

Supplementary Material

Hyperattenuins A–I, Bioactive Polyprenylated Acylphloroglucinols from *Hypericum attenuatum* Choisy

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Figure S1. ^1H NMR spectrum (400 MHz) of compound **1** in CDCl_3 .

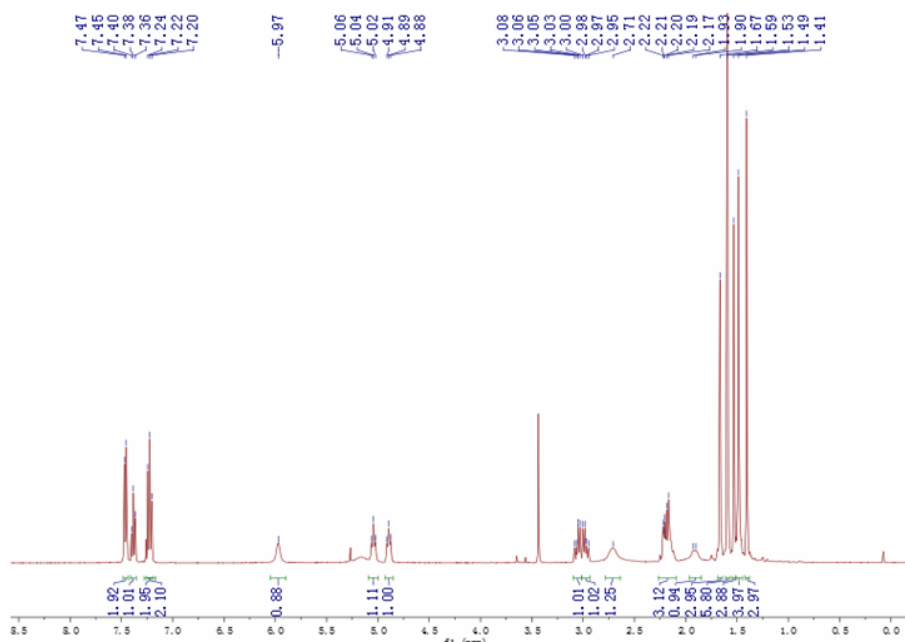


Figure S2. ^{13}C NMR spectrum (100 MHz) of compound **1** in CDCl_3 .

