Article

Structure, Absolute Configuration, and antiproliferative activity of abietane and icetexane diterpenoids from *Salvia ballotiflora*

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Supporting Information

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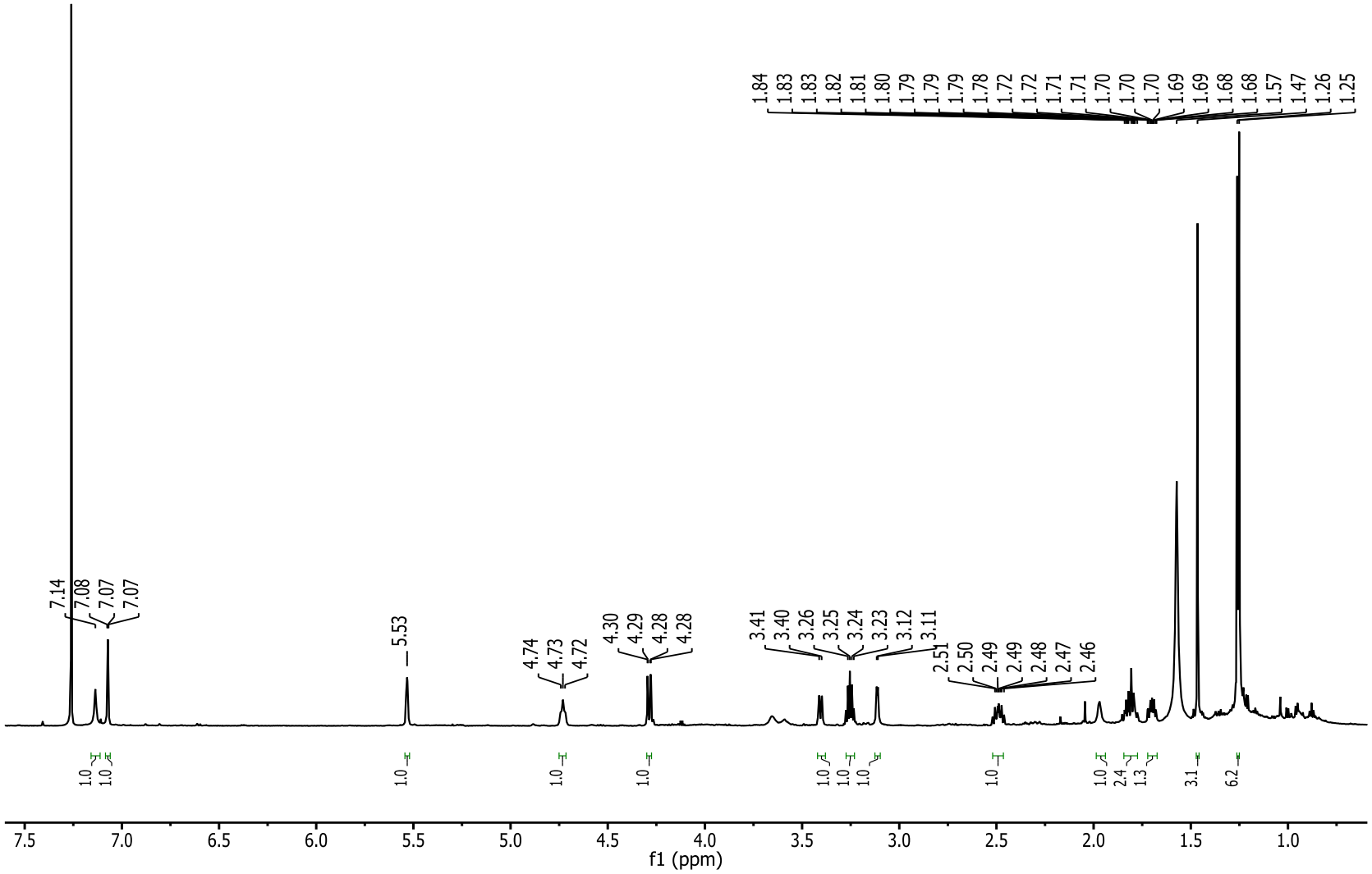


Figure S1. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **1**

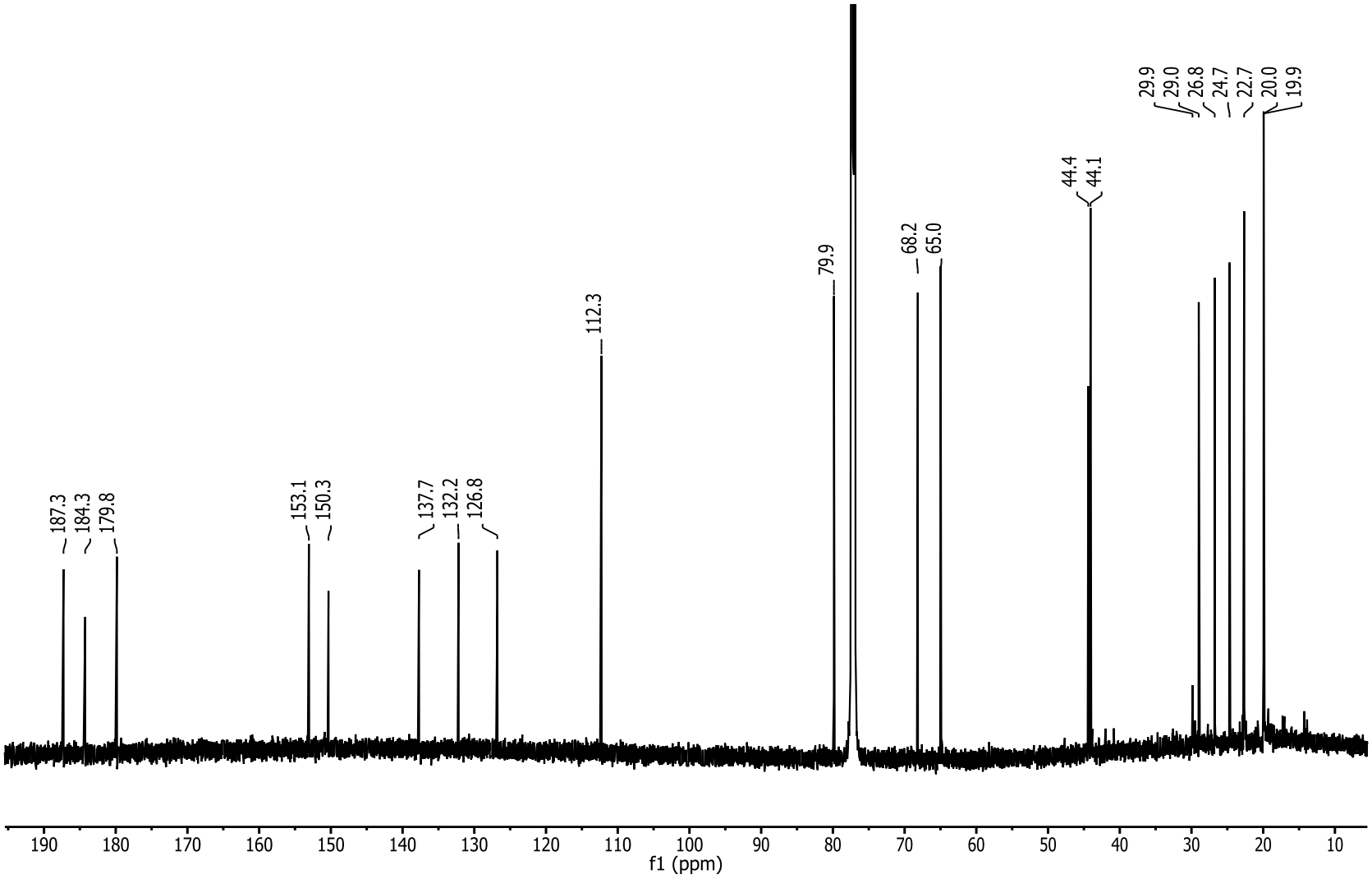


Figure S2. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **1**

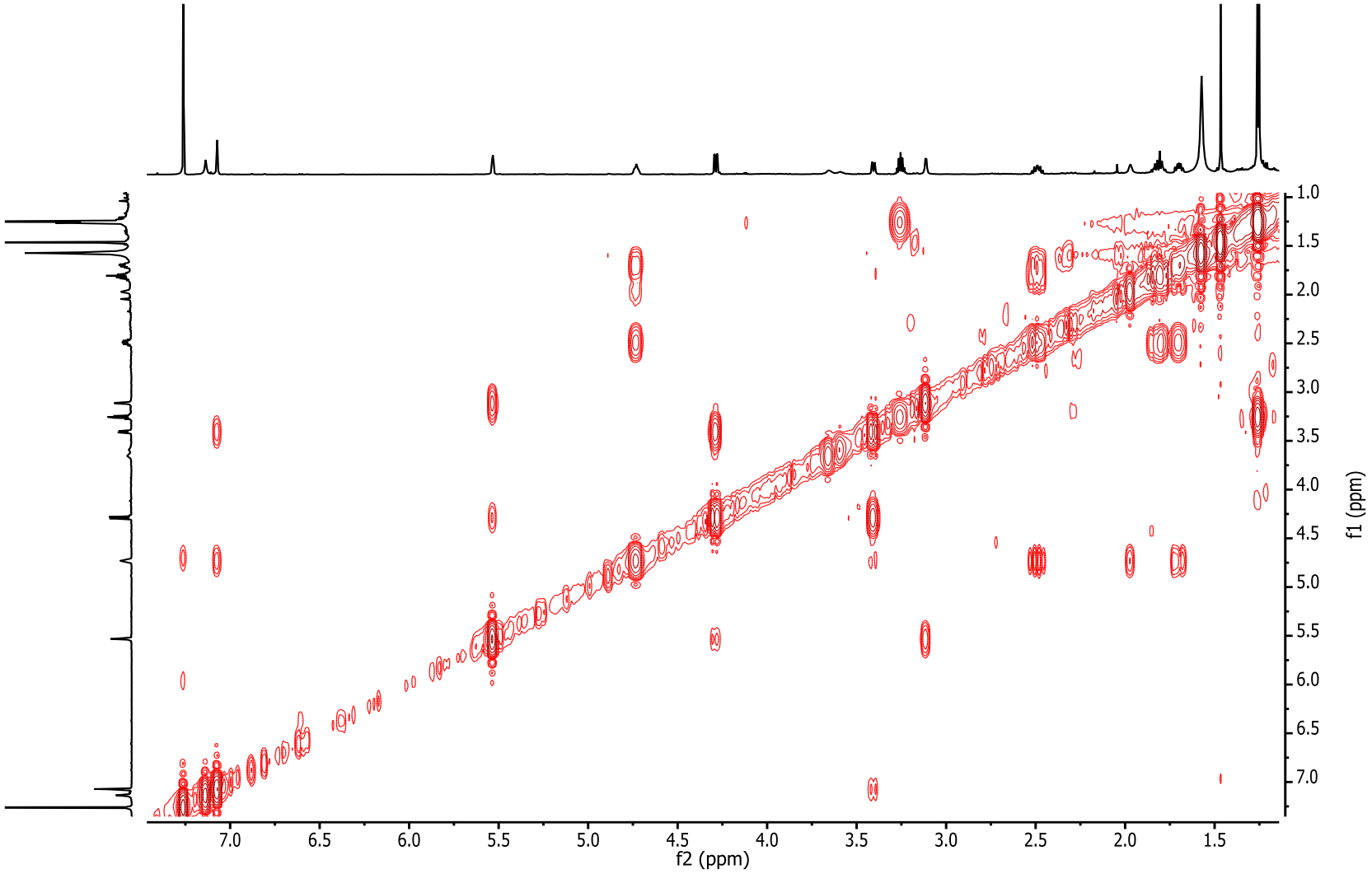


Figure S3. COSY NMR ($CDCl_3$, 700 MHz) spectrum of **1**

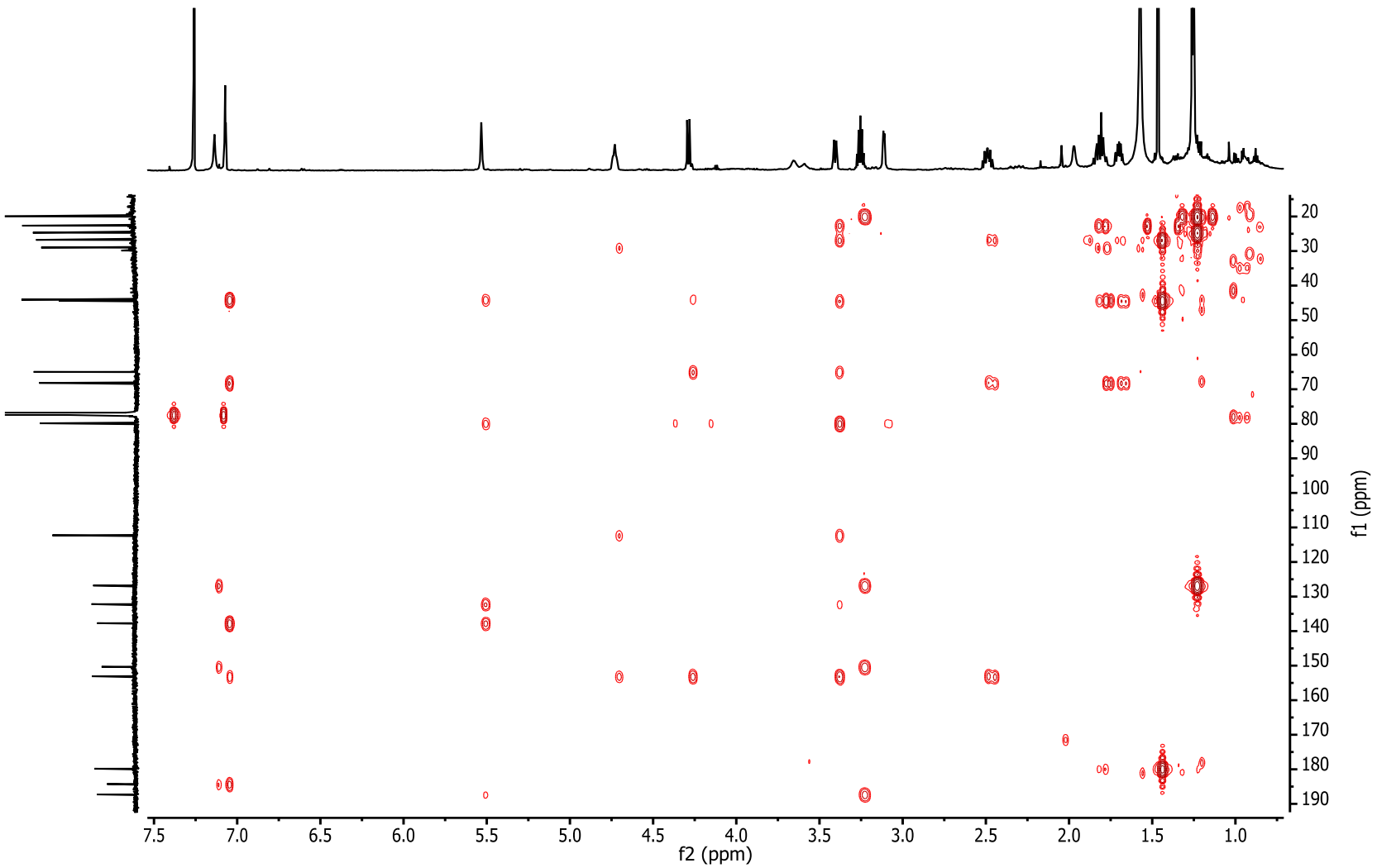


Figure S4. HMBC NMR ($CDCl_3$, 700 MHz) spectrum of **1**.

