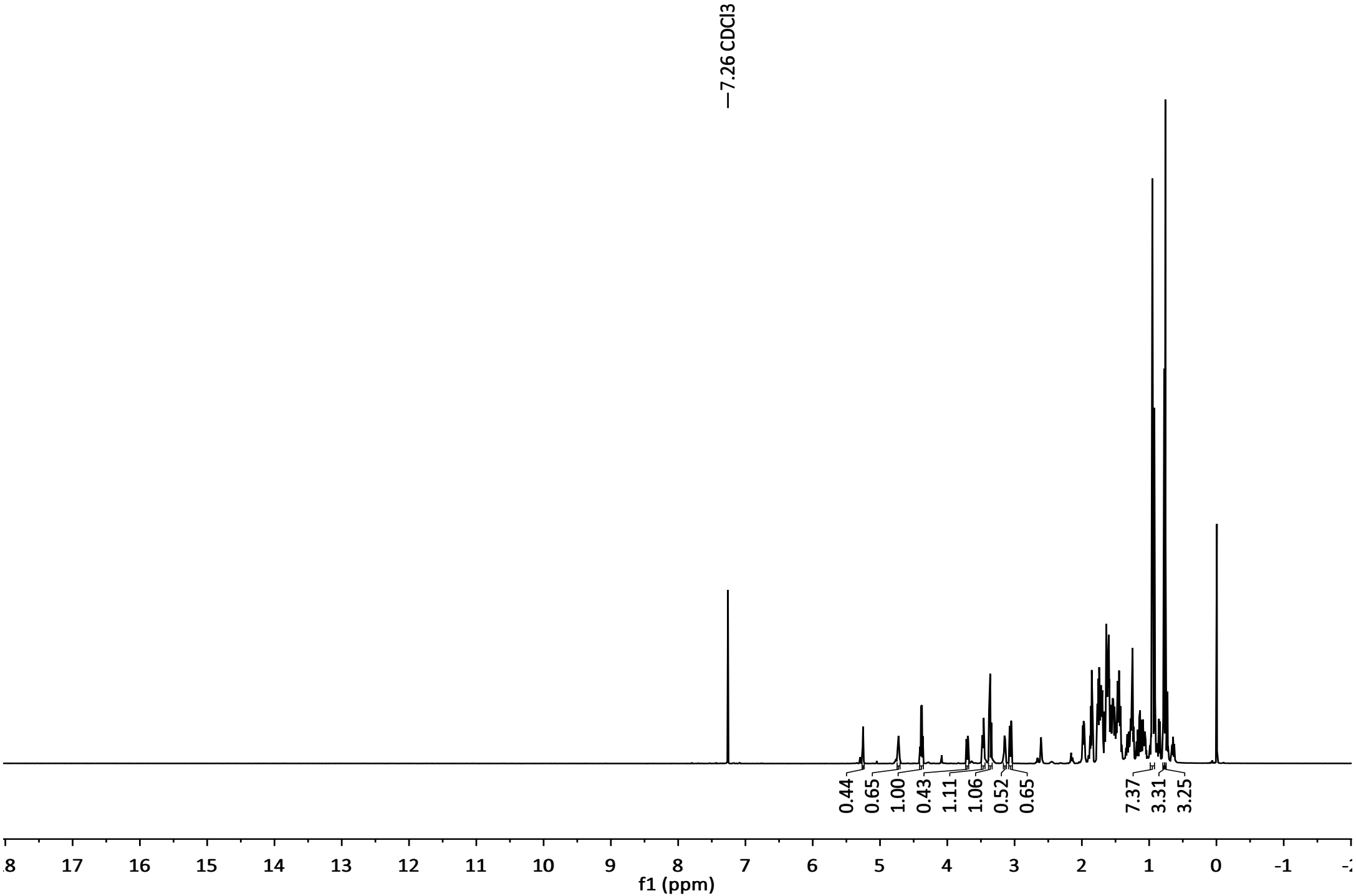

Figure S69. ^{1}H NMR spectrum of compound **21a** (600 MHz, $CDCl_3$)

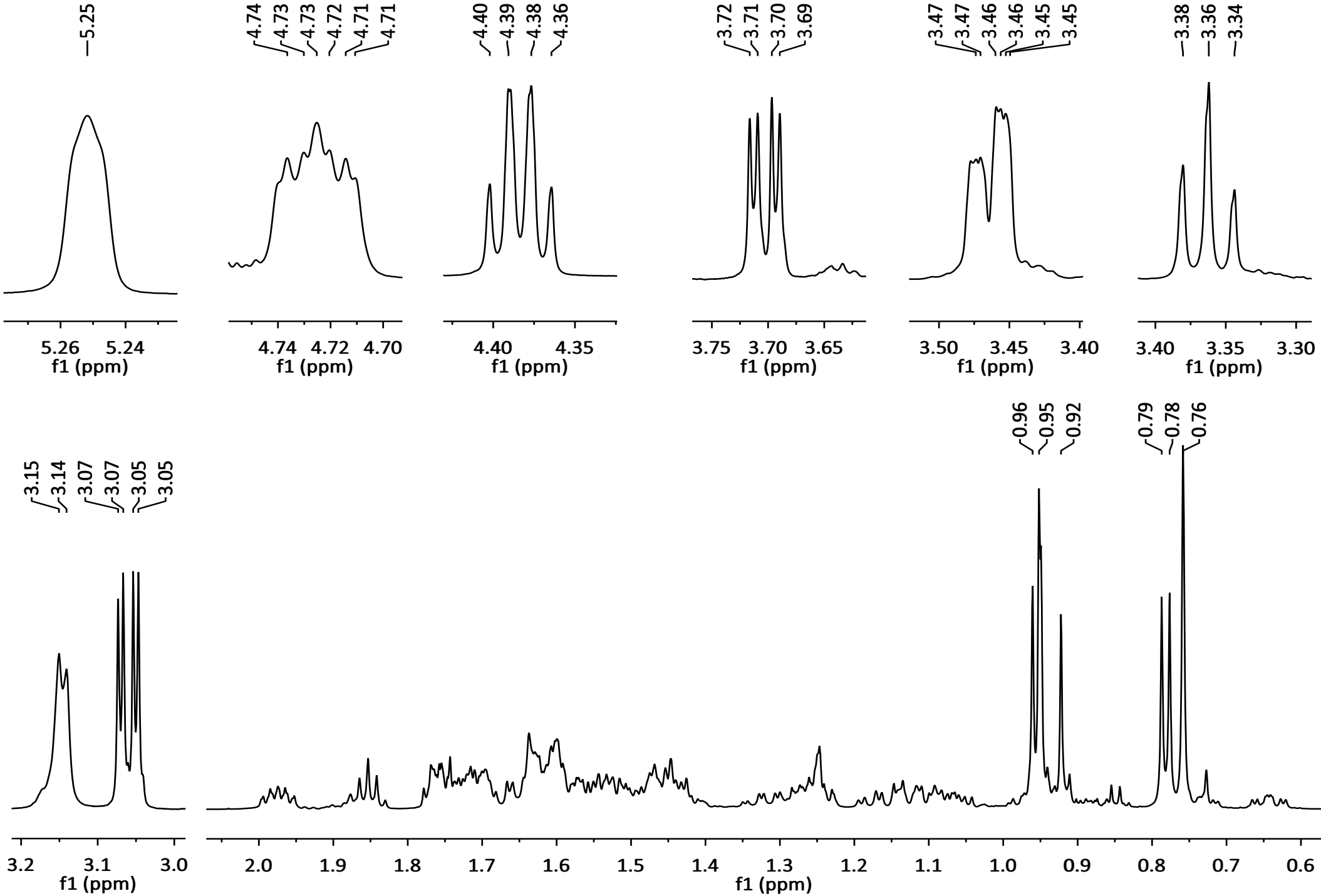

Figure S70. Sections for ^{1}H NMR spectrum of compound **21a** (600 MHz, $CDCl_3$)

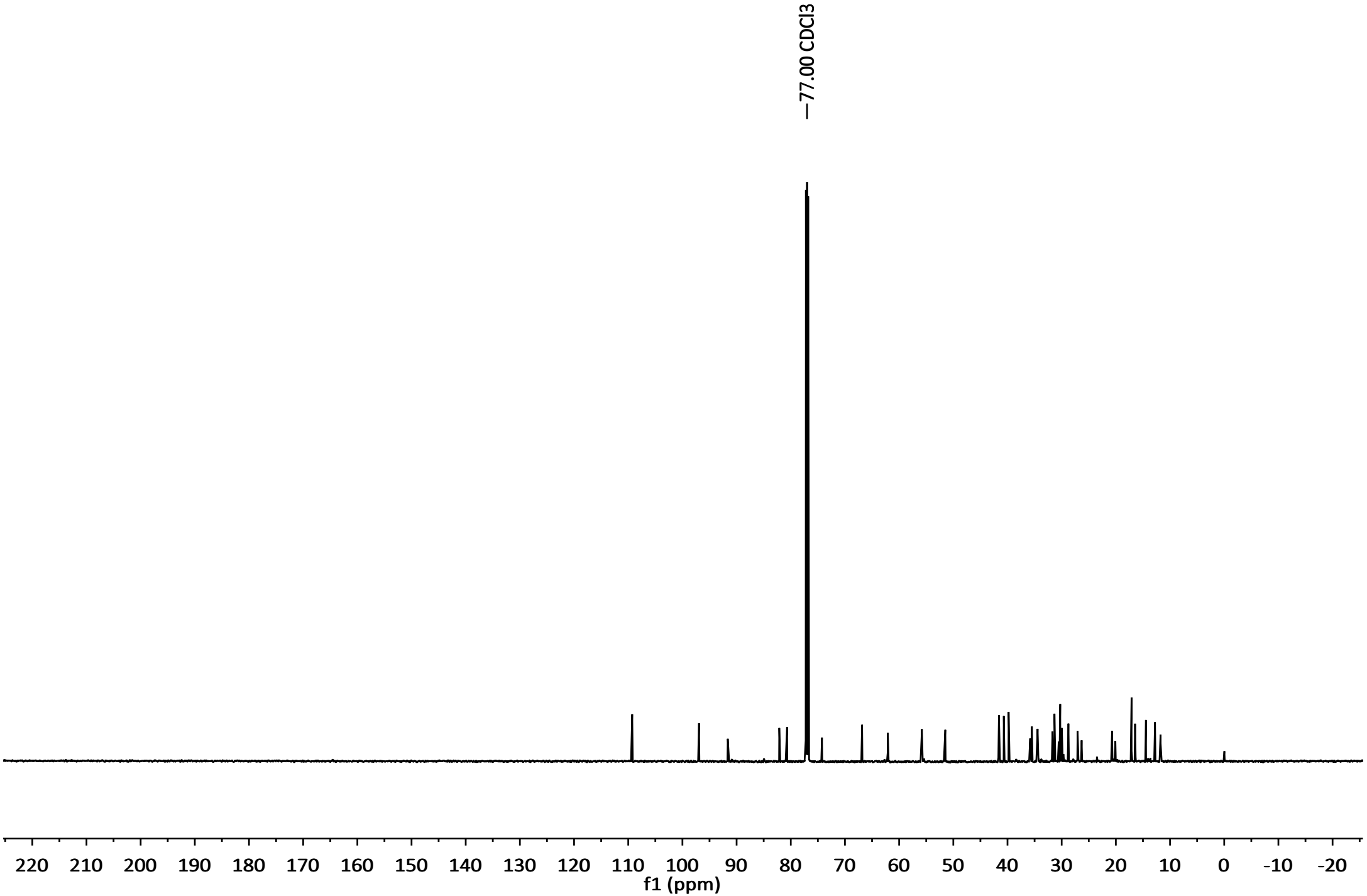

Figure S71. $^{13}C\{^{1}H\}$ NMR spectrum of compound **21a** (150 MHz, $CDCl_3$)

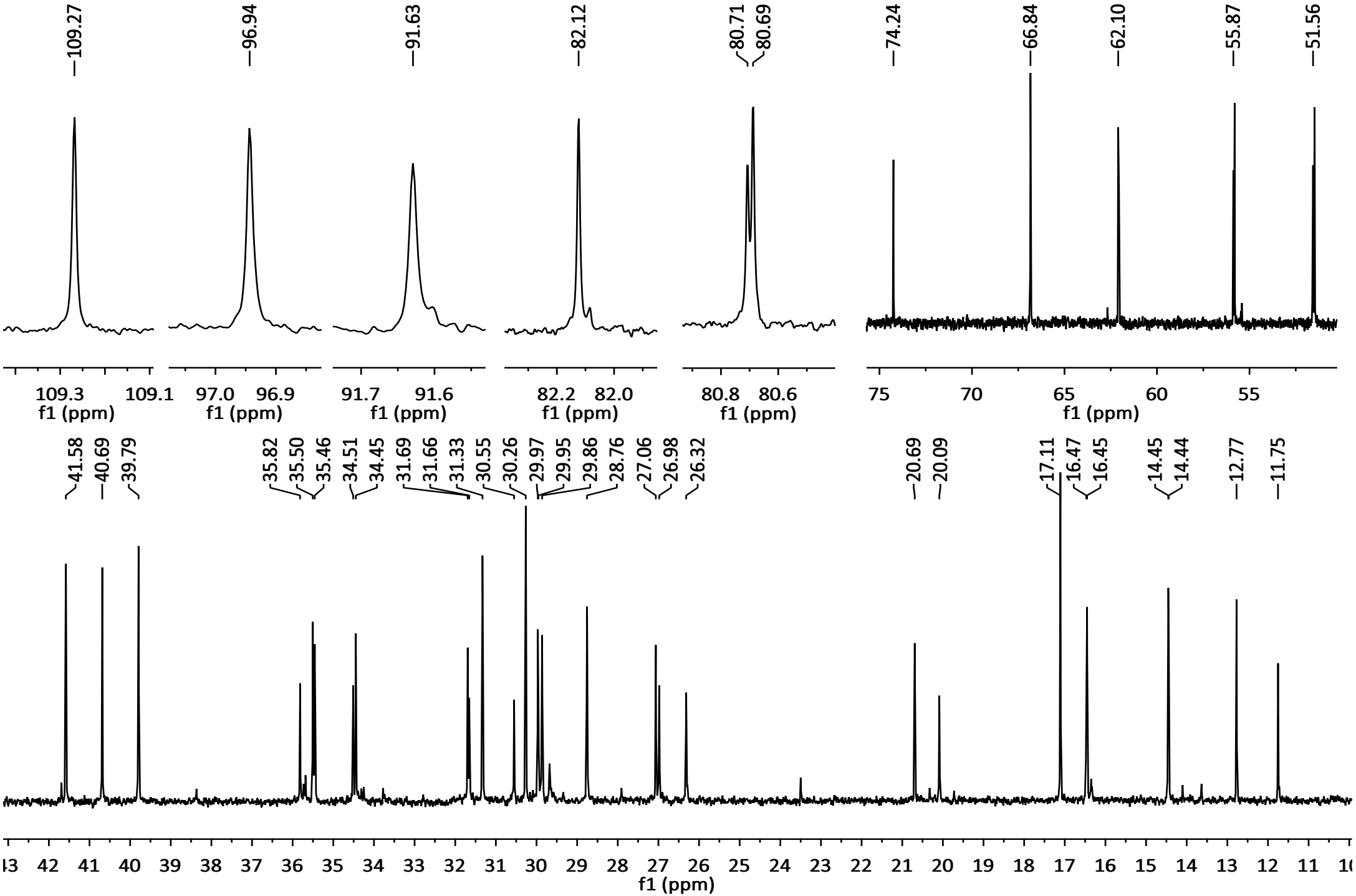

Figure S72. $^{13}C\{^{1}H\}$ NMR spectrum of compound **21a** (150 MHz, $CDCl_3$)

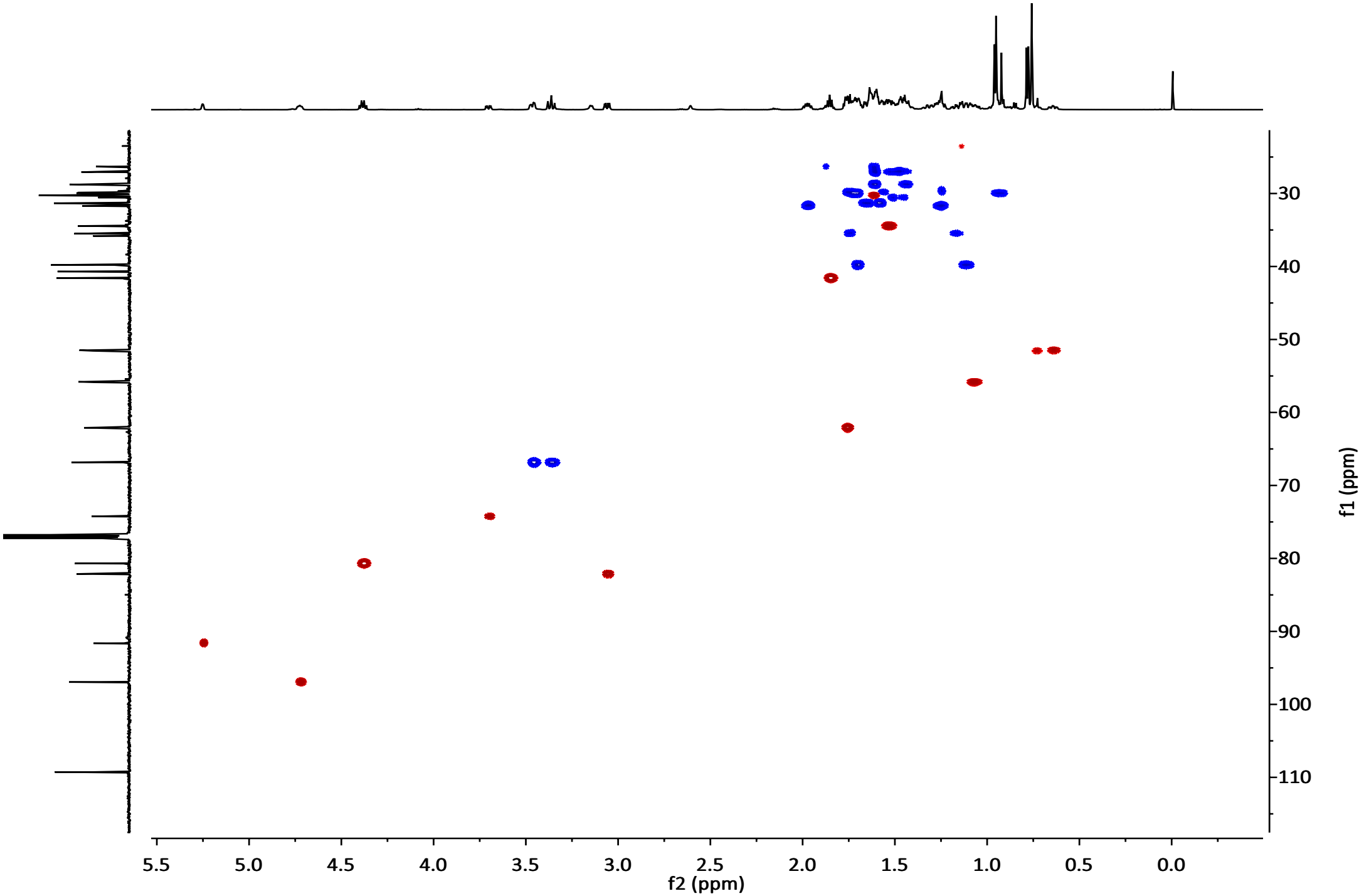

Figure S73. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21a** (600 MHz, $CDCl_3$)

