Supplementary Information

Miniolins A–C, Novel Isomeric Furanones Induced by Epigenetic Manipulation on *Penicillium minioluteum*

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‡ H.-Y. Tang and Q. Zhang contributed equally

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CONTENTS

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

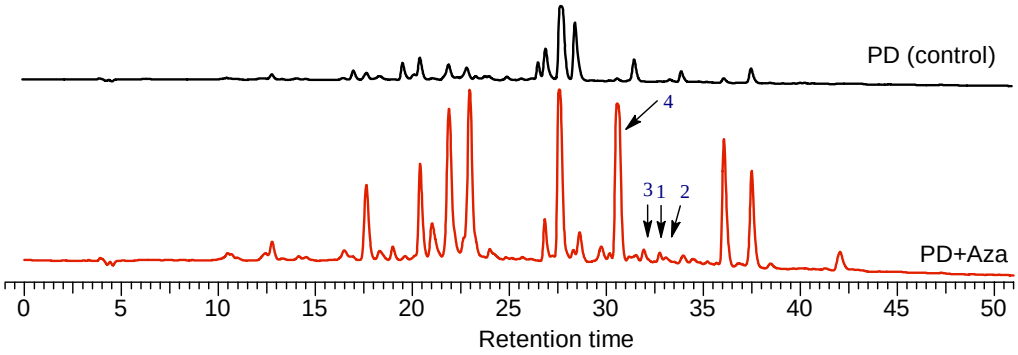
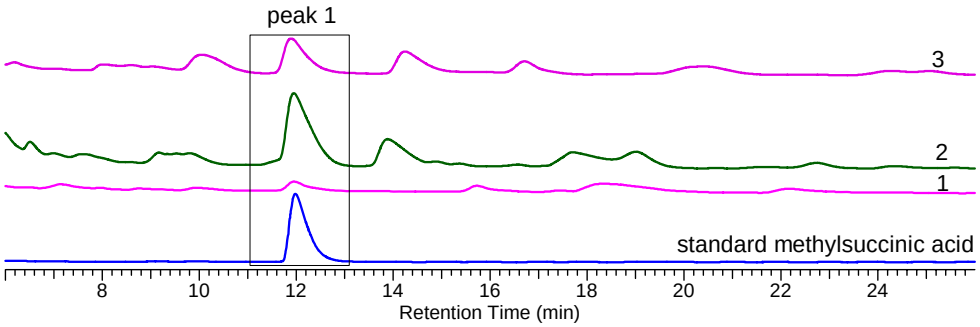


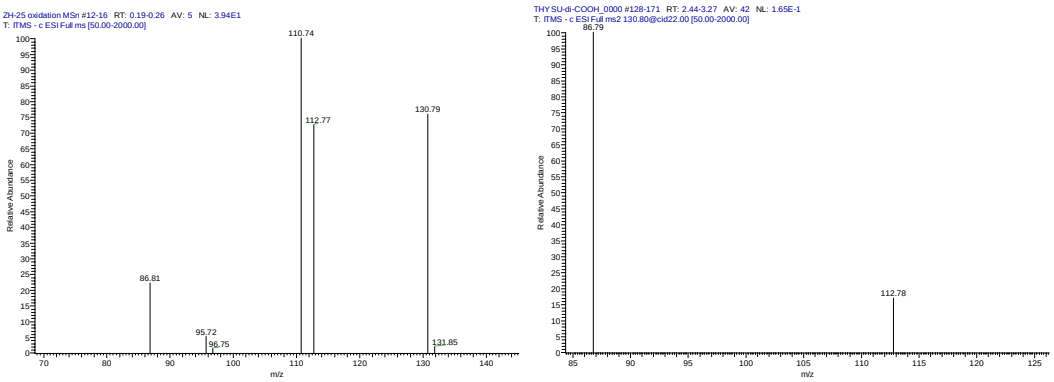
Figure S2. LC/MS^2 analysis of oxidation products of compounds 1-3

(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/H_2O with 0.1% TFA; Temperature: 25 ^{O}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

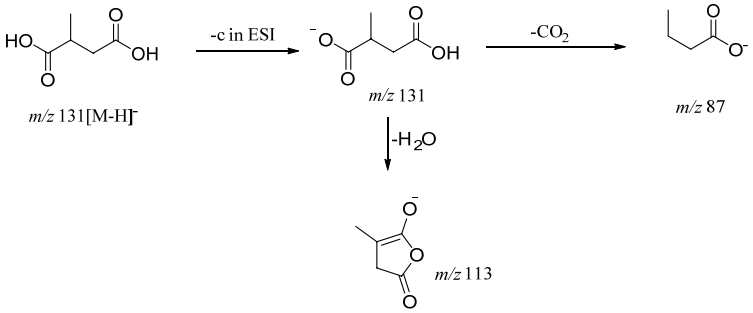


Figure S3. ^{1}H NMR of 1 in $CDCl_3$ (500 MHz)

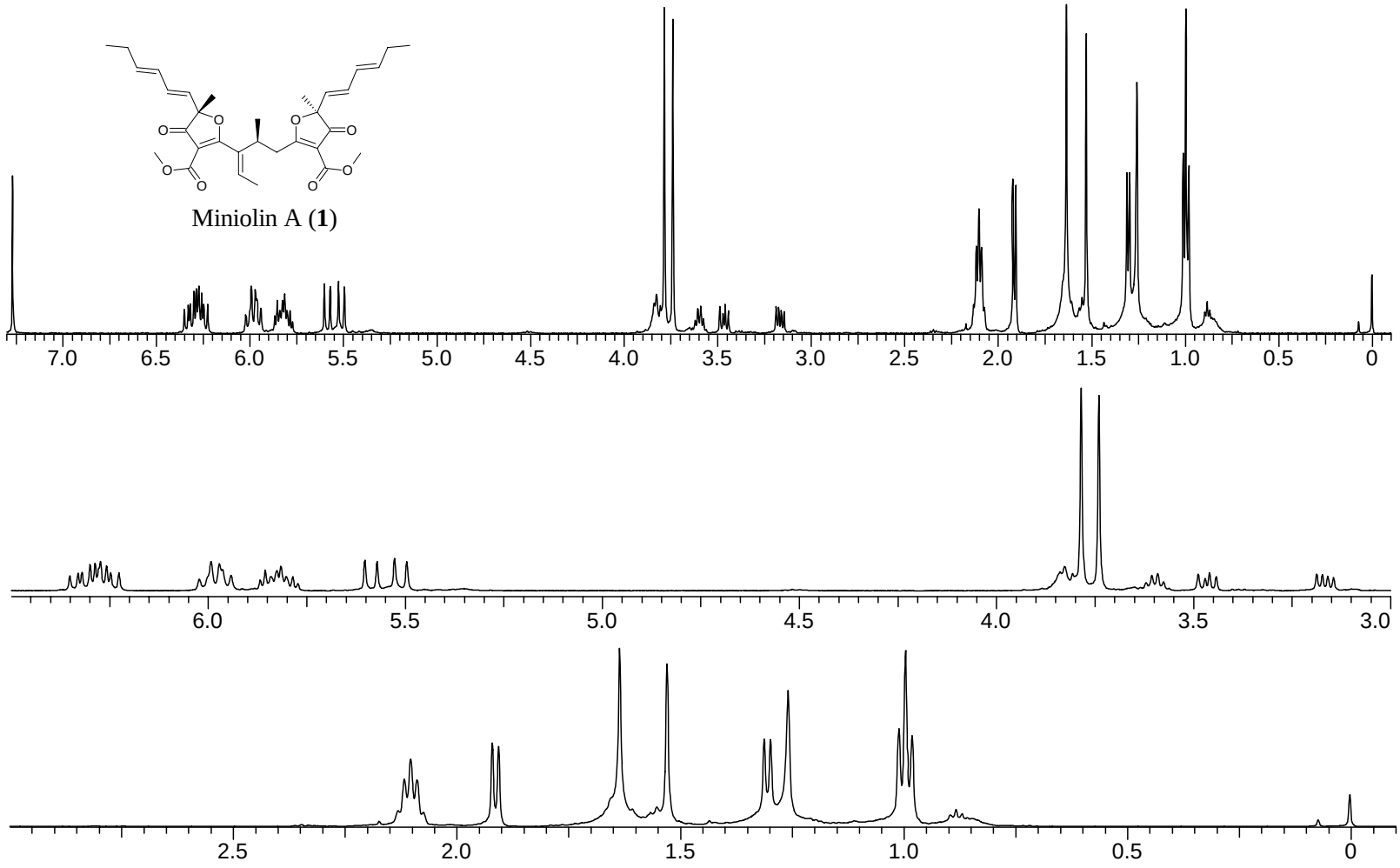


Figure S4. ^{13}C NMR and DEPT of 1 in $CDCl_3$ (125 MHz)