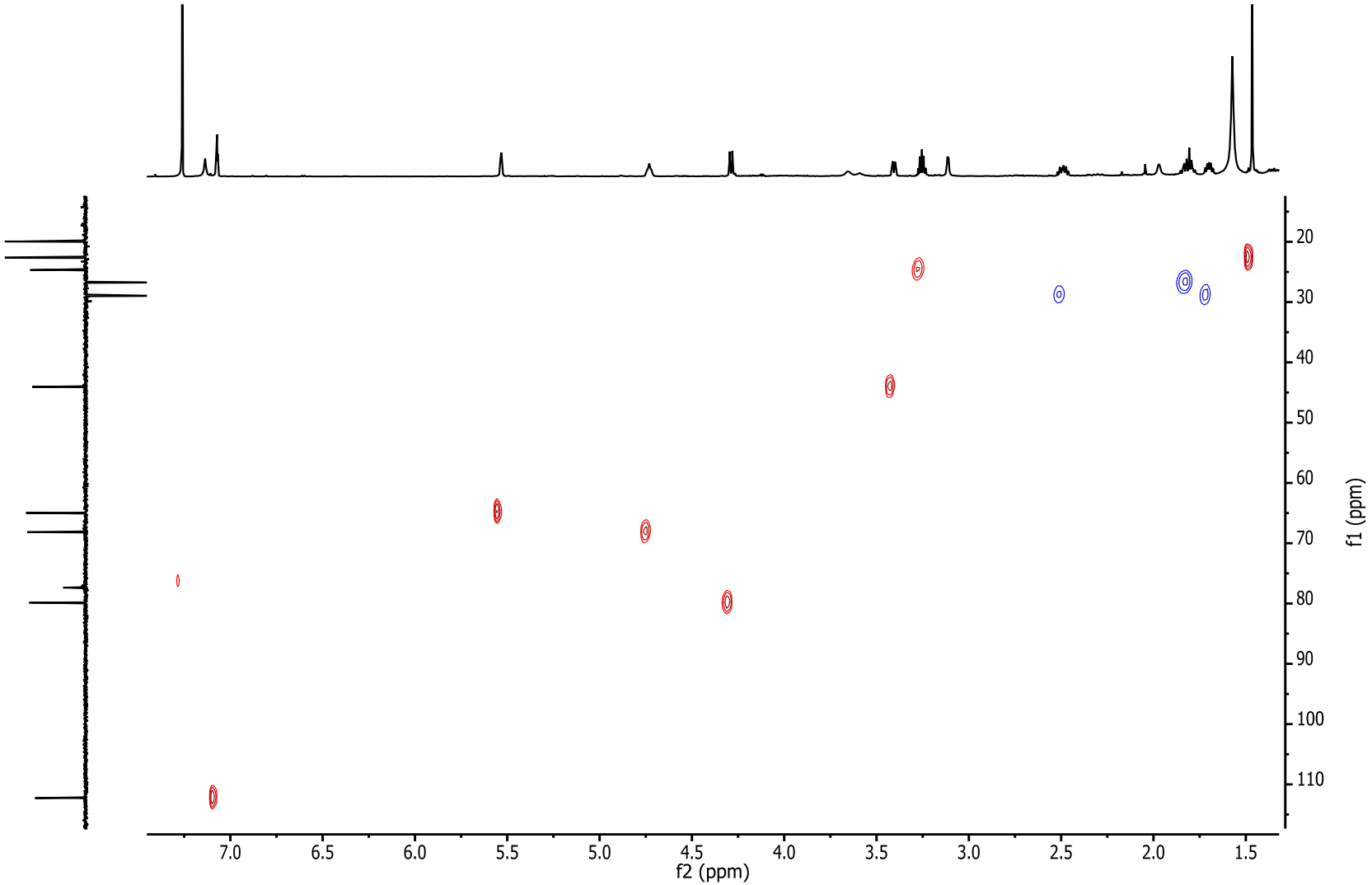


Figure S5. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **1**

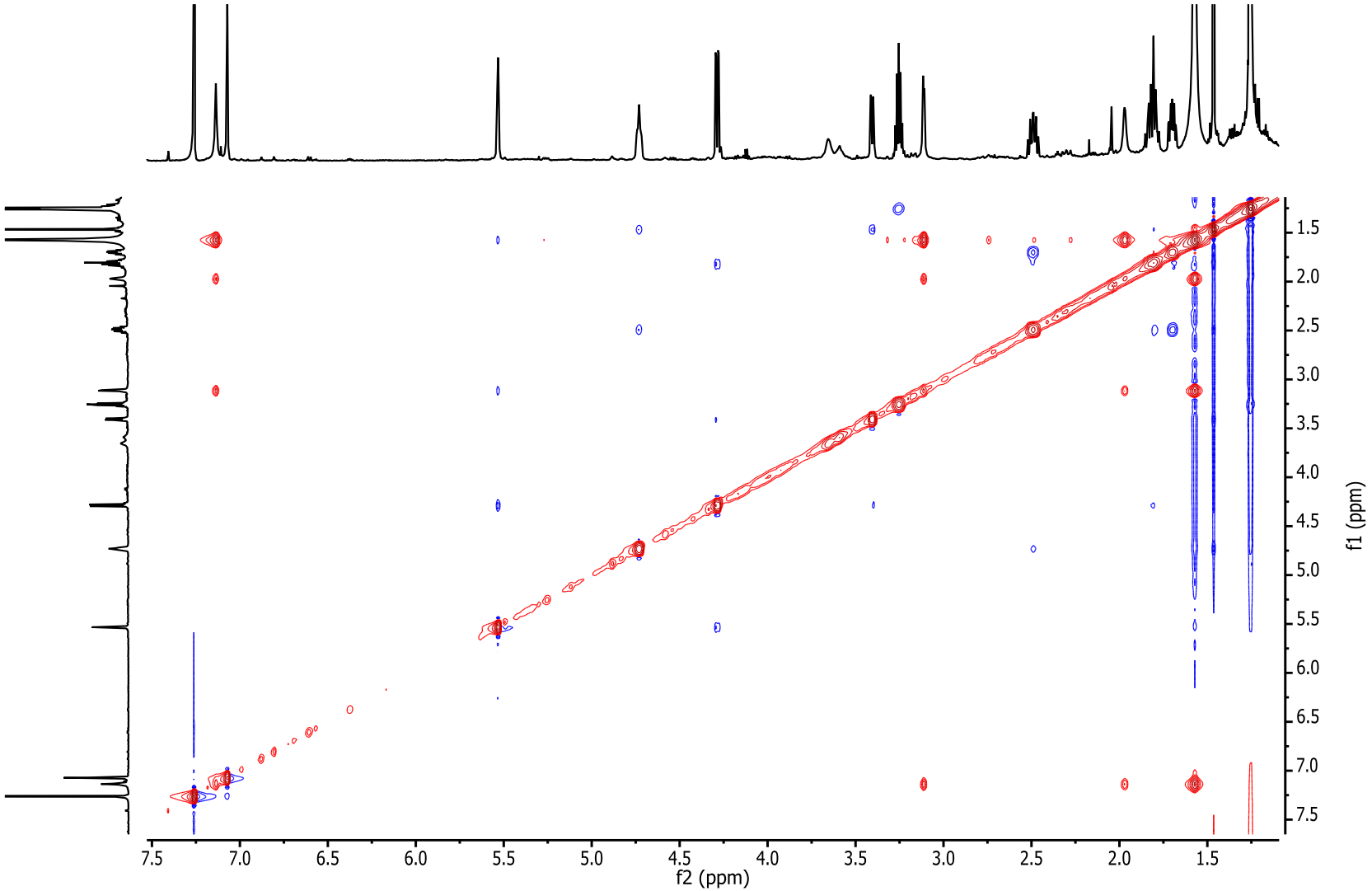
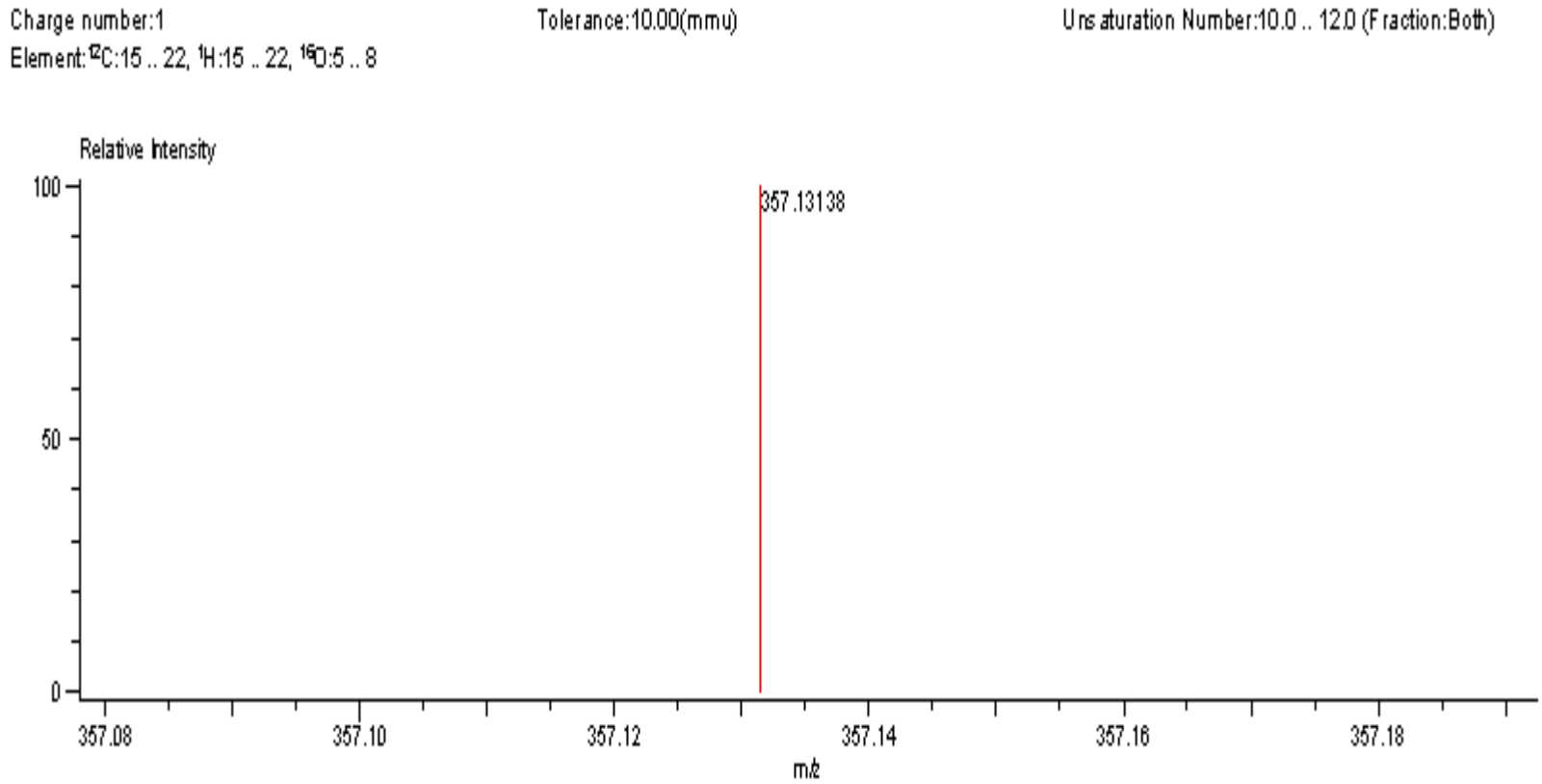


Figure S6. NOESY NMR ($CDCl_3$, 700 MHz) spectrum of **1**



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
357.13138	210041.35	357.13381	-2.43	-6.80	$^{12}C_{20}{}^{1}H_{21}{}^{16}O_{6}$	10.5

