

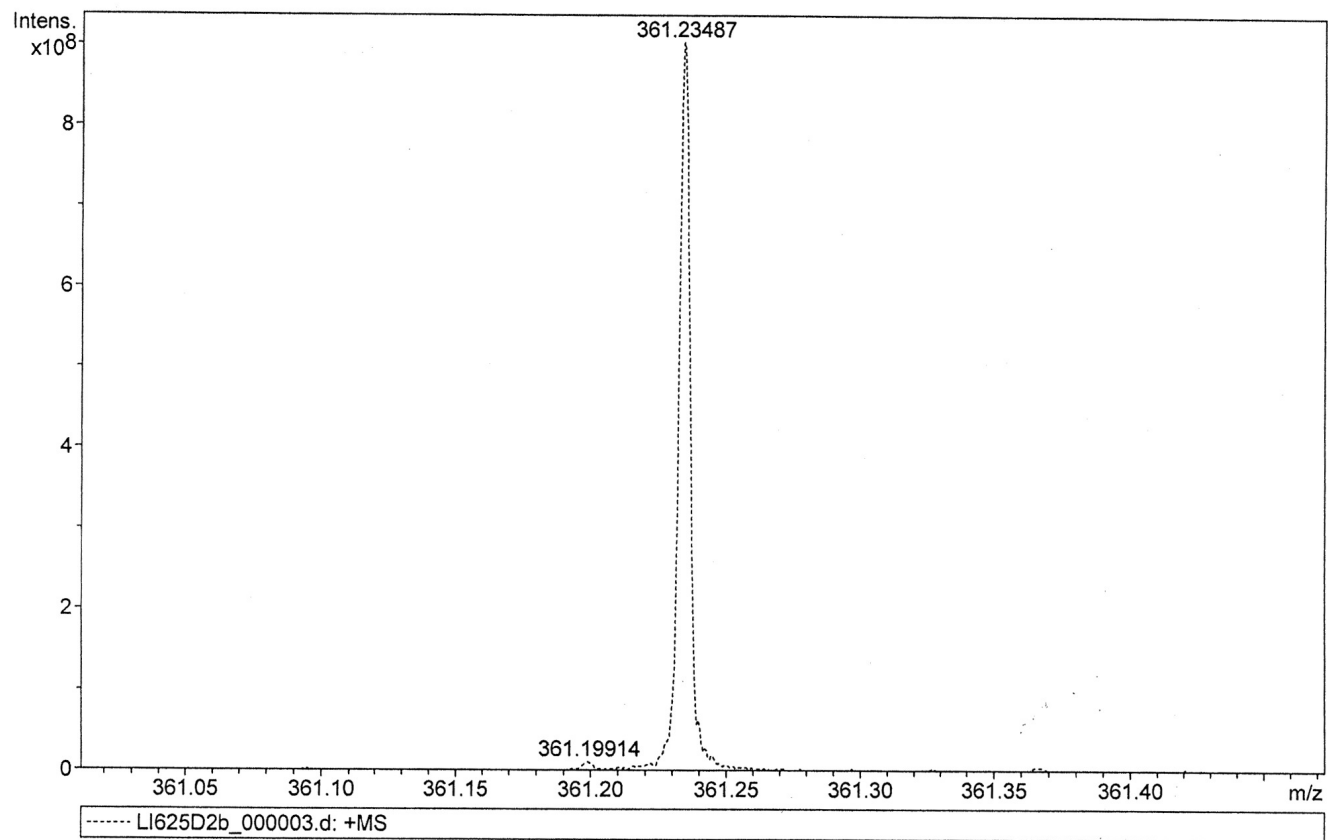
Bioactive Capnosanes and Cembranes from the Soft Coral

Klyxum Flaccidum

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Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
361.23487	1	C ₂₀ H ₃₄ NaO ₄	100.00	361.23493	0.06	0.17	8.7	3.5	even	ok

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

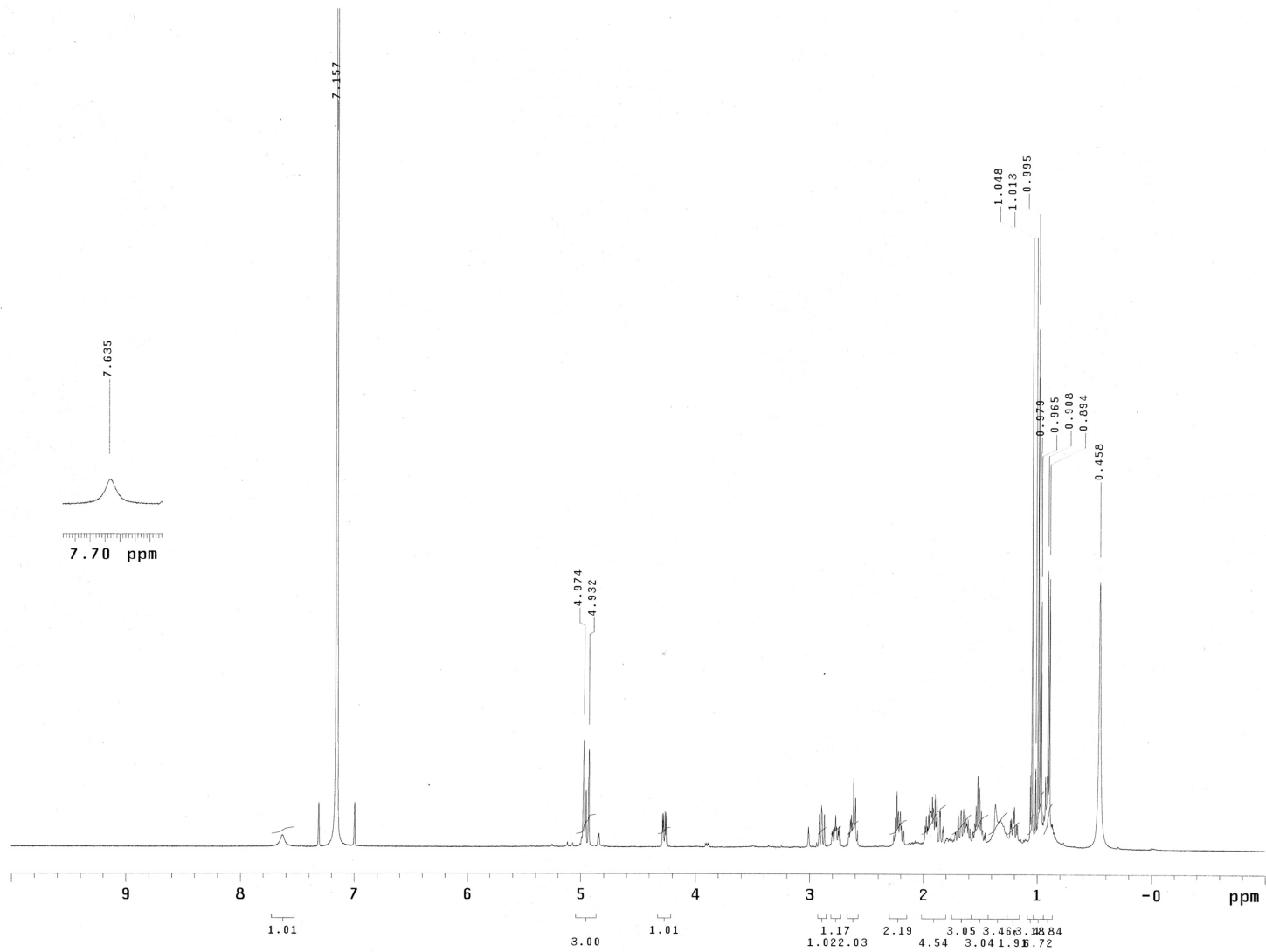


Figure S2. ^1H NMR spectrum of **1** in C_6D_6 at 500 MHz.

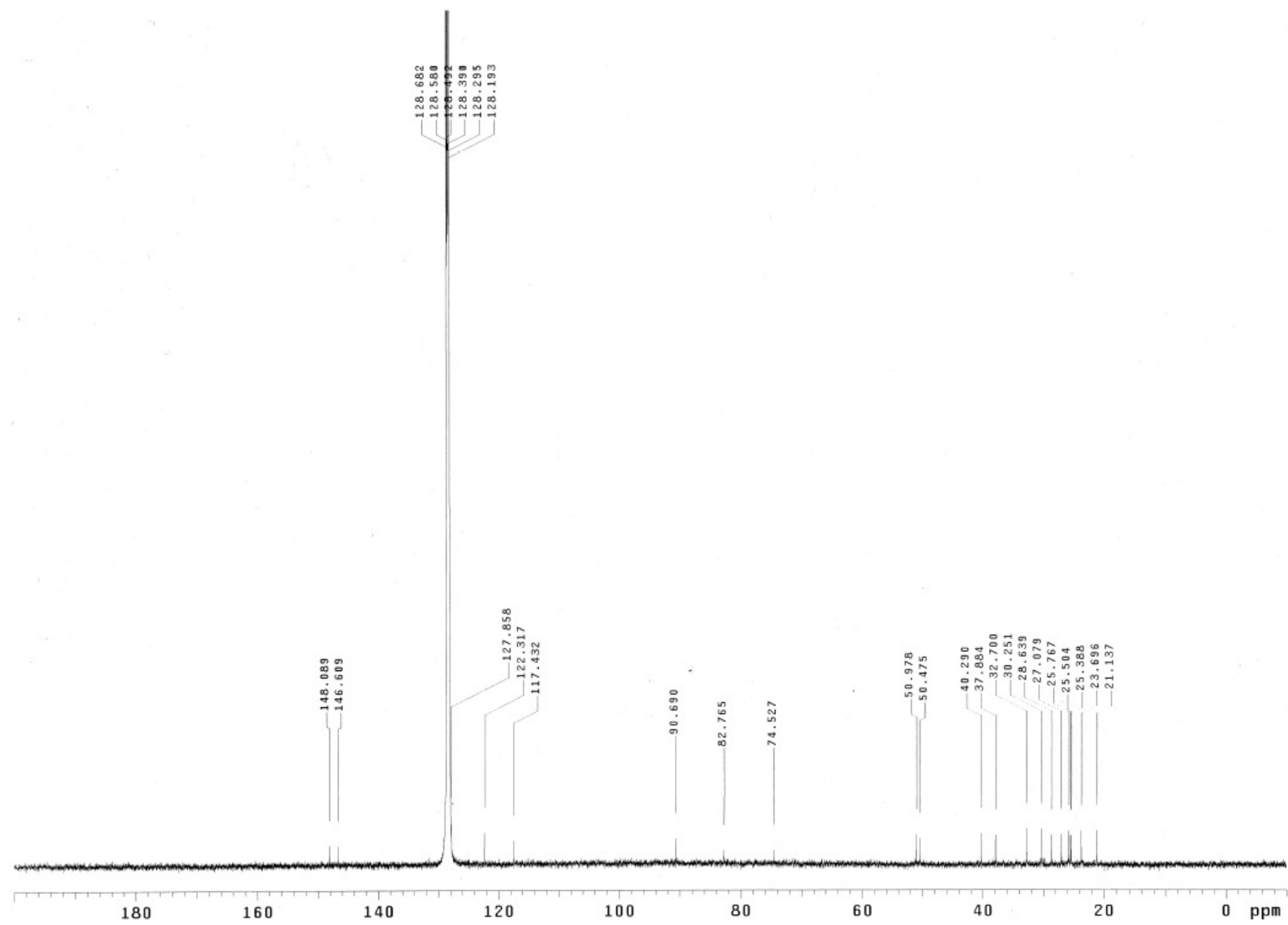


Figure S3. ^{13}C NMR spectrum of **1** in C_6D_6 at 125 MHz.

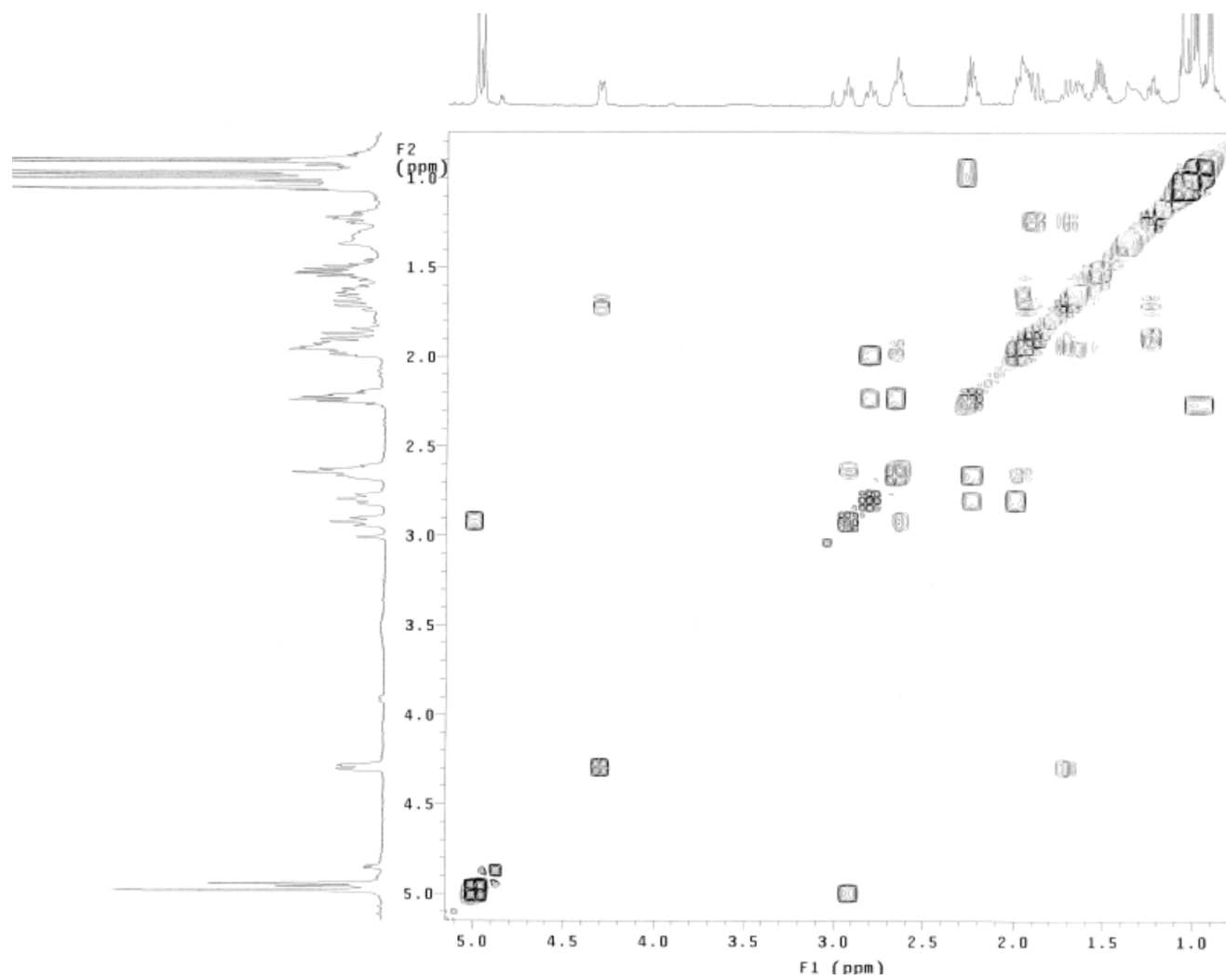


Figure S4. ^1H - ^1H COSY spectrum of **1** in C_6D_6 .

