Terpenoids and Norlignans from *Metasequoia glyptostroboides*

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Supporting information

List of Supporting Information

- 1D, 2D NMR and HRFABMS spectra of metaseglyptorin A (**1**) (Figure S1-S7);
- 1D, 2D NMR and HREIMS spectra of metasequoic acid C (**2**) (Figure S8-S14);
- 1D NMR and HRESIMS spectra of 12α-hydroxy-8,15-isopimaradien-18-oic acid (**3**) (Figure S15-S17);
- 1D, 2D NMR and HRESIMS spectra of (–) acora-2,4(14),8-trien-15-oic acid (**4**) (Figure S18-24);
- 1D NMR and HRESIMS spectra of metasequirin D (**5**) (Figure S25-27);
- 1D, 2DNMR and HRESIMS spectra of metasequirin E (**6**) (Figure S28-S34);
- 1D NMR and HRESIMS spectra of metasequirin F (**7**) (Figure S35-S37);
- ^{1}H NMR spectra of compound **8** (Figure S38);
- ^{1}H and COSY NMR spectra of **9a** and **9b** (Figure S39-S42).
- Structures of the known compounds (page 43, 44)

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Figure S1. ^{1}H NMR Spectrum of Compound **1**.

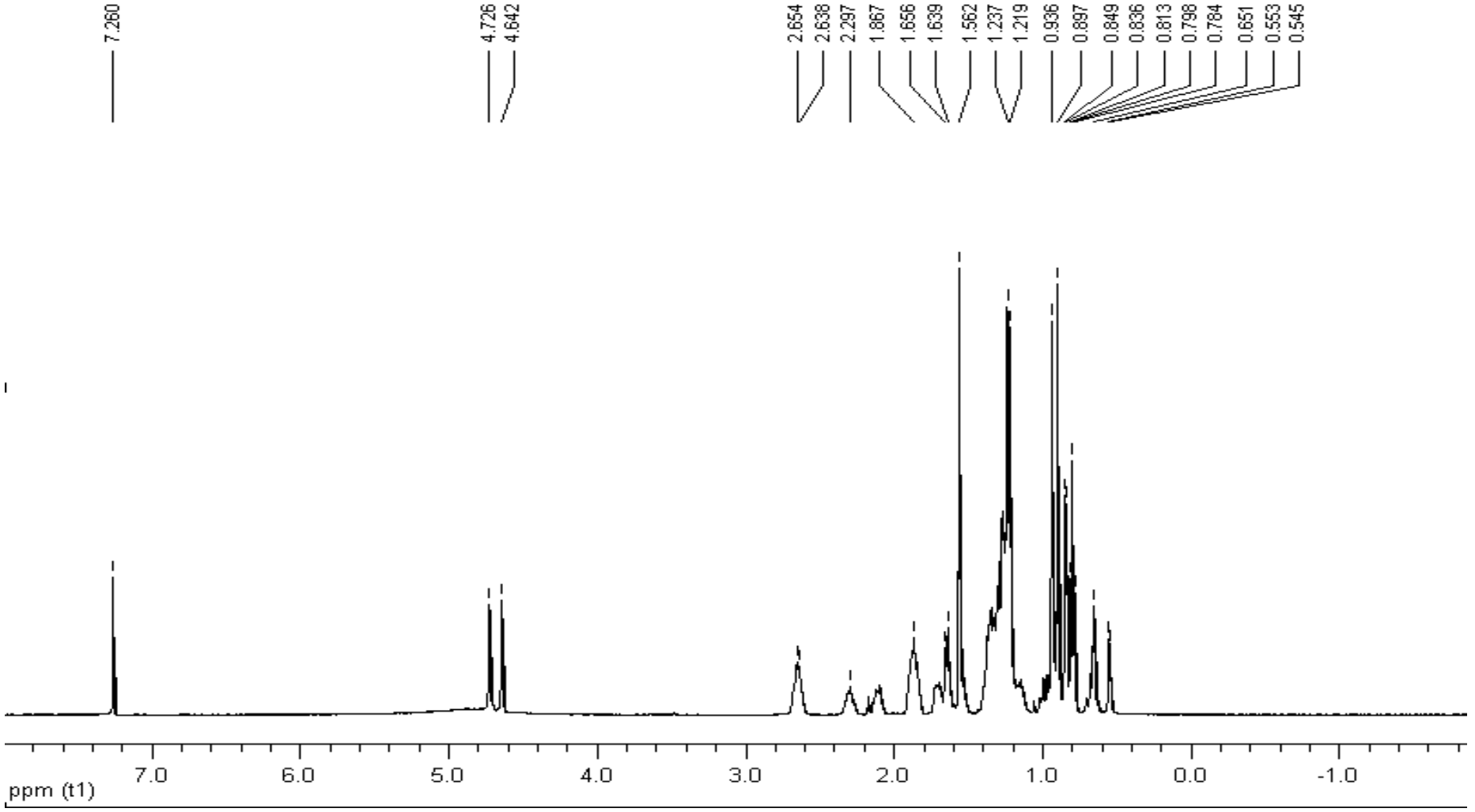


Figure S2. ^{13}C NMR Spectrum of Compound **1**.

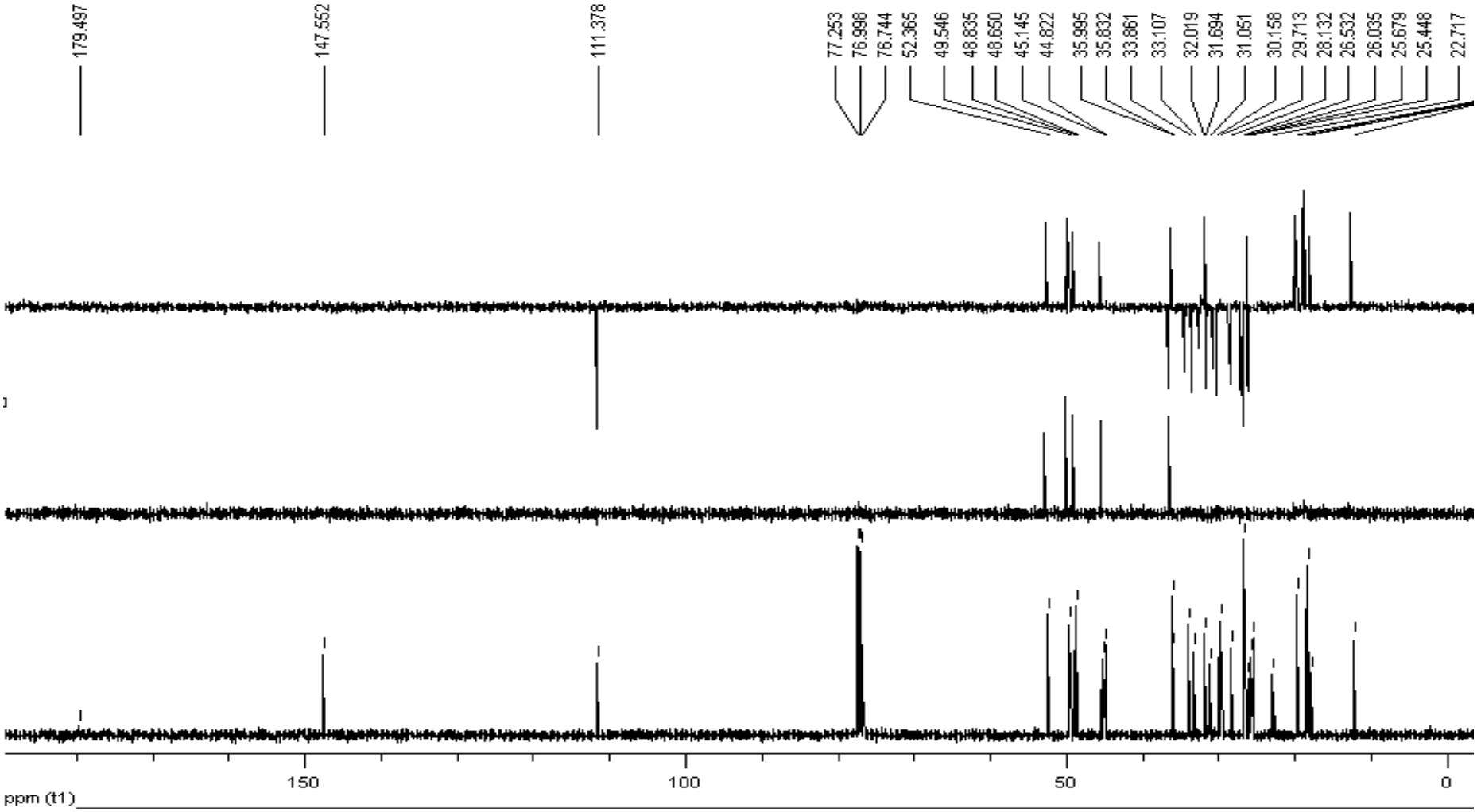


Figure S3. HSQC Spectrum of Compound **1**.

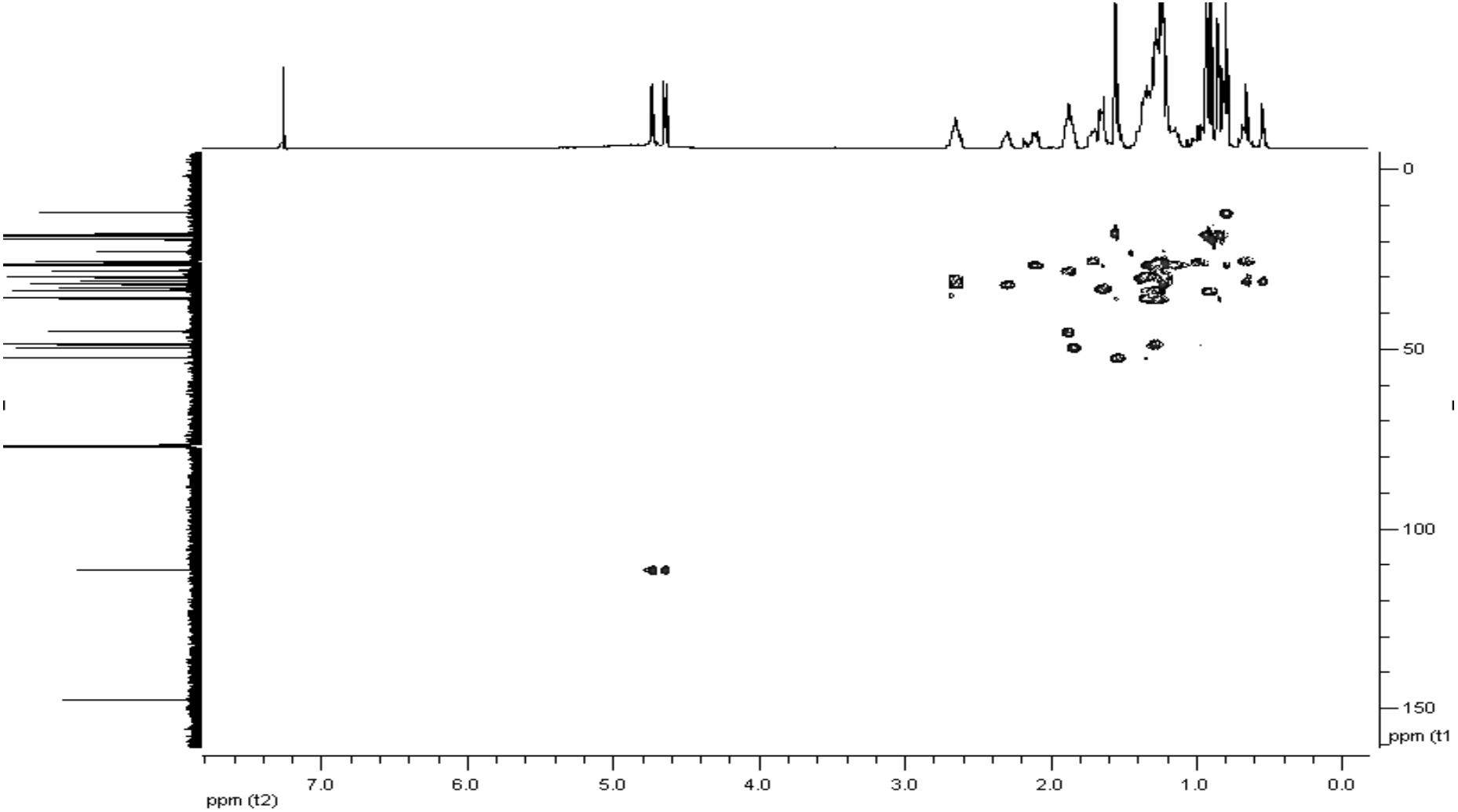


Figure S4. COSY Spectrum of Compound **1**.

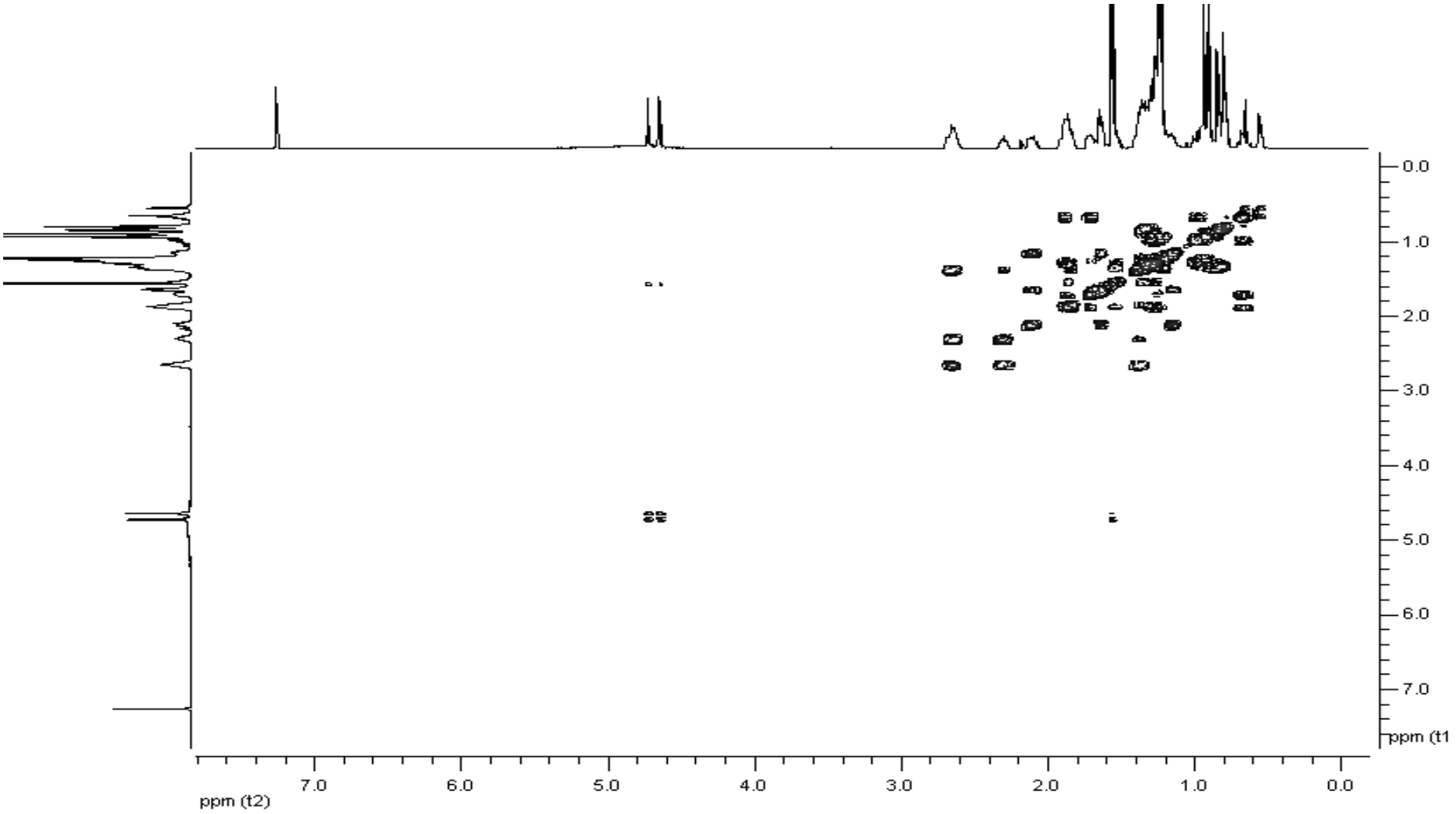


Figure S5. HMBC Spectrum of Compound **1**.

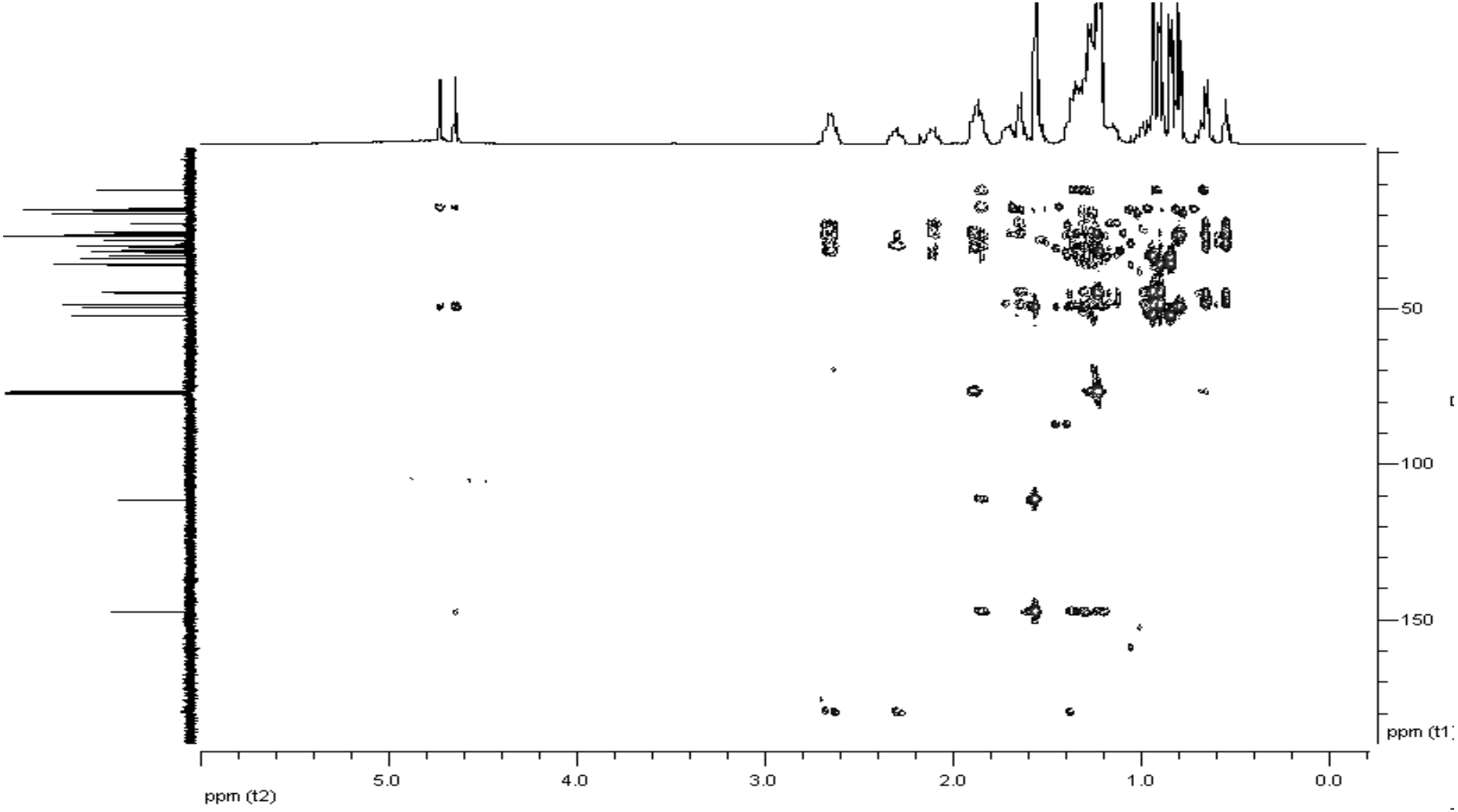


Figure S6. ROESY Spectrum of Compound **1**.

