

Supplementary Information

Miniolins A–C, Novel Isomeric Furanones Induced by Epigenetic

Manipulation on *Penicillium minioluteum*

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Figure S1. HPLC profiles of culture extracts from *P. minioluteum* cultivated in PD media (upper) and PD media with 500 μ M Aza (bottom)

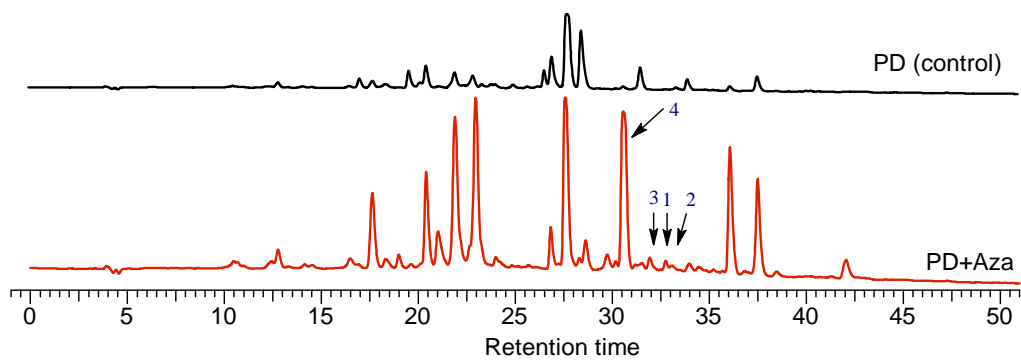
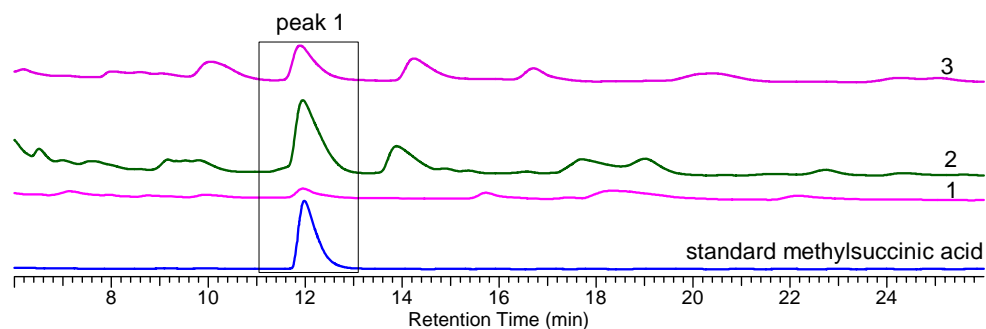


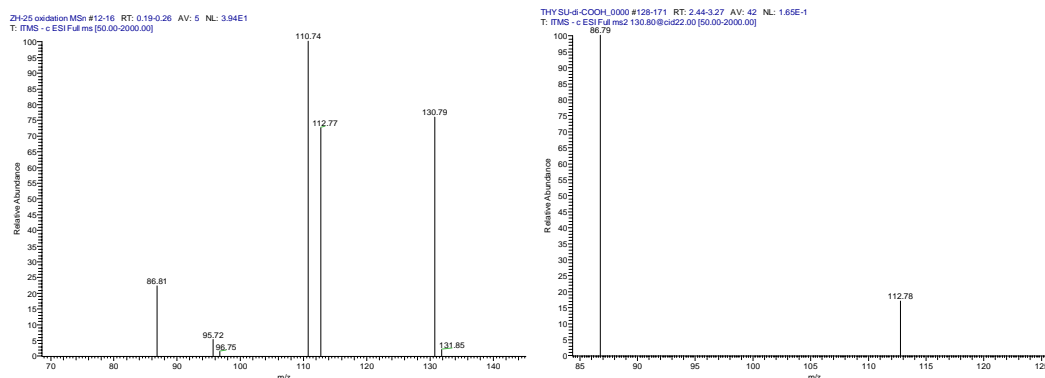
Figure S2.LC/MS² analysis of oxidation products of compounds 1-3

(1) HPLC Profile of oxidation products from compounds 1-3 on an Agilent TC-18 column



Column: Agilent TC-18 column 250×4.6 mm; Elution solvent: 10% MeOH/H₂O with 0.1% TFA; Temperature: 25 °C; Detector: UV @210nm

(2) Full MS and MS/MS of peak 1 from negative ESI source



(3) Proposed MS/MS fragmentation pathway of the methylsuccinic acid

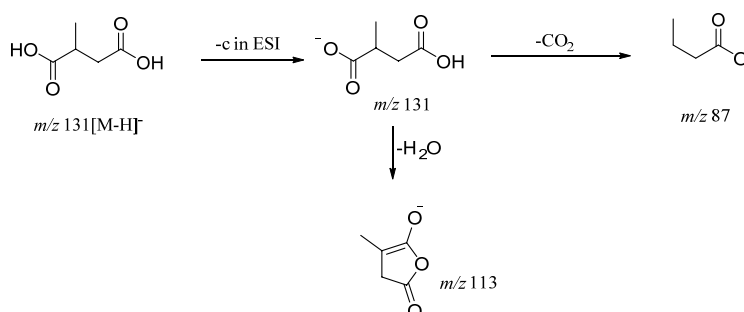


Figure S3. ^1H NMR of **1** in CDCl_3 (500 MHz)

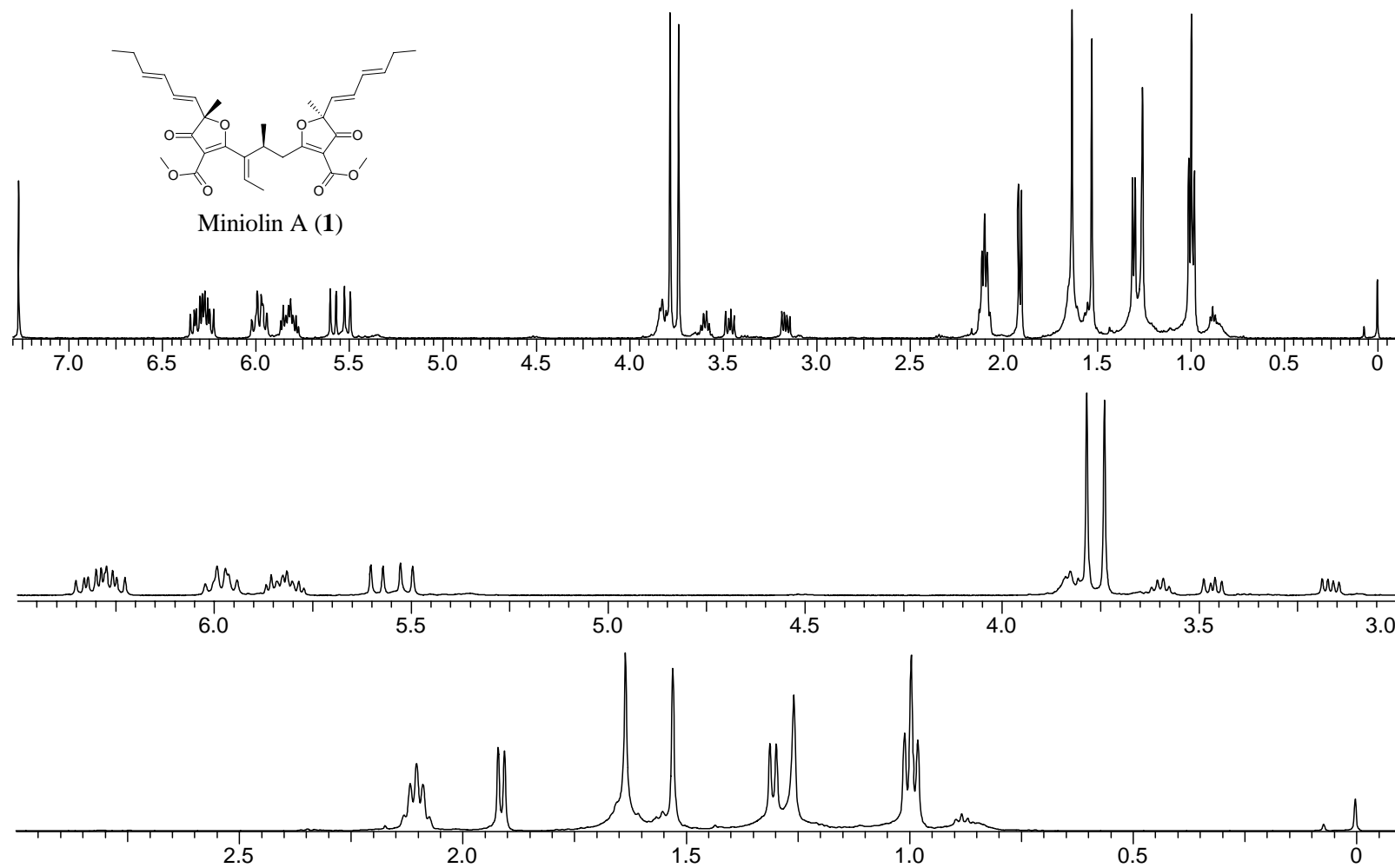


Figure S4. ^{13}C NMR and DEPT of **1** in CDCl_3 (125 MHz)

