

Supplementary Information

Antileukemic Scalarane Sesterterpenoids and Meroditerpenoid from *Carteriospongia (Phyllospongia) sp.*, Induce Apoptosis via Dual Inhibitory Effects on Topoisomerase II and Hsp90

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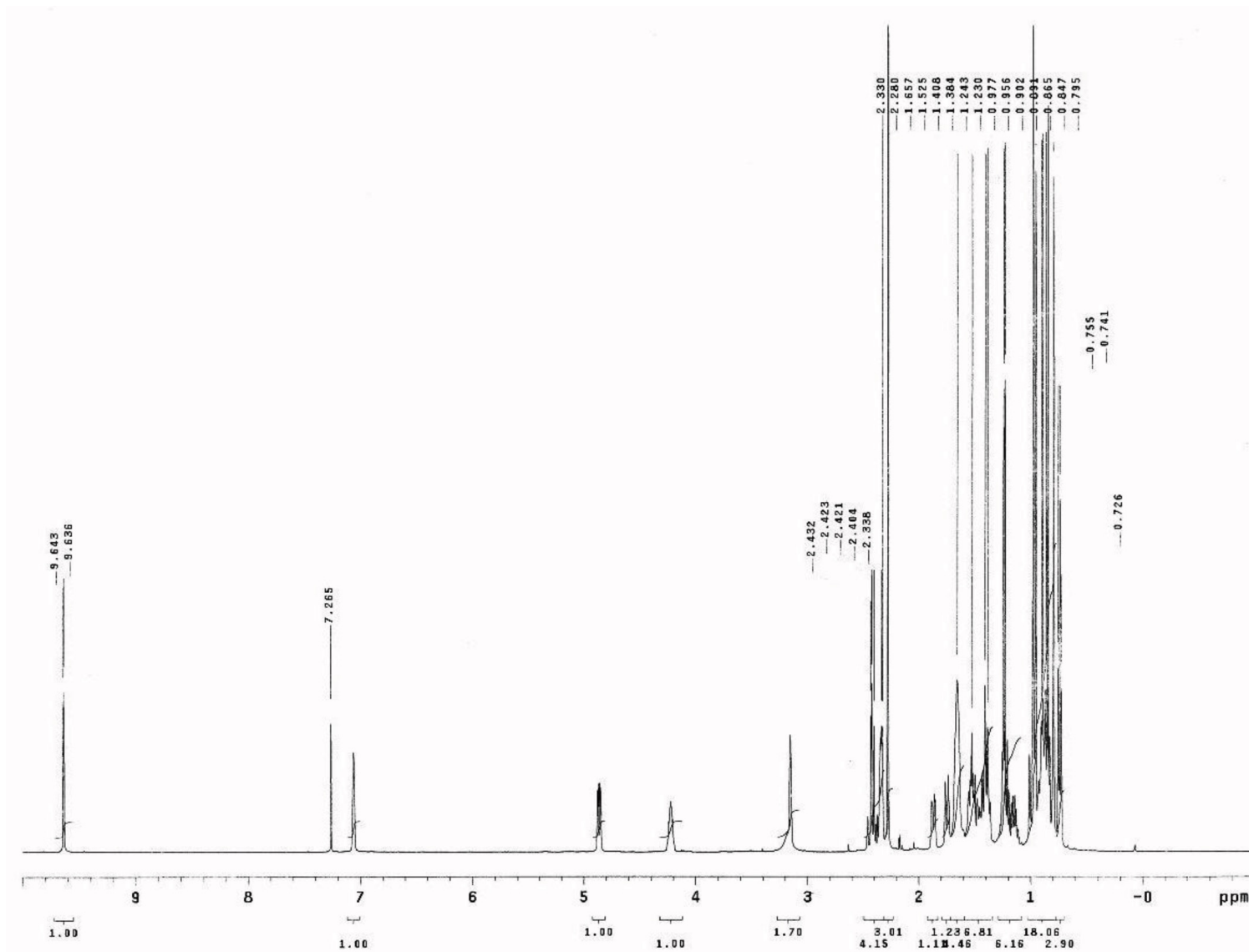


Figure S1: ^1H NMR (500 MHz, CDCl_3) spectrum of **1**.

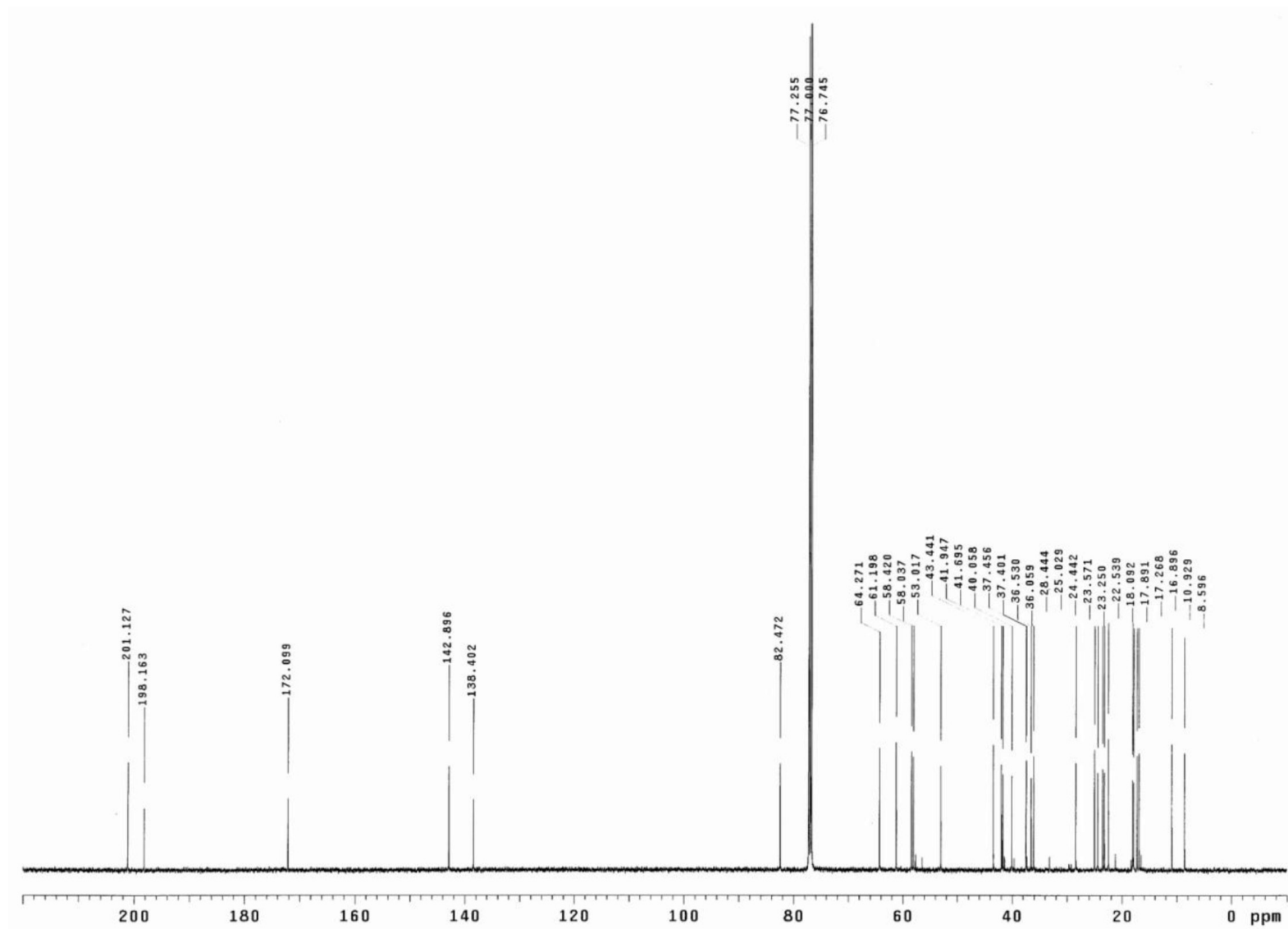


Figure S2: ¹³C NMR (125 MHz, CDCl₃) spectrum of 1.

