

Supplementary data for

New E:B-friedo-Hopane Type Triterpenoids from *Euphorbia peplus* with Simiarendiol Possessing Significant Cytostatic Activity against HeLa Cells by Induction of Apoptosis and S/G2 Cell Cycle Arrest

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Table S1. The preliminary cytotoxic screening results for compounds **1–12** at 30 μM

Compds.	HeLa	A549	MCF-7	MDA-MB-231
1	46.98%	40.23%	22.60%	46.01%
2	96.82%	98.52%	94.44%	80.22%
3	-6.82%	6.32%	-4.61%	-3.09%
4	3.78%	12.12%	23.34%	29.44%
5	27.22%	23.36%	-1.74%	23.57%
6	42.41%	-16.16%	1.36%	2.85%
7	47.25%	17.07%	3.68%	10.63%
8	15.77%	28.09%	13.56%	21.63%
9	-12.59%	10.32%	1.45%	20.21%
10	9.63%	-15.30%	10.94%	5.52%
11	44.02%	12.36%	23.41%	47.55%
12	-0.24%	-3.75%	0.38%	19.12%

Table S2. Re-optimized conformers, energies and proportions for **1**

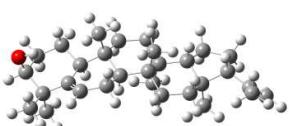
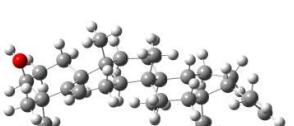
Number	Conformer	Energy (hartree)	Energy (kcal/mol)	Proportion (%)
1		-1247.5965011	-782879.280405261	39.47
2		-1247.5952798	-782878.514027298	10.81
3		-1247.5930675	-782877.125786925	1.04
4		-1247.5956592	-782878.752104592	16.17
5		-1247.5959064	-782878.907225064	21.01
6		-1247.5953387	-782878.550987637	11.51

Table S3. Re-optimized conformers, energies and proportions for **3**

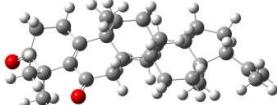
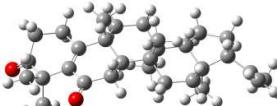
Number	Conformer	Energy (hartree)	Energy (kcal/mol)	Proportion (%)
1		-1320.4351139	-828586.238323389	67.93
2		-1320.4340493	-828585.570276243	21.97
3		-1320.4316955	-828584.093243205	1.81
4		-1320.4331291	-828584.992841541	8.28

Table S4. Re-optimized conformers, energies and proportions for **5**

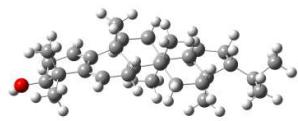
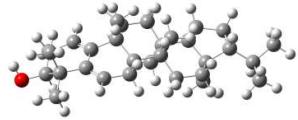
Number	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1247.6113009	-782888.567427759	23.85
2		-1247.6118684	-782888.923539684	43.53
3		-1247.6115965	-782888.752919715	32.63

