

Aquaculture Soft Coral *Lobophytum crassum* as a Producer of Anti-Proliferative Cembranoids

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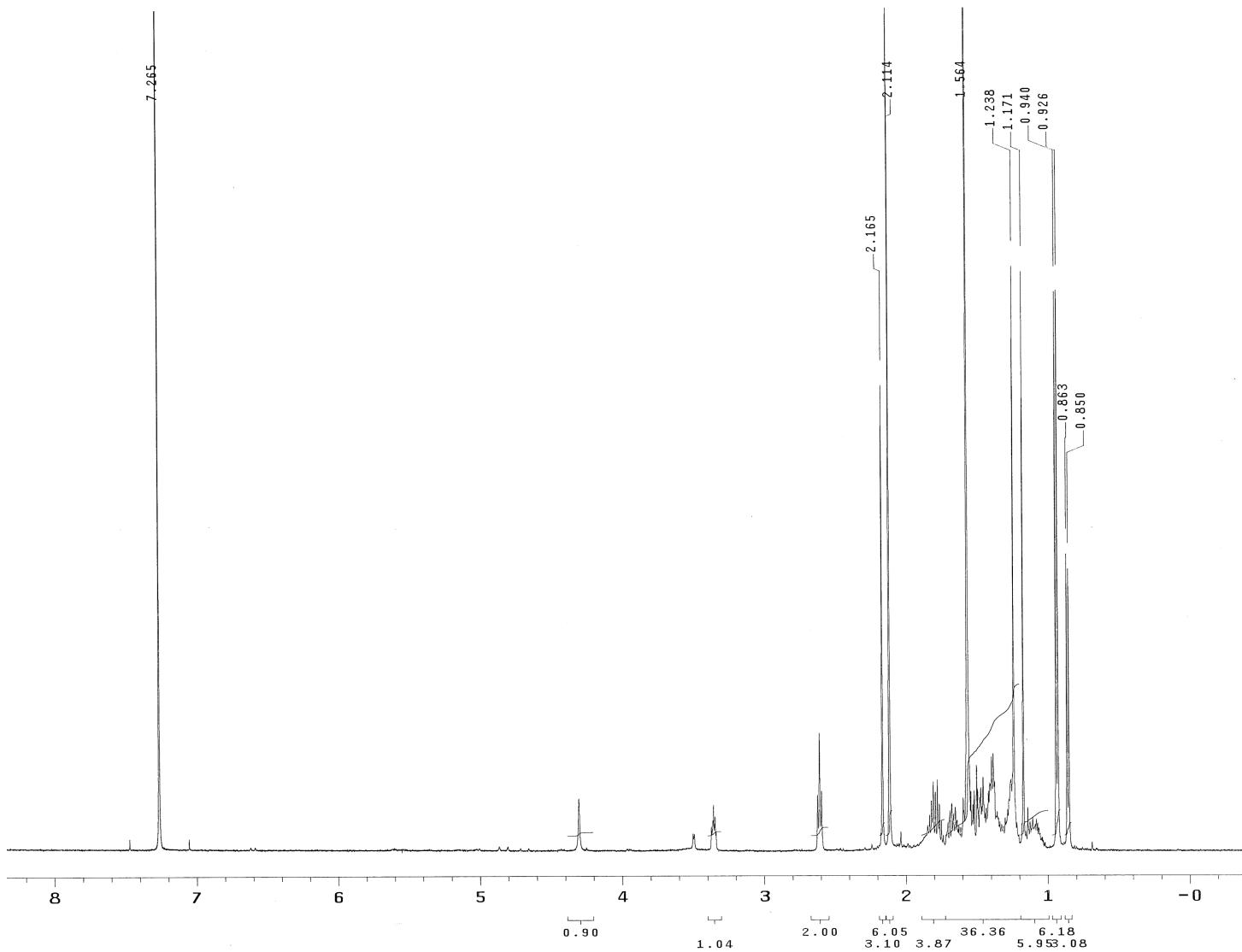


Figure S1: ^1H NMR (500 MHz, CDCl_3) spectrum of **1**.

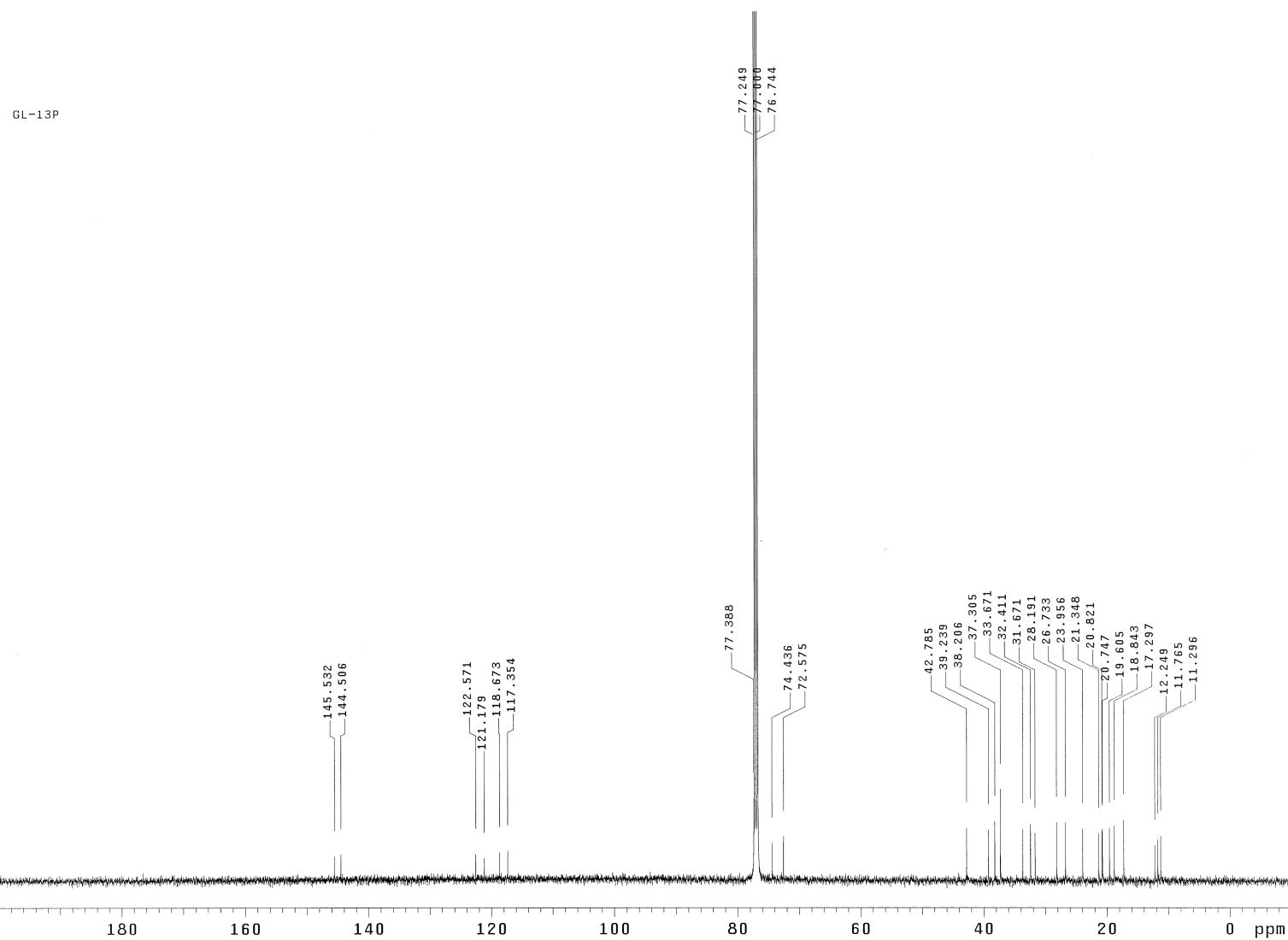
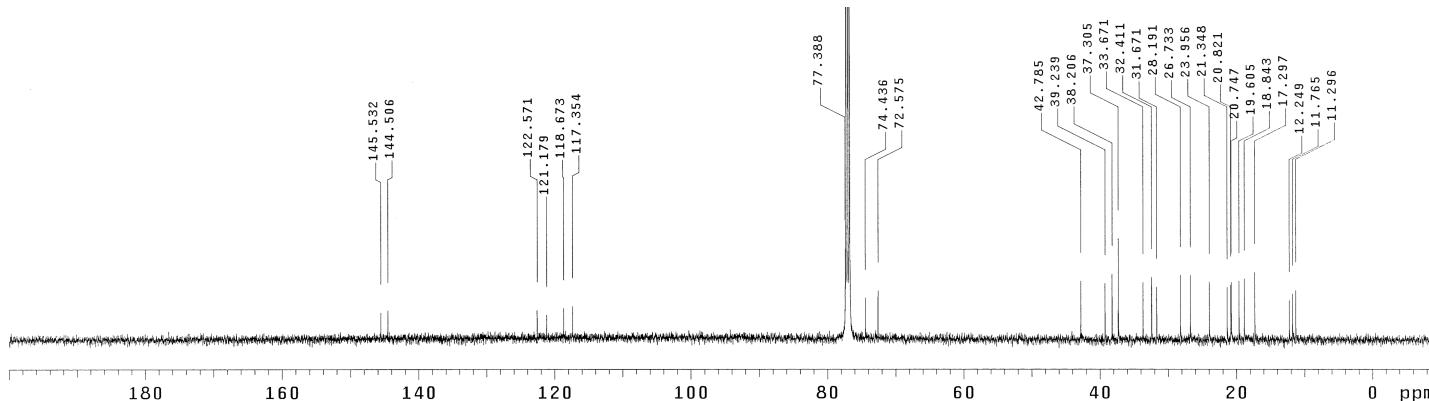


Figure S2: ^{13}C NMR (125 MHz, CDCl_3) spectrum of **1**.



CH carbons

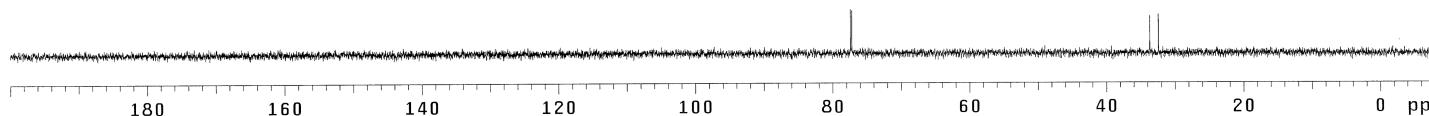


Figure S3: DEPT NMR (125 MHz, CDCl₃) spectrum of **1**.

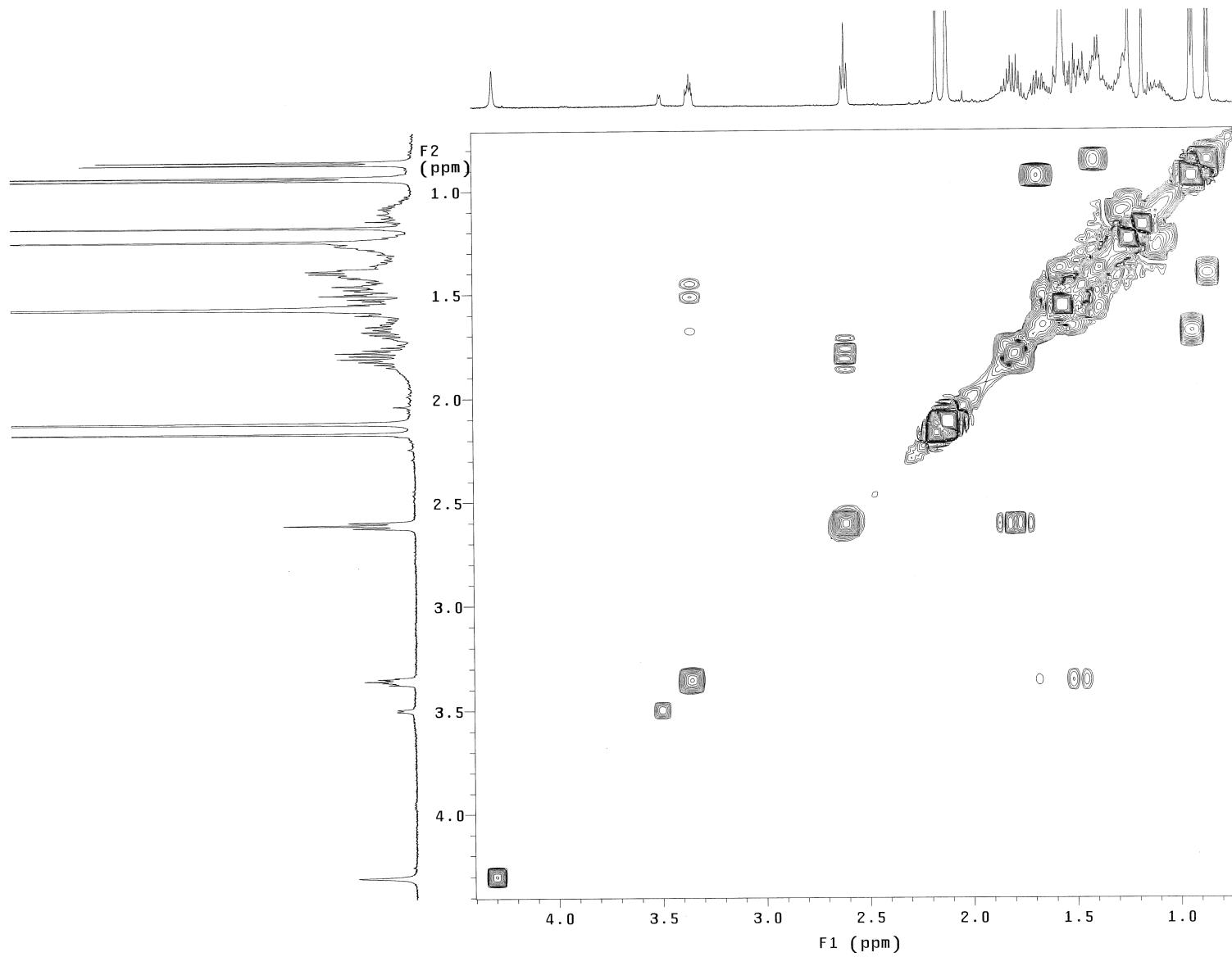


Figure S4: COSY NMR (500 MHz, CDCl_3) spectrum of **1**.