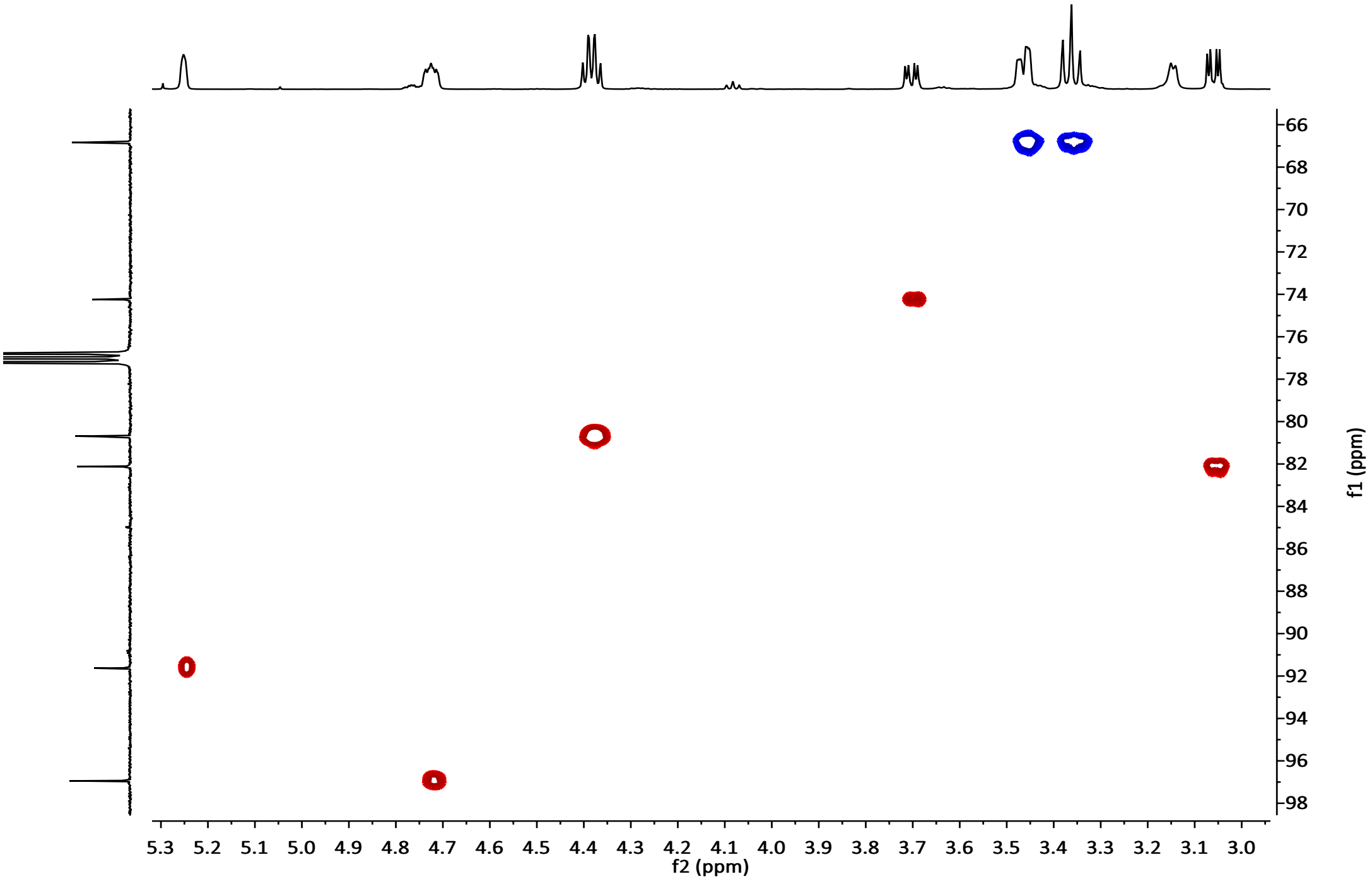

Figure S74. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21a** (600 MHz, $CDCl_3$)

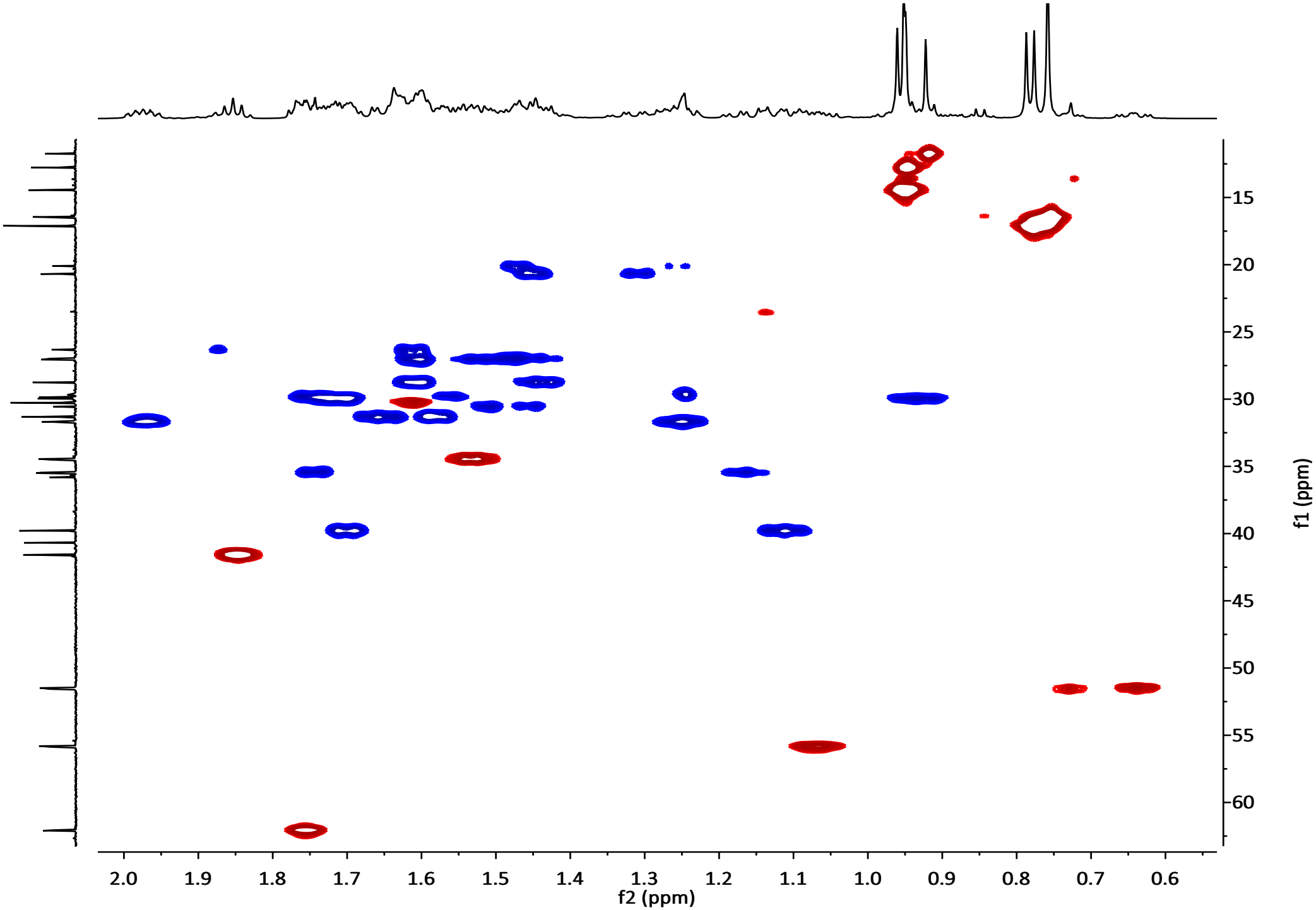

Figure S75. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21a** (600 MHz, $CDCl_3$)

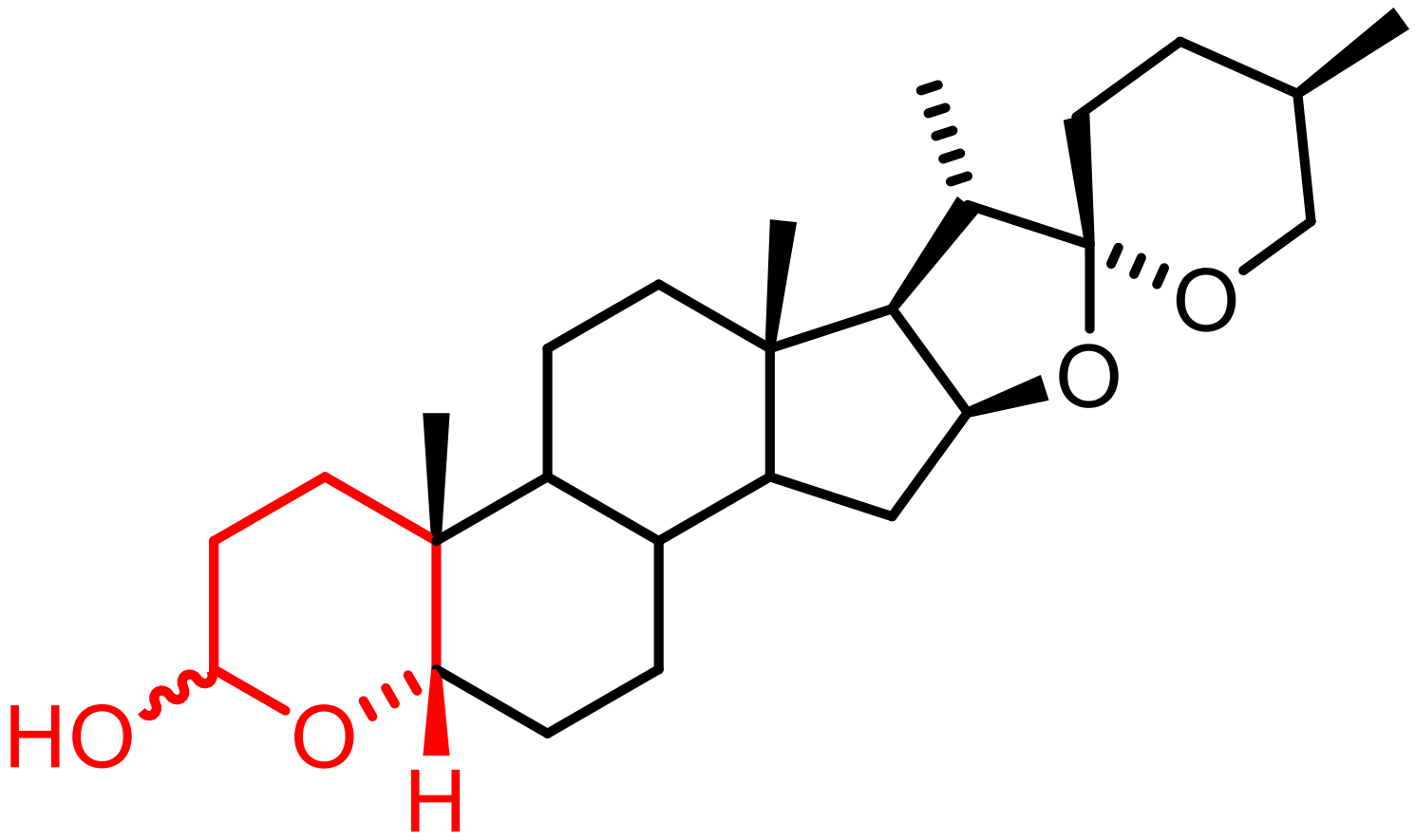

Figure S76. (25R)-4-oxa-5β-spirostan-3ε-ol **(21b)**

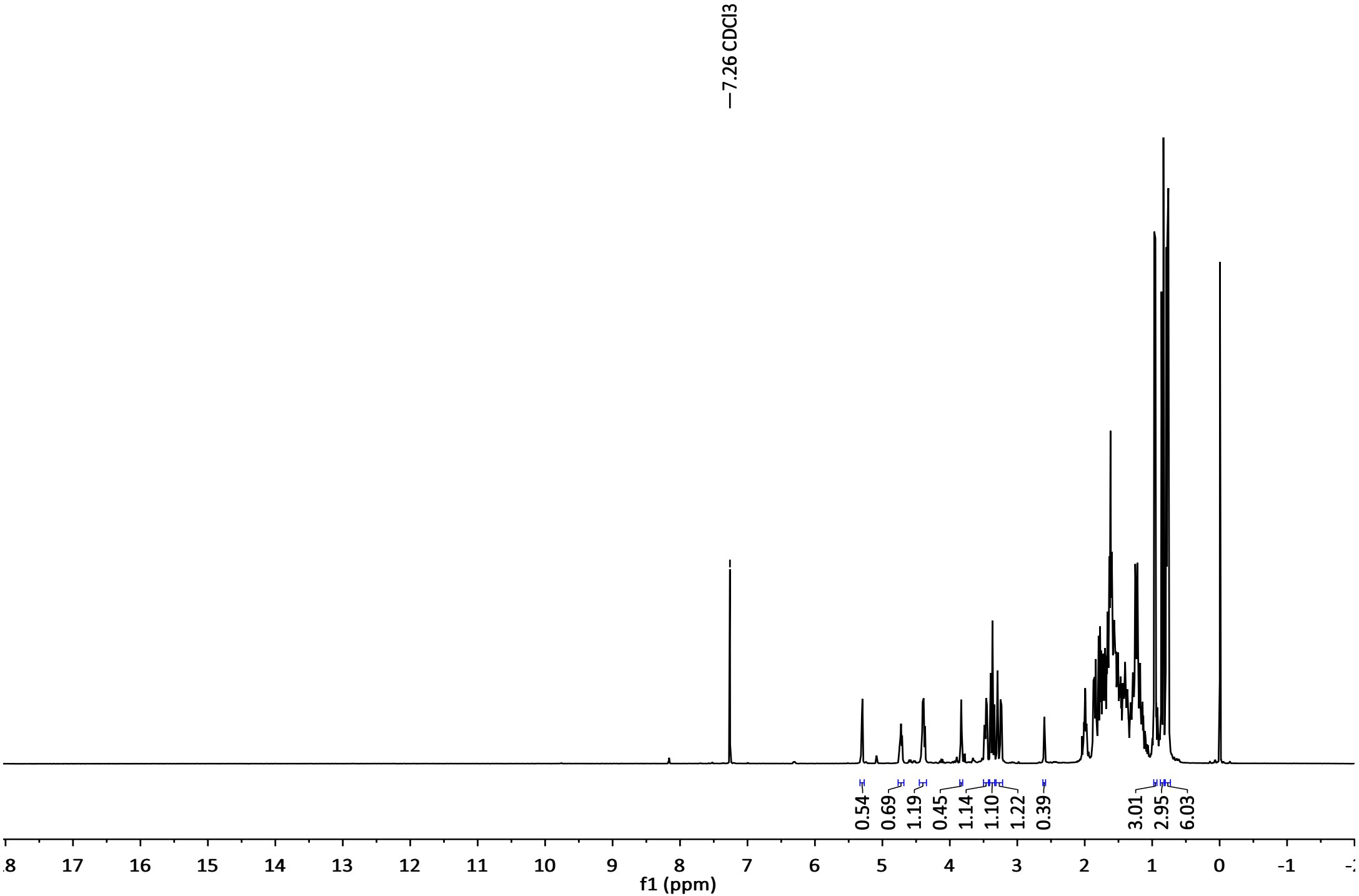

Figure S77. ^{1}H NMR spectrum of compound **21b** (400 MHz, $CDCl_3$)

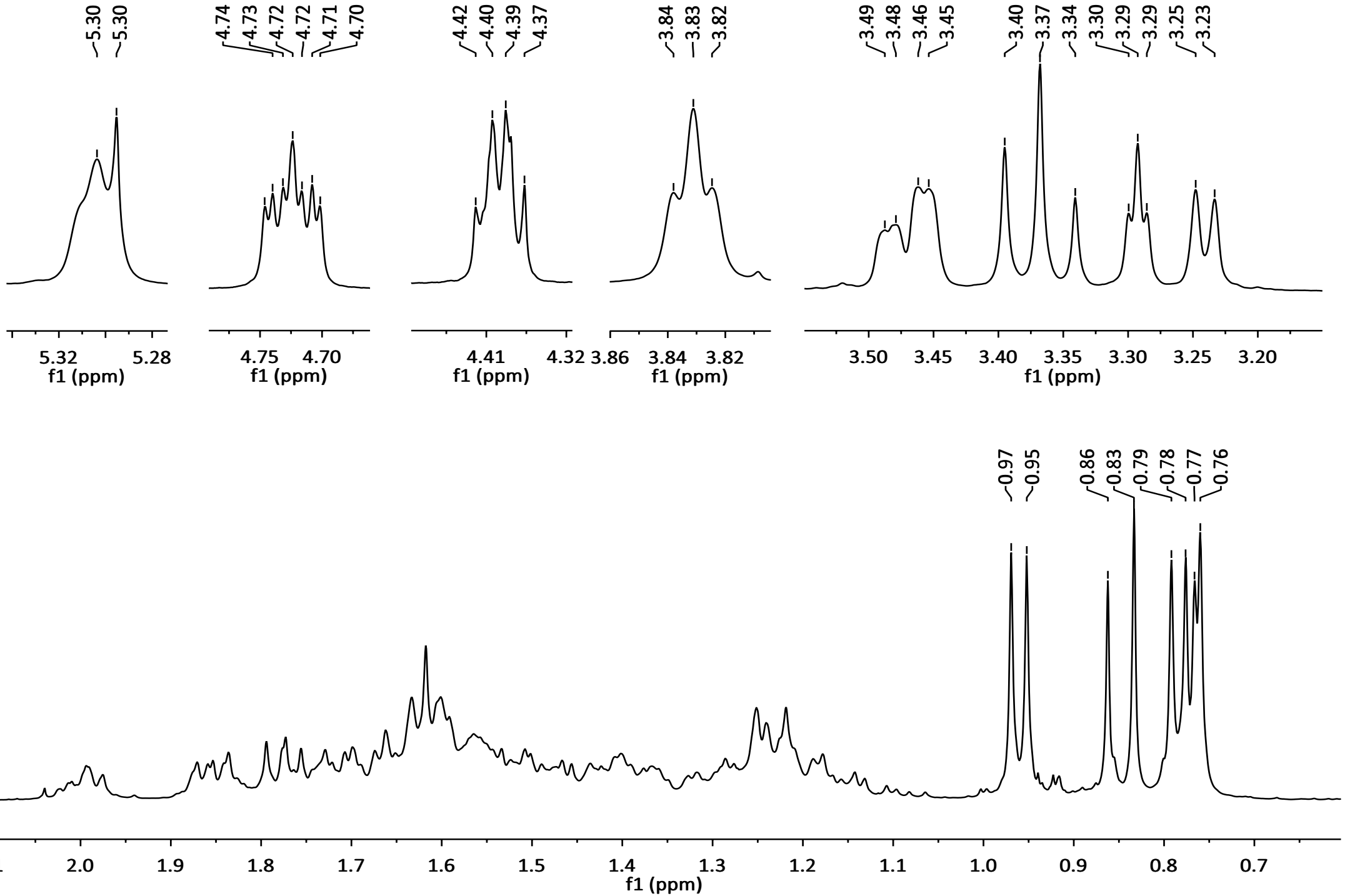

Figure S78. Sections for ^{1}H NMR spectrum of compound **21b** (400 MHz, $CDCl_3$)