Figure S7. HR-DART-MS of **1**

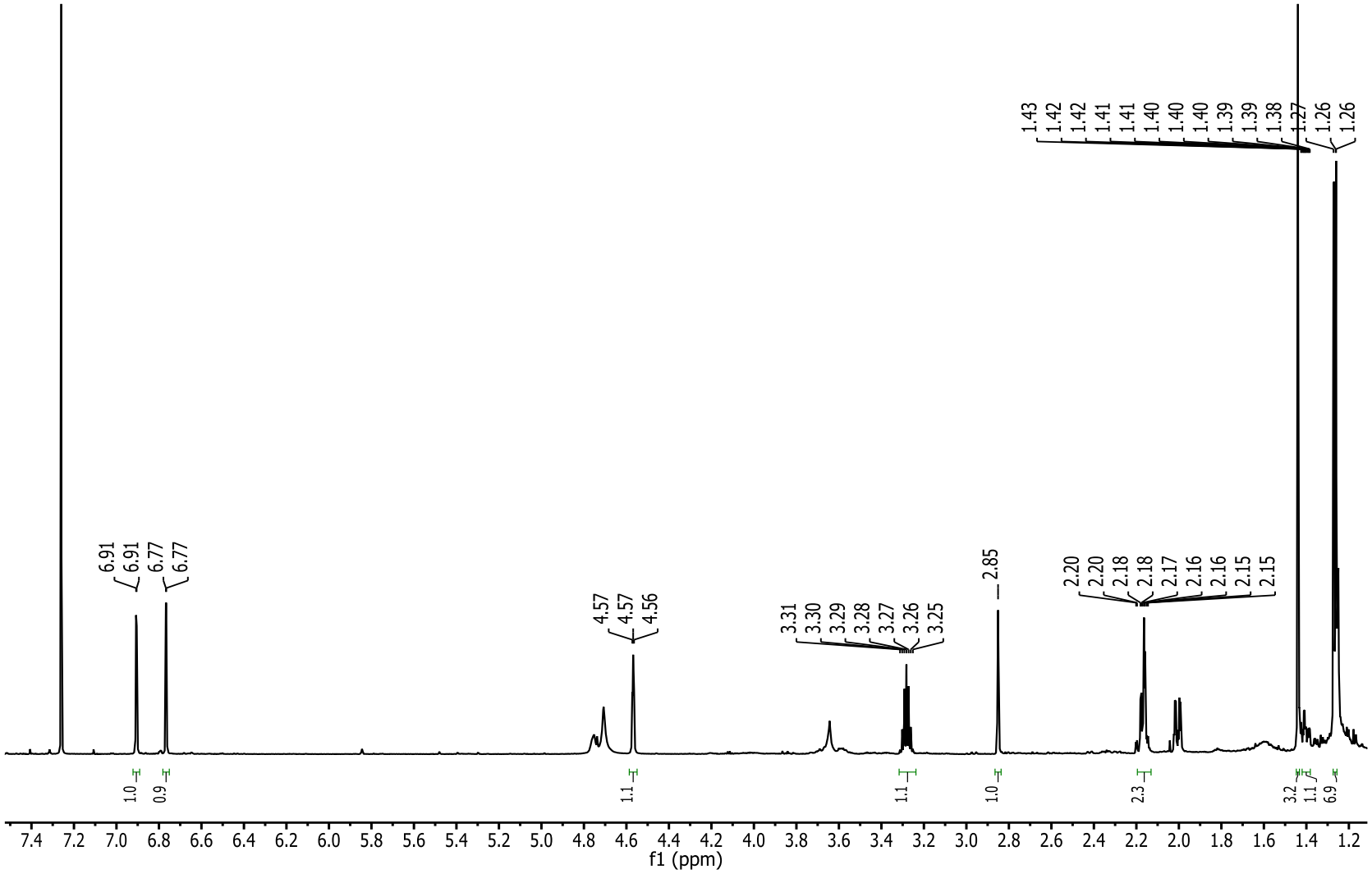


Figure S8. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **2**

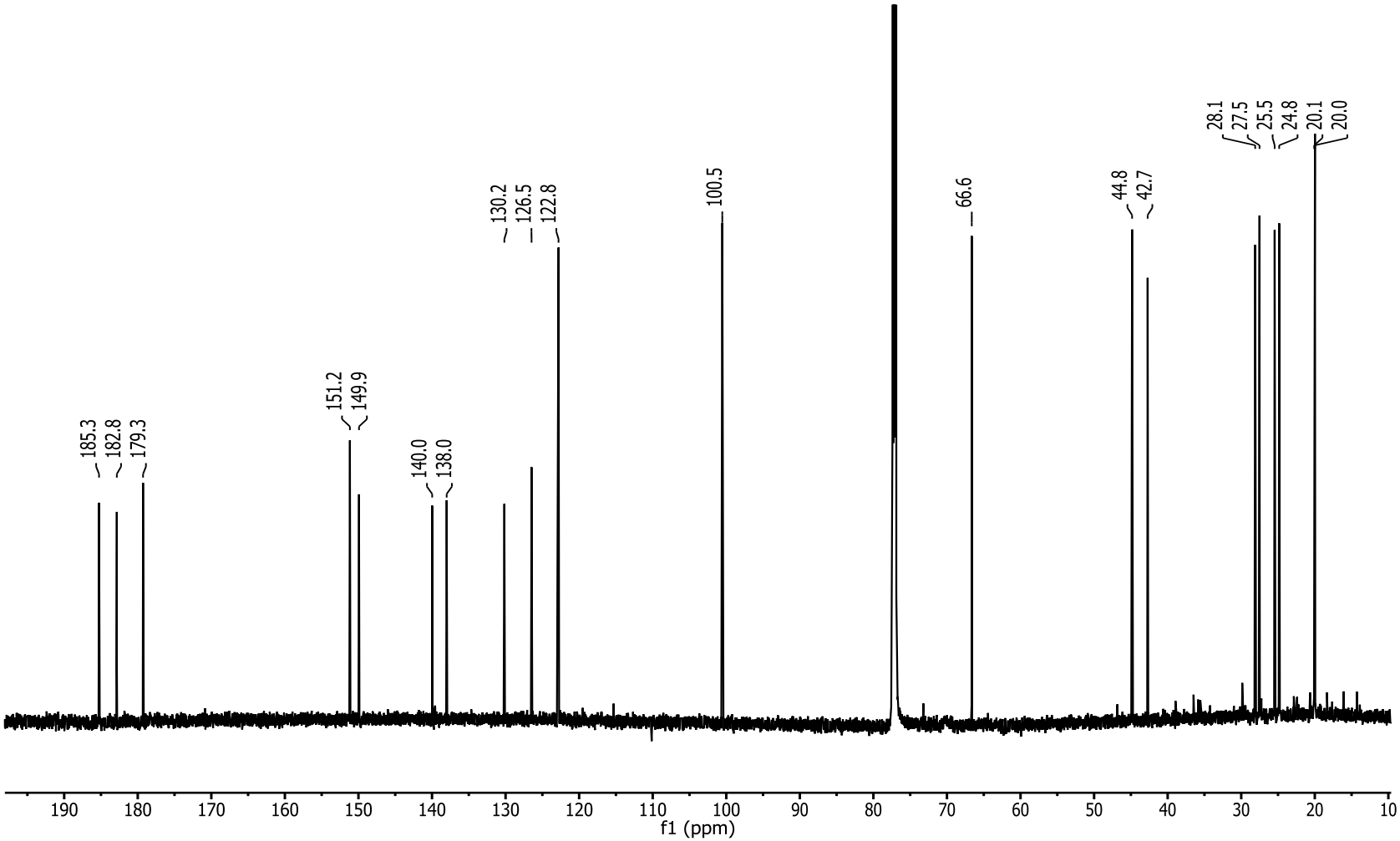


Figure S9. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **2**

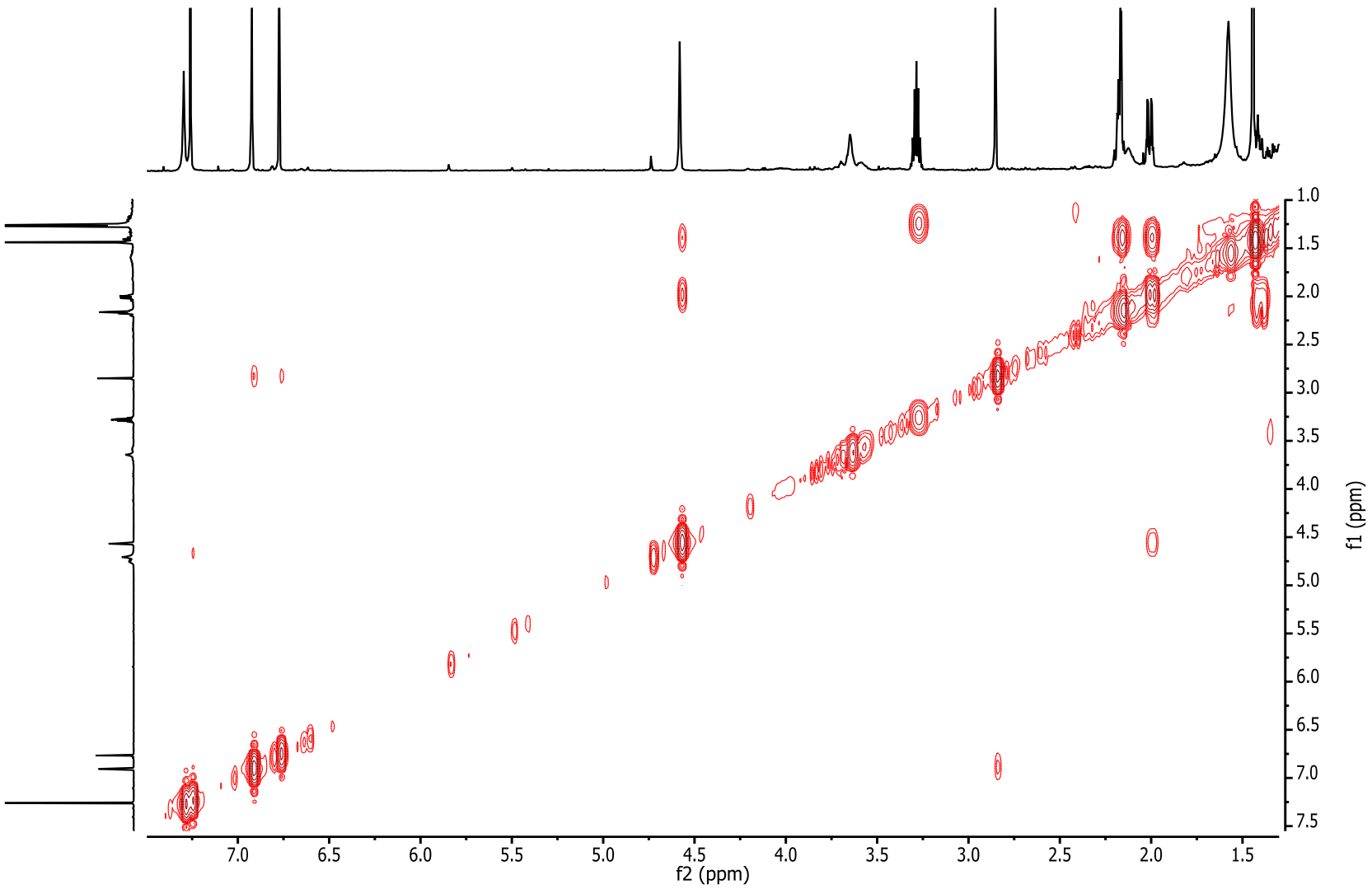


Figure S10. COSY NMR ($CDCl_3$, 700 MHz) spectrum of **2**

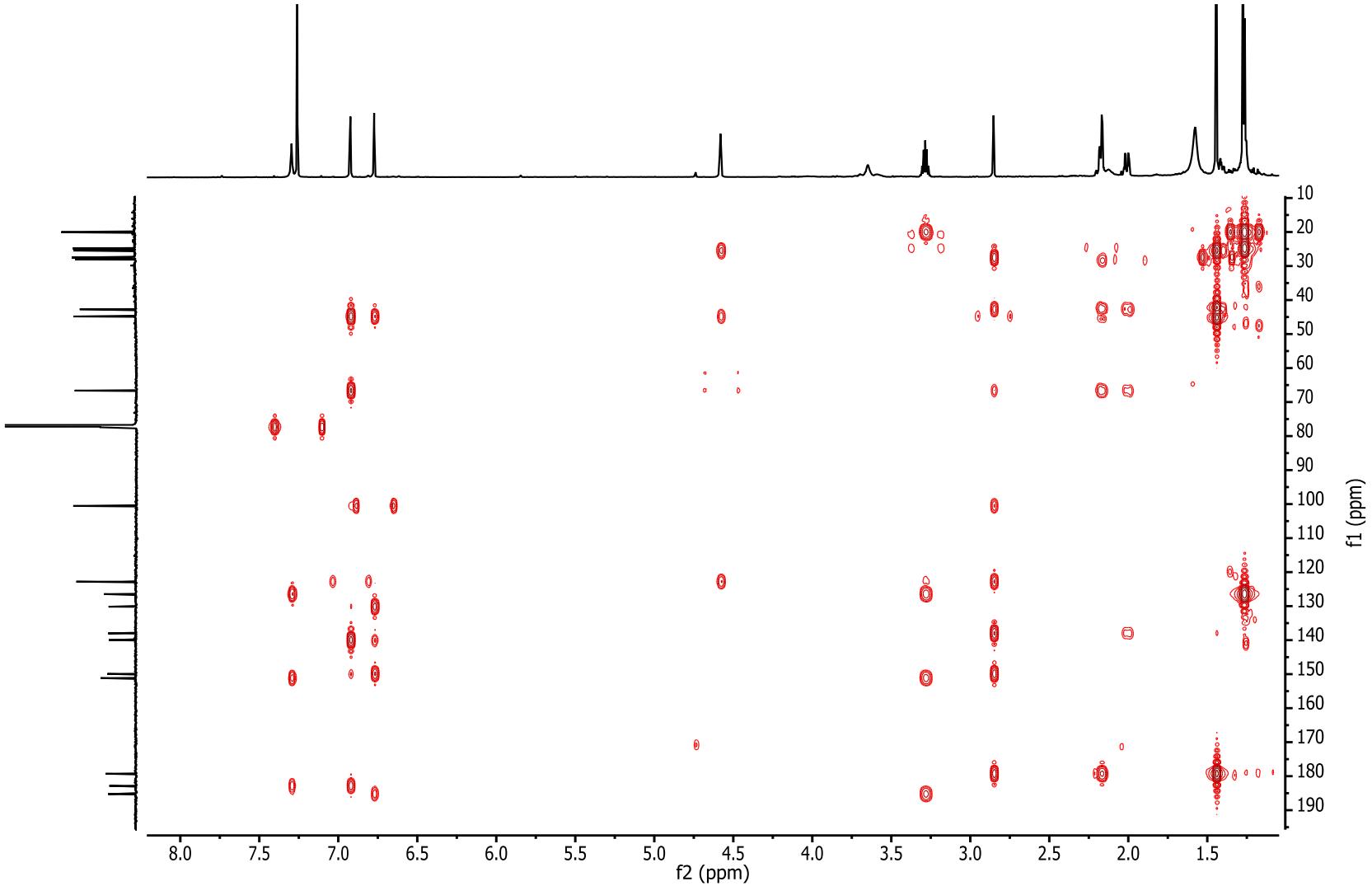


Figure S11. HMBC NMR ($CDCl_3$, 700 MHz) spectrum of **2**

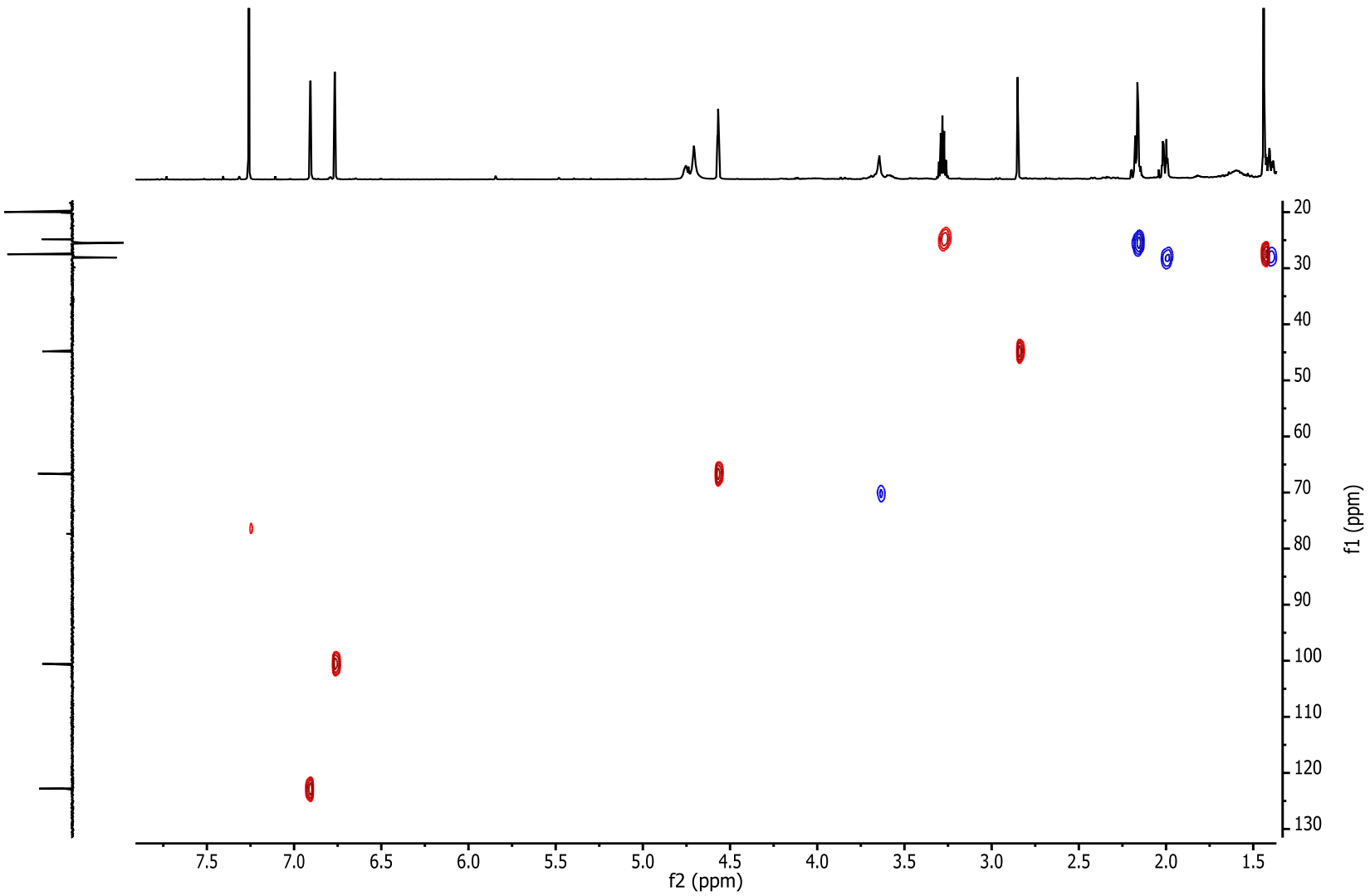


Figure S12. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **2**

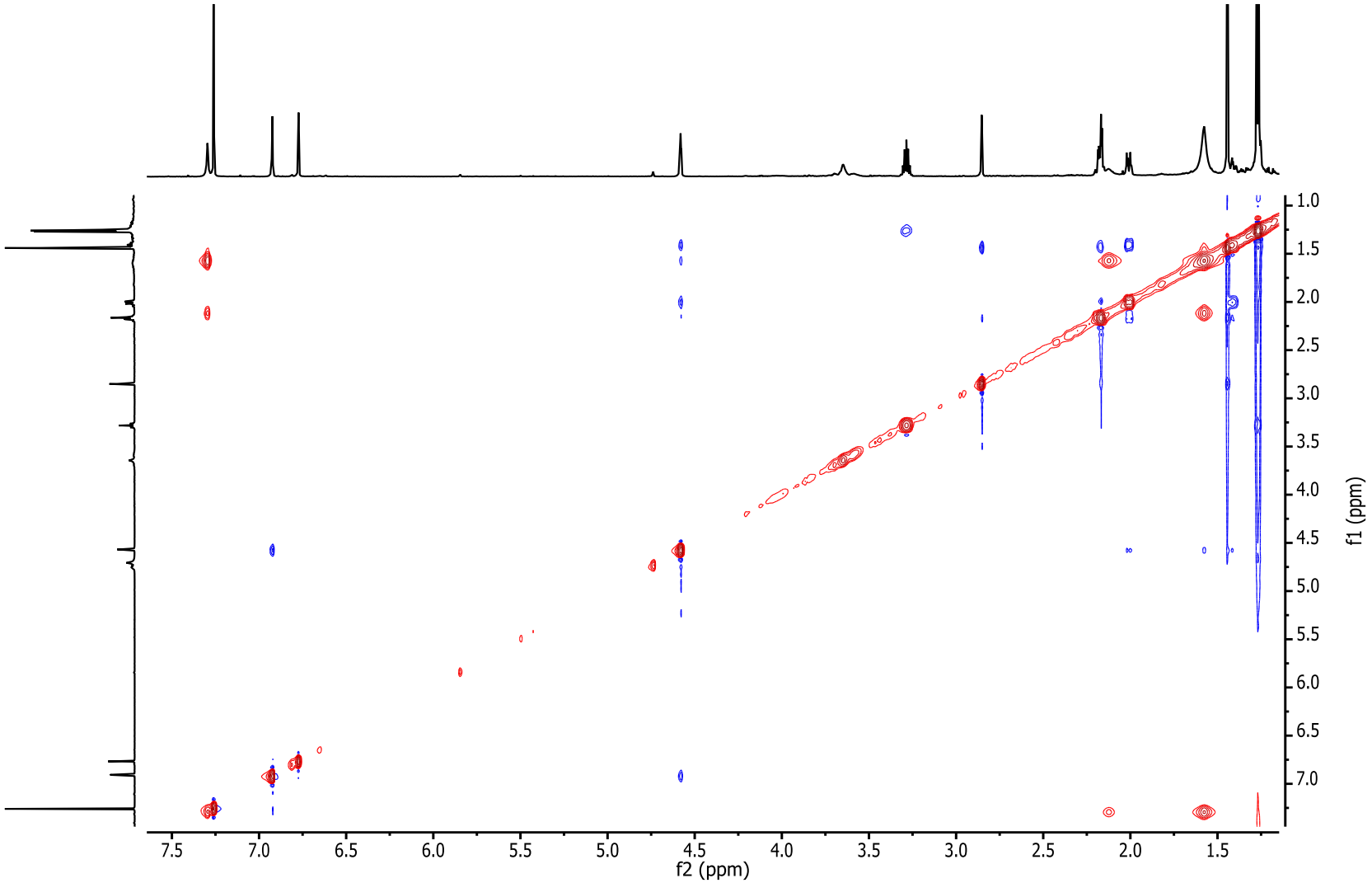
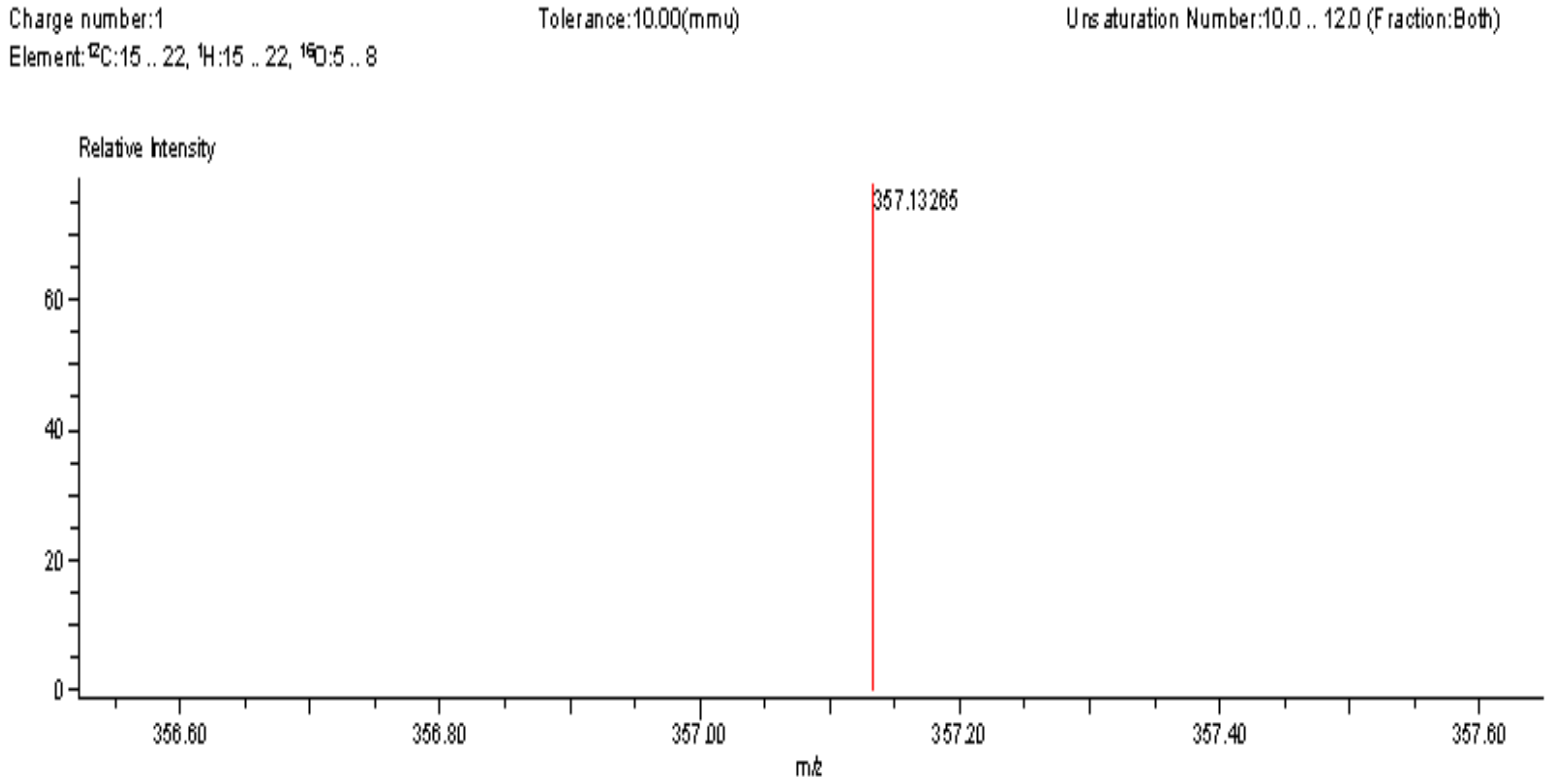


Figure S13. NOESY NMR ($CDCl_3$, 700 MHz) spectrum of **2**



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
357.13265	137196.12	357.13381	-1.16	-3.26	$^{12}C_{20}{}^{1}H_{21}{}^{16}O_{6}$	10.5