Figure S1. ^1H NMR spectrum of **1** in CDCl_3

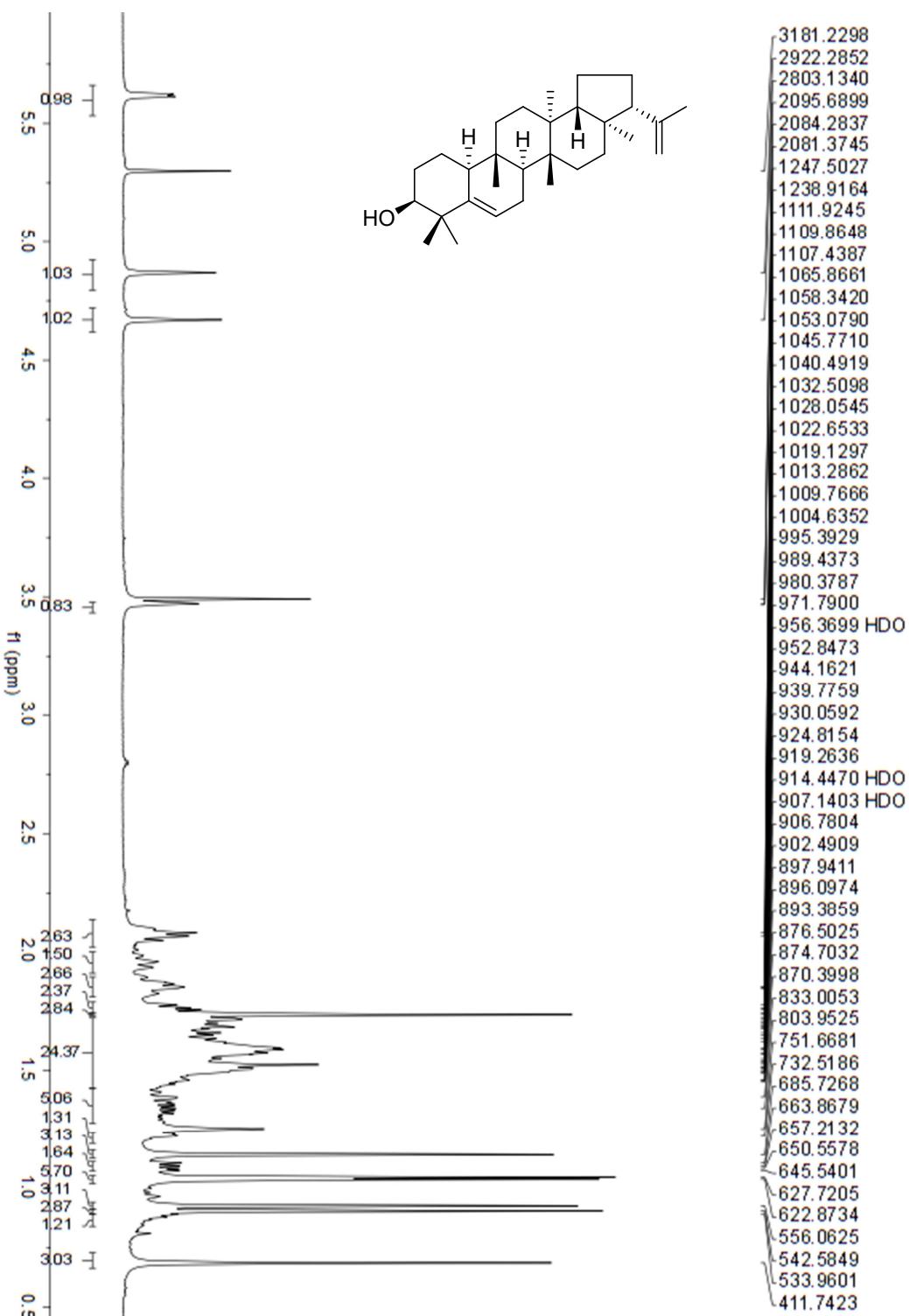


Figure S2. ^{13}C NMR spectrum of **1** in CDCl_3

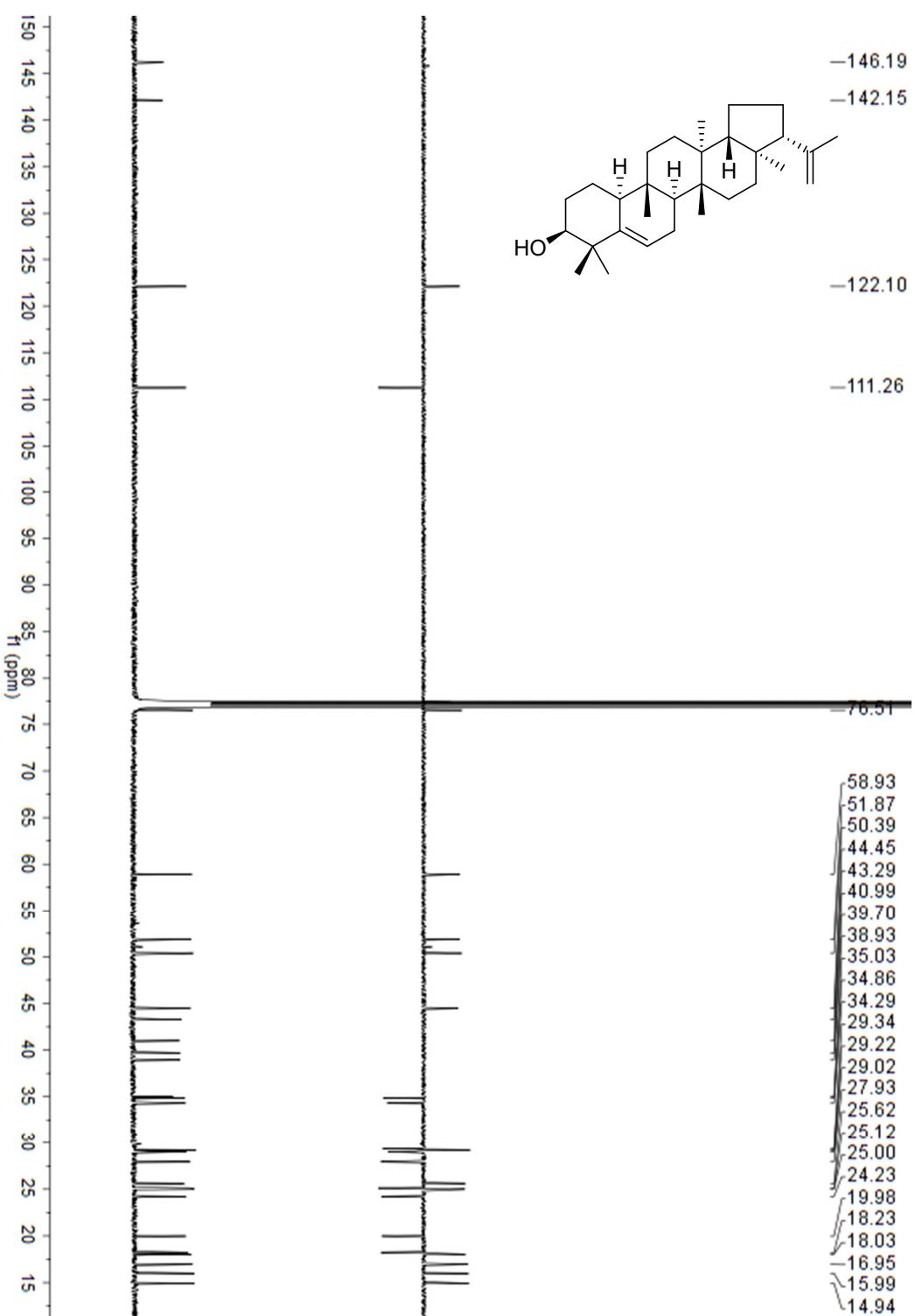


Figure S3. ^1H - ^1H COSY NMR spectrum of **1** in CDCl_3

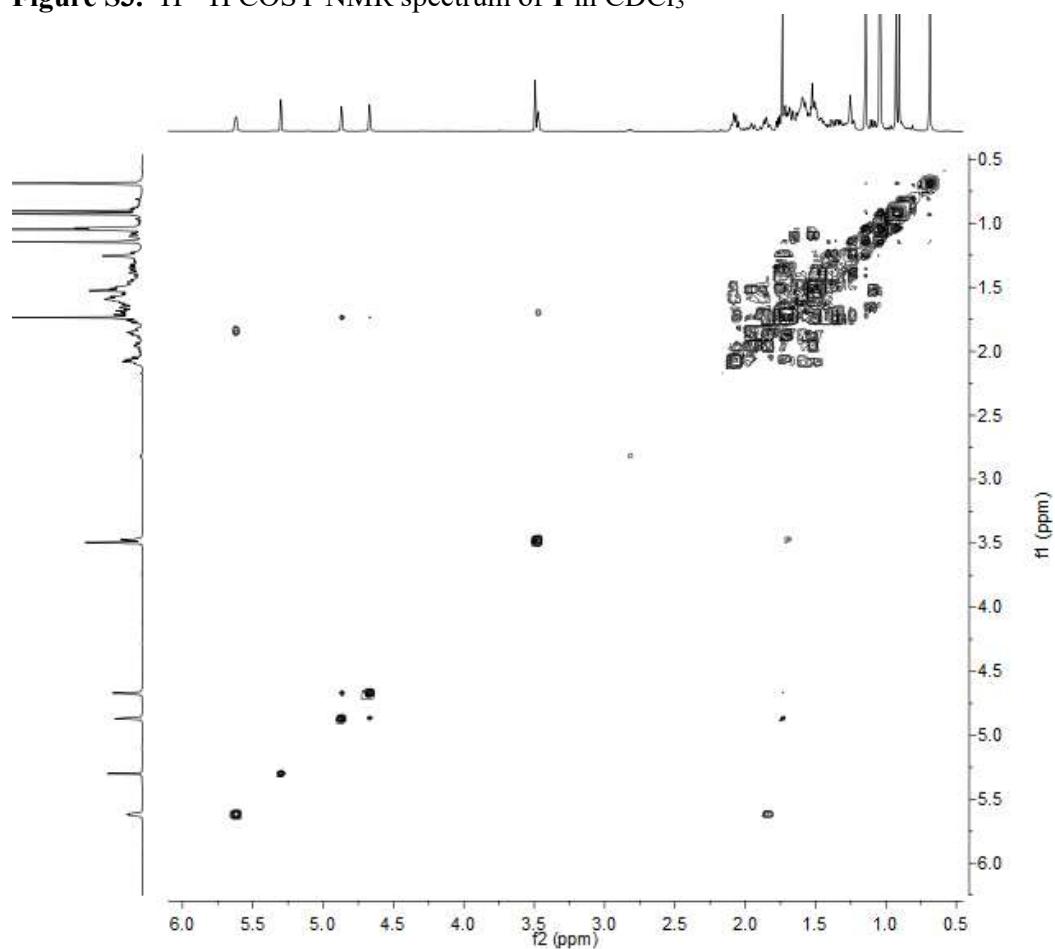


Figure S4. HSQC NMR spectrum of **1** in CDCl_3

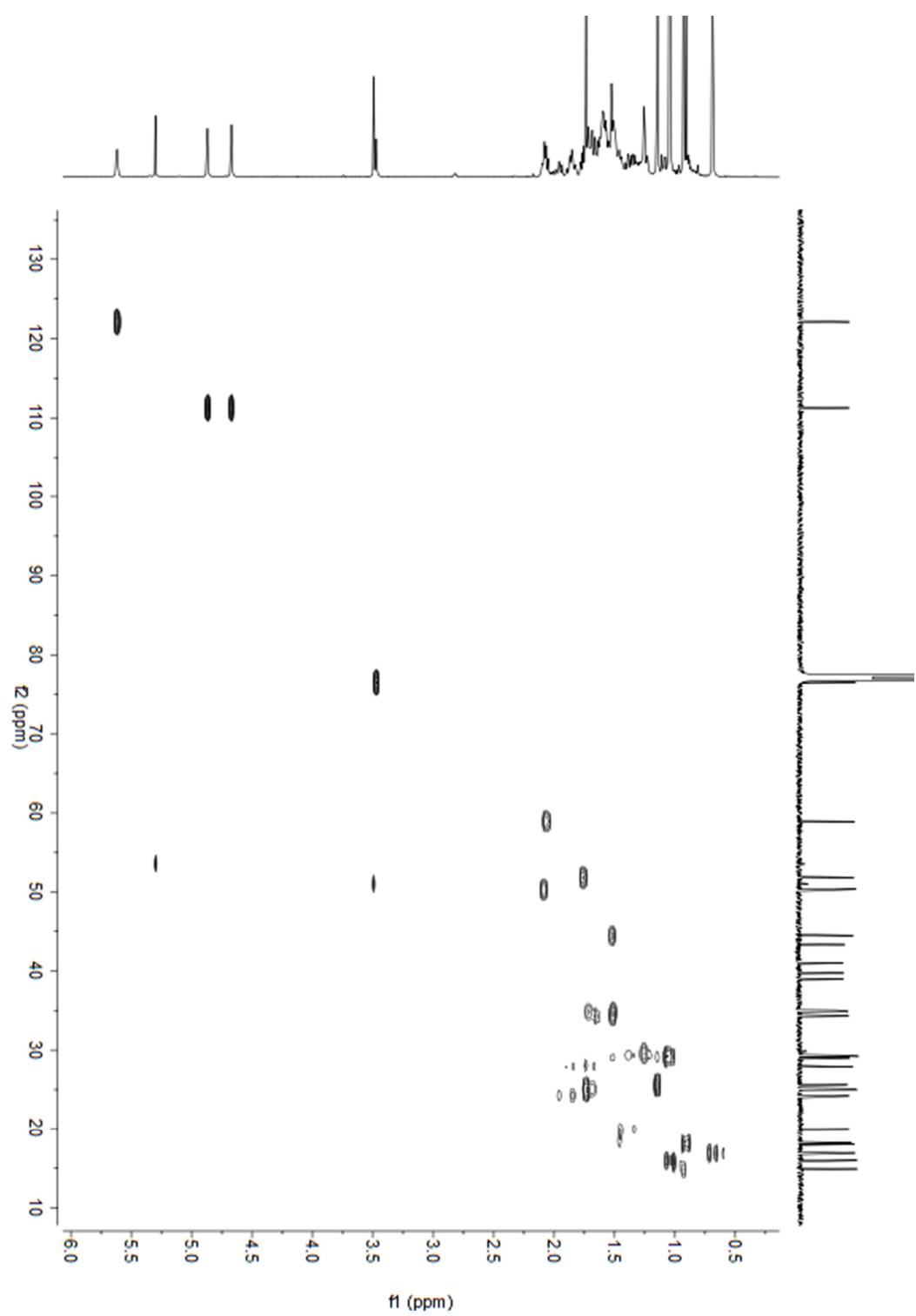


Figure S5. HMBC NMR spectrum of **1** in CDCl_3

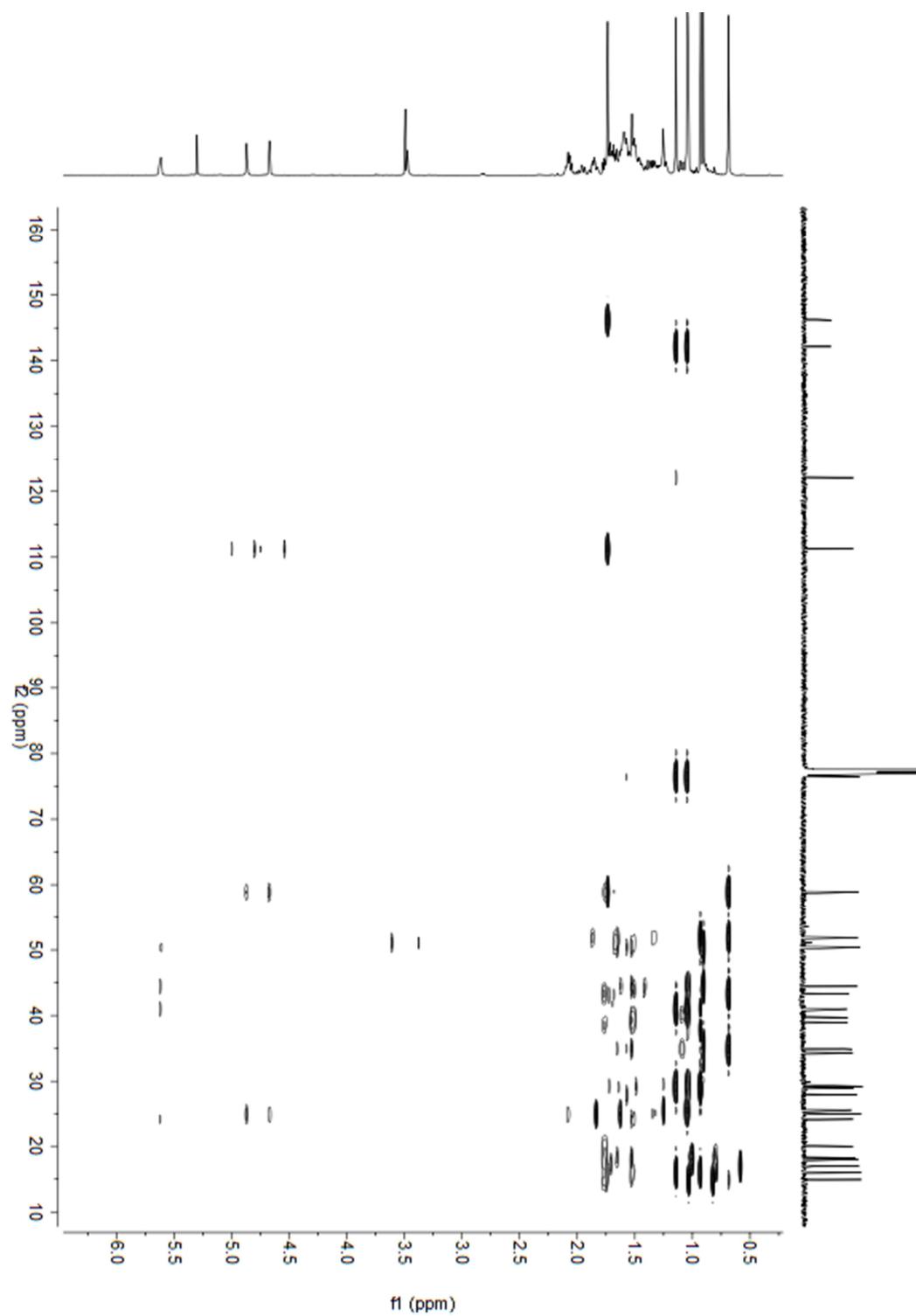


Figure S6. ROESY NMR spectrum of **1** in CDCl_3

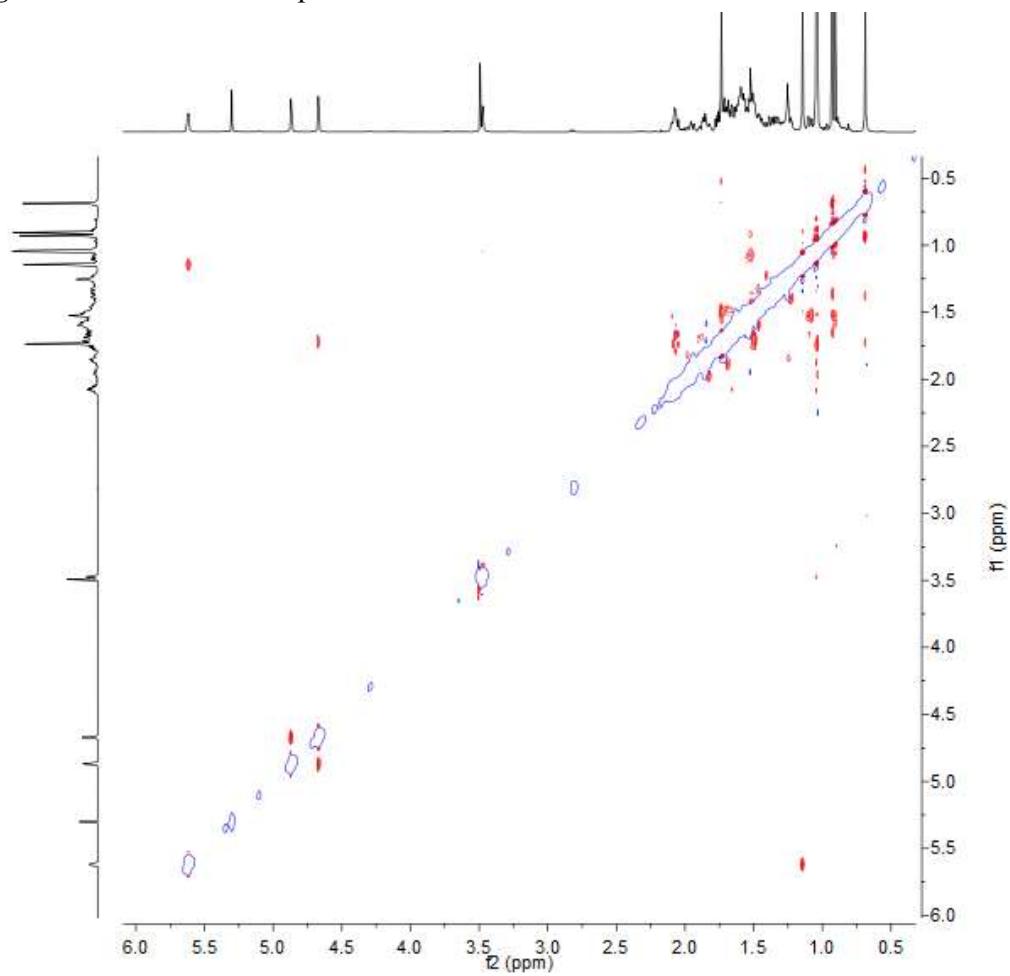