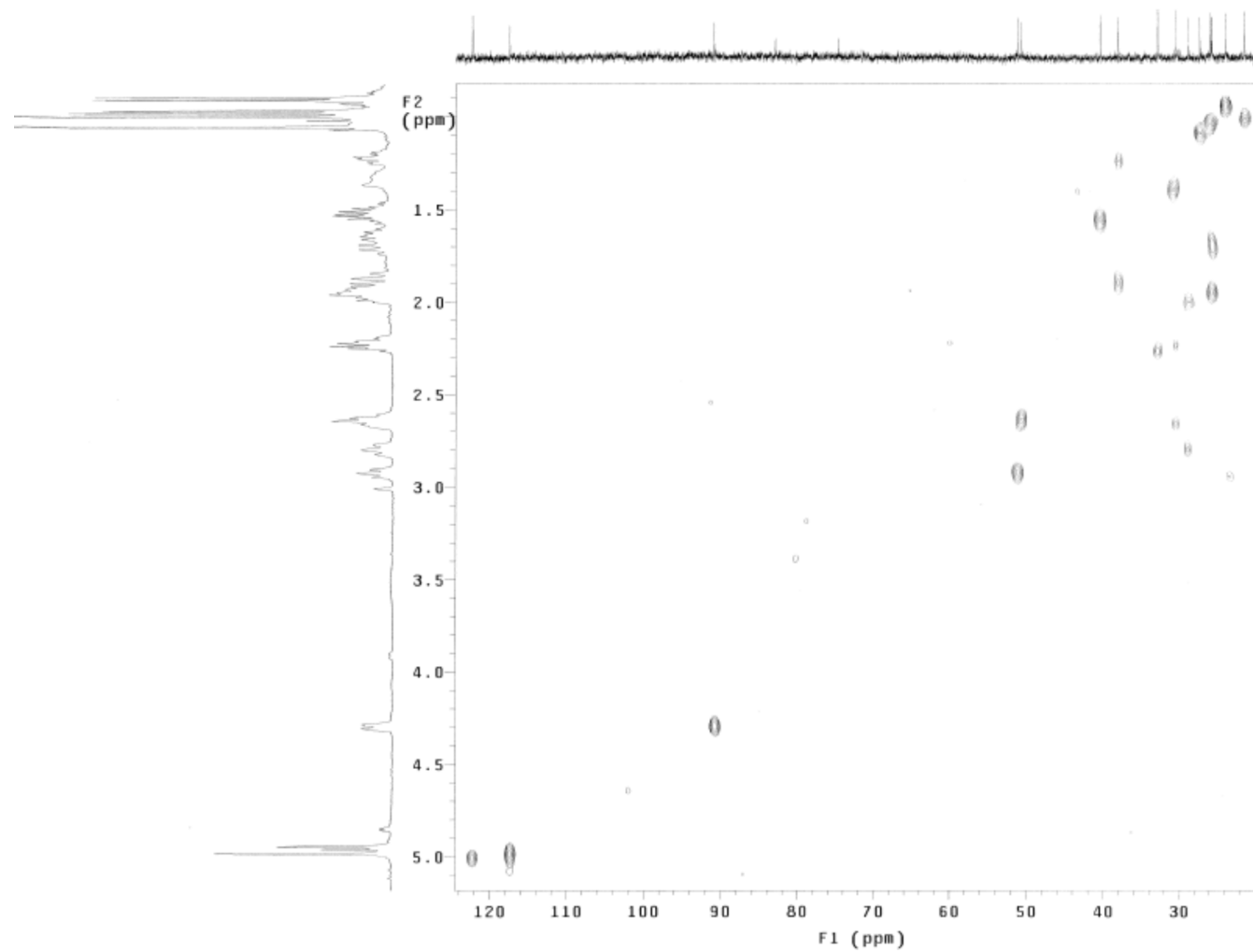


Figure S5. HSQC spectrum of **1** in C_6D_6 .

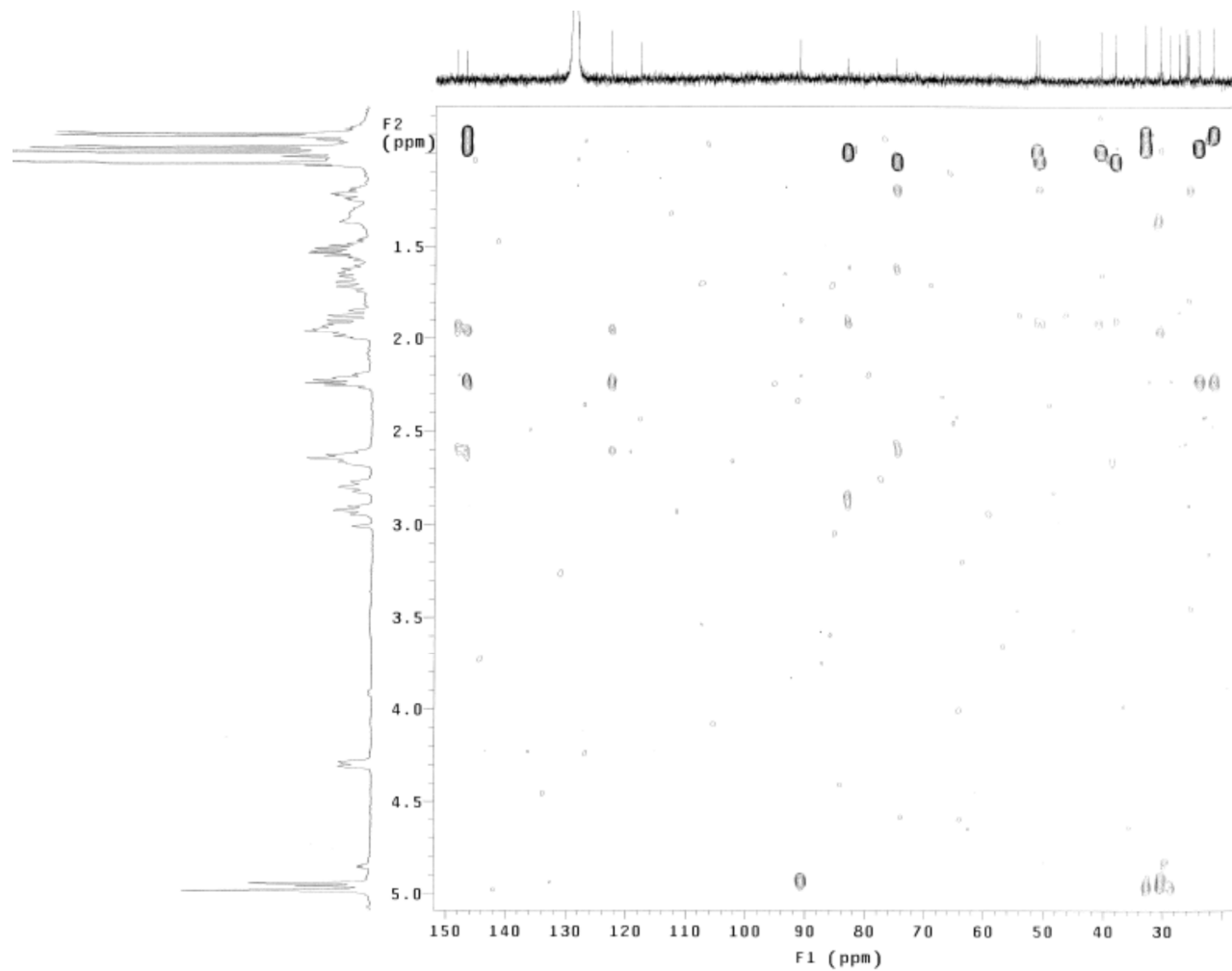


Figure S6. HMBC spectrum of **1** in C_6D_6 .