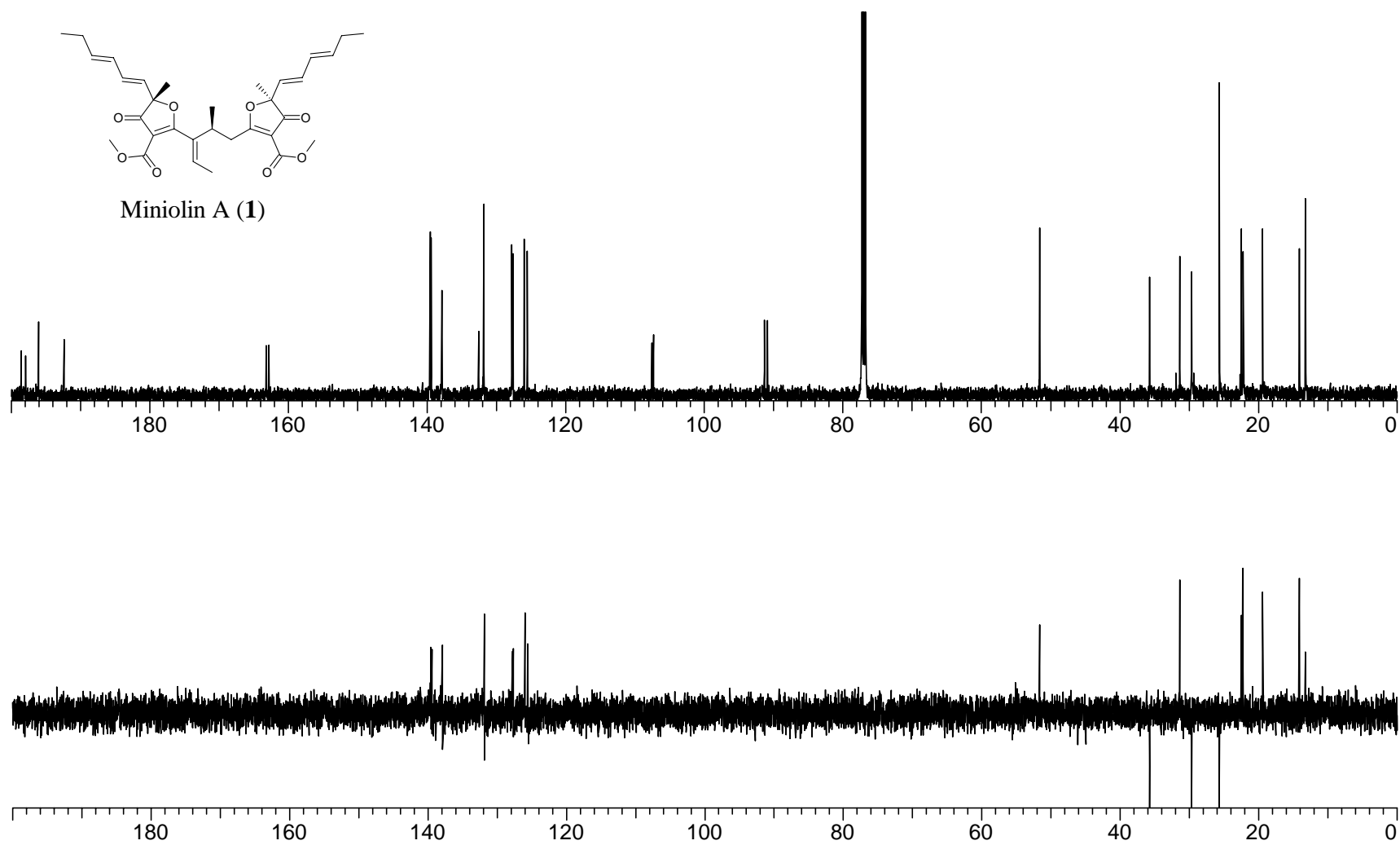


Figure S5. HSQC spectrum of 1

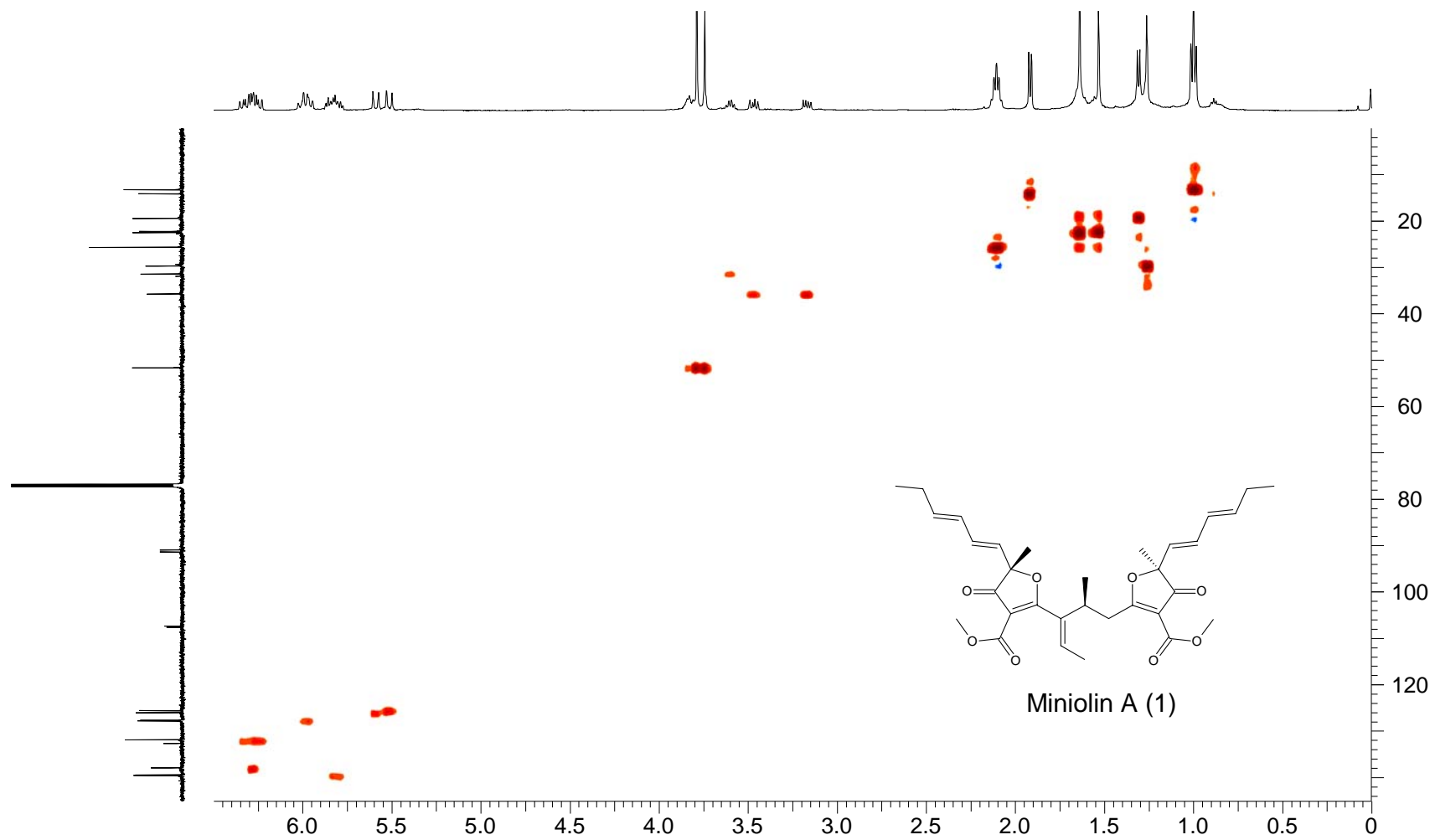


Figure S6. ^1H - ^1H COSY spectrum of **1**

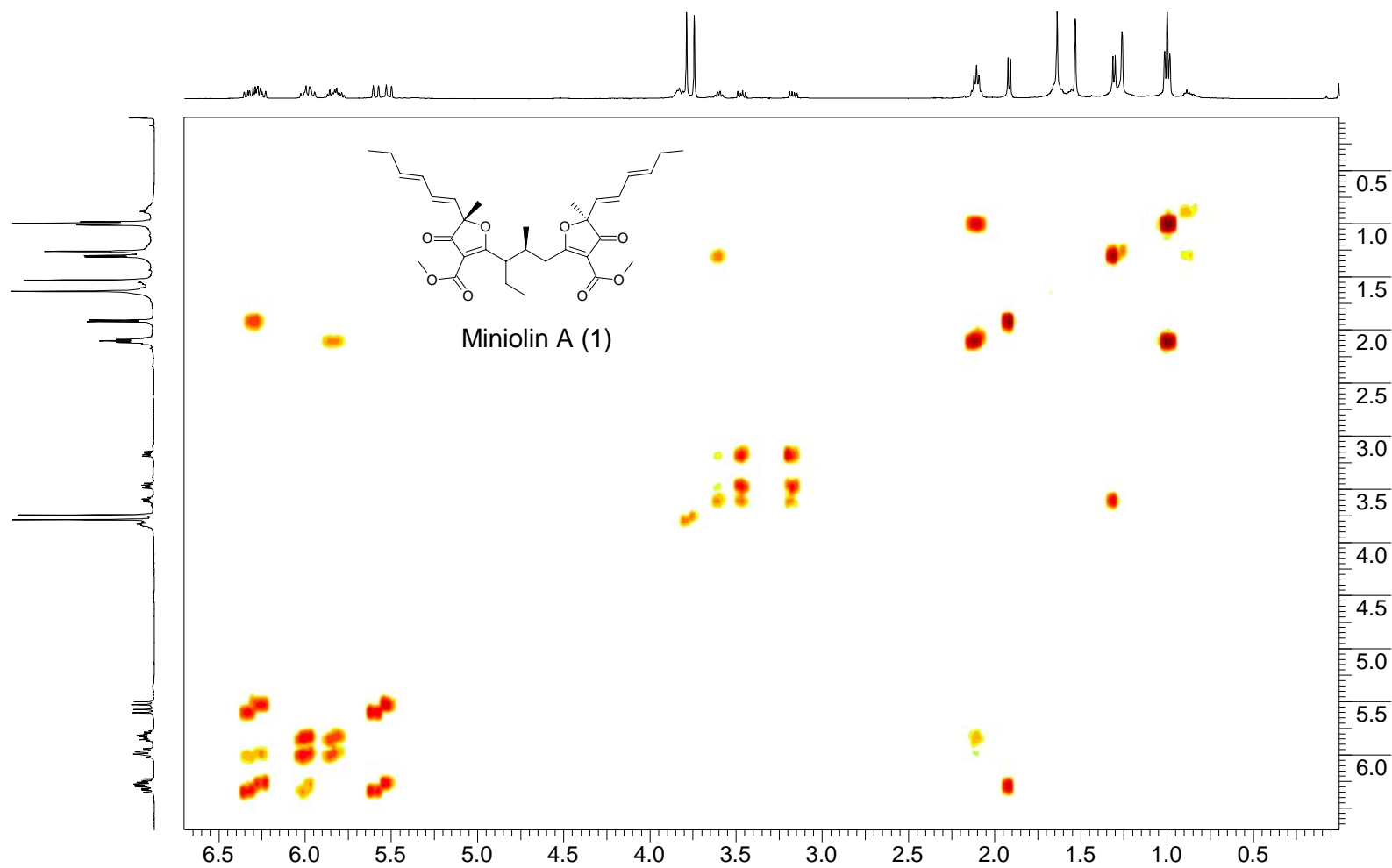
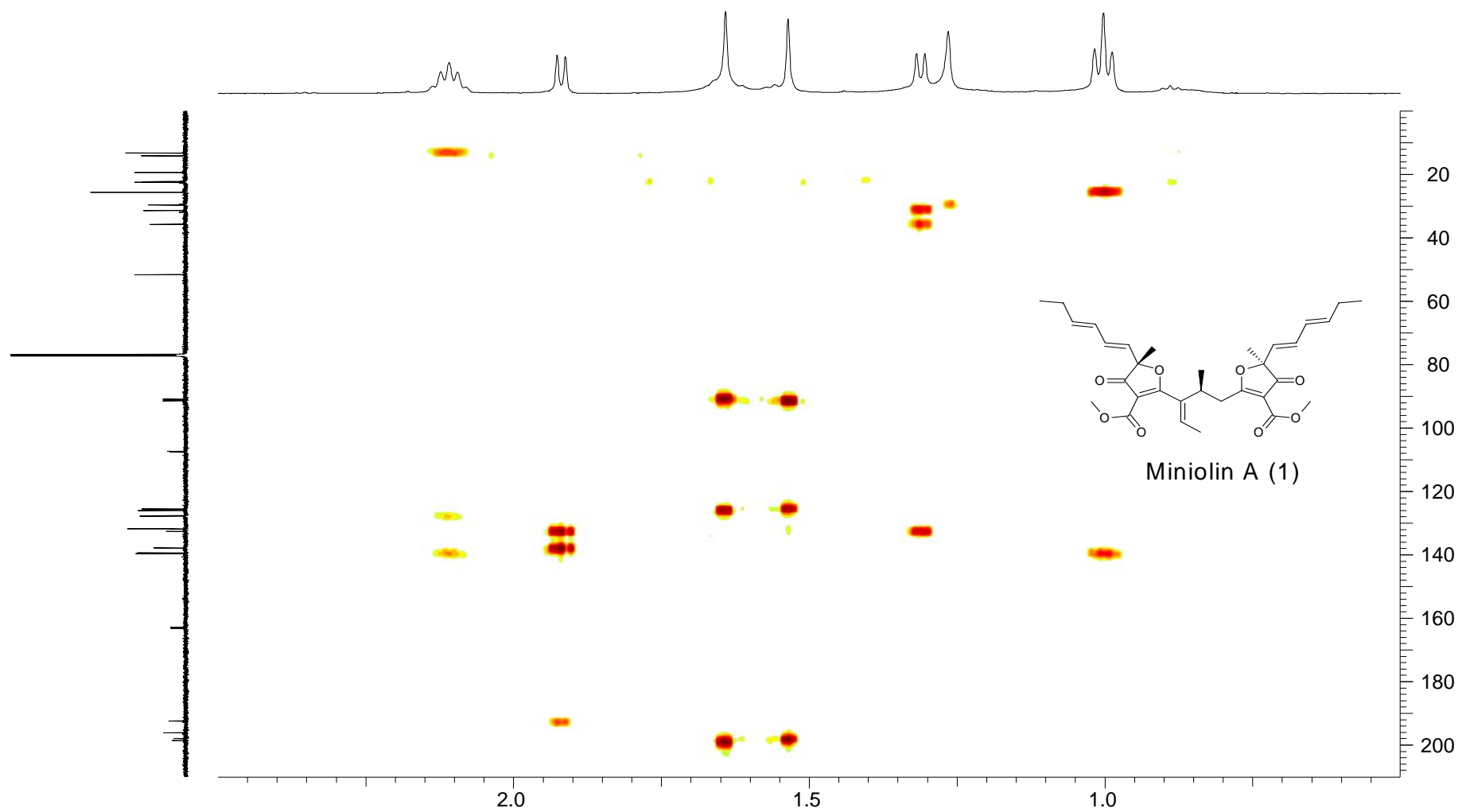
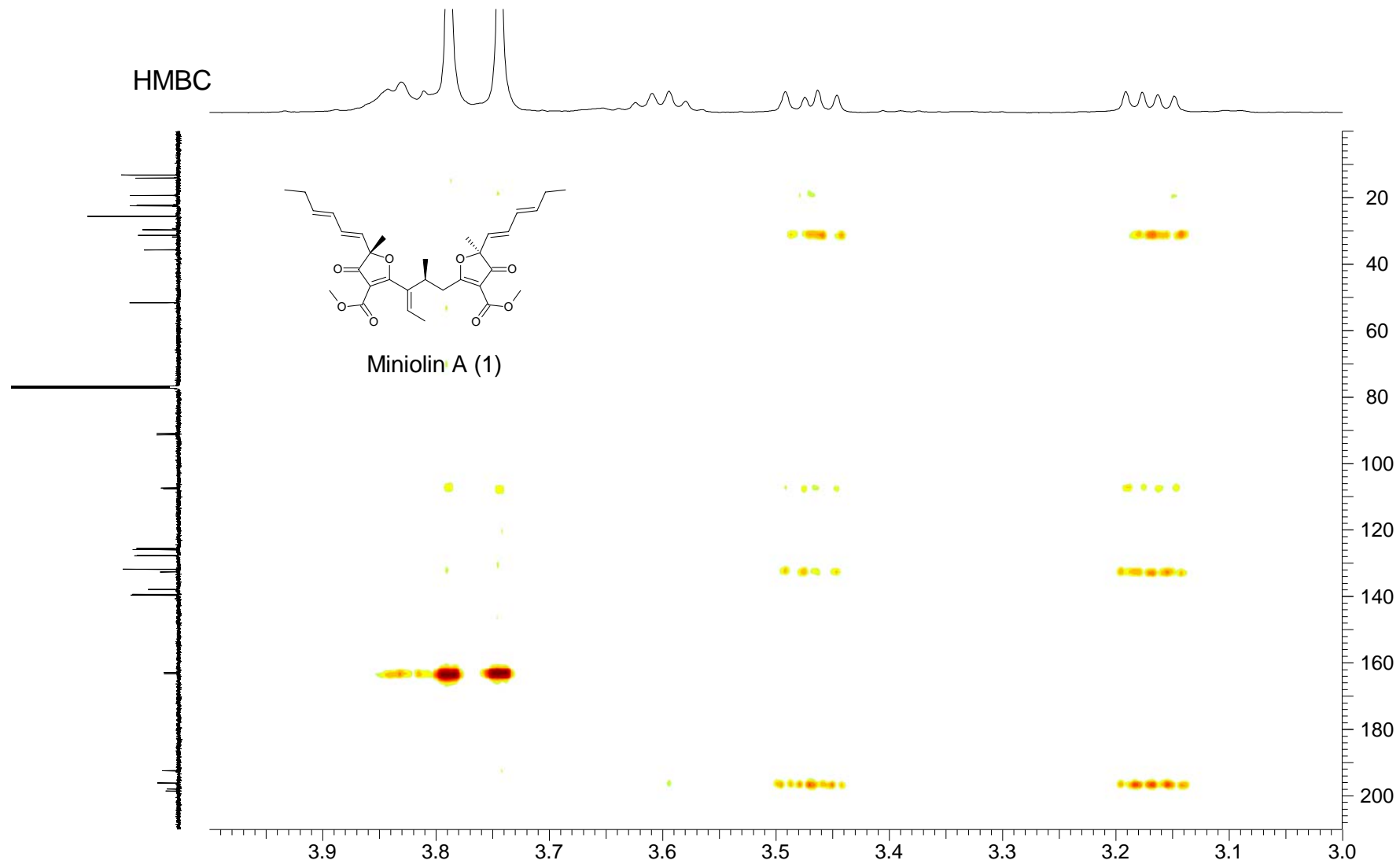
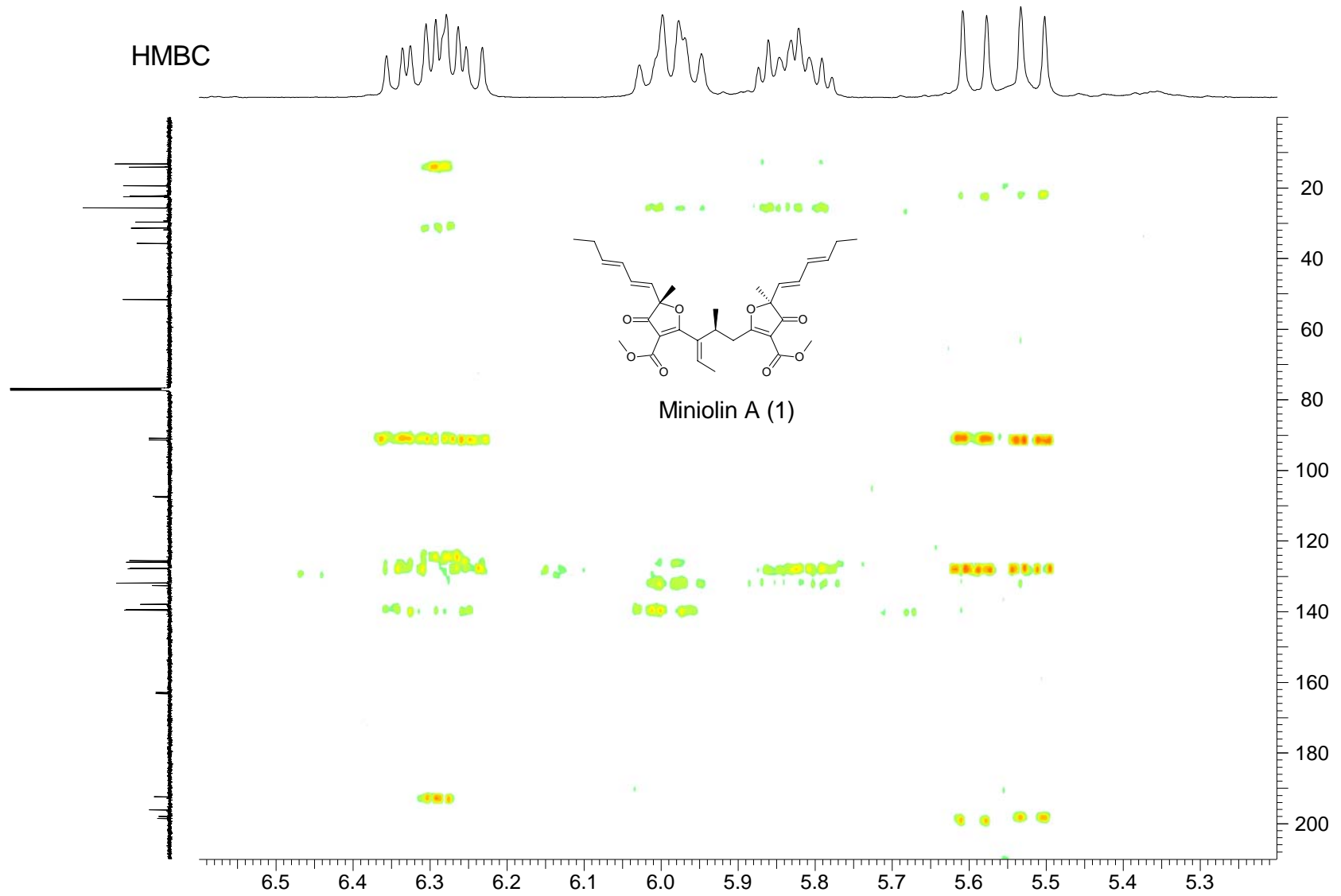


Figure S7. HMBC spectrum of 1





HMBC



Miniolin A (1)

Figure S8. NOESY spectrum of 1

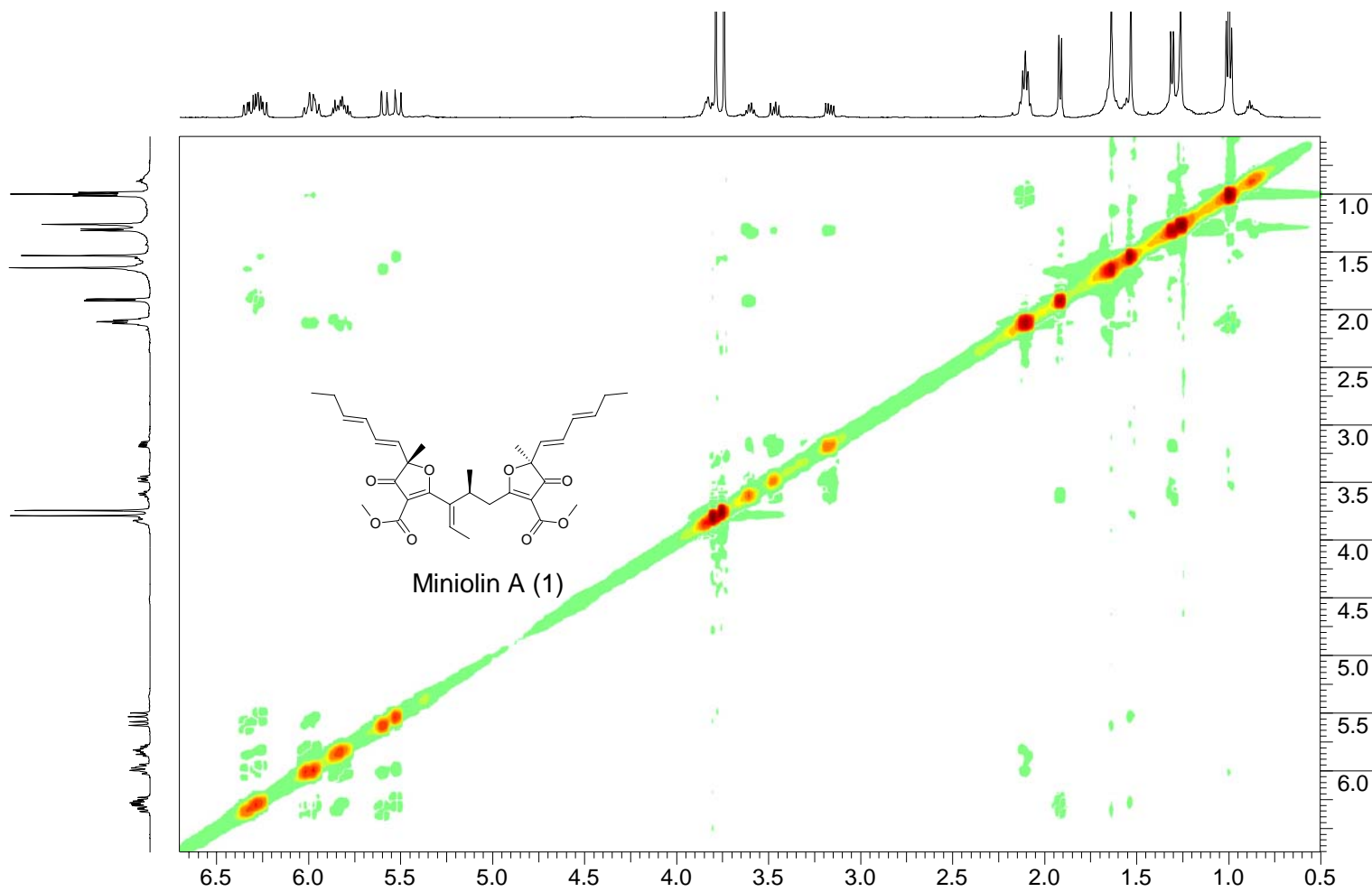


Figure S9. Positive ESIMS spectrum of 1

ZH-25 #84-104 RT: 0.36-0.45 AV: 21 NL: 1.65E4
T: ITMS + c ESI Full ms [50.00-2000.00]

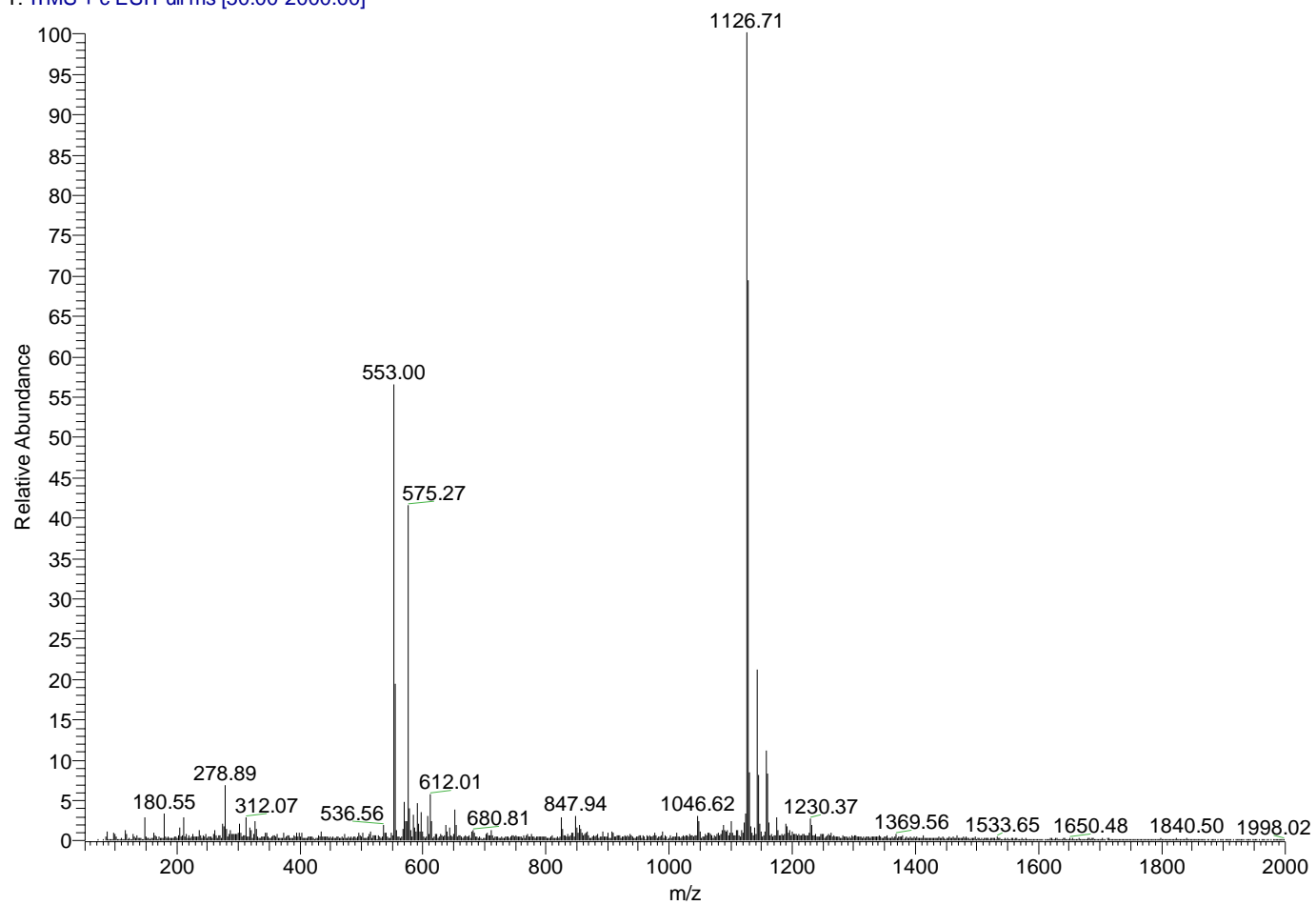
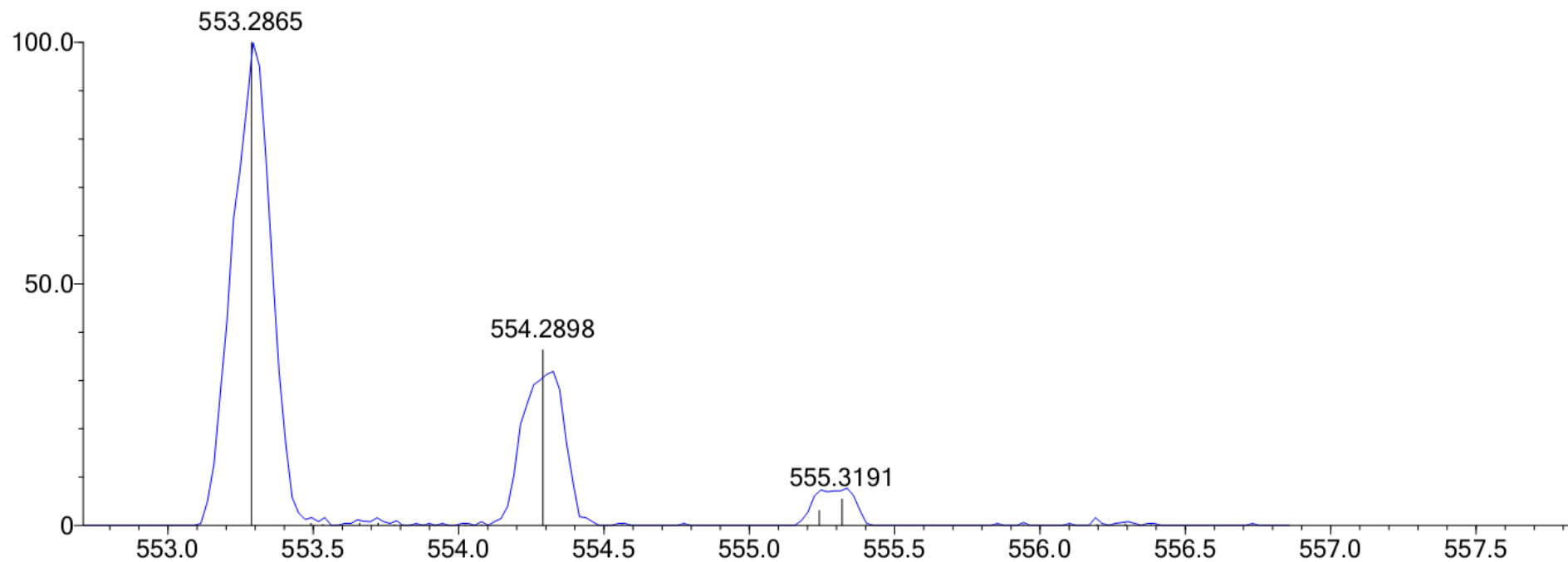


