Supplementary information

New Cembranoids and a Biscembranoid Peroxide from the Soft Coral *Sarcophyton cherbonnieri*

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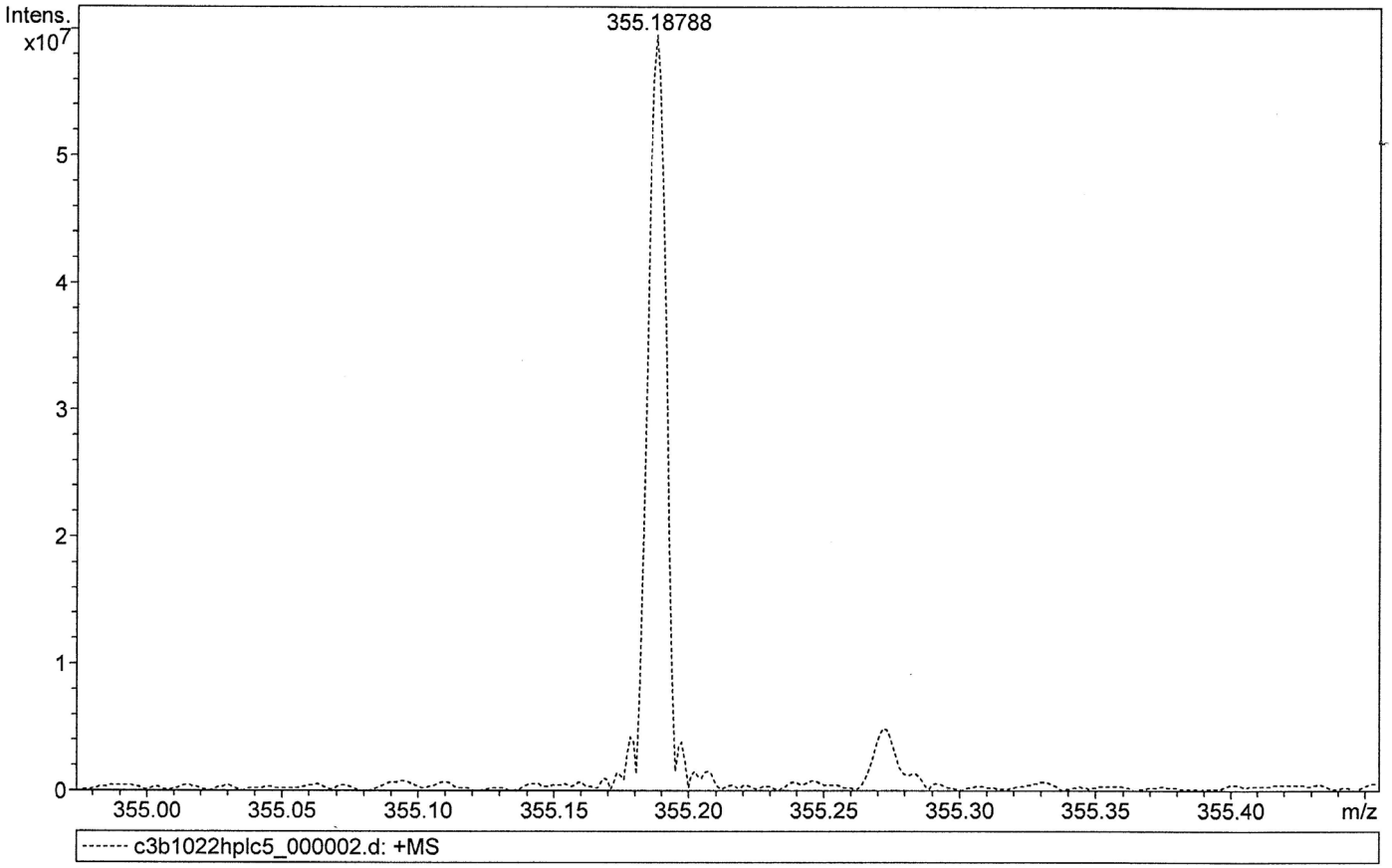


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
355.18788	1	C 20 H 28 Na O 4	100.00	355.18798	0.10	0.29	5.9	6.5	even	ok