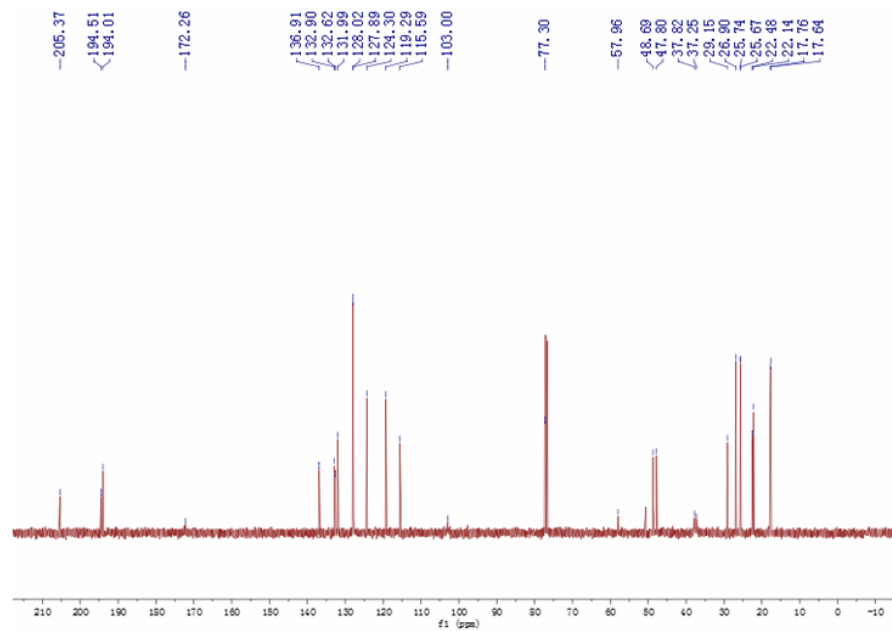


Figure S3. DEPT-135 spectrum (100 MHz) of compound **1** in CDCl₃

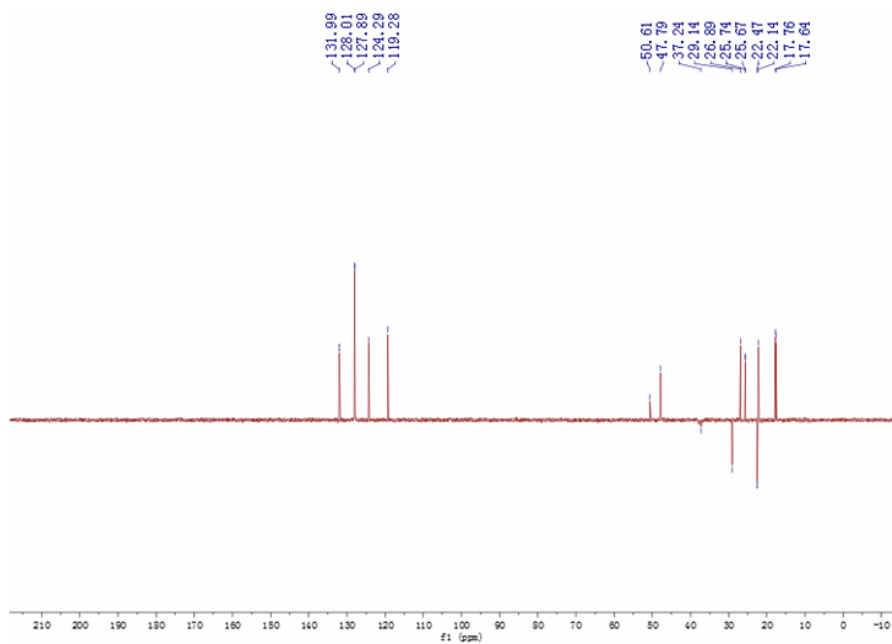


Figure S4. HSQC spectrum of compound **1** in CDCl₃

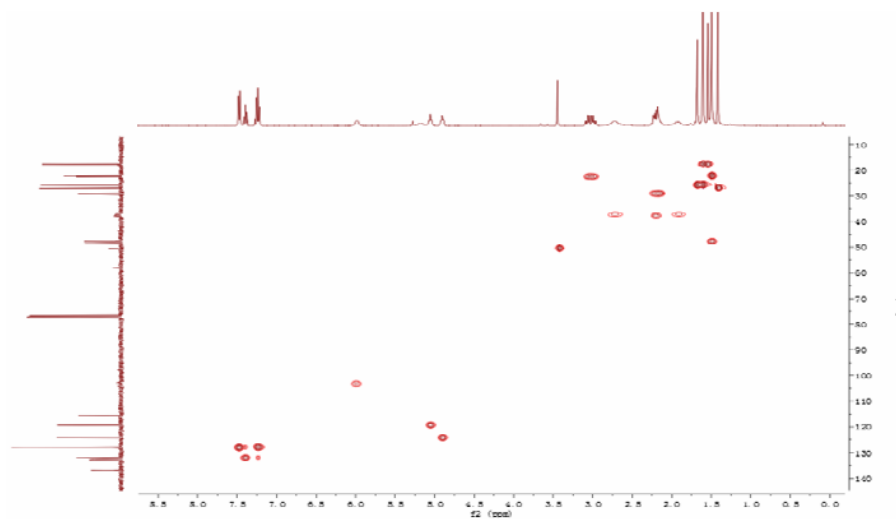


Figure S5. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3

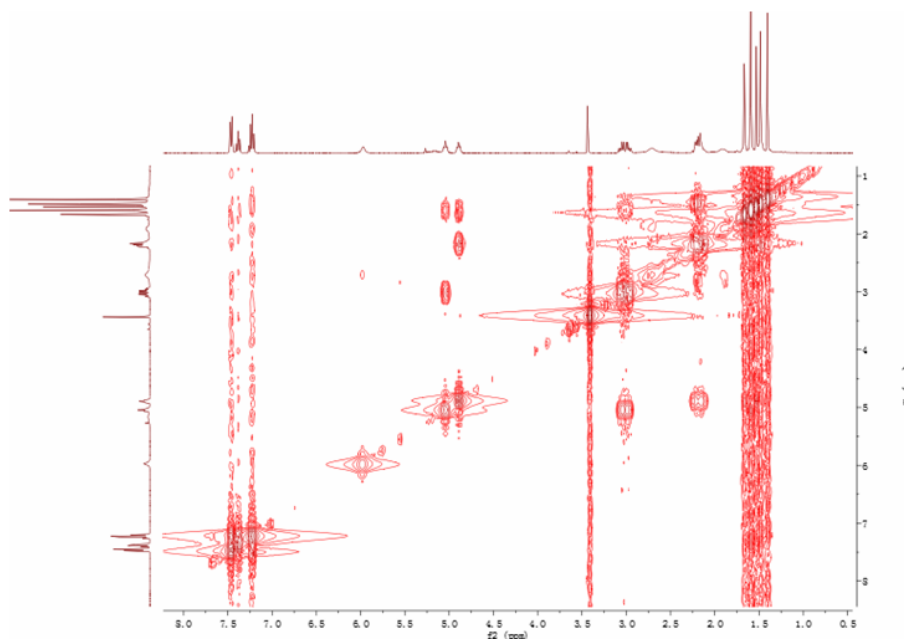


