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The supplementary file

Three new coordination geometries of homoleptic Zn complexes of curcuminoids and their high antiproliferative potential

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Table S1. Crystallographic data of compounds.

	5a	5b	7	8
Empirical formula	$C_{54.96}H_{57.58}N_{1.65}O_{18}Zn$	$C_{52}H_{52}O_{17}SZn$	$C_{51}H_{60}N_2O_{13}Zn$	$C_{79}H_{77}N_3O_{22}Zn$
Formula weight	1094.72	1046.36	974.38	1485.80
Temperature/K	298(2)	296(2)	298(2)	100(2)
Crystal system	triclinic	triclinic	Monoclinic	triclinic
Space group	P-1	P-1	C2/c	P-1
a/Å	7.7998(19)	7.4706(2)	31.514(8)	10.5643(5)
b/Å	11.640(3)	11.7637(4)	17.306(5)	12.4244(5)
c/Å	15.758(4)	30.7699(10)	10.282(3)	30.5143(14)
α/°	76.704(8)	81.6770(10)	90	91.7948(10)
β/°	88.171(7)	86.8260(10)	98.828(8)	92.0579(10)
γ/°	79.407(8)	79.6230(10)	90	114.7808(9)
Volume/Å^3	1368.5(6)	2630.68(14)	5541(3)	3629.3(3)
Z	1	2	4	2
ρ_{calc}g/cm^3	1.328	1.321	1.168	1.360
μ/mm^{-1}	0.522	0.576	0.501	0.418
F(000)	573.0	1092.0	2056.0	1556.0
Crystal size/mm^3	0.399 × 0.231 × 0.16	0.202 × 0.175 × 0.043	0.34 × 0.264 × 0.2	0.173 × 0.11 × 0.041
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.986 to 51.362	4.146 to 50.71	4.576 to 52.042	1.338 to 52.744
Index ranges	-9 ≤ h ≤ 9, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19	-8 ≤ h ≤ 8, -14 ≤ k ≤ 14, -36 ≤ l ≤ 37	-38 ≤ h ≤ 38, -21 ≤ k ≤ 21, -12 ≤ l ≤ 12	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -38 ≤ l ≤ 38
Reflections collected	28466	43039	21277	62044
Independent reflections	5180 [R_{int} = 0.0732, R_{sigma} = 0.0505]	9550 [R_{int} = 0.0736, R_{sigma} = 0.0594	5445 [R_{int} = 0.0717, R_{sigma} = 0.0789]	14846 [R_{int} = 0.0399, R_{sigma} = 0.0336]
Data/restraints/parameters	5180/66/392	9550/90/676	5445/232/387	14846/462/1104
Goodness-of-fit on F^2	1.020	1.054	0.995	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0818, wR_2 = 0.2106	R_1 = 0.0685, wR_2 = 0.1517	R_1 = 0.0779, wR_2 = 0.2045	R_1 = 0.0470, wR_2 = 0.1096
Final R indexes [all data]	R_1 = 0.1254, wR_2 = 0.2448	R_1 = 0.1073, wR_2 = 0.1714	R_1 = 0.1649, wR_2 = 0.2588	R_1 = 0.0614, wR_2 = 0.1176
Largest diff. peak/hole / e Å^{-3}	0.41/-0.46	1.35/-0.49	0.48/-0.23	0.68/-0.67

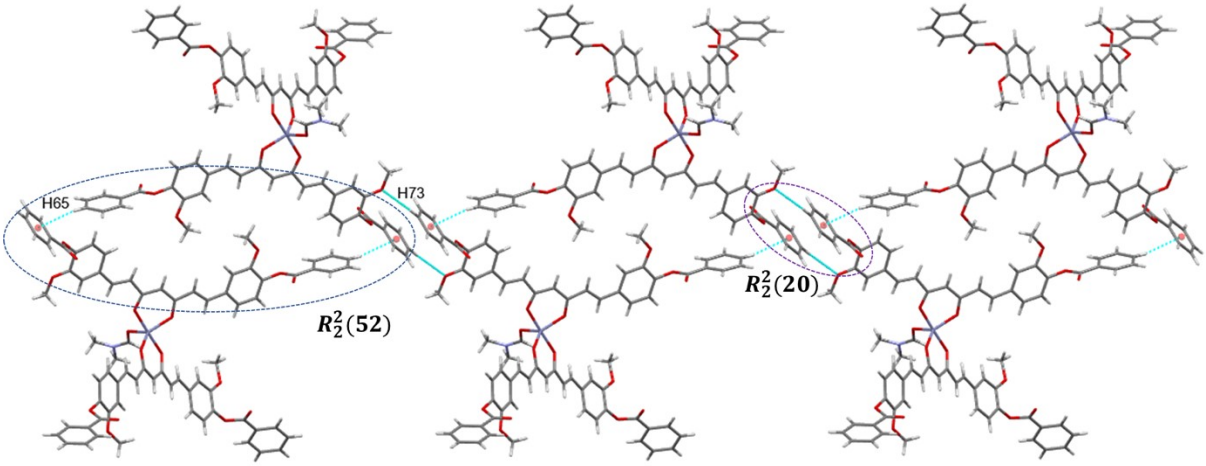
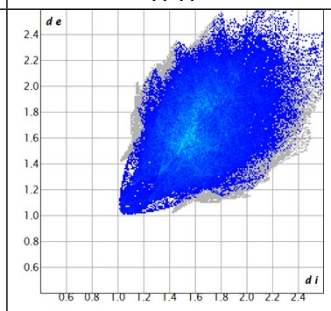
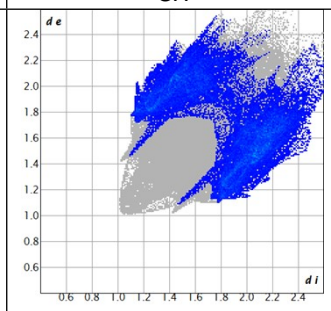
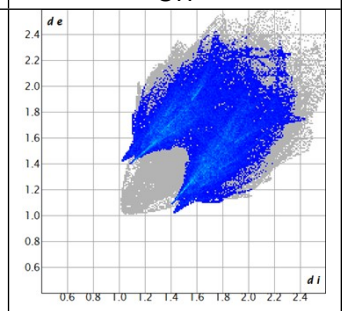
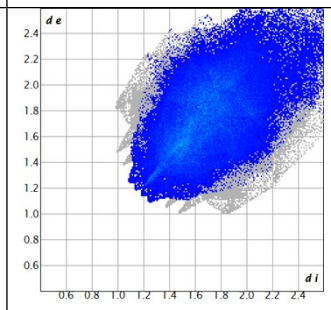
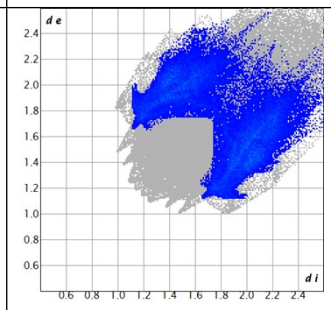
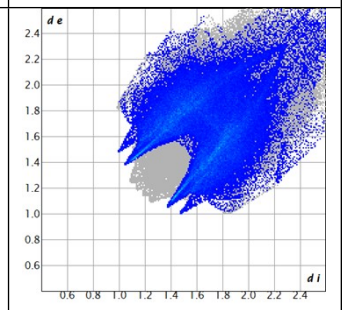
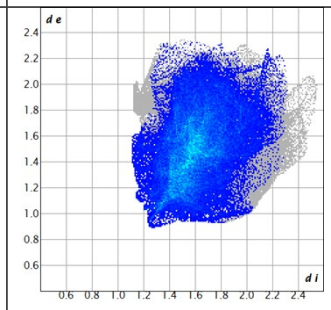
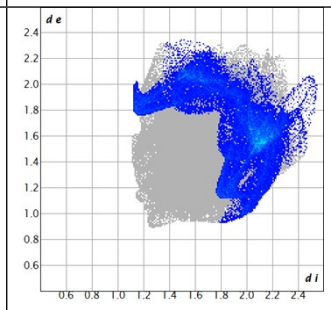
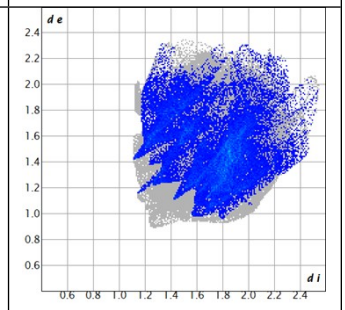
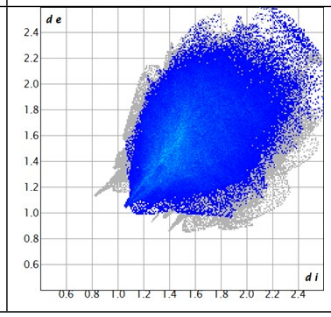
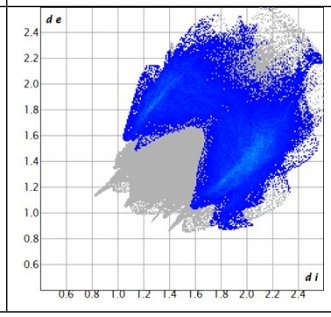
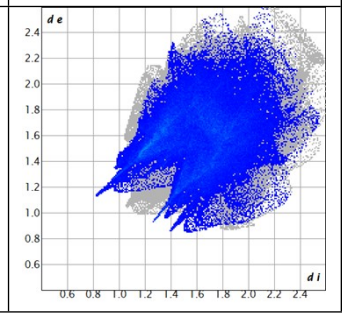


Fig S1. 2D supramolecular interactions for compound 7 supported via by C-H···O and C-H···π interactions forming rings of 20 and 52 members $R_2^2(20)$ and $R_2^2(52)$.

Table S2. Contribution of different types of contacts.

	H-H	CH	OH
5a			
5b			
7			
8			

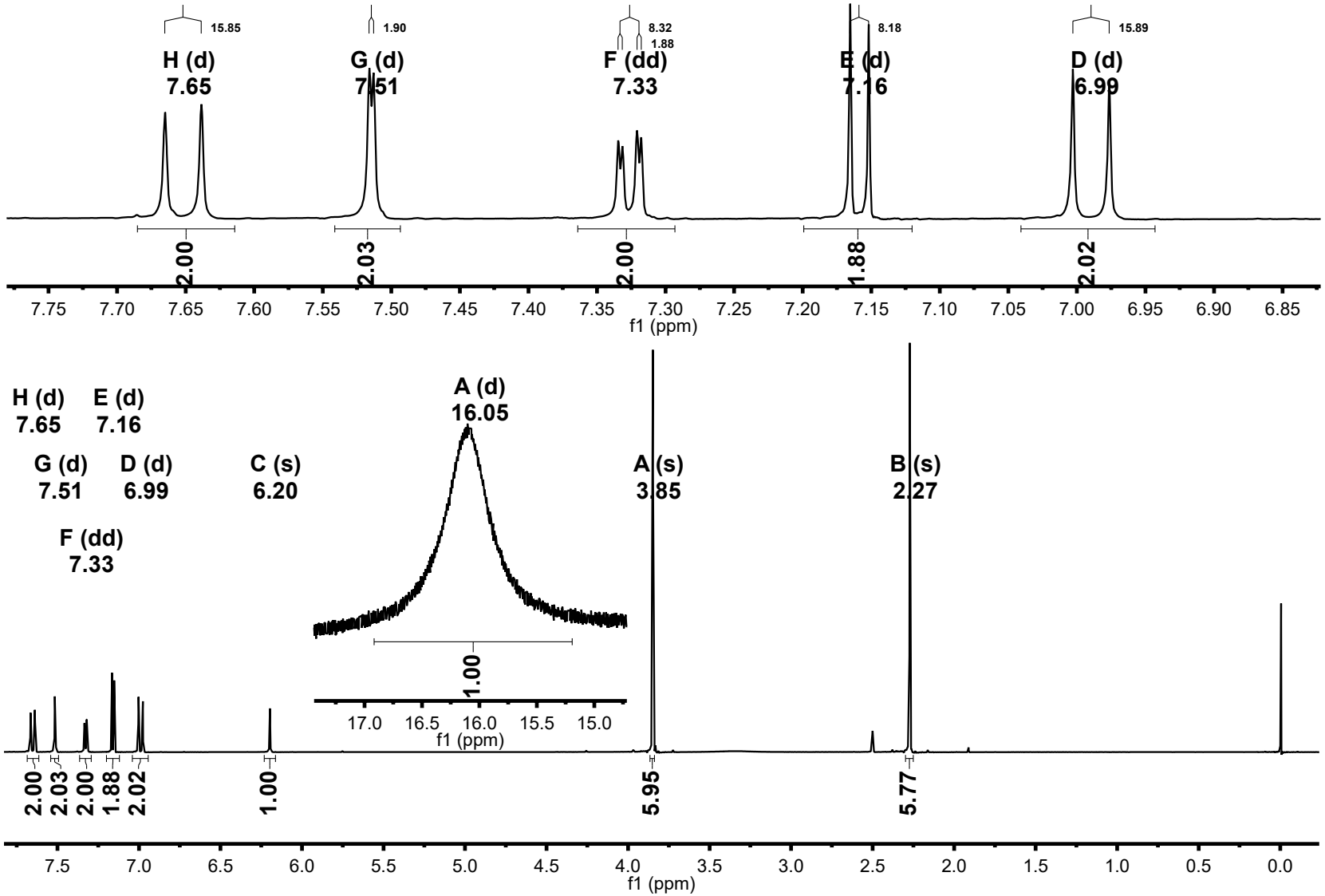


Fig S2. 500 MHz ^{1}H NMR spectrum of DAC.

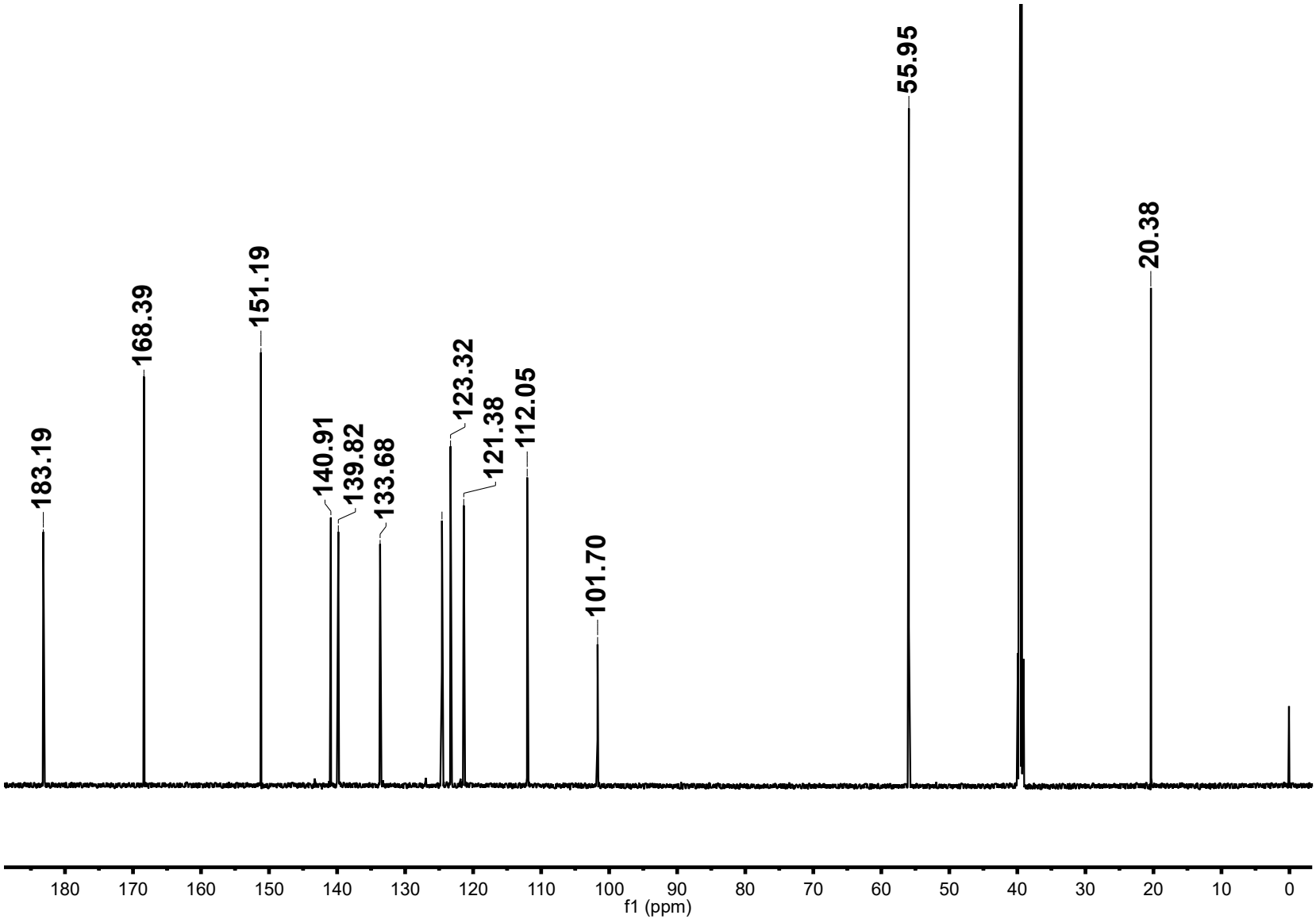


Fig S3. 125 MHz ^{13}C NMR spectrum of DAC.

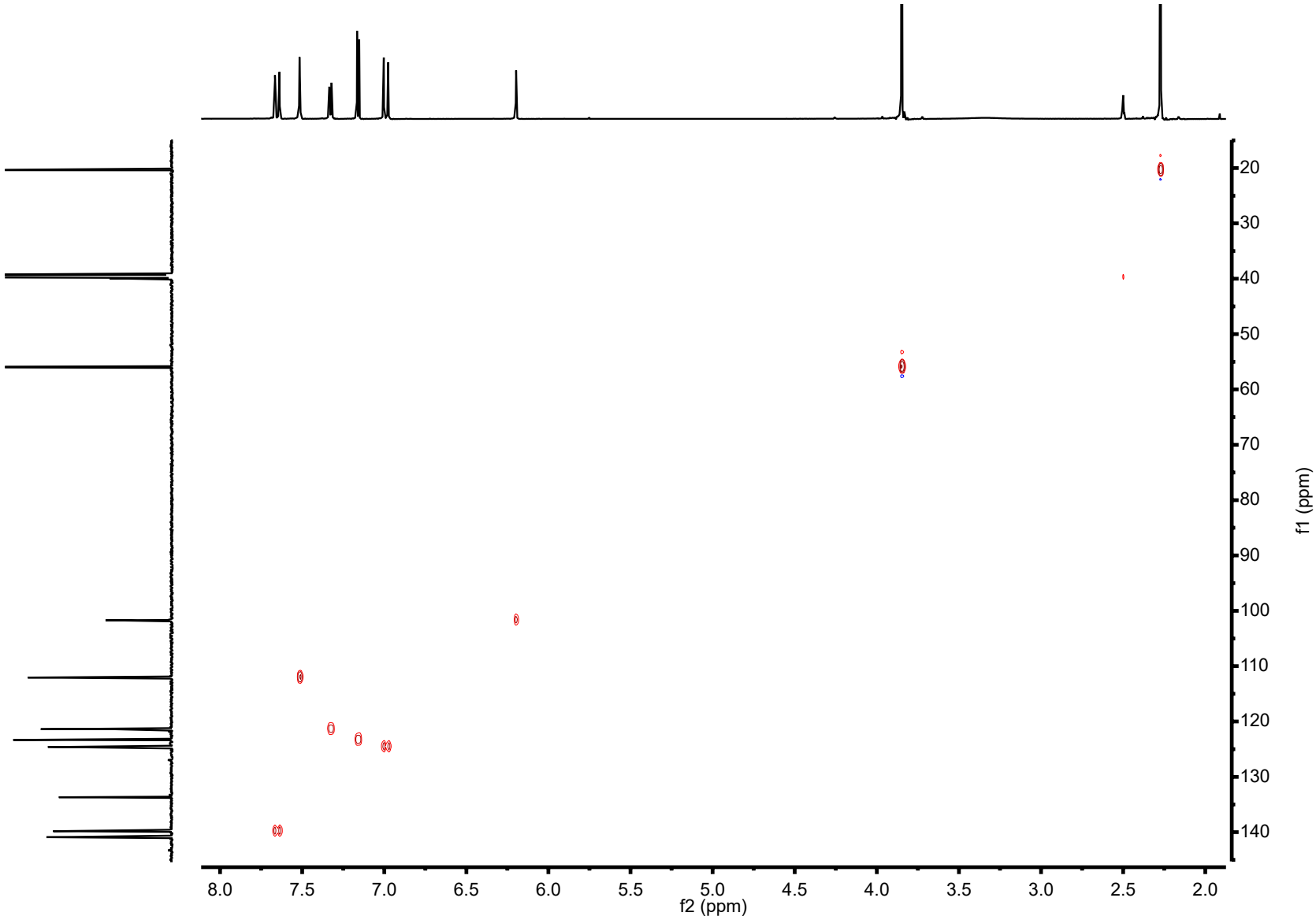


Fig S4. 500 MHz HSQC NMR spectrum of DAC.

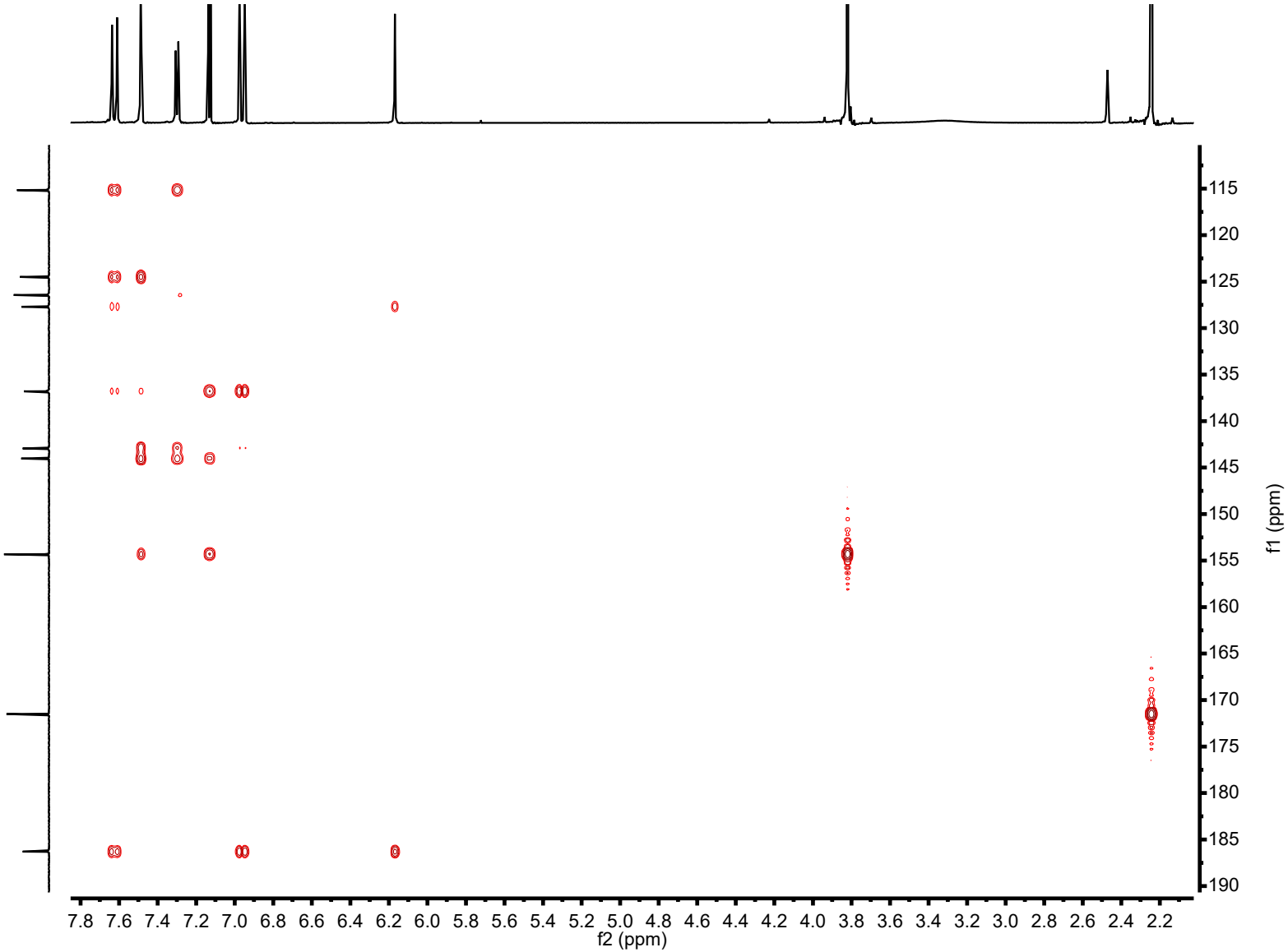


Fig S5. 500 MHz HMBC NMR spectrum of DAC.