Figure S1. HRESIMS spectrum of **1**

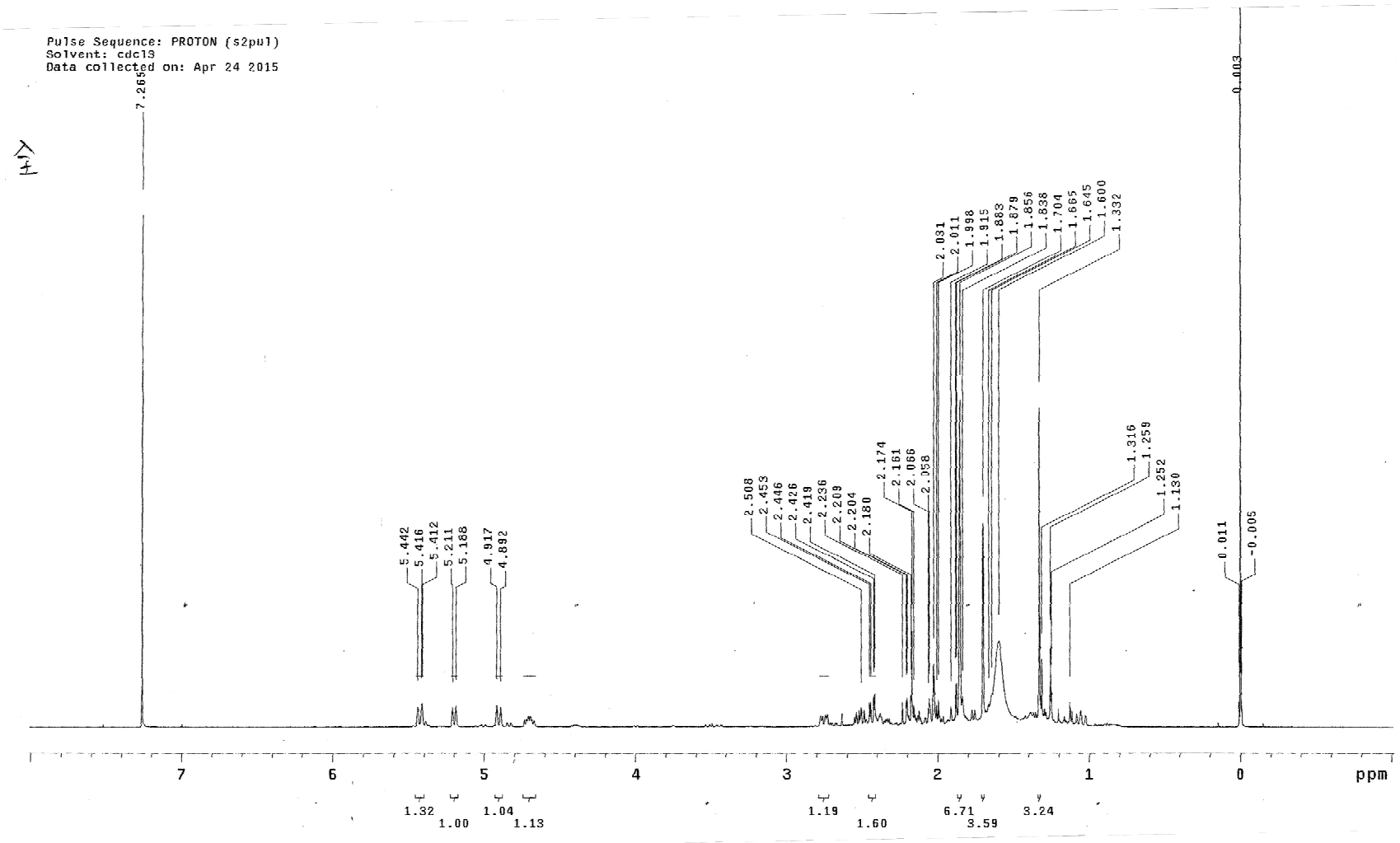


Figure S2. ^{1}H NMR spectrum of **1** in $CDCl_3$

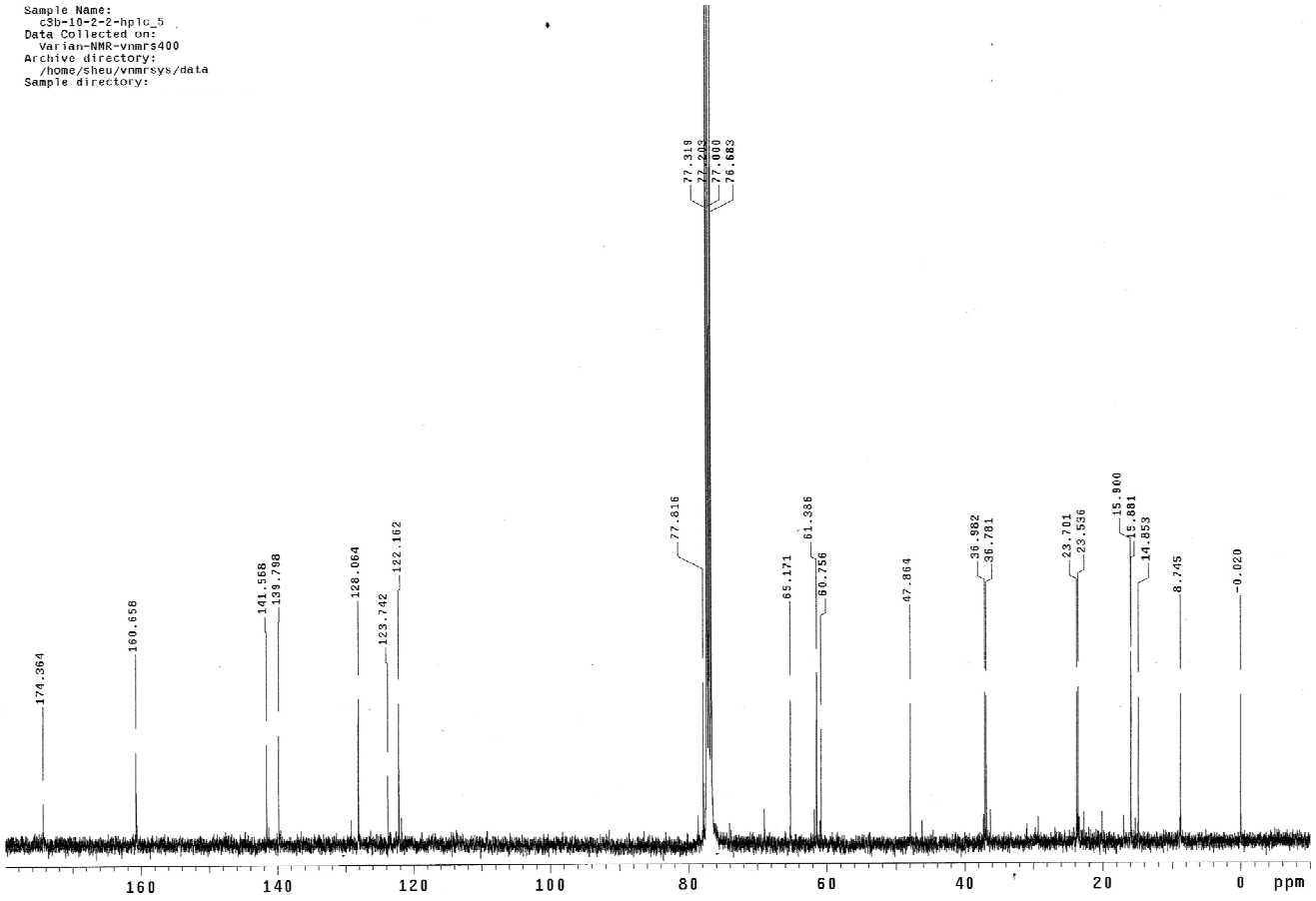


Figure S3. ^{13}C NMR spectrum of **1** in $CDCl_3$

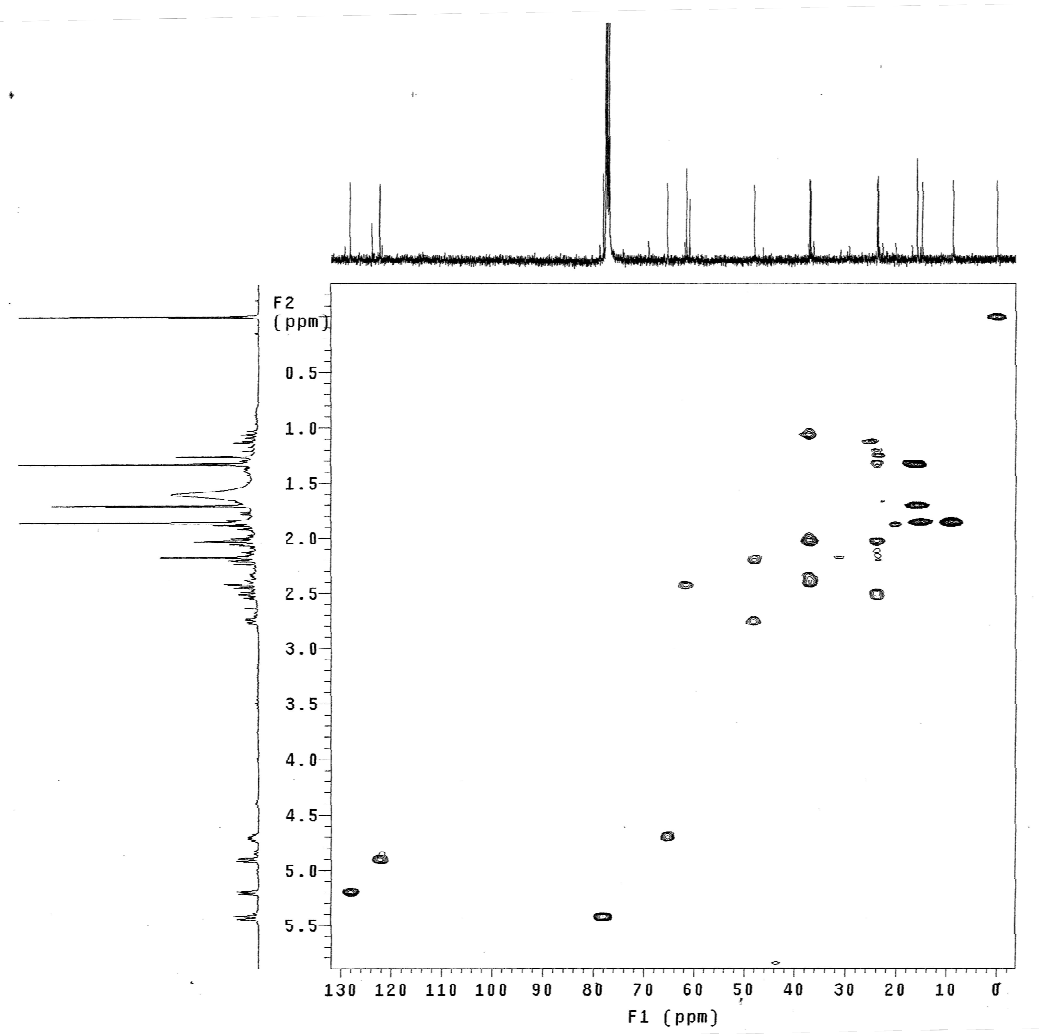


Figure S4. HSQC spectrum of **1** in $CDCl_3$

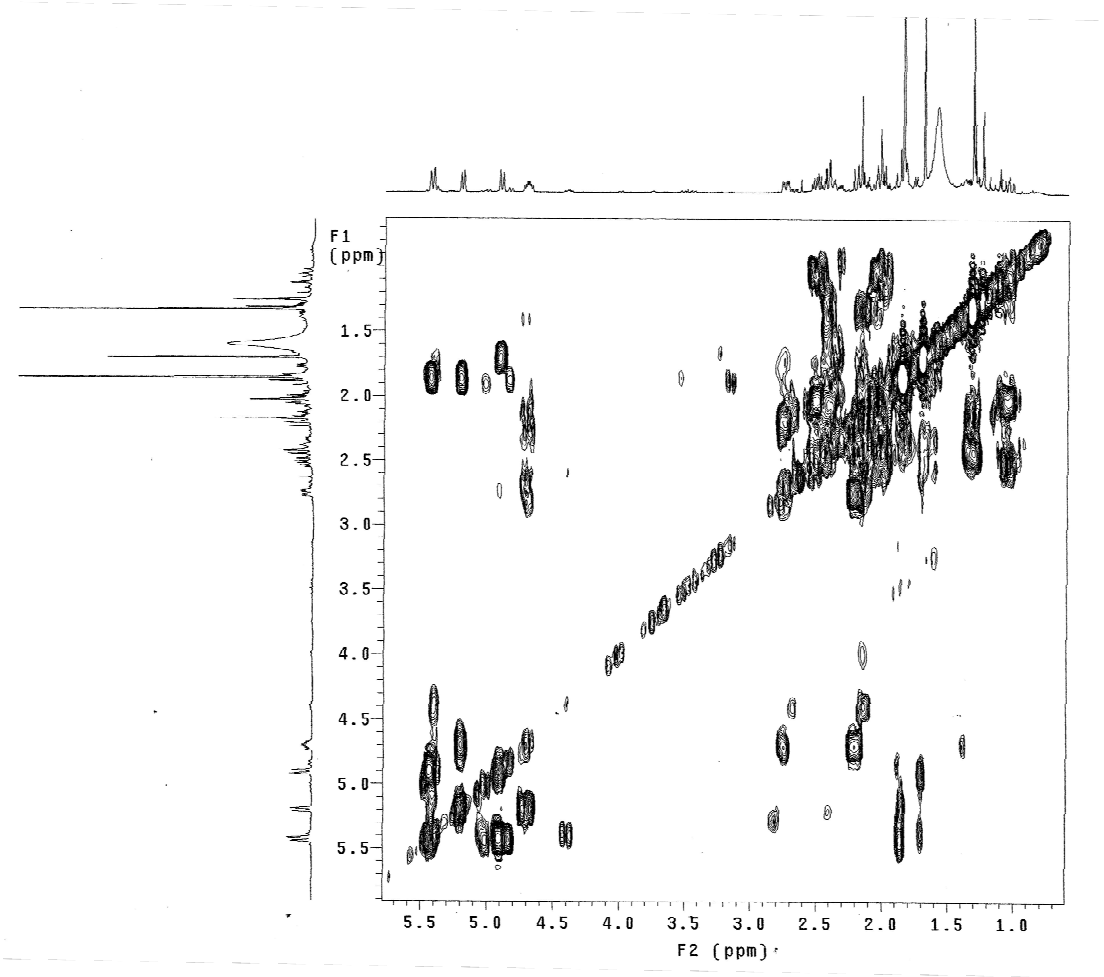


Figure S5. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$

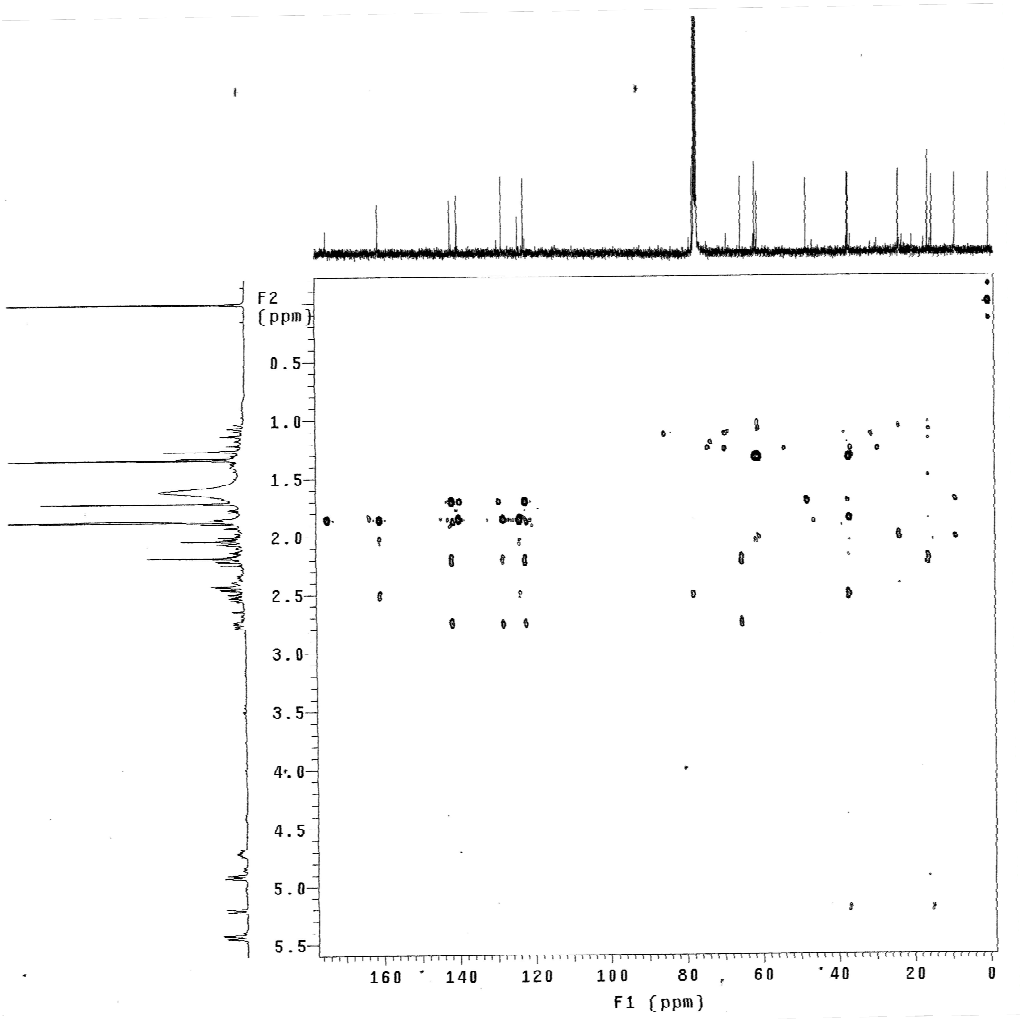


Figure S6. HMBC spectrum of **1** in $CDCl_3$

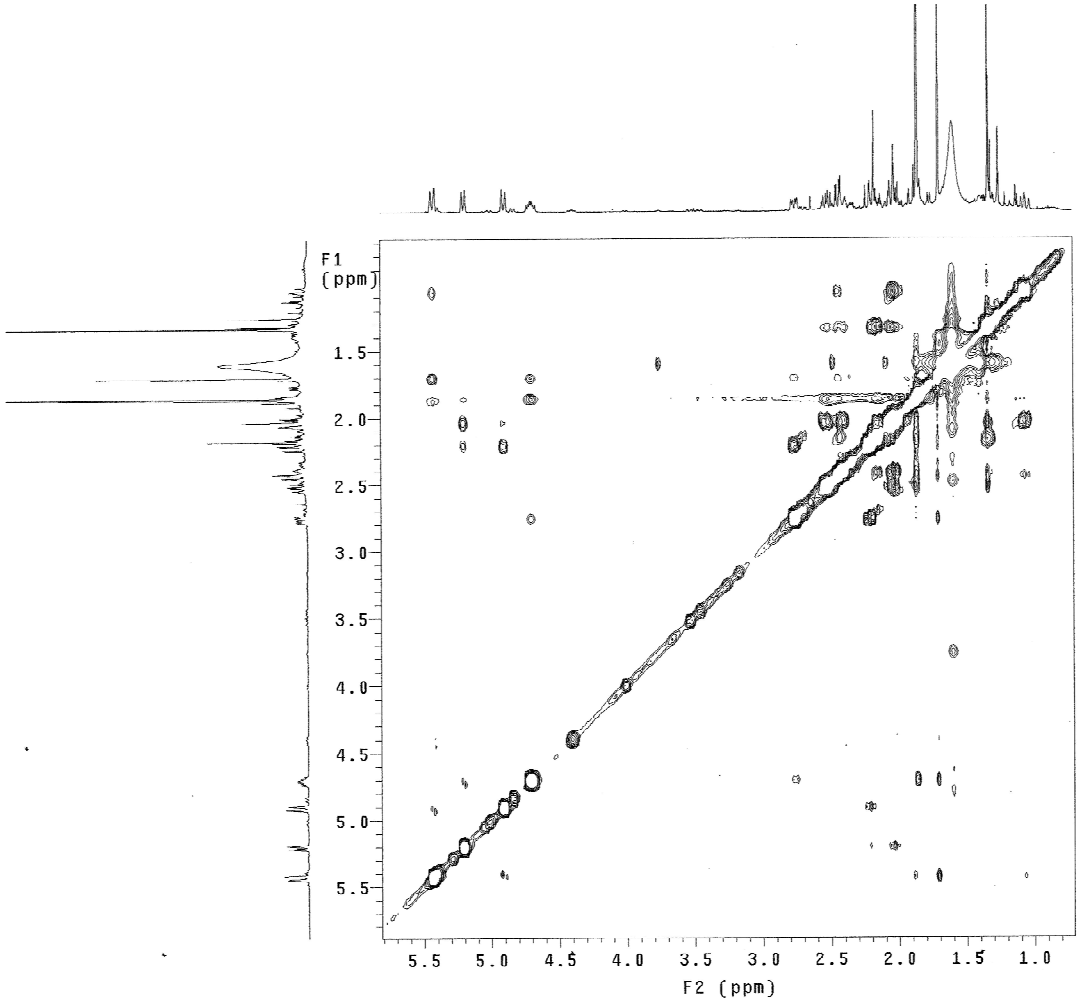
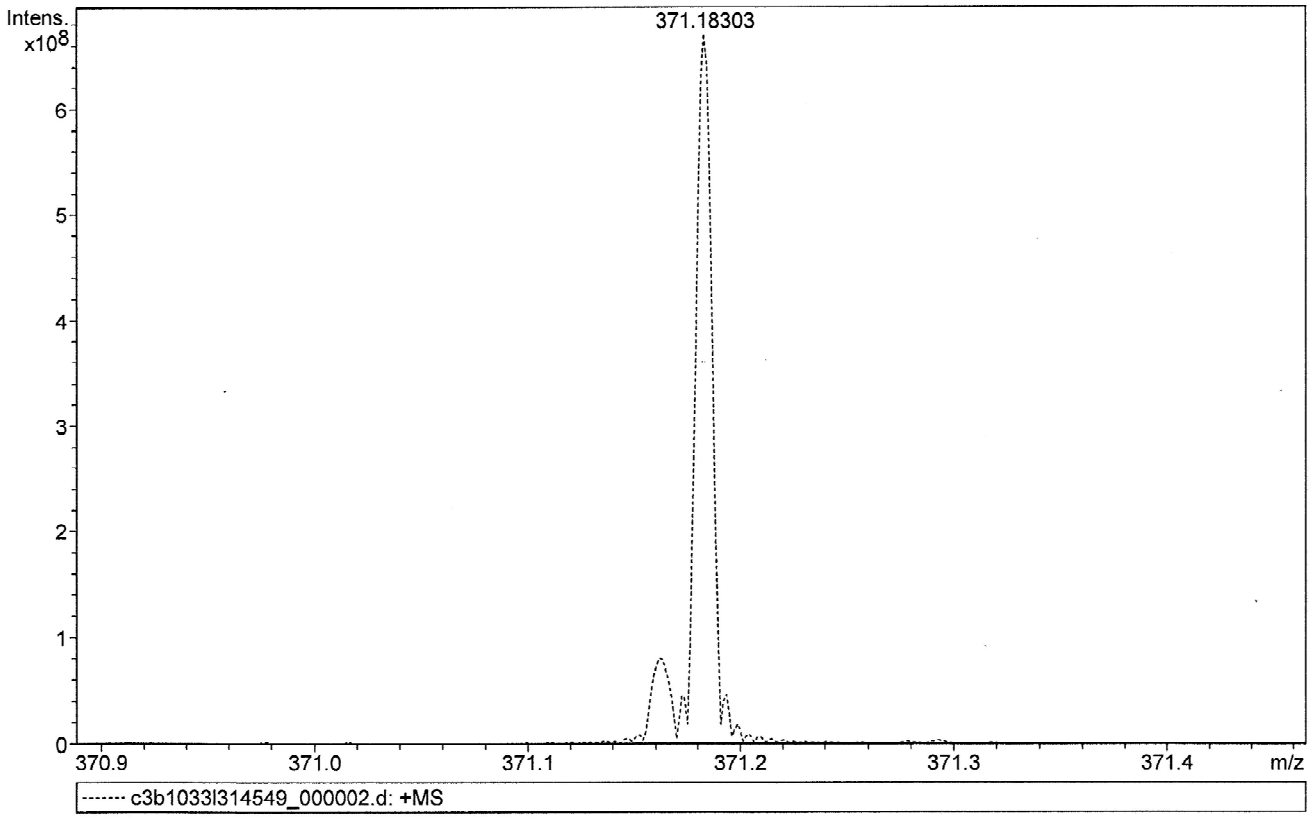


Figure S7. NOESY spectrum of **1** in $CDCl_3$



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
371.18303	1	C 20 H 28 Na O 5	100.00	371.18290	-0.14	-0.37	6.2	6.5	even	ok