Figure S7. (+)-HRESIMS spectrum of **1**

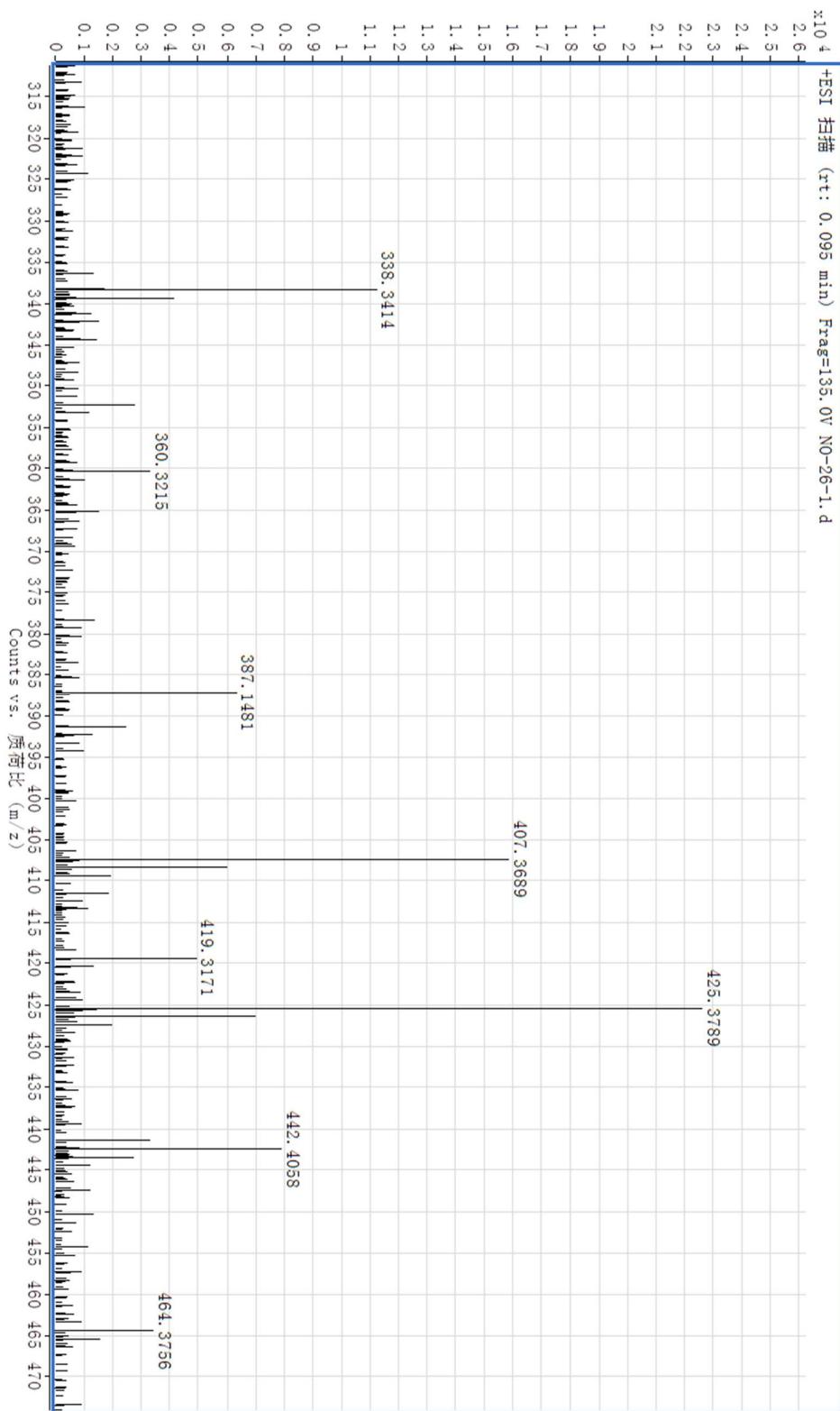


Figure S8. ^1H NMR spectrum of **2** in CDCl_3

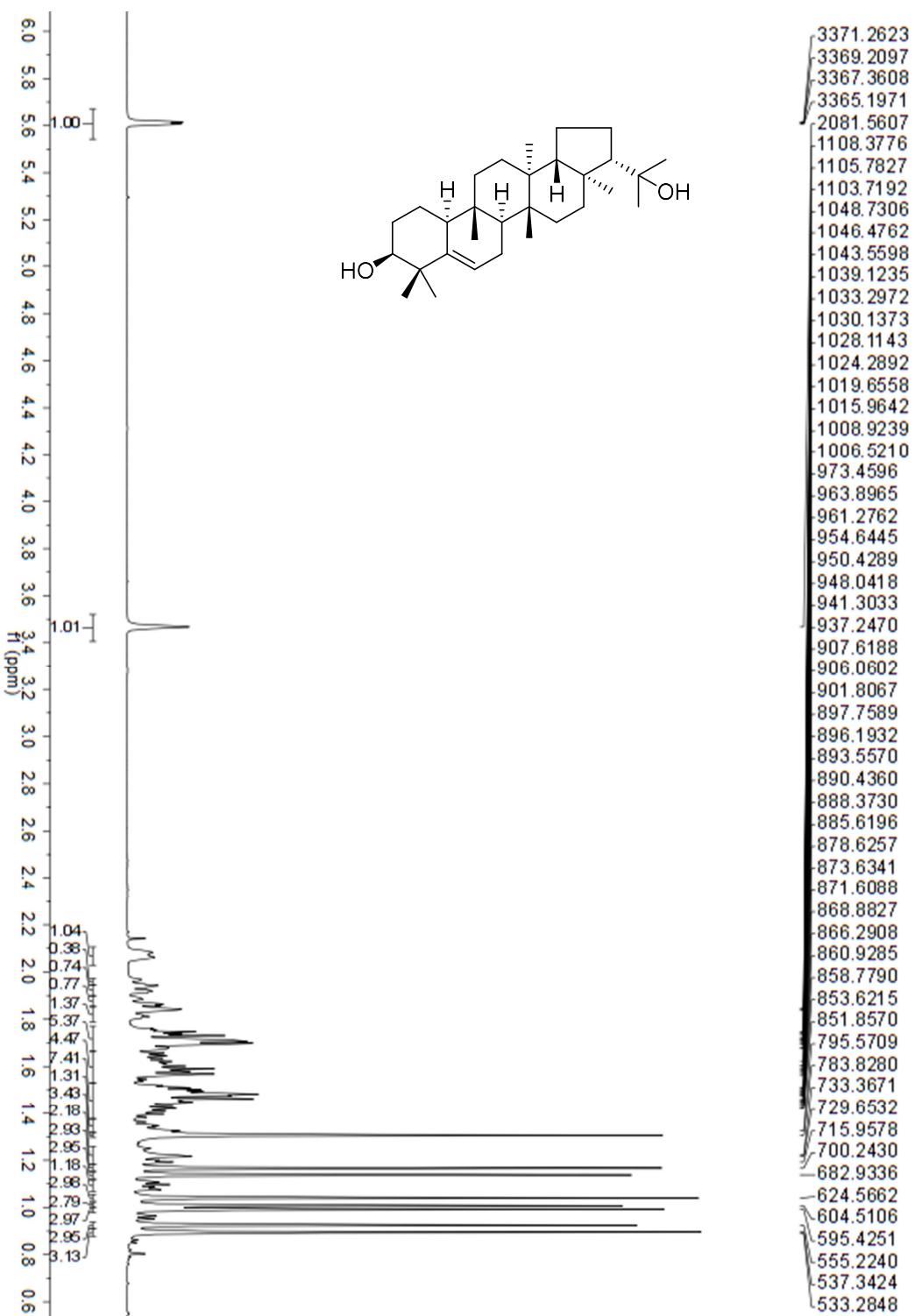


Figure S9. ^{13}C NMR spectrum of **2** in CDCl_3

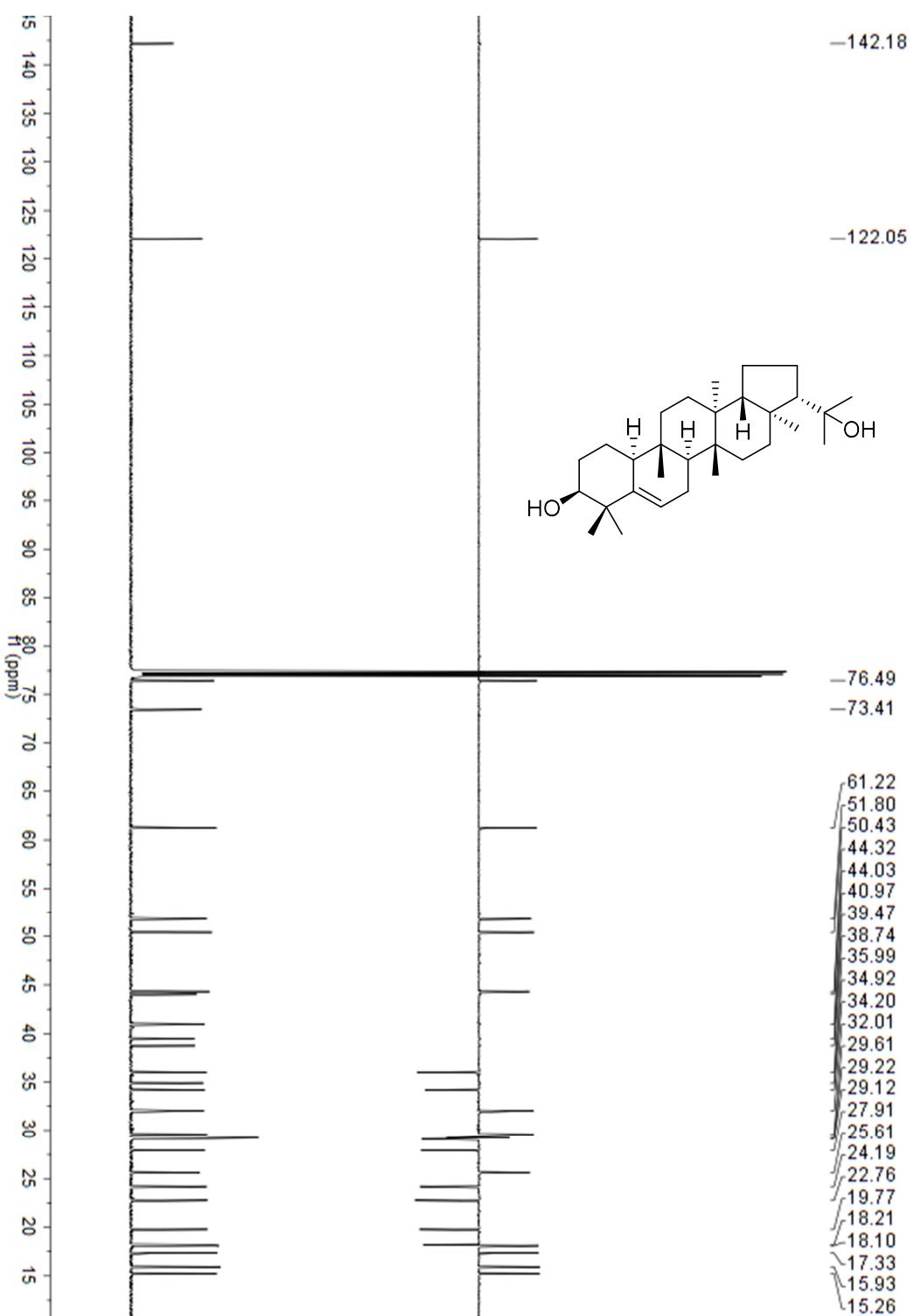


Figure S10. ^1H - ^1H COSY NMR spectrum of **2** in CDCl_3

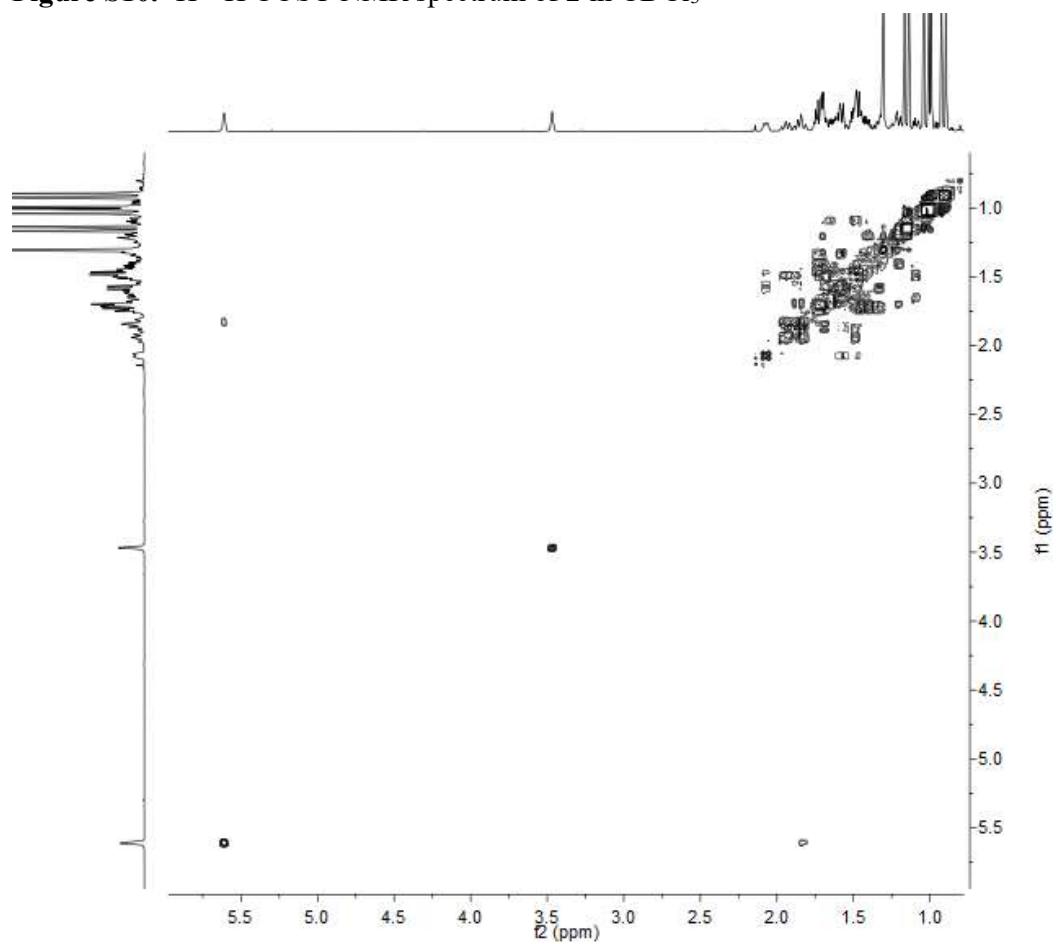


Figure S11. HSQC NMR spectrum of **2** in CDCl_3

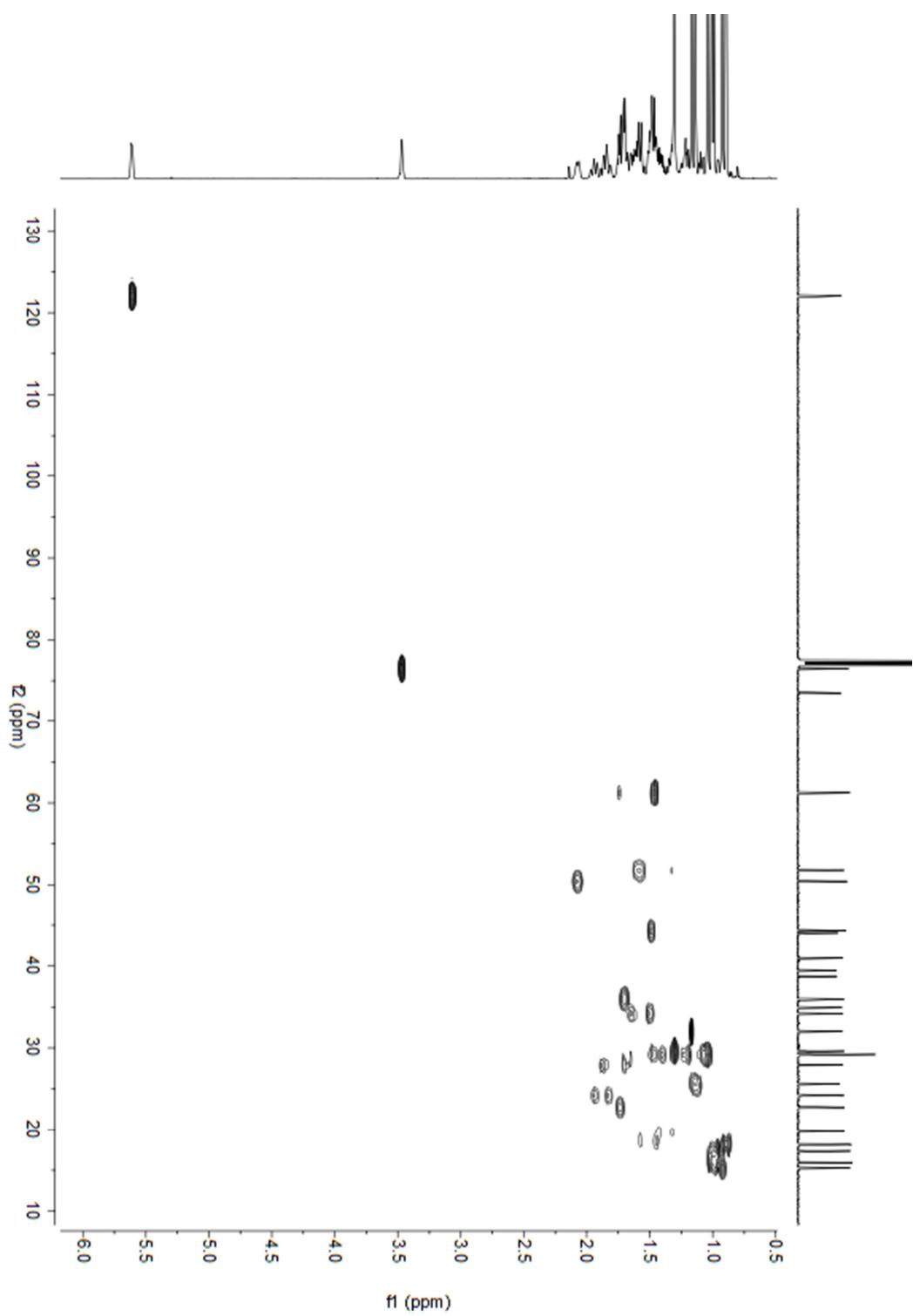


Figure S12. HMBC NMR spectrum of **2** in CDCl_3

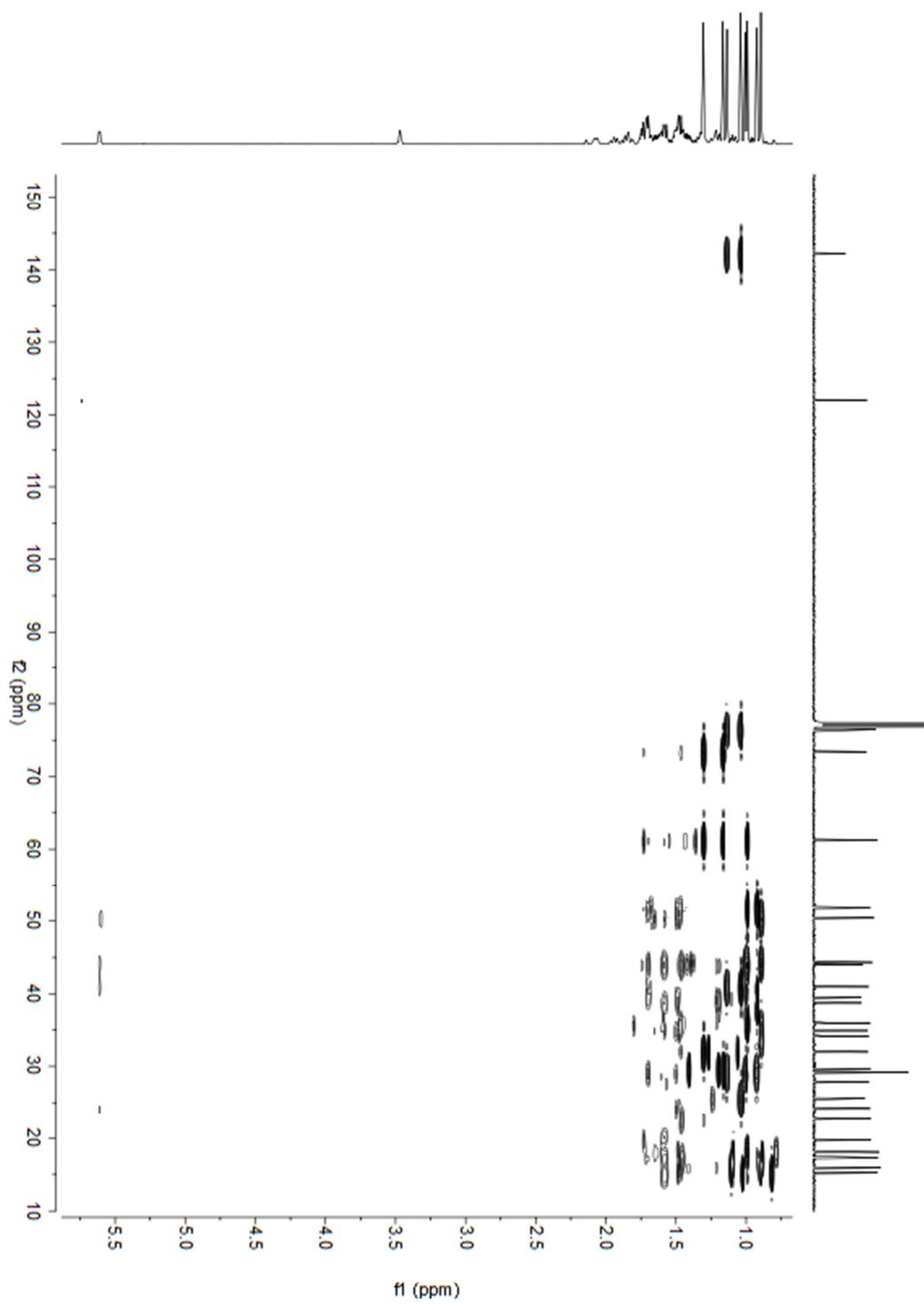