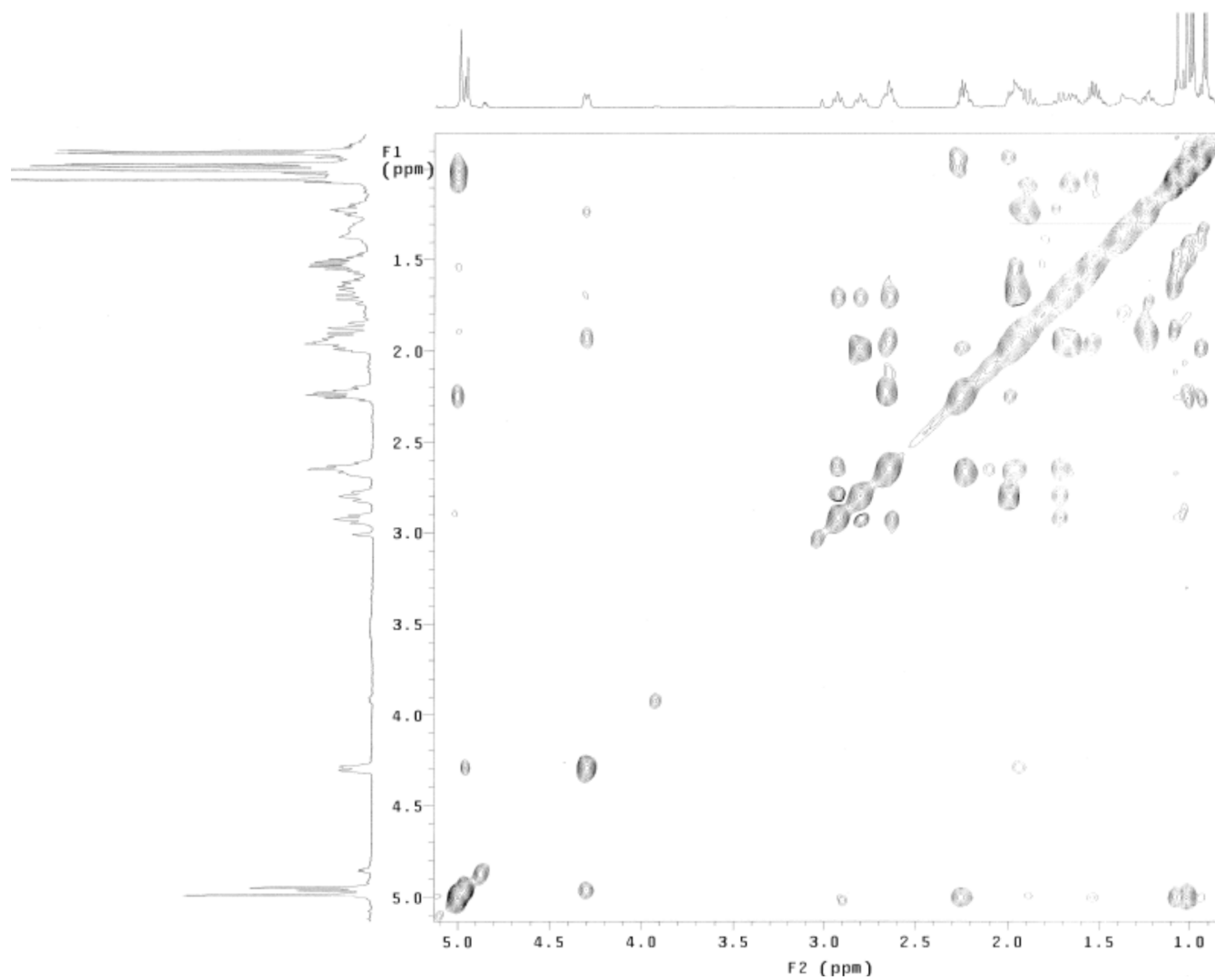
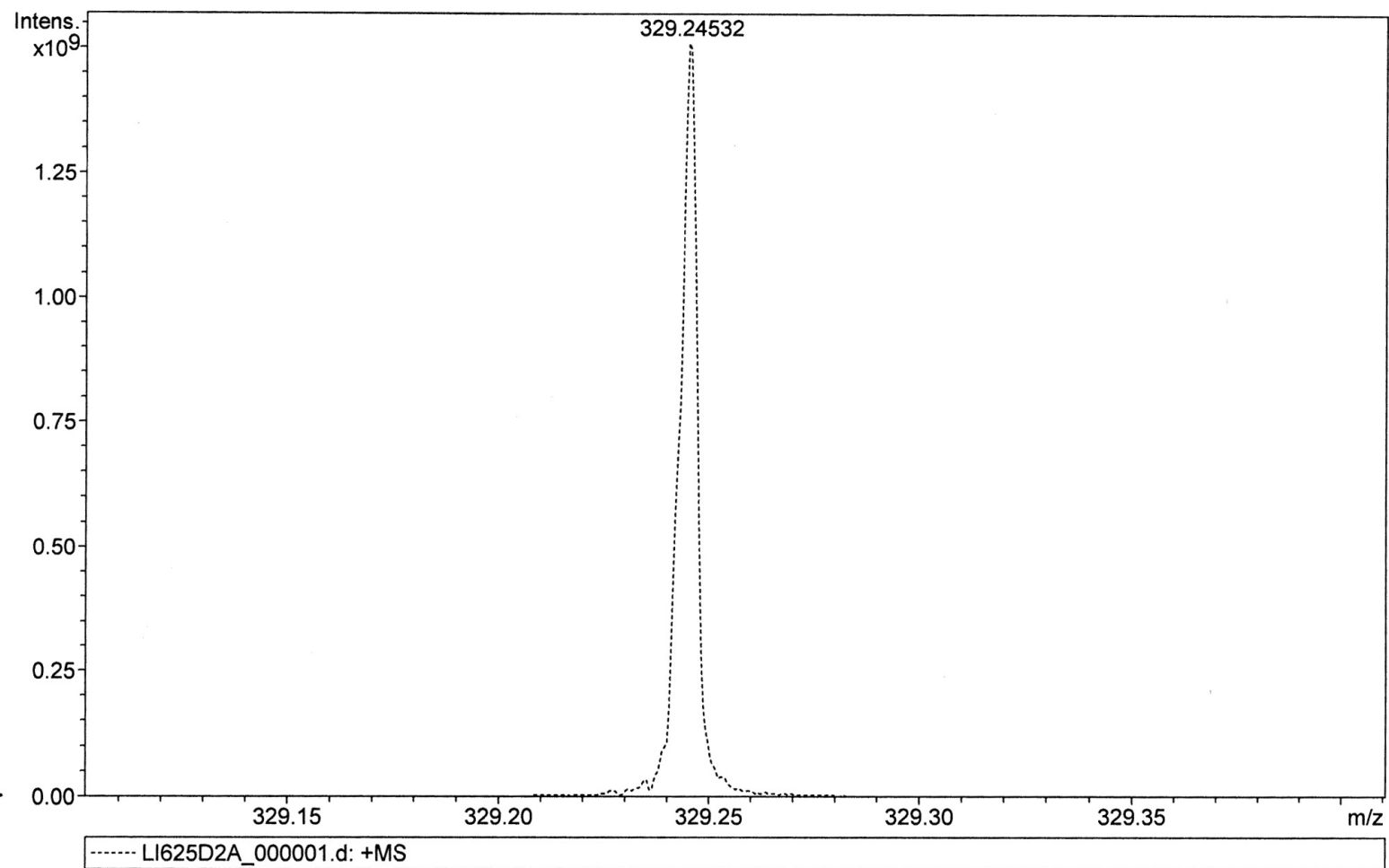
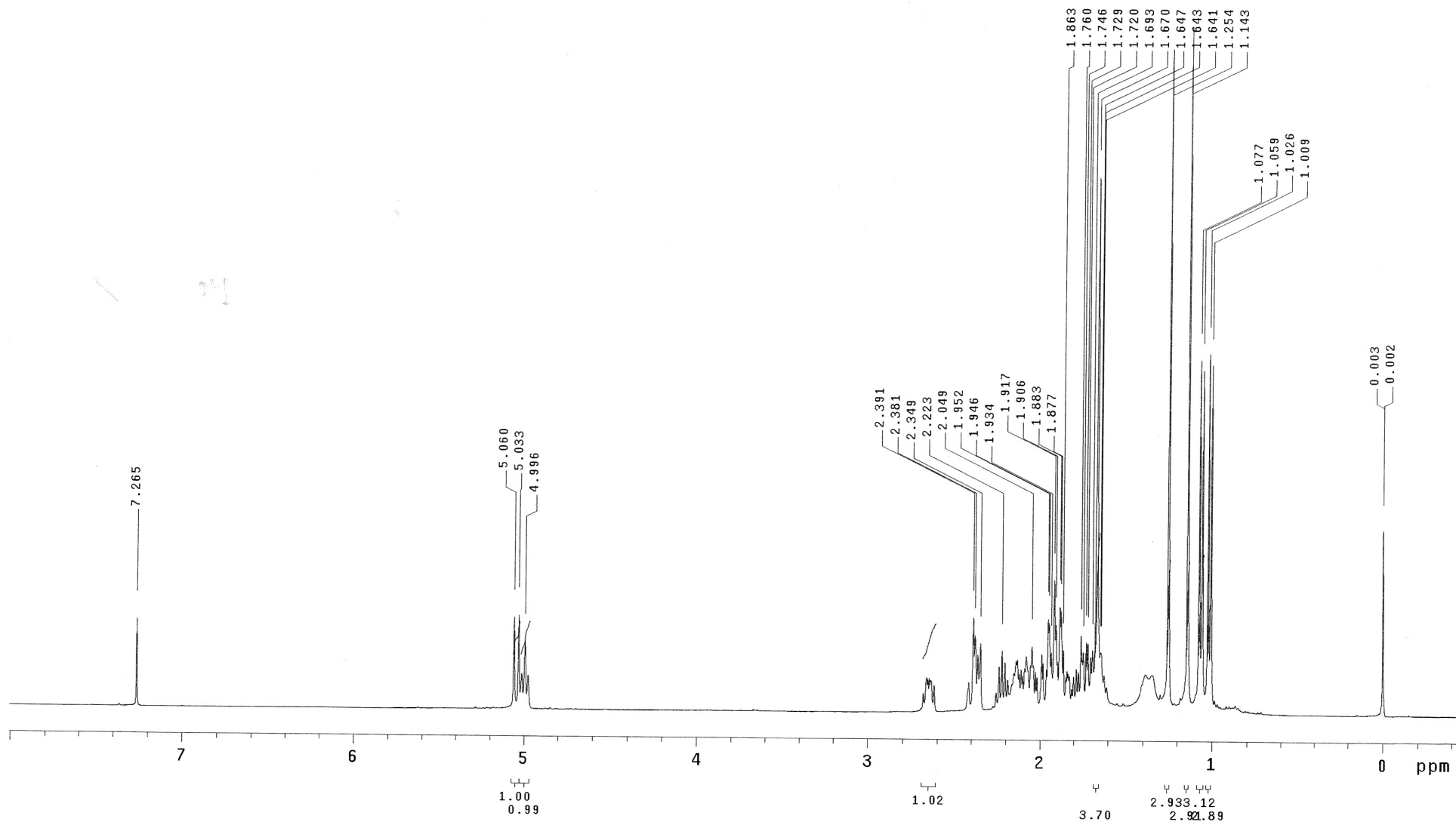


Figure S7 NOESY spectrum of **1** in C_6D_6 .



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
329.24532	1	C ₂₀ H ₃₄ NaO ₂	100.00	329.24510	-0.22	-0.66	3.2	3.5	even	ok

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



Figure

S9. ¹H NMR spectrum of **2** in CDCl₃ at 400 MHz.

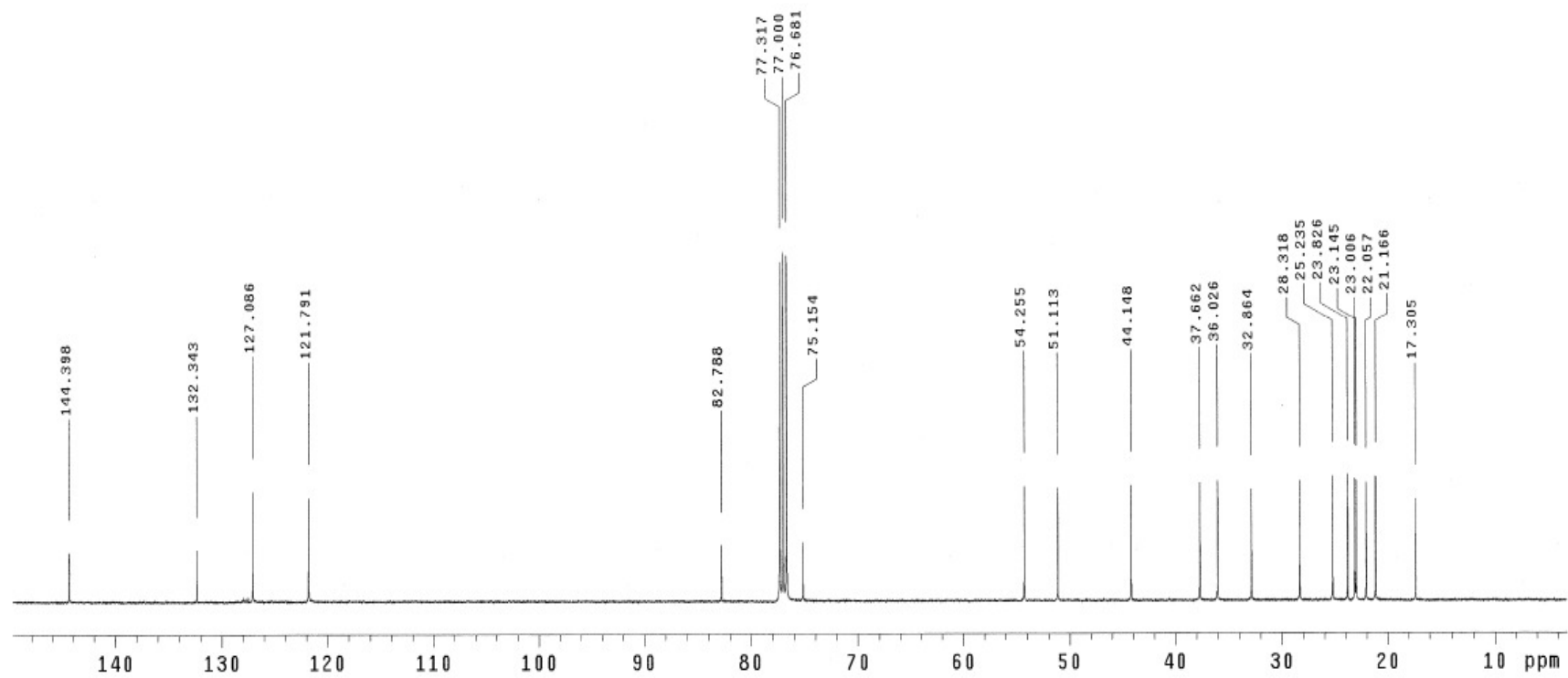


Figure S10. ¹³C NMR spectrum of **2** in CDCl₃ at 100 MHz.

LI6-25-d-2-d(2)

Sample Name:
LI6-25-d-2-a-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
LI6-25-d-2-a-2_20140112_01
Fidfile: gCOSY_01

Pulse Sequence: gCOSY
Solvent: cdc13
Data collected on: Jan 13 2014

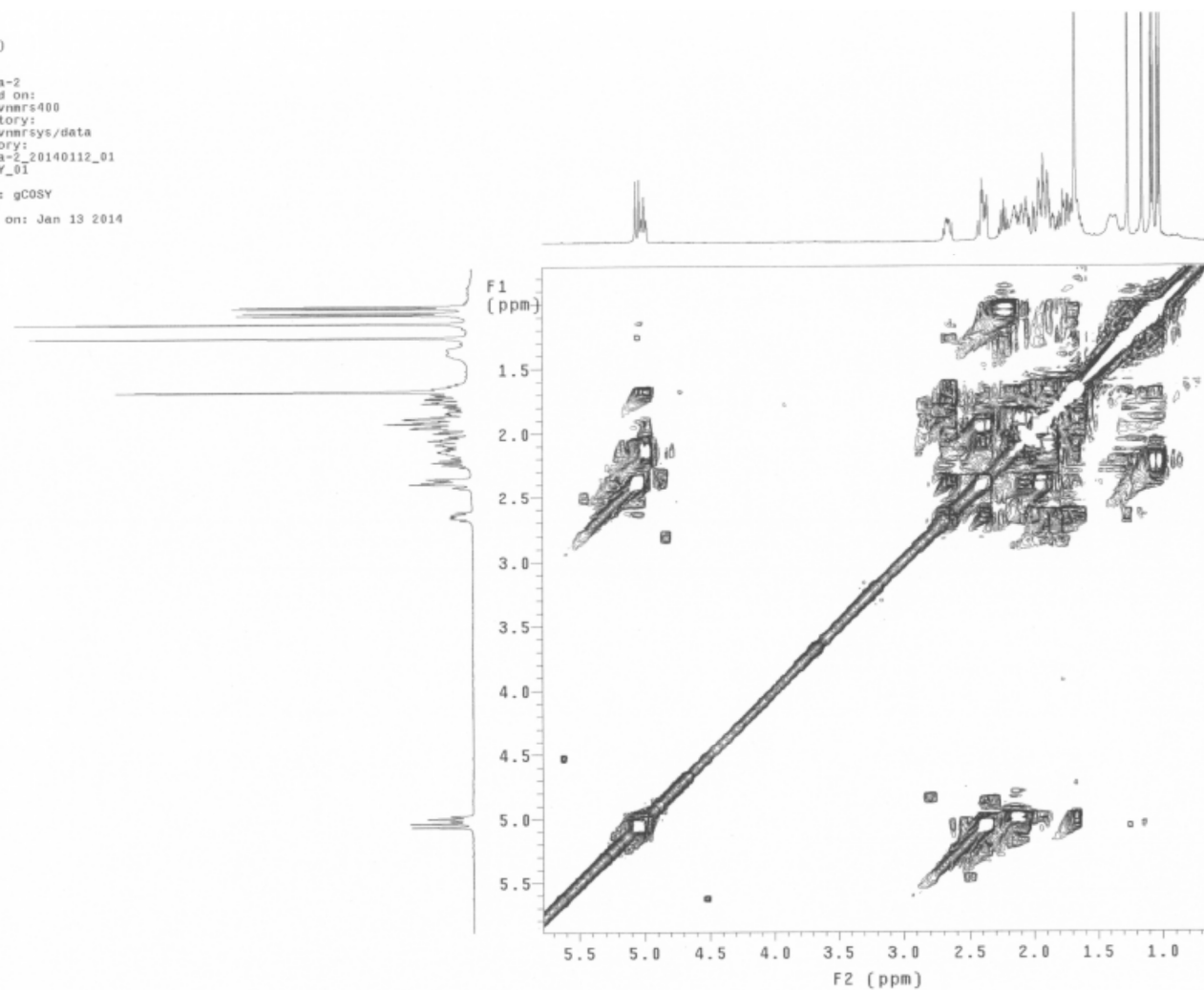


Figure S11. ^1H - ^1H COSY spectrum of **2** in CDCl_3 .