Figure S8. HRESIMS spectrum of **2**

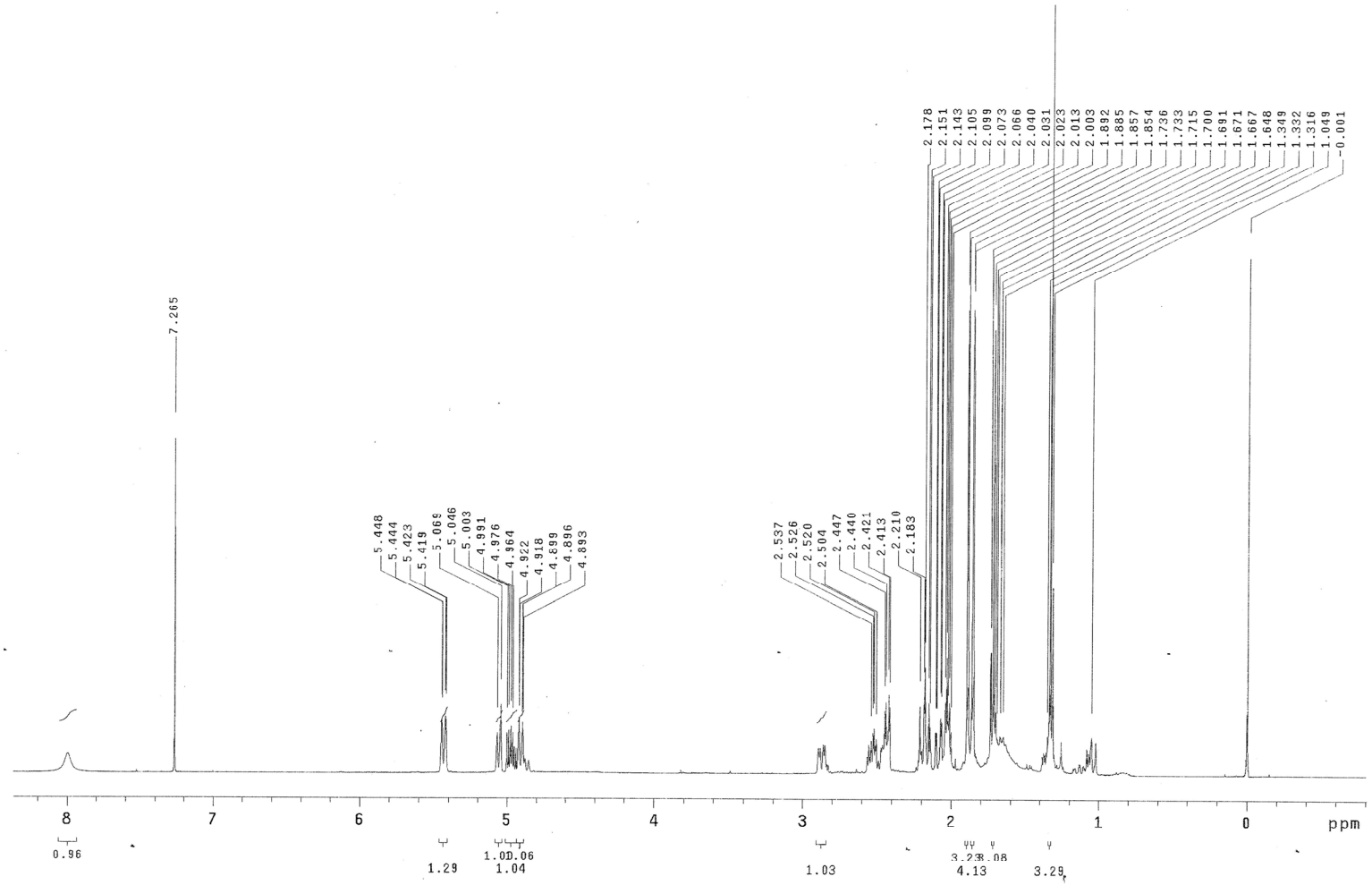


Figure S9. ^{1}H NMR spectrum of **2** in $CDCl_3$

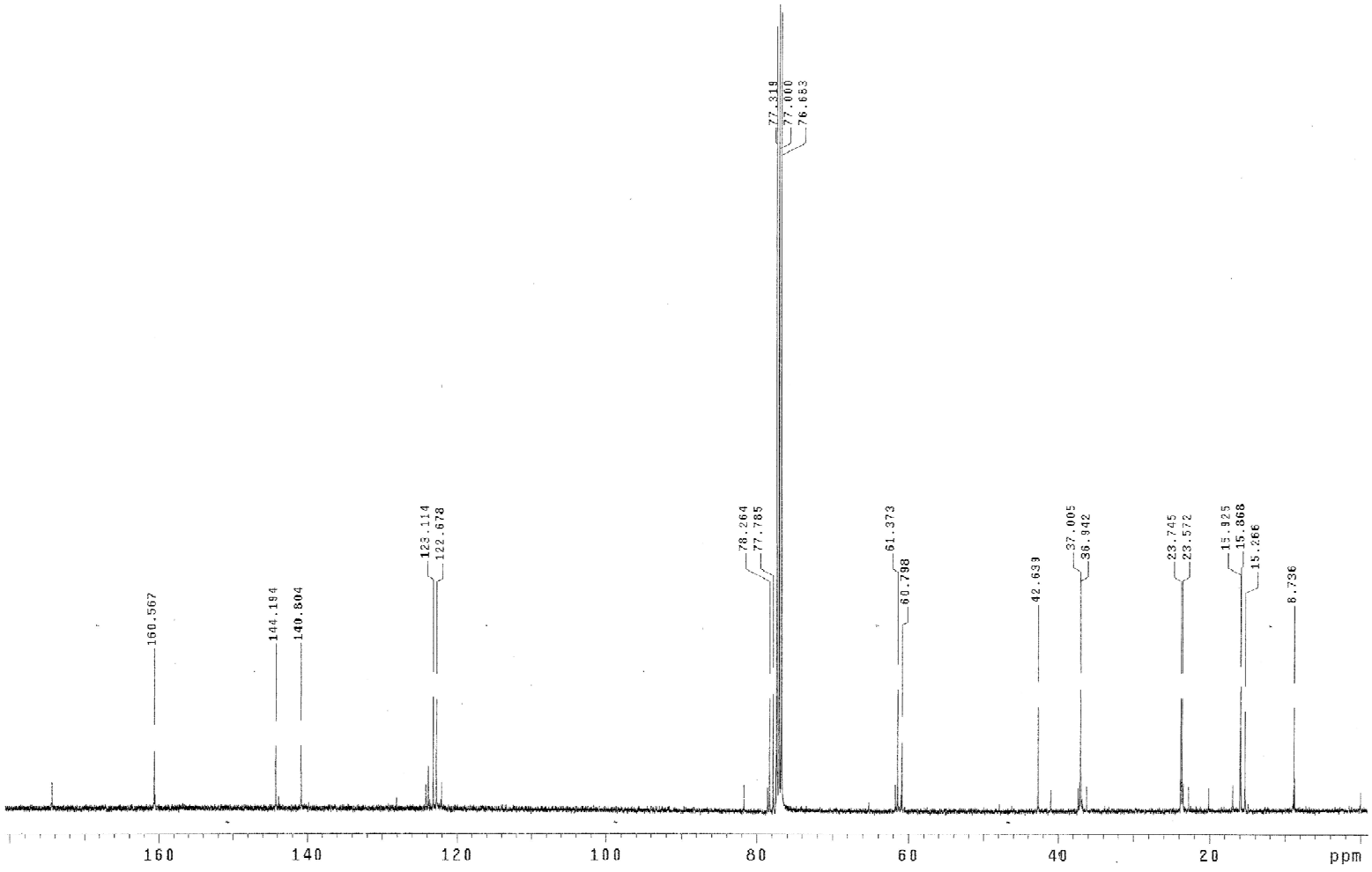


Figure S10. ^{13}C NMR spectrum of **2** in $CDCl_3$

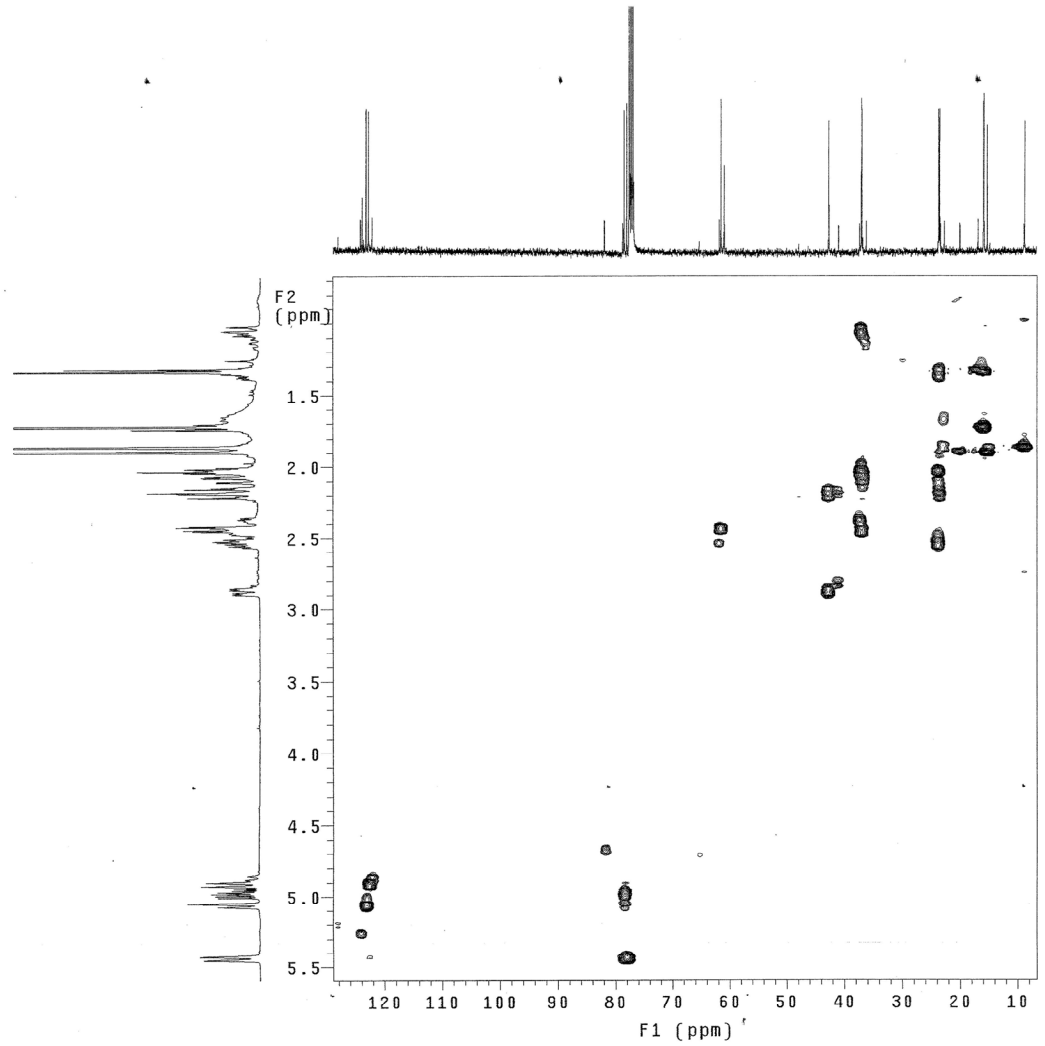


Figure S11. HSQC spectrum of **2** in $CDCl_3$

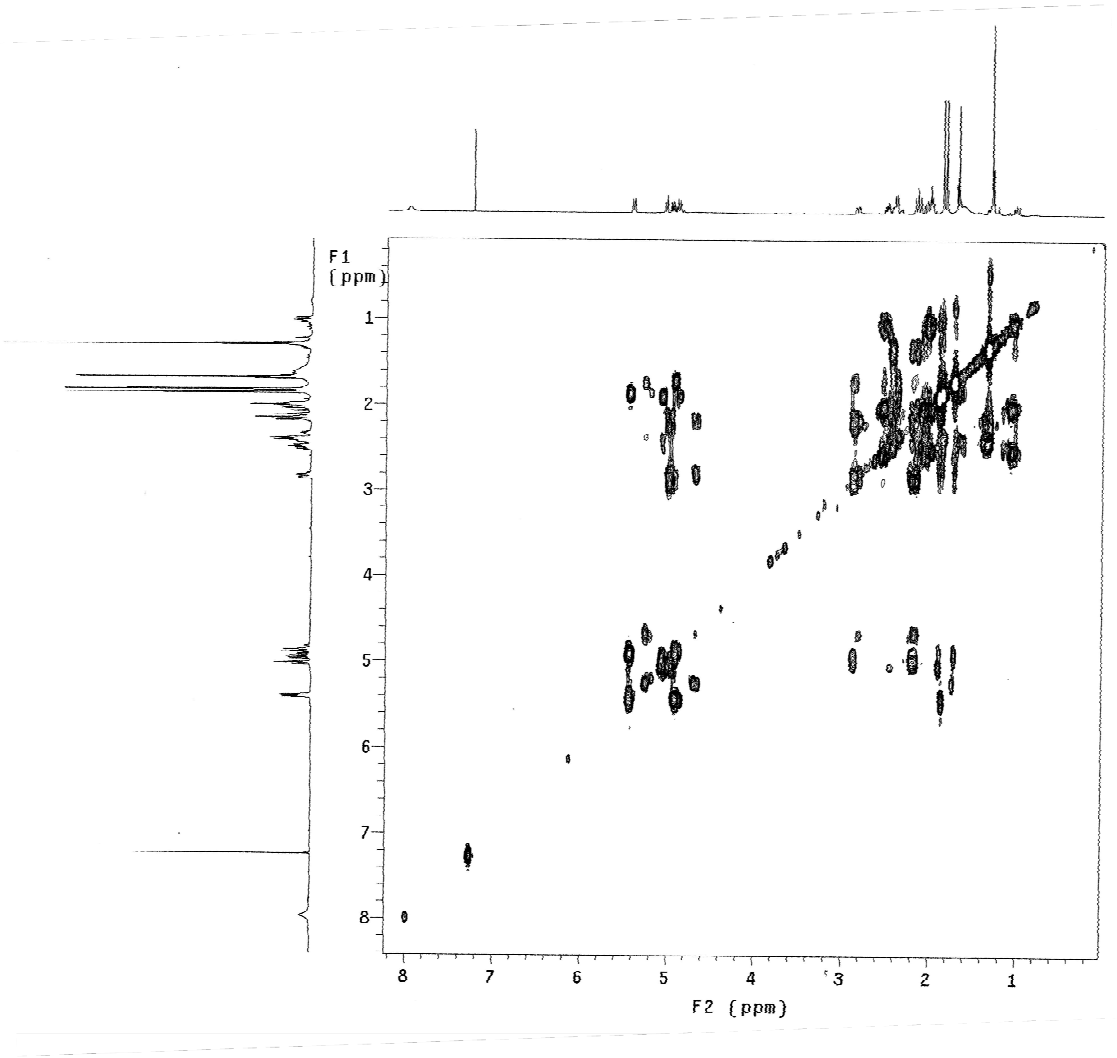


Figure S12. ^{1}H-^{1}H COSY spectrum of **2** in $CDCl_3$

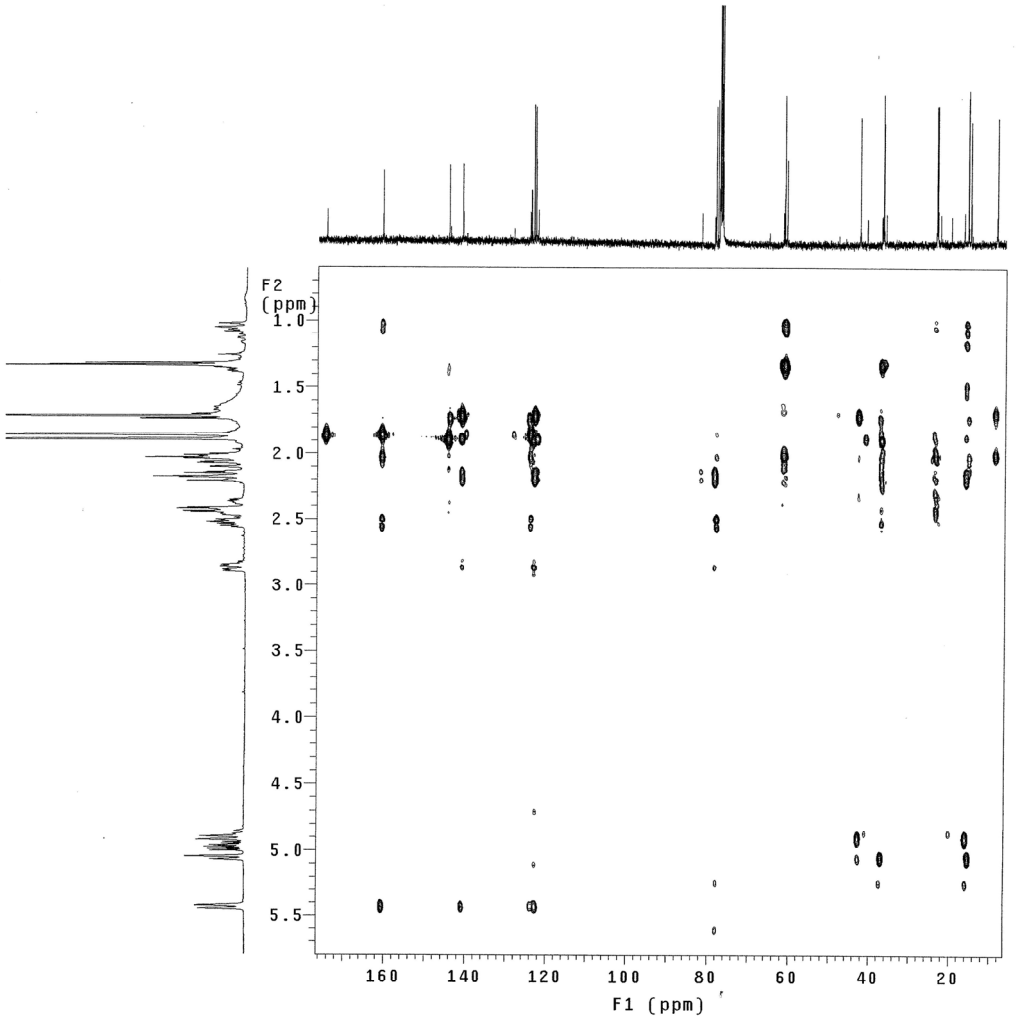


Figure S13. HMBC spectrum of **2** in C_6D_6

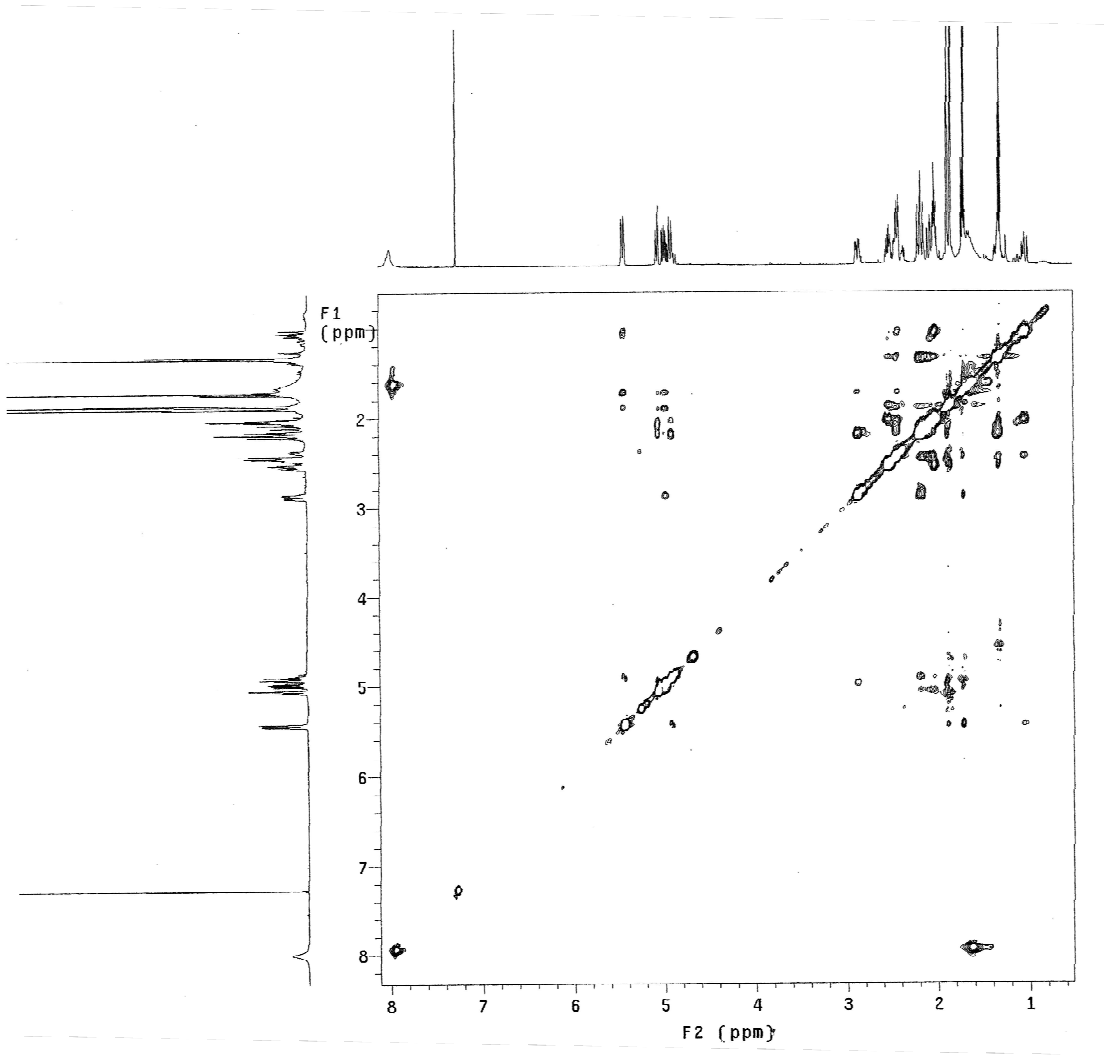
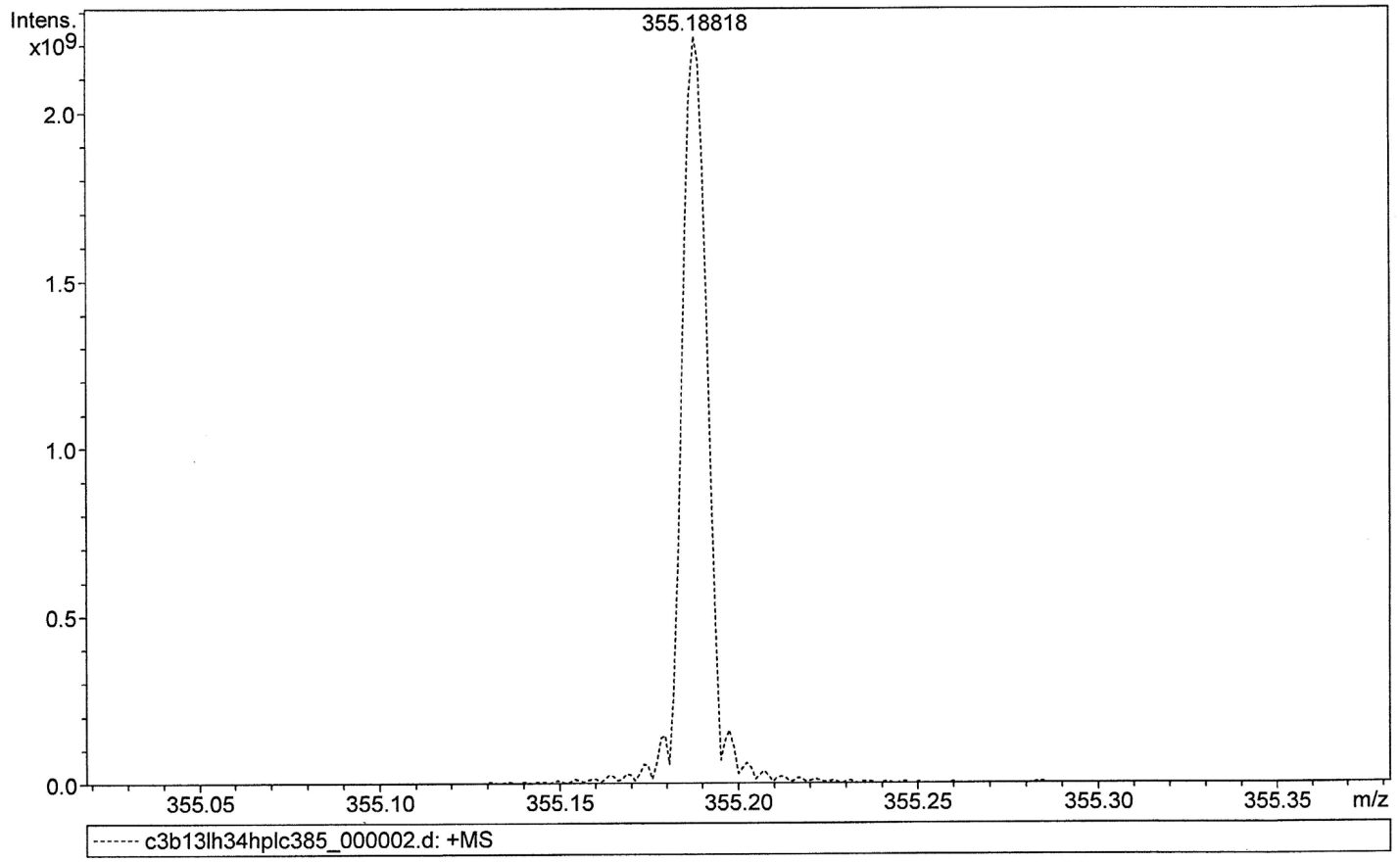


Figure S14. NOESY spectrum of **2** in C_6D_6



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
355.18818	1	C 20 H 28 Na O 4	100.00	355.18798	-0.20	-0.57	6.3	6.5	even	ok

