An Anti-inflammatory 2,4-Cyclized-3,4-Secospongian Diterpenoid and Furanoterpene-related Metabolites of a Marine Sponge *Spongia* sp. from the Red Sea

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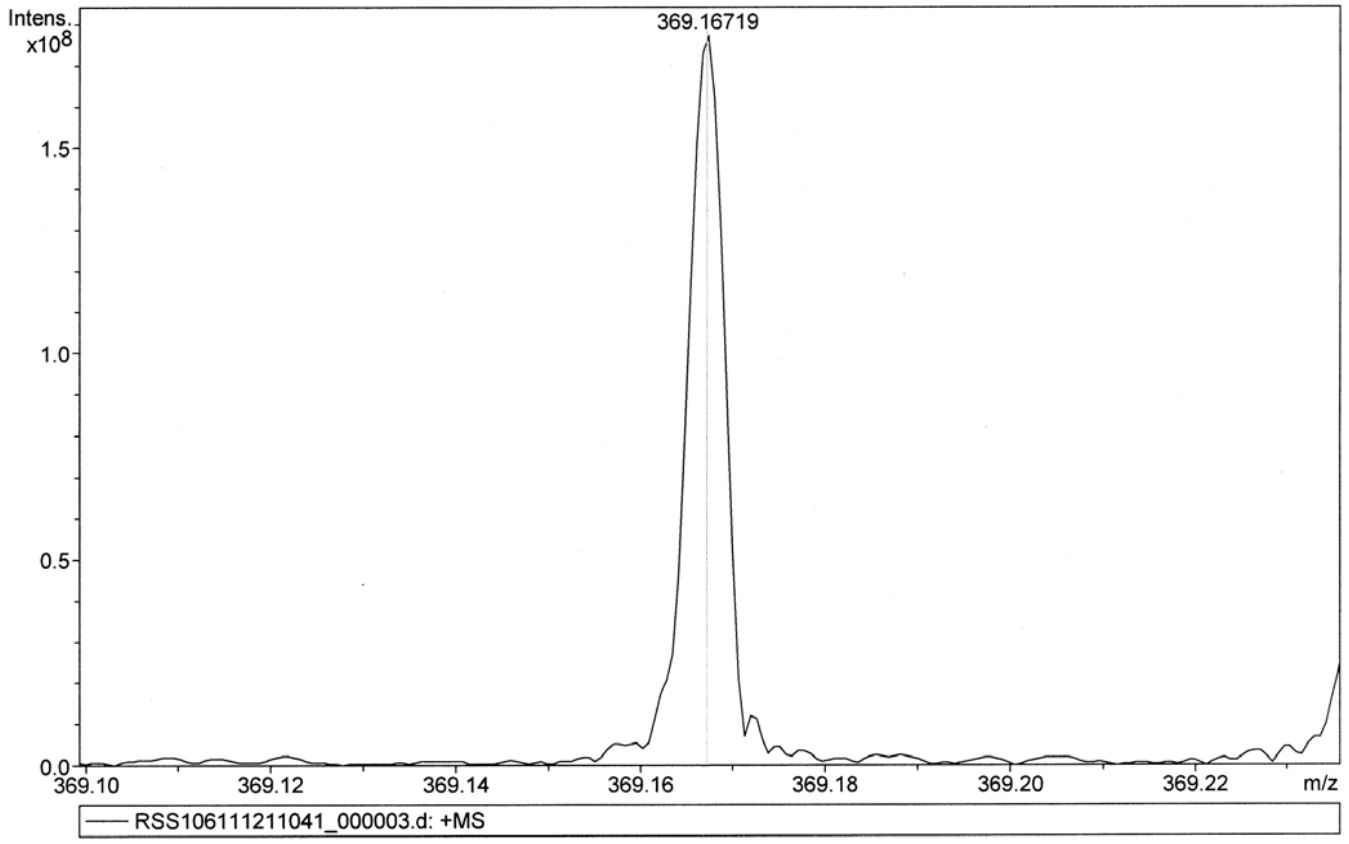

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Figure S1. HRESIMS spectrum of compound **1**.

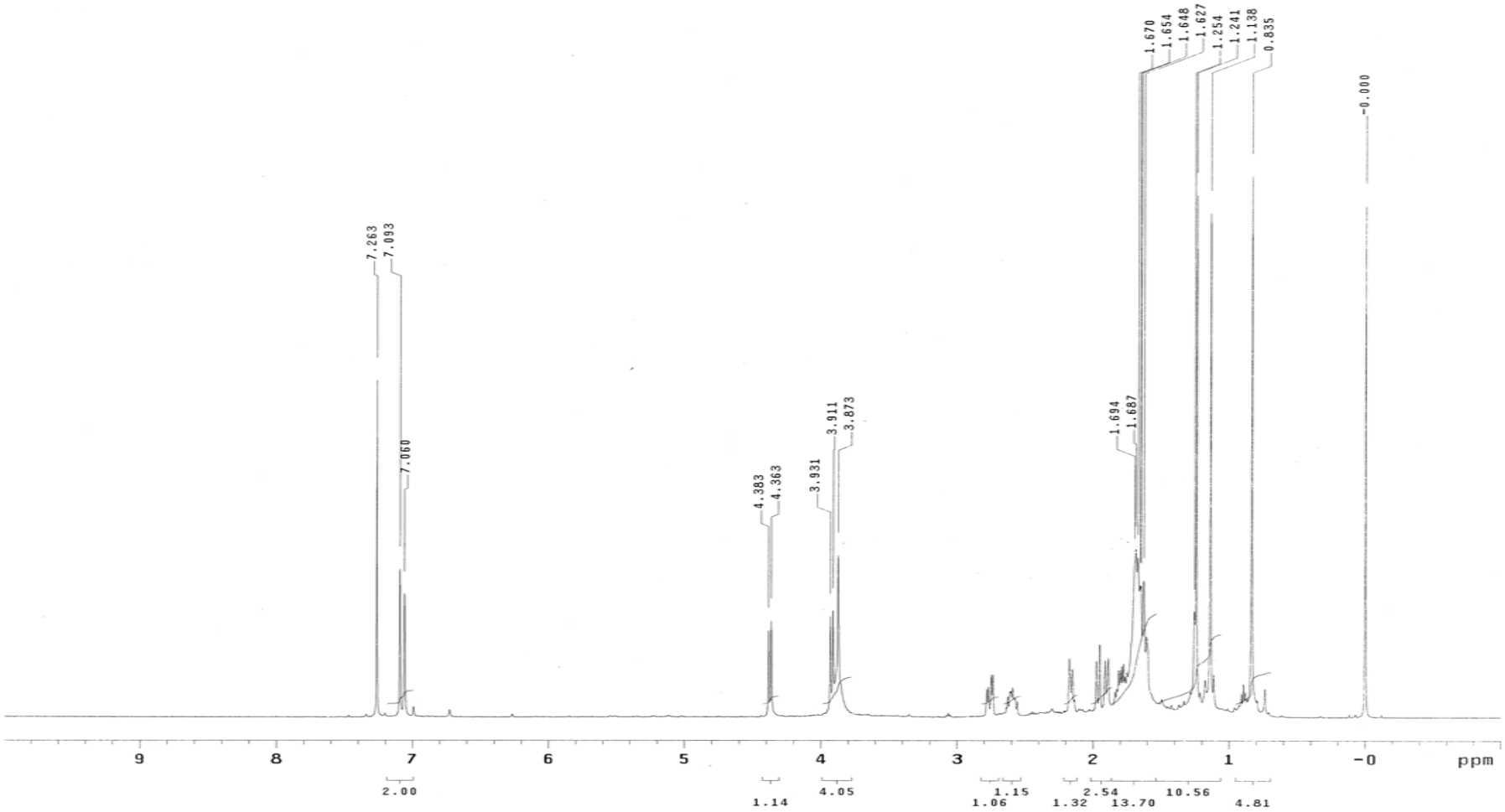


Figure S2. ^{1}H NMR spectrum (500 MHz) of compound **1** in $CDCl_3$.

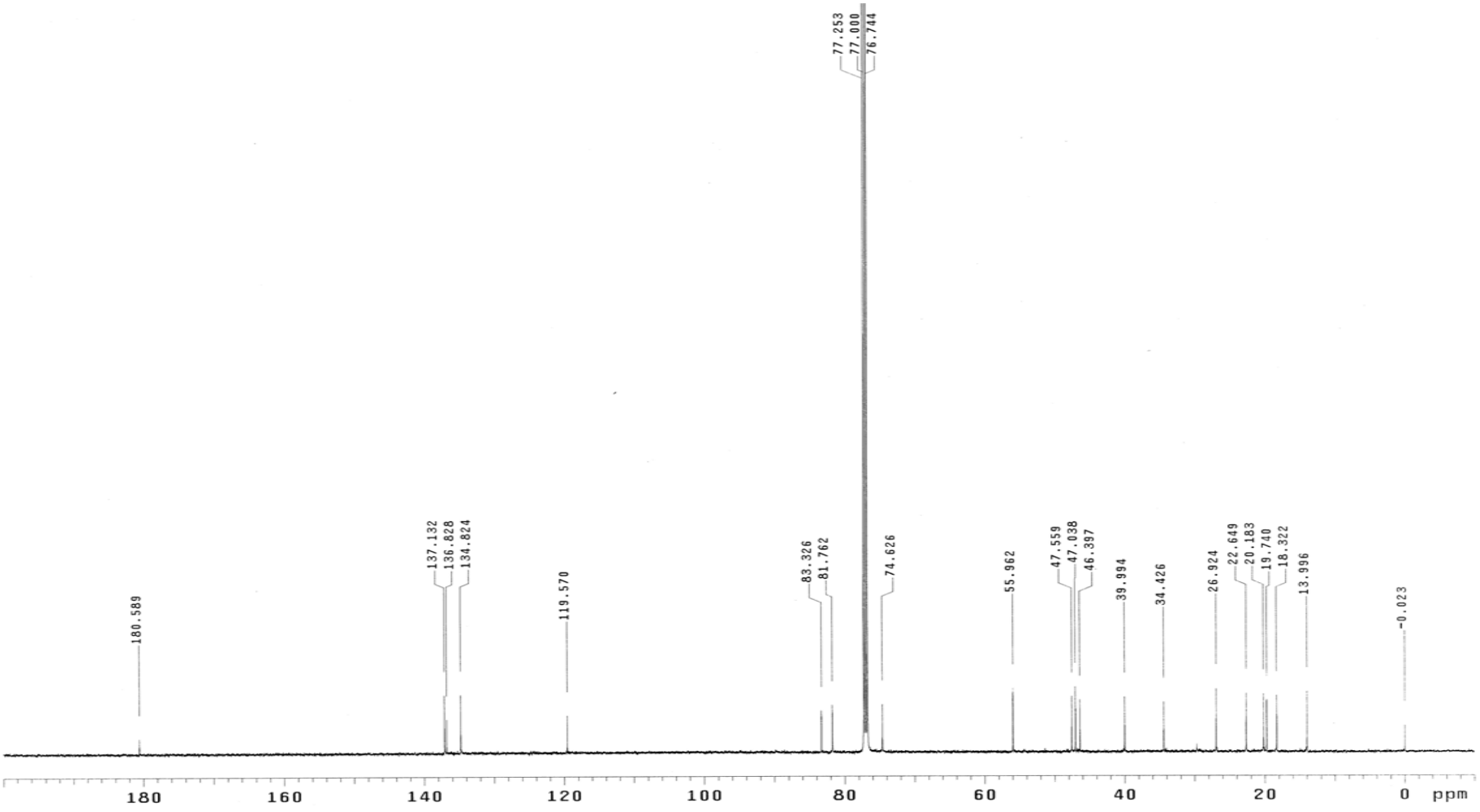


Figure S3. ^{13}C NMR spectrum (125 MHz) of compound **1** in $CDCl_3$.

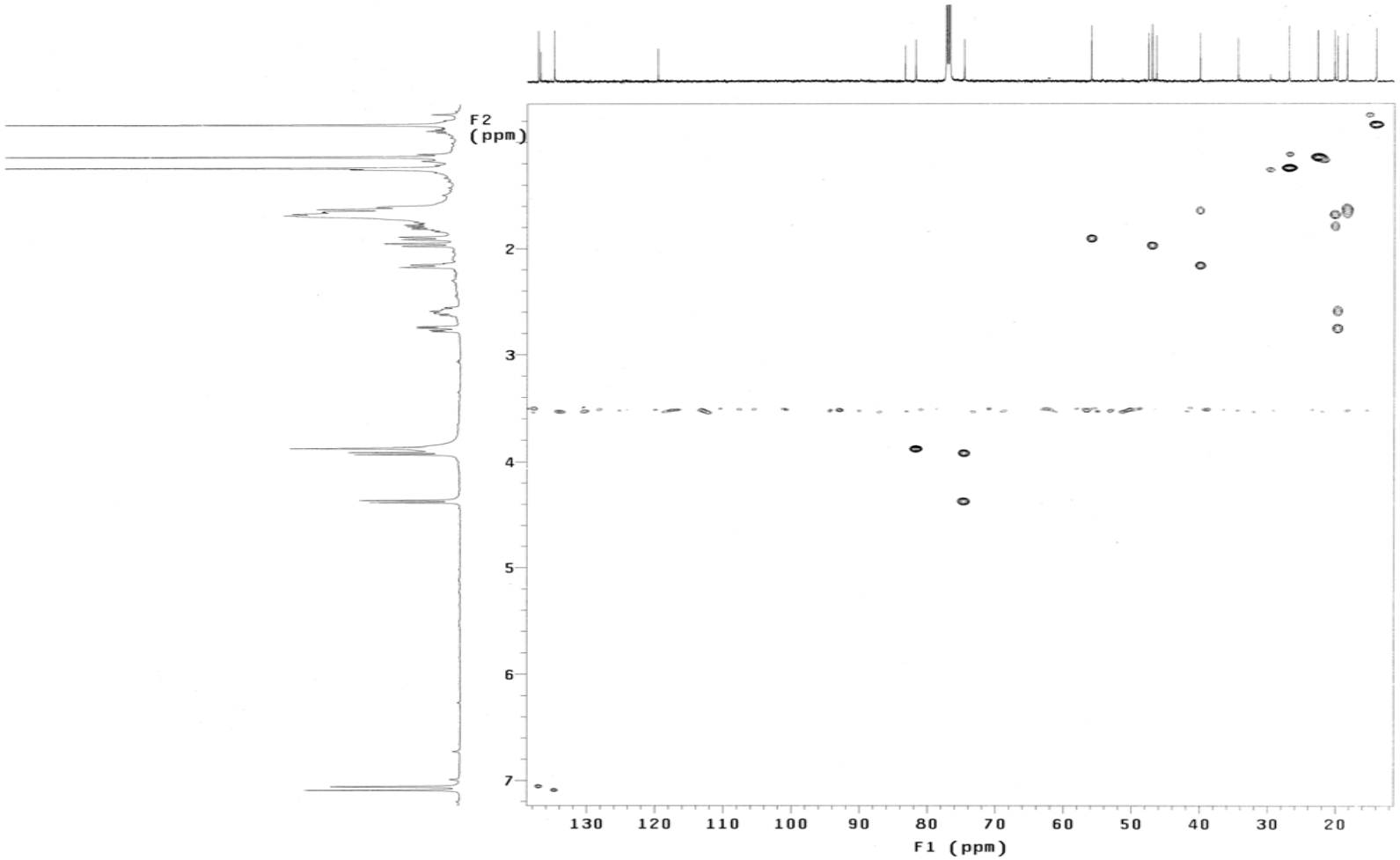


Figure S4. HSQC spectrum of **1** in $CDCl_3$.