Figure S14. HR-DART-MS of **2**

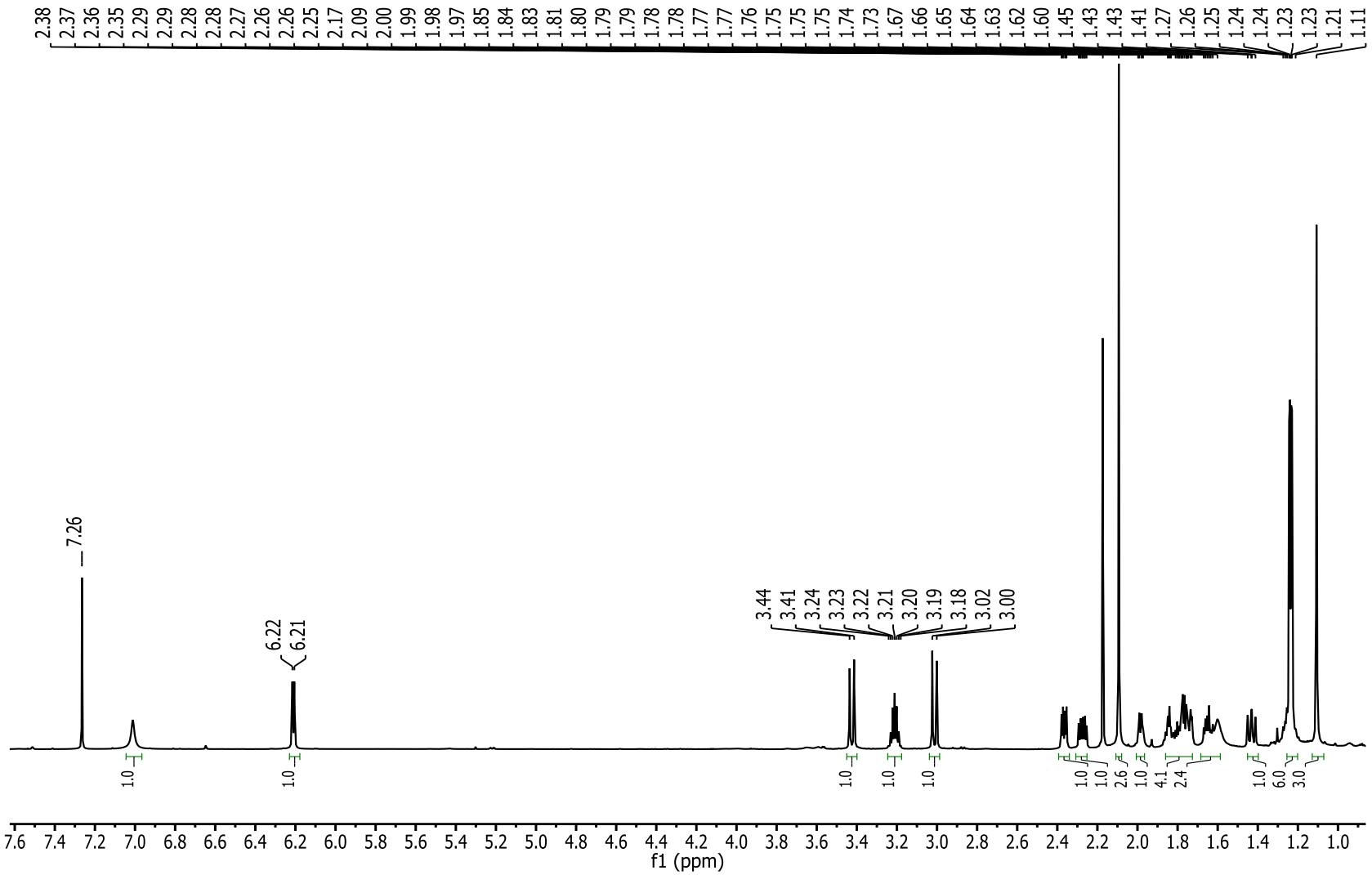


Figure S15. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **3**

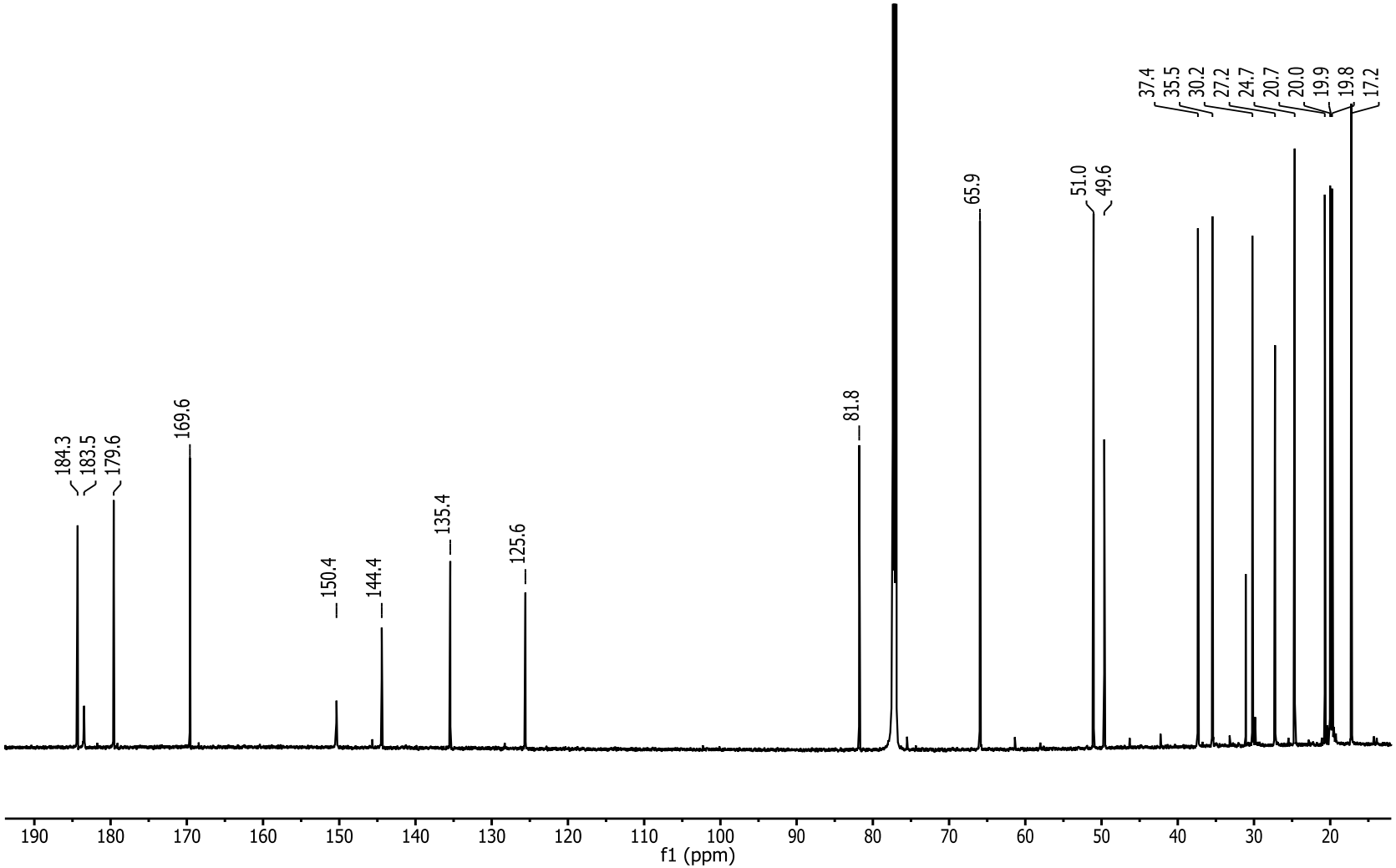


Figure S16. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **3**

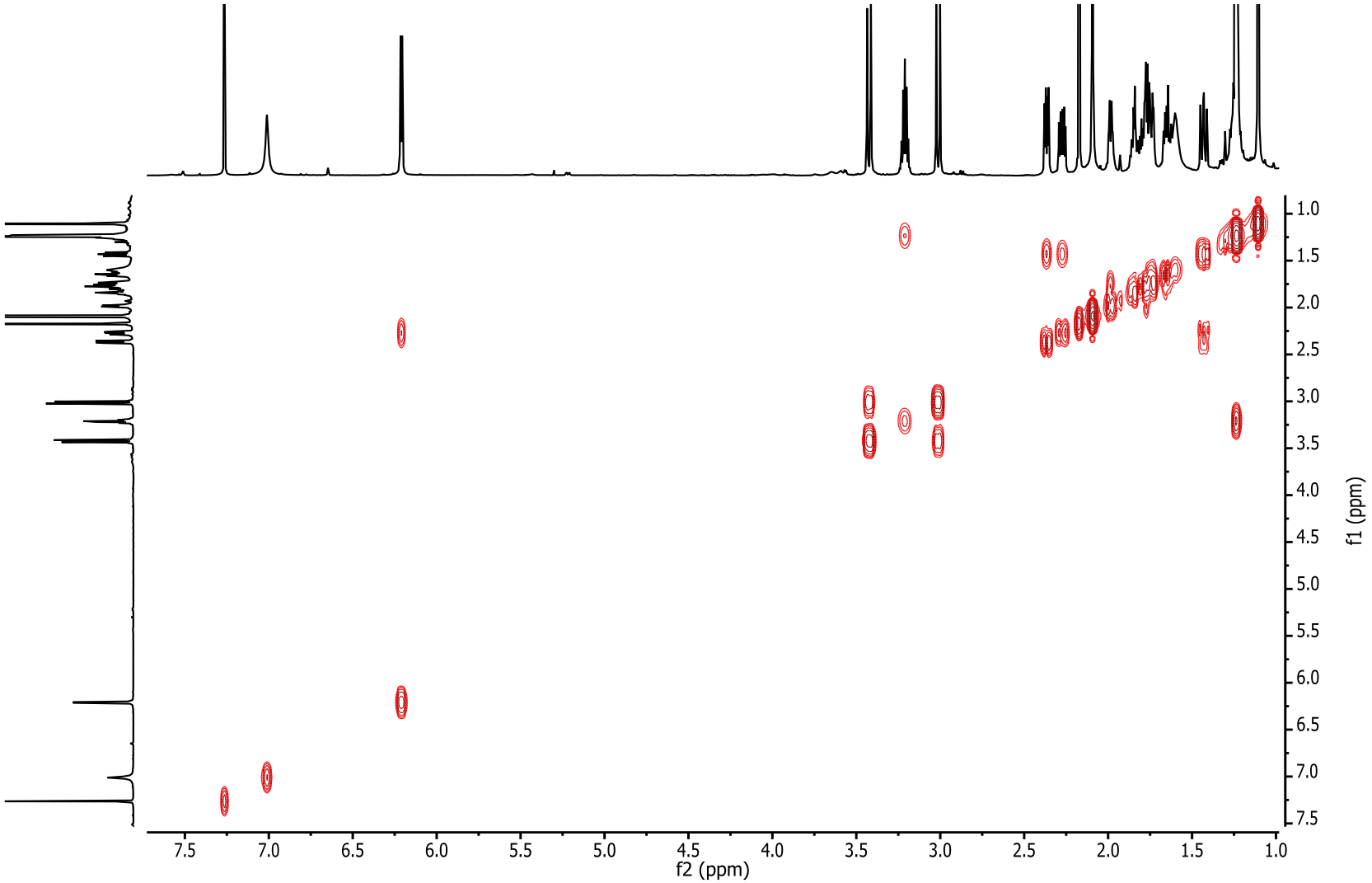


Figure S17. COSY NMR ($CDCl_3$, 700 MHz) spectrum of **3**

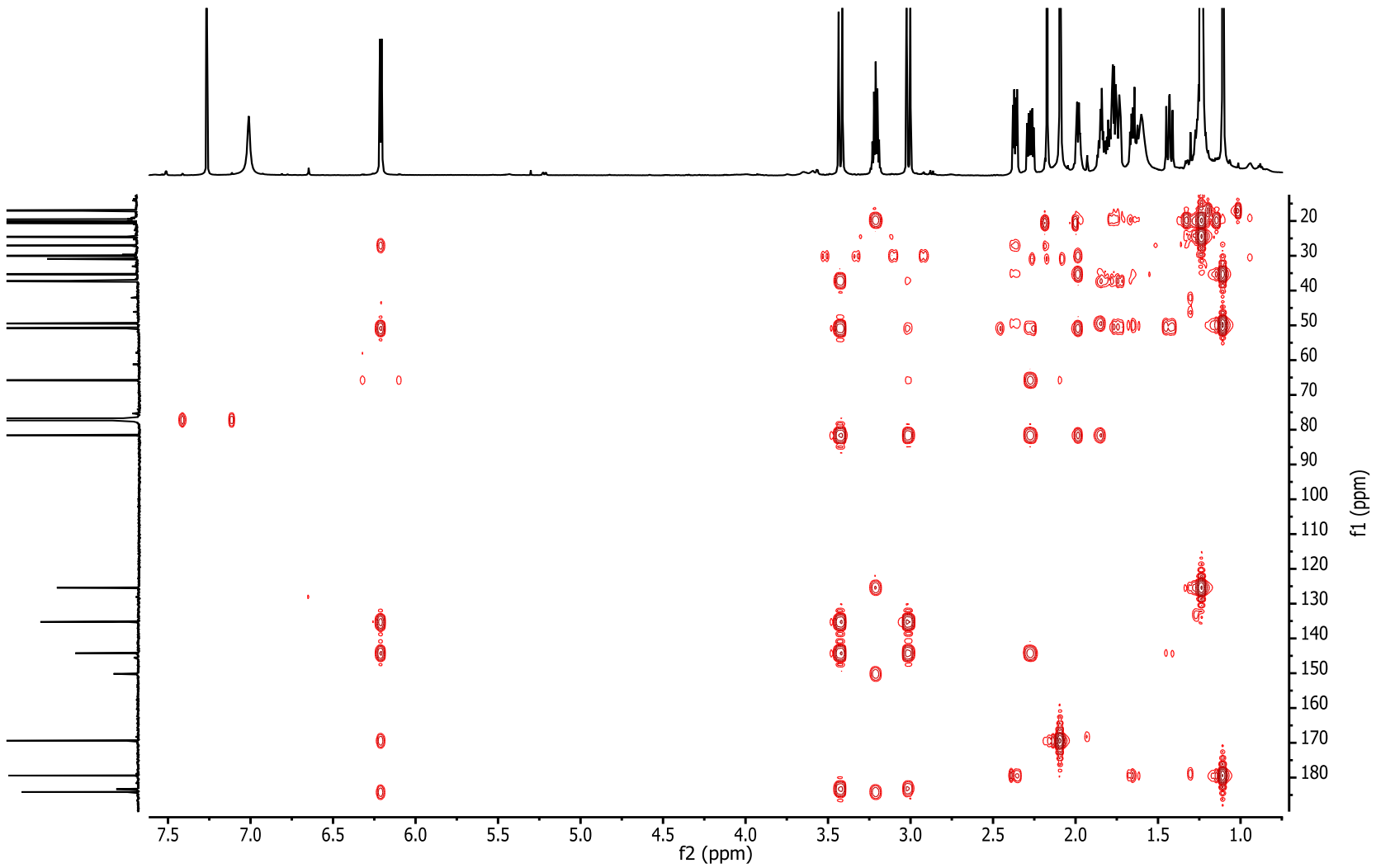


Figure S18. HMBC NMR ($CDCl_3$, 700 MHz) spectrum of **3**

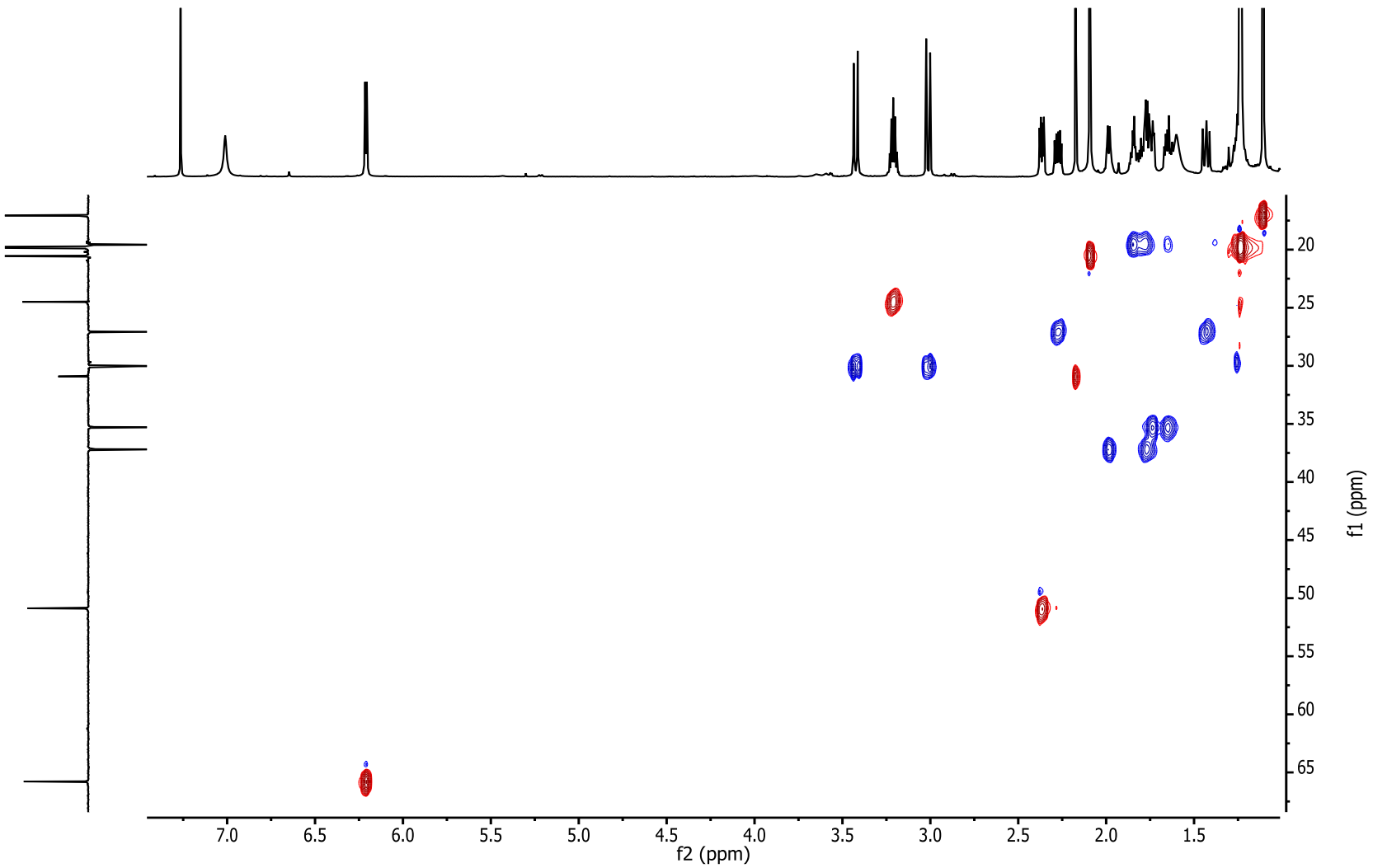


Figure S19. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **3**

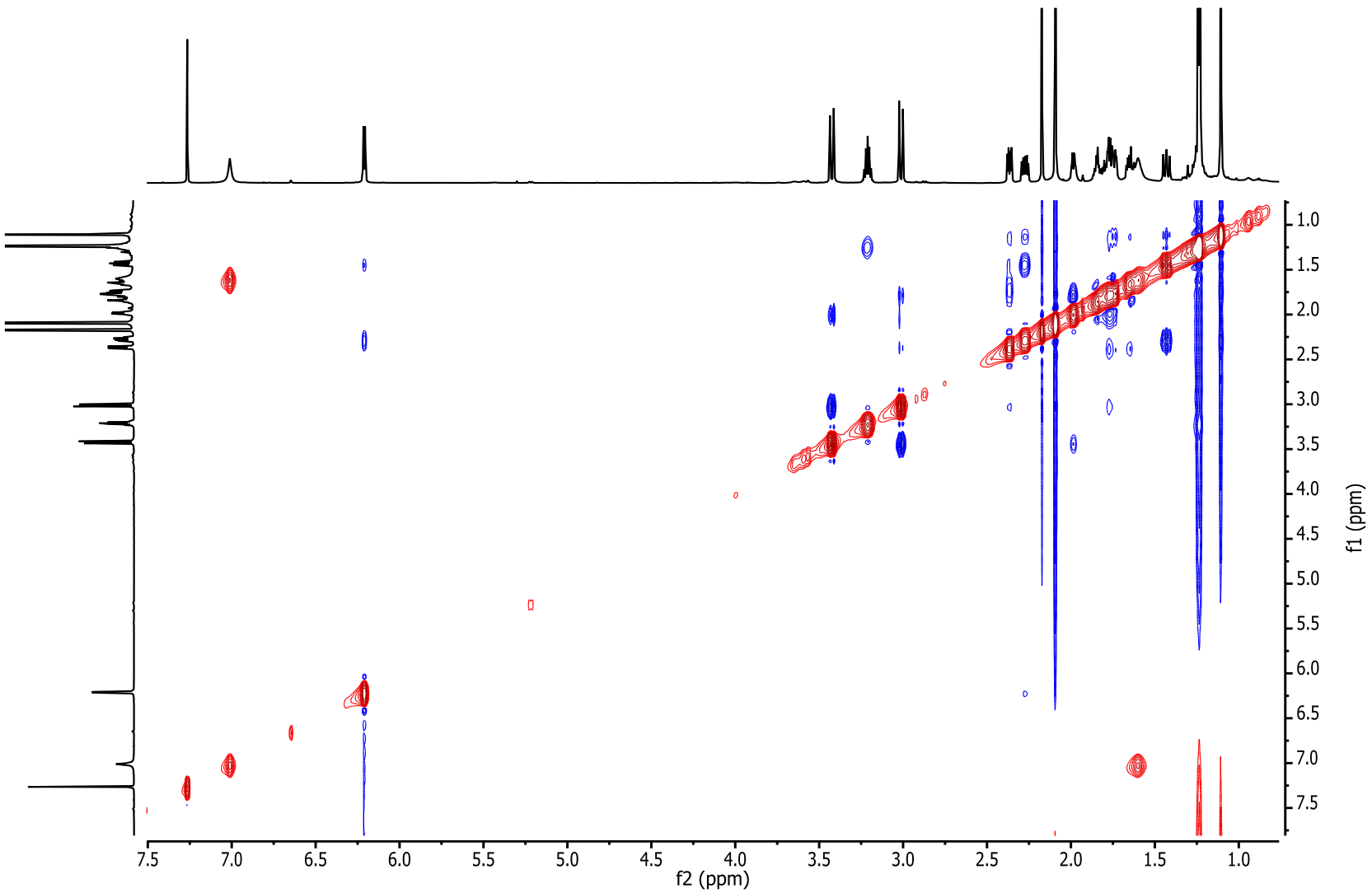
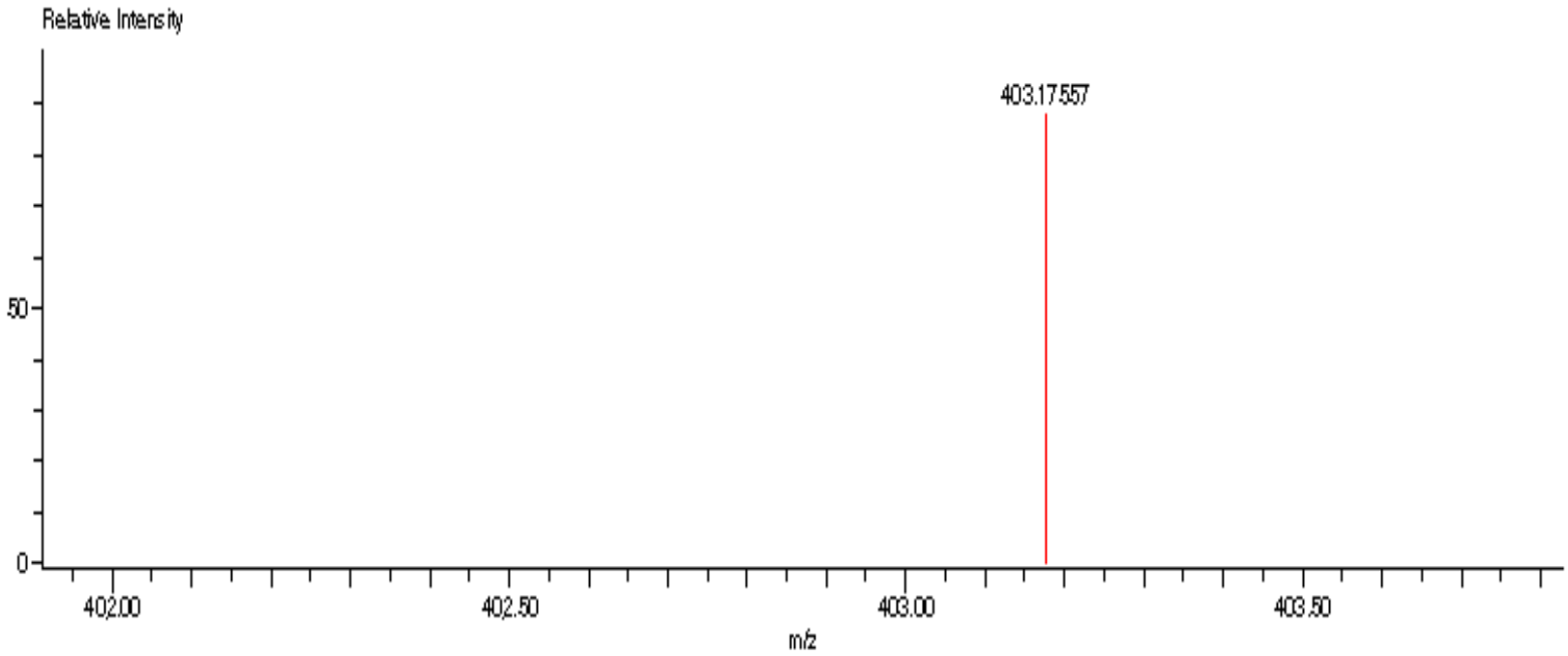


Figure S20. NOESY NMR ($CDCl_3$, 700 MHz) spectrum of **3**

Charge number:1 Tolerance:5.00(mmu) Unsaturation Number:8.0 .. 12.0 (Fraction:Both)

Element:^{12}C:20 .. 25, ^{1}H:25 .. 30, ^{16}O:5 .. 8



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
403.17557	76201.60	403.17568	-0.11	-0.27	$^{12}C_{22}{}^{1}H_{27}{}^{16}O_{7}$	9.5