Figure S10. HR ESIMS spectrum of 1



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	16.12	[M+H] ⁺	C ₃₂ H ₄₀ O ₈	553.2796	553.2865	6.9	12.47	48.26	13.0

Figure S11. IR spectrum of 1

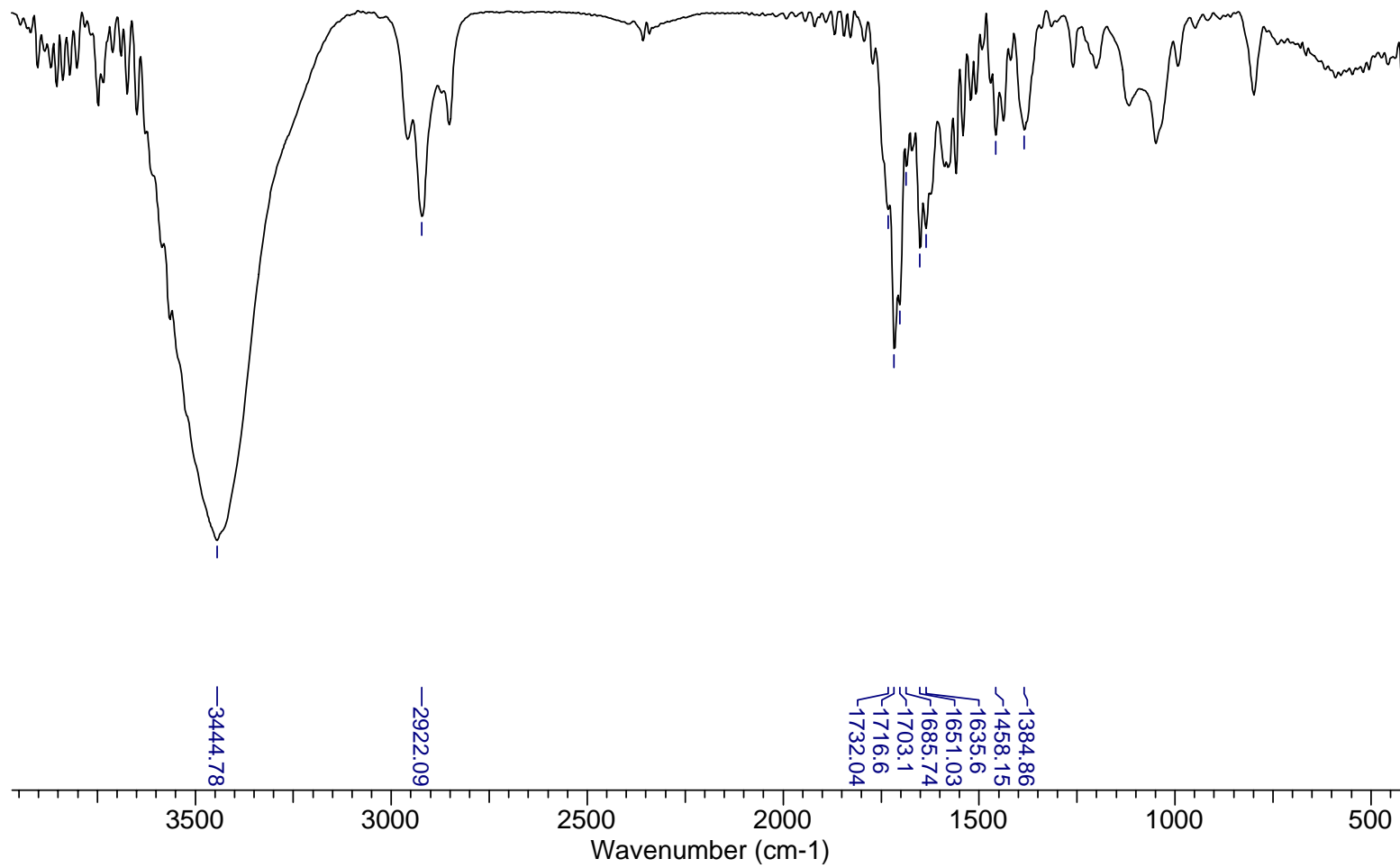


Figure S12. UV and CD spectra of 1

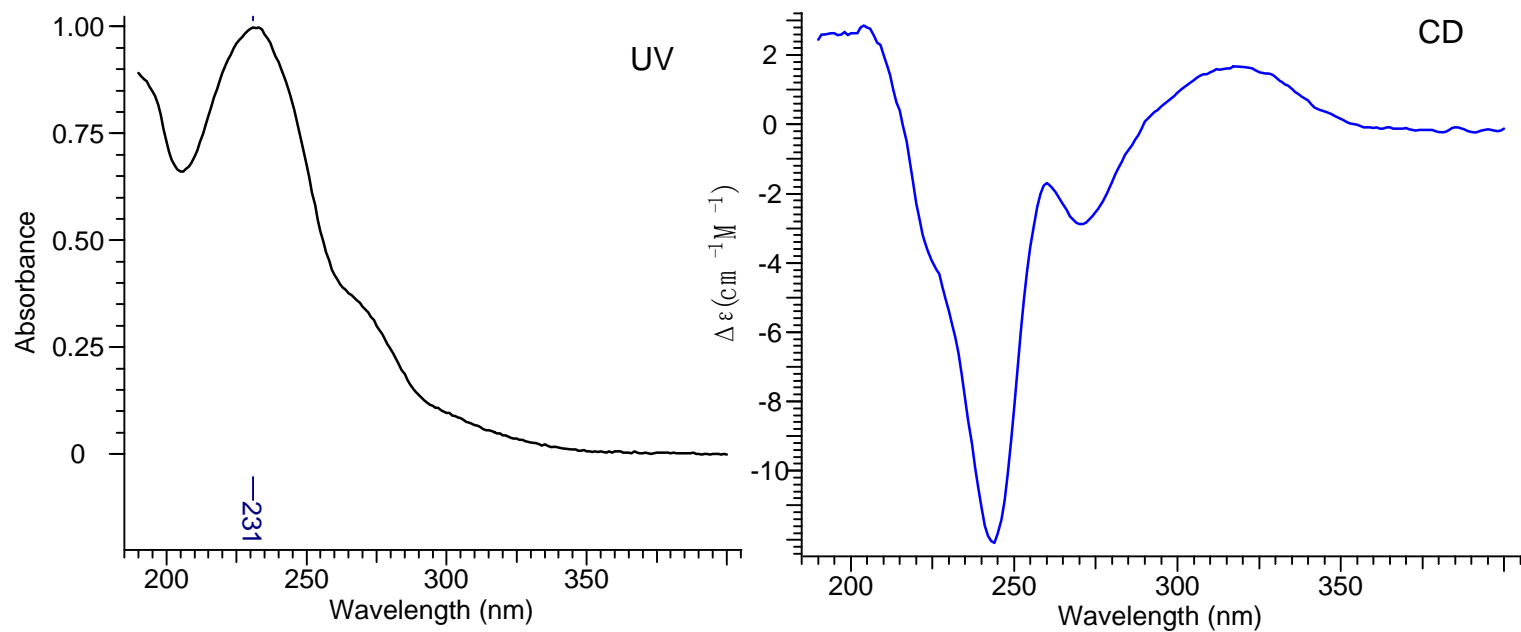


Figure S13. ^1H NMR spectrum of **2** in CDCl_3 (500 MHz)

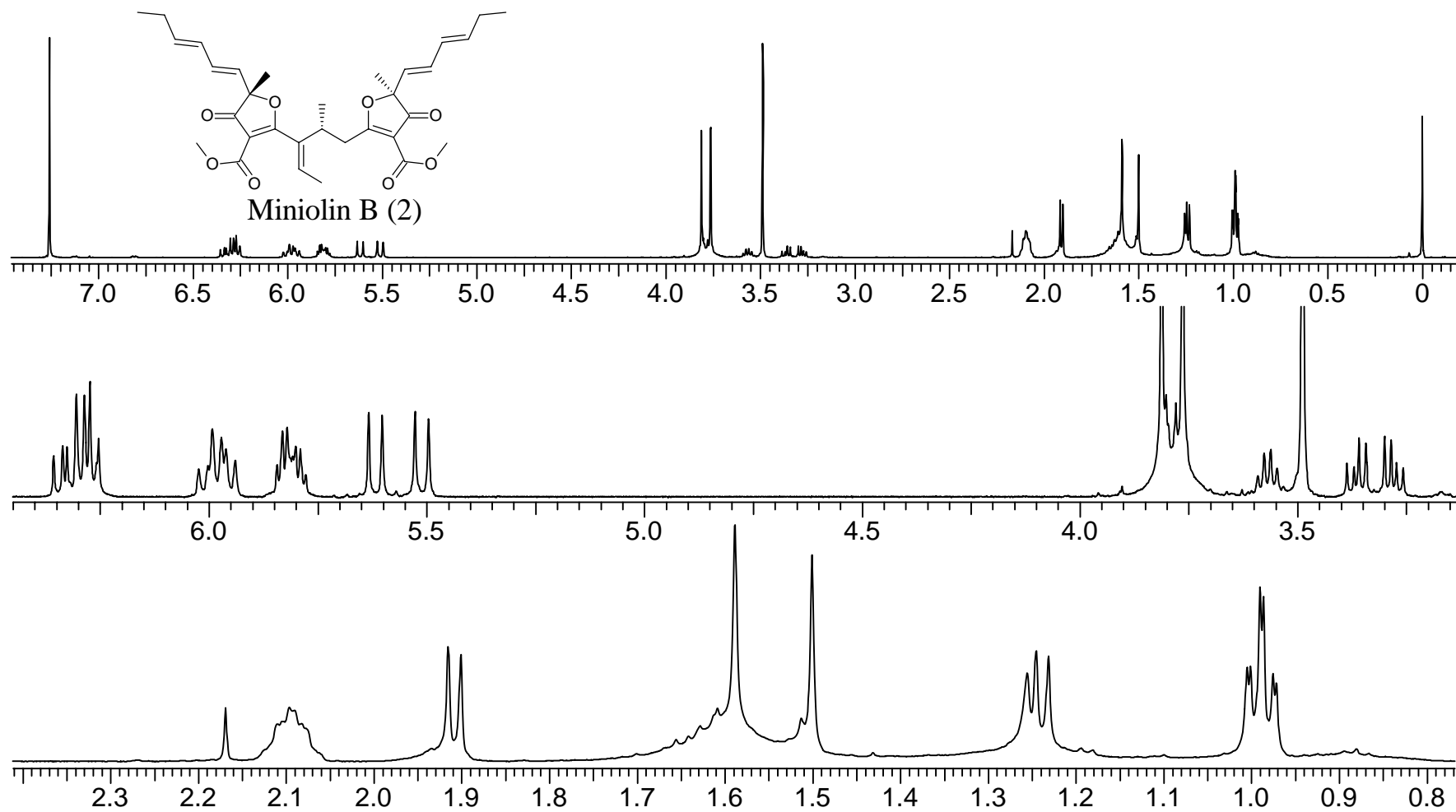


Figure S14. ^{13}C NMR and DEPT of 2 in CDCl_3 (125 MHz)