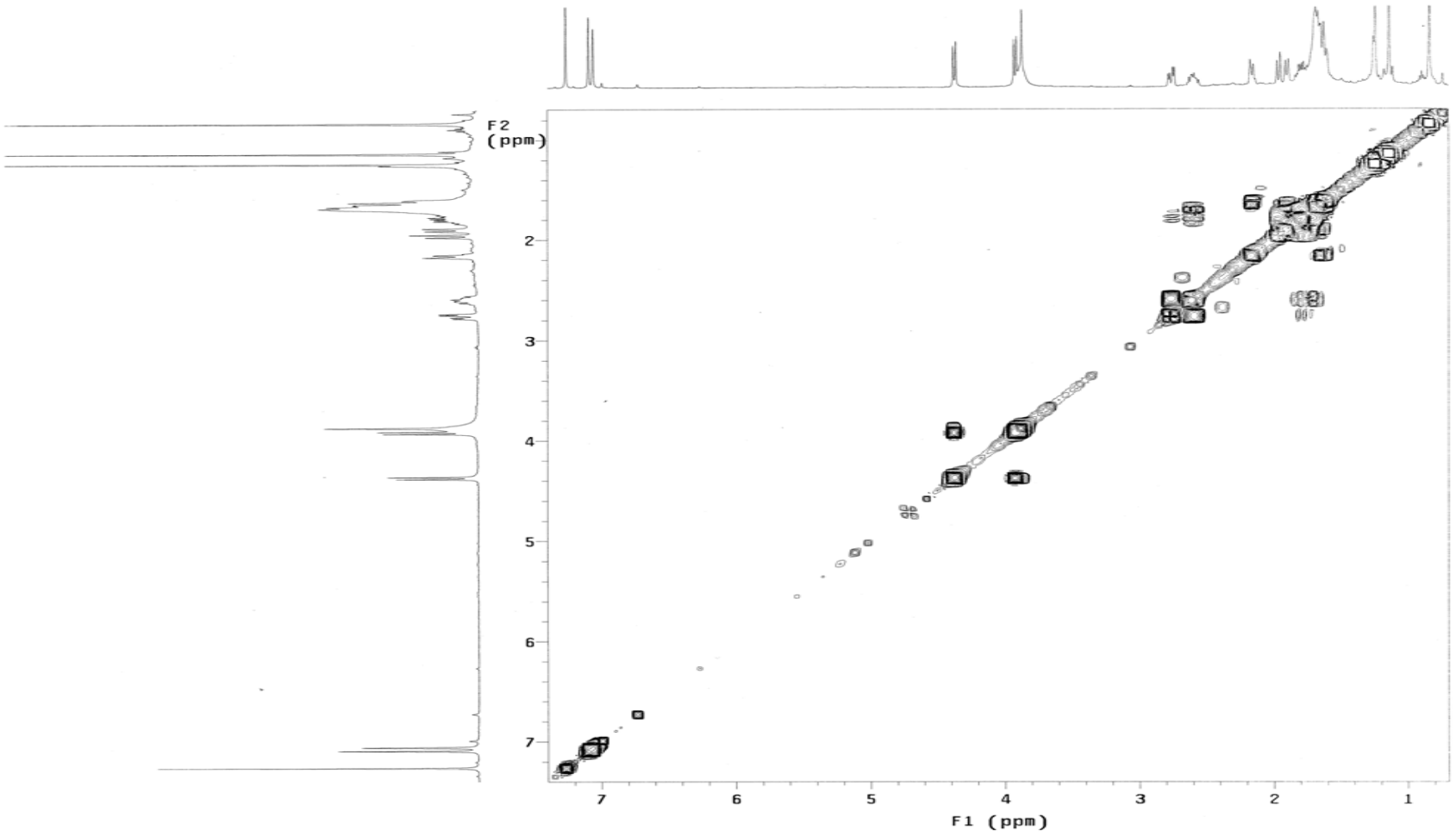


Figure S5. ^{1}H -^{1}H COSY spectrum of **1** in $CDCl_3$.

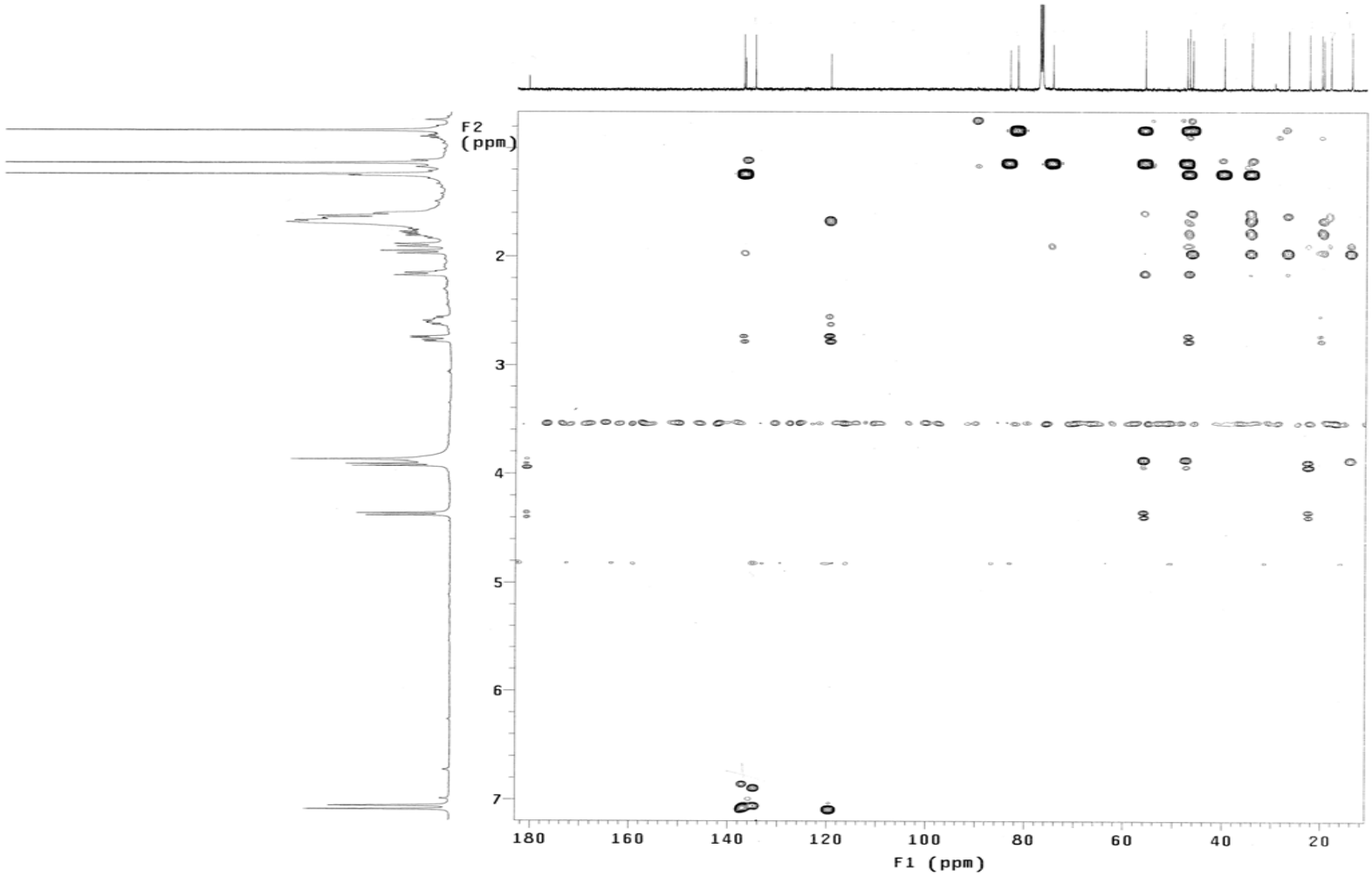


Figure S6. HMBC spectrum of **1** in $CDCl_3$.

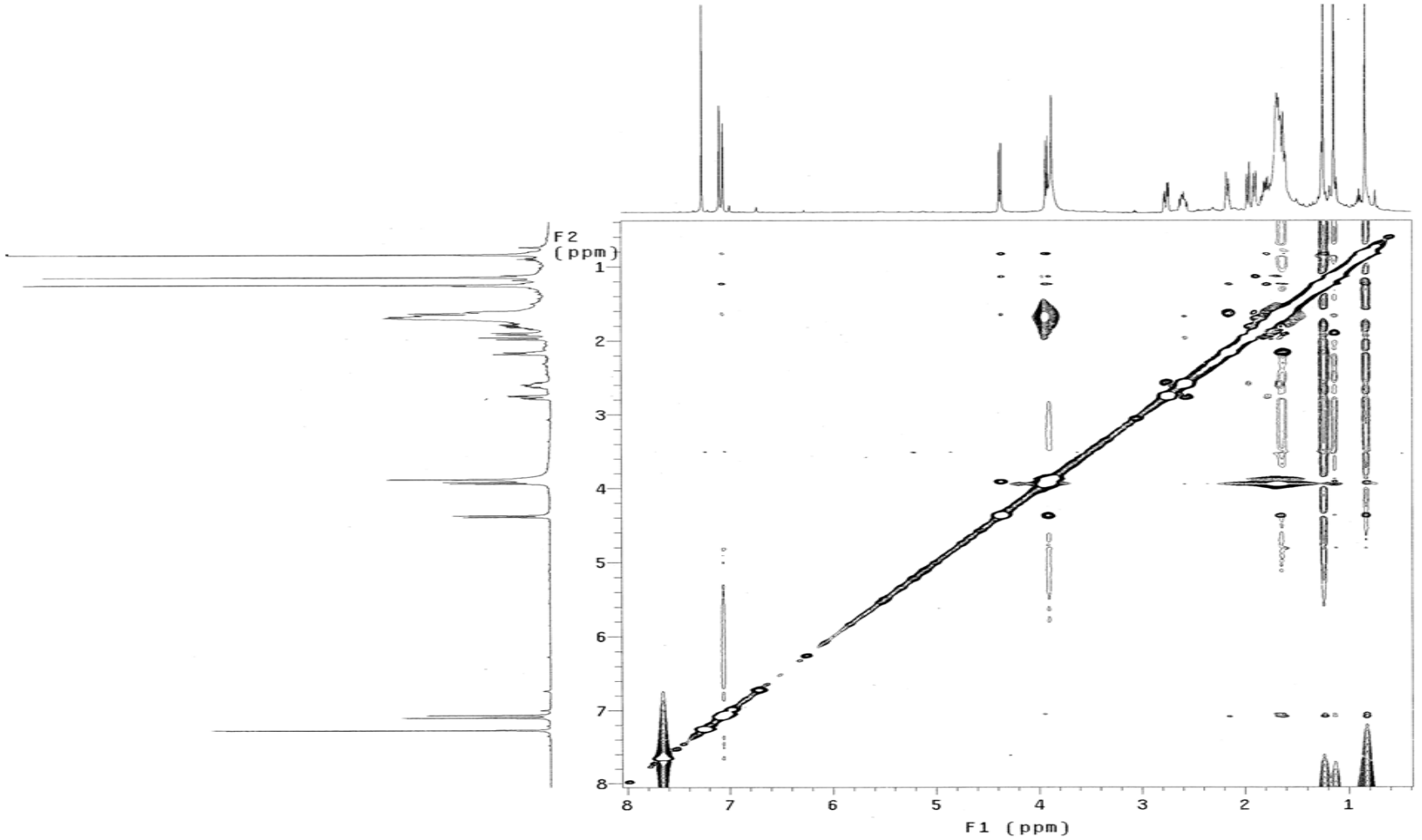
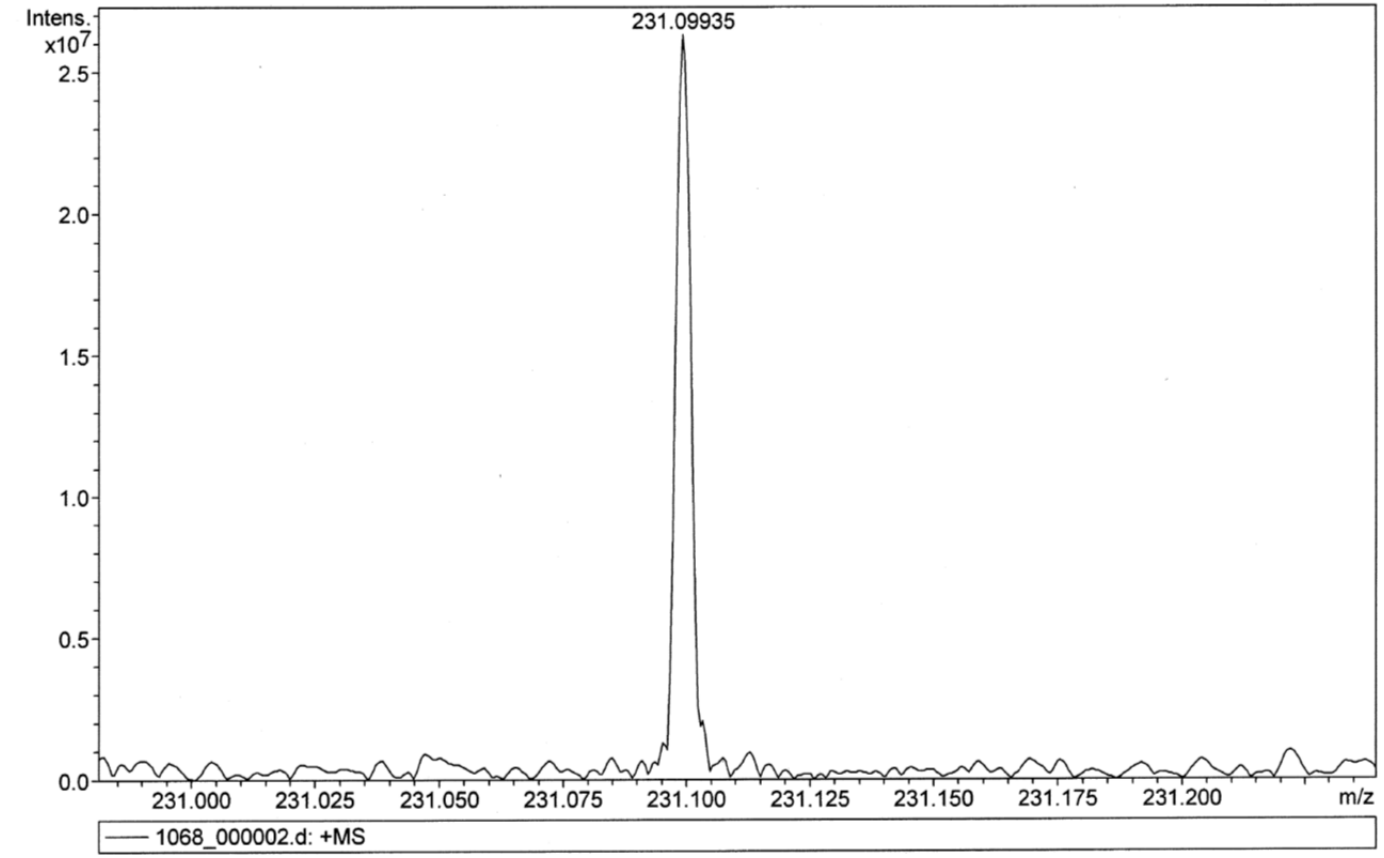


Figure S7. NOESY spectrum of **1** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
231.09935	1	C 12 H 16 Na O 3	100.00	231.09917	-0.18	-0.80	9.1	4.5	even	ok

Figure S8. HRESIMS spectrum of **2**.

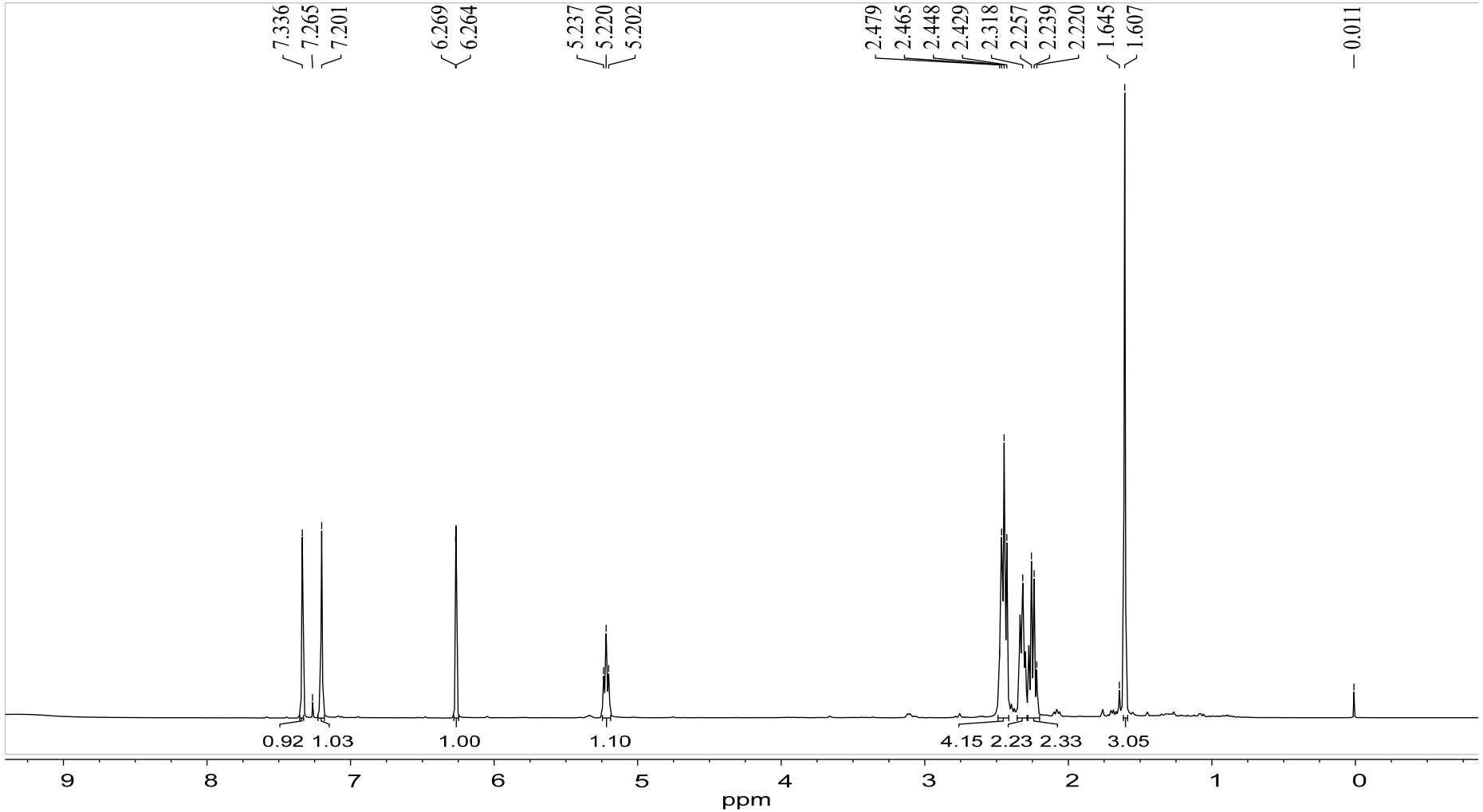


Figure S9. ^{1}H NMR spectrum (400 MHz) of compound **2** in $CDCl_3$.