Figure S6. HMBC spectrum of compound **1** in CDCl_3

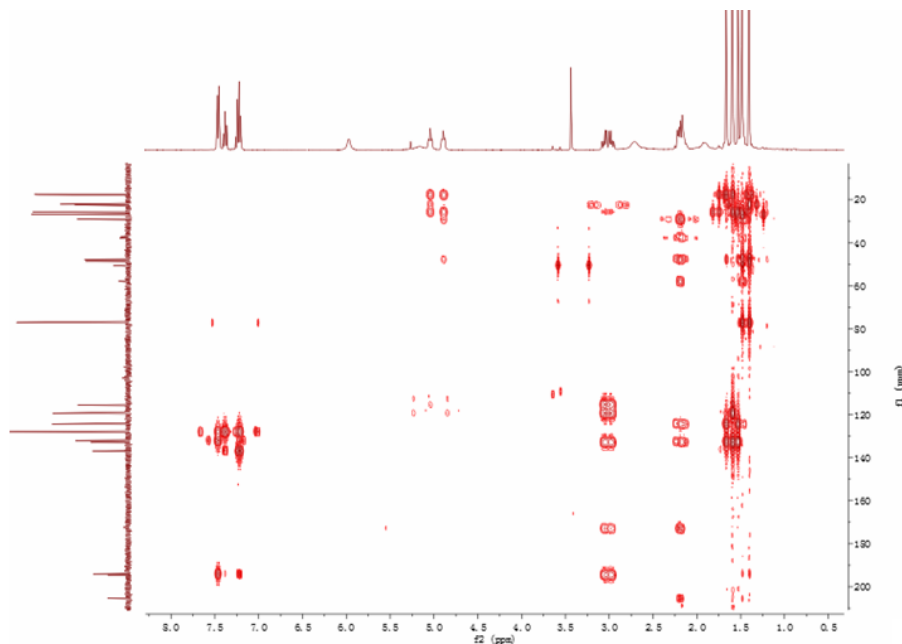


Figure S7. NOESY spectrum of compound **1** in CDCl₃

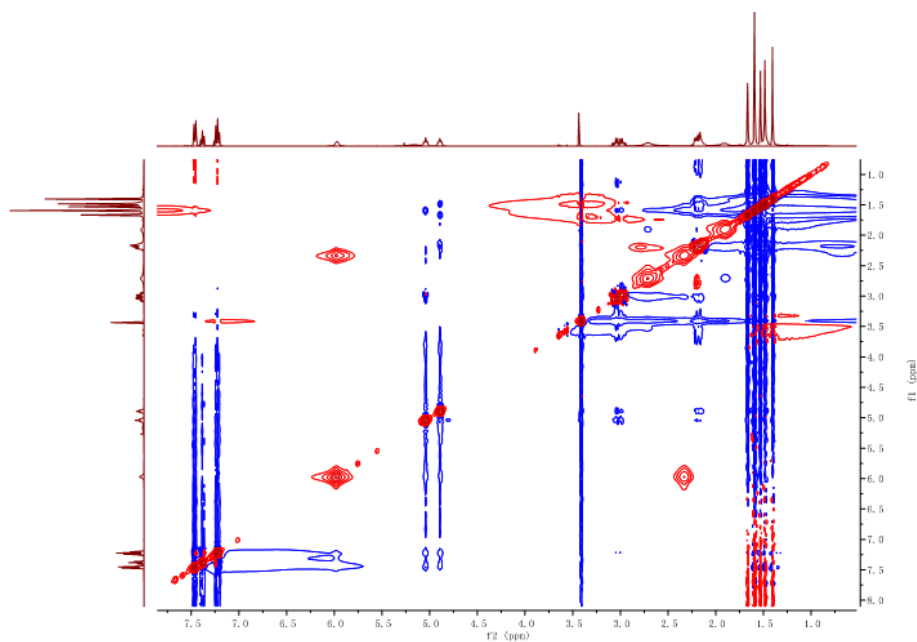


Figure S8. HRESIMS spectrum of compound **1**

Idy1-59-9 #16 RT: 0.23 AV: 1 NL: 1.17E7
T: FTMS + p ESI Full ms [50.00-1500.00]