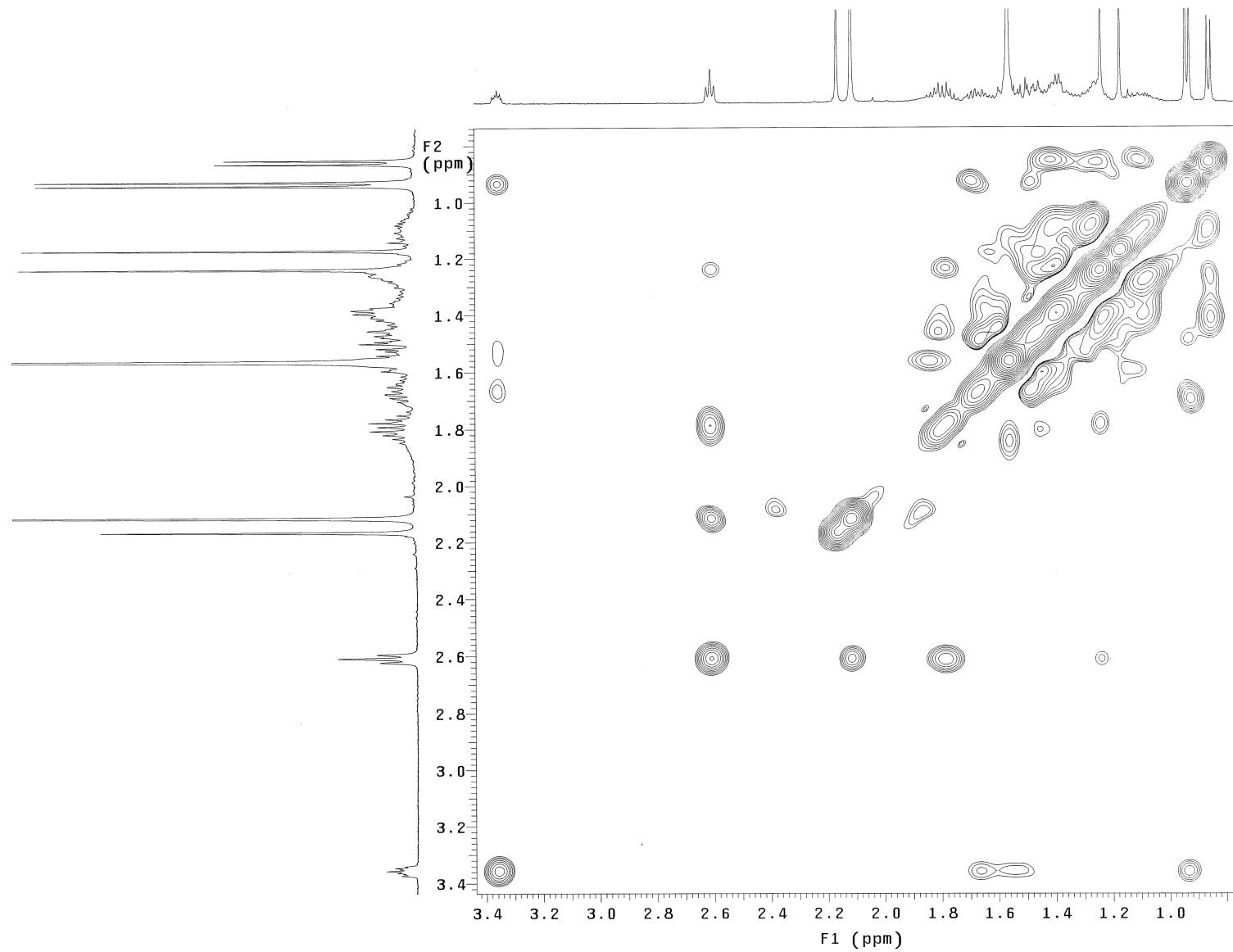


Figure S5: NOESY NMR (500 MHz, CDCl_3) spectrum of **1**.

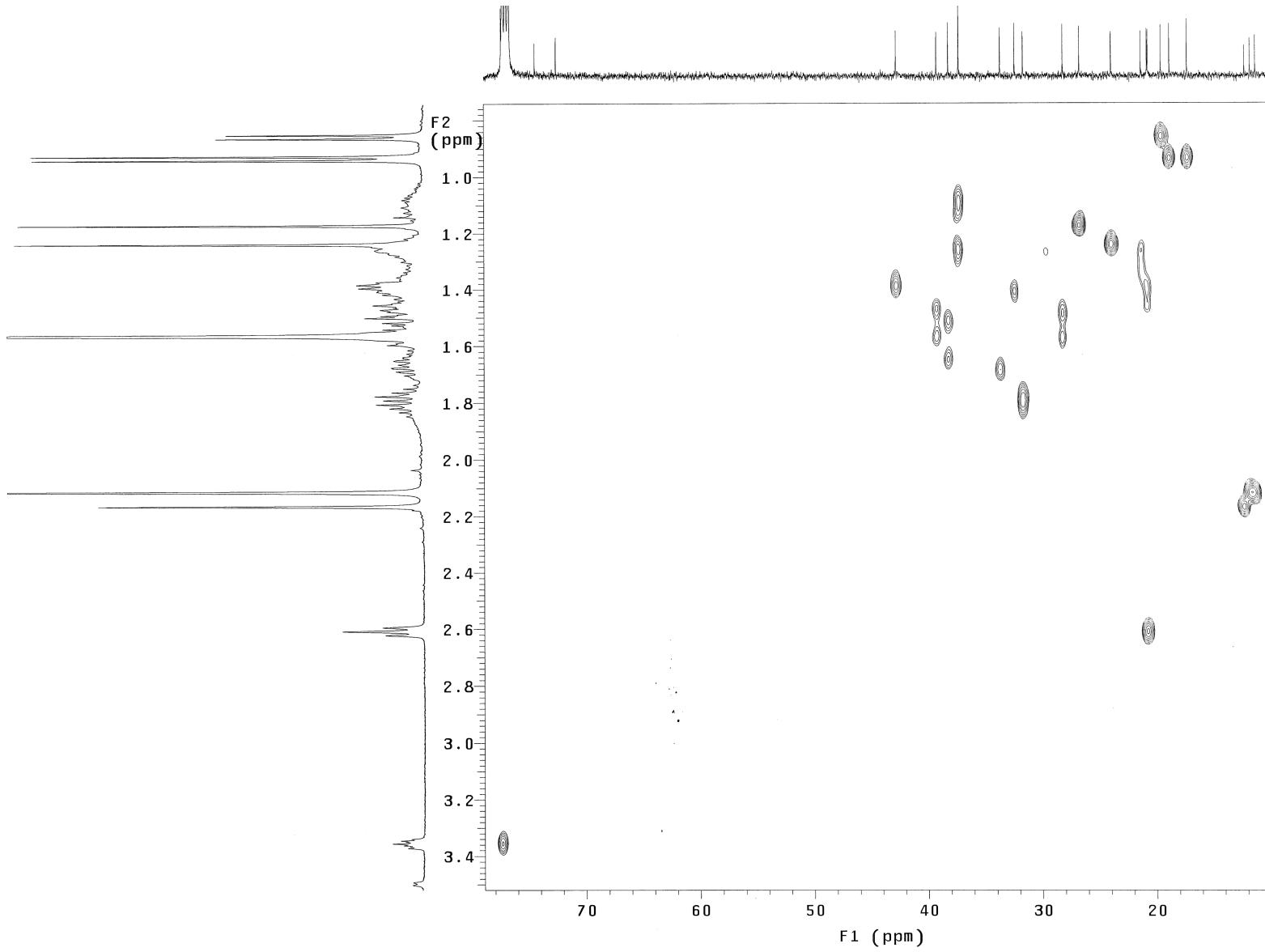


Figure S6: HSQC NMR (500 MHz, CDCl₃) spectrum of 1.

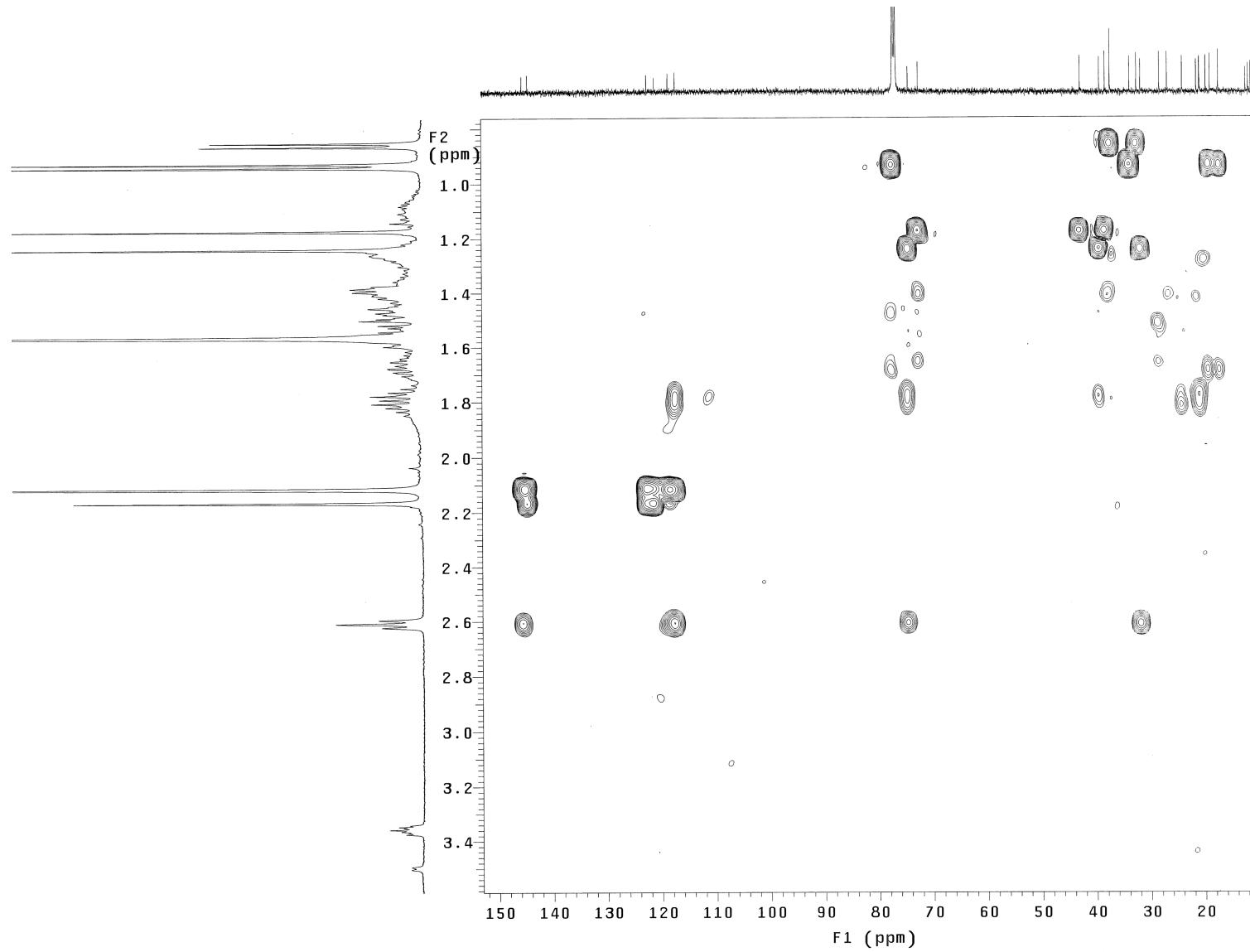
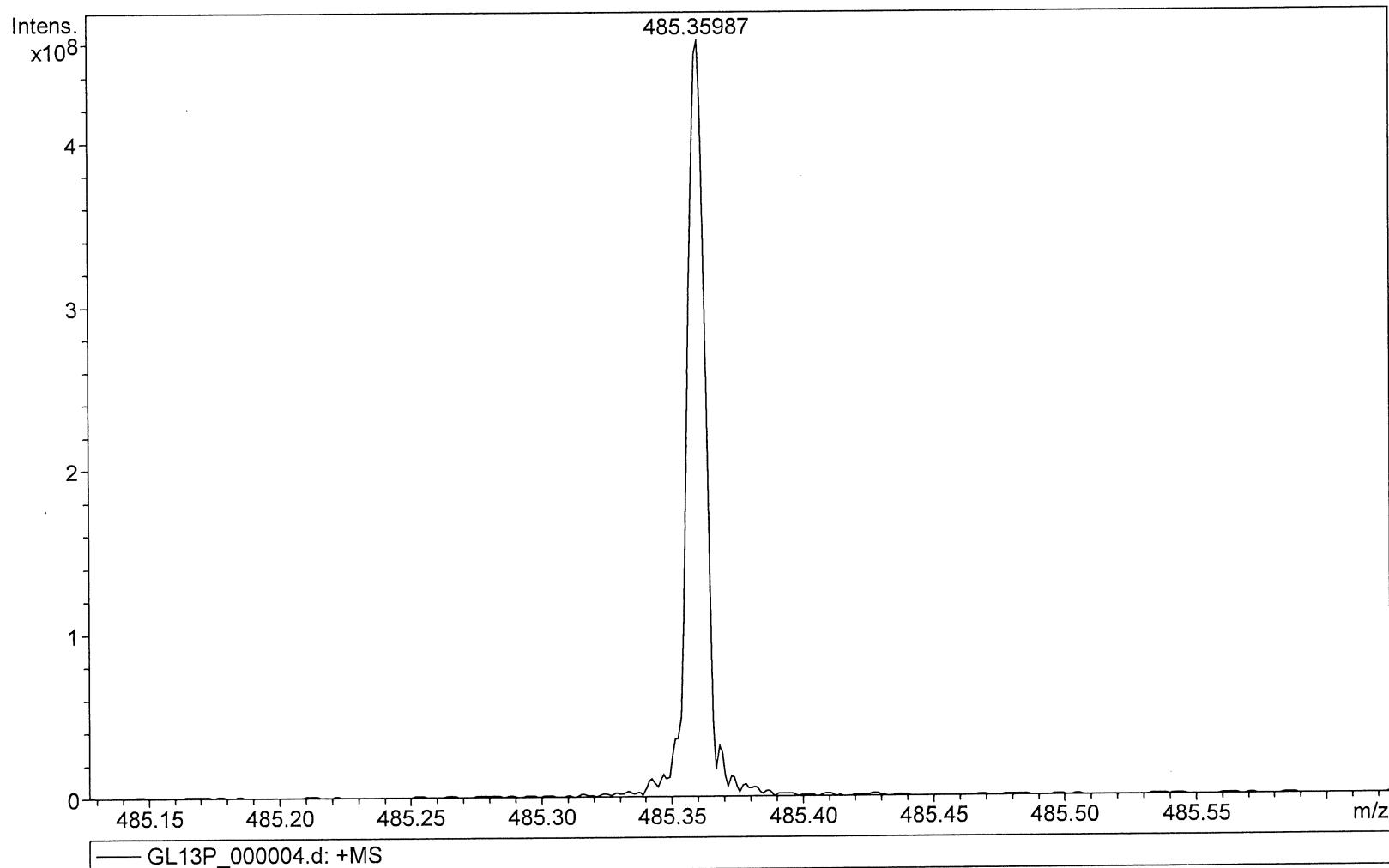