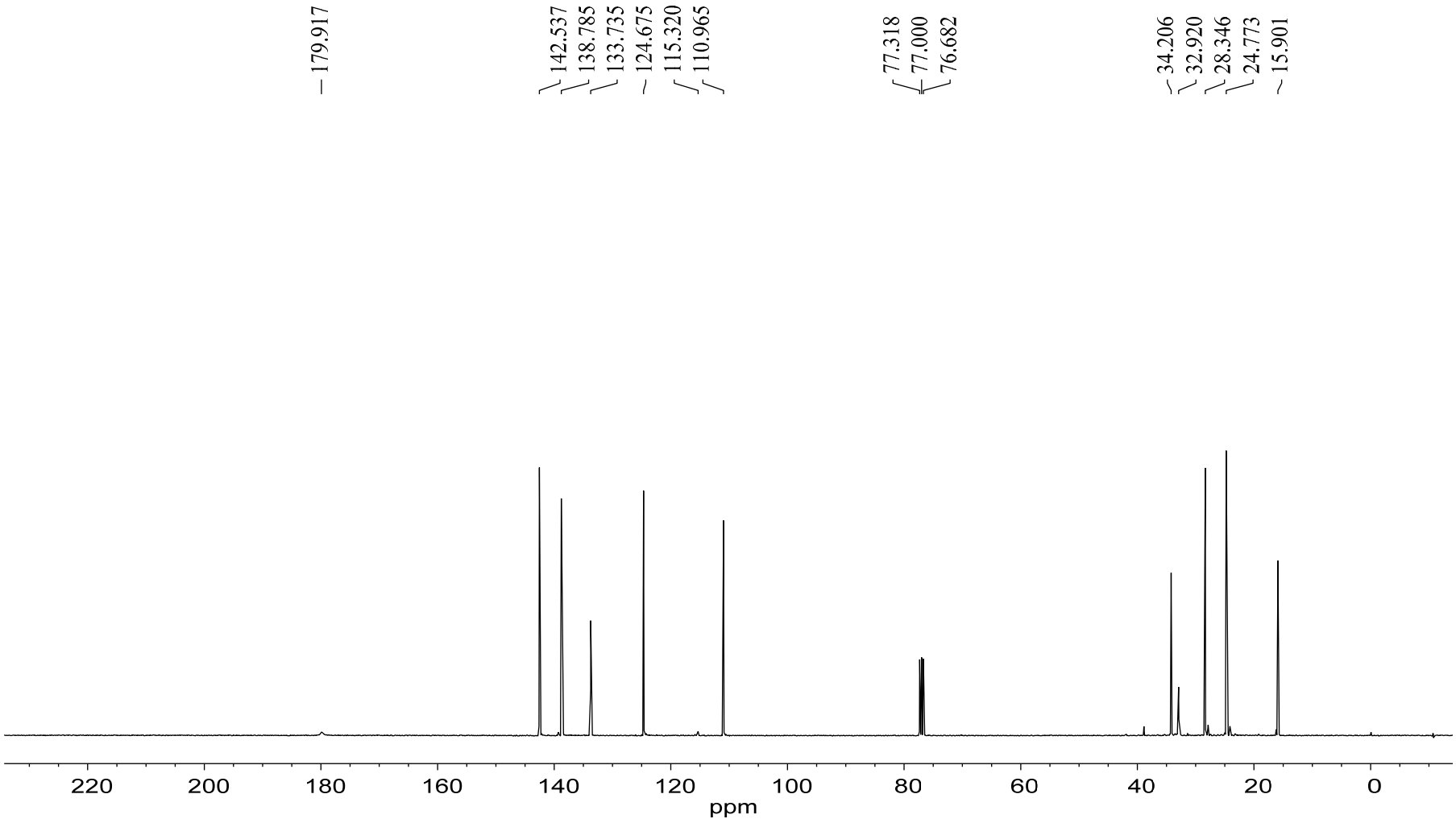


Figure S10. ^{13}C NMR spectrum (100 MHz) of compound **2** in $CDCl_3$.

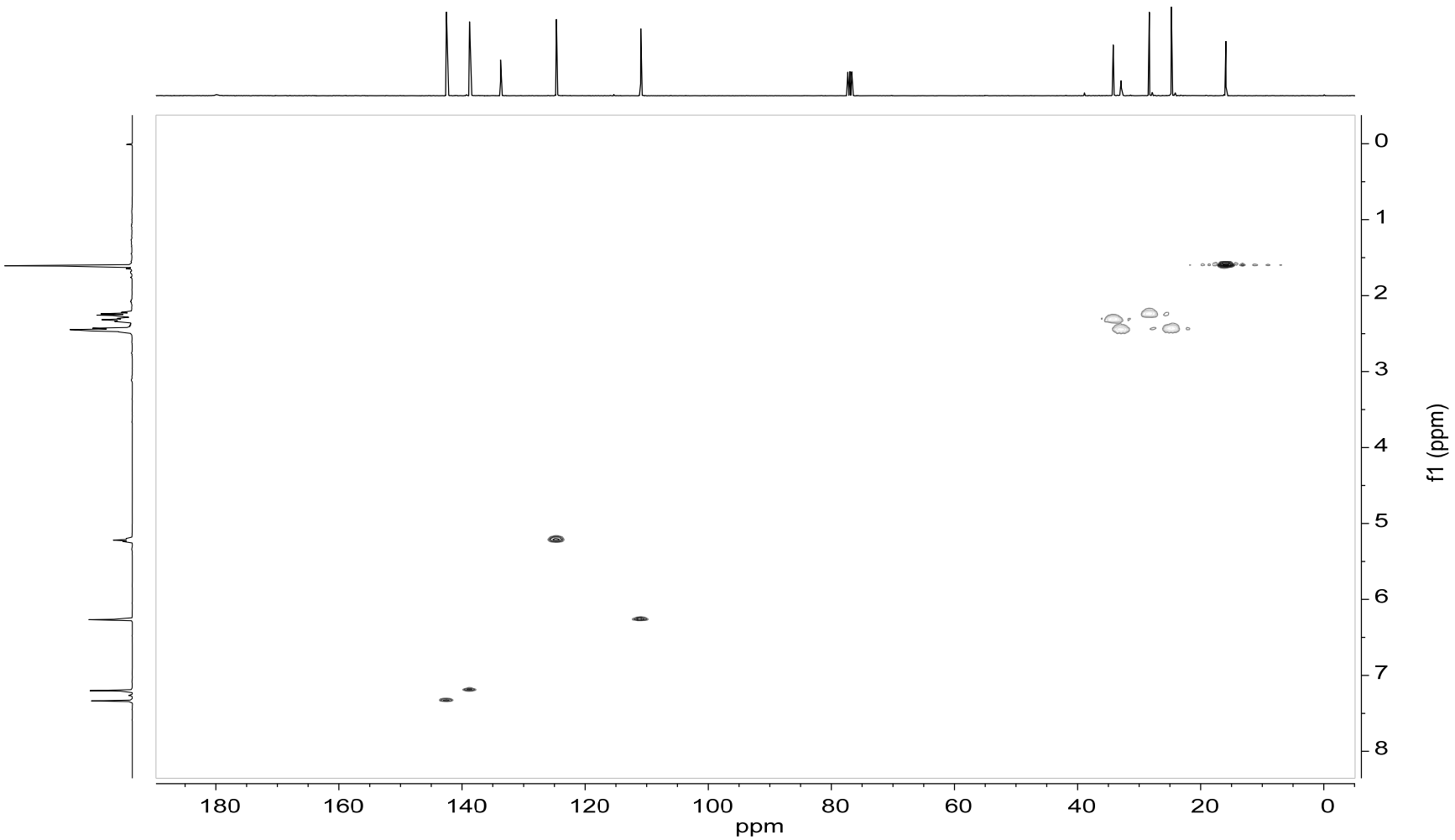


Figure S11. HSQC spectrum of **2** in $CDCl_3$.

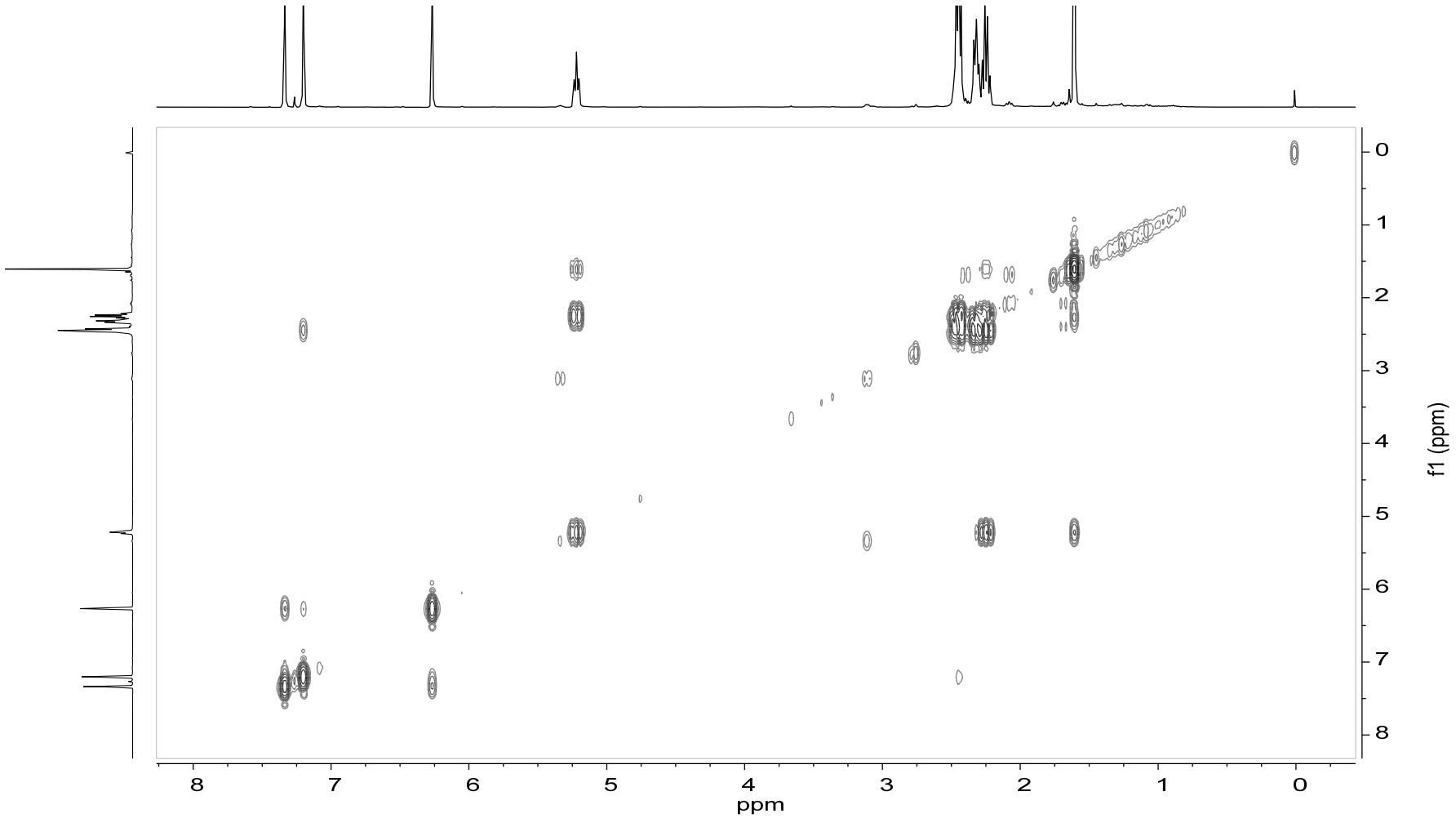


Figure S12. ^{1}H -^{1}H COSY spectrum of **2** in $CDCl_3$.

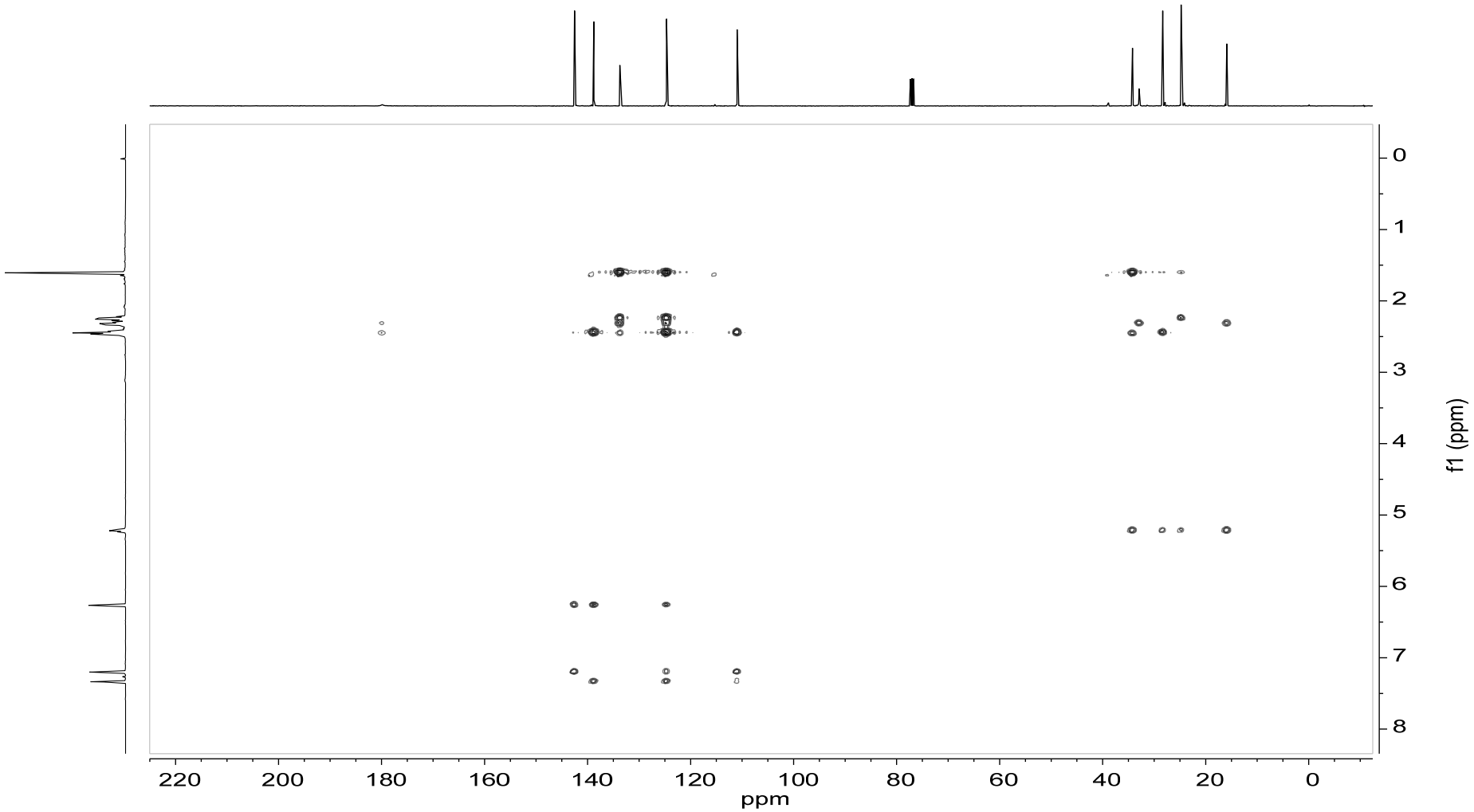


Figure S13. HMBC spectrum of **2** in $CDCl_3$.