Figure S13. ROESY NMR spectrum of **2** in CDCl_3

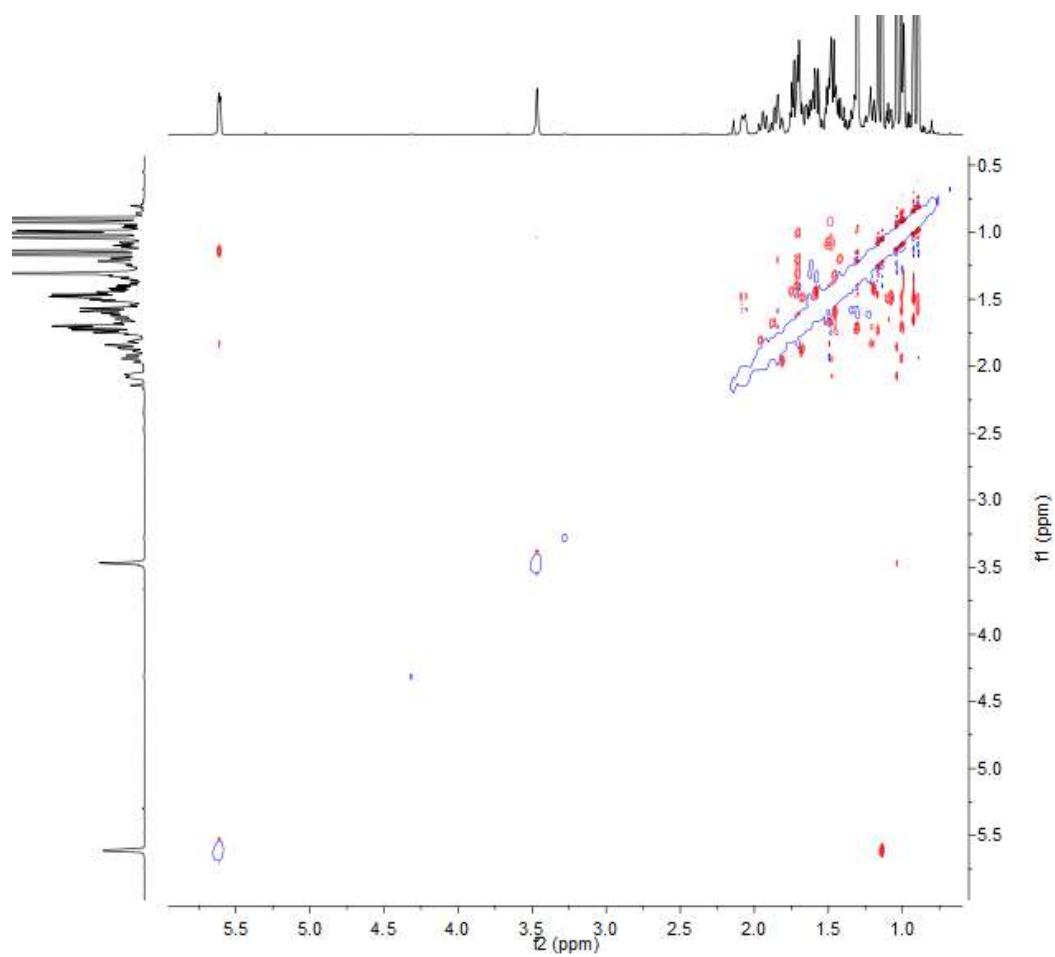


Figure S14. (+)-LRESIMS spectrum of **2**

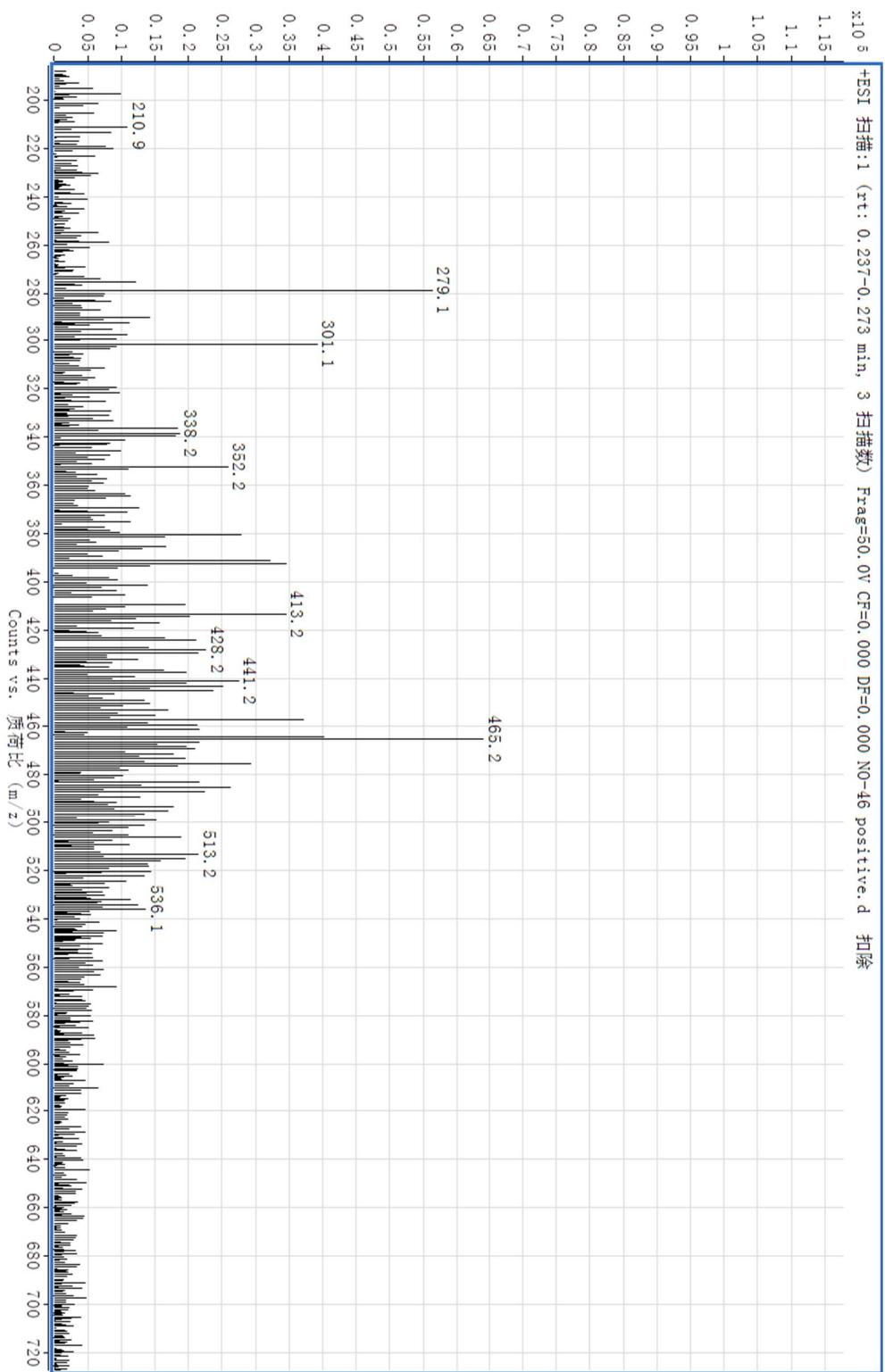


Figure S15. (+)-HRESIMS spectrum of 2

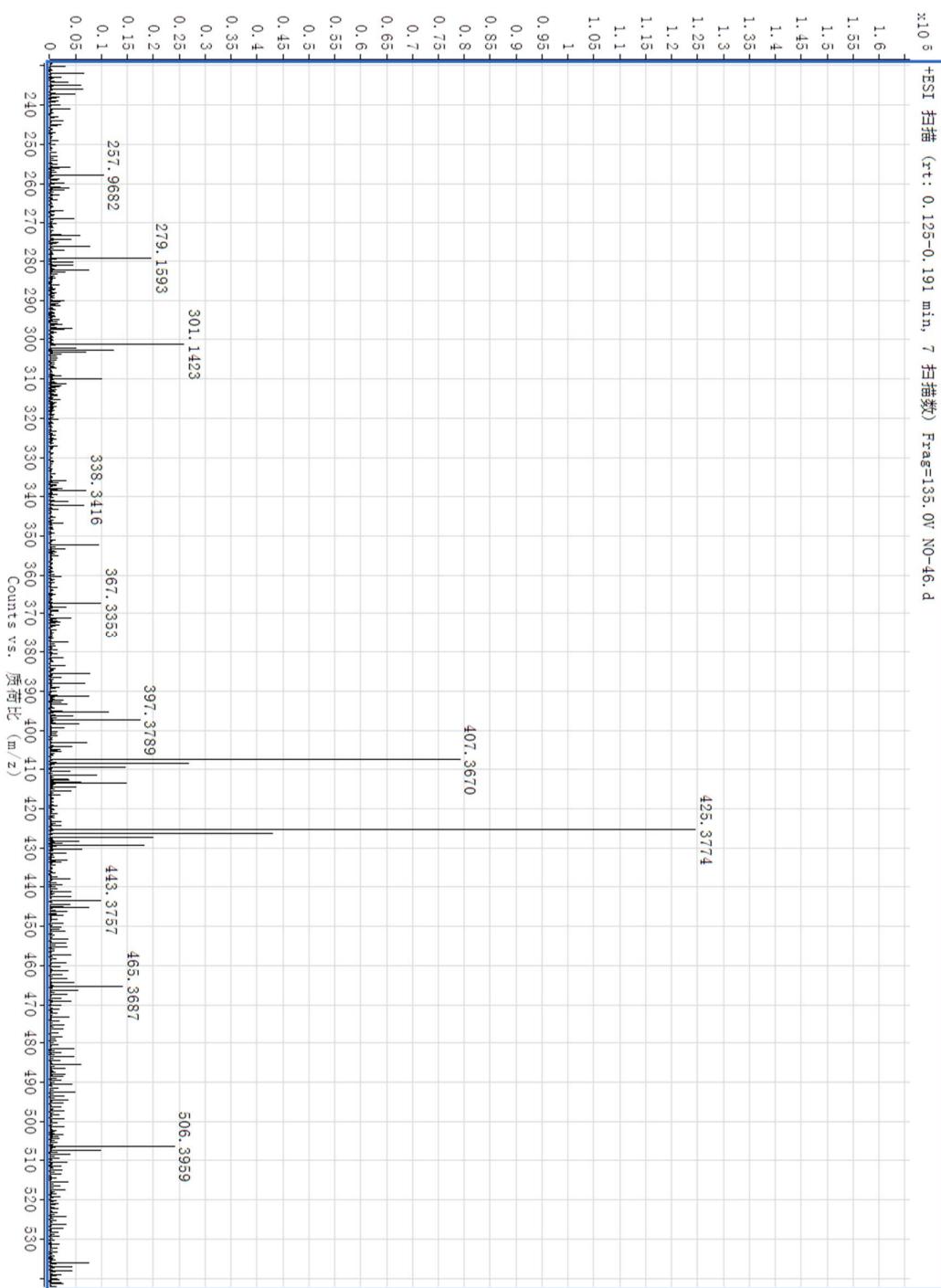


Figure S16. ^1H NMR spectrum of **3** in CDCl_3

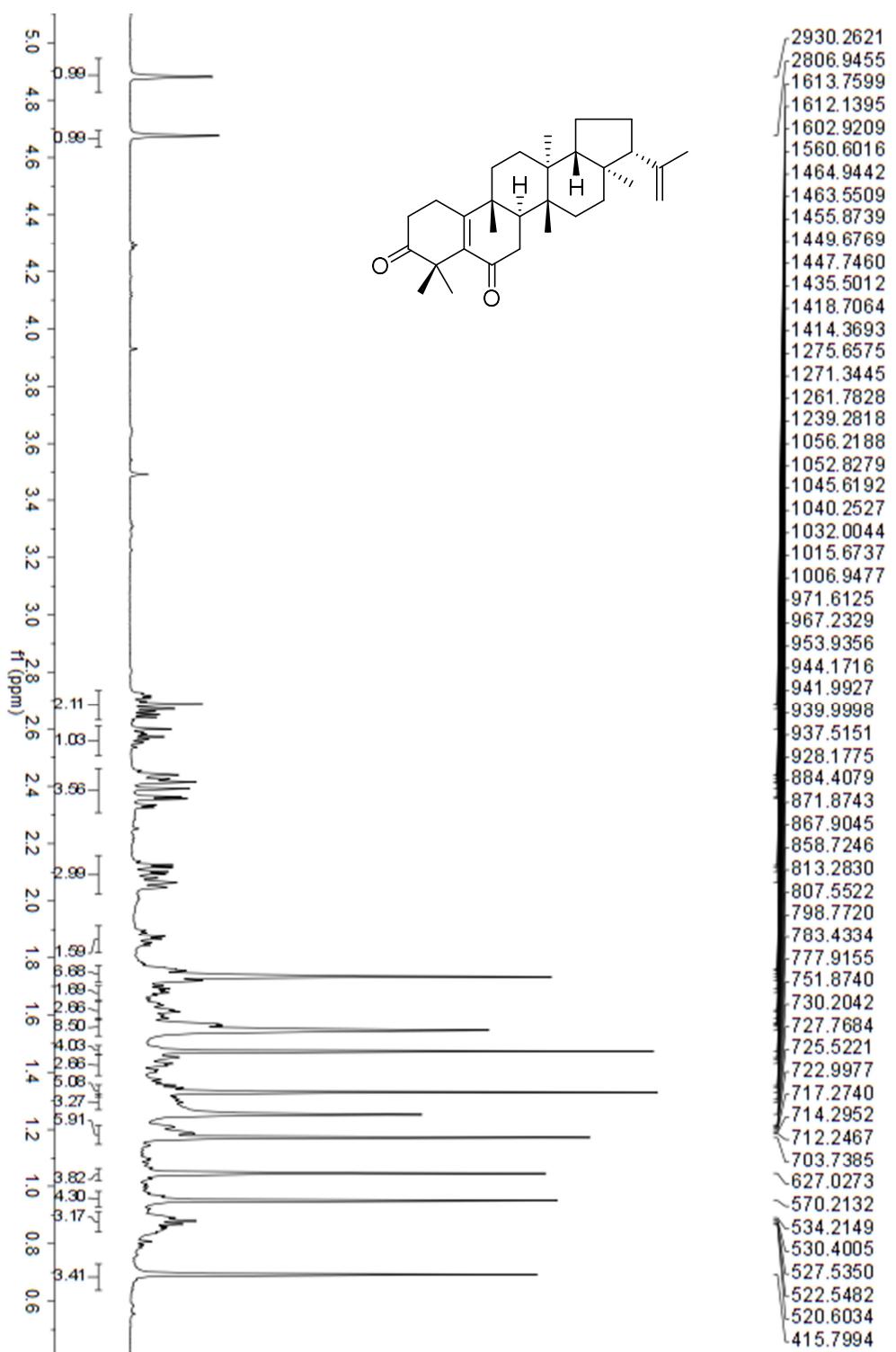


Figure S17. ^{13}C NMR spectrum of **3** in CDCl_3

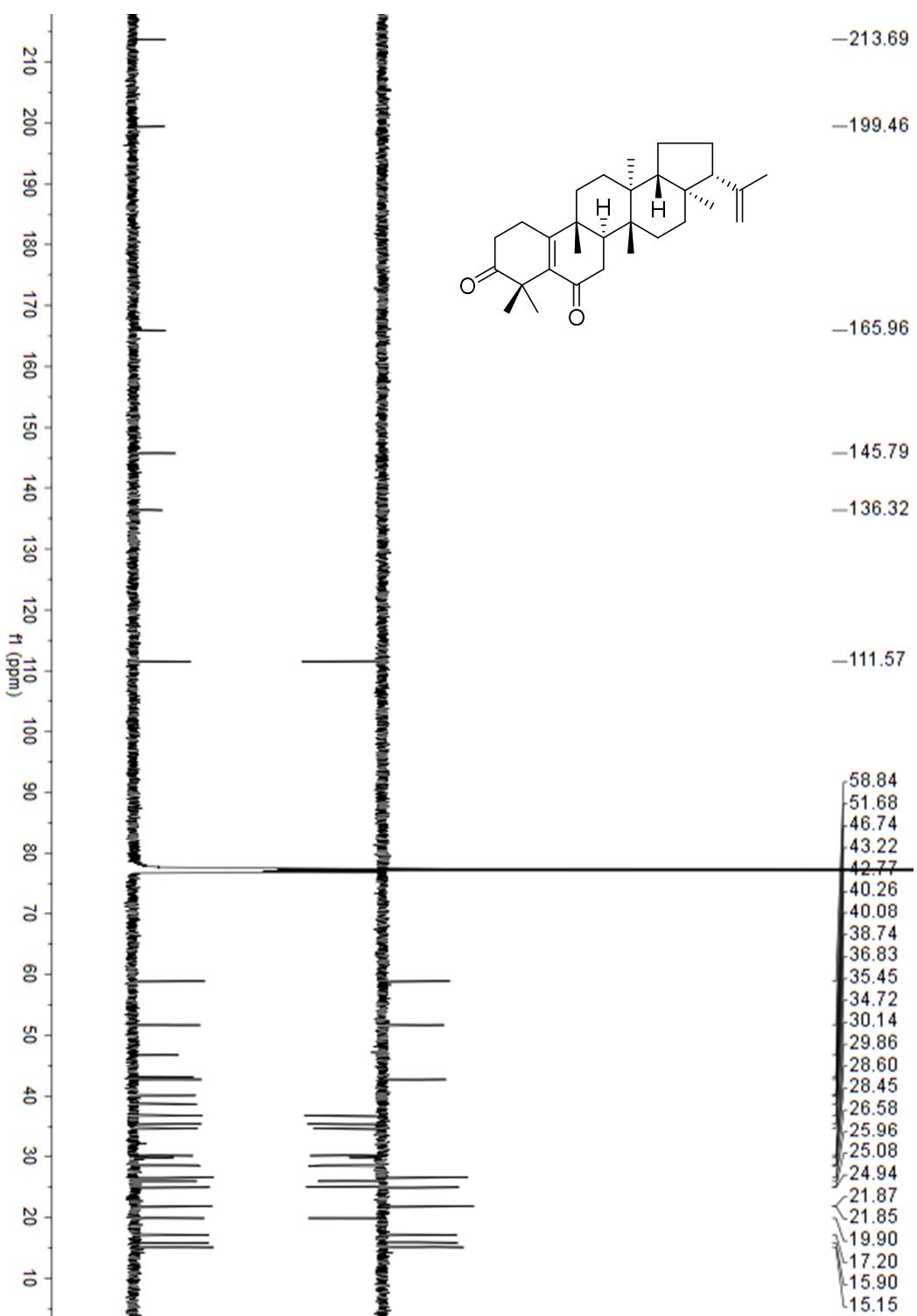


Figure S18. ^1H - ^1H COSY NMR spectrum of **3** in CDCl_3

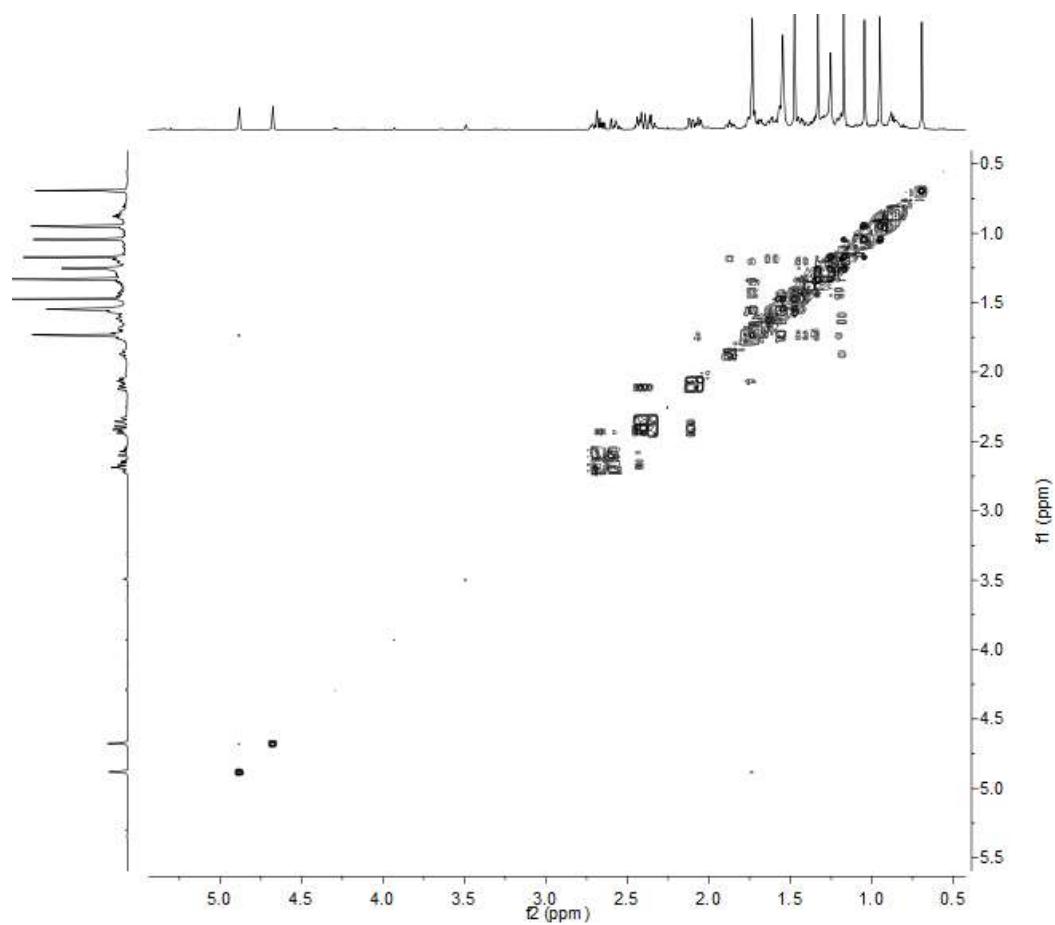