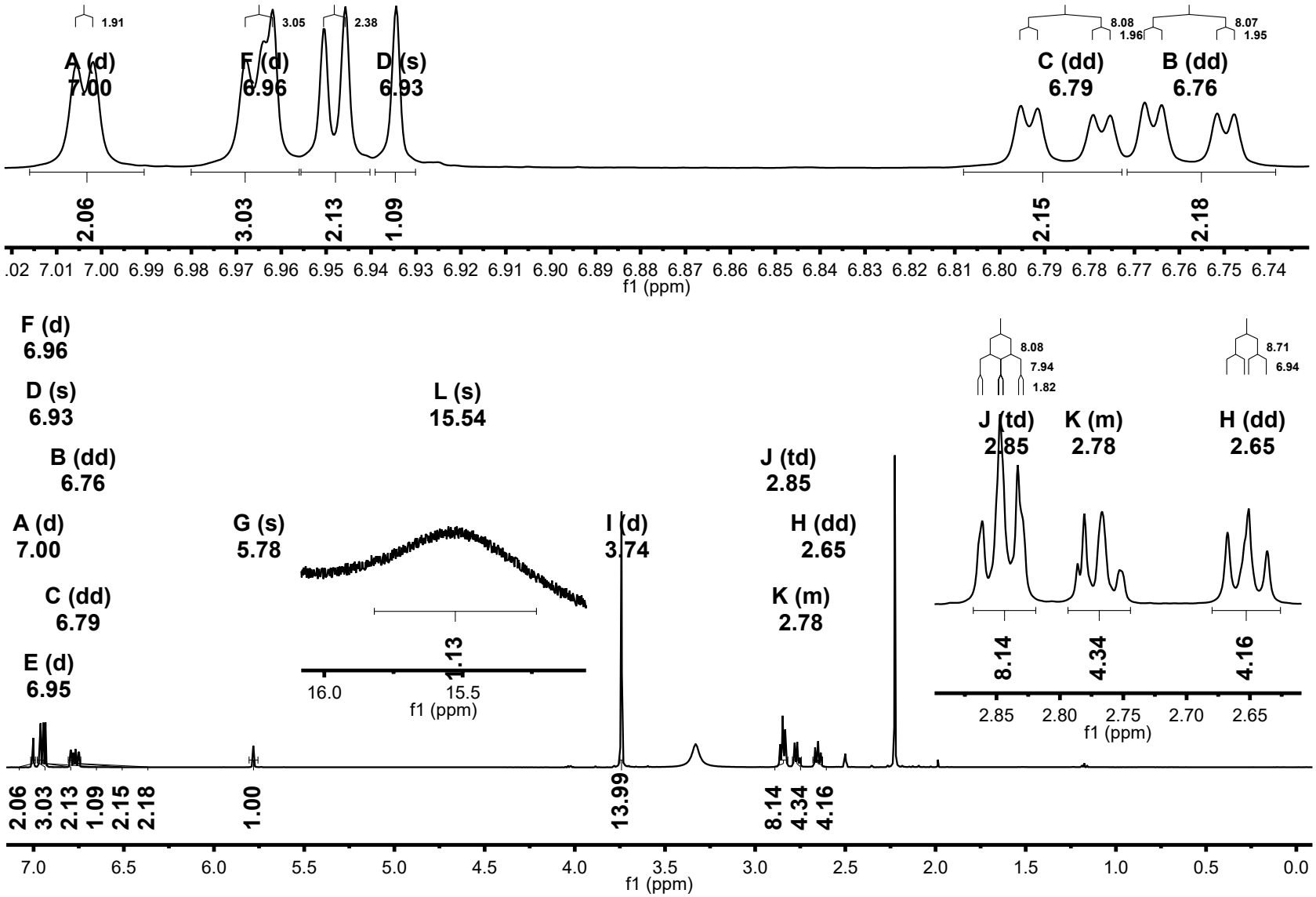


Fig S6. 500 MHz ^{1}H NMR spectrum of DACH.

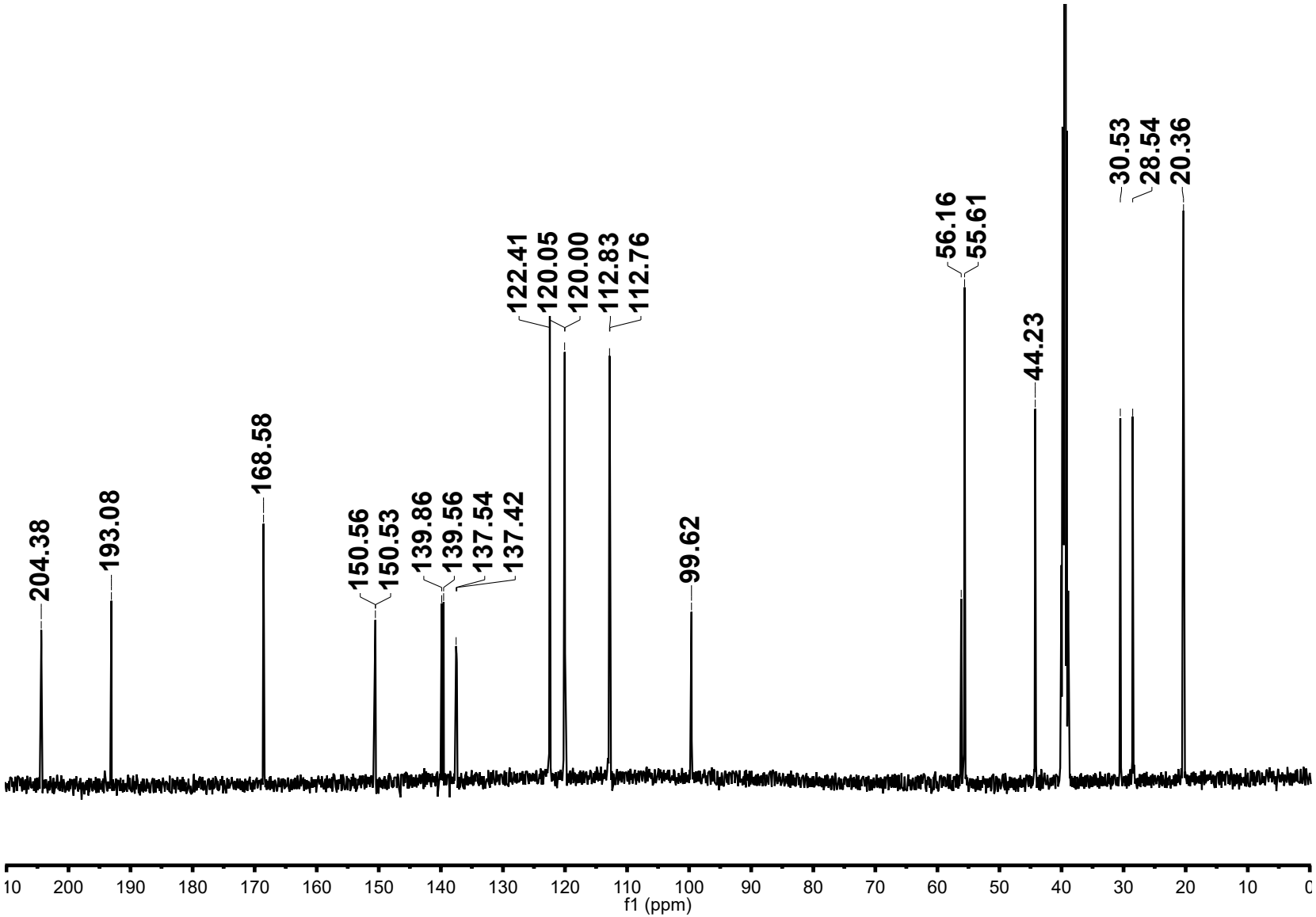


Fig S7. 125 MHz ^{13}C NMR spectrum of DACH.

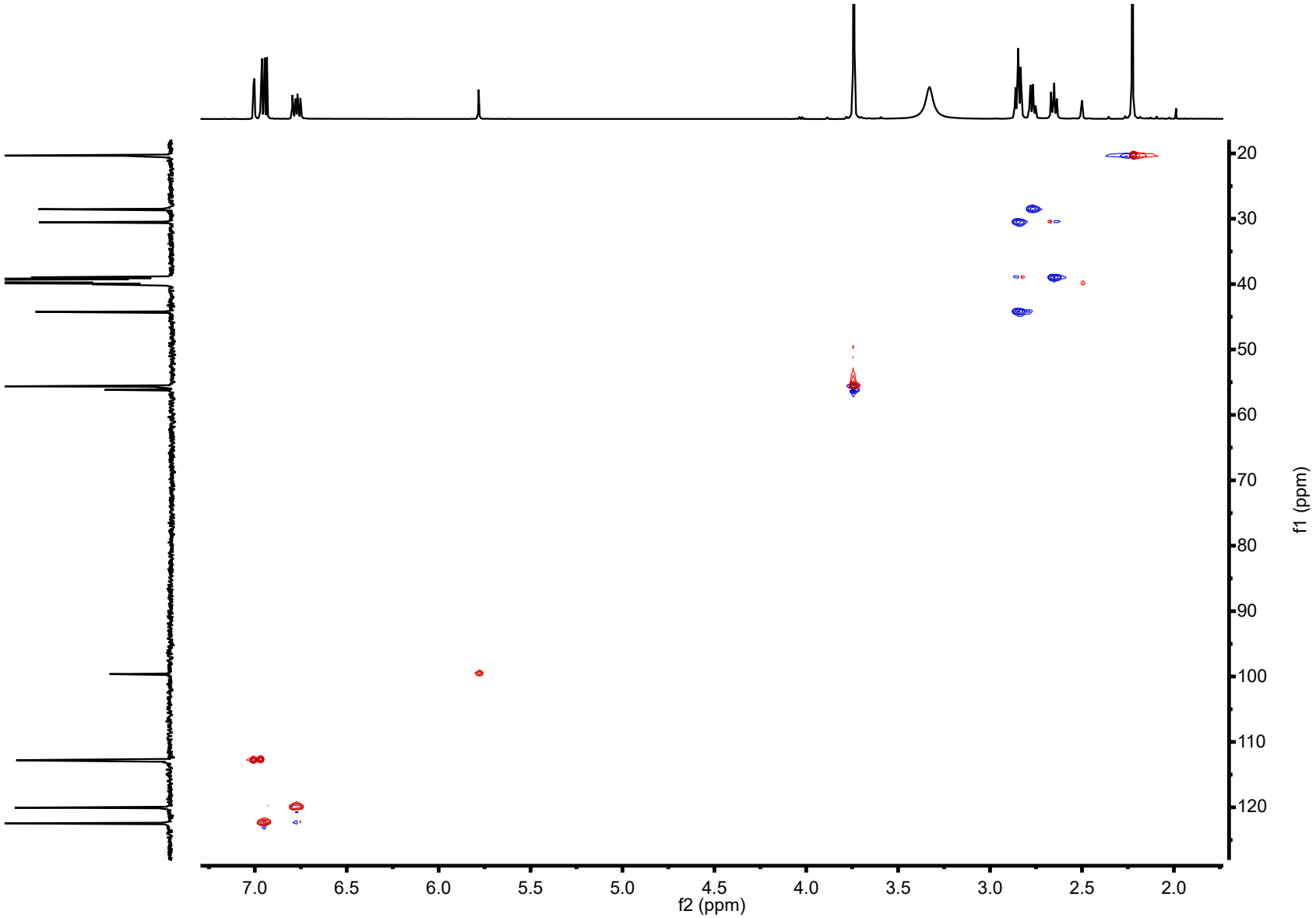


Fig S8. 500 MHz HSQC NMR spectrum of DACH.

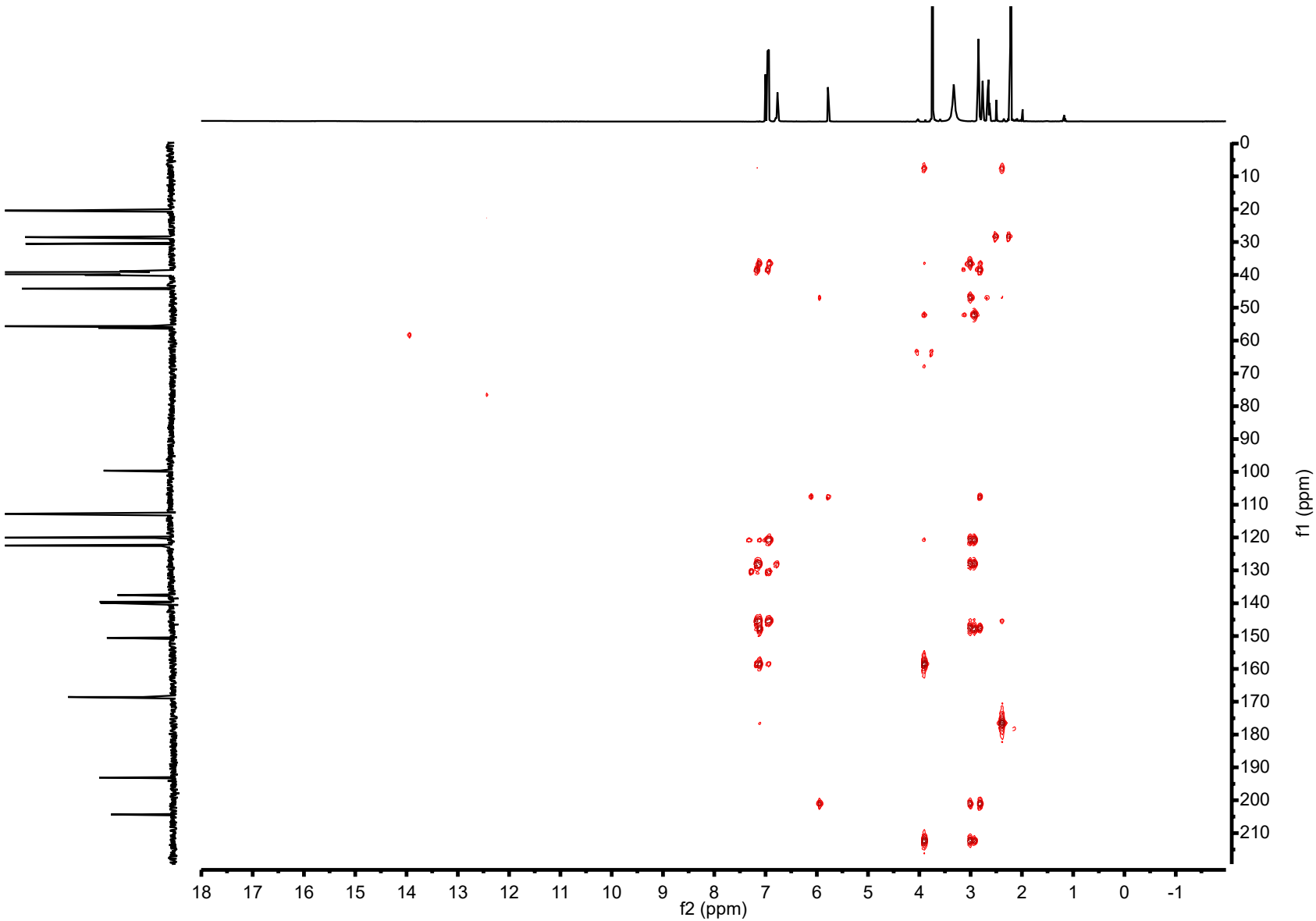


Fig S9. 500 MHz HMBC NMR spectrum of DACH.

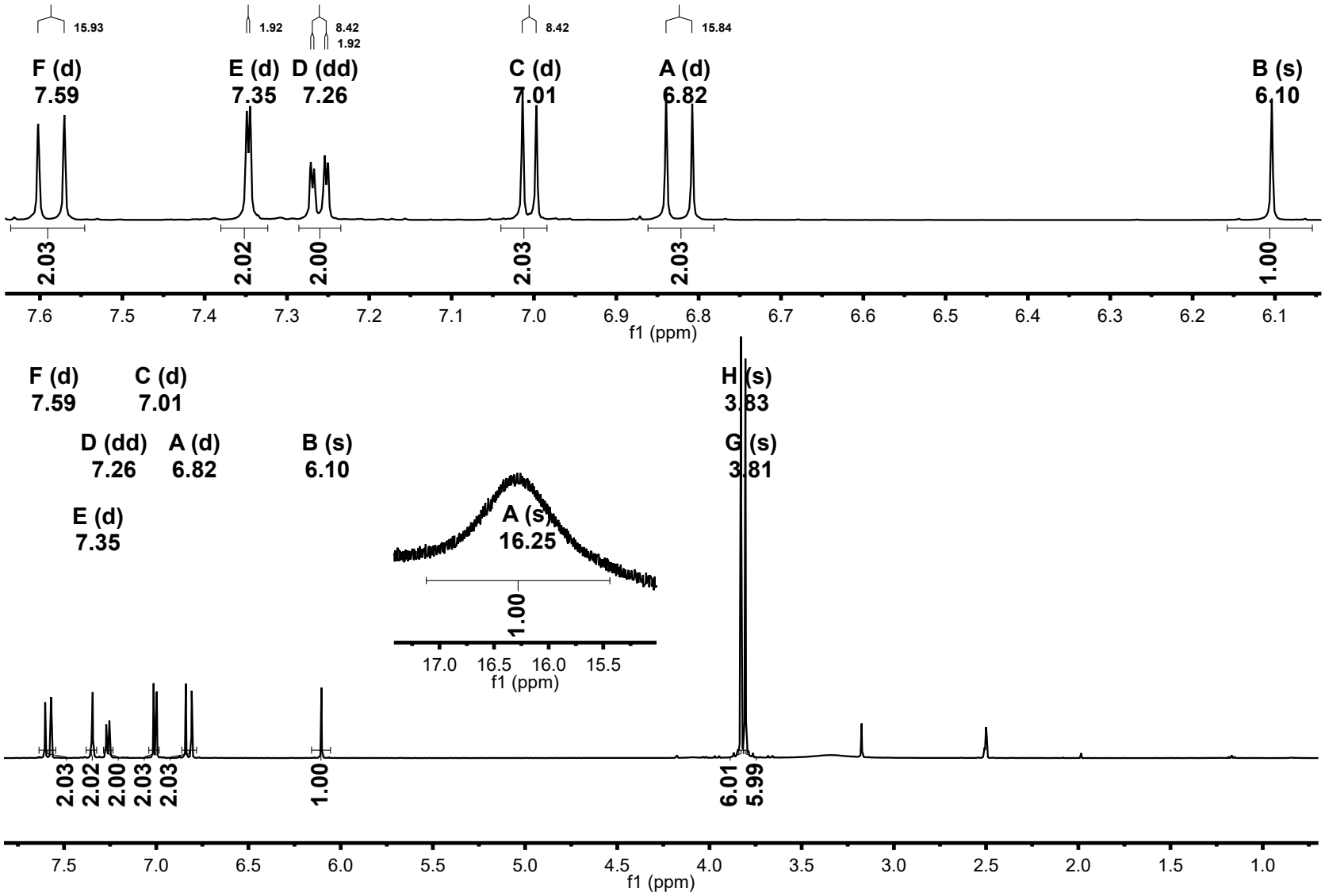


Fig S10. 500 MHz ^{1}H NMR spectrum of DiMeOC.

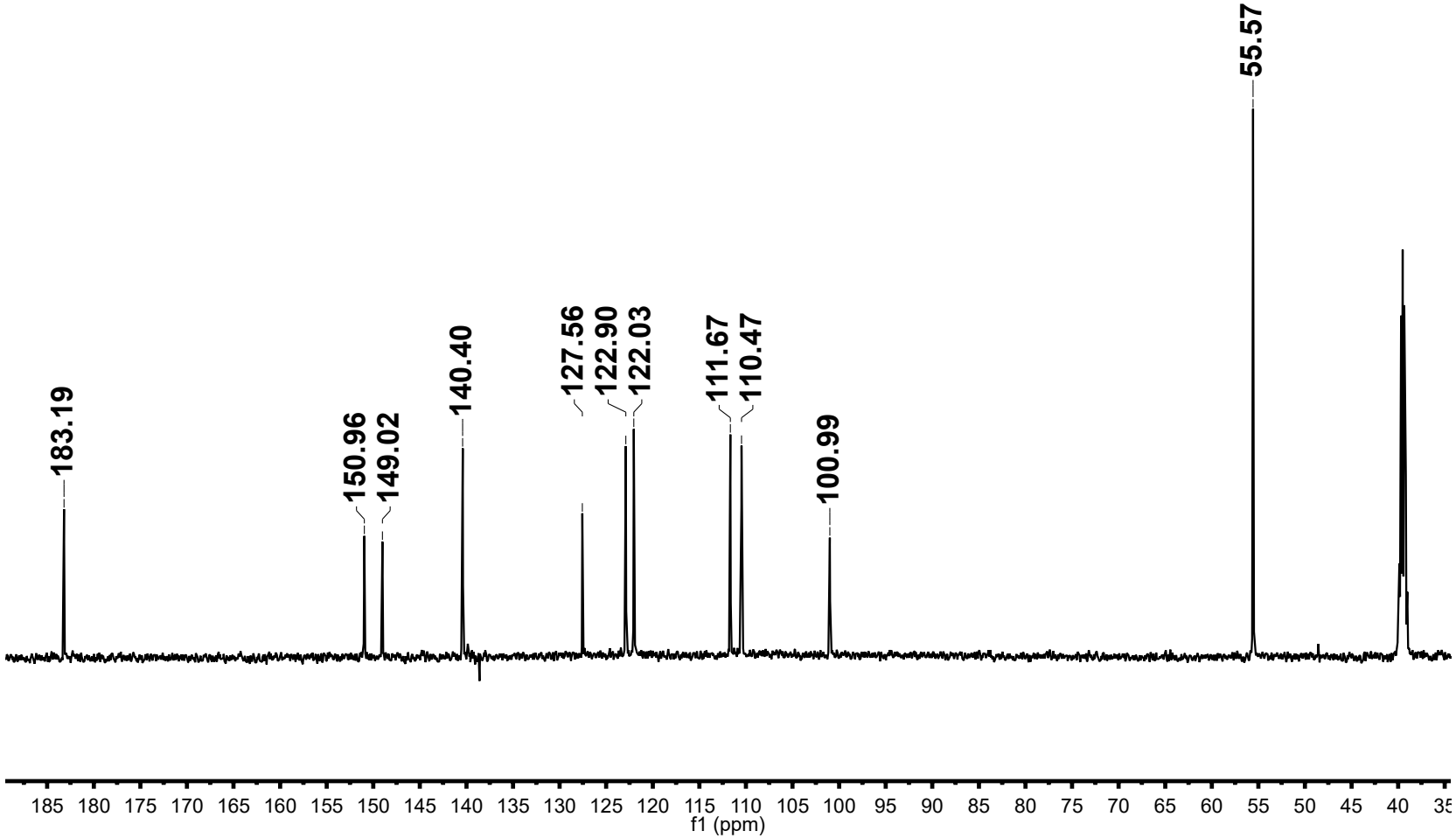


Fig S11. 125 MHz ^{13}C NMR spectrum of DIMeOC.

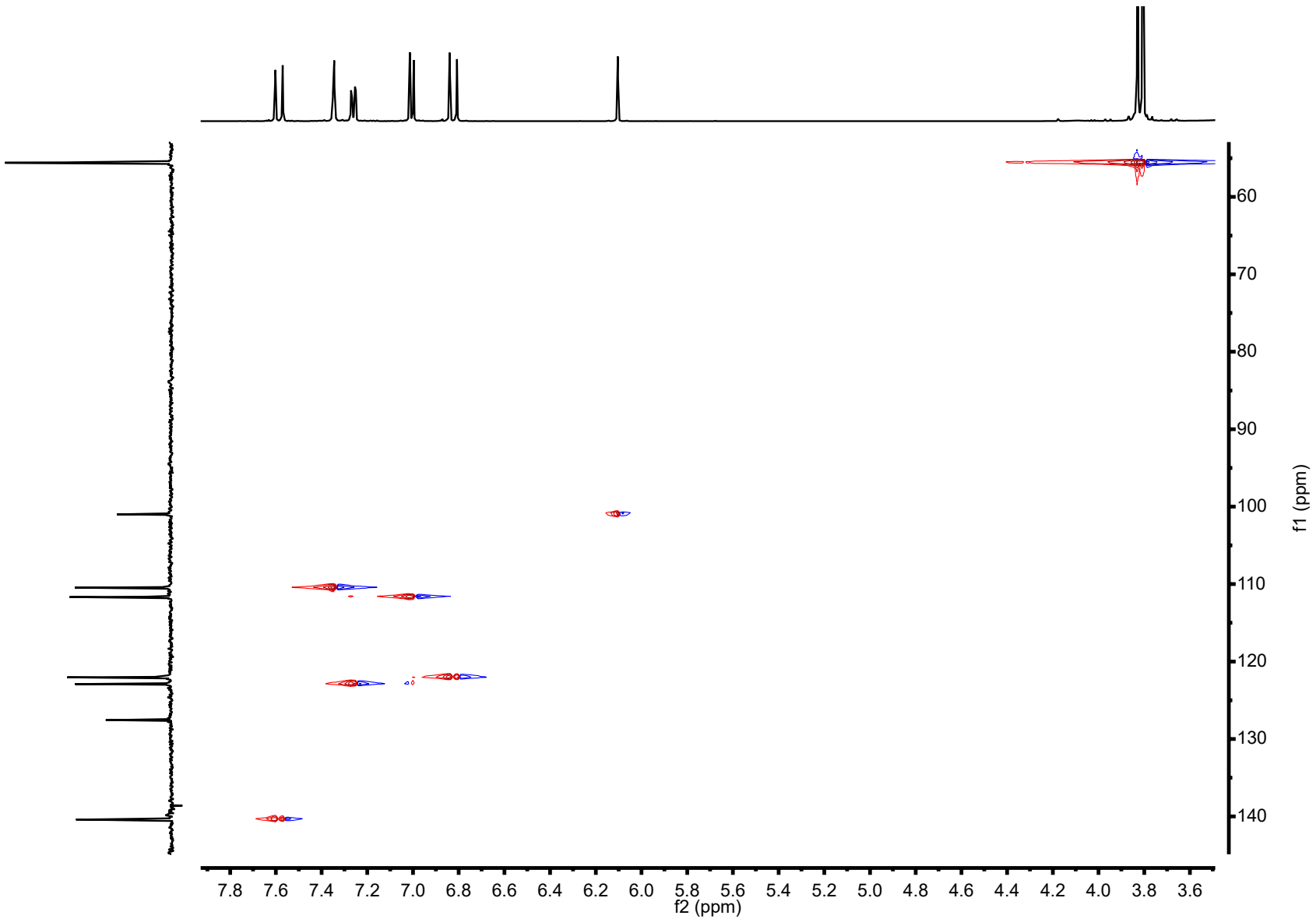


Fig S12. 500 MHz HSQC NMR spectrum of DiMeOC.