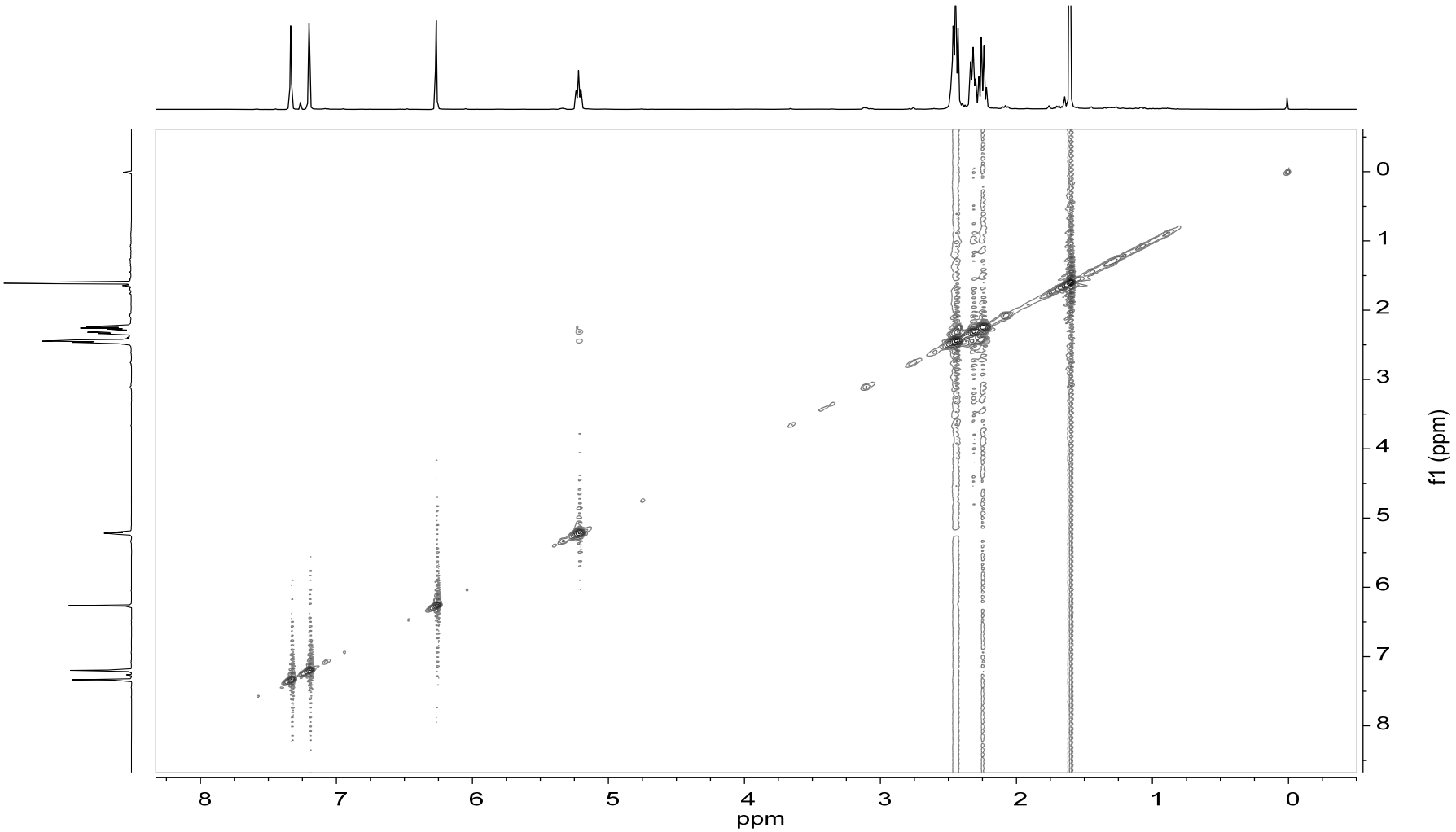
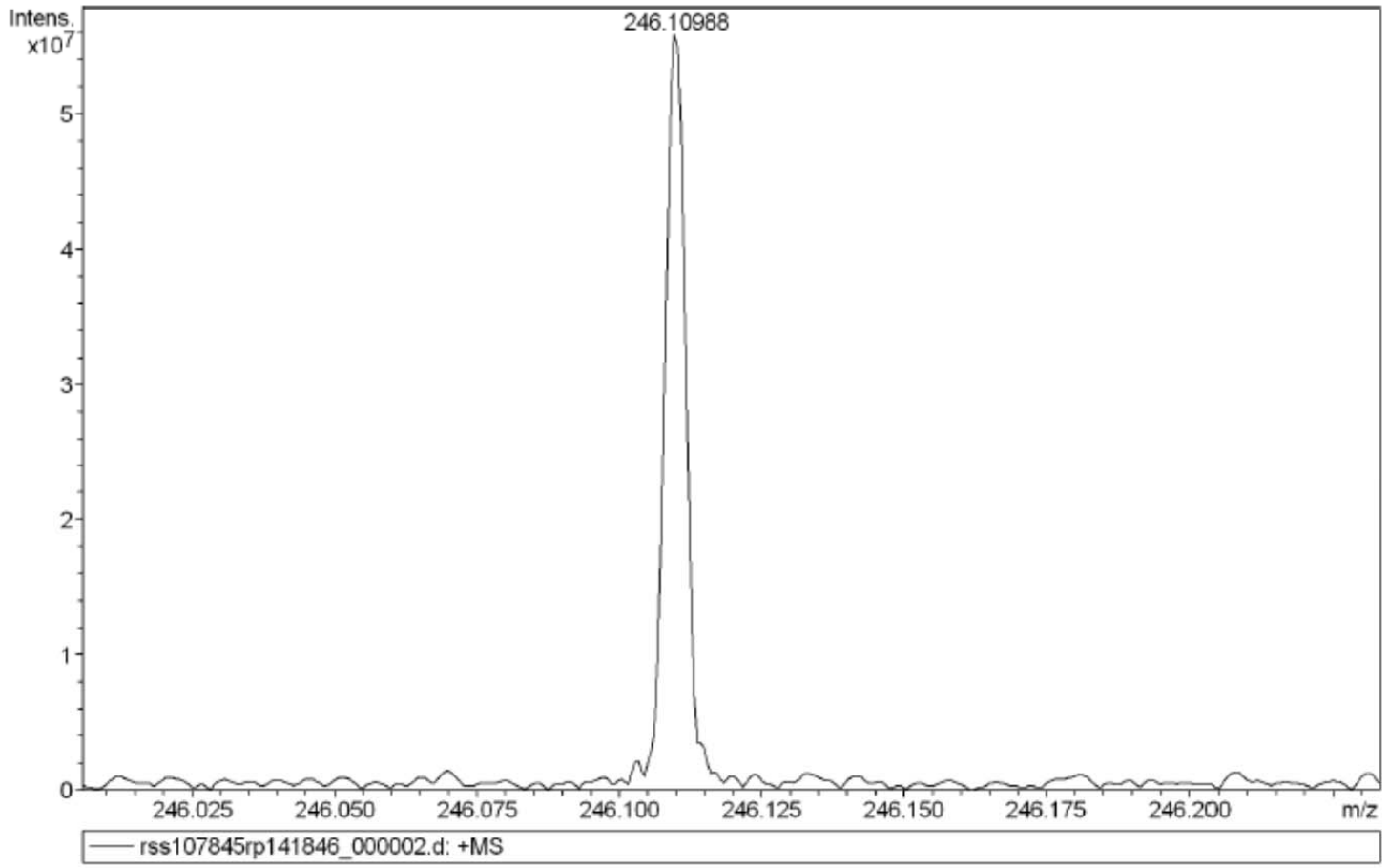


Figure S14. NOESY spectrum of **2** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
246.10988	1	C 12 H 17 N Na O 3	100.00	246.11006	0.18	0.74	12.1	4.5	even	ok

Figure S15. HRESIMS spectrum of compound **3**.

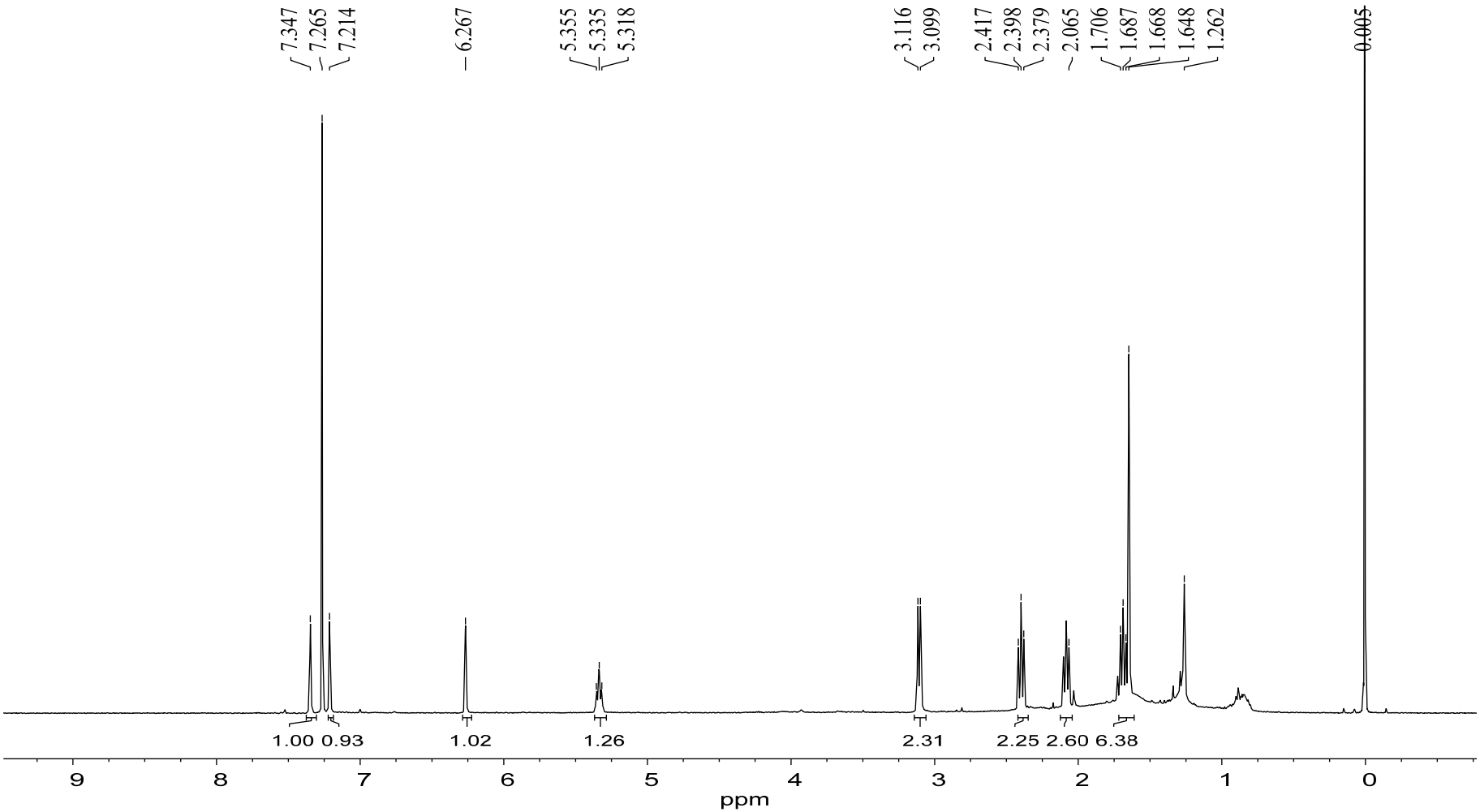


Figure S16. ^{1}H NMR spectrum (400 MHz) of compound **3** in $CDCl_3$.

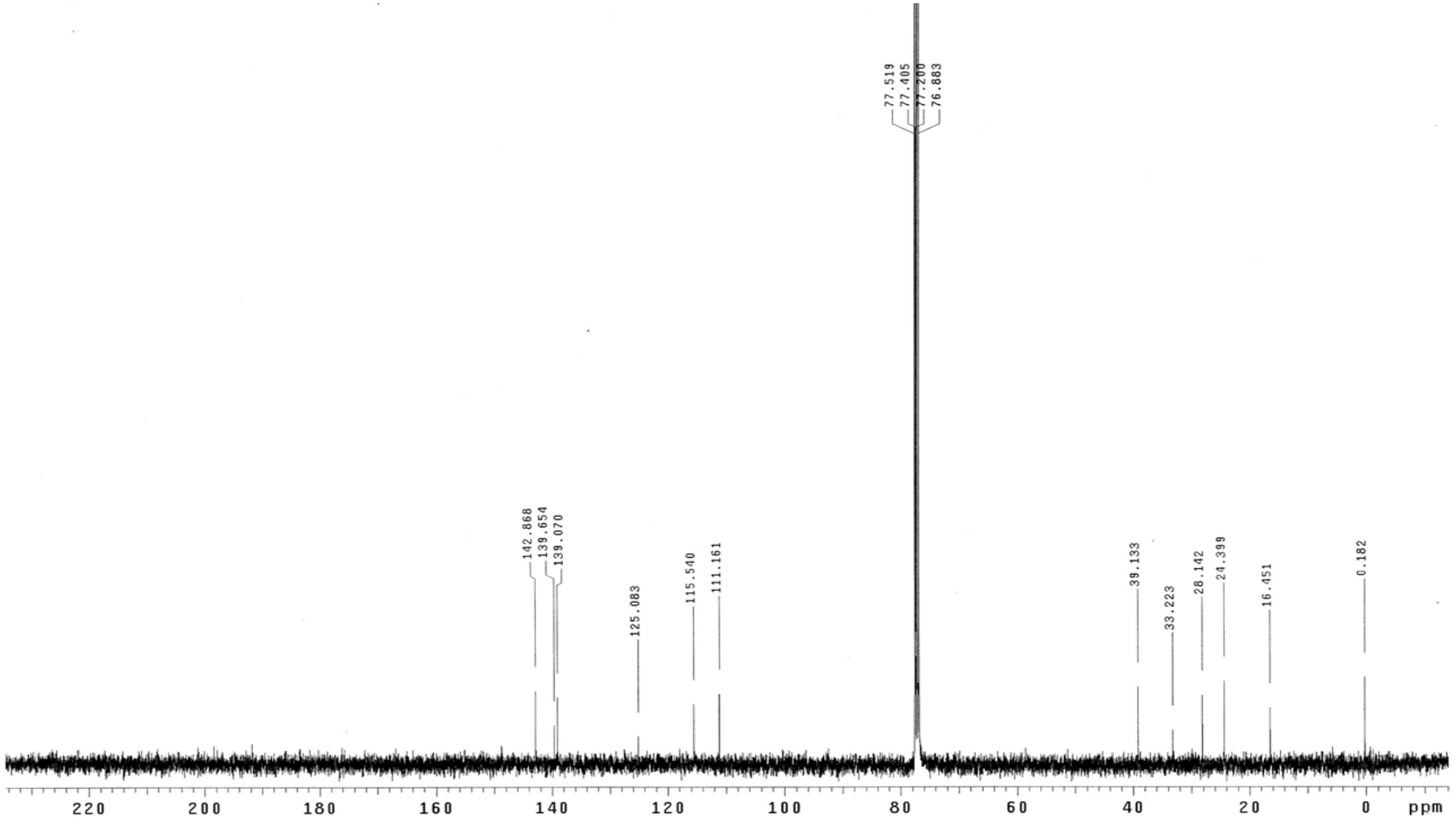


Figure S17. ^{13}C NMR spectrum (100 MHz) of compound **3** in $CDCl_3$.