Figure S19. HSQC NMR spectrum of **3** in CDCl_3

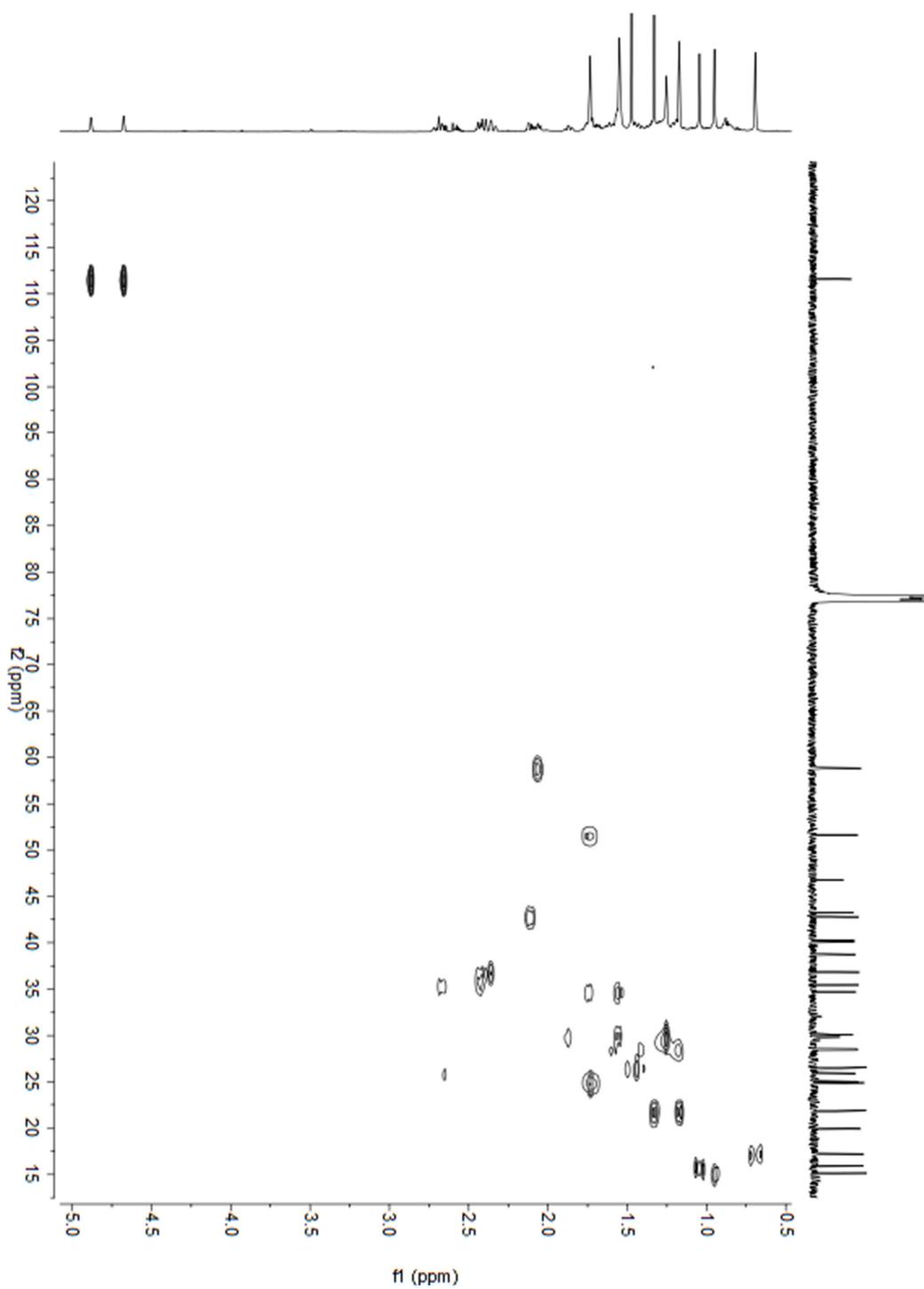


Figure S20. HMBC NMR spectrum of **3** in CDCl_3

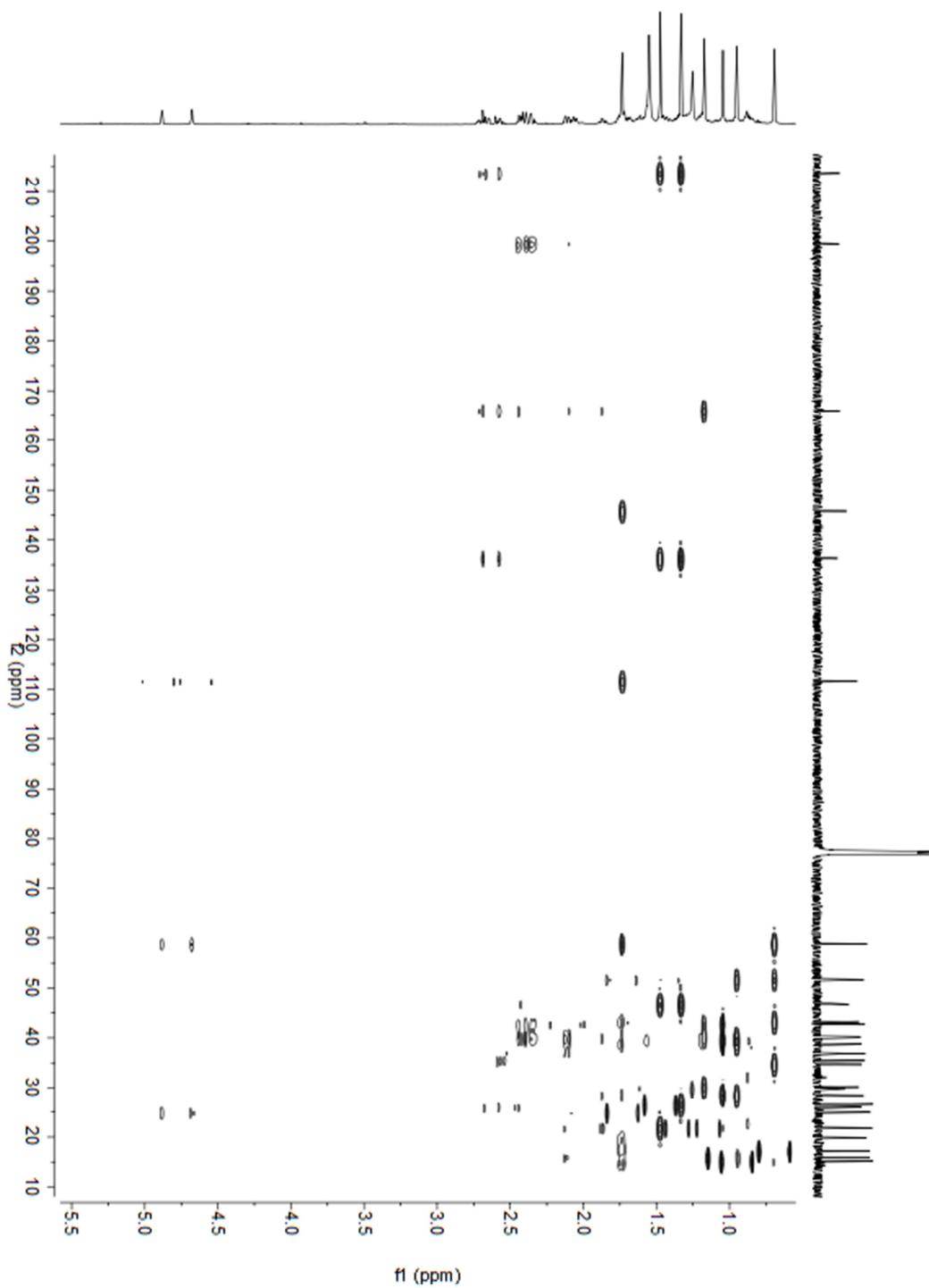


Figure S21. ROESY NMR spectrum of **3** in CDCl_3

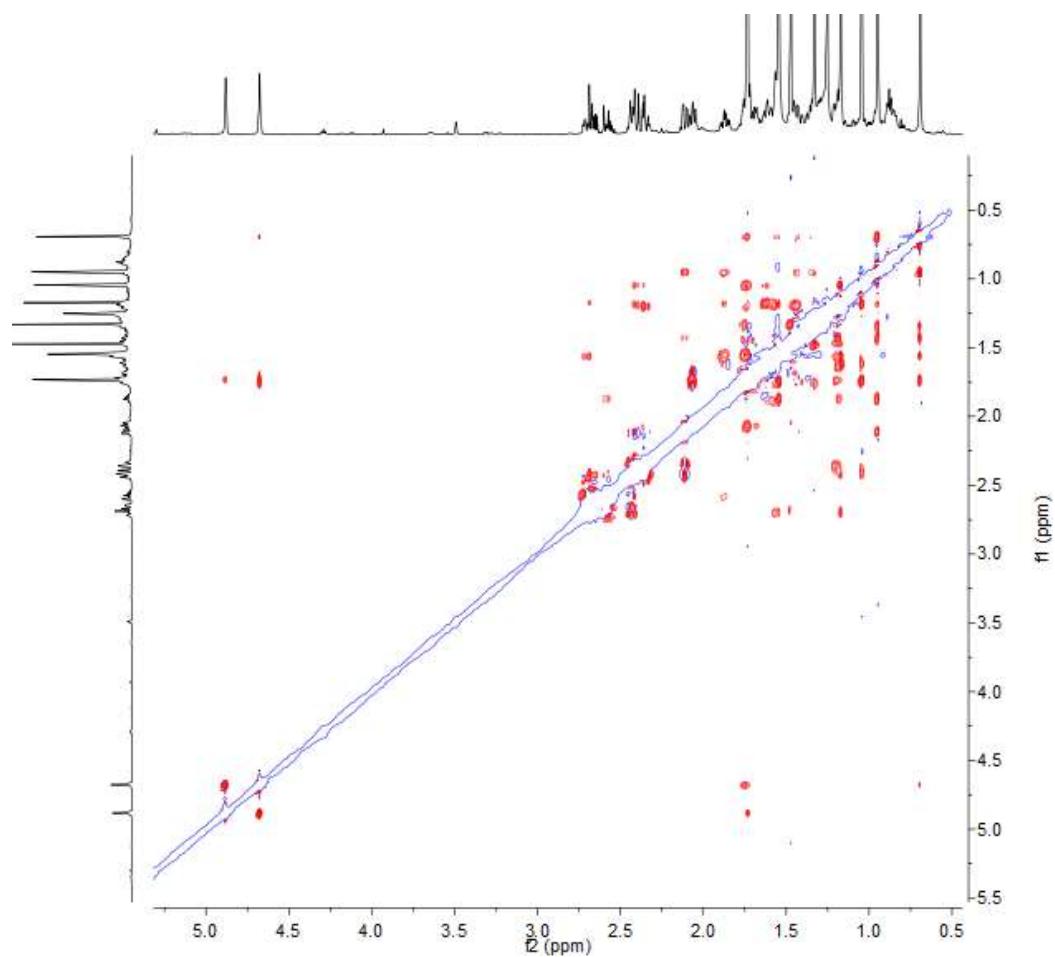


Figure S22. (+)-LRESIMS spectrum of 3

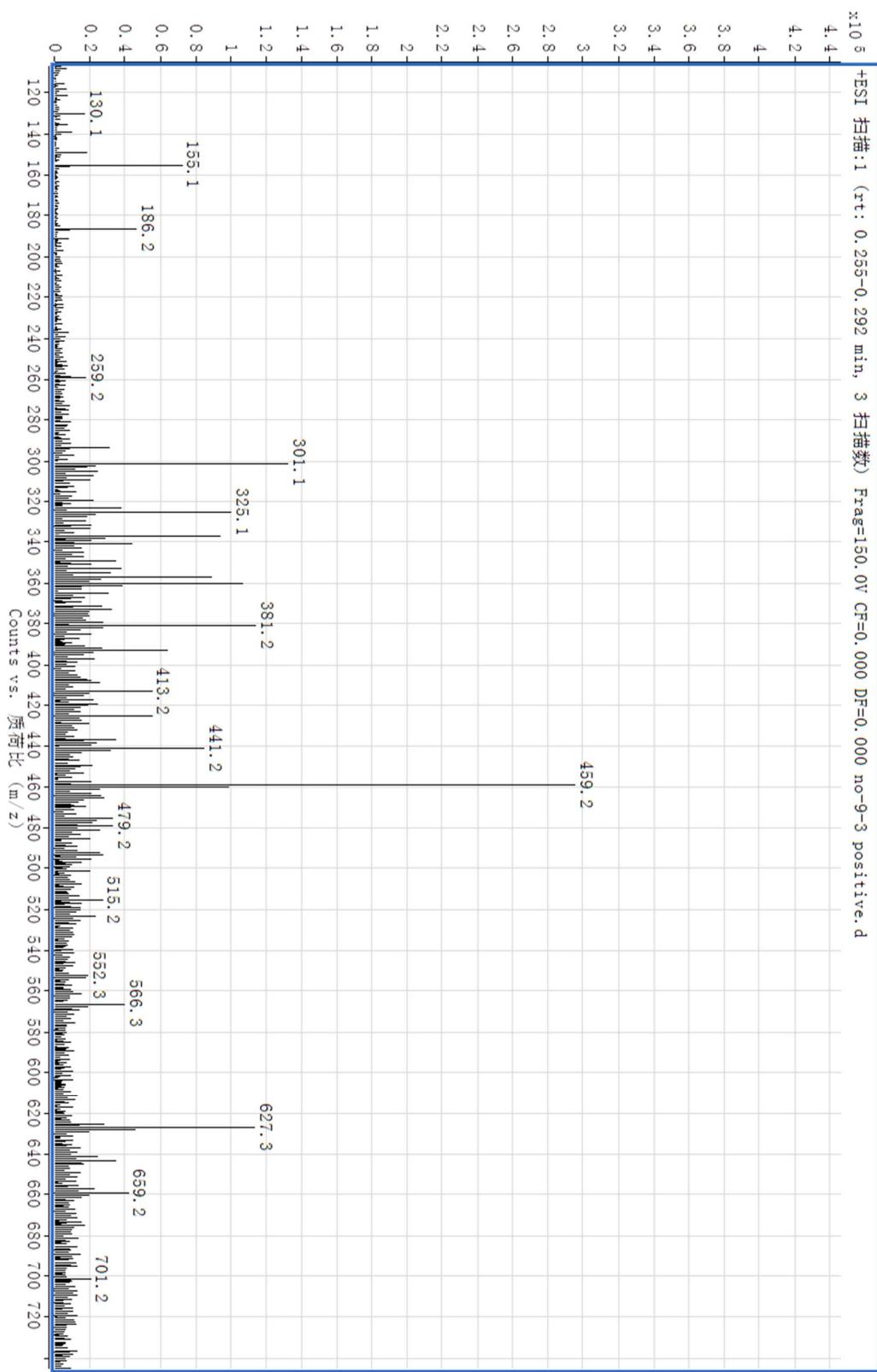


Figure S23. (+)-HRESIMS spectrum of 3

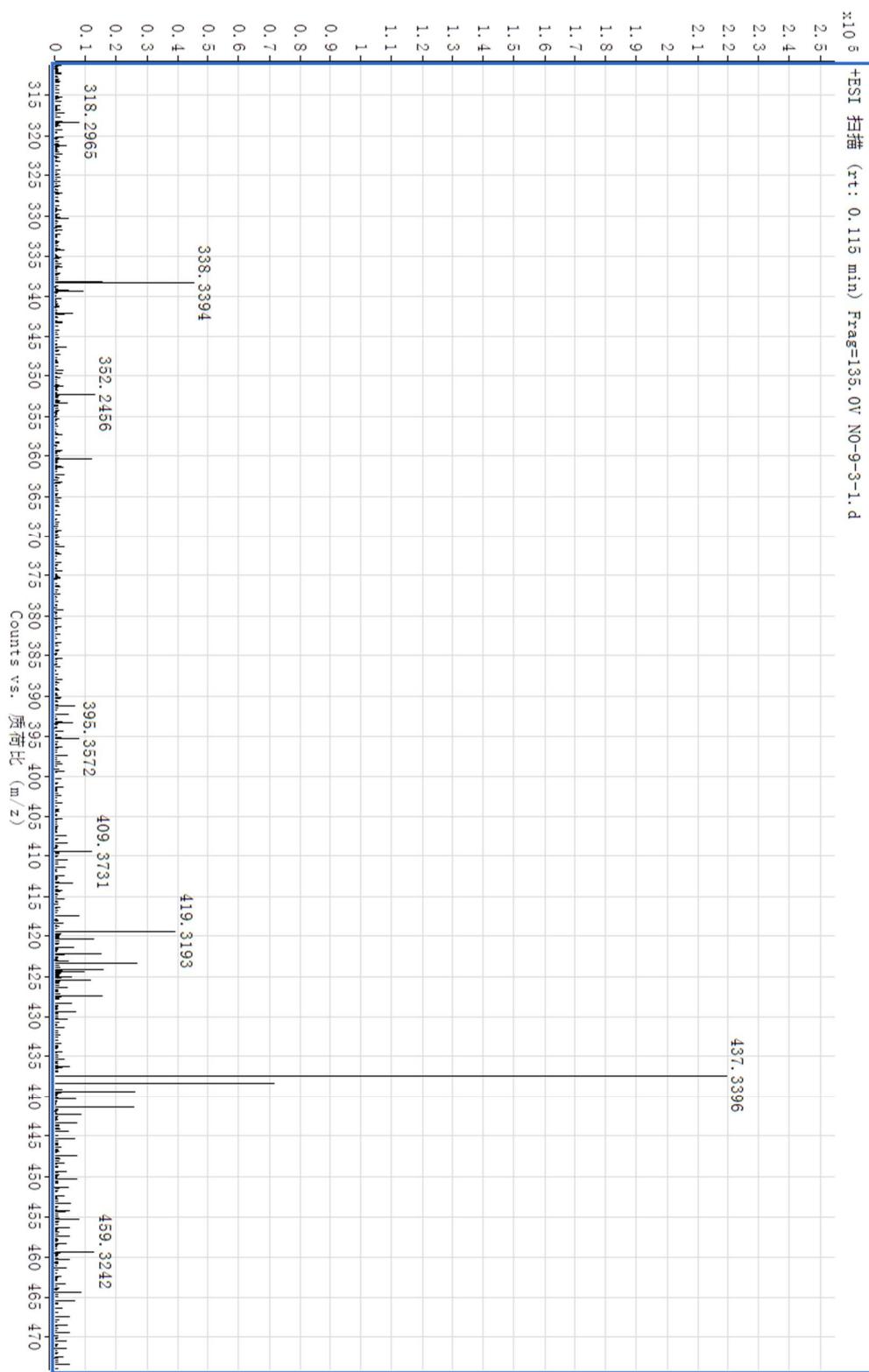


Figure S24. UV spectrum of **3**

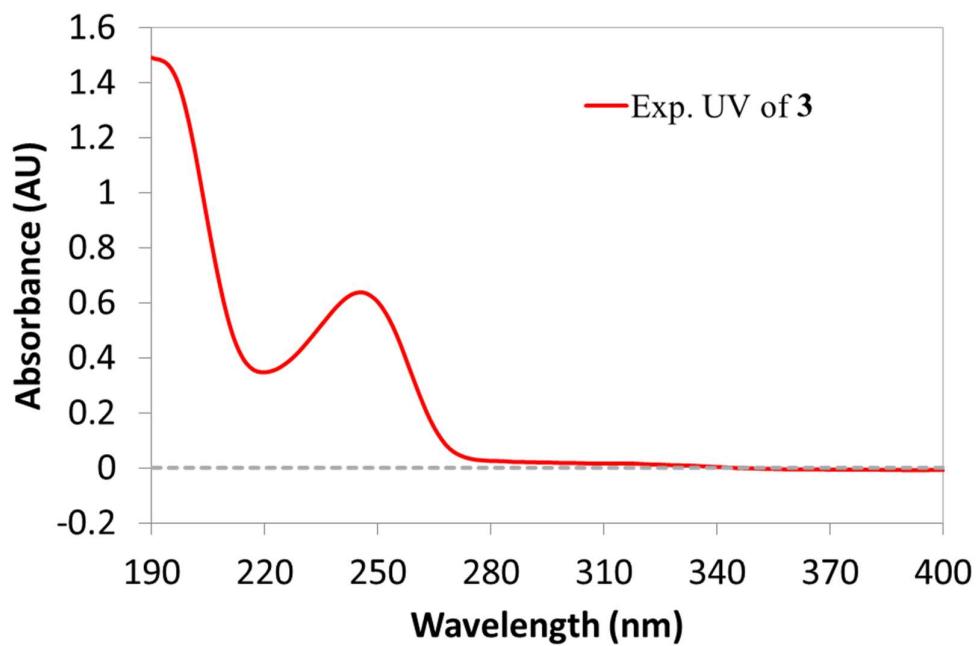