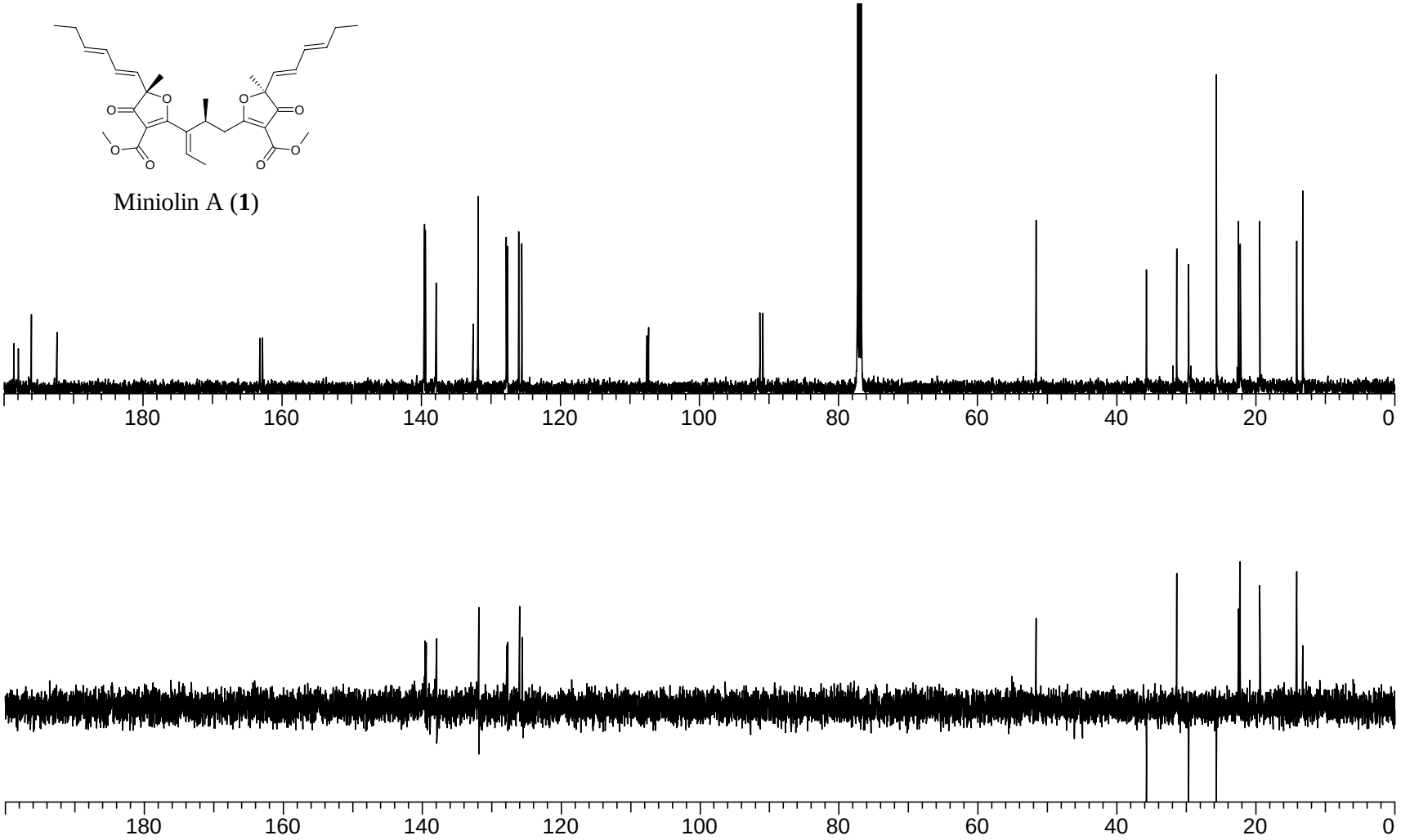


Figure S5. HSQC spectrum of 1

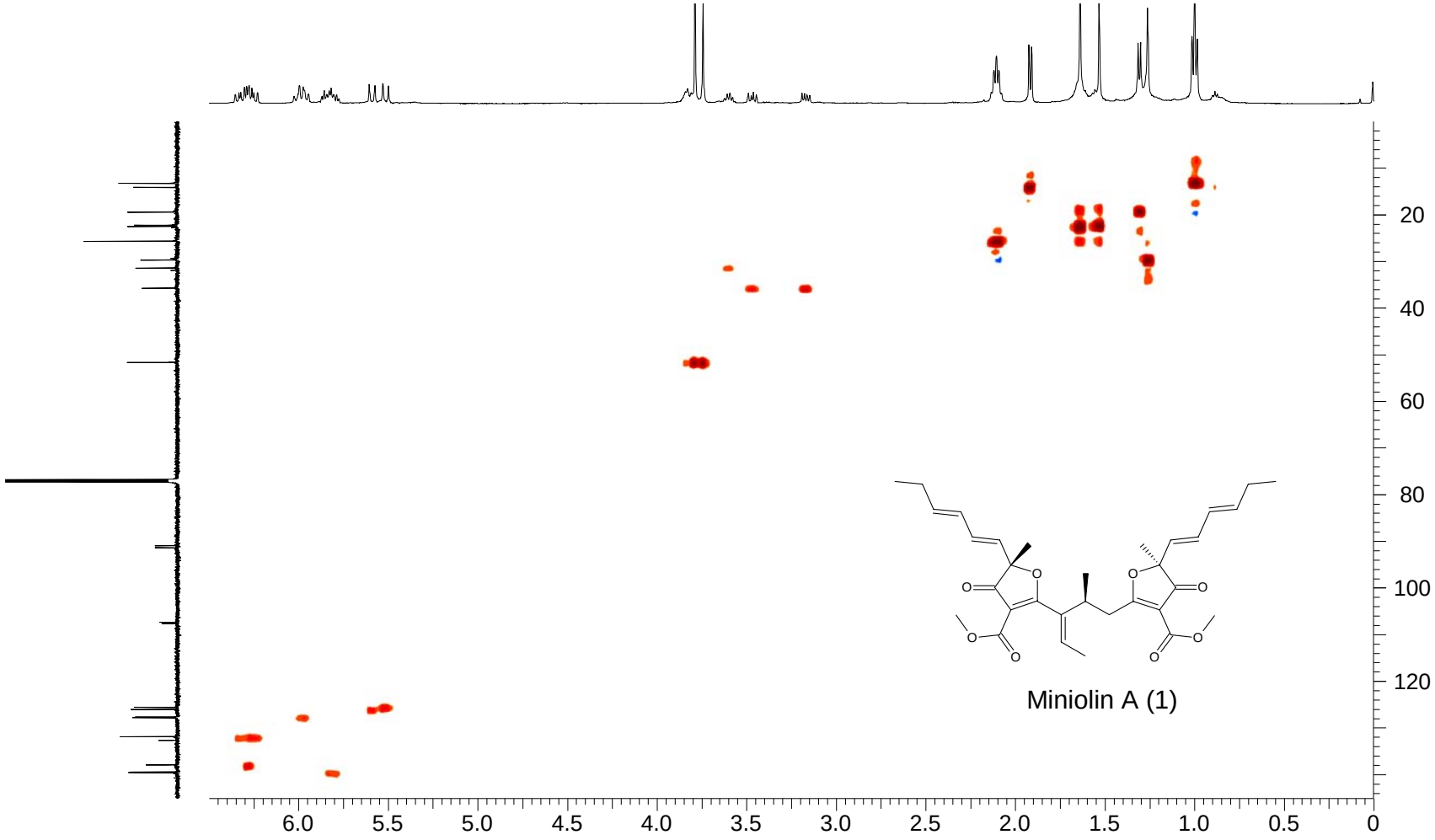


Figure S6. ^{1}H-^{1}H COSY spectrum of 1

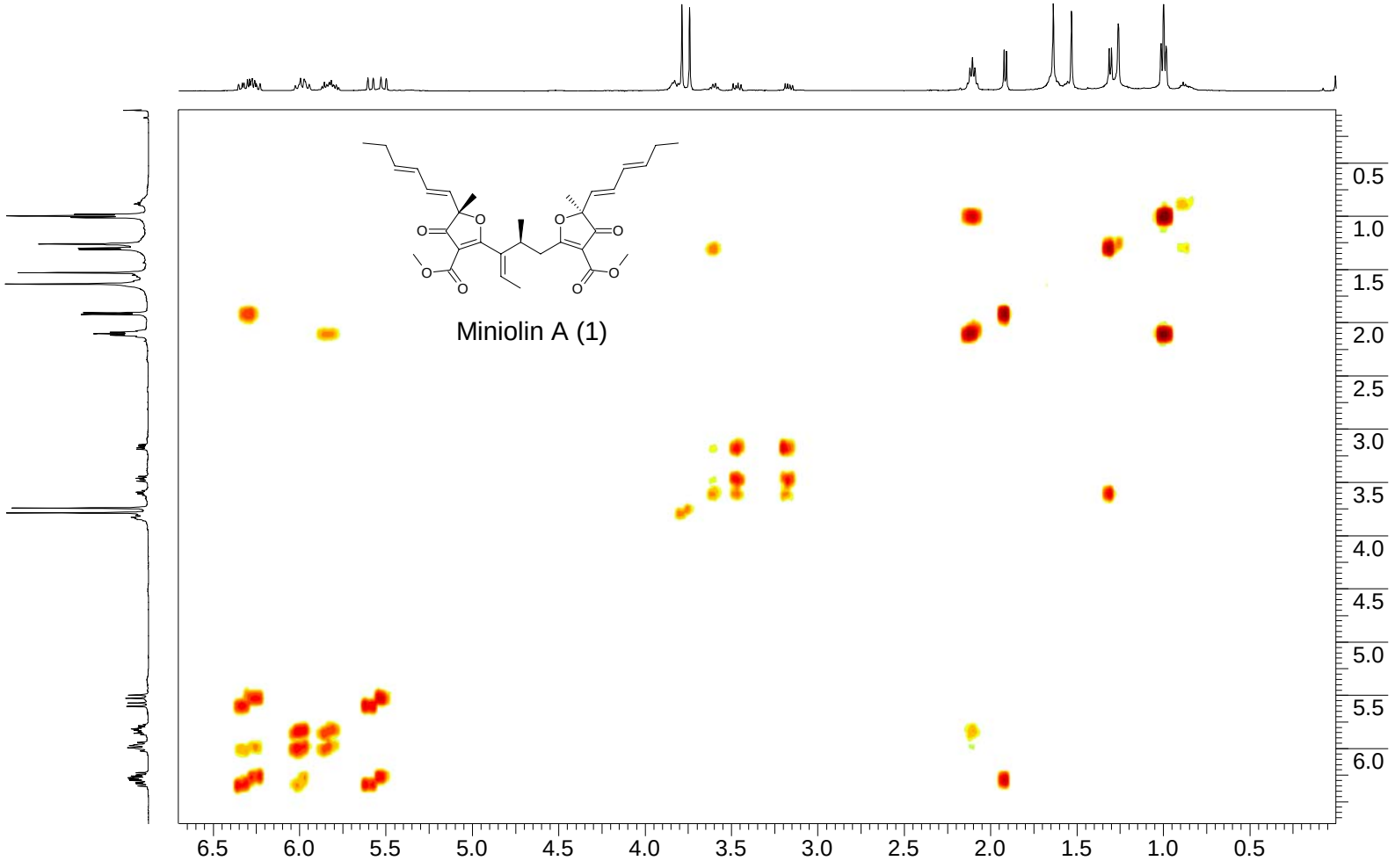
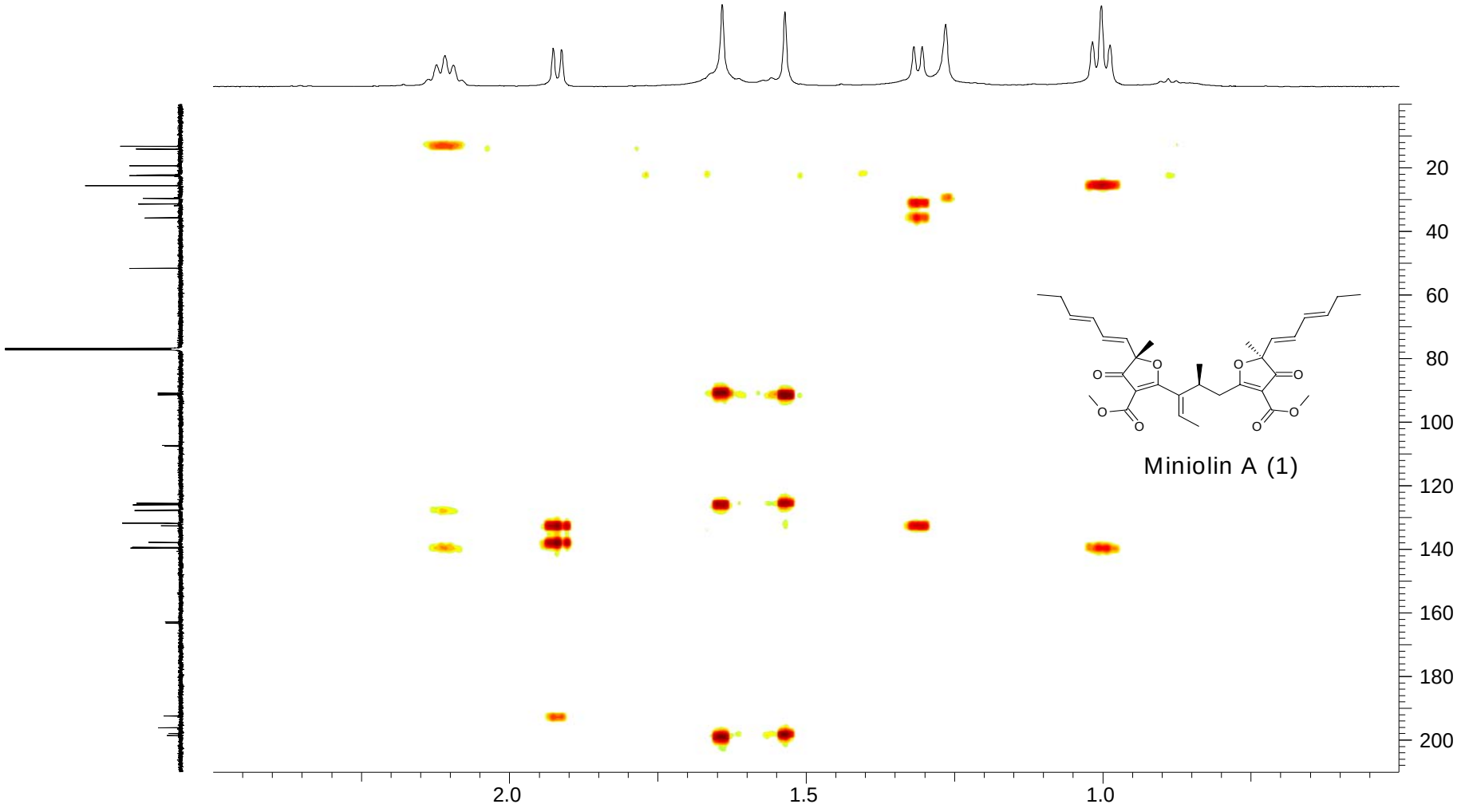
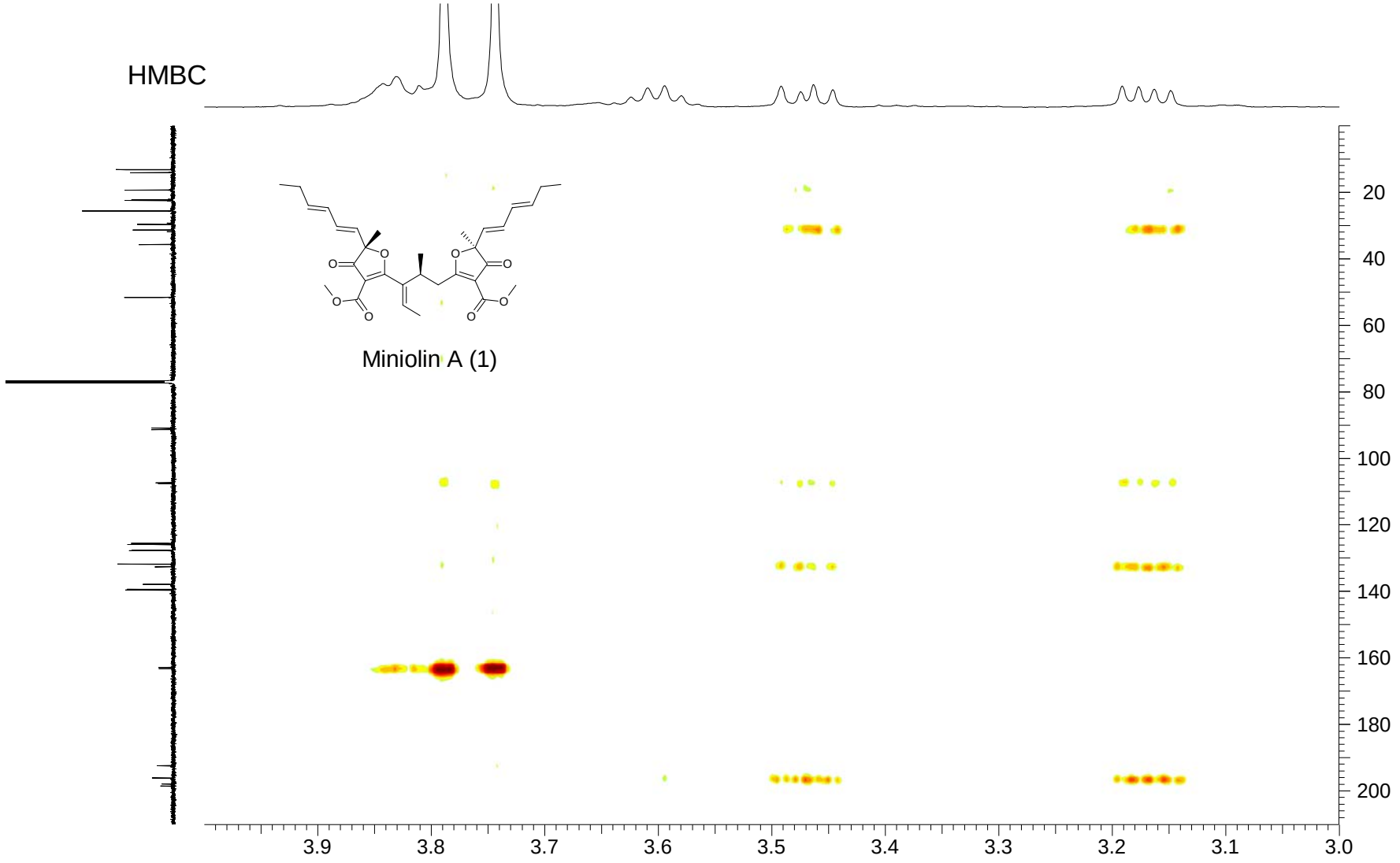


Figure S7. HMBC spectrum of 1

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40
60
80
100
120
140
160
180
200
3.9
3.8
3.7
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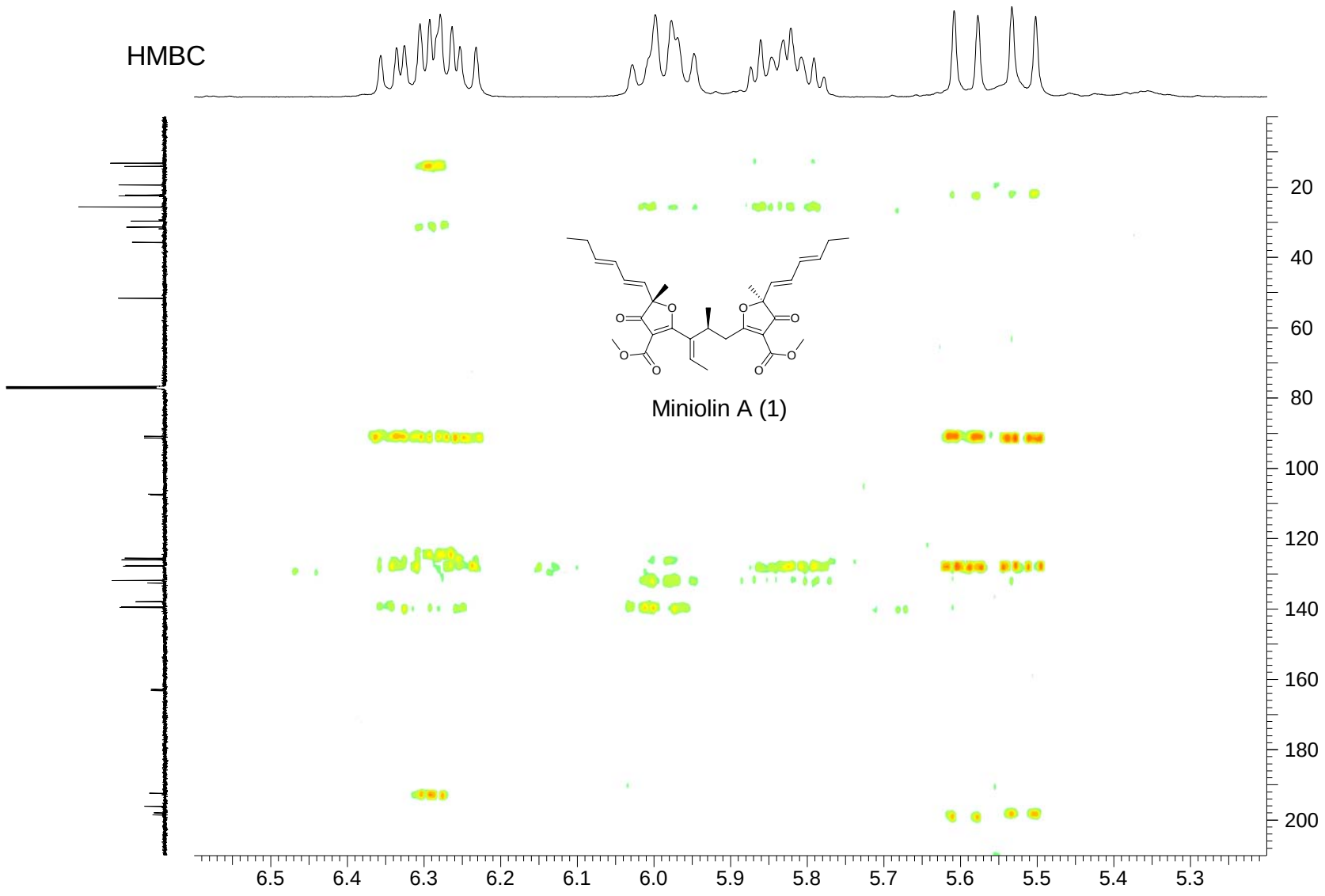
3.5
3.4
3.3
3.2
3.1
3.0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Miniolin A (1)
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40
60
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100
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180
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6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3

Figure S8. NOESY spectrum of 1

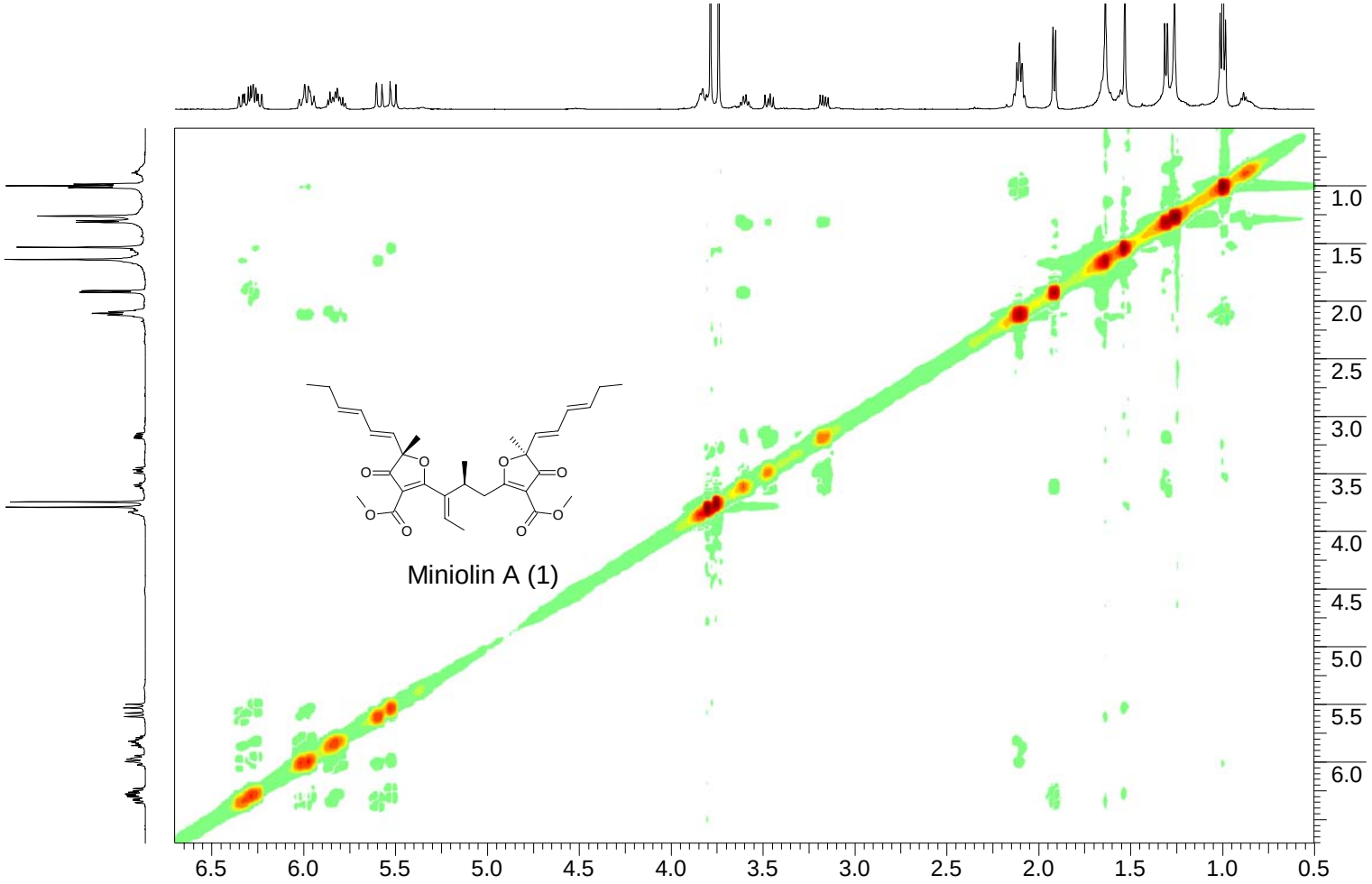


Figure S9. Positive ESIMS spectrum of 1

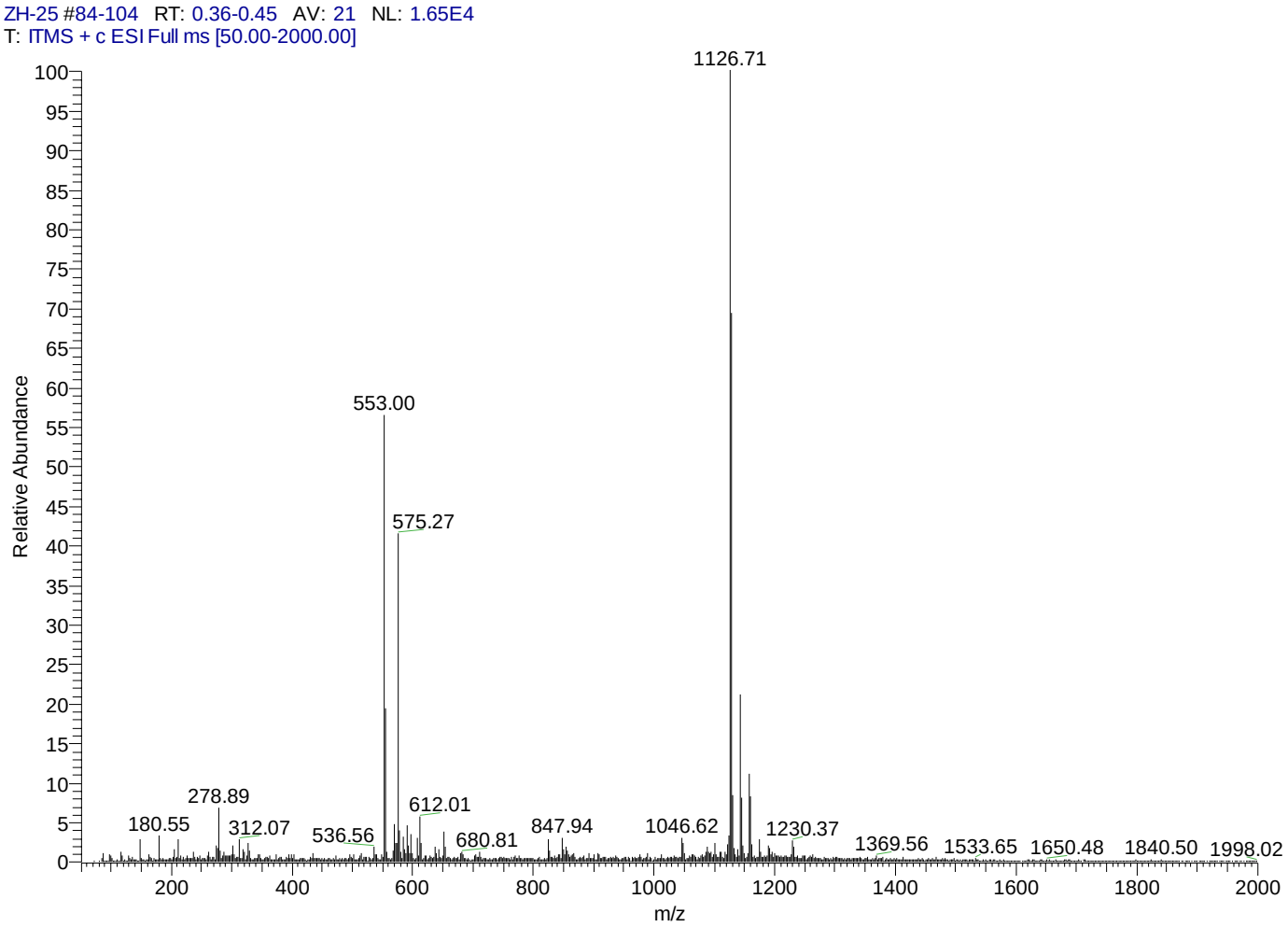
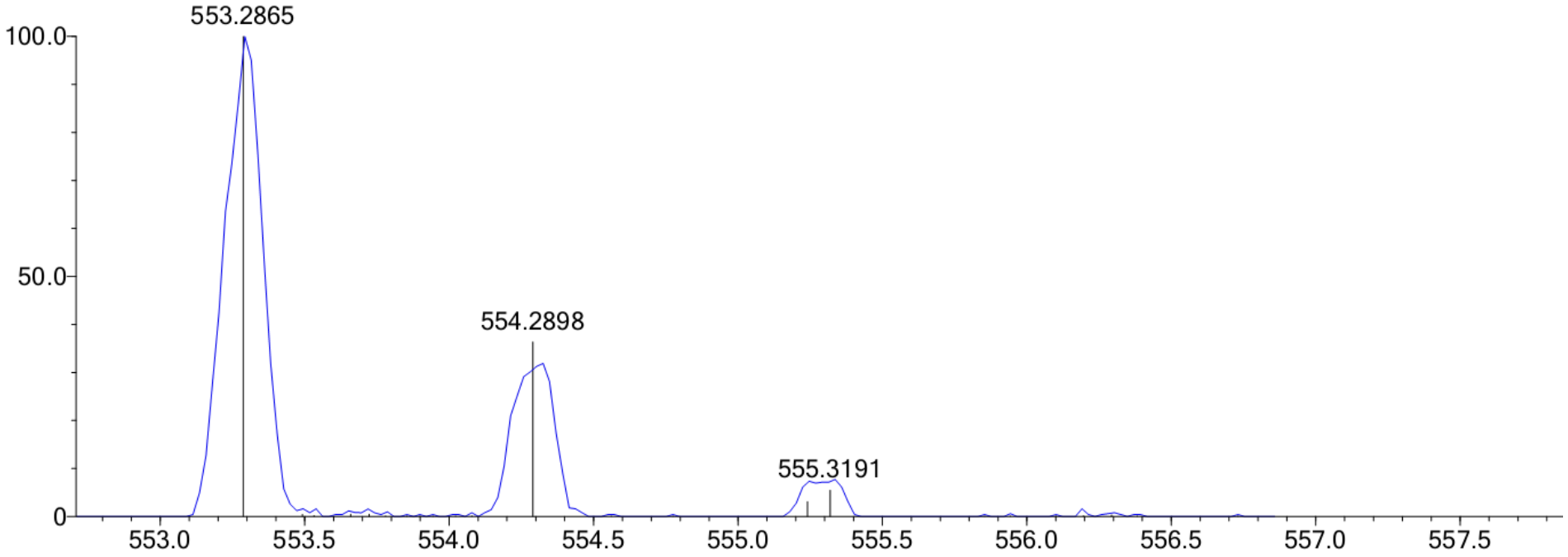