Figure S21. HR-DART-MS of **3**

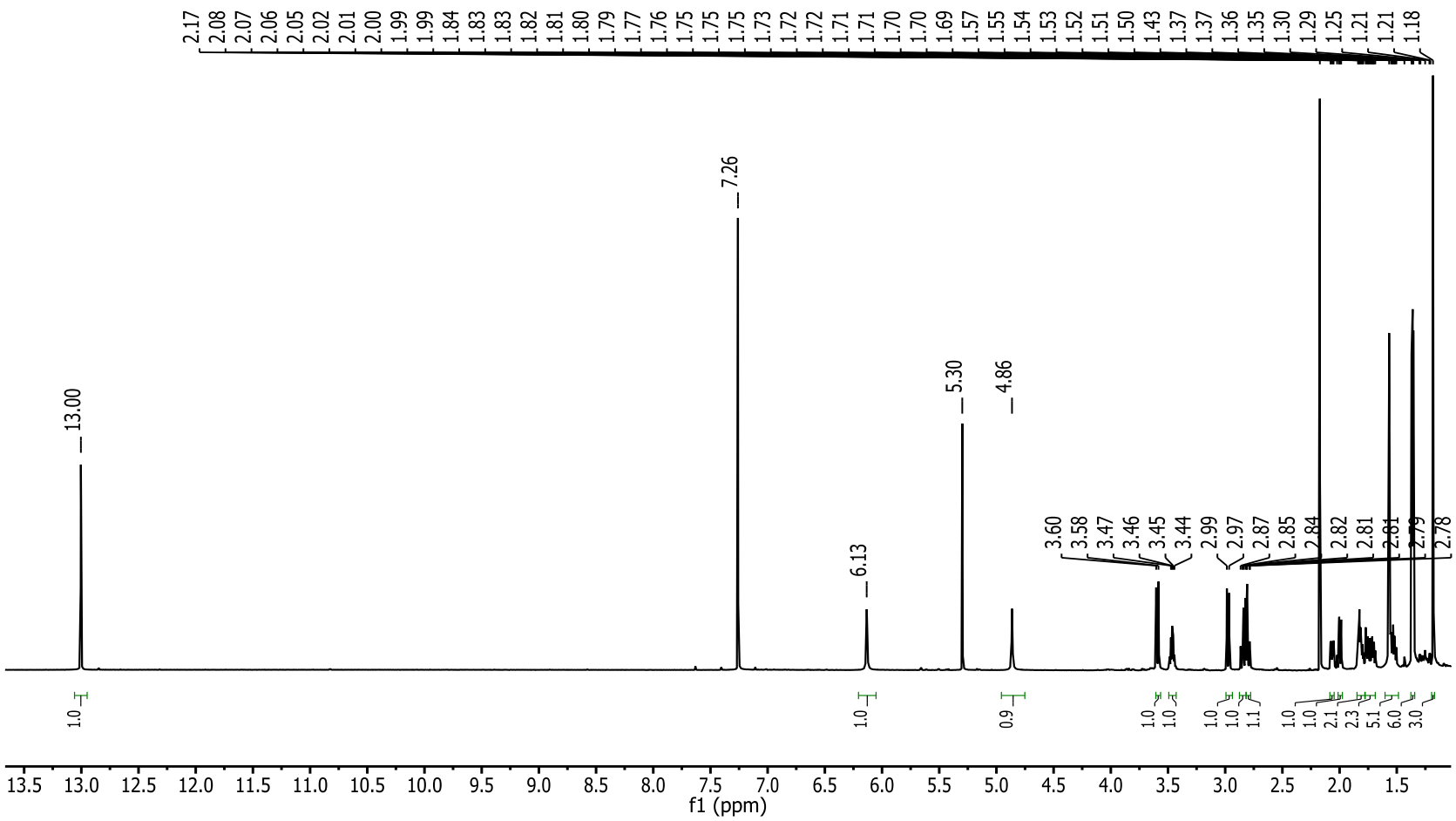


Figure S22. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **4**

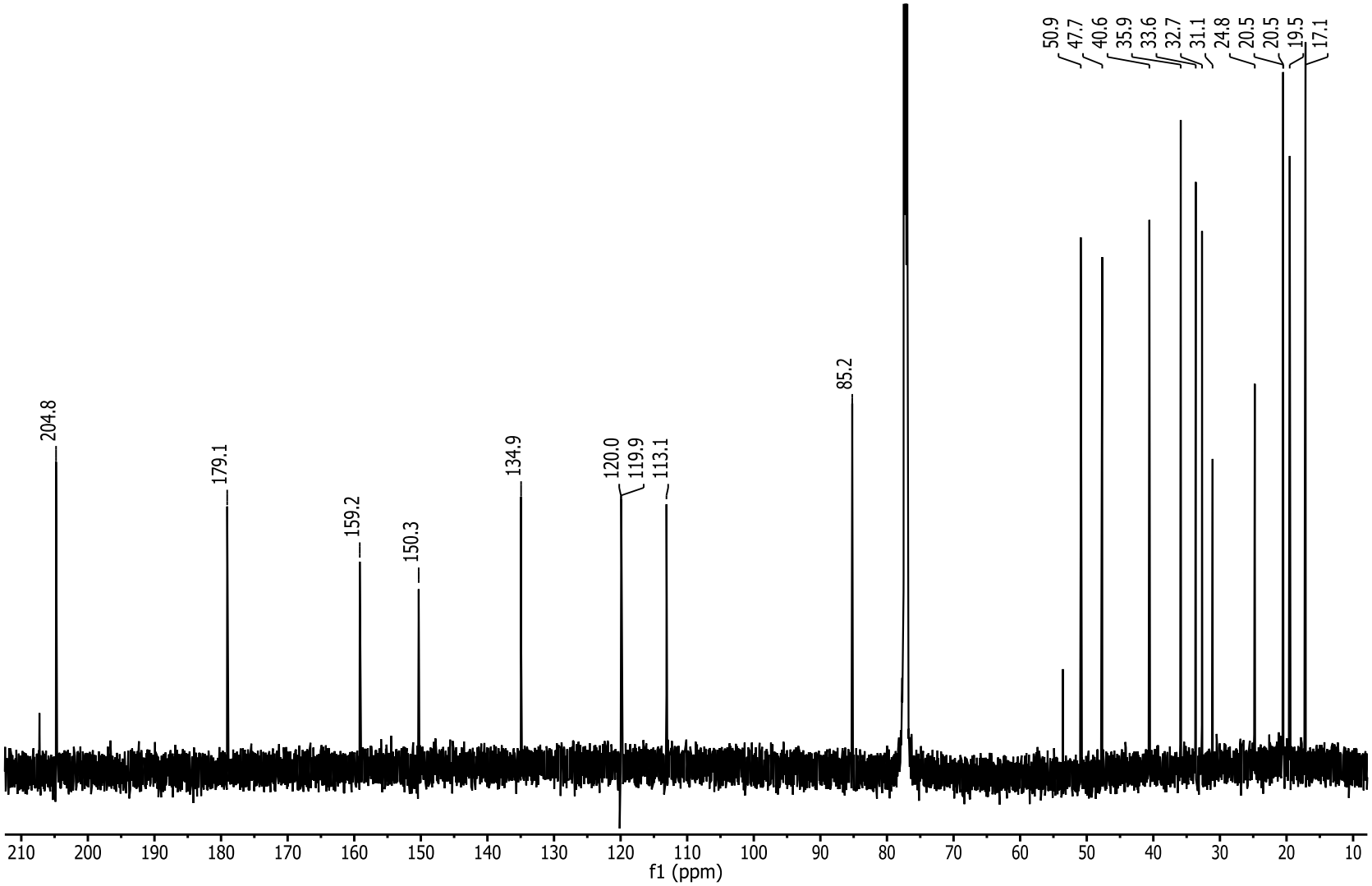


Figure S23. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **4**

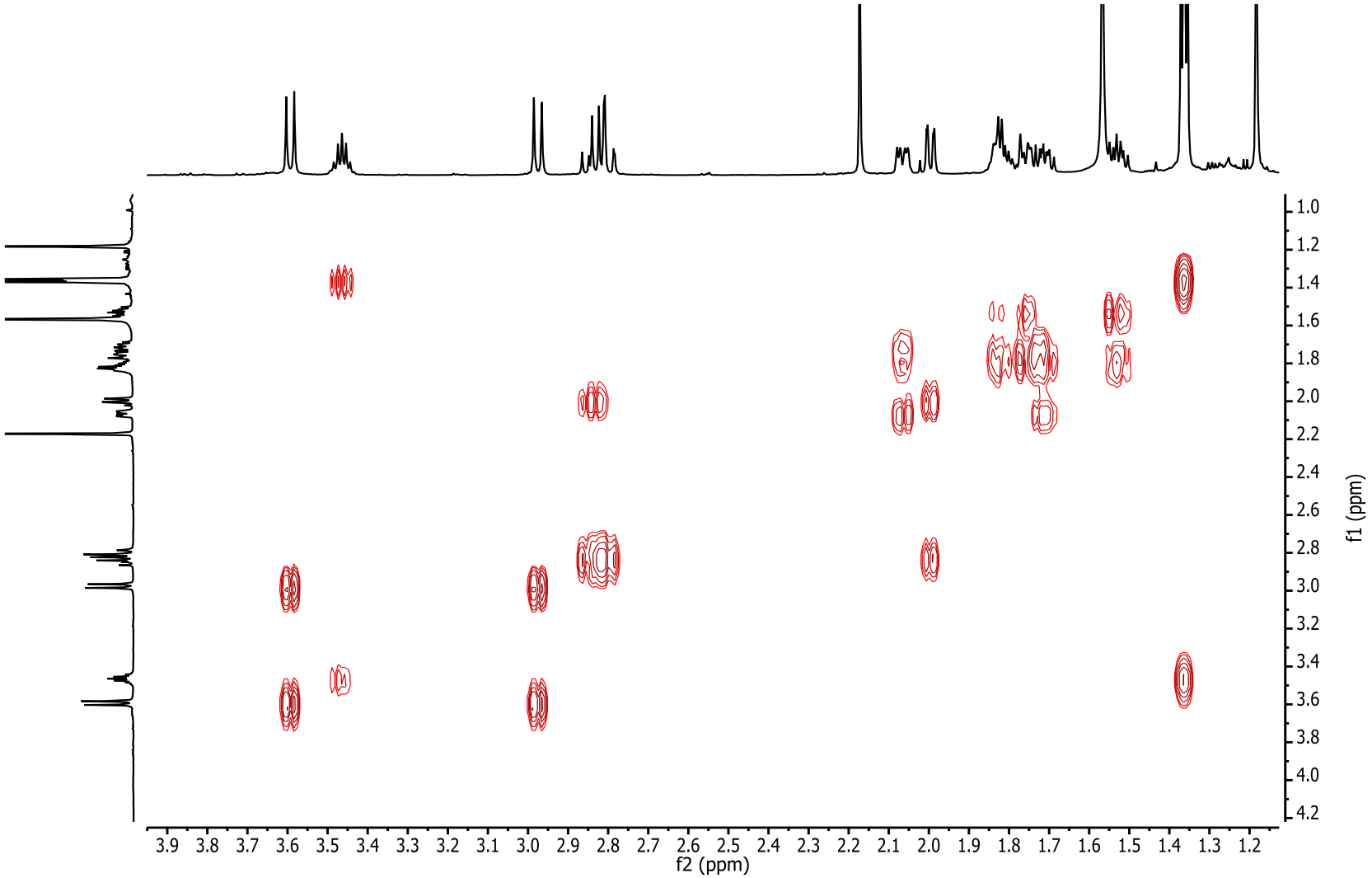


Figure S24. COSY NMR ($CDCl_3$, 700 MHz) spectrum of **4**

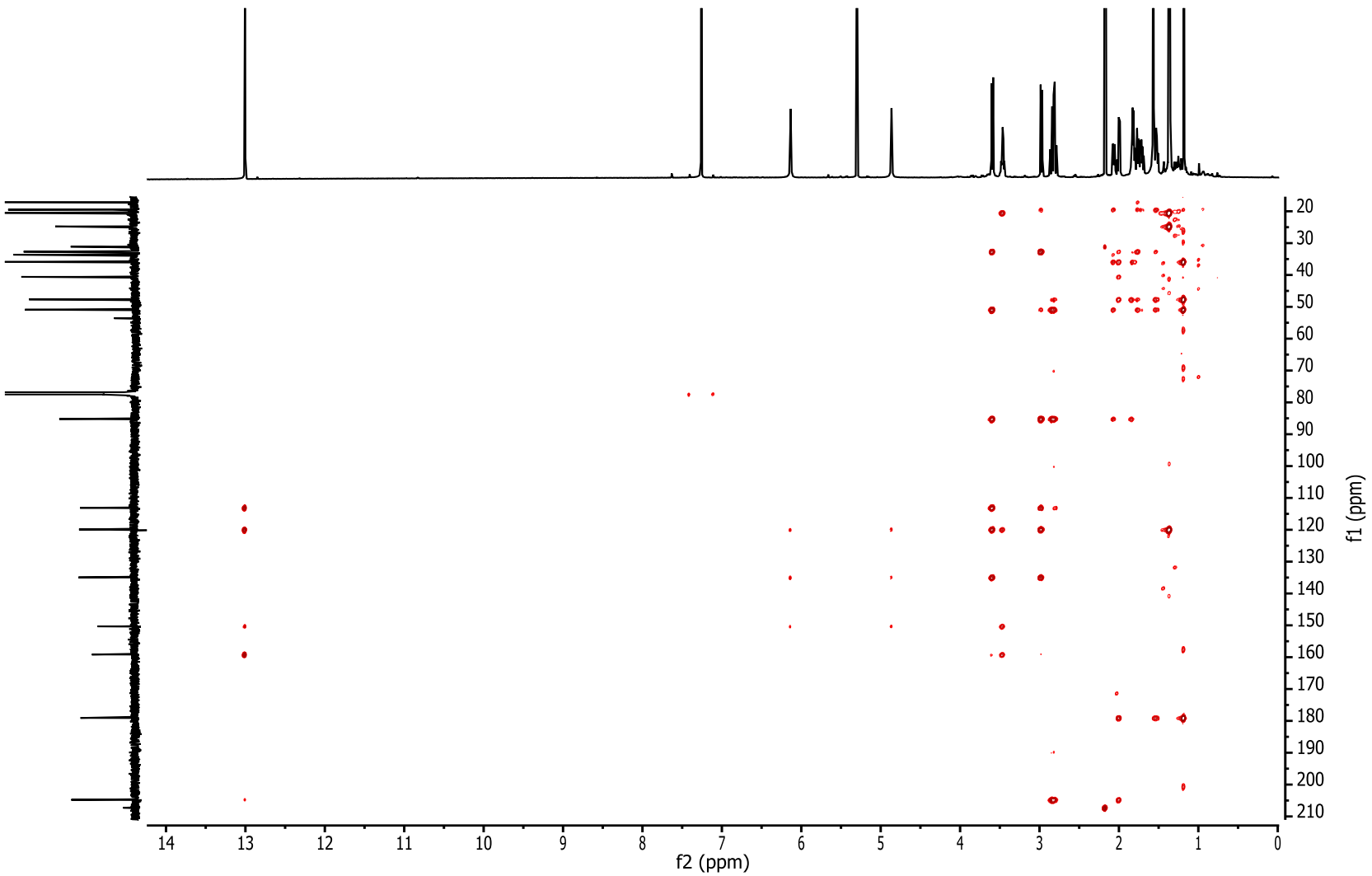


Figure S25. HMBC NMR ($CDCl_3$, 700 MHz) spectrum of **4**

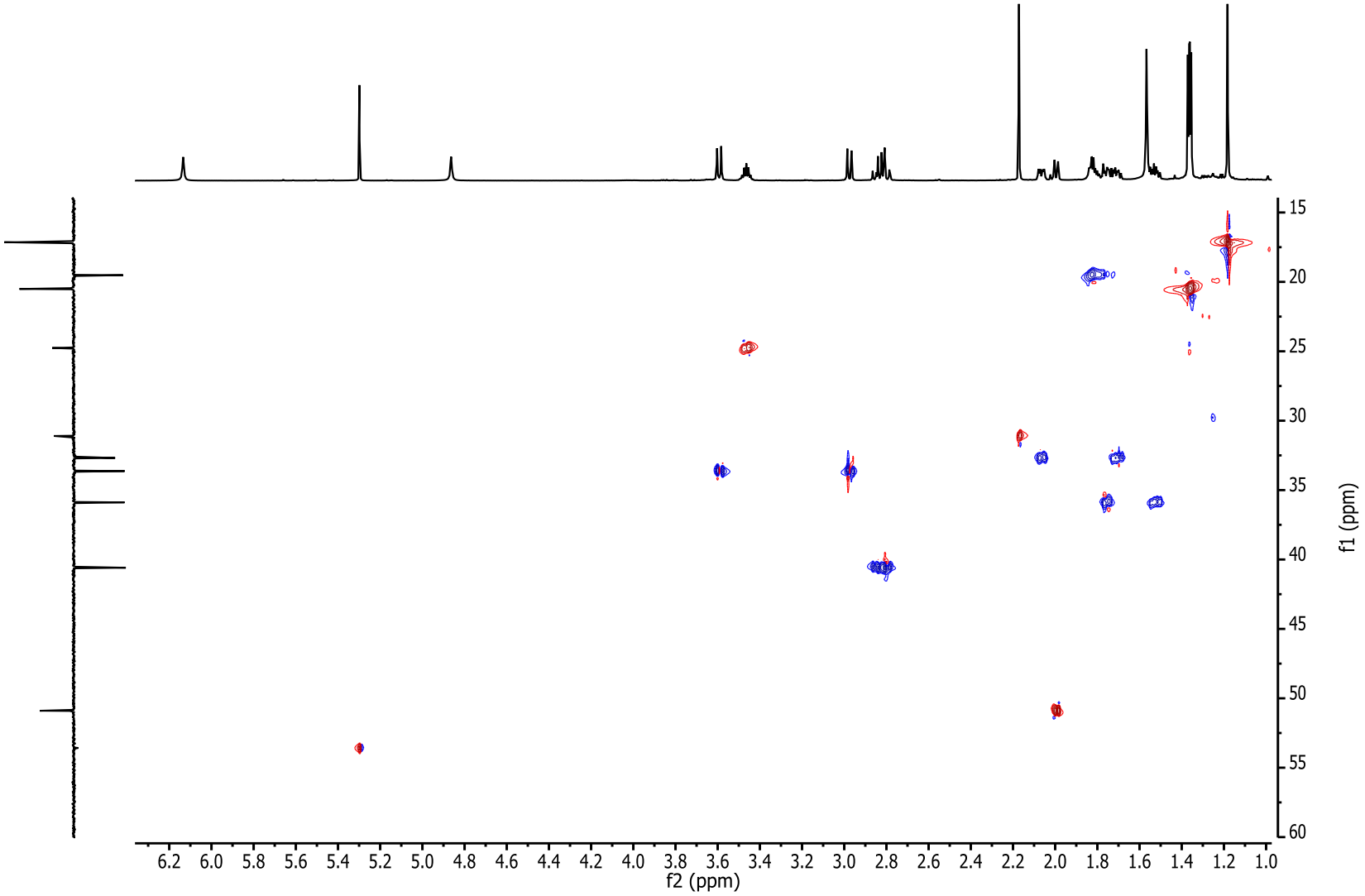


Figure S26. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **4**

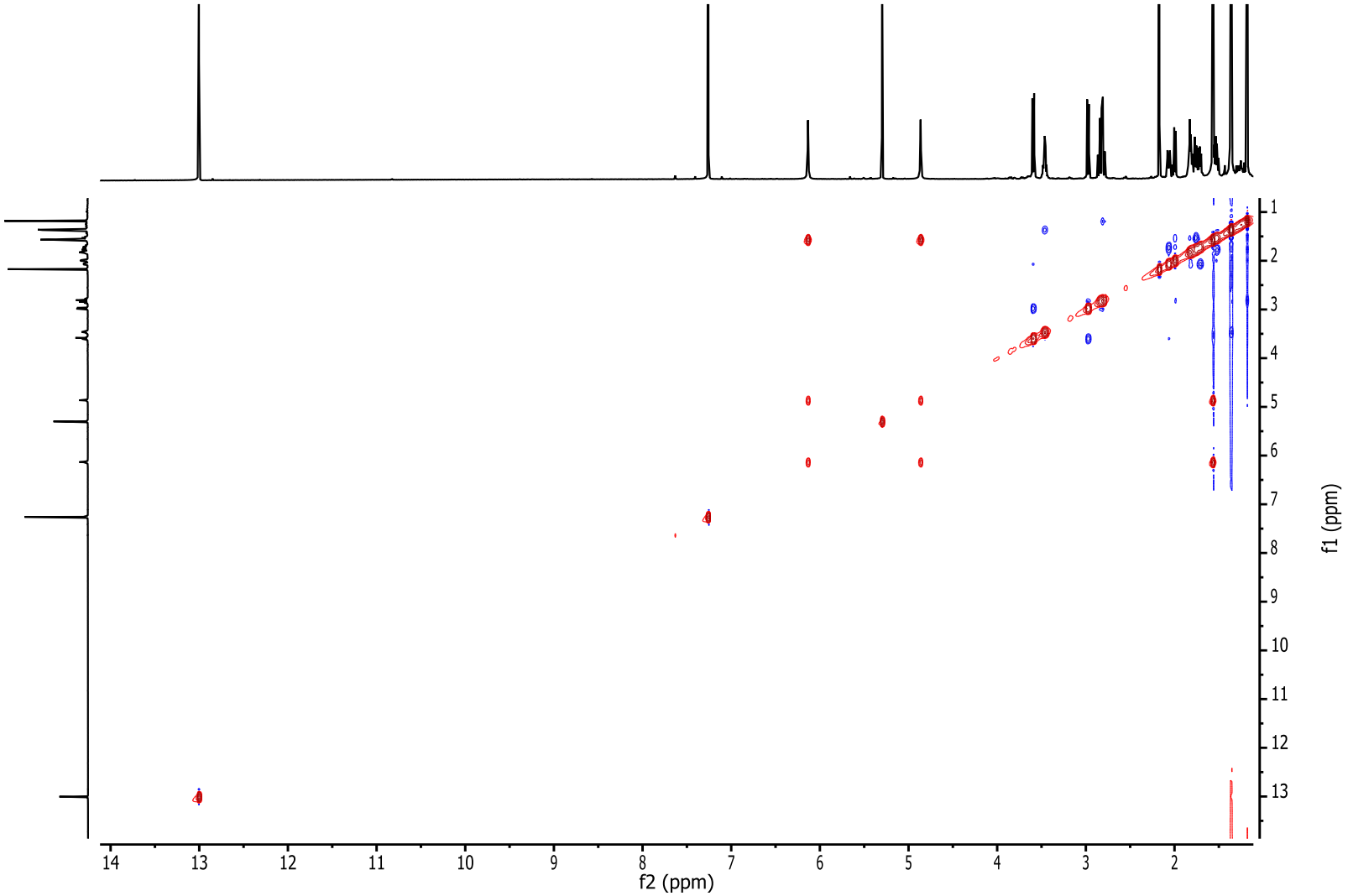
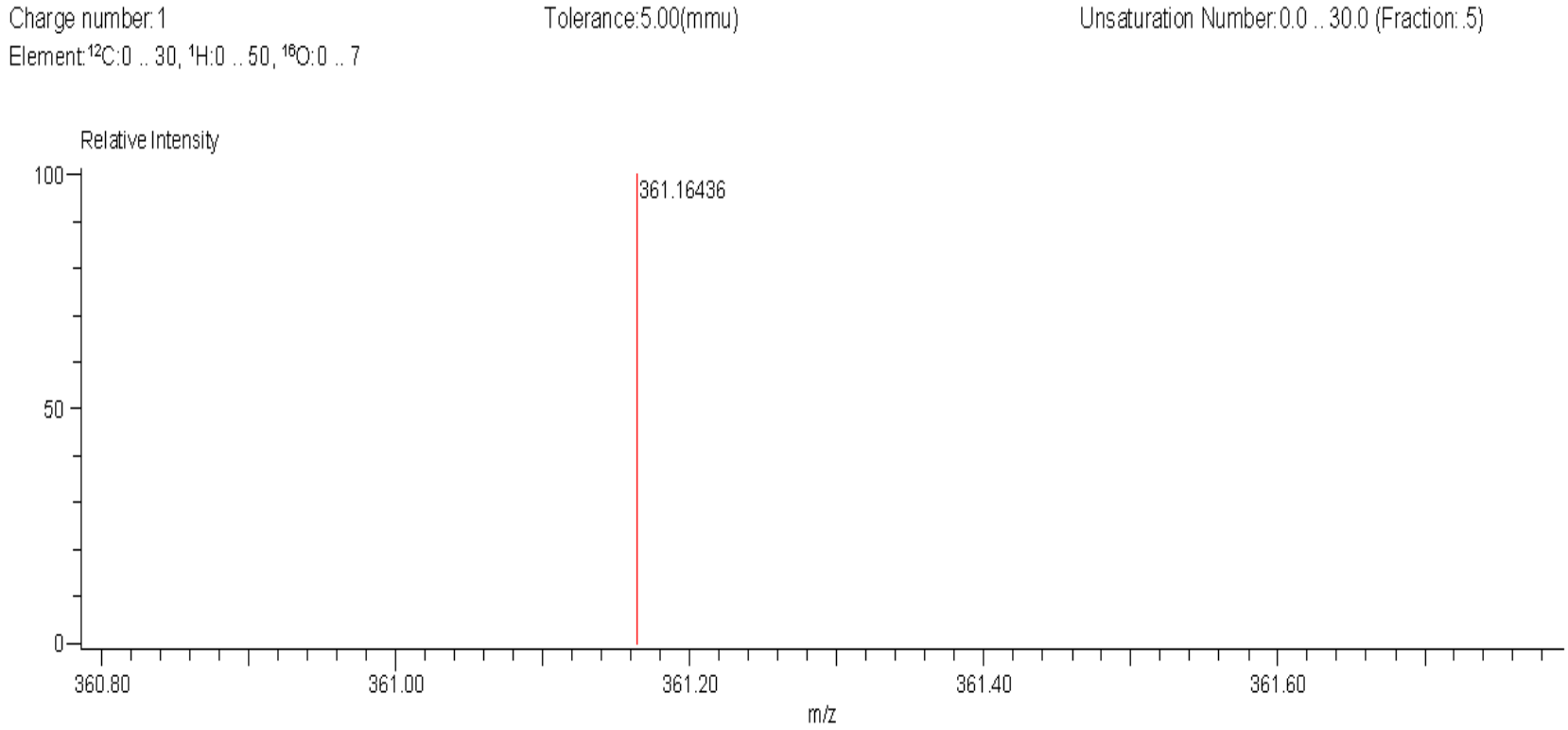


Figure S27. NOESY NMR ($CDCl_3$, 700 MHz) spectrum of **4**



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
361.16436	63640.89	361.16511	-0.76	-2.09	$^{12}C_{20}{}^{1}H_{25}{}^{16}O_{6}$	8.5