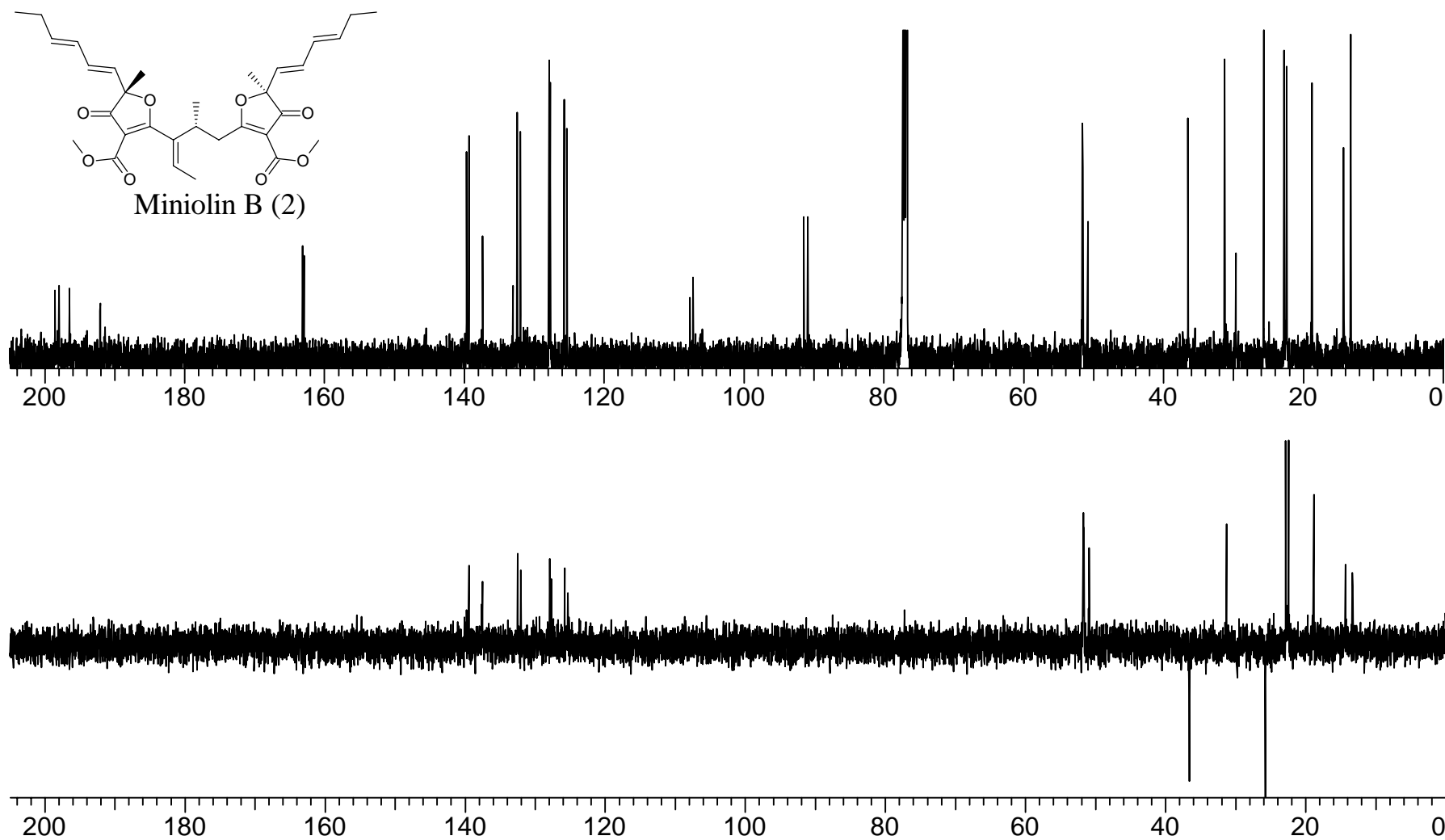


Figure S15. HSQC spectrum of 2

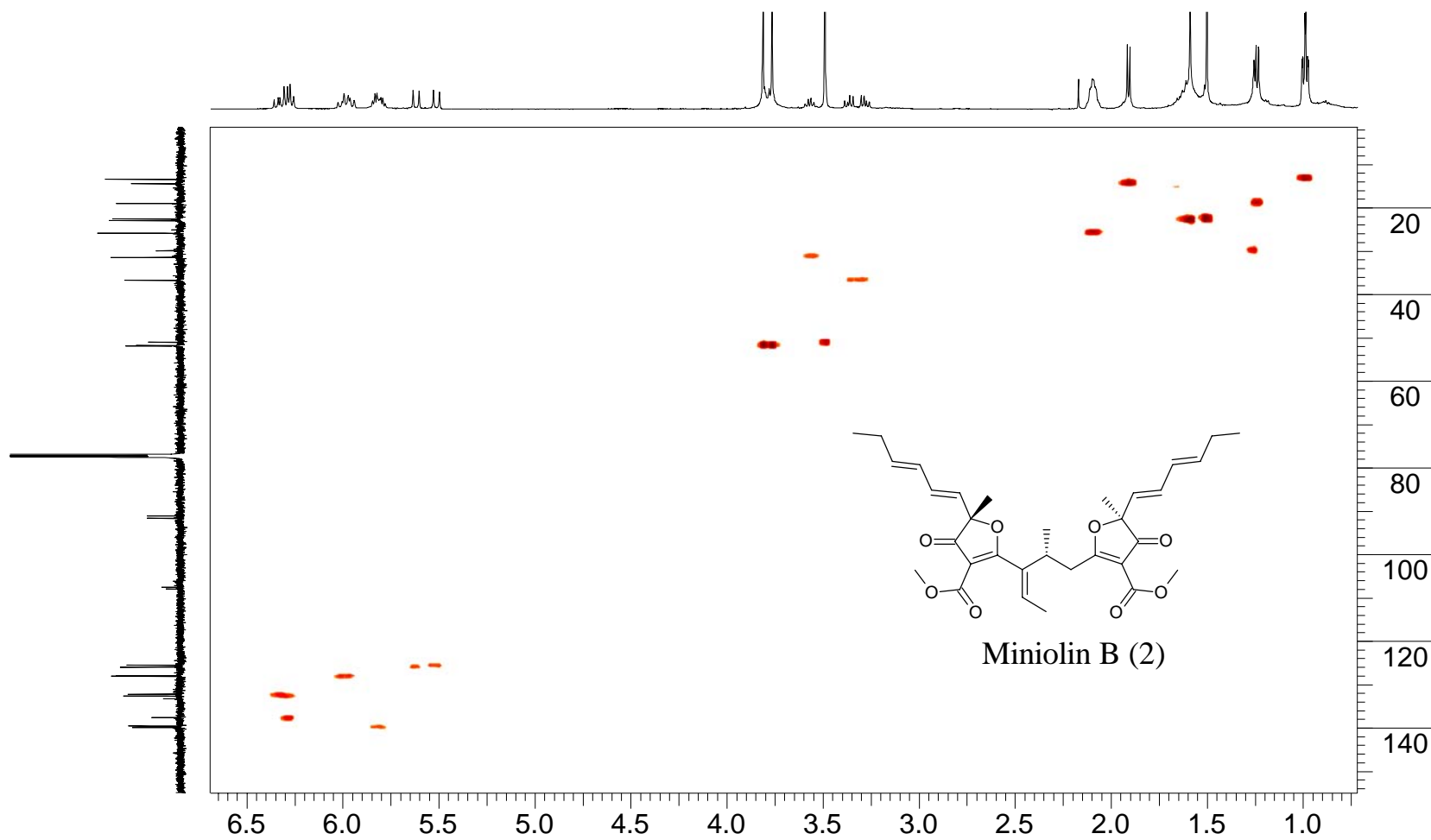


Figure S16. ^1H - ^1H COSY spectrum of 2

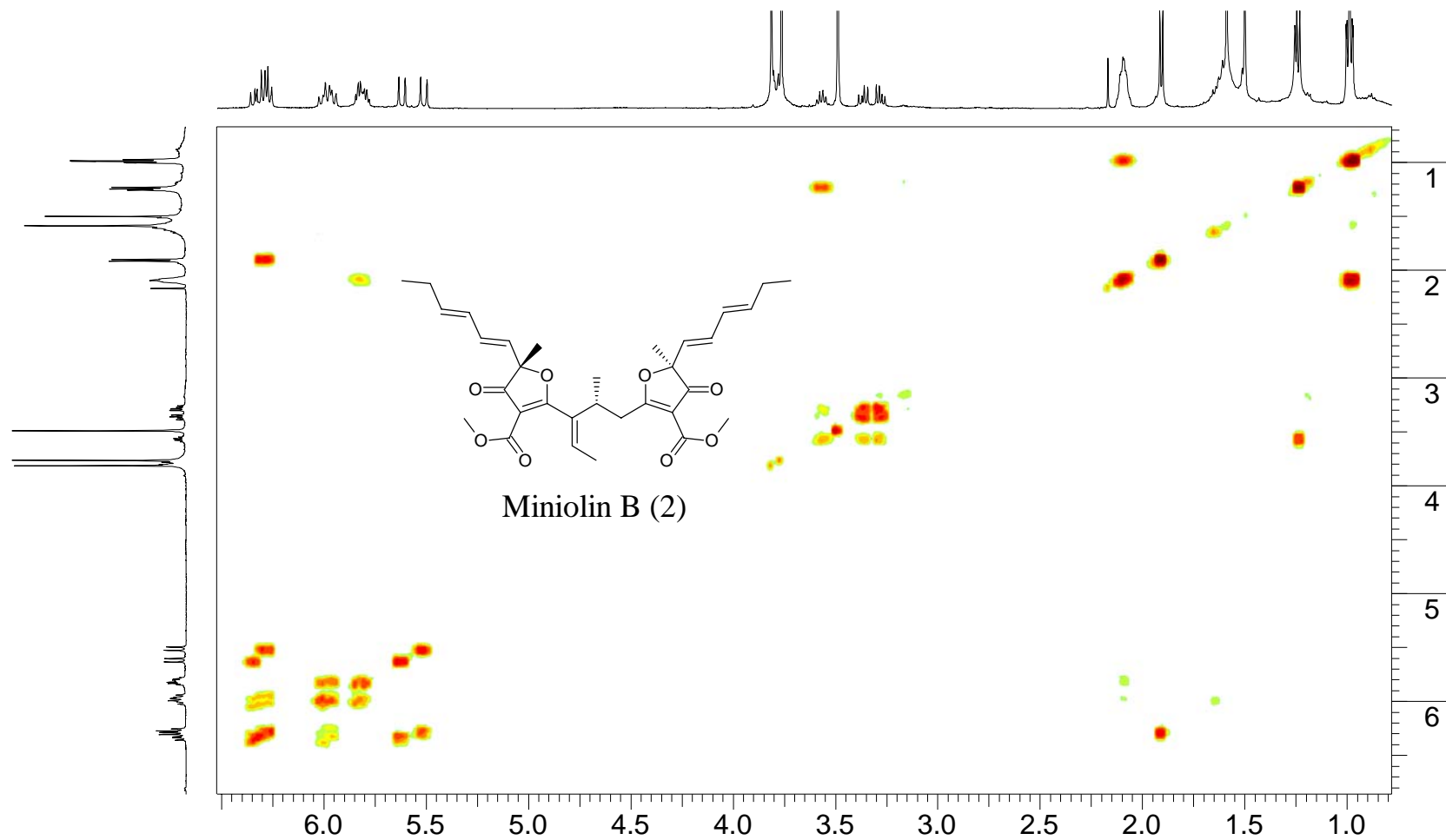
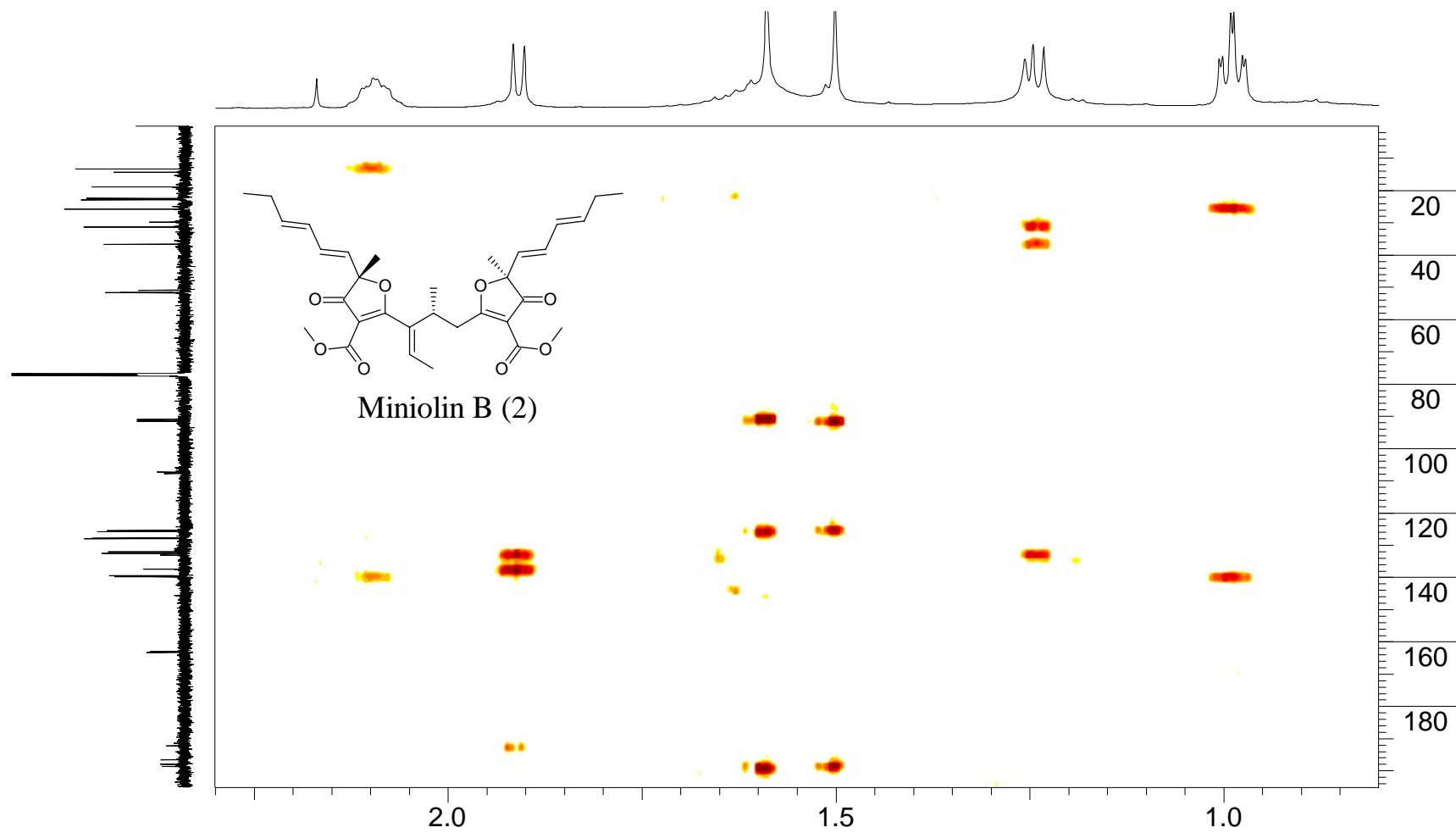
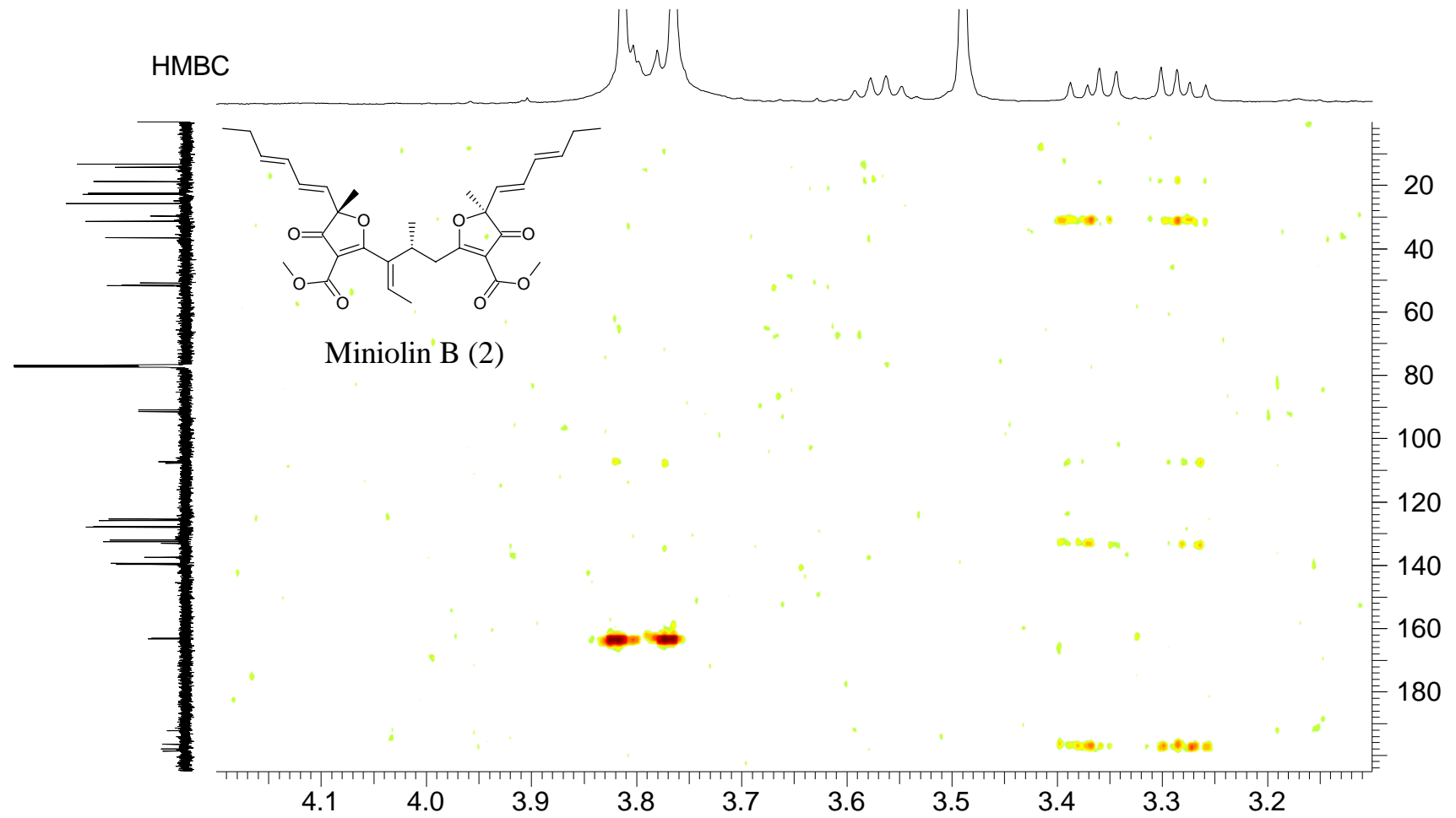


Figure S17. HMBC spectrum of 2





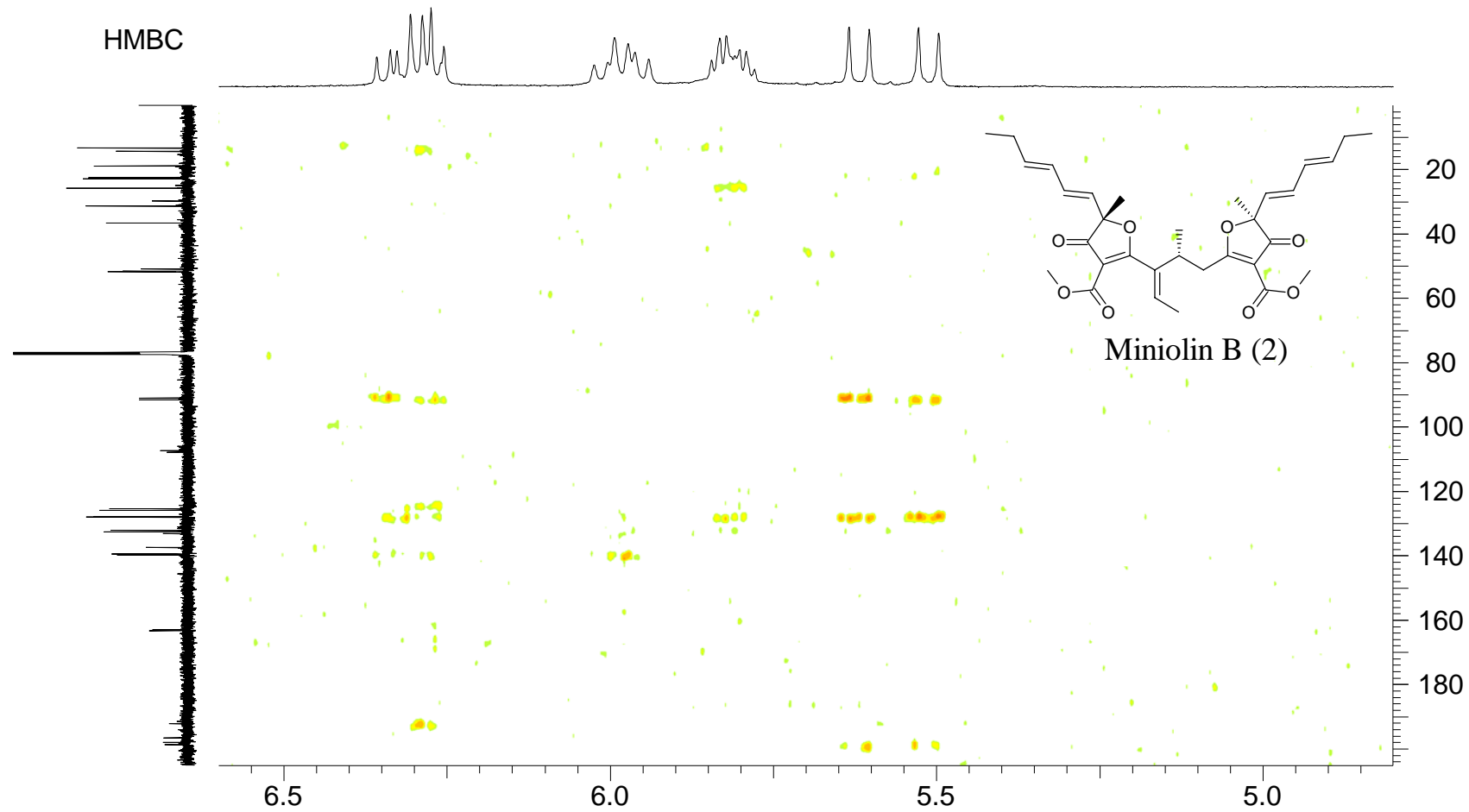


Figure S18. NOESY spectrum of 2

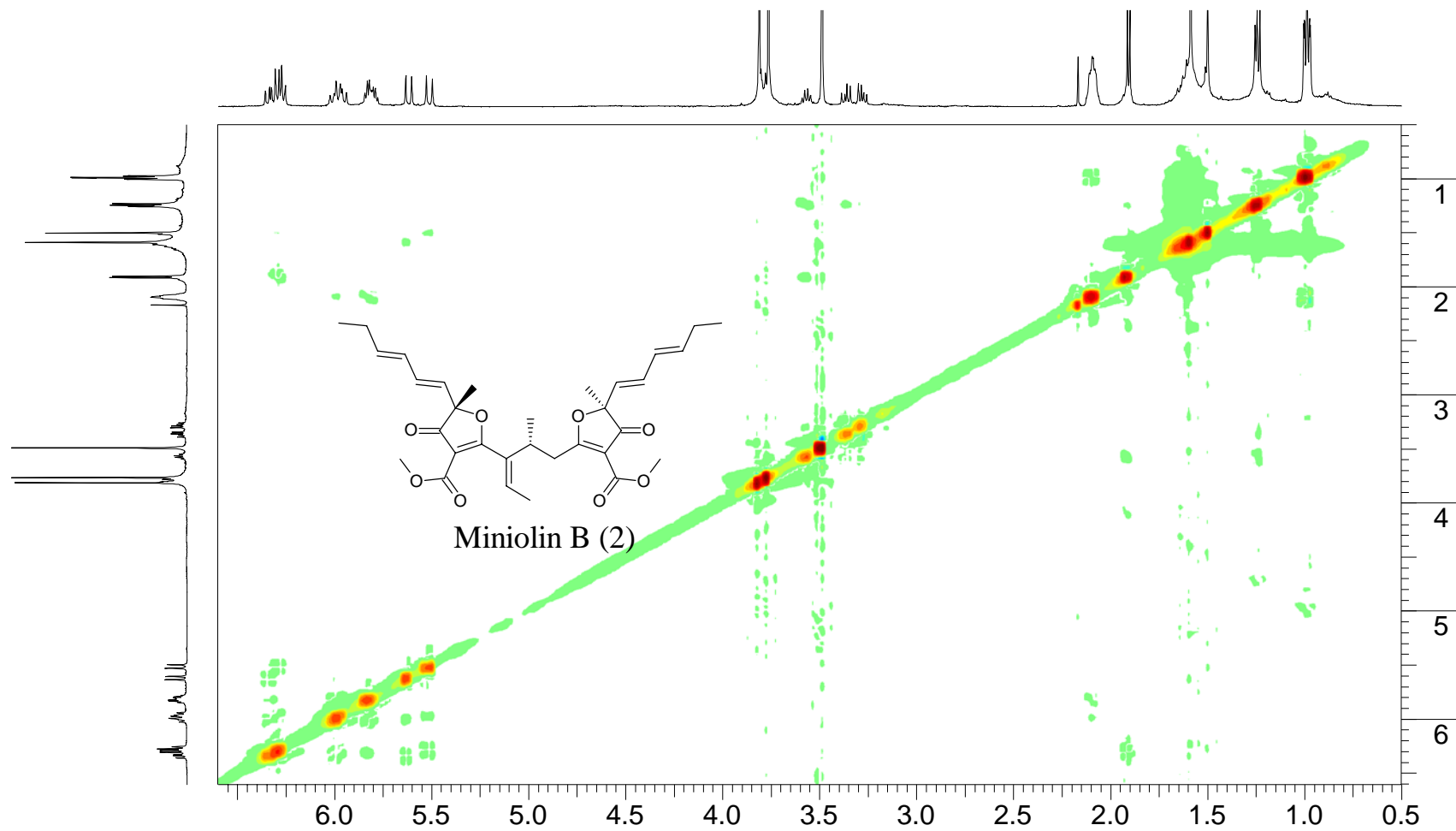


Figure S19. Positive ESIMS spectrum of 2

ZH-26 #17-20 RT: 0.07-0.08 AV: 4 NL: 1.28E4
T: ITMS + c ESI Full ms [50.00-2000.00]