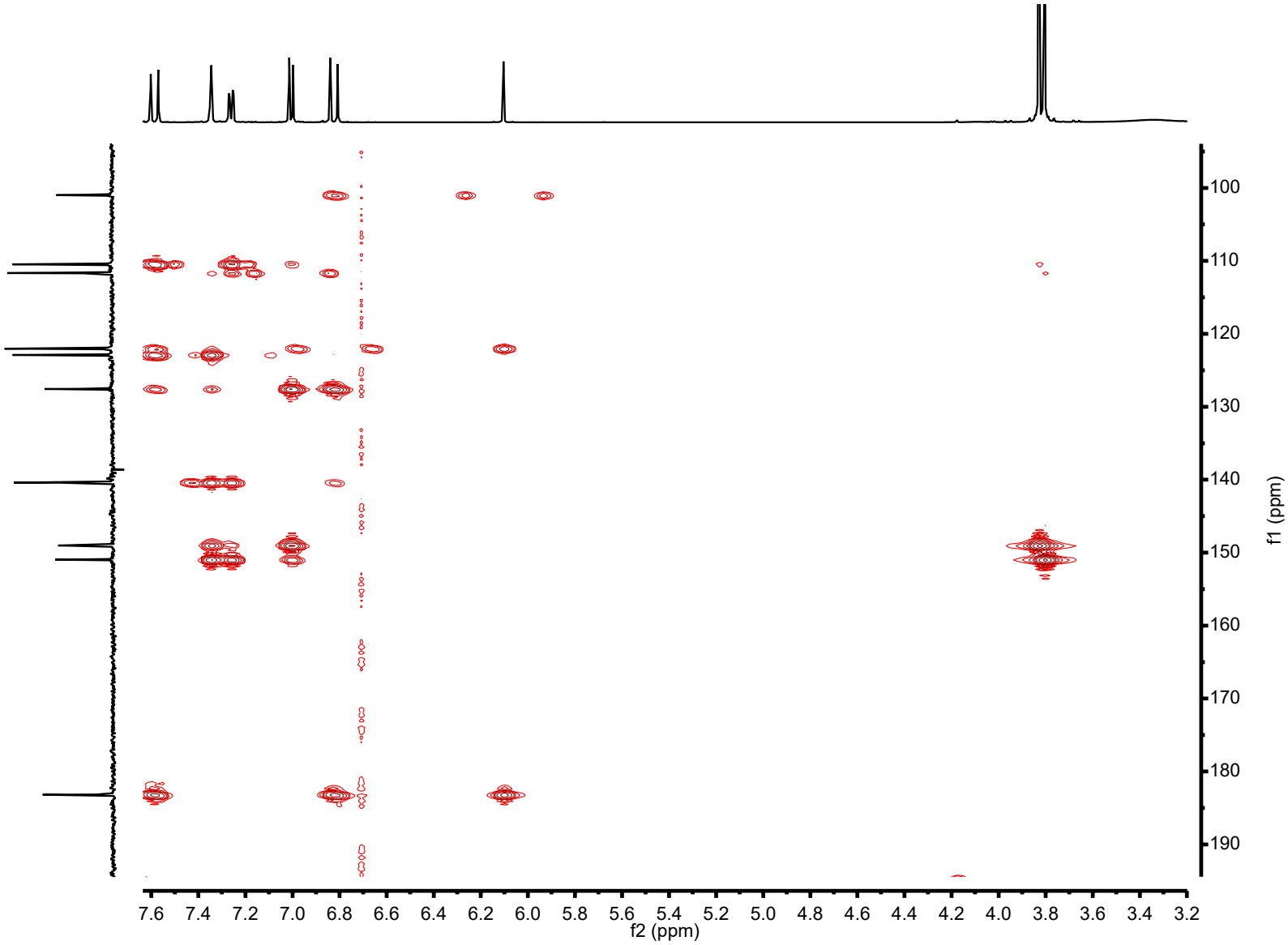


Fig S13. 500 MHz HMBC NMR spectrum of DiMeOC.

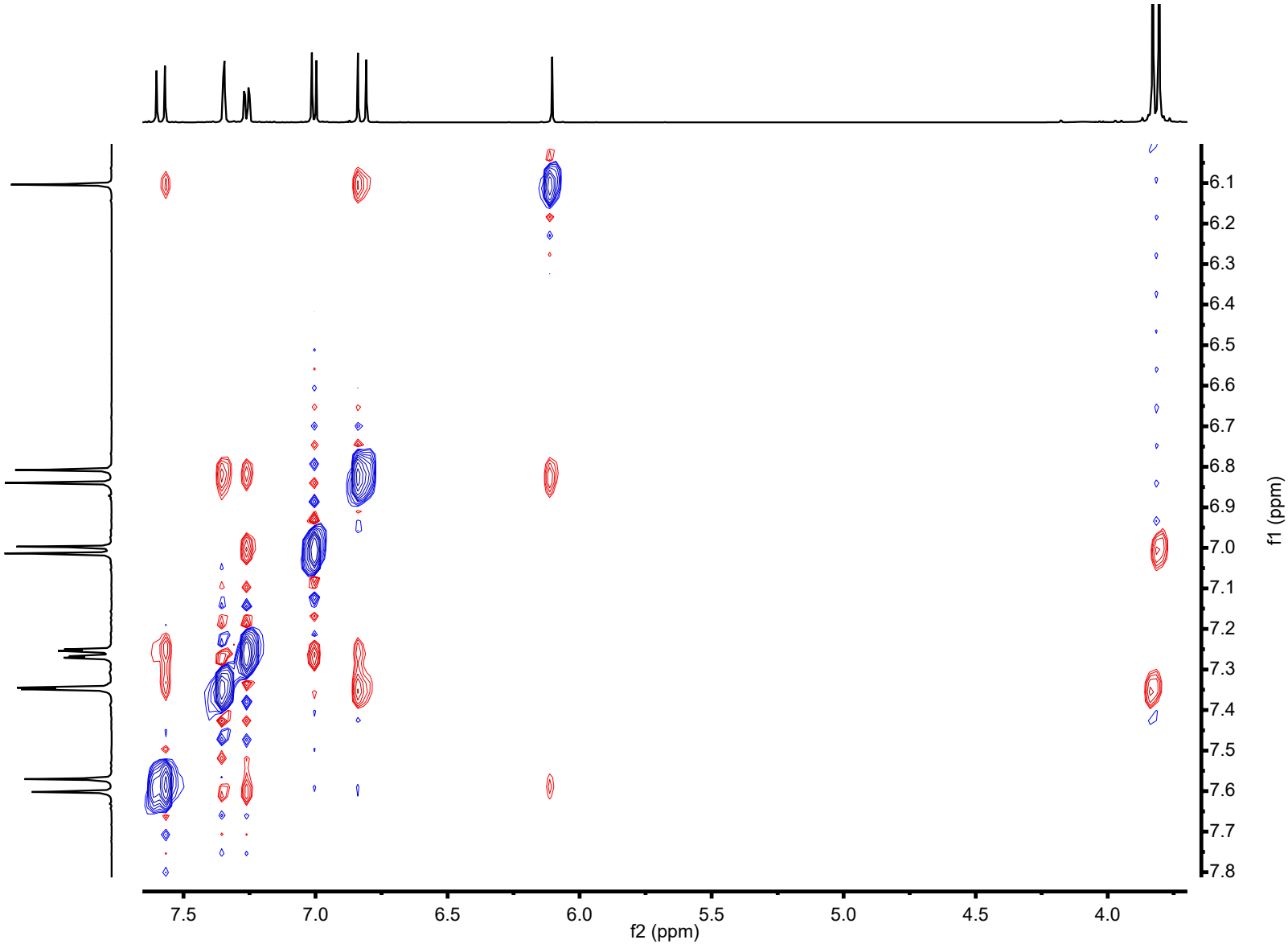


Fig S14. 500 MHz ROESY NMR spectrum of DiMeOC.

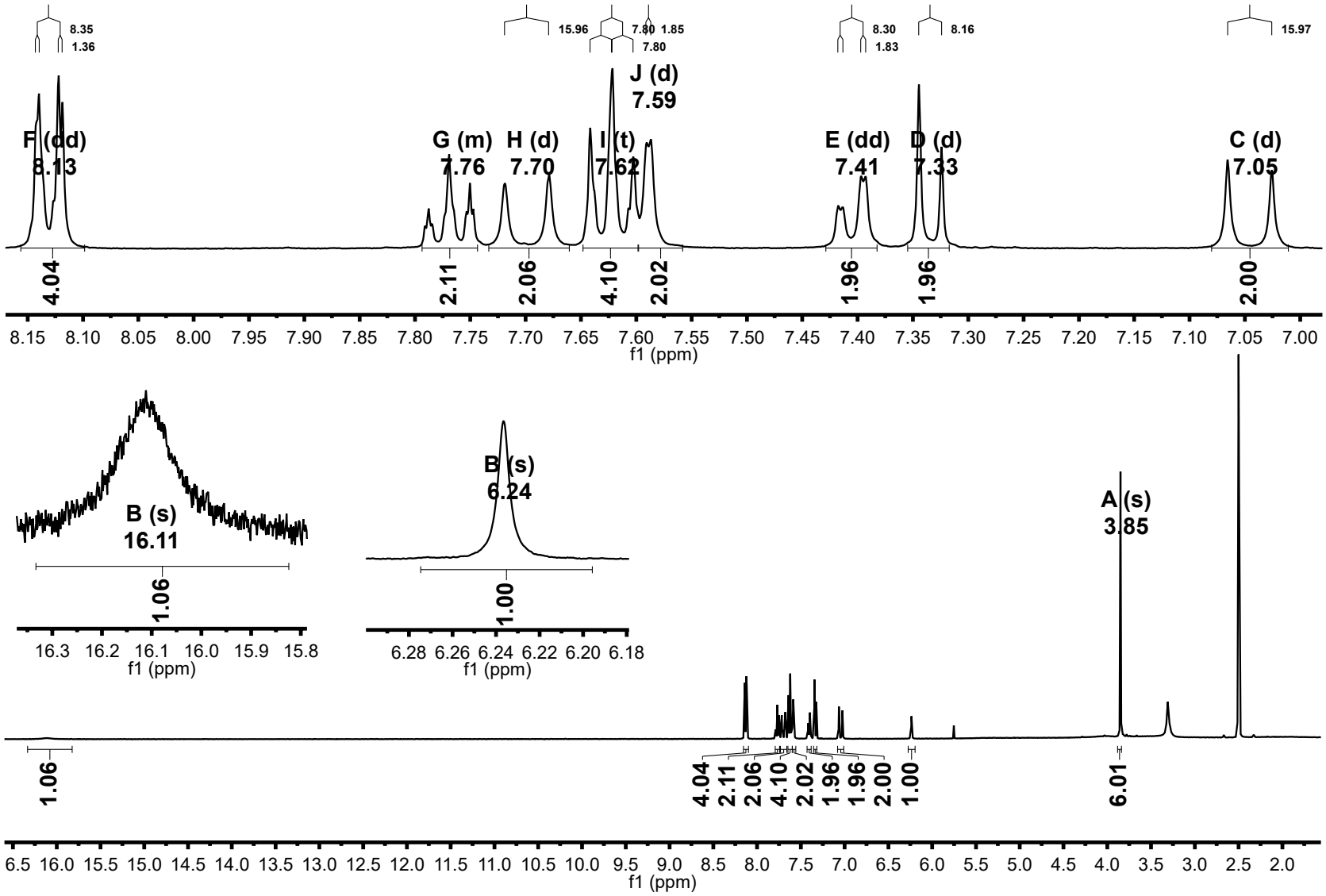


Fig S15. 500 MHz ^{1}H NMR spectrum of DiBzOC.

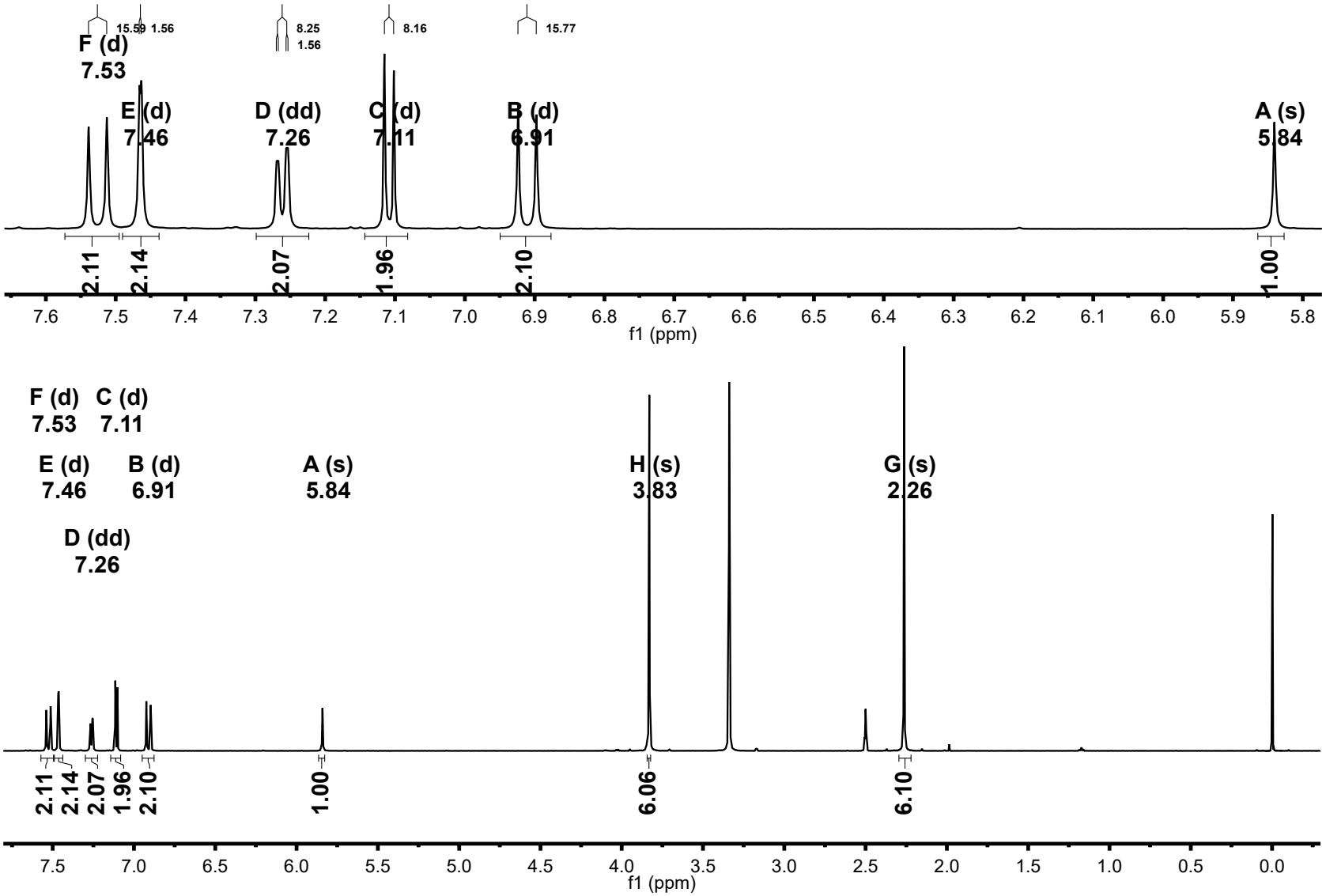


Fig S16. 500 MHz ^{1}H NMR spectrum of DAC-Zn.

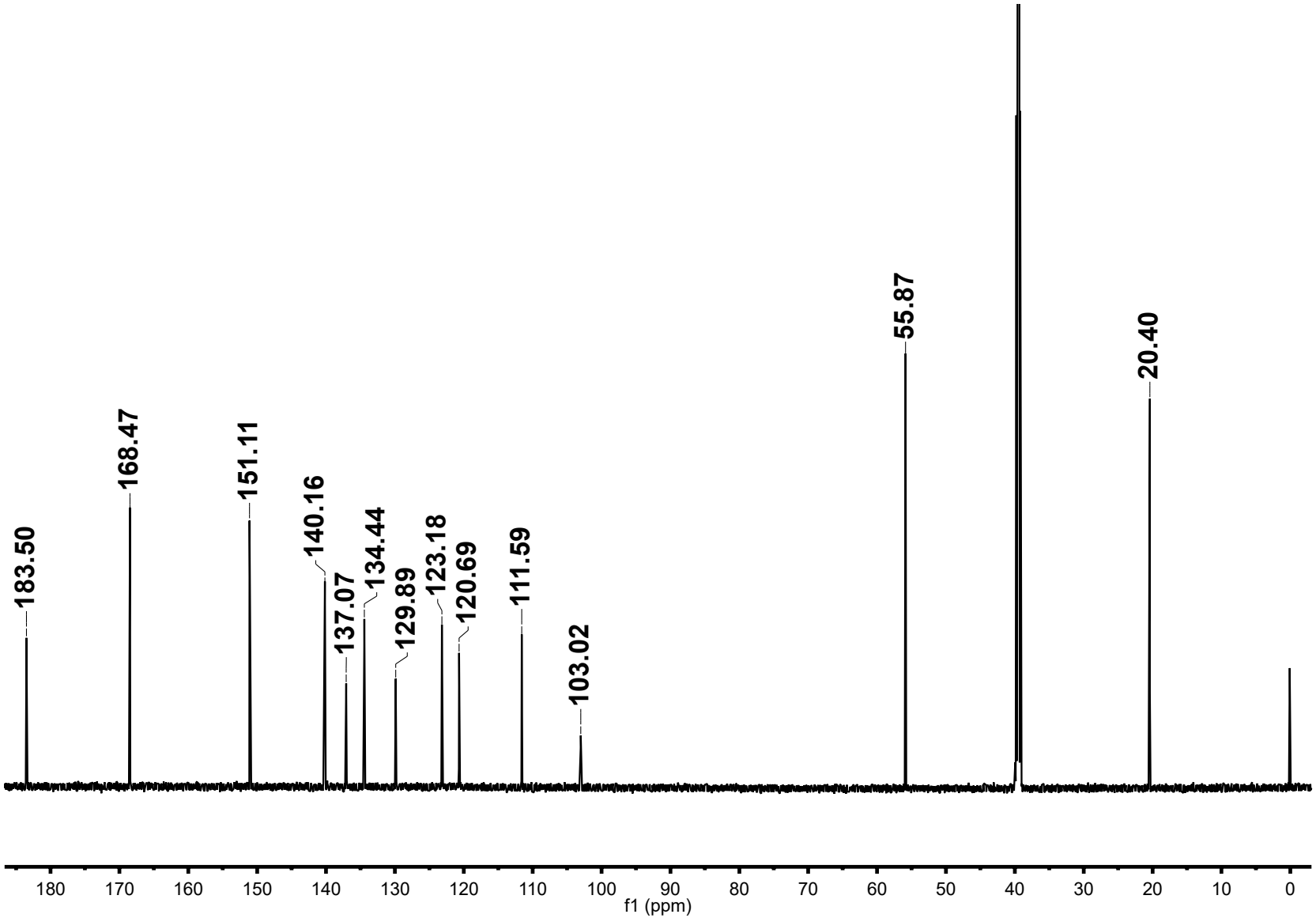


Fig S17. 125 MHz ^{13}C NMR spectrum of DAC-Zn.

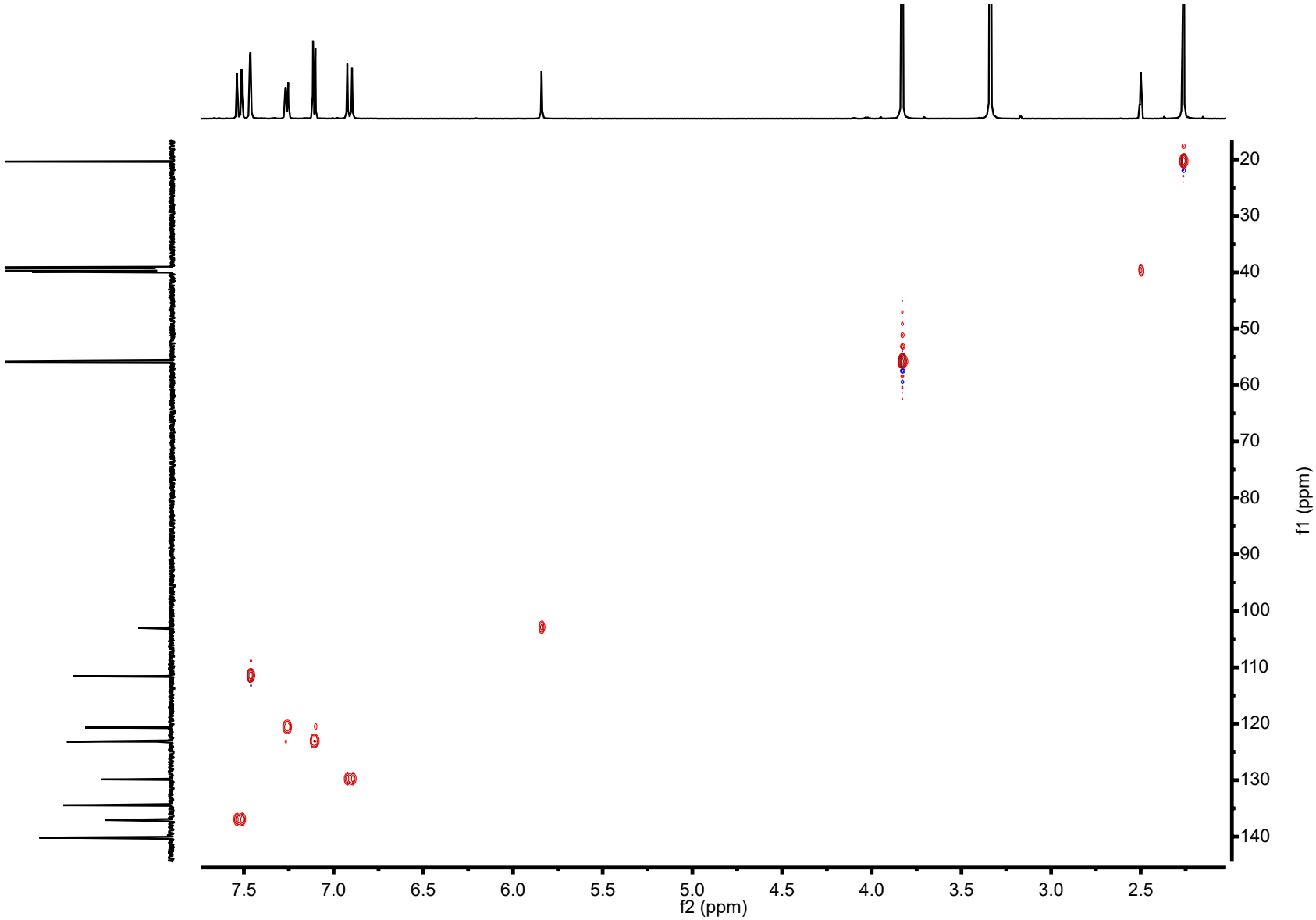


Fig S18. 500 MHz HSQC NMR spectrum of DAC-Zn.

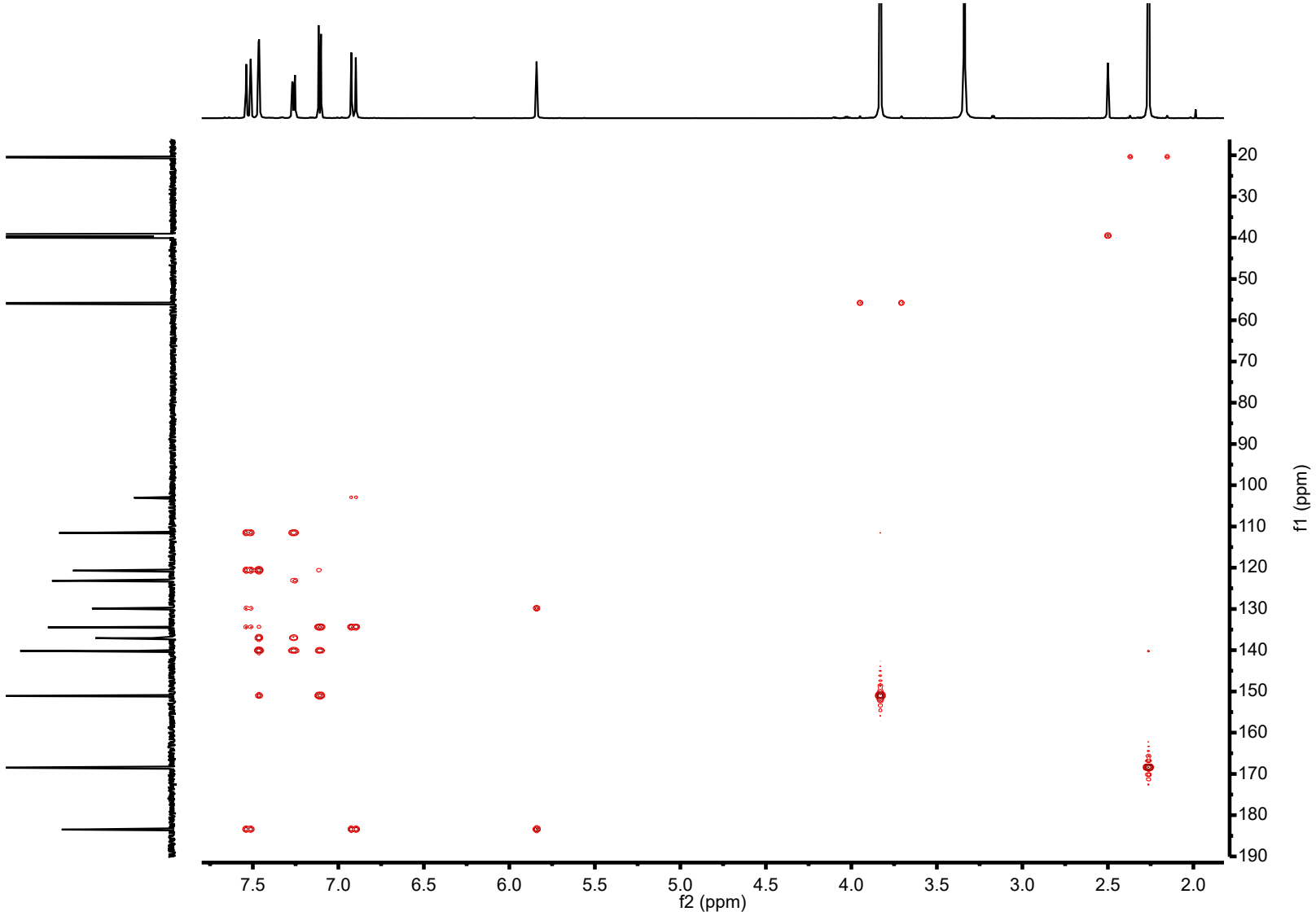


Fig S19. 500 MHz HMBC NMR spectrum of DAC-Zn.