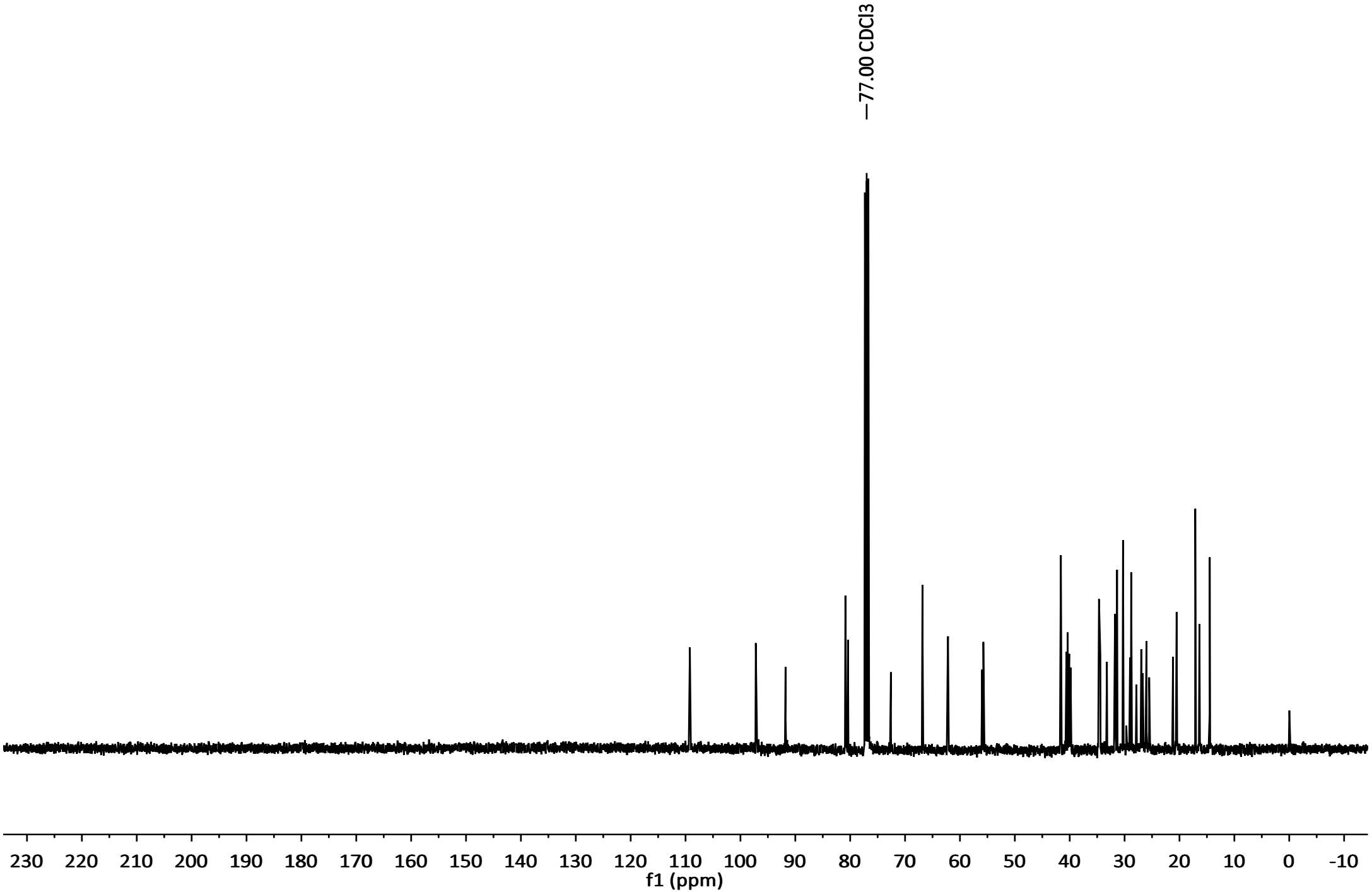

Figure S79. $^{13}C\{^{1}H\}$ NMR spectrum of compound **21b** (100 MHz, $CDCl_3$)

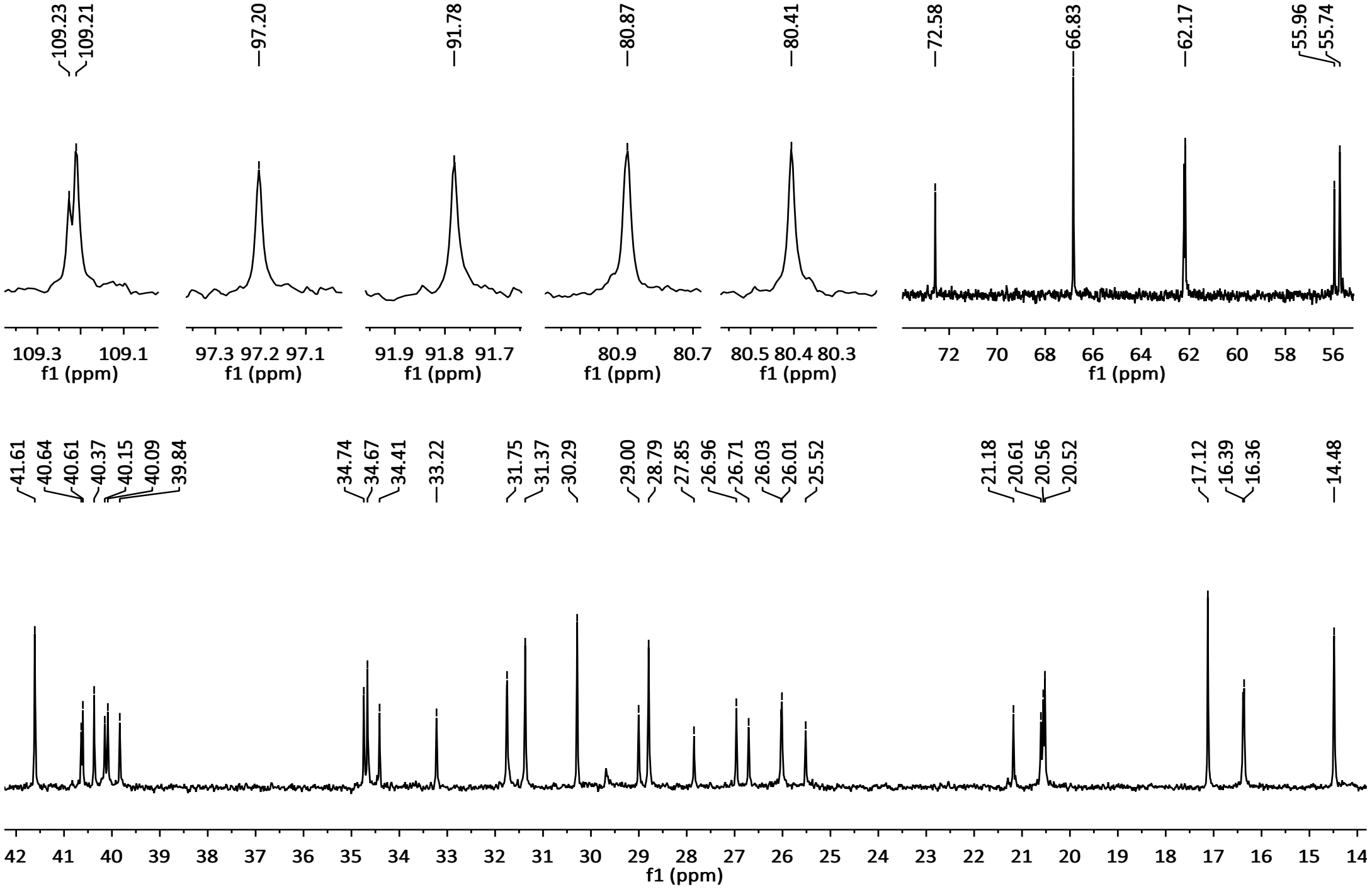

Figure S80. Sections for $^{13}C\{^{1}H\}$ NMR spectrum of compound **21b** (100 MHz, $CDCl_3$)

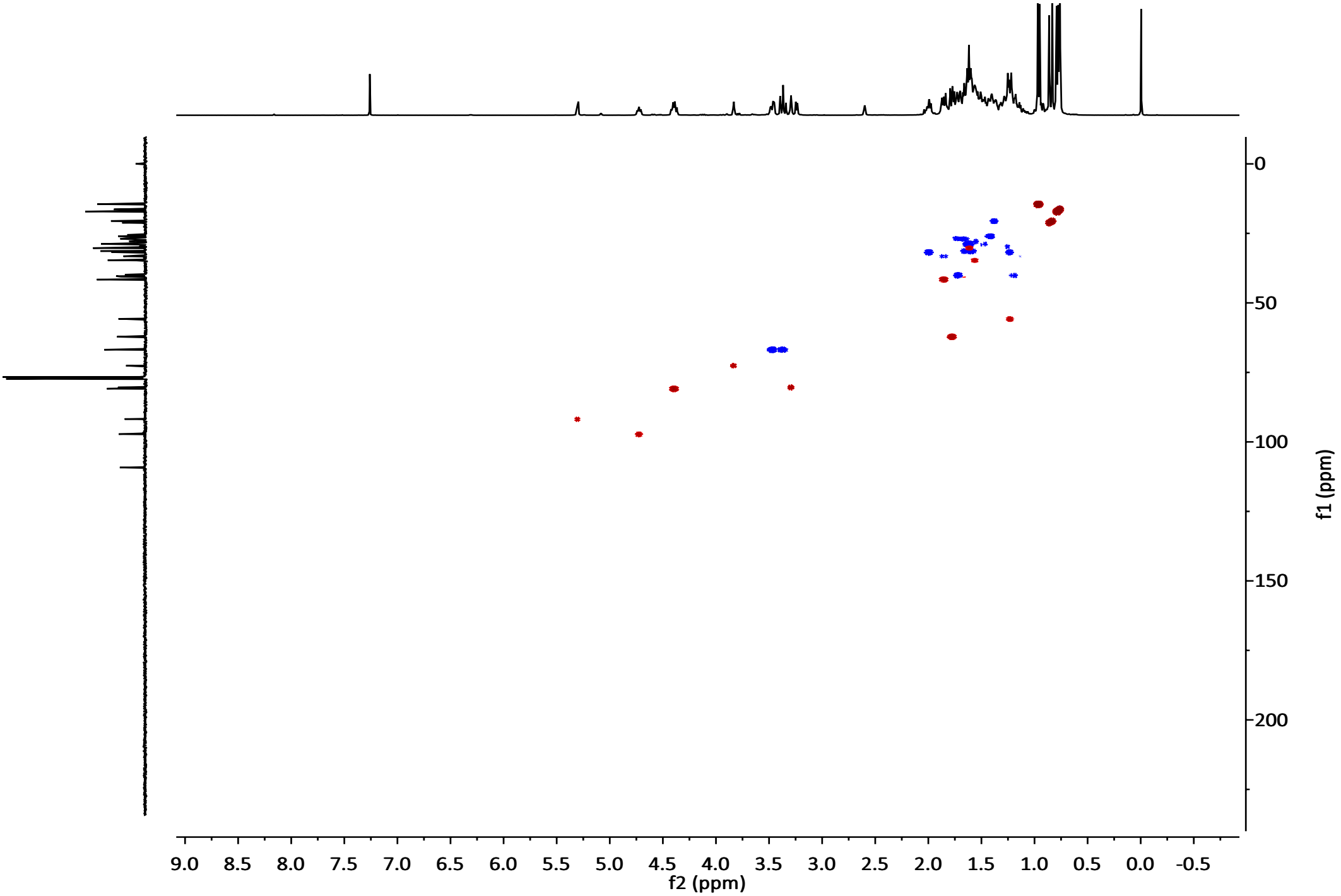

Figure S81. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21b** (400 MHz, $CDCl_3$)

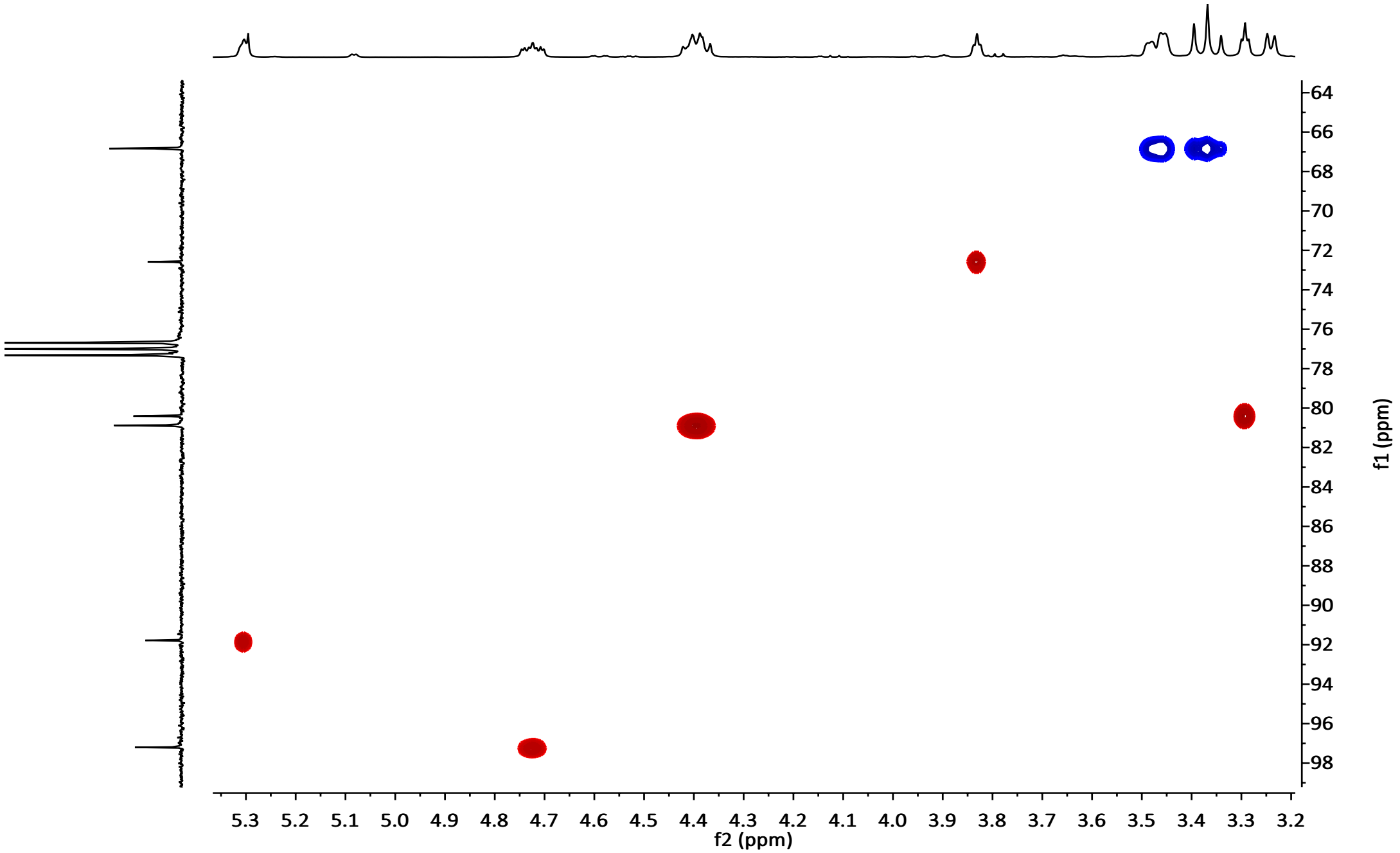

Figure S82. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21b** (400 MHz, $CDCl_3$)

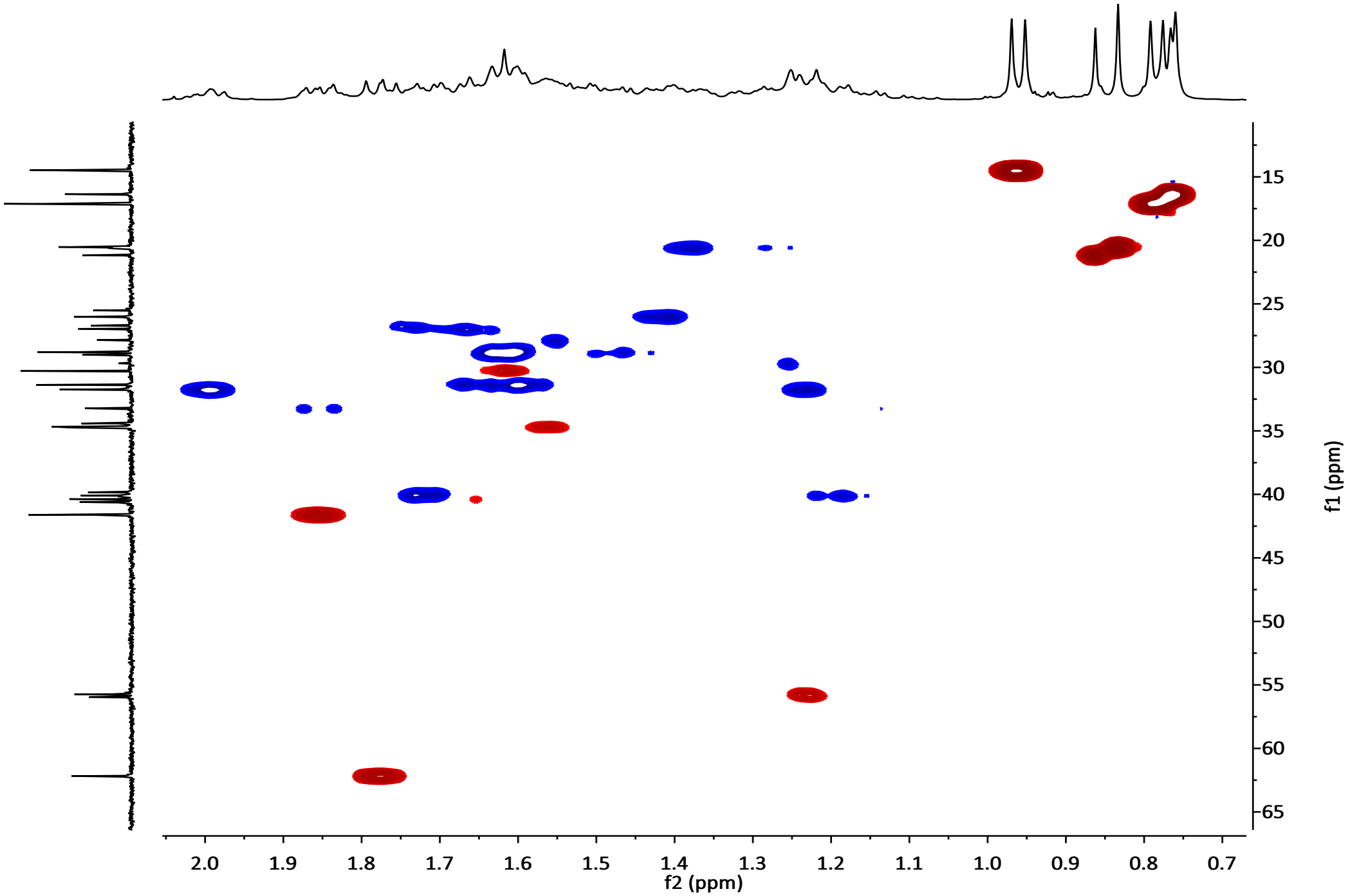

Figure S83. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **21b** (400 MHz, $CDCl_3$)