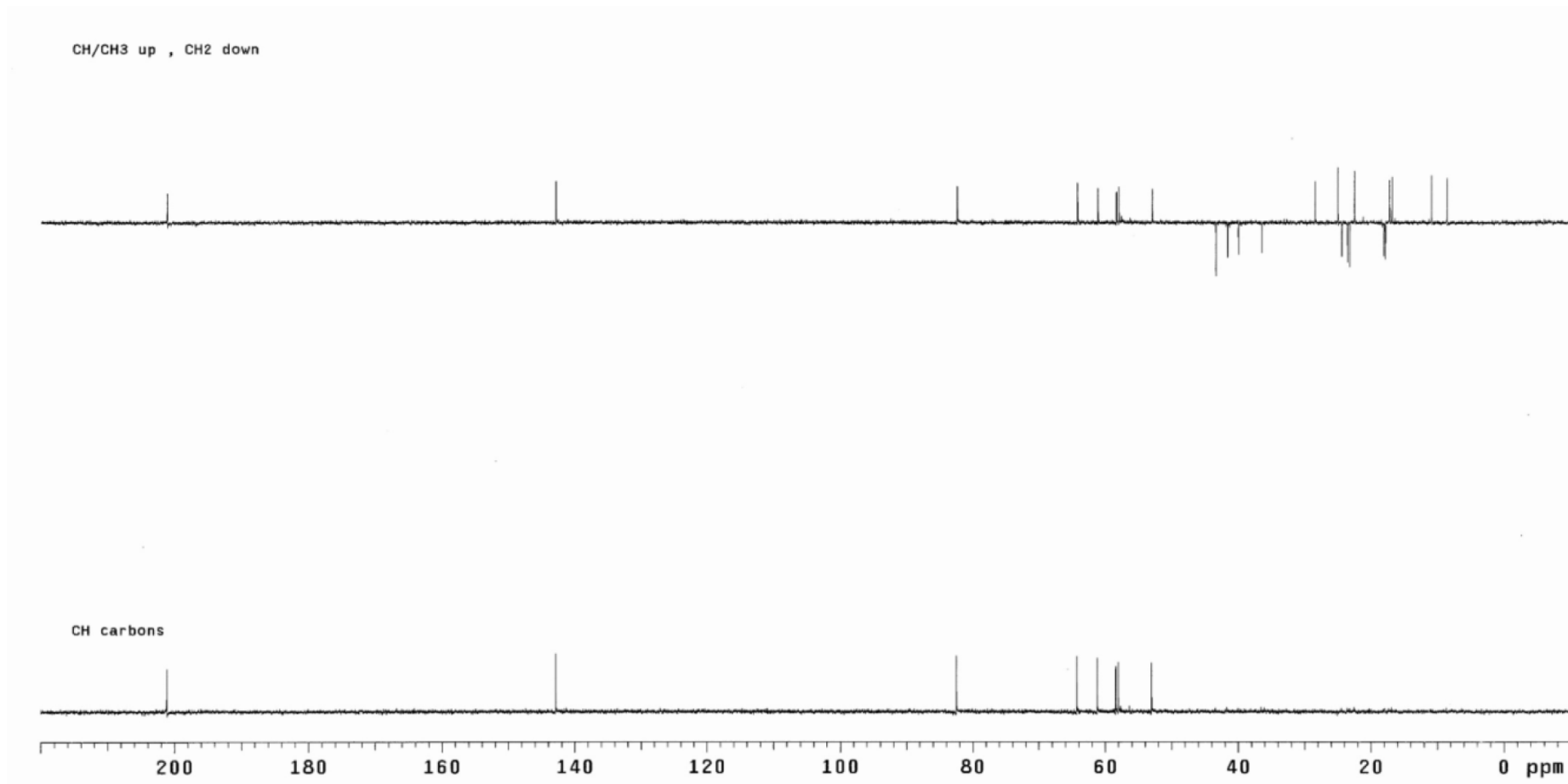


Figure S3: DEPT NMR (125 MHz, CDCl₃) spectrum of **1**.

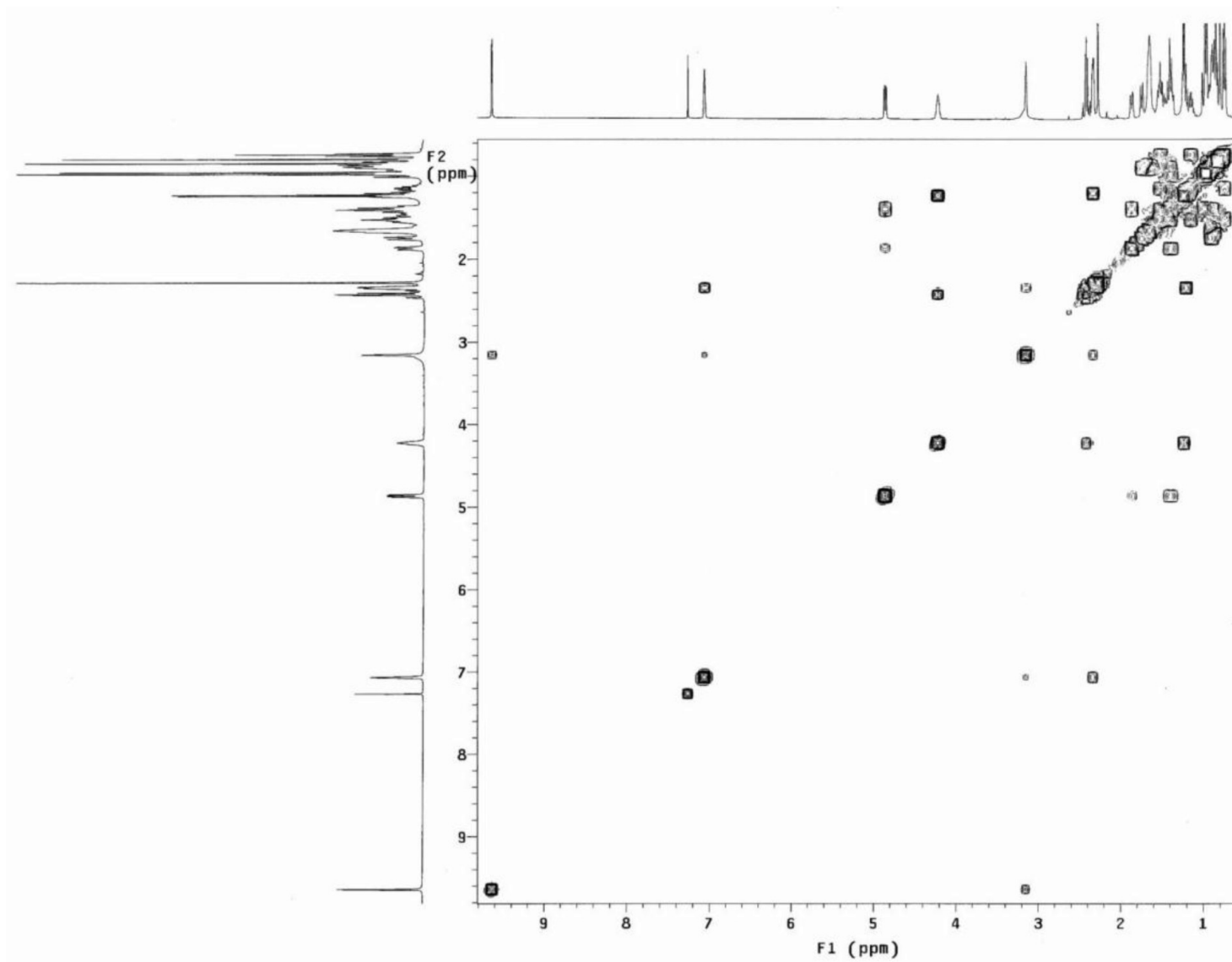


Figure S4: COSY NMR (500 MHz, CDCl₃) spectrum of **1**.

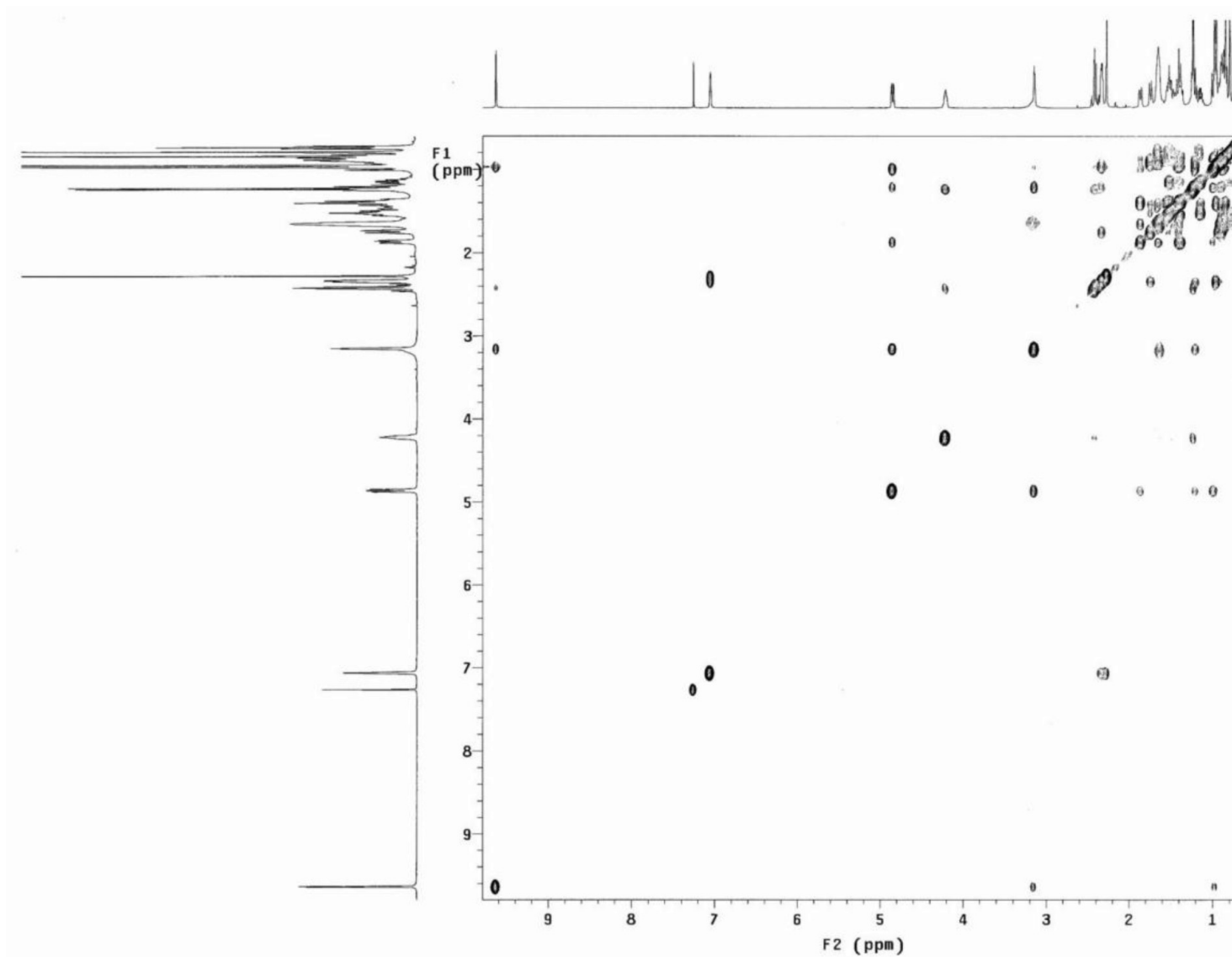


Figure S5: NOESY NMR (500 MHz, CDCl₃) spectrum of **1**.