Figure S7: HMBC NMR (500 MHz, CDCl_3) spectrum of **1**.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
485.35987	1	C 29 H 50 Na O 4	100.00	485.36013	0.26	0.54	3.9	4.5	even	ok

Figure S8: HRESIMS spectrum of **1**.

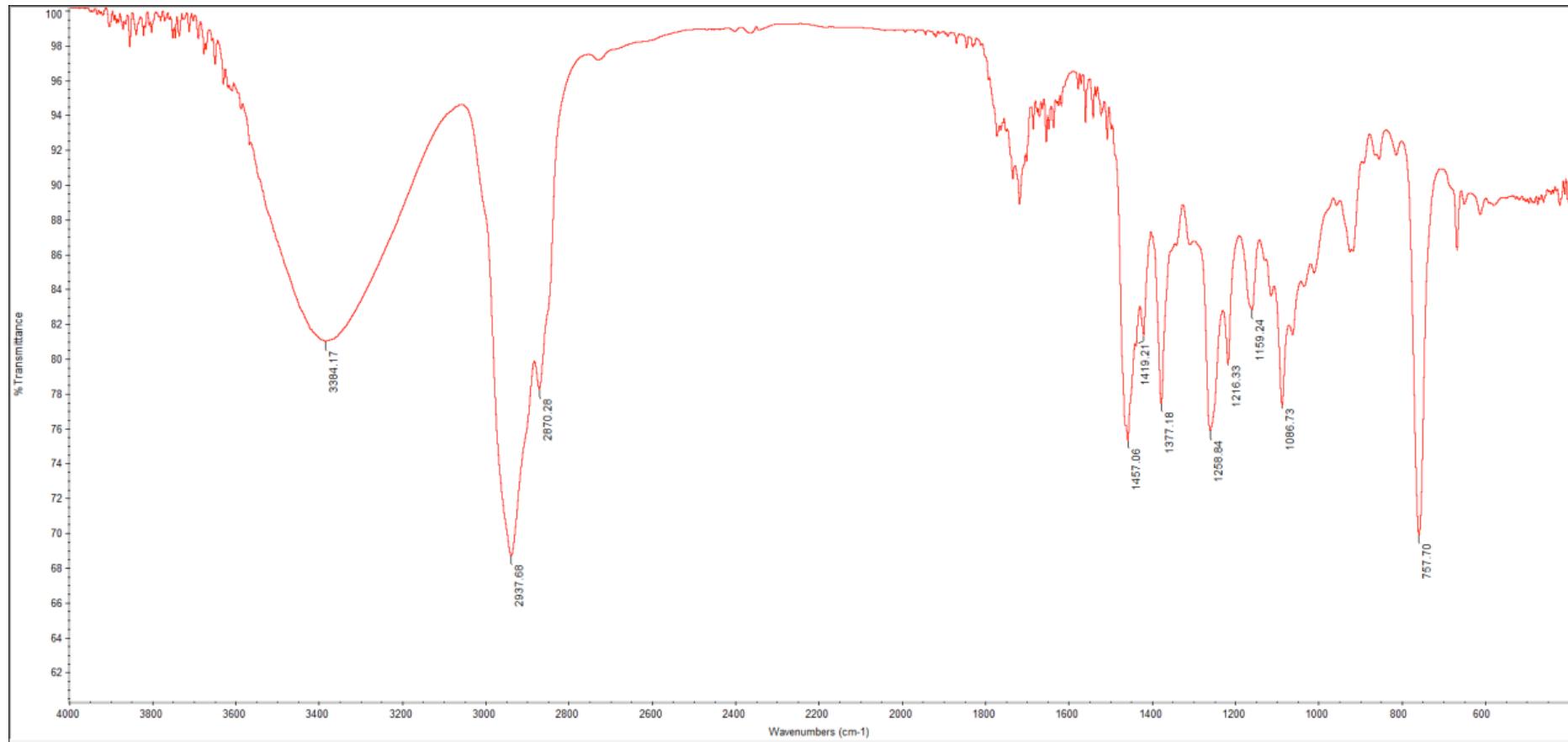


Figure S9: IR spectrum of 1.

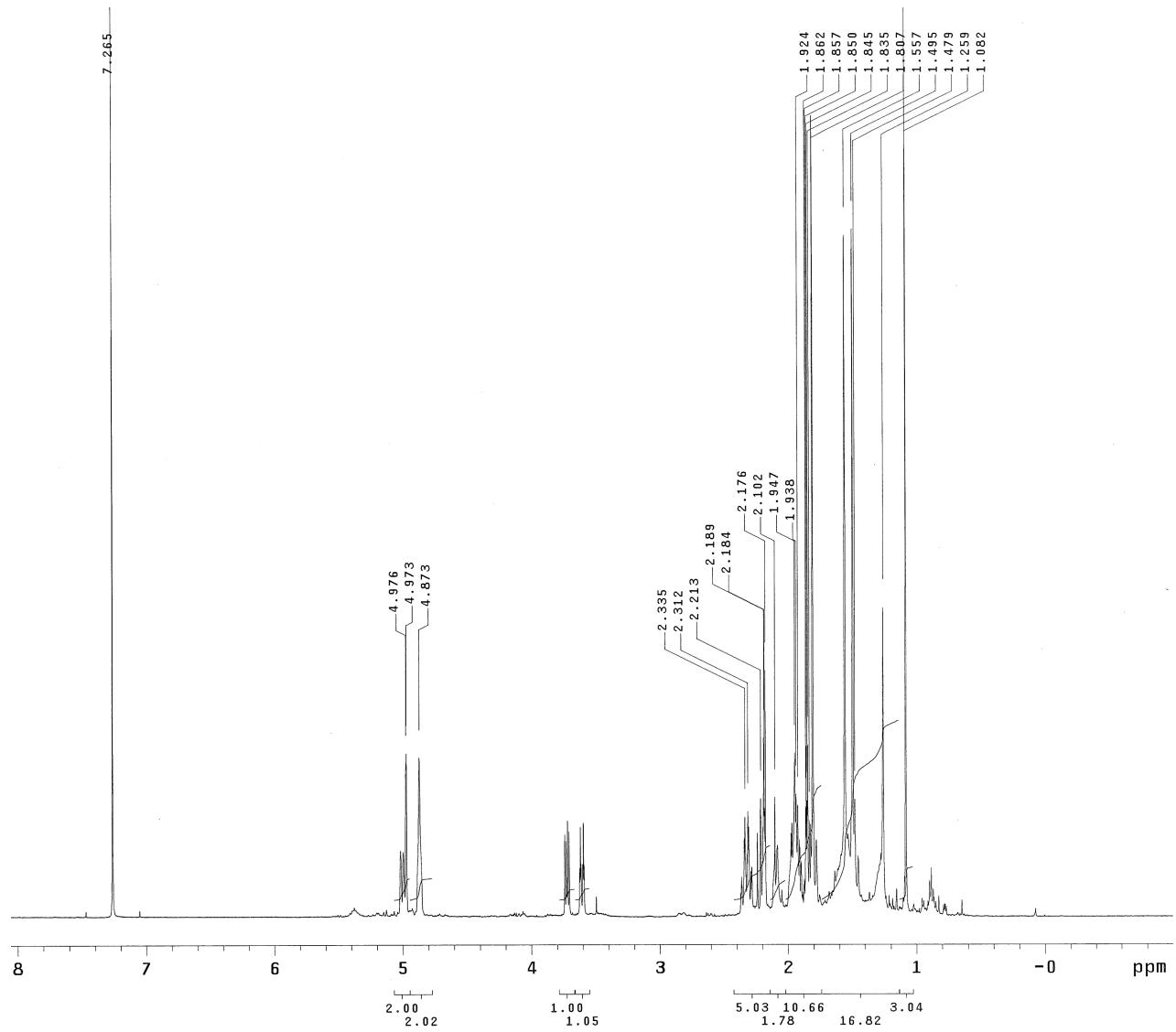


Figure S10: ^1H NMR (500 MHz, CDCl_3) spectrum of **2**.