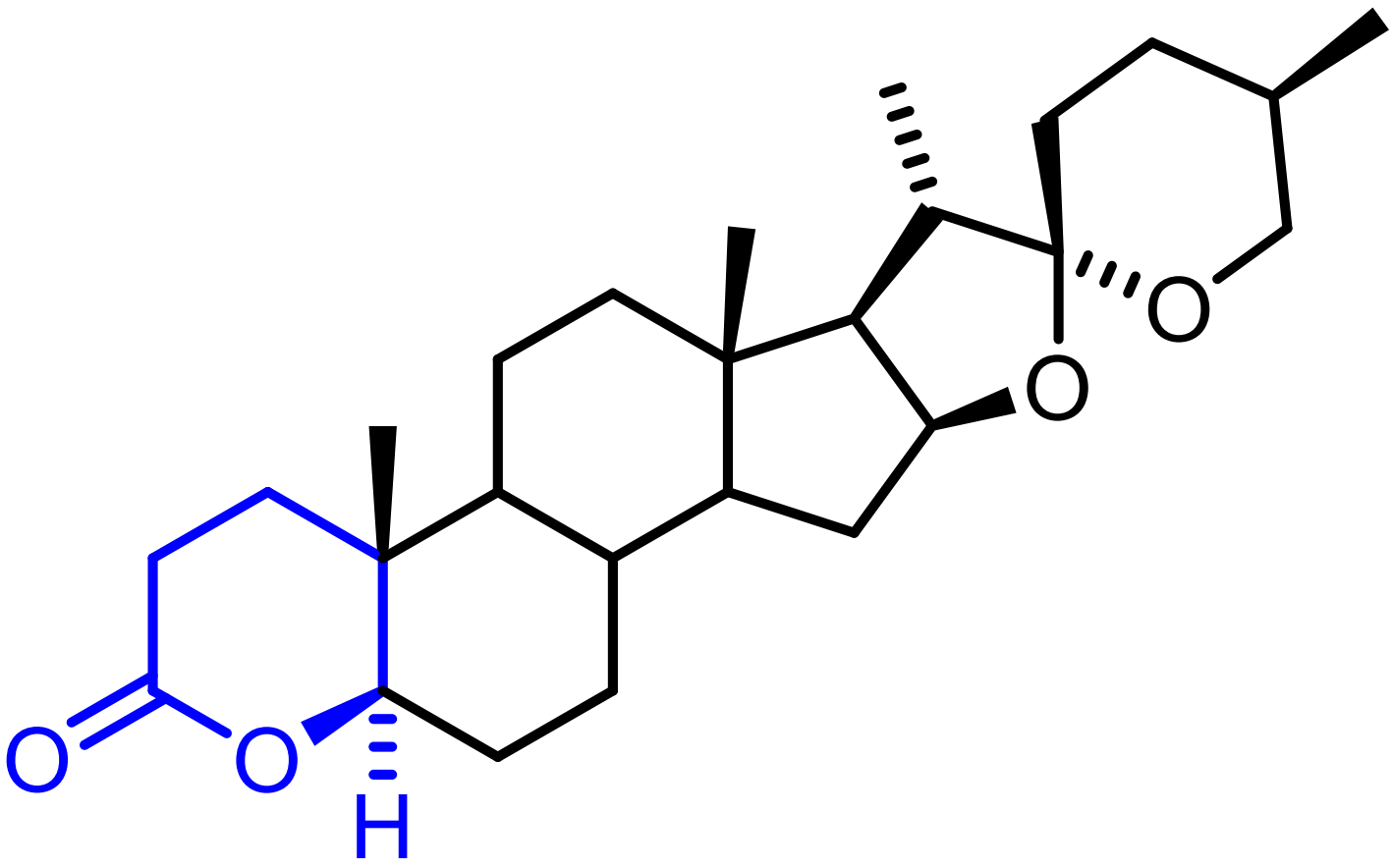

Figure S84. (25R)-4-Oxa-5α-spirostan-3-one **(20a)**

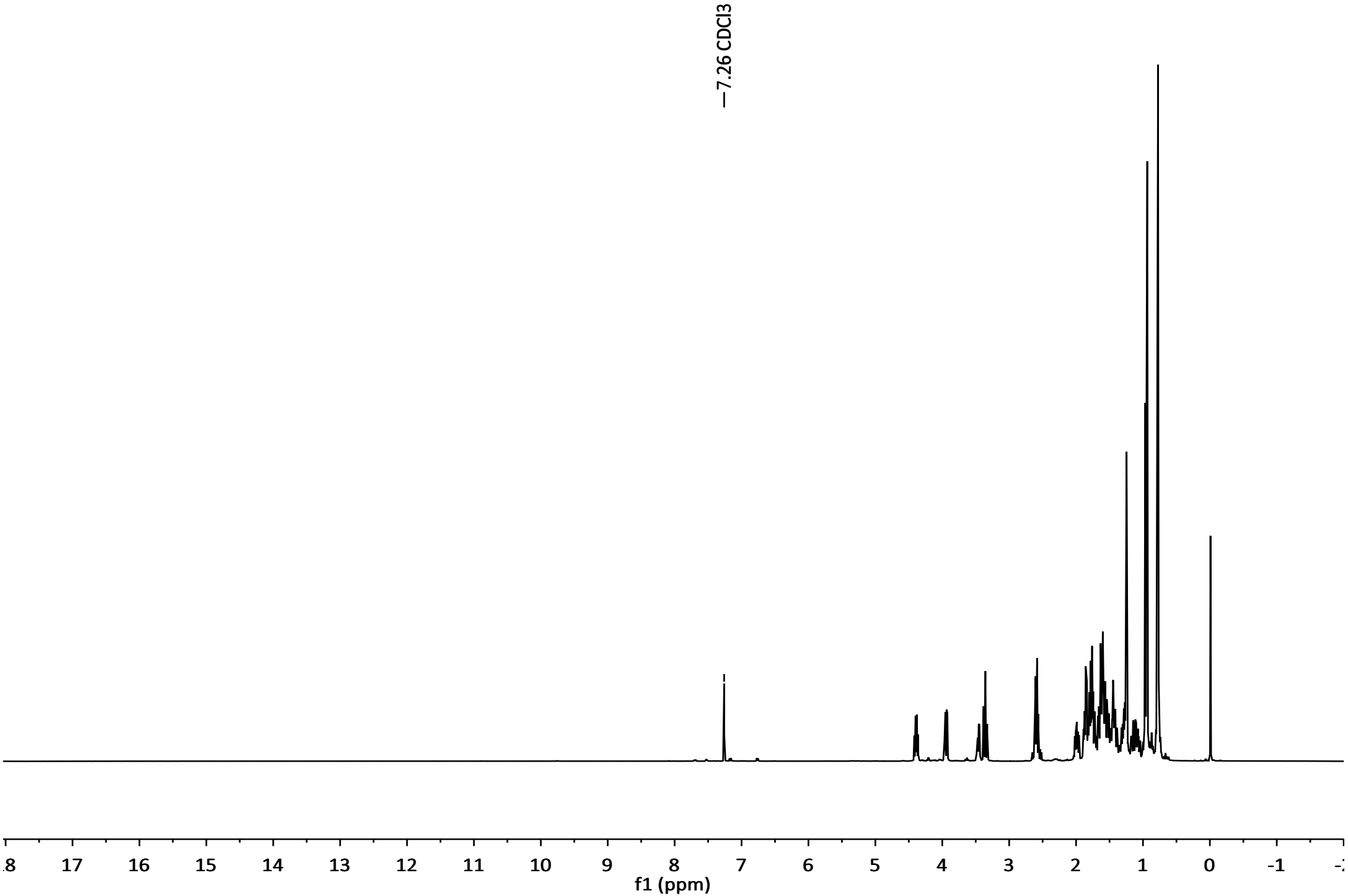

Figure S85. ^{1}H NMR spectrum of compound **20a** (400 MHz, $CDCl_3$)

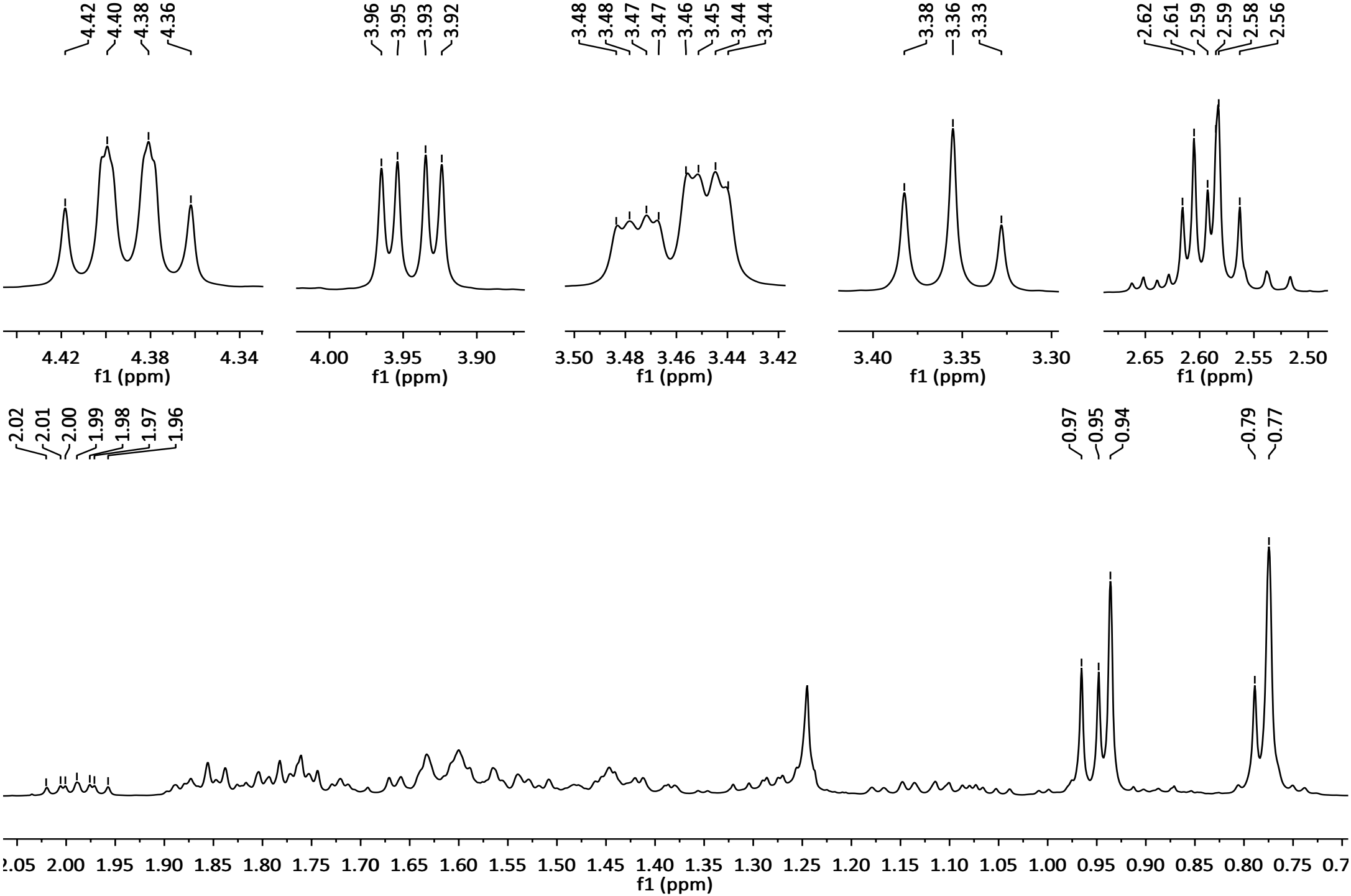

Figure S86. Sections for ^{1}H NMR spectrum of compound **20a** (400 MHz, $CDCl_3$)

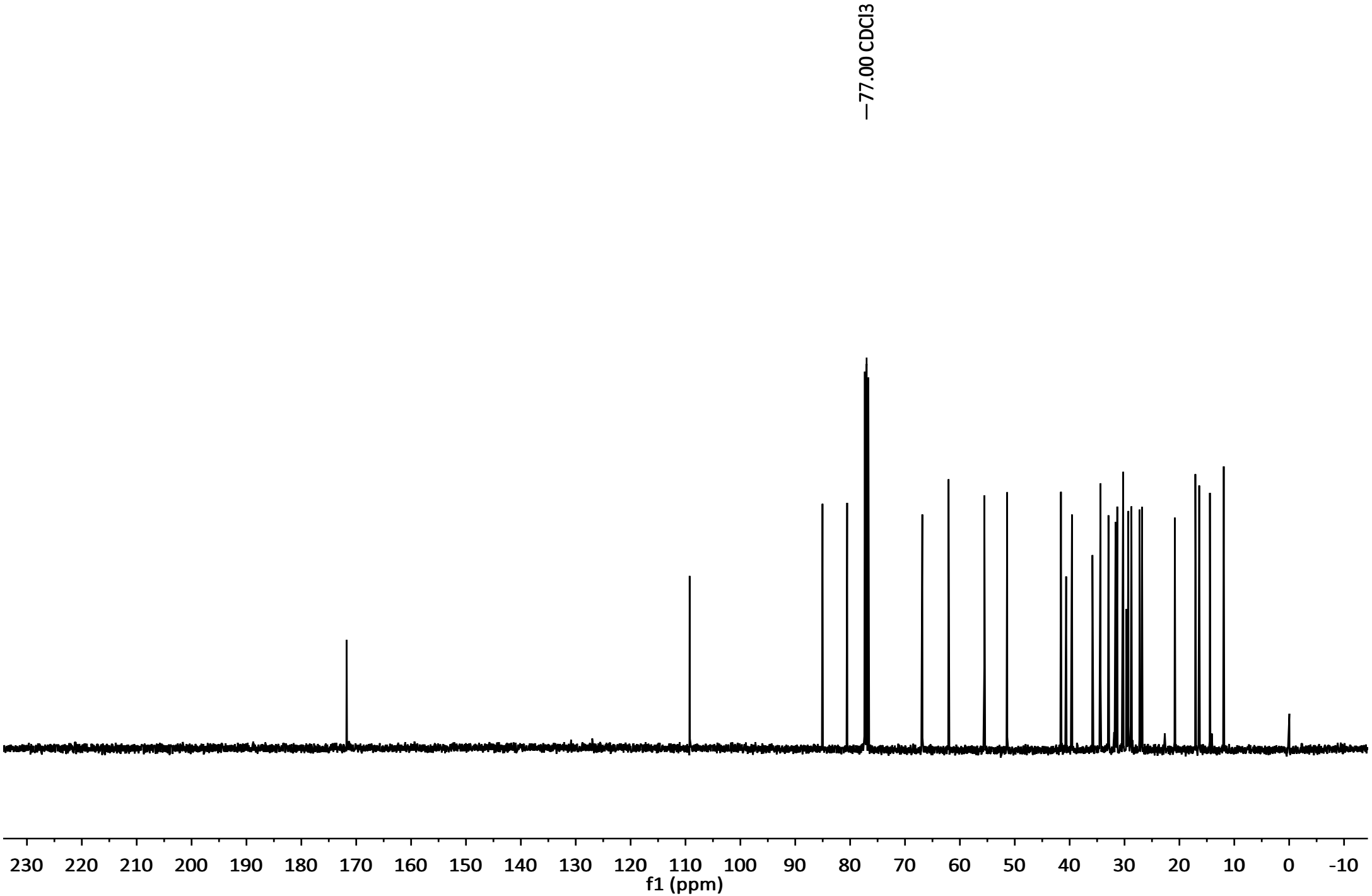

Figure S87. ^{13}C {^{1}H} NMR spectrum of compound **20a** (100 MHz, $CDCl_3$)

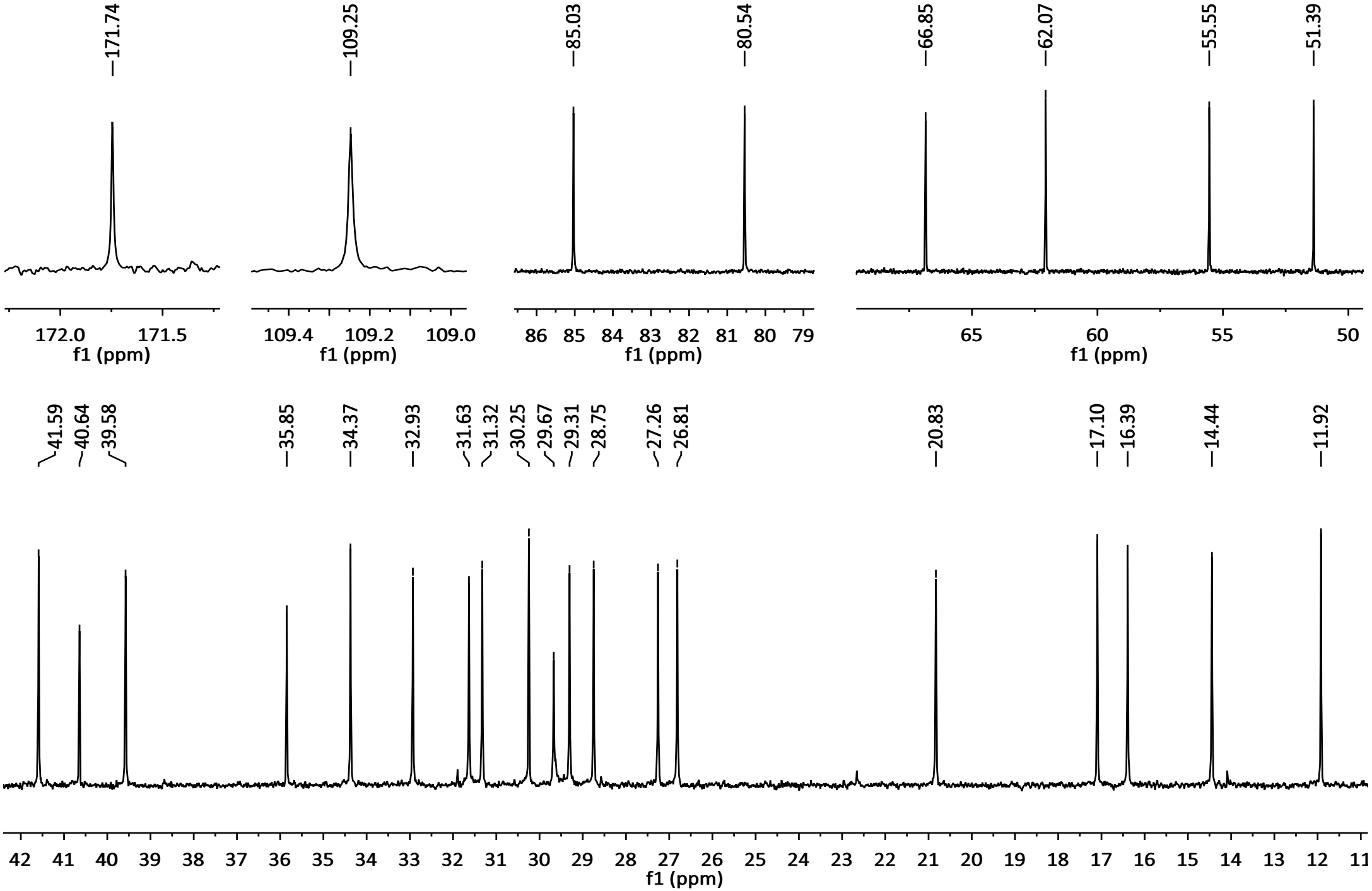

Figure S88. Sections for ^{13}C {^{1}H} NMR spectrum of compound **20a** (100 MHz, $CDCl_3$)

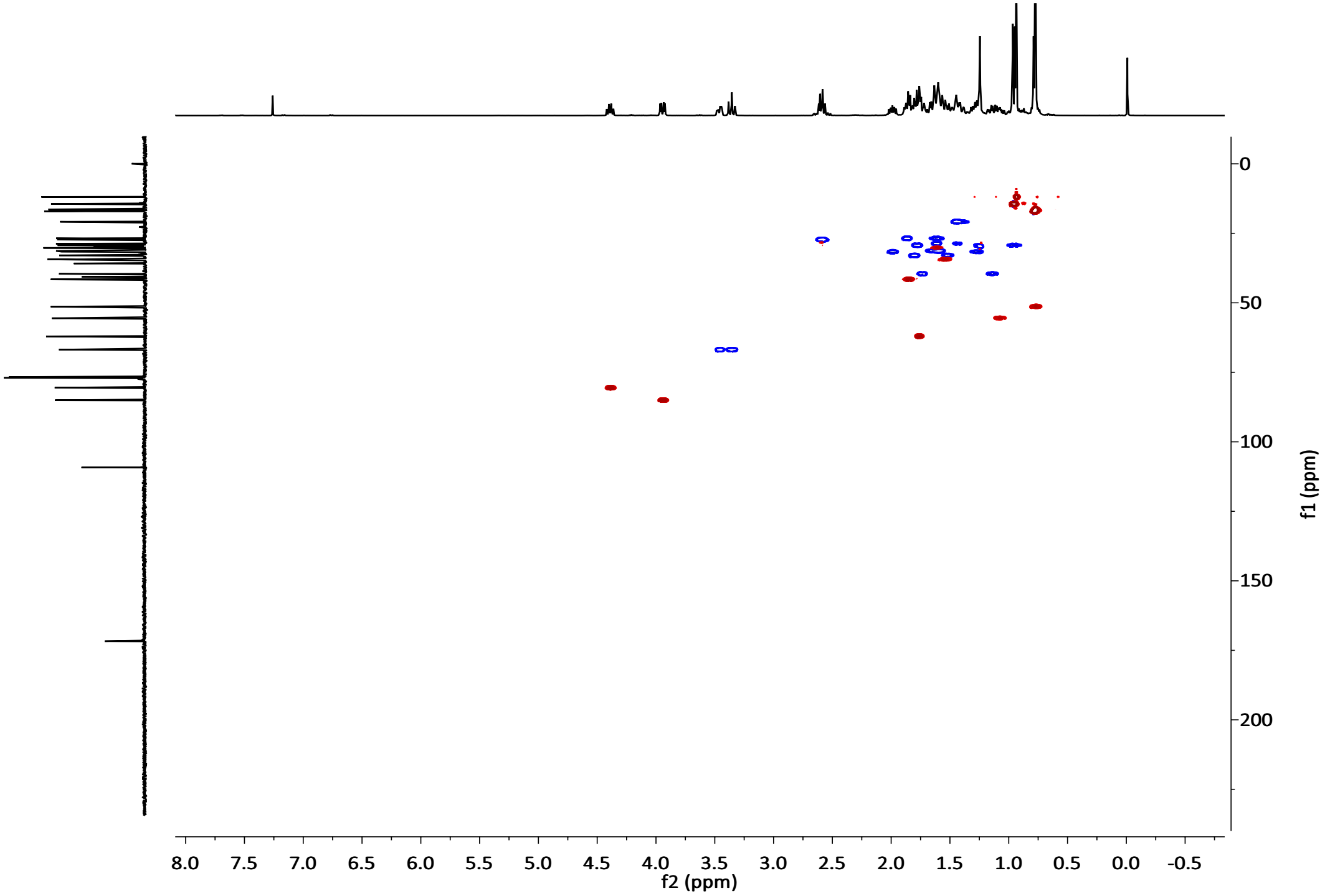

Figure S89. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20a** (400 MHz, $CDCl_3$)