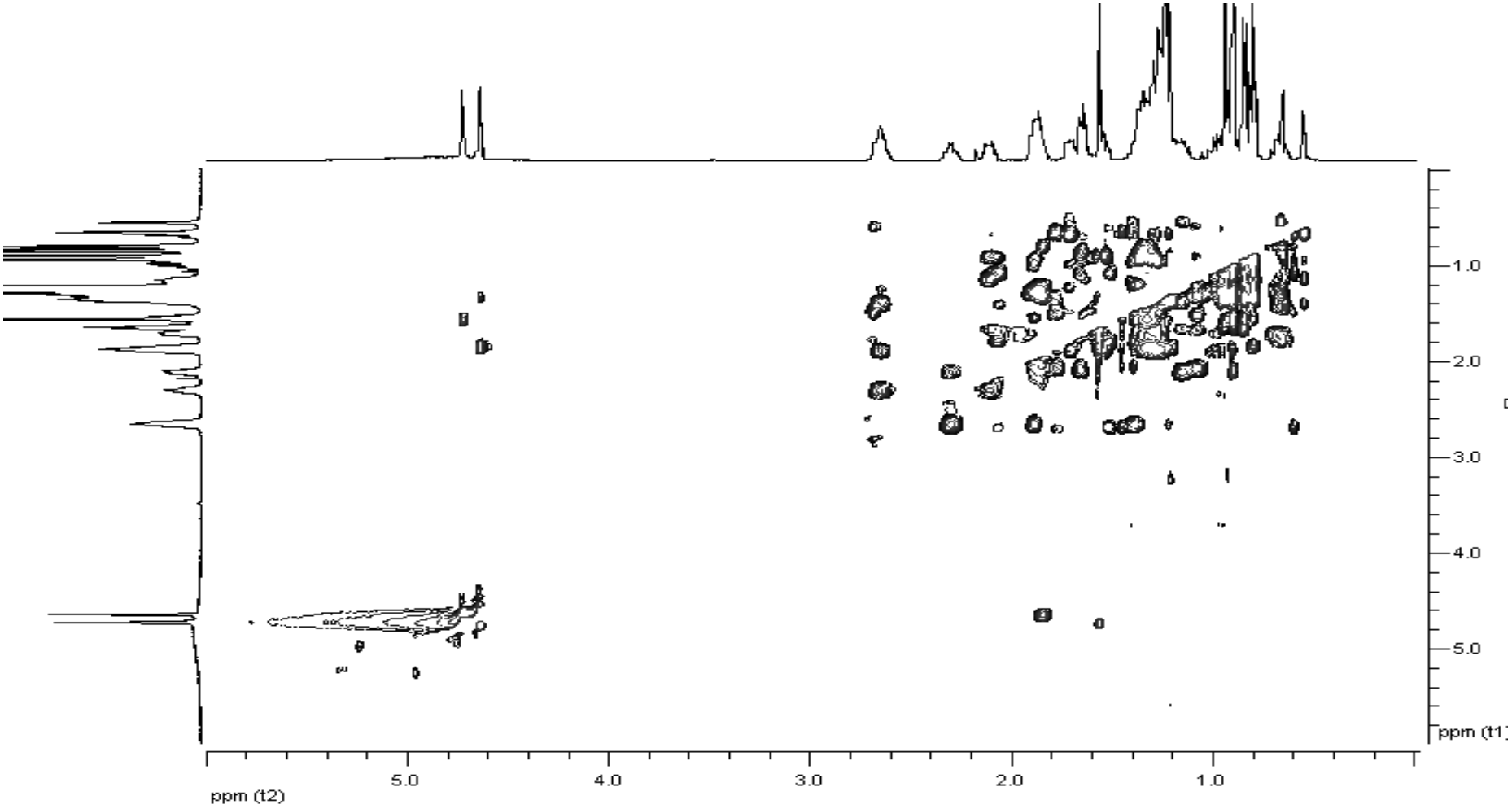


Figure S7. HRFABMS Spectrum of Compound **1**.

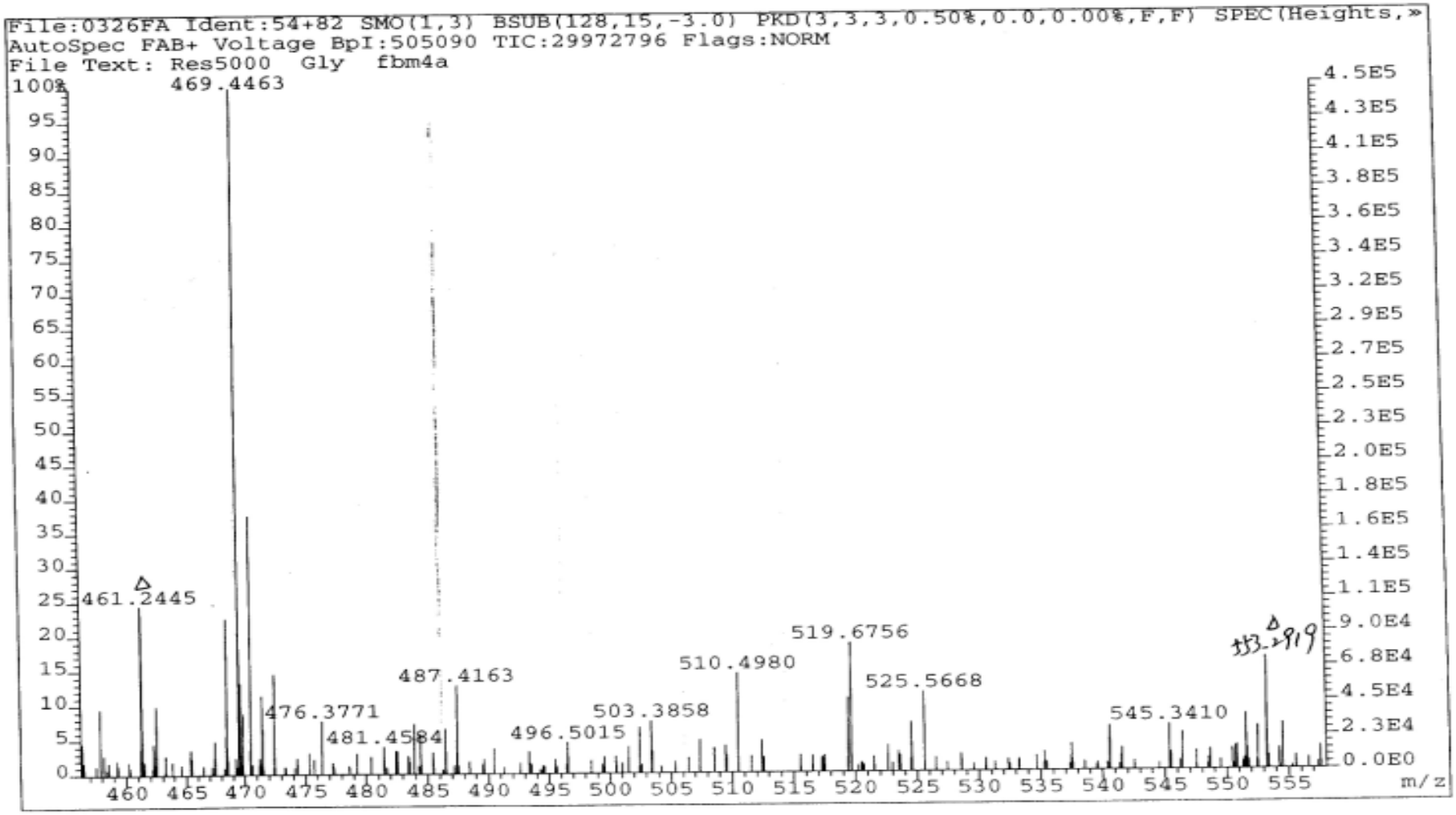


Figure S8. ^{1}H NMR Spectrum of Compound **2**.

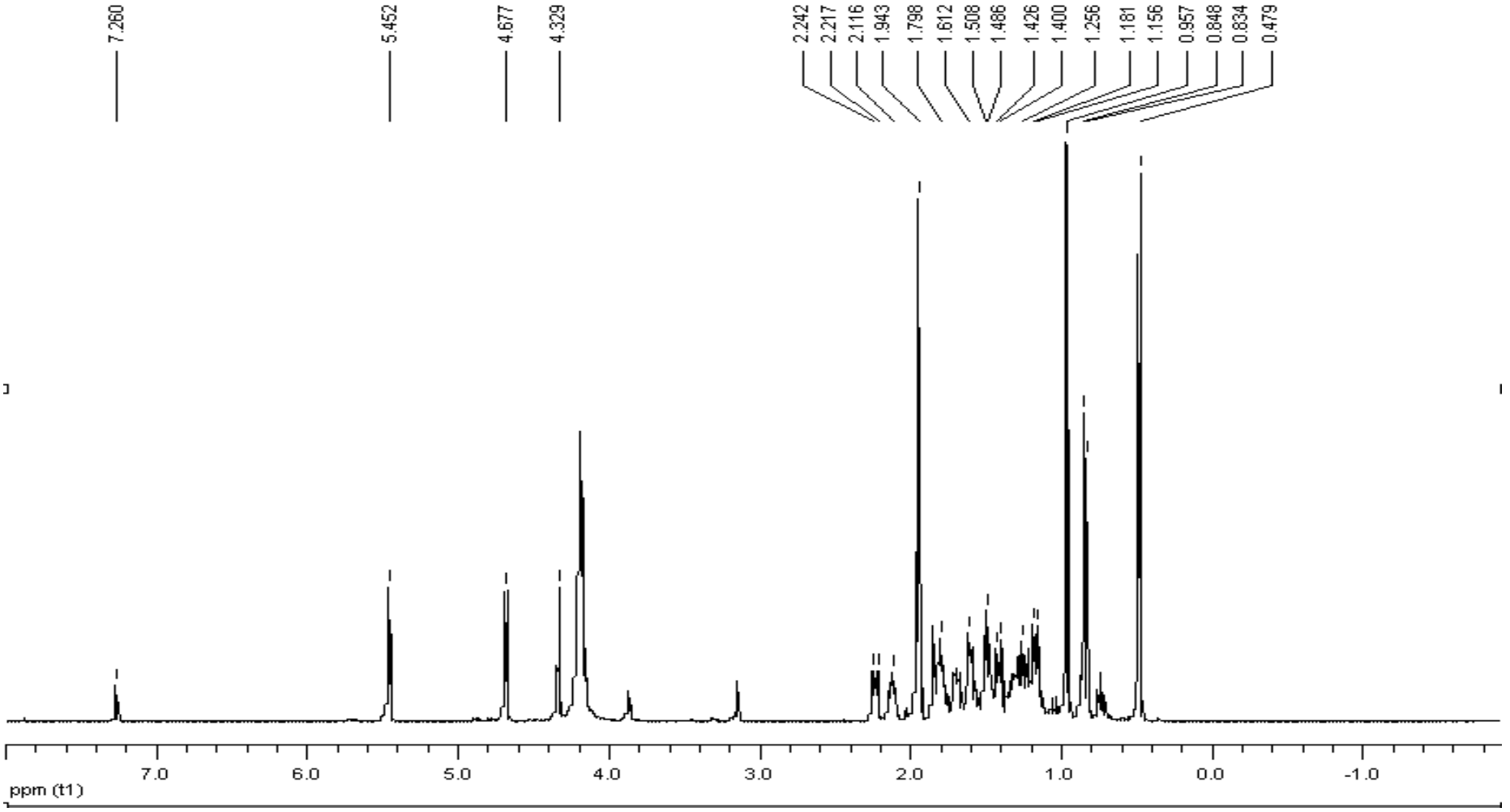


Figure S9. ^{13}C NMR Spectrum of Compound **2**.

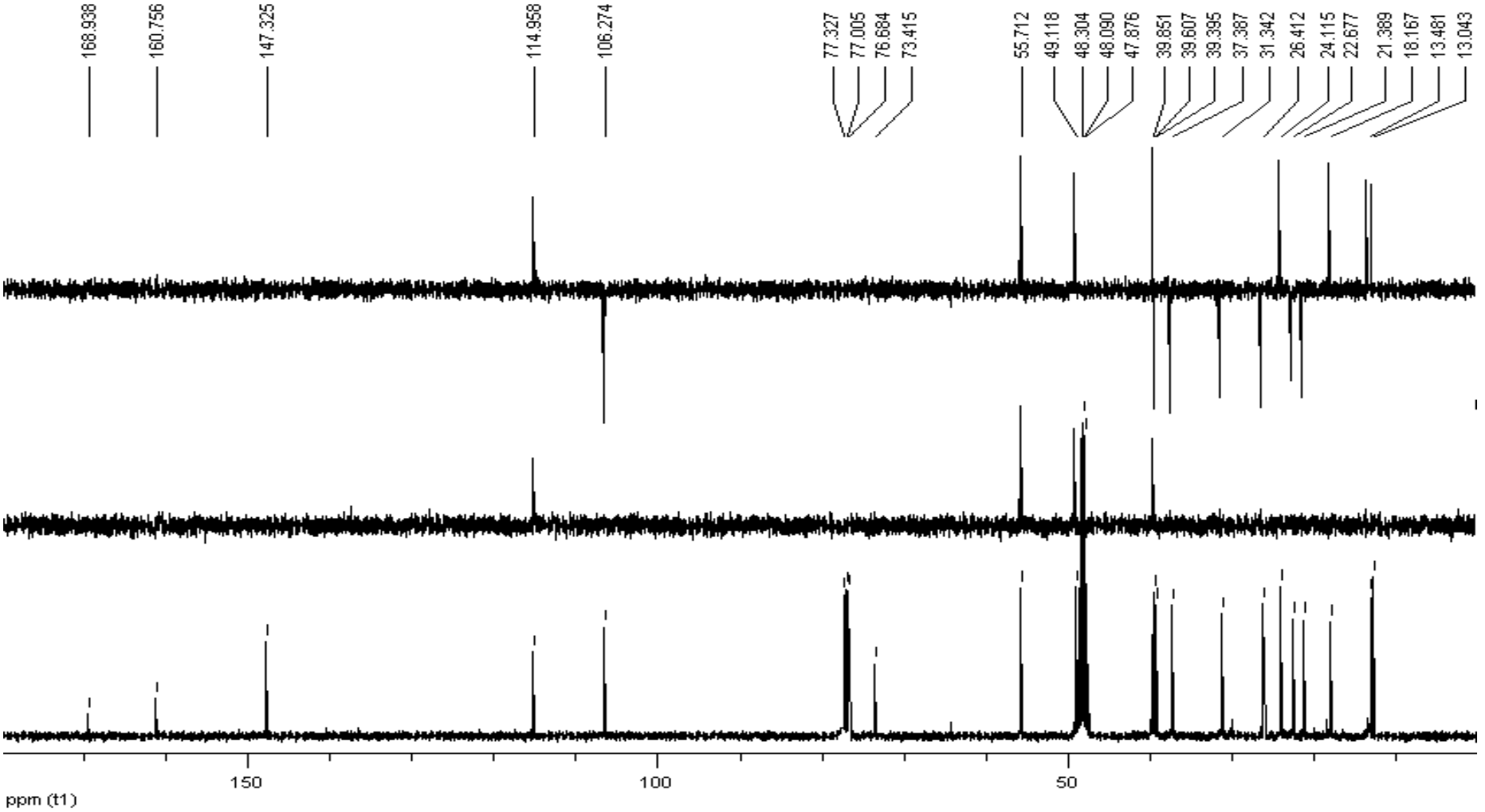


Figure S10. HSQC Spectrum of Compound **2**.

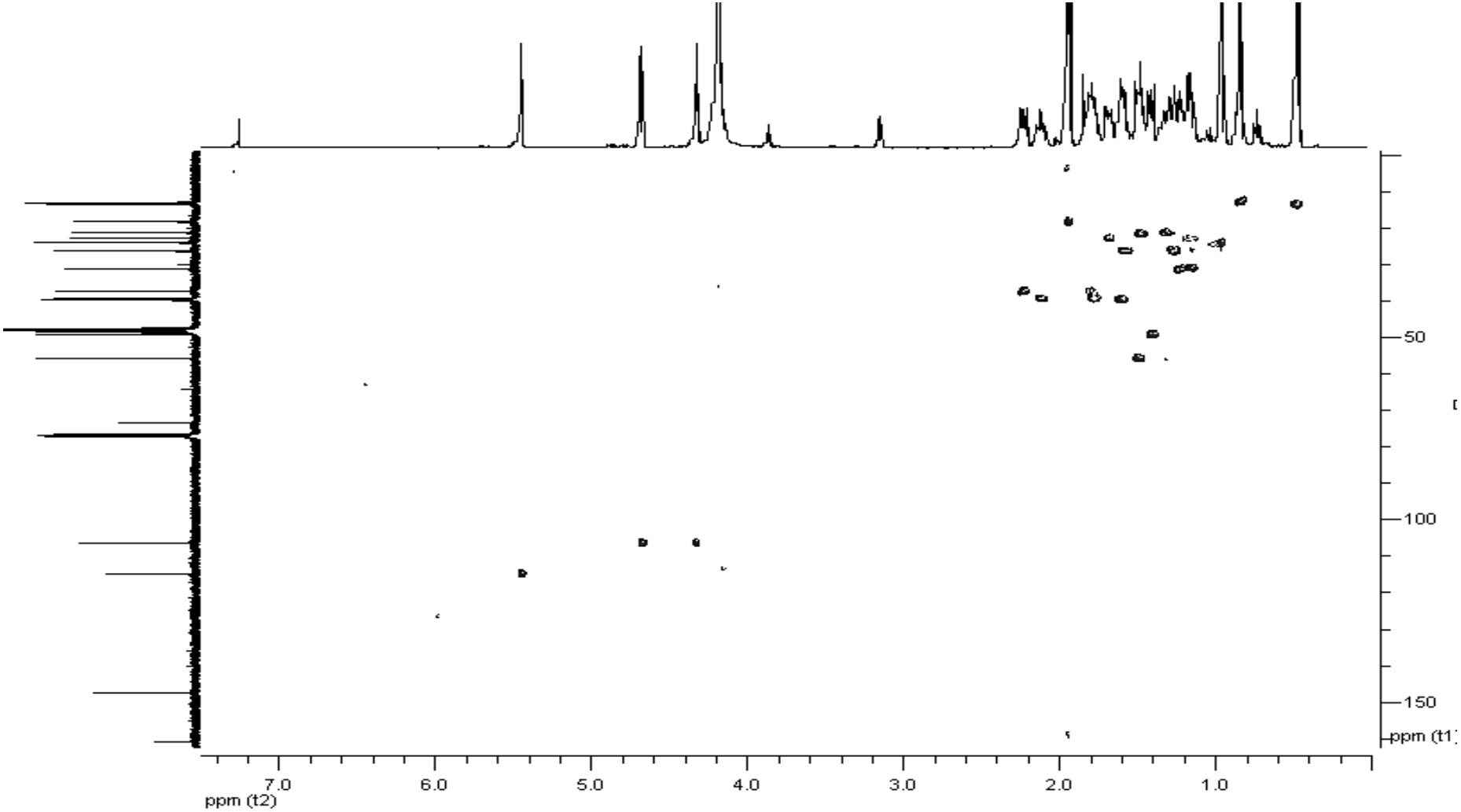


Figure S11. COSY Spectrum of Compound **2**.