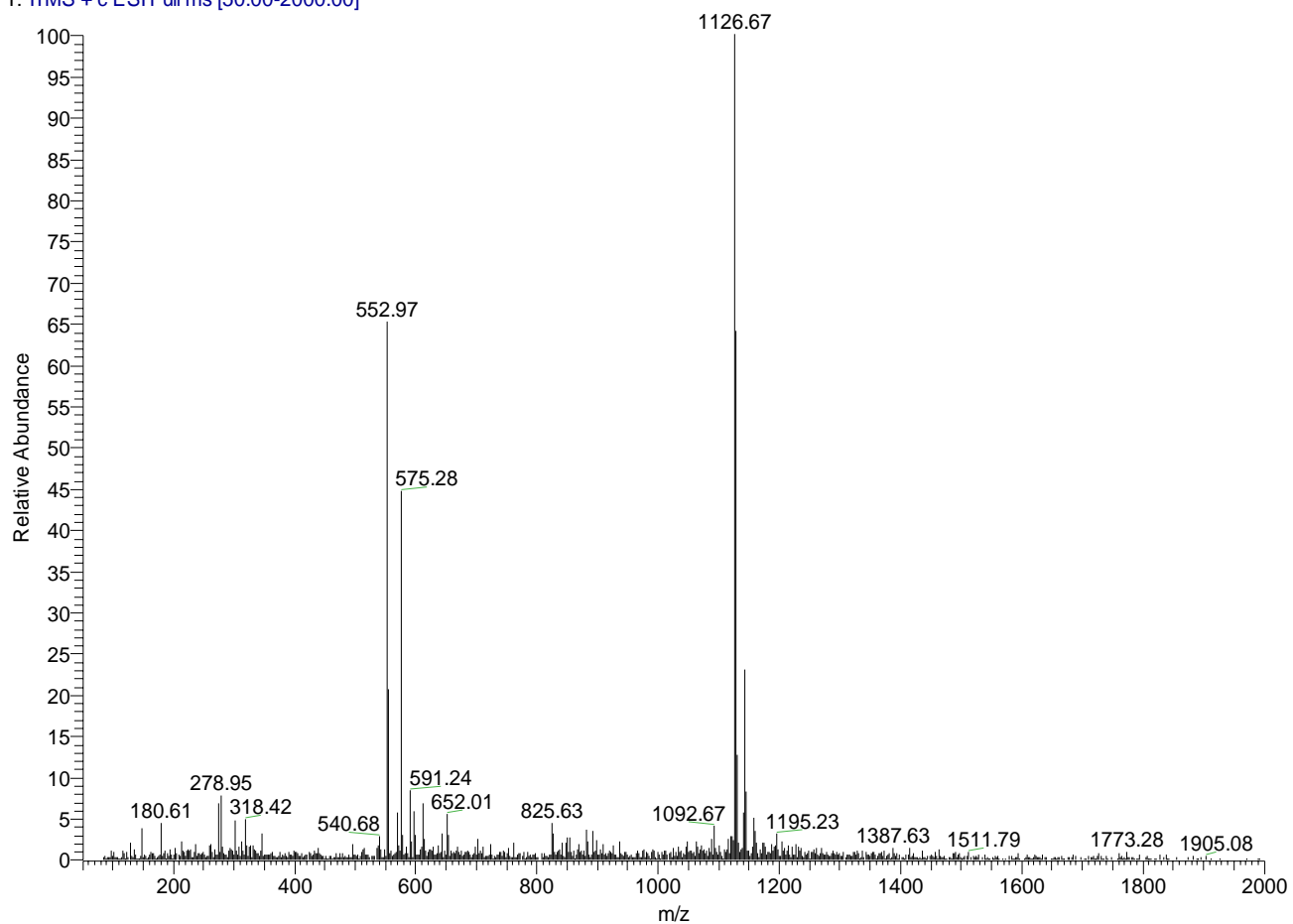
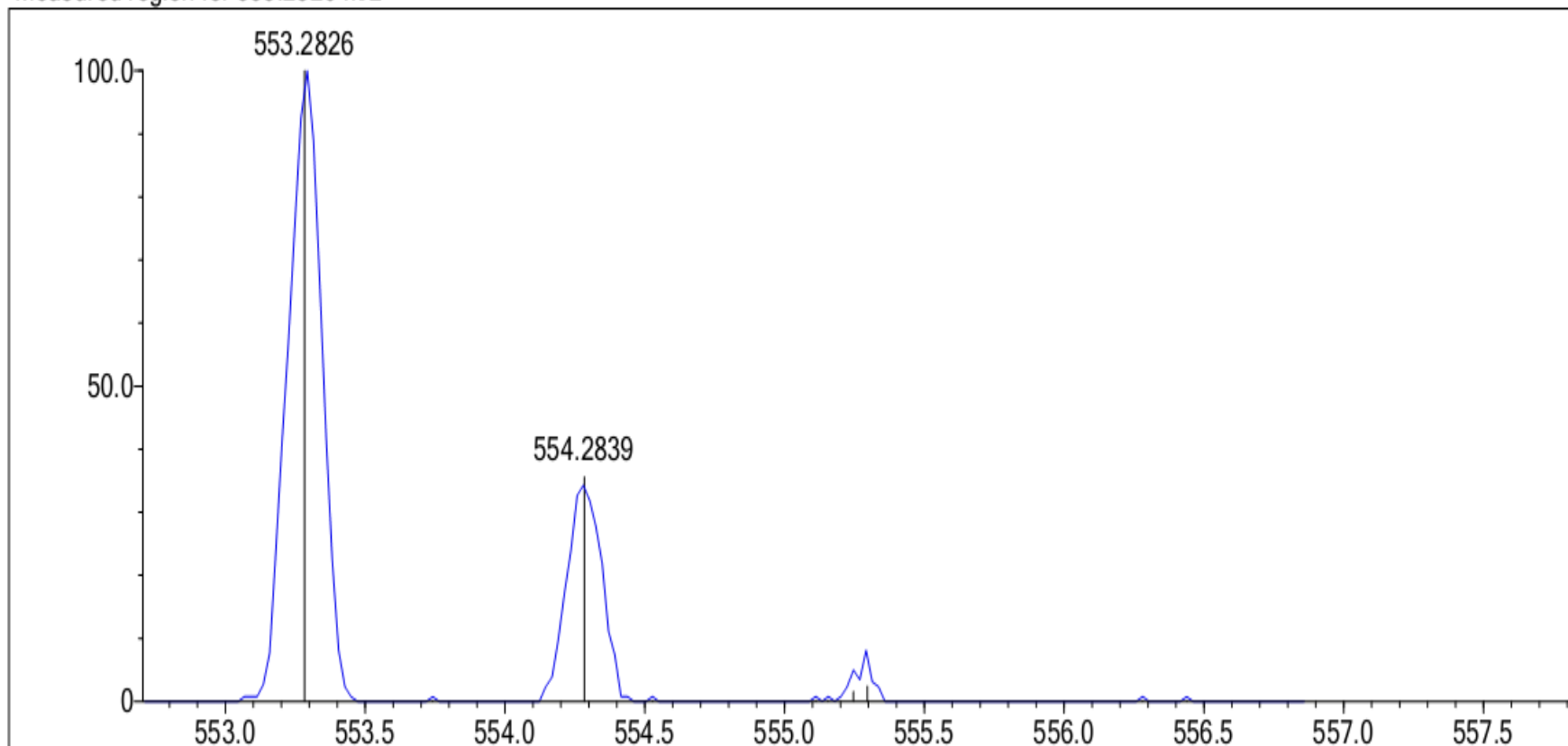


Figure S20. HR ESIMS spectrum of 2

Measured region for 553.2826 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.32	[M+H] ⁺	C ₃₂ H ₄₀ O ₈	553.2796	553.2826	3.0	5.42	97.11	13.0

Figure S21. IR spectrum of 2

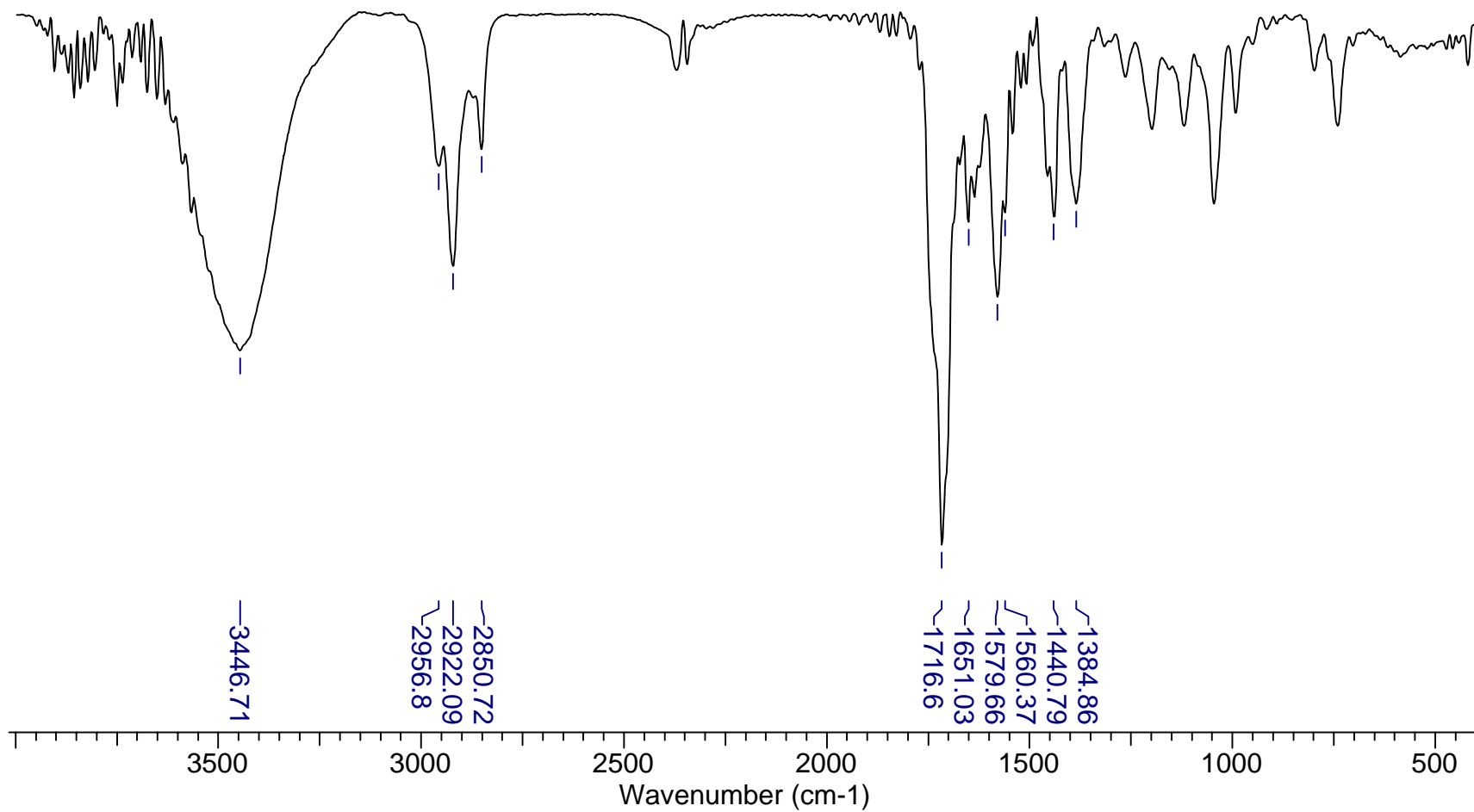


Figure S22. UV and CD spectra of 2

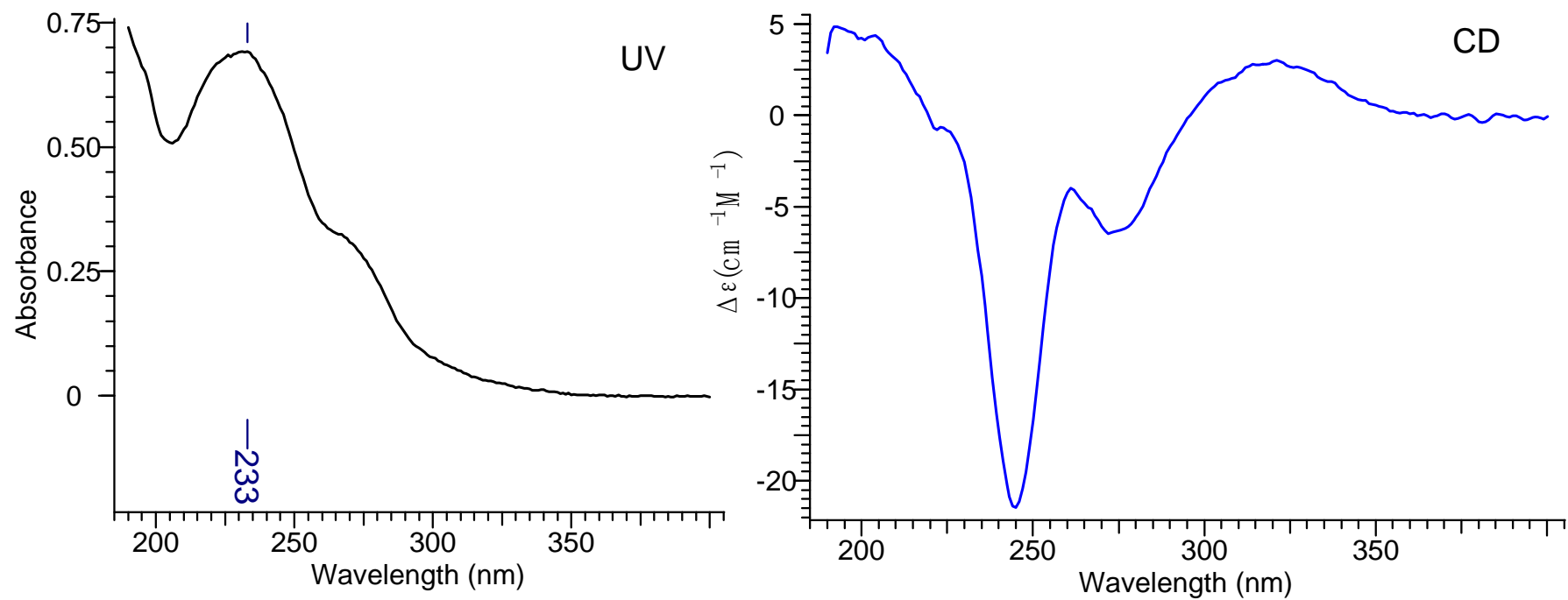


Figure S23. ^1H NMR spectrum of 3 in CDCl_3 (500 MHz)

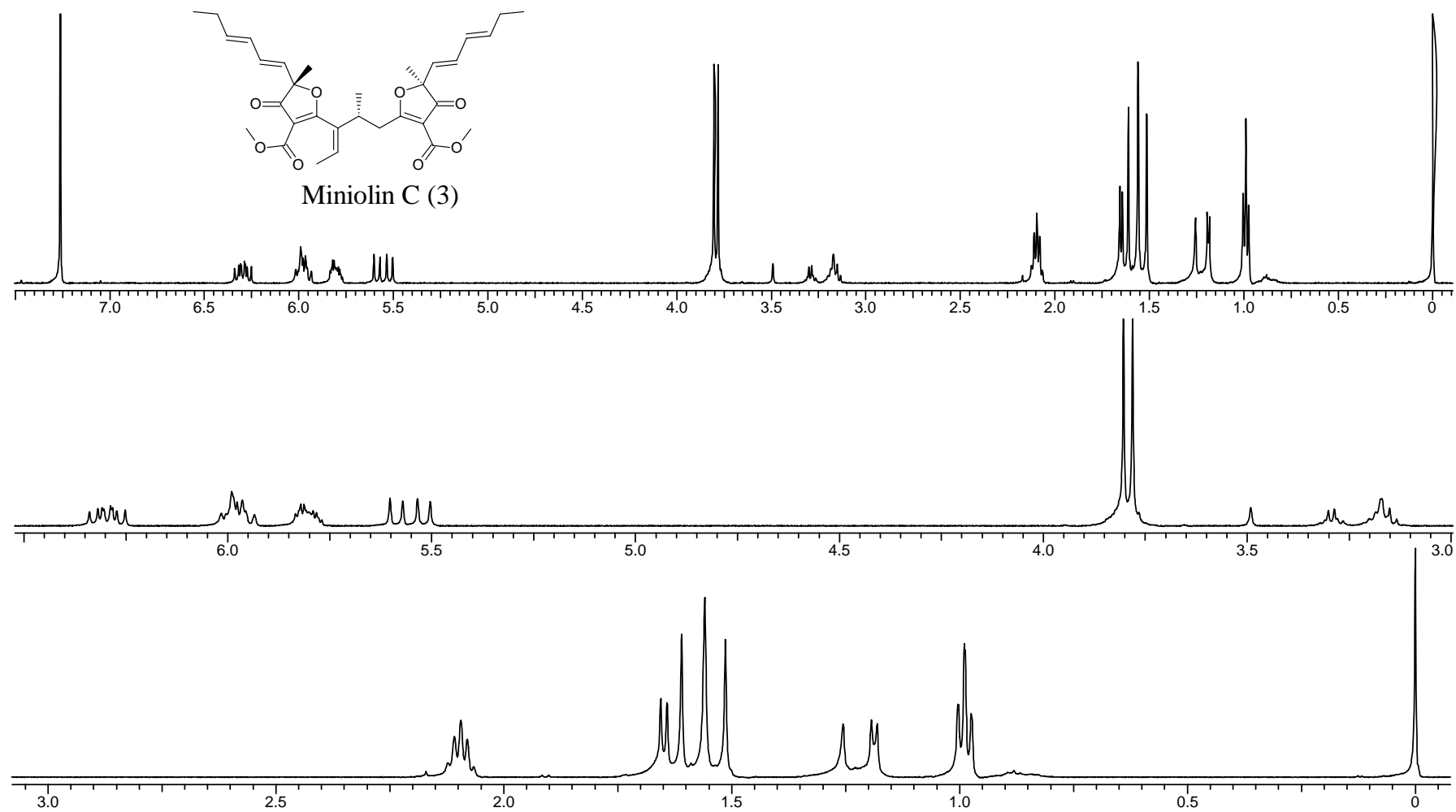


Figure S24. ^{13}C NMR and DEPT spectrum of 3 in CDCl_3 (125 MHz)