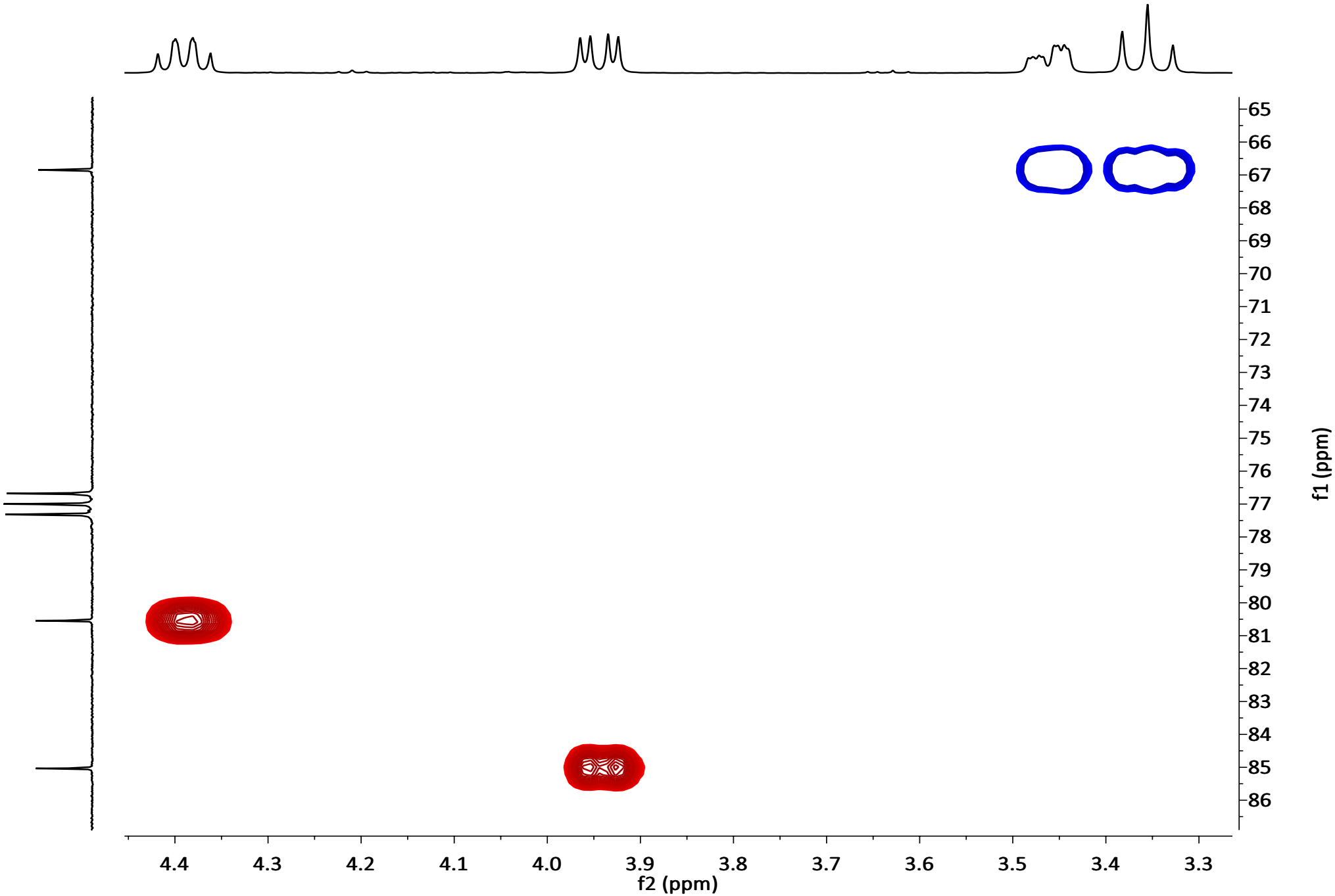

Figure S90. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20a** (400 MHz, $CDCl_3$)

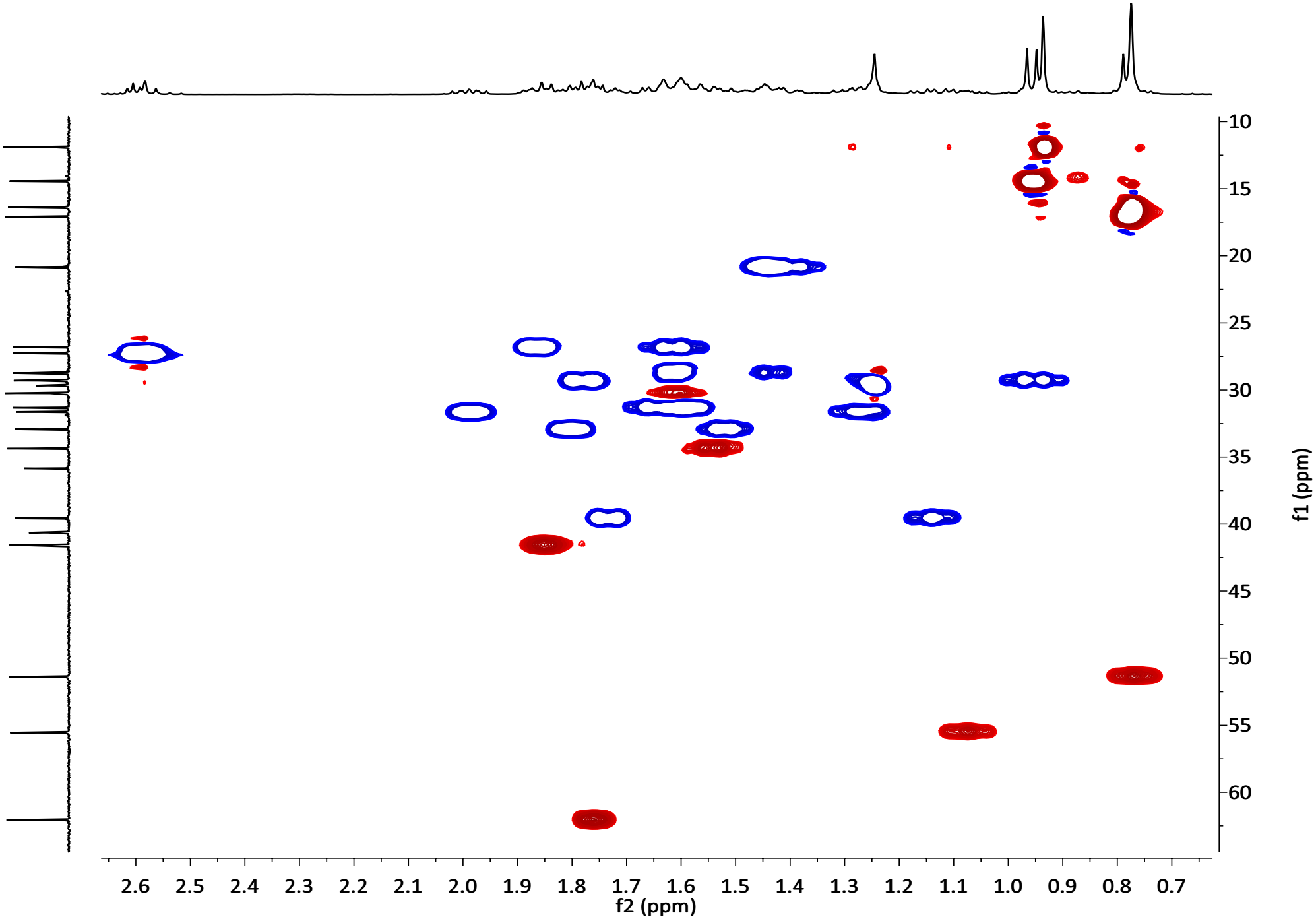

Figure S91. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20a** (400 MHz, $CDCl_3$)

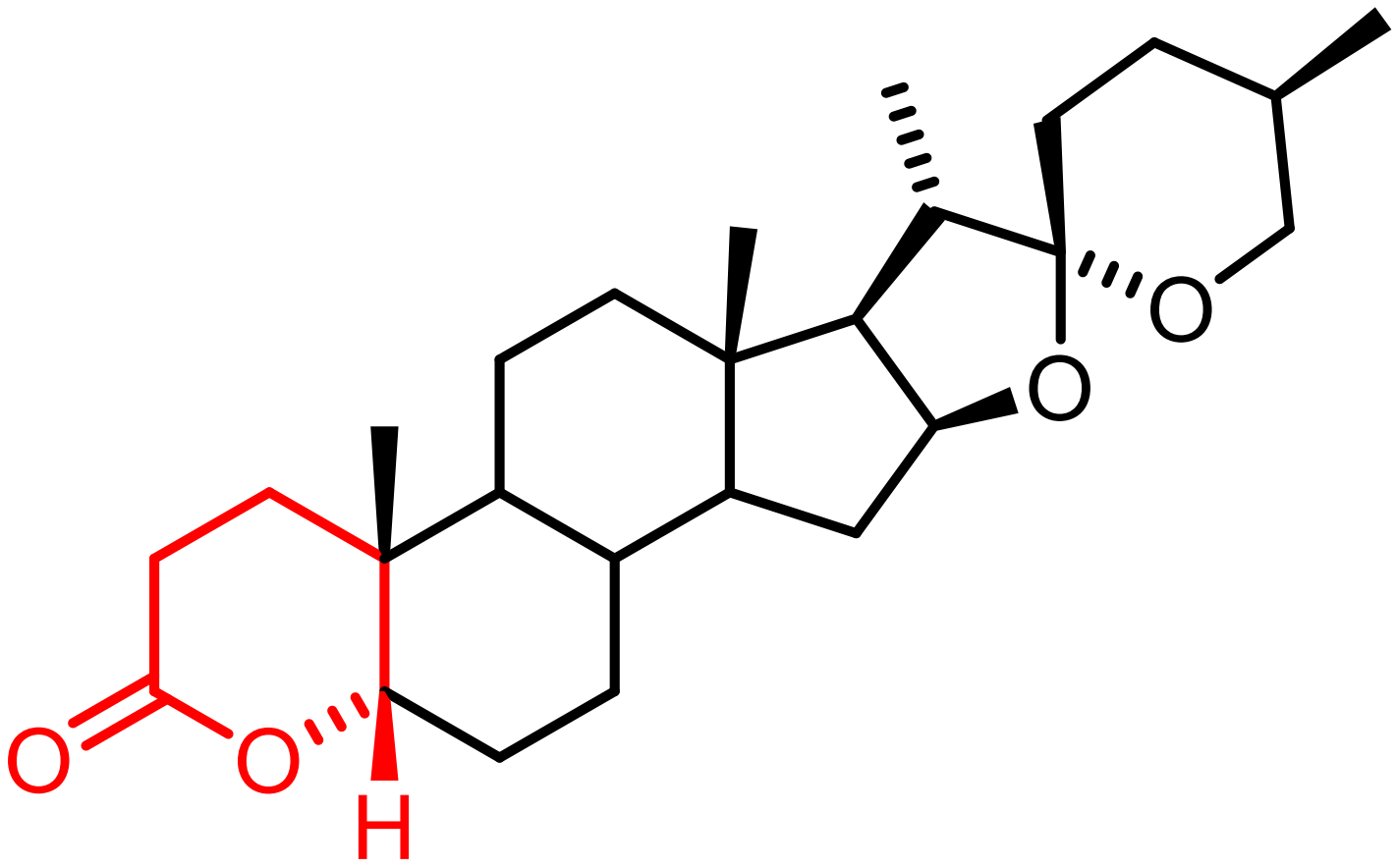

Figure S92. (25R)-4-Oxa-5β-spirostan-3-one **(20b)**

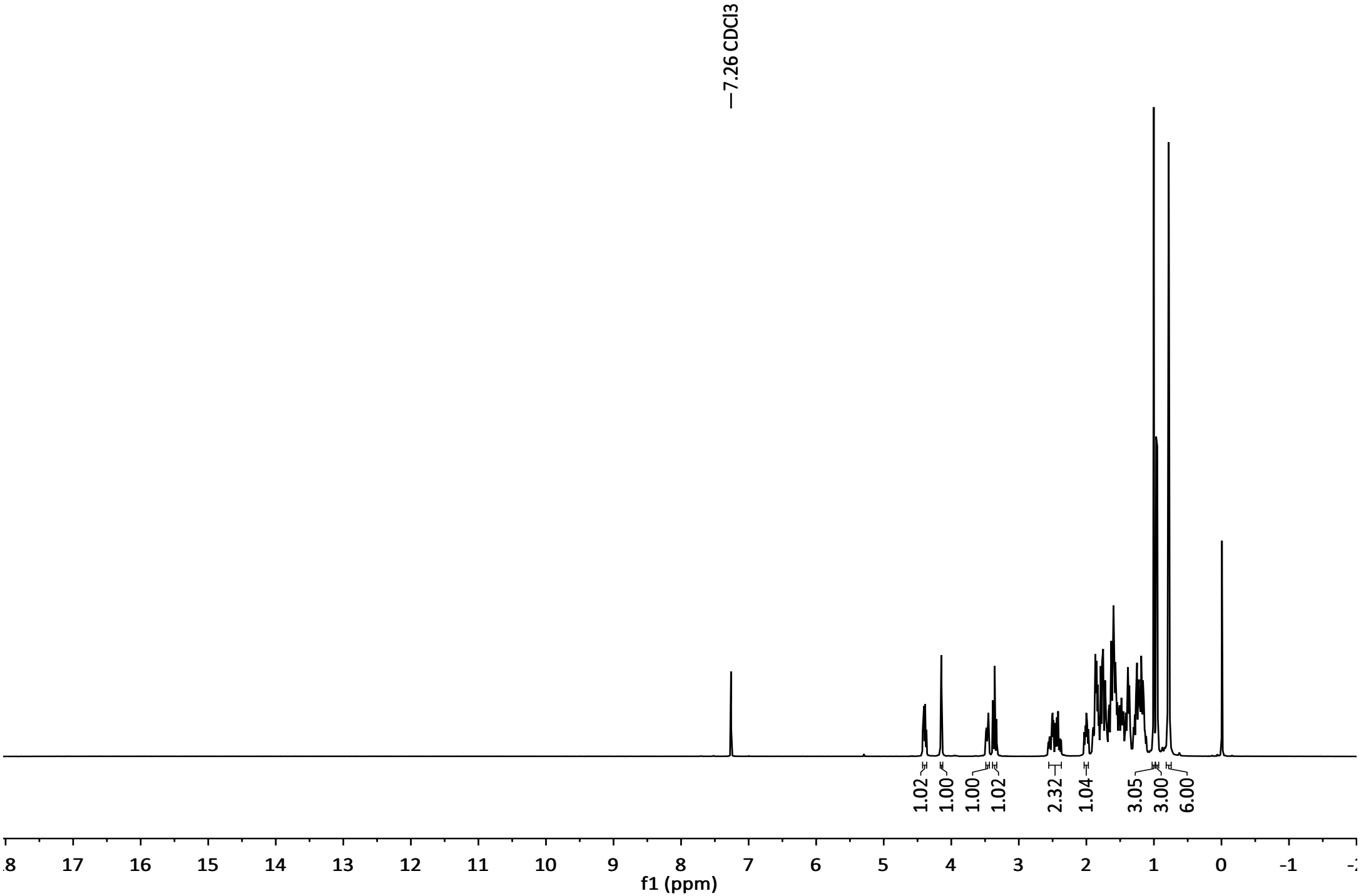

Figure S93. ^{1}H NMR spectrum of compound **20b** (400 MHz, $CDCl_3$)

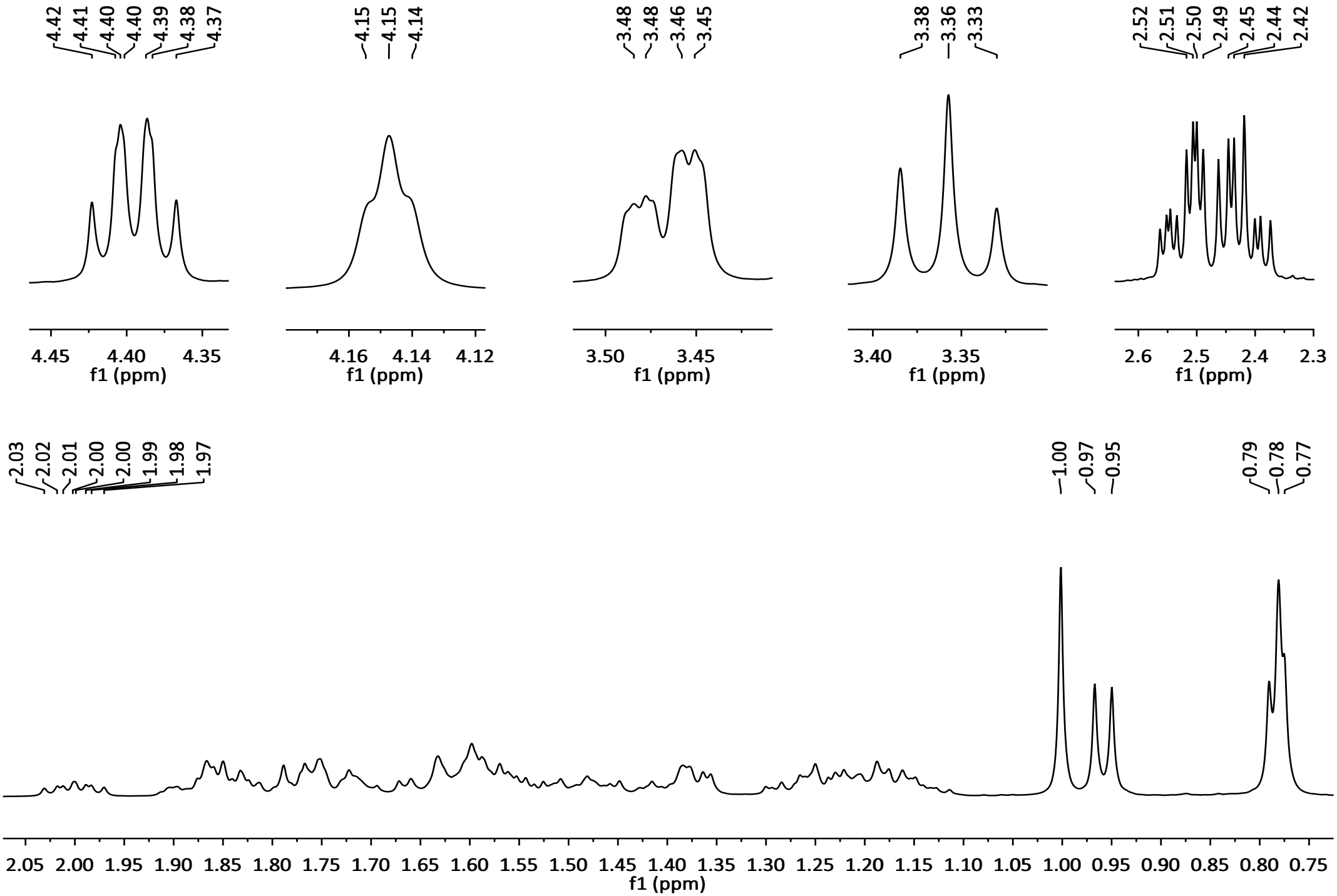

Figure S94. Sections for ^{1}H NMR spectrum of compound **20b** (400 MHz, $CDCl_3$)