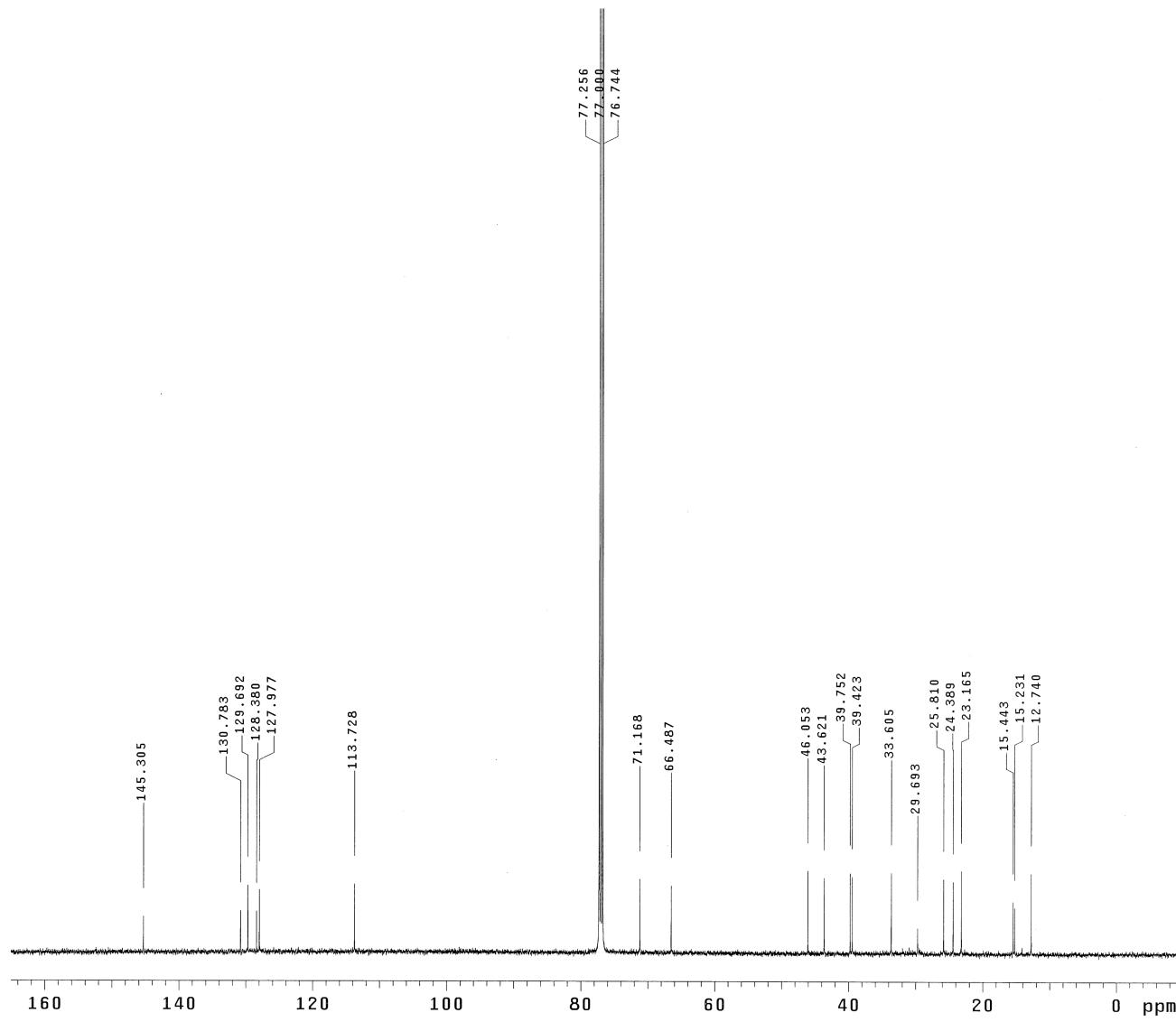


Figure S11: ^{13}C NMR (125 MHz, CDCl_3) spectrum of **2**.

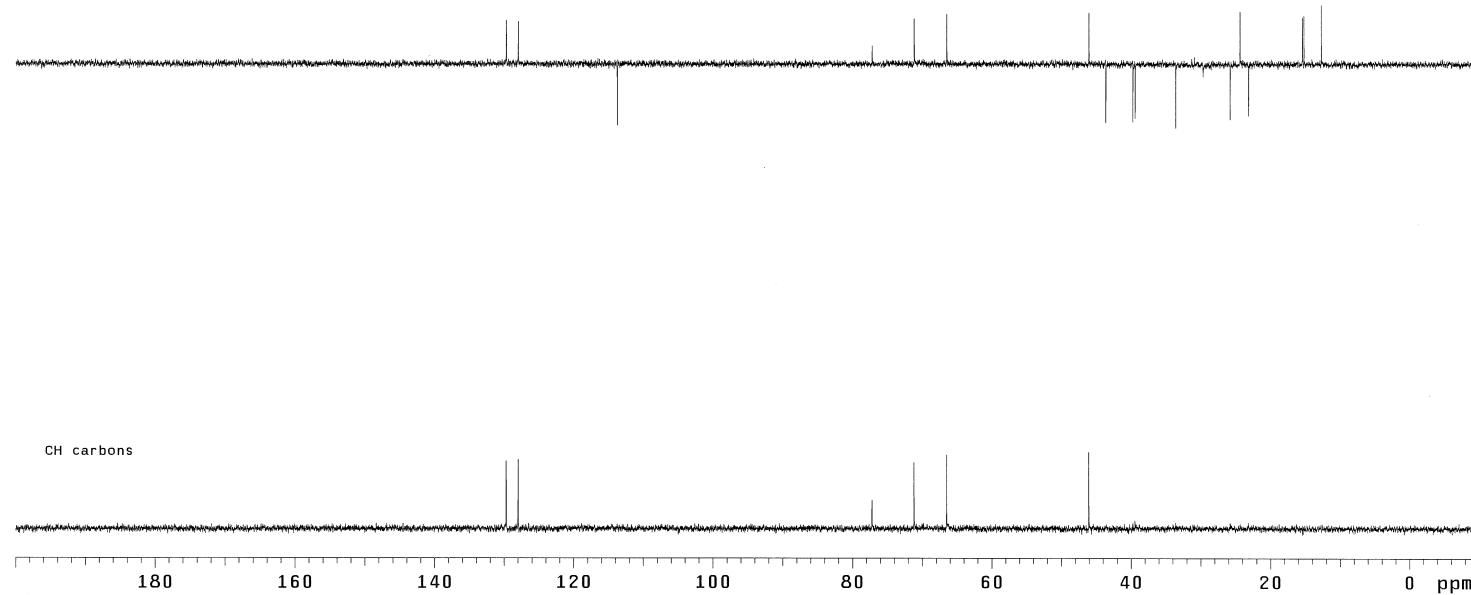
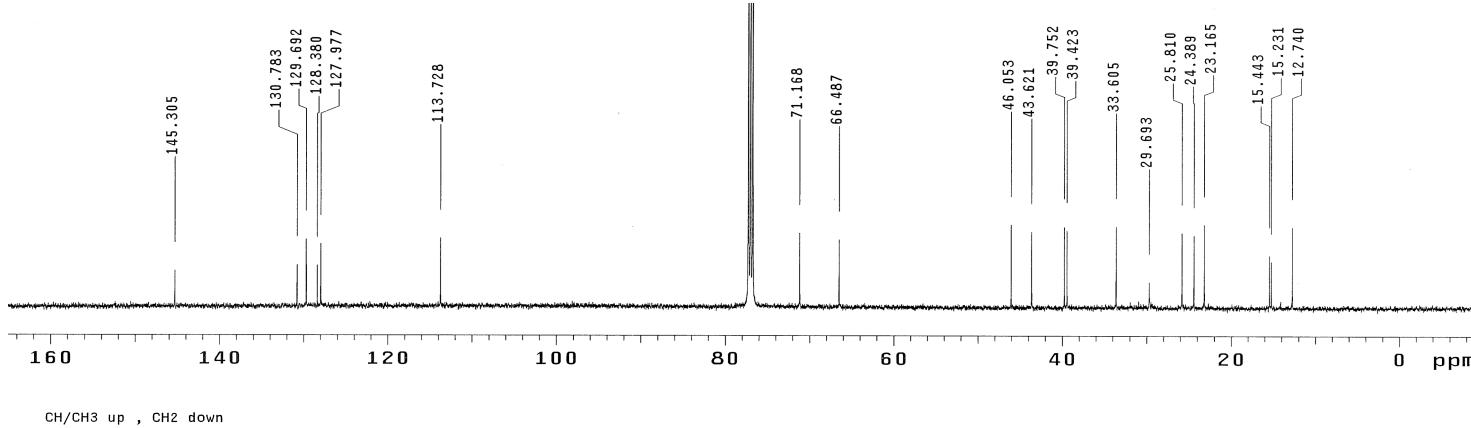


Figure S12: DEPT NMR (125 MHz, CDCl₃) spectrum of **2**.

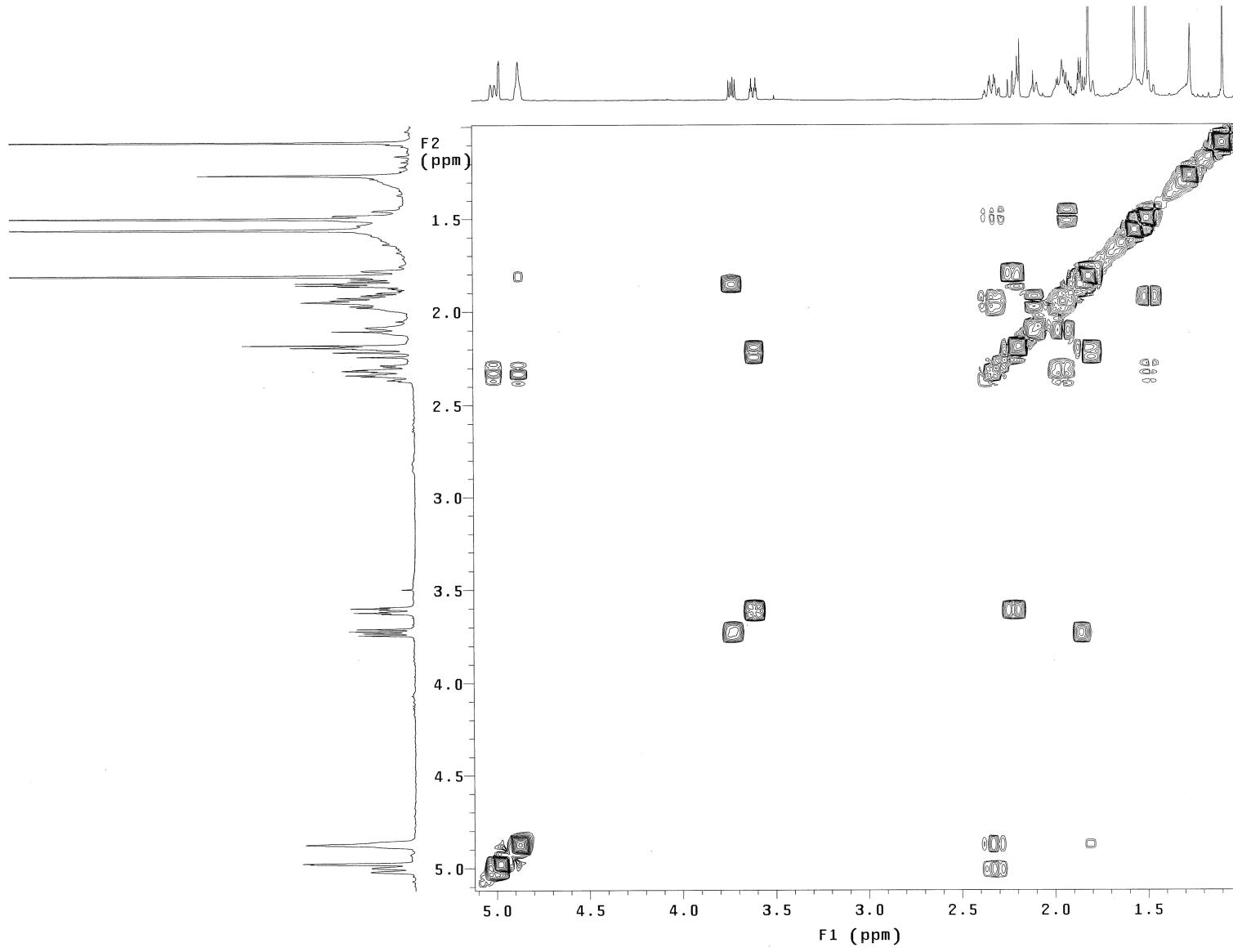


Figure S13: COSY NMR (500 MHz, CDCl_3) spectrum of 2.

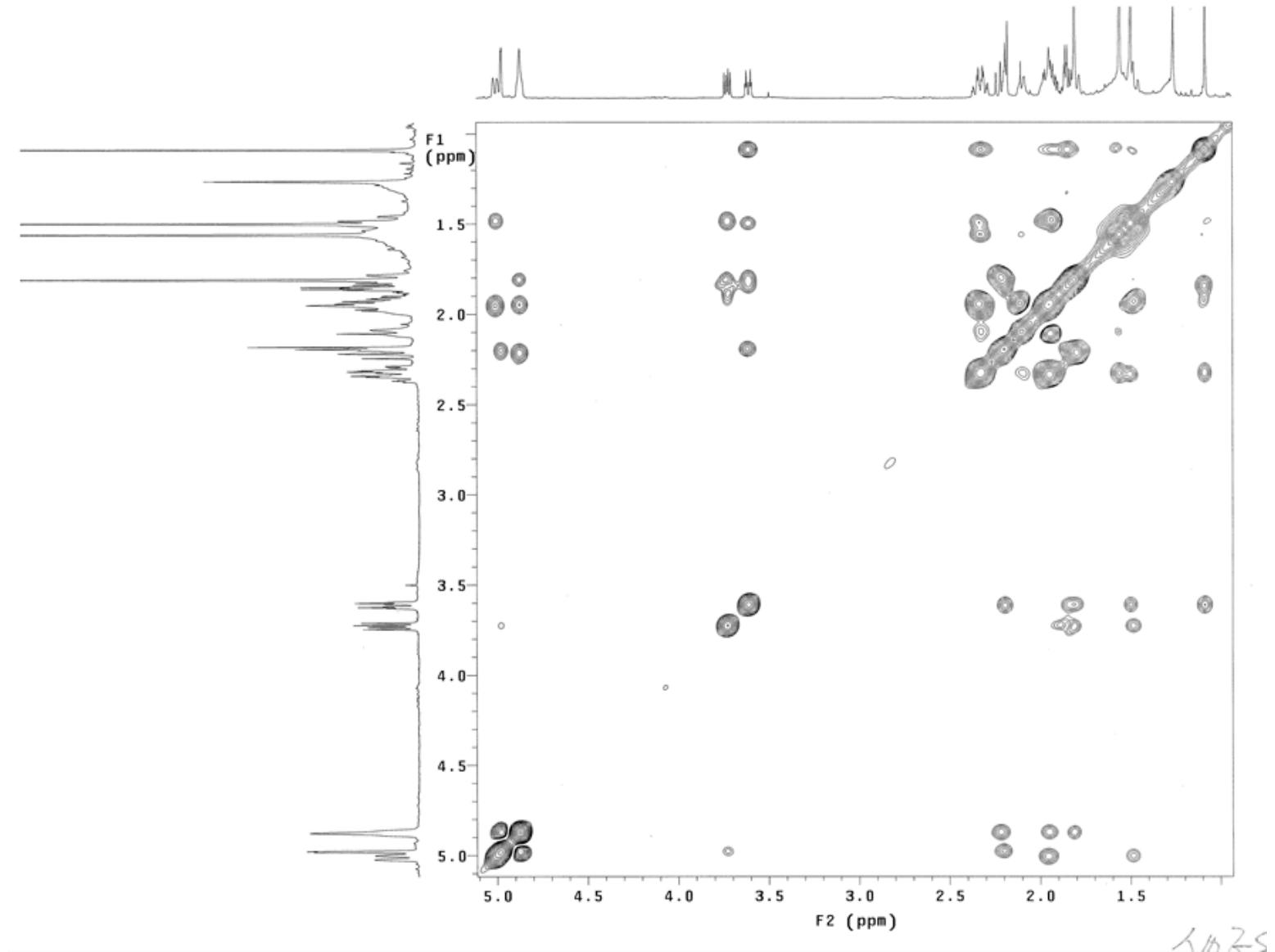


Figure S14: NOESY NMR (500 MHz, CDCl_3) spectrum of **2**.