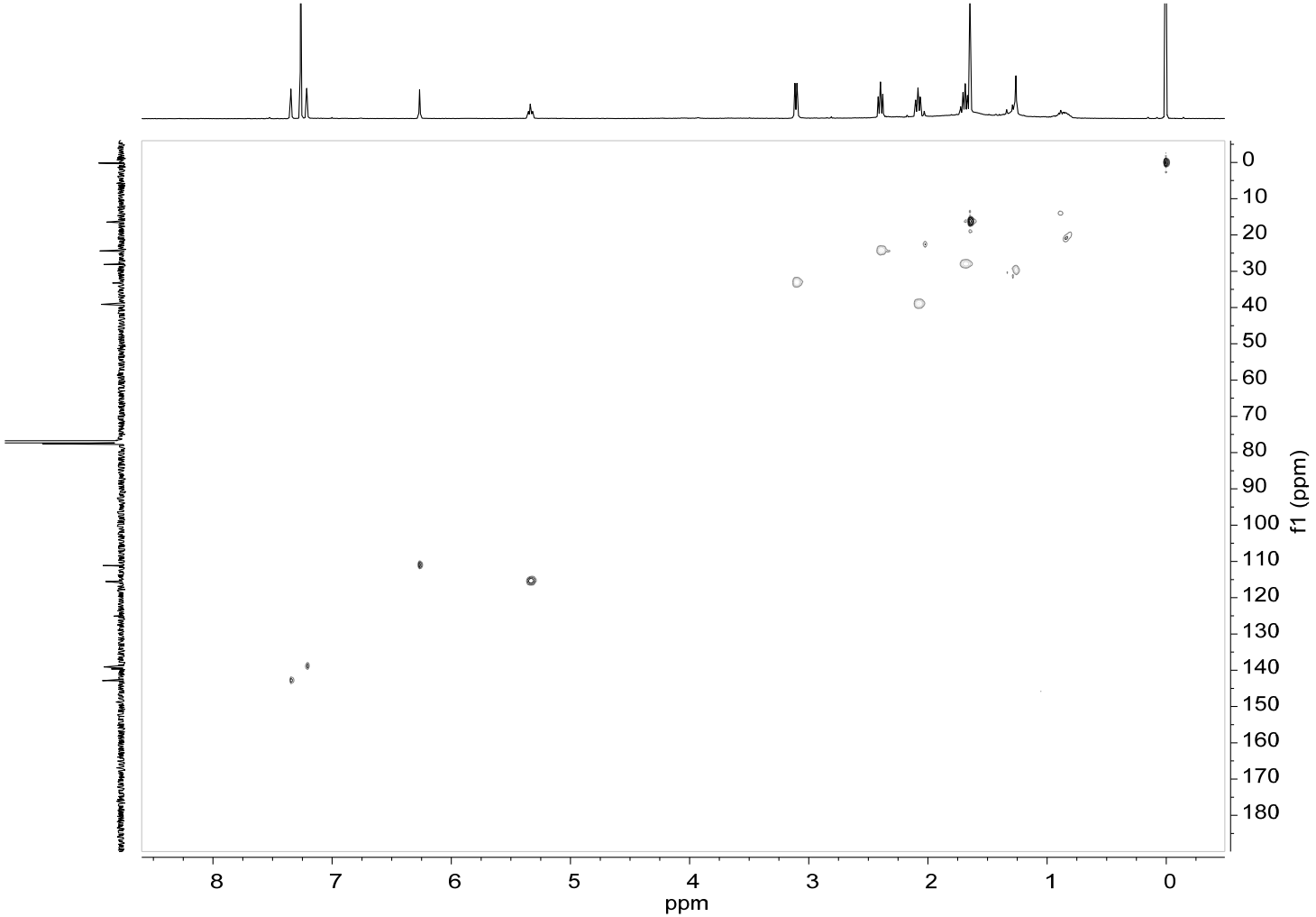


Figure S18. HSQC spectrum of **3** in $CDCl_3$.

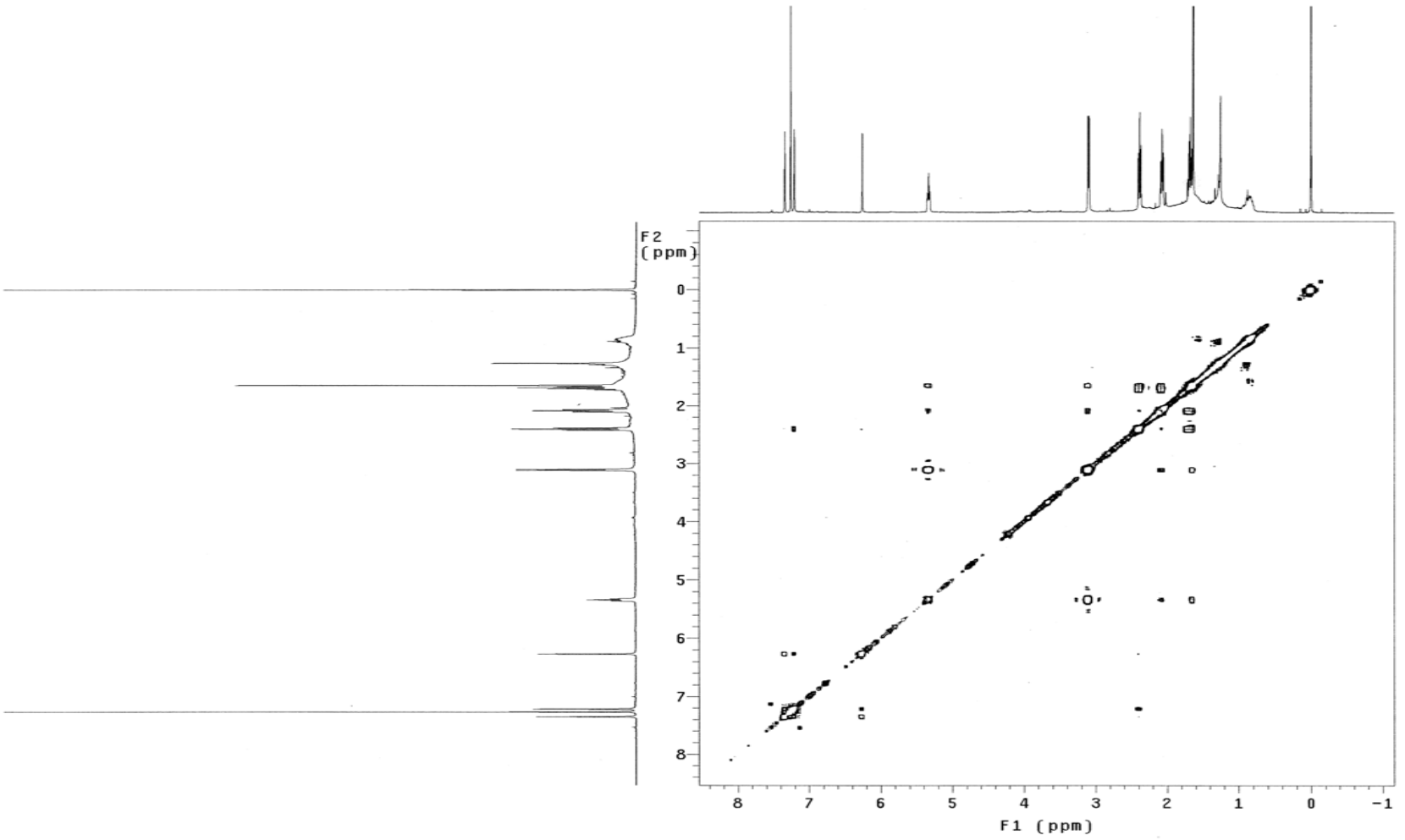


Figure S19. ^{1}H -^{1}H COSY spectrum of **3** in $CDCl_3$.

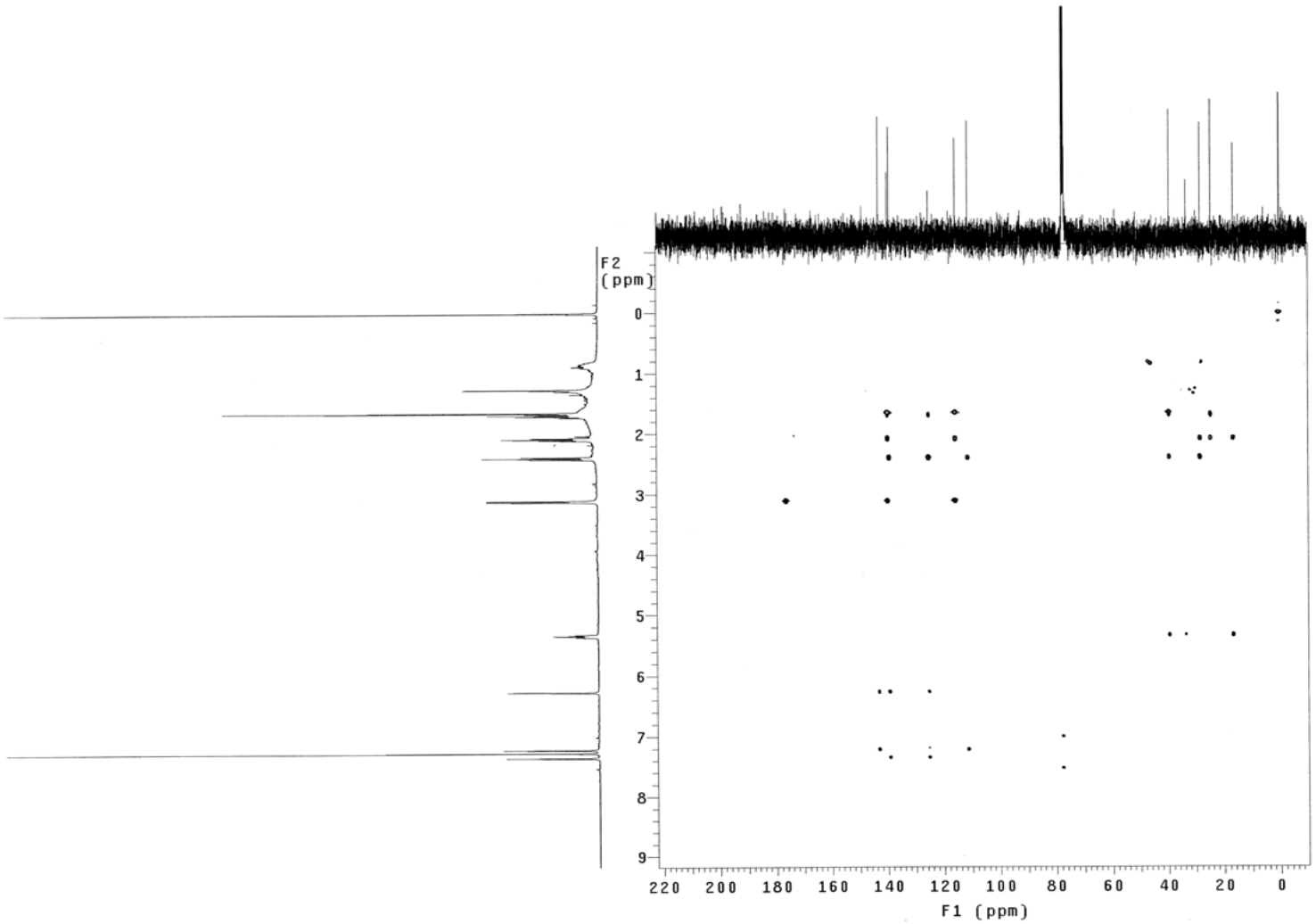


Figure S20. HMBC spectrum of **3** in $CDCl_3$.

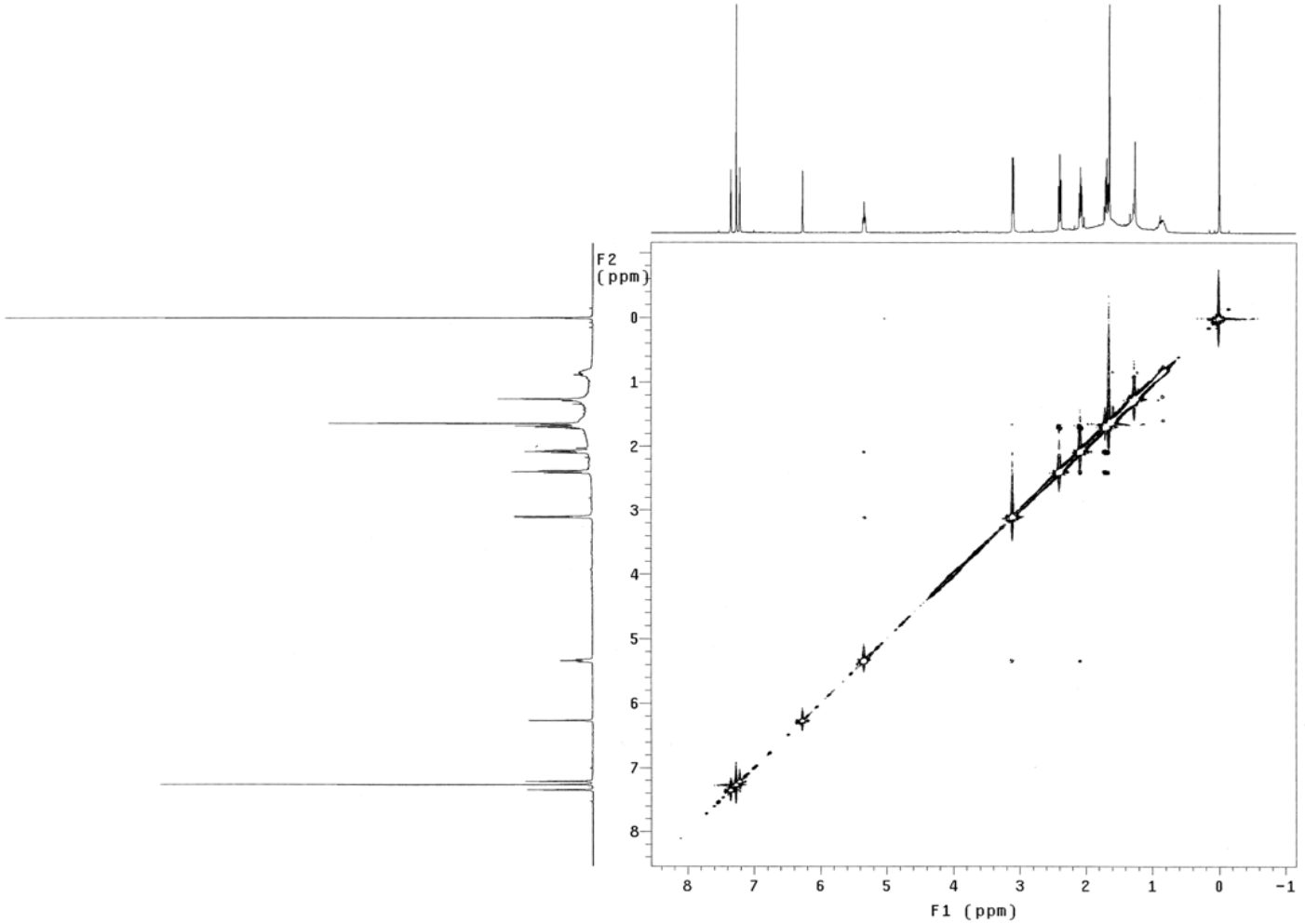
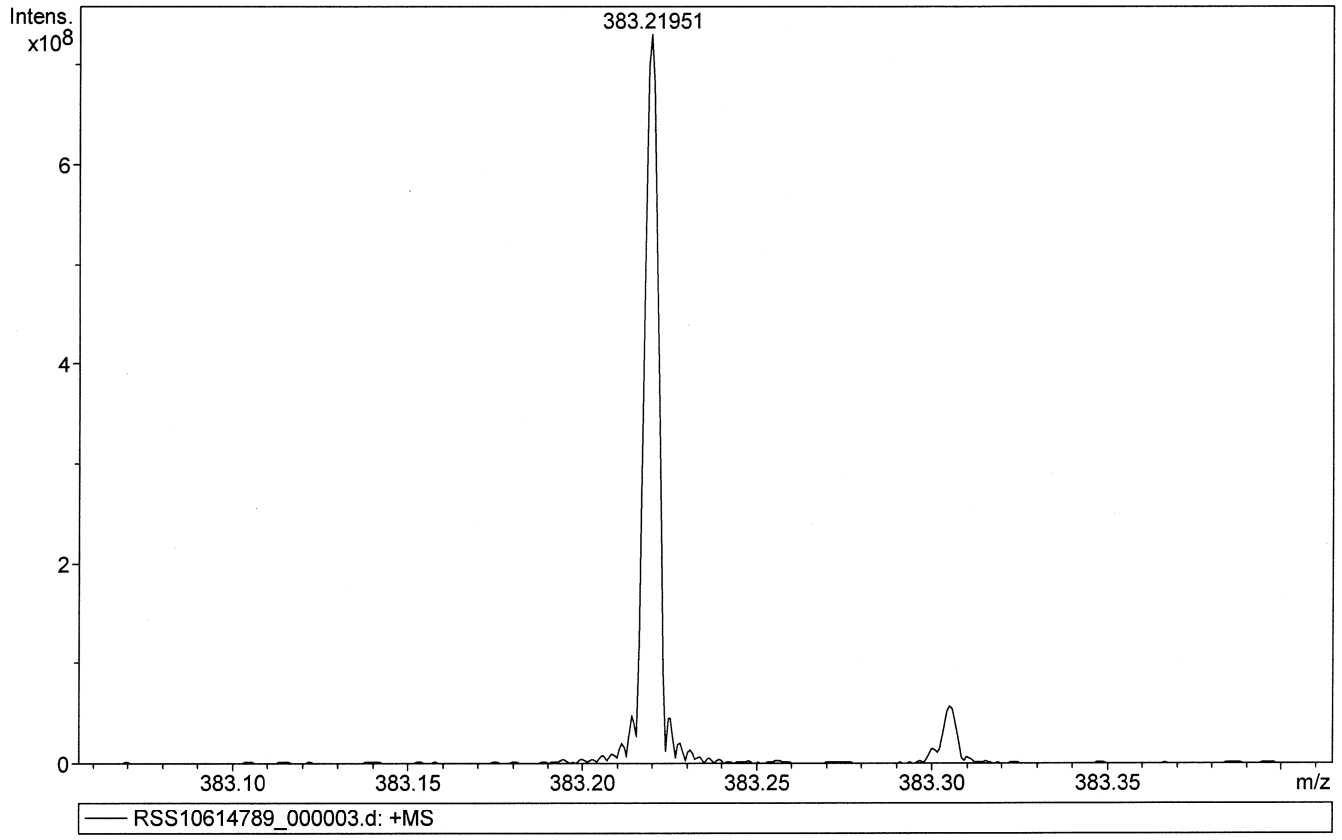


Figure S21. NOESY spectrum of **3** in $CDCl_3$.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
383.21951	1	C 22 H 32 Na O 4	100.00	383.21928	-0.23	-0.61	8.9	6.5	even	ok

Figure S22. HRESIMS spectrum of compound **4**.