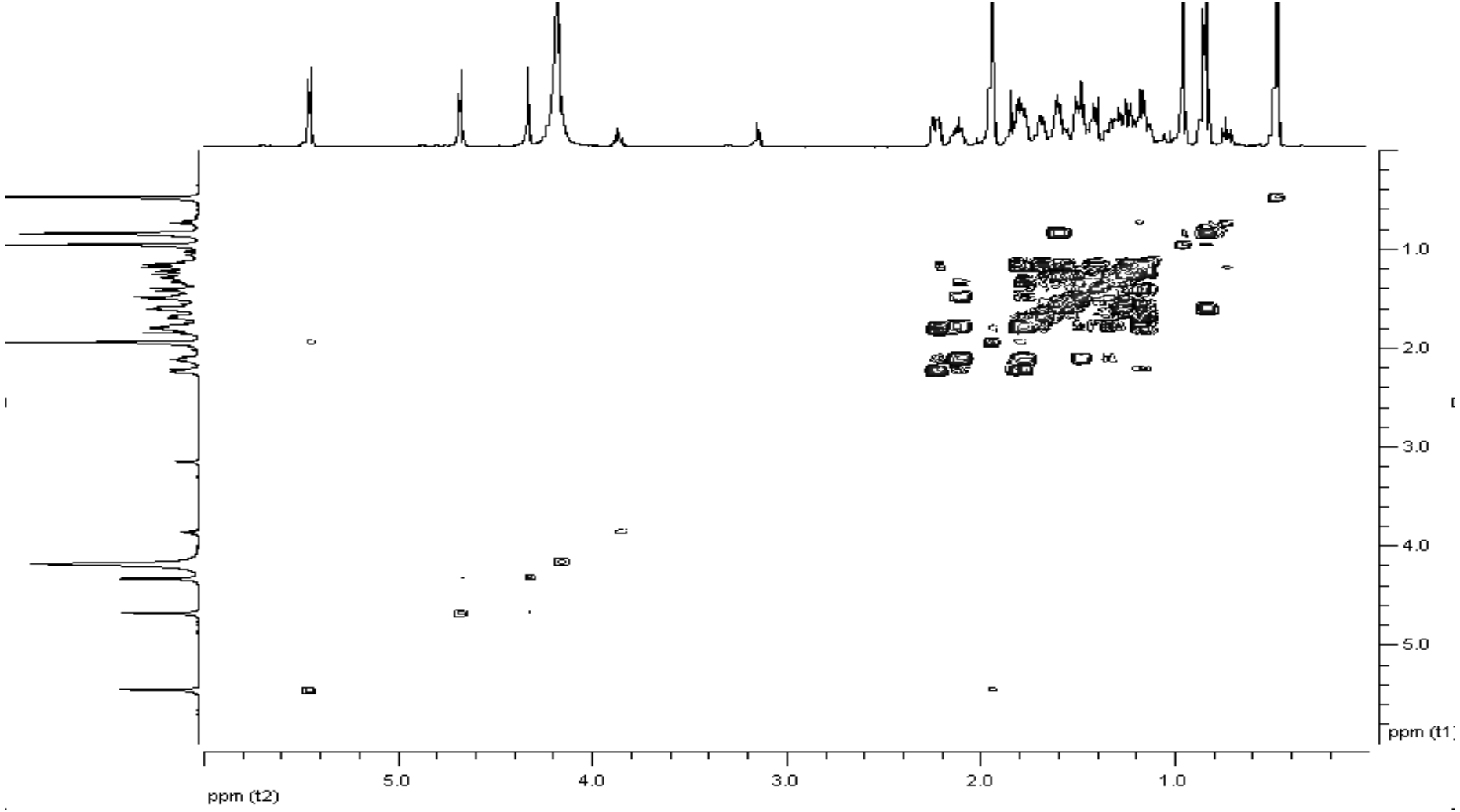


Figure S12. HMBC Spectrum of Compound **2**.

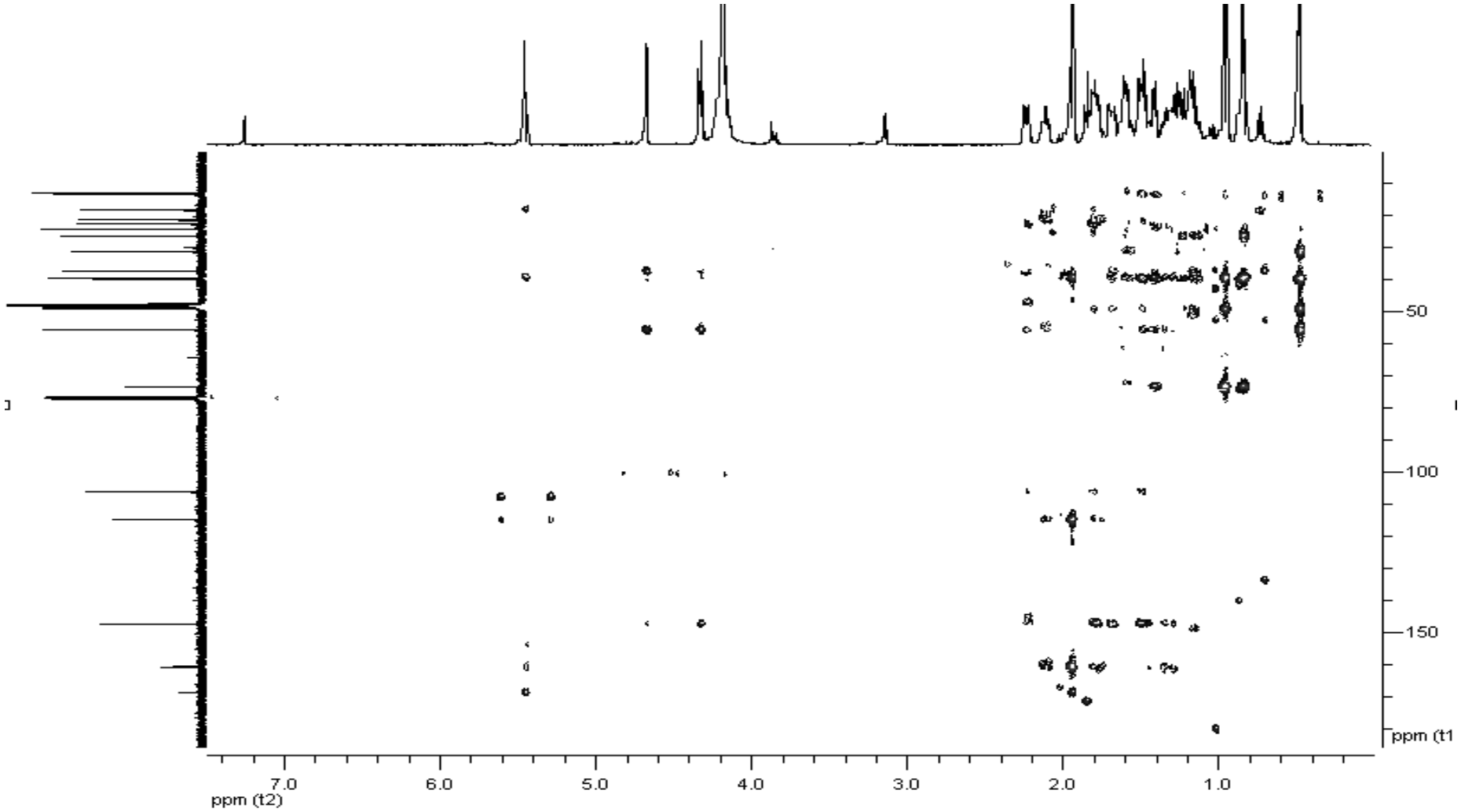


Figure S13. ROESY Spectrum of Compound **2**.

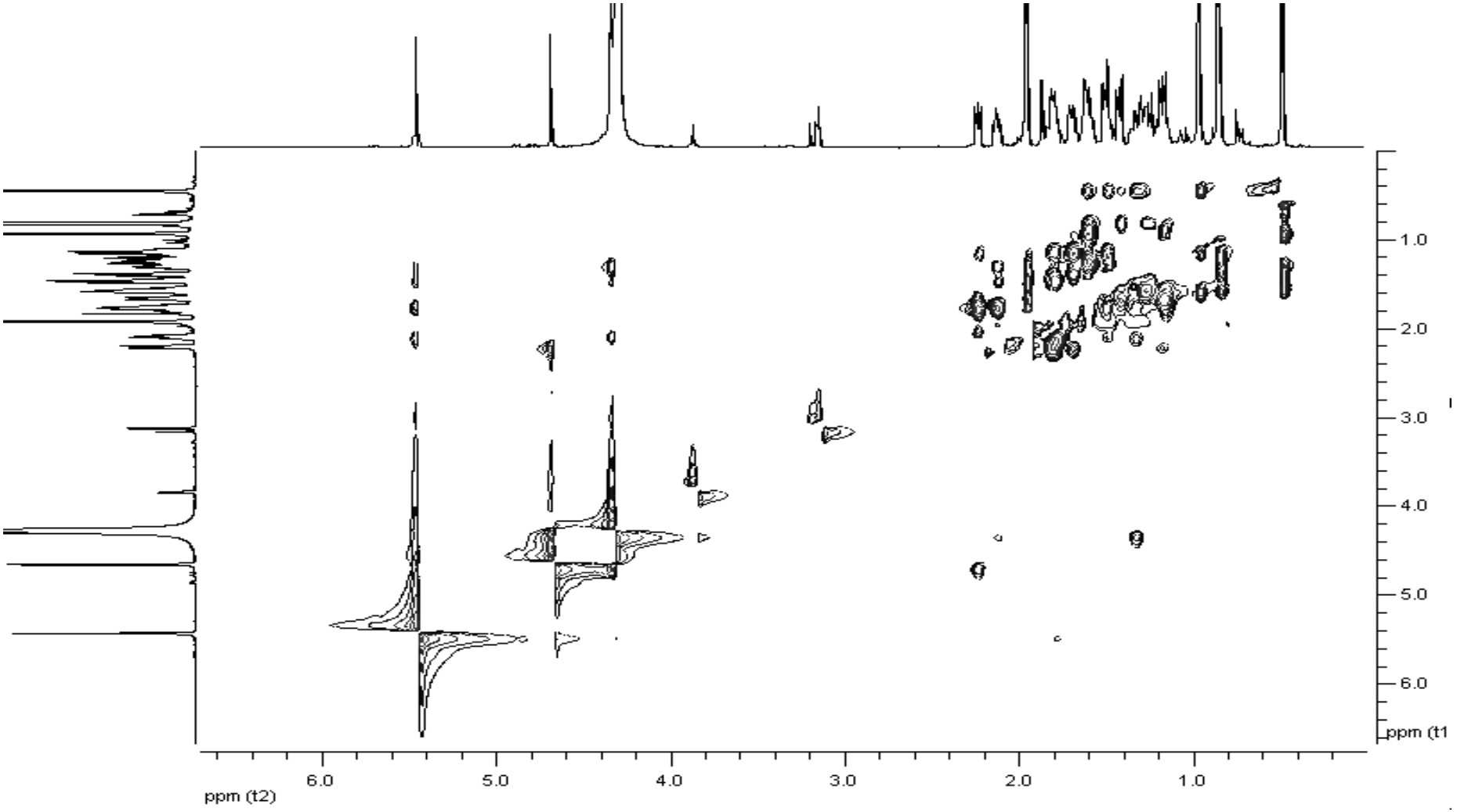
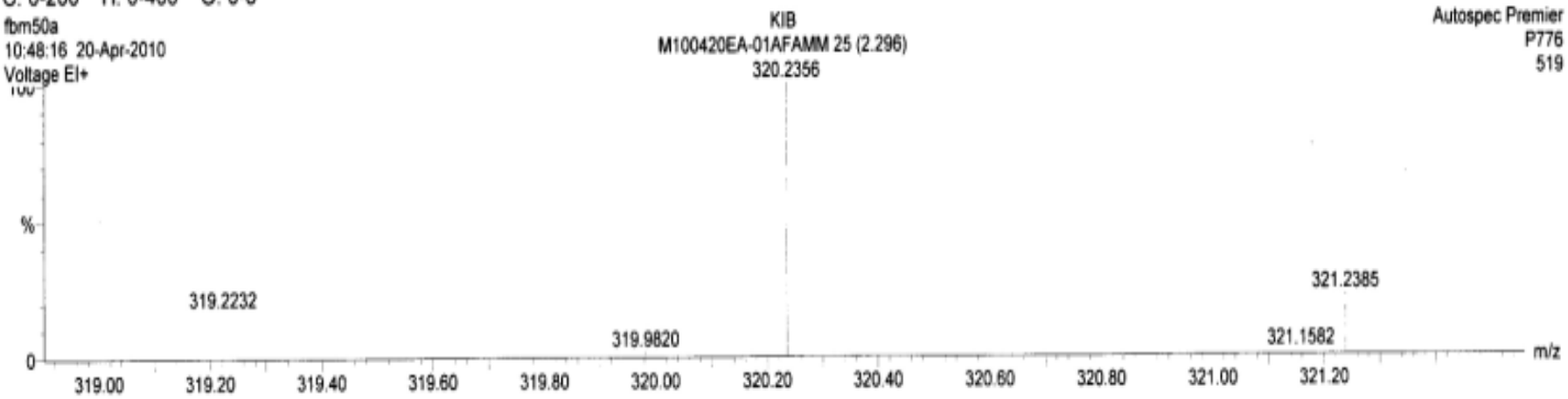


Figure S14. HREIMS Spectrum of Compound **2**.

Single Mass Analysis (displaying only valid results)
Tolerance = 100.0 PPM / DBE: min = 0.5, max = 40.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
25 formula(e) evaluated with 3 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 0-5



Minimum:				0.5		
Maximum:		10.0	100.0	40.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
320.2356	320.2351	0.5	1.6	5.0	2773092.0	C20 H32 O3
	320.2504	-14.8	-46.2	9.0	2773110.3	C24 H32
	320.2140	21.6	67.5	10.0	2773111.5	C23 H28 O

Figure S15. ^{1}H NMR Spectrum of Compound **3**.

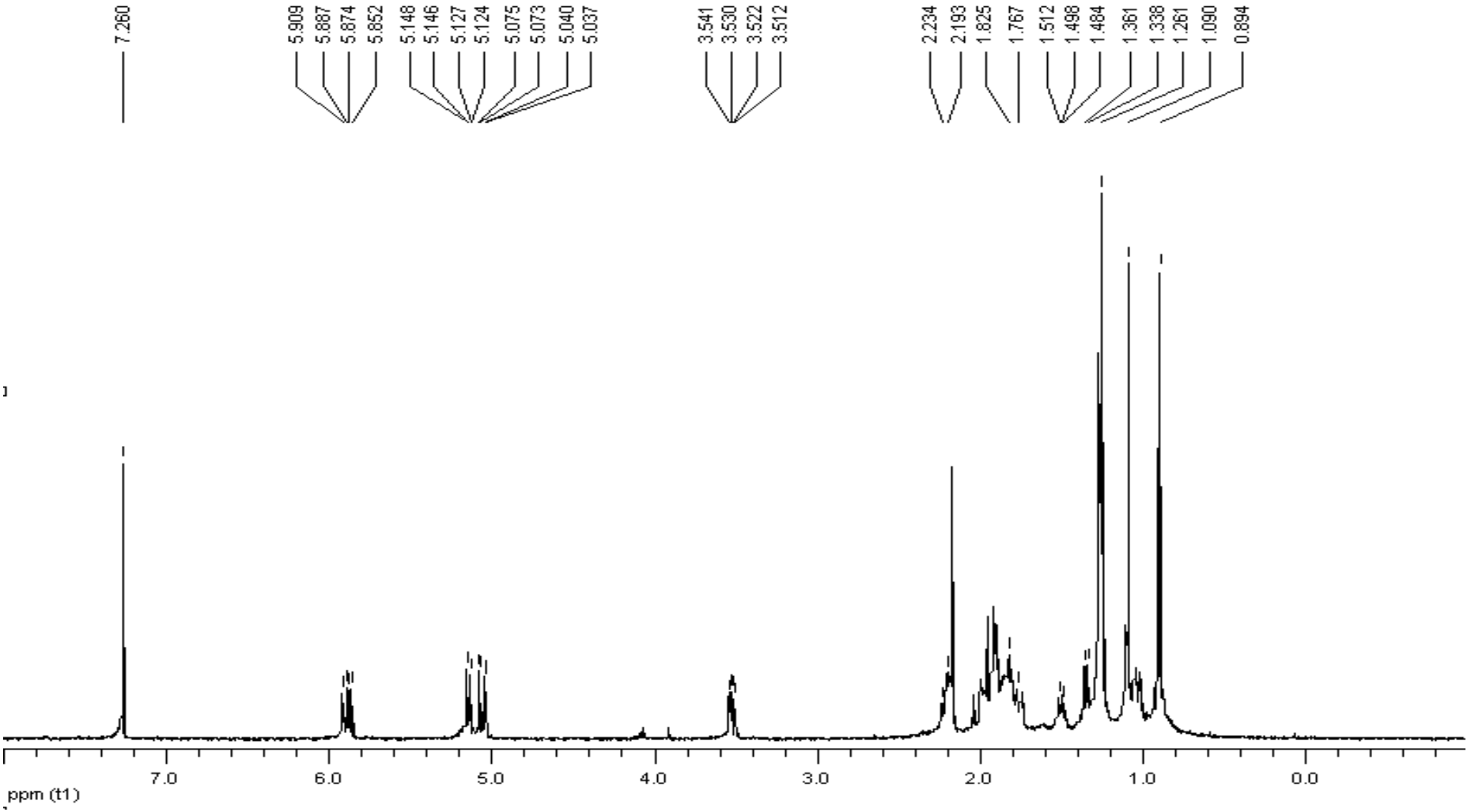


Figure S16. ^{13}C NMR Spectrum of Compound **3**.

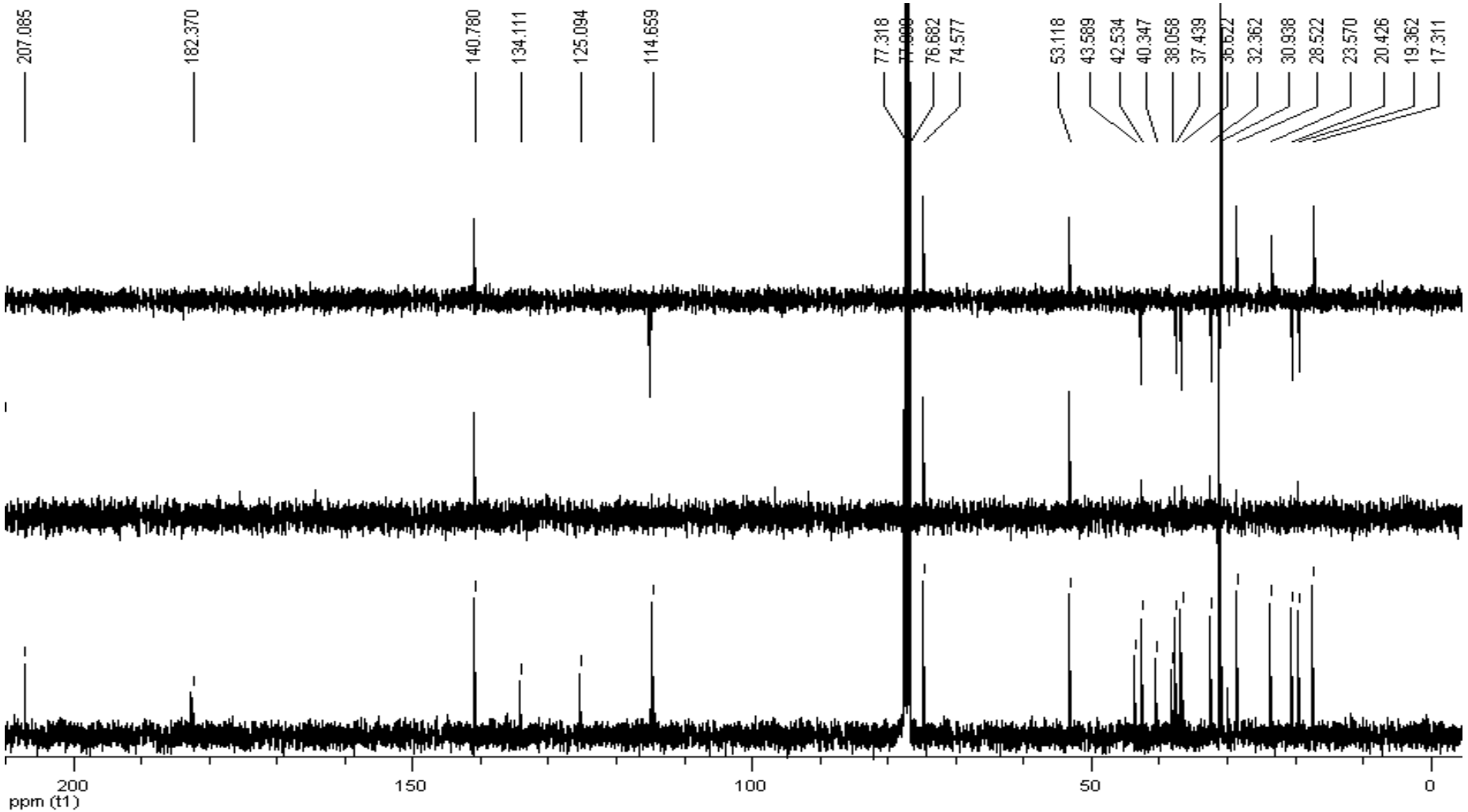


Figure S17. HRESIMS Spectrum of Compound **3**.