Figure S15. HRESIMS spectrum of **3**

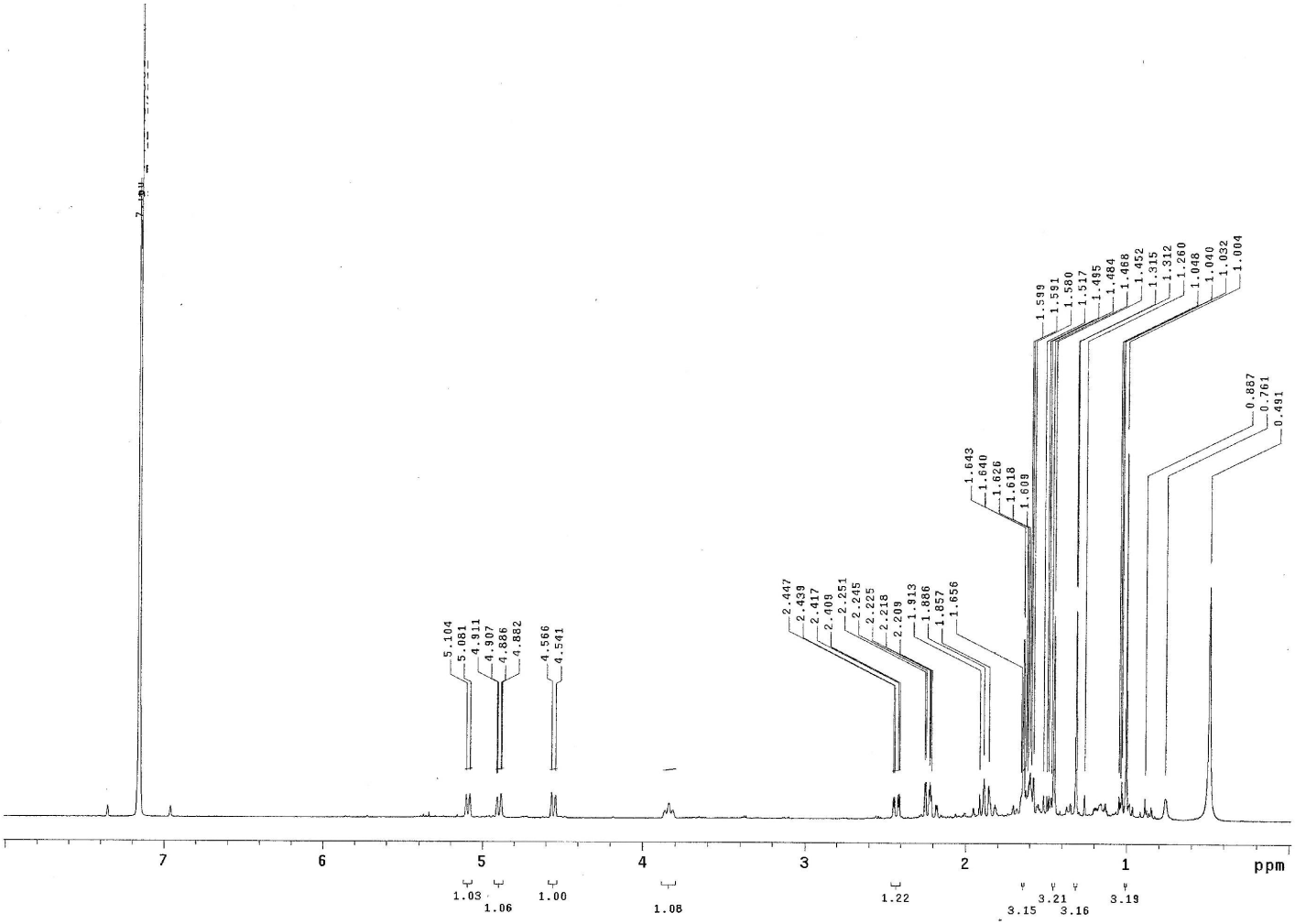


Figure S16. ^{1}H NMR spectrum of **3** in C_6D_6

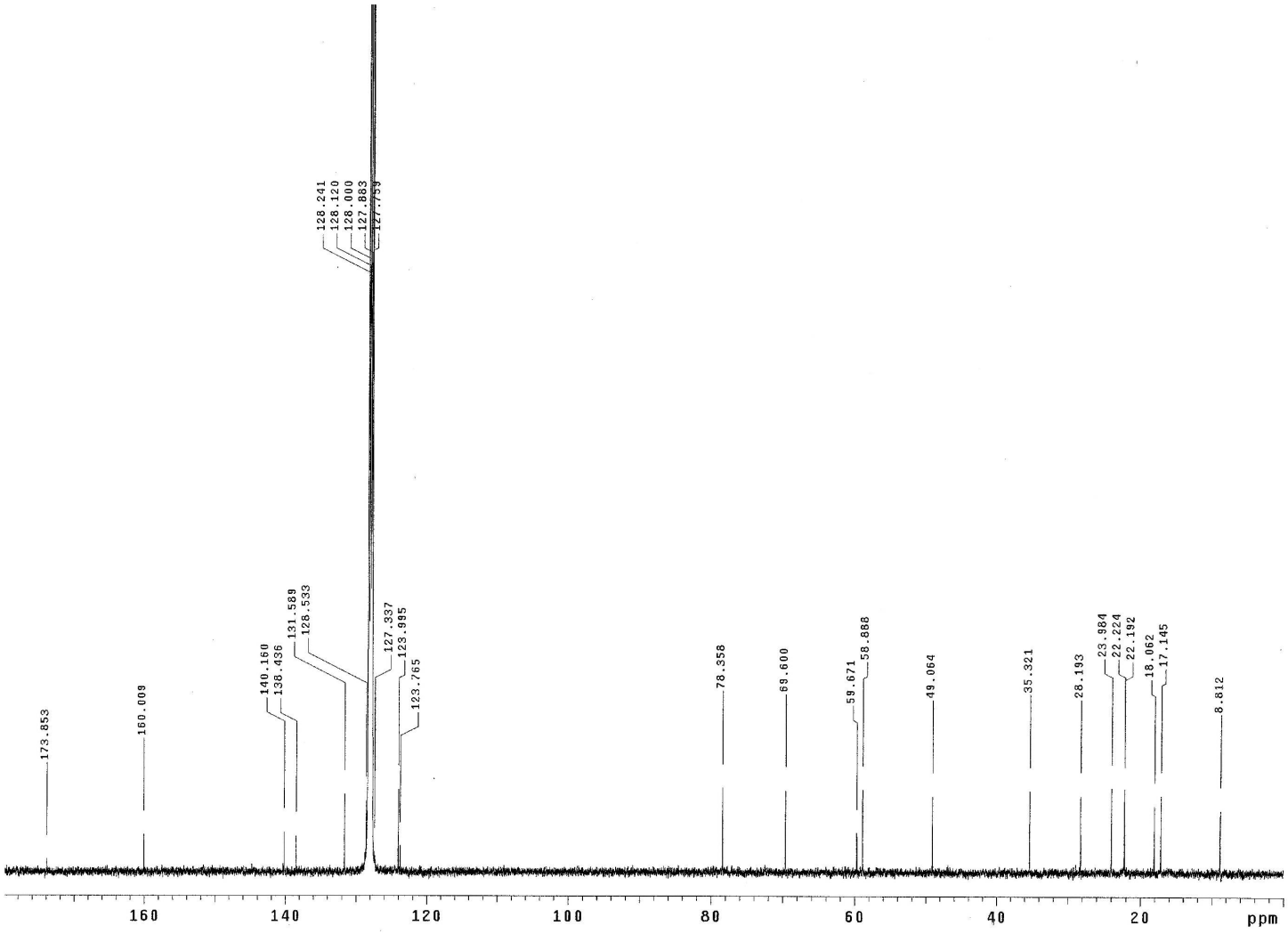


Figure S17. ^{13}C NMR spectrum of **3** in C_6D_6

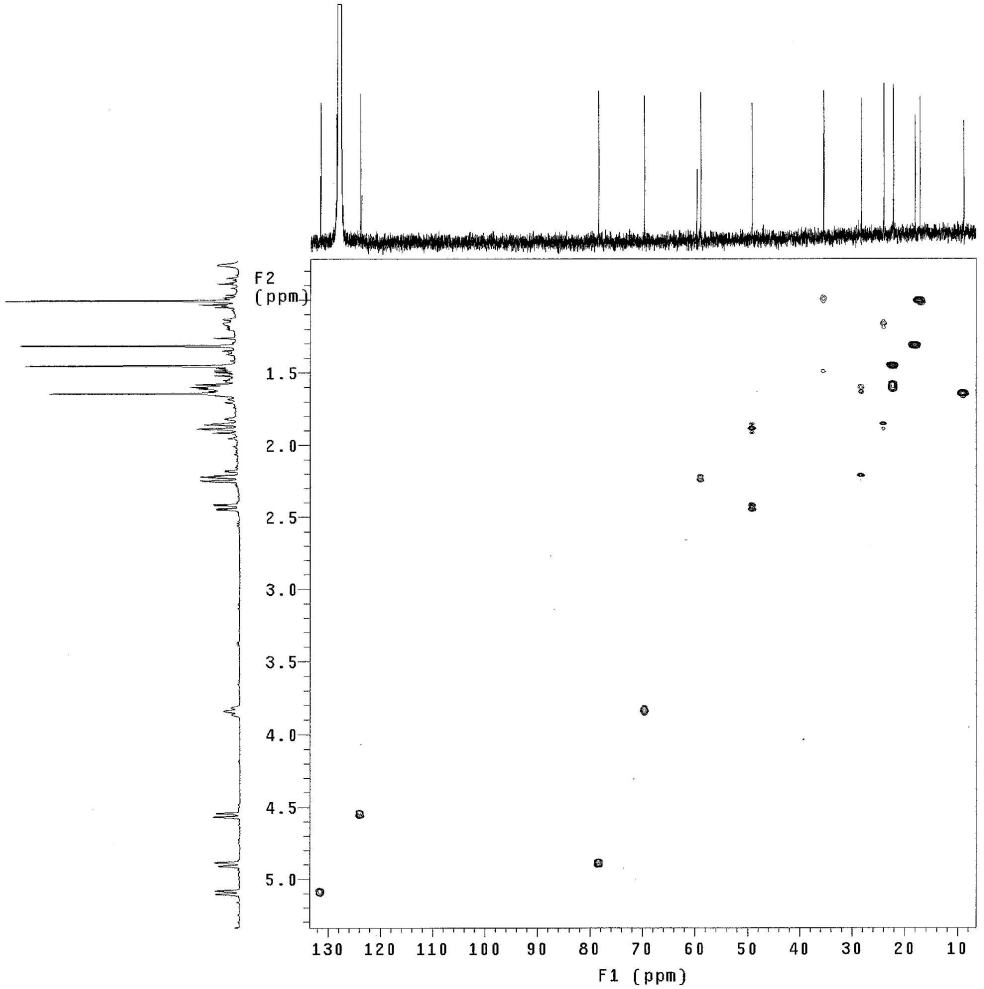


Figure S18. HSQC spectrum of **3** in C_6D_6

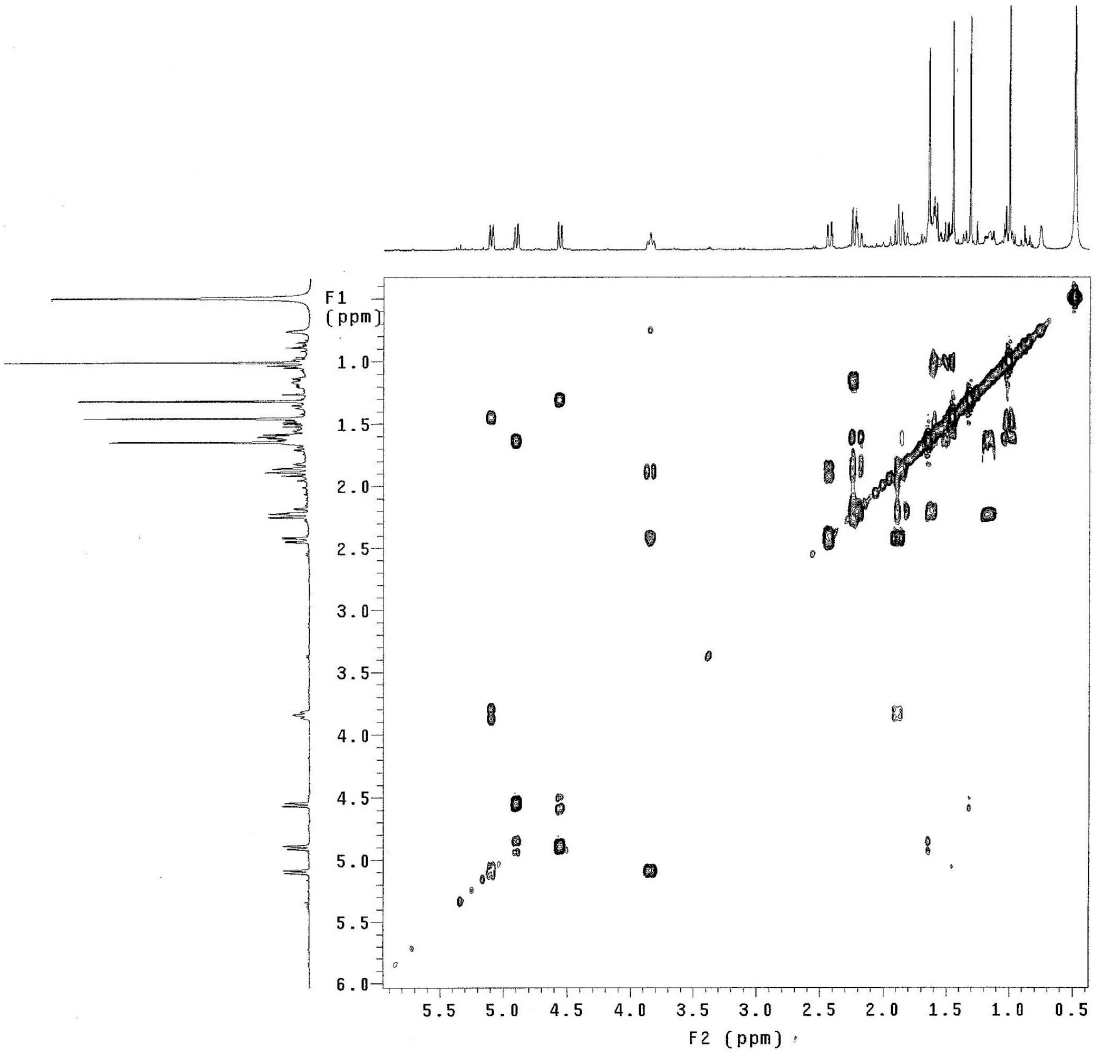


Figure S19. ^{1}H-^{1}H COSY spectrum of **3** in C_6D_6

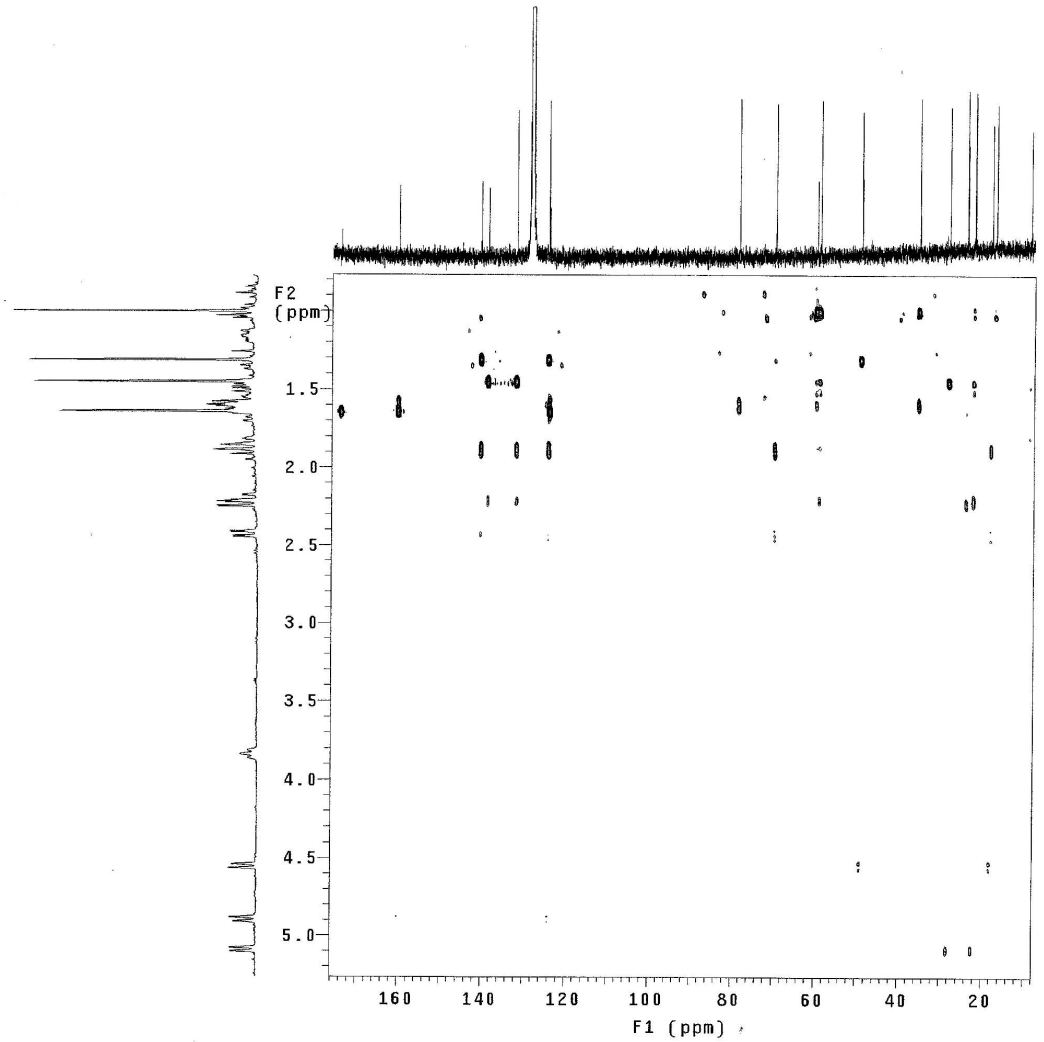


Figure S20. HMBC spectrum of **3** in C_6D_6

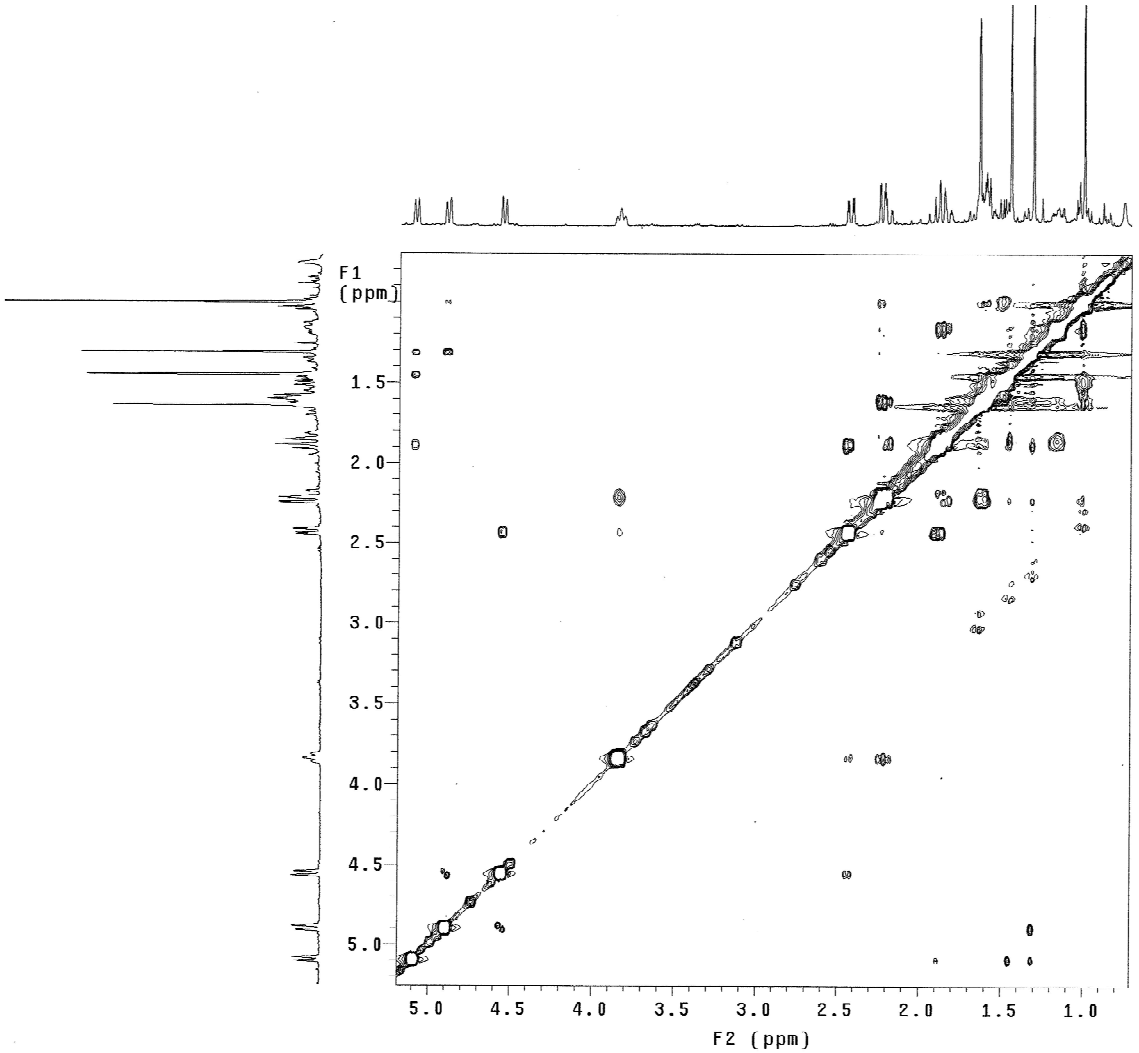
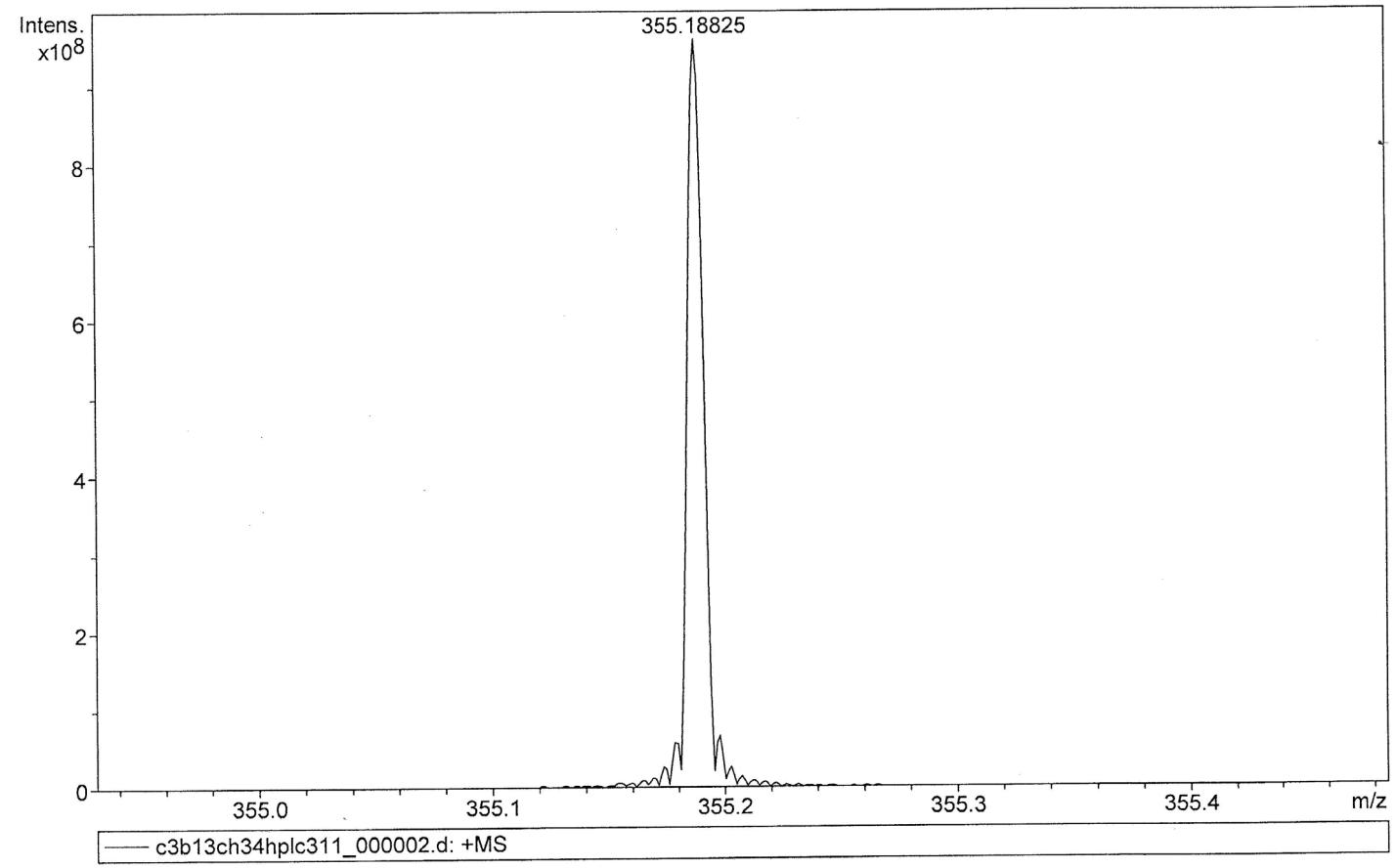


Figure S21. NOESY spectrum of **3** in C_6D_6



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
355.18825	1	C 20 H 28 Na O 4	100.00	355.18798	-0.27	-0.75	13.1	6.5	even	ok