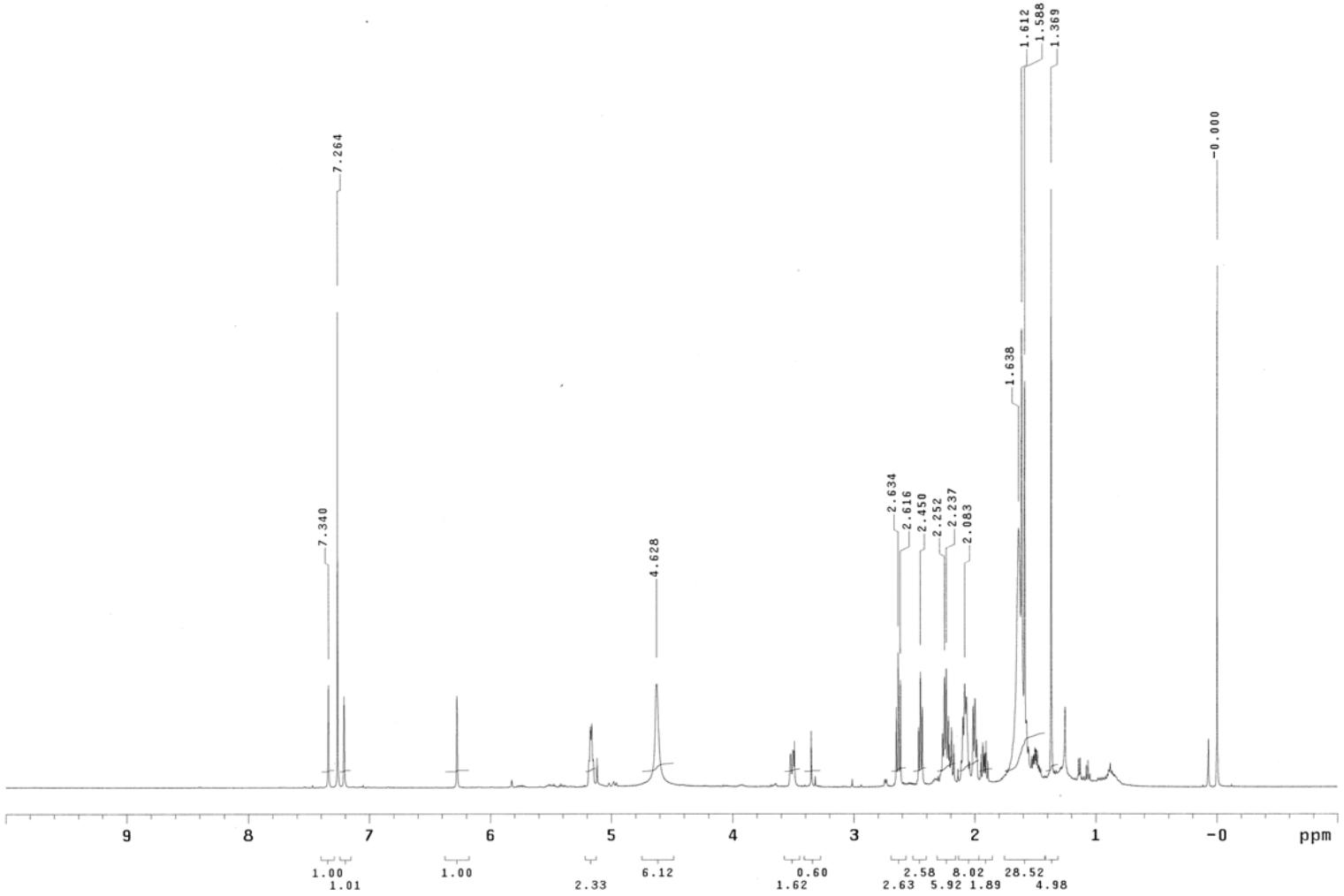


Figure S23. ^{1}H NMR spectrum (500 MHz) of compound **4** in $CDCl_3$.

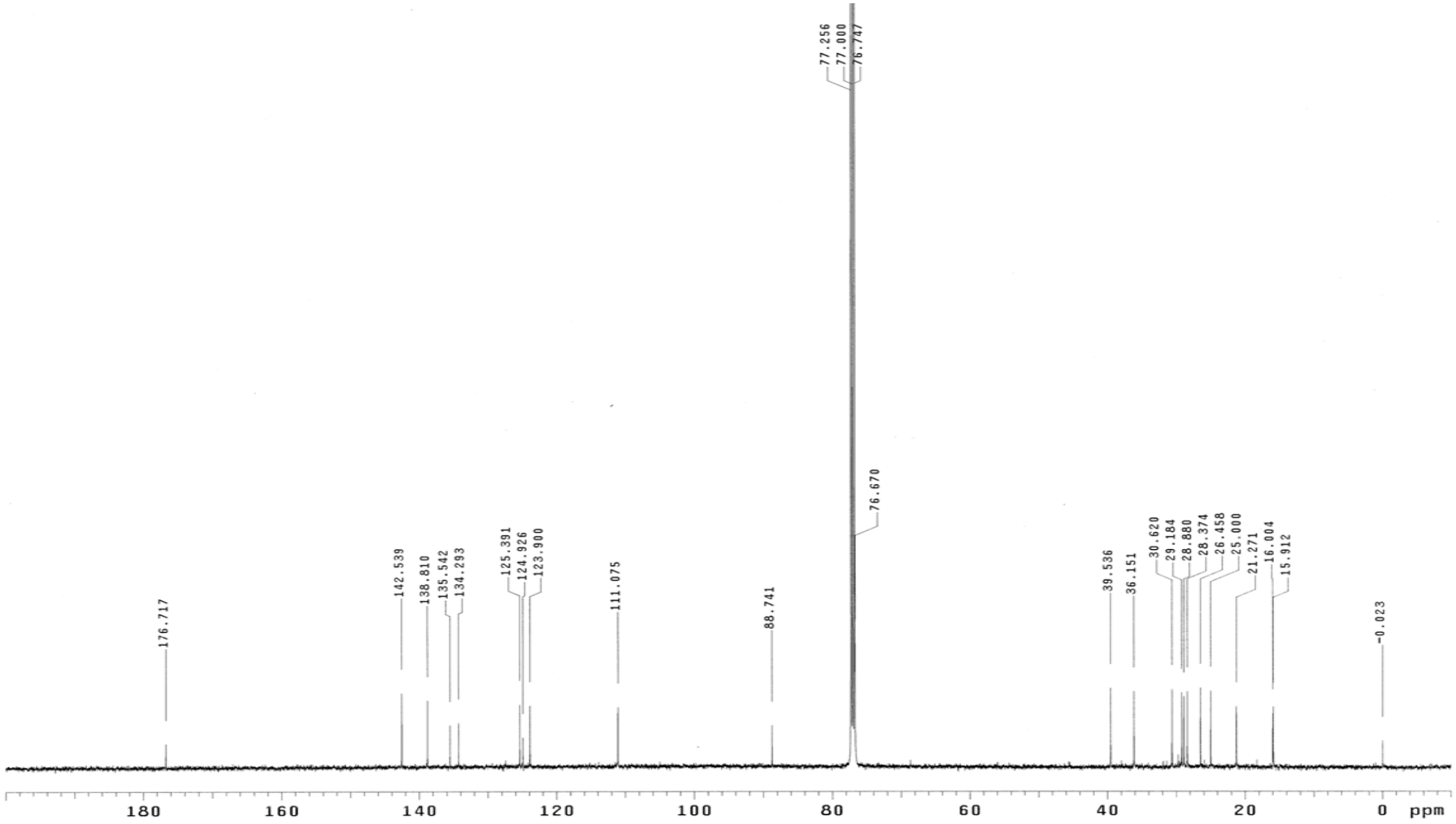


Figure S24. ^{13}C NMR spectrum (125 MHz) of compound **4** in $CDCl_3$.

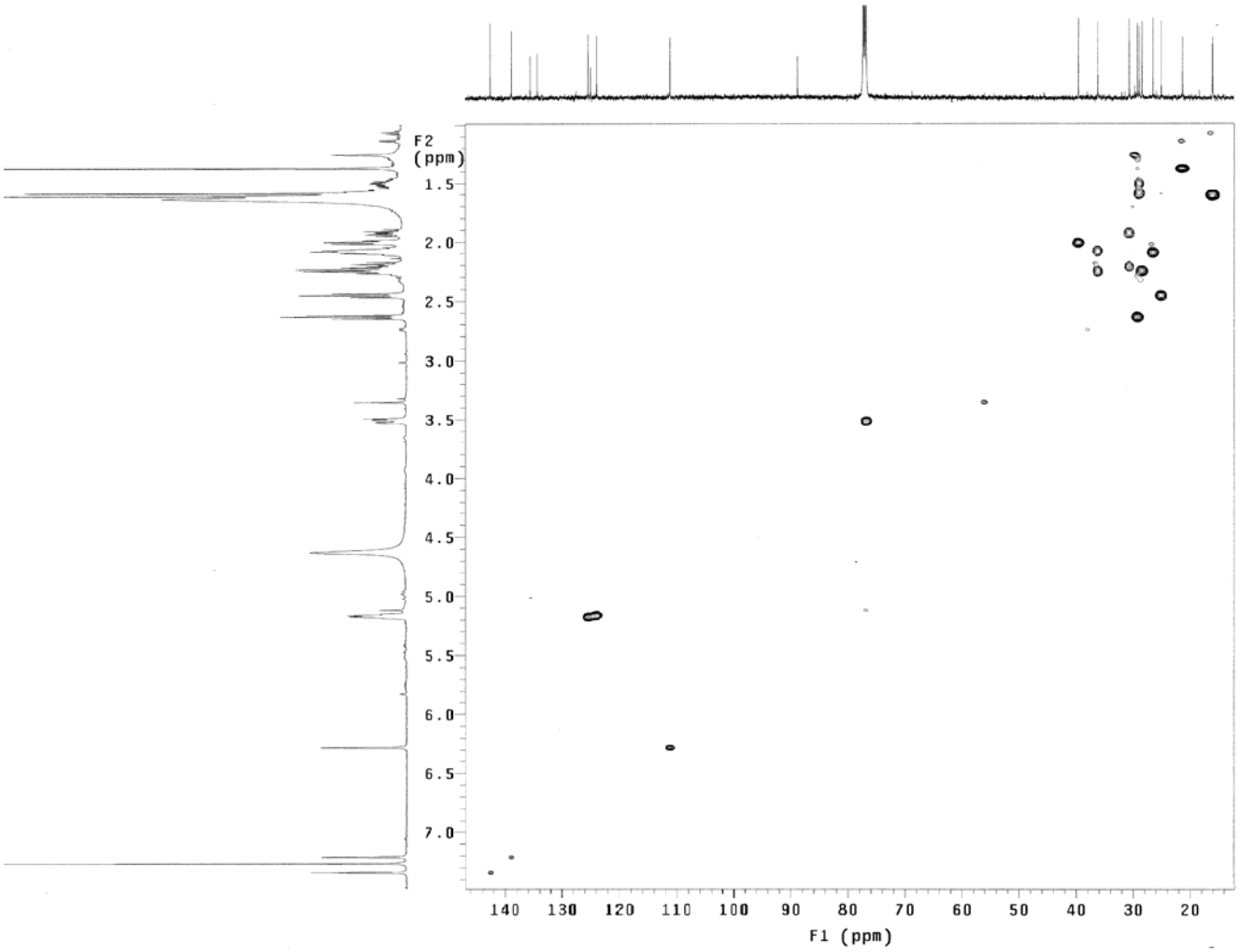


Figure S25. HSQC spectrum of **4** in $CDCl_3$.

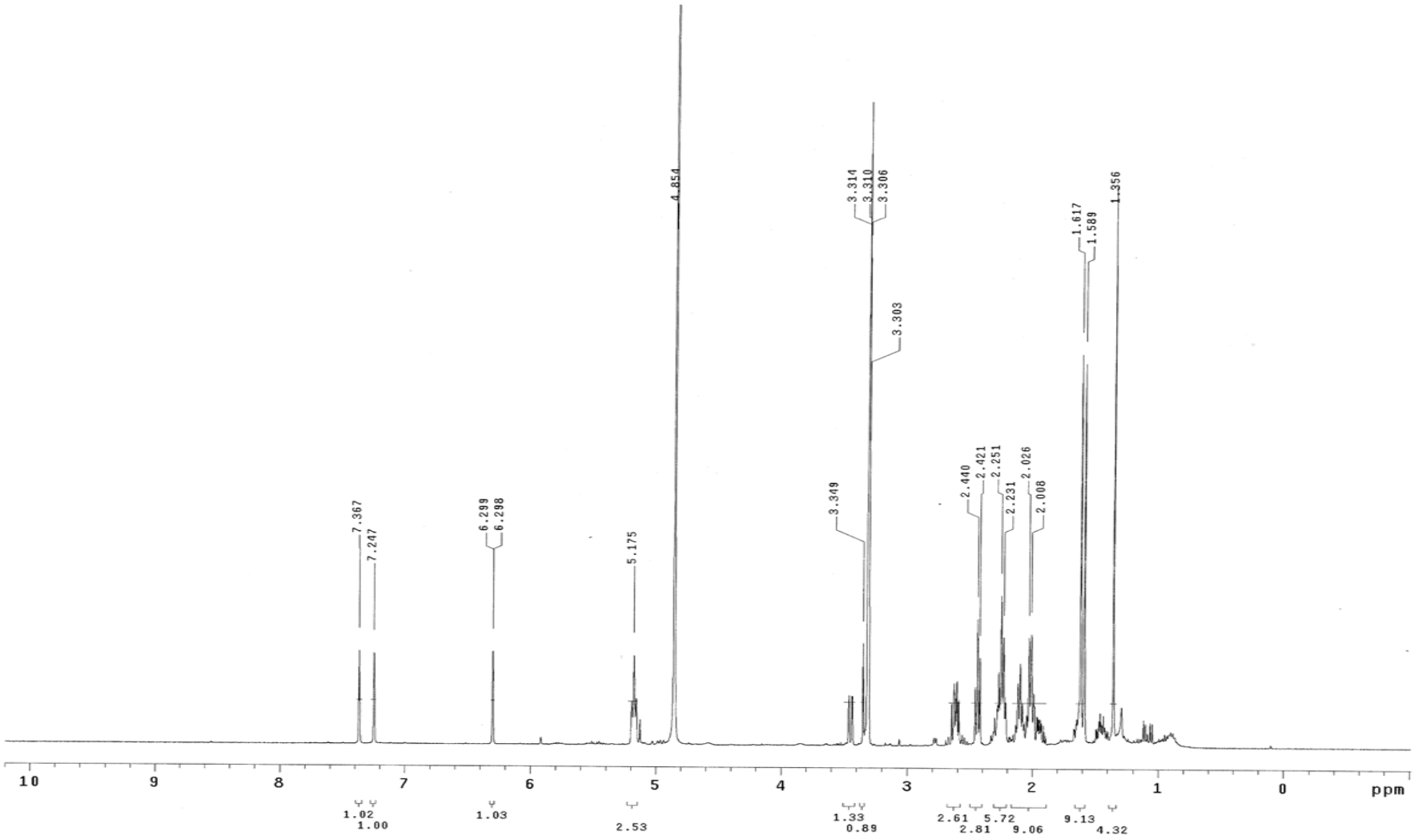


Figure S26. ^{1}H NMR spectrum (400 MHz) of compound **4** in CD_3OD.