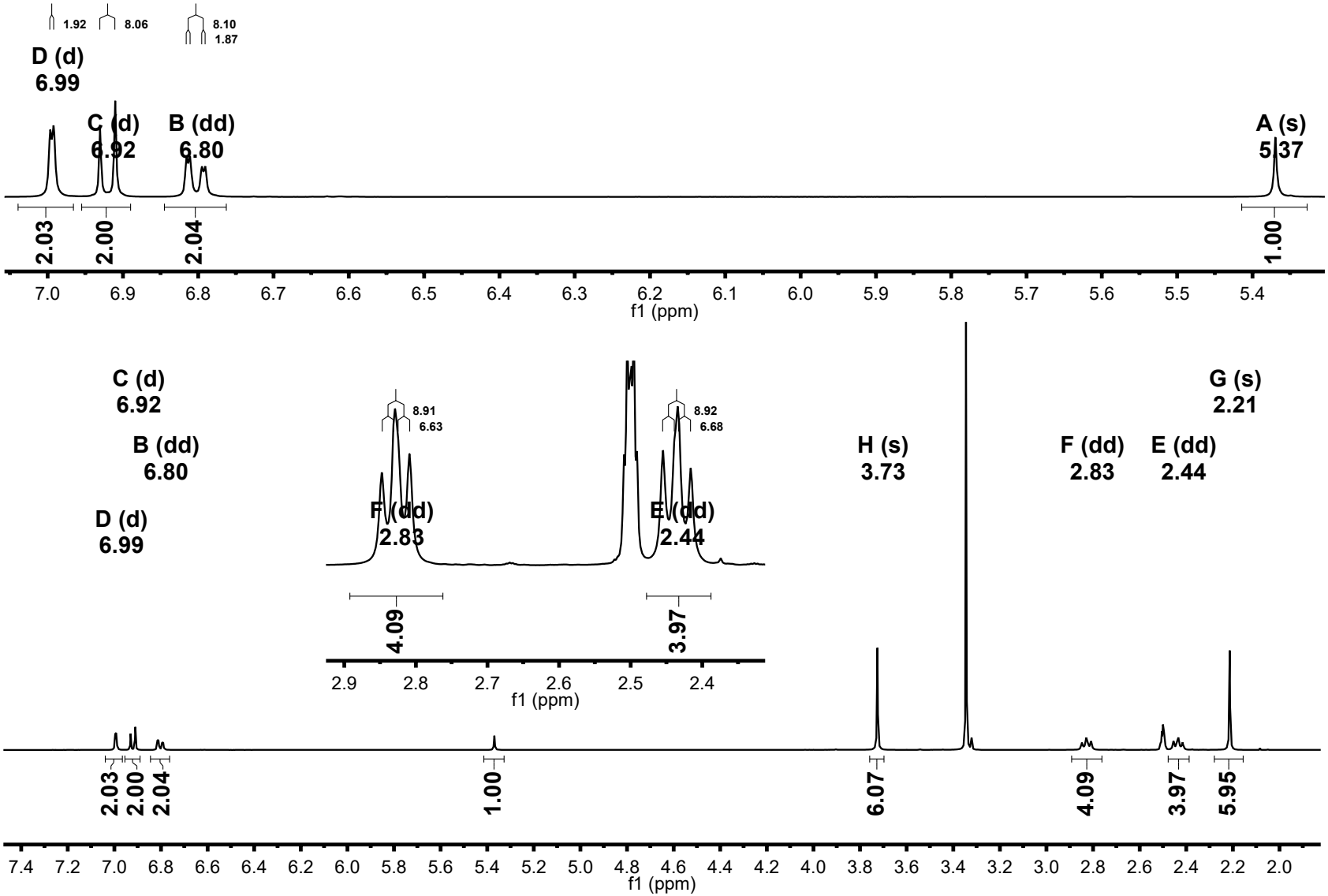


Fig S20. 500 MHz ^{1}H NMR spectrum of DACH-Zn.

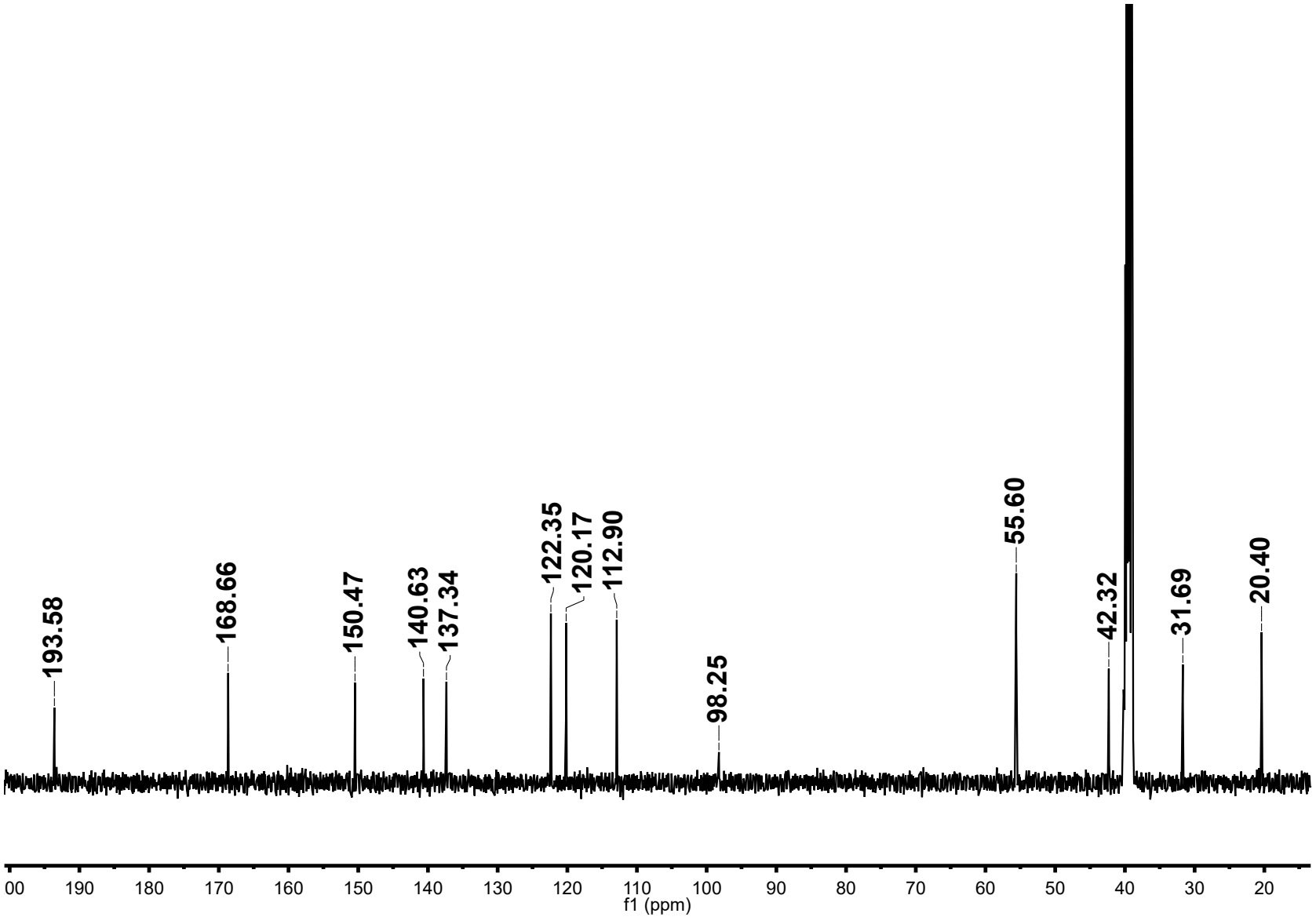


Fig S21. 125 MHz ^{13}C NMR spectrum of DACH-Zn.

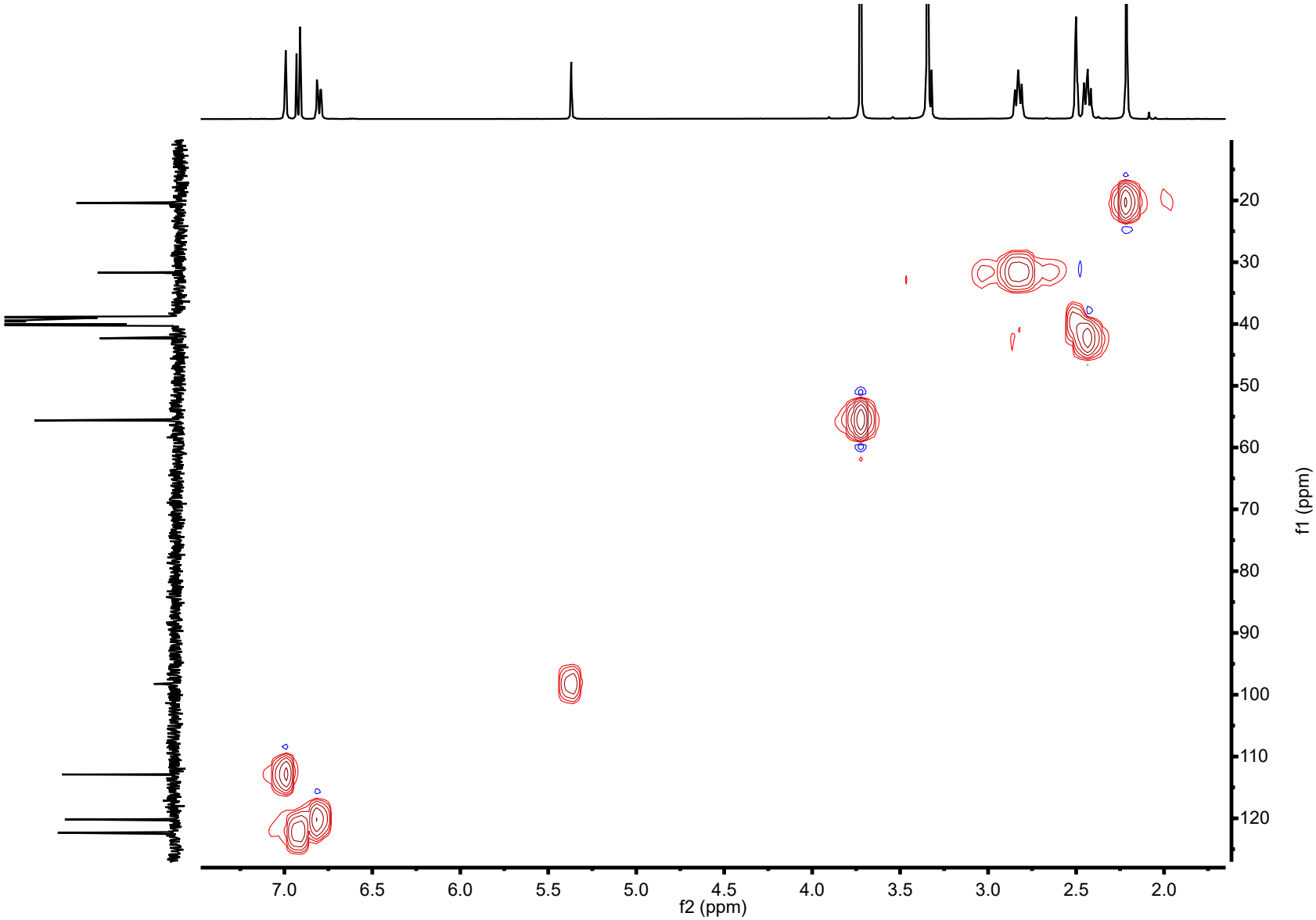


Fig S22. 500 MHz HSQC NMR spectrum of DACH-Zn.

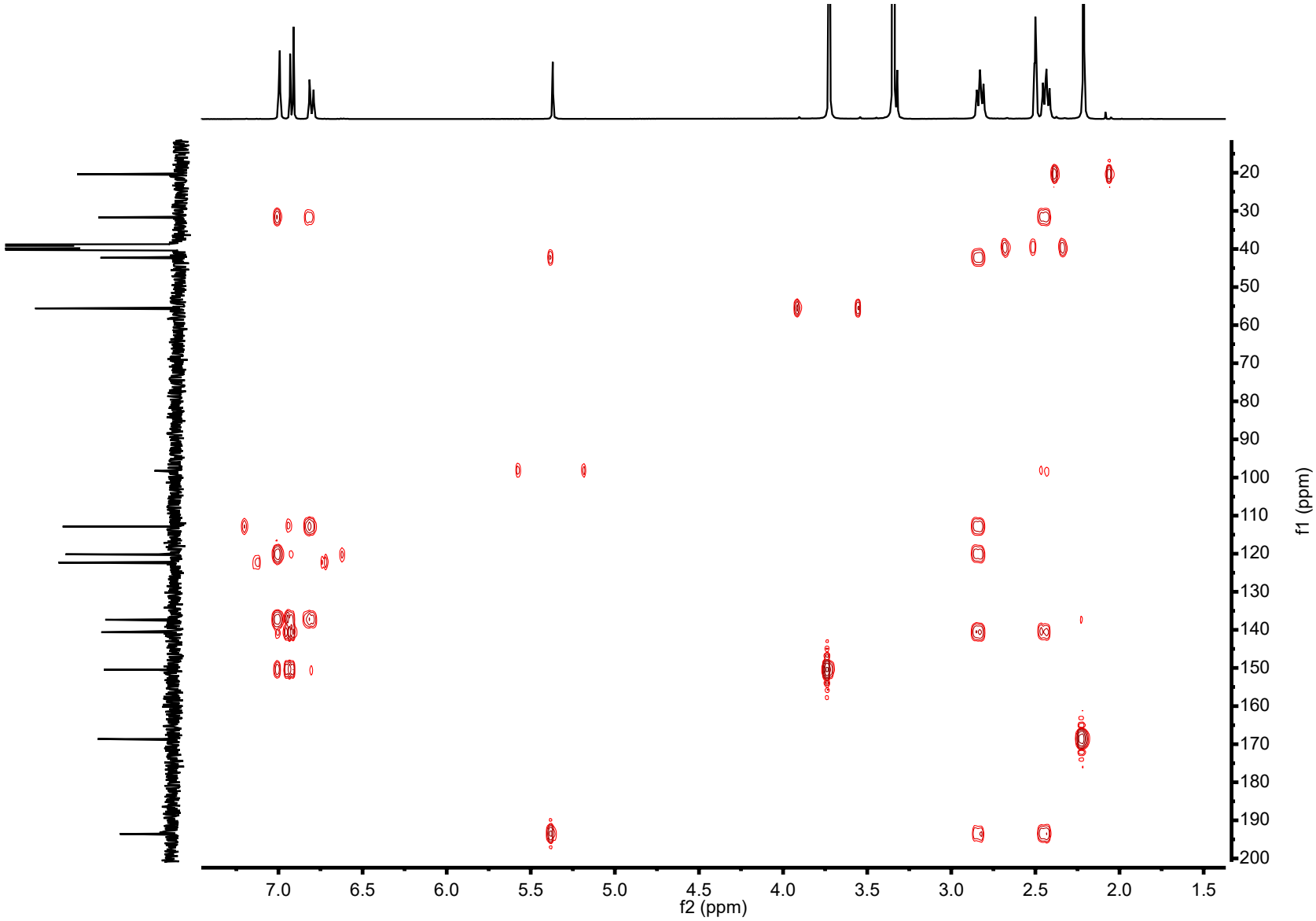


Fig S23. 500 MHz HMBC NMR spectrum of DACH-Zn.

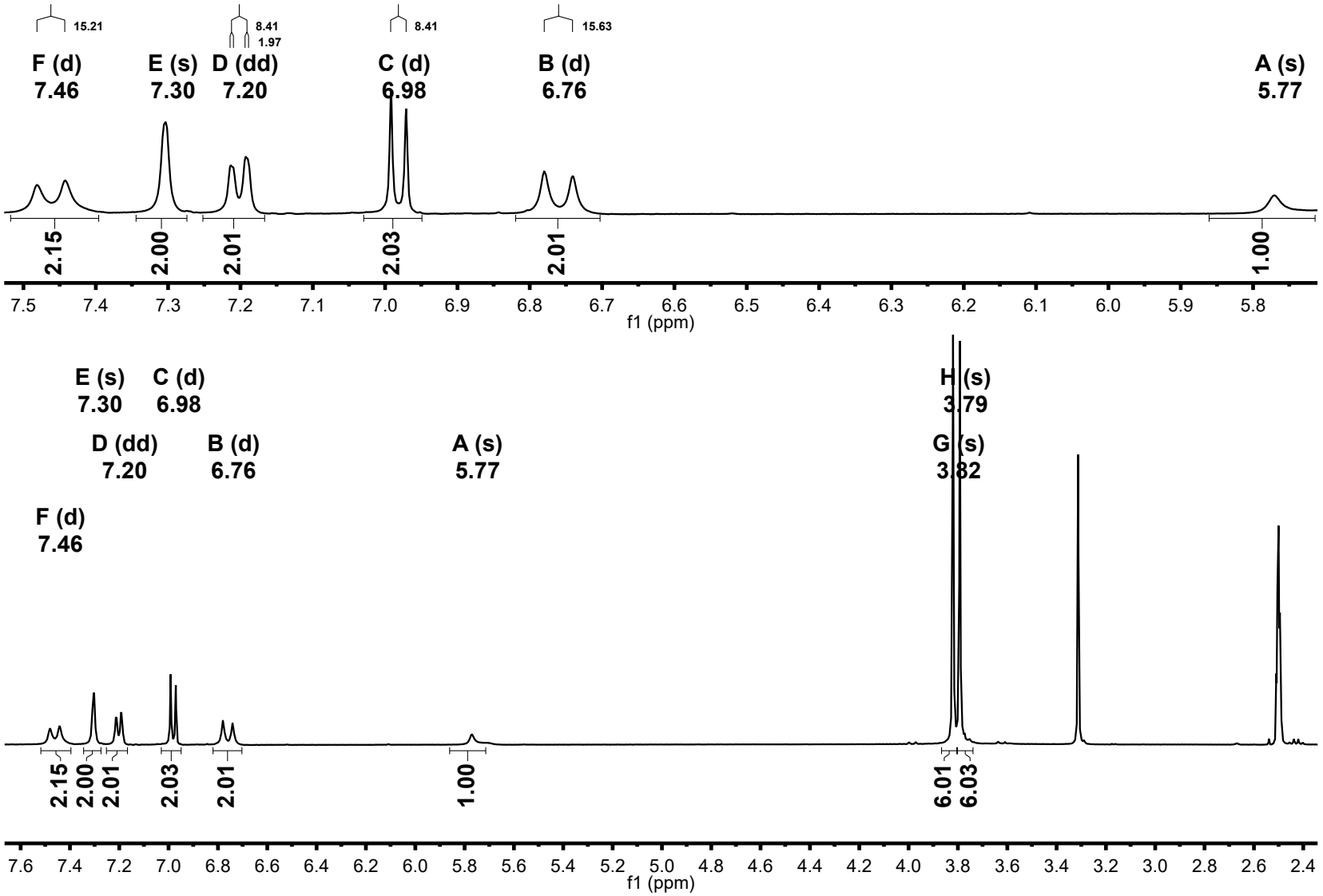


Fig S24. 500 MHz ^{1}H NMR spectrum of DiMeOC-Zn.

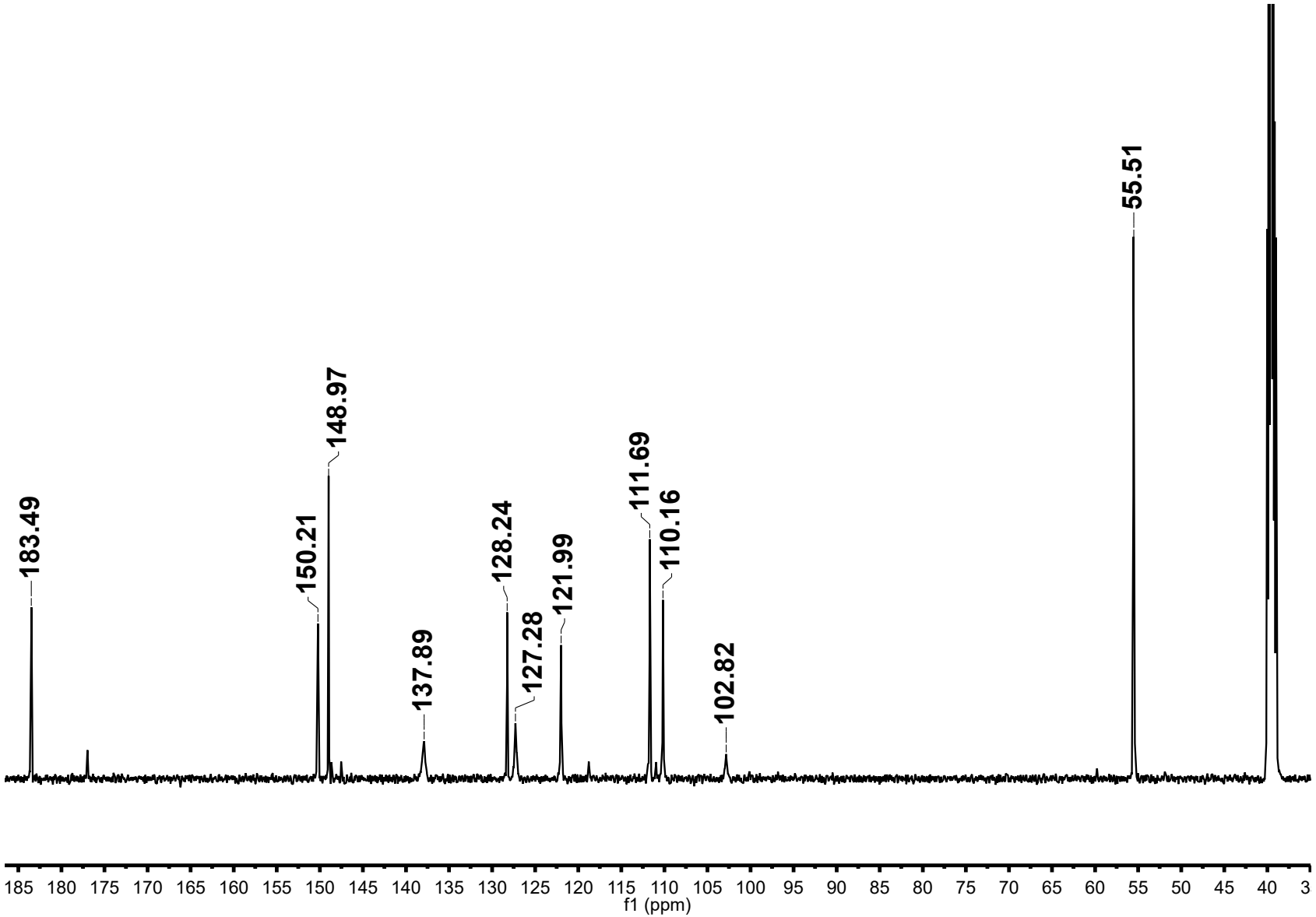


Fig S25. 125 MHz ^{13}C NMR spectrum of DiMeOC-Zn.

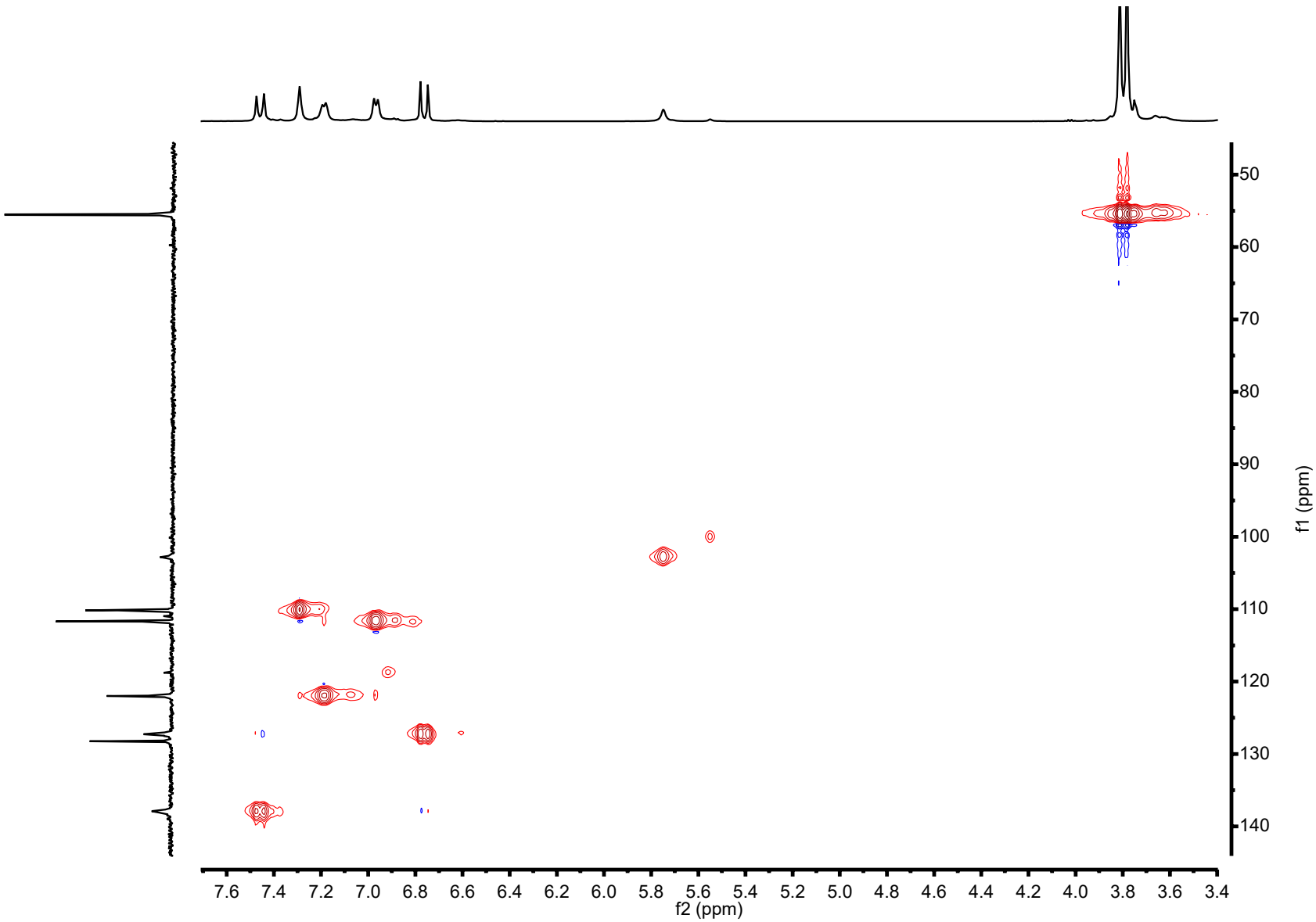


Fig S26. 500 MHz HSQC NMR spectrum of DiMeOC-Zn.