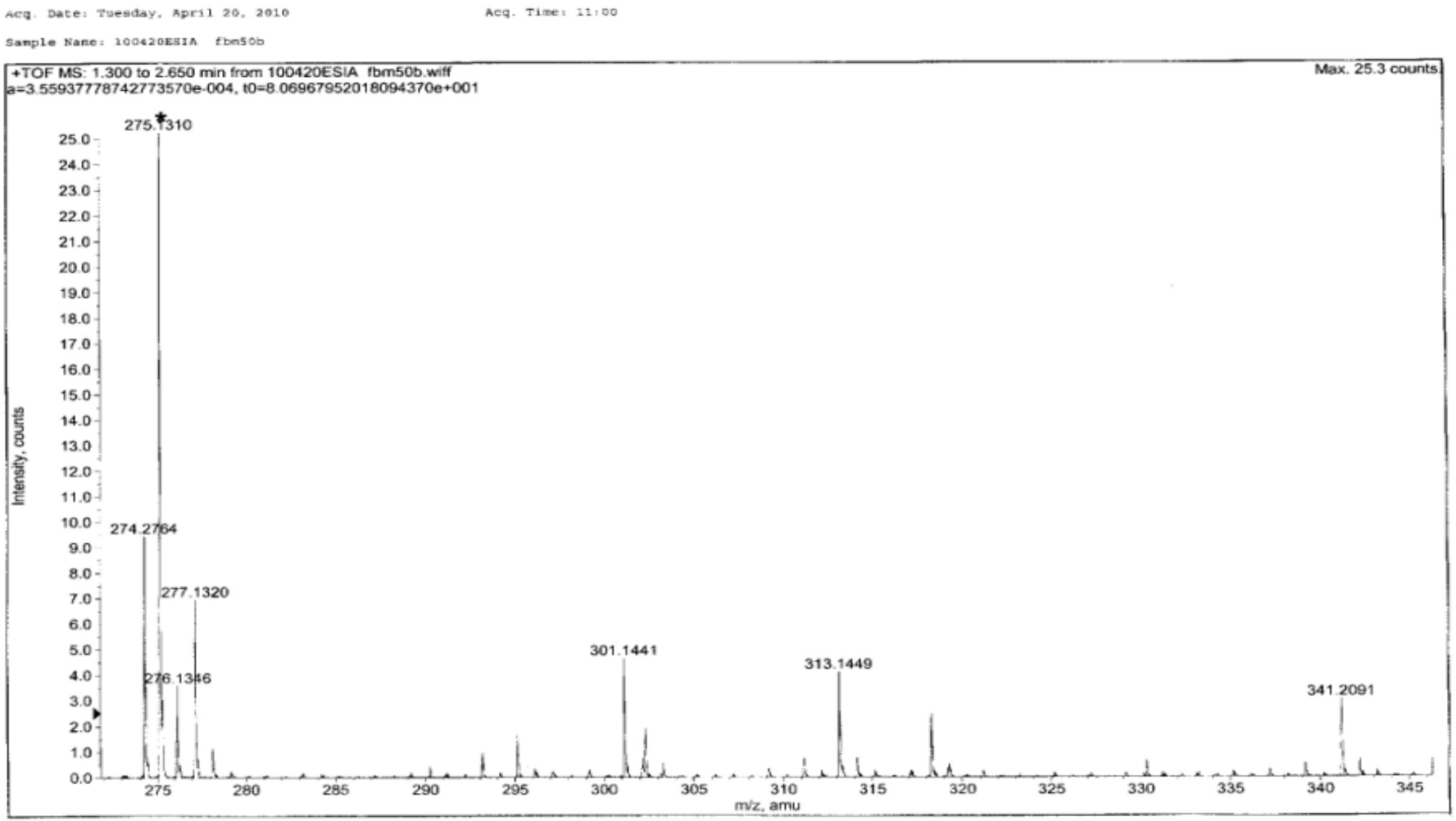


Figure S18. ^{1}H NMR Spectrum of Compound **4**.

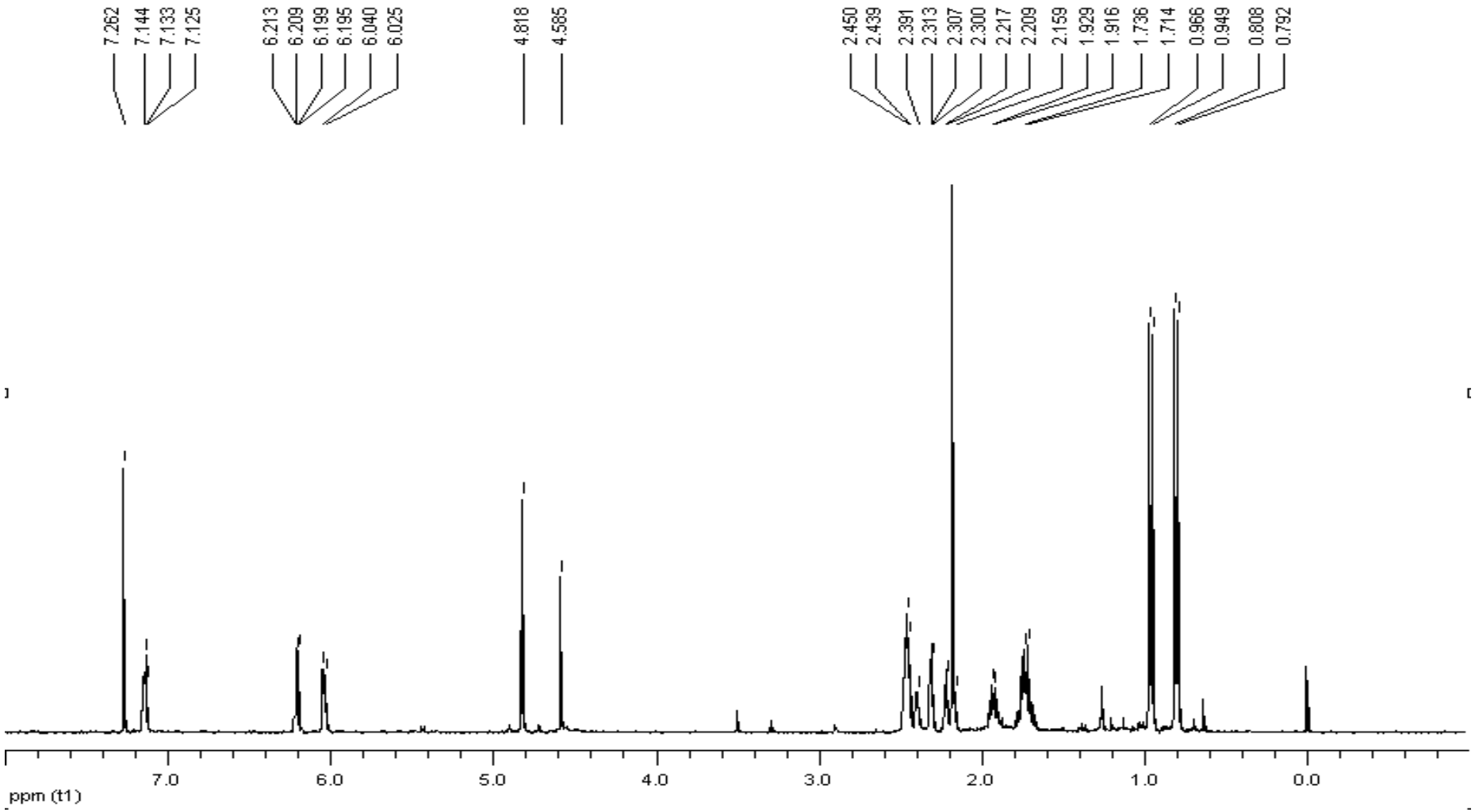


Figure S19. ^{13}C NMR Spectrum of Compound **4**.

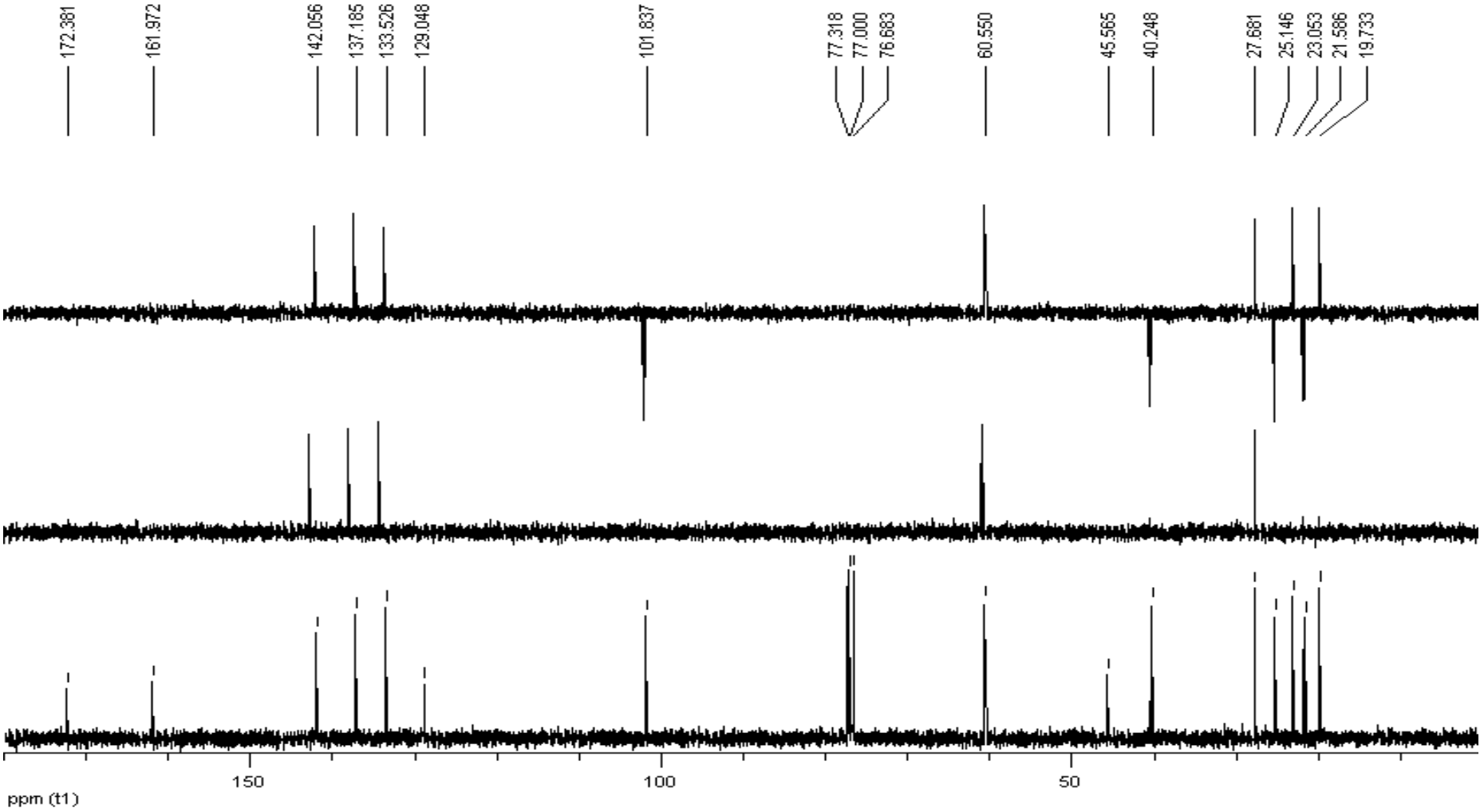


Figure S20. HSQC Spectrum of Compound **4**.

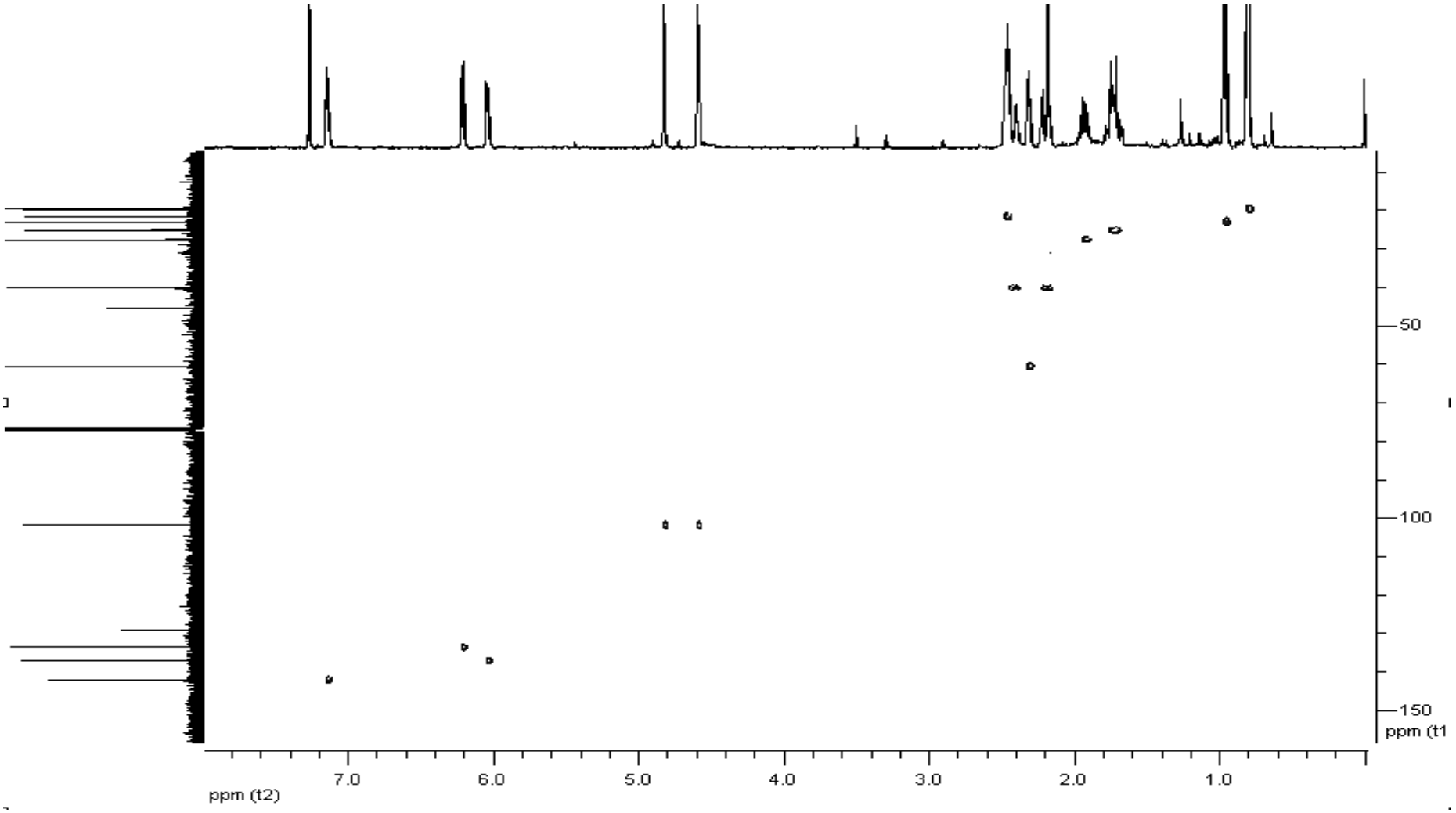


Figure S21. COSY Spectrum of Compound **4**.

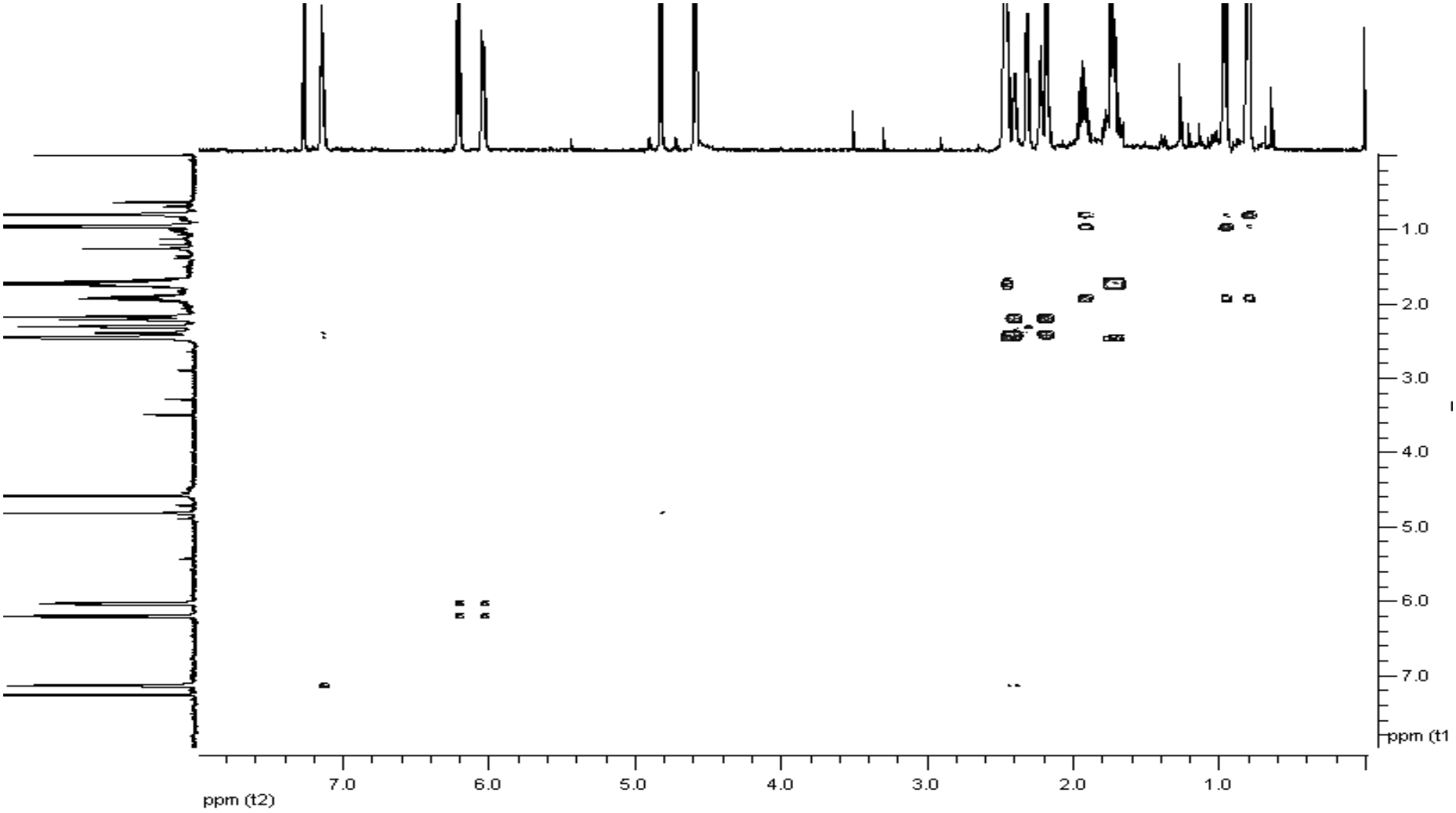


Figure S22. HMBC Spectrum of Compound **4**.