Figure S10. HR ESIMS spectrum of 1



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	16.12	[M+H]+	C32 H40 O8	553.2796	553.2865	6.9	12.47	48.26	13.0

Figure S11. IR spectrum of 1

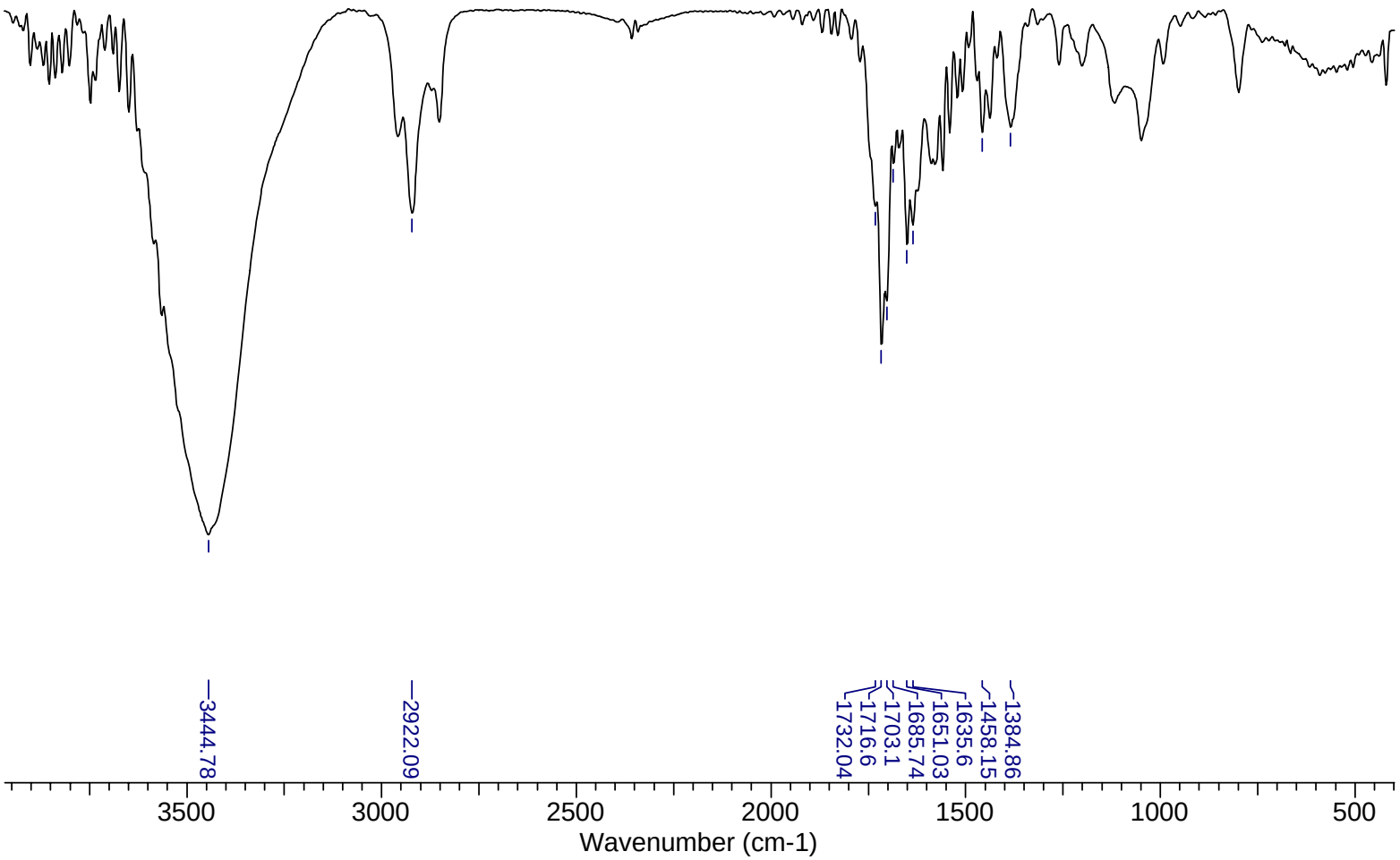


Figure S12. UV and CD spectra of 1

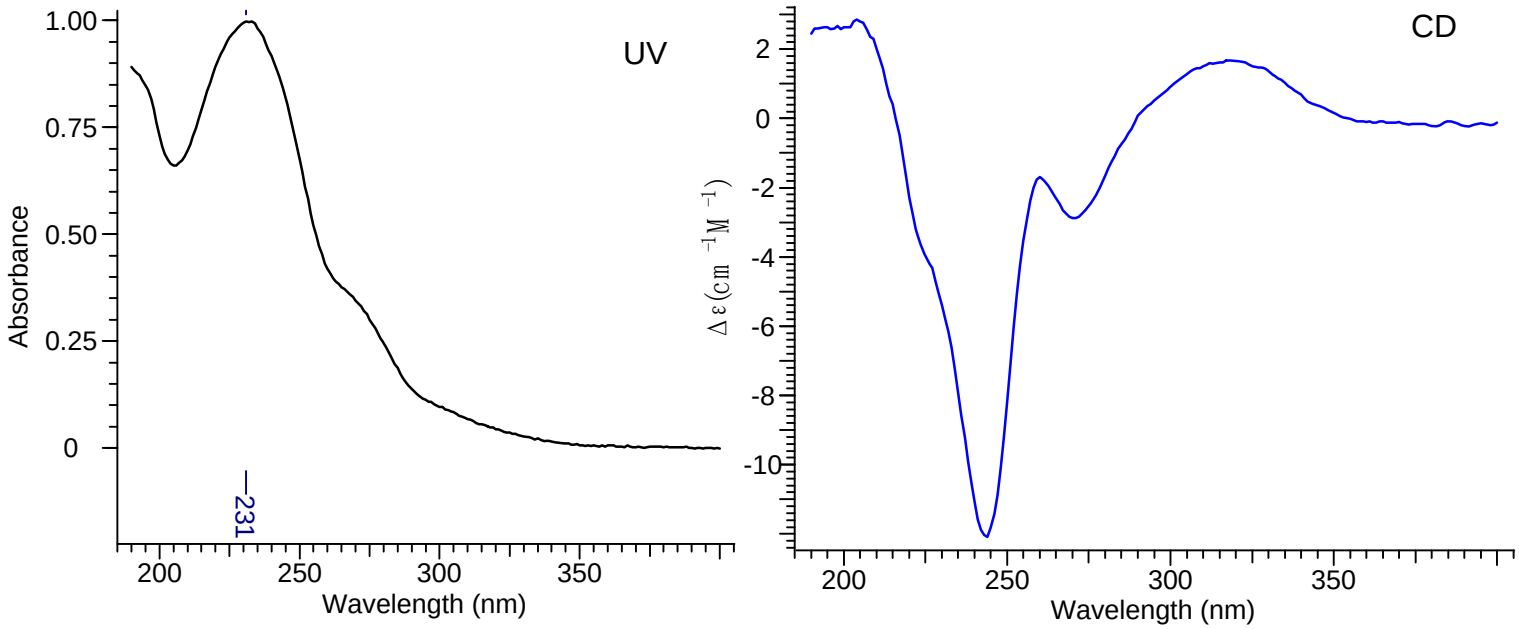


Figure S13. ^{1}**H NMR spectrum of 2 in** $CDCl_3$ **(500 MHz)**

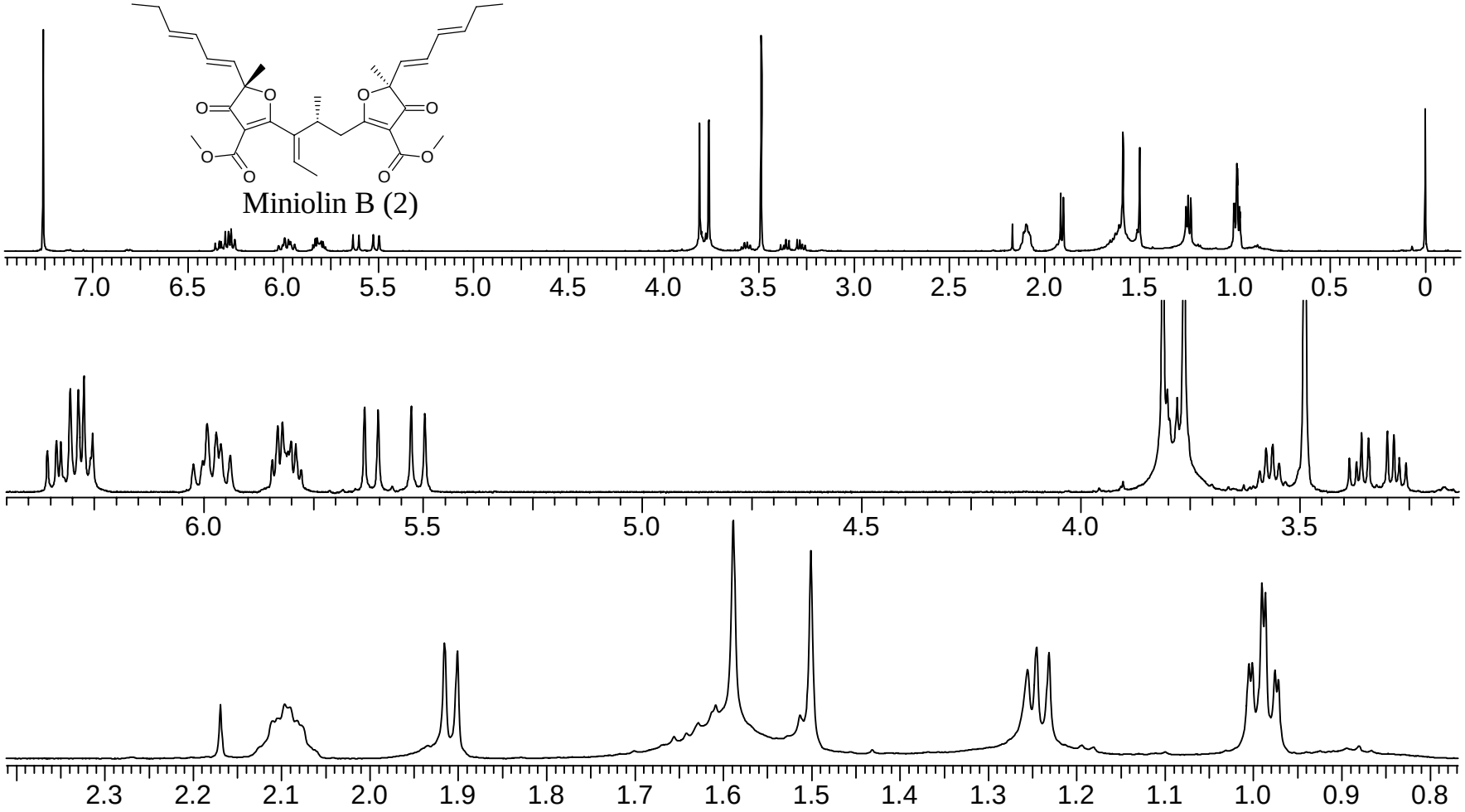


Figure S14. ^{13}C NMR and DEPT of 2 in $CDCl_3$ (125 MHz)