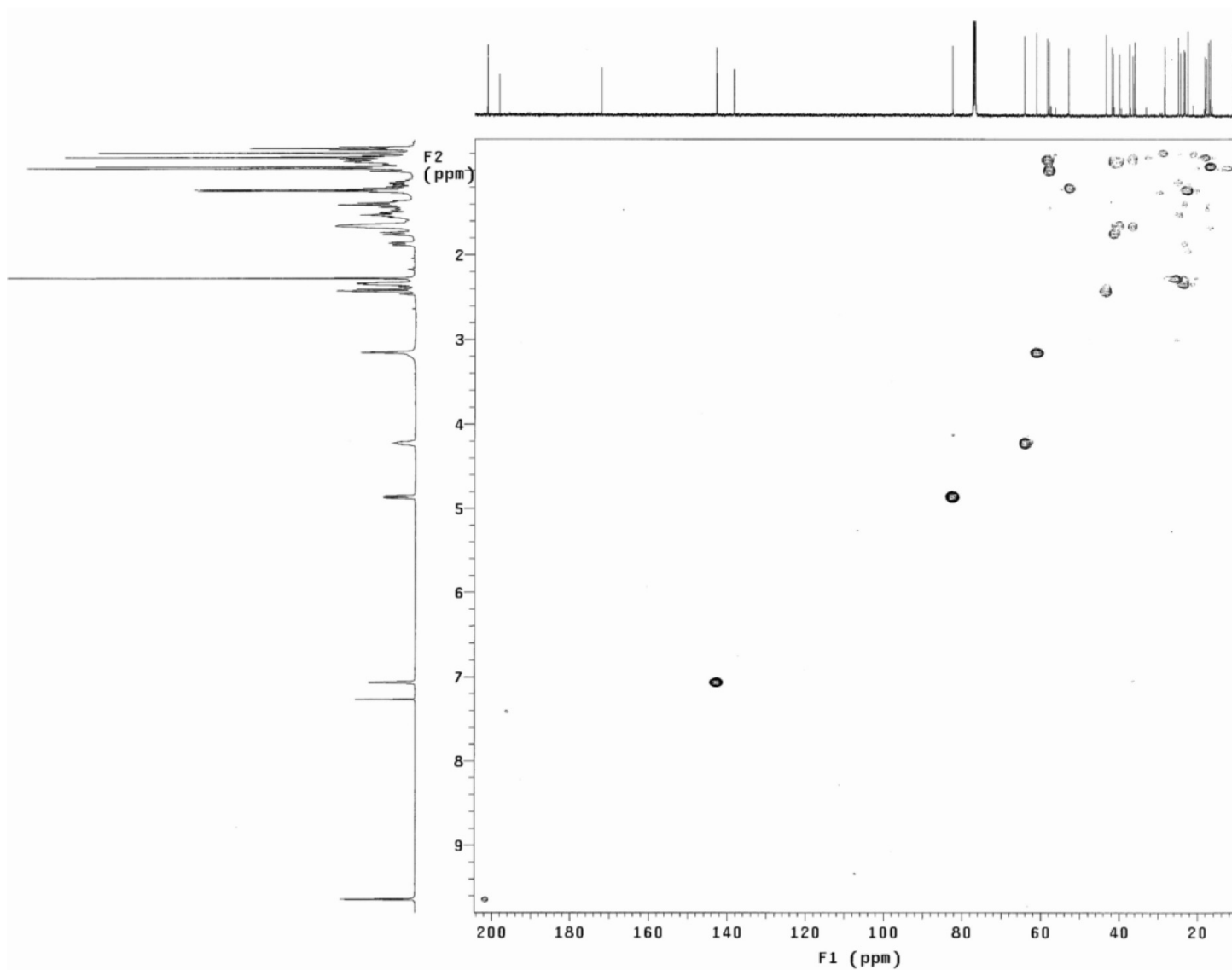


Figure S6: HSQC NMR (500 MHz, CDCl_3) spectrum of **1**.

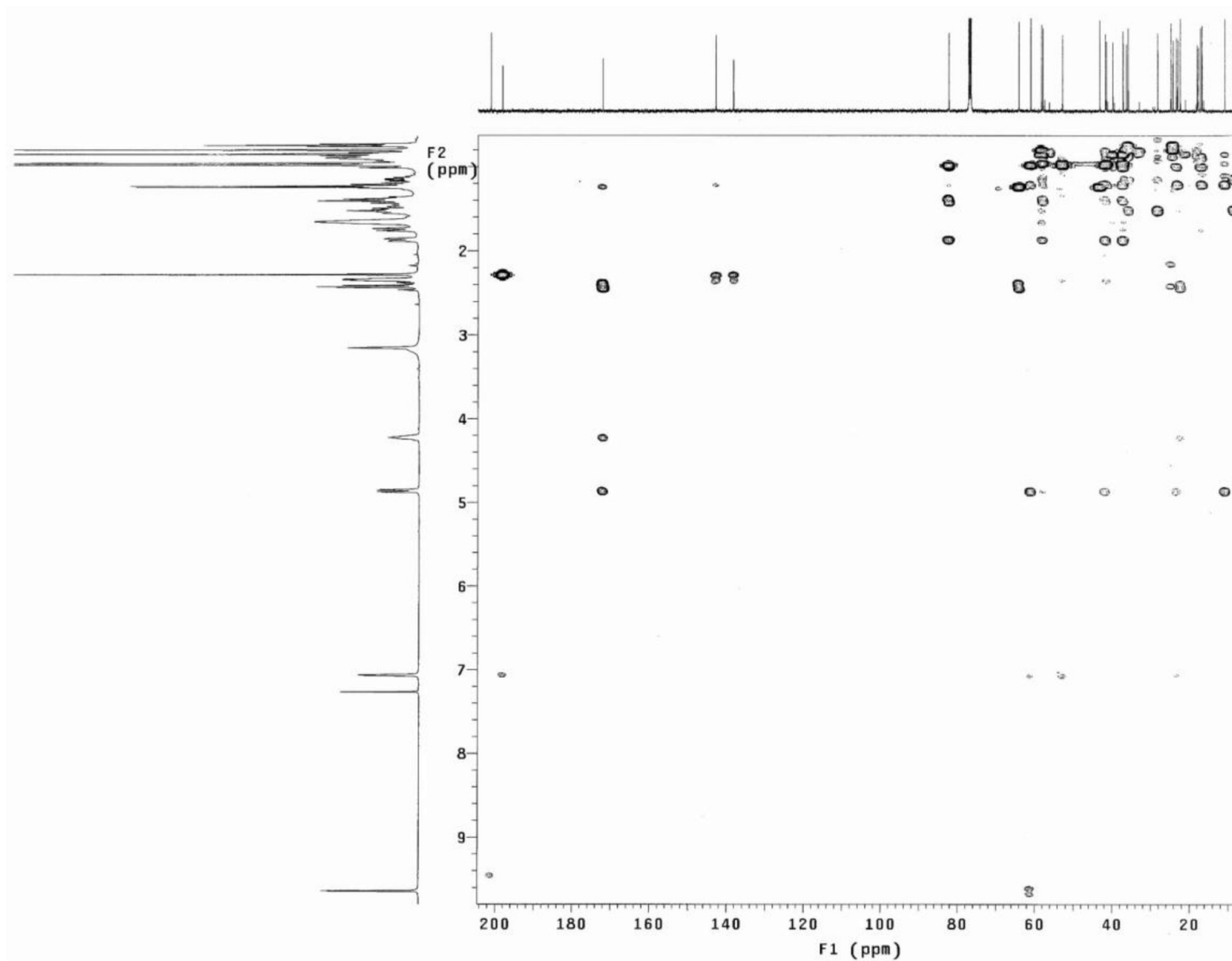


Figure S7: HMBC NMR (500 MHz, CDCl_3) spectrum of **1**.