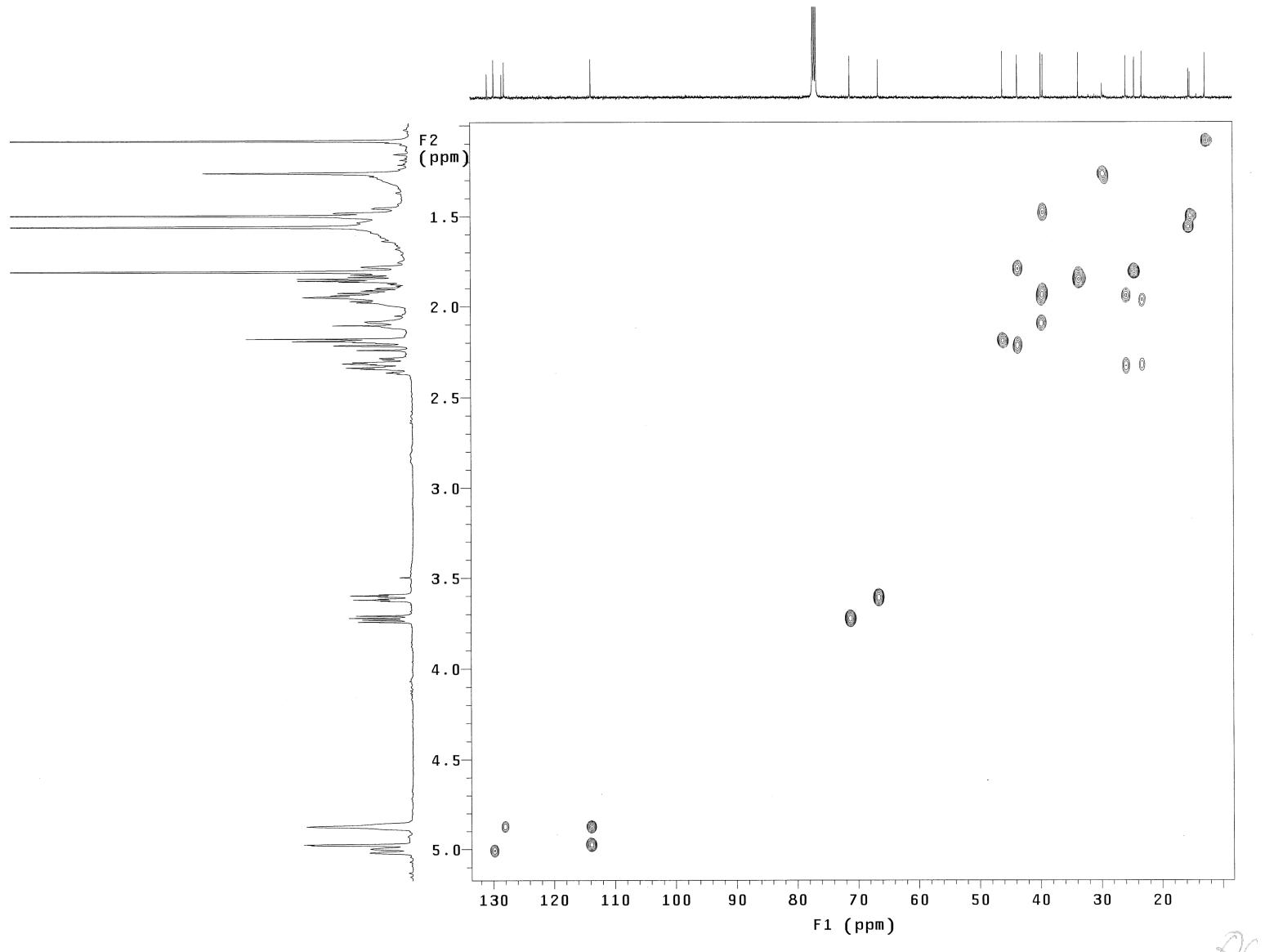


Figure S15: HSQC NMR (500 MHz, CDCl₃) spectrum of 2.

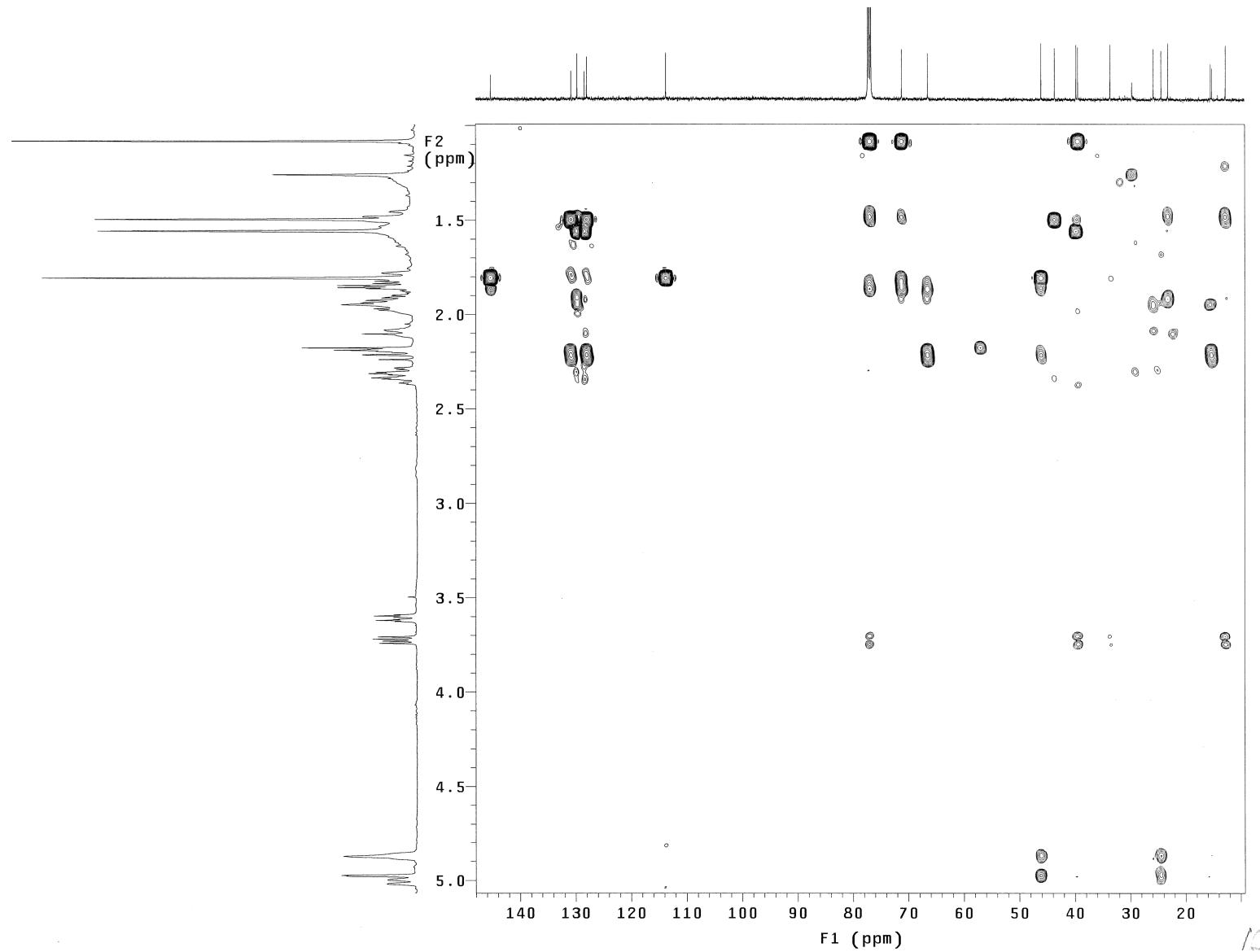
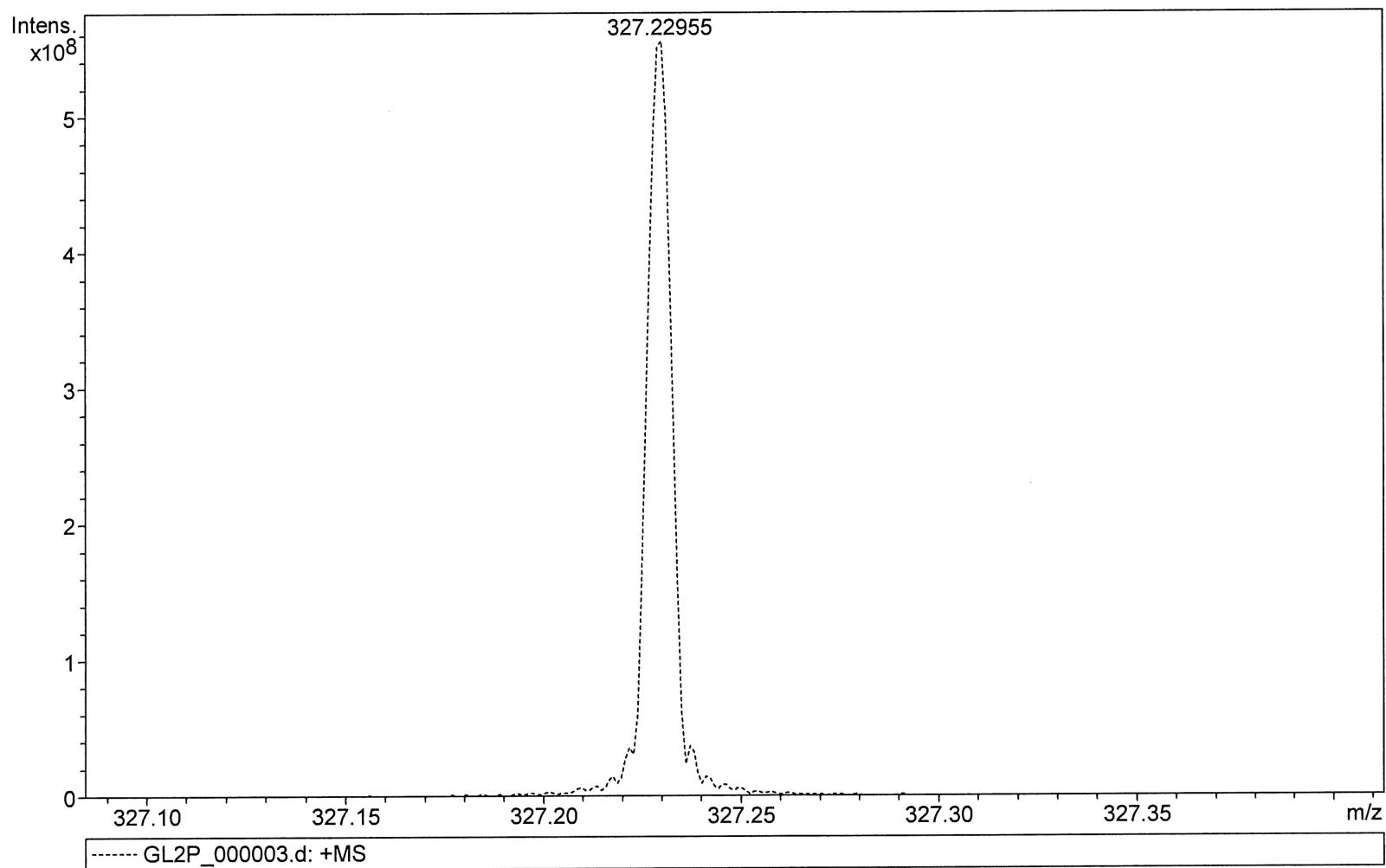


Figure S16: HMBC NMR (500 MHz, CDCl₃) spectrum of **2**.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	$m\Sigma$	rdb	e^- Conf	N-Rule
327.22955	1	C 20 H 32 Na O 2	100.00	327.22945	-0.10	-0.30	4.3	4.5	even	ok

Figure S17: HRESIMS spectrum of **2**.