Figure S22. HREIMS spectrum of **4**

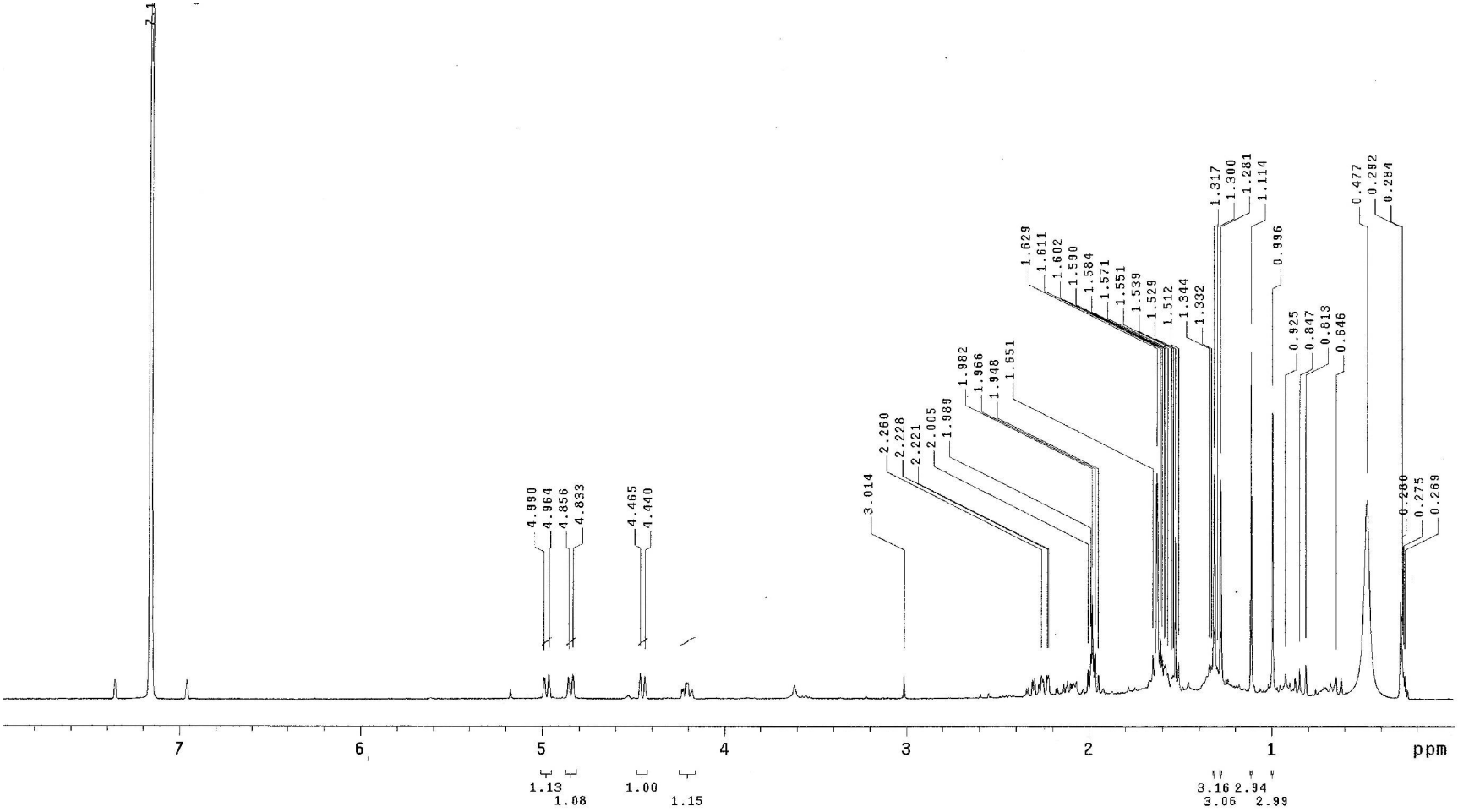


Figure S23. ^{1}H NMR spectrum of **4** in C_6D_6

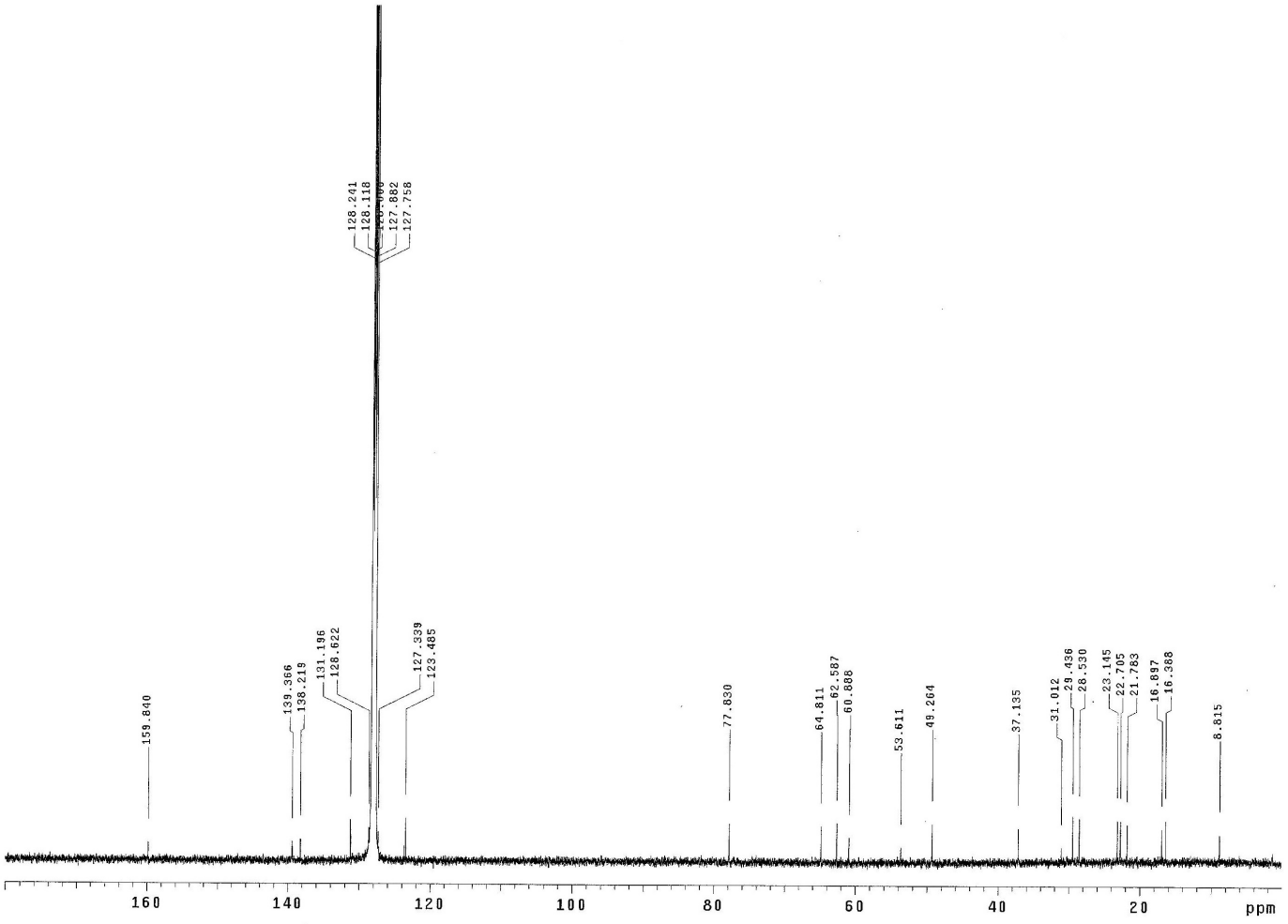


Figure S24. ^{13}C NMR spectrum of **4** in C_6D_6

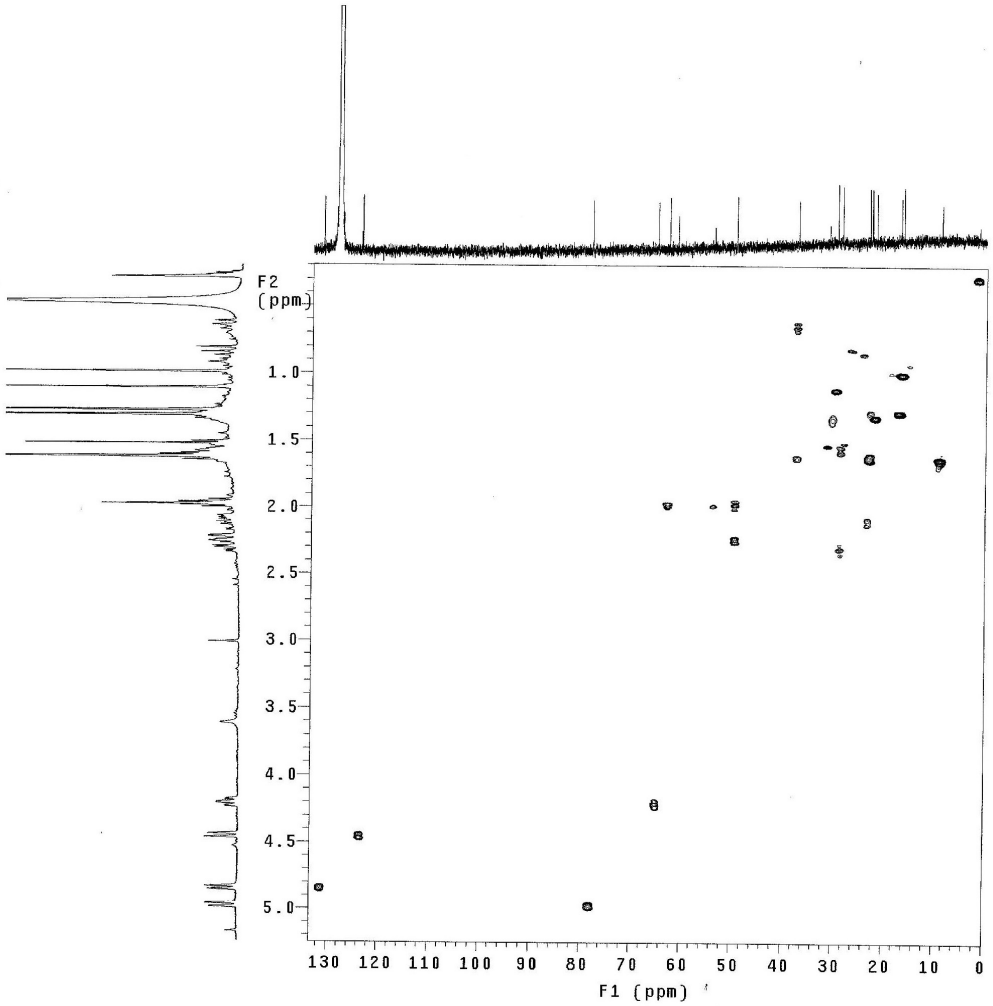


Figure S25. HSQC spectrum of **4** in C_6D_6

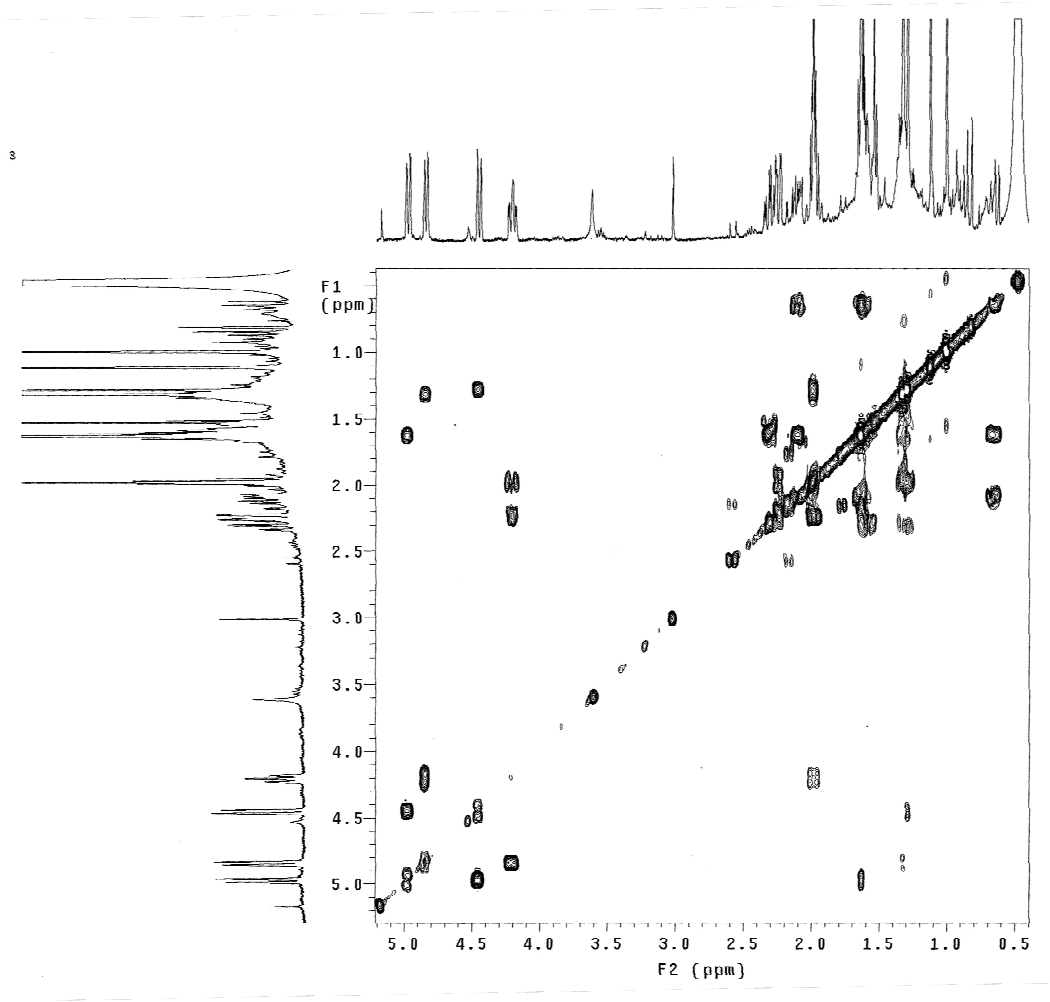


Figure S26. ^{1}H-^{1}H COSY spectrum of **4** in C_6D_6

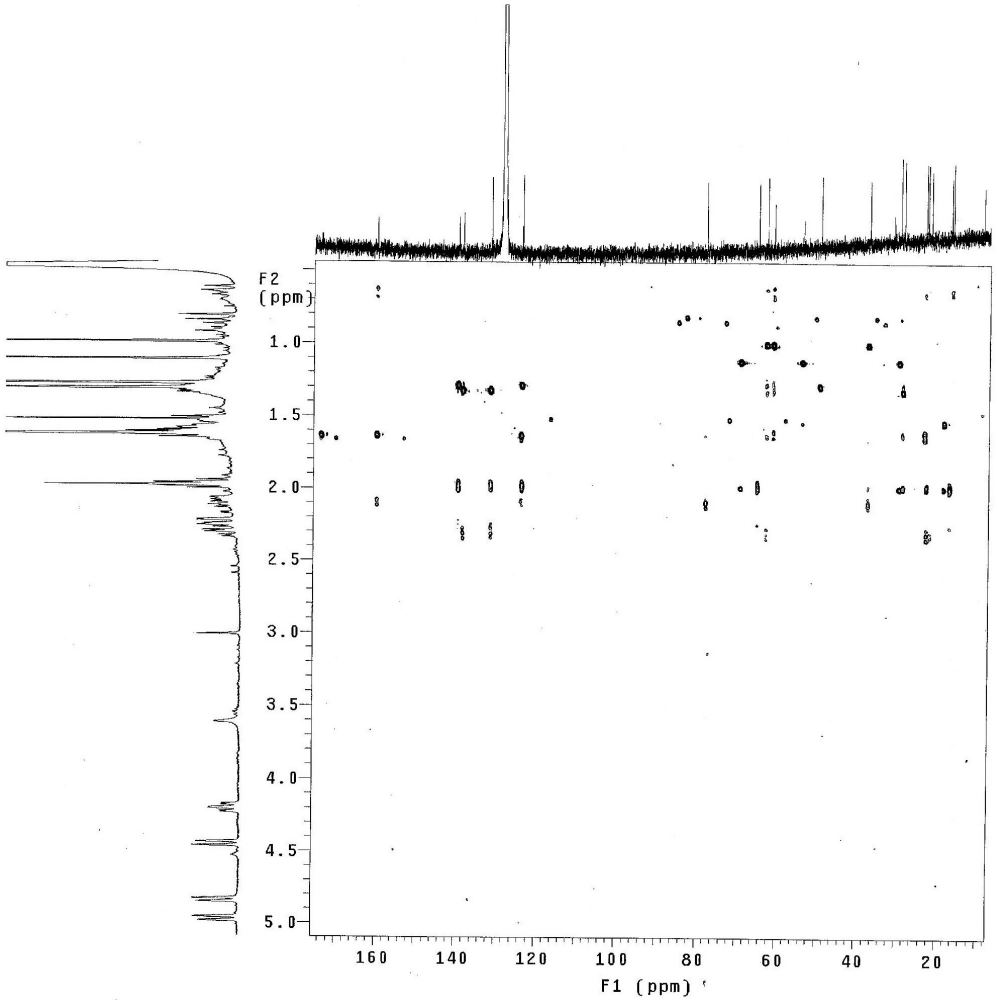


Figure S27. HMBC spectrum of **4** in C_6D_6

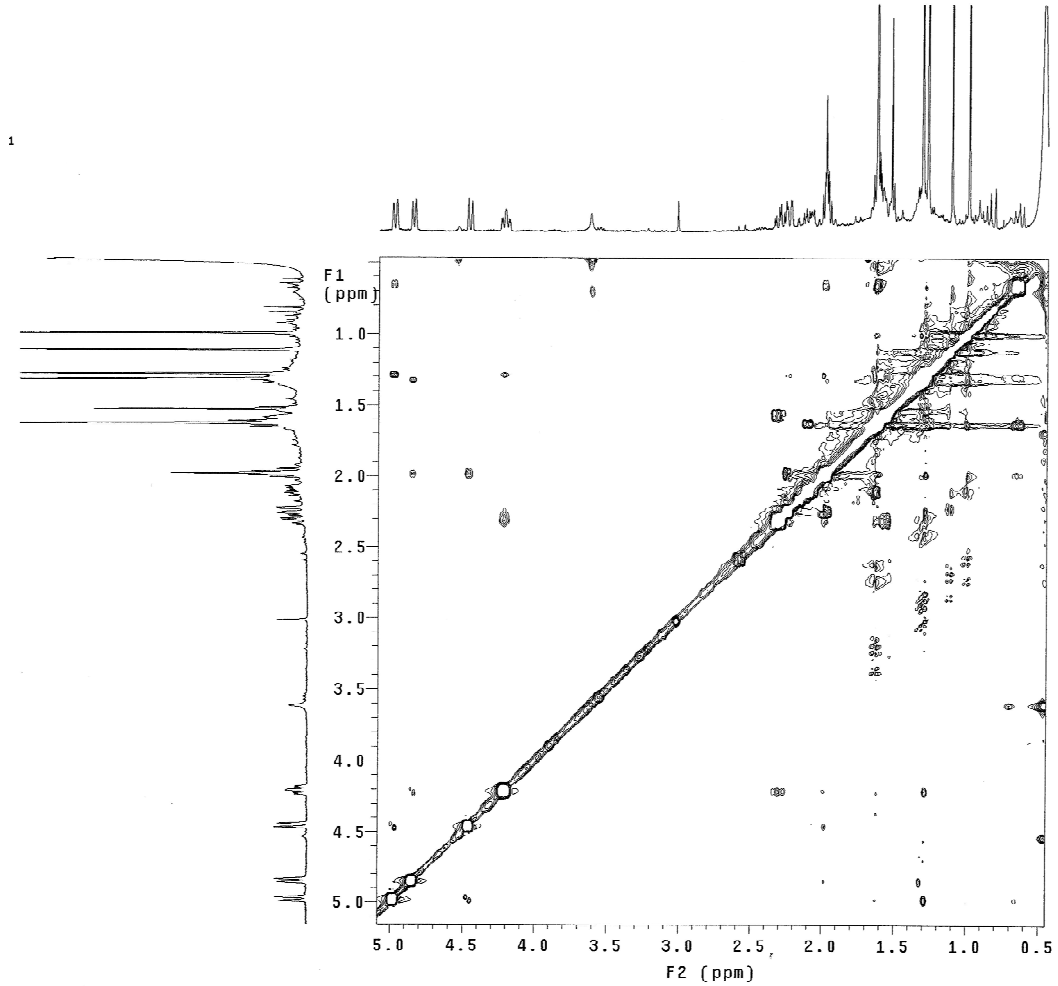
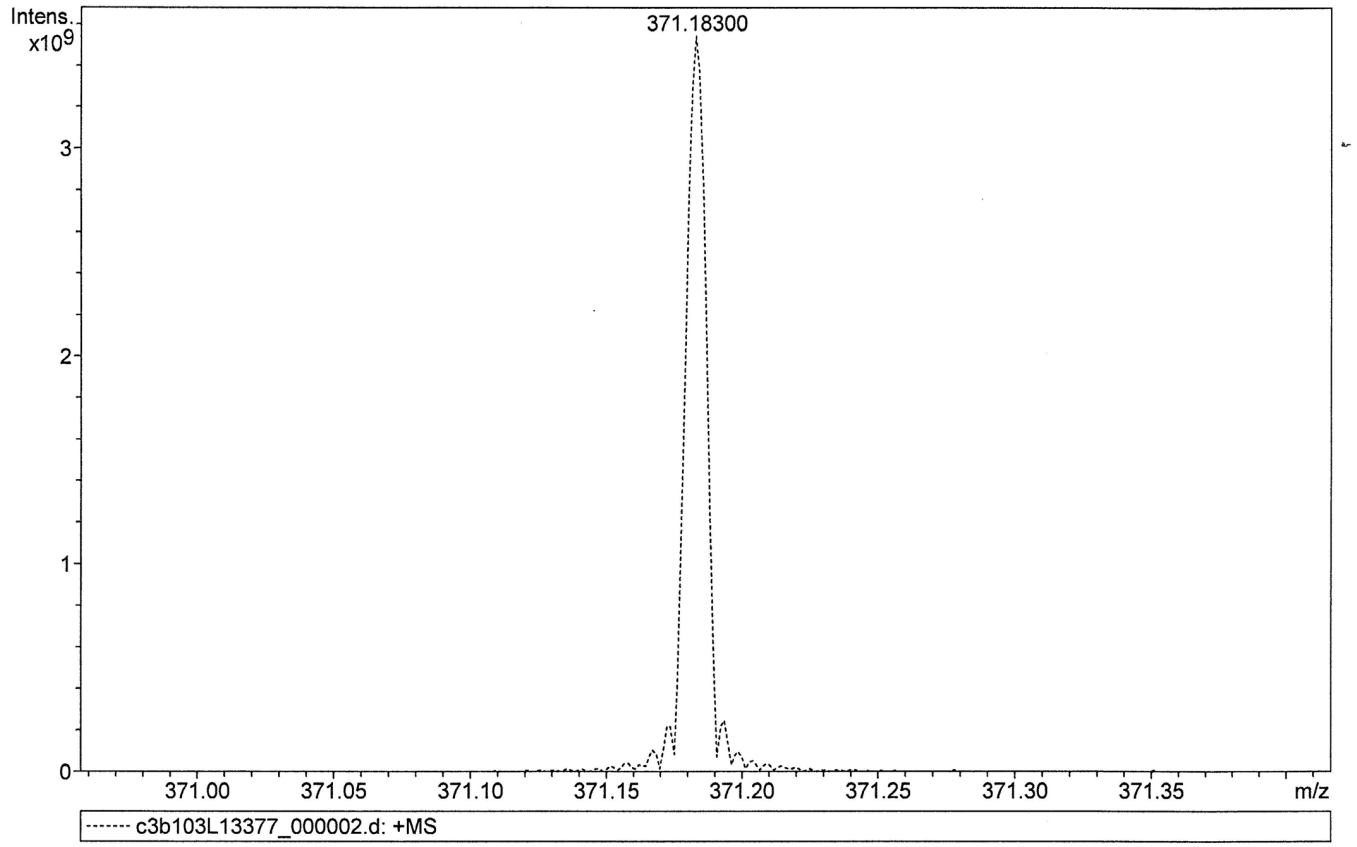


Figure S28. NOESY spectrum of **4** in C_6D_6



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
371.18300	1	C 20 H 28 Na O 5	100.00	371.18290	-0.11	-0.29	6.6	6.5	even	ok