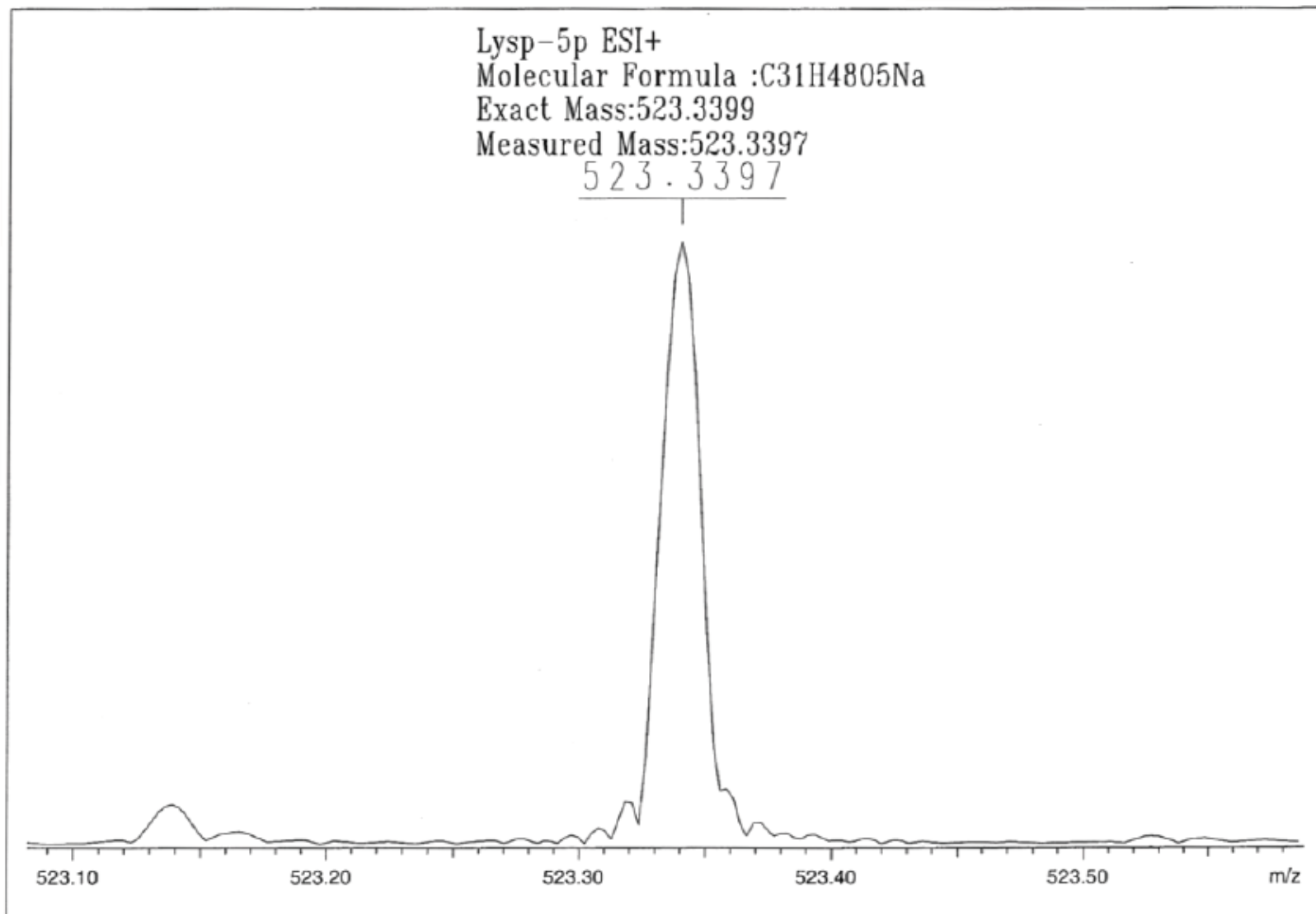


Figure S8: HRESIMS spectrum of **1**.

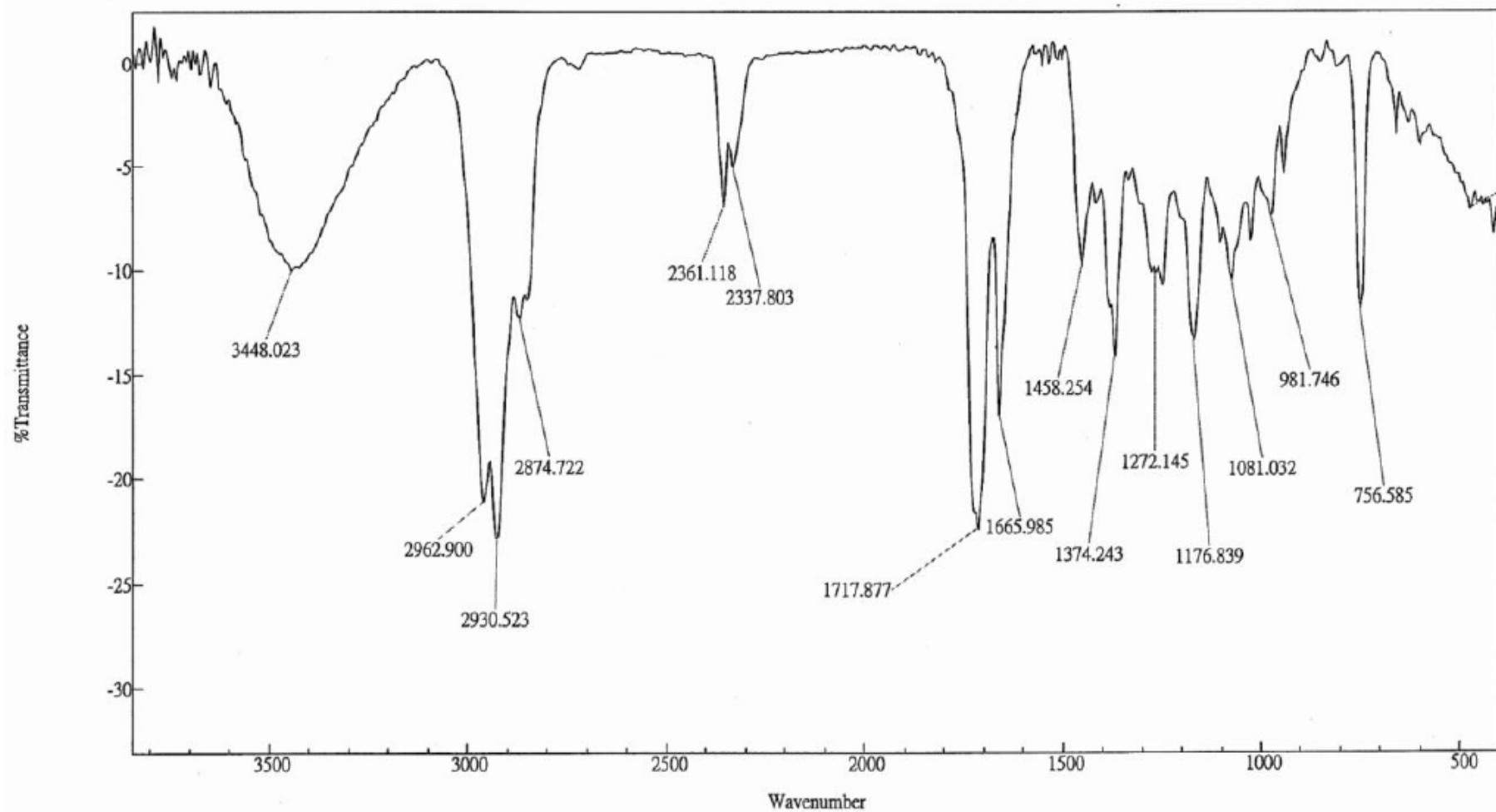


Figure S9: IR spectrum of **1**.

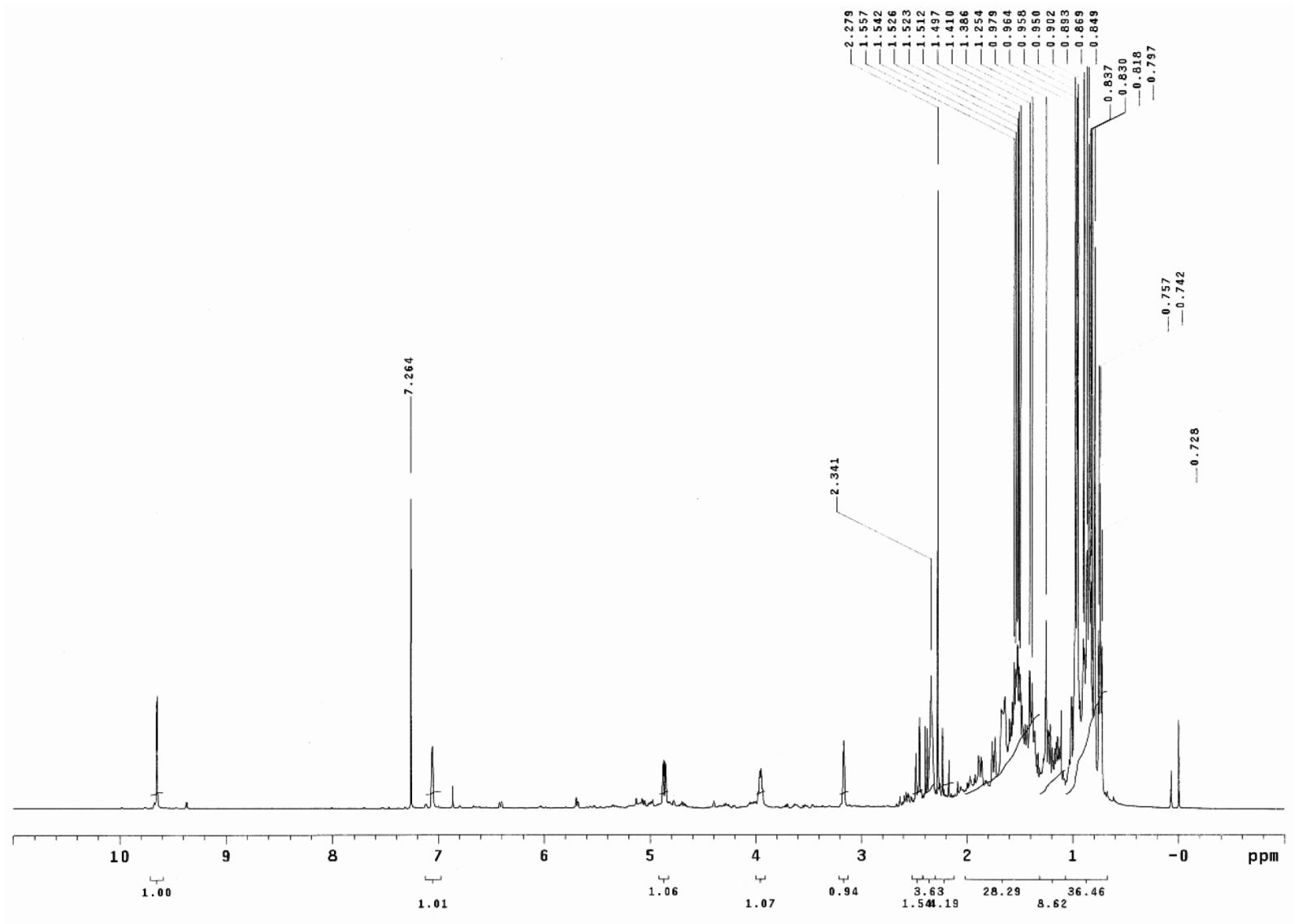


Figure S10: ¹H NMR (500 MHz, CDCl₃) spectrum of **2**.