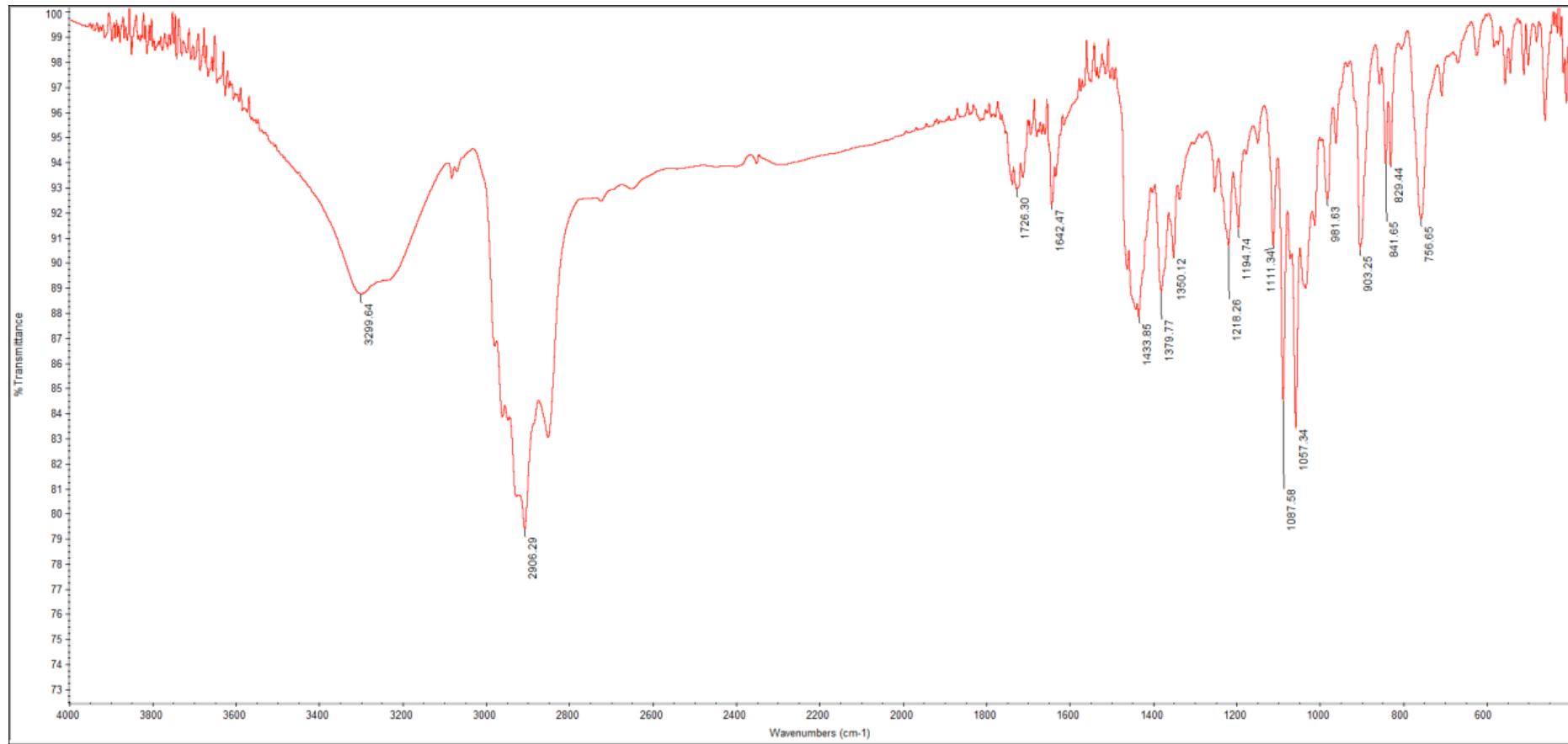


Figure S18: IR spectrum of 2.

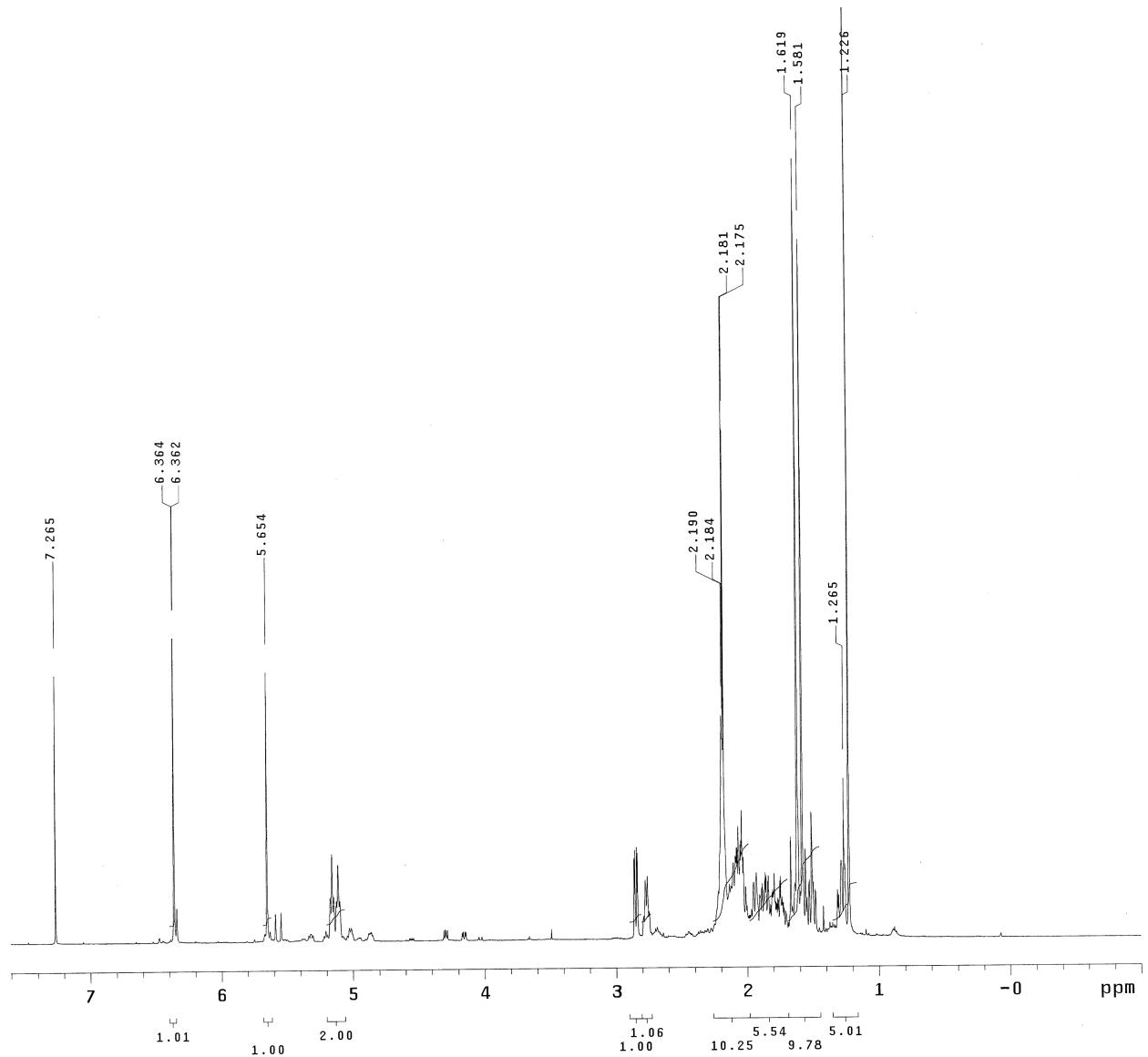


Figure S19: ^1H NMR (500 MHz, CDCl_3) spectrum of 3.

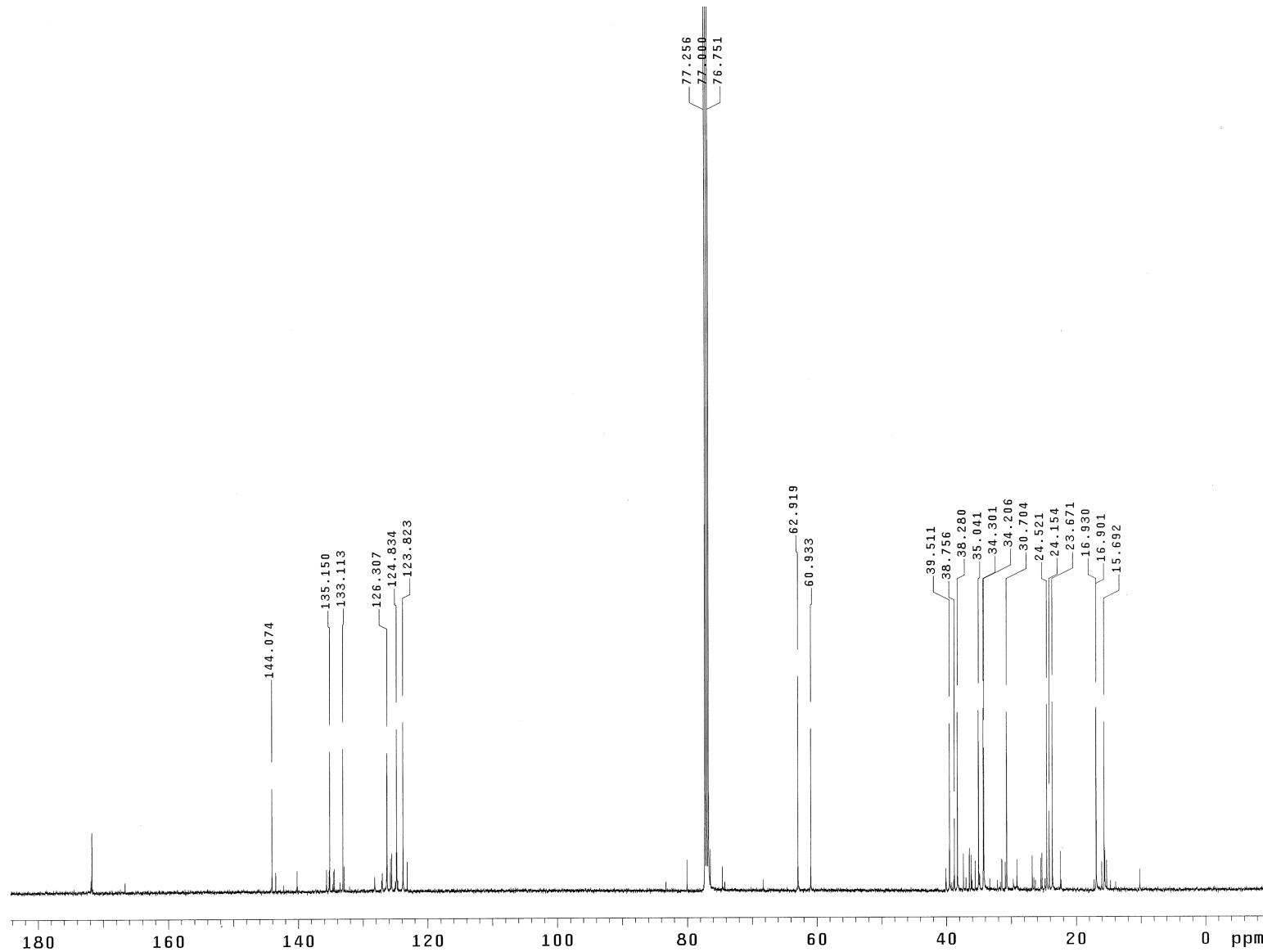
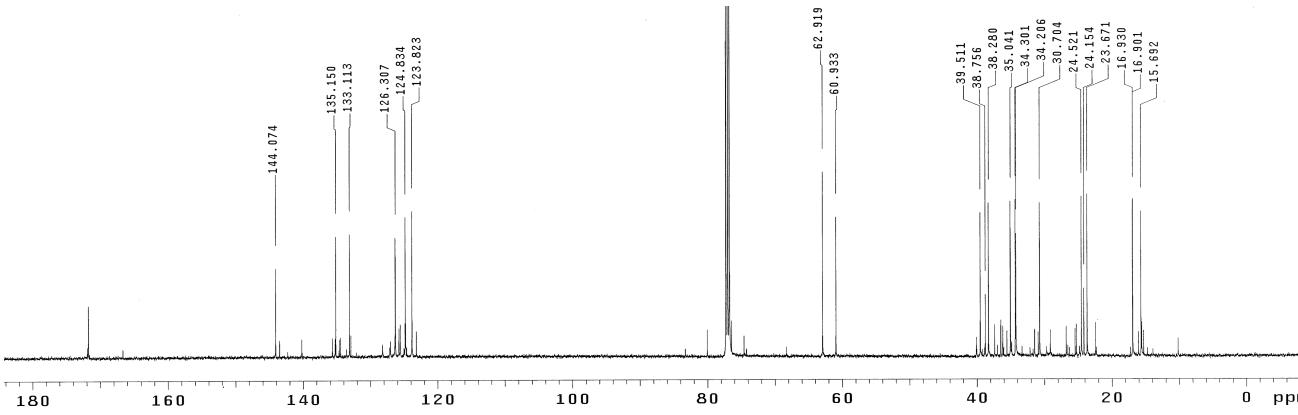
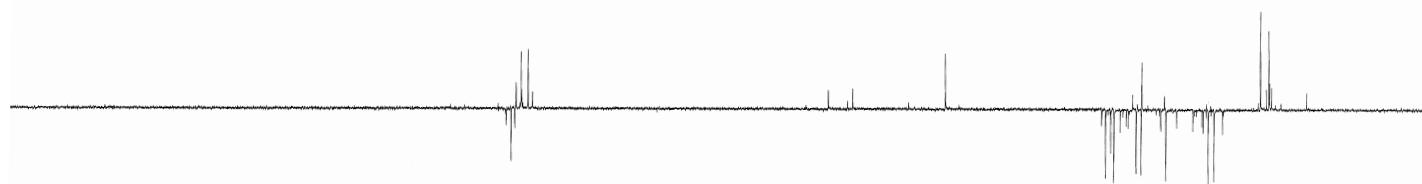


Figure S20: ^{13}C NMR (125 MHz, CDCl_3) spectrum of 3.