Figure S29. HREIMS spectrum of **5**

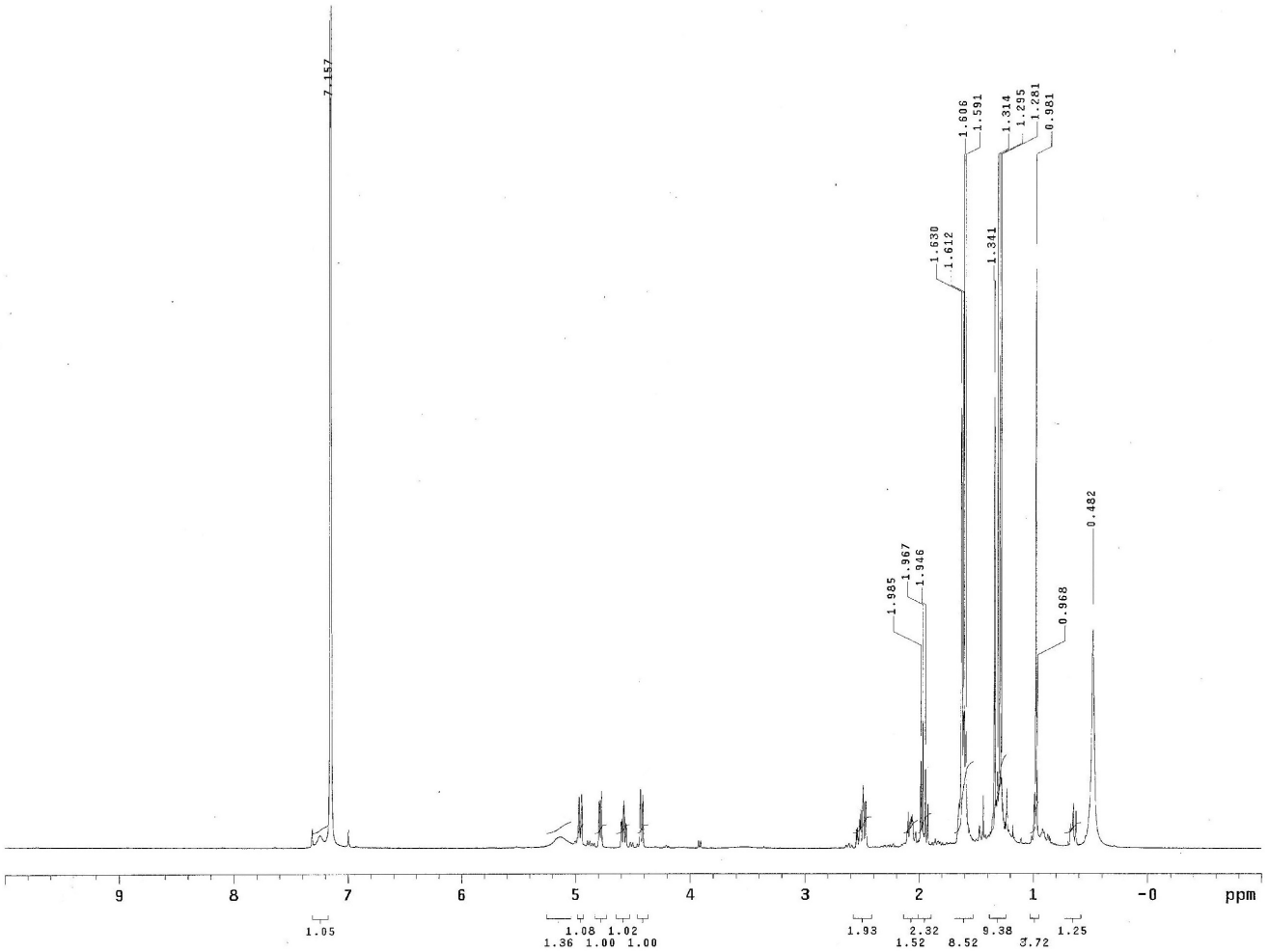


Figure S30. ^{1}H NMR spectrum of **5** in C_6D_6

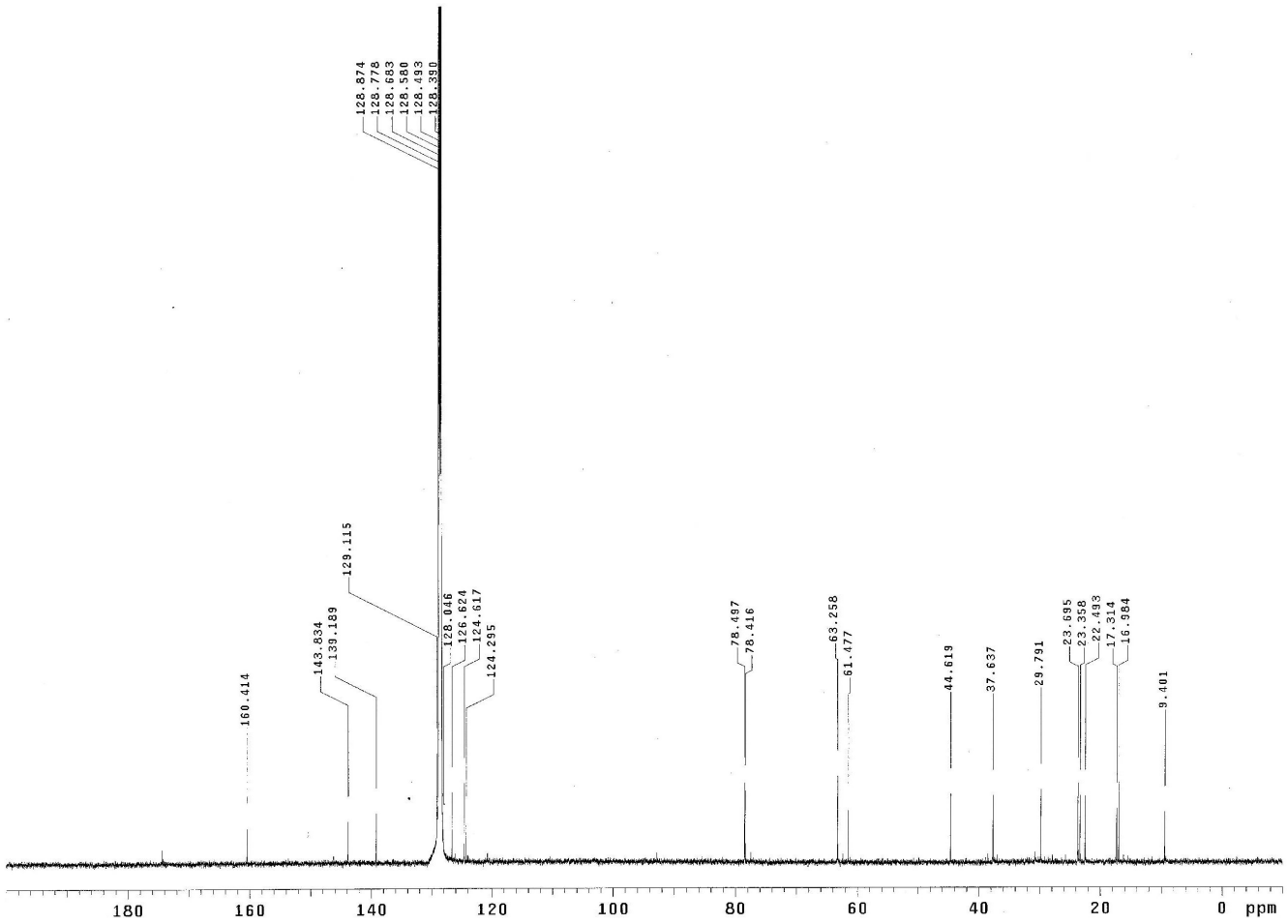


Figure S31. ^{13}C NMR spectrum of **5** in C_6D_6

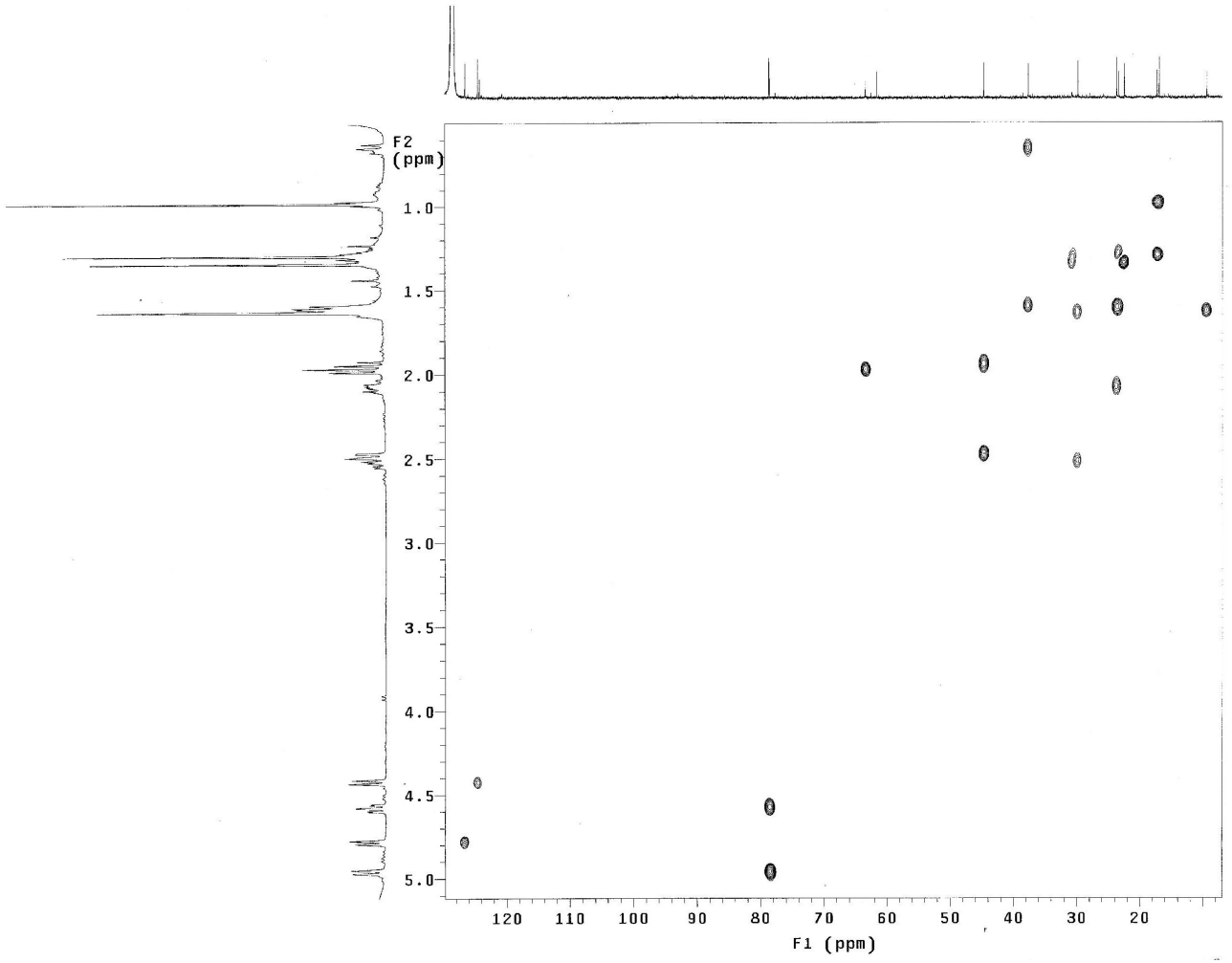


Figure S32. HSQC spectrum of **5** in C_6D_6

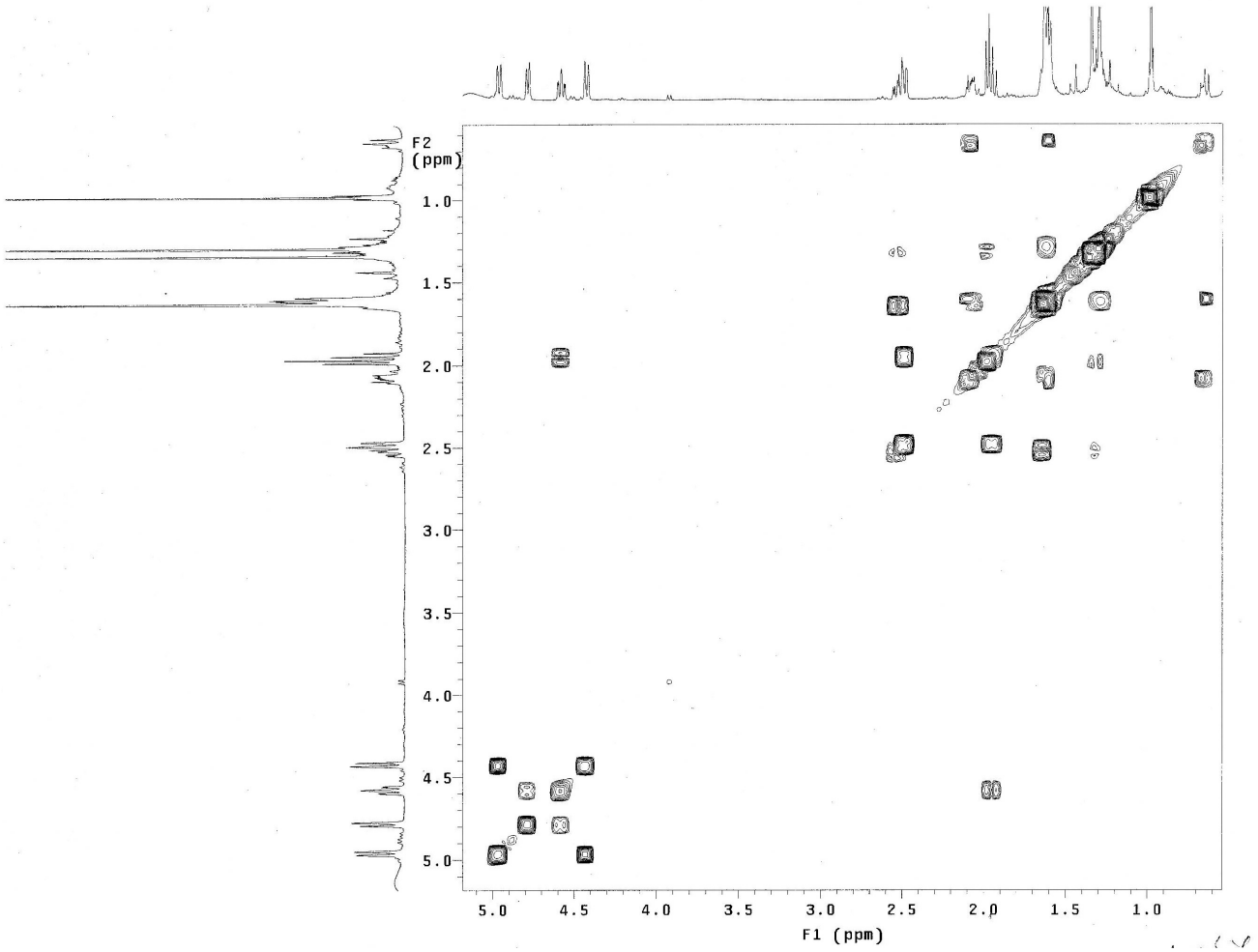


Figure S33. ^{1}H-^{1}H COSY spectrum of **5** in C_6D_6

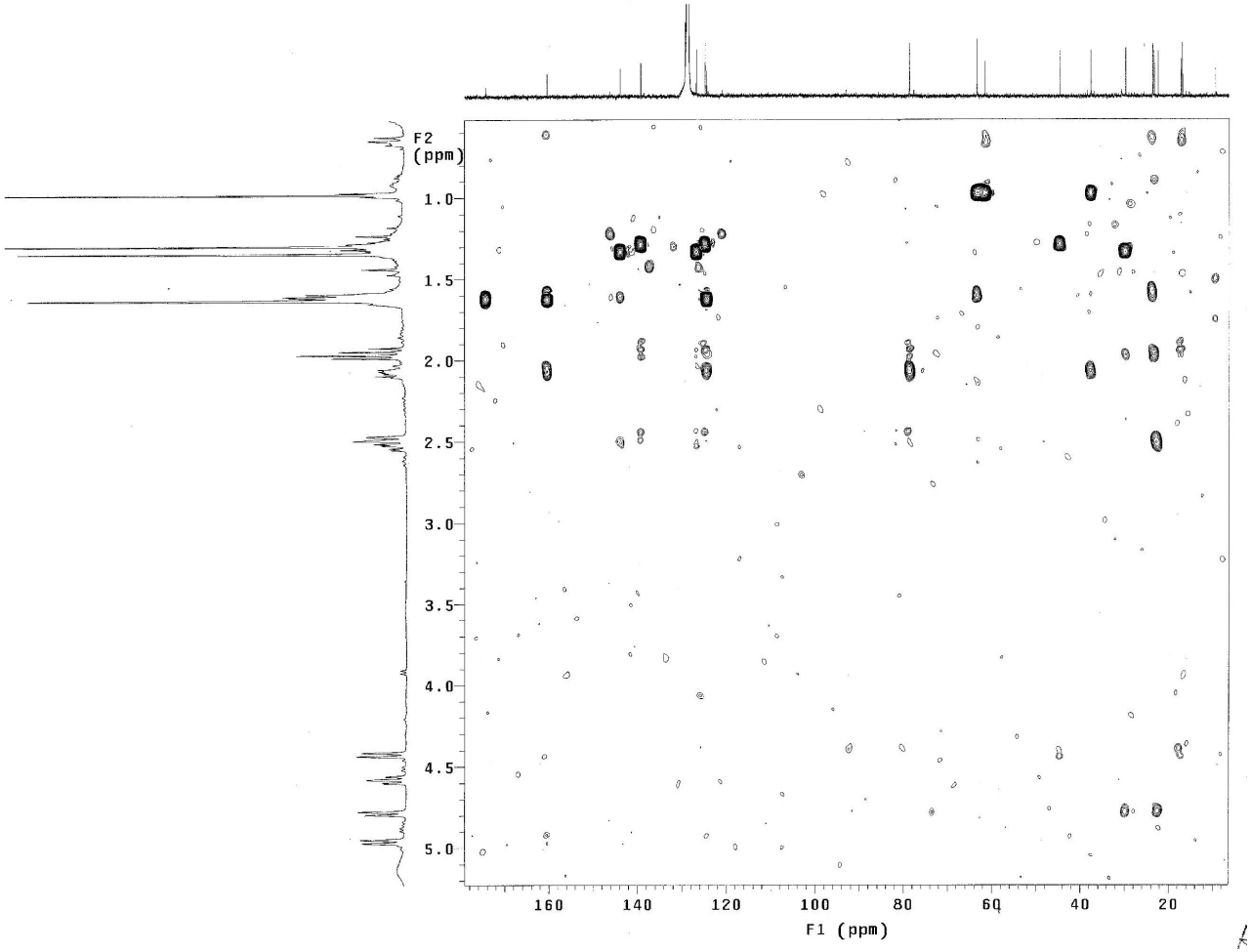


Figure S34. HMBC spectrum of **5** in C_6D_6

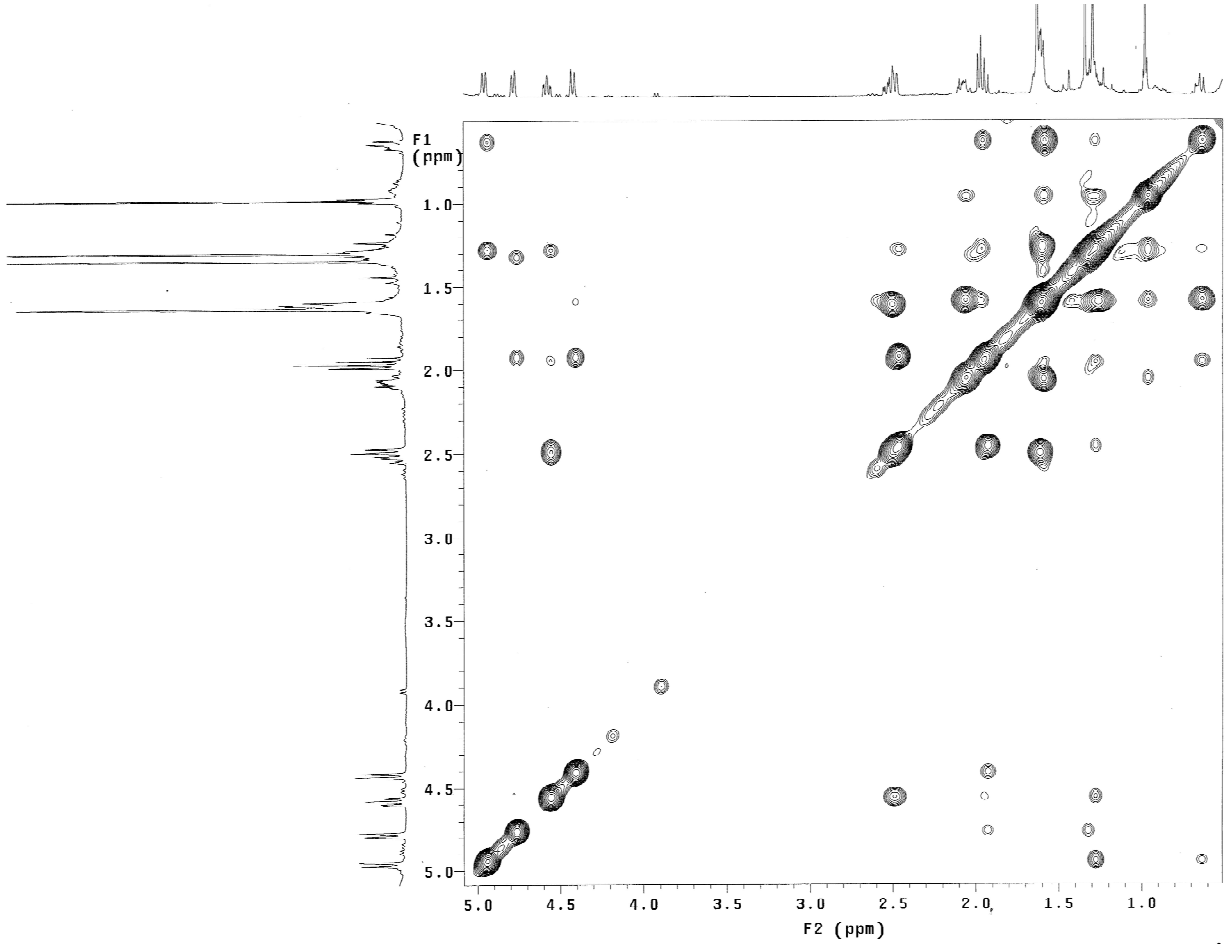
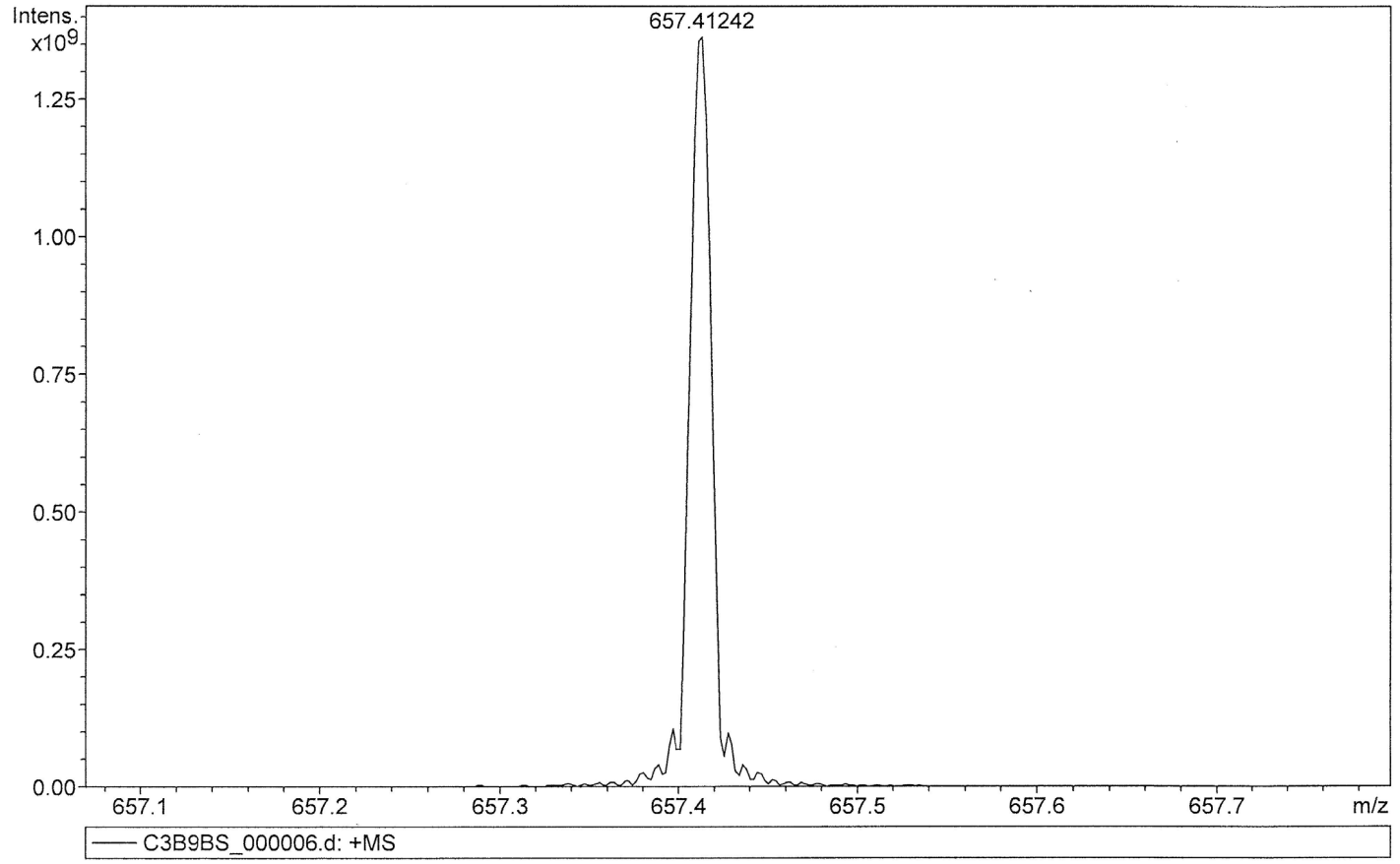