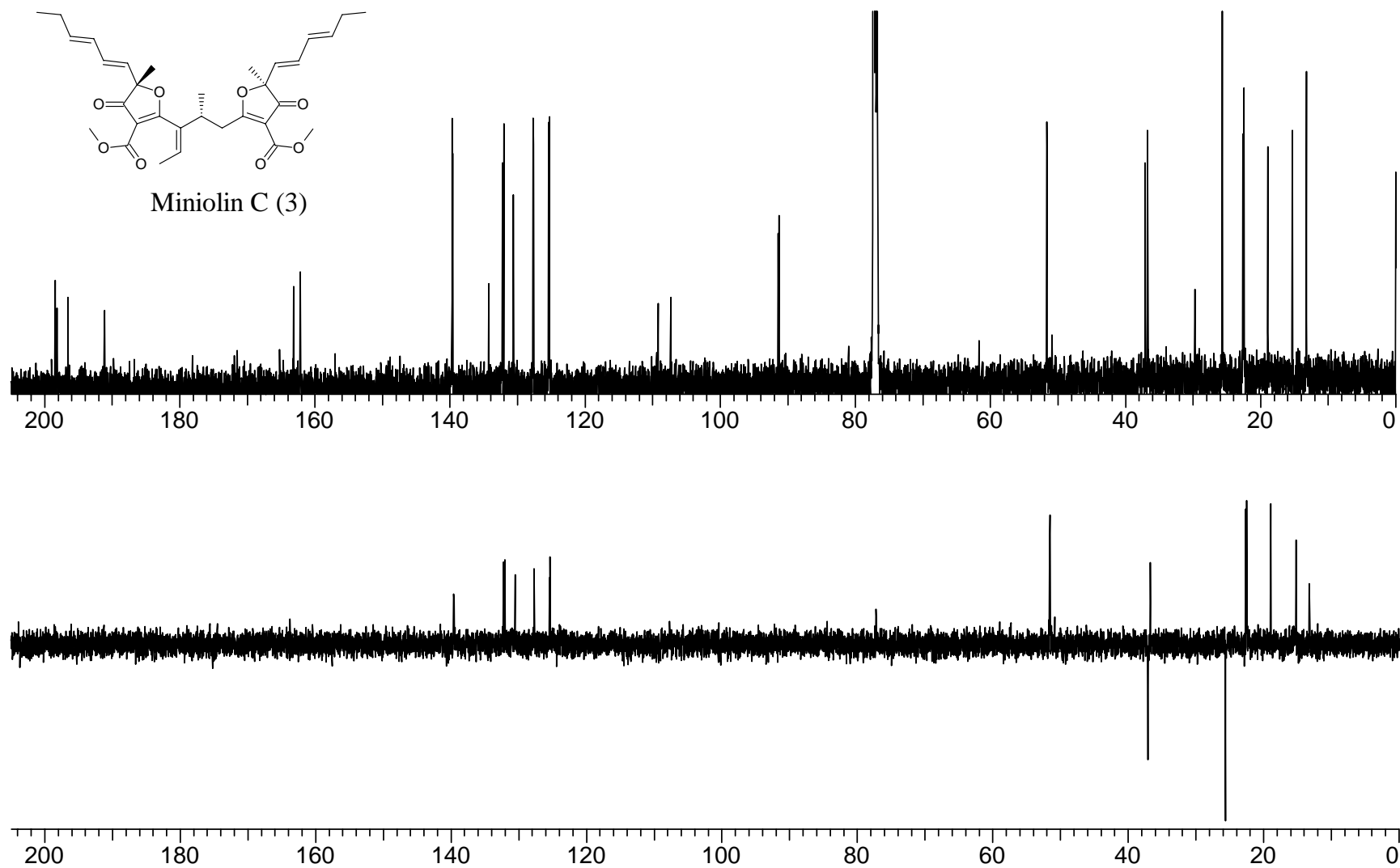


Figure S25. HSQC spectrum of 3

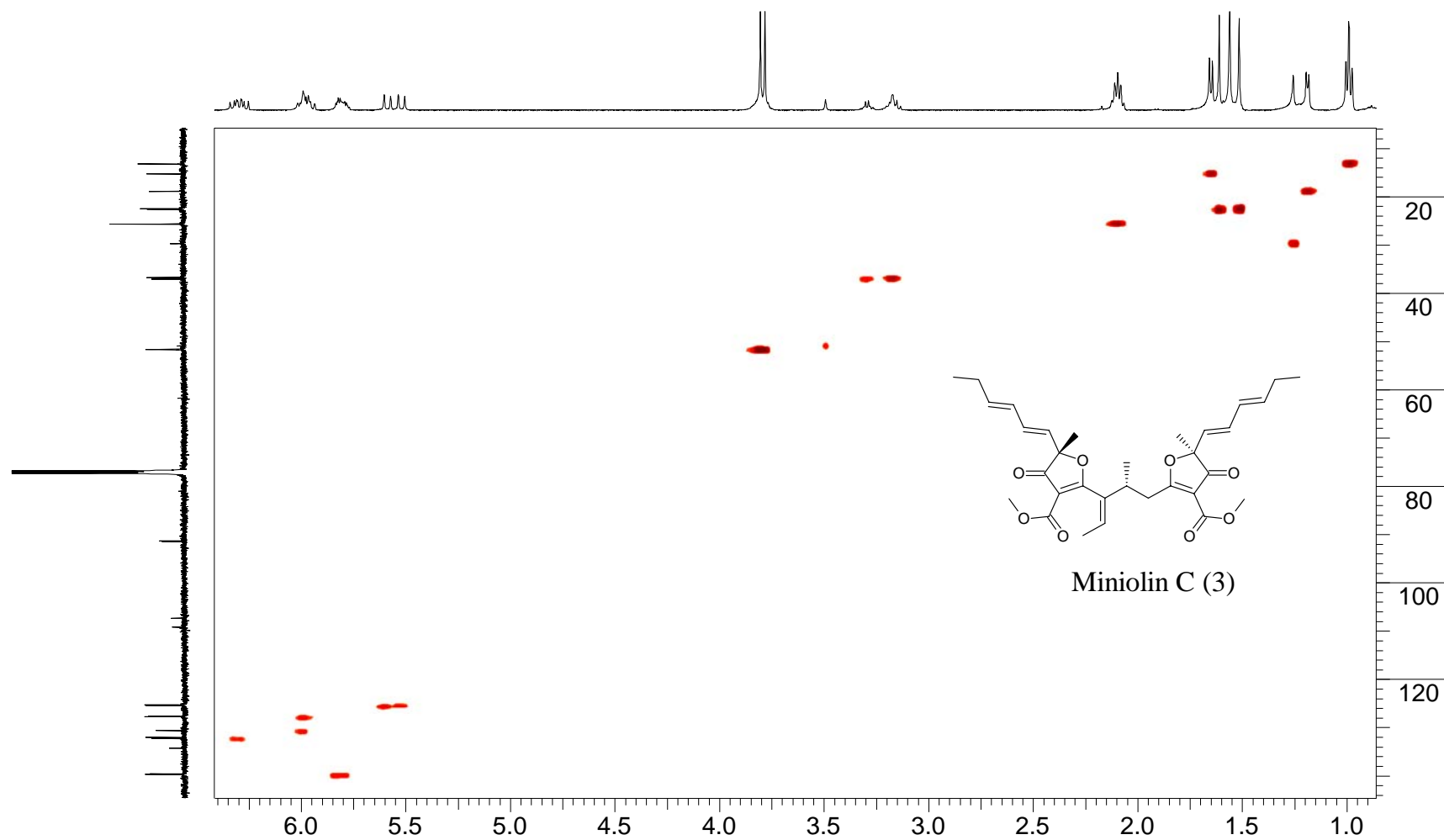


Figure S26. ^1H - ^1H COSY spectrum of 3

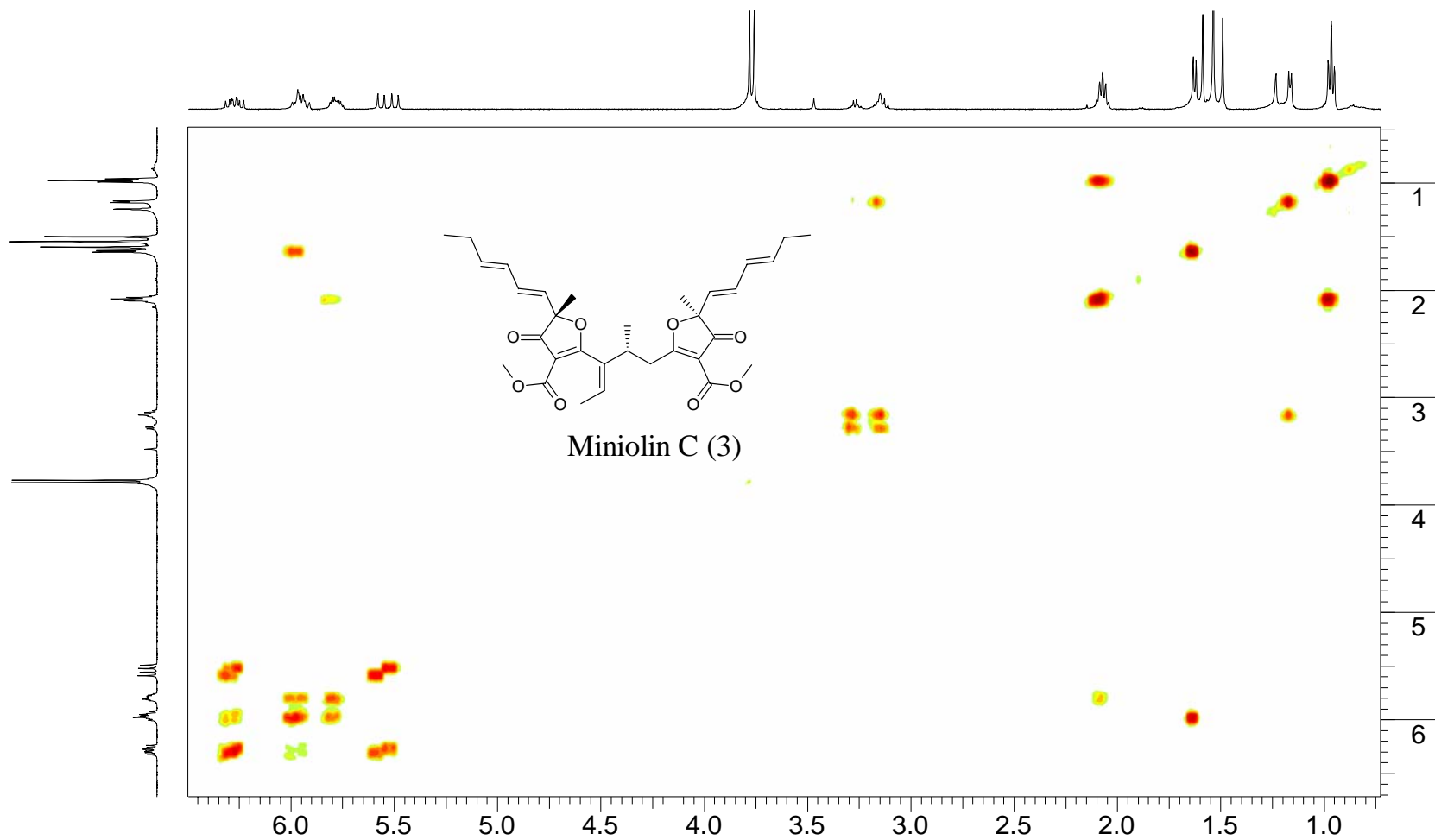
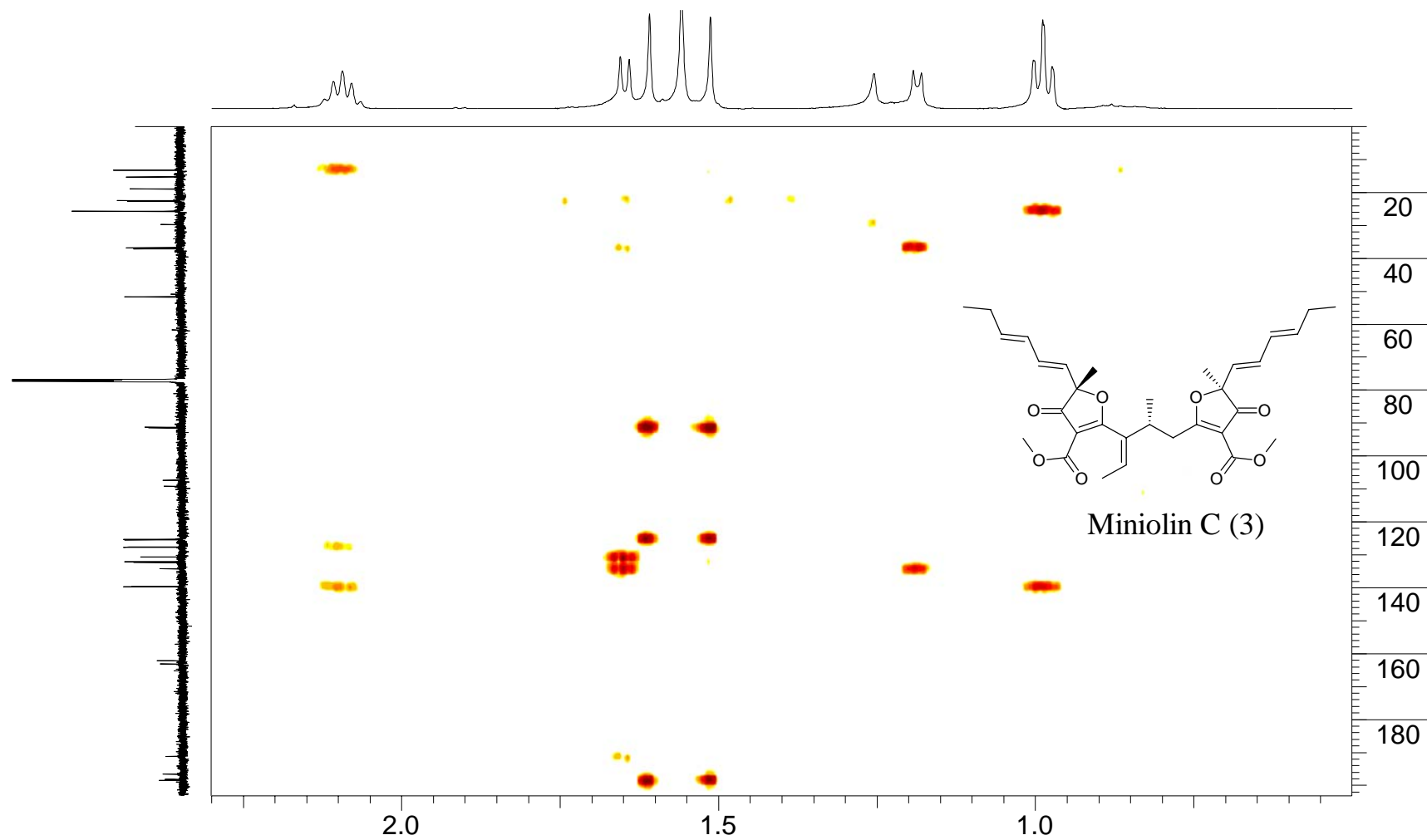
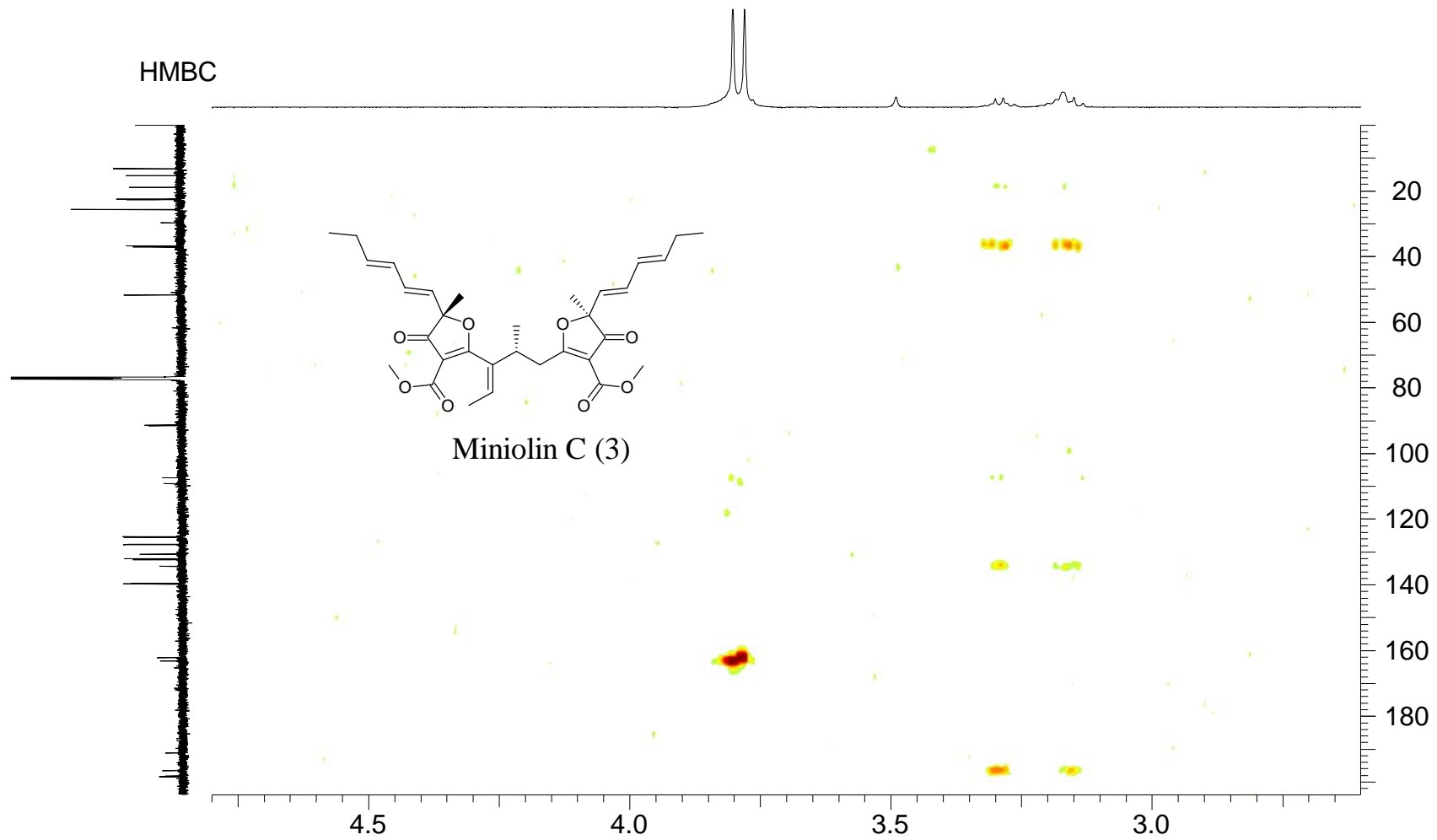