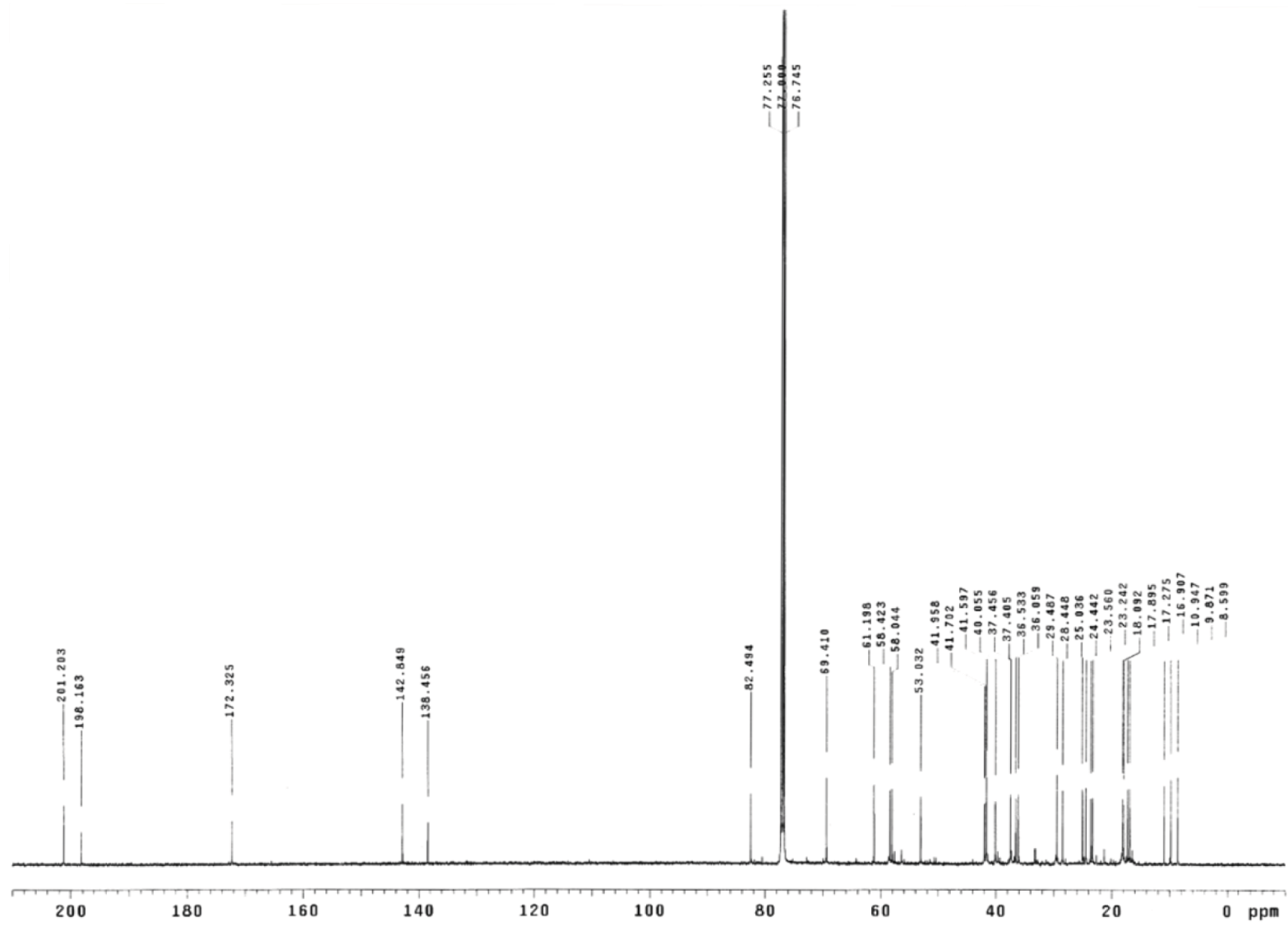


Figure S11: ^{13}C NMR (125 MHz, CDCl_3) spectrum of **2**.

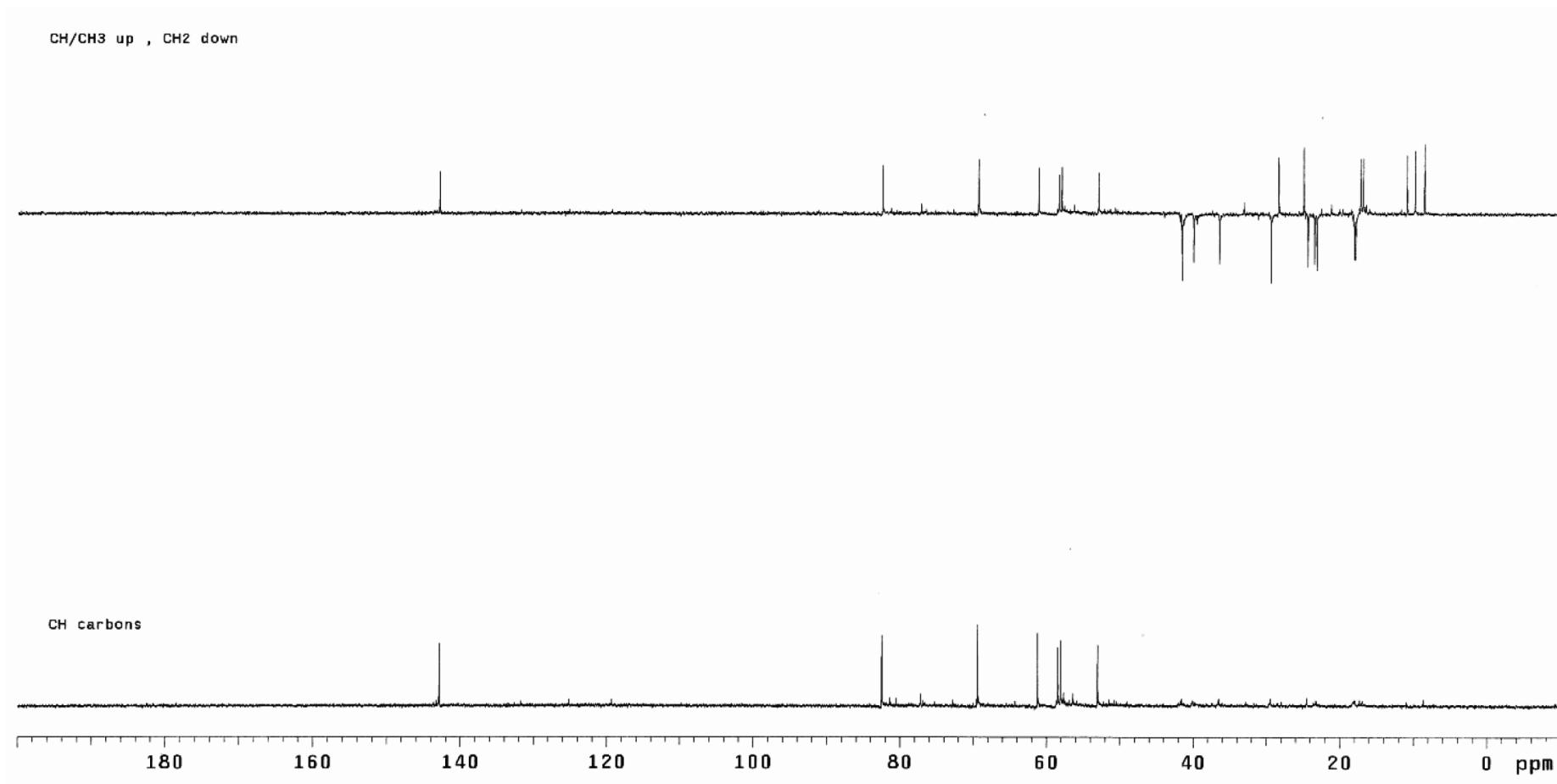


Figure S12: DEPT NMR (125 MHz, CDCl₃) spectrum of **2**.