Figure S25. ^1H NMR spectrum of **4** in CDCl_3

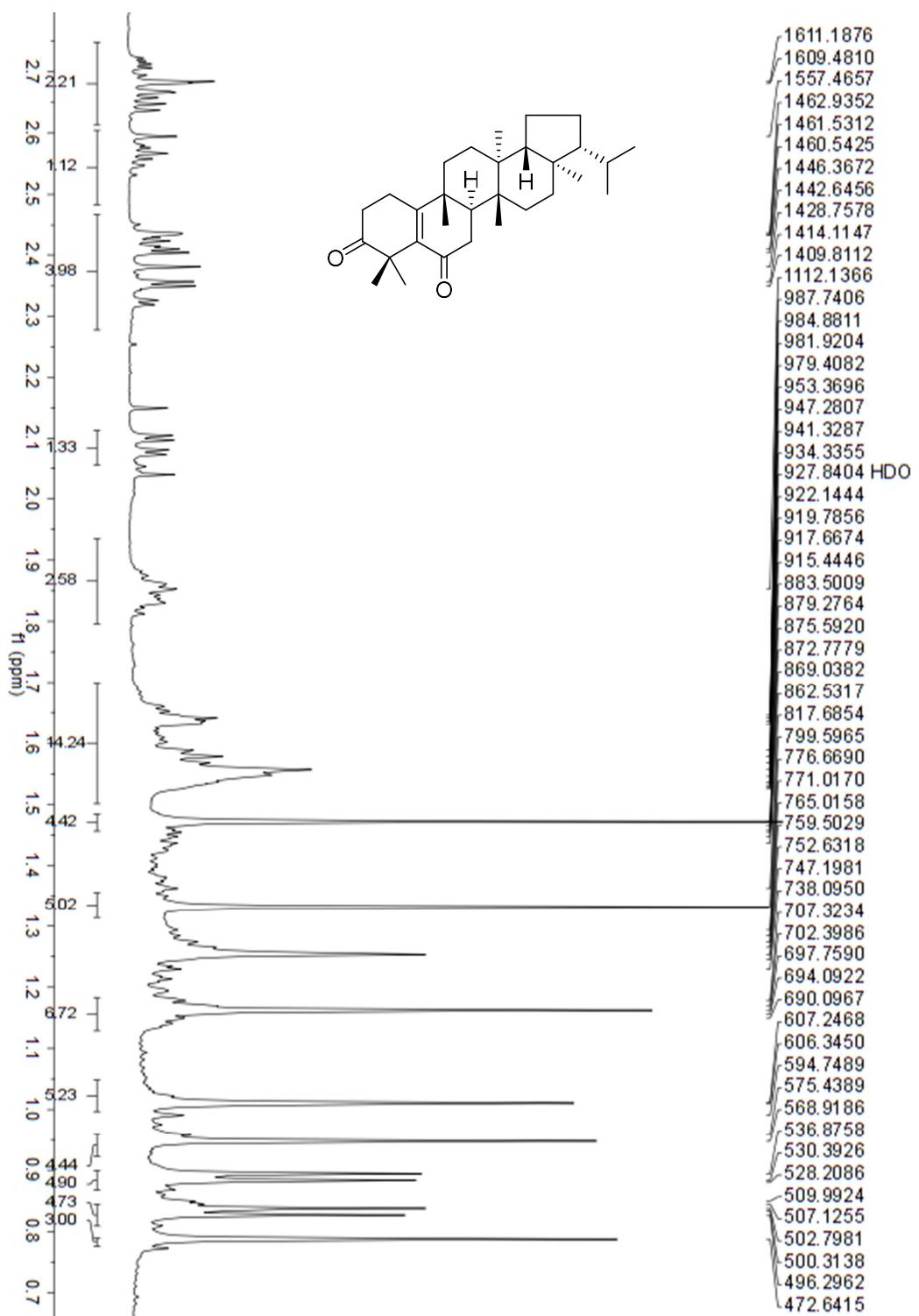


Figure S26. ^{13}C NMR spectrum of **4** in CDCl_3

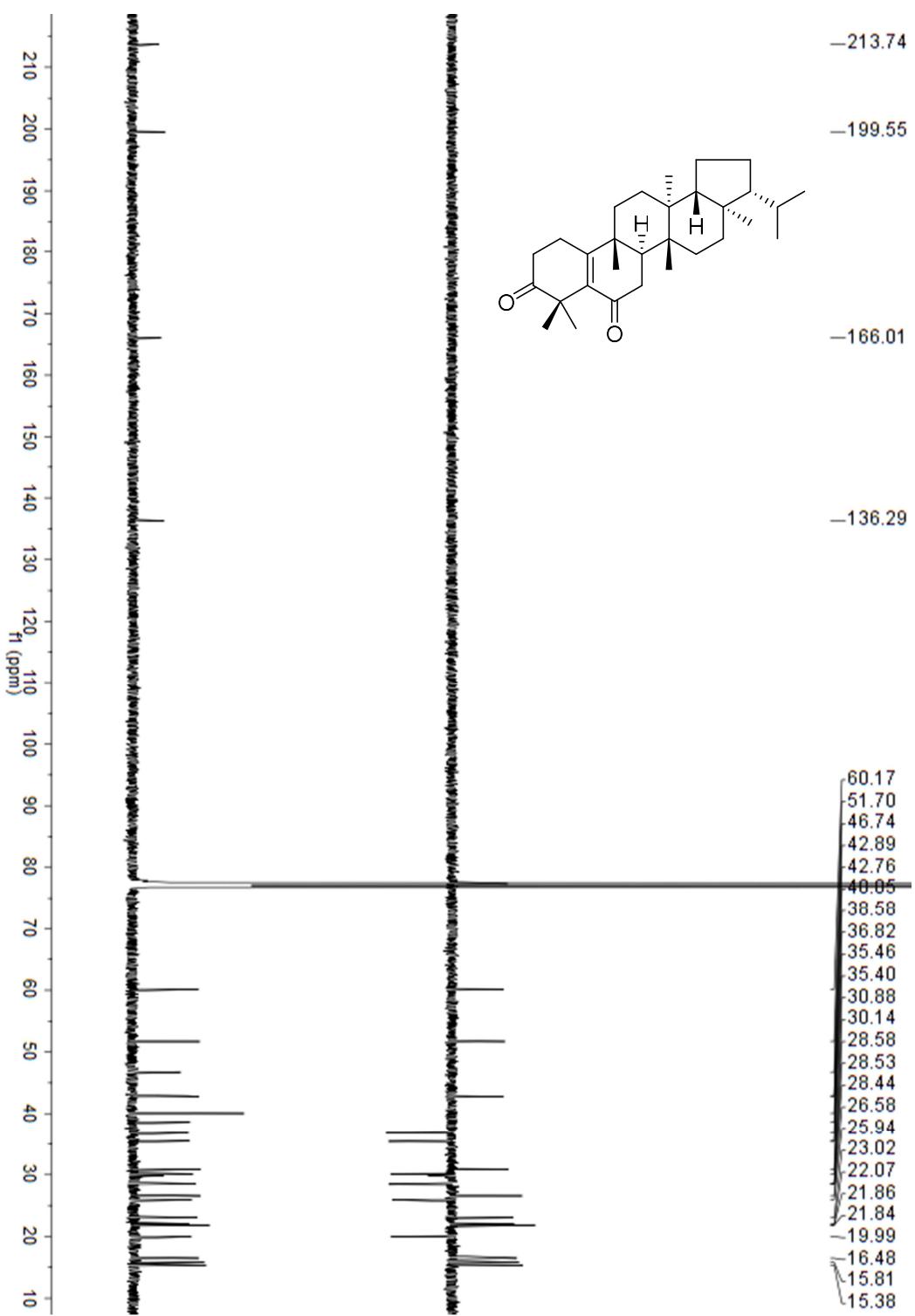


Figure S27. ^1H - ^1H COSY NMR spectrum of **4** in CDCl_3

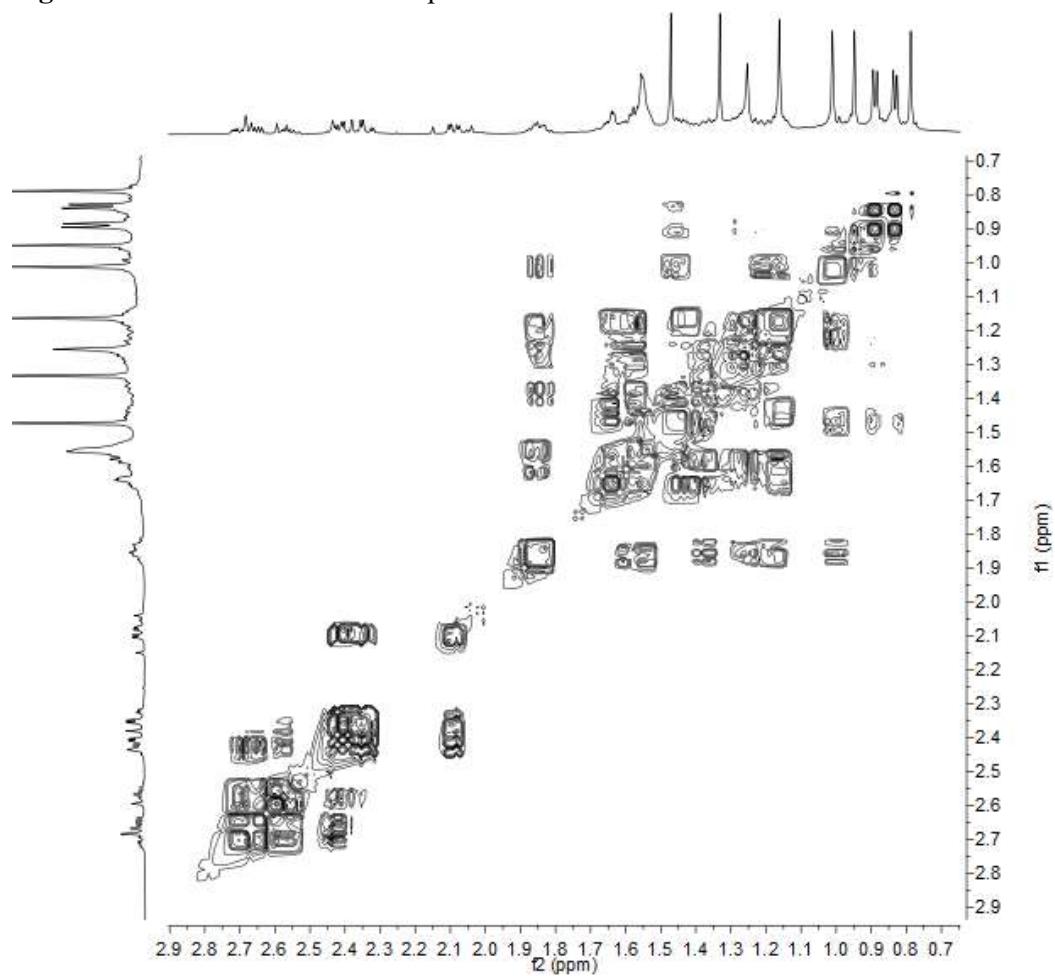


Figure S28. HSQC NMR spectrum of **4** in CDCl_3

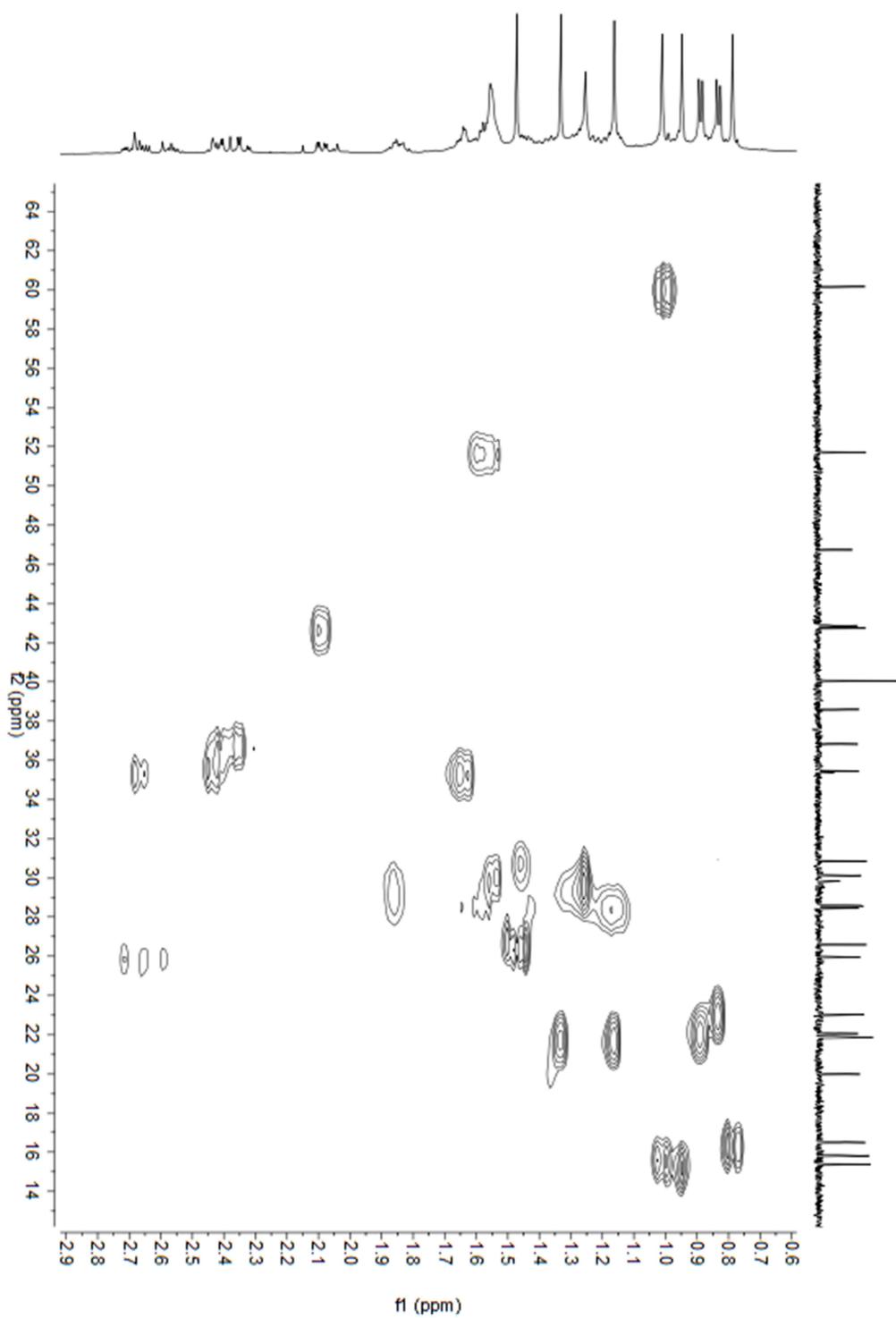


Figure S29. HMBC NMR spectrum of **4** in CDCl_3

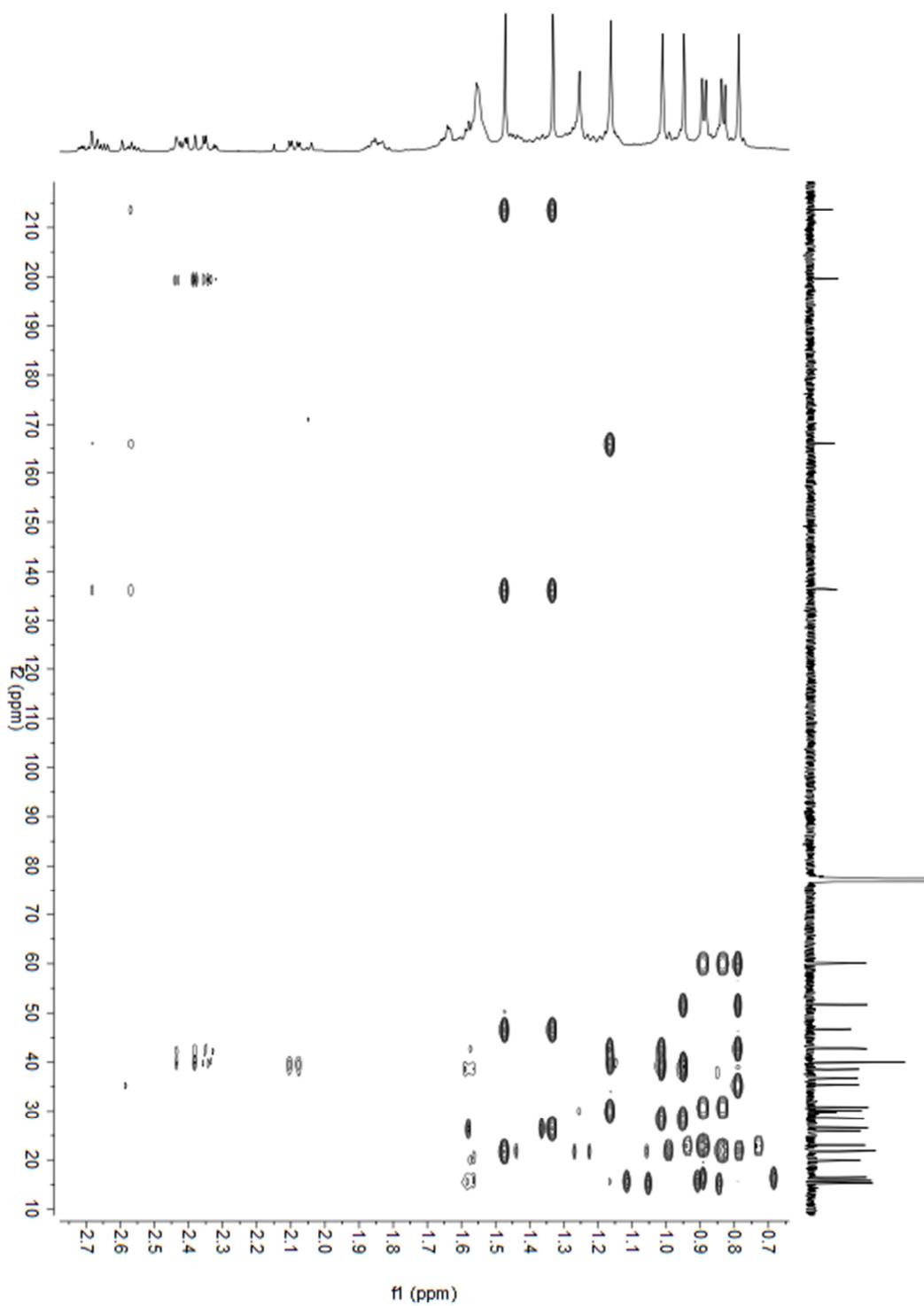


Figure S30. ROESY NMR spectrum of **4** in CDCl_3

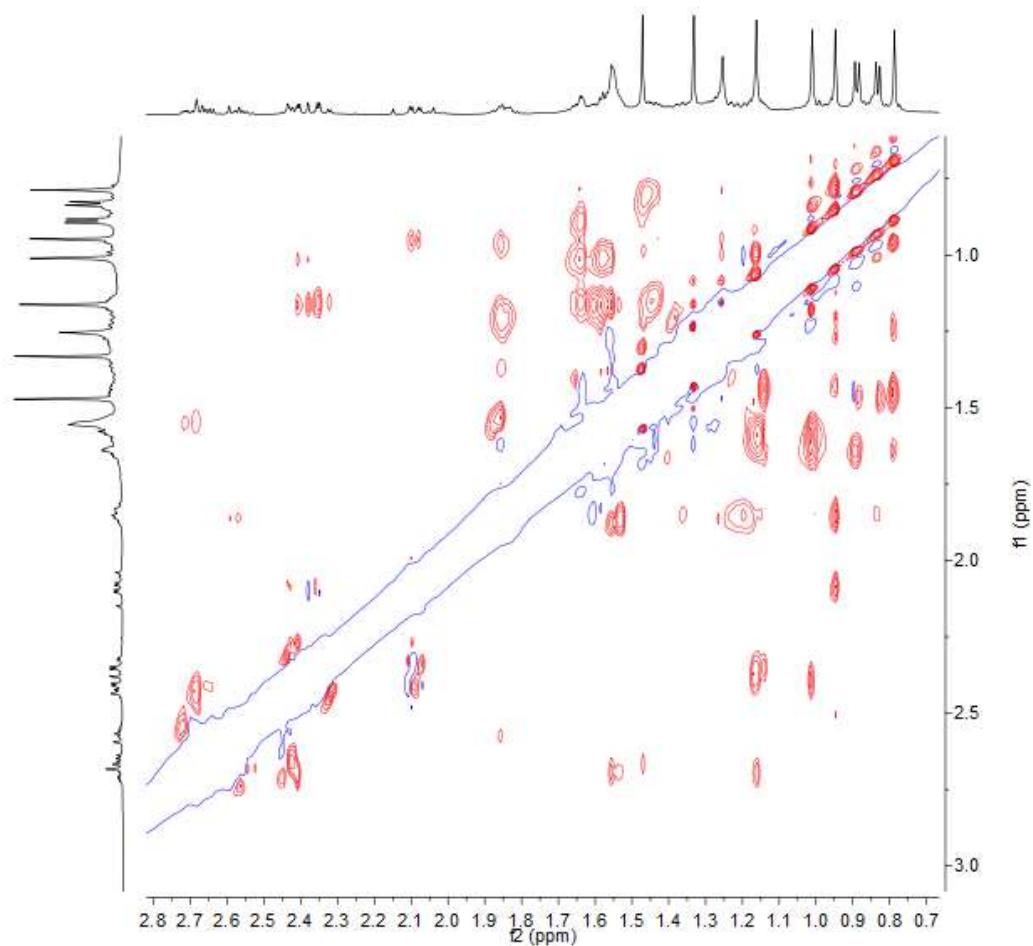