Figure S35. NOESY spectrum of **5** in C_6D_6



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
657.41242	1	C 40 H 58 Na O 6	100.00	657.41256	0.14	0.22	16.2	11.5	even	ok

Figure S36. HRESIMS spectrum of **6**

FT-MS

Analysis Info

Analysis Name	D:\Data\a1\C3B9BS_000006.d	11/6/2015 10:45:00 AM
Method	broadband first signal	
Sample Name	C3b-9bs	Instrument: FT-MS solariX
Comment	ESI Positive	

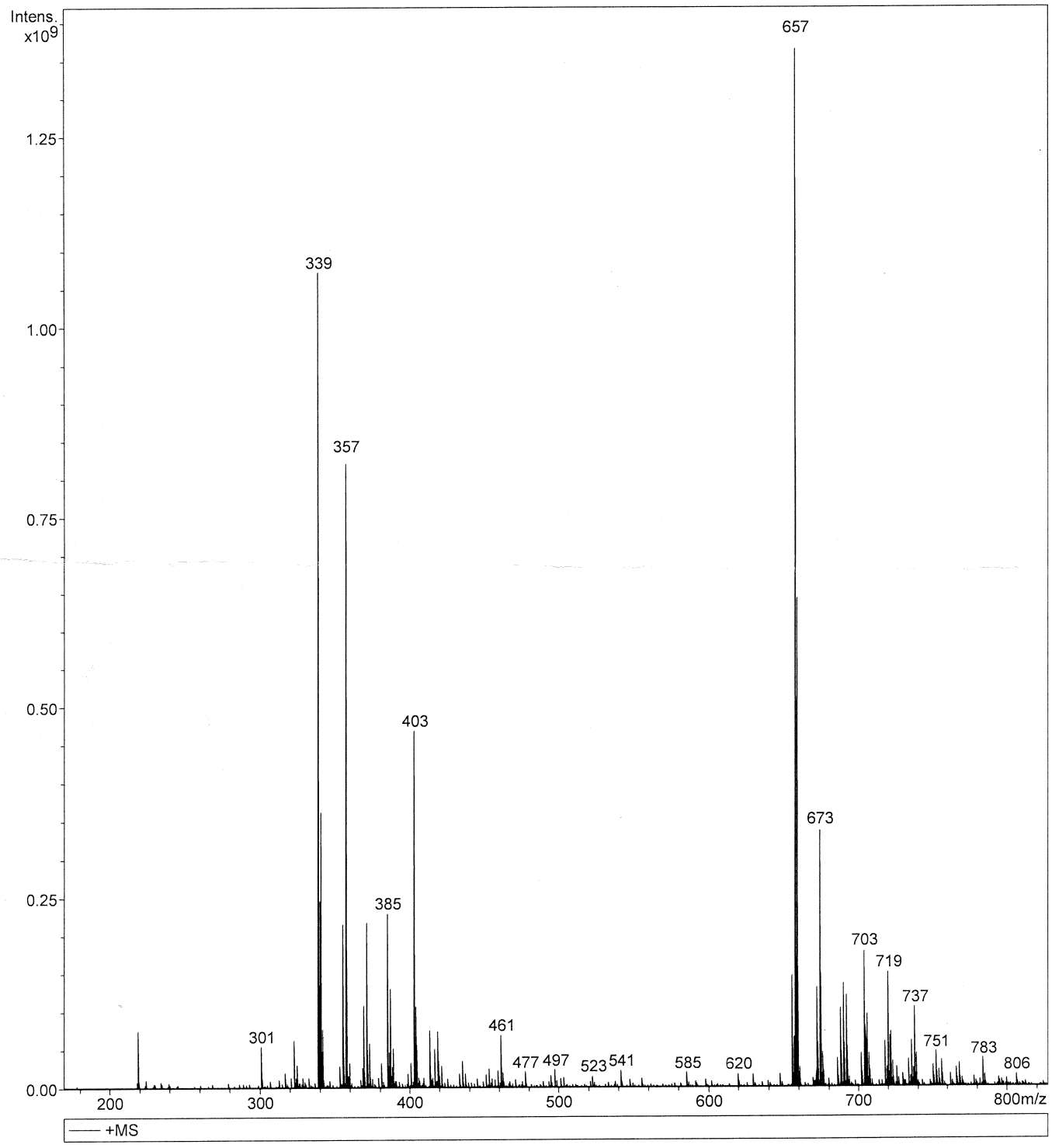


Figure S37. ESIMS of **6**

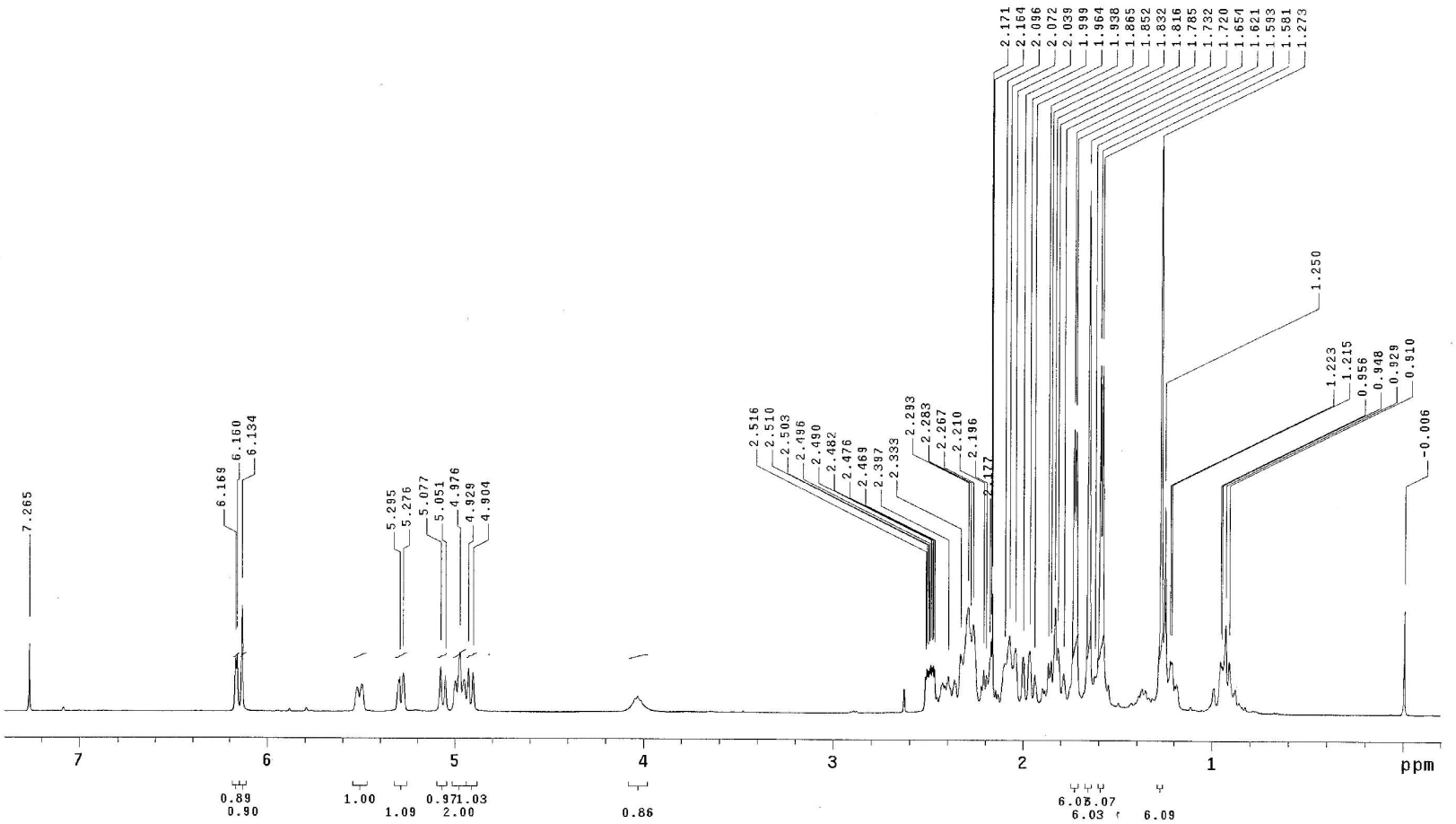


Figure S38. ^{1}H NMR spectrum of **6** in $CDCl_3$

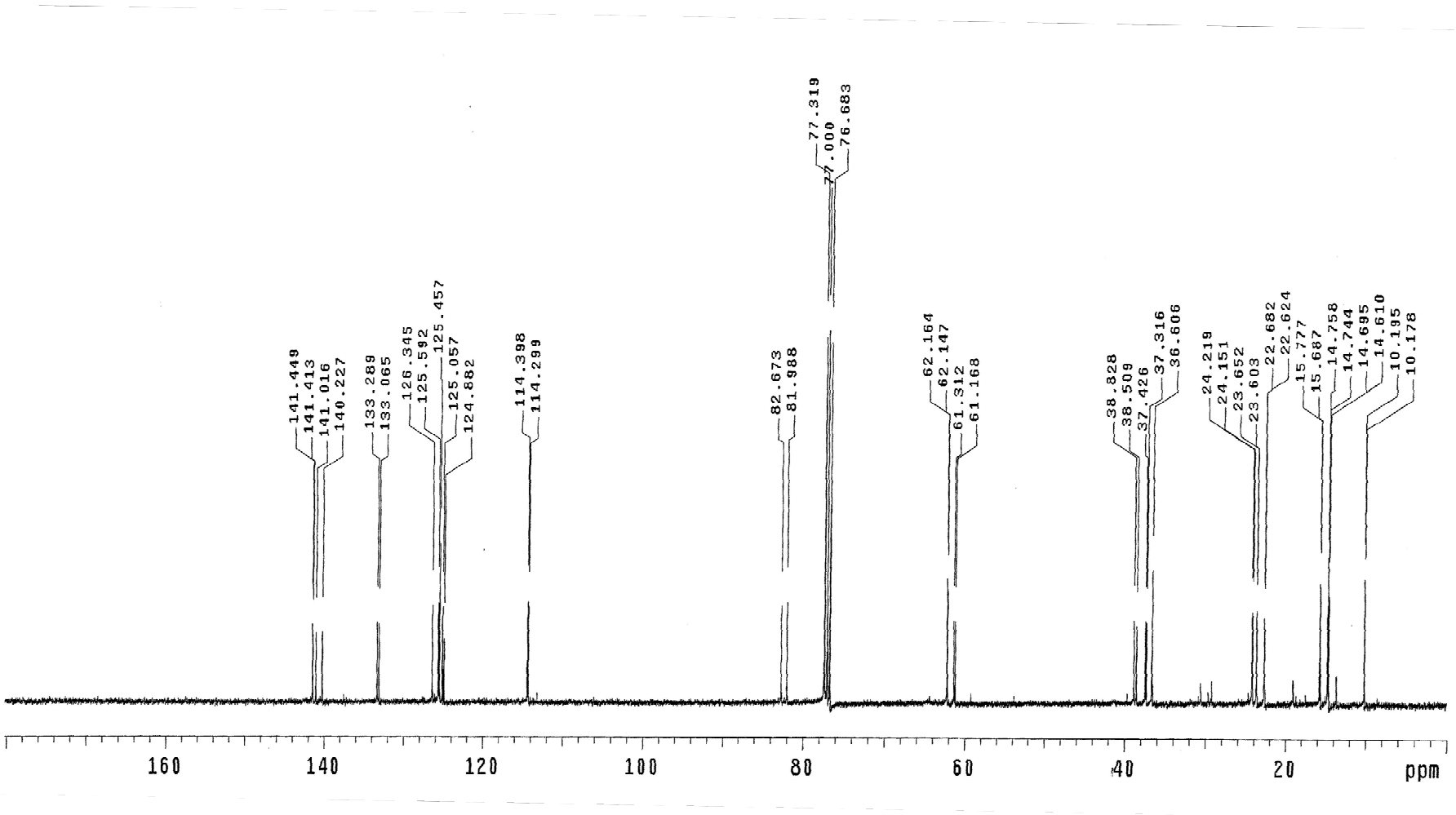


Figure S39. ^{13}C NMR spectrum of **6** in $CDCl_3$

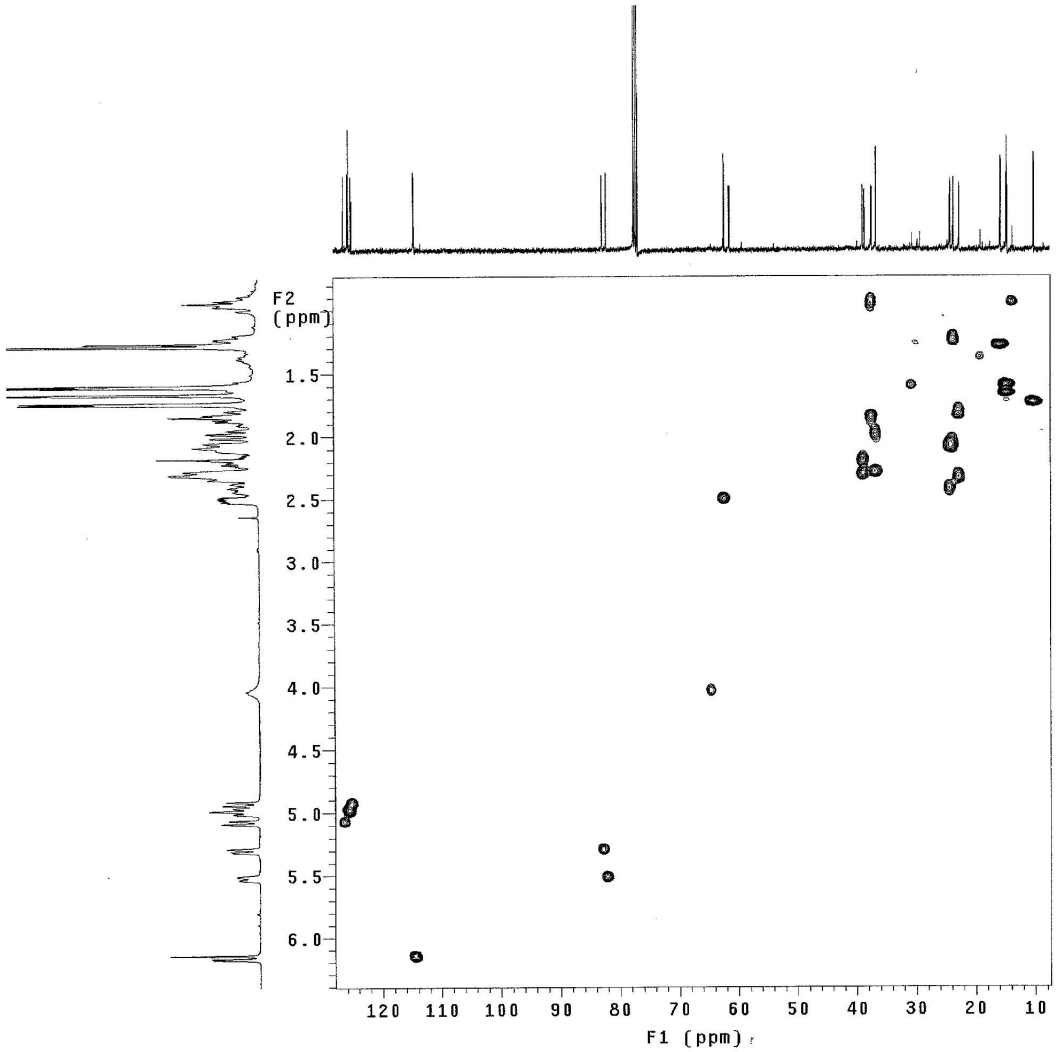


Figure S40. HSQC spectrum of **6** in $CDCl_3$

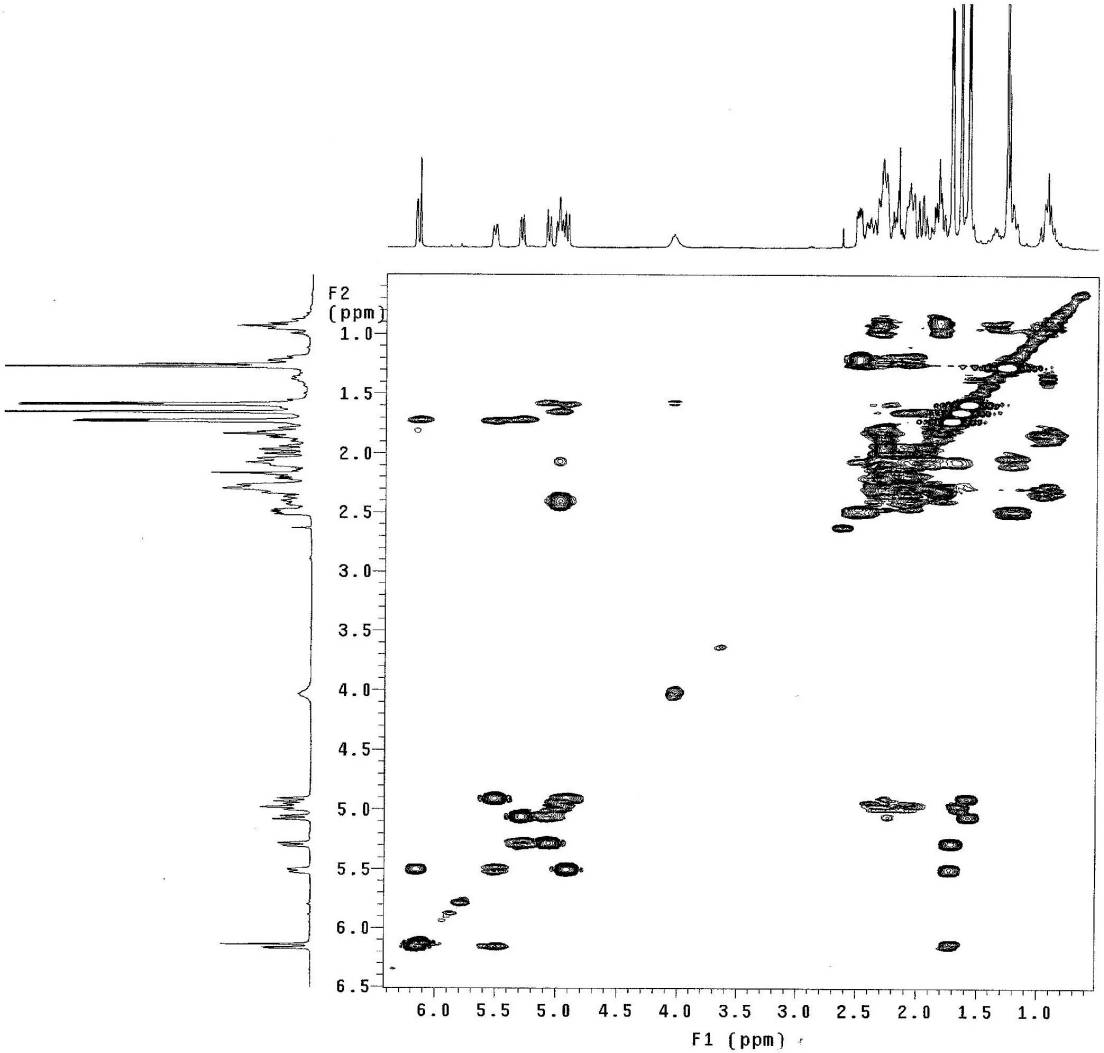


Figure S41. ^{1}H-^{1}H COSY spectrum of **6** in $CDCl_3$