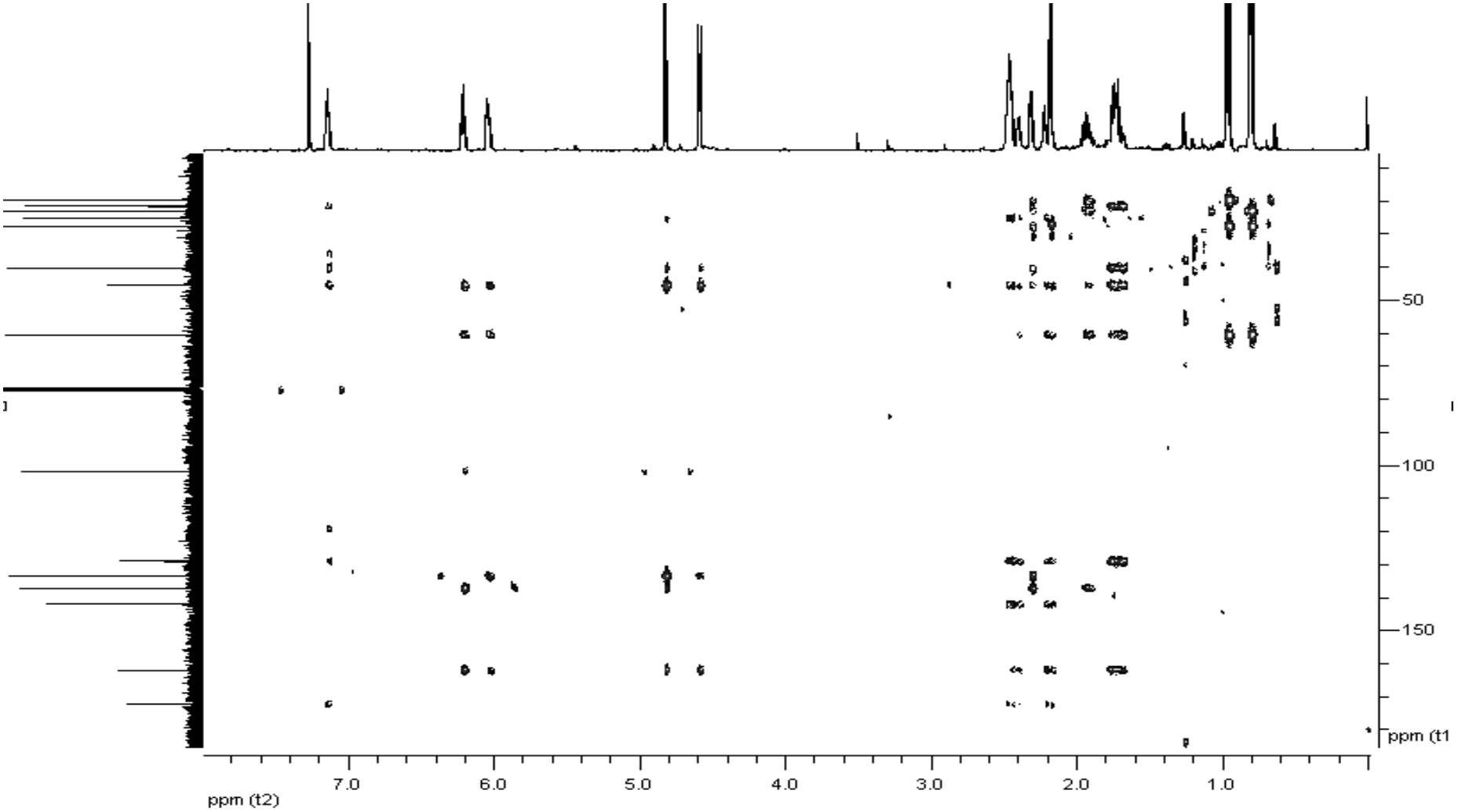


Figure S23. ROESY Spectrum of Compound **4**.

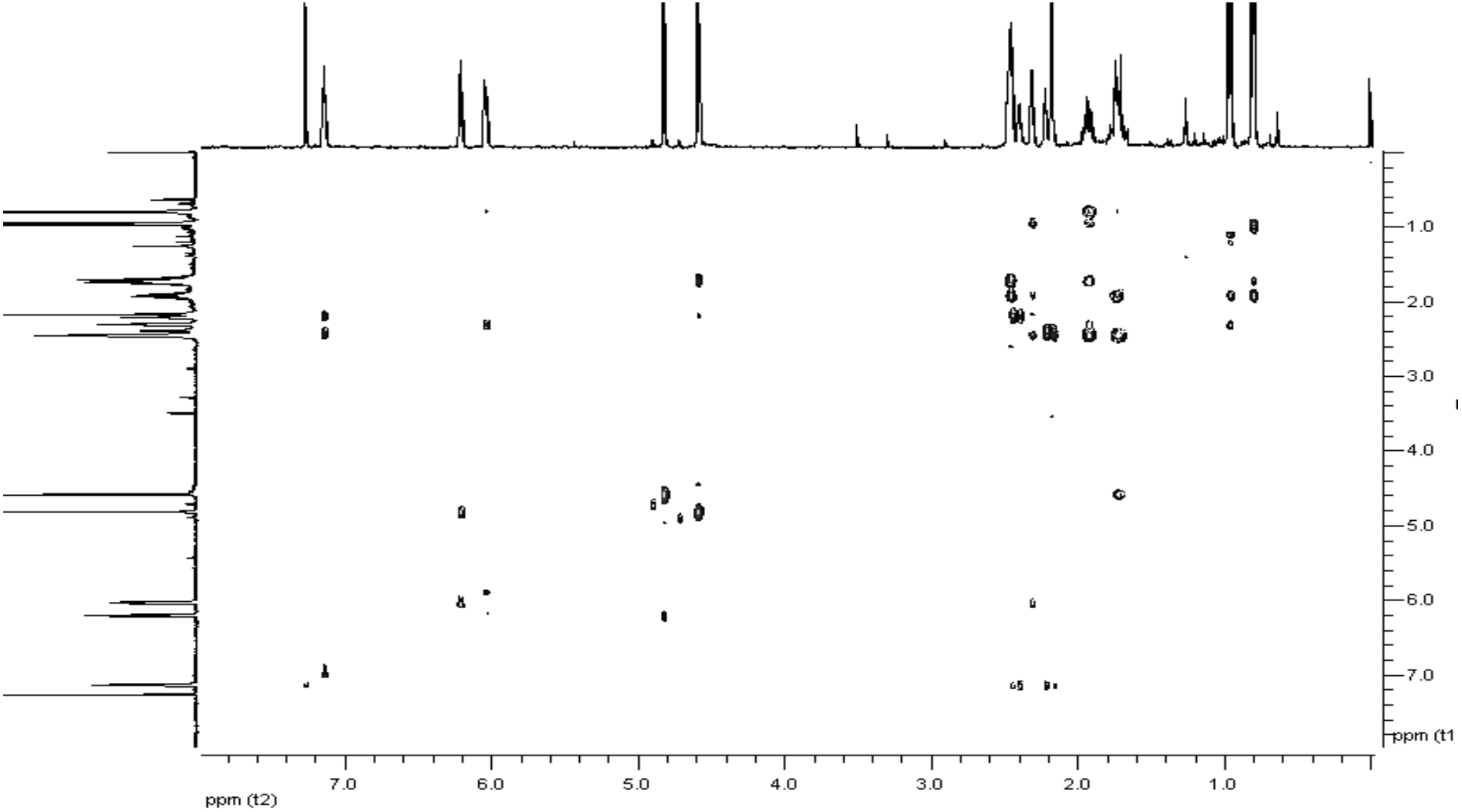


Figure S24. HRESIMS Spectrum of Compound **4**.

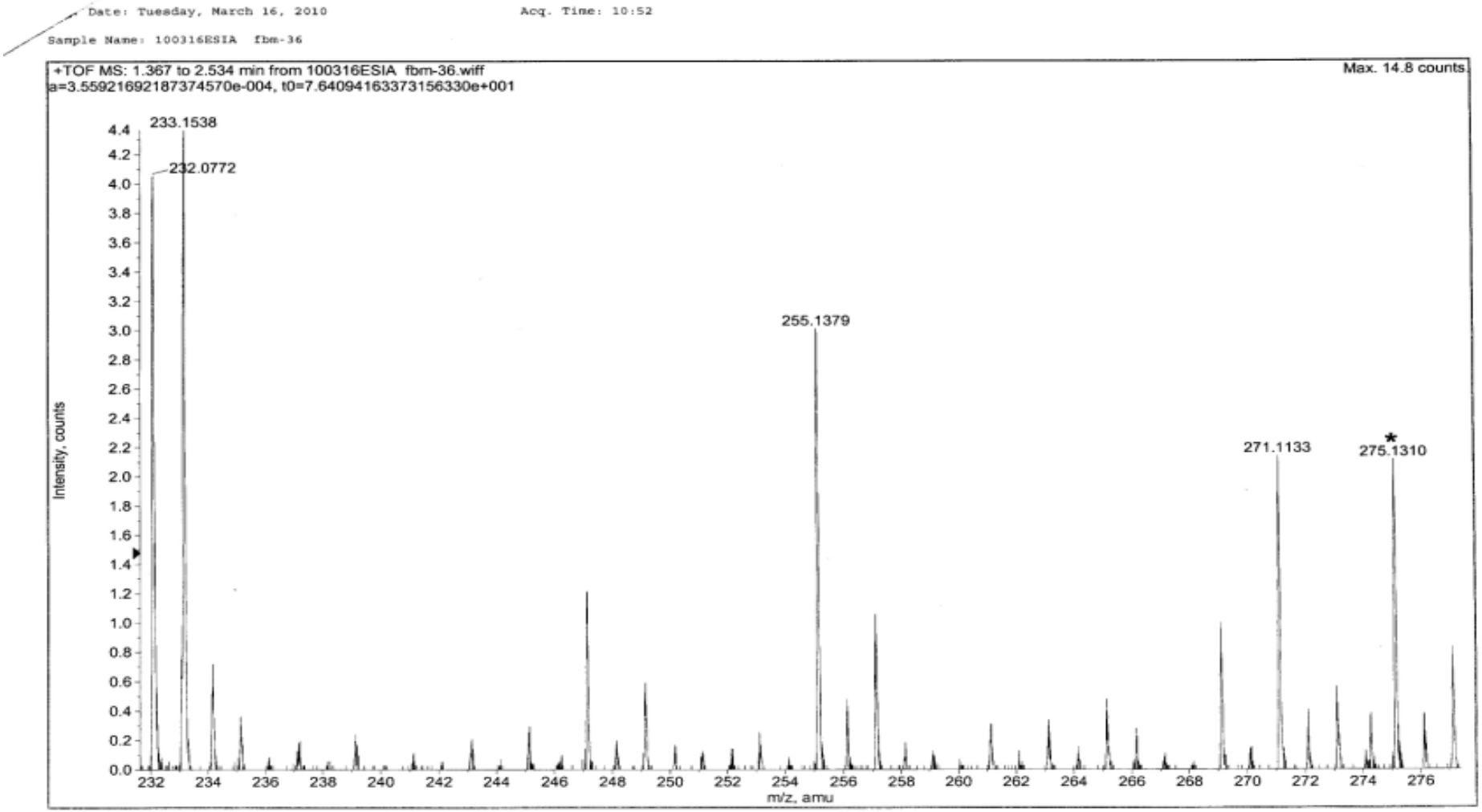


Figure S25. ^{1}H NMR Spectrum of Compound **5**.

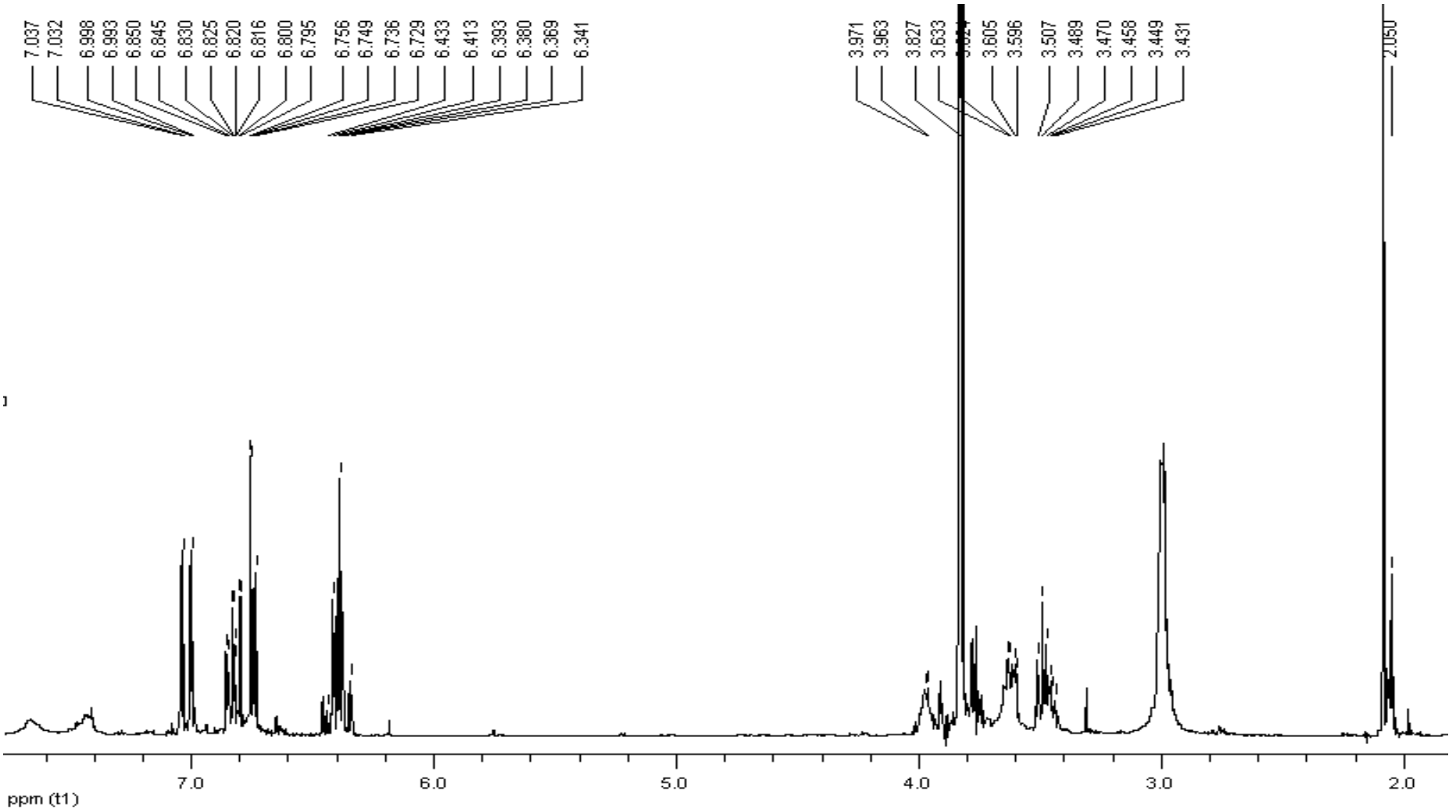


Figure S26. ^{13}C NMR Spectrum of Compound **5**.

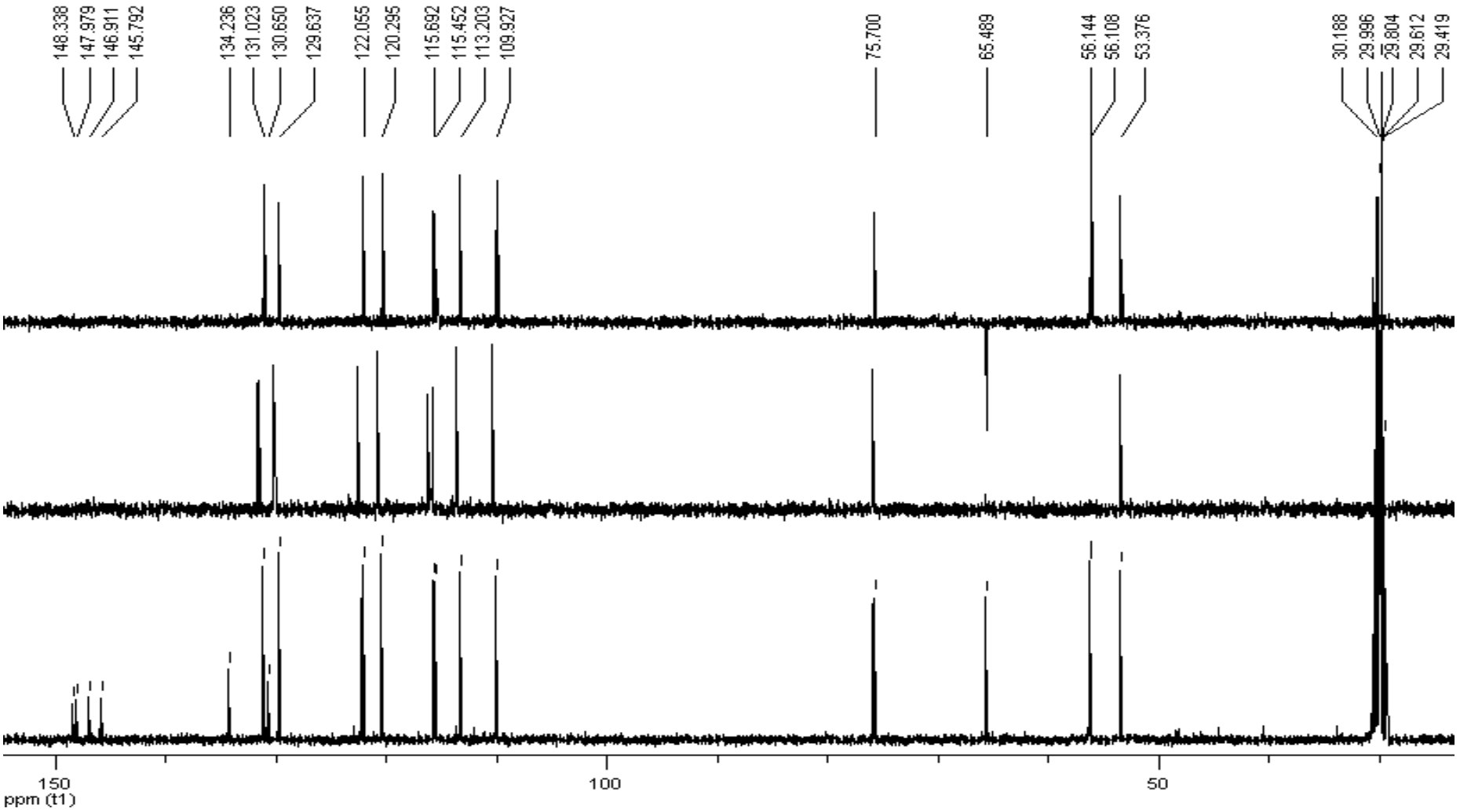


Figure S27. HRESIMS Spectrum of Compound **5**.

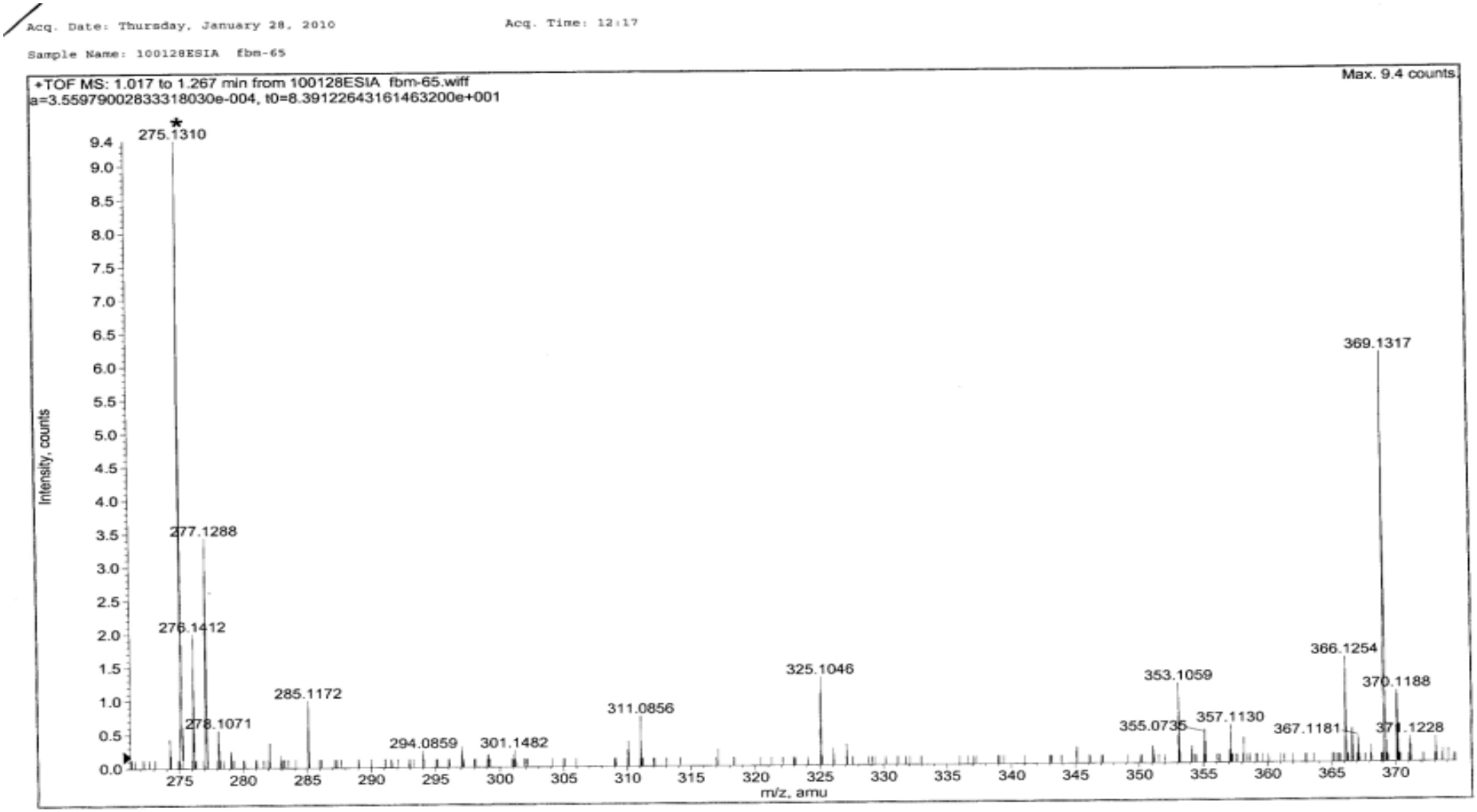


Figure S28. ^{1}H NMR Spectrum of Compound **6**.