LI6-25-d-2-a(2)

Sample Name:
LI6-25-d-2-a-2
Data Collected On:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
LI6-25-d-2-a-2_20140112_01
Fidfile: HSQCAD_01

Pulse Sequence: HSQCAD
Solvent: cdc13
Data collected on: Jan 13 2014

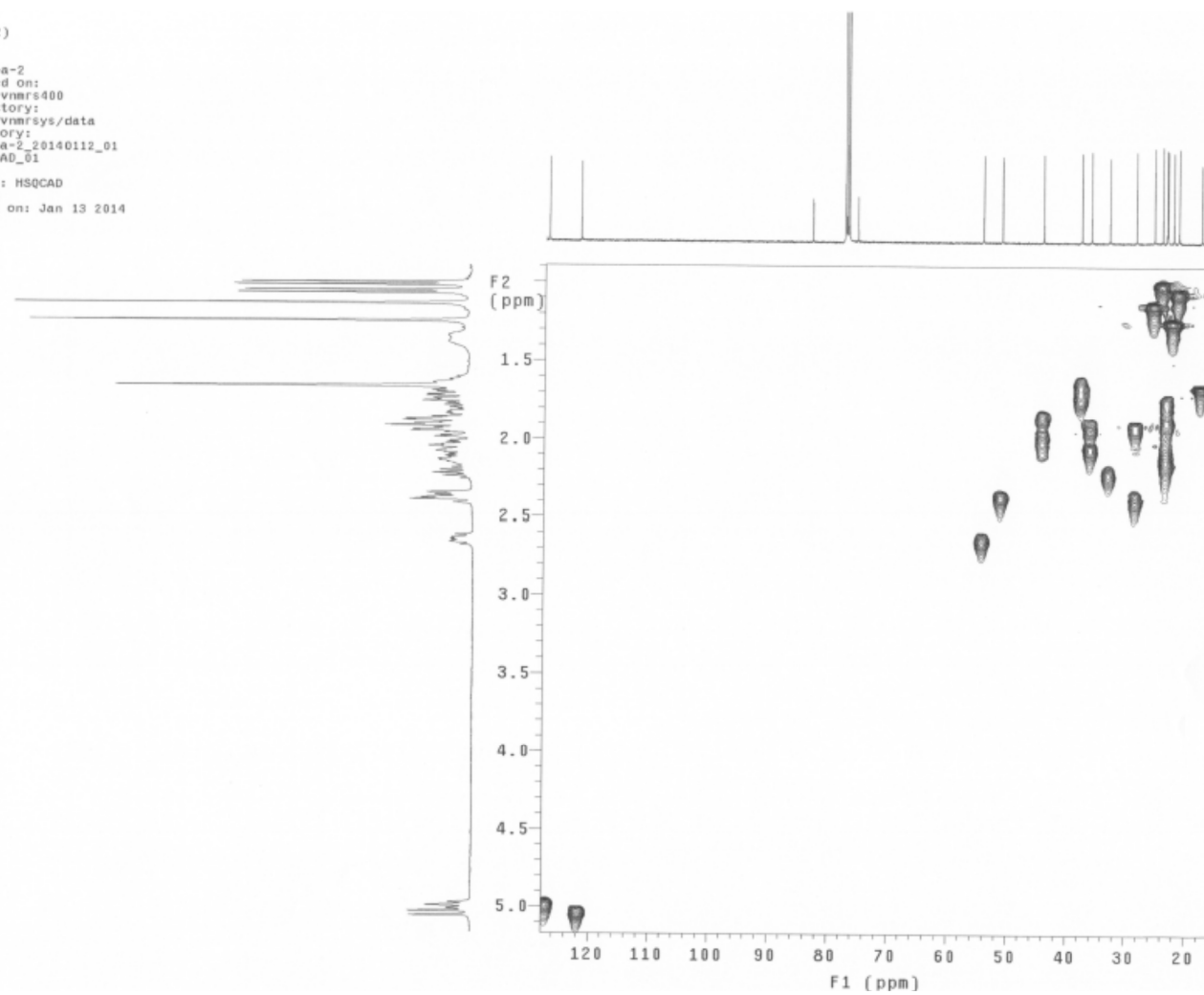


Figure S12. HSQC spectrum of **2** in CDCl_3 .

LI6-25-d-2-a(2)

Sample Name:
LI6-25-d-2-a-2
Data Collected on:
Varian-NMR-vnmrs400
Archive directory:
/home/sheu/vnmrsys/data
Sample directory:
LI6-25-d-2-a-2_20140112_01
FidFile: gHMBCAD_01

Pulse Sequence: gHMBCAD
Solvent: cdcl3
Date collected on: Jan 13 2014

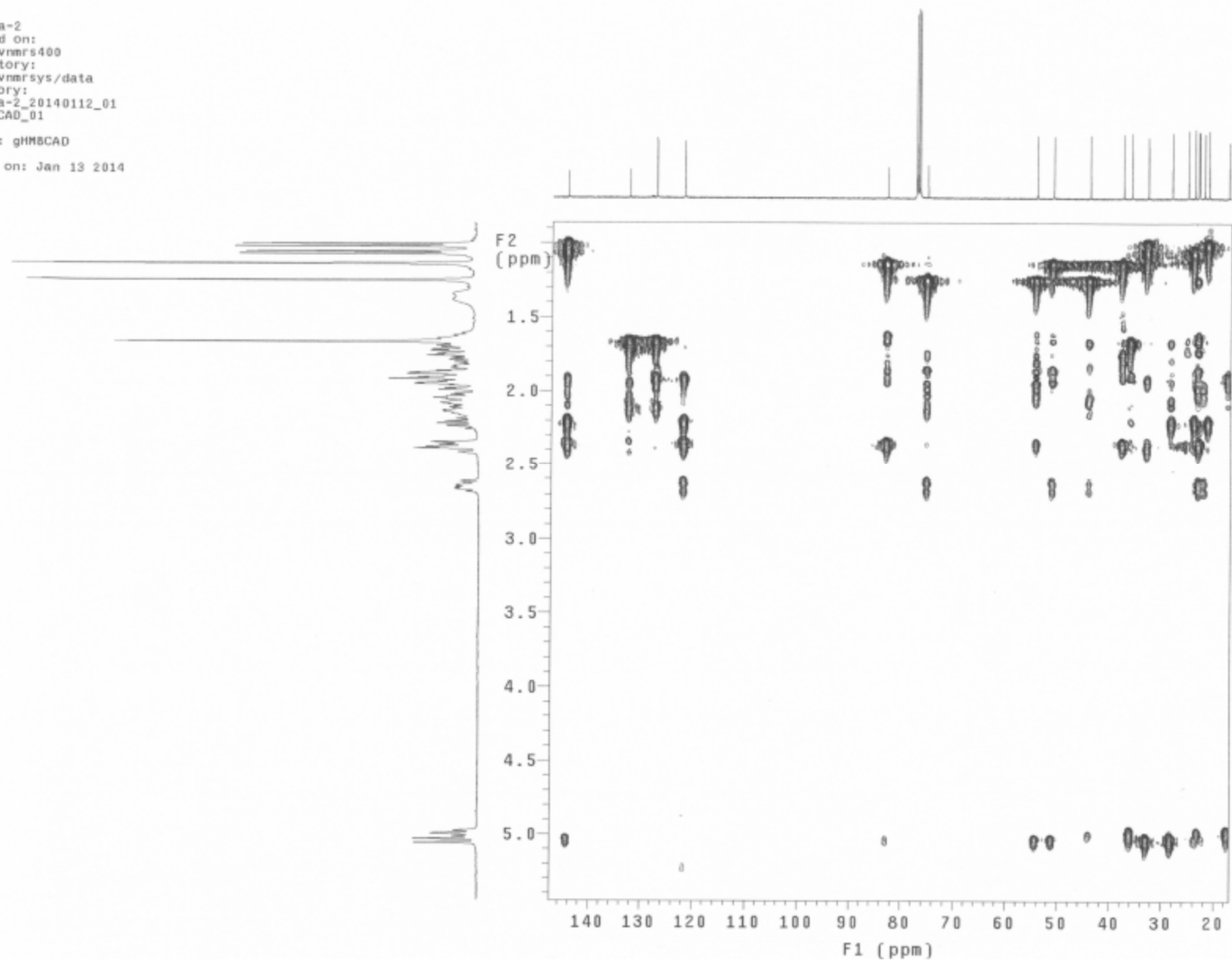


Figure S13. HMBC spectrum of **2** in CDCl₃.