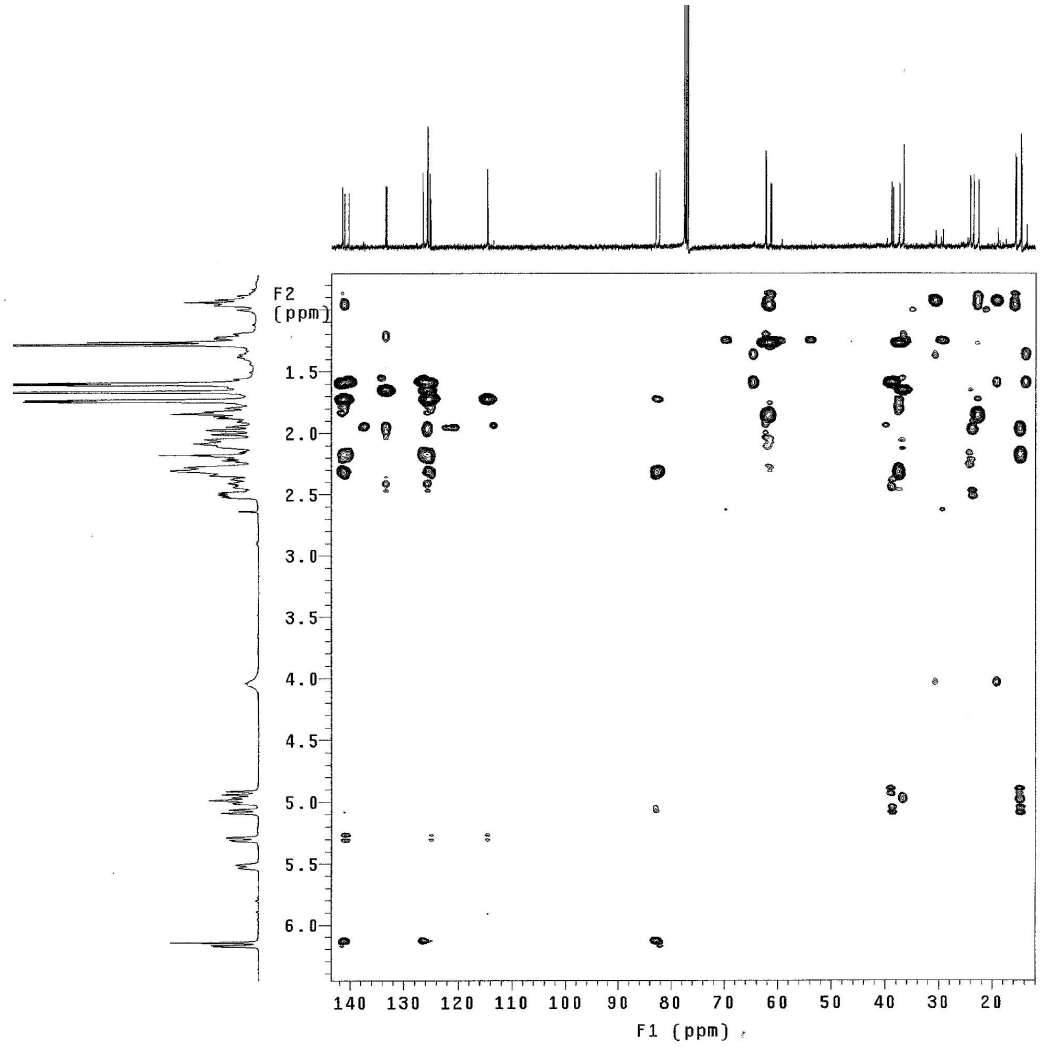


Figure S42 HMBC spectrum of **6** in $CDCl_3$

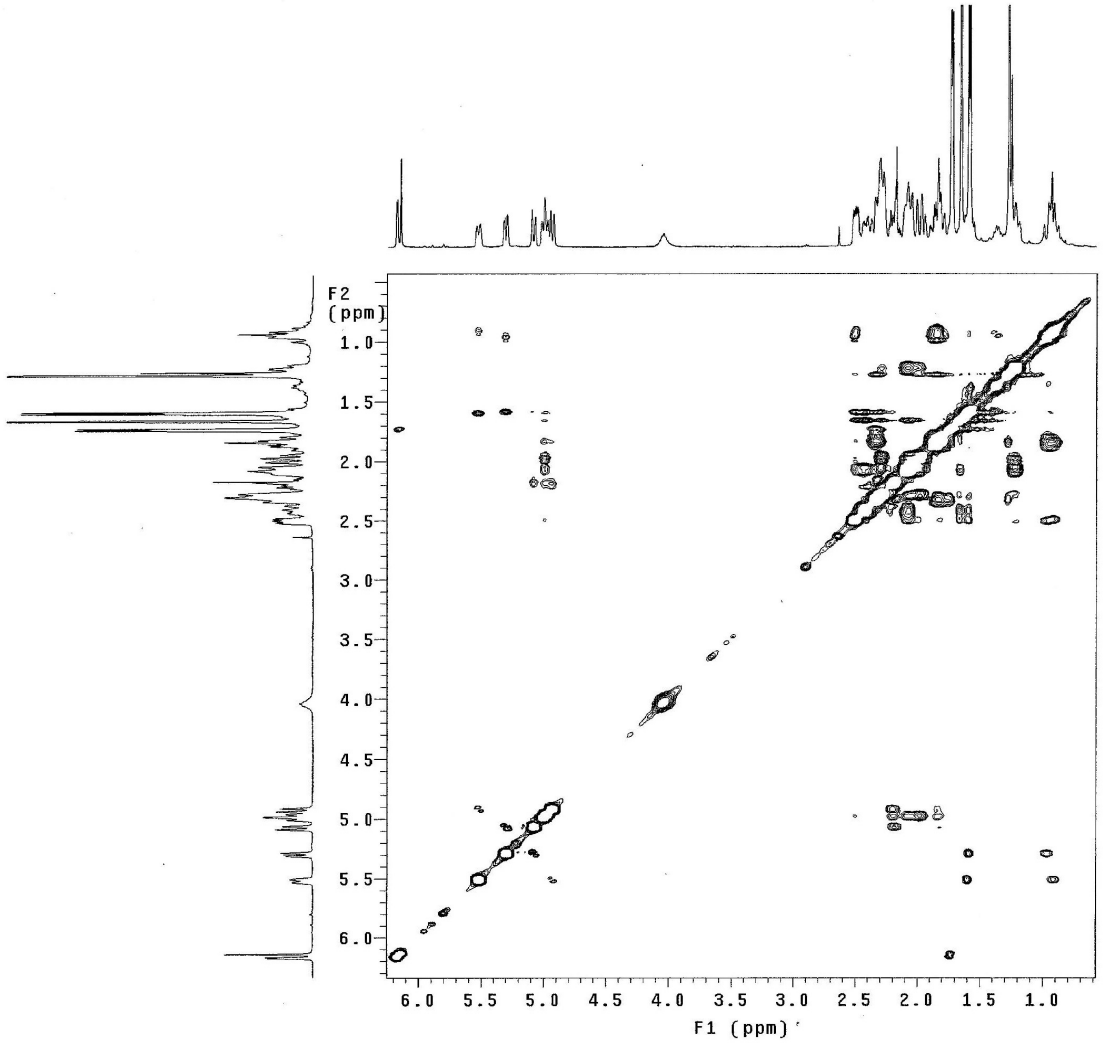


Figure S43. NOESY spectrum of **6** in $CDCl_3$

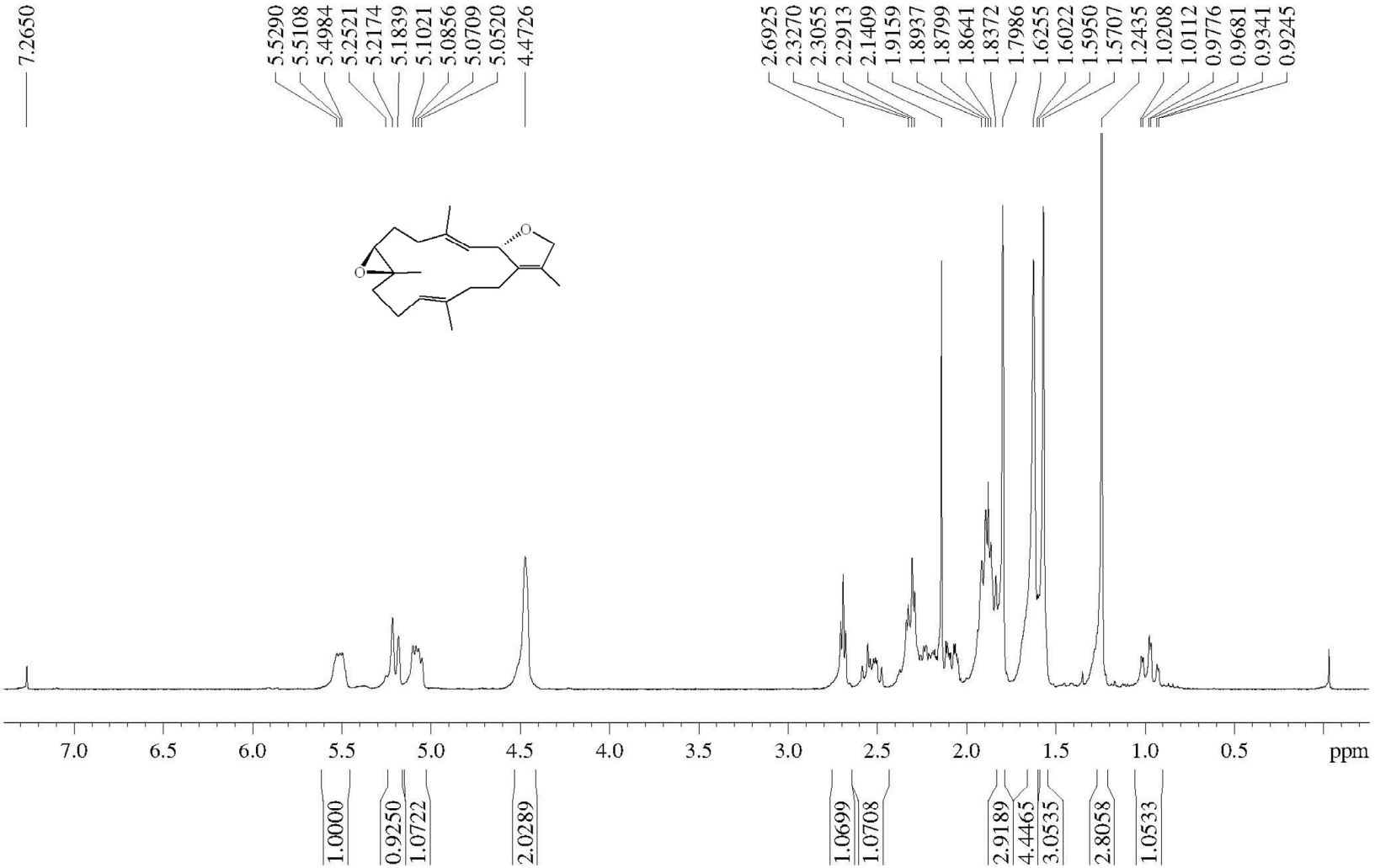


Figure S44. ^{1}H NMR spectrum of (+)-sarcophytoxide in $CDCl_3$ before treatment with acetone and silica gel under air

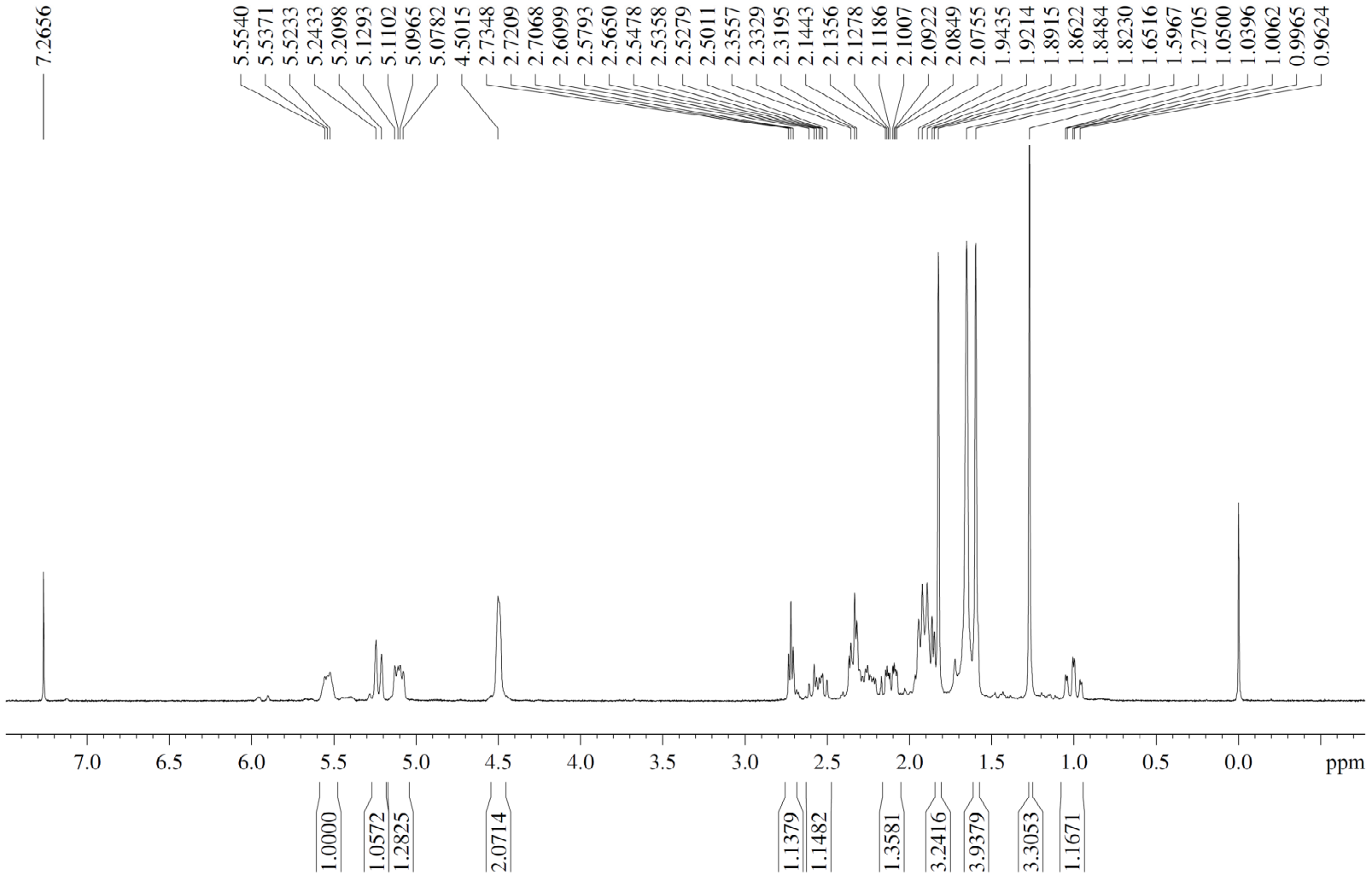


Figure S45. ^{1}H NMR spectrum of (+)-sarcophytoxide in $CDCl_3$ after treatment with acetone and silica gel under air

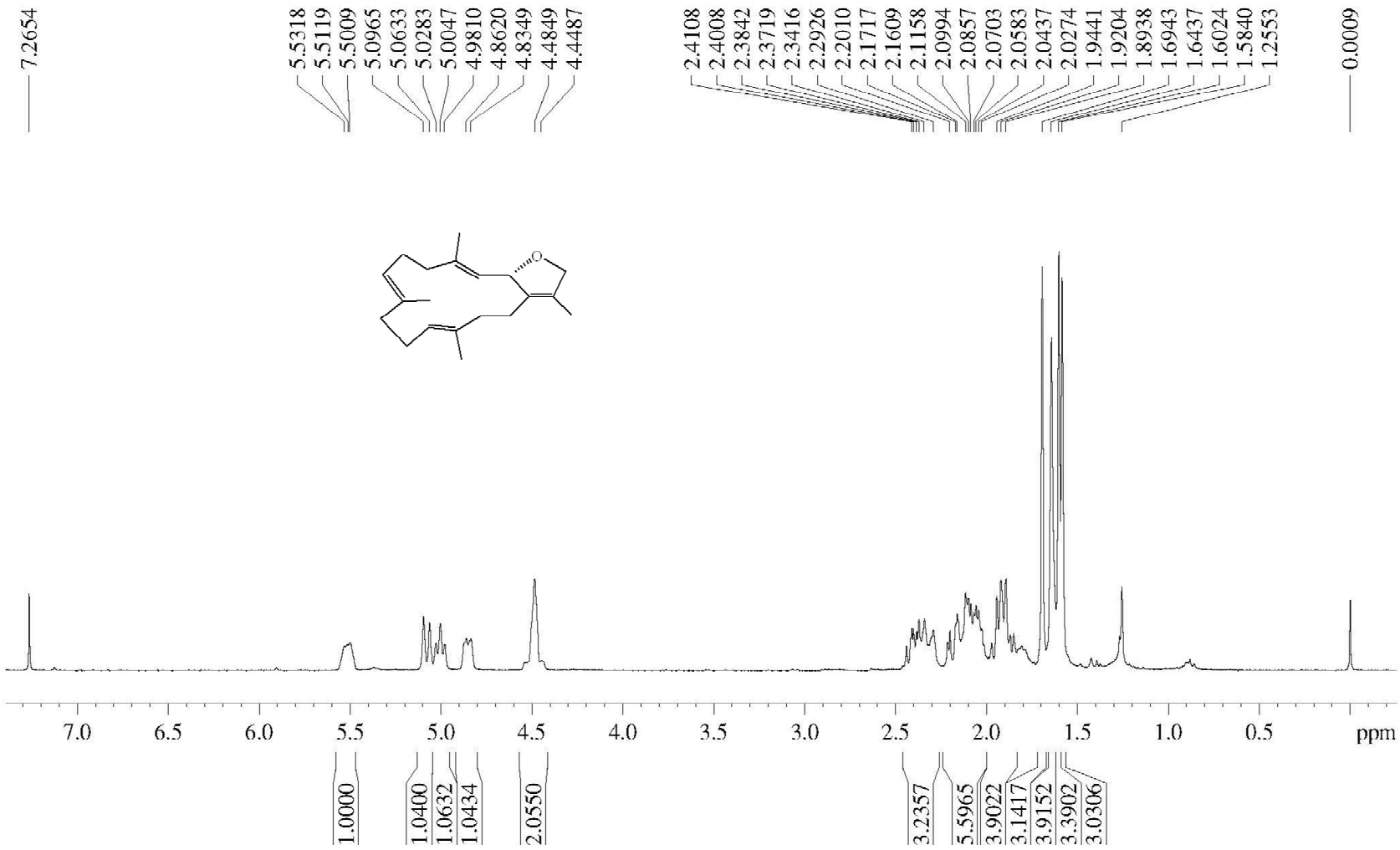


Figure S46. ^{1}H NMR spectrum of sarcophytonin A in $CDCl_3$ before treatment with acetone and silica gel under air

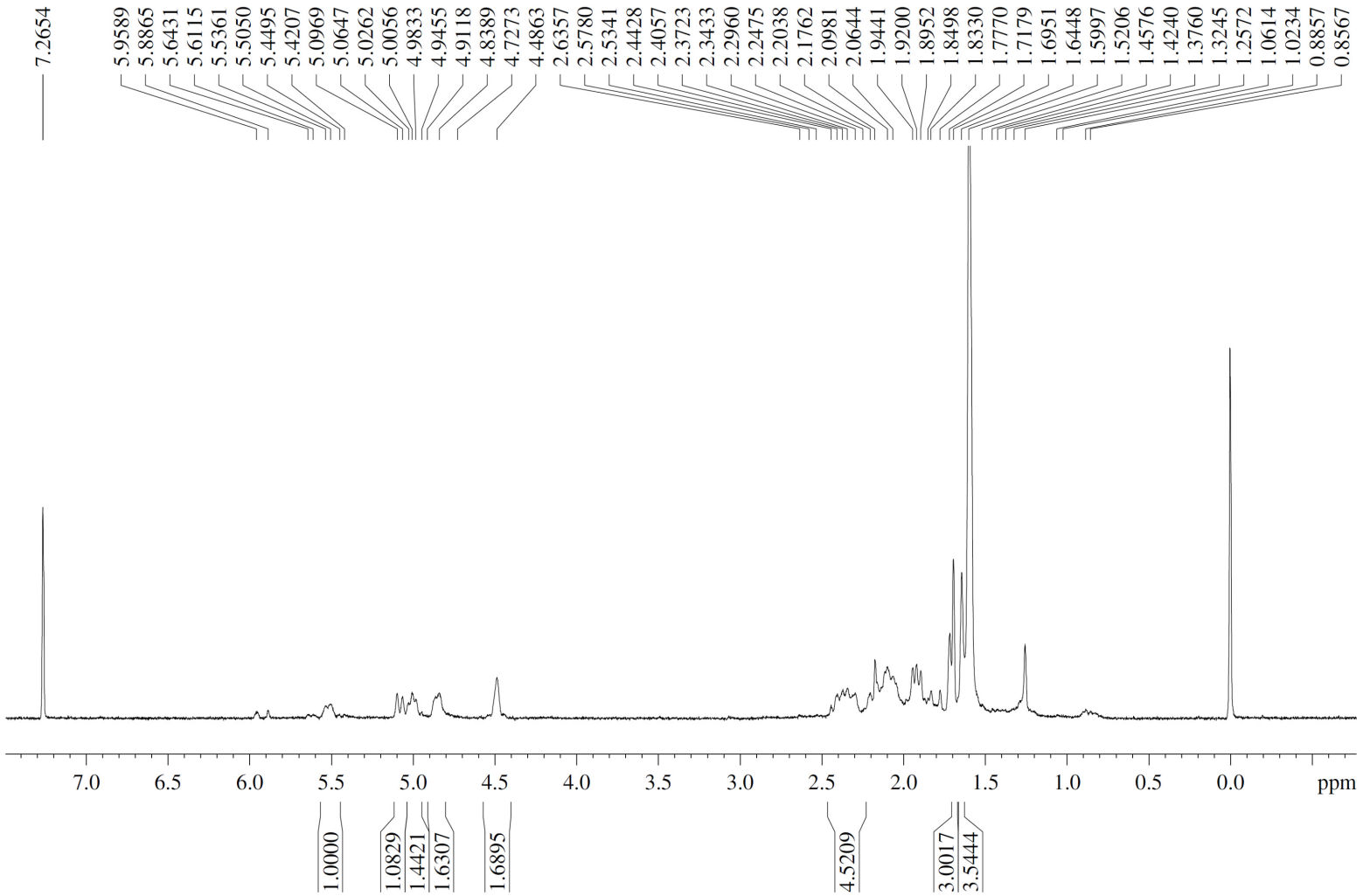


Figure S47. ^{1}H NMR spectrum of sarcophytonin A in $CDCl_3$ after treatment with acetone and silica gel under air