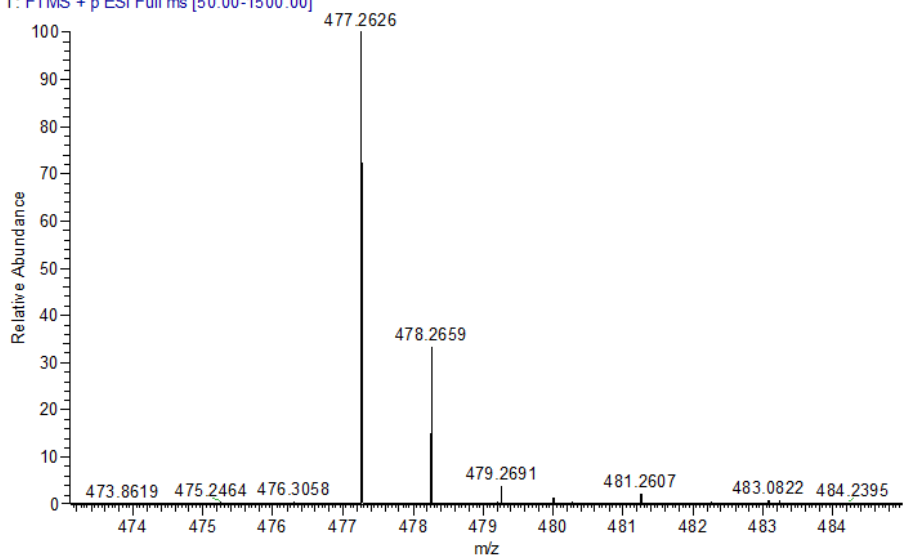


Figure S9. UV spectrum of compound **1**

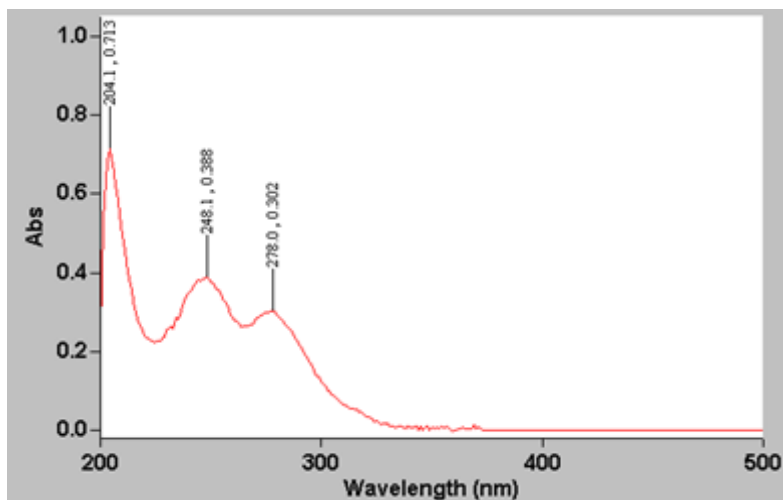


Figure S10. IR (KBr) spectrum of compound **1**

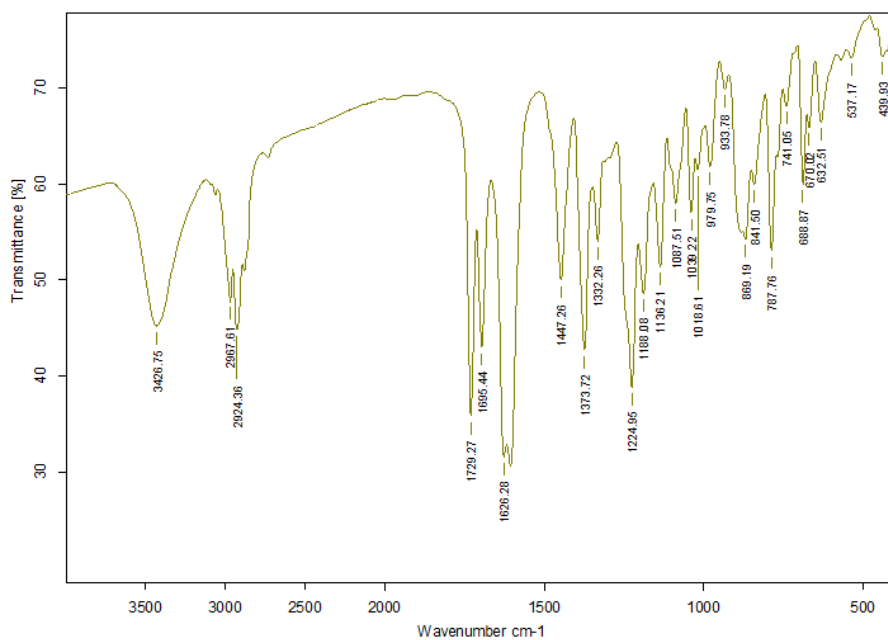


Figure S11. ^1H NMR spectrum (400 MHz) of compound **2** in CDCl_3