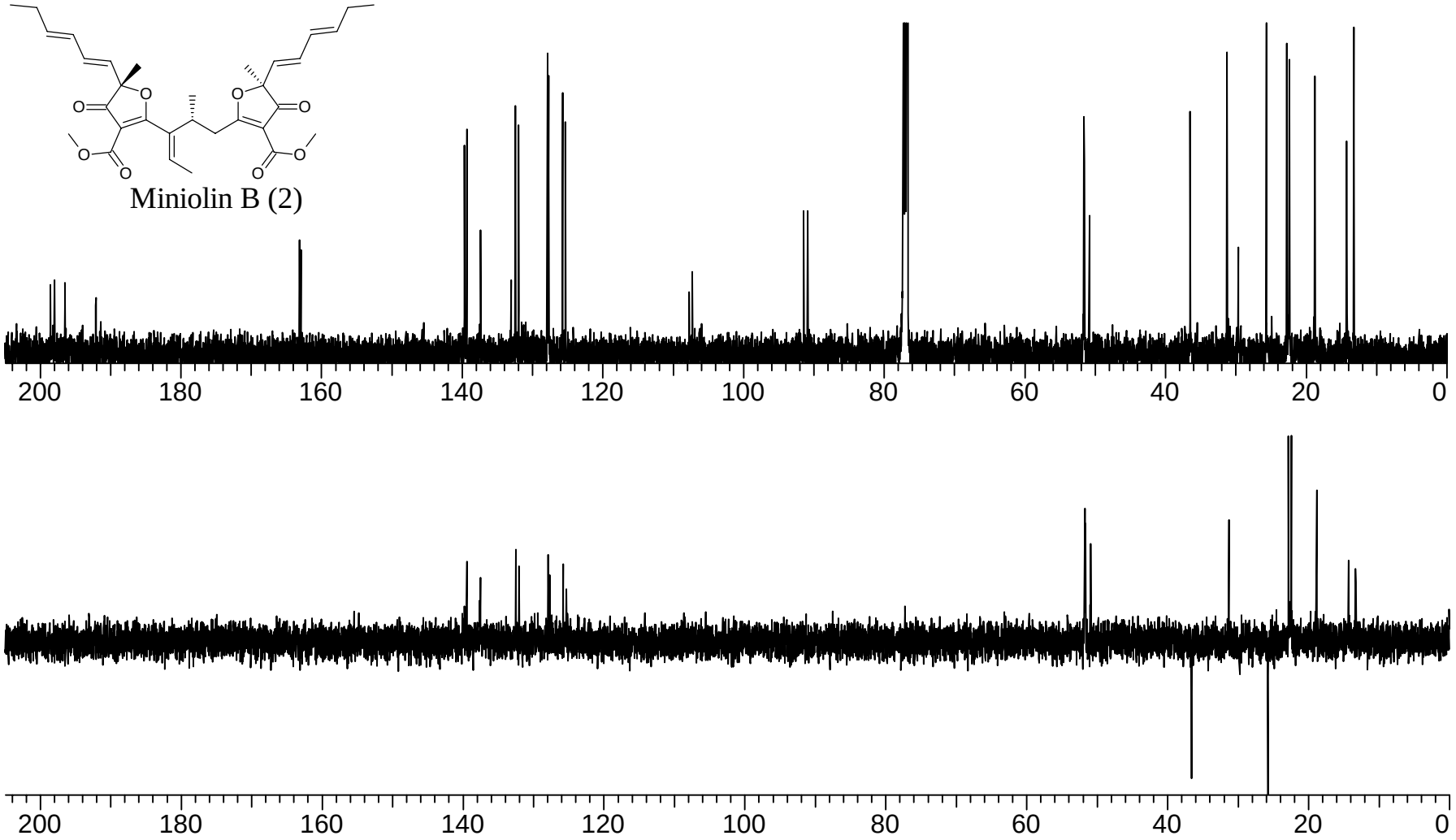


Figure S15. HSQC spectrum of 2

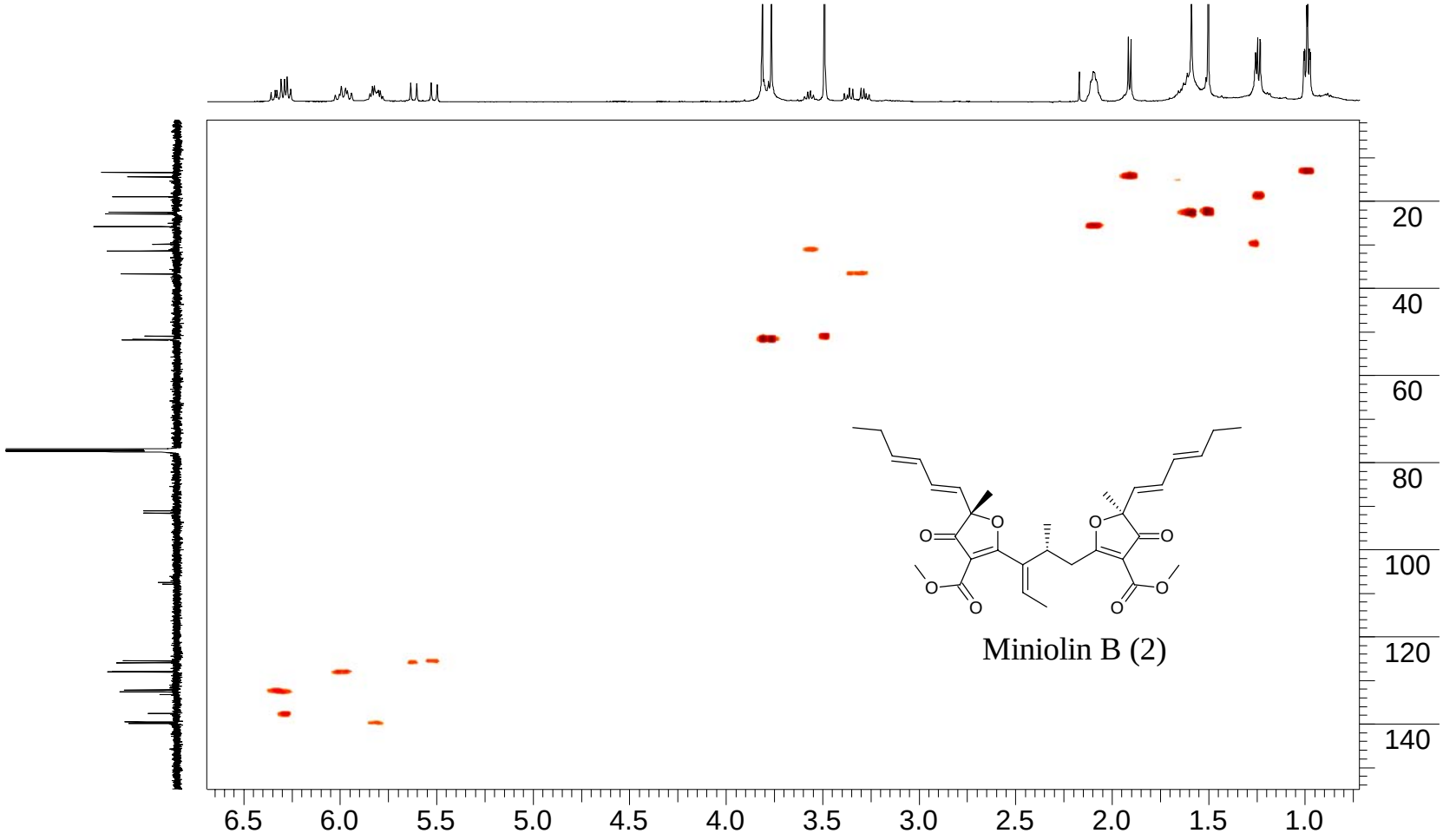


Figure S16. ^{1}H-^{1}H COSY spectrum of 2

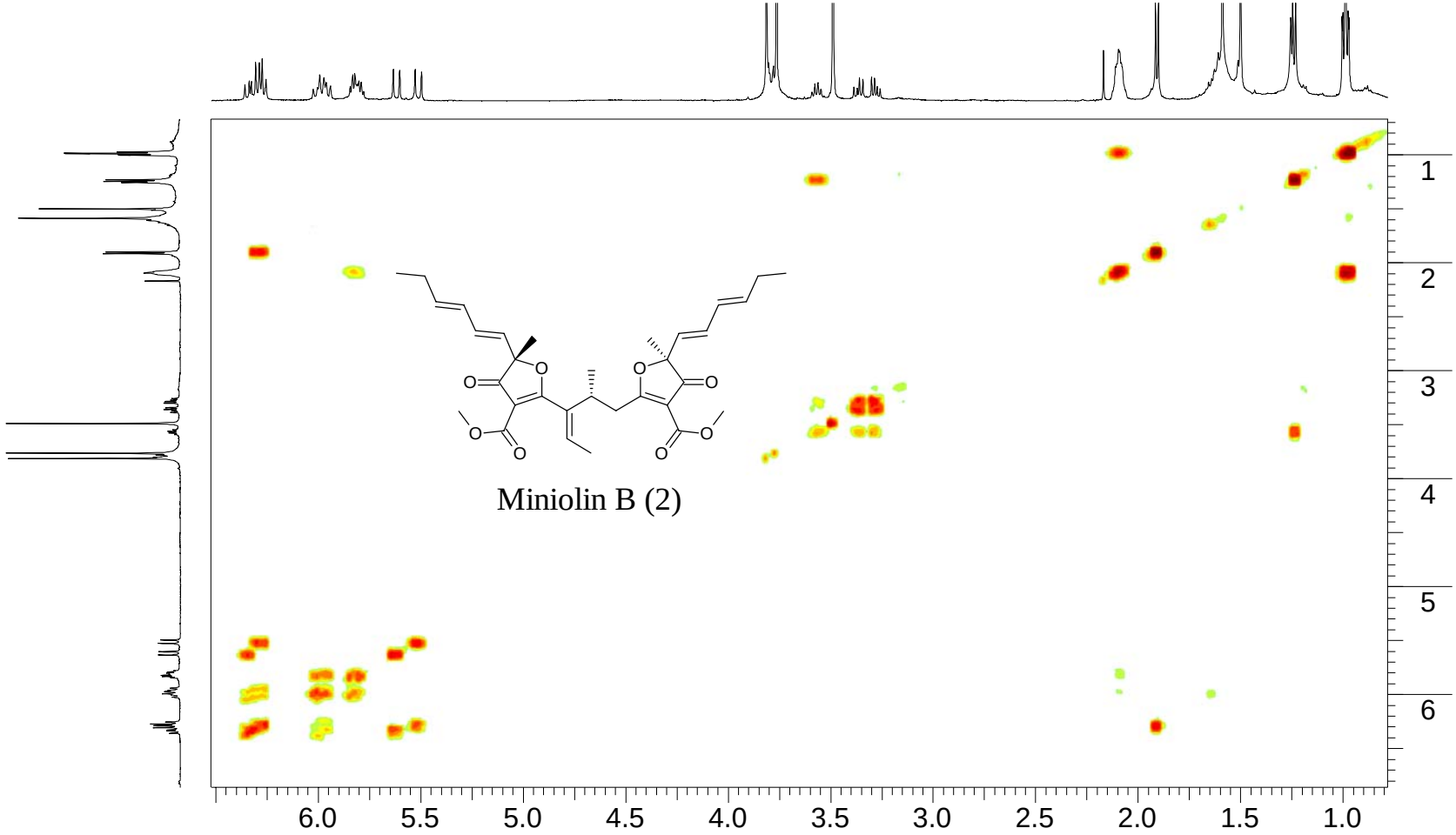
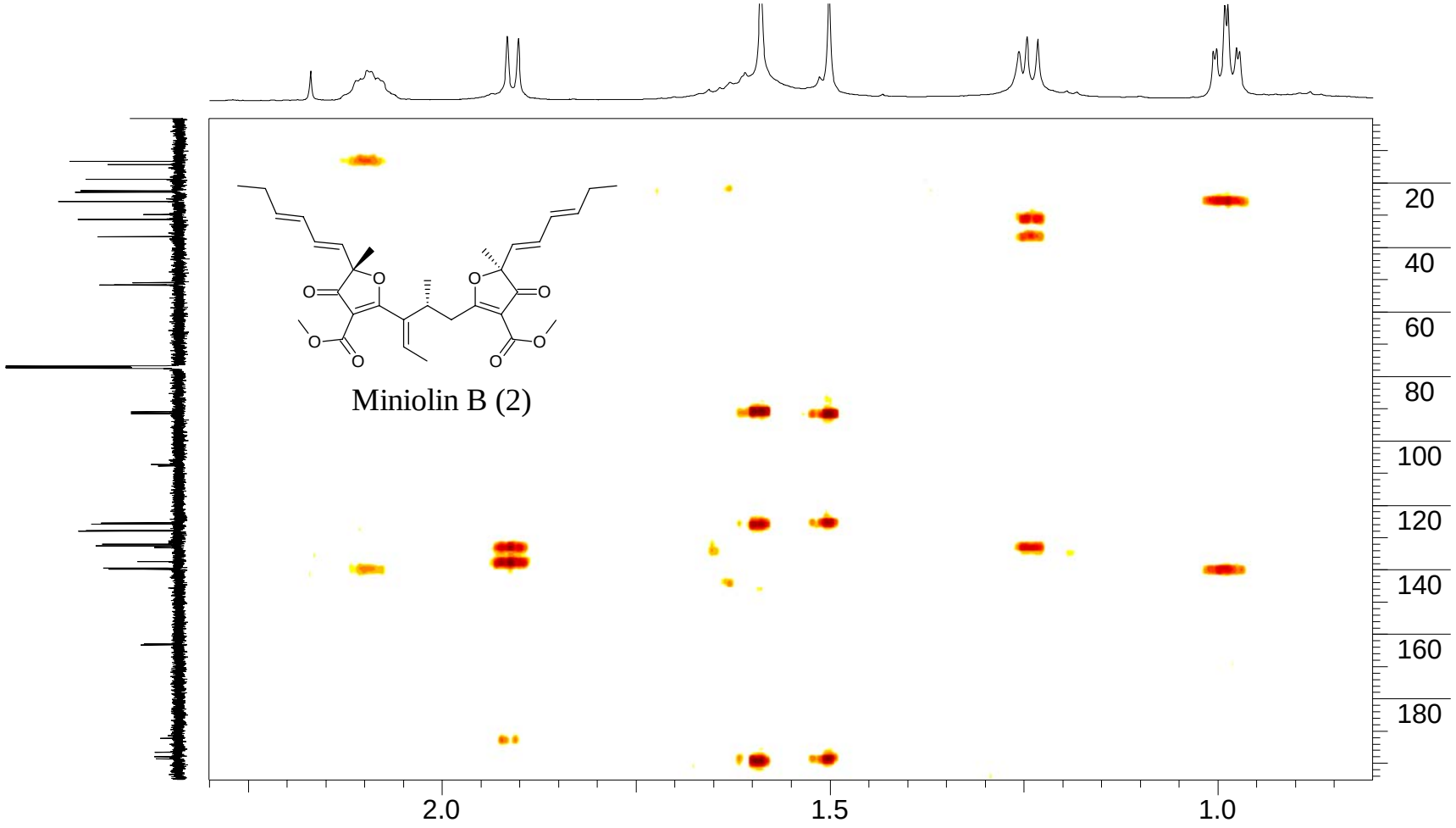
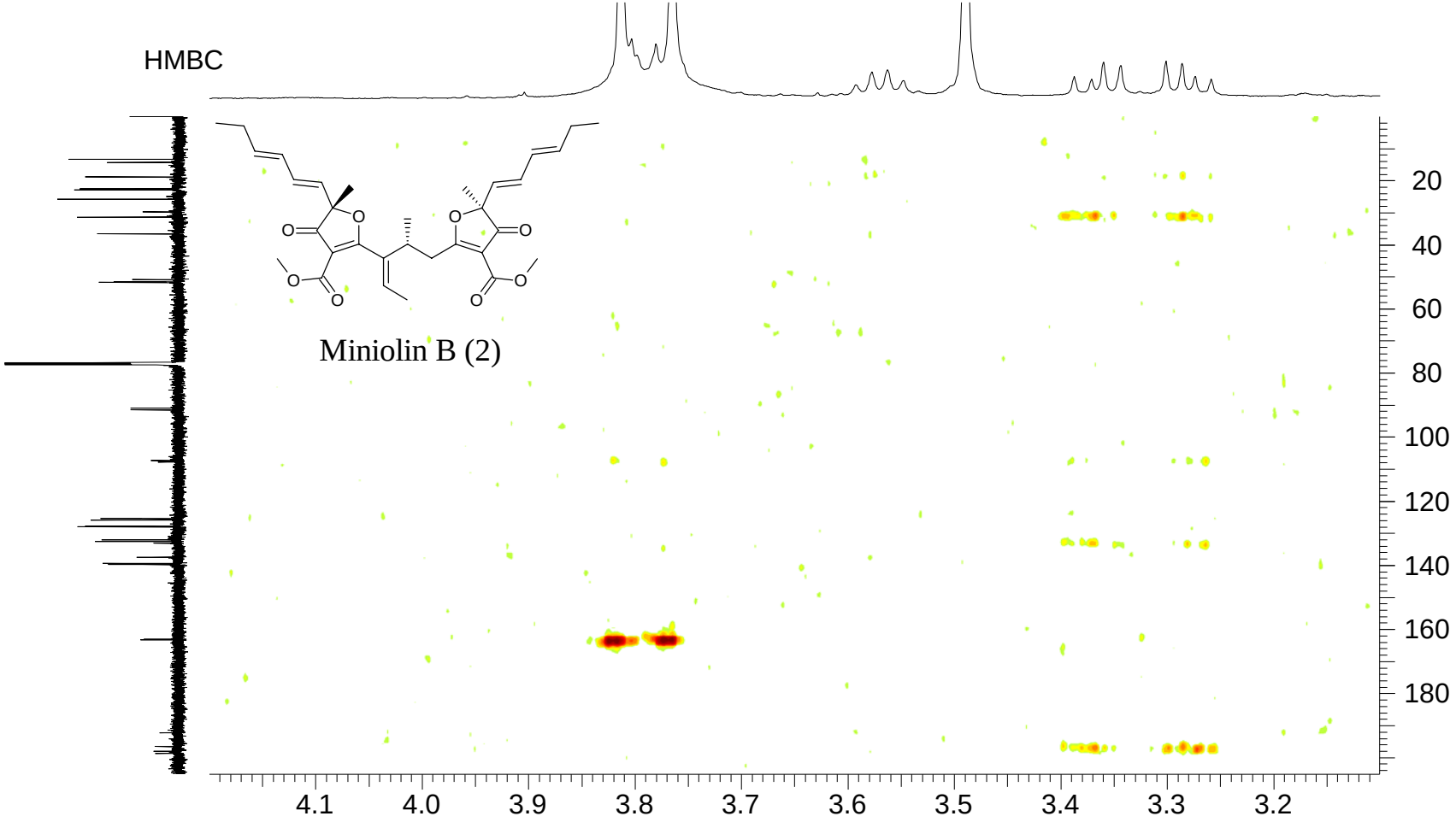


Figure S17. HMBC spectrum of 2

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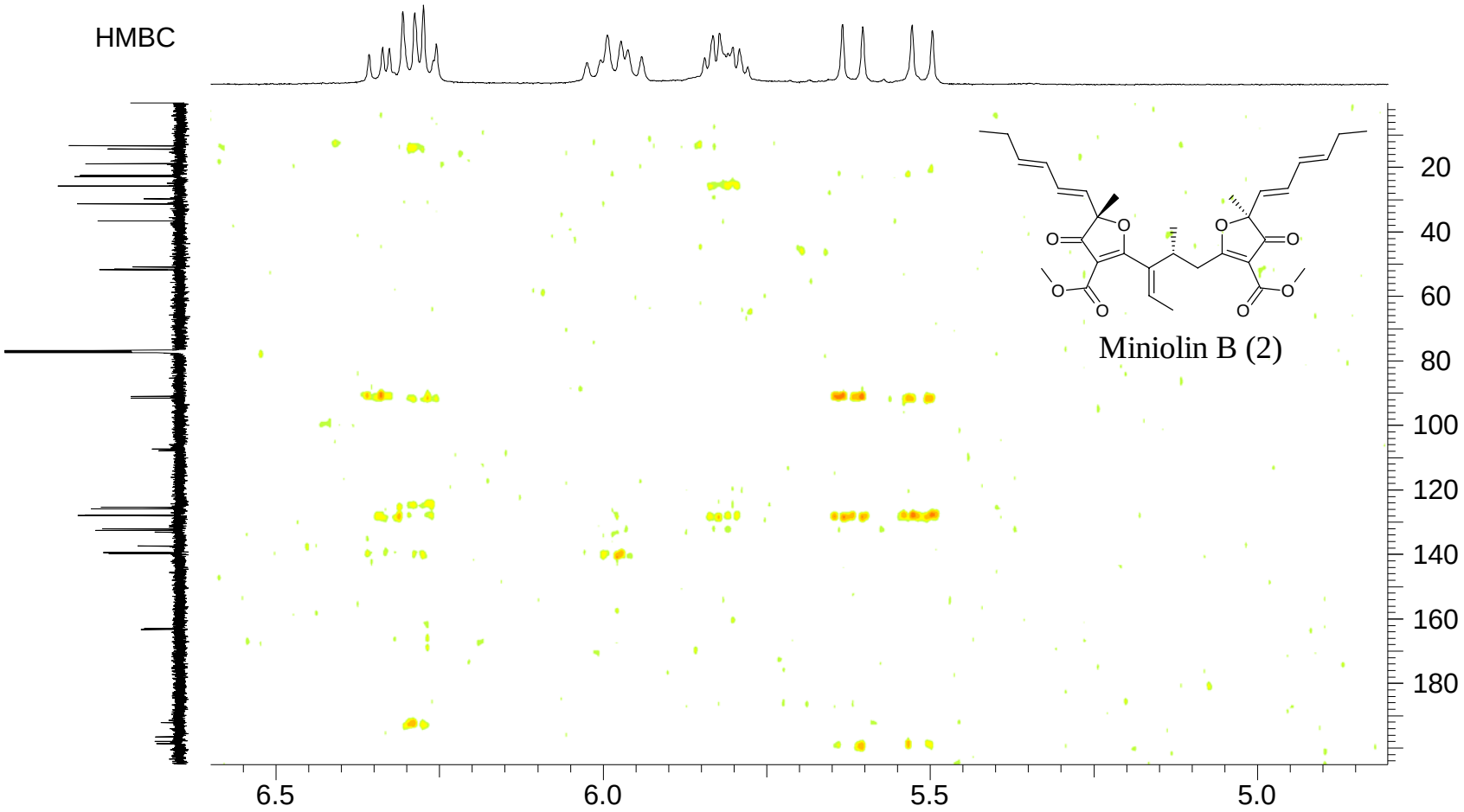
Miniolin B (2)
20
40
60
80
100
120
140
160
180
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2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Miniolin B (2)
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100
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140
160
180
6.5
6.0
5.5
5.0