Figure S28. HR-DART-MS of **4**

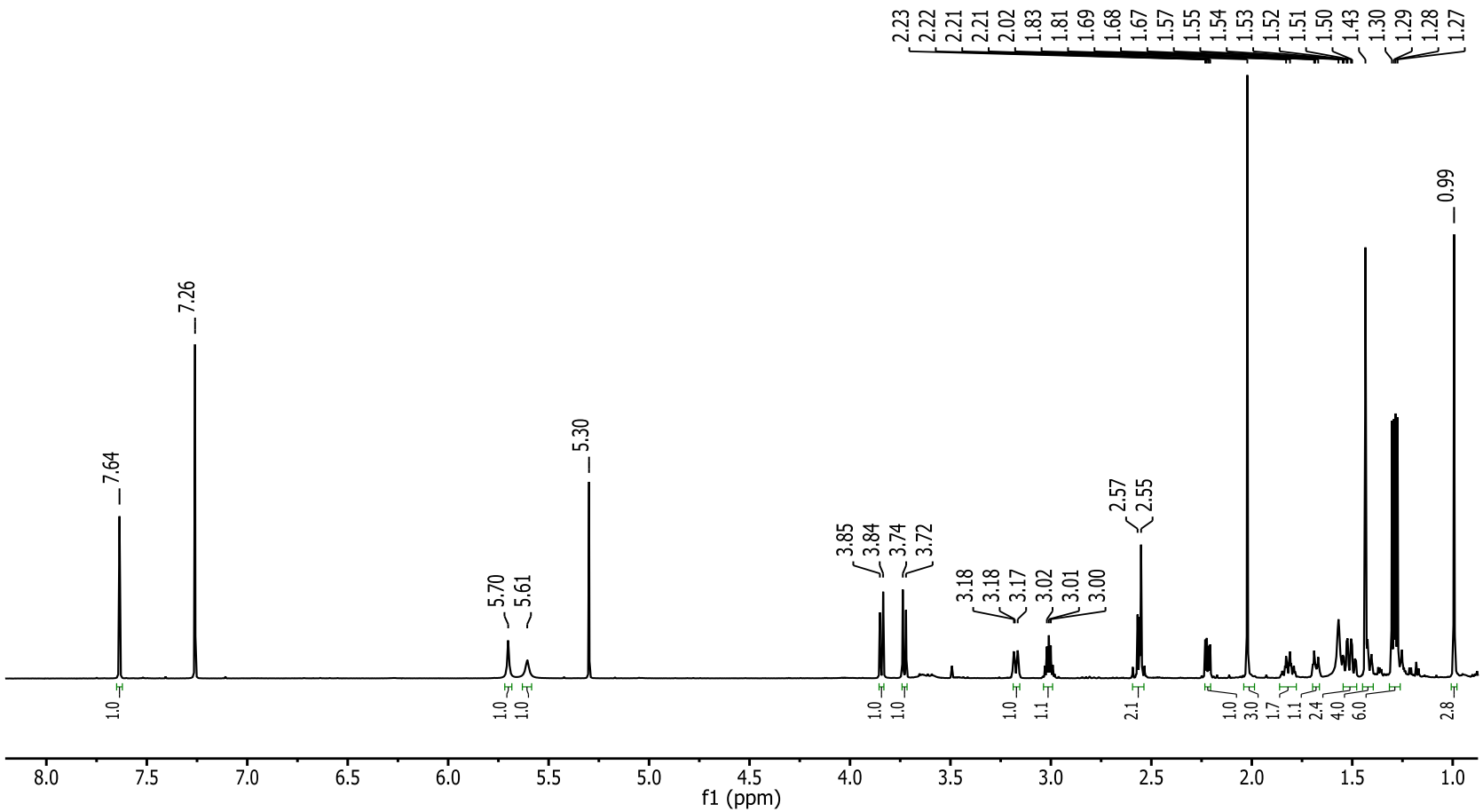


Figure S29. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **5**

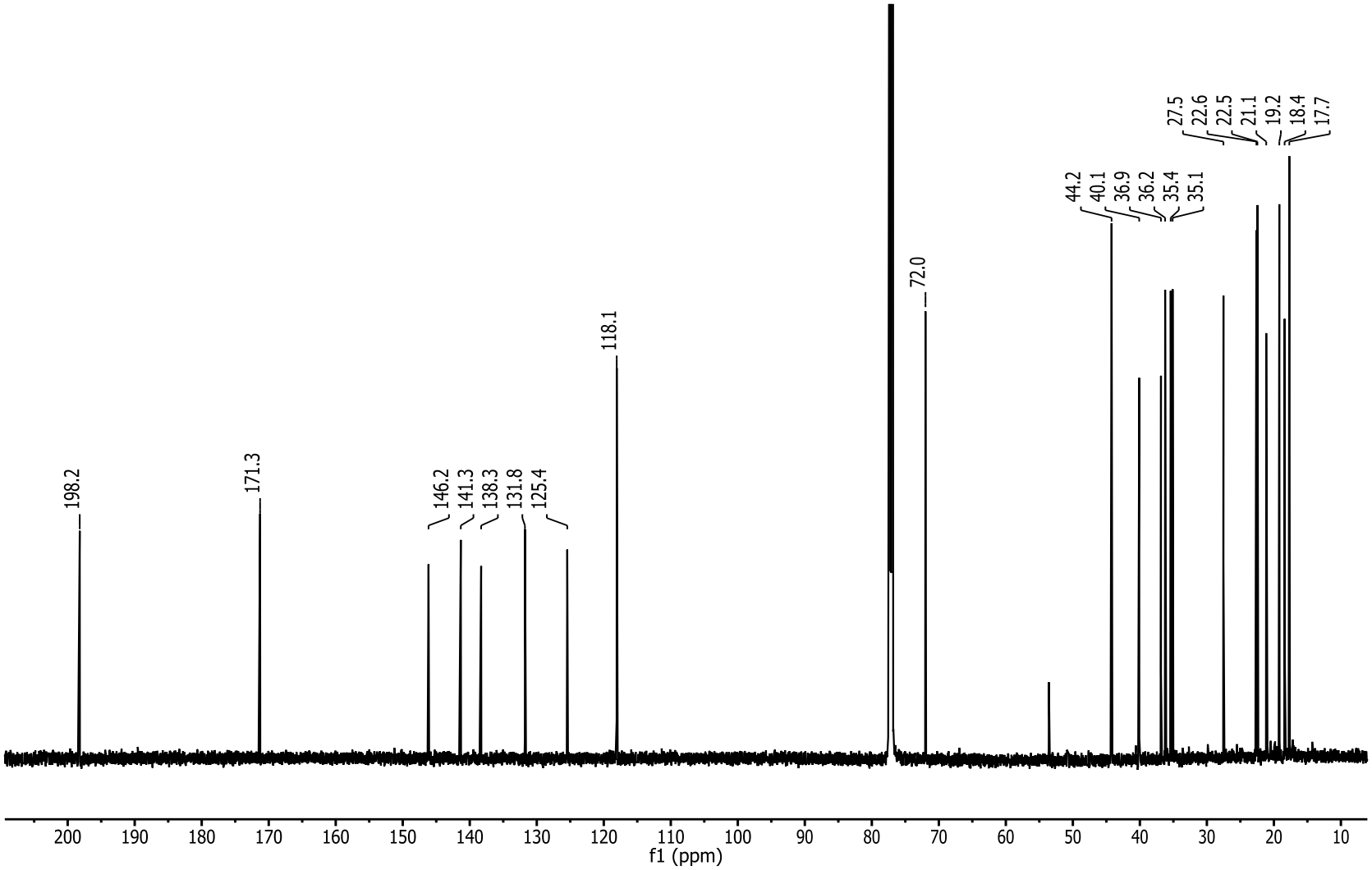


Figure S30. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **5**

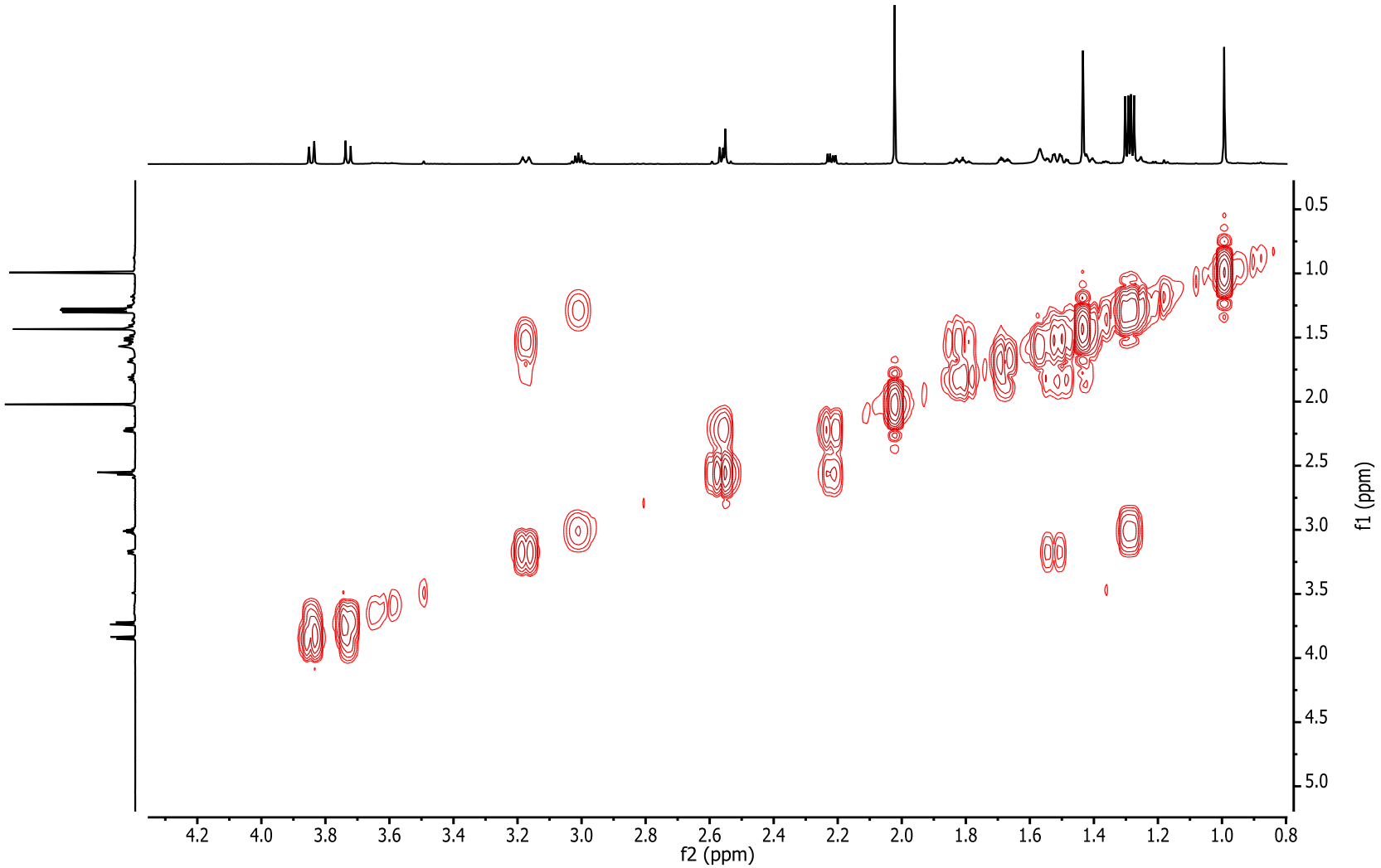


Figure S31. COSY NMR ($CDCl_3$, 700 MHz) spectrum of **5**

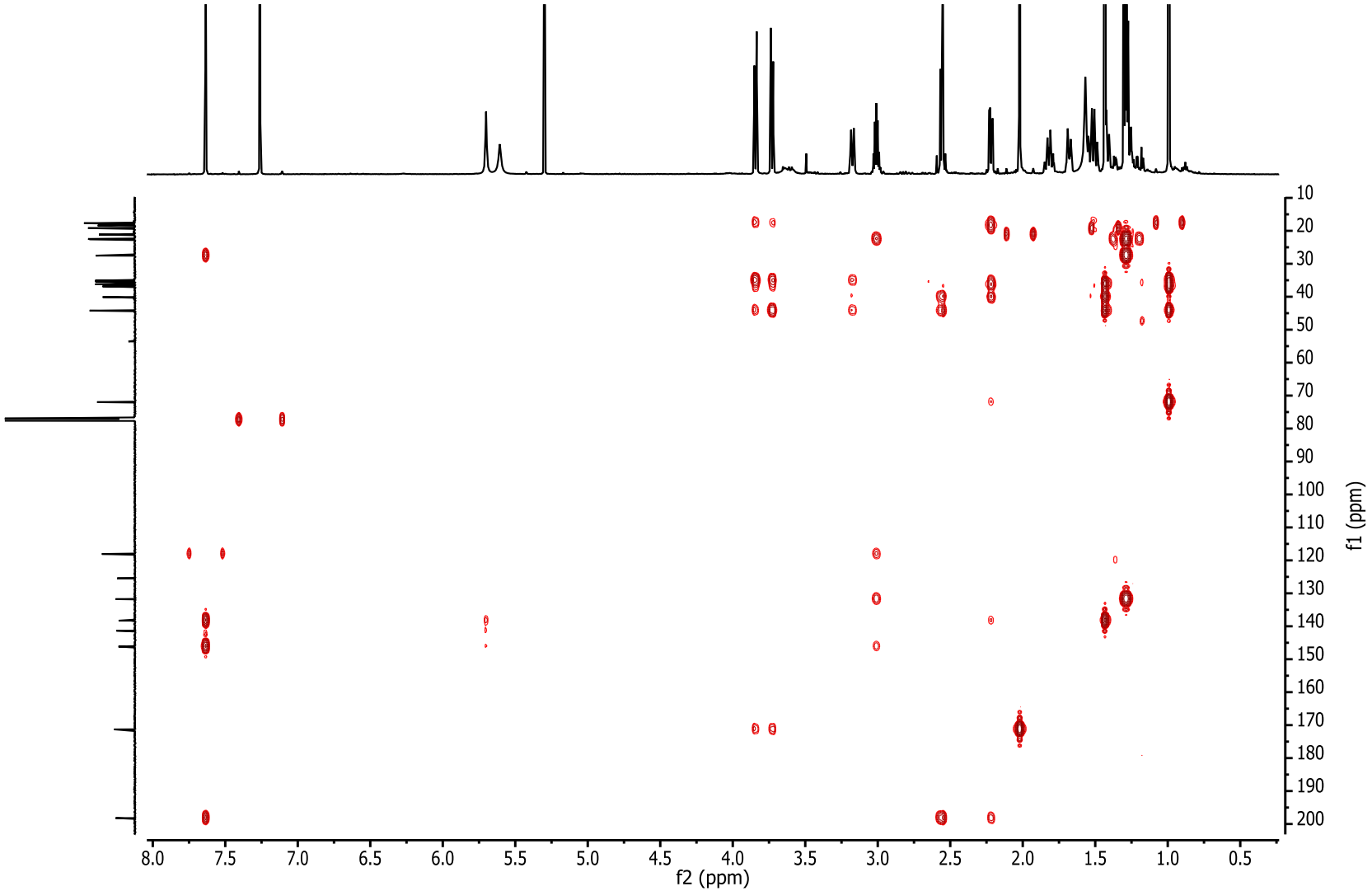


Figure S32. HMBC NMR ($CDCl_3$, 700 MHz) spectrum of **5**

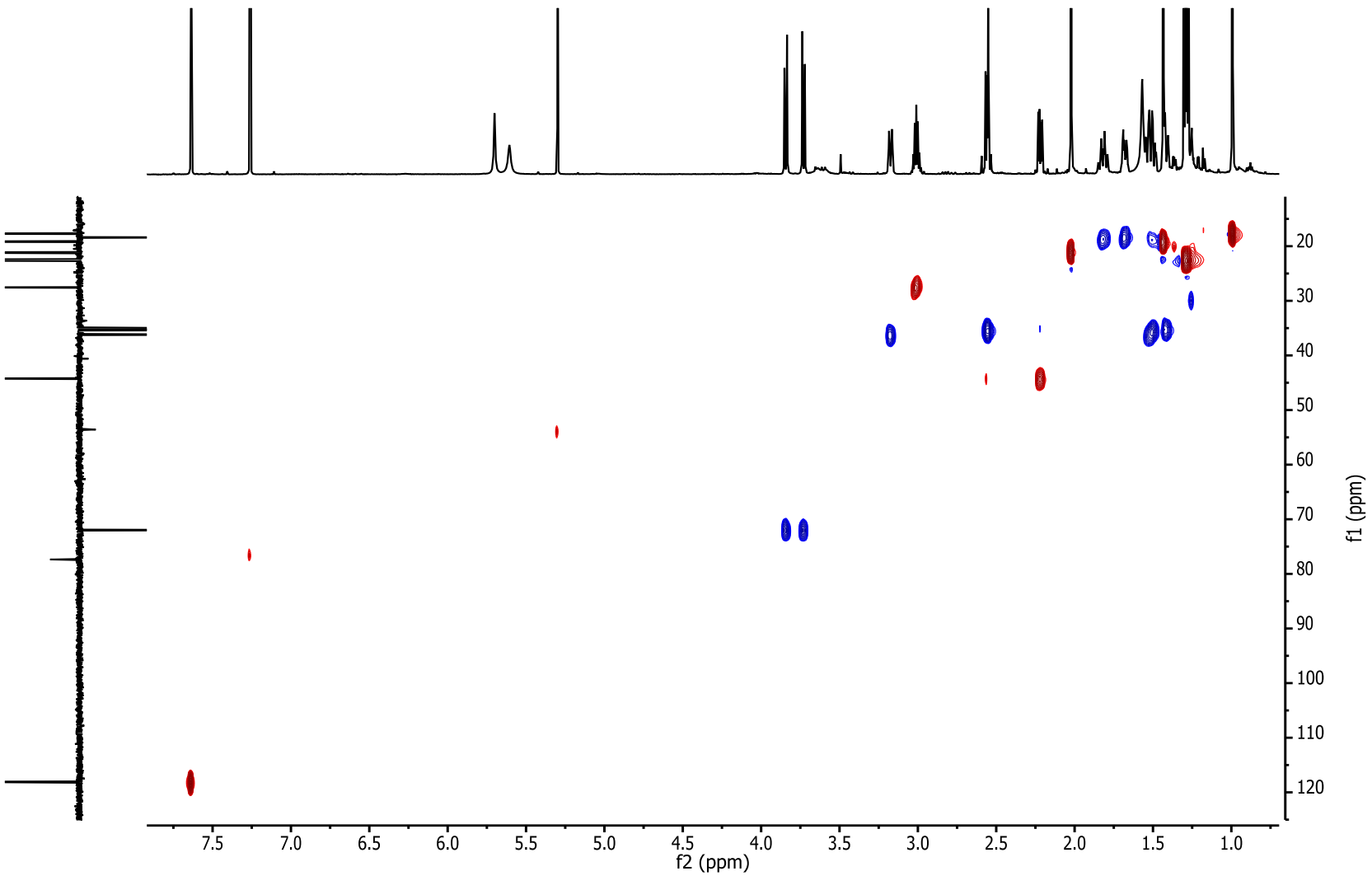


Figure S33. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **5**

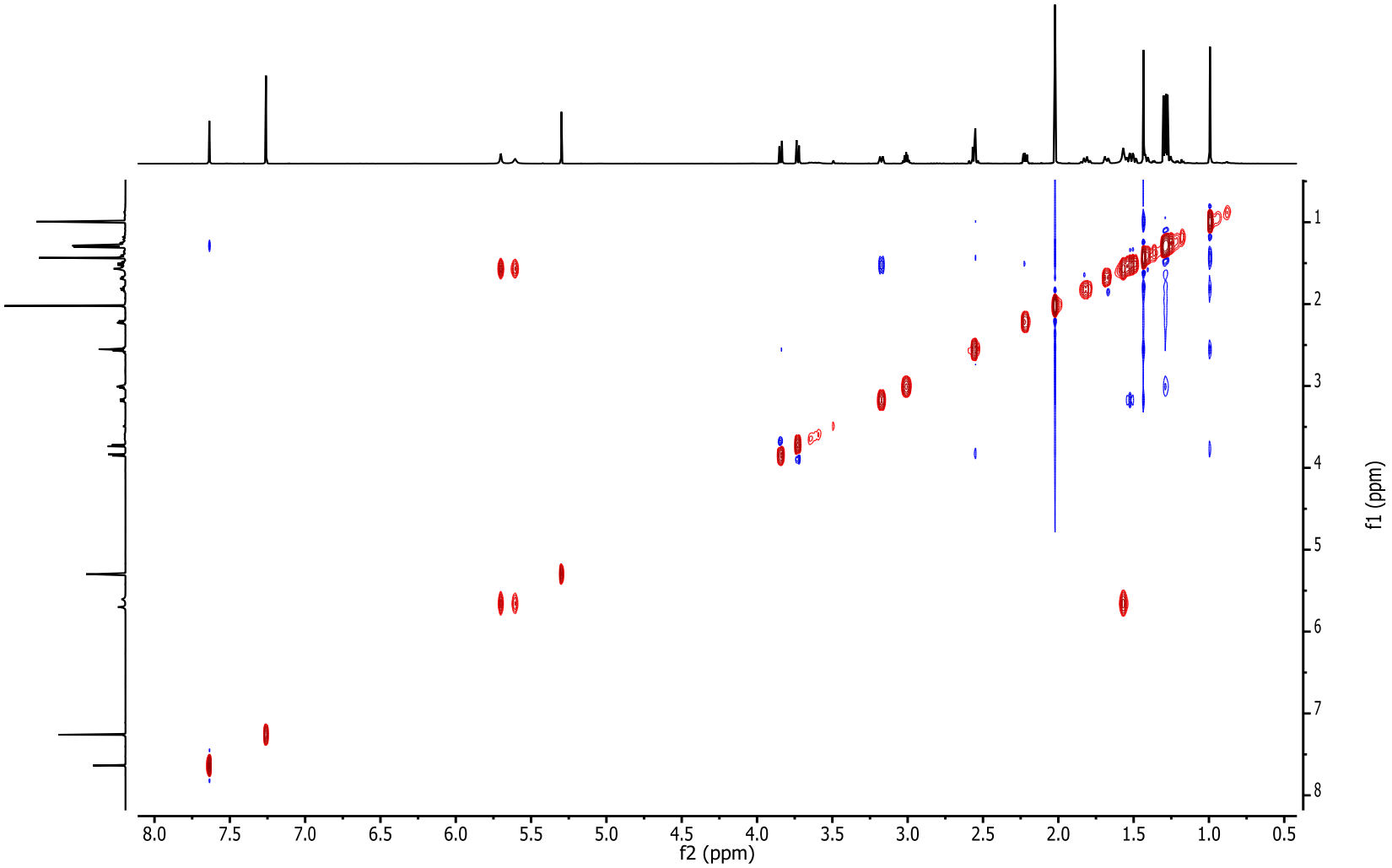
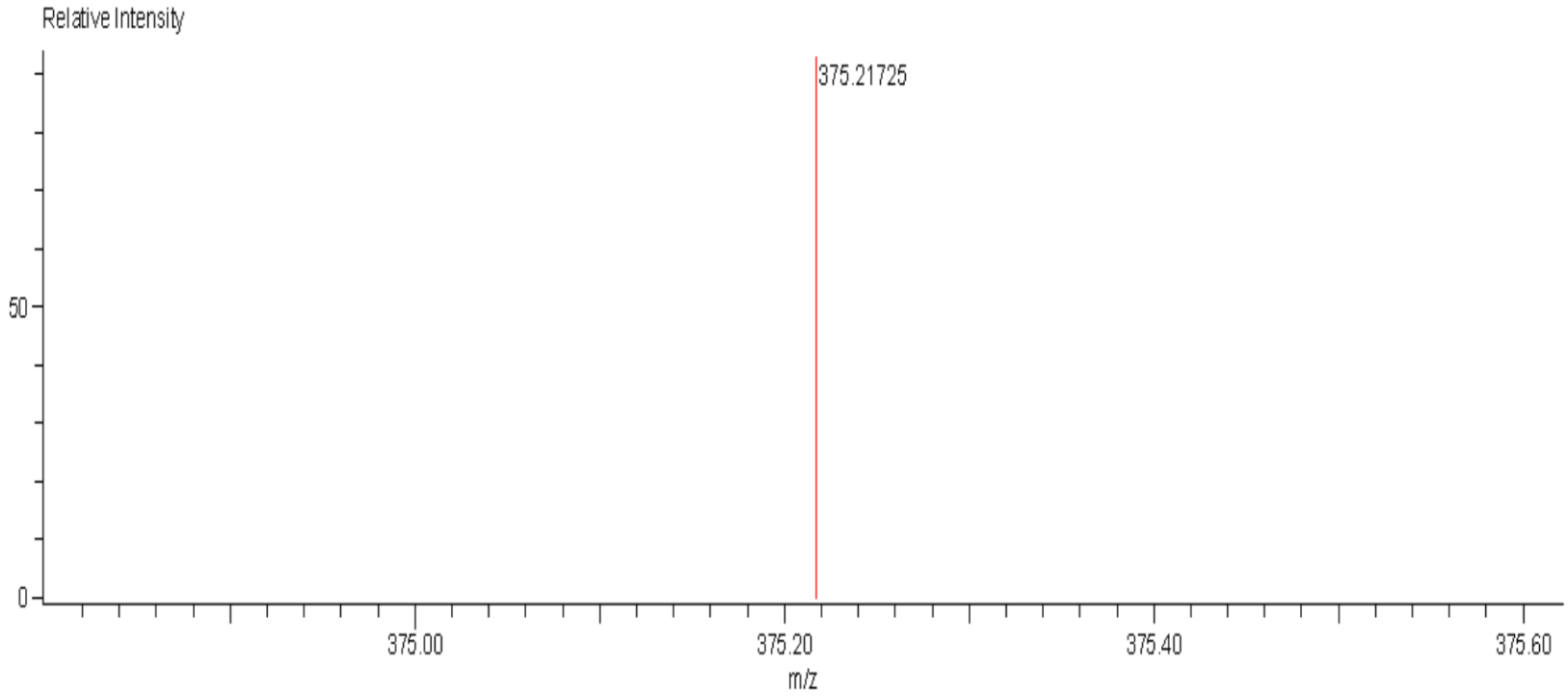


Figure S34. NOESY NMR ($CDCl_3$, 700 MHz) spectrum of **5**

Charge number:1 Tolerance:5.00(mmu) Unsaturation Number:5.0 .. 10.0 (Fraction:Both)

Element:^{12}C:20 .. 25, ^{1}H:30 .. 35, ^{16}O:4 .. 7



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
375.21725	125046.05	375.21715	0.10	0.27	$^{12}C_{22}{}^{1}H_{31}{}^{16}O_5$	7.5