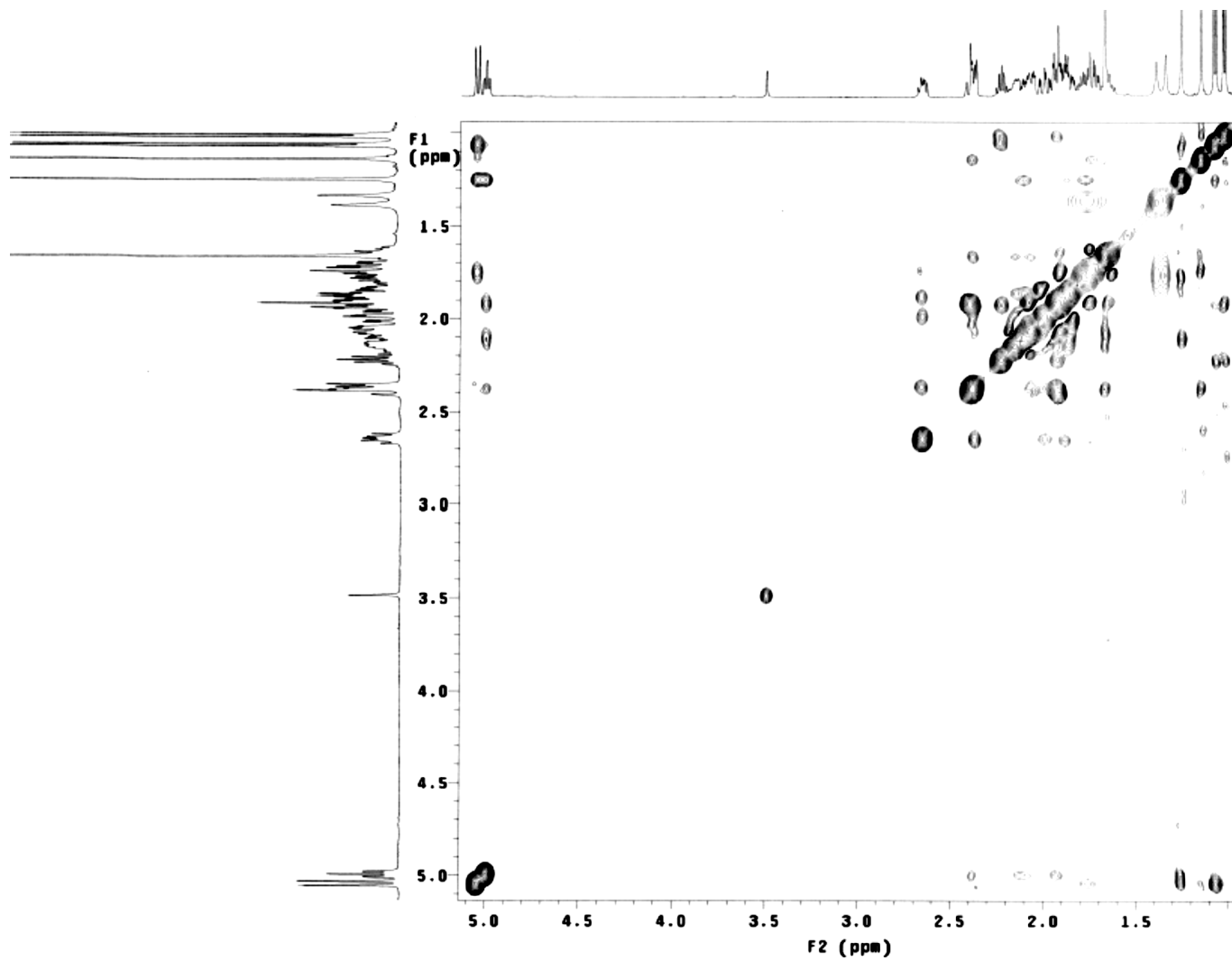
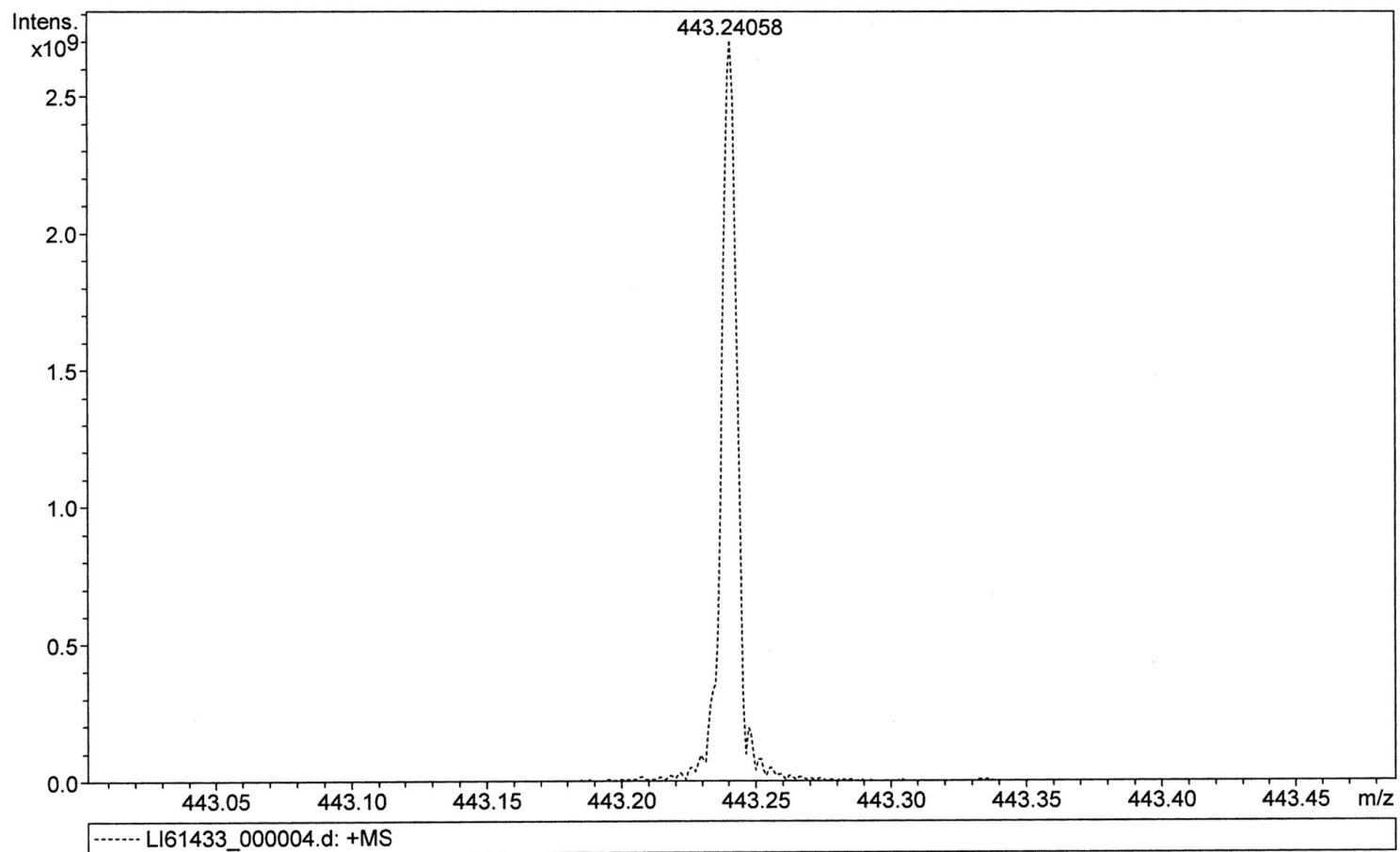


Figure S14. NOESY spectrum of **2** in CDCl₃.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
443.24058	1	C ₂₄ H ₃₆ NaO ₆	100.00	443.24041	-0.17	-0.38	9.9	6.5	even	ok

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

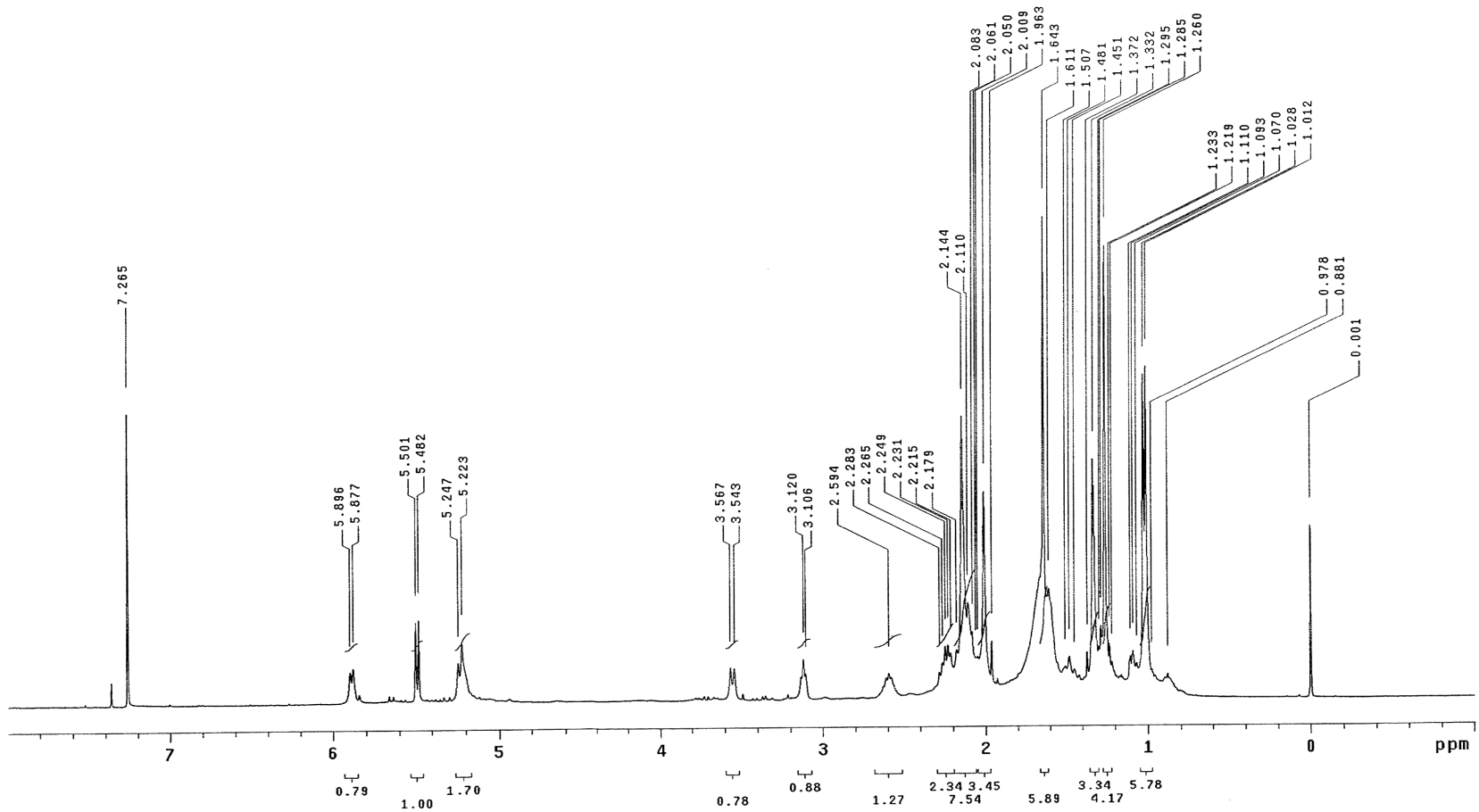


Figure S16. ¹H NMR spectrum of **3** in CDCl₃ at 400 MHz.

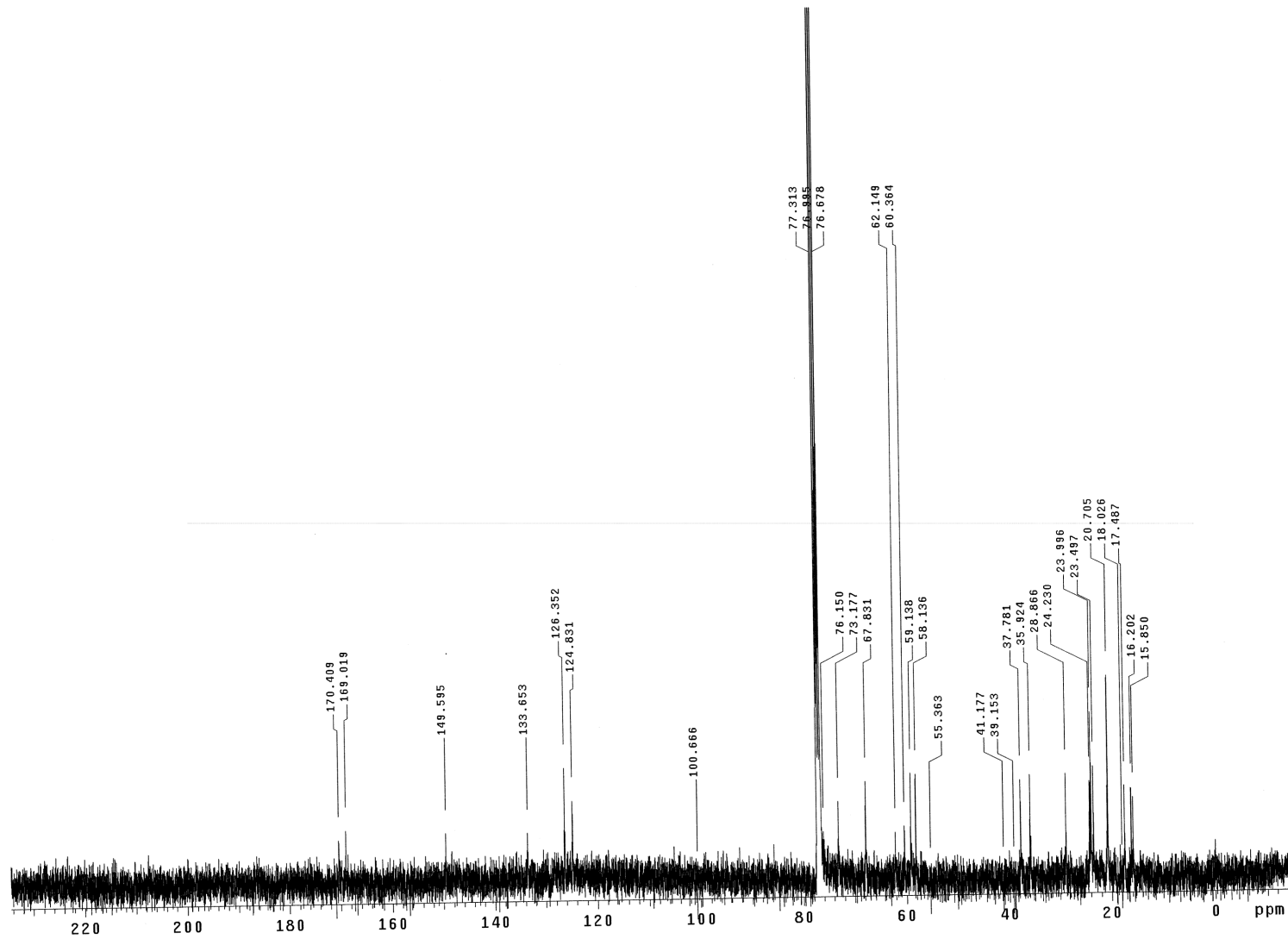


Figure S17. ^{13}C NMR spectrum of **3** in CDCl_3 at 100 MHz.