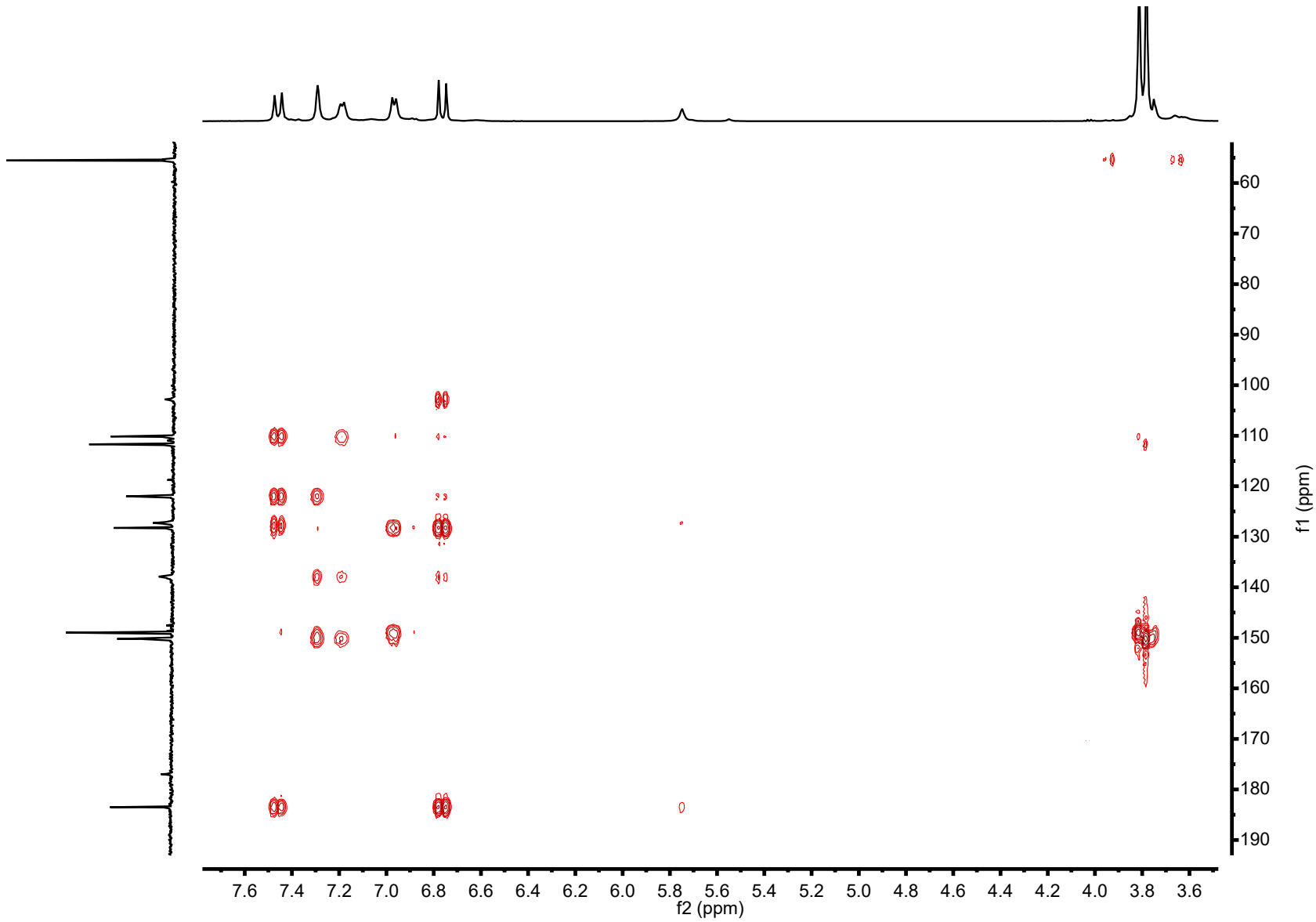


Fig S27. 500 MHz HMBC NMR spectrum of DiMeOC-Zn.

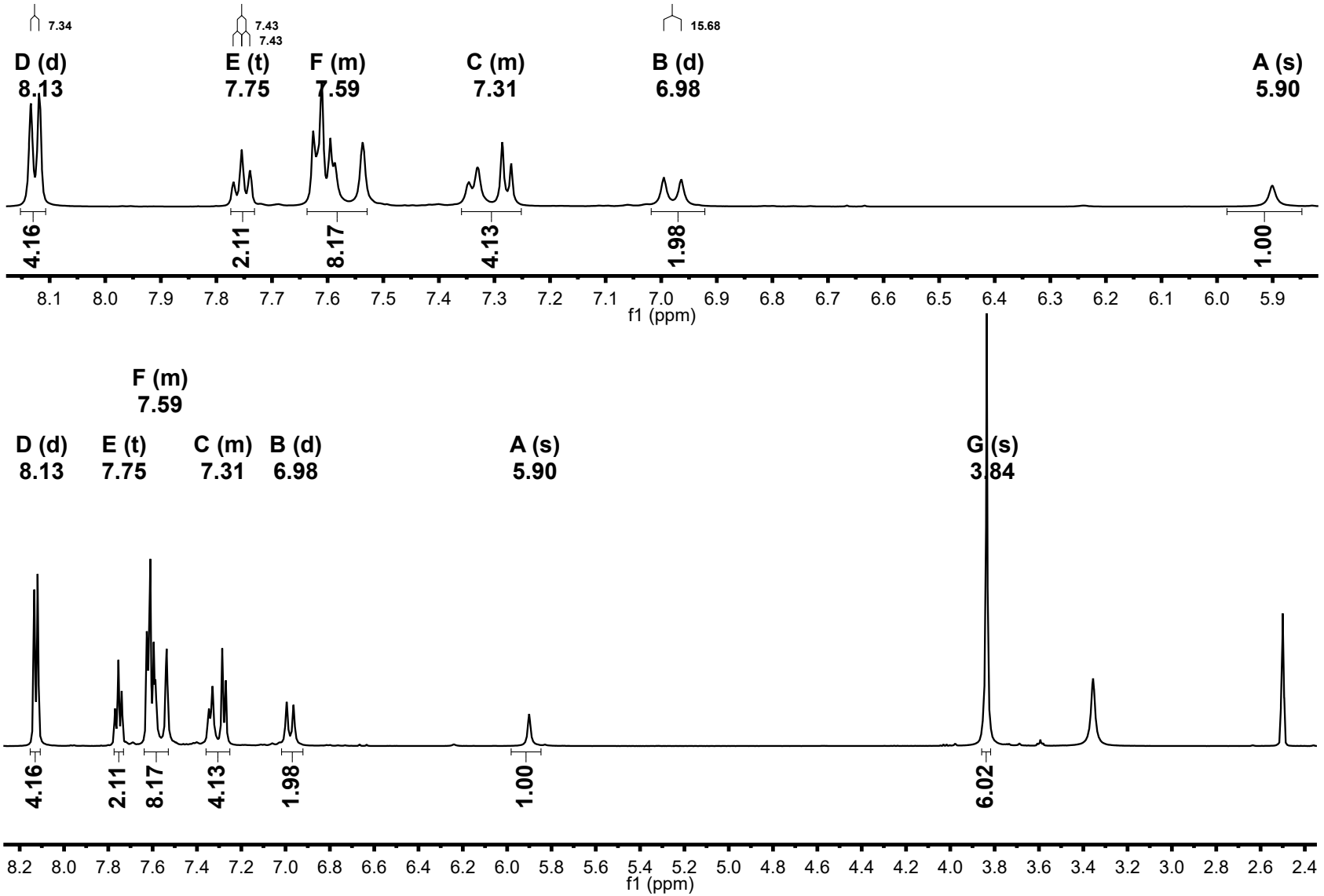


Fig S28. 500 MHz ^{1}H NMR spectrum of DiBzOC-Zn.

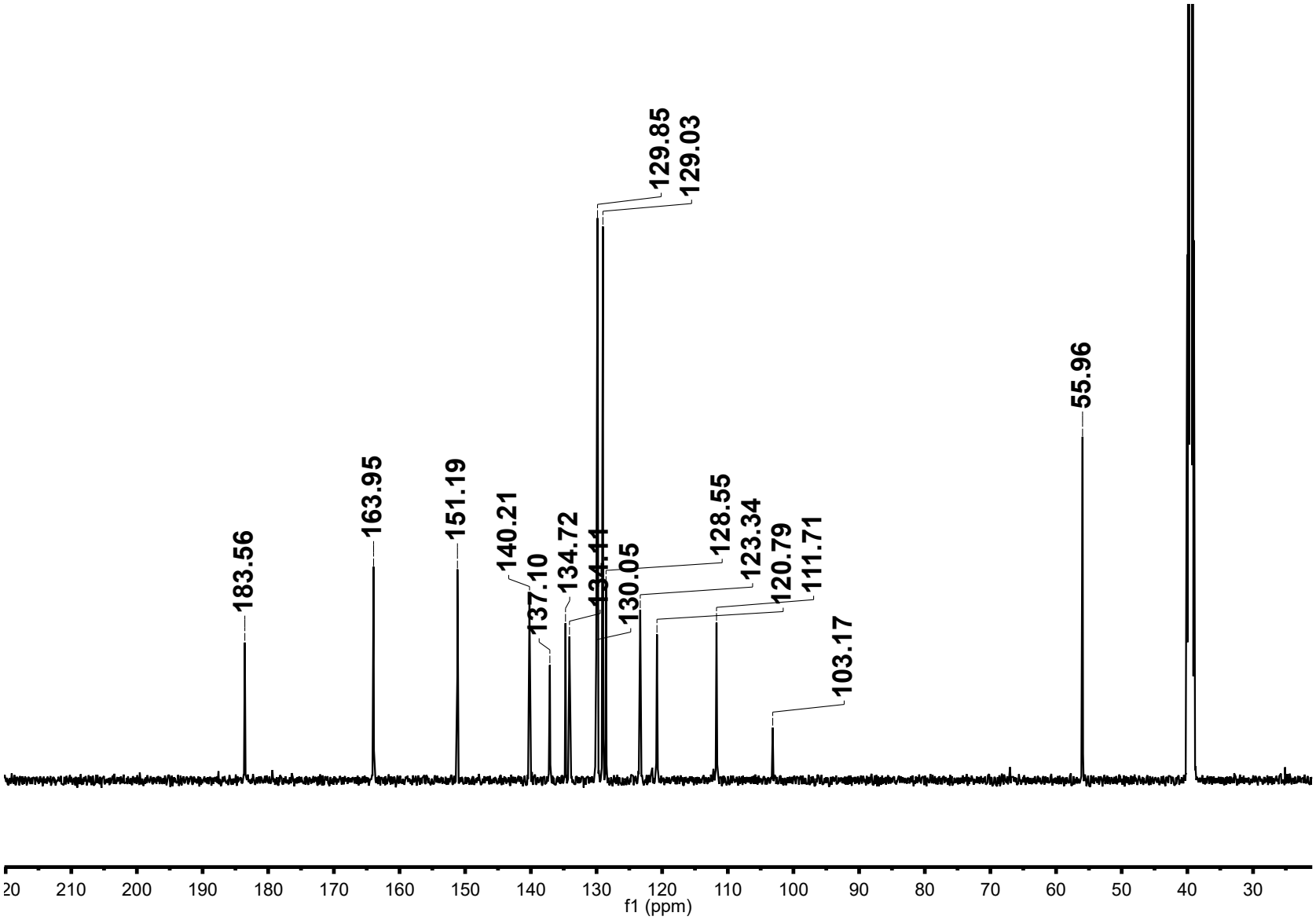


Fig S29. 125 MHz ^{13}C NMR spectrum of DiBzOC-Zn.

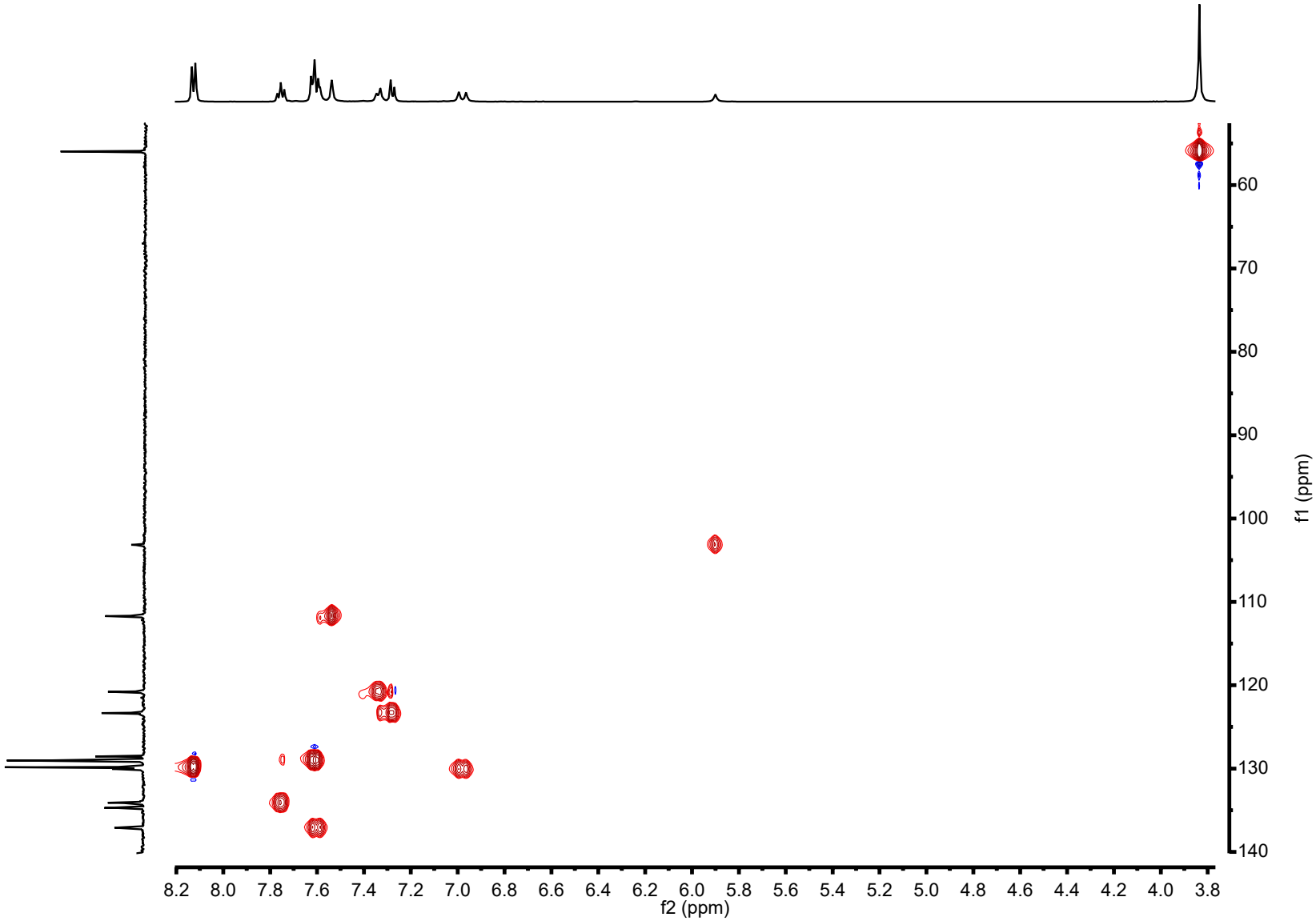


Fig S30. 500 MHz HSQC NMR spectrum of DiBzO-Zn.

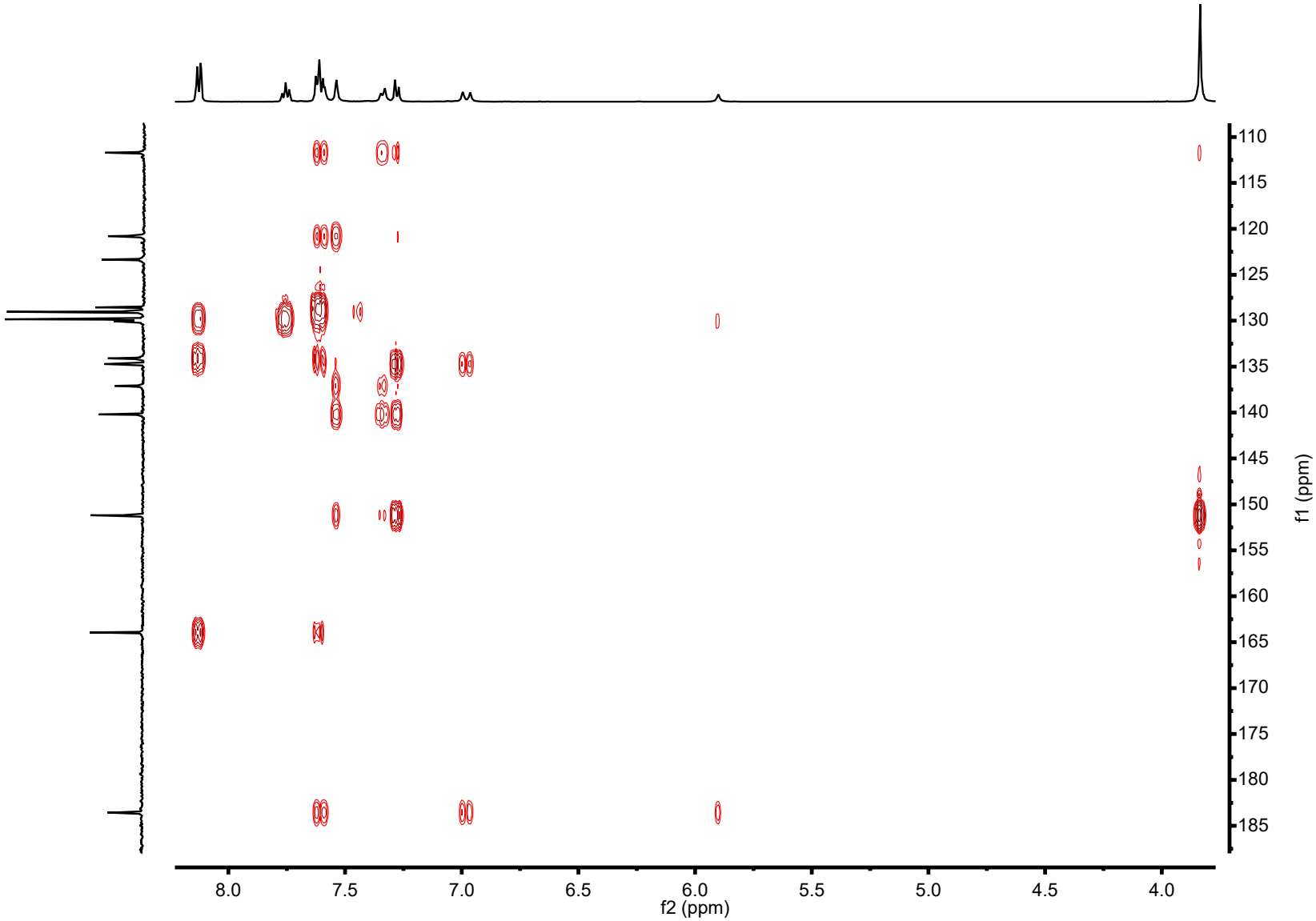


Fig S31. 500 MHz HMBC NMR spectrum of DiBzOC-Zn.

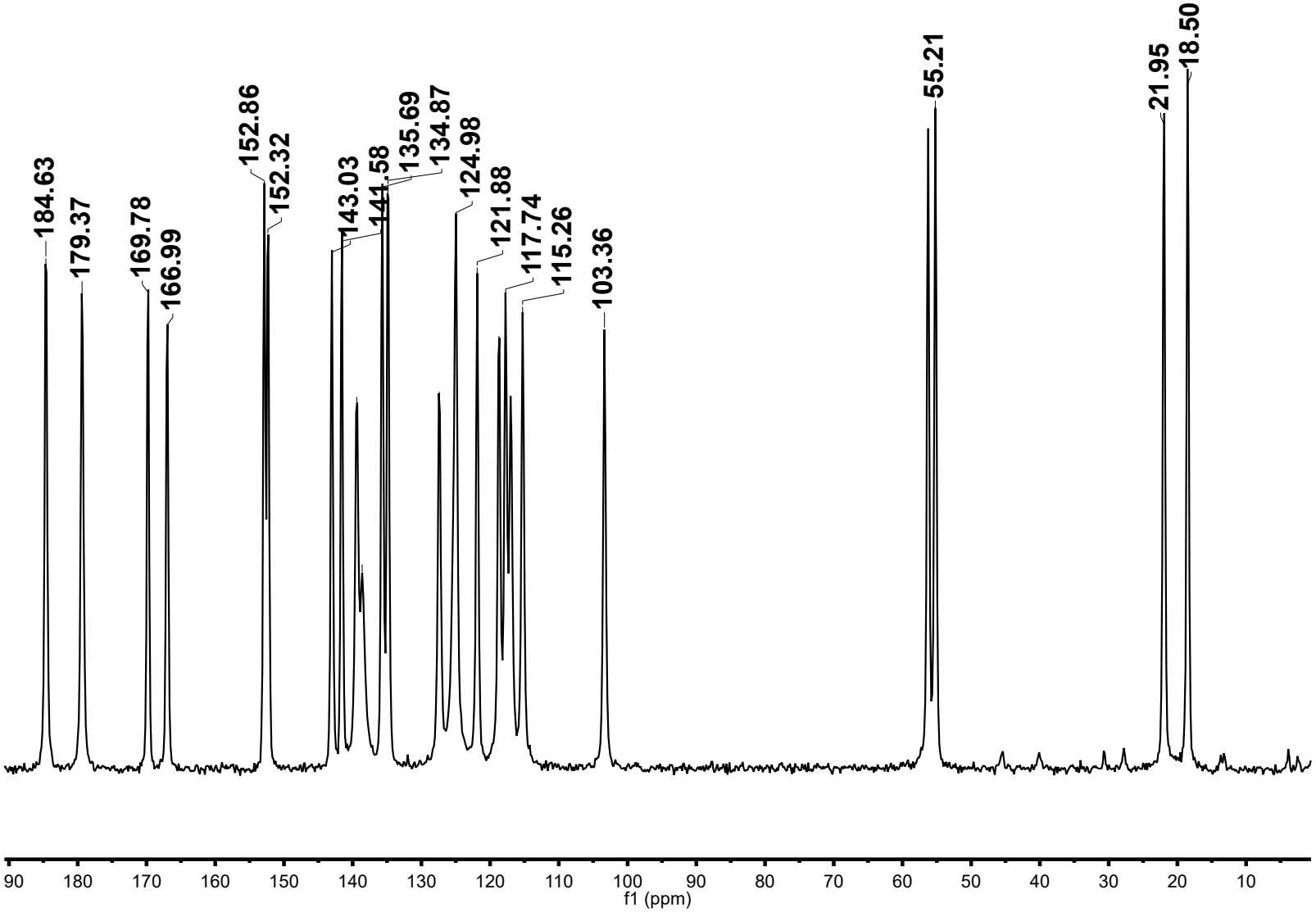


Fig S32. 100 MHz ^{13}C ssNMR spectrum of DAC.

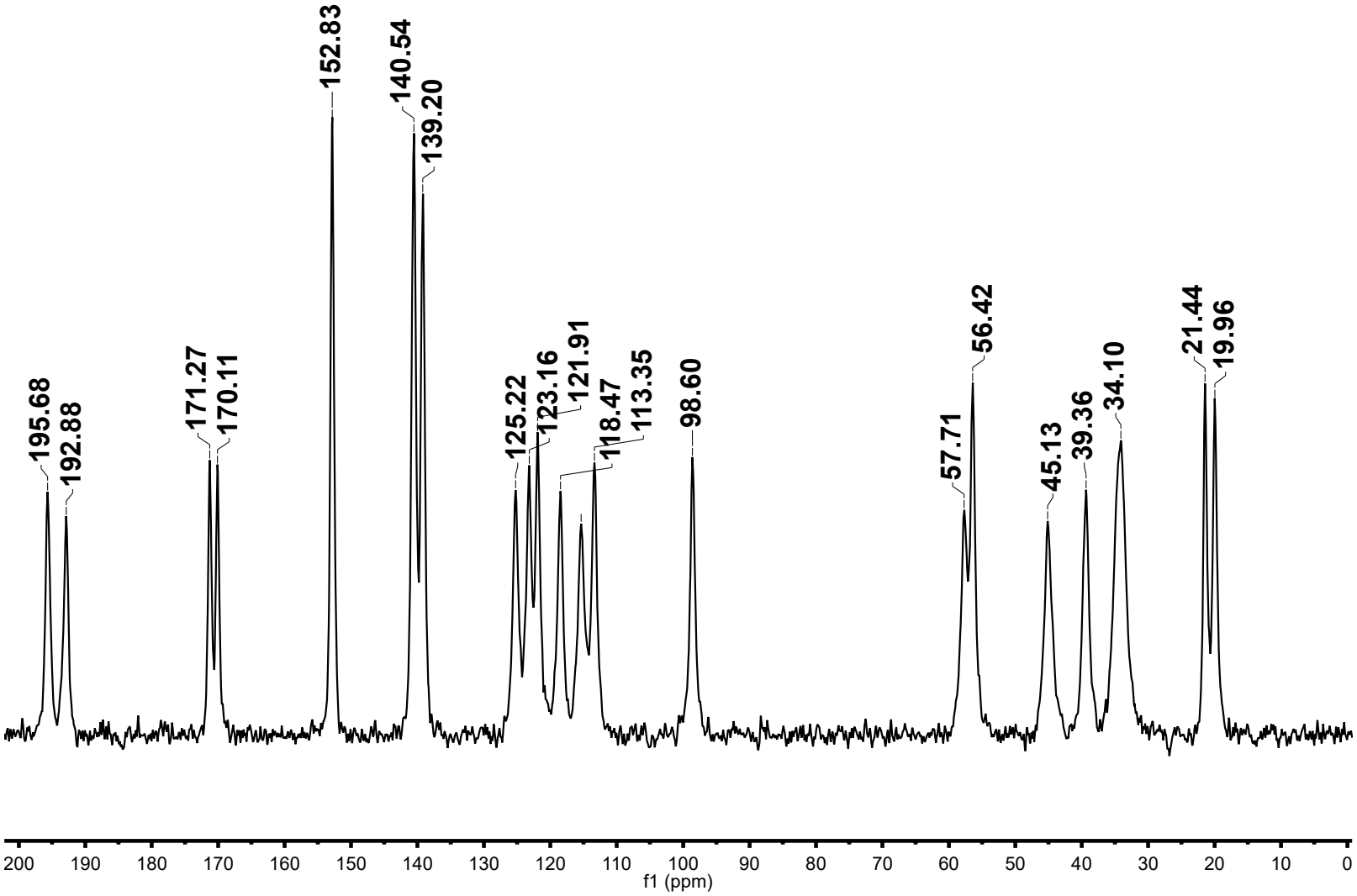


Fig S33. 150 MHz ^{13}C ssNMR spectrum of DACH.