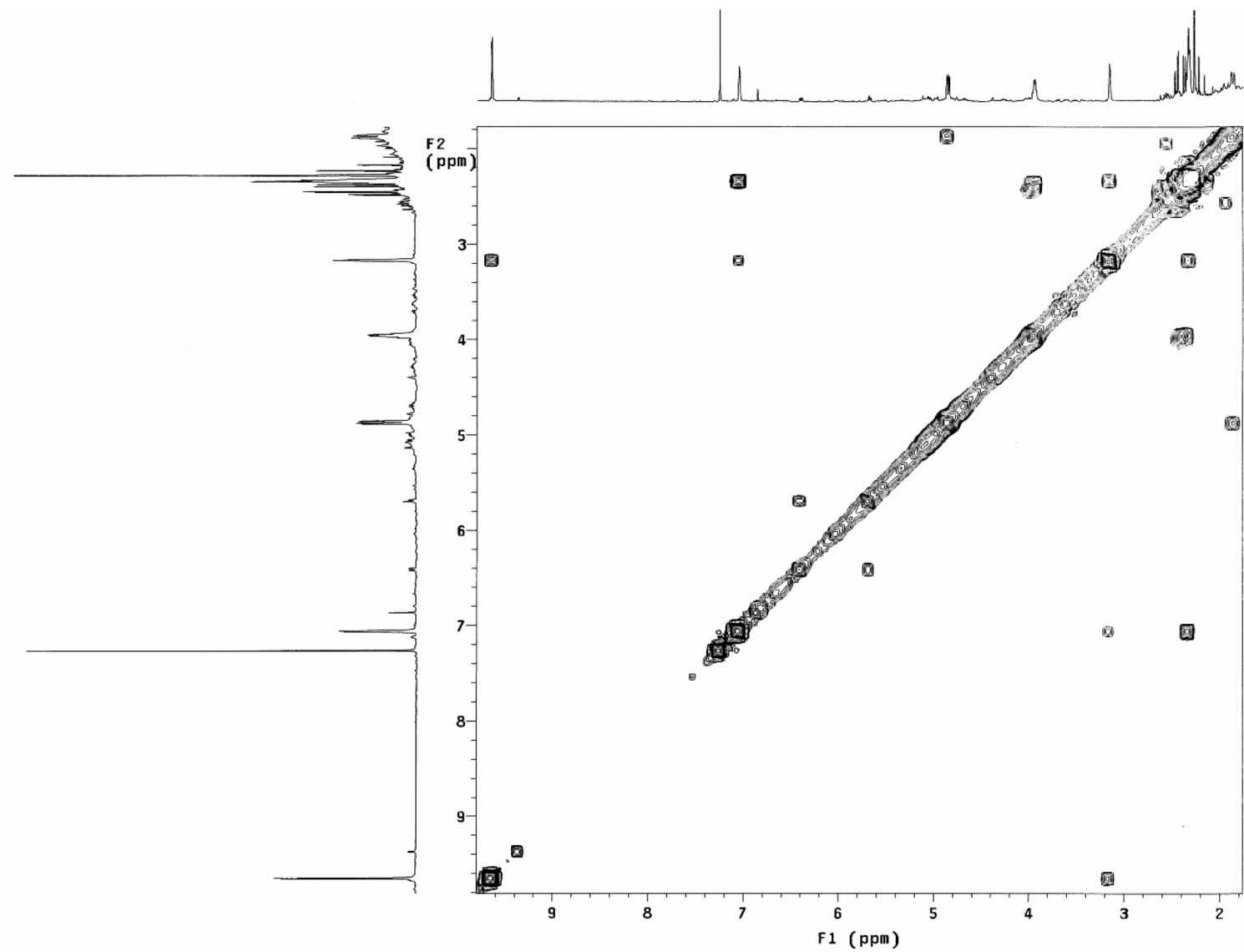


Figure S13: COSY NMR (500 MHz, CDCl₃) spectrum of **2**.

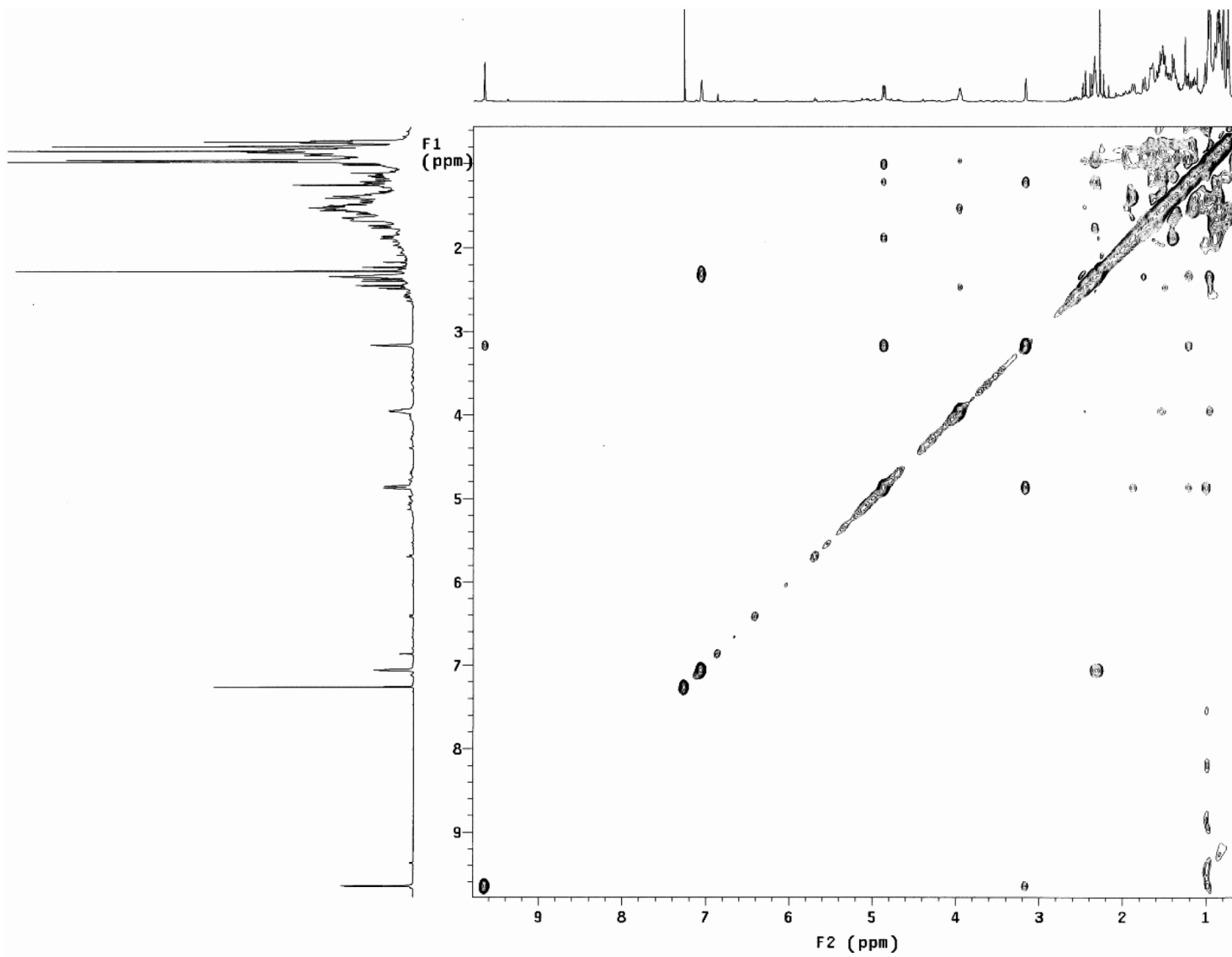


Figure S14: NOESY NMR (500 MHz, CDCl_3) spectrum of **2**.

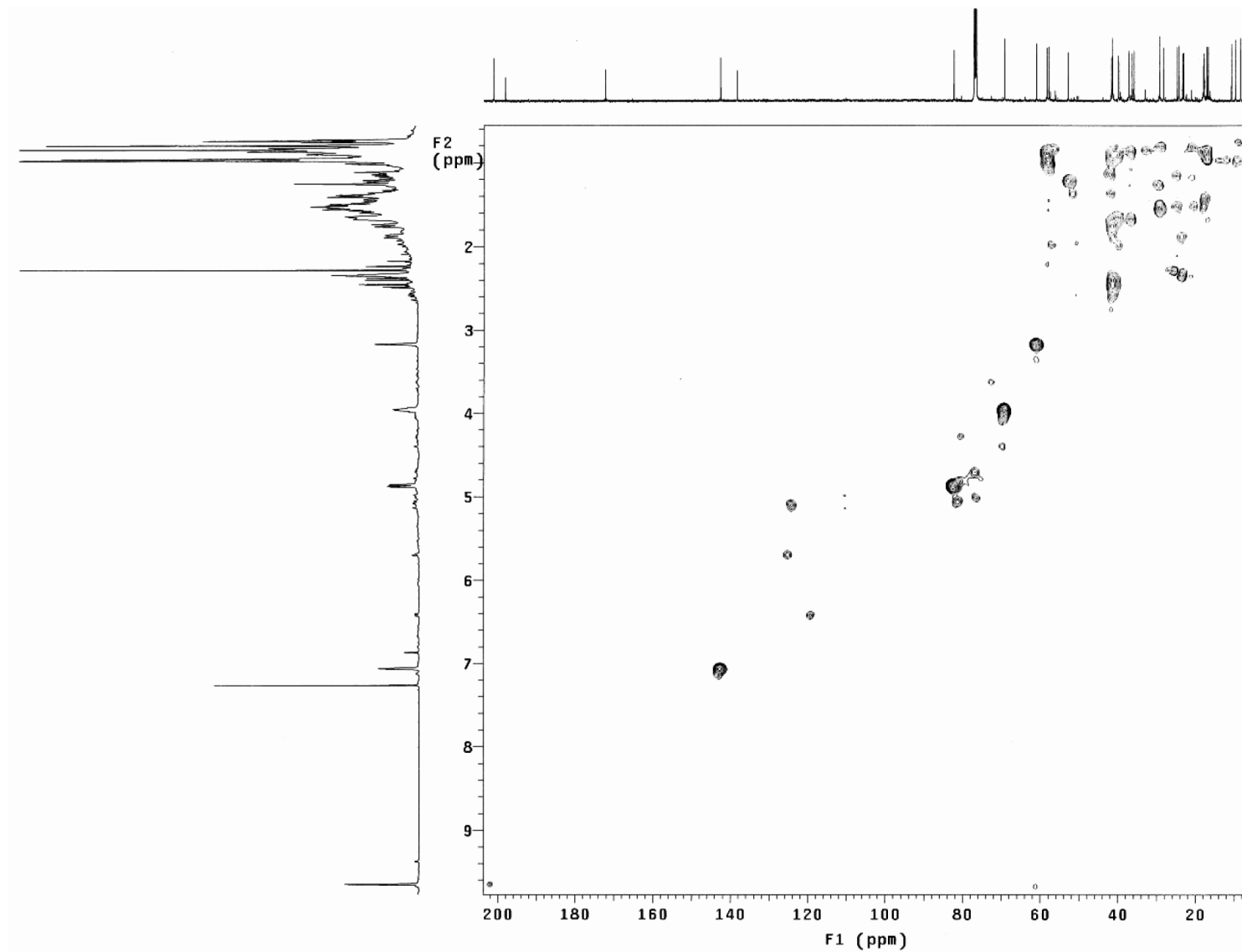


Figure S15: HSQC NMR (500 MHz, CDCl₃) spectrum of **2**.