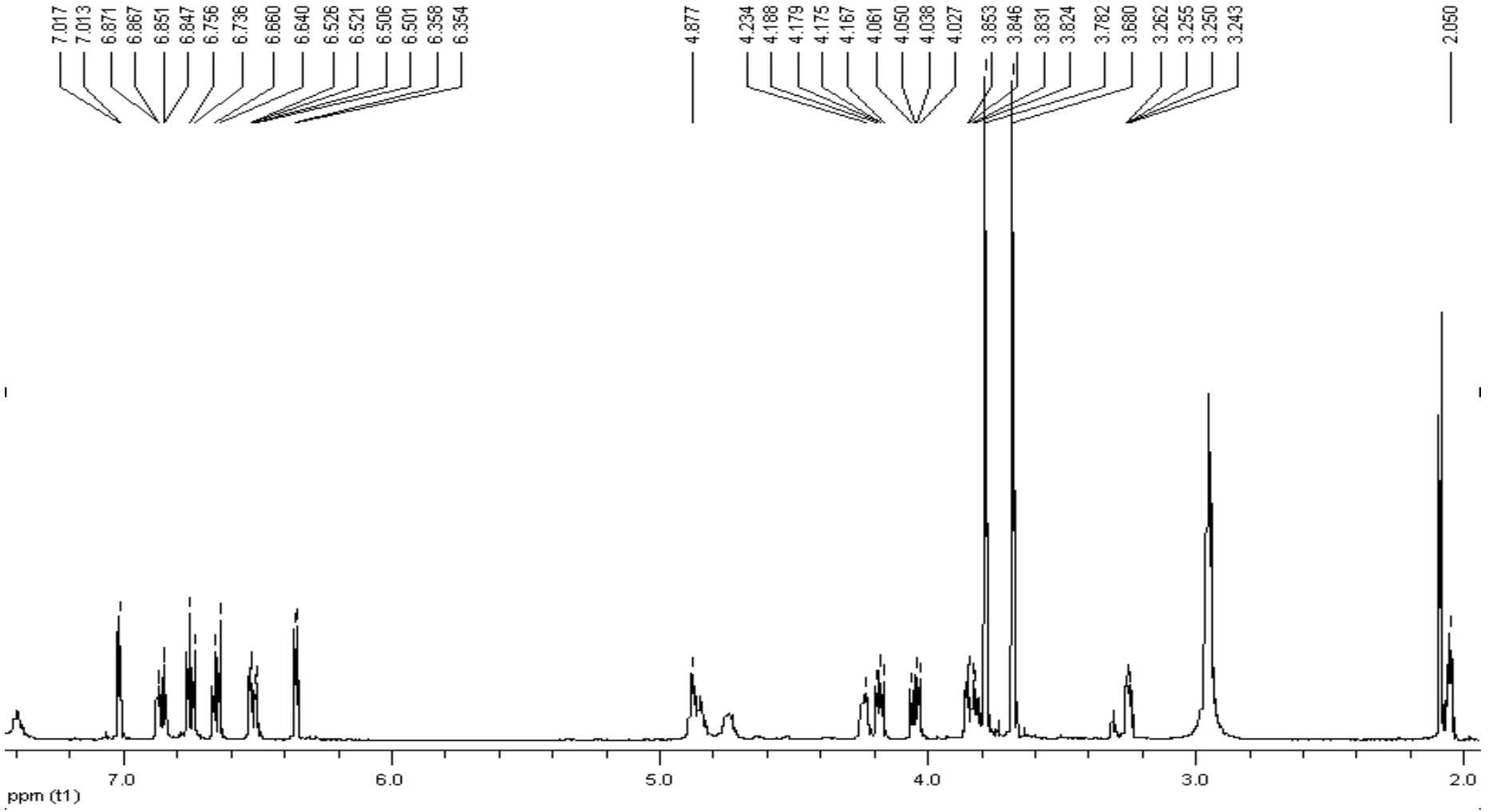


Figure S29. ^{13}C NMR Spectrum of Compound **6**.

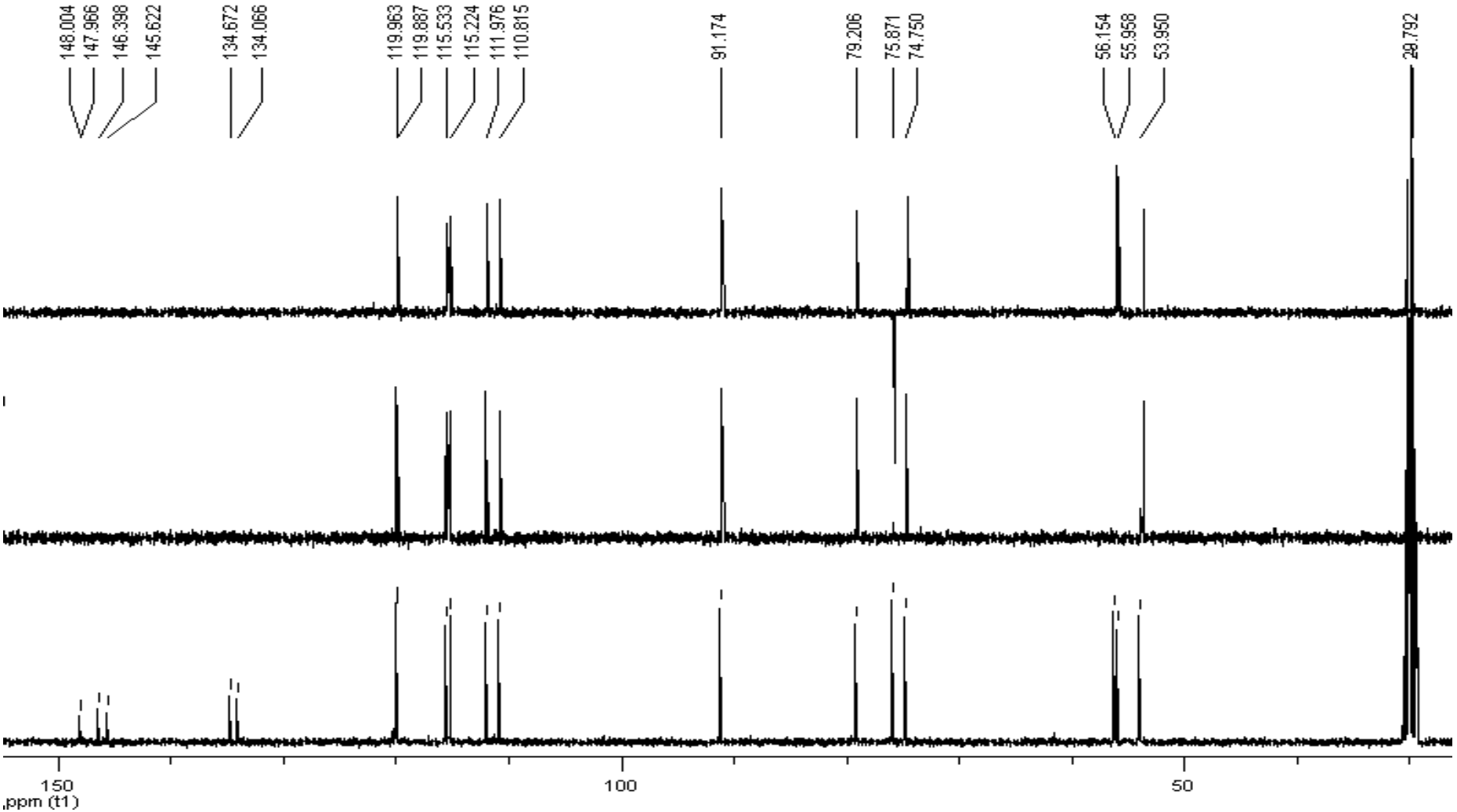


Figure S30. HSQC Spectrum of Compound **6**.

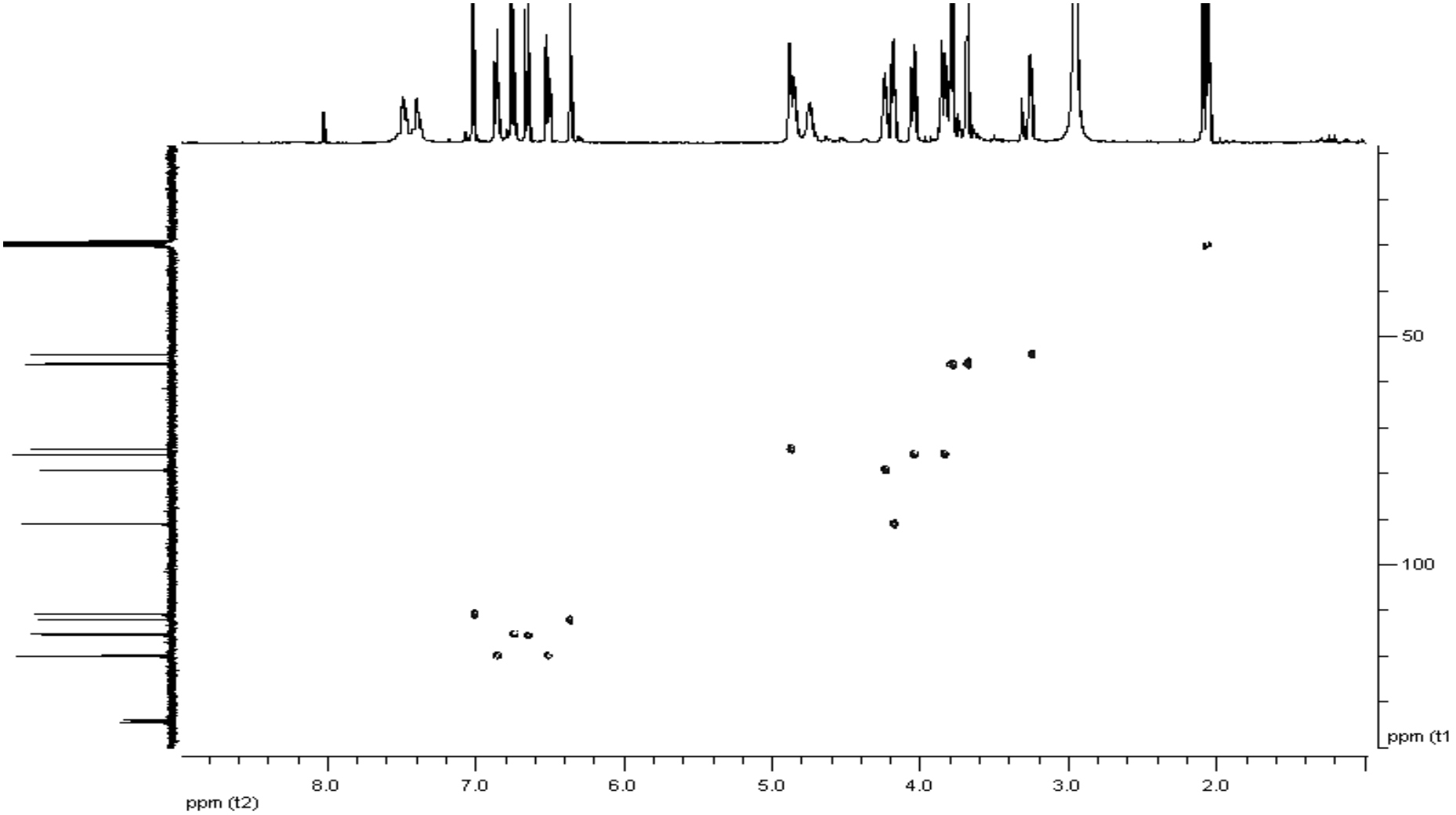


Figure S31. COSY Spectrum of Compound **6**.

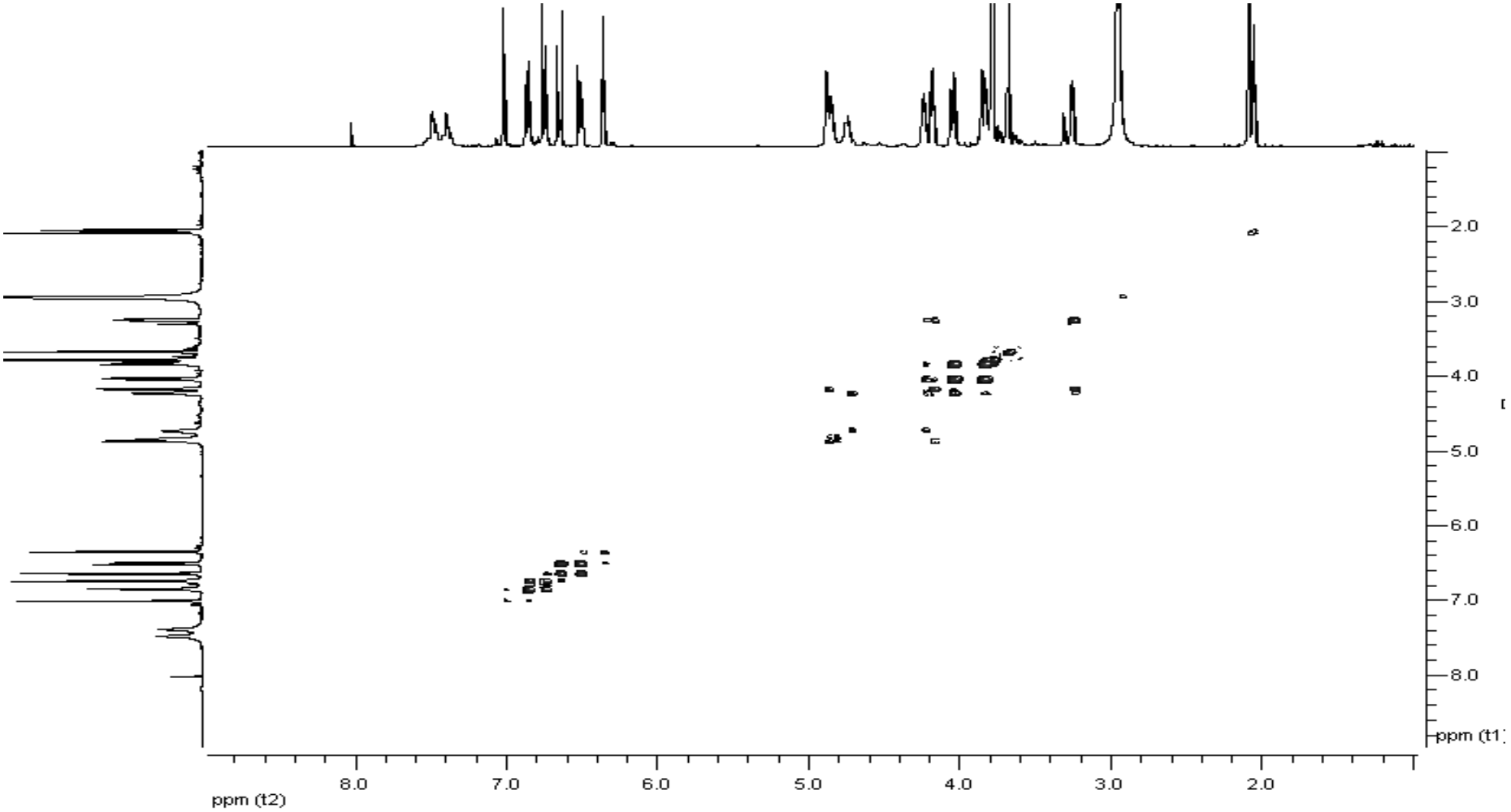


Figure S32. HMBC Spectrum of Compound **6**.

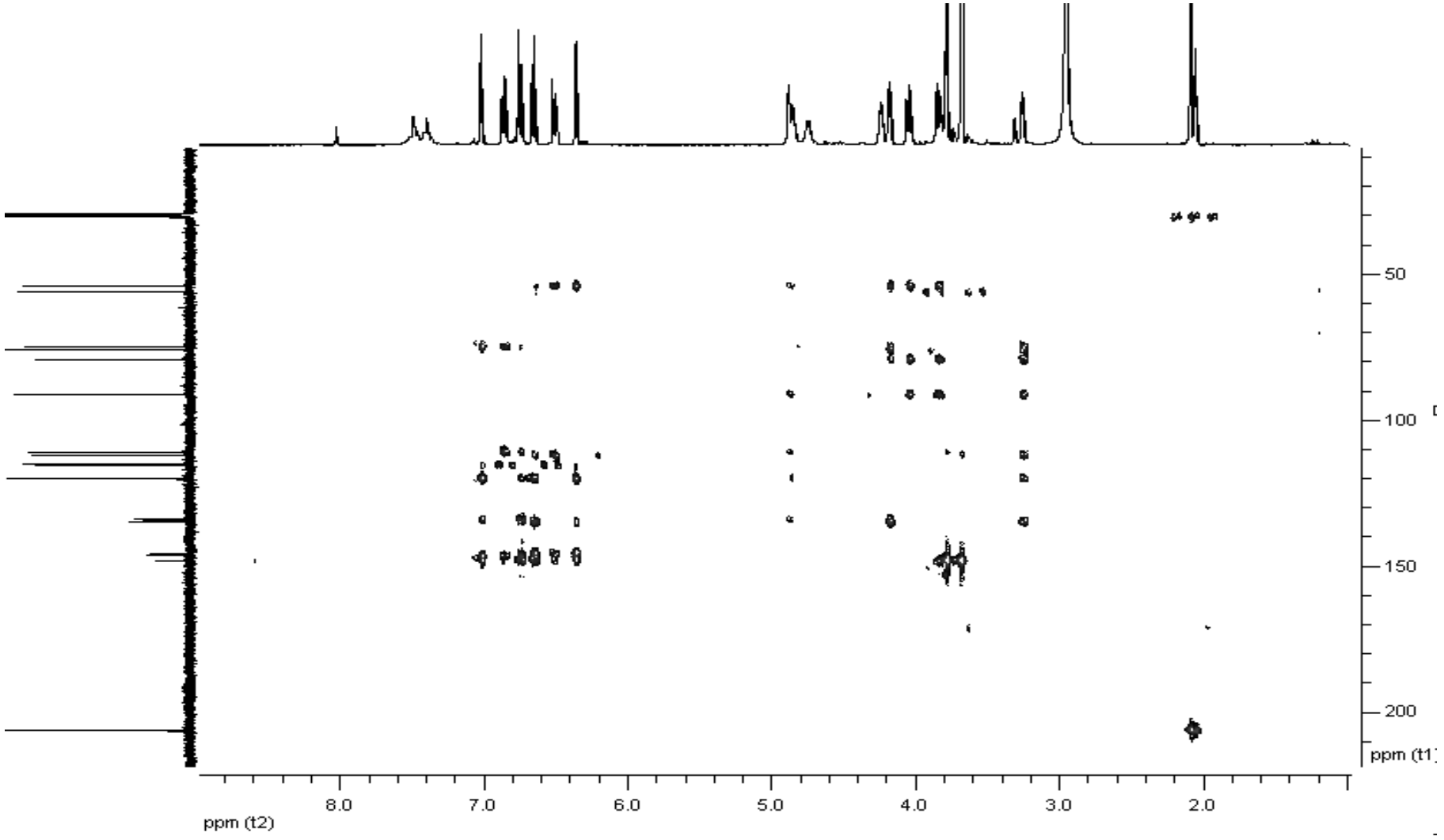


Figure S33. ROESY Spectrum of Compound **6**.