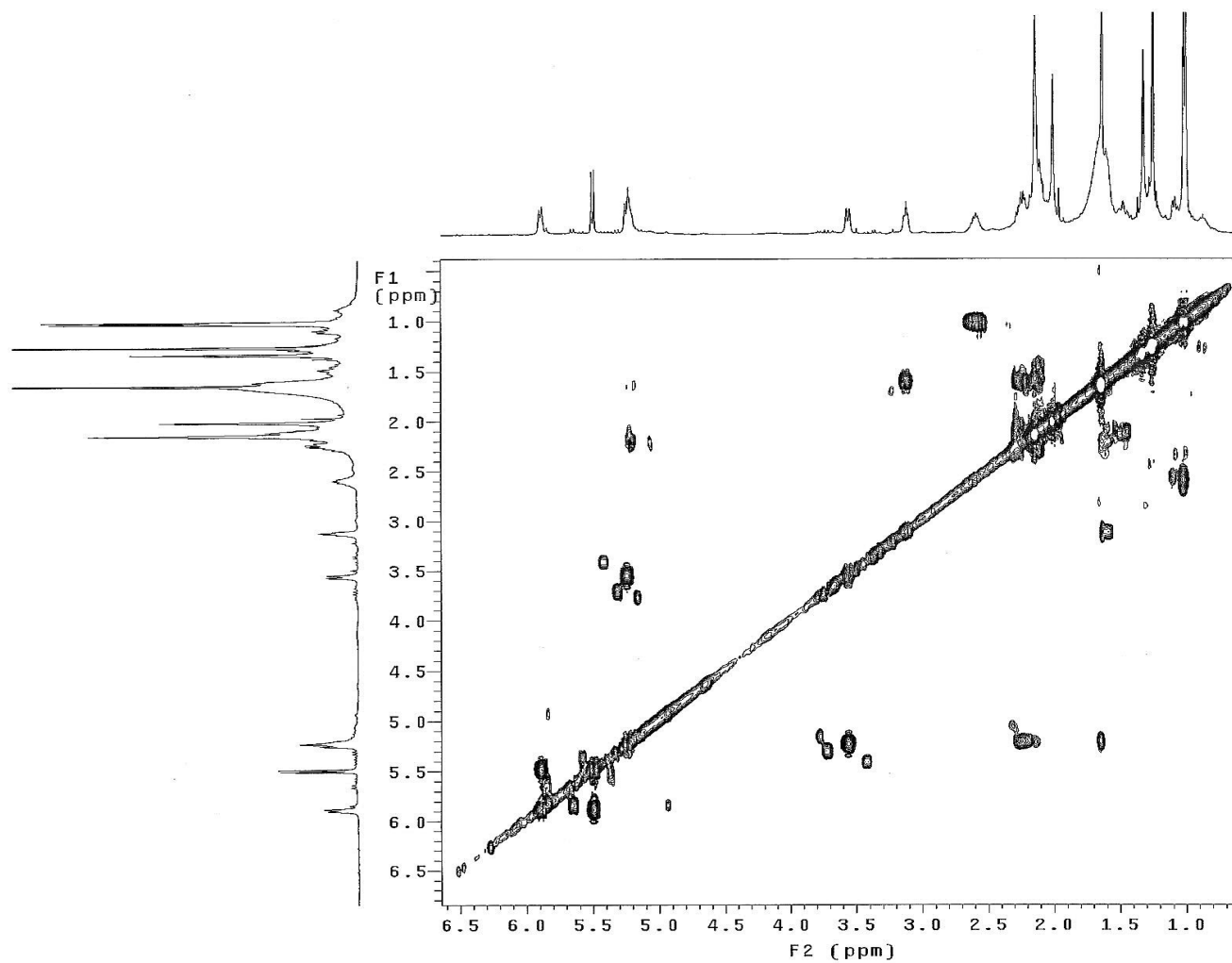


Figure S18. ^1H - ^1H COSY spectrum of **3** in CDCl_3 .

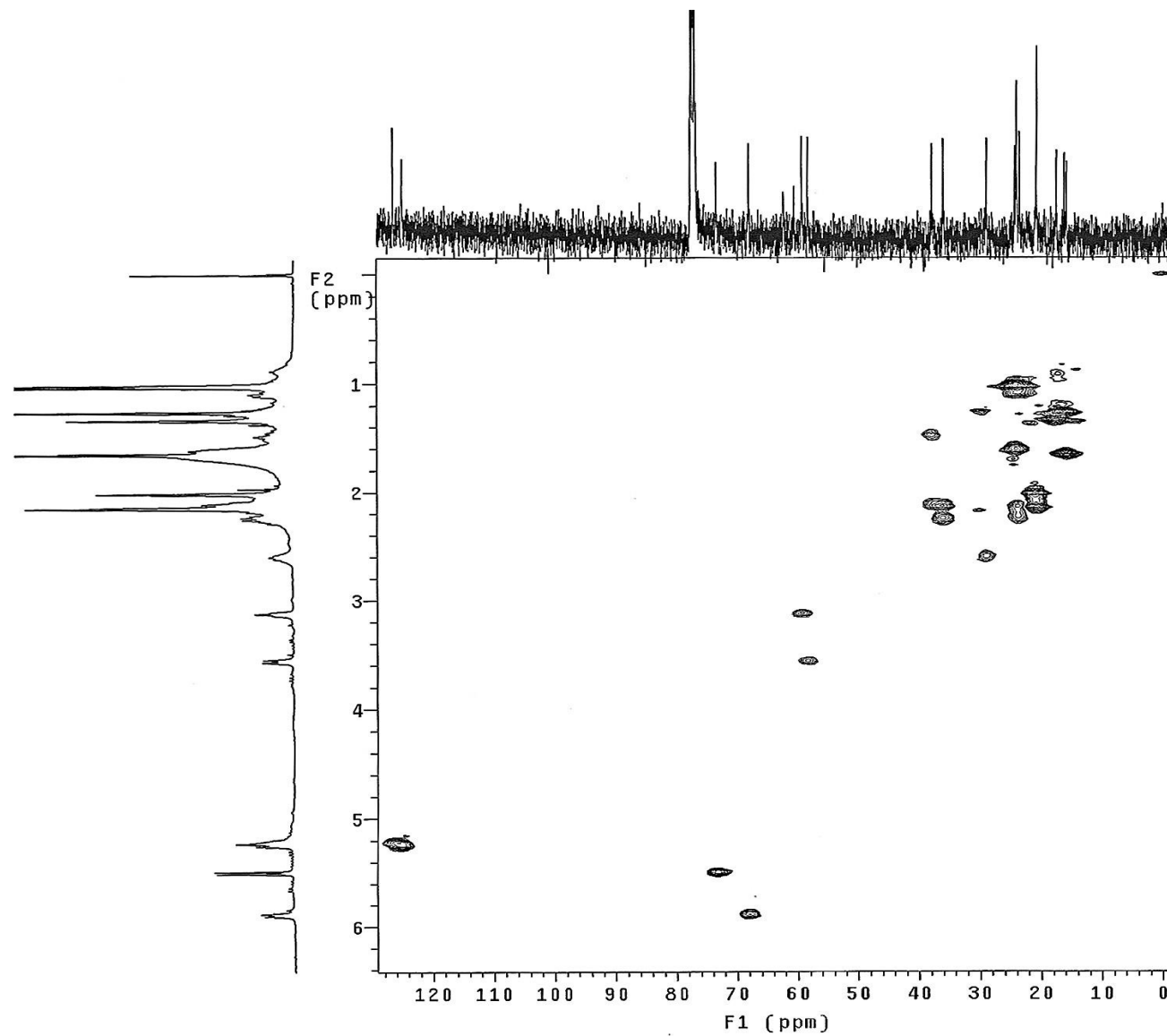


Figure S19. HSQC spectrum of **3** in CDCl₃.

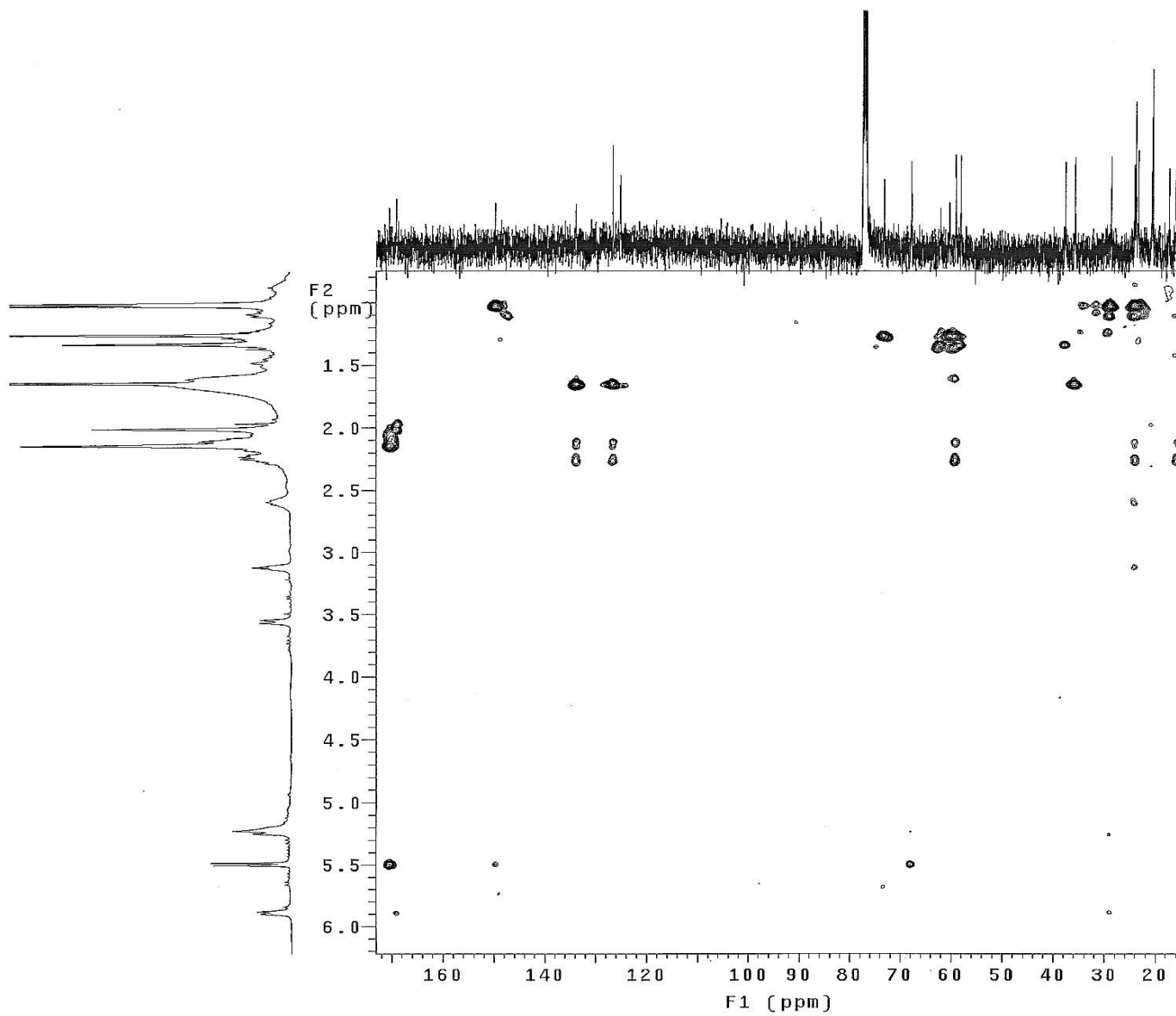


Figure S20. HMBC spectrum of **3** in CDCl₃.