Figure S18. NOESY spectrum of 2

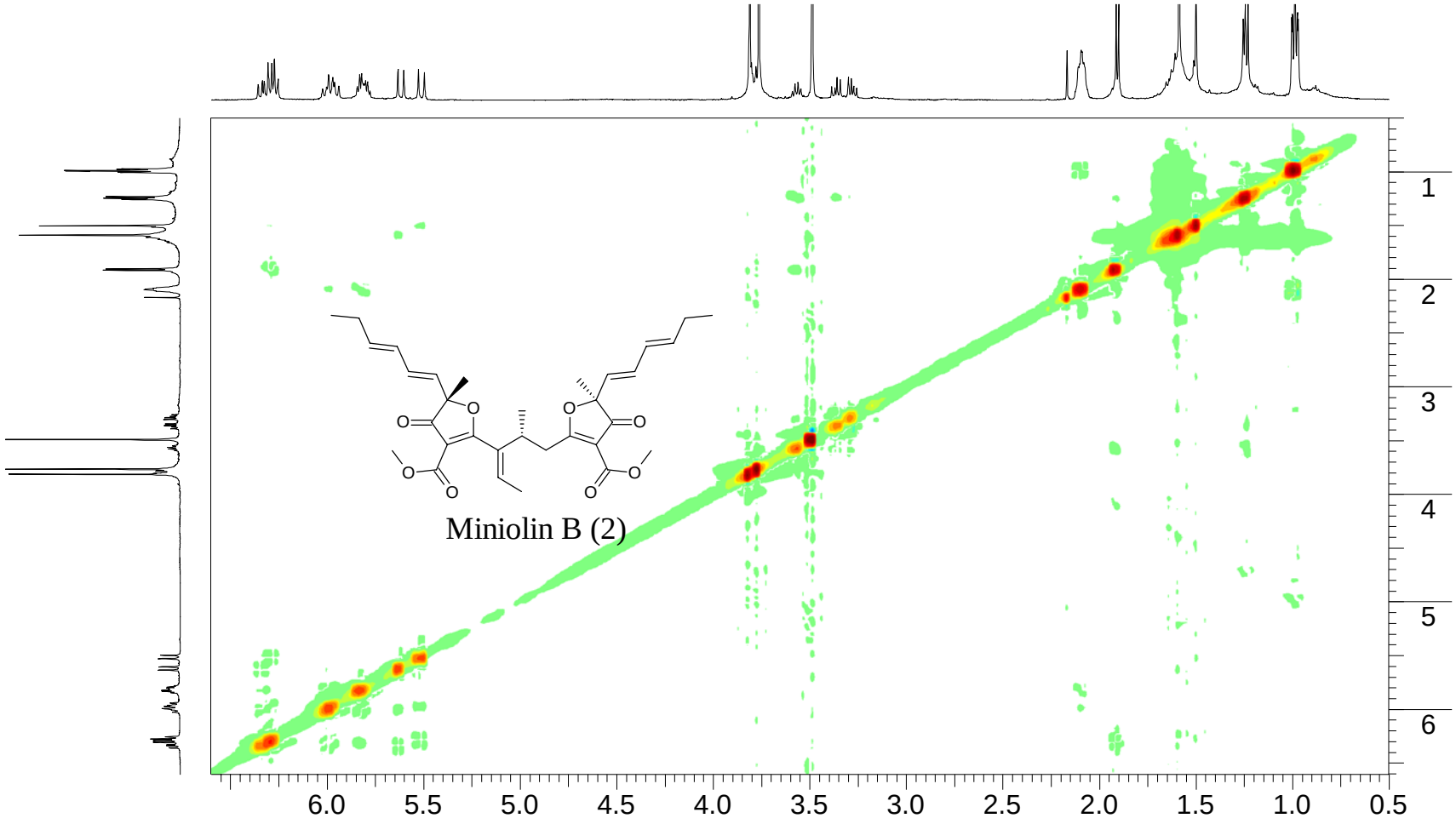


Figure S19. Positive ESIMS spectrum of 2

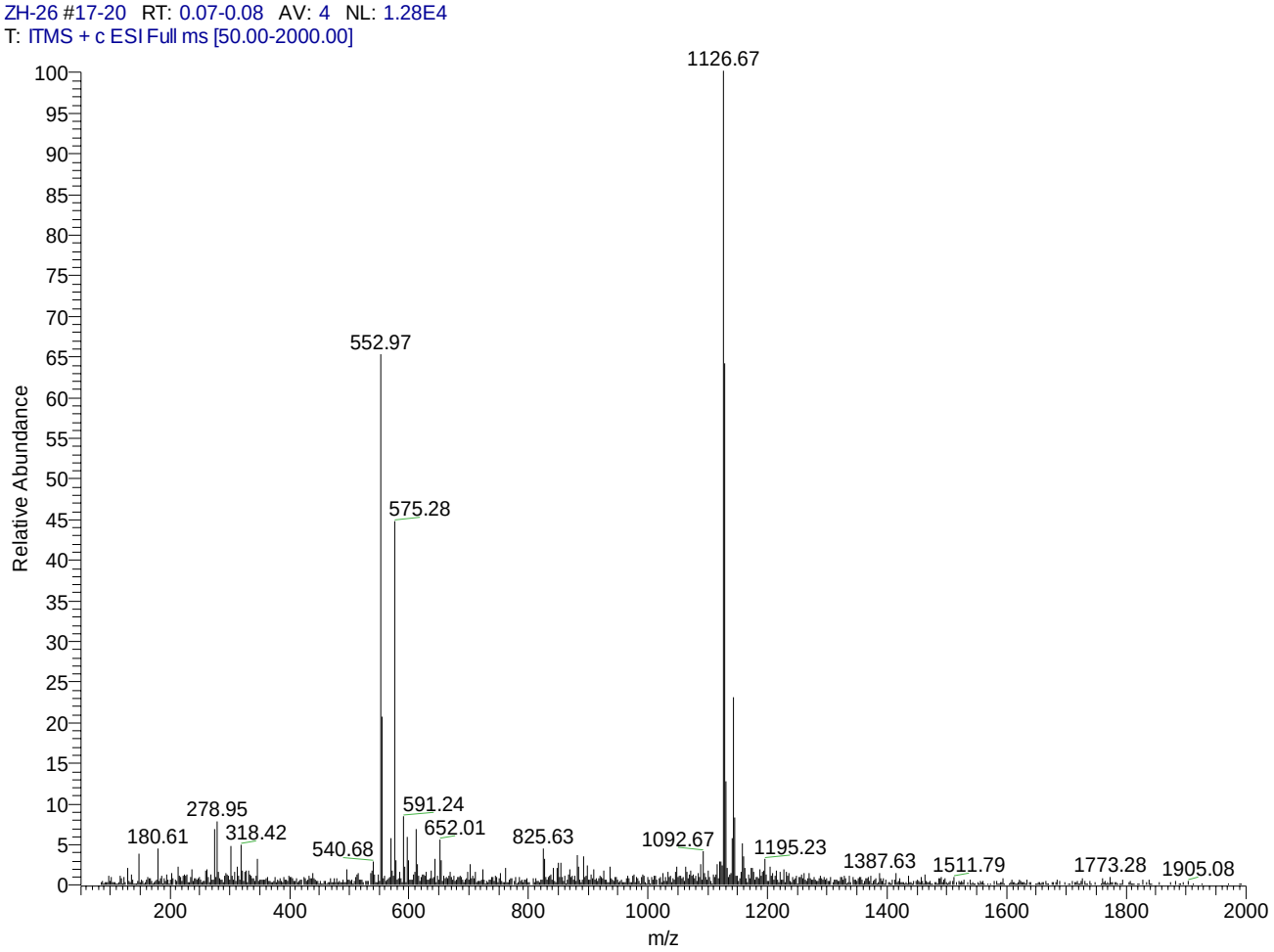
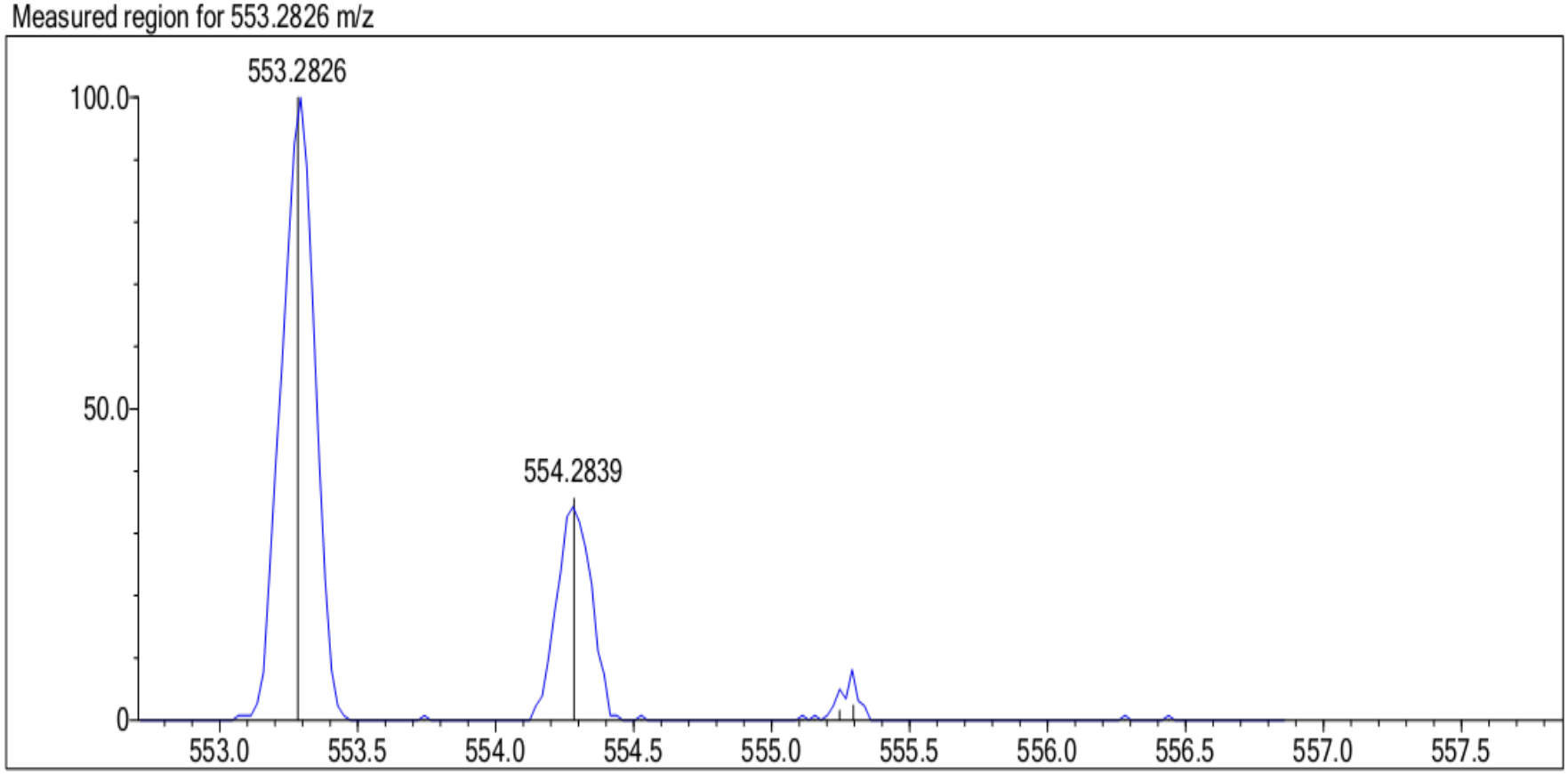


Figure S20. HR ESIMS spectrum of 2



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.32	[M+H]+	C32 H40 O8	553.2796	553.2826	3.0	5.42	97.11	13.0

Figure S21. IR spectrum of 2

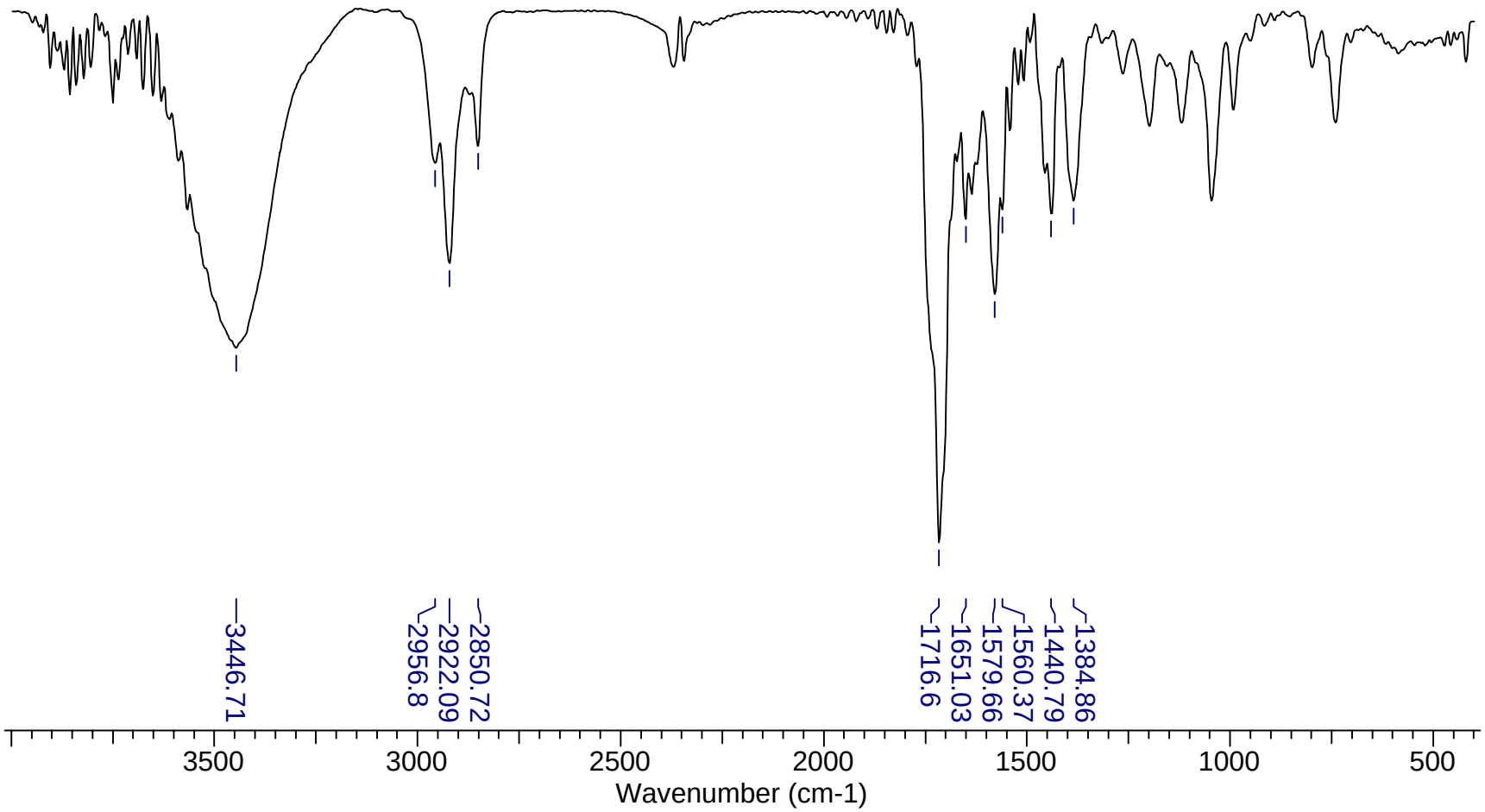


Figure S22. UV and CD spectra of 2

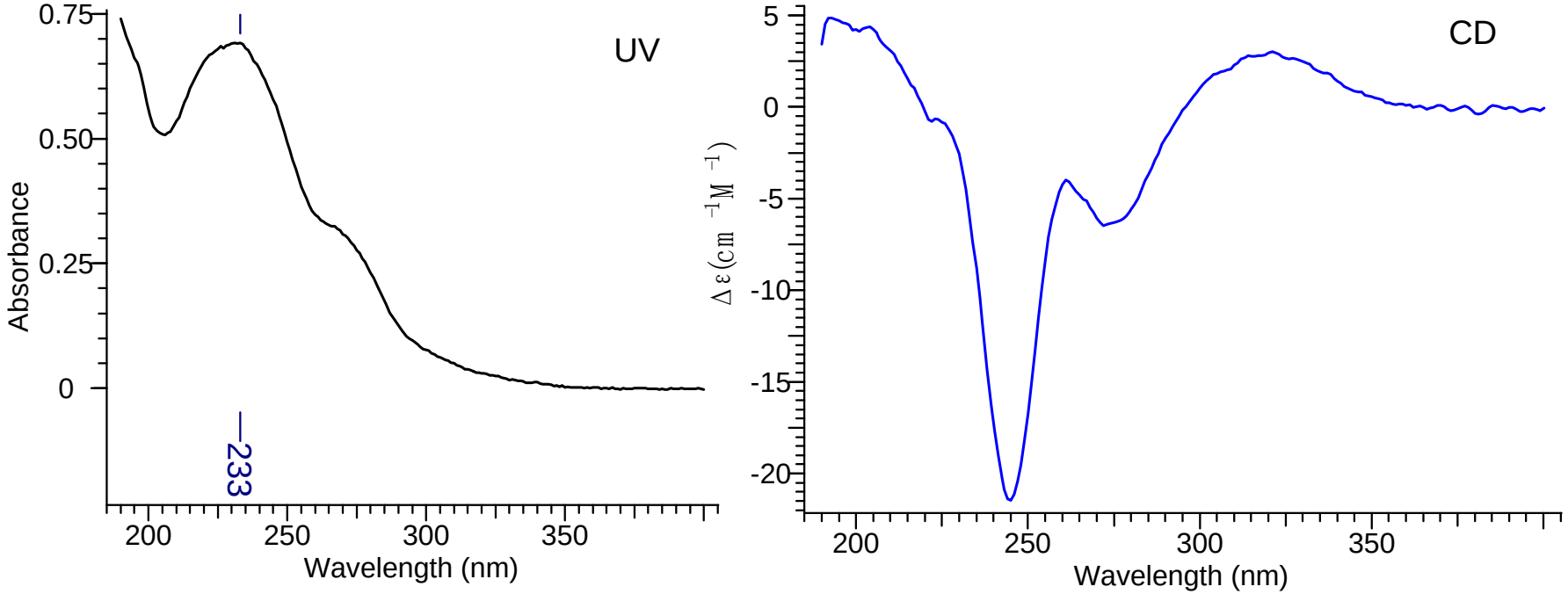


Figure S23. ^{1}**H NMR spectrum of 3 in** $CDCl_3$ **(500 MHz)**

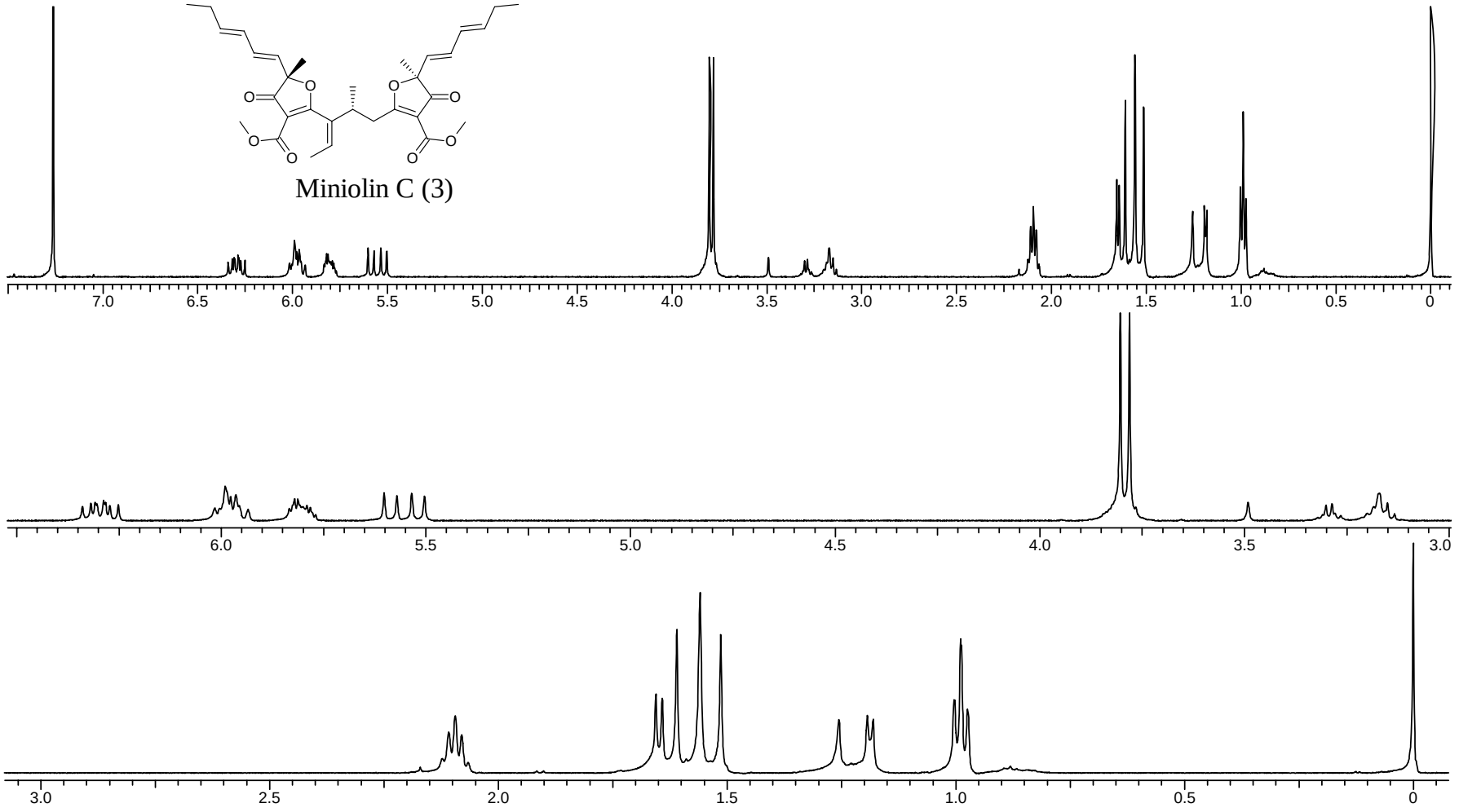


Figure S24. ^{13}C NMR and DEPT spectrum of 3 in $CDCl_3$ (125 MHz)