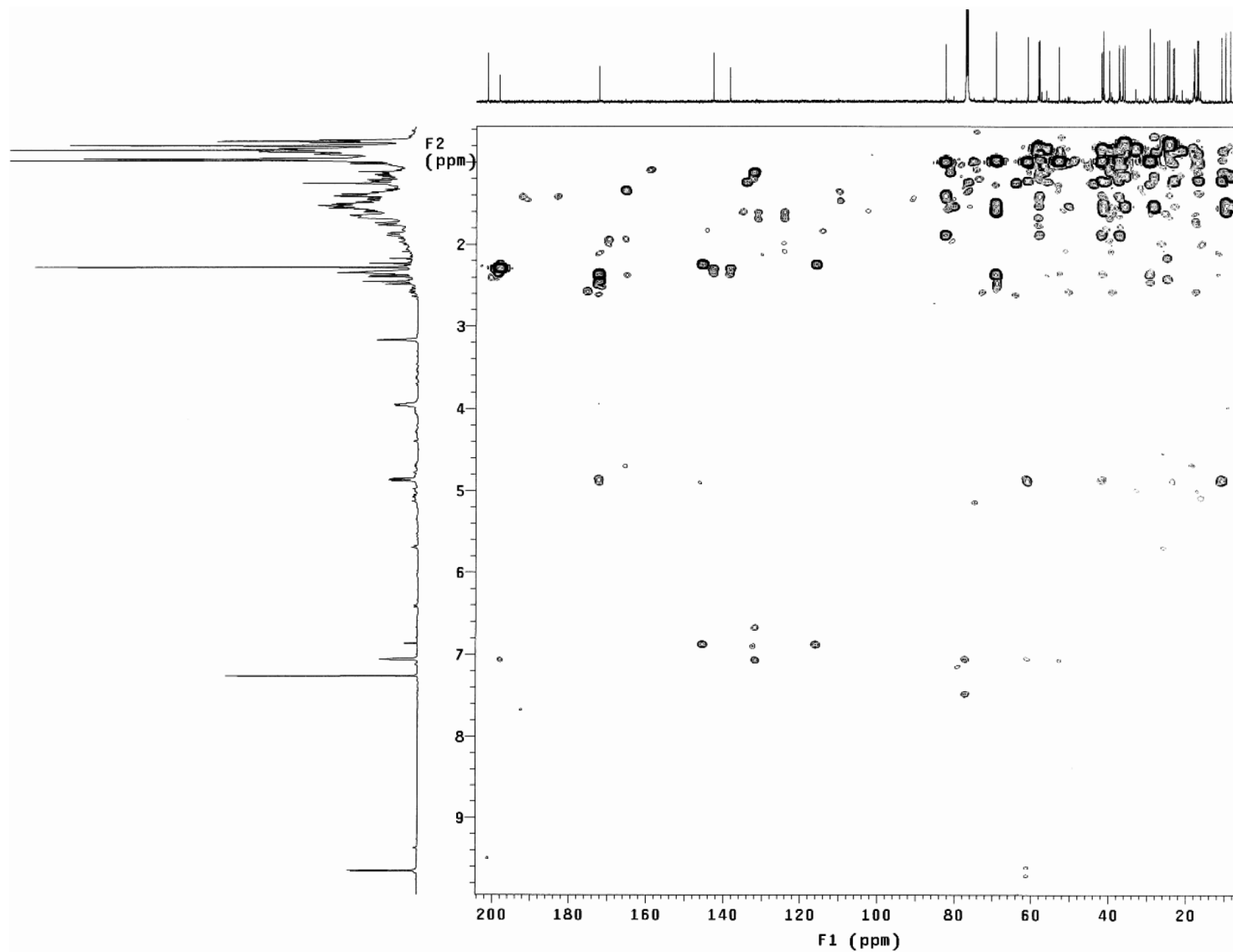


Figure S16: HMBC NMR (500 MHz, CDCl_3) spectrum of **2**.

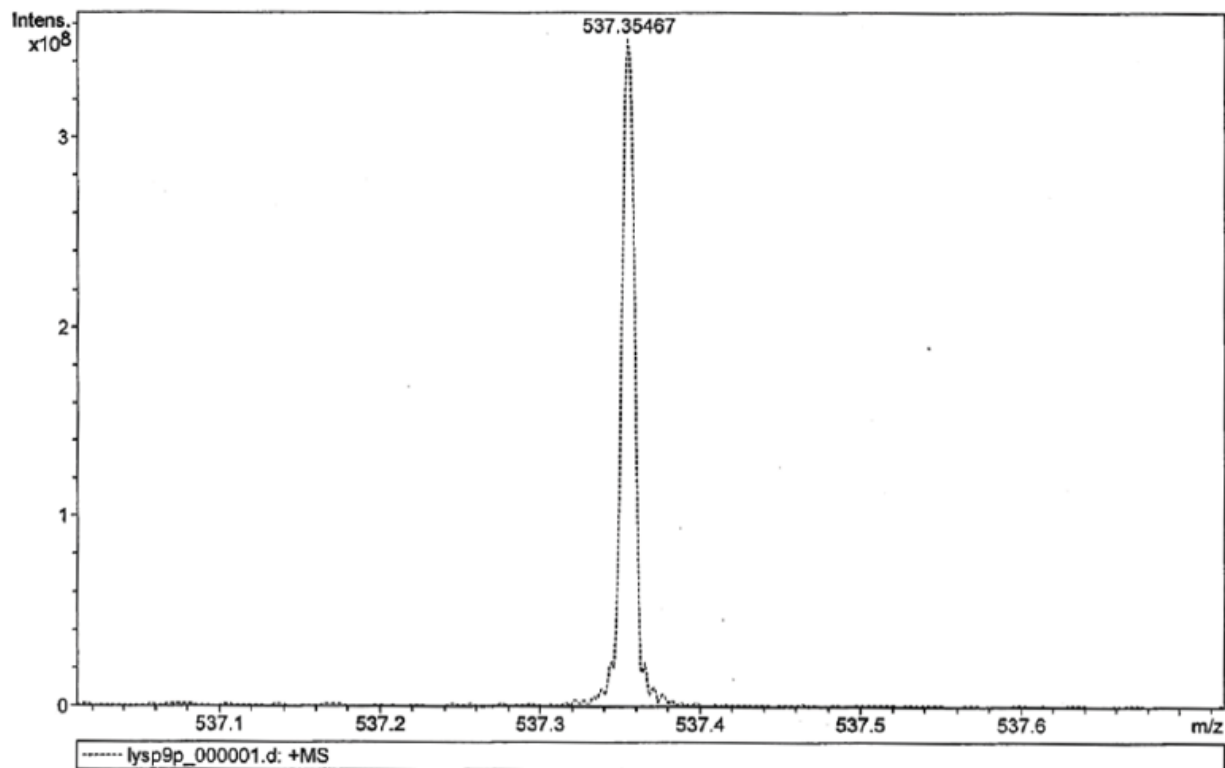
Mass Spectrum SmartFormula Report

Analysis Info

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Method broadband first signal
Sample Name Lysp-9p
Comment ESI Positive

12/20/2013 10:40:21 AM

Instrument: FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
537.35467	1	C ₃₂ H ₅₀ NaO ₅	100.00	537.35505	0.37	0.70	4.8	7.5	even	ok

Figure S17: HRESIMS spectrum of 2.