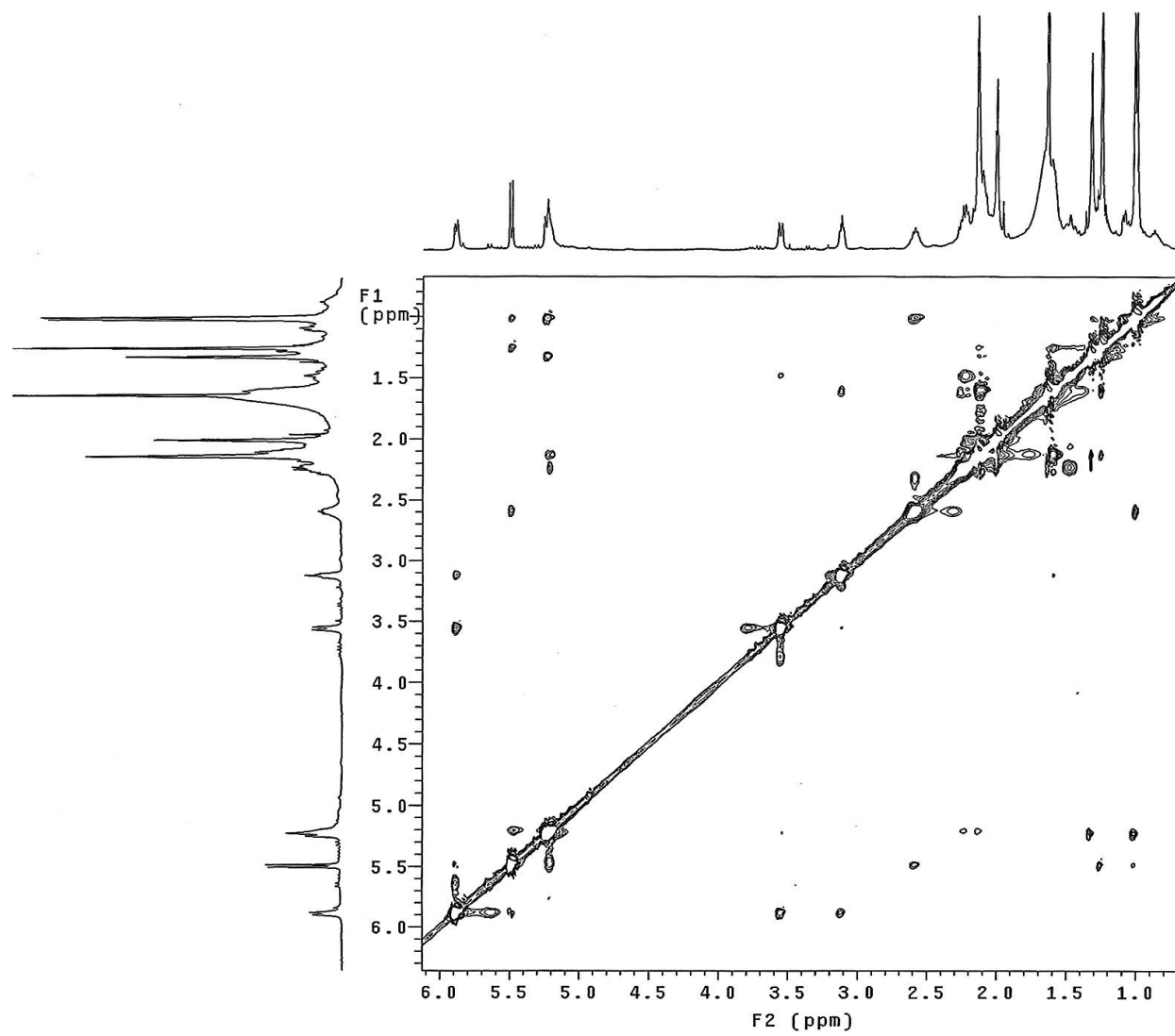
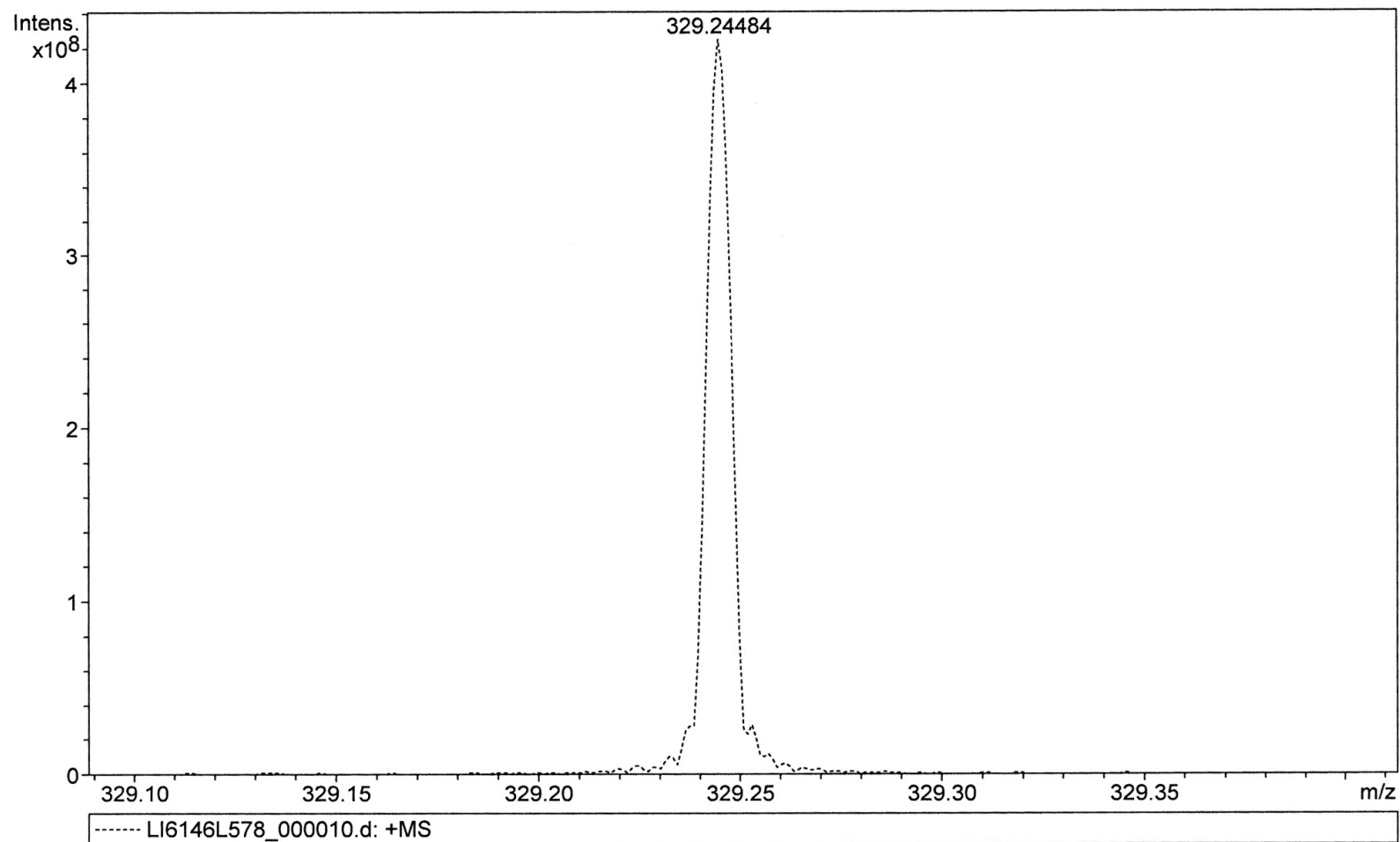


Figure S21. NOESY spectrum of **3** in CDCl₃.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
329.24484	1	C ₂₀ H ₃₄ NaO ₂	100.00	329.24510	0.27	0.81	3.6	3.5	even	ok

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

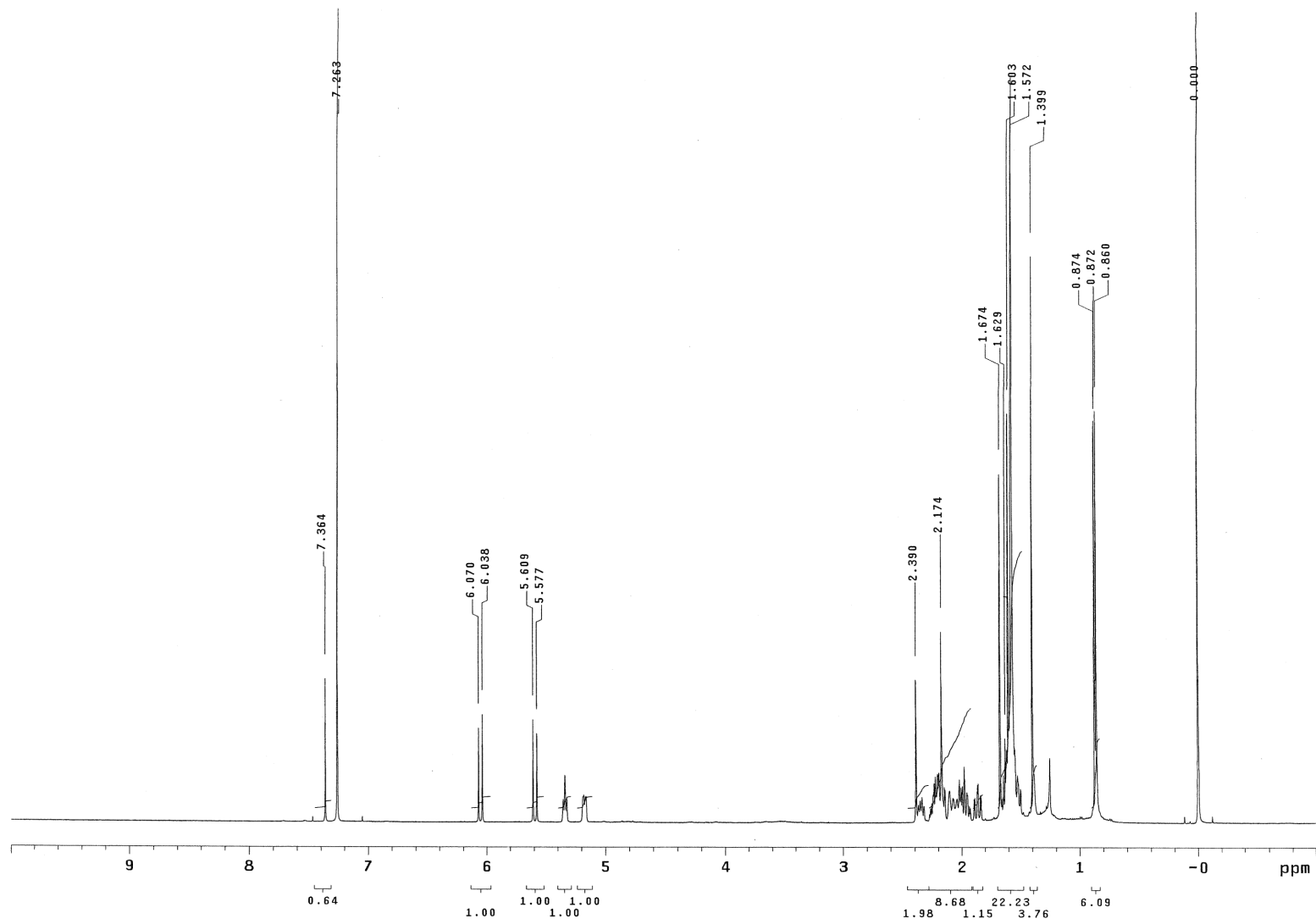


Figure S23. ¹H NMR spectrum of **4** in CDCl₃ at 500 MHz.

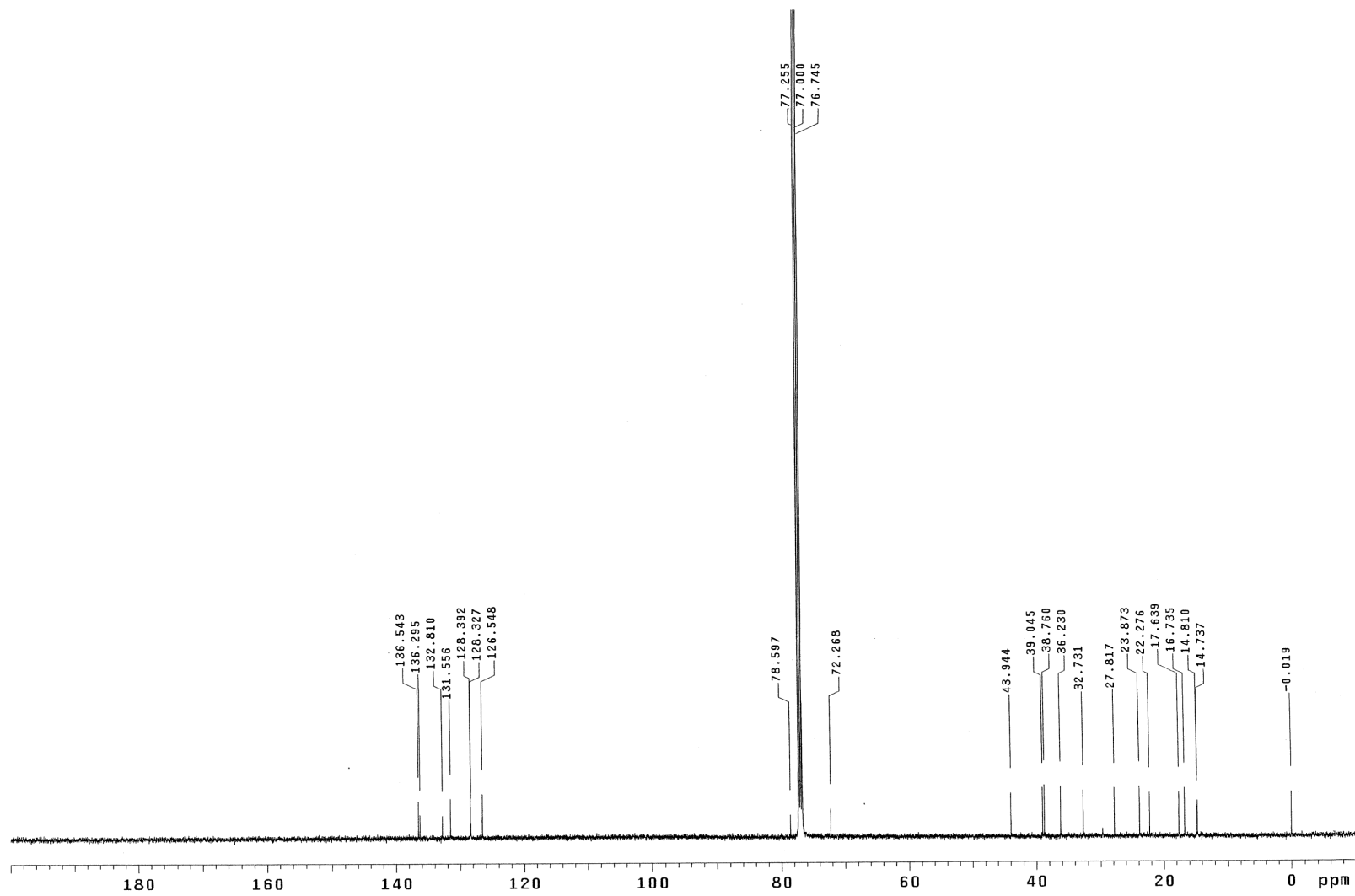


Figure S24. ^{13}C NMR spectrum of **4** in CDCl_3 at 125 MHz.