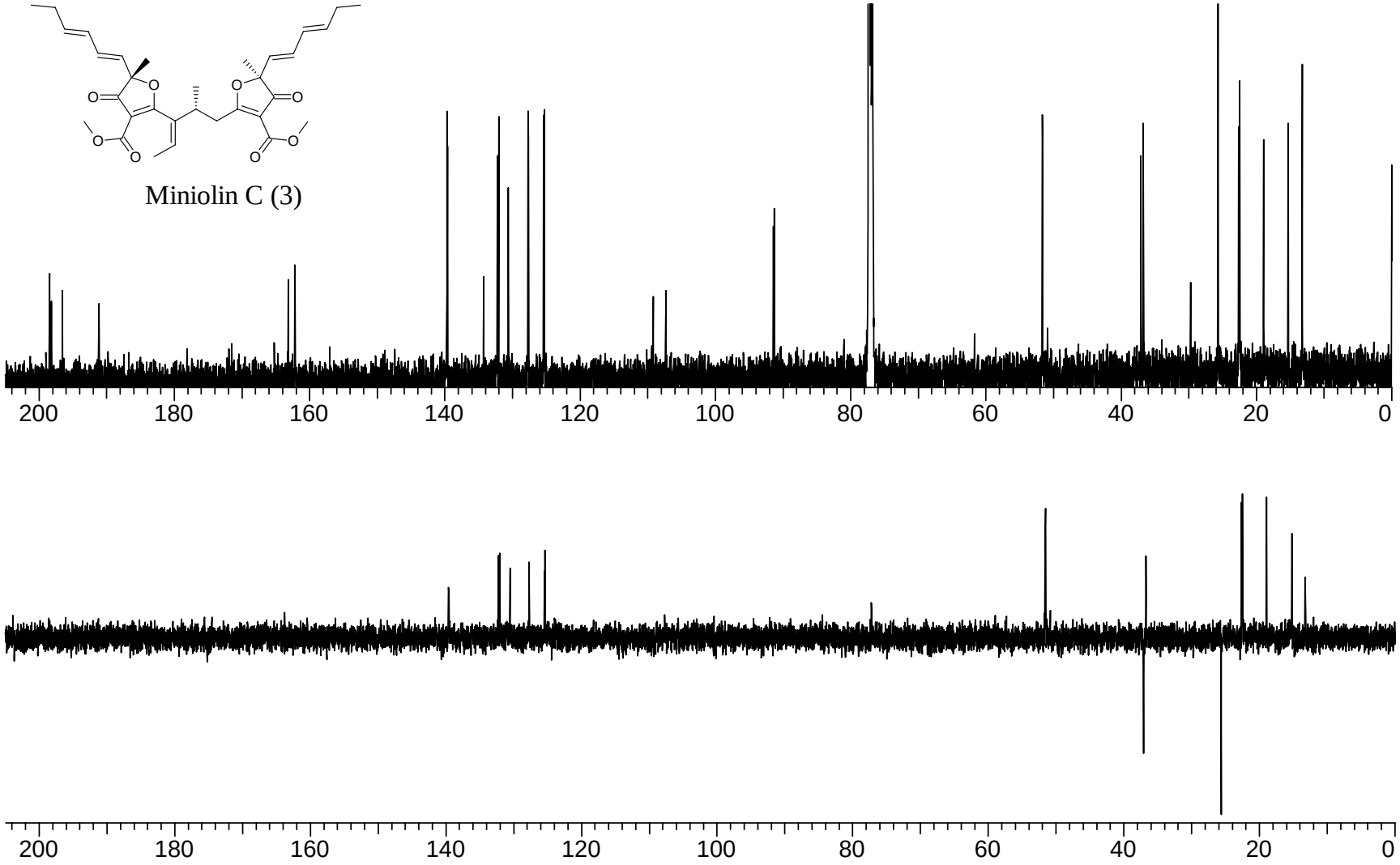


Figure S25. HSQC spectrum of 3

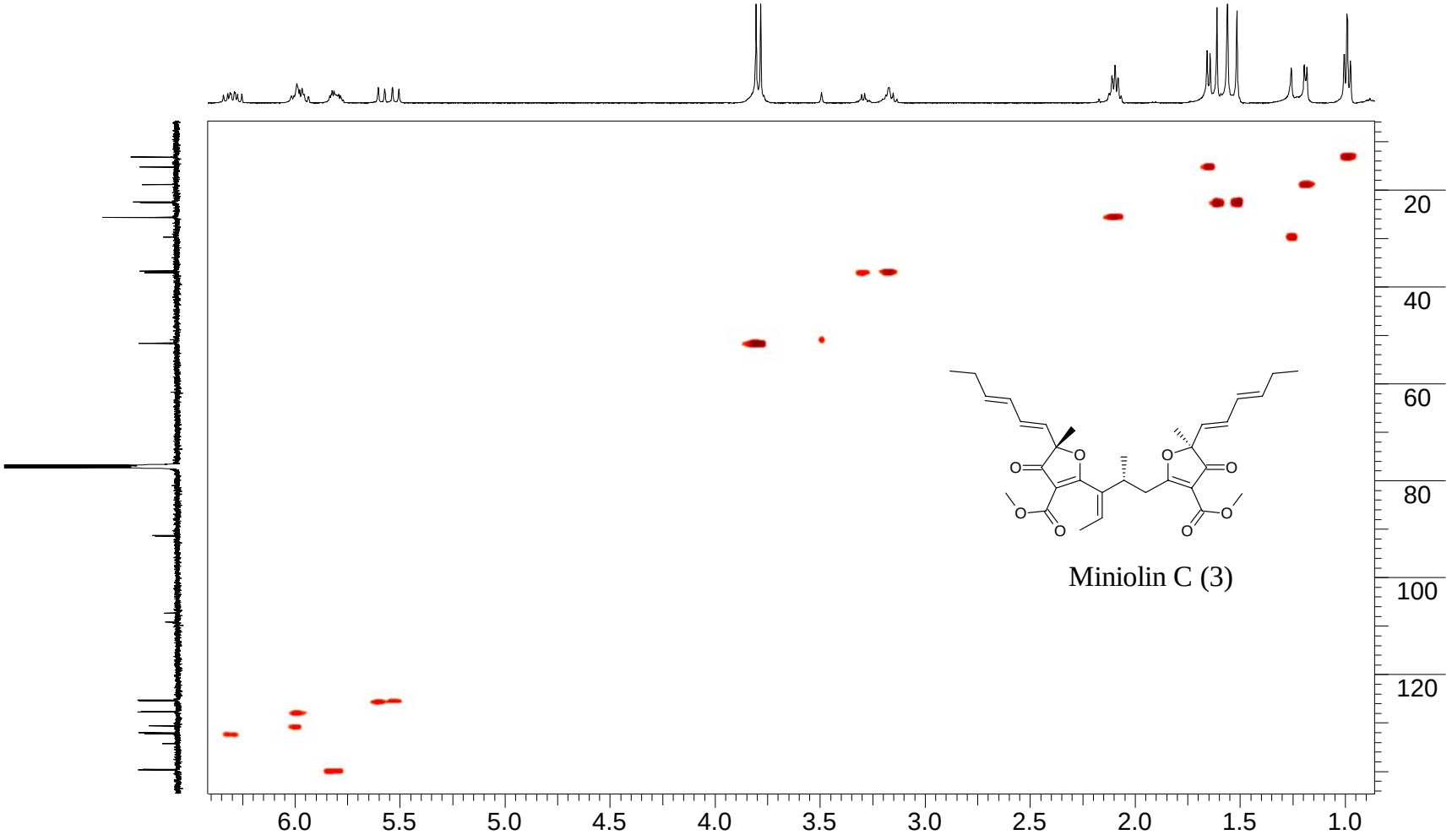


Figure S26. ^{1}H-^{1}H COSY spectrum of 3

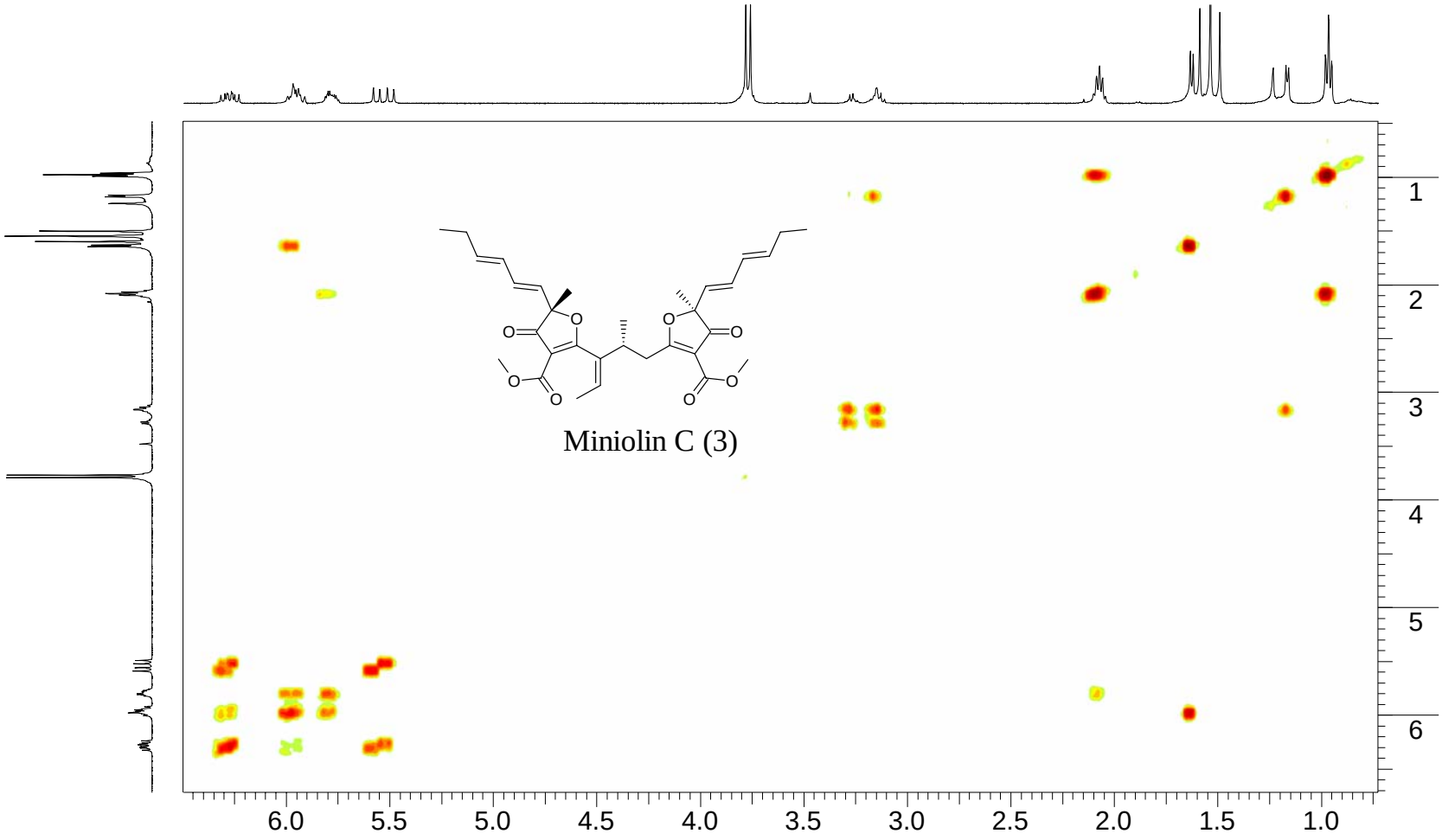
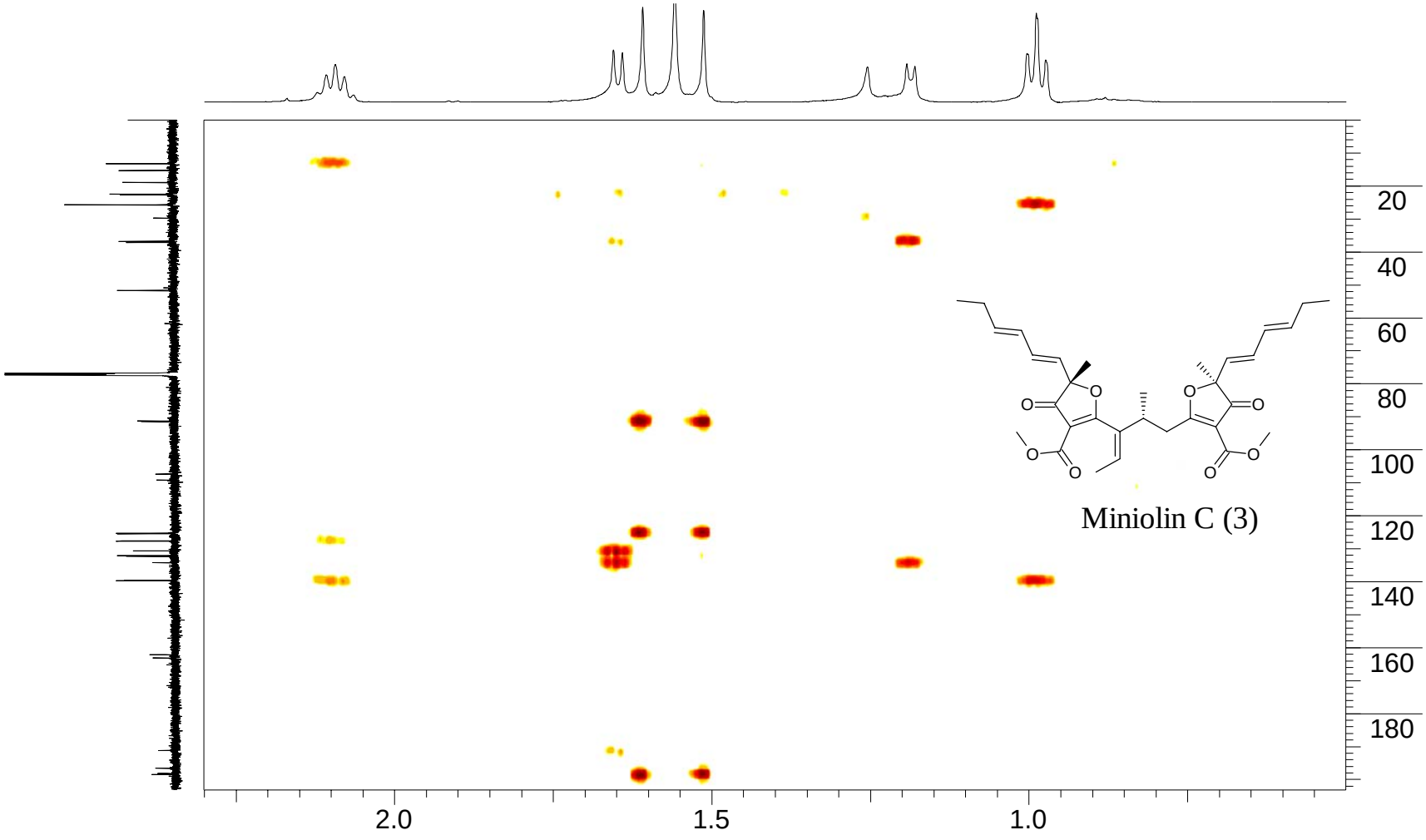
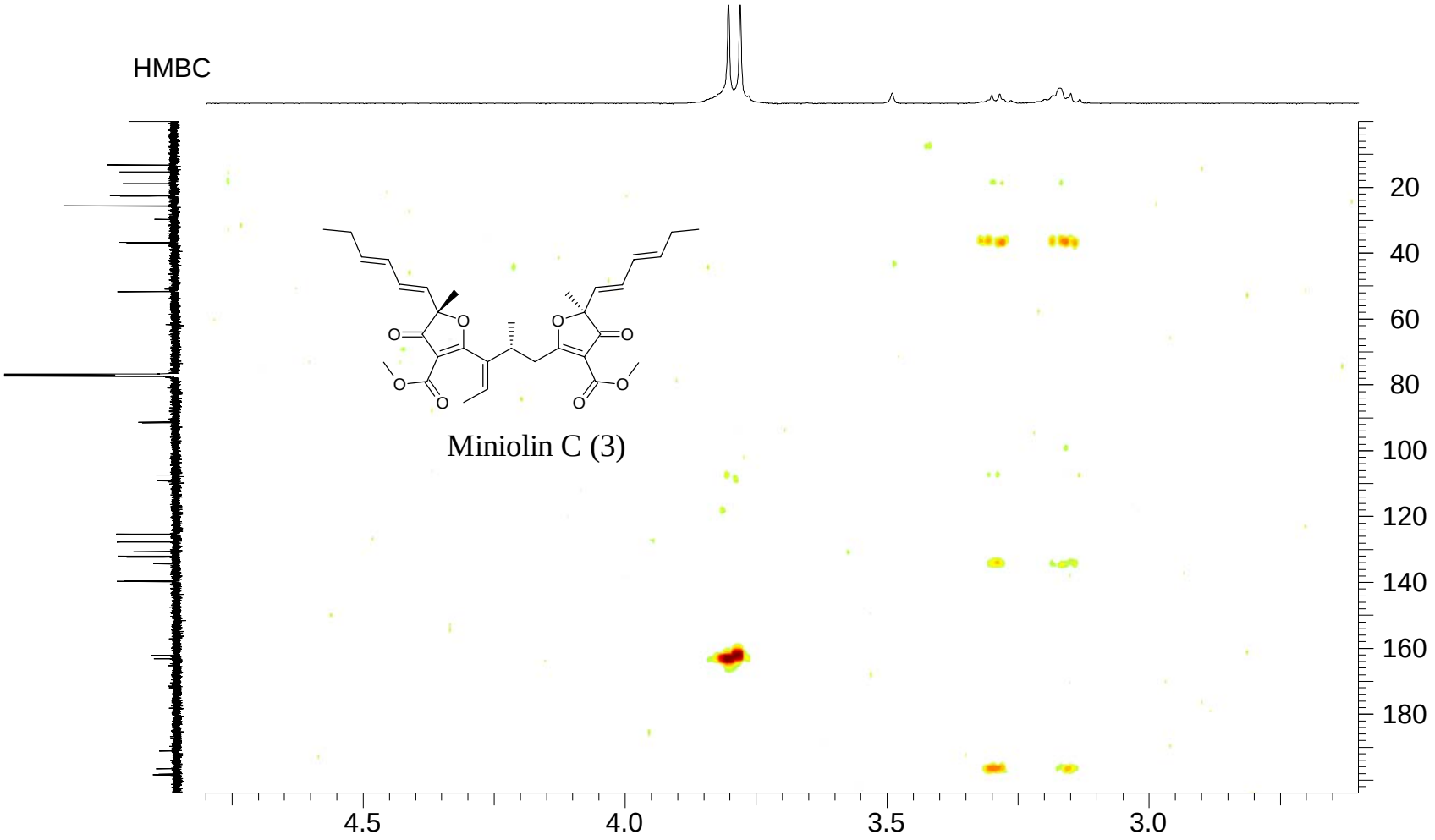


Figure S27. HMBC spectrum of 3

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Miniolin C (3)
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80
100
120
140
160
180
4.5
4.0
3.5
3.0