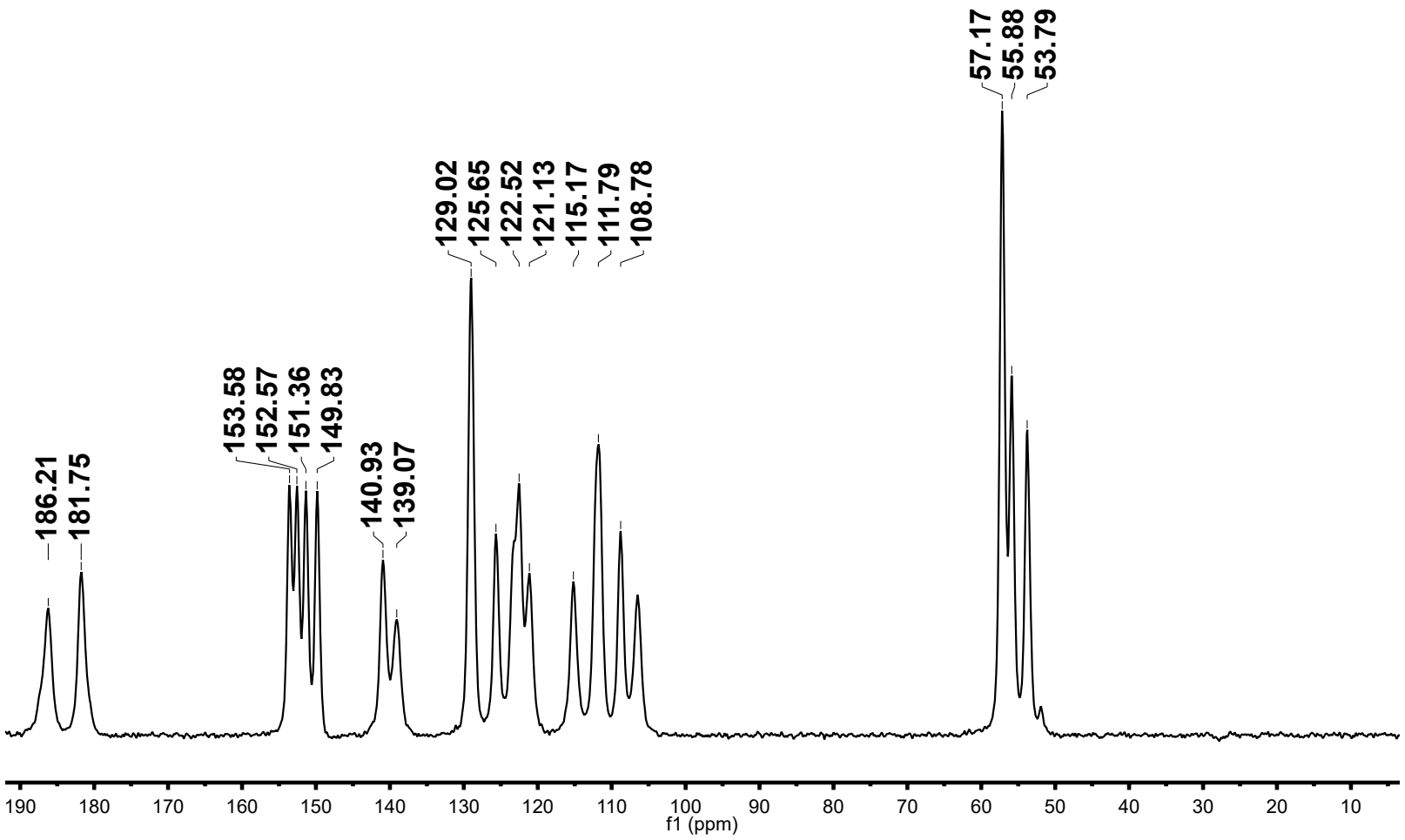


Fig S34. 150 MHz ^{13}C ssNMR spectrum of DiMeOC.

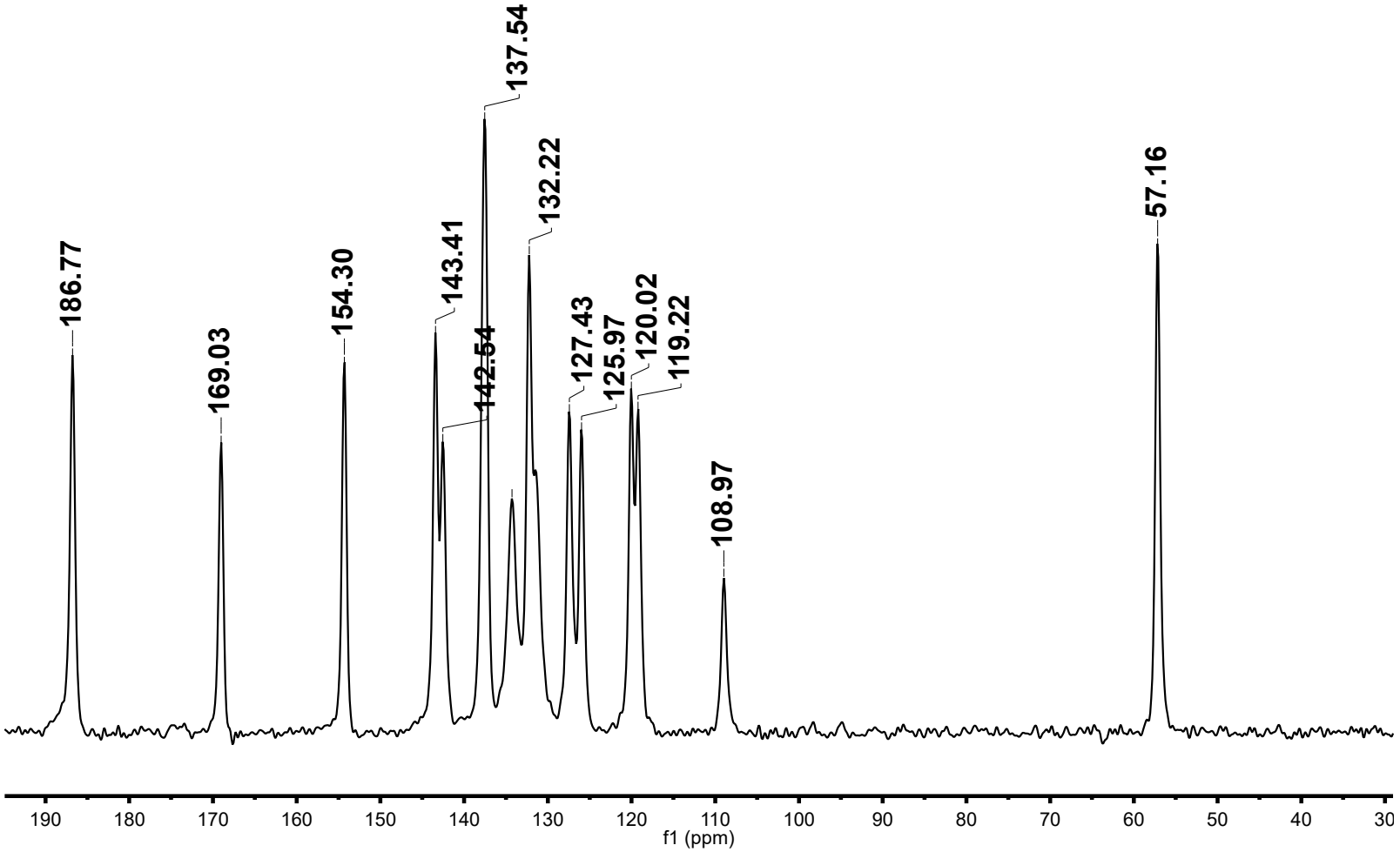


Fig S35. 150 MHz ^{13}C ssNMR spectrum of DiBzOC.

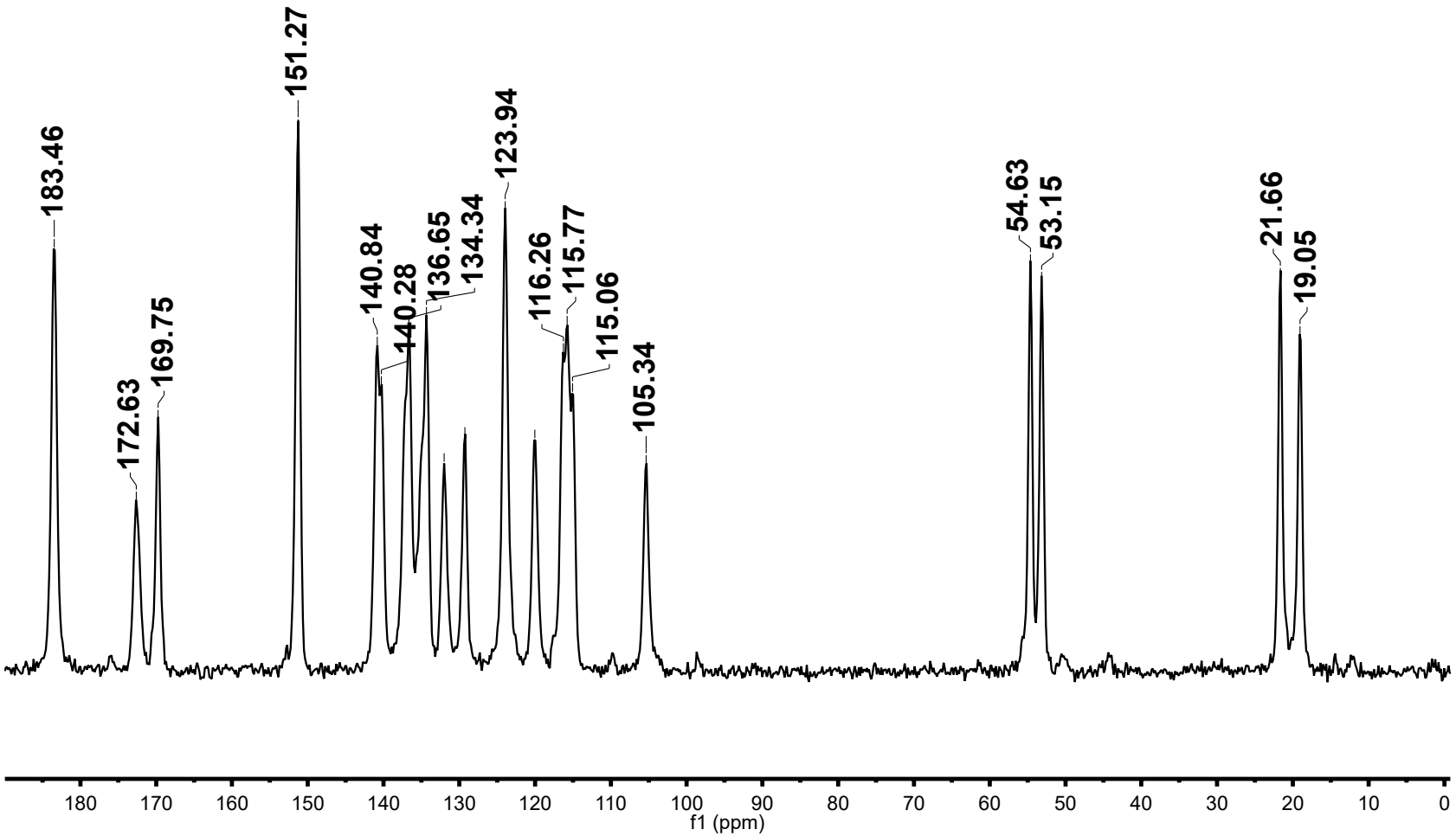


Fig S36. 100 MHz ^{13}C ssNMR spectrum of DAC-Zn.

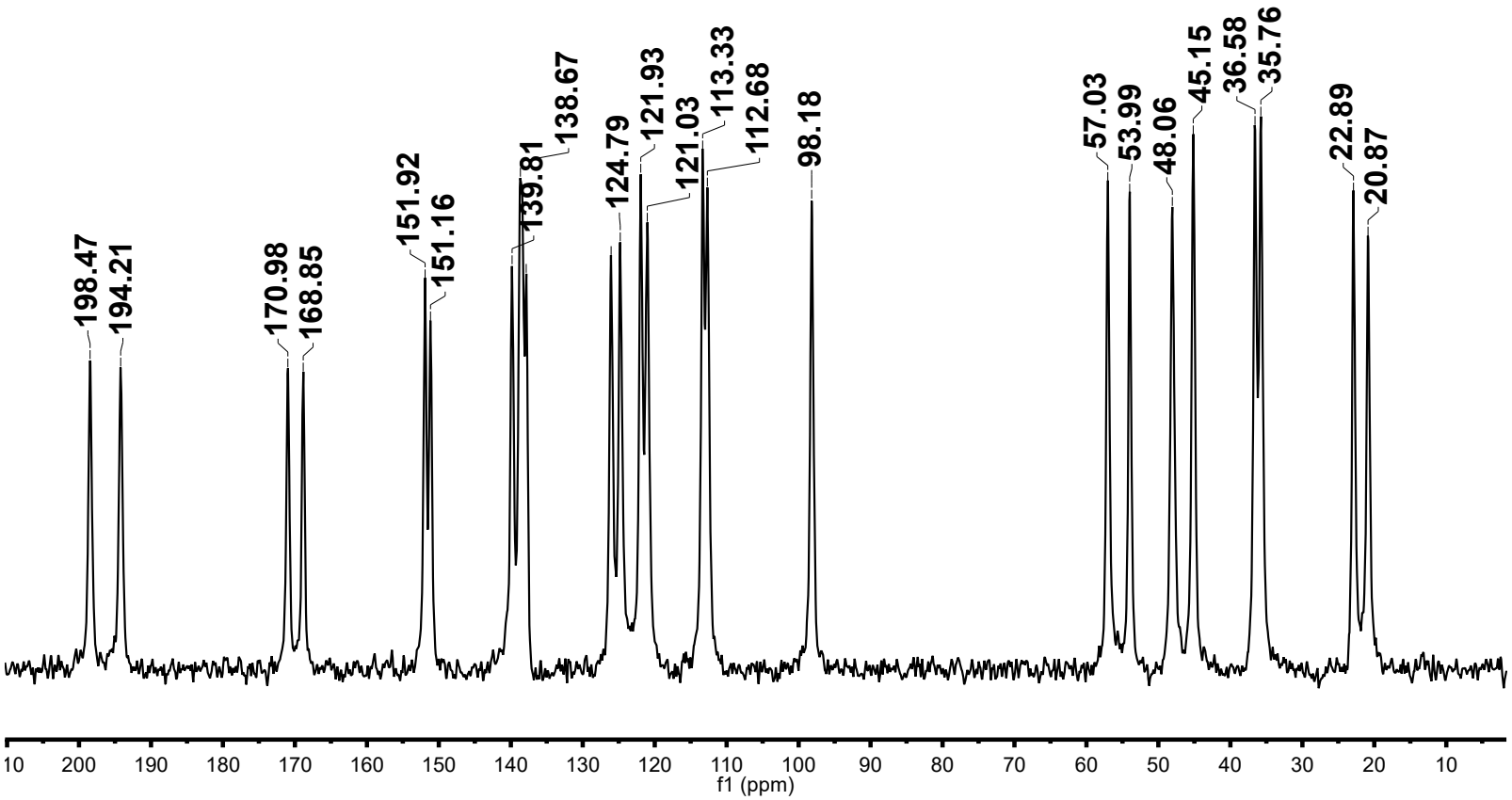


Fig S37. 150 MHz ^{13}C ssNMR spectrum of DACH-Zn.

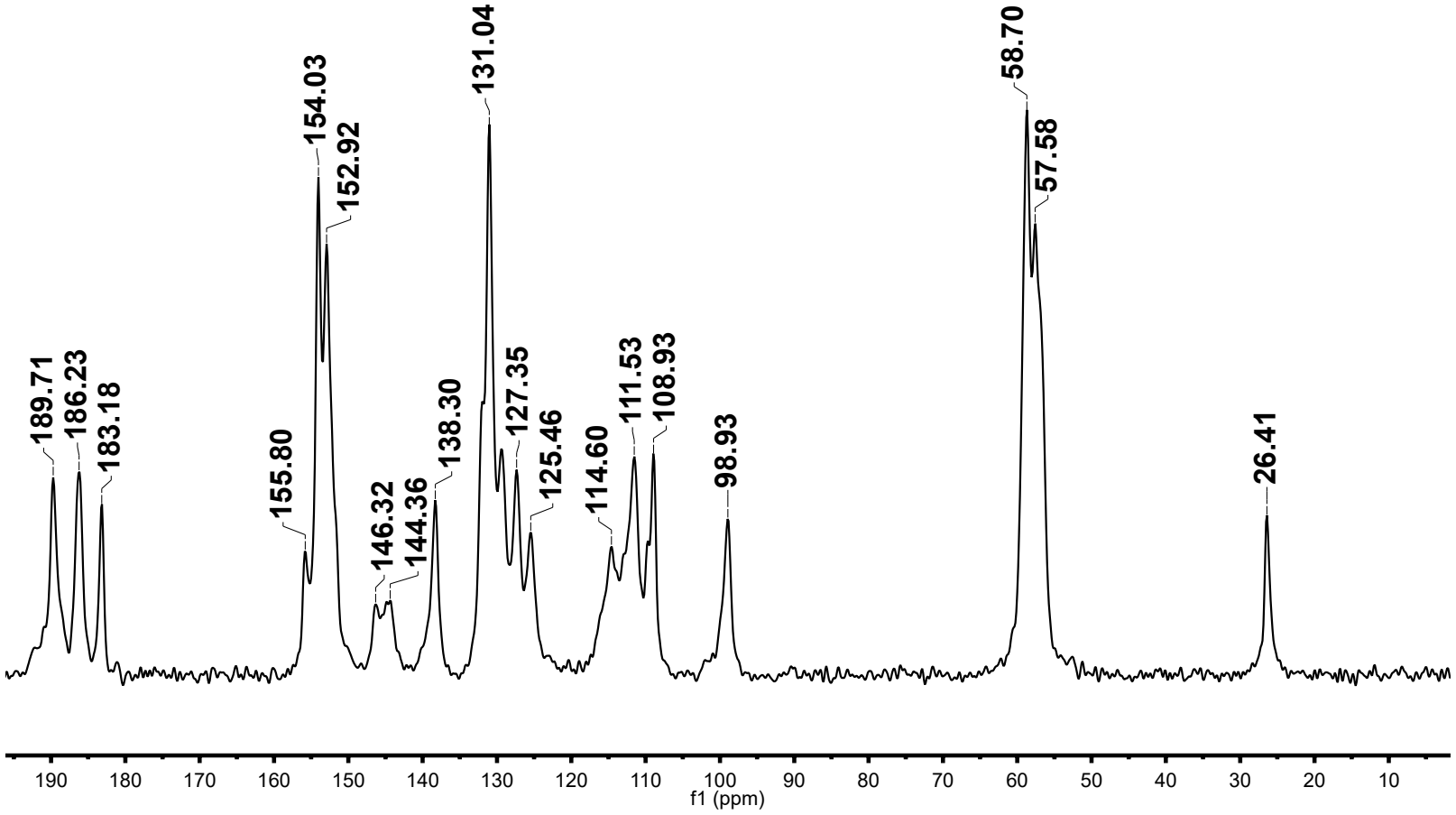


Fig S38. 150 MHz ^{13}C ssNMR spectrum of DiMeOC-Zn.

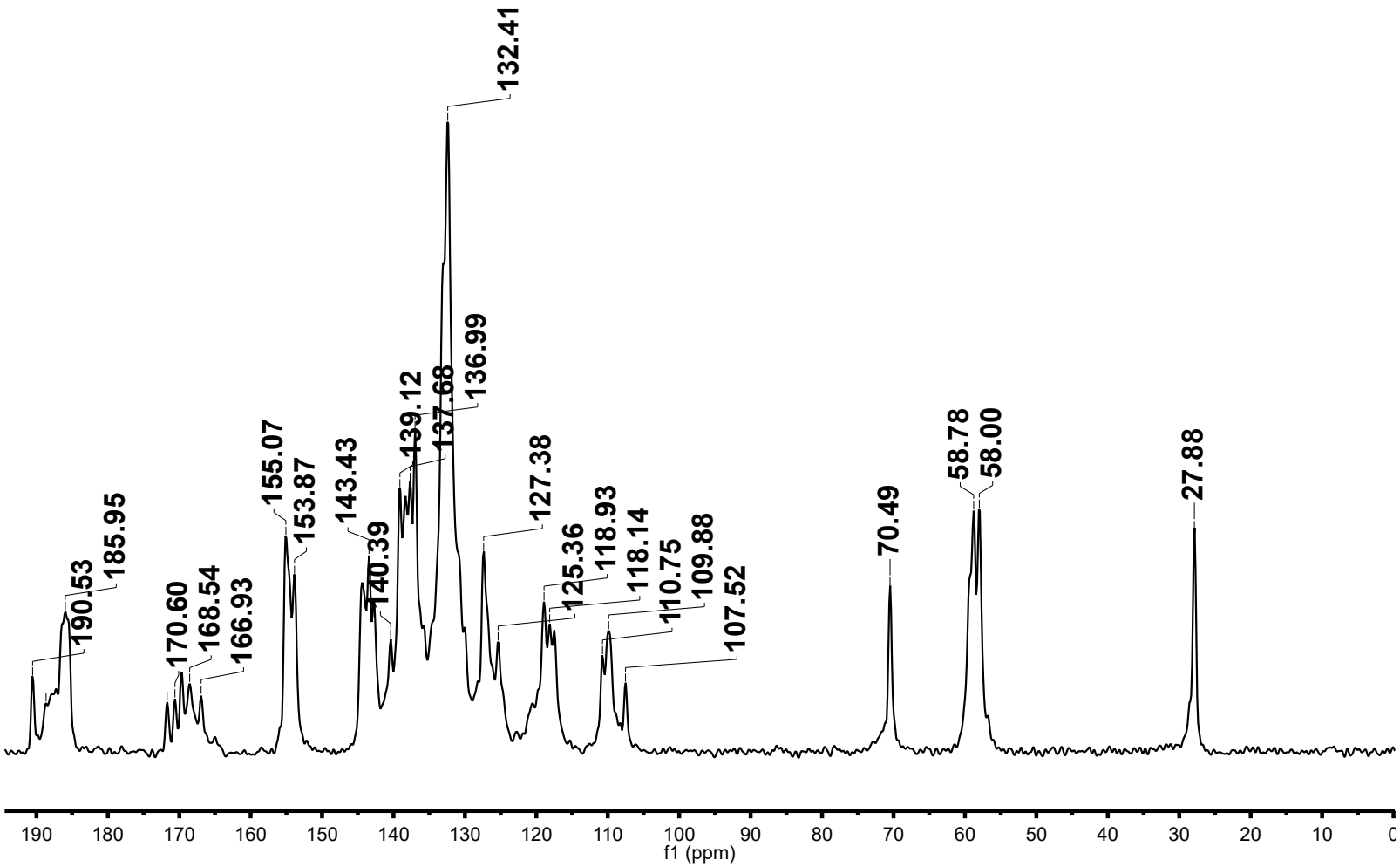


Fig S39. 150 MHz ^{13}C ssNMR spectrum of DiBzOC-Zn.

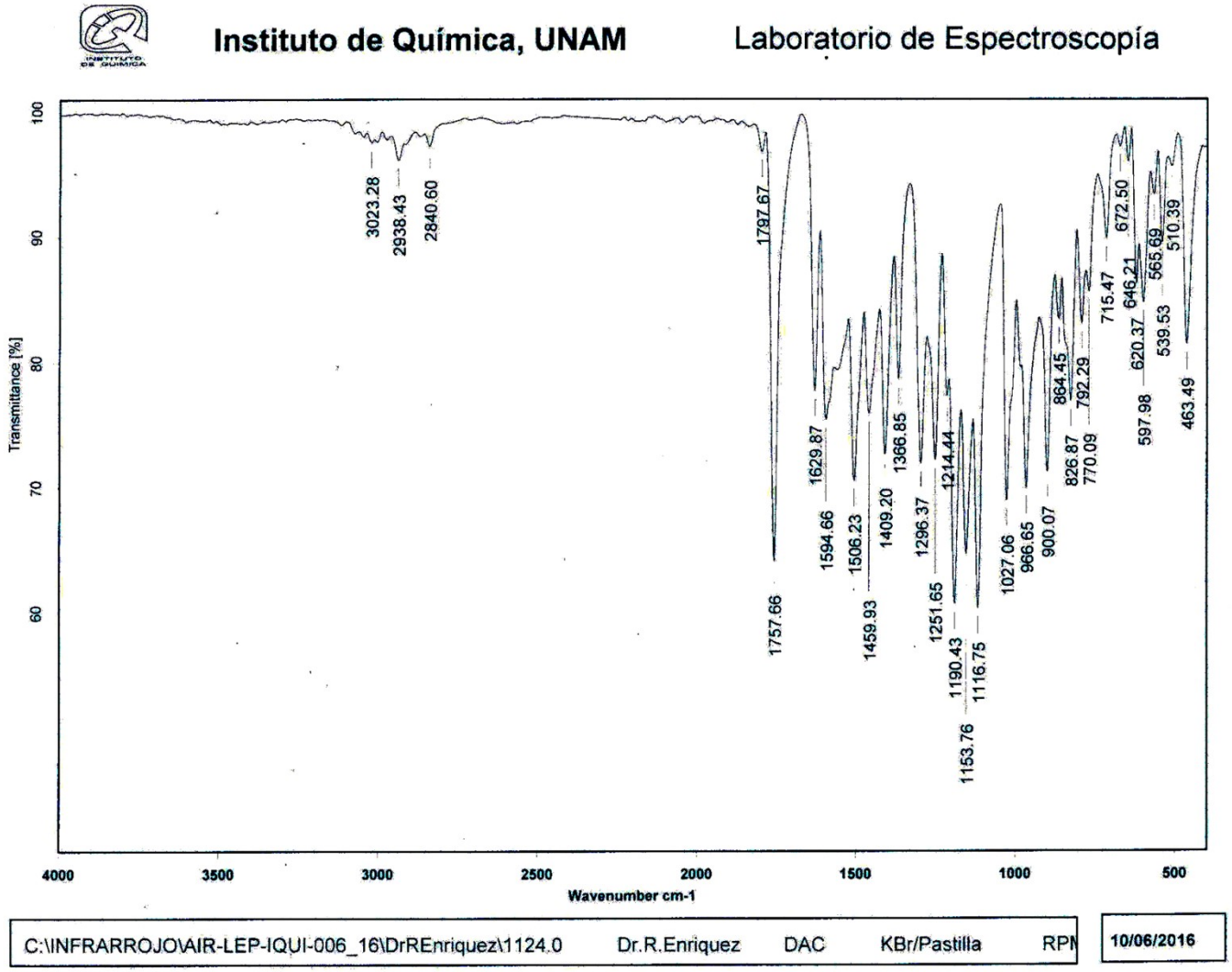


Fig S40. IR Spectrum of DAC.