Figure S27. HMBC spectrum of 3





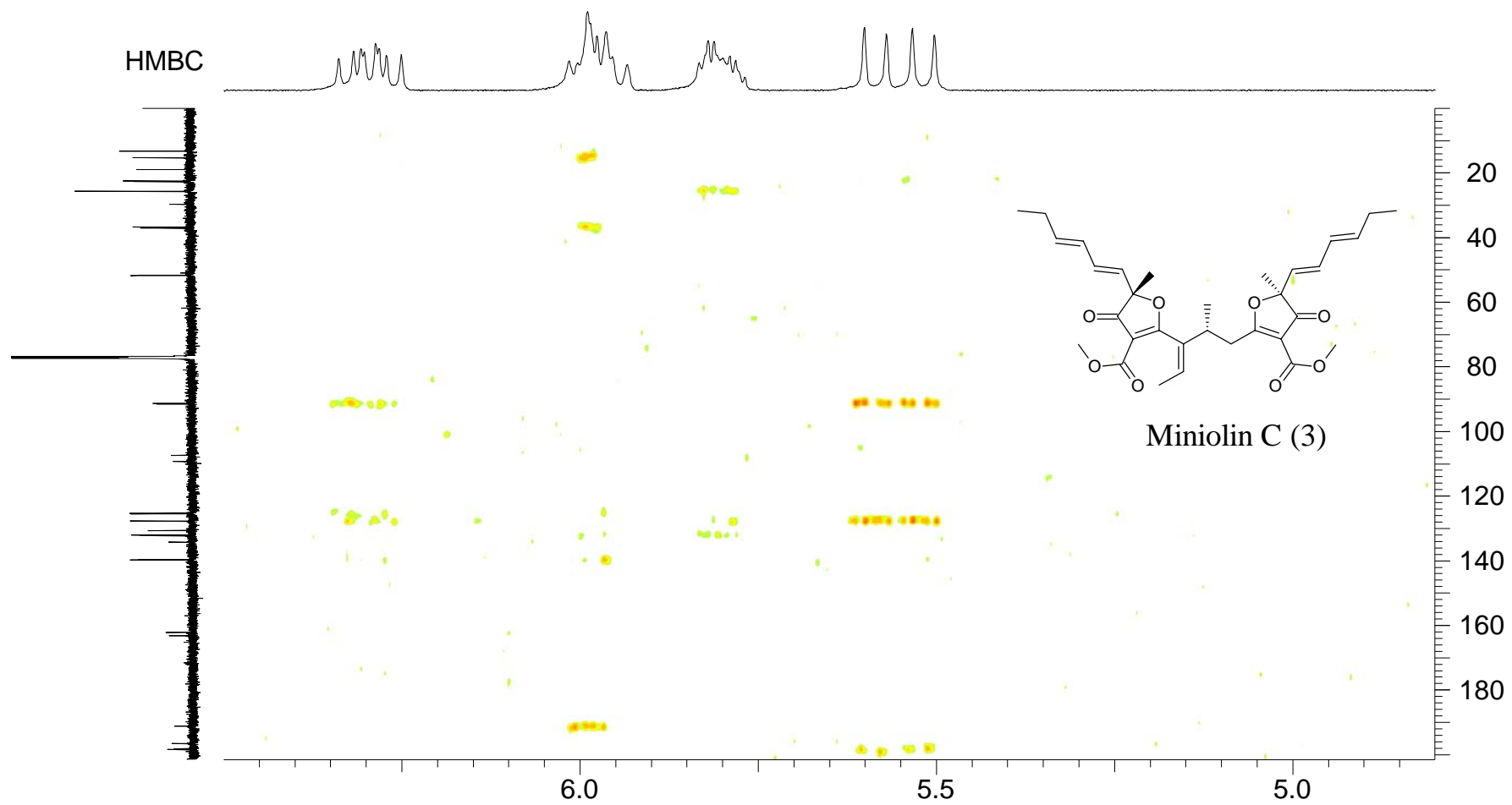


Figure S28. NOESY spectrum of 3

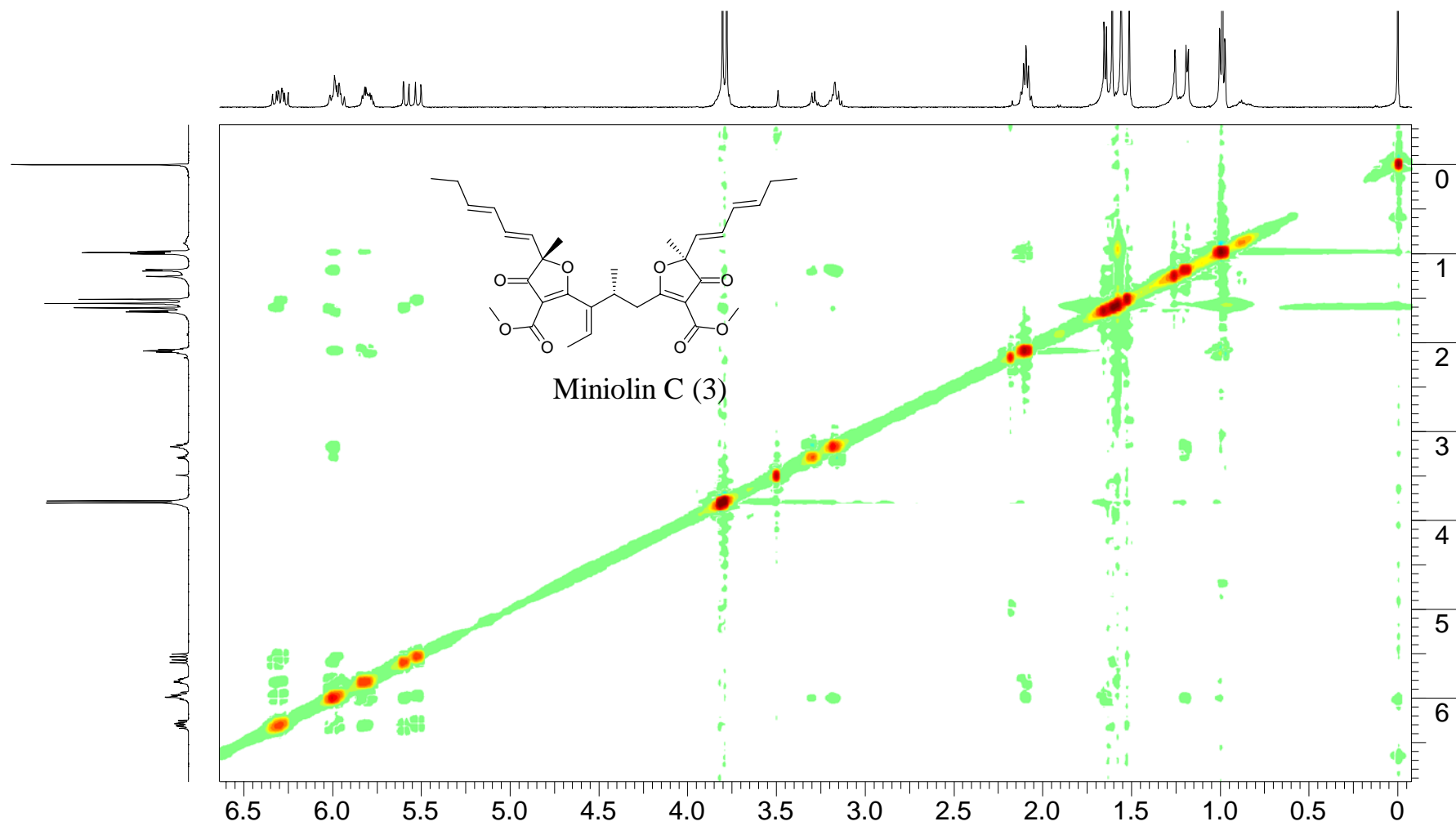


Figure S29. Positive ESIMS spectrum of 3

ZH28 #9-13 RT: 0.03-0.05 AV: 5 NL: 1.21E4
T: ITMS + c ESI sid=35.00 Full ms [50.00-2000.00]

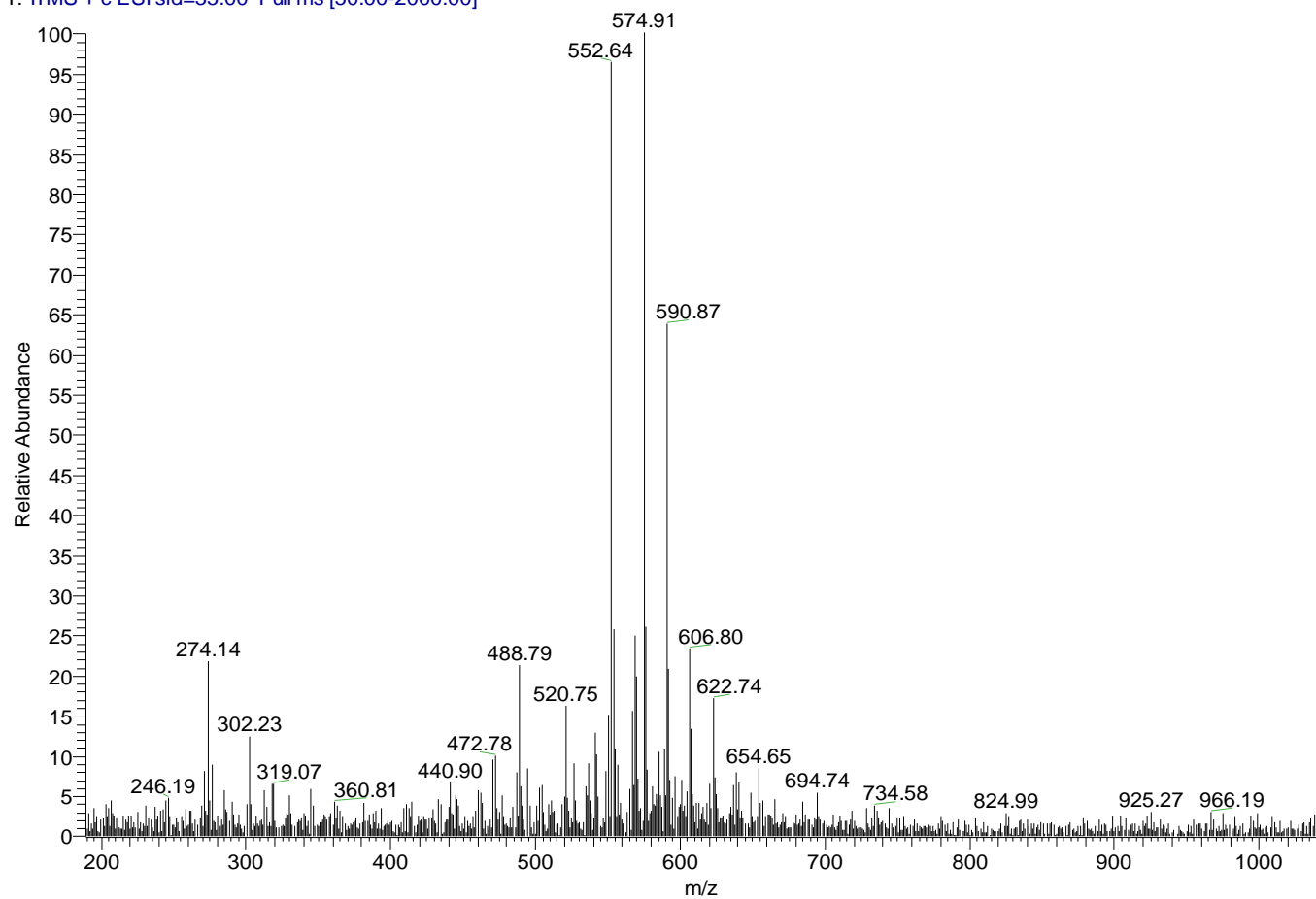
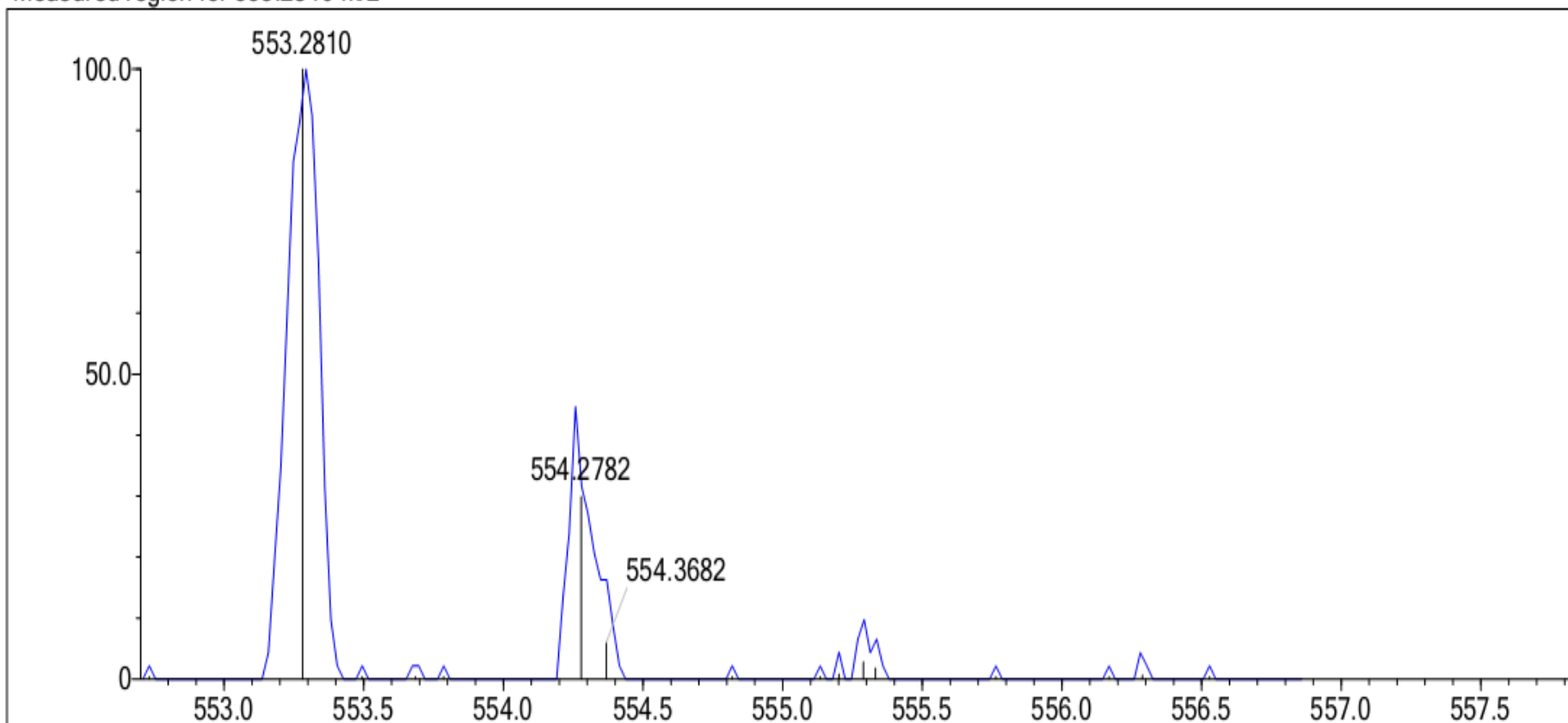


Figure S30. HR ESIMS spectrum of 3

Measured region for 553.2810 m/z



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	57.74	[M+H] ⁺	C ₃₂ H ₄₀ O ₈	553.2796	553.2810	1.4	2.53	60.03	13.0

Figure S31. IR spectrum of 3

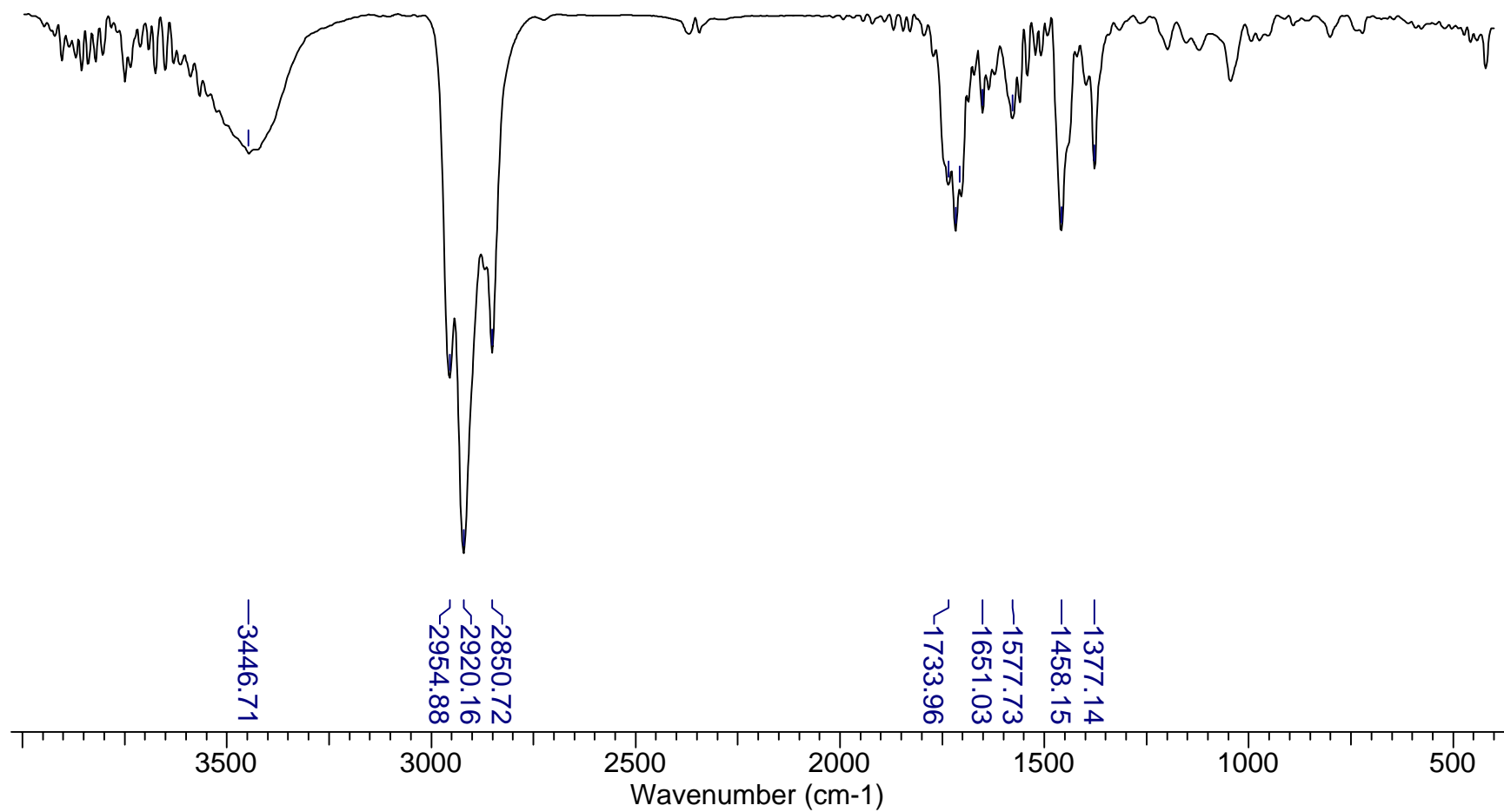


Figure S32. UV and CD spectra of 3

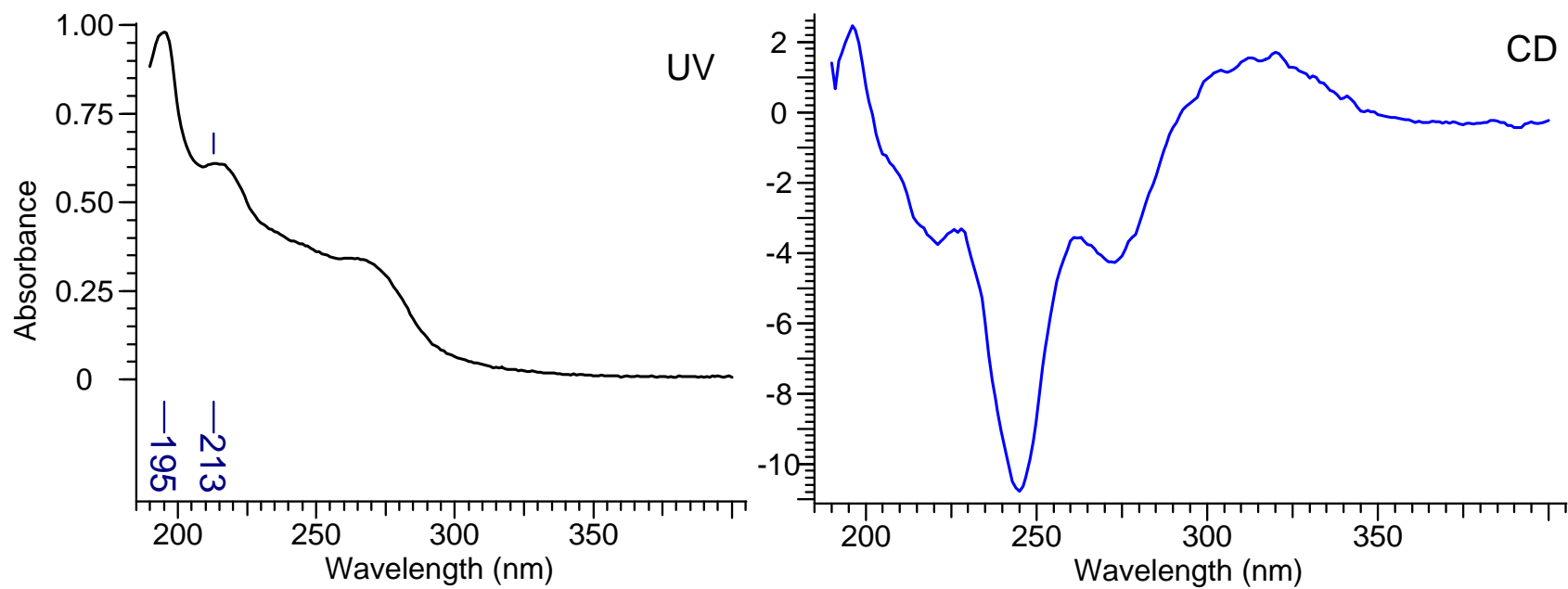


Figure S33. ^1H NMR spectrum of 4 in CDCl_3 (400 MHz)