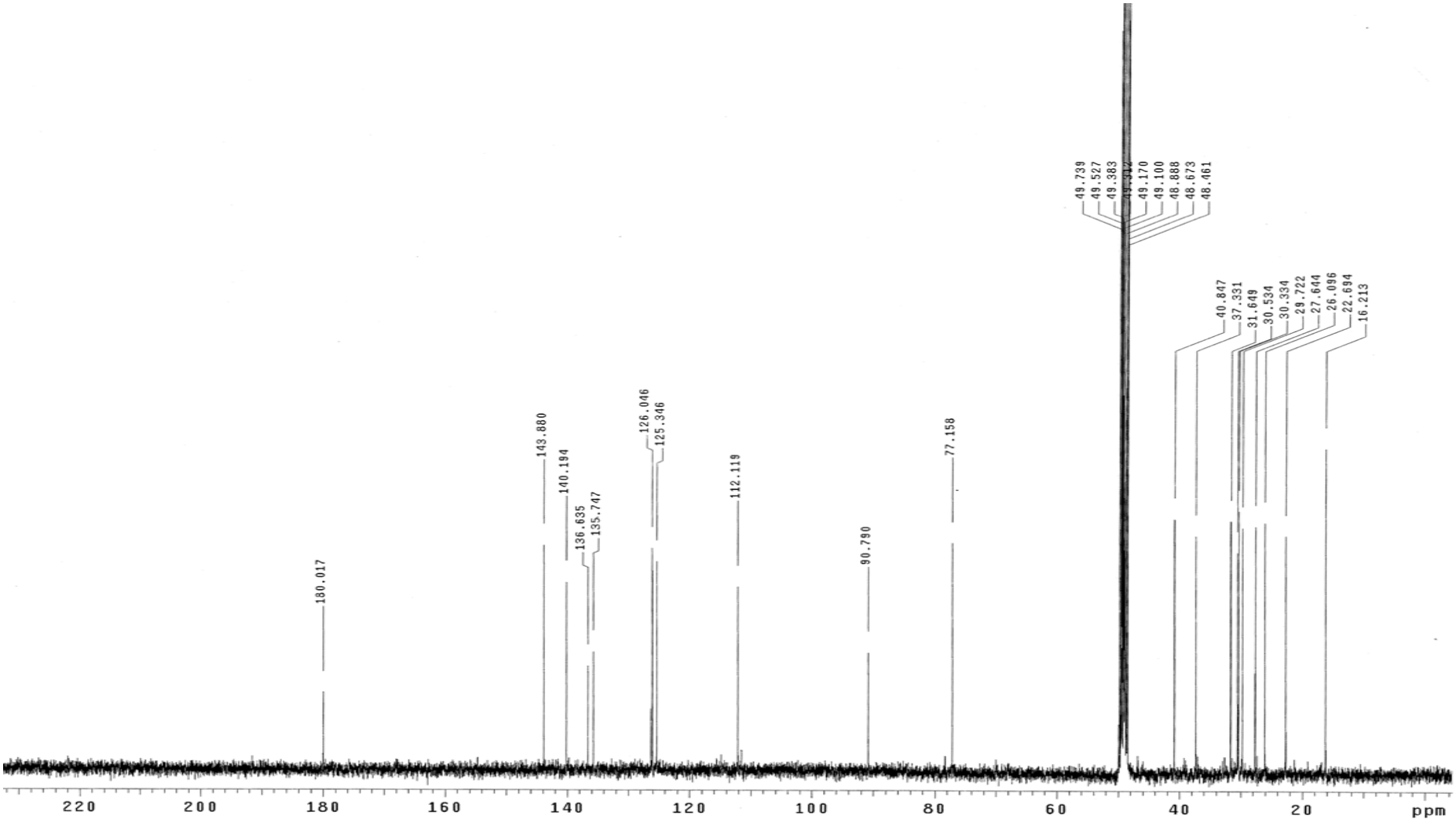


Figure S27. ^{13}C NMR spectrum (100 MHz) of compound **4** in CD_3OD.

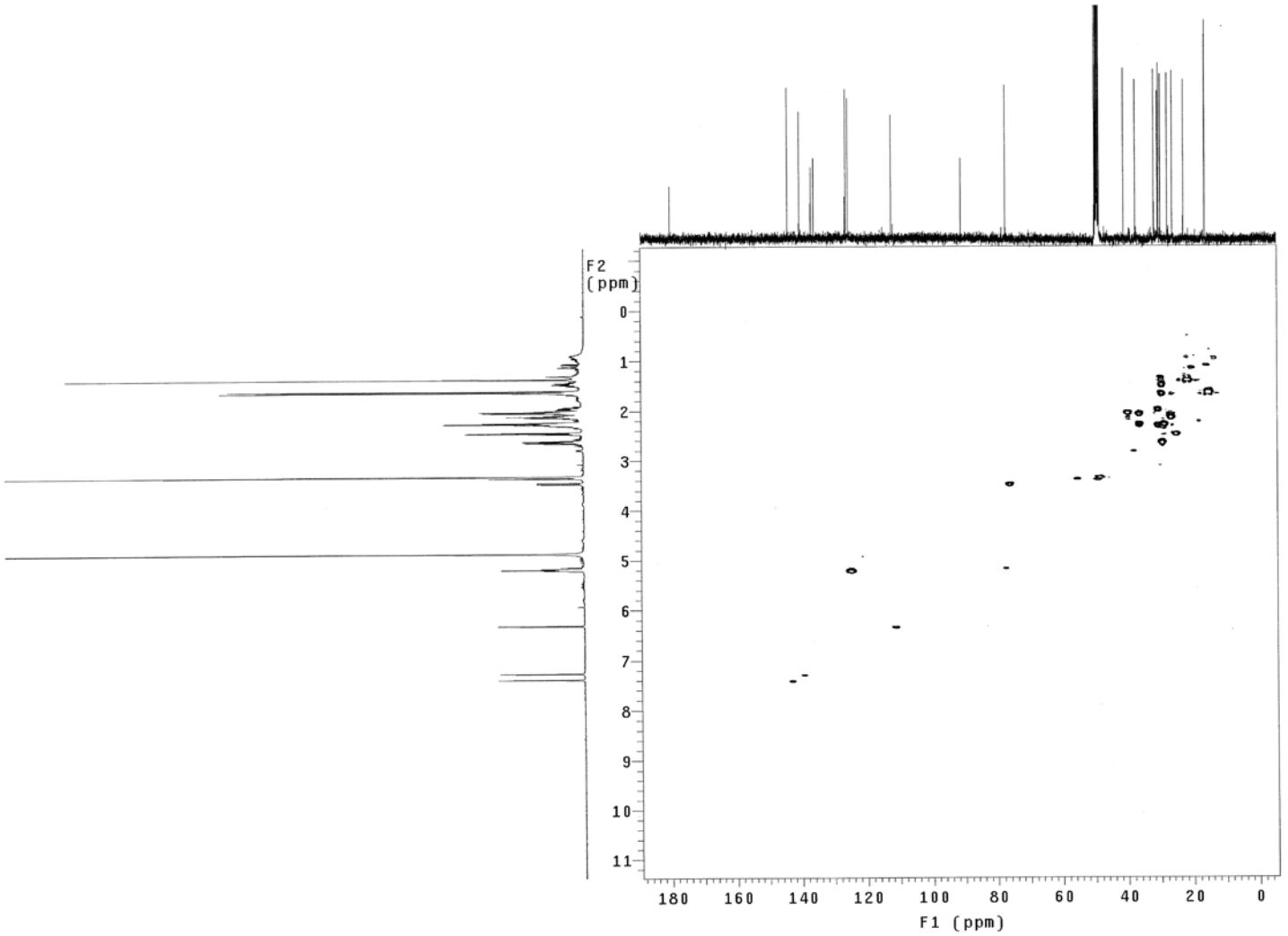


Figure S28. HSQC spectrum of **4** in CD_3OD.

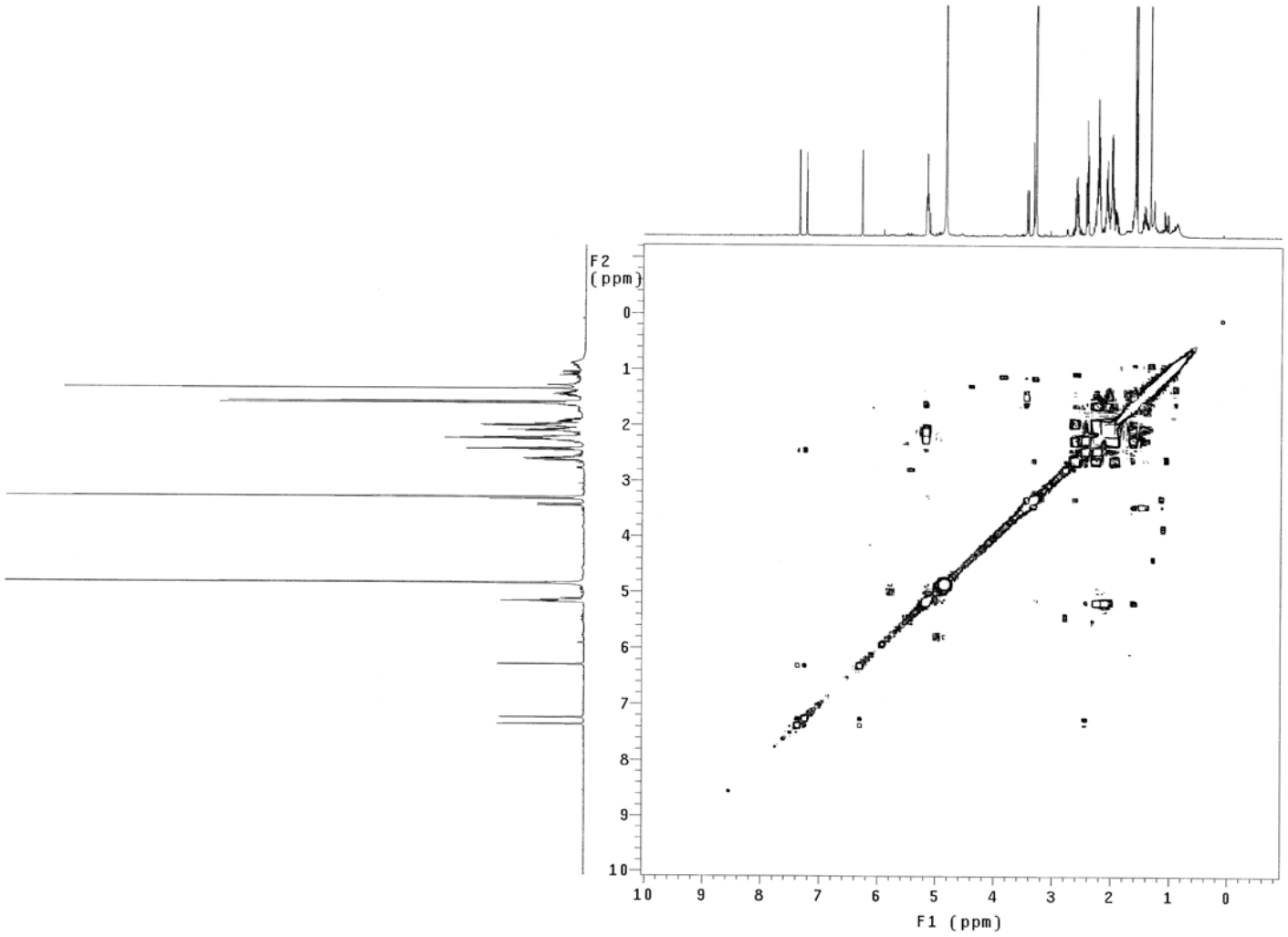


Figure S29. ^{1}H -^{1}H COSY spectrum of **4** in CD_3OD.

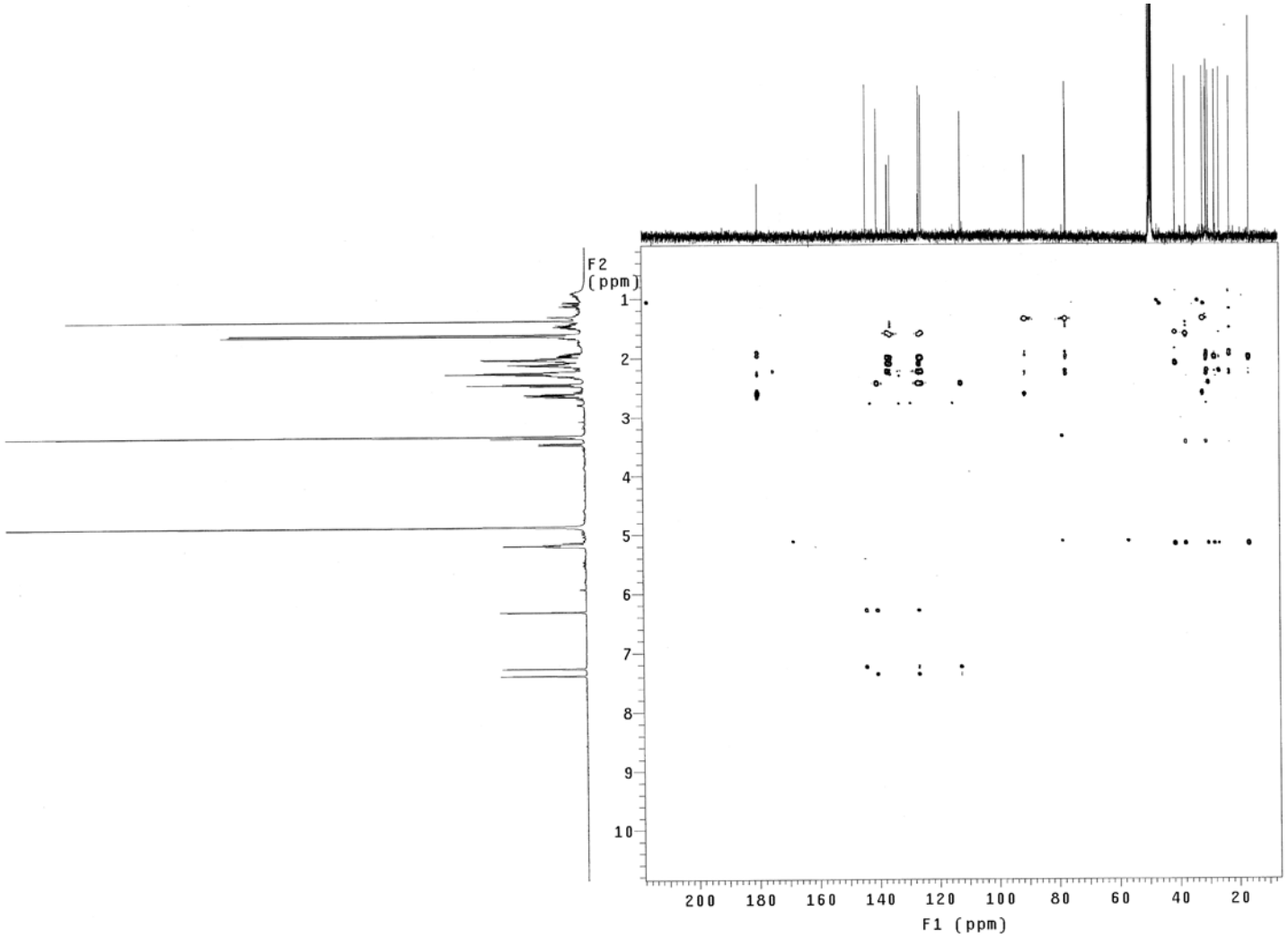


Figure S30. HMBC spectrum of **4** in in CD_3OD.