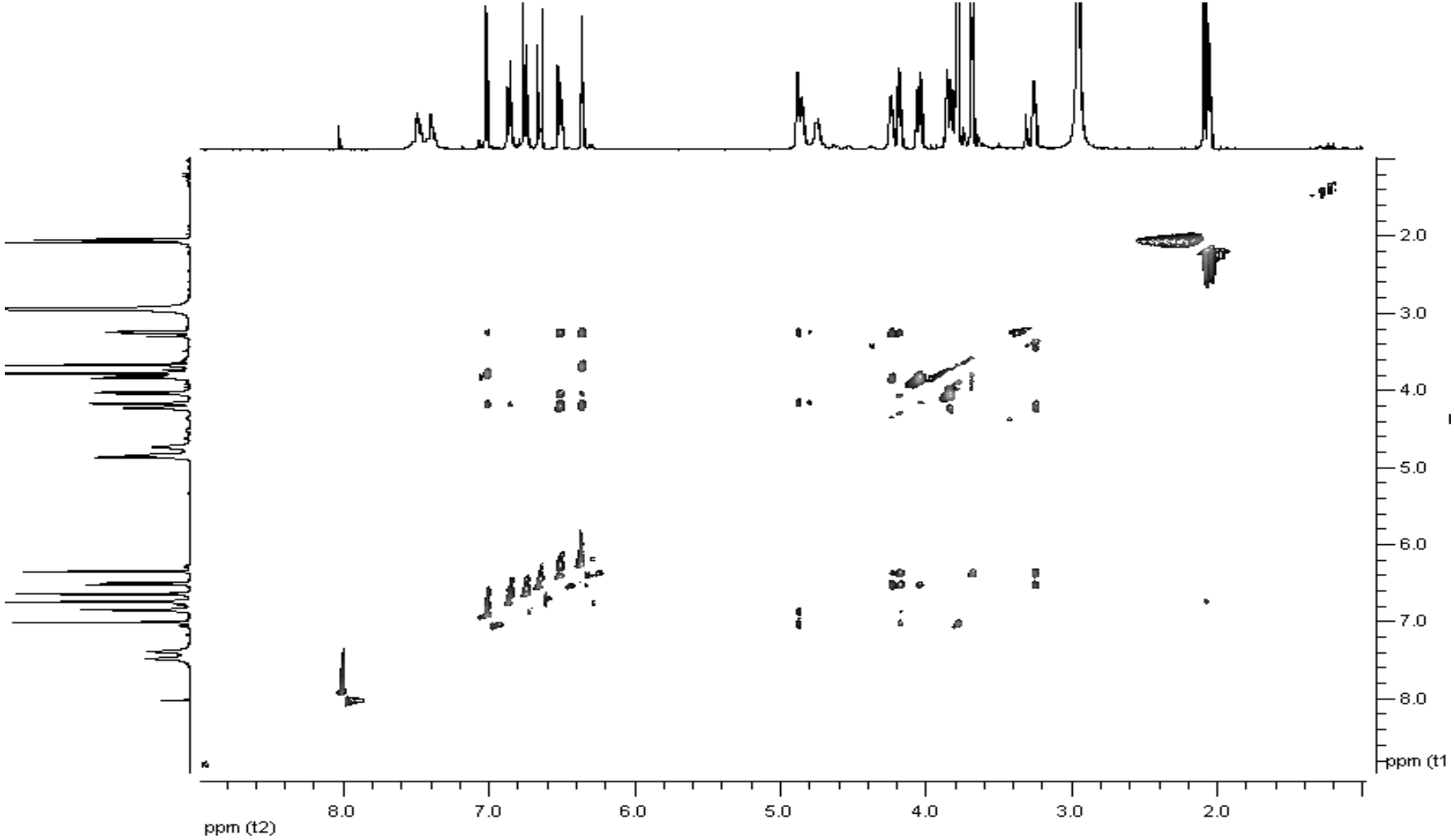


Figure S34. HRESIMS Spectrum of Compound **6**.

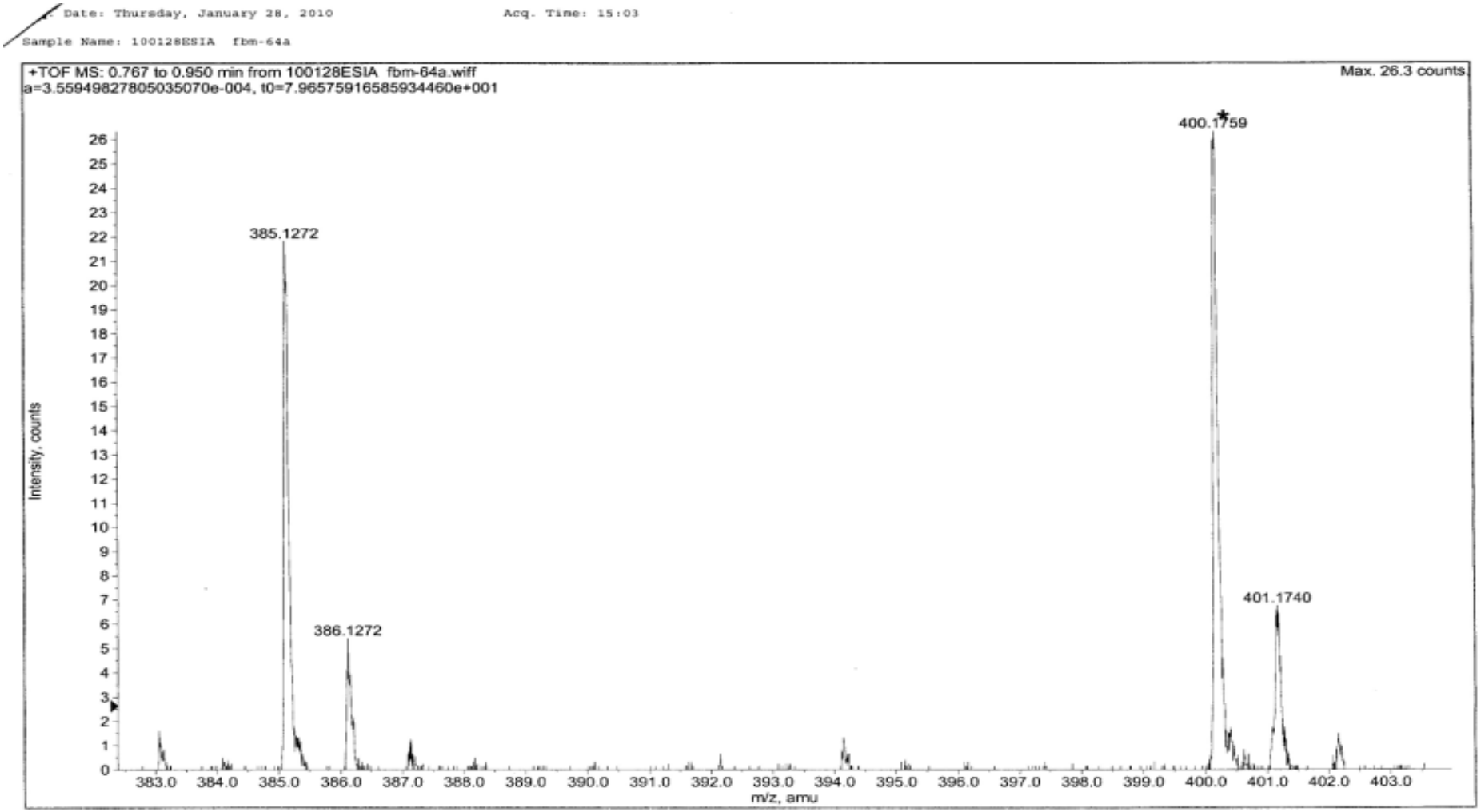


Figure S35. ^{1}H NMR Spectrum of Compound **7**.

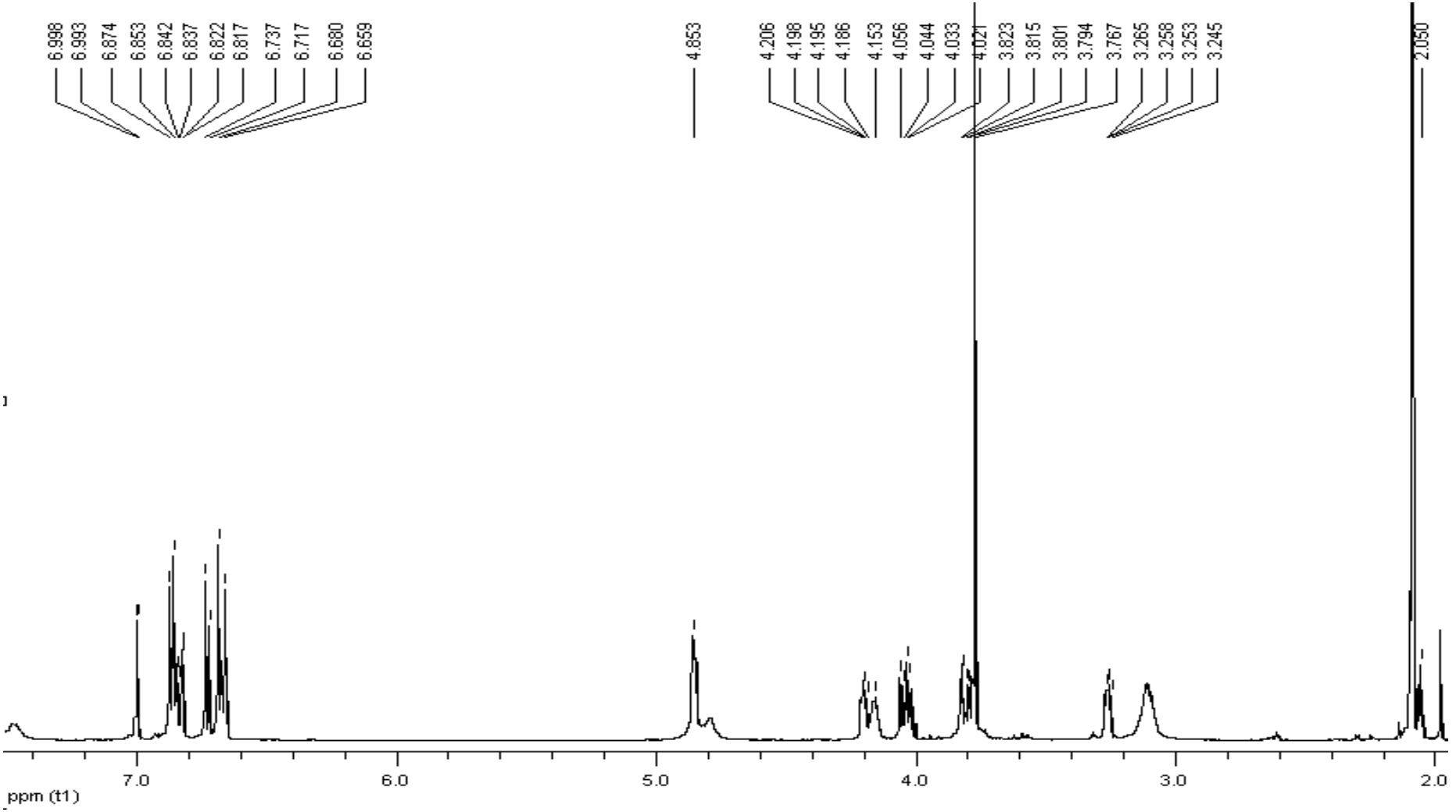


Figure S36. ^{13}C NMR Spectrum of Compound **7**.

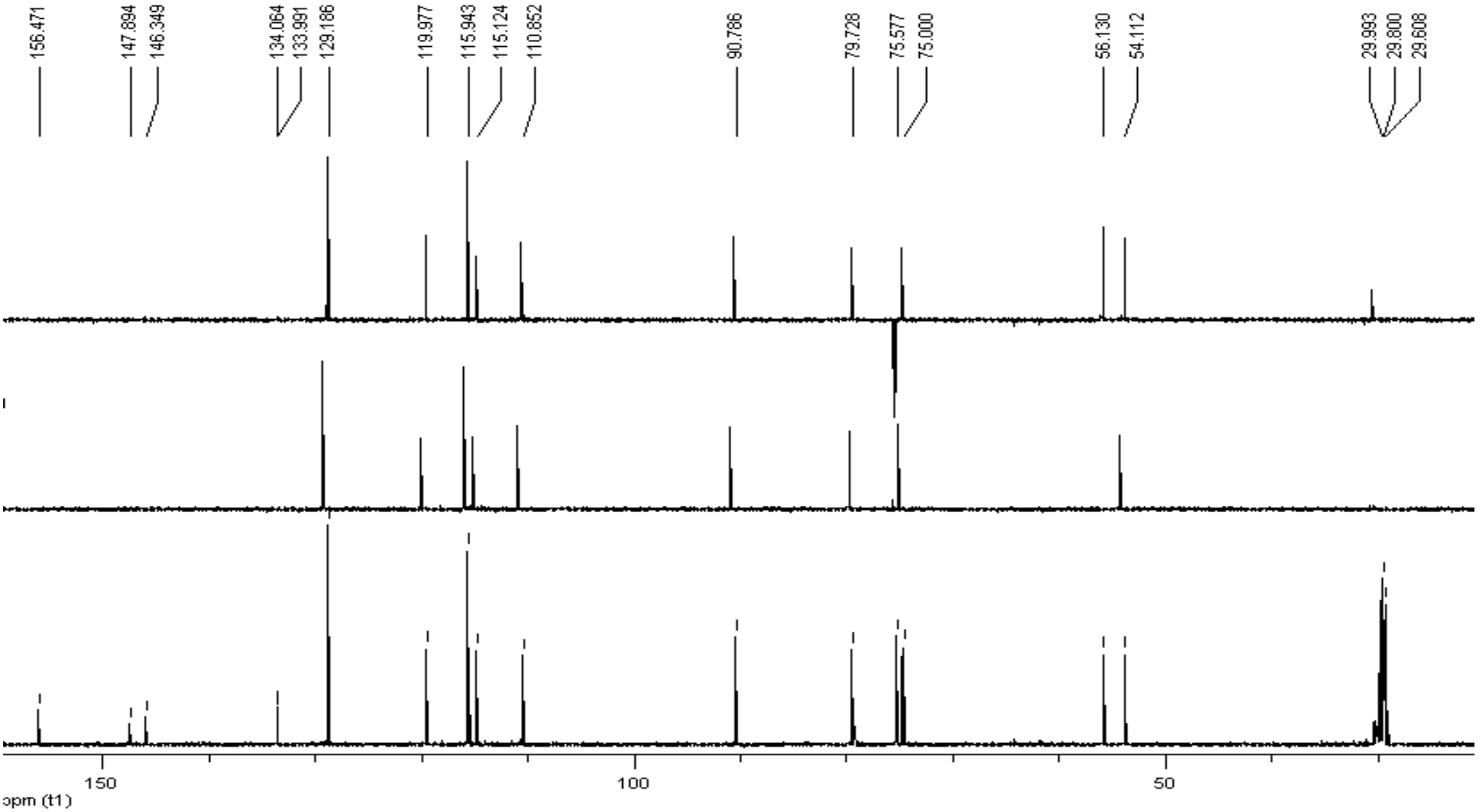


Figure S37. HRESIMS Spectrum of Compound **7**.

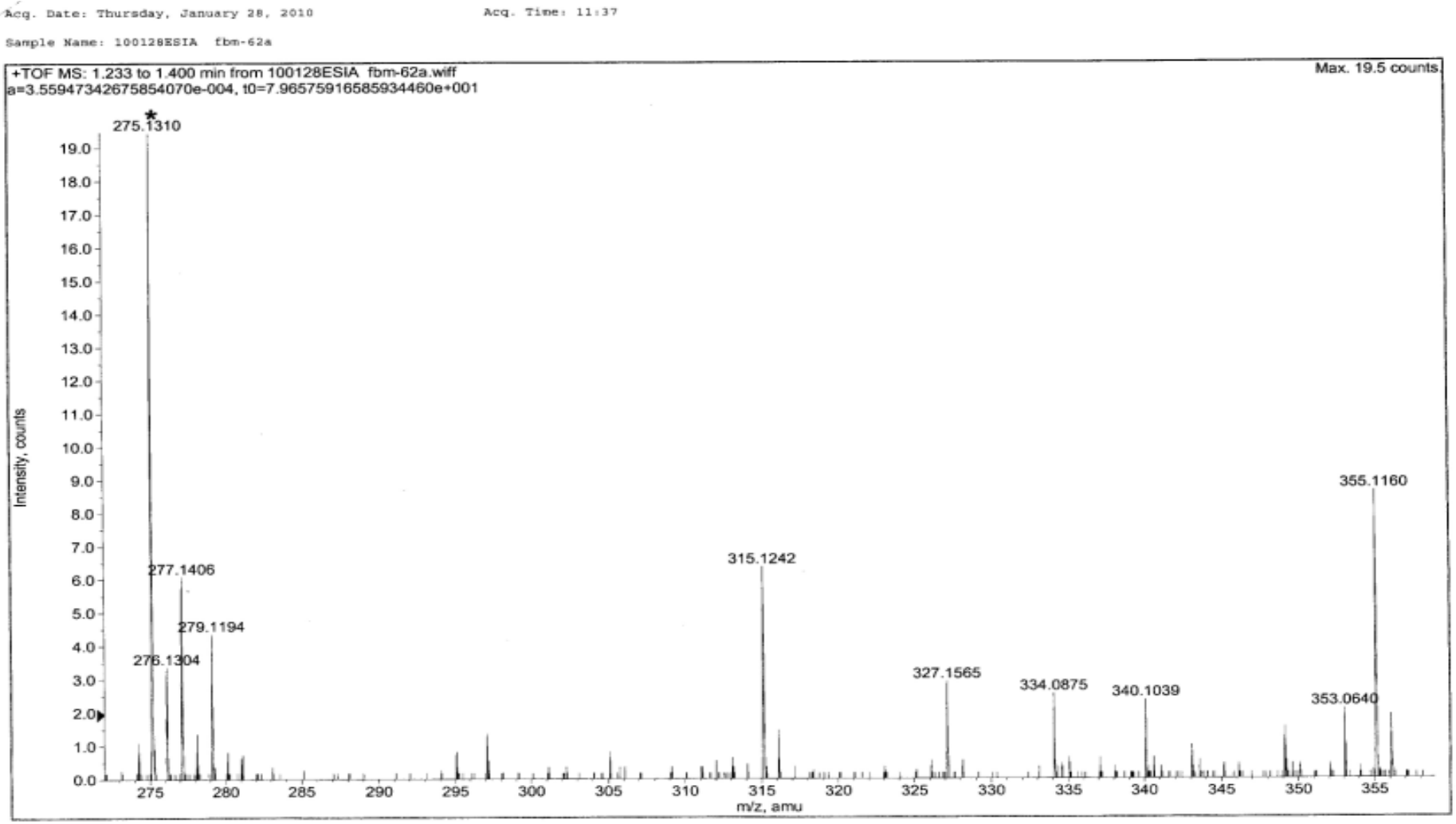


Figure S38. ^{1}H NMR Spectrum of Compound **8**.

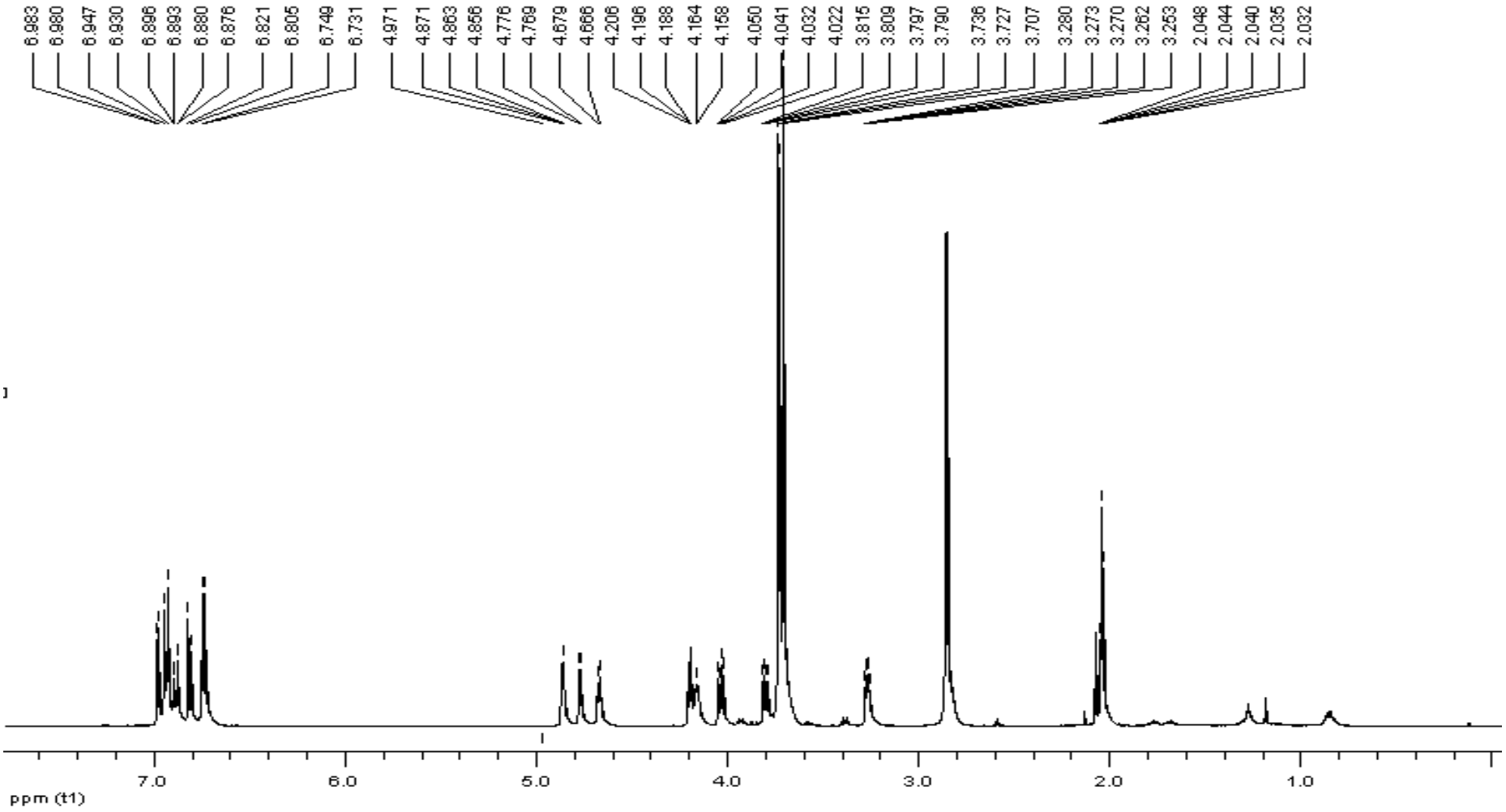


Figure S39. ^{1}H NMR Spectrum of Compound **9a**.