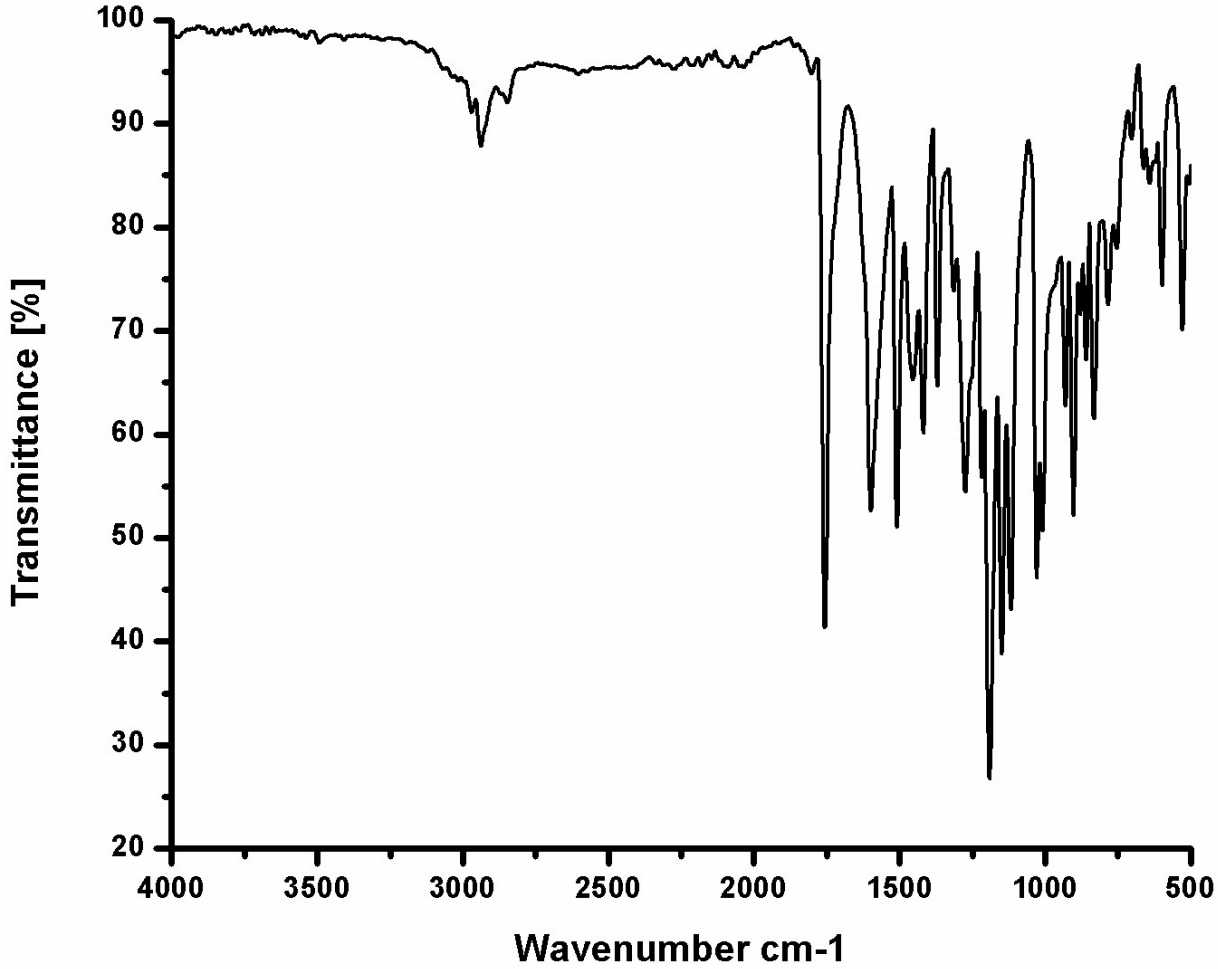


Fig S41. IR Spectrum of DACH.

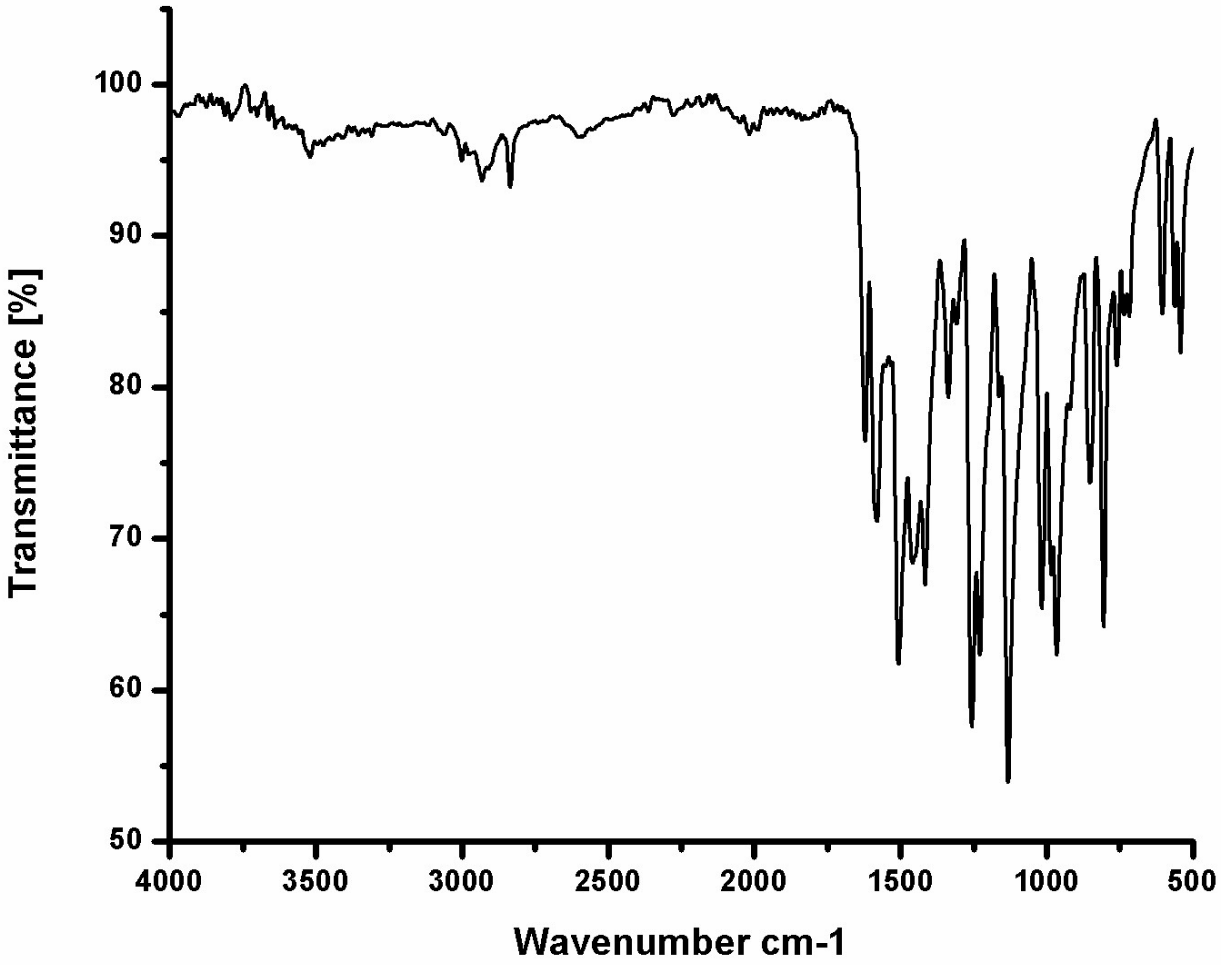


Fig S42. IR Spectrum of DiMeOC.

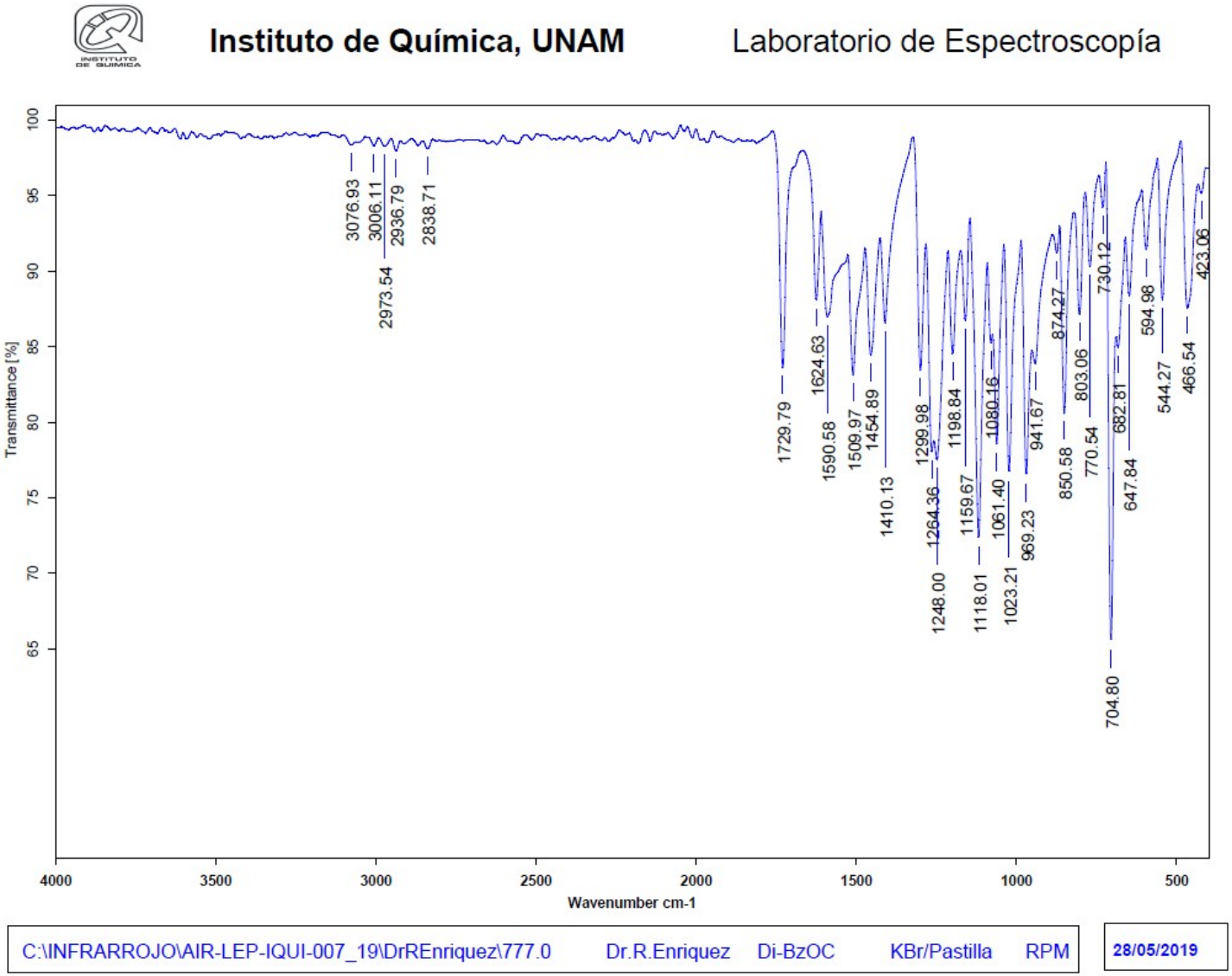


Fig S43. IR Spectrum of DiBzOC.

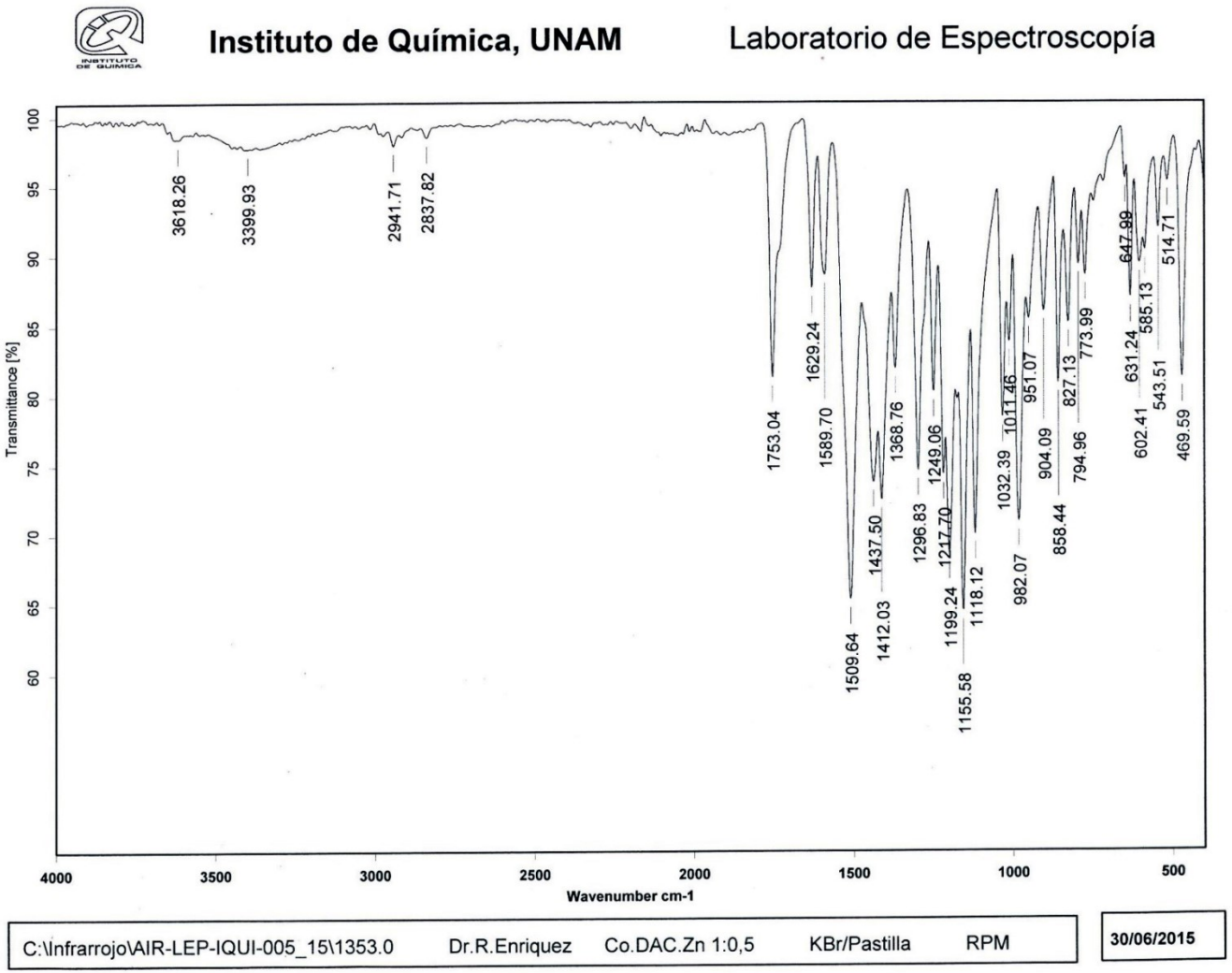


Fig S44. IR Spectrum of DAC-Zn.

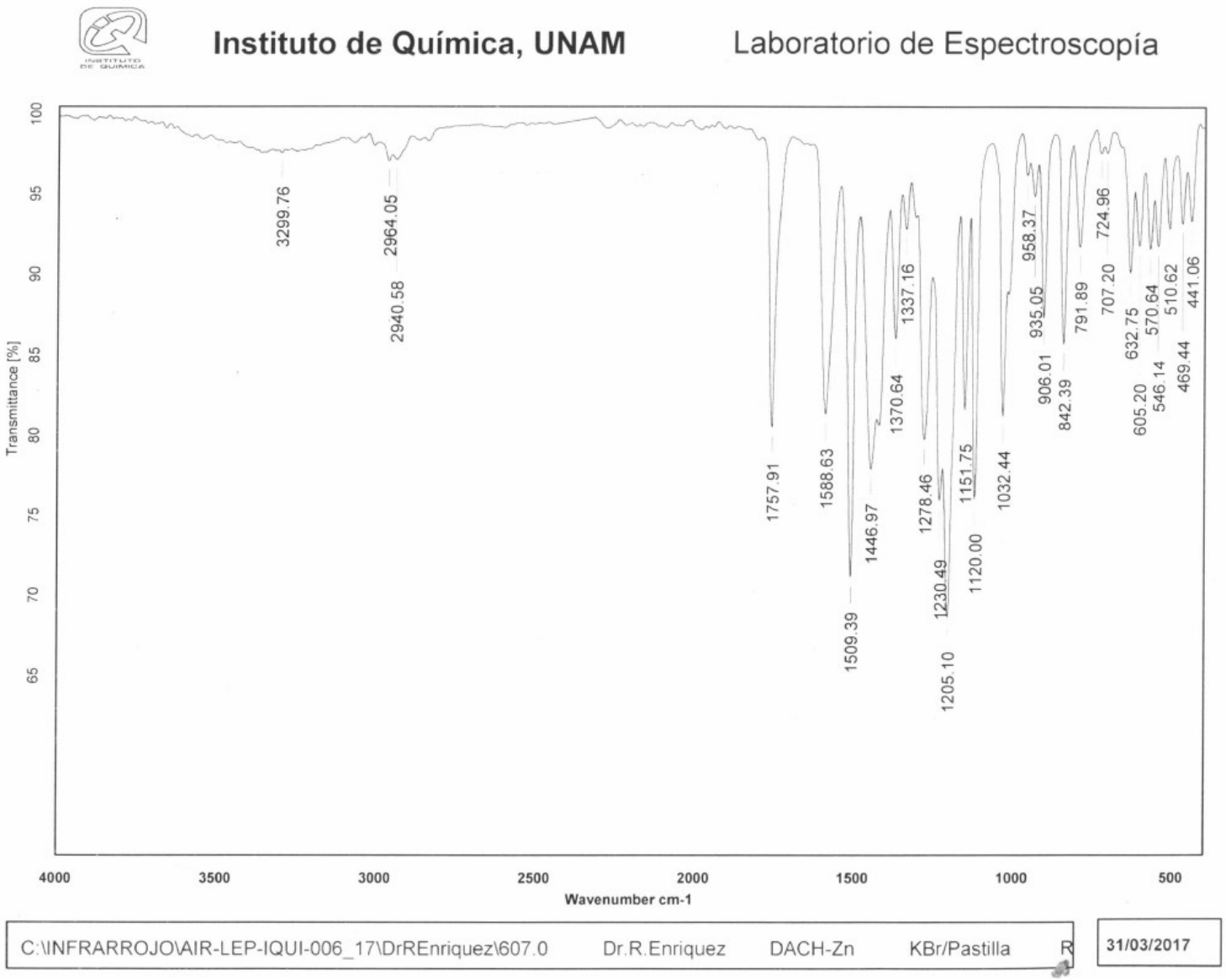


Fig S45. IR Spectrum of DACH-Zn.

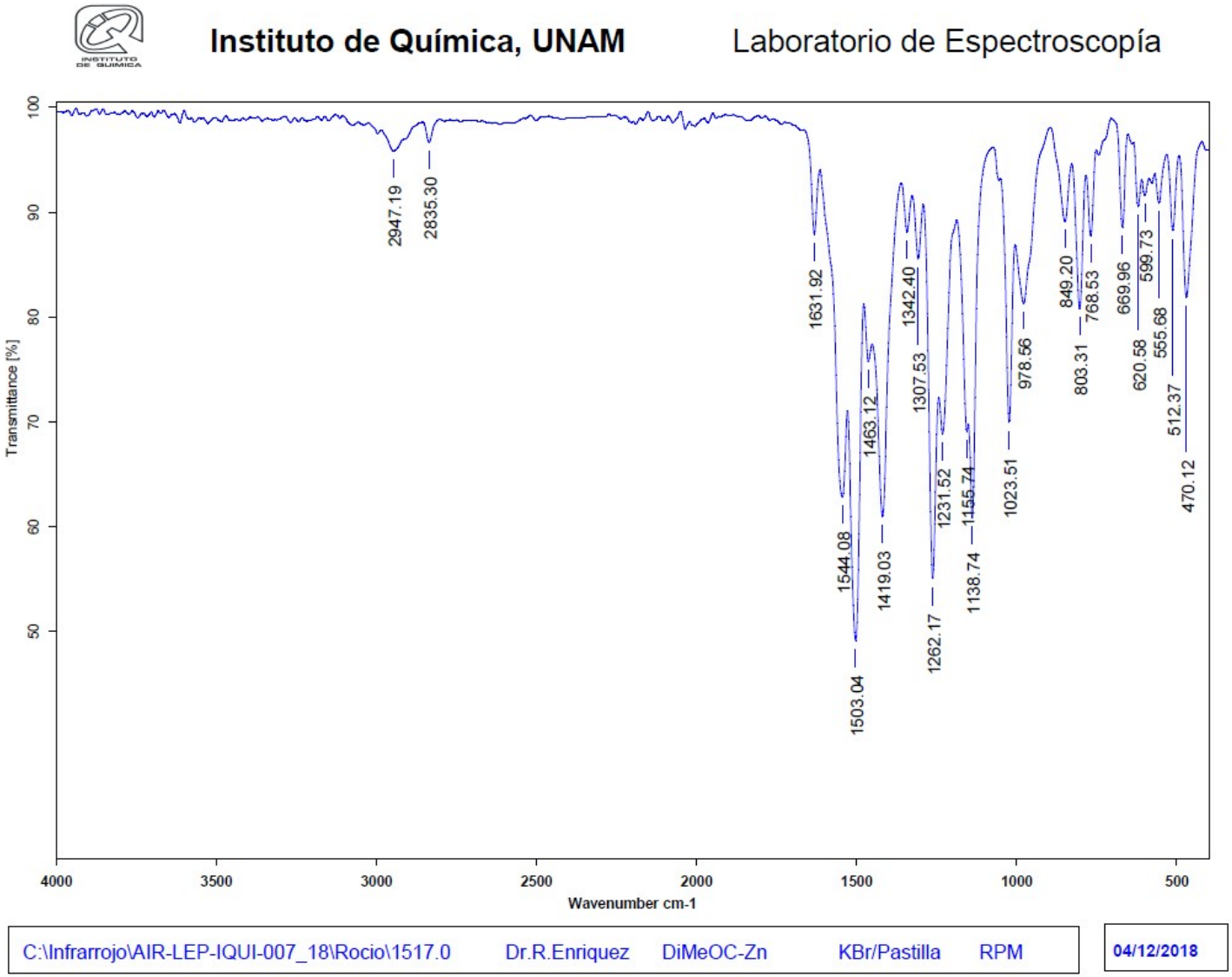


Fig S46. IR Spectrum of DiMeOC-Zn.

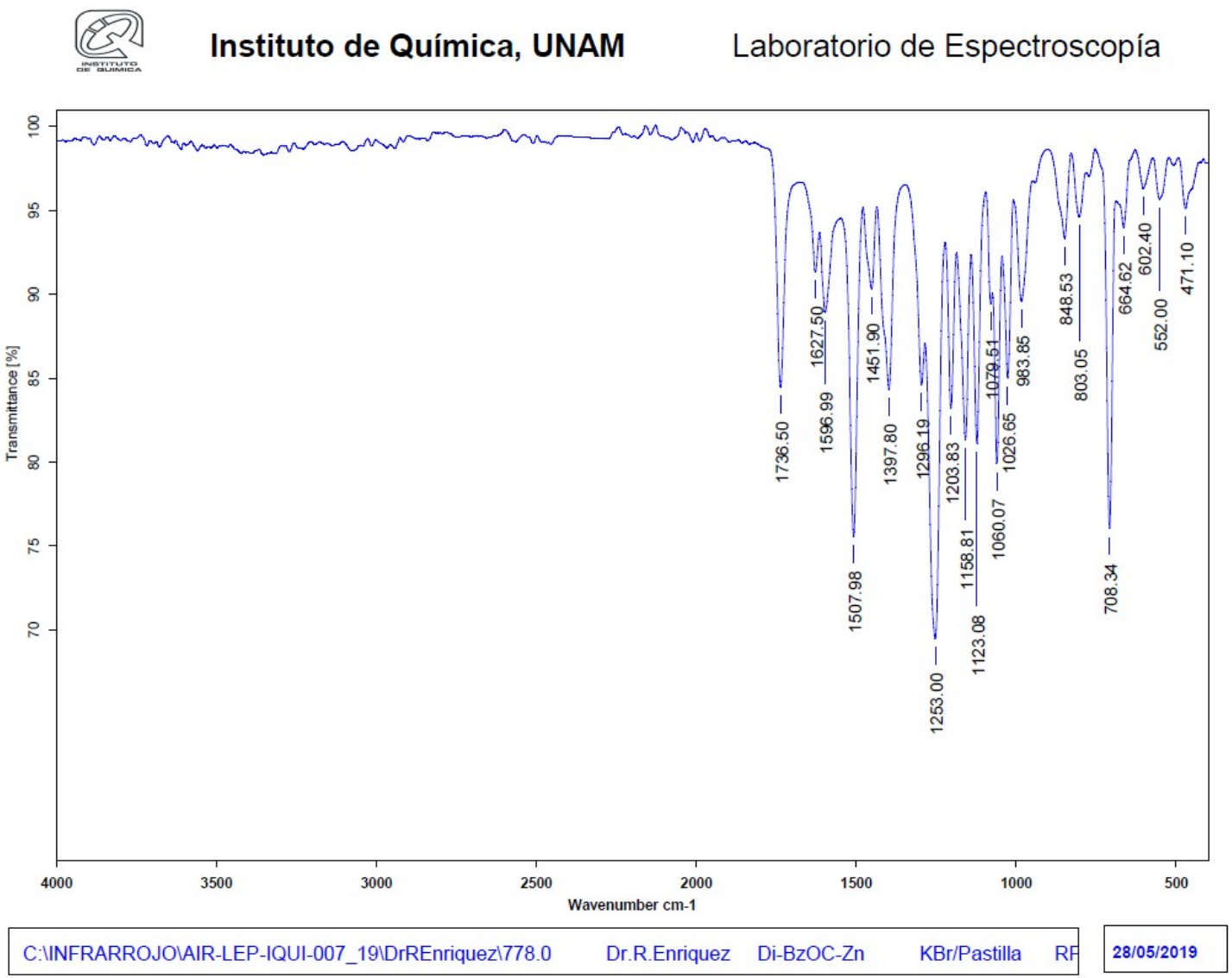


Fig S47. IR Spectrum of DiBzOC-Zn.