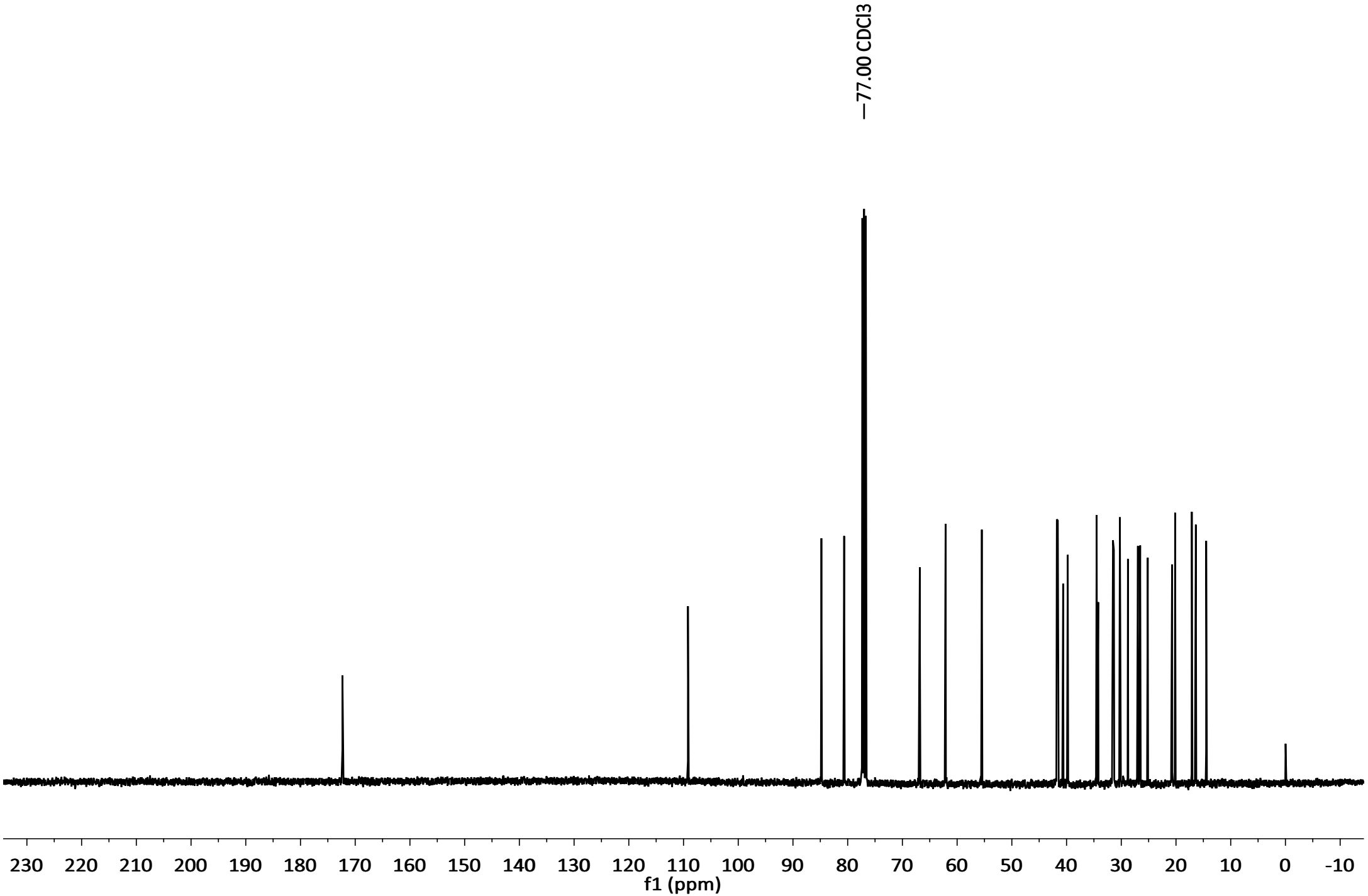

Figure S95. $^{13}C\{^{1}H\}$ NMR spectrum of compound **20b** (100 MHz, $CDCl_3$)

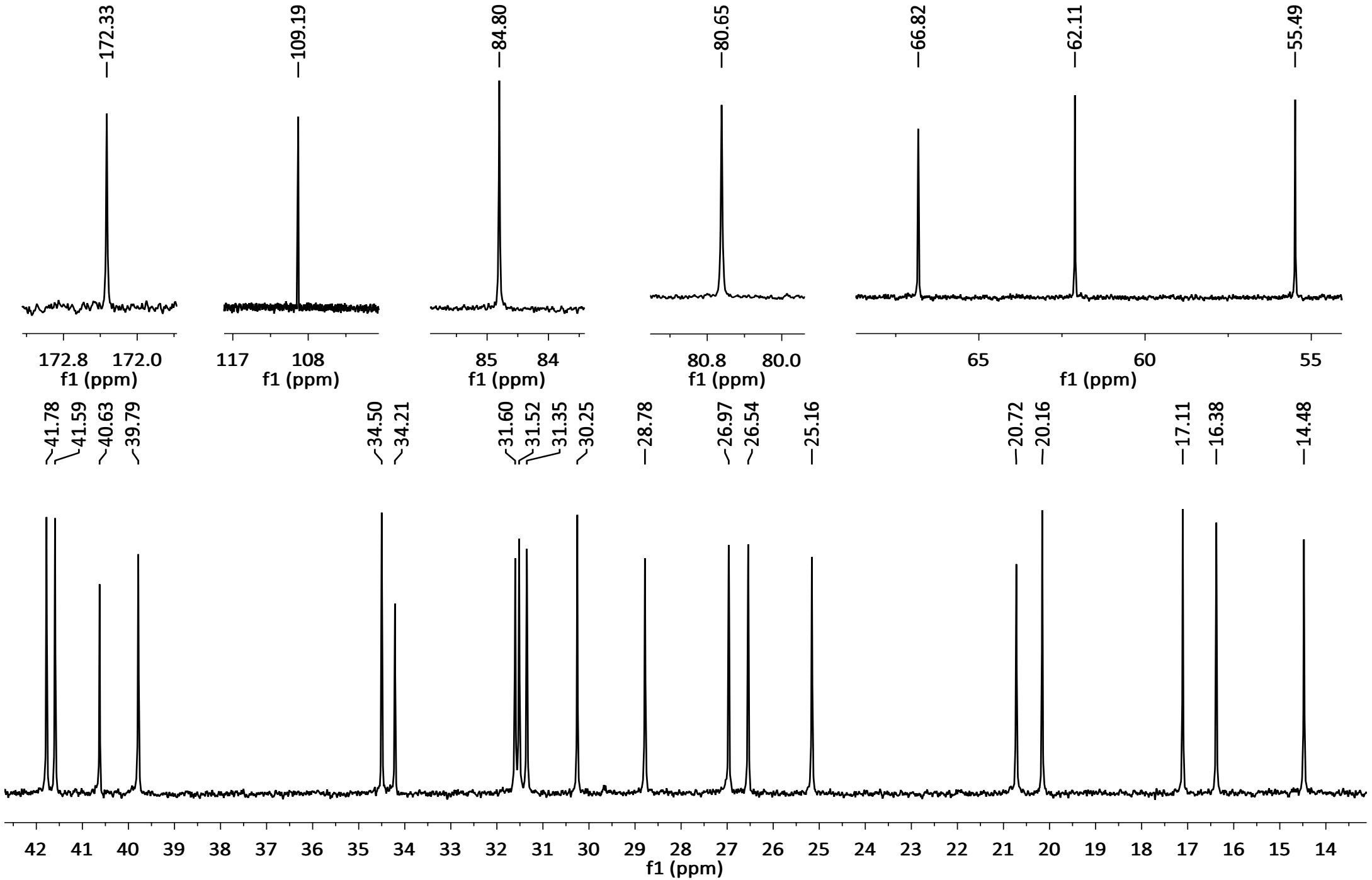

Figure S96. Sections for $^{13}C\{^{1}H\}$ NMR spectrum of compound **20b** (100 MHz, $CDCl_3$)

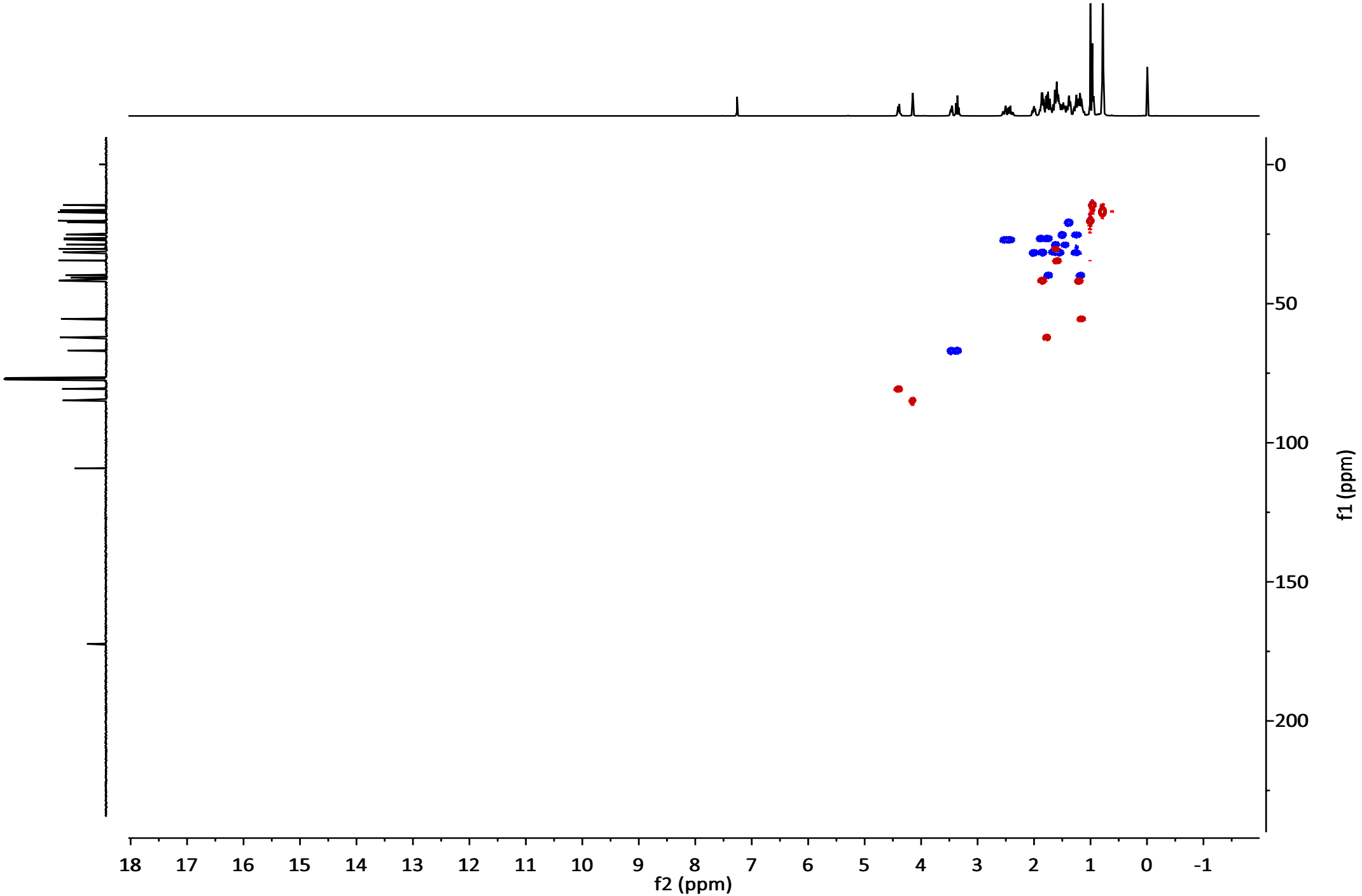

Figure S97. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20b** (400 MHz, $CDCl_3$)

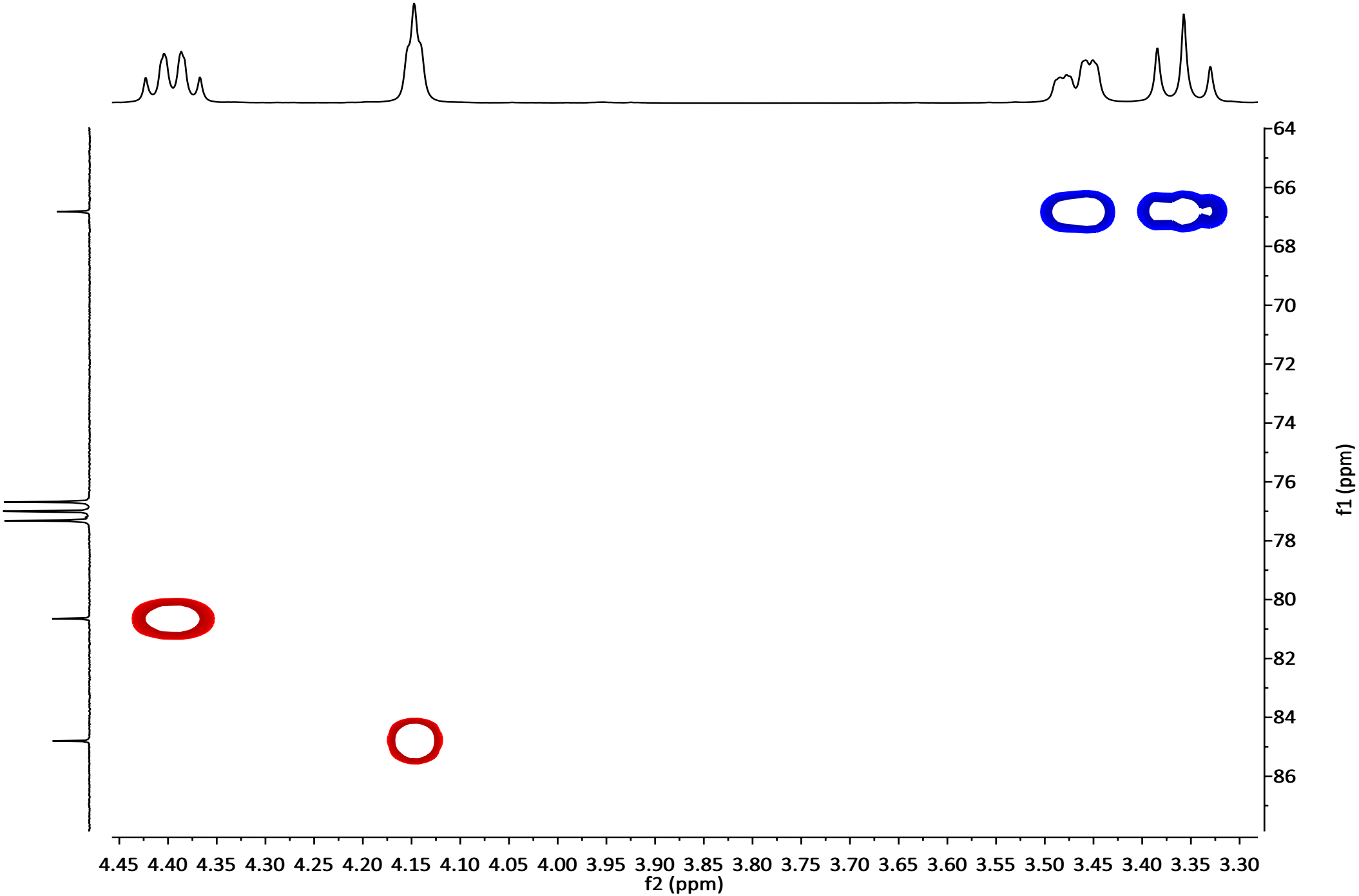

Figure S98. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20b** (400 MHz, $CDCl_3$)

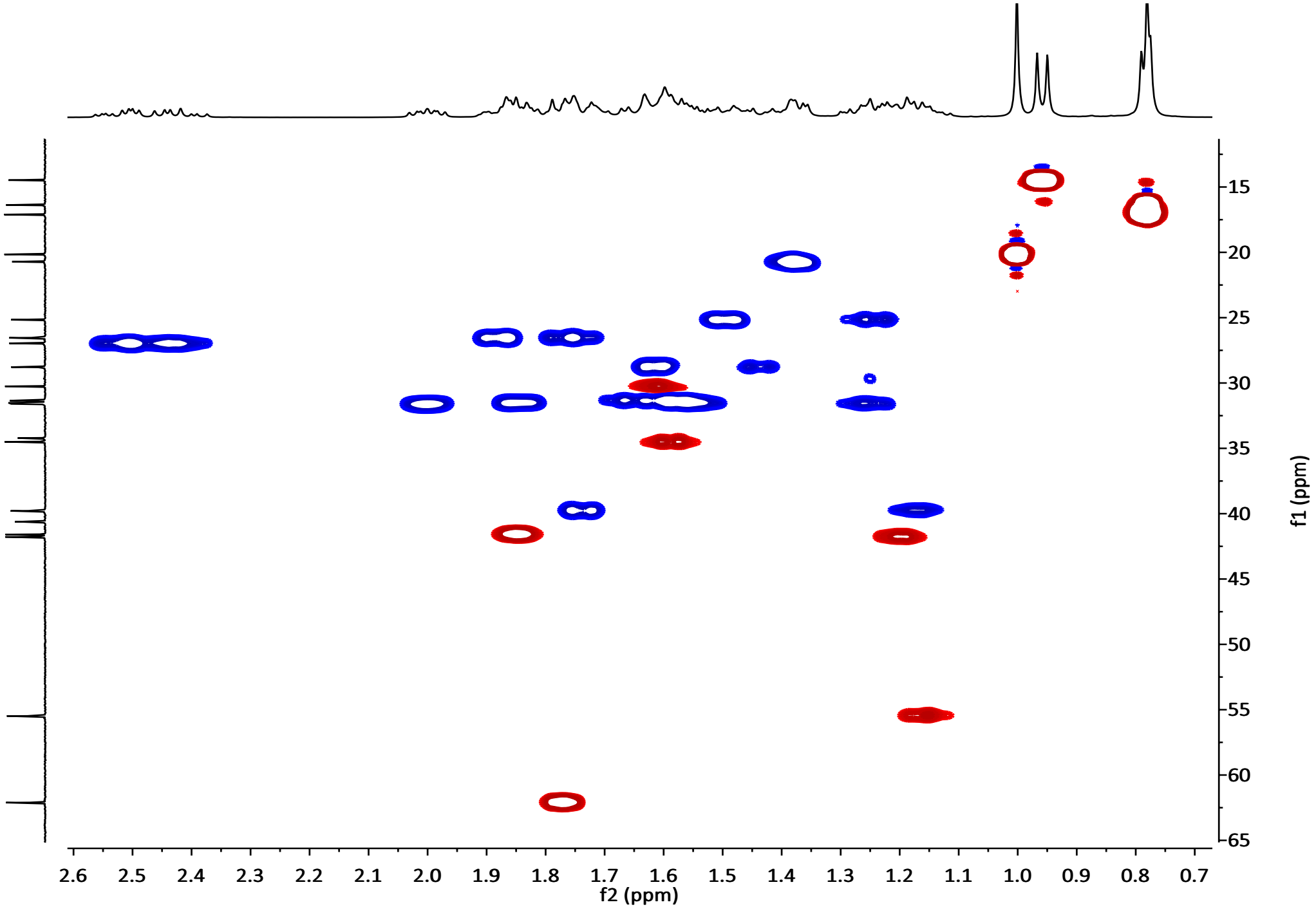

Figure S99. Section for ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR spectrum of compound **20b** (400 MHz, $CDCl_3$)

X-Ray data

Table S-1. Selected bond lengths [Å], angles [°] and torsion angles [°] for compounds **20a** and **20b**.