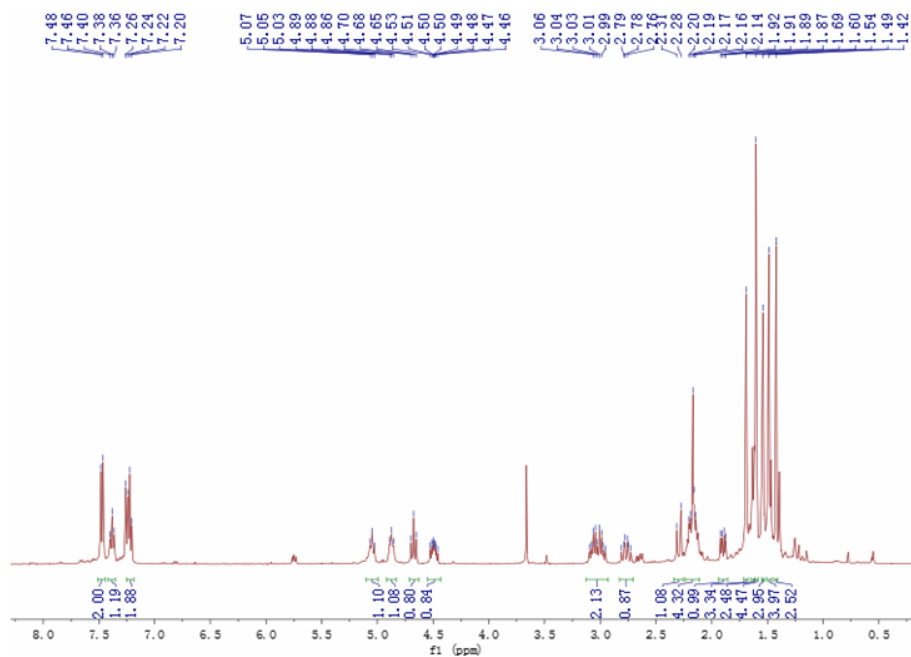


Figure S12. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3

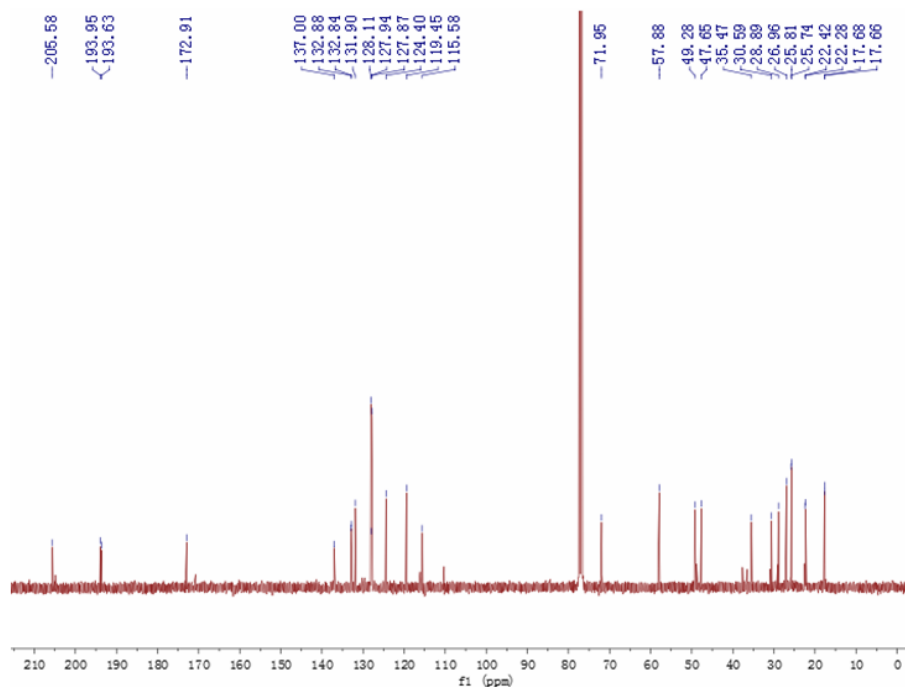


Figure S13. DEPT-135 spectrum (100 MHz) of compound **2** in CDCl₃