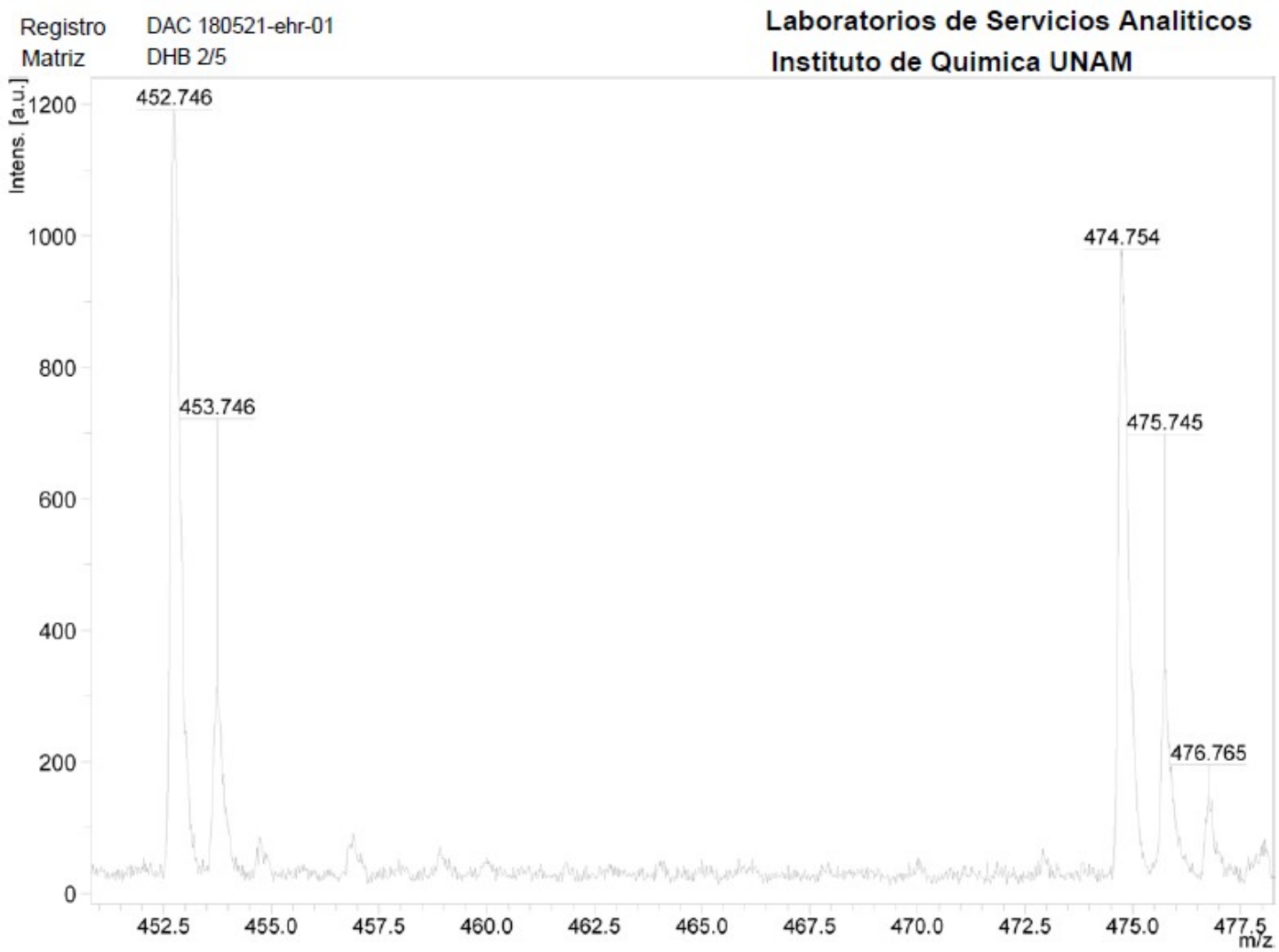


Fig S48. Mass Spectrum of DAC.

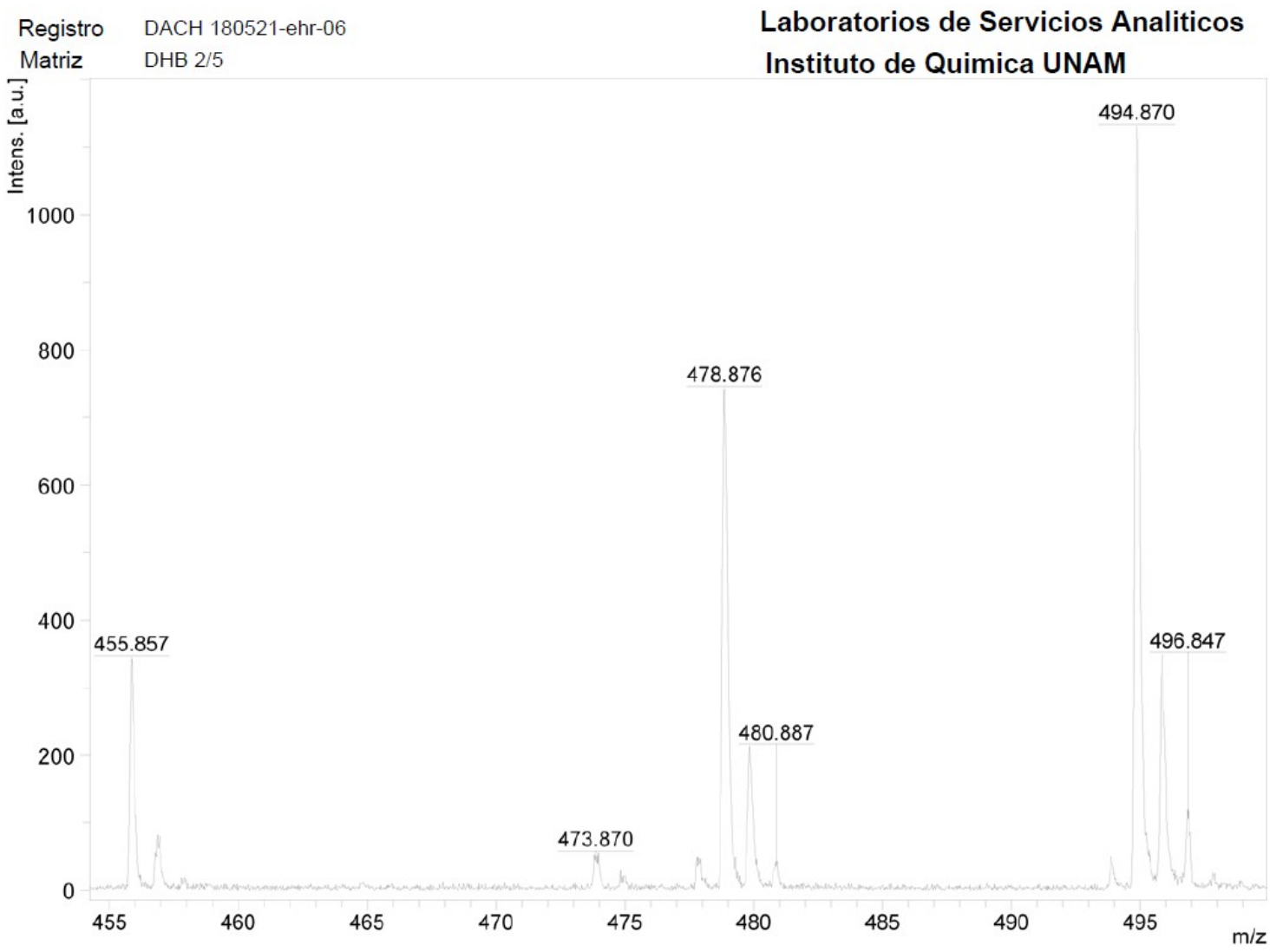


Fig S49. Mass Spectrum of DACH.

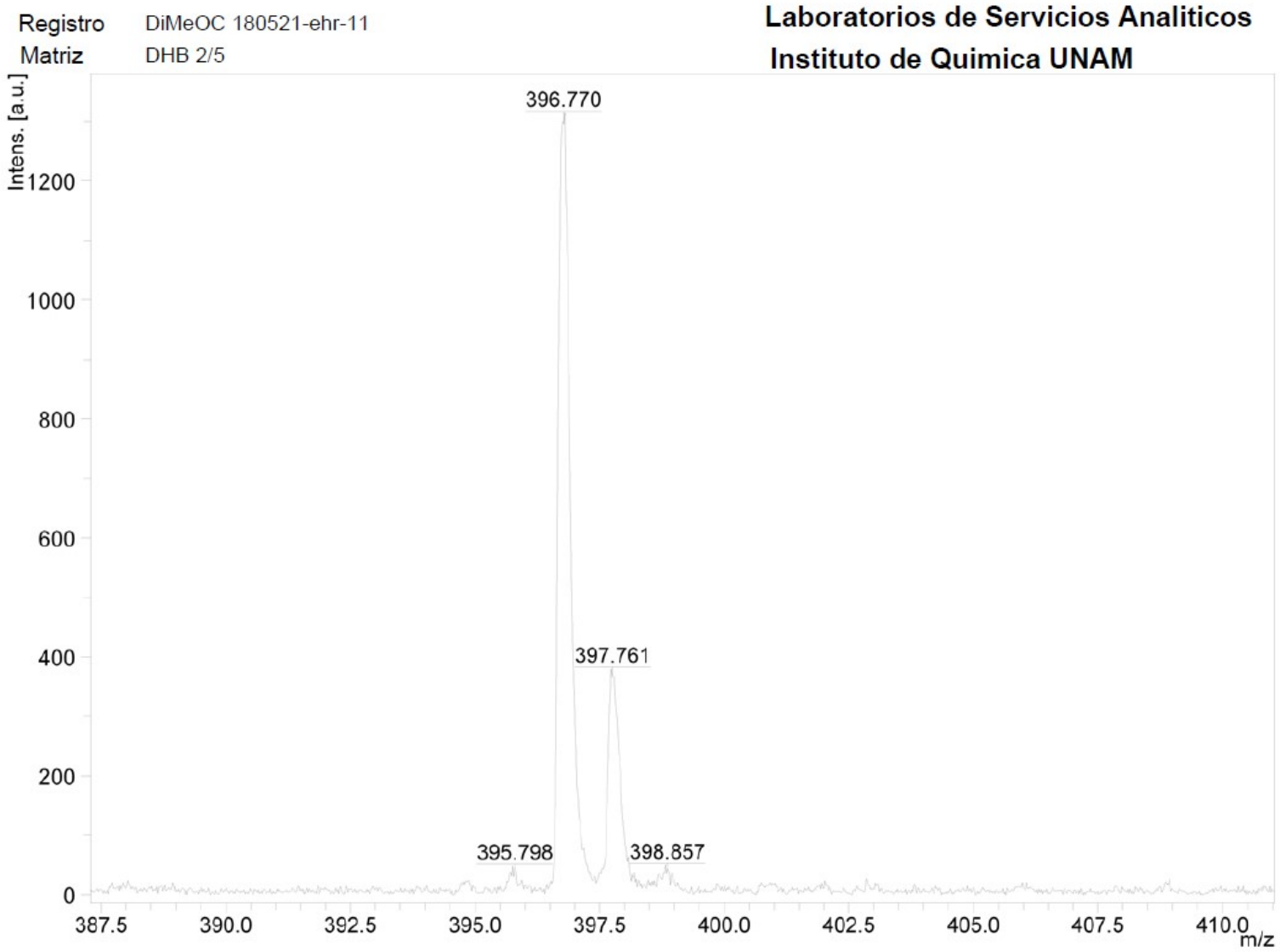


Fig S50. Mass Spectrum of DiMeOC.

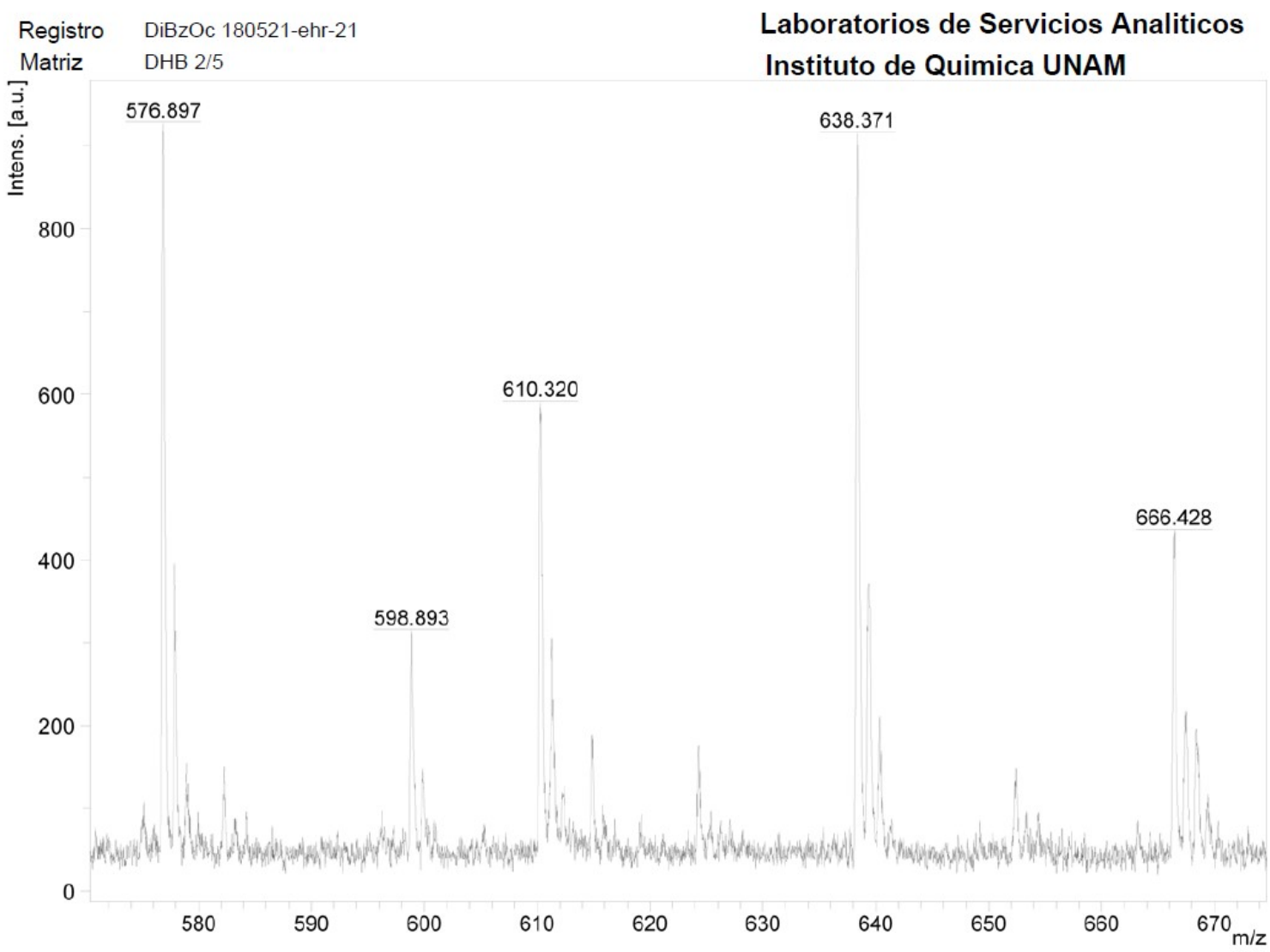


Fig S51. Mass Spectrum of DiBzOC.

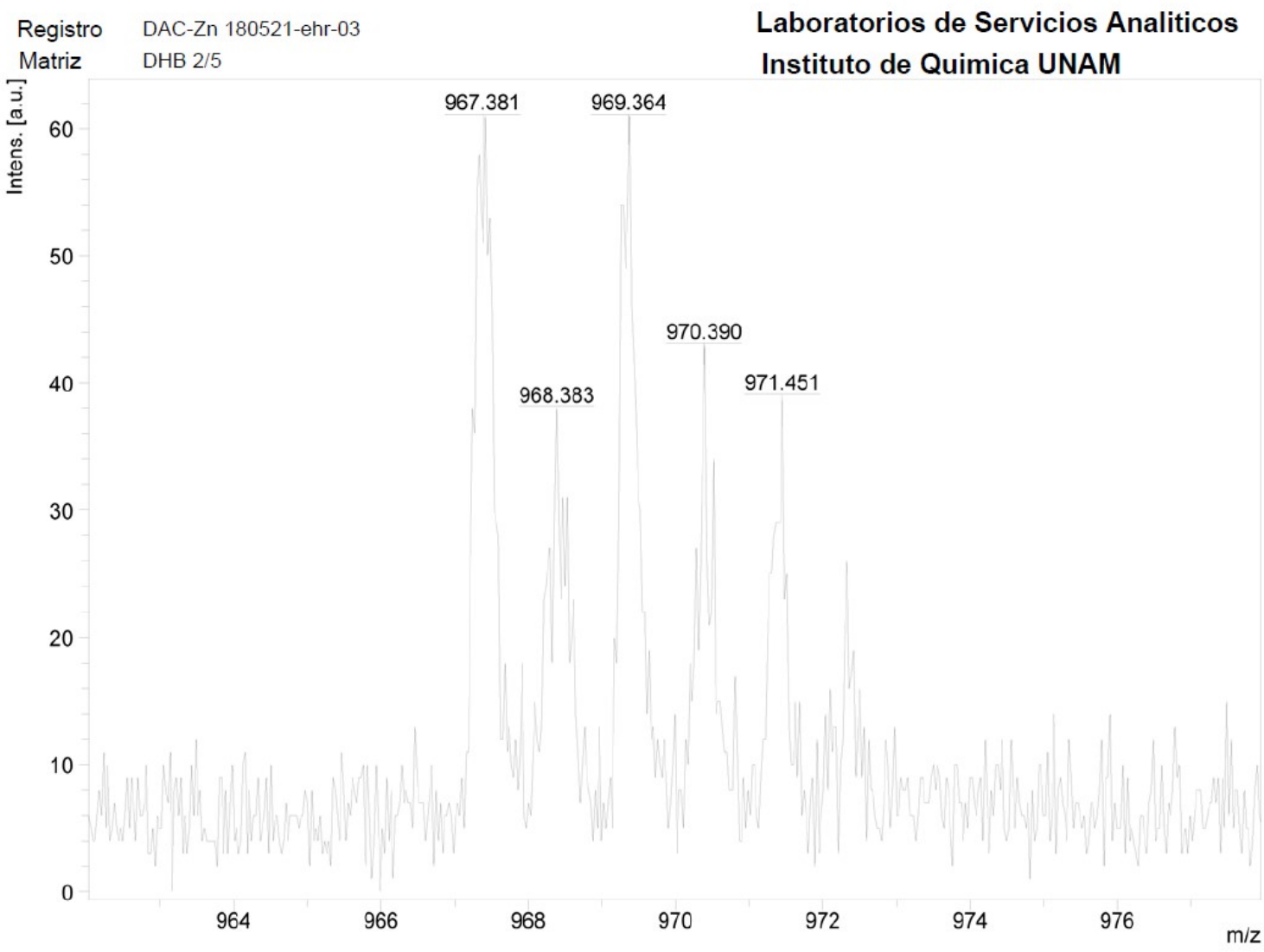


Fig S52. Mass Spectrum of DAC-Zn.

Data : Dr Enriquez Raul-151 Date : 29-Jul-2022 15:54
Instrument : MStation
Sample : 2258_DACH-Zn
Note : Operator name: Carmen Garcia
Inlet : Direct Ion Mode : FAB+
RT : 0.58 min Scan# : (24,31)
Elements : C 50/0, H 55/0, O 16/0, Zn 1/0
Mass Tolerance : 1000ppm, 10mmu if m/z > 10
Unsaturation (U.S.) : 0.0 - 50.0

	Observed m/z	Int%						
	975.2803	100.00						
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	O	Zn
1	975.2782	+2.2 / +2.1		23.5	50	55	16	1

Fig S53. Mass Spectrum of DACH-Zn.

Data : Dr Enriquez Raul-149 Date : 06-Feb-2020 09:46
Instrument : MStation
Sample : 0179 DiMeOC-Zn
Note : Operador: Carmen Garcia
Inlet : Direct Ion Mode : FAB+
RT : 14.90 min Scan# : (220,240)
Elements : C 46/0, H 50/0, O 12/0, Zn 1/0
Mass Tolerance : 1000ppm, 5mmu if m/z > 5
Unsaturation (U.S.) : 0.0 - 30.0

	Observed m/z	Int%						
	855.2322	100.00						
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	O	Zn
1	855.2359	-4.3 /	-3.7	23.5	46	47	12	1

Fig S54. Mass Spectrum of DiMeOC-Zn.

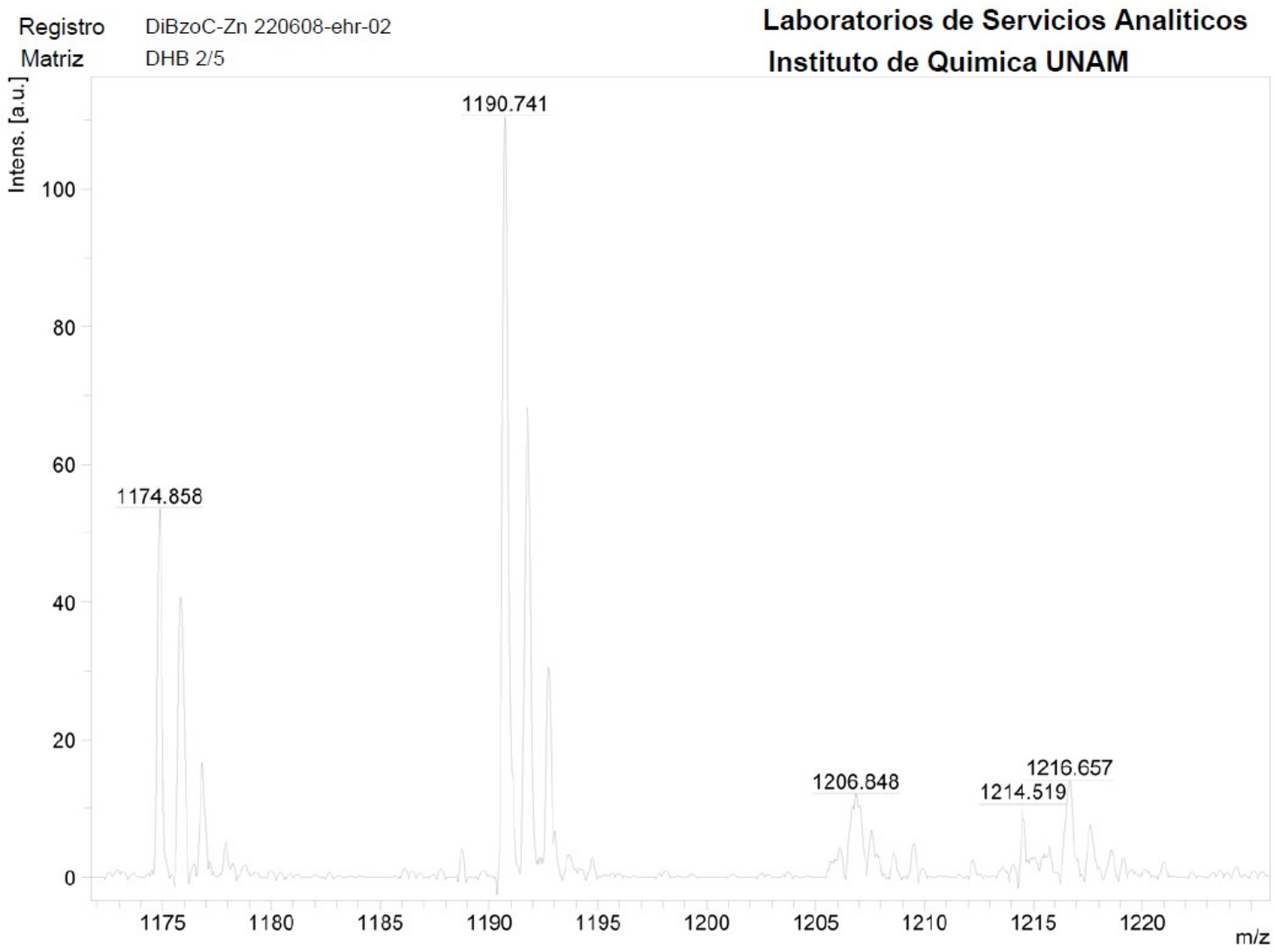


Fig S55. Mass Spectrum of DiBzOC-Zn.