20a		**20b**	
Bond	[Å]	Bond	[Å]
(1)-C(2)	1.547(3)	C(1)-C(2)	1.523(4)
C(2)-C(3)	1.506(3)	C(2)-C(3)	1.499(4)
C(3)-O(1)	1.201(3)	C(3)-O(1)	1.207(3)
C(3)-O(4)	1.347(3)	C(3)-O(4)	1.352(3)
C(5)-O(4)	1.465(2)	C(5)-O(4)	1.480(3)
C(5)-C(6)	1.514(3)	C(5)-C(6)	1.514(4)
C(5)-C(10)	1.537(3)	C(5)-C(10)	1.533(4)
Angle	[°]	Angle	[°]
C(2)-C(1)-C(10)	112.86(18)	C(2)-C(1)-C(10)	111.9(2)
C(3)-C(2)-C(1)	113.9(2)	C(3)-C(2)-C(1)	115.2(2)
O(1)-C(3)-O(4)	120.3(2)	O(1)-C(3)-O(4)	117.7(3)
O(4)-C(3)-C(2)	115.24(18)	O(4)-C(3)-C(2)	119.3(2)
O(4)-C(5)-C(6)	106.64(16)	O(4)-C(5)-C(6)	104.4(2)
O(4)-C(5)-C(10)	110.05(16)	O(4)-C(5)-C(10)	112.5(2)
C(3)-O(4)-C(5)	117.35(16)	C(3)-O(4)-C(5)	123.1(2)
Torsion angle	[°]	Torsion angle	[°]
C(10)-C(1)-C(2)-C(3)	27.0(3)	C(10)-C(1)-C(2)-C(3)	42.7(3)
C(1)-C(2)-C(3)-O(4)	-48.3(3)	C(1)-C(2)-C(3)-O(4)	-18.7(4)
O(4)-C(5)-C(10)-C(1)	-64.6(2)	O(4)-C(5)-C(10)-C(1)	54.7(3)
C(6)-C(5)-O(4)-C(3)	173.06(18)	C(6)-C(5)-O(4)-C(3)	-159.5(2)

Table S-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **20a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2799(3)	11024(1)	2809(1)	41(1)
O(2)	6229(2)	5337(1)	4503(1)	23(1)
O(3)	6165(2)	5345(1)	5598(1)	22(1)
O(4)	3681(2)	9745(1)	2366(1)	27(1)
C(1)	175(3)	9019(2)	2328(1)	28(1)
C(2)	585(4)	9862(2)	2725(1)	31(1)
C(3)	2398(4)	10264(2)	2632(1)	30(1)
C(5)	3306(3)	8882(2)	2023(1)	24(1)
C(6)	5058(3)	8372(2)	2024(1)	26(1)
C(7)	5536(3)	8028(2)	2677(1)	22(1)
C(8)	4046(3)	7448(2)	2962(1)	19(1)
C(9)	2280(3)	7990(2)	2968(1)	19(1)
C(10)	1752(3)	8345(2)	2307(1)	22(1)
C(11)	793(3)	7454(2)	3302(1)	21(1)
C(12)	1320(3)	7159(2)	3967(1)	21(1)
C(13)	3034(3)	6592(2)	3963(1)	17(1)
C(14)	4478(3)	7166(2)	3632(1)	19(1)
C(15)	6195(3)	6630(2)	3763(1)	23(1)
C(16)	5932(3)	6312(2)	4437(1)	21(1)
C(17)	3945(3)	6443(2)	4608(1)	18(1)
C(18)	2715(4)	5668(2)	3627(1)	23(1)
C(19)	1261(4)	7559(2)	1857(1)	30(1)
C(20)	3491(3)	5590(2)	5010(1)	21(1)
C(21)	2683(3)	5824(2)	5647(1)	26(1)
C(22)	5257(3)	5056(2)	5040(1)	21(1)
C(23)	5113(4)	4016(2)	5023(1)	28(1)
C(24)	6945(4)	3567(2)	5078(1)	31(1)
C(25)	7920(4)	3923(2)	5656(1)	27(1)
C(26)	7925(3)	4968(2)	5643(1)	24(1)
C(27)	9820(4)	3569(2)	5698(2)	36(1)

Table S-3. Bond lengths [Å] and angles [°] for **20a**.

O(1)-C(3)	1.207(3)
O(2)-C(22)	1.420(3)
O(2)-C(16)	1.443(3)
O(3)-C(26)	1.438(3)
O(3)-C(22)	1.438(3)
O(4)-C(3)	1.352(3)
O(4)-C(5)	1.480(3)
C(1)-C(2)	1.523(4)
C(1)-C(10)	1.541(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.499(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(5)-C(6)	1.514(4)
C(5)-C(10)	1.533(4)
C(5)-H(5)	1.0000
C(6)-C(7)	1.527(4)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.530(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(14)	1.524(4)
C(8)-C(9)	1.547(3)
C(8)-H(8)	1.0000
C(9)-C(11)	1.539(3)
C(9)-C(10)	1.556(4)
C(9)-H(9)	1.0000
C(10)-C(19)	1.539(4)
C(11)-C(12)	1.537(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.533(3)

C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(18)	1.543(3)
C(13)-C(14)	1.544(3)
C(13)-C(17)	1.553(3)
C(14)-C(15)	1.536(3)
C(14)-H(14)	1.0000
C(15)-C(16)	1.527(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.552(3)
C(16)-H(16)	1.0000
C(17)-C(20)	1.548(3)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.528(4)
C(20)-C(22)	1.542(3)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.519(4)
C(23)-C(24)	1.532(4)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.528(4)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.521(4)
C(25)-C(27)	1.524(4)
C(25)-H(25)	1.0000

C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800

C(22)-O(2)-C(16)	106.32(18)
C(26)-O(3)-C(22)	112.50(19)
C(3)-O(4)-C(5)	123.1(2)
C(2)-C(1)-C(10)	111.9(2)
C(2)-C(1)-H(1A)	109.2
C(10)-C(1)-H(1A)	109.2
C(2)-C(1)-H(1B)	109.2
C(10)-C(1)-H(1B)	109.2
H(1A)-C(1)-H(1B)	107.9
C(3)-C(2)-C(1)	115.2(2)
C(3)-C(2)-H(2A)	108.5
C(1)-C(2)-H(2A)	108.5
C(3)-C(2)-H(2B)	108.5
C(1)-C(2)-H(2B)	108.5
H(2A)-C(2)-H(2B)	107.5
O(1)-C(3)-O(4)	117.7(3)
O(1)-C(3)-C(2)	123.0(3)
O(4)-C(3)-C(2)	119.3(2)
O(4)-C(5)-C(6)	104.4(2)
O(4)-C(5)-C(10)	112.5(2)
C(6)-C(5)-C(10)	114.5(2)
O(4)-C(5)-H(5)	108.4
C(6)-C(5)-H(5)	108.4
C(10)-C(5)-H(5)	108.4
C(5)-C(6)-C(7)	111.6(2)
C(5)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0

C(6)-C(7)-C(8)	111.8(2)
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
C(14)-C(8)-C(7)	111.4(2)
C(14)-C(8)-C(9)	108.2(2)
C(7)-C(8)-C(9)	110.69(19)
C(14)-C(8)-H(8)	108.8
C(7)-C(8)-H(8)	108.8
C(9)-C(8)-H(8)	108.8
C(11)-C(9)-C(8)	111.85(19)
C(11)-C(9)-C(10)	113.7(2)
C(8)-C(9)-C(10)	112.4(2)
C(11)-C(9)-H(9)	106.1
C(8)-C(9)-H(9)	106.1
C(10)-C(9)-H(9)	106.1
C(5)-C(10)-C(19)	108.4(2)
C(5)-C(10)-C(1)	106.0(2)
C(19)-C(10)-C(1)	107.8(2)
C(5)-C(10)-C(9)	109.5(2)
C(19)-C(10)-C(9)	112.4(2)
C(1)-C(10)-C(9)	112.4(2)
C(12)-C(11)-C(9)	112.4(2)
C(12)-C(11)-H(11A)	109.1
C(9)-C(11)-H(11A)	109.1
C(12)-C(11)-H(11B)	109.1
C(9)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.9
C(13)-C(12)-C(11)	111.3(2)
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12B)	109.4
C(11)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0

C(12)-C(13)-C(18)	109.9(2)
C(12)-C(13)-C(14)	107.7(2)
C(18)-C(13)-C(14)	111.6(2)
C(12)-C(13)-C(17)	116.3(2)
C(18)-C(13)-C(17)	111.1(2)
C(14)-C(13)-C(17)	99.85(18)
C(8)-C(14)-C(15)	119.2(2)
C(8)-C(14)-C(13)	115.2(2)
C(15)-C(14)-C(13)	103.6(2)
C(8)-C(14)-H(14)	105.9
C(15)-C(14)-H(14)	105.9
C(13)-C(14)-H(14)	105.9
C(16)-C(15)-C(14)	102.5(2)
C(16)-C(15)-H(15A)	111.3
C(14)-C(15)-H(15A)	111.3
C(16)-C(15)-H(15B)	111.3
C(14)-C(15)-H(15B)	111.3
H(15A)-C(15)-H(15B)	109.2
O(2)-C(16)-C(15)	111.7(2)
O(2)-C(16)-C(17)	104.31(19)
C(15)-C(16)-C(17)	108.0(2)
O(2)-C(16)-H(16)	110.9
C(15)-C(16)-H(16)	110.9
C(17)-C(16)-H(16)	110.9
C(20)-C(17)-C(16)	104.19(19)
C(20)-C(17)-C(13)	120.4(2)
C(16)-C(17)-C(13)	103.61(19)
C(20)-C(17)-H(17)	109.3
C(16)-C(17)-H(17)	109.3
C(13)-C(17)-H(17)	109.3
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(22)	114.8(2)
C(21)-C(20)-C(17)	113.8(2)
C(22)-C(20)-C(17)	103.65(19)
C(21)-C(20)-H(20)	108.1
C(22)-C(20)-H(20)	108.1
C(17)-C(20)-H(20)	108.1
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(2)-C(22)-O(3)	109.93(18)
O(2)-C(22)-C(23)	107.8(2)
O(3)-C(22)-C(23)	110.1(2)
O(2)-C(22)-C(20)	105.5(2)
O(3)-C(22)-C(20)	107.3(2)
C(23)-C(22)-C(20)	116.1(2)
C(22)-C(23)-C(24)	111.1(2)
C(22)-C(23)-H(23A)	109.4
C(24)-C(23)-H(23A)	109.4
C(22)-C(23)-H(23B)	109.4
C(24)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0
C(25)-C(24)-C(23)	110.4(2)
C(25)-C(24)-H(24A)	109.6
C(23)-C(24)-H(24A)	109.6
C(25)-C(24)-H(24B)	109.6
C(23)-C(24)-H(24B)	109.6
H(24A)-C(24)-H(24B)	108.1

C(26)-C(25)-C(27)	109.7(2)
C(26)-C(25)-C(24)	109.0(2)
C(27)-C(25)-C(24)	112.6(2)
C(26)-C(25)-H(25)	108.5
C(27)-C(25)-H(25)	108.5
C(24)-C(25)-H(25)	108.5
O(3)-C(26)-C(25)	112.3(2)
O(3)-C(26)-H(26A)	109.1
C(25)-C(26)-H(26A)	109.1
O(3)-C(26)-H(26B)	109.1
C(25)-C(26)-H(26B)	109.1
H(26A)-C(26)-H(26B)	107.9
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **20a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	66(2)	24(1)	33(1)	-1(1)	12(1)	-5(1)
O(2)	26(1)	21(1)	21(1)	1(1)	2(1)	5(1)
O(3)	23(1)	22(1)	21(1)	-2(1)	-4(1)	2(1)
O(4)	32(1)	19(1)	29(1)	3(1)	2(1)	-2(1)
C(1)	25(1)	33(2)	27(2)	11(1)	-3(1)	0(1)
C(2)	33(2)	31(2)	28(2)	9(1)	3(1)	9(1)
C(3)	43(2)	26(2)	20(1)	9(1)	1(1)	3(1)
C(5)	30(1)	23(1)	19(1)	2(1)	0(1)	-3(1)
C(6)	28(1)	25(1)	25(2)	3(1)	6(1)	-3(1)
C(7)	22(1)	21(1)	24(2)	0(1)	3(1)	0(1)
C(8)	20(1)	16(1)	20(1)	-1(1)	2(1)	0(1)
C(9)	20(1)	16(1)	19(1)	-1(1)	-2(1)	-1(1)
C(10)	24(1)	23(1)	19(1)	2(1)	-2(1)	-1(1)
C(11)	18(1)	24(1)	20(1)	0(1)	0(1)	0(1)
C(12)	20(1)	23(1)	19(1)	1(1)	1(1)	-2(1)
C(13)	17(1)	17(1)	17(1)	-1(1)	1(1)	1(1)
C(14)	19(1)	17(1)	20(1)	-3(1)	1(1)	-1(1)
C(15)	19(1)	25(1)	24(2)	3(1)	2(1)	1(1)
C(16)	20(1)	19(1)	23(1)	-2(1)	0(1)	1(1)
C(17)	20(1)	16(1)	18(1)	-4(1)	0(1)	-2(1)
C(18)	29(1)	20(1)	21(1)	-1(1)	-2(1)	-5(1)
C(19)	36(2)	34(2)	22(2)	1(1)	-5(1)	-8(1)
C(20)	21(1)	20(1)	21(1)	-1(1)	-2(1)	-2(1)
C(21)	25(1)	29(1)	23(1)	2(1)	0(1)	1(1)
C(22)	26(1)	19(1)	19(1)	-1(1)	-1(1)	-1(1)
C(23)	35(1)	21(1)	29(2)	-1(1)	-7(1)	-2(1)
C(24)	43(2)	18(1)	31(2)	-2(1)	-7(1)	5(1)
C(25)	31(1)	25(1)	25(2)	2(1)	-2(1)	5(1)
C(26)	25(1)	24(1)	22(1)	-1(1)	-2(1)	1(1)
C(27)	38(2)	29(2)	40(2)	2(1)	-3(1)	9(1)

Table S-5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **20b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3867(1)	9908(3)	5410(1)	19(1)
C(1B)	-3305(1)	1619(3)	760(1)	23(1)
C(2)	4686(2)	9346(4)	5986(1)	31(1)
C(2B)	-4312(2)	2154(4)	503(1)	26(1)
C(3)	5089(1)	7503(3)	5896(1)	21(1)
C(3B)	-4610(2)	2568(3)	-216(1)	25(1)
C(5)	3530(1)	6593(3)	5515(1)	18(1)
C(5B)	-3237(1)	4308(3)	57(1)	18(1)
C(6)	3018(2)	4845(3)	5247(1)	21(1)
C(6B)	-2728(1)	5548(3)	-286(1)	21(1)
C(7)	2002(1)	5256(3)	5032(1)	20(1)
C(7B)	-1865(1)	6227(3)	214(1)	18(1)
C(8)	1763(1)	6850(3)	4542(1)	15(1)
C(8B)	-1272(1)	4616(3)	552(1)	15(1)
C(9)	2319(1)	8593(3)	4824(1)	14(1)
C(9B)	-1814(1)	3288(3)	867(1)	16(1)
C(10)	3354(1)	8224(3)	5034(1)	15(1)
C(10B)	-2707(1)	2588(3)	385(1)	17(1)
C(11)	2050(1)	10272(3)	4366(1)	19(1)
C(11B)	-1214(1)	1706(3)	1241(1)	22(1)
C(12)	1026(1)	10665(3)	4180(1)	18(1)
C(12B)	-385(1)	2444(3)	1766(1)	21(1)
C(13)	486(1)	8955(3)	3873(1)	14(1)
C(13B)	171(1)	3759(3)	1471(1)	16(1)
C(14)	761(1)	7341(3)	4365(1)	14(1)
C(14B)	-462(1)	5304(3)	1095(1)	15(1)
C(15)	53(1)	5849(3)	4081(1)	20(1)
C(15B)	193(1)	6732(3)	952(1)	19(1)
C(16)	-819(1)	6993(3)	3845(1)	18(1)
C(16B)	928(1)	6793(3)	1613(1)	17(1)
C(17)	-544(1)	9053(3)	3793(1)	16(1)

C(17B)	867(1)	4956(3)	1979(1)	16(1)
C(18)	674(1)	8508(3)	3219(1)	19(1)
C(18B)	623(1)	2681(3)	1028(1)	21(1)
C(19)	3709(1)	7804(3)	4445(1)	21(1)
C(19B)	-2541(2)	1262(3)	-131(1)	22(1)
C(20)	-1201(1)	9720(3)	3140(1)	18(1)
C(20B)	1858(1)	4330(3)	2251(1)	17(1)
C(21)	-1660(2)	11574(3)	3168(1)	26(1)
C(21B)	2105(2)	3663(3)	2959(1)	23(1)
C(22)	-1848(1)	8077(3)	2920(1)	18(1)
C(22B)	2395(1)	6005(3)	2120(1)	17(1)
C(23)	-2210(1)	7790(3)	2188(1)	20(1)
C(23B)	3300(1)	5567(3)	2004(1)	21(1)
C(24)	-2854(1)	6136(3)	2028(1)	22(1)
C(24B)	3795(2)	7331(3)	1920(1)	24(1)
C(25)	-3596(1)	6317(3)	2370(1)	21(1)
C(25B)	3884(2)	8636(3)	2495(1)	25(1)
C(26)	-3177(1)	6743(3)	3090(1)	22(1)
C(26B)	2951(2)	8948(3)	2580(1)	23(1)
C(27)	-4164(2)	4558(4)	2285(1)	30(1)
C(27B)	4315(2)	10477(4)	2400(2)	37(1)
O(1)	5885(1)	7213(3)	6012(1)	38(1)
O(1B)	-5289(1)	2003(3)	-603(1)	37(1)
O(2)	-1330(1)	6490(2)	3191(1)	18(1)
O(2B)	1827(1)	6824(2)	1540(1)	18(1)
O(3)	-2578(1)	8307(2)	3200(1)	20(1)
O(3B)	2512(1)	7241(2)	2660(1)	20(1)
O(4)	4492(1)	6112(2)	5706(1)	24(1)
O(4B)	-4067(1)	3726(2)	-429(1)	21(1)

Table S-6. Bond lengths [Å] and angles [°] for **20b**.

C(1)-C(2)	1.547(3)
C(1)-C(10)	1.548(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(1B)-C(2B)	1.544(3)
C(1B)-C(10B)	1.551(3)
C(1B)-H(1BA)	0.9900
C(1B)-H(1BB)	0.9900
C(2)-C(3)	1.506(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2B)-C(3B)	1.502(3)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
C(3)-O(1)	1.201(3)
C(3)-O(4)	1.347(3)
C(3B)-O(1B)	1.208(3)
C(3B)-O(4B)	1.351(3)
C(5)-O(4)	1.465(2)
C(5)-C(6)	1.514(3)
C(5)-C(10)	1.537(3)
C(5)-H(5)	1.0000
C(5B)-O(4B)	1.463(2)
C(5B)-C(6B)	1.511(3)
C(5B)-C(10B)	1.544(3)
C(5B)-H(5B)	1.0000
C(6)-C(7)	1.533(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(6B)-C(7B)	1.532(3)
C(6B)-H(6BA)	0.9900
C(6B)-H(6BB)	0.9900
C(7)-C(8)	1.530(3)
C(7)-H(7A)	0.9900

C(7)-H(7B)	0.9900
C(7B)-C(8B)	1.530(3)
C(7B)-H(7BA)	0.9900
C(7B)-H(7BB)	0.9900
C(8)-C(14)	1.526(3)
C(8)-C(9)	1.548(3)
C(8)-H(8)	1.0000
C(8B)-C(14B)	1.527(3)
C(8B)-C(9B)	1.548(3)
C(8B)-H(8B)	1.0000
C(9)-C(11)	1.539(3)
C(9)-C(10)	1.554(3)
C(9)-H(9)	1.0000
C(9B)-C(11B)	1.545(3)
C(9B)-C(10B)	1.552(3)
C(9B)-H(9B)	1.0000
C(10)-C(19)	1.537(3)
C(10B)-C(19B)	1.536(3)
C(11)-C(12)	1.543(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(11B)-C(12B)	1.537(3)
C(11B)-H(11C)	0.9900
C(11B)-H(11D)	0.9900
C(12)-C(13)	1.531(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(12B)-C(13B)	1.531(3)
C(12B)-H(12C)	0.9900
C(12B)-H(12D)	0.9900
C(13)-C(18)	1.539(3)
C(13)-C(14)	1.547(3)
C(13)-C(17)	1.552(3)
C(13B)-C(18B)	1.540(3)
C(13B)-C(14B)	1.550(3)
C(13B)-C(17B)	1.555(3)

C(14)-C(15)	1.534(3)
C(14)-H(14)	1.0000
C(14B)-C(15B)	1.535(3)
C(14B)-H(14B)	1.0000
C(15)-C(16)	1.538(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(15B)-C(16B)	1.540(3)
C(15B)-H(15C)	0.9900
C(15B)-H(15D)	0.9900
C(16)-O(2)	1.442(2)
C(16)-C(17)	1.561(3)
C(16)-H(16)	1.0000
C(16B)-O(2B)	1.439(2)
C(16B)-C(17B)	1.558(3)
C(16B)-H(16B)	1.0000
C(17)-C(20)	1.550(3)
C(17)-H(17)	1.0000
C(17B)-C(20B)	1.543(3)
C(17B)-H(17B)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20)-C(21)	1.525(3)
C(20)-C(22)	1.538(3)
C(20)-H(20)	1.0000
C(20B)-C(21B)	1.530(3)