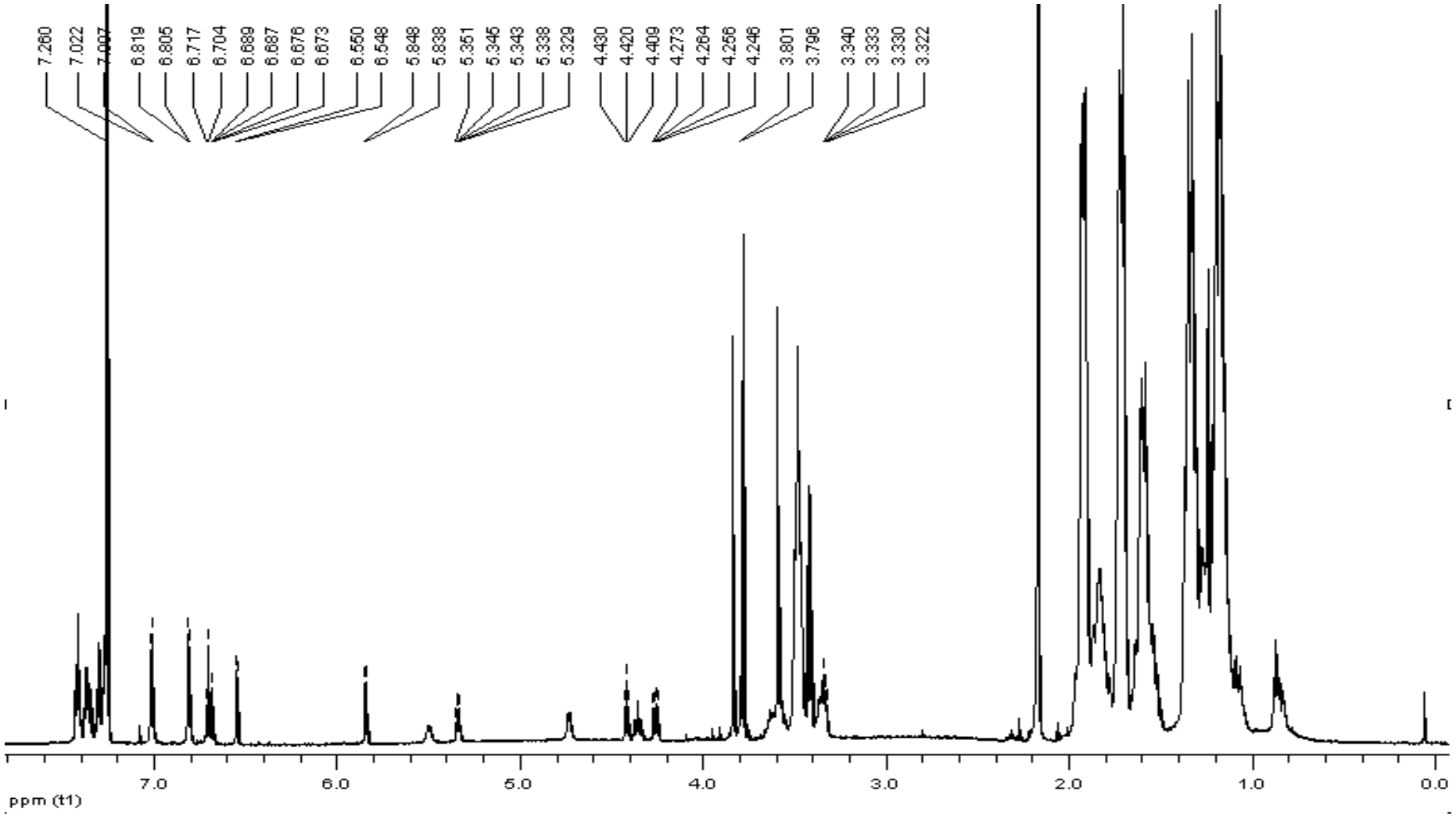


Figure S40. COSY Spectrum of Compound **9a**.

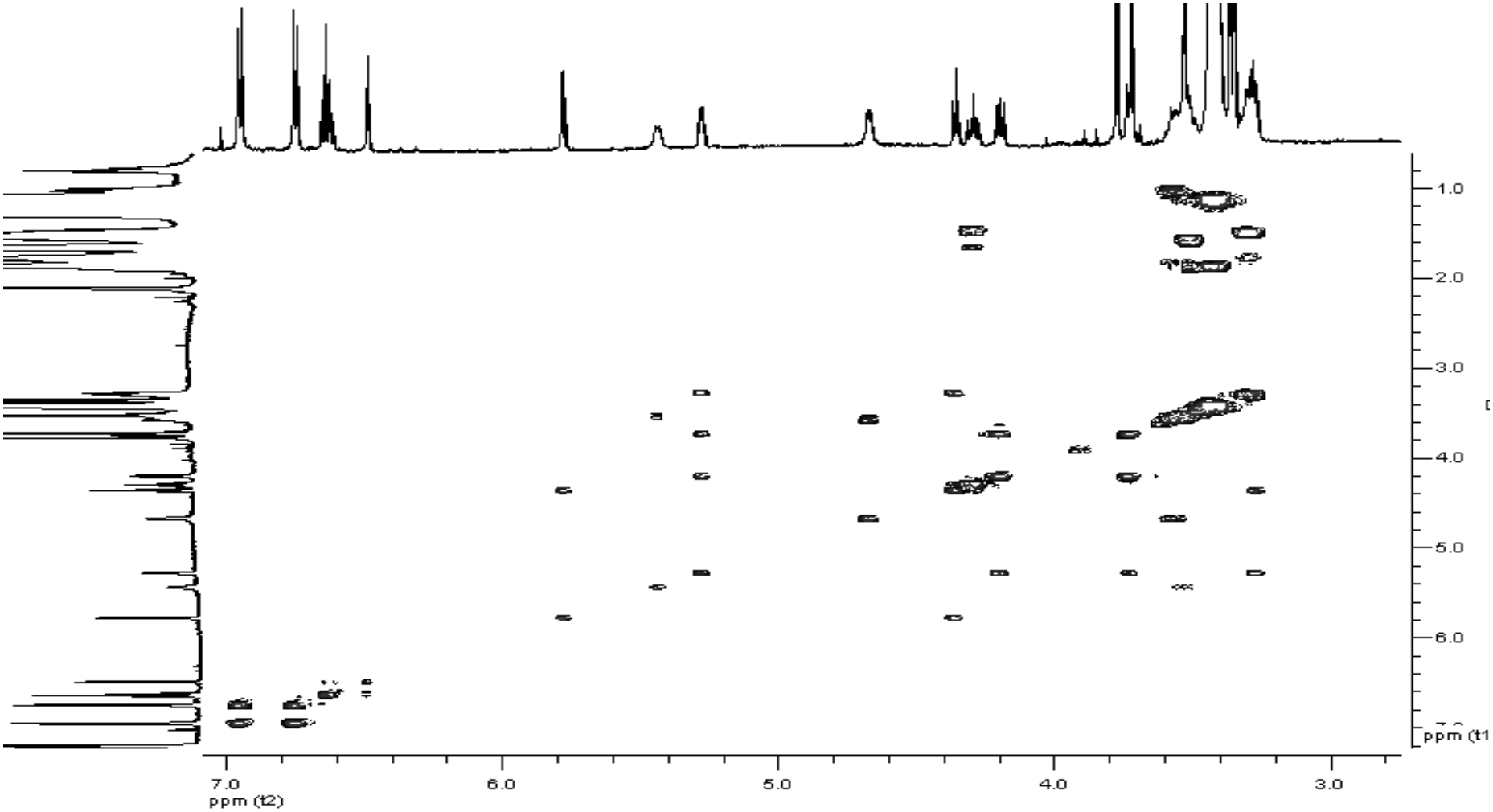


Figure S41. ^{1}H NMR Spectrum of Compound **9b**.

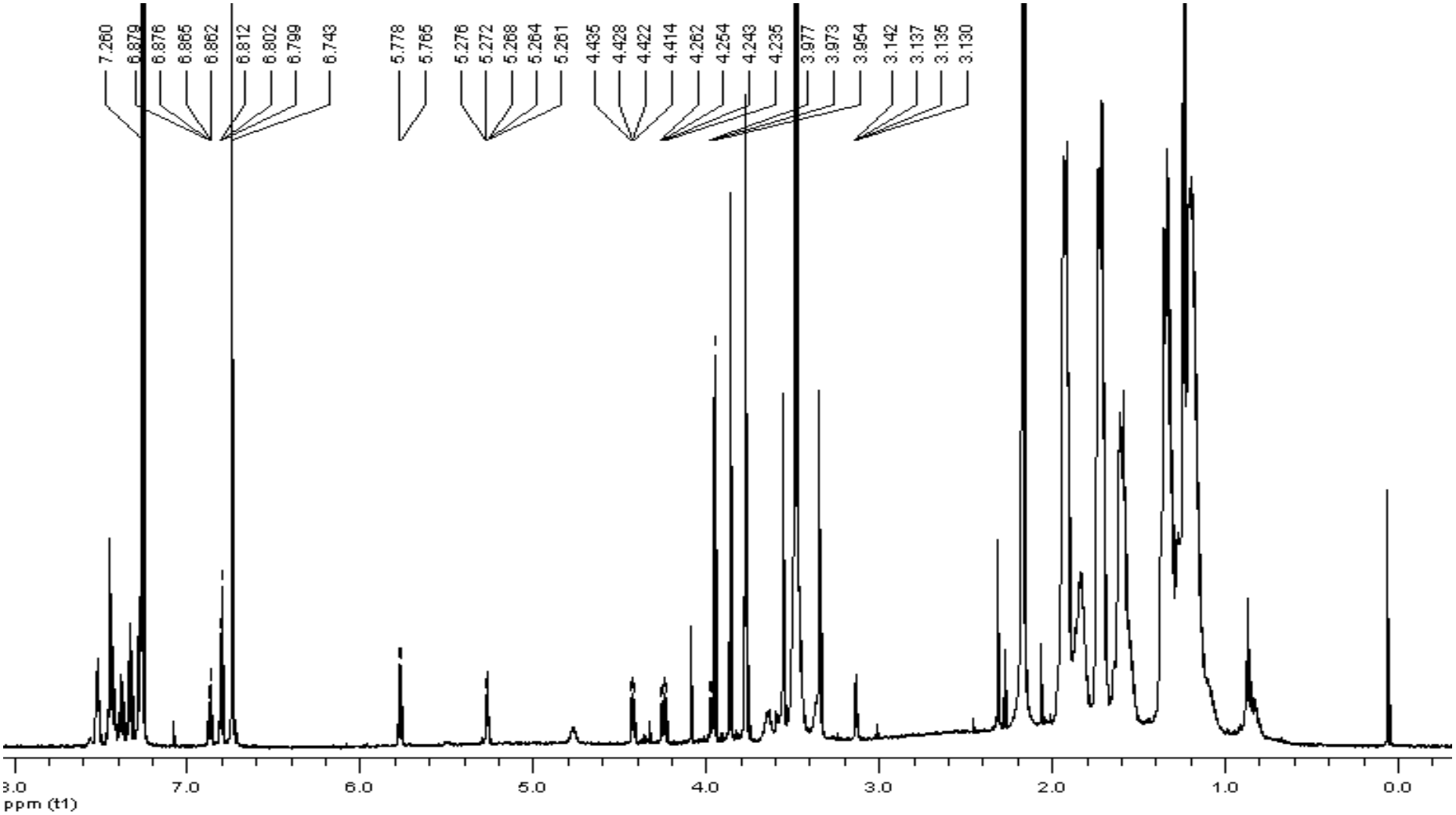


Figure S42. COSY Spectrum of Compound **9b**.

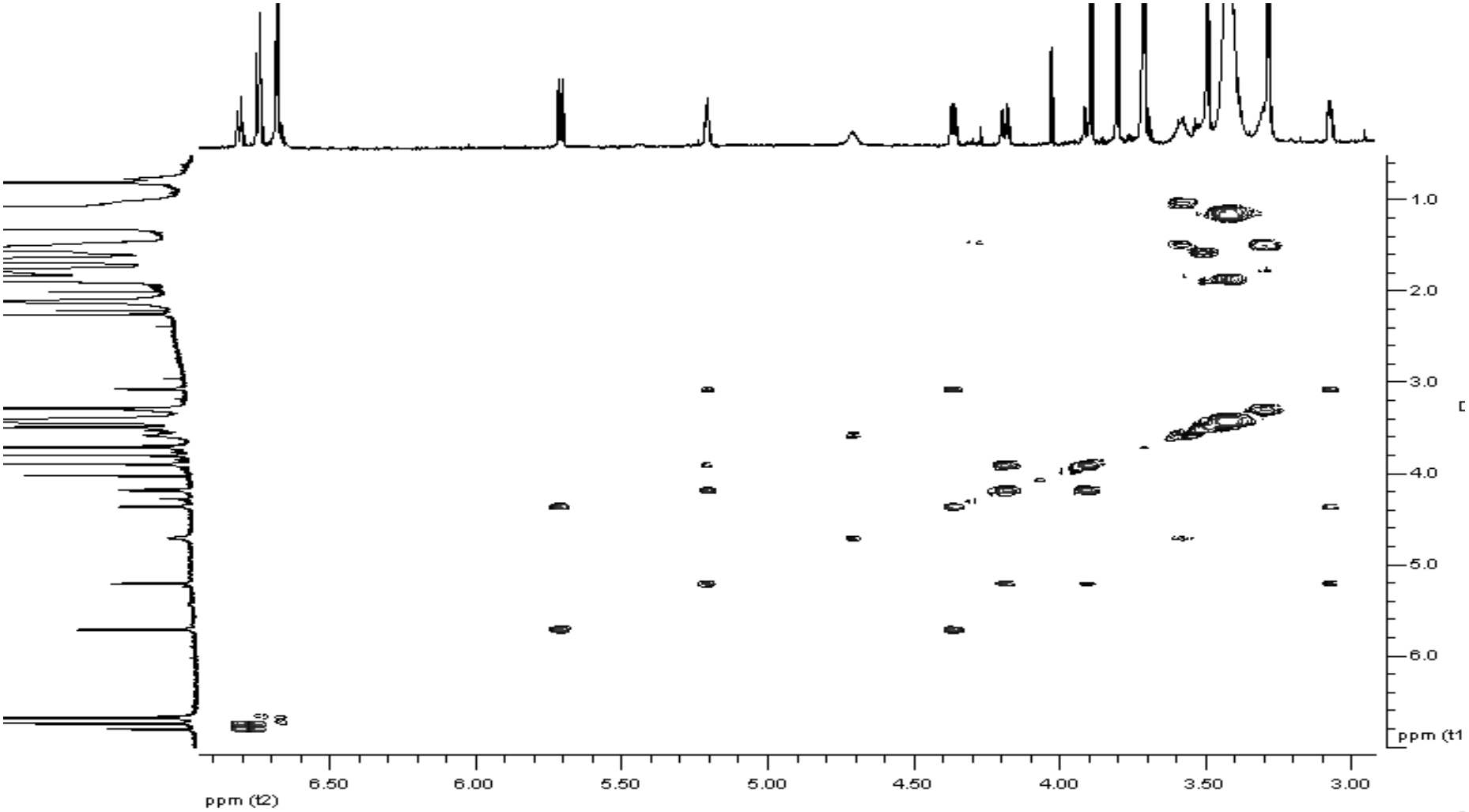
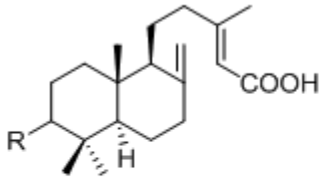
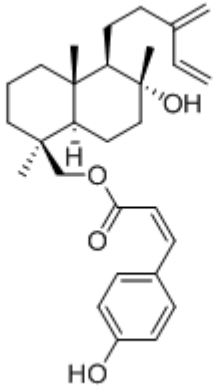


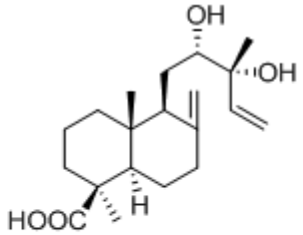
Figure S43. Structures of the known terpenoids.



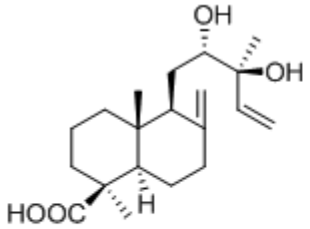
3-Hydroxylabda-8(20),13-dien-15-oic acid R = OH
3-Acetoxylabda-8(20),13-dien-15-oic acid R = $OCOCH_3$



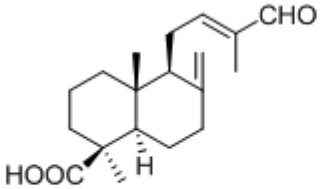
8α-Hydroxylabda-13(16),14-dien-19-yl-*cis*-4-hydroxycinnamate



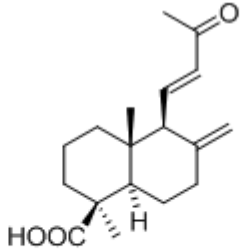
12*S*,13*R*-Dihydroxylabda-8(17),14-dien-19-oic acid



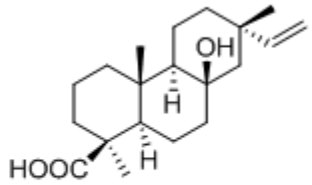
12*S*,13*S*-Dihydroxylabda-8(17),14-dien-19-oic acid



15-Norlabda-8(20),12*E*-diene-14-carboxaldehyde-19-oic acid

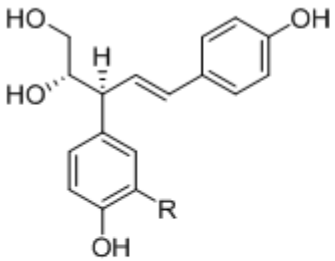


15,16-Bisnor-13-oxo-8(17),11*E*-labdadien-19-oic acid

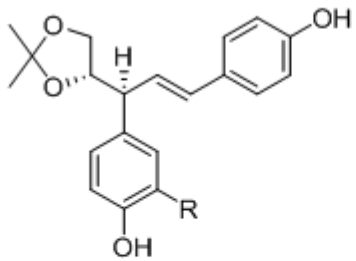


8β-Hydroxy-isopimar-15-en-19-oic acid

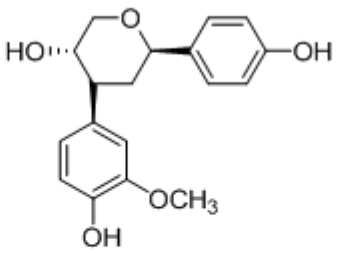
Figure S44. Structures of the known norlignans.



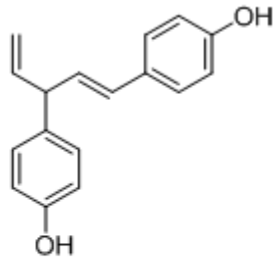
Agatharesinol R = H
Sequirin C R = OH
Sequosempervirin B R = OCH_3



Agatharesinol acetonide R = H
Sequosempervirin D R = OCH_3



Sequosempervirin F



Hinokiresinol