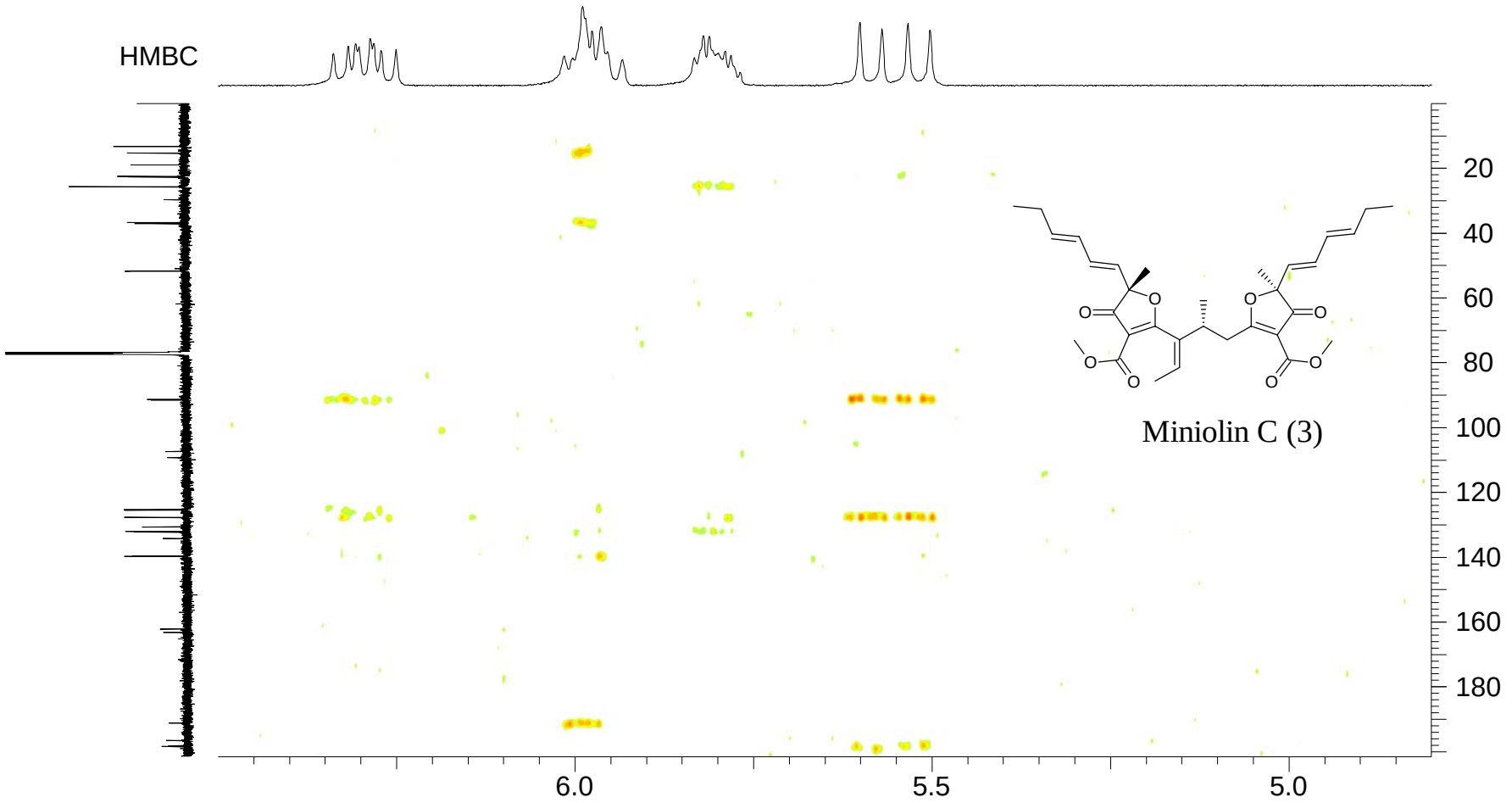

HMBC
20
40
60
80
100
120
140
160
180
6.0
5.5
5.0
Miniolin C (3)

Figure S28. NOESY spectrum of 3

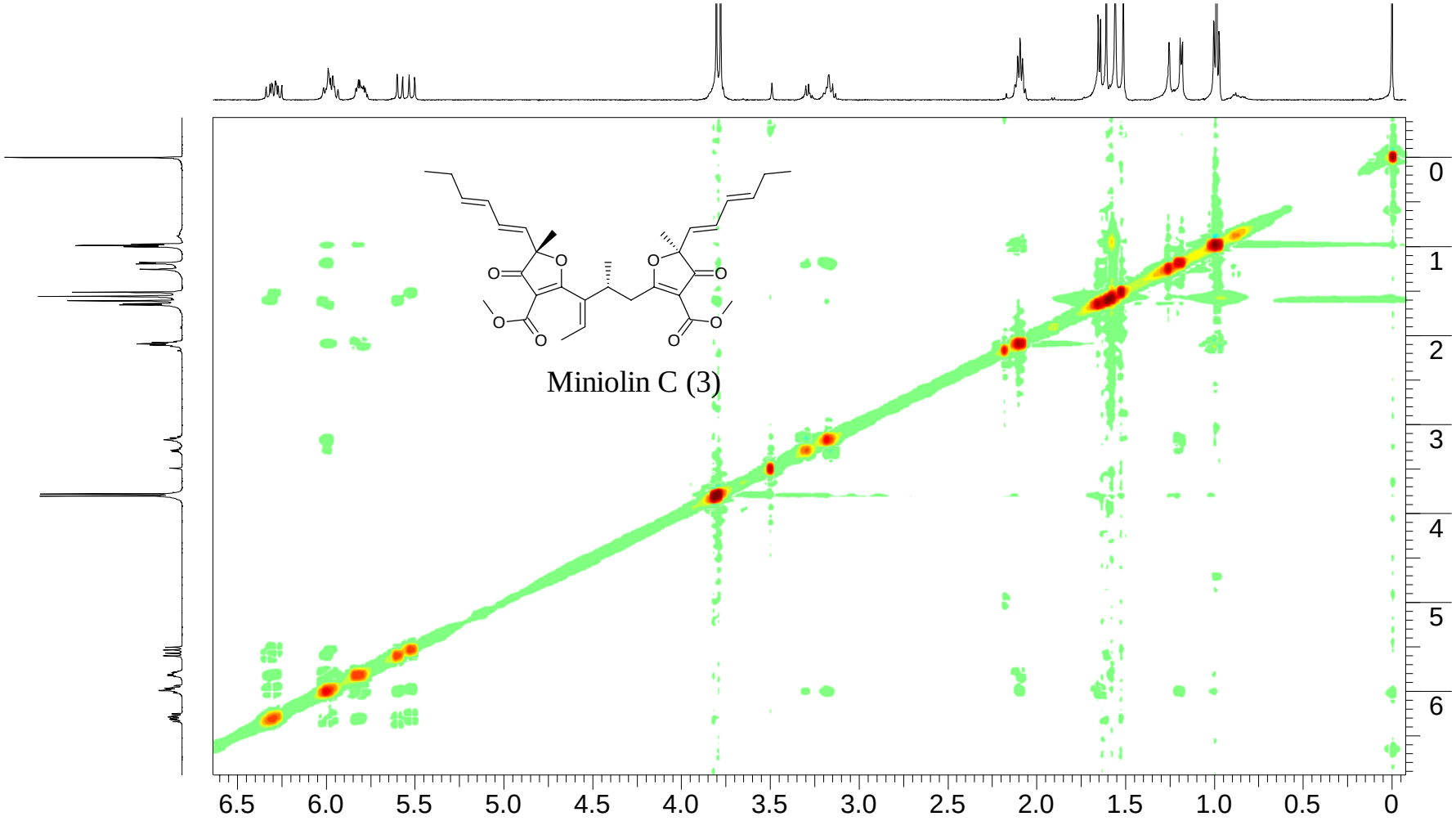


Figure S29. Positive ESIMS spectrum of 3

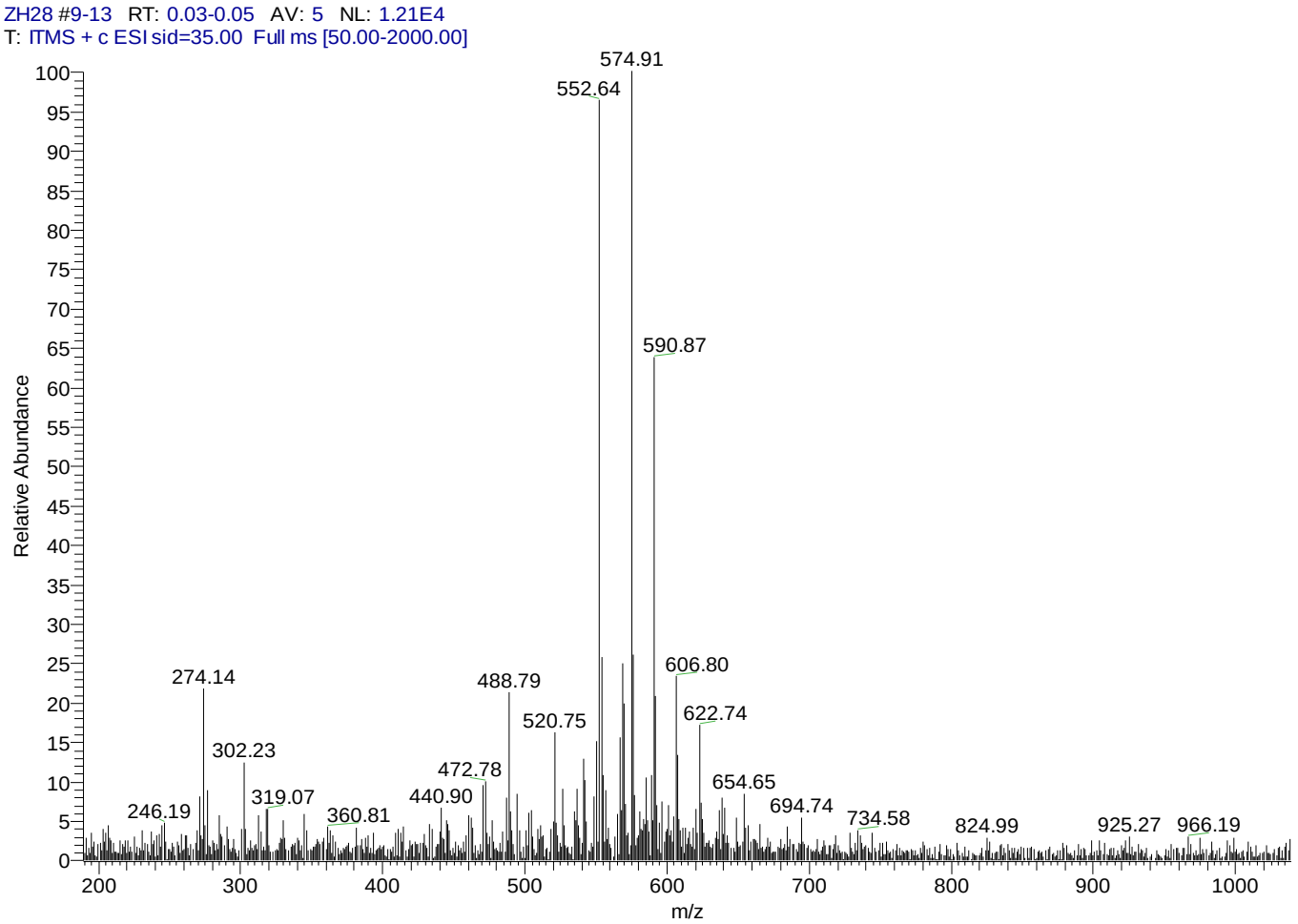
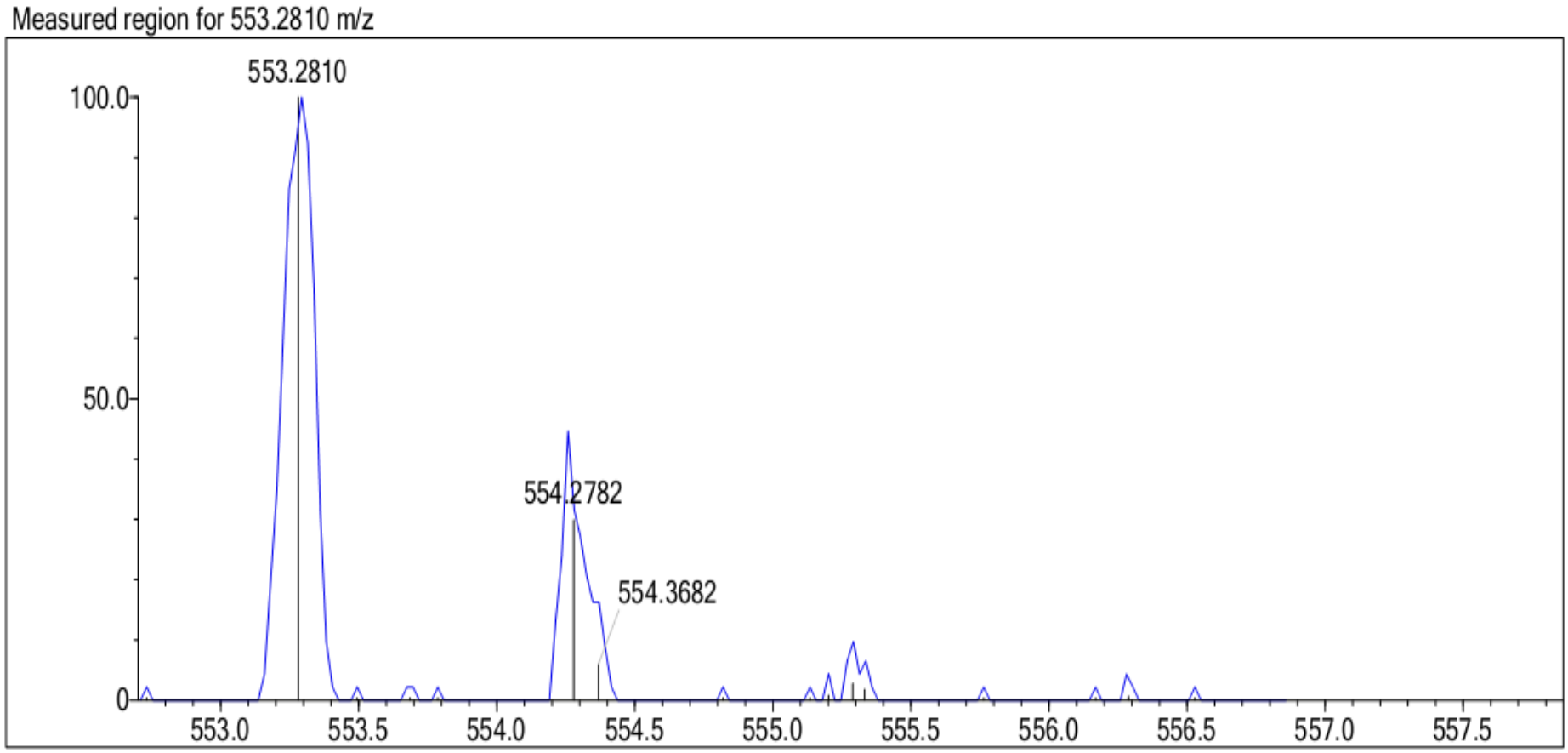


Figure S30. HR ESIMS spectrum of 3



Rank	Score	Ion	Formula (M)	Pred. m/z	Meas. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	57.74	[M+H]+	C32 H40 O8	553.2796	553.2810	1.4	2.53	60.03	13.0