C(20B)-C(22B)	1.537(3)
C(20B)-H(20B)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22)-O(2)	1.424(2)
C(22)-O(3)	1.428(2)
C(22)-C(23)	1.519(3)
C(22B)-O(2B)	1.428(2)
C(22B)-O(3B)	1.429(3)
C(22B)-C(23B)	1.520(3)
C(23)-C(24)	1.530(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(23B)-C(24B)	1.523(3)
C(23B)-H(23C)	0.9900
C(23B)-H(23D)	0.9900
C(24)-C(25)	1.530(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(24B)-C(25B)	1.523(3)
C(24B)-H(24C)	0.9900
C(24B)-H(24D)	0.9900
C(25)-C(26)	1.520(3)
C(25)-C(27)	1.526(3)
C(25)-H(25)	1.0000
C(25B)-C(26B)	1.519(3)
C(25B)-C(27B)	1.527(3)
C(25B)-H(25B)	1.0000
C(26)-O(3)	1.437(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(26B)-O(3B)	1.441(3)

C(26B)-H(26C)	0.9900
C(26B)-H(26D)	0.9900
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(2)-C(1)-C(10)	112.86(18)
C(2)-C(1)-H(1A)	109.0
C(10)-C(1)-H(1A)	109.0
C(2)-C(1)-H(1B)	109.0
C(10)-C(1)-H(1B)	109.0
H(1A)-C(1)-H(1B)	107.8
C(2B)-C(1B)-C(10B)	112.93(18)
C(2B)-C(1B)-H(1BA)	109.0
C(10B)-C(1B)-H(1BA)	109.0
C(2B)-C(1B)-H(1BB)	109.0
C(10B)-C(1B)-H(1BB)	109.0
H(1BA)-C(1B)-H(1BB)	107.8
C(3)-C(2)-C(1)	113.9(2)
C(3)-C(2)-H(2A)	108.8
C(1)-C(2)-H(2A)	108.8
C(3)-C(2)-H(2B)	108.8
C(1)-C(2)-H(2B)	108.8
H(2A)-C(2)-H(2B)	107.7
C(3B)-C(2B)-C(1B)	113.52(18)
C(3B)-C(2B)-H(2BA)	108.9
C(1B)-C(2B)-H(2BA)	108.9
C(3B)-C(2B)-H(2BB)	108.9
C(1B)-C(2B)-H(2BB)	108.9
H(2BA)-C(2B)-H(2BB)	107.7
O(1)-C(3)-O(4)	120.3(2)
O(1)-C(3)-C(2)	124.3(2)
O(4)-C(3)-C(2)	115.24(18)
O(1B)-C(3B)-O(4B)	118.7(2)

O(1B)-C(3B)-C(2B)	125.9(2)
O(4B)-C(3B)-C(2B)	115.38(19)
O(4)-C(5)-C(6)	106.64(16)
O(4)-C(5)-C(10)	110.05(16)
C(6)-C(5)-C(10)	114.41(16)
O(4)-C(5)-H(5)	108.5
C(6)-C(5)-H(5)	108.5
C(10)-C(5)-H(5)	108.5
O(4B)-C(5B)-C(6B)	107.40(16)
O(4B)-C(5B)-C(10B)	109.59(17)
C(6B)-C(5B)-C(10B)	114.61(17)
O(4B)-C(5B)-H(5B)	108.4
C(6B)-C(5B)-H(5B)	108.4
C(10B)-C(5B)-H(5B)	108.4
C(5)-C(6)-C(7)	109.37(17)
C(5)-C(6)-H(6A)	109.8
C(7)-C(6)-H(6A)	109.8
C(5)-C(6)-H(6B)	109.8
C(7)-C(6)-H(6B)	109.8
H(6A)-C(6)-H(6B)	108.2
C(5B)-C(6B)-C(7B)	108.75(17)
C(5B)-C(6B)-H(6BA)	109.9
C(7B)-C(6B)-H(6BA)	109.9
C(5B)-C(6B)-H(6BB)	109.9
C(7B)-C(6B)-H(6BB)	109.9
H(6BA)-C(6B)-H(6BB)	108.3
C(8)-C(7)-C(6)	112.26(17)
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
C(8B)-C(7B)-C(6B)	111.76(17)
C(8B)-C(7B)-H(7BA)	109.3
C(6B)-C(7B)-H(7BA)	109.3
C(8B)-C(7B)-H(7BB)	109.3

C(6B)-C(7B)-H(7BB)	109.3
H(7BA)-C(7B)-H(7BB)	107.9
C(14)-C(8)-C(7)	112.06(16)
C(14)-C(8)-C(9)	108.53(16)
C(7)-C(8)-C(9)	110.34(16)
C(14)-C(8)-H(8)	108.6
C(7)-C(8)-H(8)	108.6
C(9)-C(8)-H(8)	108.6
C(14B)-C(8B)-C(7B)	111.21(17)
C(14B)-C(8B)-C(9B)	107.42(15)
C(7B)-C(8B)-C(9B)	110.57(16)
C(14B)-C(8B)-H(8B)	109.2
C(7B)-C(8B)-H(8B)	109.2
C(9B)-C(8B)-H(8B)	109.2
C(11)-C(9)-C(8)	112.03(16)
C(11)-C(9)-C(10)	112.85(16)
C(8)-C(9)-C(10)	112.53(16)
C(11)-C(9)-H(9)	106.3
C(8)-C(9)-H(9)	106.3
C(10)-C(9)-H(9)	106.3
C(11B)-C(9B)-C(8B)	111.40(17)
C(11B)-C(9B)-C(10B)	113.02(17)
C(8B)-C(9B)-C(10B)	113.72(16)
C(11B)-C(9B)-H(9B)	106.0
C(8B)-C(9B)-H(9B)	106.0
C(10B)-C(9B)-H(9B)	106.0
C(19)-C(10)-C(5)	110.97(17)
C(19)-C(10)-C(1)	109.39(17)
C(5)-C(10)-C(1)	106.78(16)
C(19)-C(10)-C(9)	111.97(16)
C(5)-C(10)-C(9)	107.31(16)
C(1)-C(10)-C(9)	110.29(16)
C(19B)-C(10B)-C(5B)	110.57(17)
C(19B)-C(10B)-C(1B)	109.43(18)
C(5B)-C(10B)-C(1B)	106.39(16)
C(19B)-C(10B)-C(9B)	112.46(17)

C(5B)-C(10B)-C(9B)	107.18(16)
C(1B)-C(10B)-C(9B)	110.61(16)
C(9)-C(11)-C(12)	112.37(17)
C(9)-C(11)-H(11A)	109.1
C(12)-C(11)-H(11A)	109.1
C(9)-C(11)-H(11B)	109.1
C(12)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.9
C(12B)-C(11B)-C(9B)	111.90(18)
C(12B)-C(11B)-H(11C)	109.2
C(9B)-C(11B)-H(11C)	109.2
C(12B)-C(11B)-H(11D)	109.2
C(9B)-C(11B)-H(11D)	109.2
H(11C)-C(11B)-H(11D)	107.9
C(13)-C(12)-C(11)	110.81(17)
C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(13B)-C(12B)-C(11B)	111.29(17)
C(13B)-C(12B)-H(12C)	109.4
C(11B)-C(12B)-H(12C)	109.4
C(13B)-C(12B)-H(12D)	109.4
C(11B)-C(12B)-H(12D)	109.4
H(12C)-C(12B)-H(12D)	108.0
C(12)-C(13)-C(18)	109.83(17)
C(12)-C(13)-C(14)	107.83(15)
C(18)-C(13)-C(14)	111.84(16)
C(12)-C(13)-C(17)	115.26(16)
C(18)-C(13)-C(17)	111.14(16)
C(14)-C(13)-C(17)	100.61(15)
C(12B)-C(13B)-C(18B)	110.08(18)
C(12B)-C(13B)-C(14B)	108.50(16)
C(18B)-C(13B)-C(14B)	112.01(16)
C(12B)-C(13B)-C(17B)	114.60(16)

C(18B)-C(13B)-C(17B)	111.53(16)
C(14B)-C(13B)-C(17B)	99.75(16)
C(8)-C(14)-C(15)	119.51(17)
C(8)-C(14)-C(13)	114.02(16)
C(15)-C(14)-C(13)	103.56(15)
C(8)-C(14)-H(14)	106.3
C(15)-C(14)-H(14)	106.3
C(13)-C(14)-H(14)	106.3
C(8B)-C(14B)-C(15B)	120.78(17)
C(8B)-C(14B)-C(13B)	114.73(17)
C(15B)-C(14B)-C(13B)	103.56(15)
C(8B)-C(14B)-H(14B)	105.5
C(15B)-C(14B)-H(14B)	105.5
C(13B)-C(14B)-H(14B)	105.5
C(14)-C(15)-C(16)	102.14(16)
C(14)-C(15)-H(15A)	111.3
C(16)-C(15)-H(15A)	111.3
C(14)-C(15)-H(15B)	111.3
C(16)-C(15)-H(15B)	111.3
H(15A)-C(15)-H(15B)	109.2
C(14B)-C(15B)-C(16B)	101.14(16)
C(14B)-C(15B)-H(15C)	111.5
C(16B)-C(15B)-H(15C)	111.5
C(14B)-C(15B)-H(15D)	111.5
C(16B)-C(15B)-H(15D)	111.5
H(15C)-C(15B)-H(15D)	109.4
O(2)-C(16)-C(15)	111.69(17)
O(2)-C(16)-C(17)	104.91(16)
C(15)-C(16)-C(17)	107.84(16)
O(2)-C(16)-H(16)	110.7
C(15)-C(16)-H(16)	110.7
C(17)-C(16)-H(16)	110.7
O(2B)-C(16B)-C(15B)	112.59(16)
O(2B)-C(16B)-C(17B)	105.41(15)
C(15B)-C(16B)-C(17B)	107.54(16)
O(2B)-C(16B)-H(16B)	110.4

C(15B)-C(16B)-H(16B)	110.4
C(17B)-C(16B)-H(16B)	110.4
C(20)-C(17)-C(13)	120.10(17)
C(20)-C(17)-C(16)	103.84(16)
C(13)-C(17)-C(16)	103.86(16)
C(20)-C(17)-H(17)	109.5
C(13)-C(17)-H(17)	109.5
C(16)-C(17)-H(17)	109.5
C(20B)-C(17B)-C(13B)	120.94(17)
C(20B)-C(17B)-C(16B)	104.08(16)
C(13B)-C(17B)-C(16B)	104.64(16)
C(20B)-C(17B)-H(17B)	108.8
C(13B)-C(17B)-H(17B)	108.8
C(16B)-C(17B)-H(17B)	108.8
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(13B)-C(18B)-H(18D)	109.5
C(13B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(13B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(10B)-C(19B)-H(19D)	109.5
C(10B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(10B)-C(19B)-H(19F)	109.5

H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(21)-C(20)-C(22)	115.00(17)
C(21)-C(20)-C(17)	115.53(18)
C(22)-C(20)-C(17)	103.68(16)
C(21)-C(20)-H(20)	107.4
C(22)-C(20)-H(20)	107.4
C(17)-C(20)-H(20)	107.4
C(21B)-C(20B)-C(22B)	115.58(17)
C(21B)-C(20B)-C(17B)	113.95(17)
C(22B)-C(20B)-C(17B)	103.25(16)
C(21B)-C(20B)-H(20B)	107.9
C(22B)-C(20B)-H(20B)	107.9
C(17B)-C(20B)-H(20B)	107.9
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20B)-C(21B)-H(21D)	109.5
C(20B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5
C(20B)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
O(2)-C(22)-O(3)	110.03(16)
O(2)-C(22)-C(23)	107.98(17)
O(3)-C(22)-C(23)	110.10(16)
O(2)-C(22)-C(20)	104.94(15)
O(3)-C(22)-C(20)	107.67(17)
C(23)-C(22)-C(20)	115.95(17)
O(2B)-C(22B)-O(3B)	110.30(16)
O(2B)-C(22B)-C(23B)	108.13(16)
O(3B)-C(22B)-C(23B)	110.48(17)
O(2B)-C(22B)-C(20B)	104.70(15)

O(3B)-C(22B)-C(20B)	107.37(16)
C(23B)-C(22B)-C(20B)	115.67(18)
C(22)-C(23)-C(24)	111.26(18)
C(22)-C(23)-H(23A)	109.4
C(24)-C(23)-H(23A)	109.4
C(22)-C(23)-H(23B)	109.4
C(24)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0
C(22B)-C(23B)-C(24B)	111.09(18)
C(22B)-C(23B)-H(23C)	109.4
C(24B)-C(23B)-H(23C)	109.4
C(22B)-C(23B)-H(23D)	109.4
C(24B)-C(23B)-H(23D)	109.4
H(23C)-C(23B)-H(23D)	108.0
C(25)-C(24)-C(23)	110.71(18)
C(25)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24A)	109.5
C(25)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	108.1
C(23B)-C(24B)-C(25B)	110.90(18)
C(23B)-C(24B)-H(24C)	109.5
C(25B)-C(24B)-H(24C)	109.5
C(23B)-C(24B)-H(24D)	109.5
C(25B)-C(24B)-H(24D)	109.5
H(24C)-C(24B)-H(24D)	108.0
C(26)-C(25)-C(27)	110.80(19)
C(26)-C(25)-C(24)	109.85(17)
C(27)-C(25)-C(24)	110.75(19)
C(26)-C(25)-H(25)	108.5
C(27)-C(25)-H(25)	108.5
C(24)-C(25)-H(25)	108.5
C(26B)-C(25B)-C(24B)	108.46(18)
C(26B)-C(25B)-C(27B)	110.5(2)
C(24B)-C(25B)-C(27B)	112.1(2)
C(26B)-C(25B)-H(25B)	108.6

C(24B)-C(25B)-H(25B)	108.6
C(27B)-C(25B)-H(25B)	108.6
O(3)-C(26)-C(25)	113.24(17)
O(3)-C(26)-H(26A)	108.9
C(25)-C(26)-H(26A)	108.9
O(3)-C(26)-H(26B)	108.9
C(25)-C(26)-H(26B)	108.9
H(26A)-C(26)-H(26B)	107.7
O(3B)-C(26B)-C(25B)	112.33(18)
O(3B)-C(26B)-H(26C)	109.1
C(25B)-C(26B)-H(26C)	109.1
O(3B)-C(26B)-H(26D)	109.1
C(25B)-C(26B)-H(26D)	109.1
H(26C)-C(26B)-H(26D)	107.9
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25B)-C(27B)-H(27D)	109.5
C(25B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(25B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(22)-O(2)-C(16)	106.27(15)
C(22B)-O(2B)-C(16B)	105.86(14)
C(22)-O(3)-C(26)	112.79(16)
C(22B)-O(3B)-C(26B)	113.34(16)
C(3)-O(4)-C(5)	117.35(16)
C(3B)-O(4B)-C(5B)	116.18(17)

Symmetry transformations used to generate equivalent atoms:

Table S-7. Anisotropic displacement parameters ($Å^2$x 10^3)for **20b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	18(1)	21(1)	0(1)	3(1)	-1(1)
C(1B)	20(1)	26(1)	23(1)	5(1)	4(1)	-4(1)
C(2)	25(1)	27(1)	36(1)	-3(1)	-2(1)	-3(1)
C(2B)	19(1)	33(1)	26(1)	2(1)	8(1)	-7(1)
C(3)	17(1)	26(1)	17(1)	-1(1)	1(1)	1(1)
C(3B)	17(1)	26(1)	30(1)	2(1)	5(1)	-2(1)
C(5)	14(1)	17(1)	20(1)	0(1)	0(1)	1(1)
C(5B)	12(1)	20(1)	19(1)	0(1)	1(1)	-1(1)
C(6)	20(1)	14(1)	26(1)	3(1)	0(1)	0(1)
C(6B)	16(1)	22(1)	21(1)	6(1)	1(1)	1(1)
C(7)	17(1)	17(1)	22(1)	3(1)	0(1)	-2(1)
C(7B)	15(1)	17(1)	20(1)	5(1)	2(1)	0(1)
C(8)	14(1)	14(1)	15(1)	0(1)	3(1)	0(1)
C(8B)	14(1)	17(1)	14(1)	2(1)	3(1)	1(1)
C(9)	15(1)	14(1)	14(1)	0(1)	5(1)	0(1)
C(9B)	15(1)	16(1)	17(1)	3(1)	4(1)	1(1)
C(10)	13(1)	15(1)	16(1)	0(1)	3(1)	1(1)
C(10B)	15(1)	18(1)	18(1)	2(1)	4(1)	0(1)
C(11)	15(1)	16(1)	24(1)	2(1)	3(1)	-1(1)
C(11B)	19(1)	19(1)	25(1)	8(1)	1(1)	-1(1)
C(12)	16(1)	14(1)	22(1)	2(1)	5(1)	1(1)
C(12B)	18(1)	22(1)	20(1)	9(1)	1(1)	0(1)
C(13)	14(1)	12(1)	15(1)	1(1)	4(1)	1(1)
C(13B)	15(1)	16(1)	14(1)	2(1)	3(1)	2(1)
C(14)	14(1)	13(1)	15(1)	0(1)	3(1)	-1(1)
C(14B)	14(1)	16(1)	16(1)	2(1)	5(1)	2(1)
C(15)	17(1)	16(1)	23(1)	5(1)	1(1)	-2(1)
C(15B)	16(1)	19(1)	20(1)	5(1)	1(1)	0(1)
C(16)	15(1)	23(1)	16(1)	3(1)	2(1)	-1(1)
C(16B)	14(1)	16(1)	19(1)	0(1)	3(1)	2(1)
C(17)	14(1)	17(1)	16(1)	1(1)	5(1)	1(1)

C(17B)	15(1)	18(1)	15(1)	1(1)	3(1)	2(1)
C(18)	19(1)	23(1)	16(1)	4(1)	6(1)	4(1)
C(18B)	19(1)	24(1)	19(1)	-2(1)	1(1)	5(1)
C(19)	17(1)	28(1)	19(1)	-2(1)	5(1)	2(1)
C(19B)	22(1)	19(1)	23(1)	-1(1)	2(1)	2(1)
C(20)	14(1)	18(1)	20(1)	4(1)	3(1)	2(1)
C(20B)	14(1)	19(1)	16(1)	0(1)	1(1)	1(1)
C(21)	21(1)	18(1)	34(1)	4(1)	1(1)	3(1)
C(21B)	20(1)	25(1)	21(1)	6(1)	0(1)	0(1)
C(22)	14(1)	20(1)	18(1)	5(1)	4(1)	3(1)
C(22B)	15(1)	19(1)	14(1)	0(1)	0(1)	2(1)
C(23)	17(1)	25(1)	16(1)	4(1)	4(1)	3(1)
C(23B)	16(1)	22(1)	25(1)	1(1)	5(1)	4(1)
C(24)	18(1)	26(1)	19(1)	-1(1)	2(1)	0(1)
C(24B)	16(1)	26(1)	29(1)	5(1)	7(1)	2(1)
C(25)	15(1)	24(1)	23(1)	1(1)	2(1)	1(1)
C(25B)	20(1)	23(1)	27(1)	3(1)	-1(1)	-4(1)
C(26)	17(1)	25(1)	24(1)	2(1)	7(1)	-4(1)
C(26B)	26(1)	18(1)	21(1)	-3(1)	2(1)	-2(1)
C(27)	21(1)	31(1)	35(1)	-3(1)	5(1)	-4(1)
C(27B)	37(2)	30(1)	44(2)	0(1)	9(1)	-12(1)
O(1)	18(1)	42(1)	48(1)	-17(1)	-3(1)	3(1)
O(1B)	24(1)	44(1)	35(1)	3(1)	-3(1)	-13(1)
O(2)	15(1)	18(1)	19(1)	3(1)	0(1)	0(1)
O(2B)	13(1)	20(1)	17(1)	3(1)	2(1)	1(1)
O(3)	16(1)	24(1)	21(1)	0(1)	7(1)	-2(1)
O(3B)	22(1)	20(1)	18(1)	-2(1)	4(1)	-1(1)
O(4)	17(1)	20(1)	29(1)	-1(1)	-5(1)	3(1)
O(4B)	14(1)	25(1)	22(1)	1(1)	1(1)	-1(1)