Figure S31. (+)-LRESIMS spectrum of 4

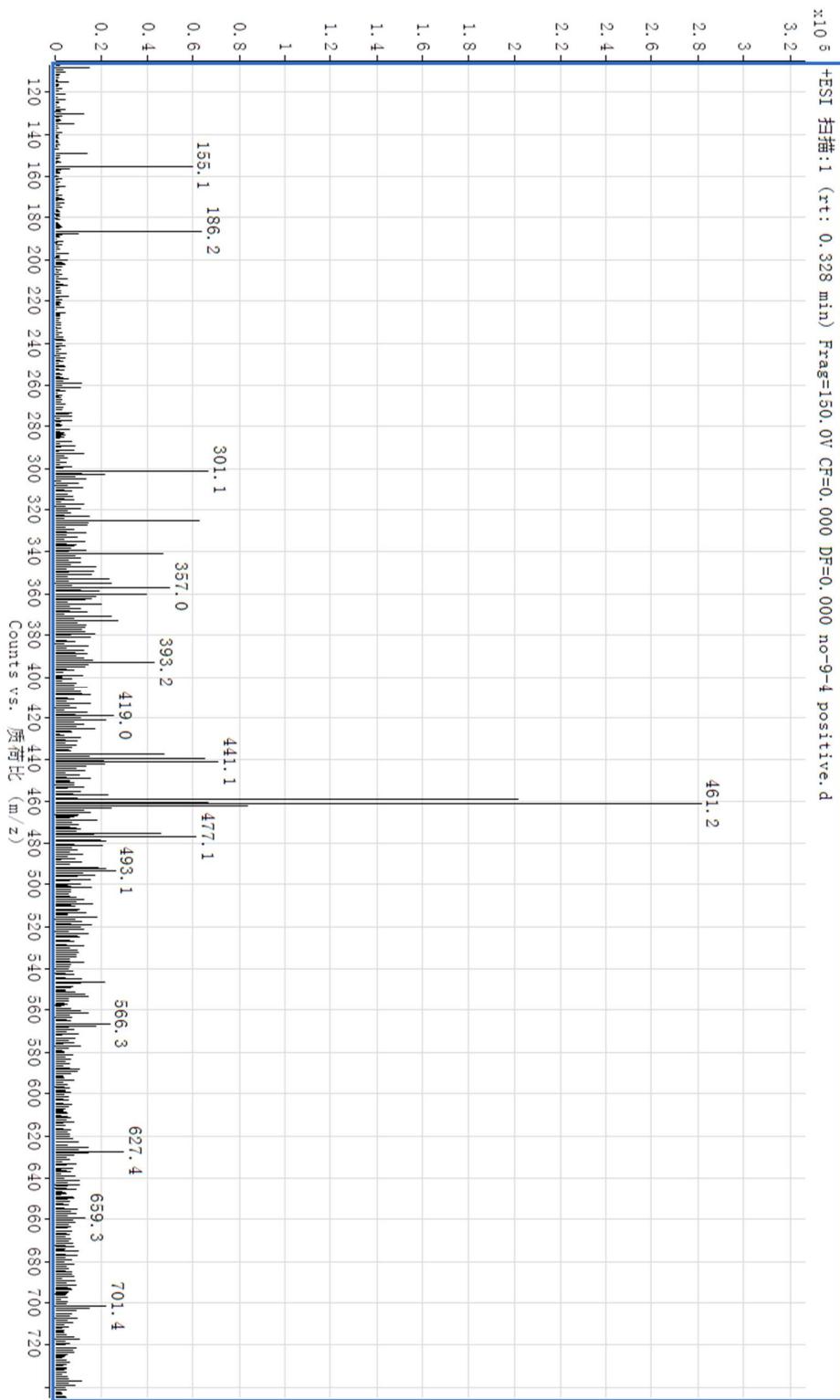


Figure S32. (+)-HRESIMS spectrum of 4

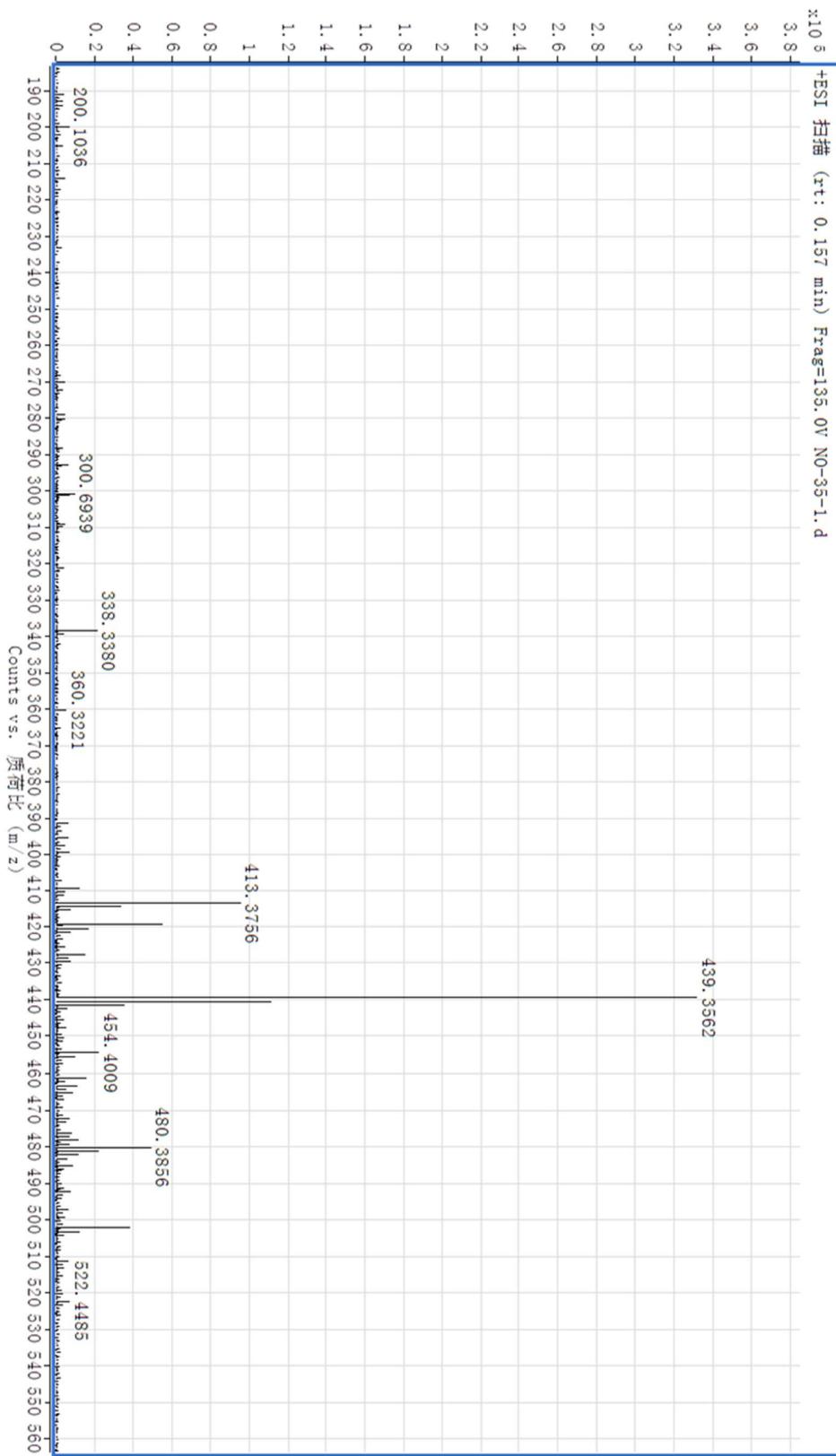


Figure S33. UV spectrum of **4**

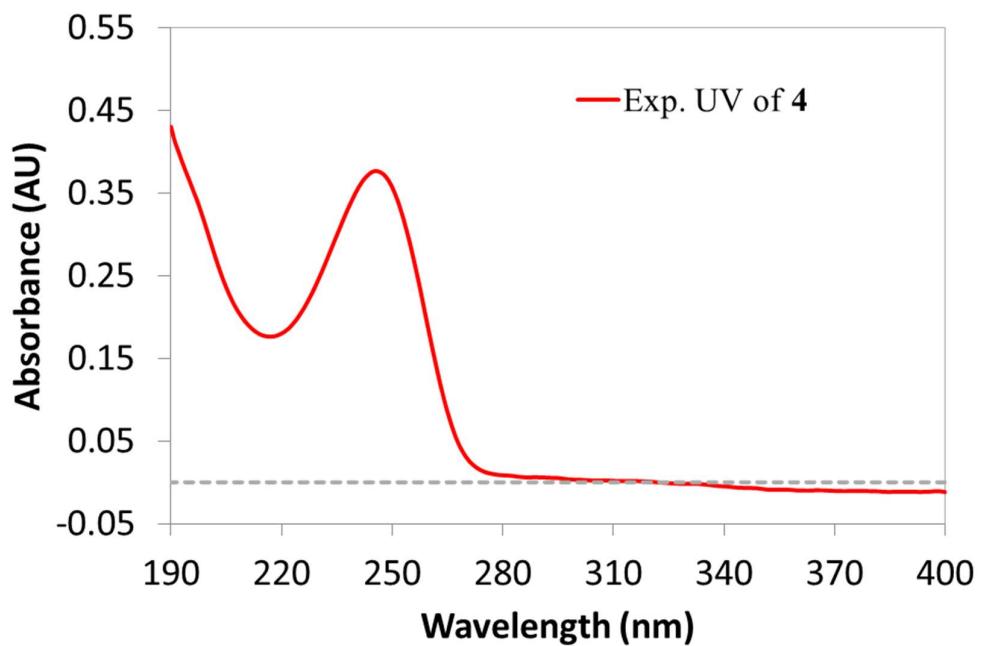


Figure S34. ^1H NMR spectrum of **5** in $\text{C}_5\text{D}_5\text{N}$

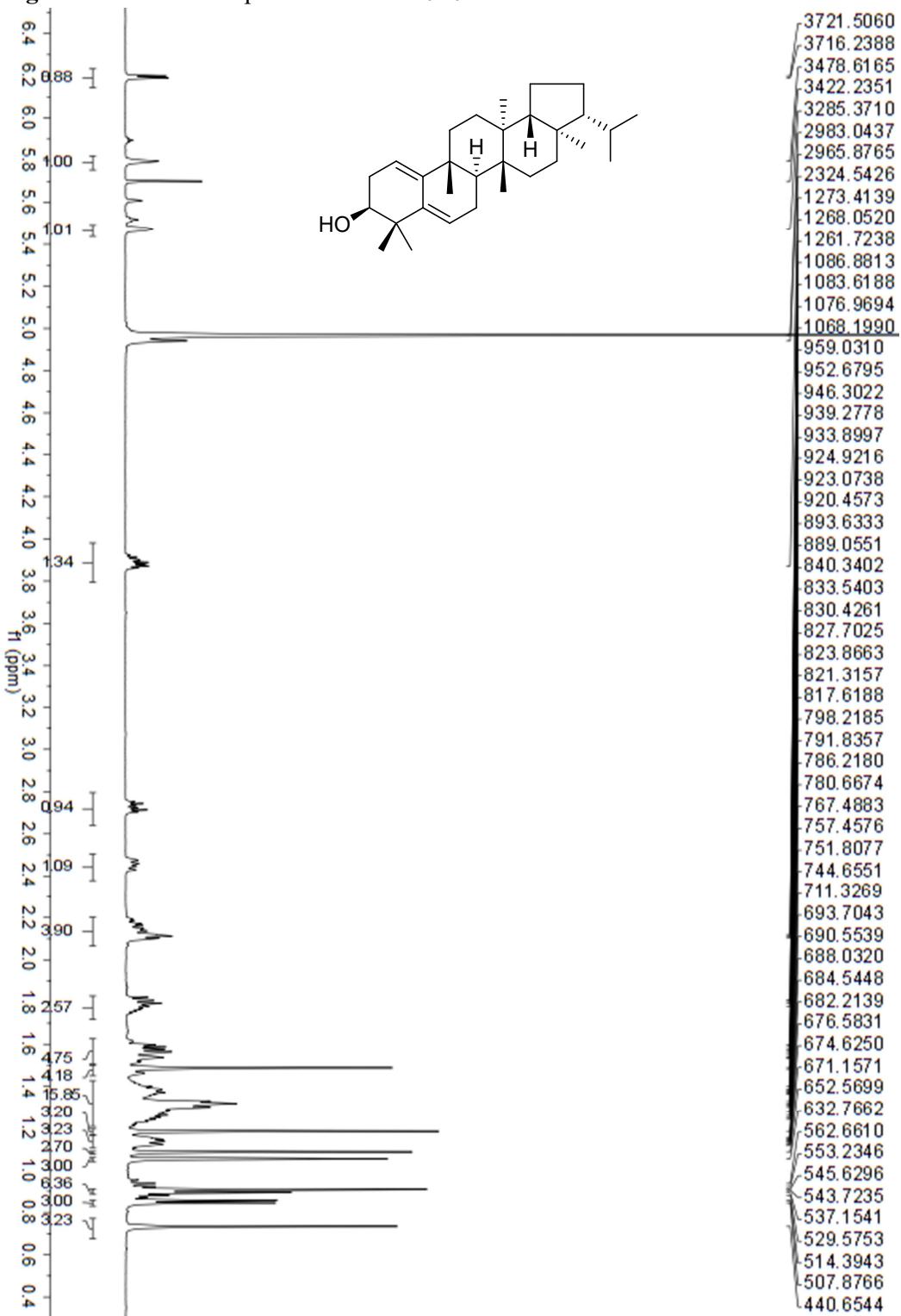


Figure S35. ^{13}C NMR spectrum of **5** in $\text{C}_5\text{D}_5\text{N}$

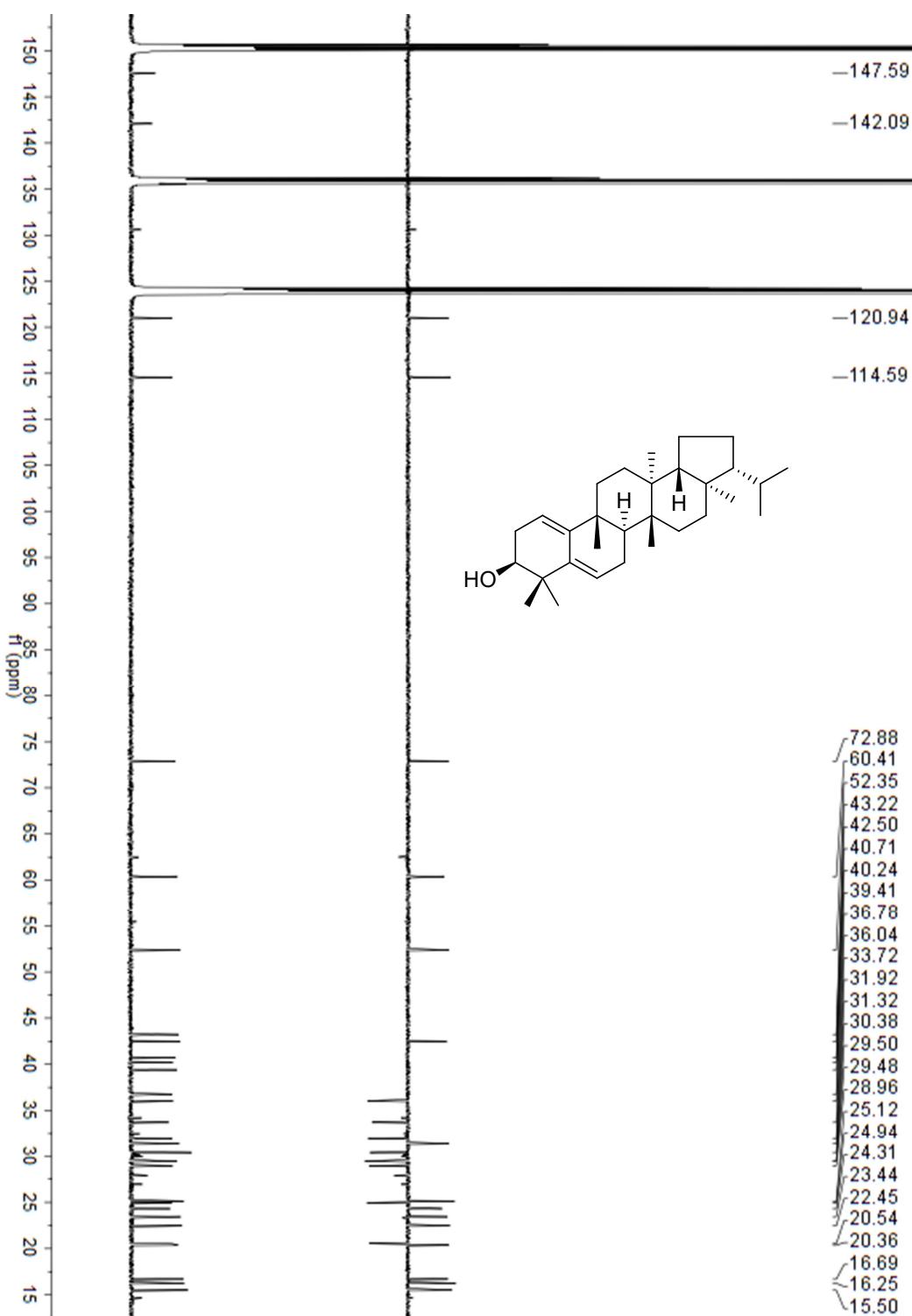


Figure S36. ^1H - ^1H COSY NMR spectrum of **5** in $\text{C}_5\text{D}_5\text{N}$