Figure S31. IR spectrum of 3

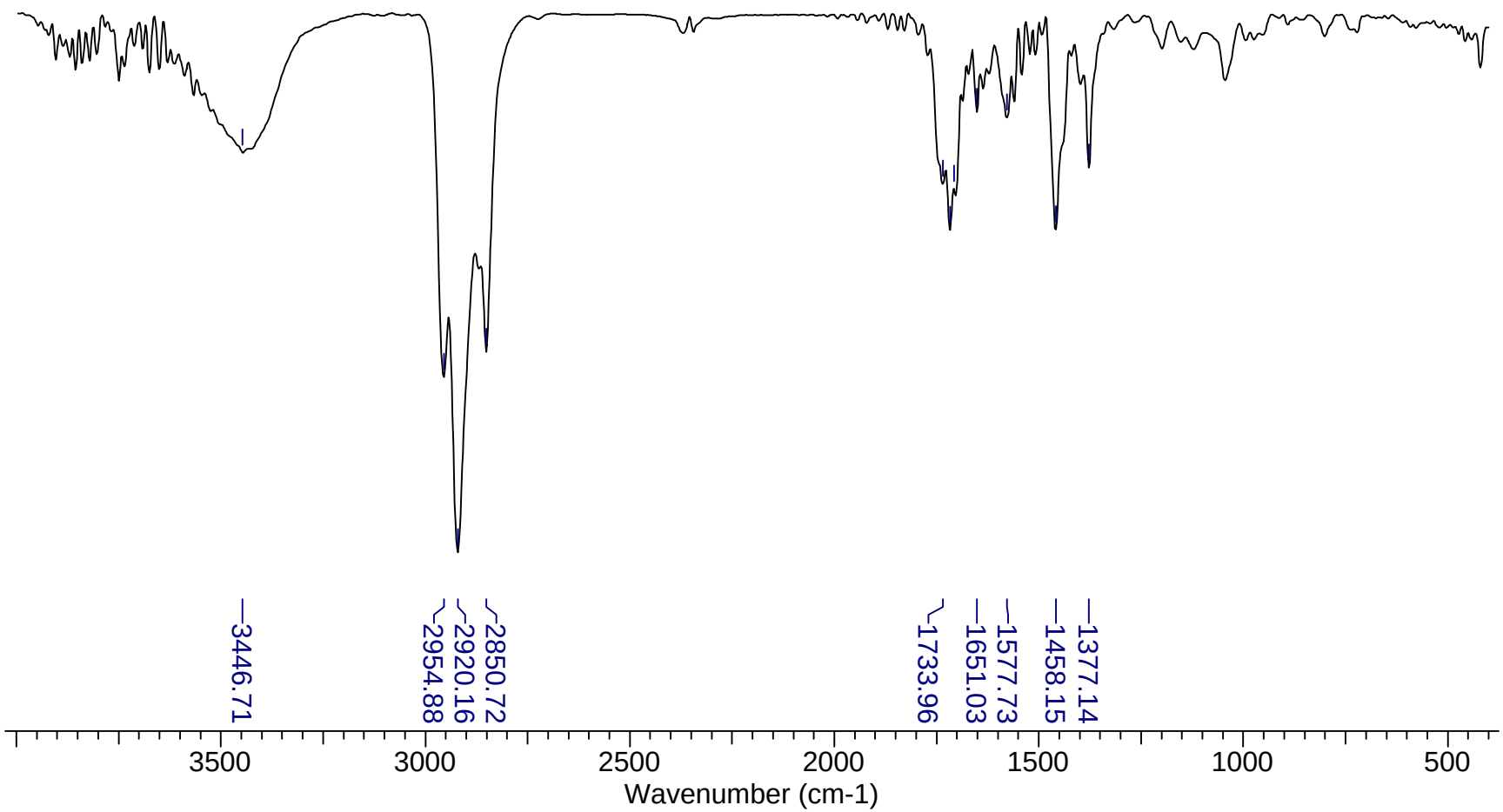


Figure S32. UV and CD spectra of 3

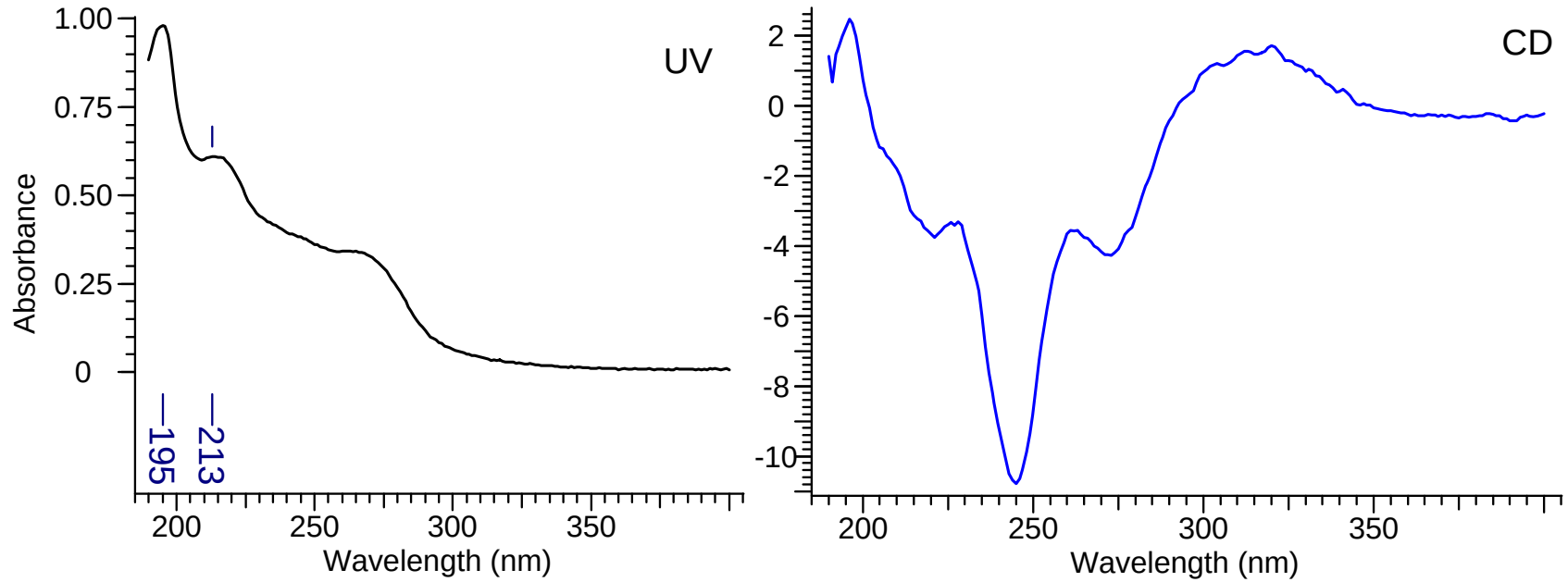
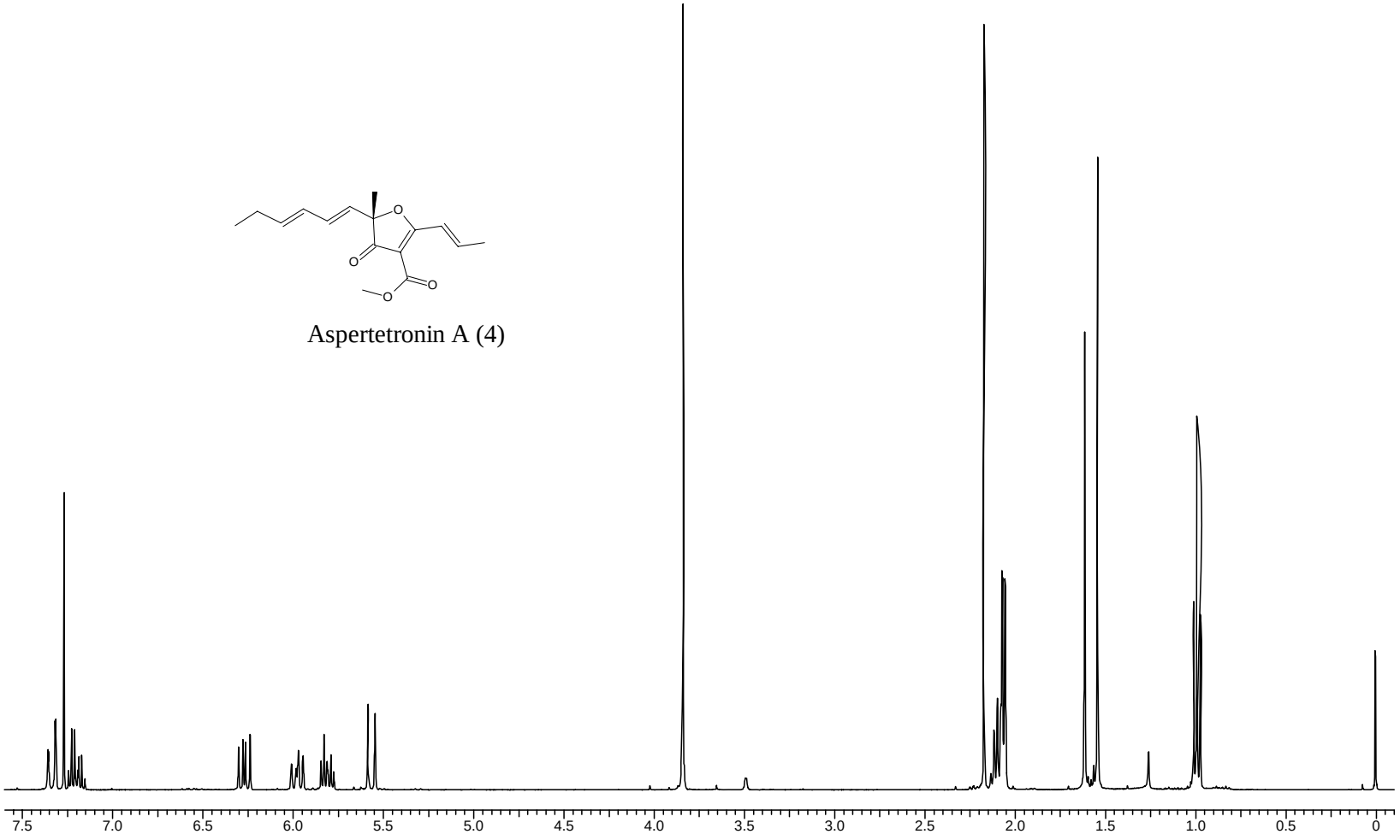


Figure S33. ^{1}**H NMR spectrum of 4 in** $CDCl_3$ **(400 MHz)**



Aspertetronin A (4)

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

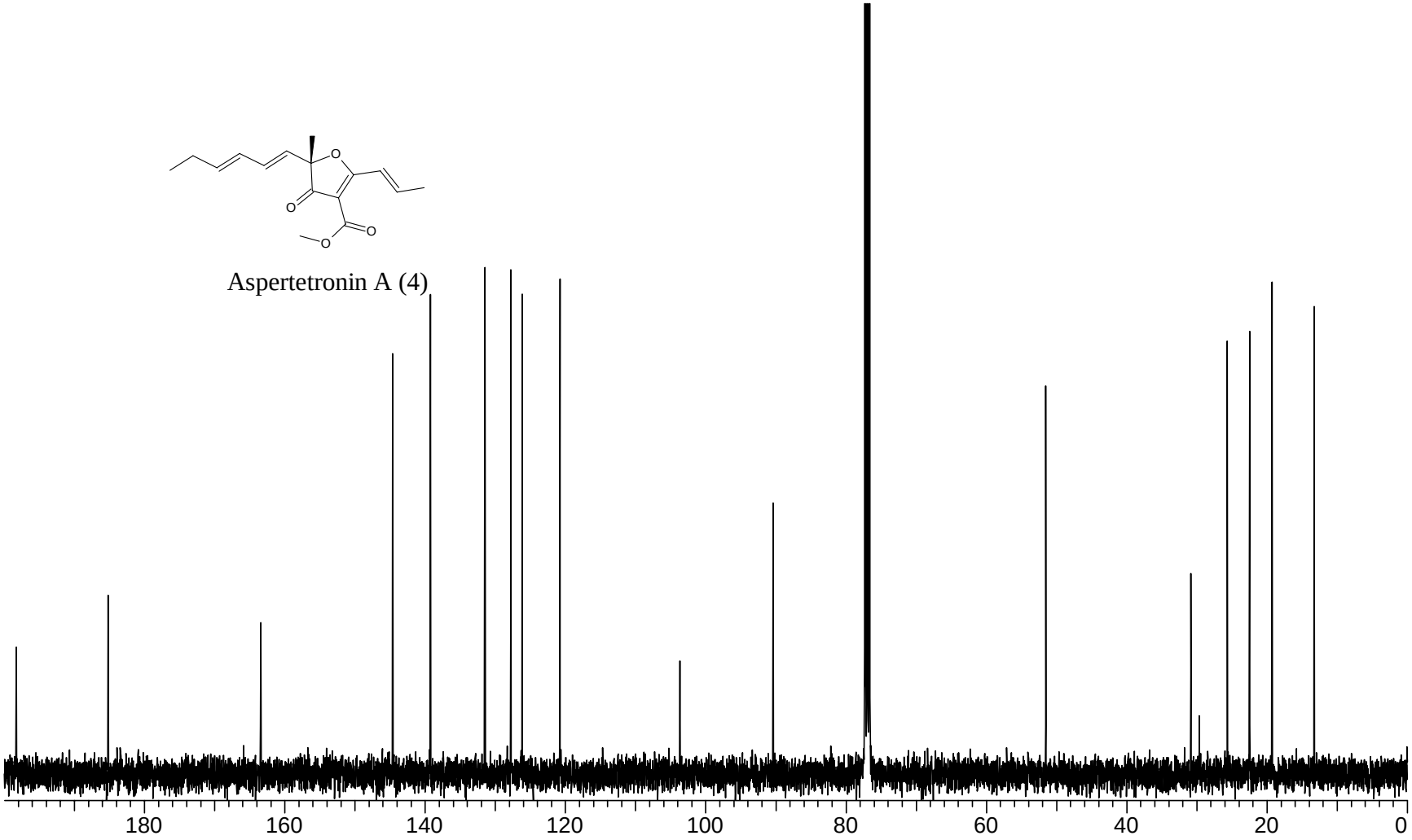


Figure S35. IR spectrum of 4

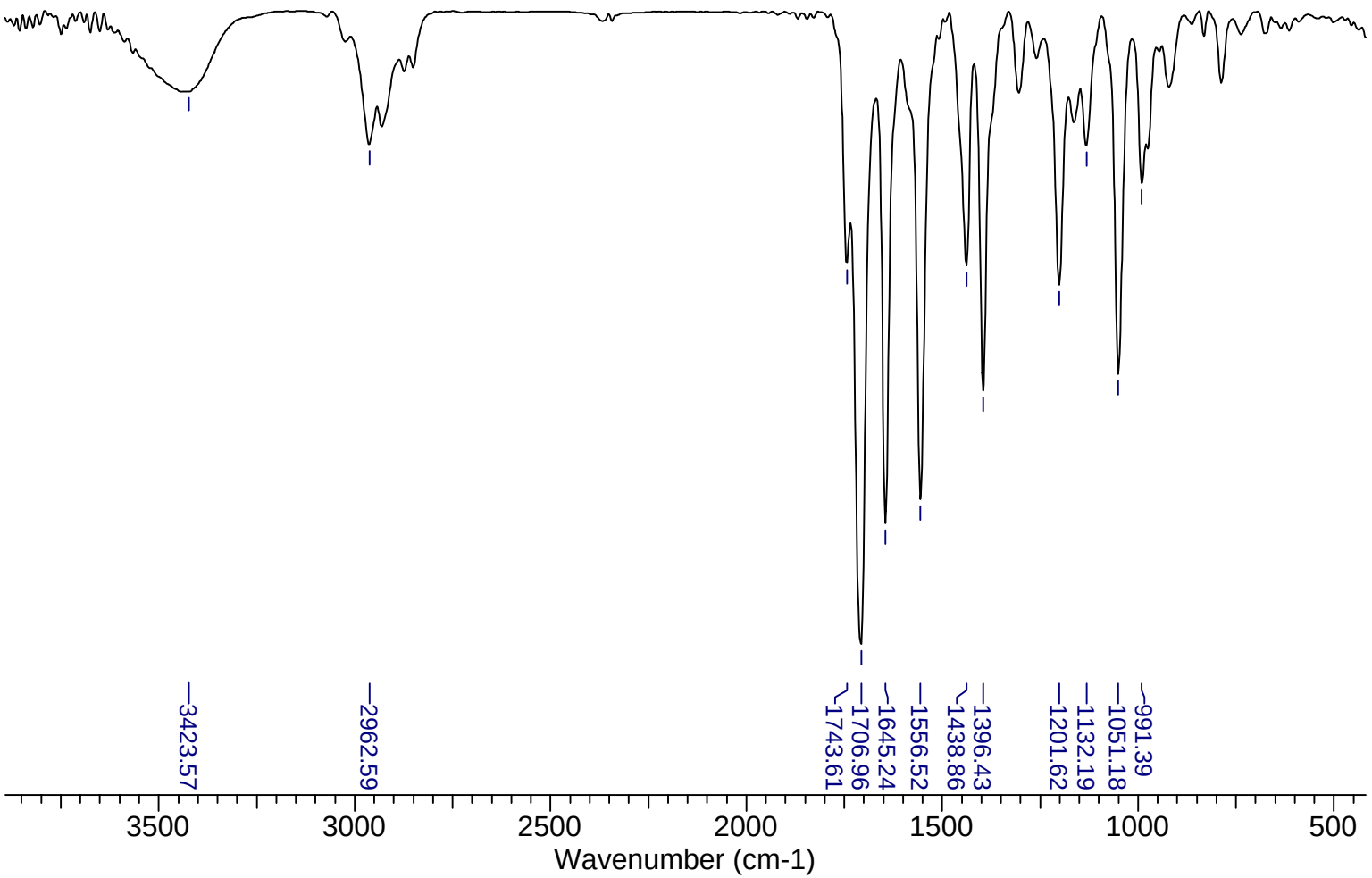


Figure S36. UV spectrum of 4

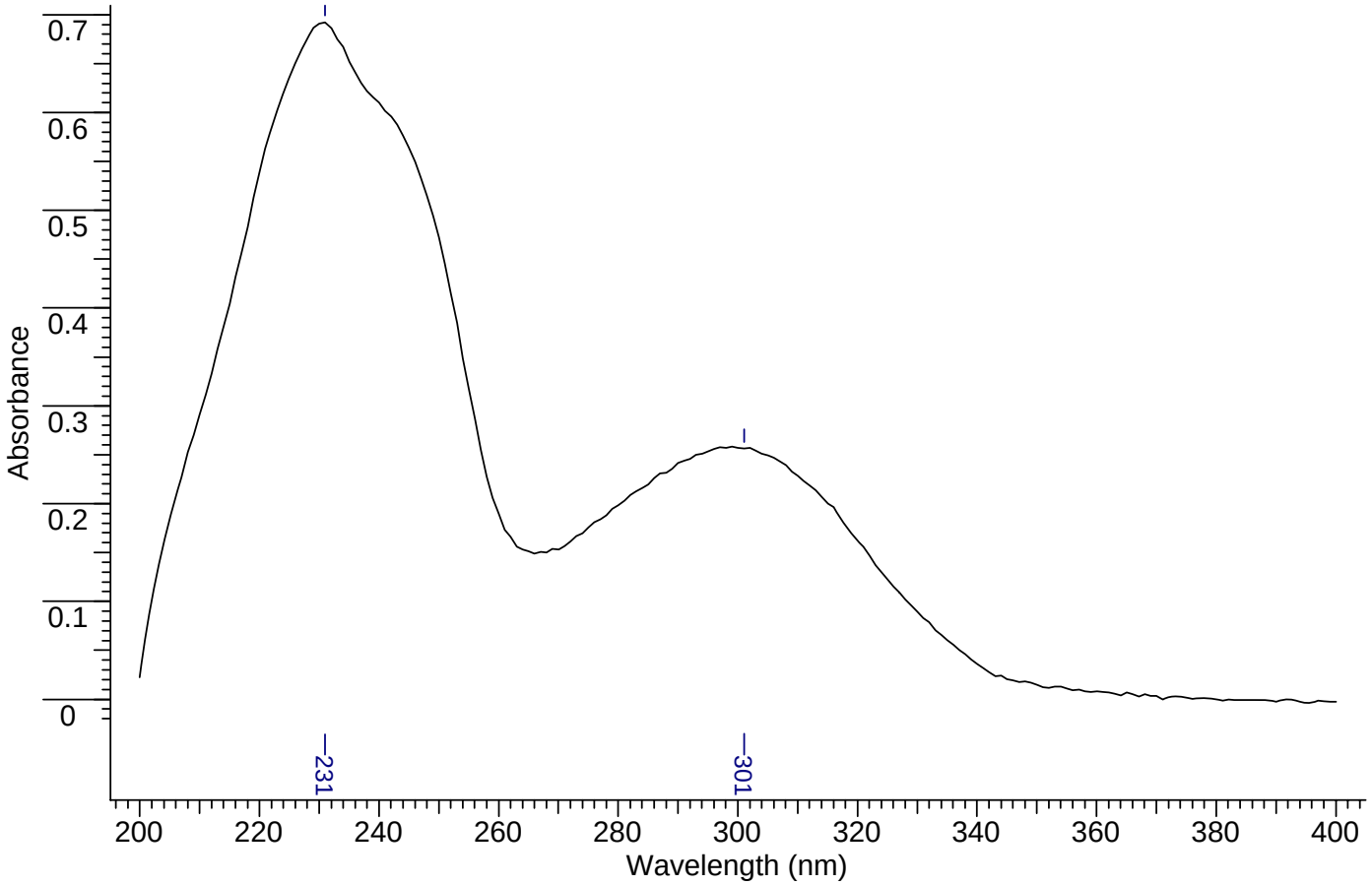


Figure S37. ESIMS of 4

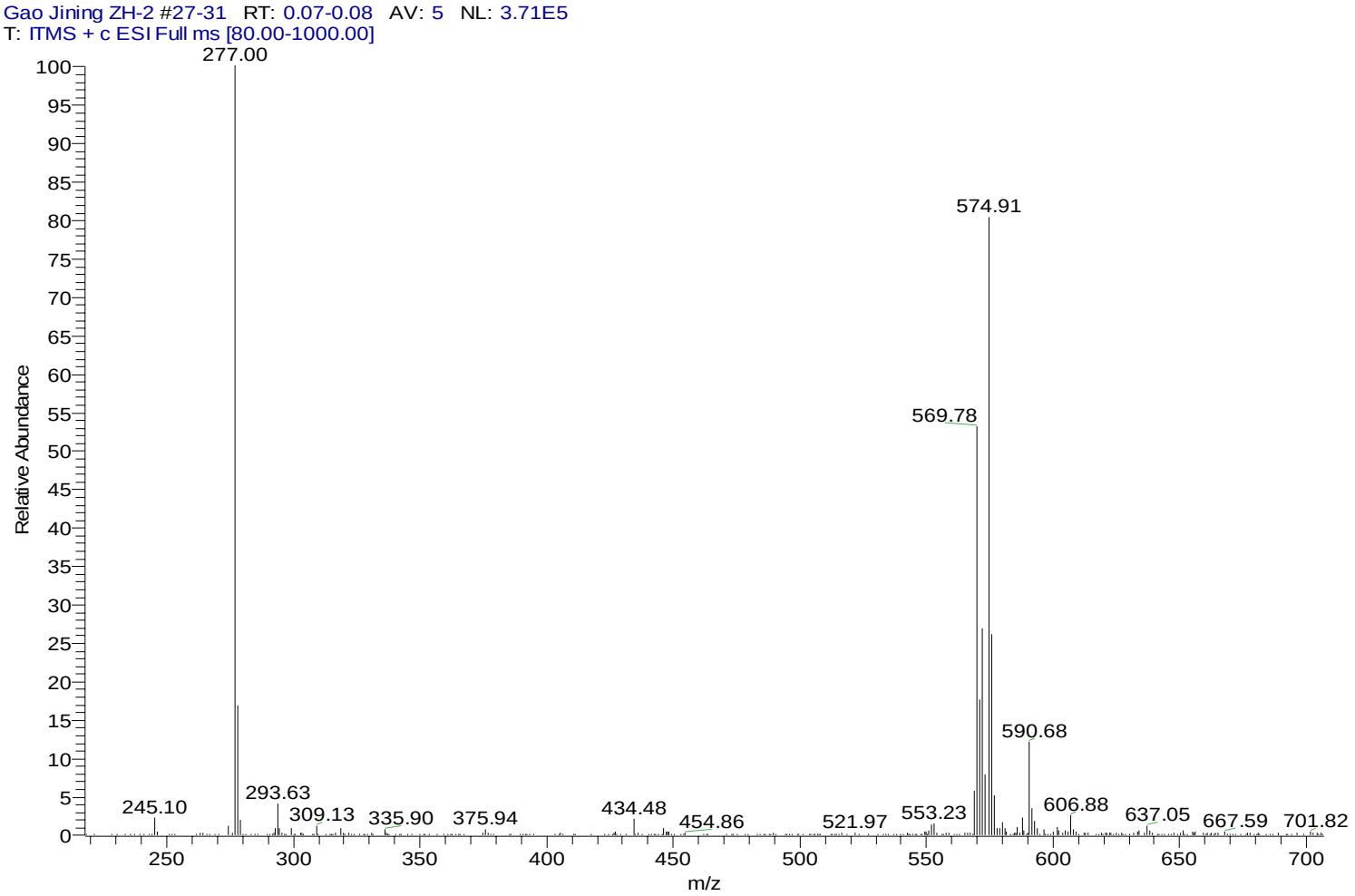


Figure S38. CD of 4