Figure S35. HR-DART-MS of **5**

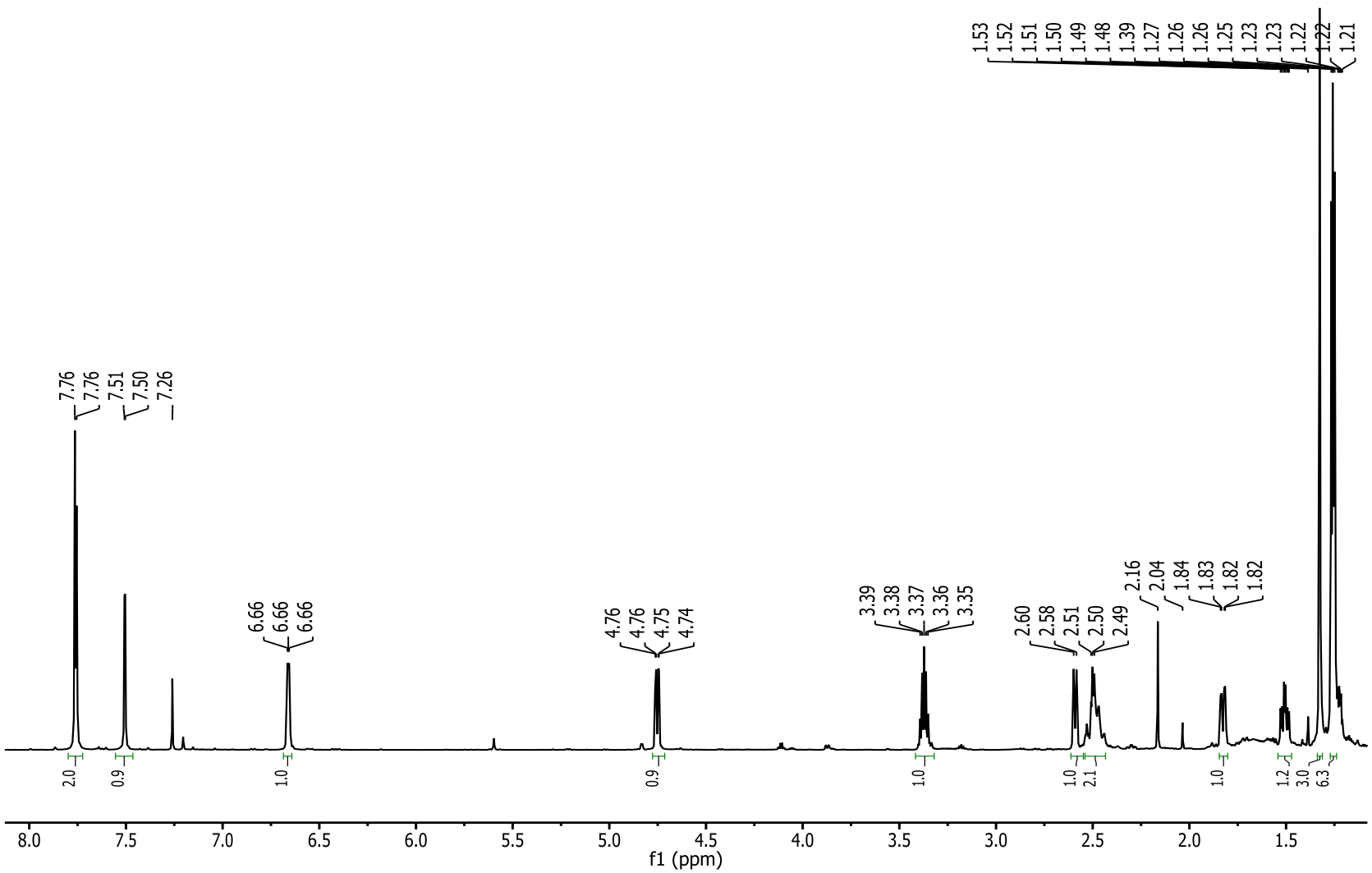


Figure S36. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **6**

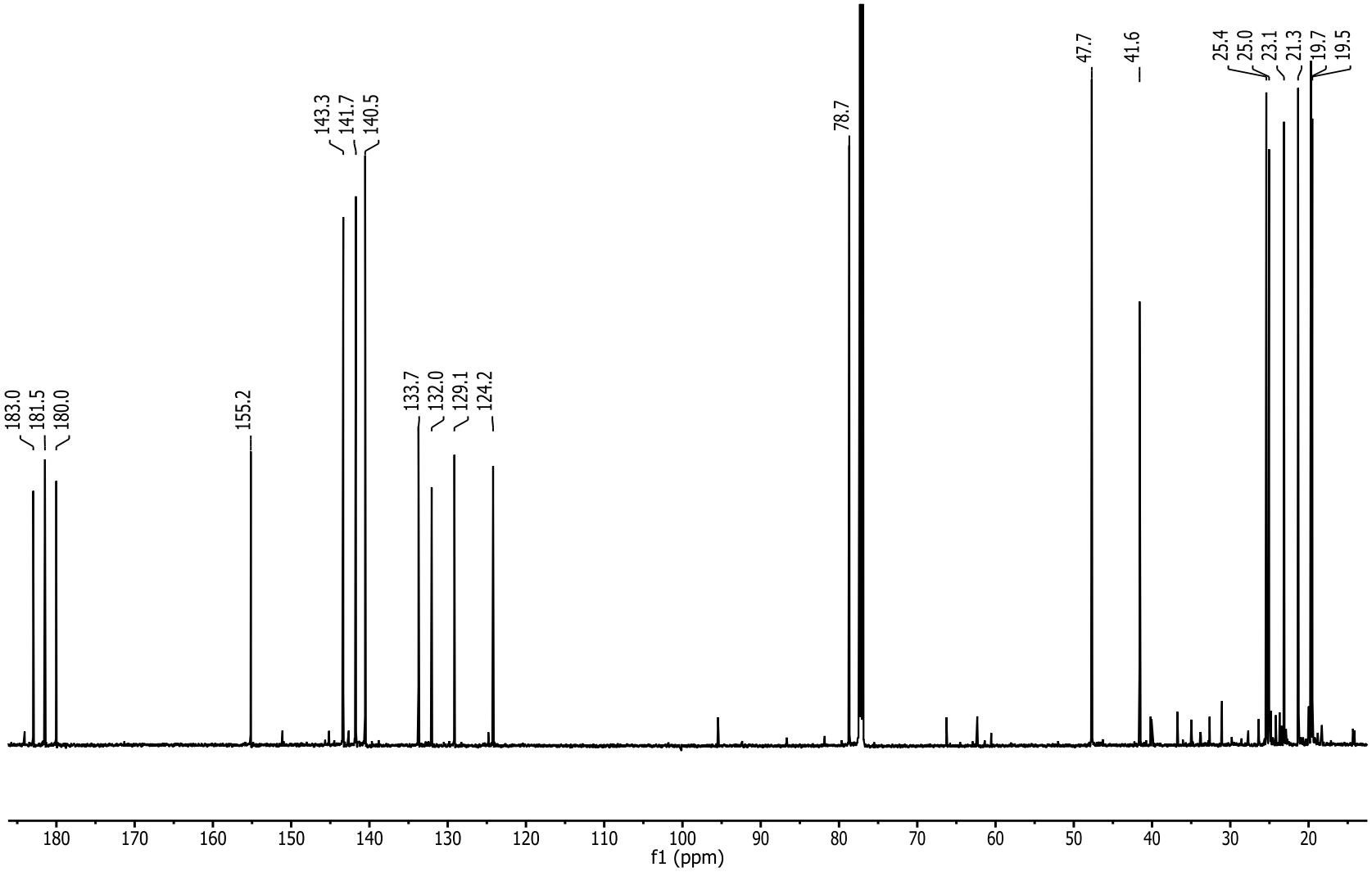


Figure S37. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **6**

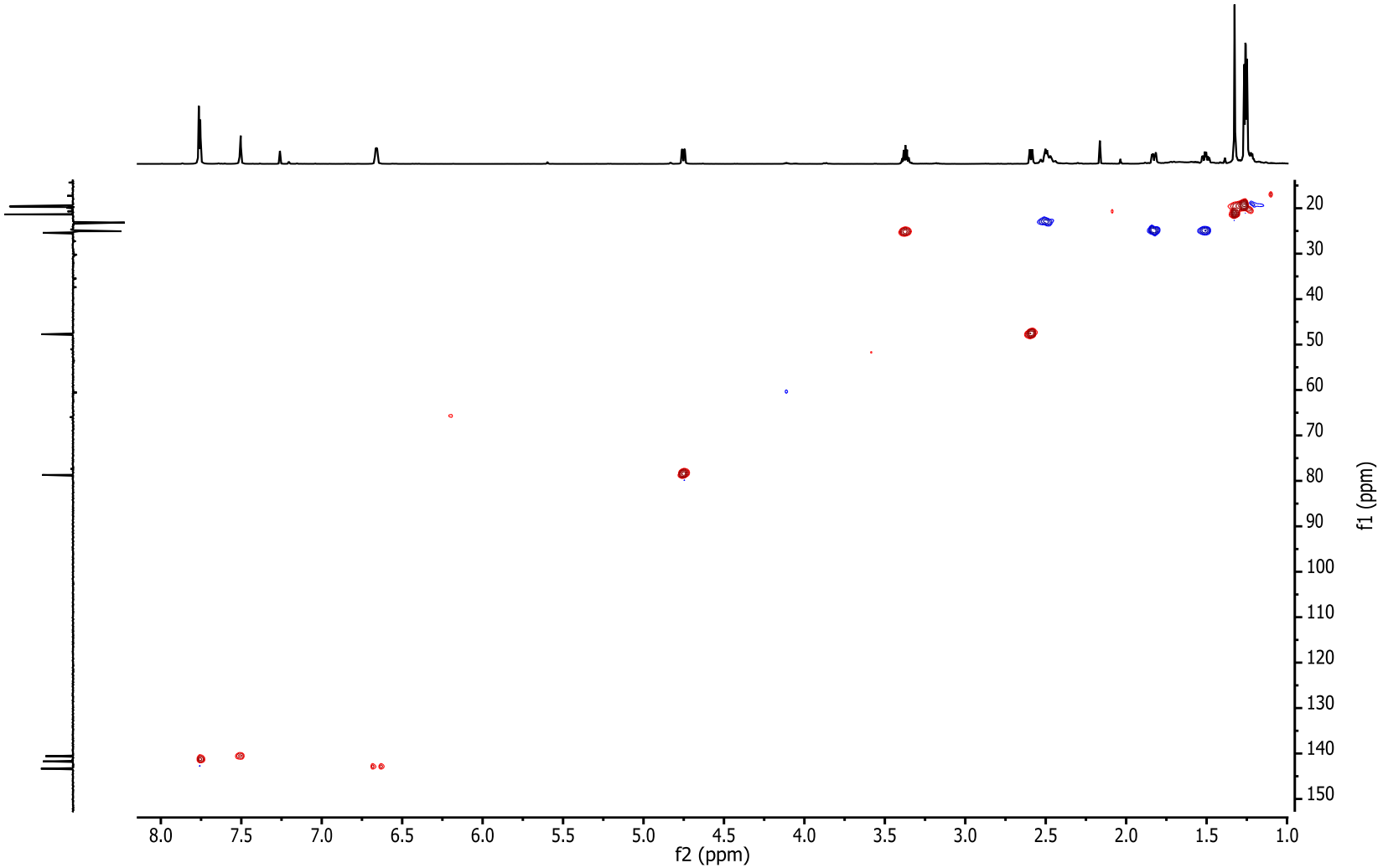


Figure S38. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **6**

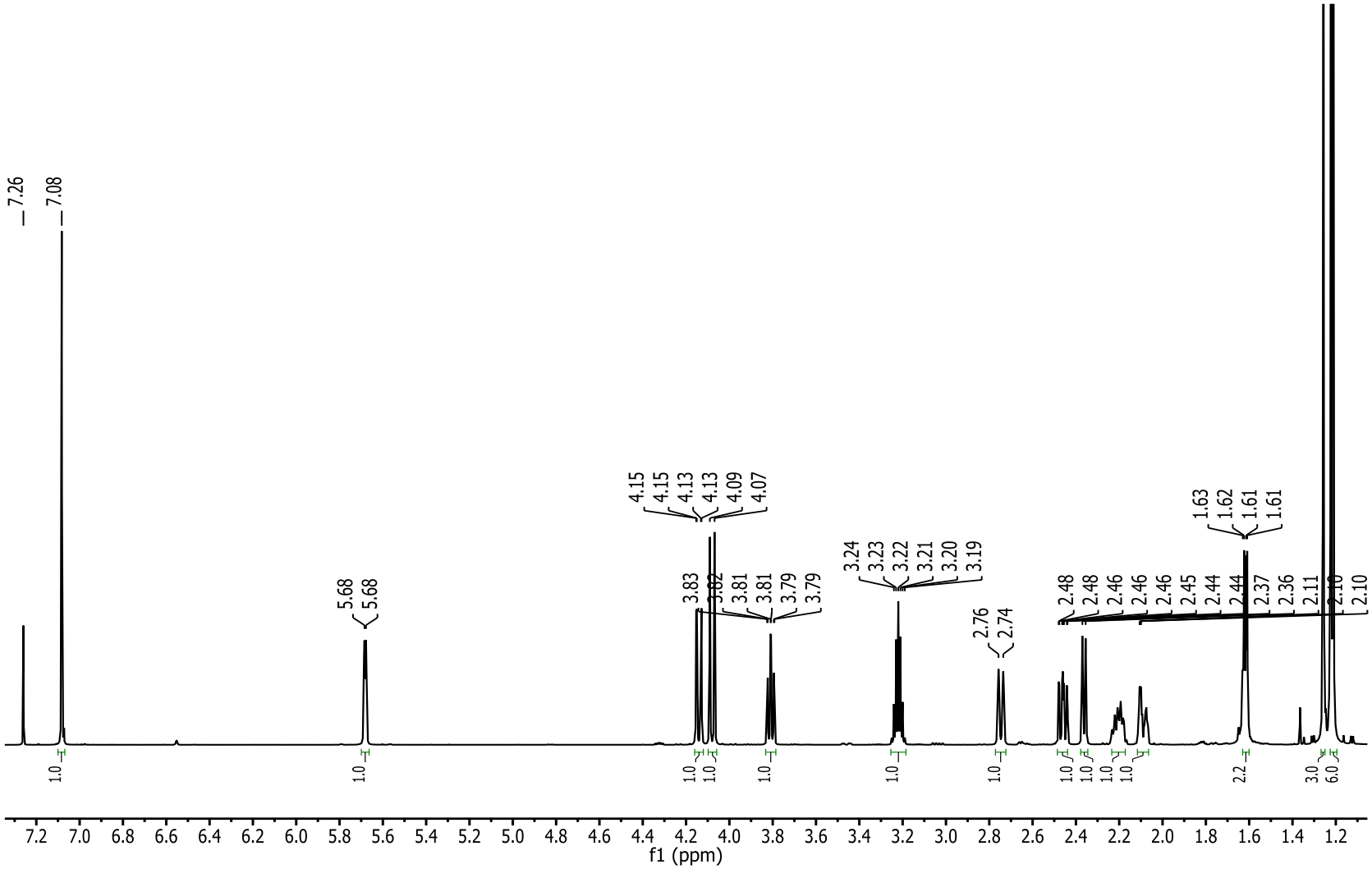


Figure S39. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **7**

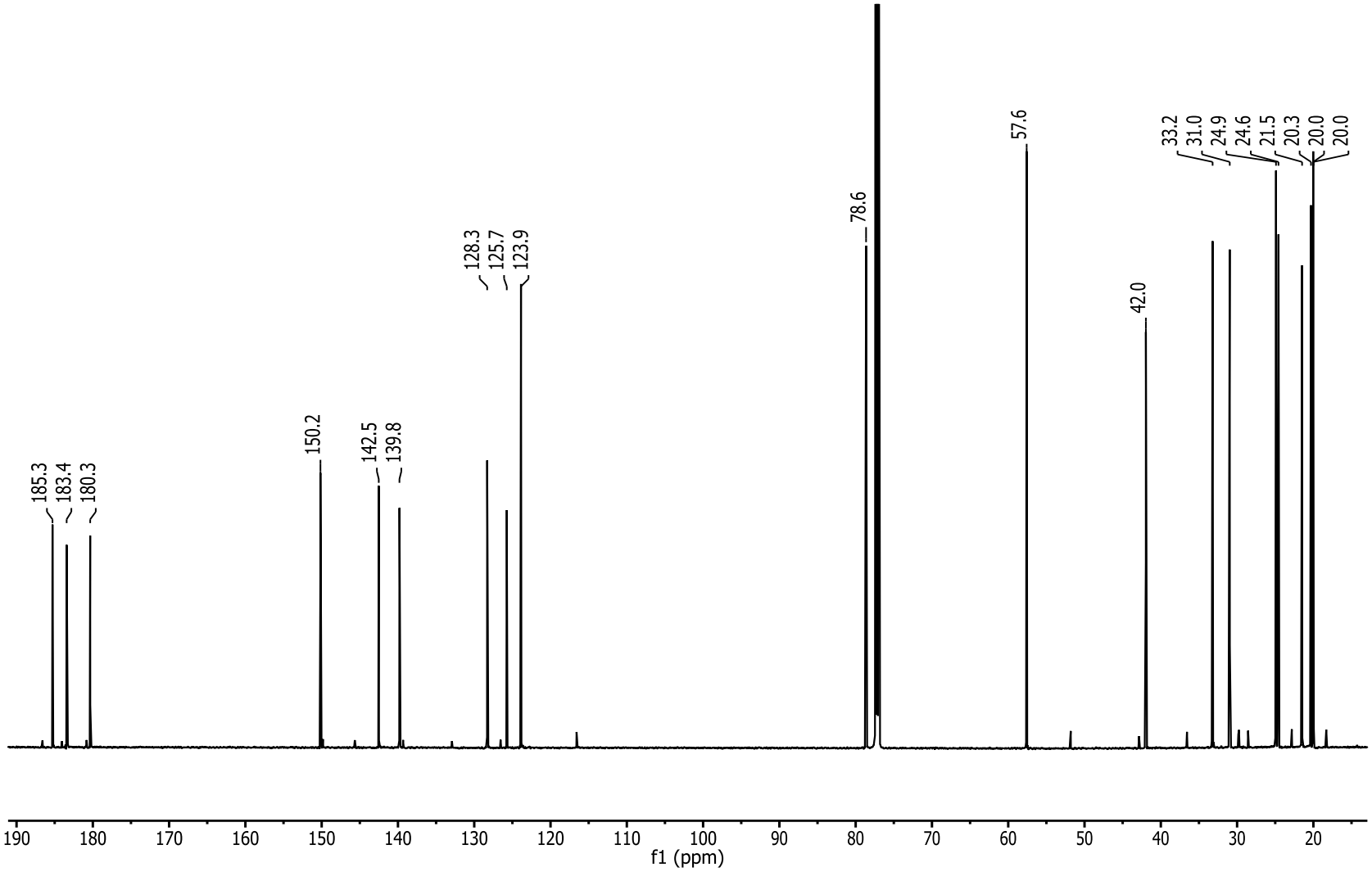


Figure S40. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **7**

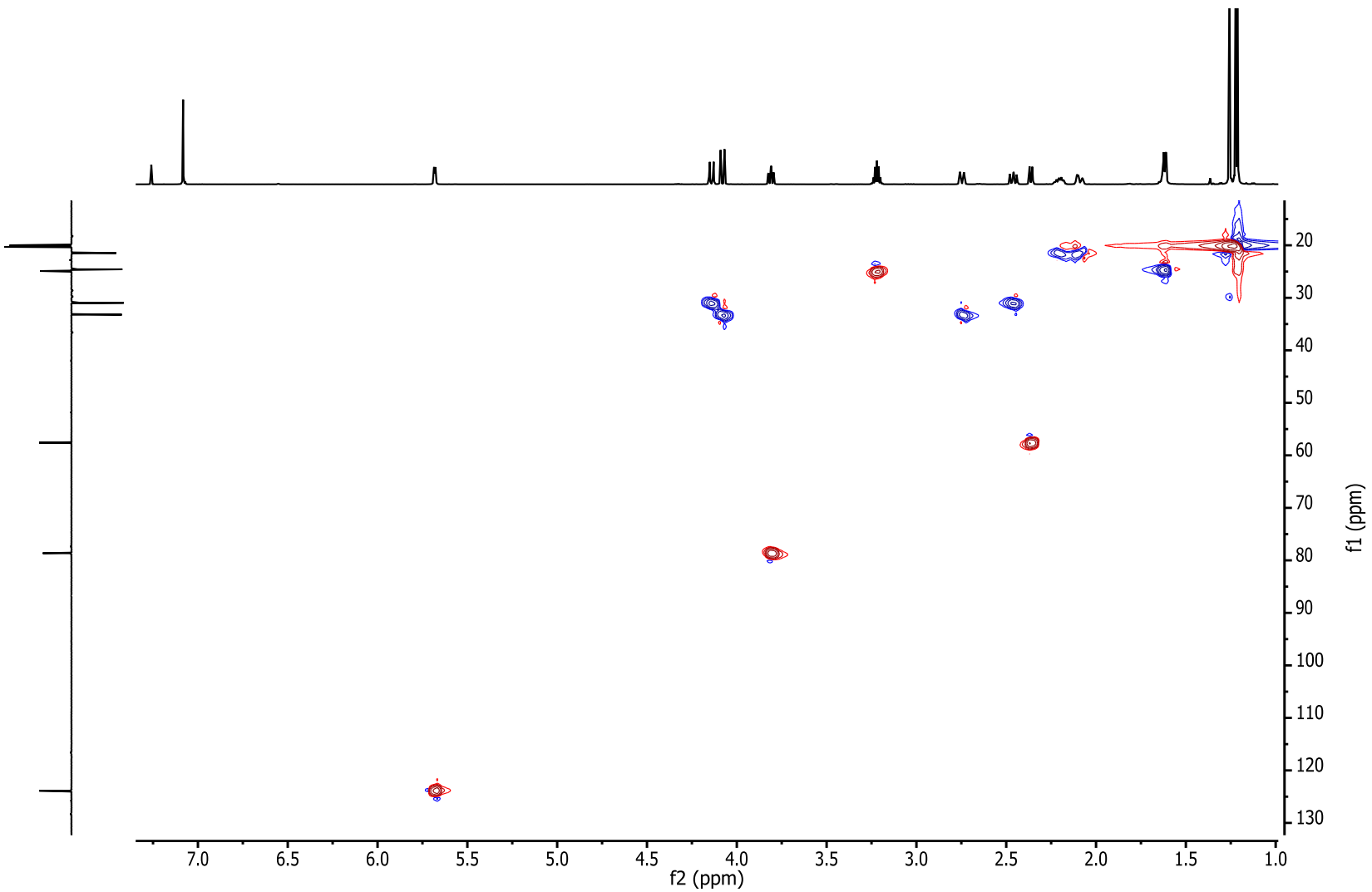


Figure S41. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **7**

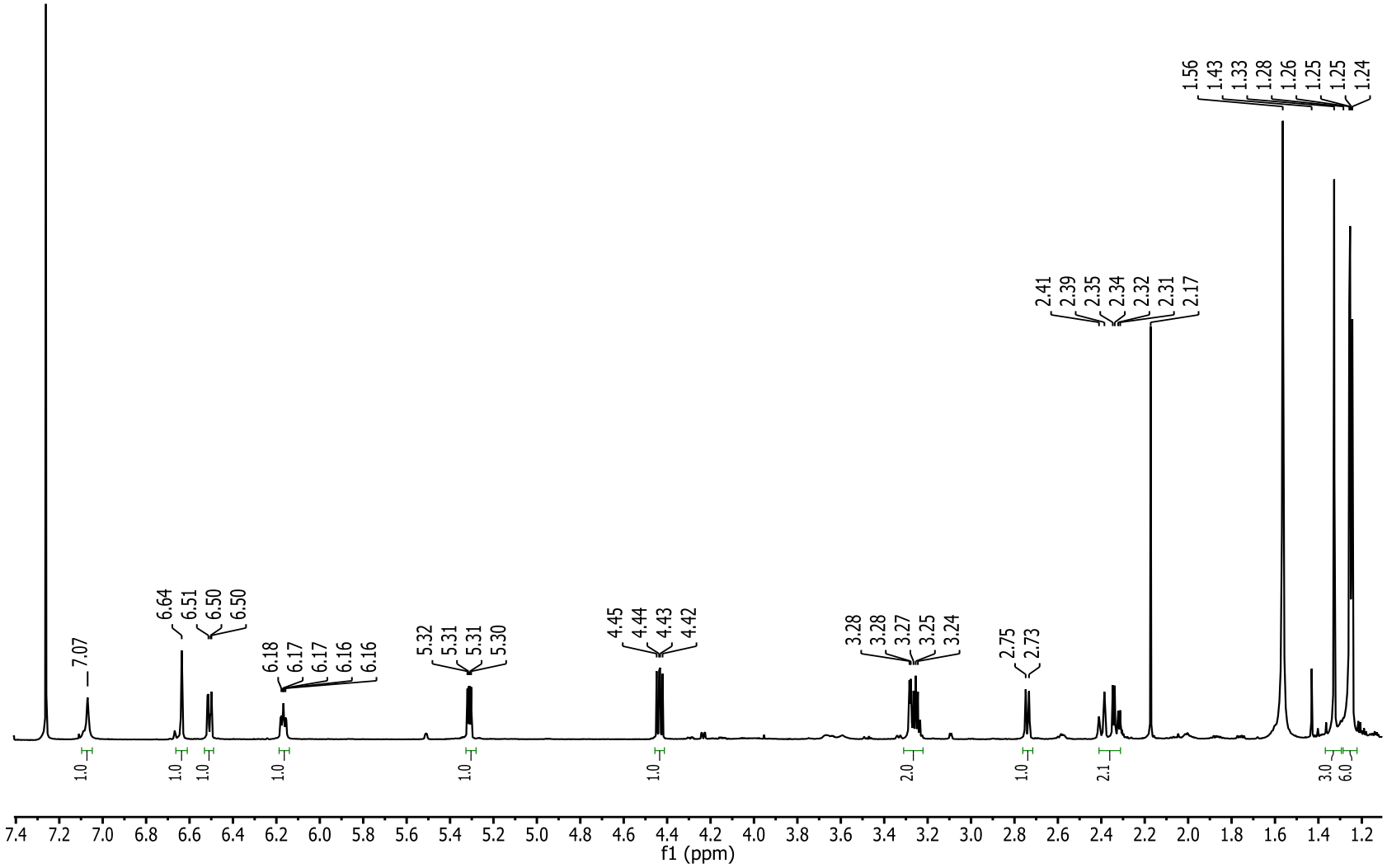


Figure S42. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **9**

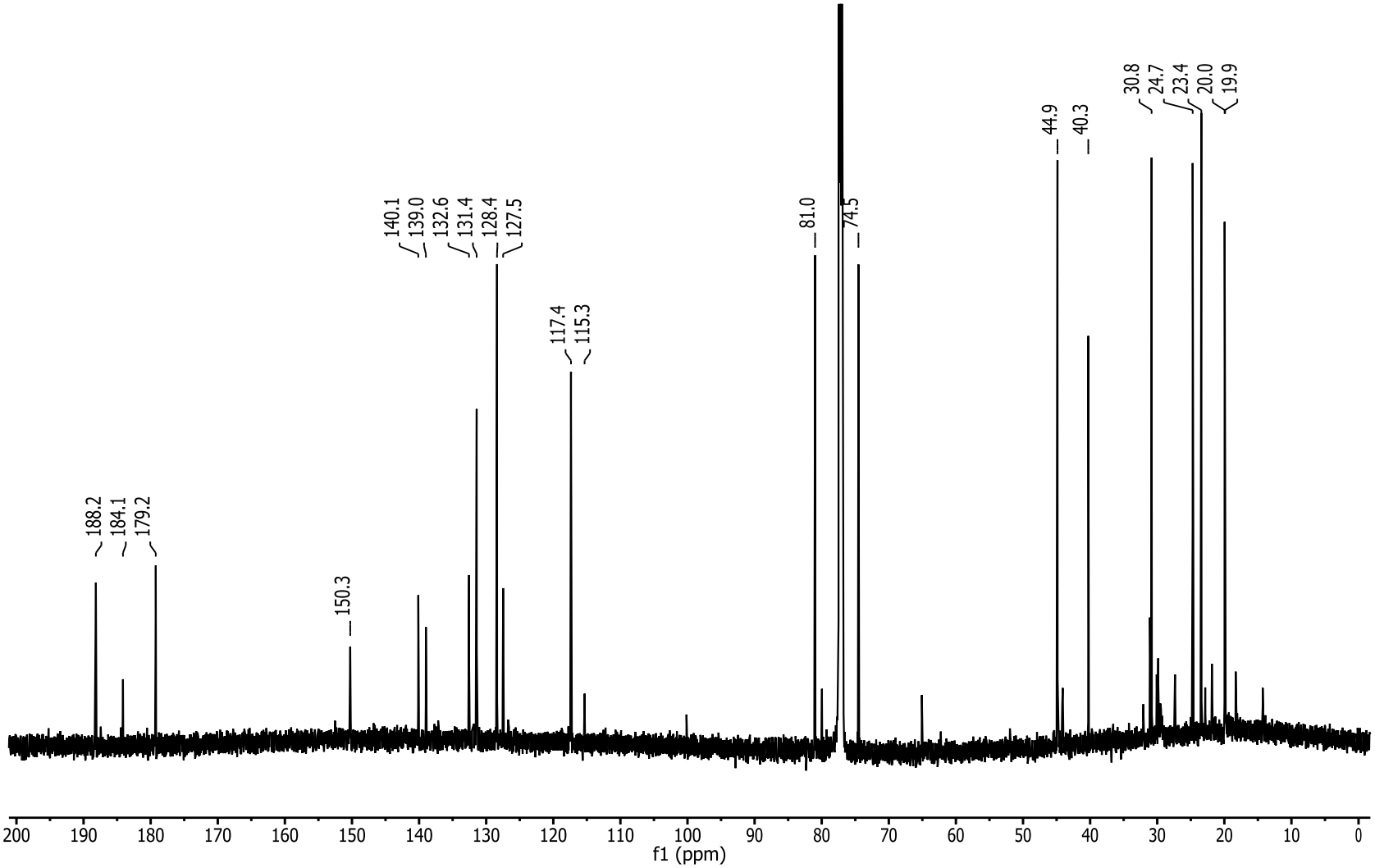


Figure S43. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **9**

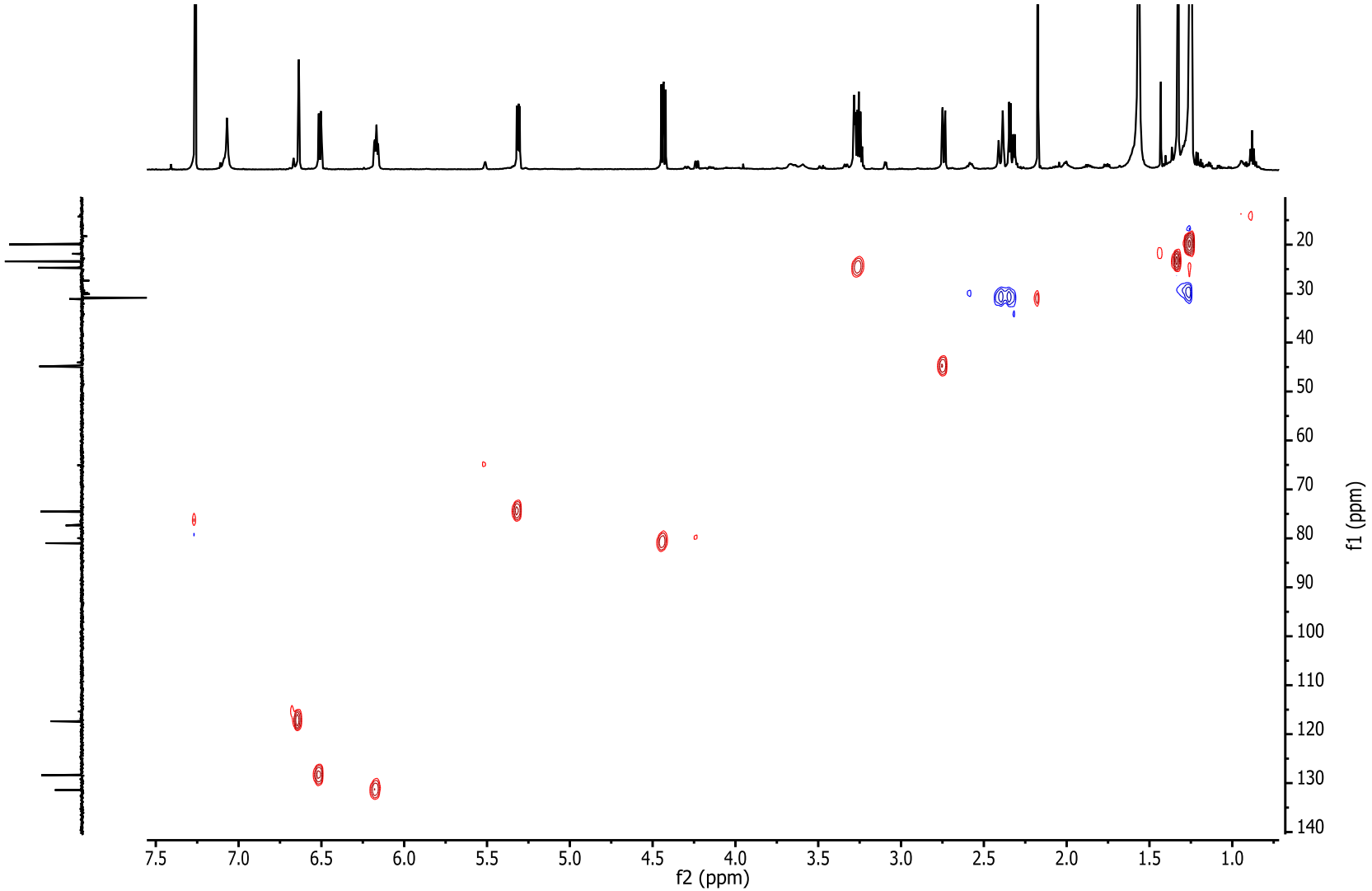


Figure S44. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **9**

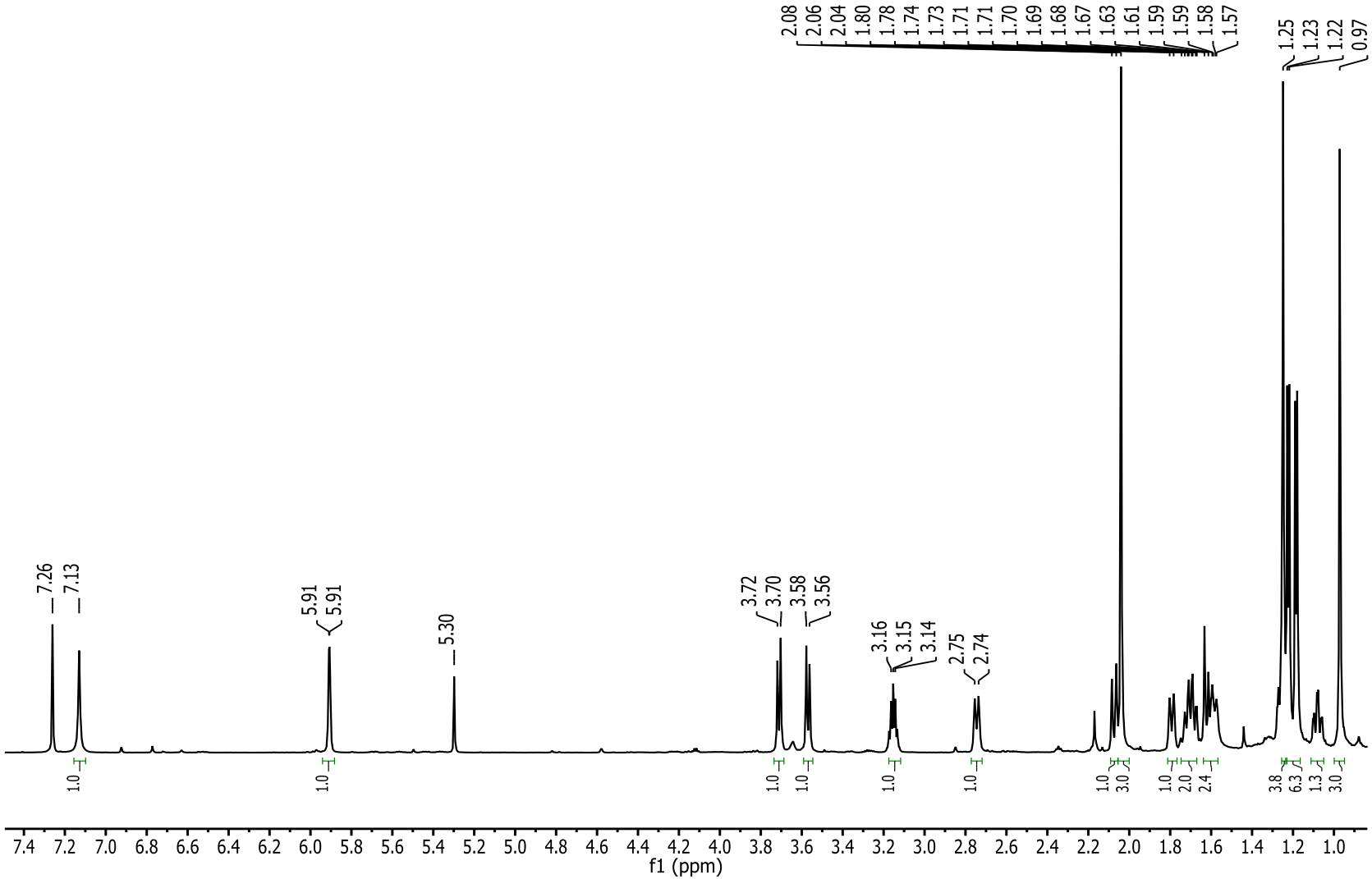


Figure S45. ^{1}H NMR ($CDCl_3$, 700 MHz) spectrum of **11**

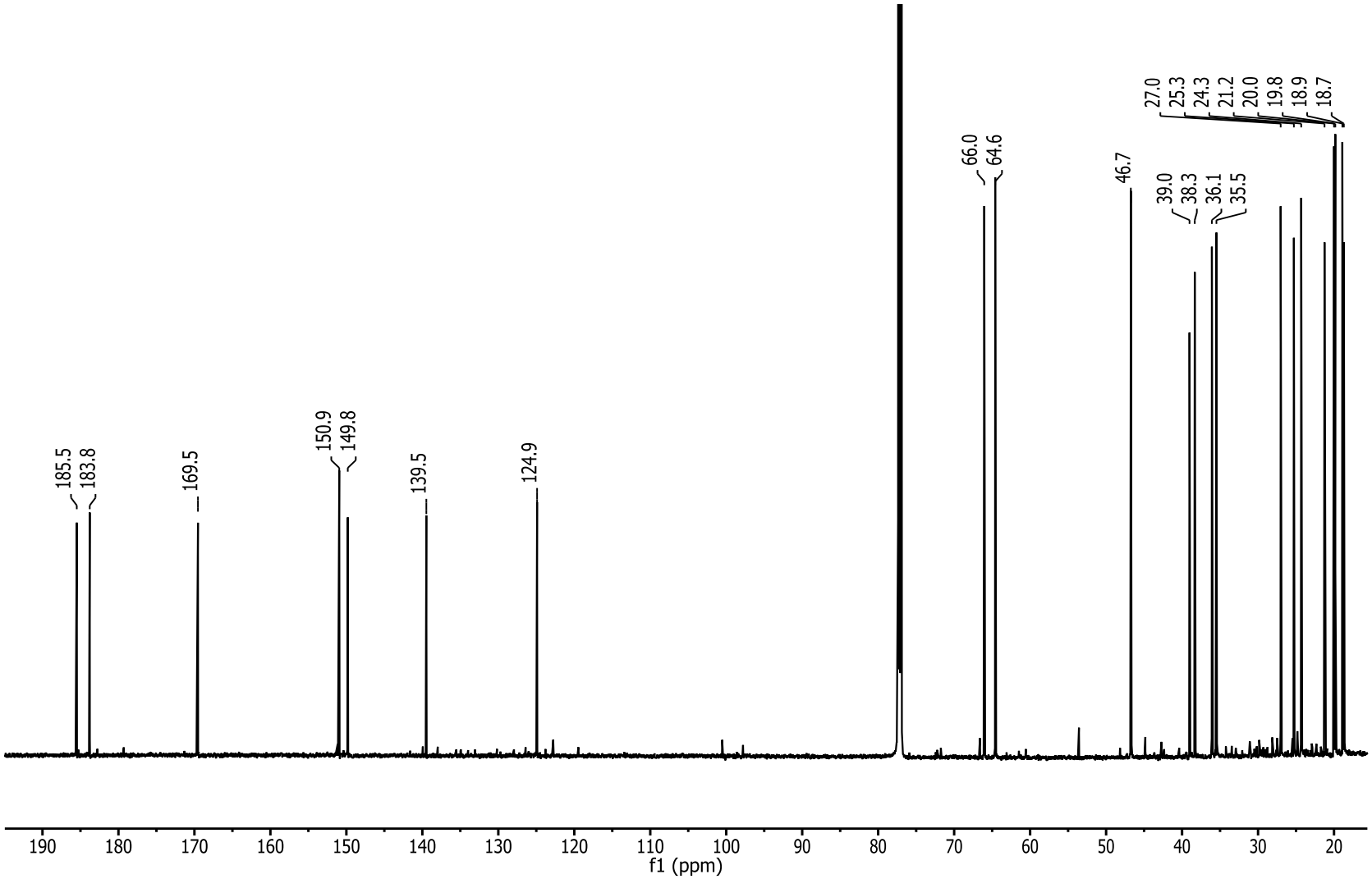