CH/CH₃ up , CH₂ down



CH carbons

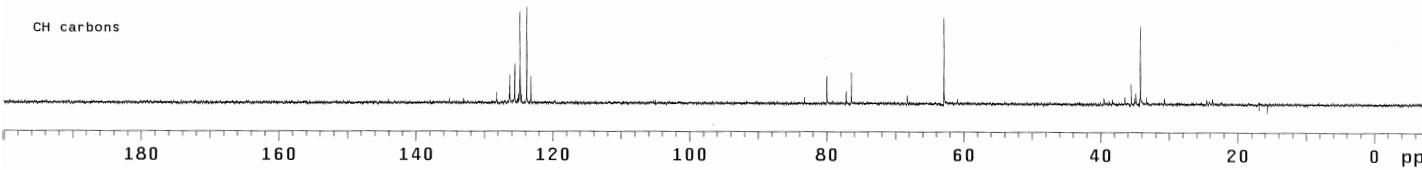


Figure S21: DEPT NMR (125 MHz, CDCl₃) spectrum of 3.

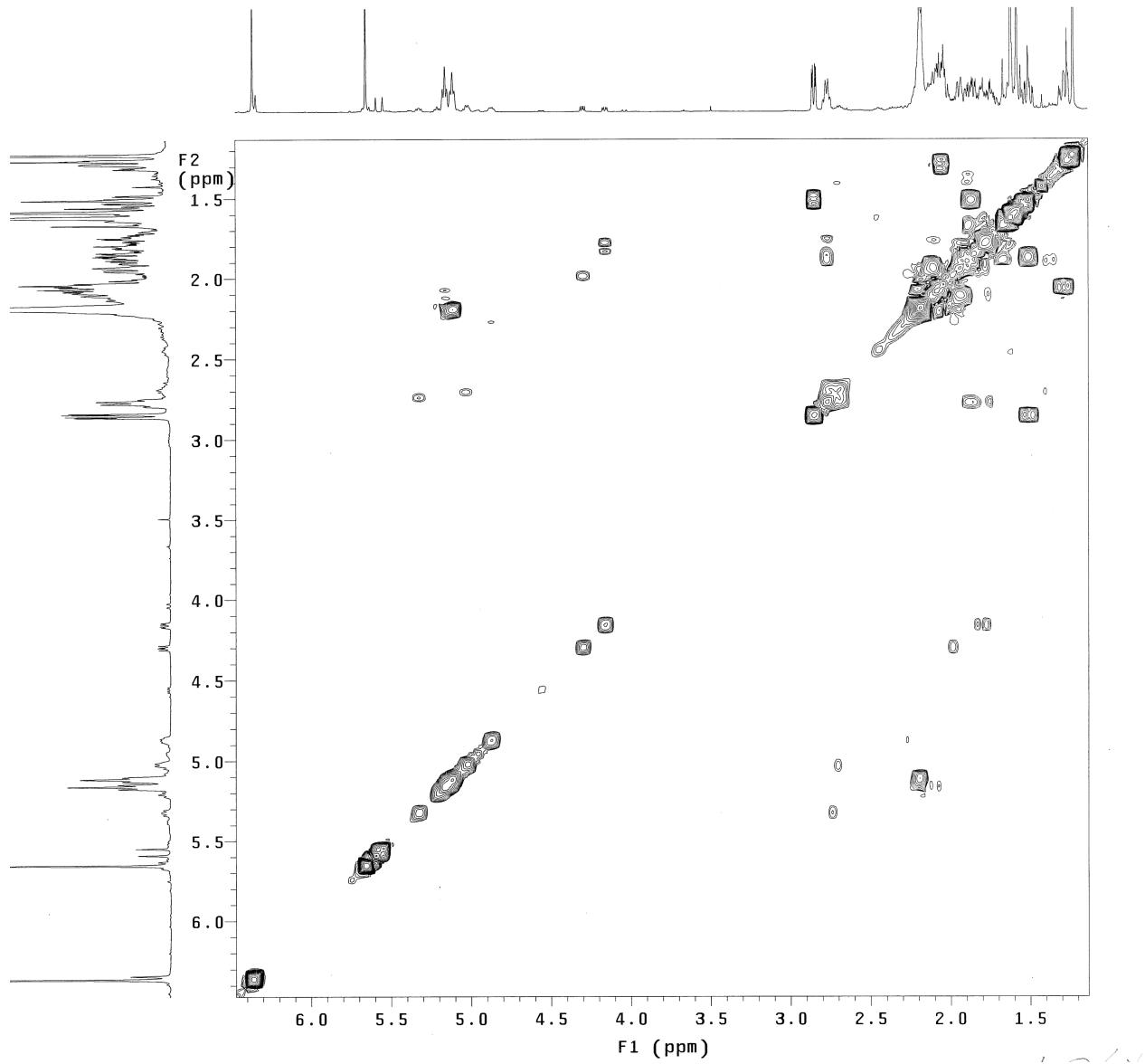


Figure S22: COSY NMR (500 MHz, CDCl_3) spectrum of 3.

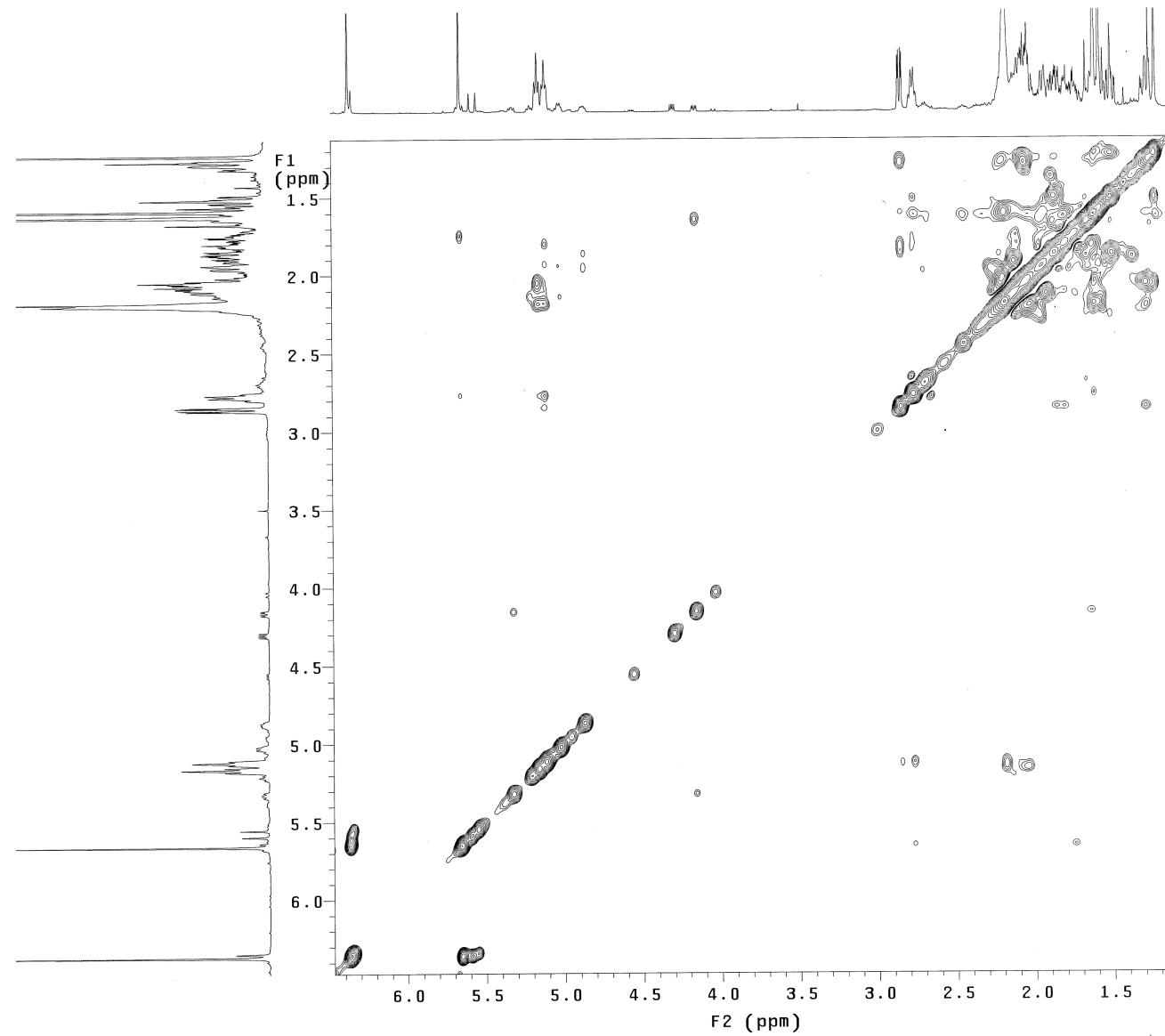


Figure S23: NOESY NMR (500 MHz, CDCl_3) spectrum of 3.

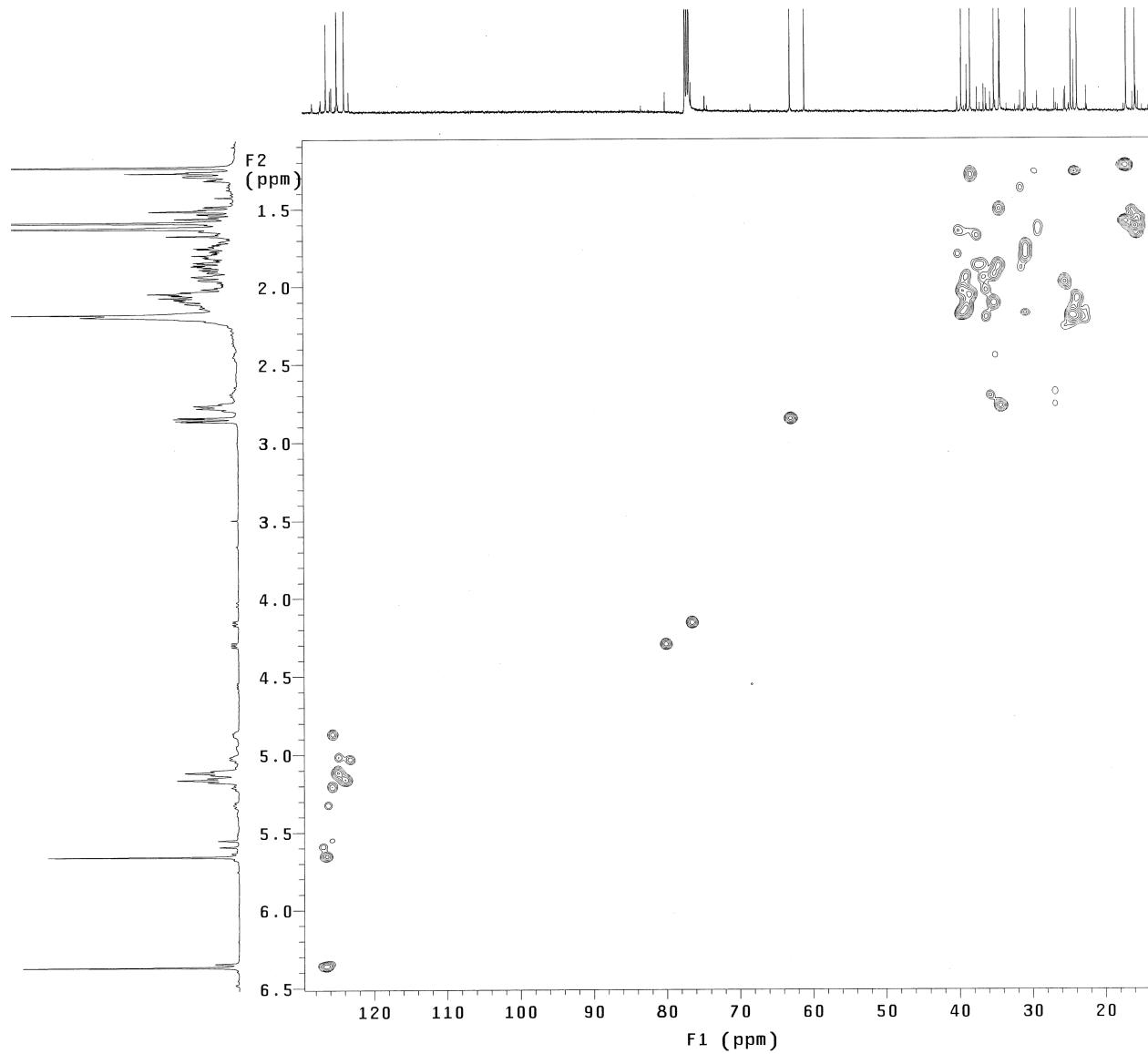


Figure S24: HSQC NMR (500 MHz, CDCl_3) spectrum of 3.