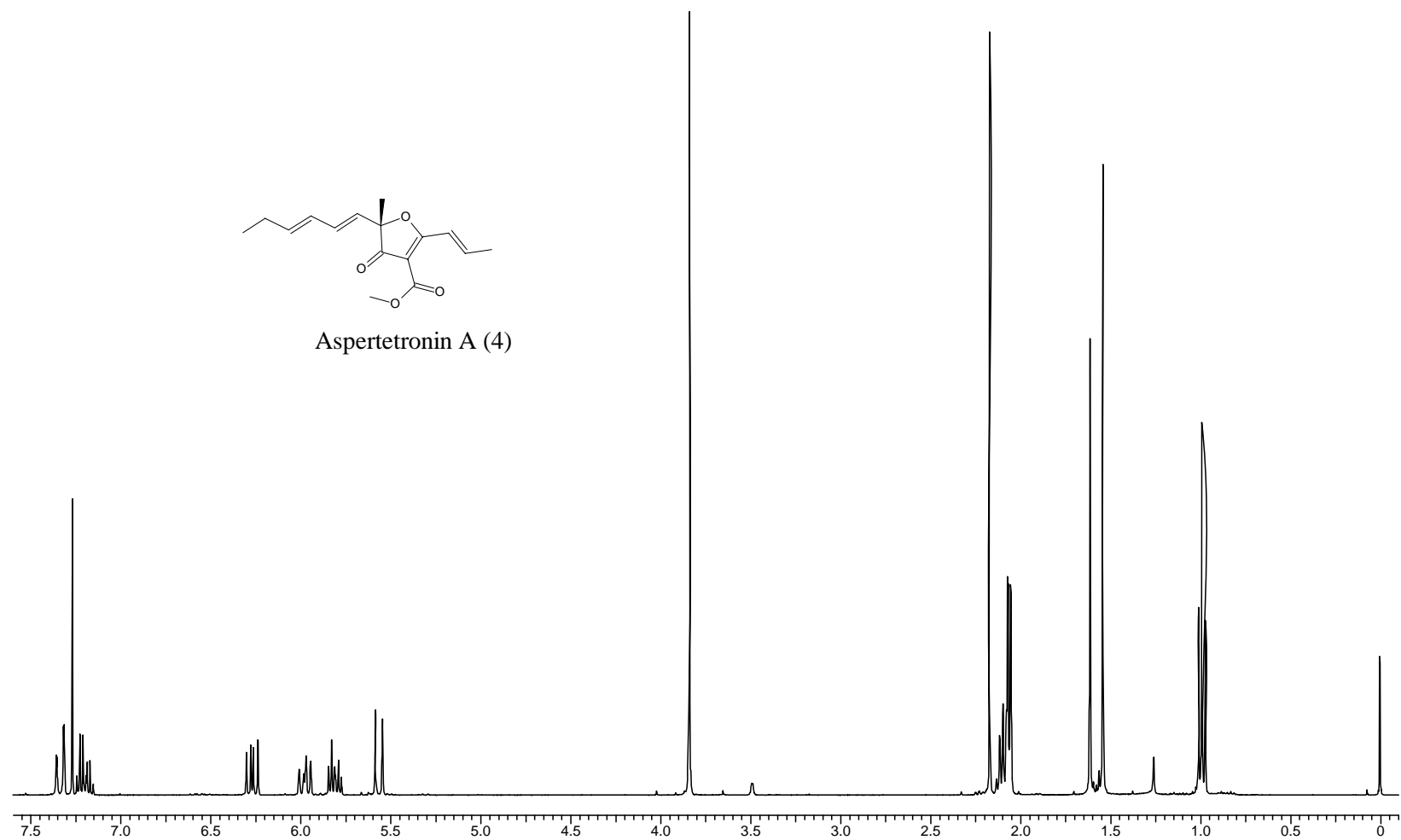


Figure S34. ^{13}C NMR spectrum of **4** in CDCl_3 (100 MHz)

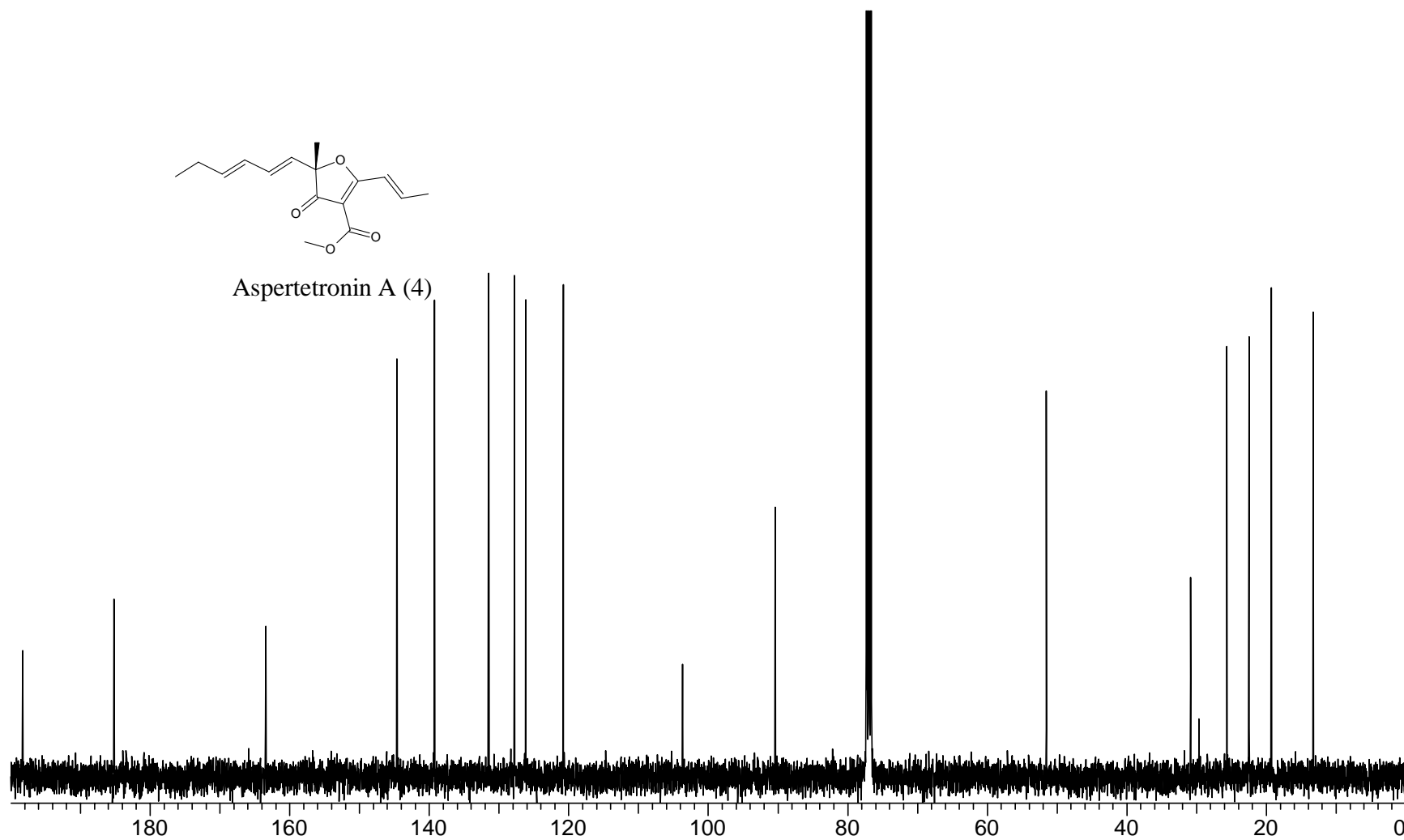


Figure S35. IR spectrum of 4

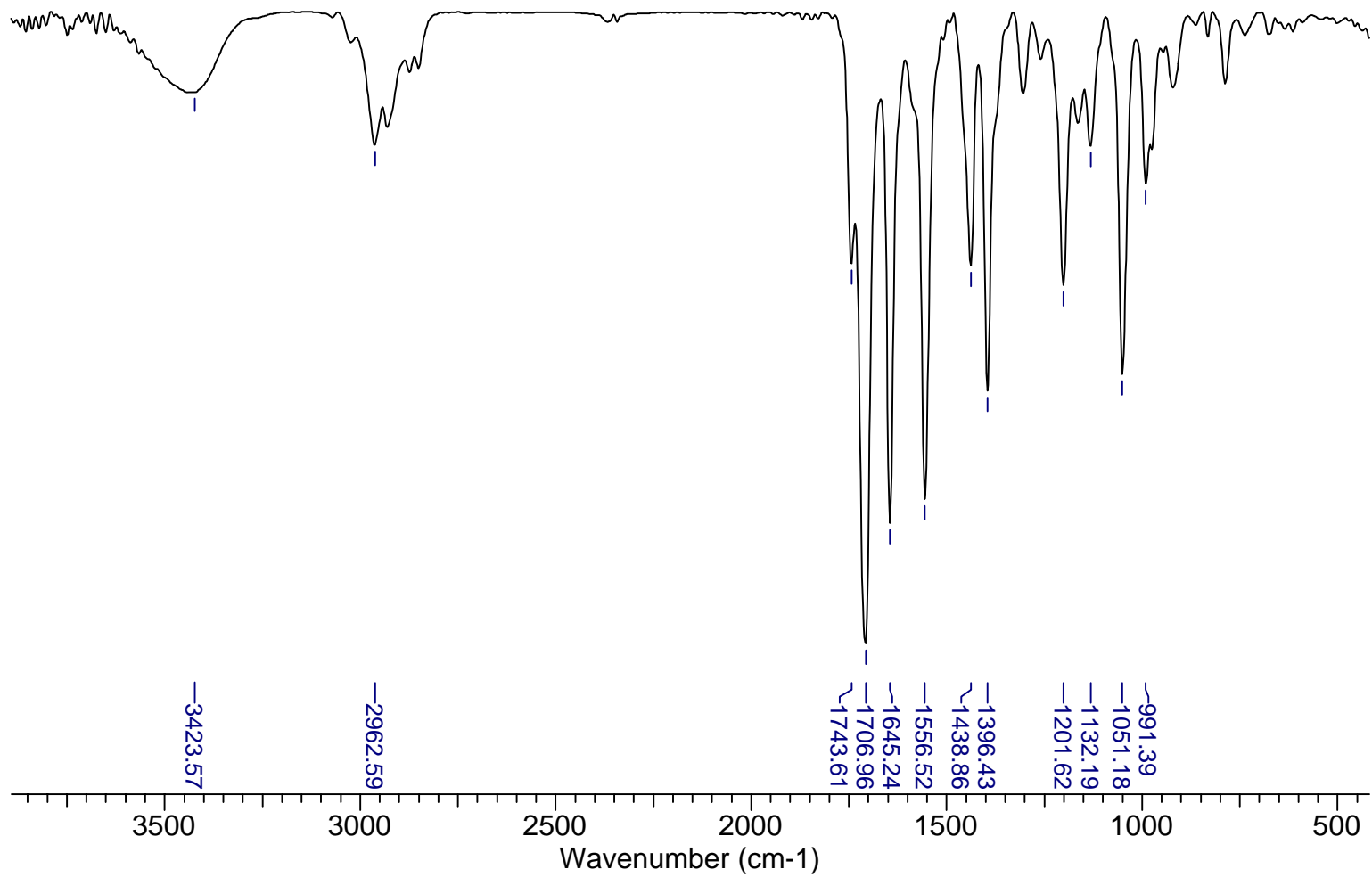


Figure S36. UV spectrum of 4

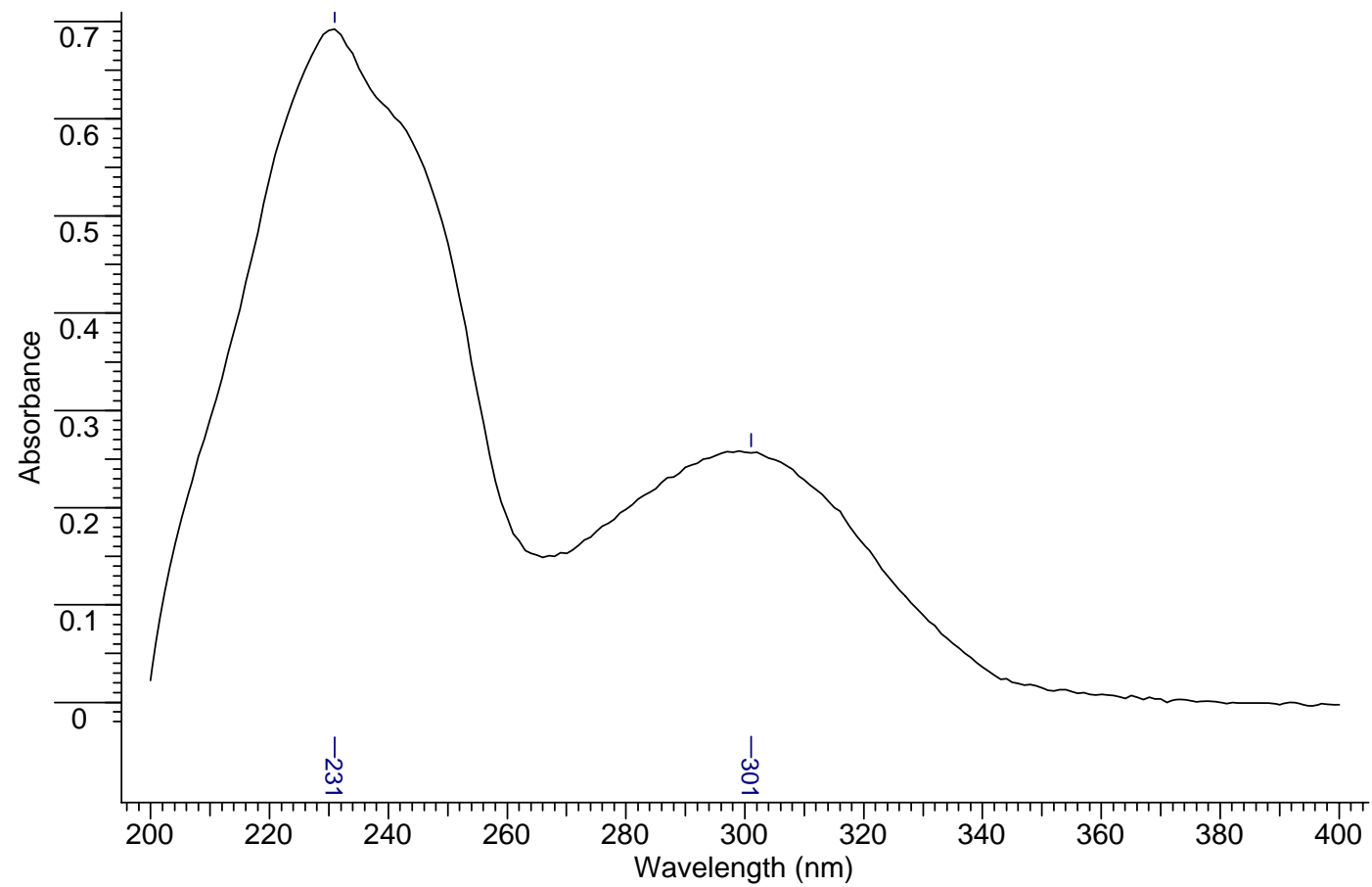


Figure S37. ESIMS of 4

Gao Jining ZH-2 #27-31 RT: 0.07-0.08 AV: 5 NL: 3.71E5
T: ITMS + c ESI Full ms [80.00-1000.00]

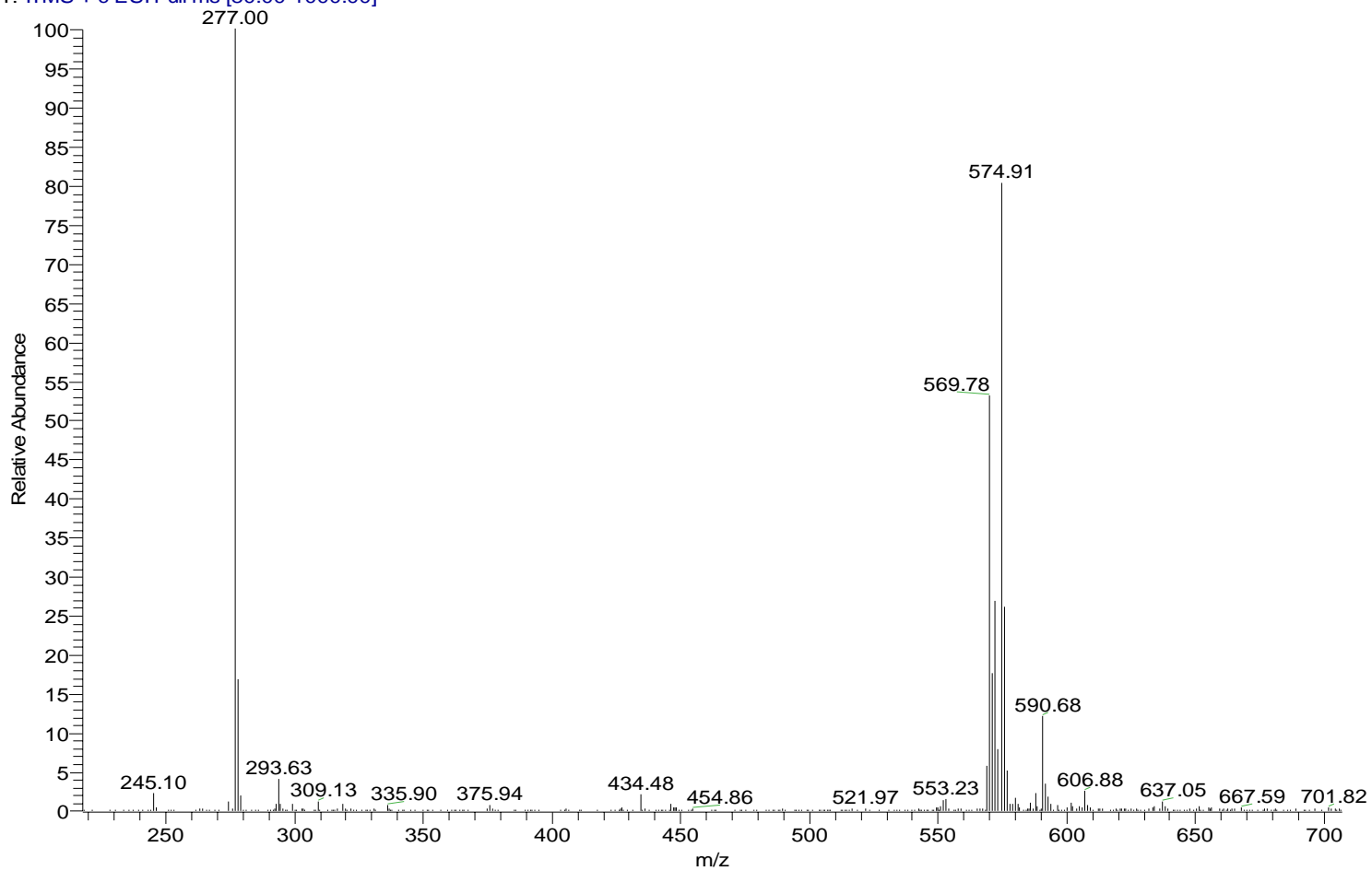


Figure S38. CD of 4