Figure S46. ^{13}C NMR ($CDCl_3$, 175 MHz) spectrum of **11**

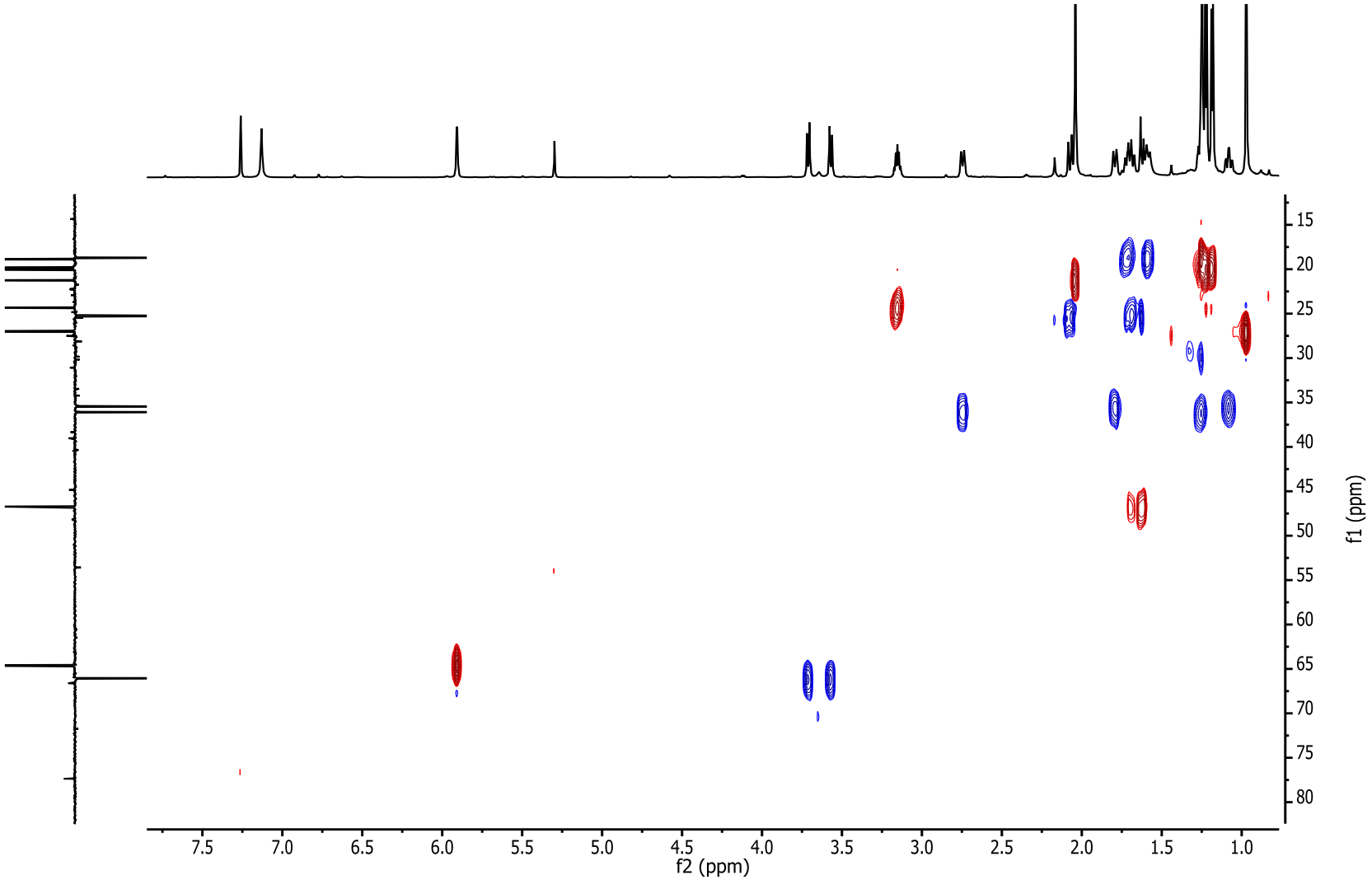


Figure S47. HSQC NMR ($CDCl_3$, 700 MHz) spectrum of **11**

Primary screening of compounds **3**, **4**, **6** - **8**, **10** on antiproliferative activity at concentration of 50.0 μM.

Compound	Antiproliferative activity (%)						
	U251	PC-3	K562	HCT-15	MCF-7	SKLU-1	FGH
3*	**65.4**	34.2	48.6	33.4	NC	**64.5**	**12.4**
4	100	80.3	100	76.7	99.0	96.9	87.0
6*	**98.4**	82.3	76.4	85.6	51.3	**100**	**46.5**
7	10.1	17.8	**63.2**	26.8	**62.6**	46.5	**NC**
8	35.8	39.6	**83.1**	29.0	**71.6**	52.9	**NC**
10	NC	NC	NC	NC	14.7	11.8	NT
Adriamicyn 0.5 μM	96.0	85.2	100	86.9	99.1	90.0	53.4

Results are represented as the mean (n = 2); U251 = human glioblastoma; PC-3 = human prostate cancer; K562 = human chronic myelogenous leukemia; HCT-15 = human colon cancer; MCF-7 = human mammary adenocarcinoma; SKLU-1 = human lung adenocarcinoma; FGH = gingival human fibroblasts; NC = No cytotoxic. NT = No tested; *Compounds tested at 1.0 μM.

Figure S48. Primary screening of compounds **3**, **4**, **6** - **8**, **10** on antiproliferative activity at concentration of 50.0 μM.