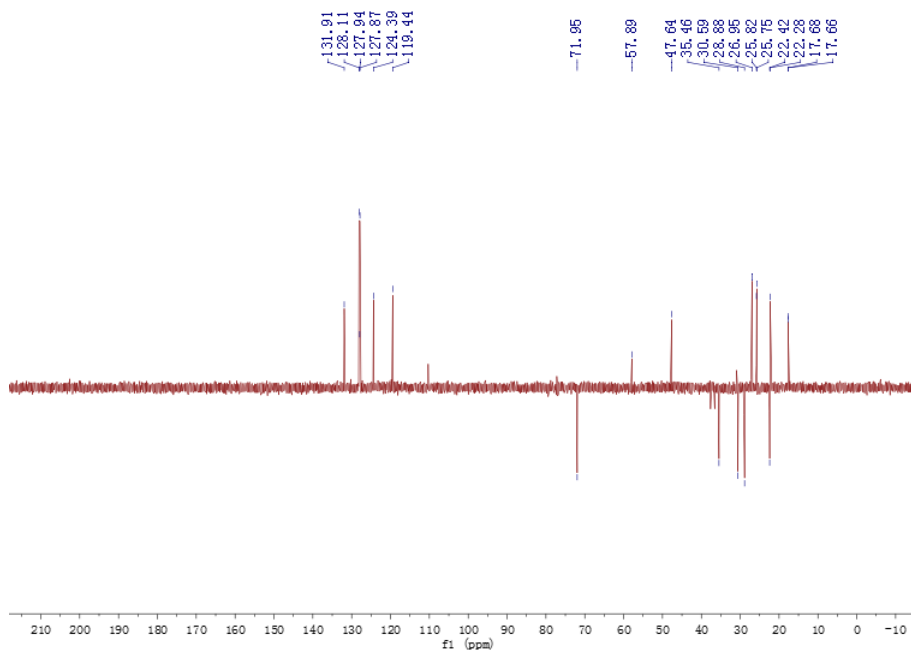


Figure S14. HSQC spectrum of compound **2** in CDCl₃

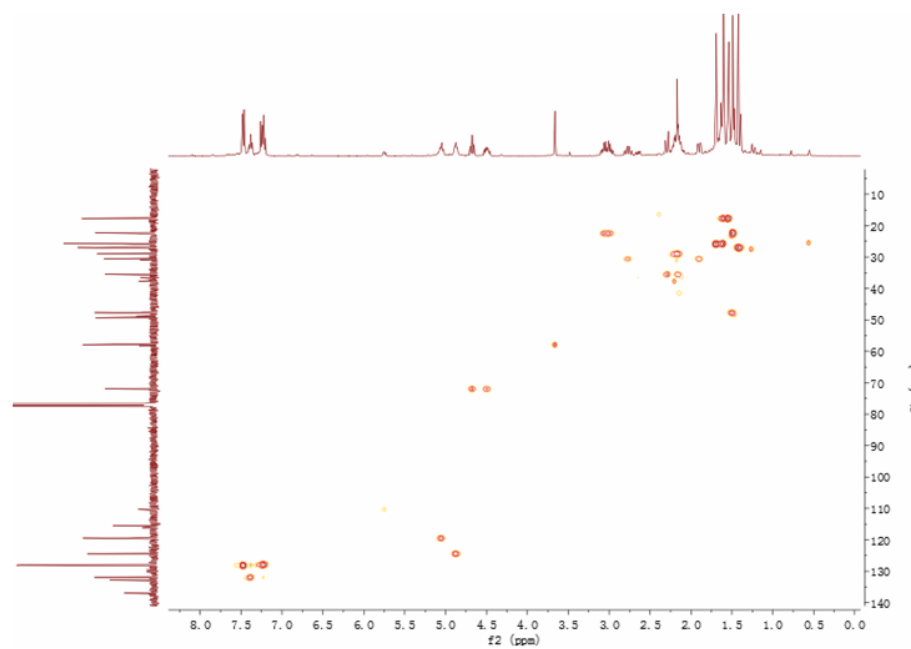


Figure S15. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3

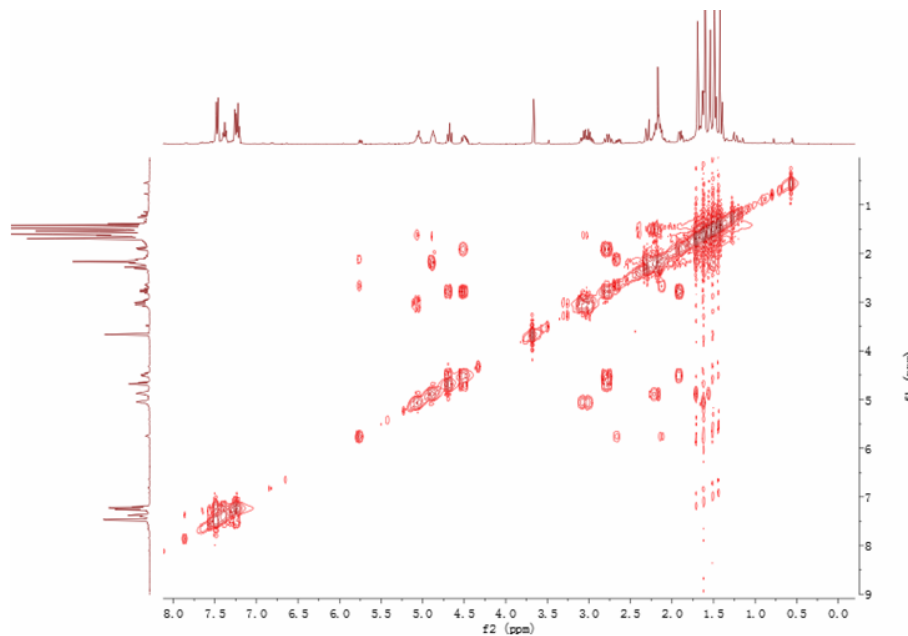