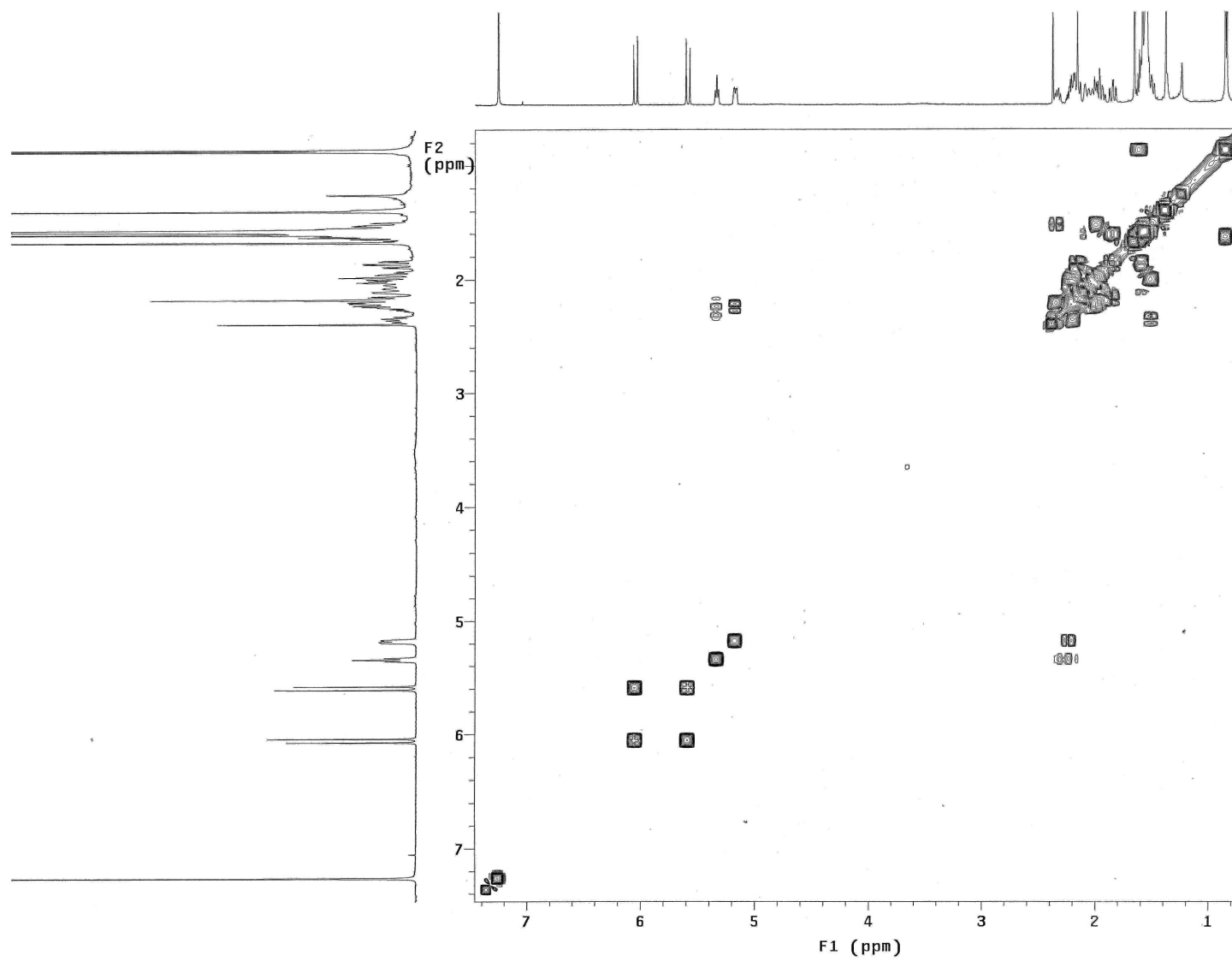


Figure S25. ^1H - ^1H COSY spectrum of **4** in CDCl_3 .

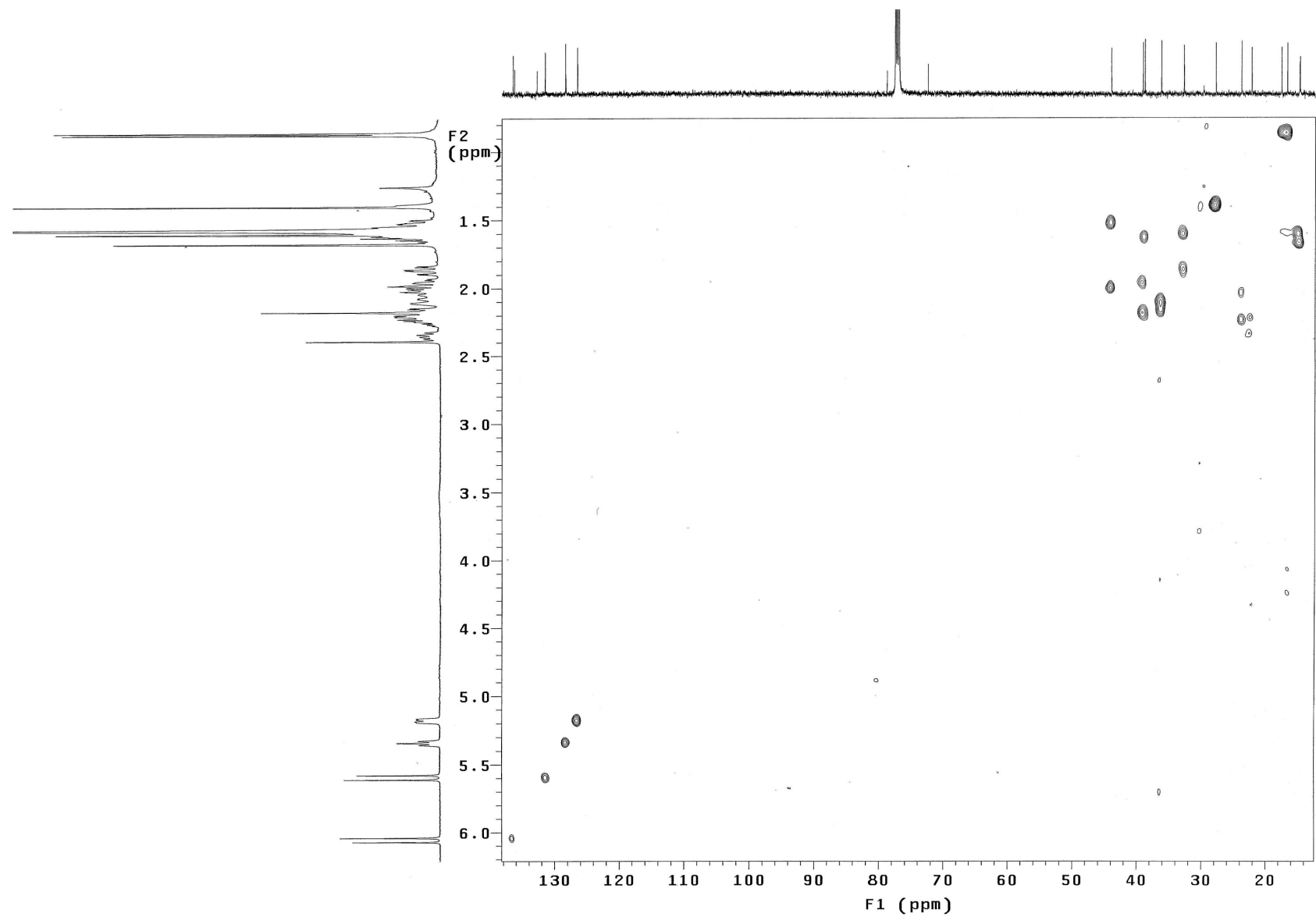


Figure S26. HSQC spectrum of **4** in CDCl₃.

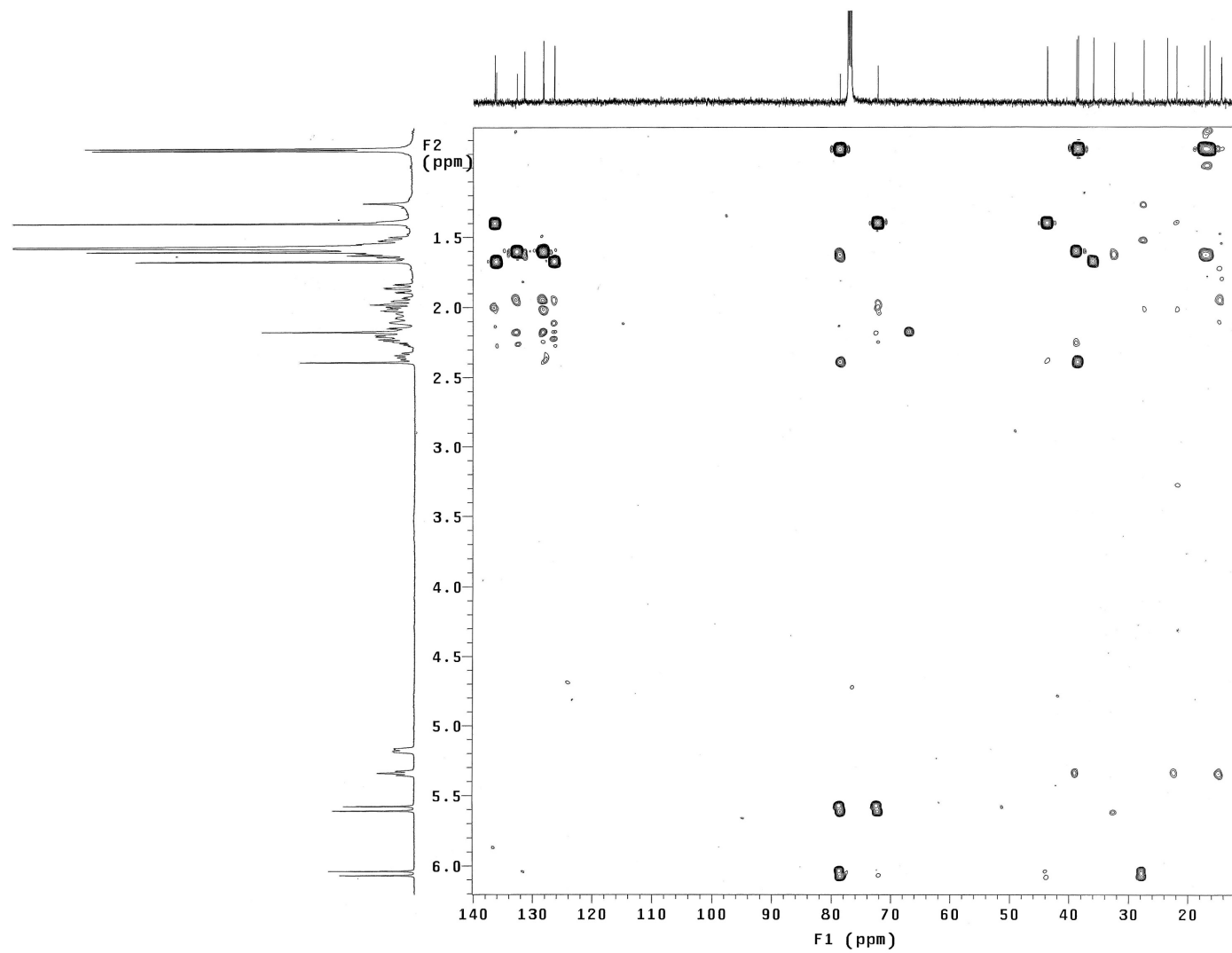


Figure S27. HMBC spectrum of 4 in CDCl₃.

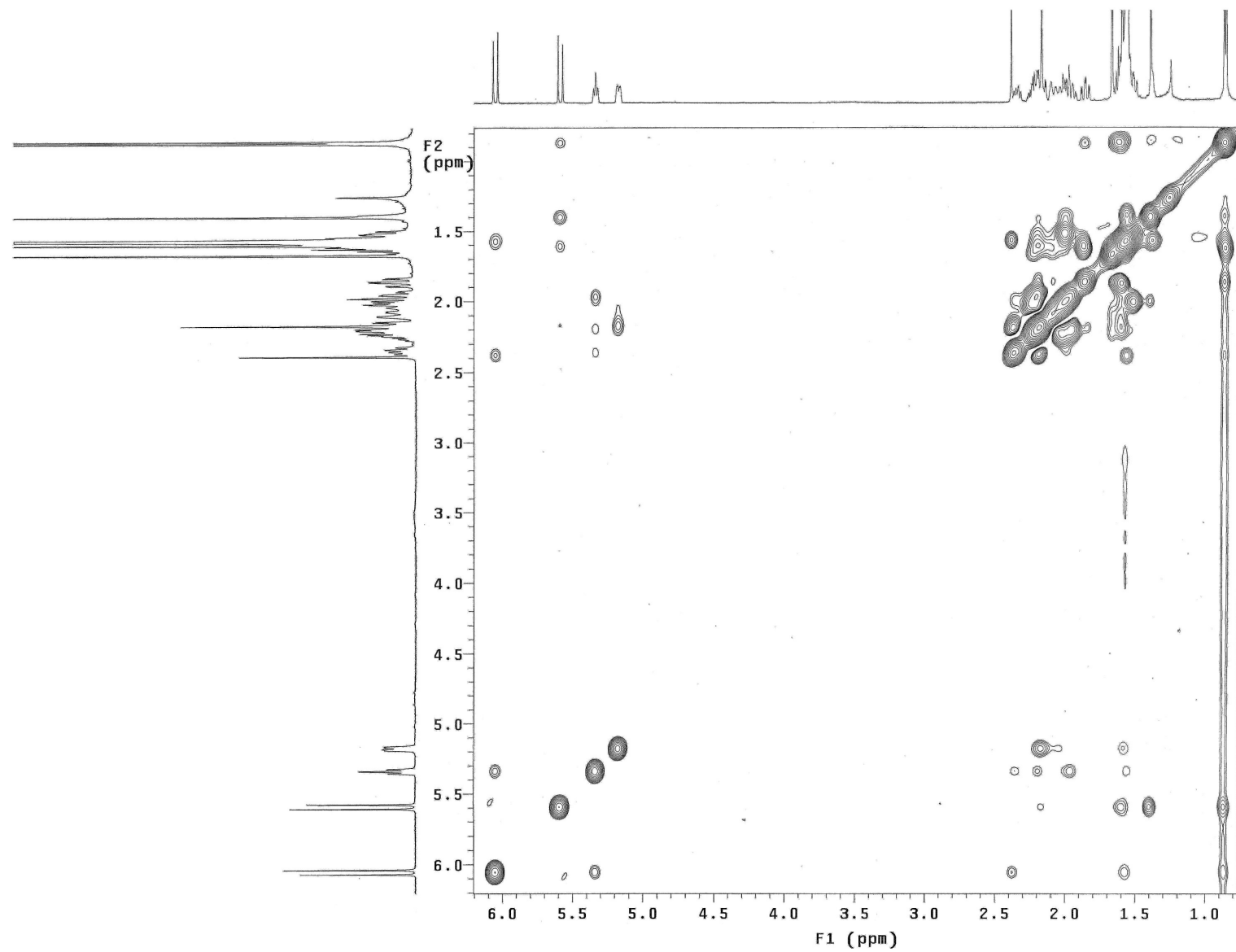


Figure S28. NOESY spectrum of **4** in CDCl₃.