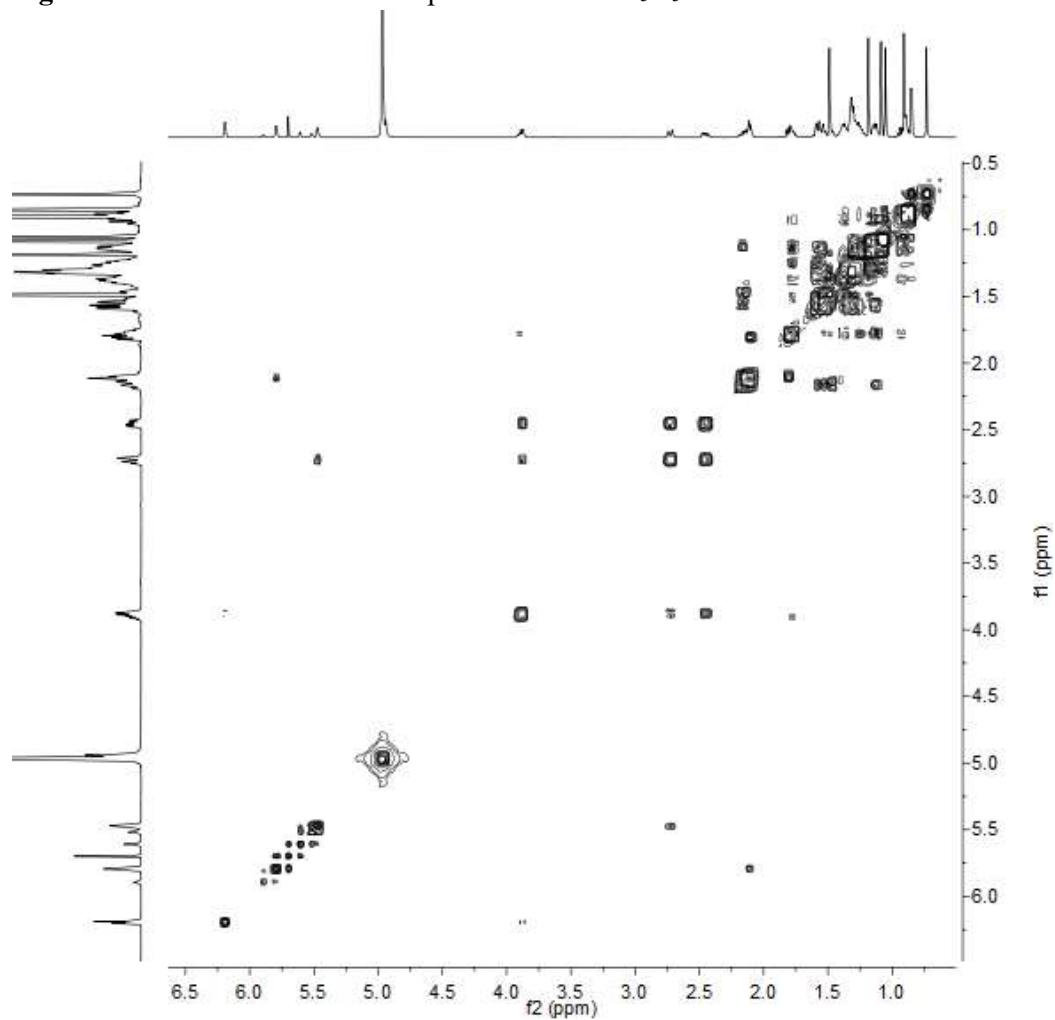


Figure S37. HSQC NMR spectrum of **5** in C₅D₅N

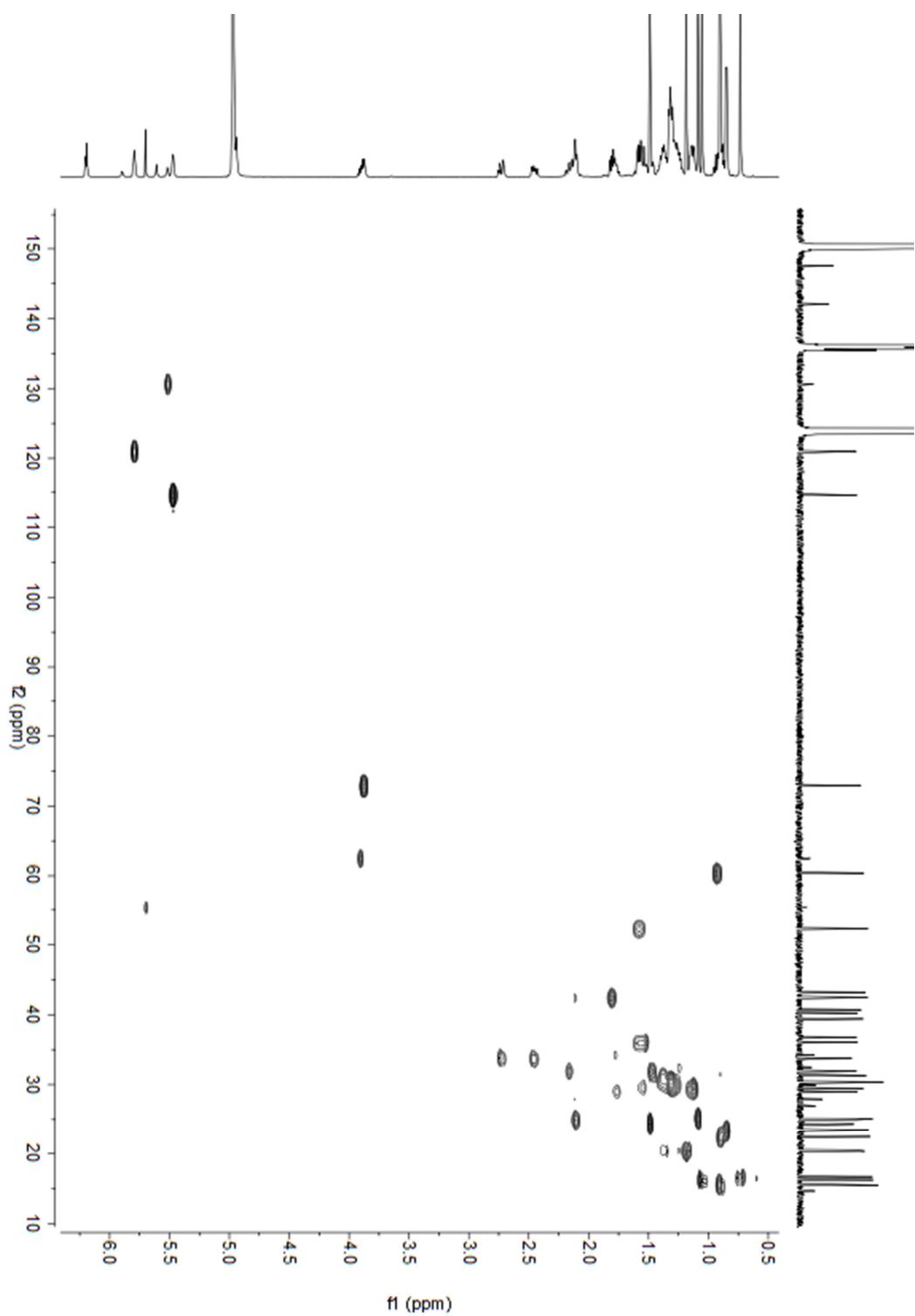


Figure S38. HMBC NMR spectrum of **5** in C₅D₅N

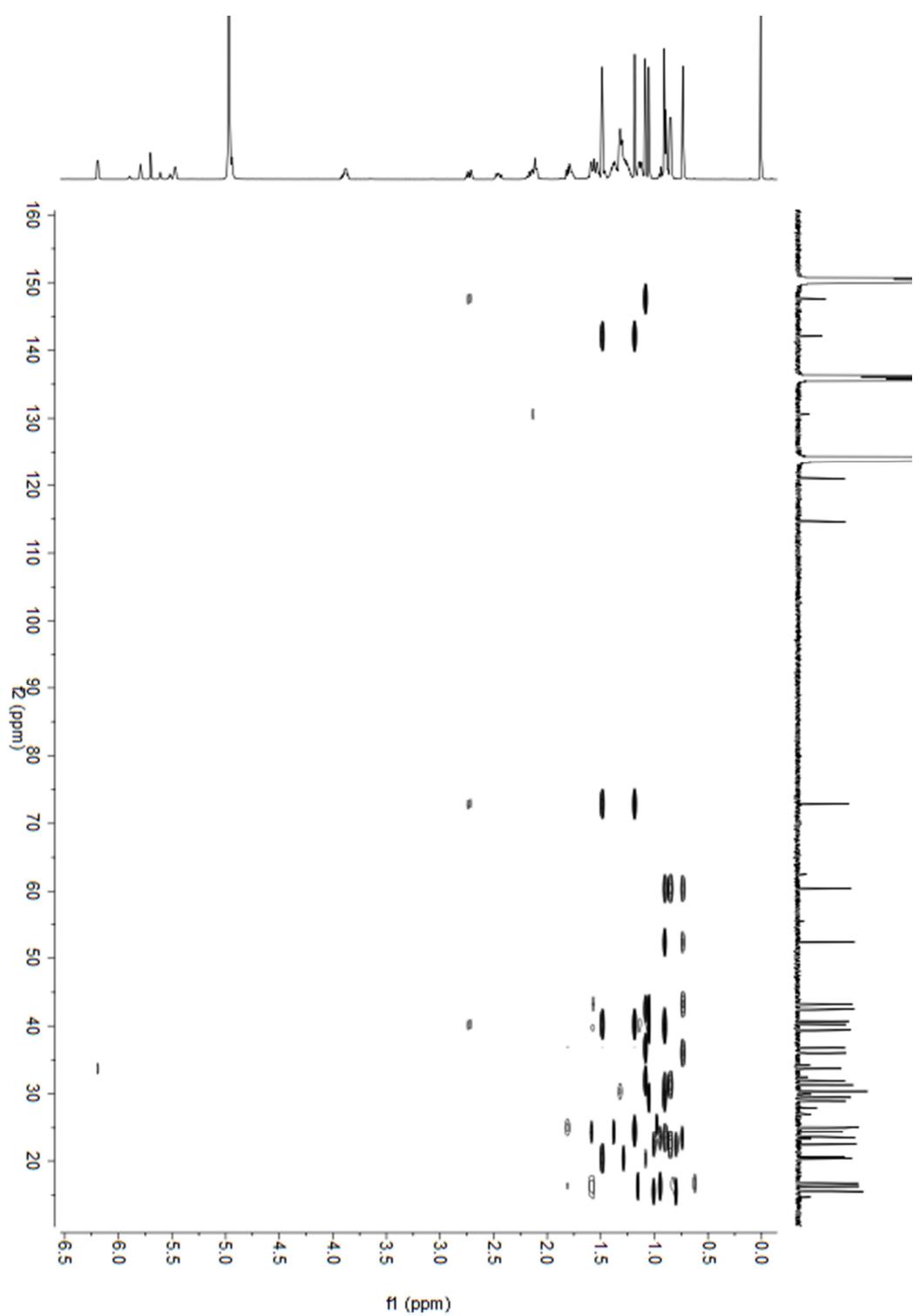


Figure S39. ROESY NMR spectrum of **5** in C₅D₅N

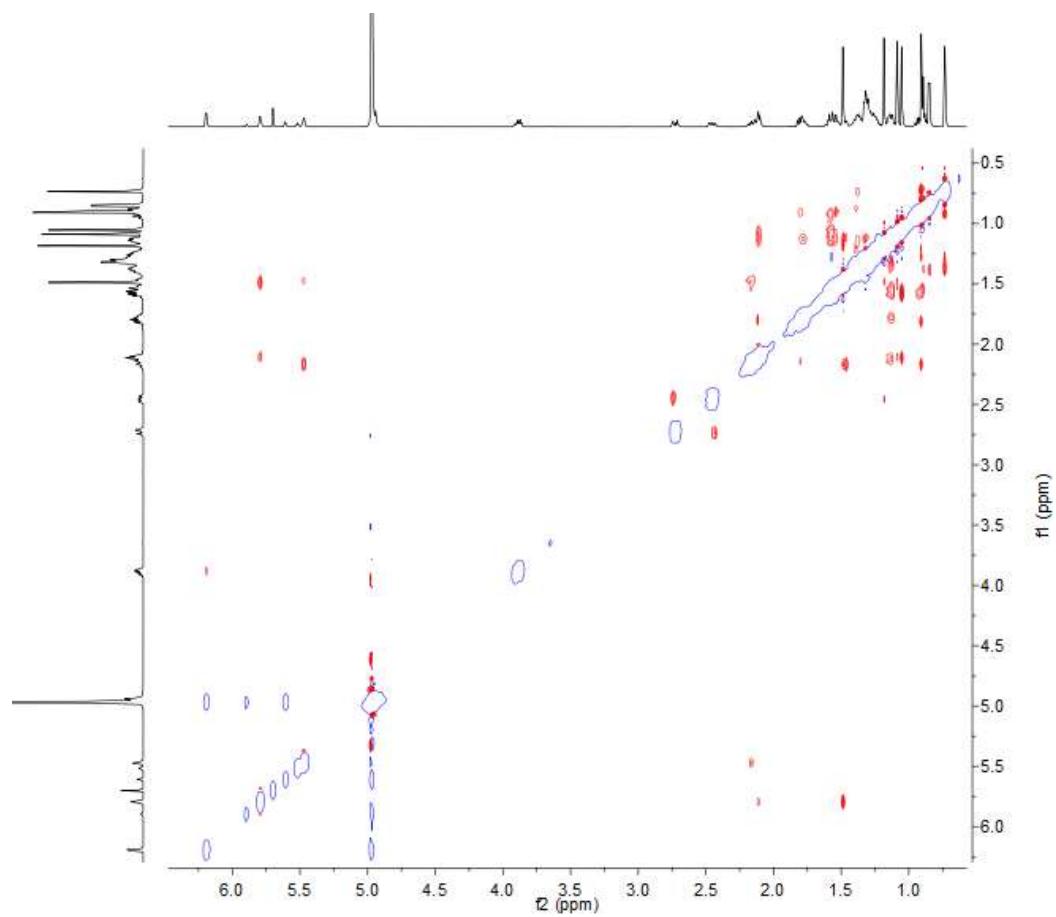


Figure S40. (+)-LRESIMS spectrum of 5

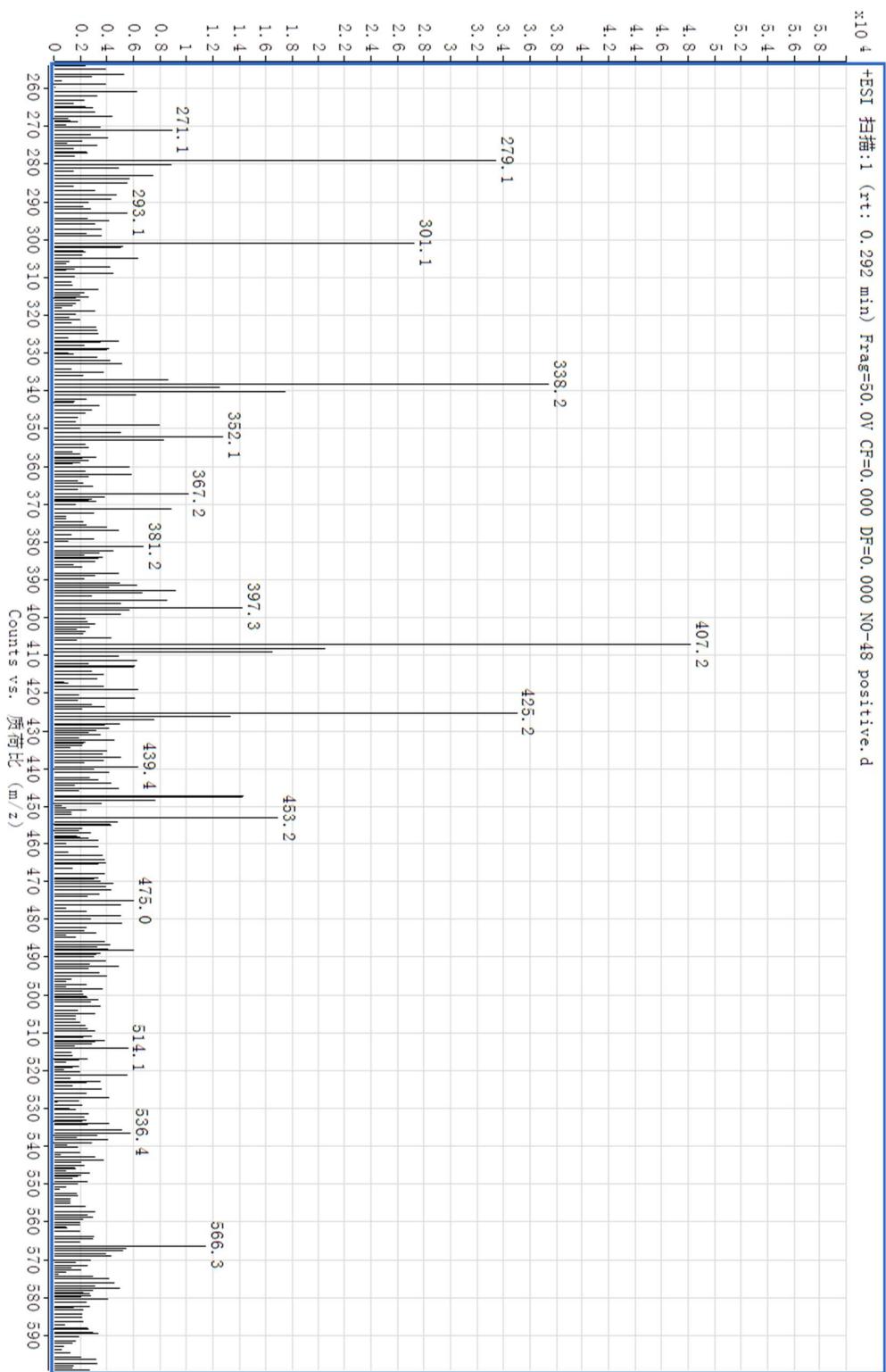


Figure S41. (+)-HRESIMS spectrum of **5**

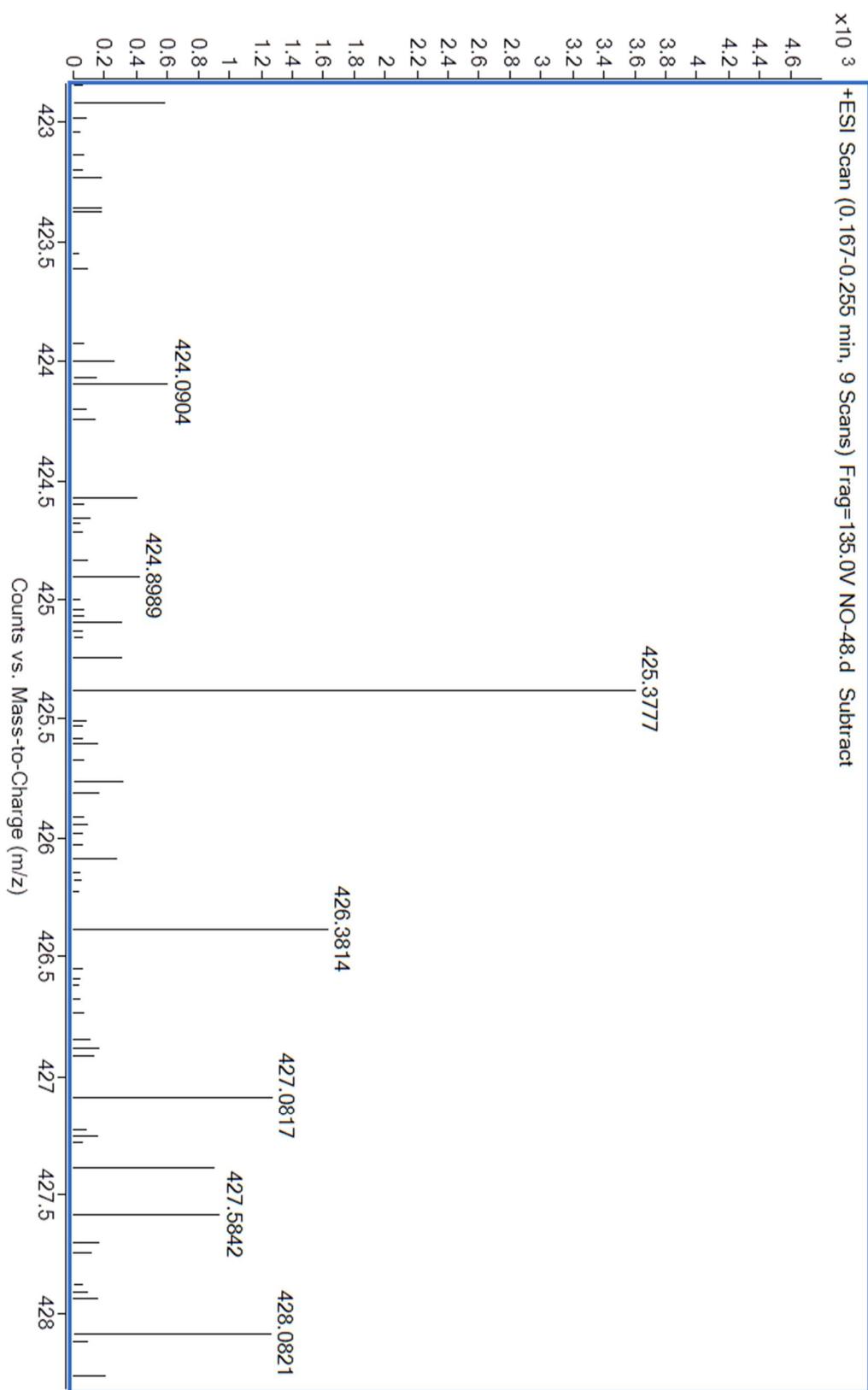


Figure S42. UV spectrum of **5**

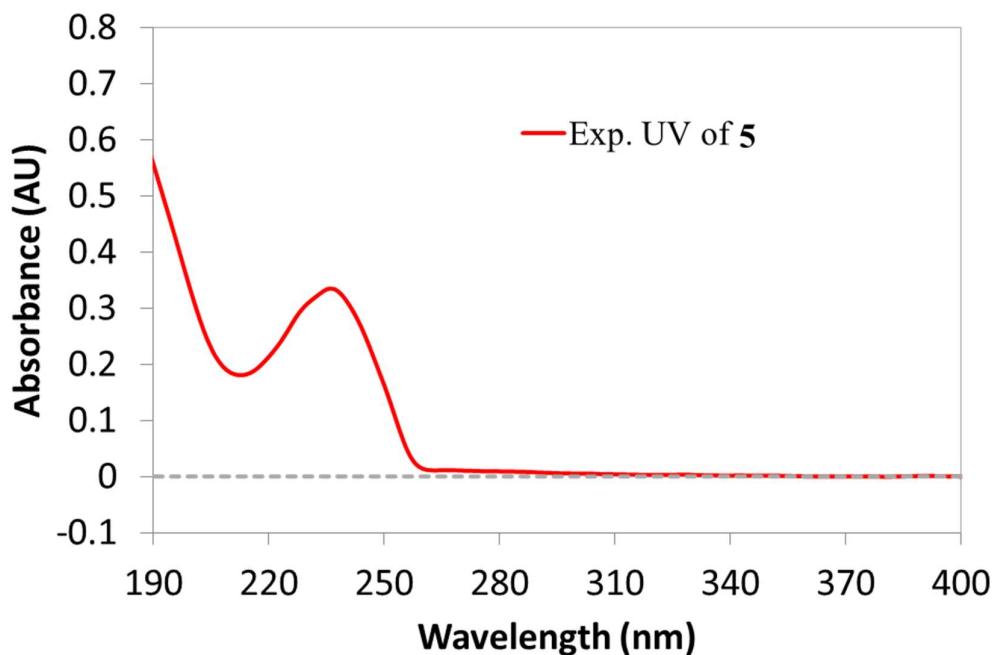


Figure S43. The HPLC analysis for the purity of compound 1

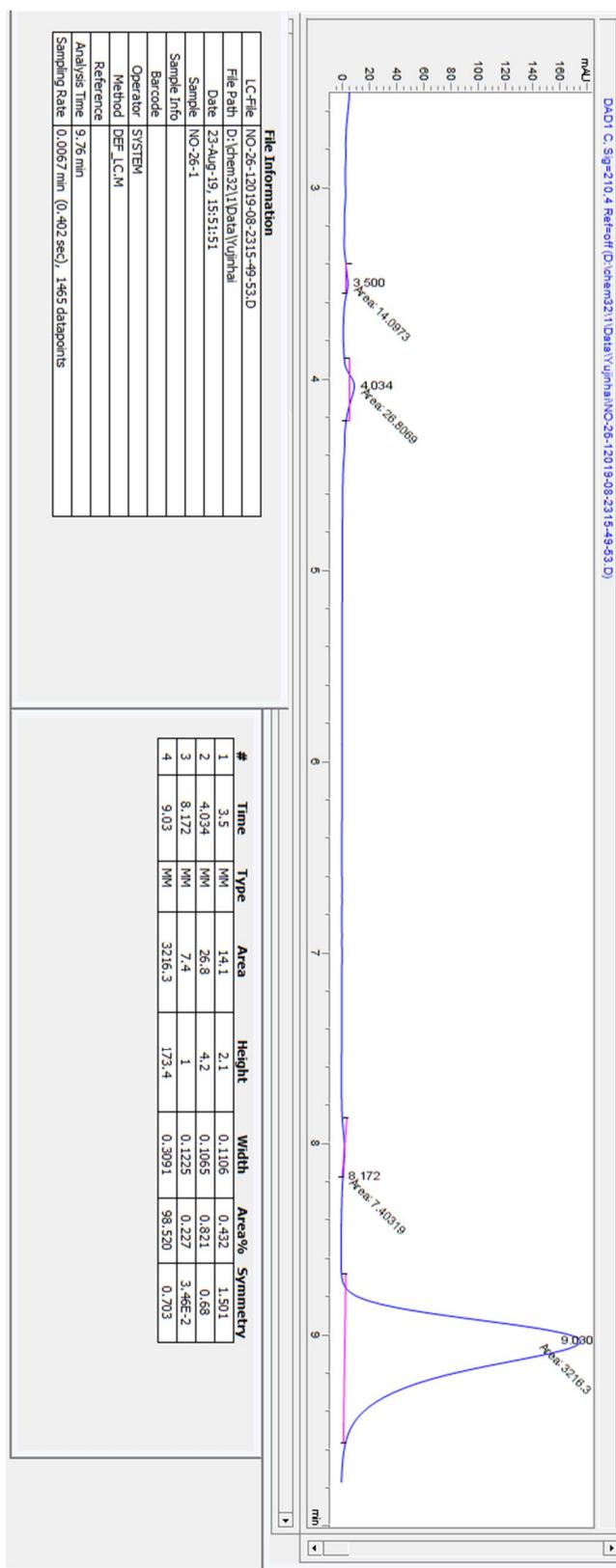


Figure S44. The HPLC analysis for the purity of compound 2

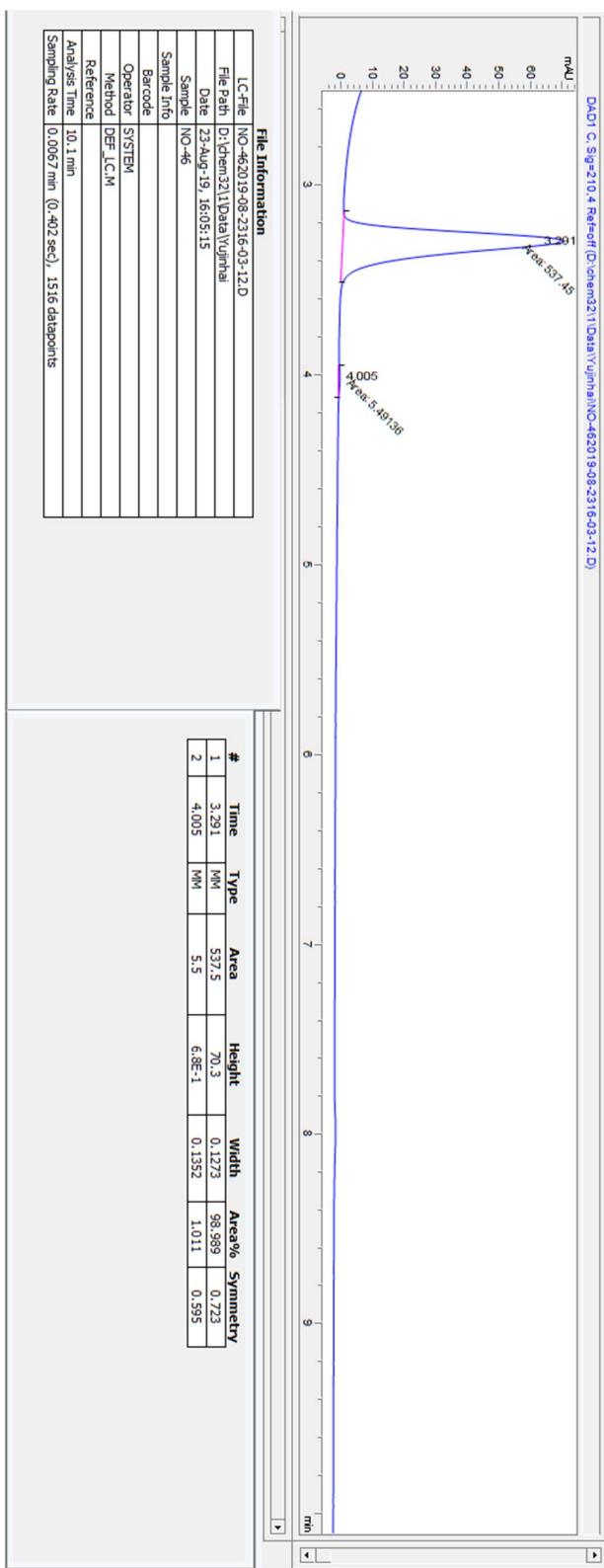


Figure S45. The HPLC analysis for the purity of compound 3

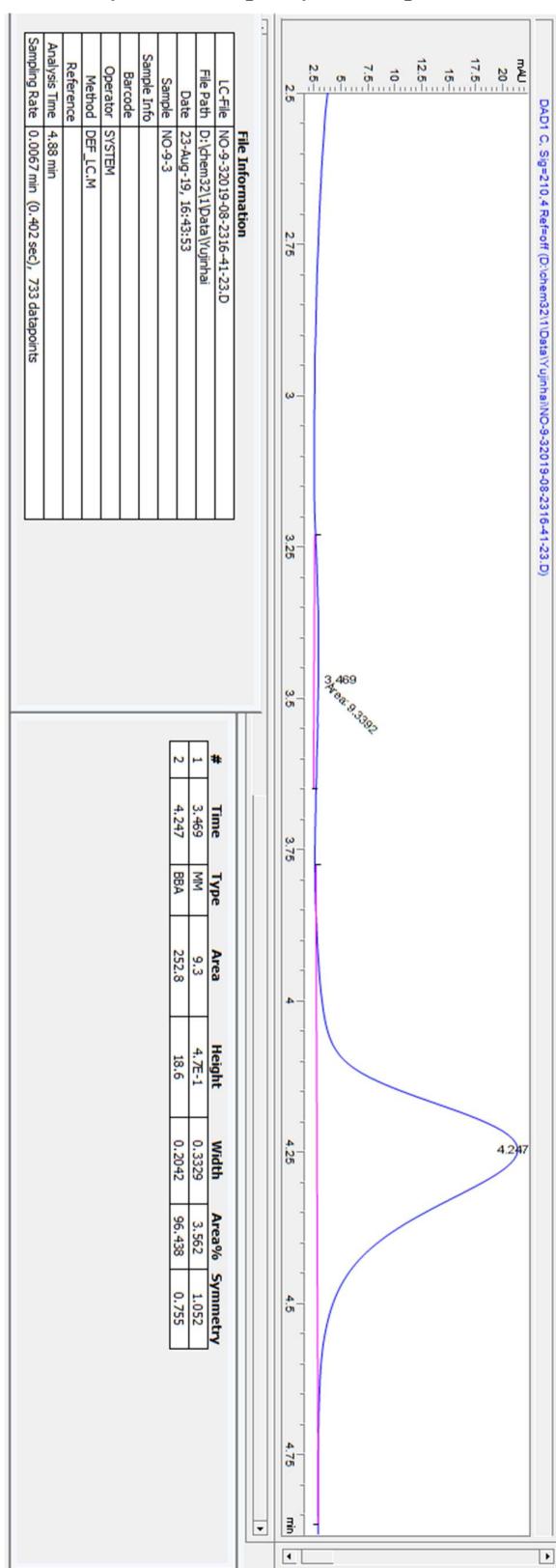


Figure S46. The HPLC analysis for the purity of compound 4

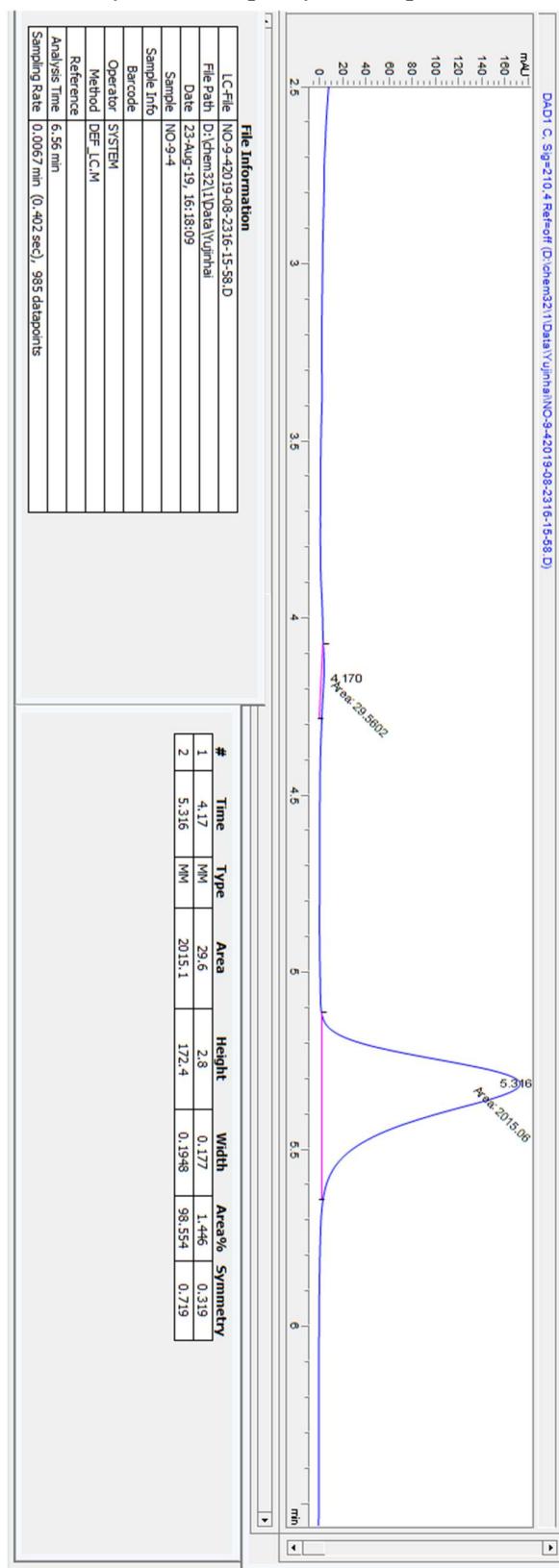


Figure S47. The HPLC analysis for the purity of compound 5