Figure S16. HMBC spectrum of compound **2** in CDCl_3

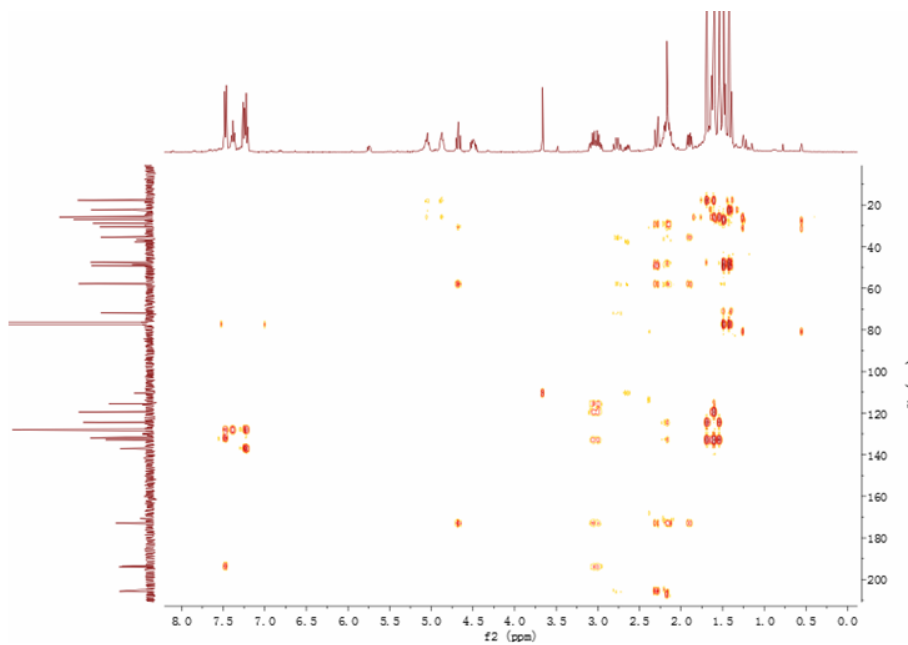


Figure S17. NOESY spectrum of compound **2** in CDCl₃

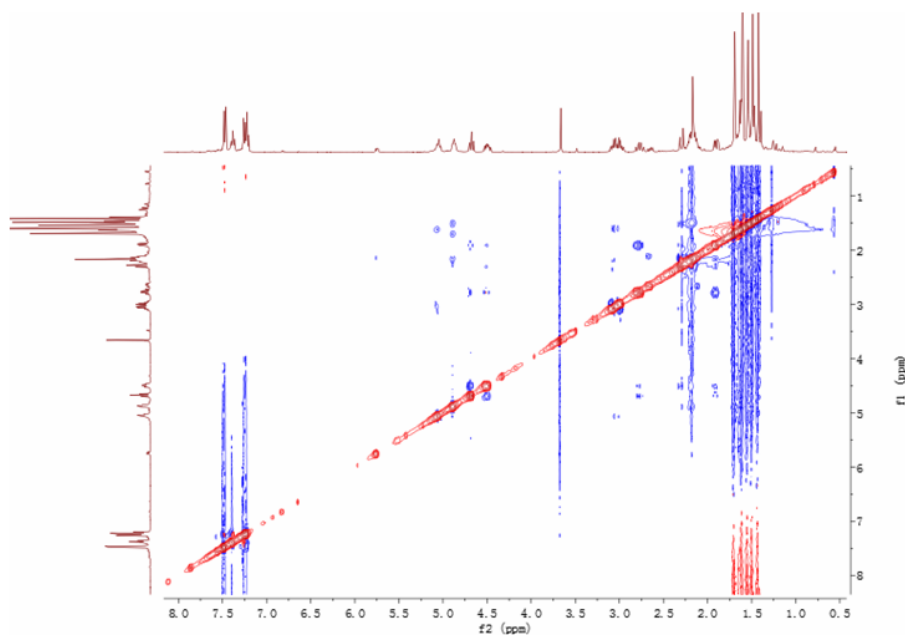


Figure S18. HRESIMS spectrum of compound **2**

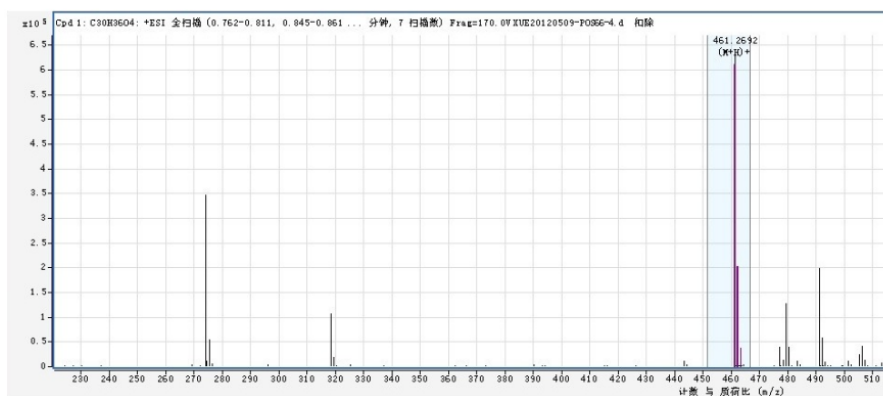