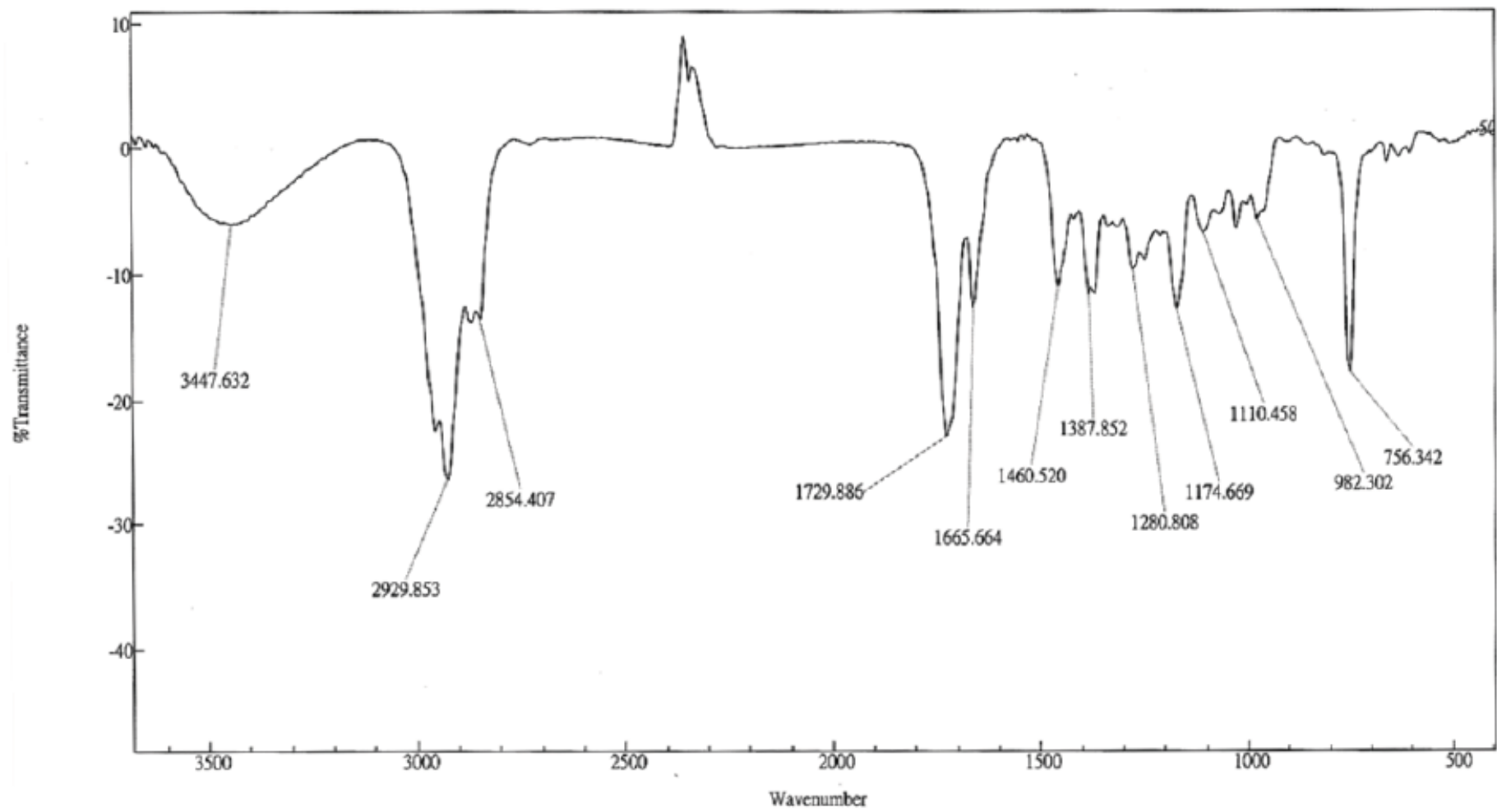


Figure S18: IR spectrum of 2.

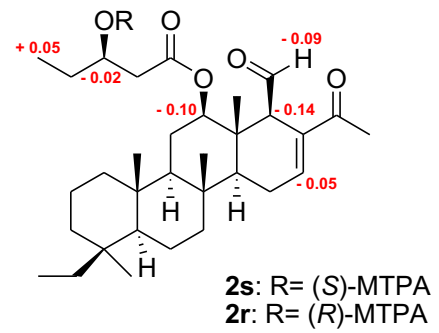


Figure S19: Values of $\Delta\delta_{S-R}$ of the MTPA esters of **2**.

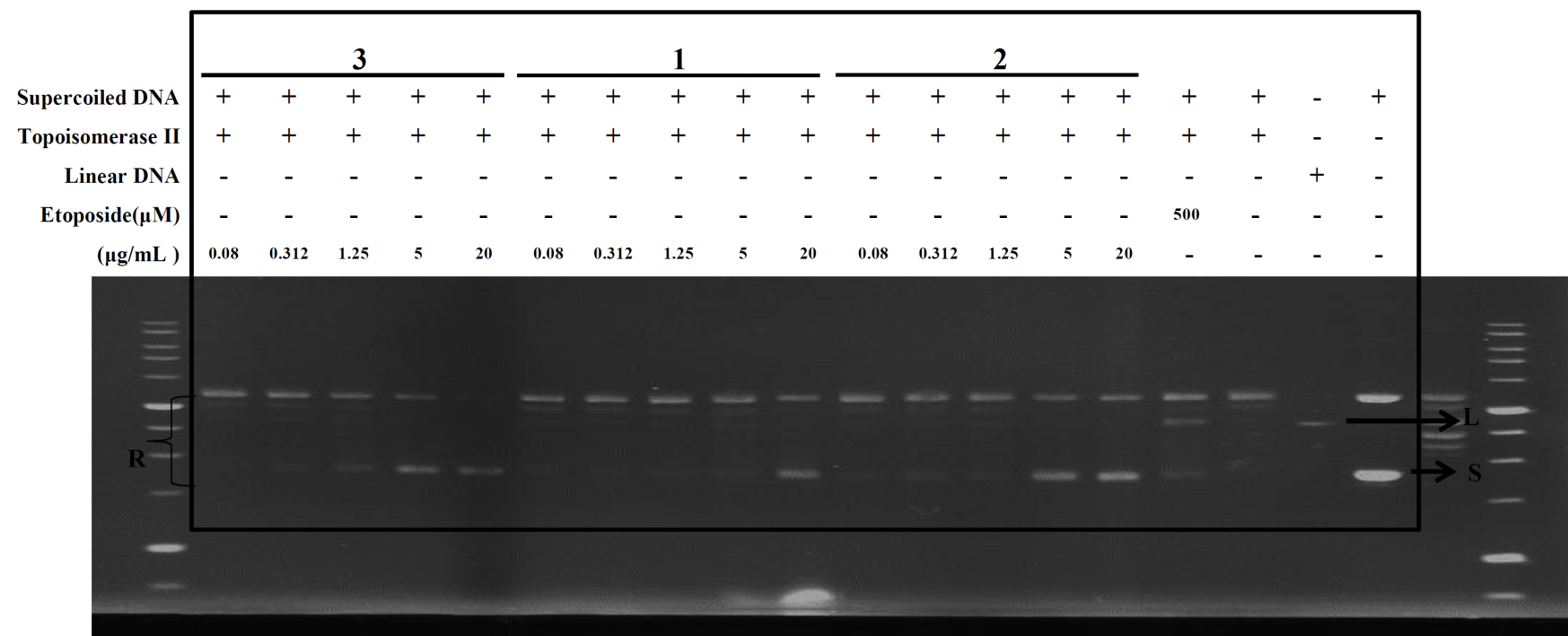


Figure S20: The full length gel of Topo II α activity.

Effect of compounds **1-3** on topo II activity. Lanes 1-5: **3** (0.08, 0.3125, 1.25, 5, and 20 $\mu\text{g/mL}$); Lanes 6-10: **1** (0.08, 0.3125, 1.25, 5, and 20 $\mu\text{g/mL}$); Lanes 11-15: **2** (0.08, 0.3125, 1.25, 5, and 20 $\mu\text{g/mL}$); Lane 16: positive control, etoposide (500 μM), as topo II poison (induction of linear DNA); Lane 17: plasmid DNA + topo II + solvent control (induction of DNA relaxation); Lane 18: Linear DNA; Lane 19: negative control plasmid DNA (supercoiled DNA)

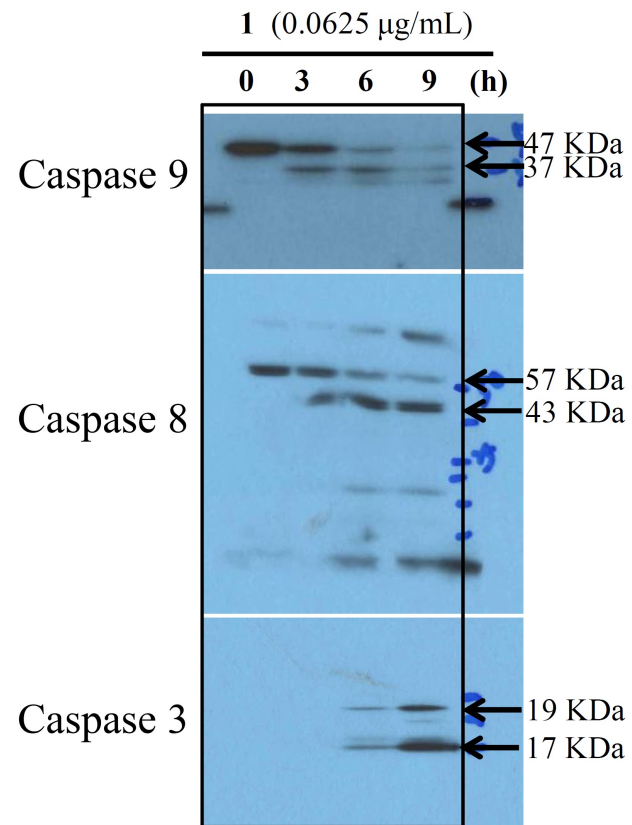


Figure S21: The full length blots of caspase 9, 8 and 3 expressions.

Molt 4 cells were treated with 0.0625 μg/mL of compound 1 for the indicated time. Western blot analysis of Caspase 9 at 47 and 37 KDa, Caspase 8 at 57 and 43 KDa, as well as Caspase 3 at 19 and 17 KDa.