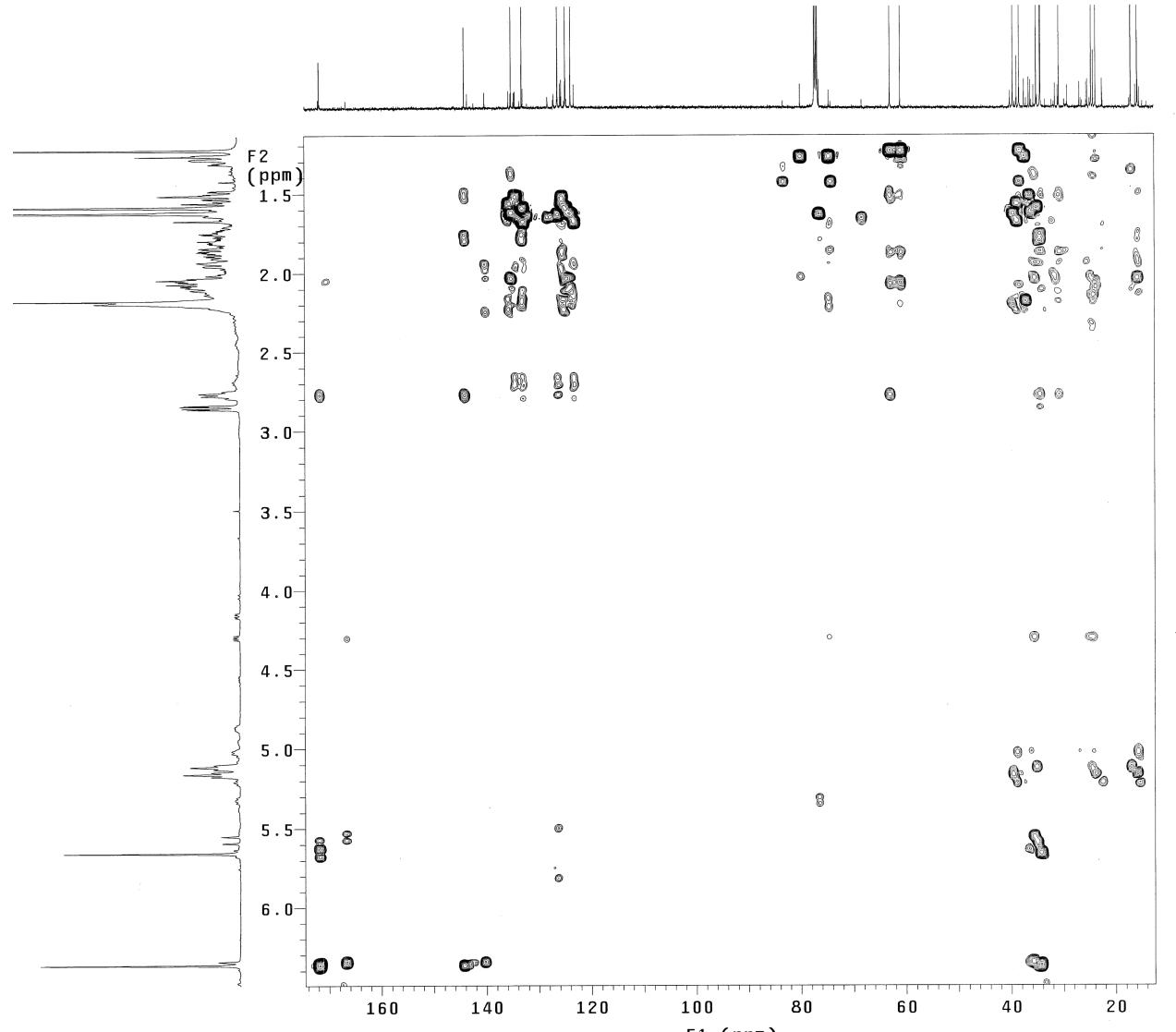
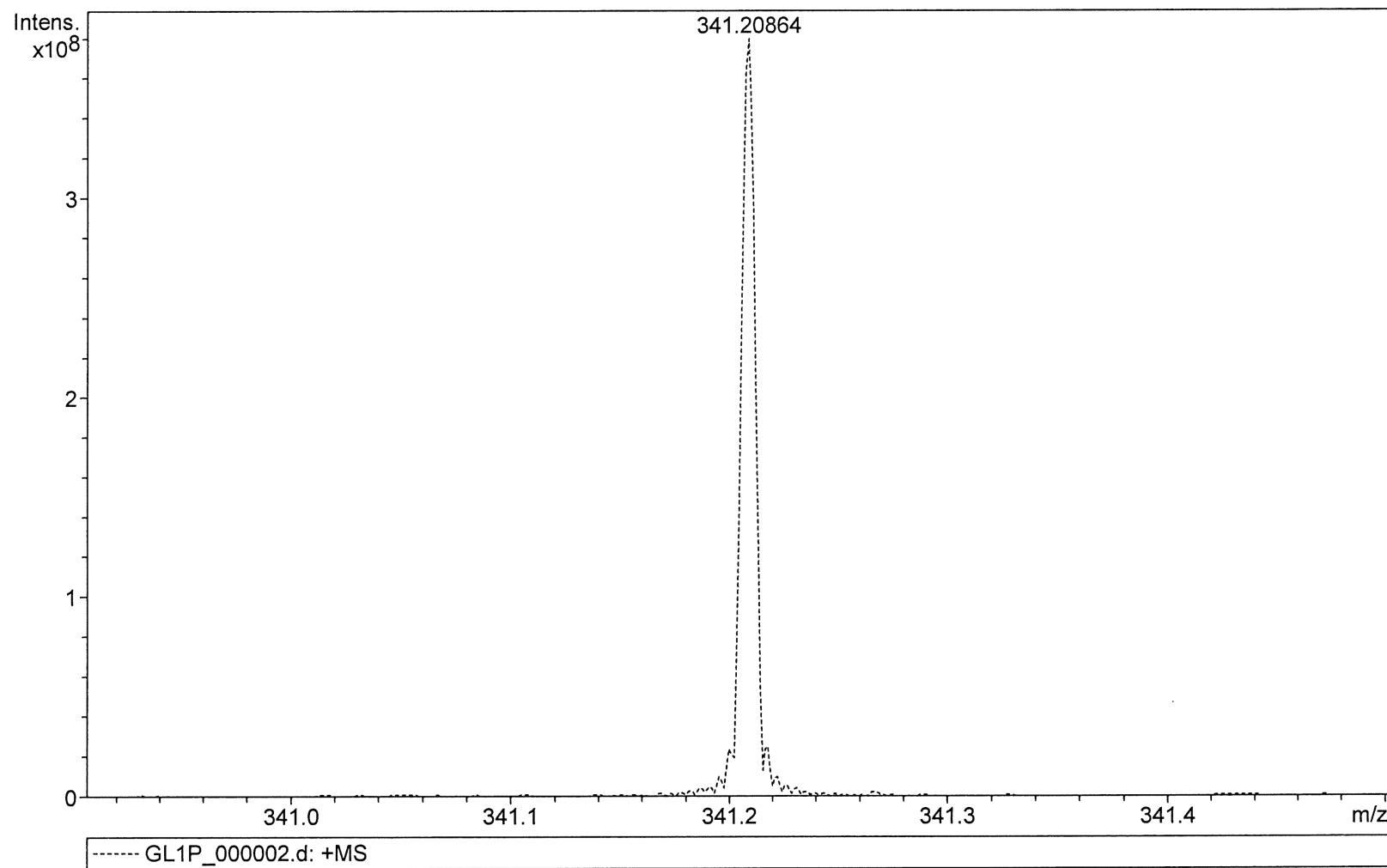


Figure S25: HMBC NMR (500 MHz, CDCl_3) spectrum of 3.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
341.20864	1	C 20 H 30 Na O 3	100.00	341.20872	0.07	0.22	5.2	5.5	even	ok

Figure S26: HRESIMS spectrum of 3.

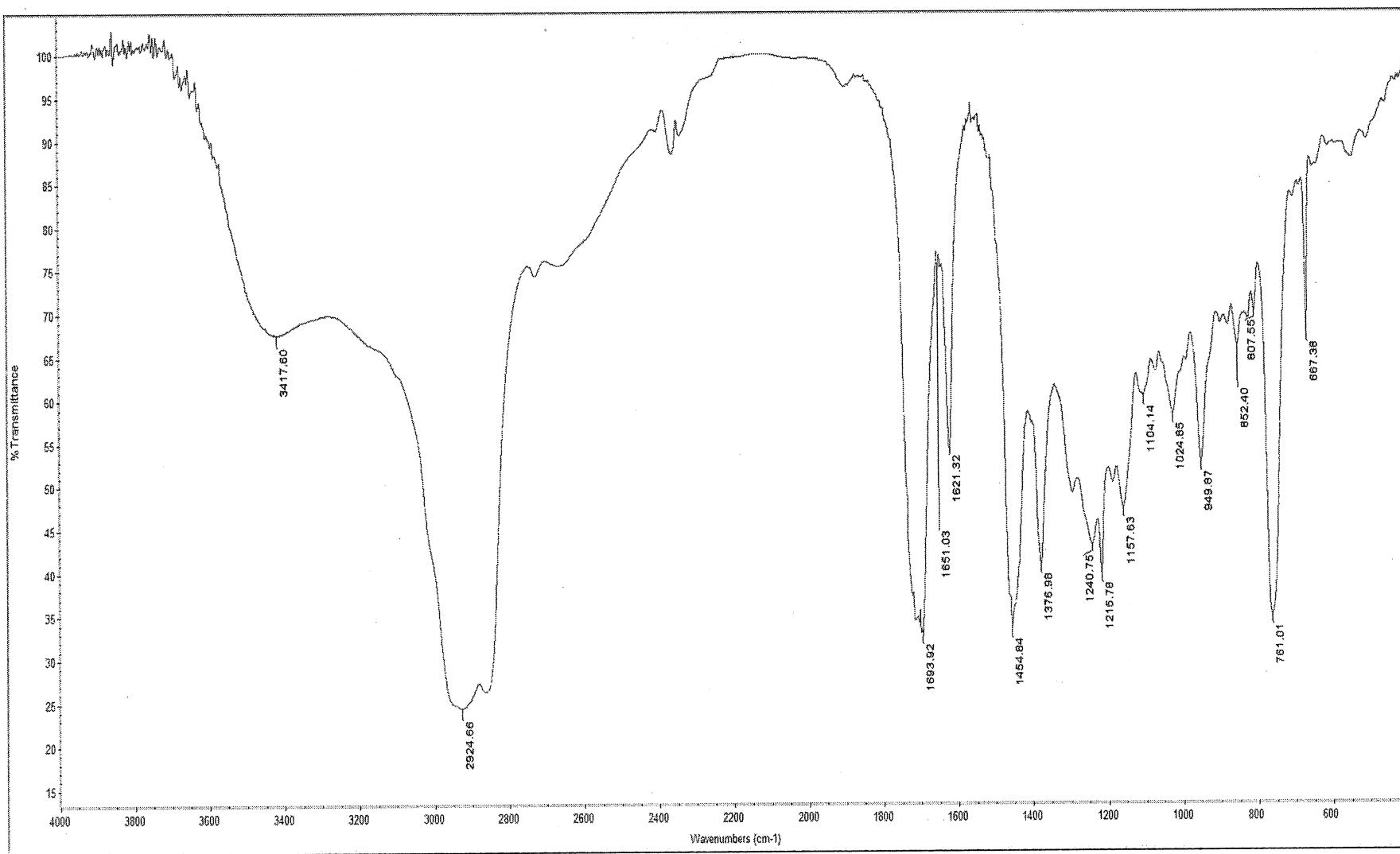


Figure S27: IR spectrum of 3.