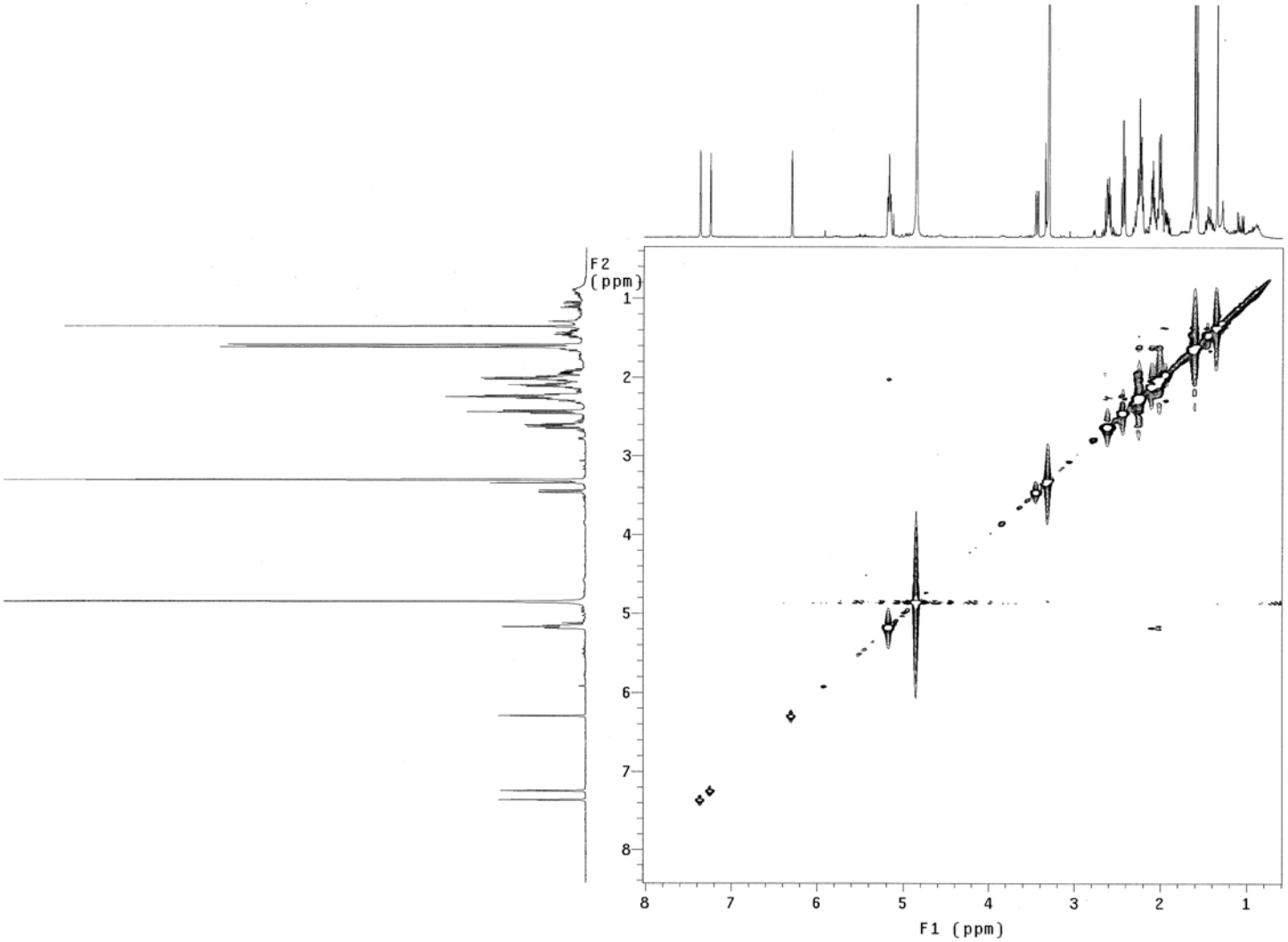
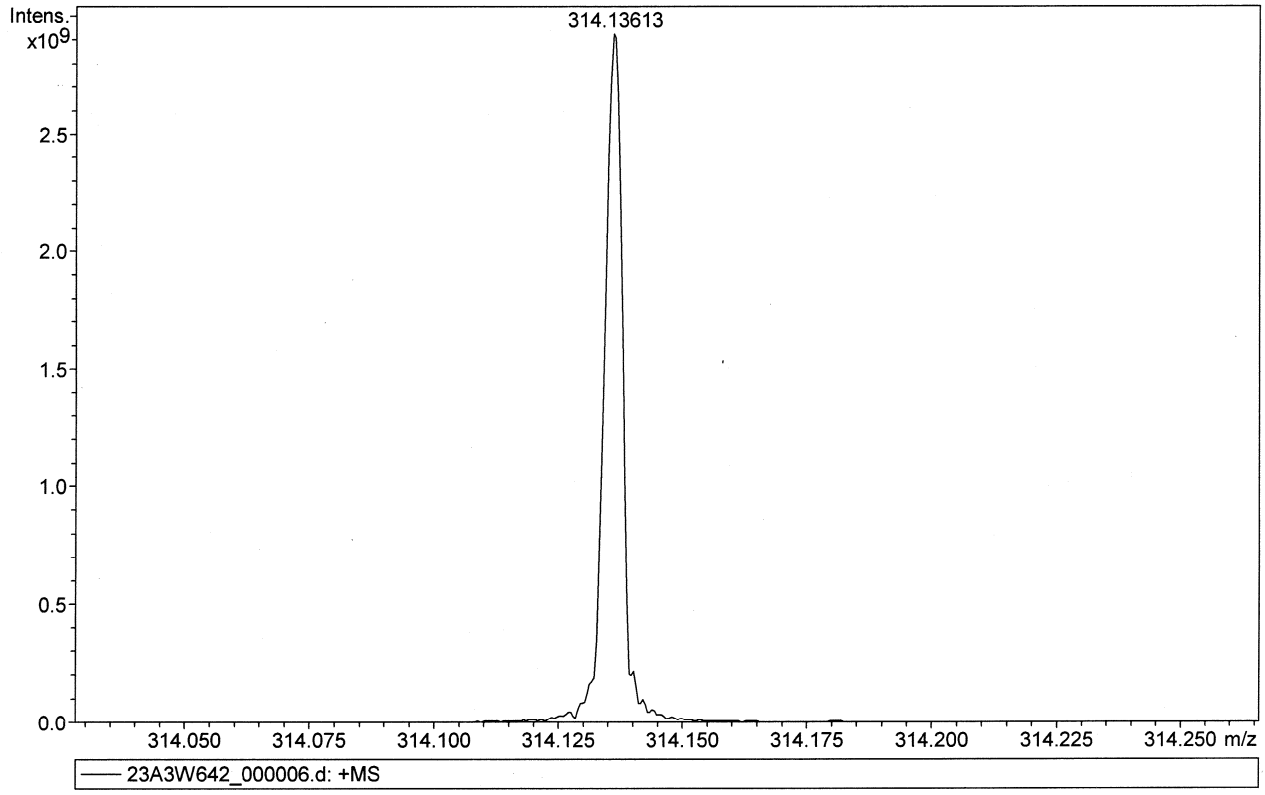


Figure S31. NOESY spectrum of **4** in in CD_3OD.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
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Figure S32. HRESIMS spectrum of **5**.

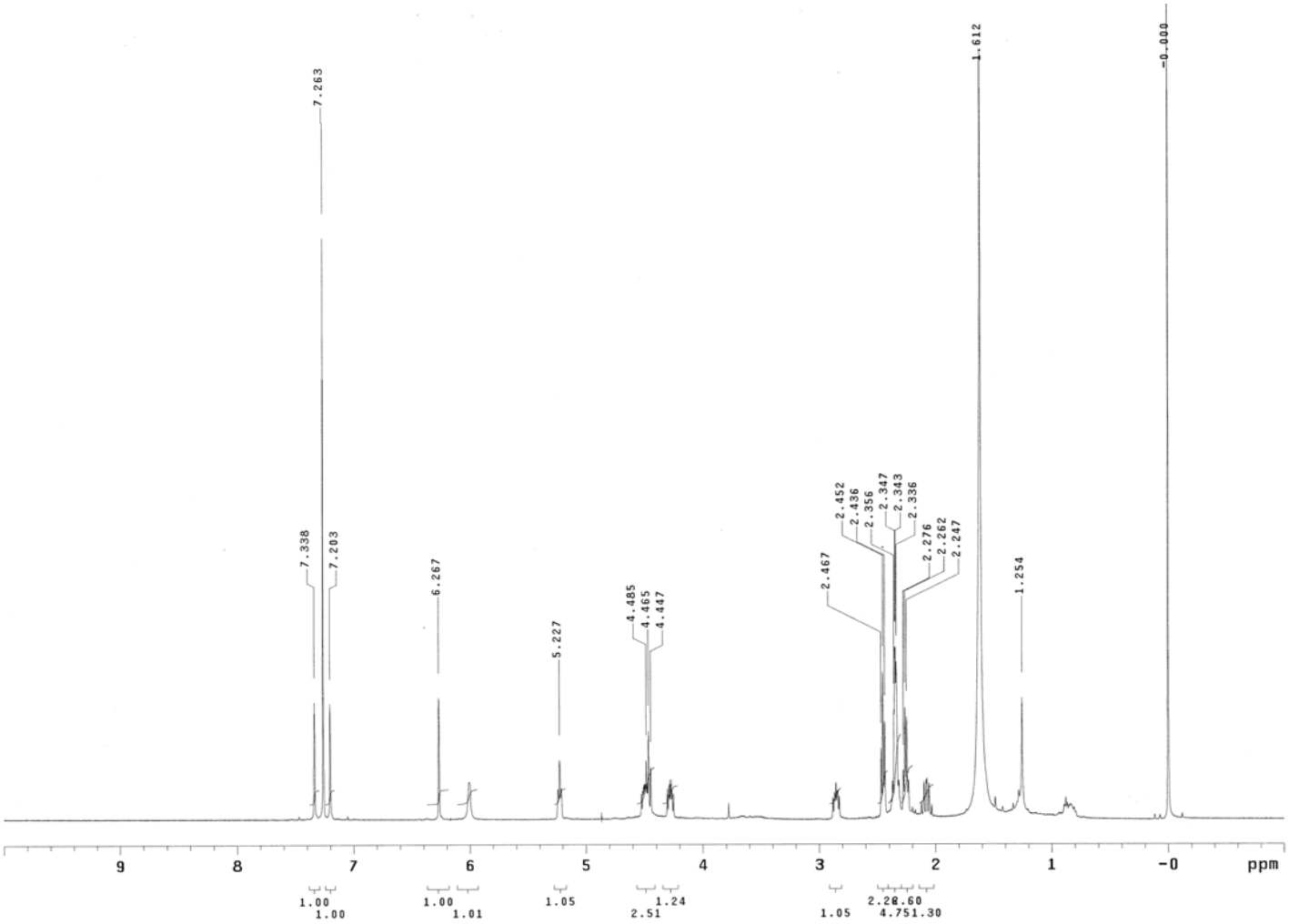

Figure S33. ^{1}H NMR spectrum of **5** in $CDCl_3$ at 500 MHz.

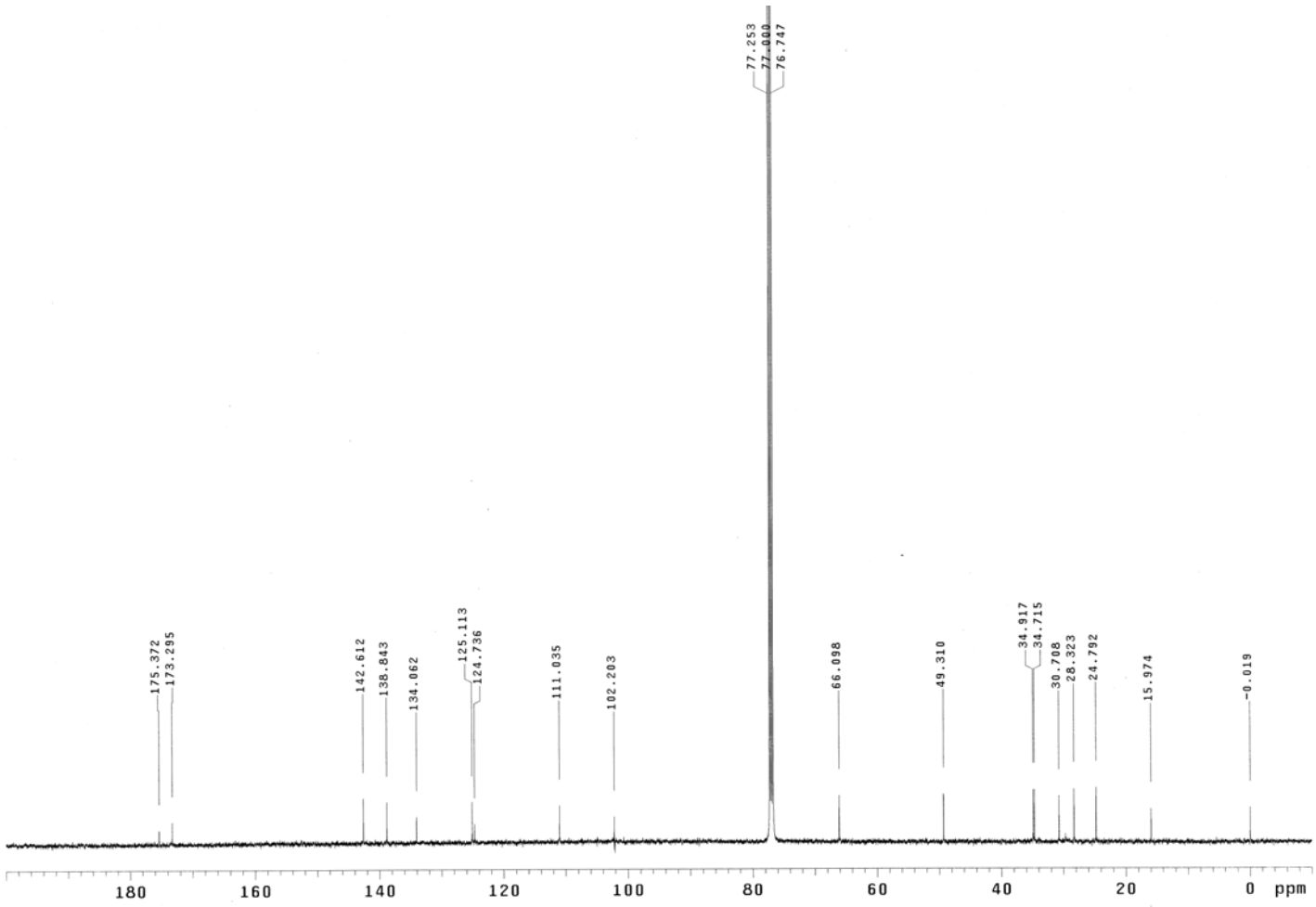

Figure S34. ^{13}C NMR spectrum of **5** in $CDCl_3$ at 125 MHz.

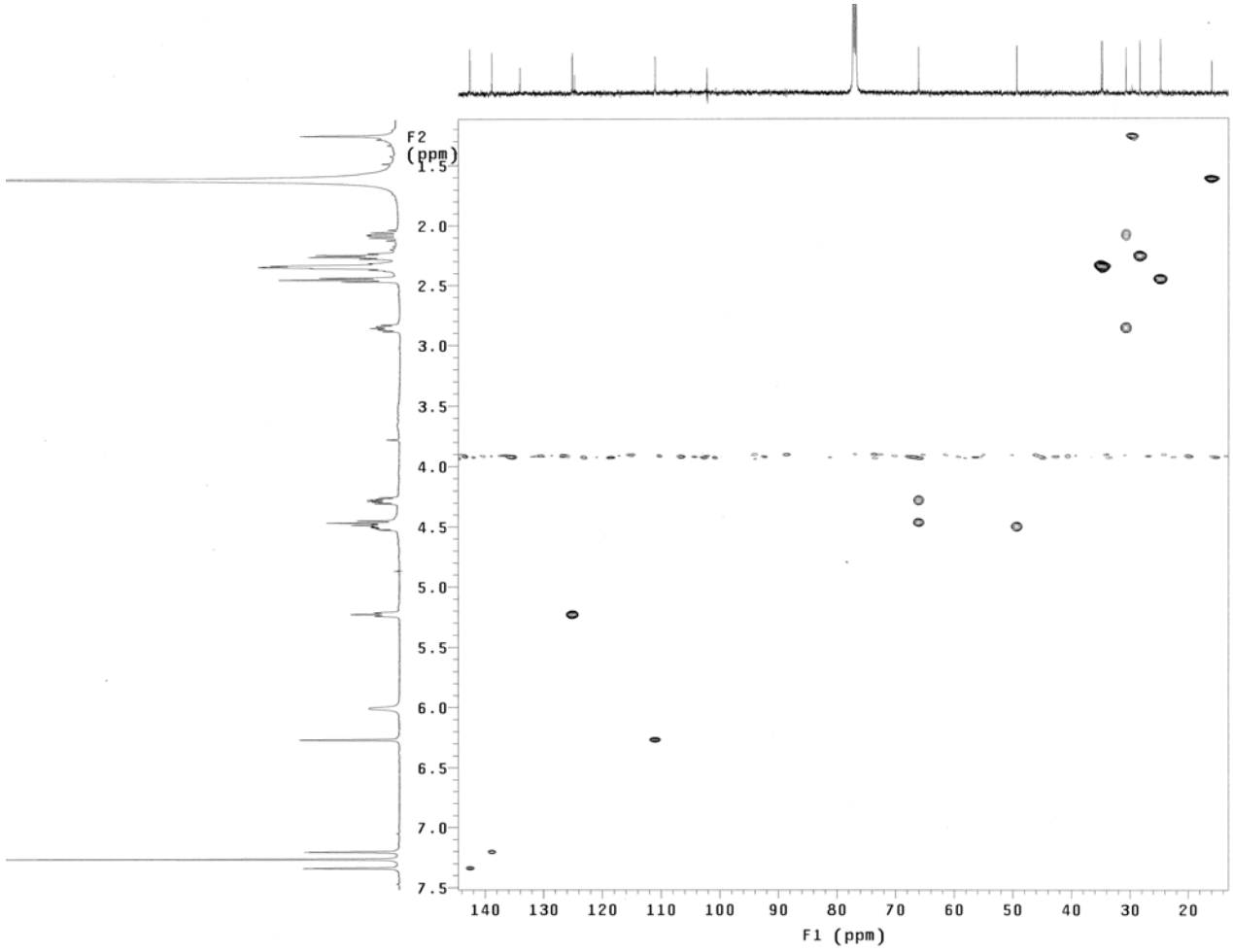

Figure S35. HSQC spectrum of **5** in $CDCl_3$.