Figure S19. UV spectrum of compound **2**

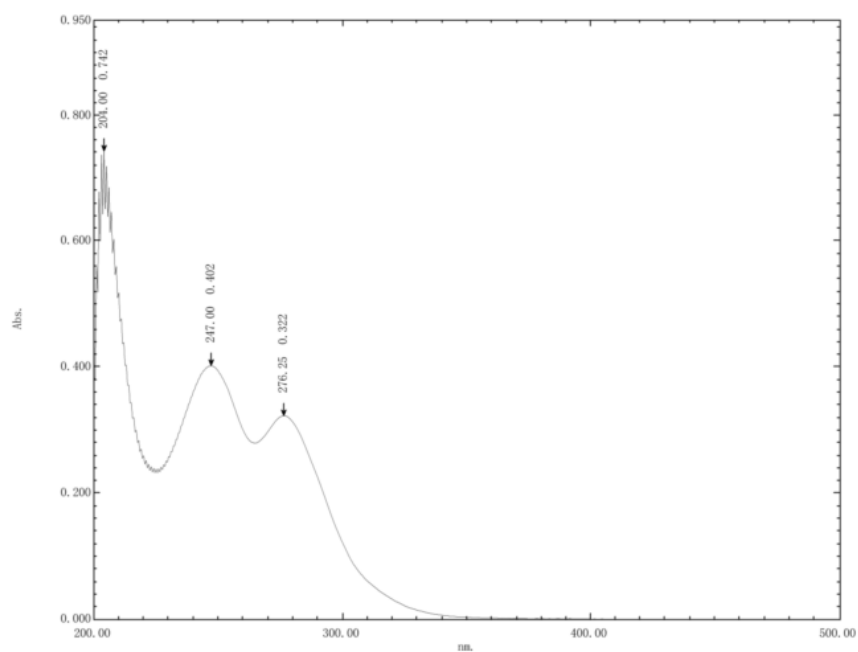


Figure S20. IR (KBr) spectrum of compound **2**

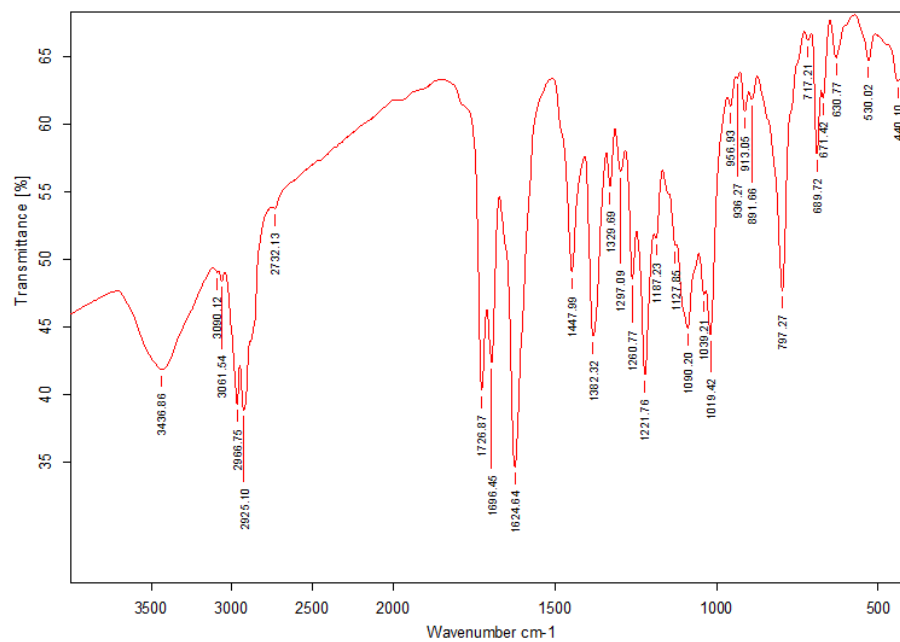


Figure S21. ^1H NMR spectrum (400 MHz) of compound **3** in CDCl_3

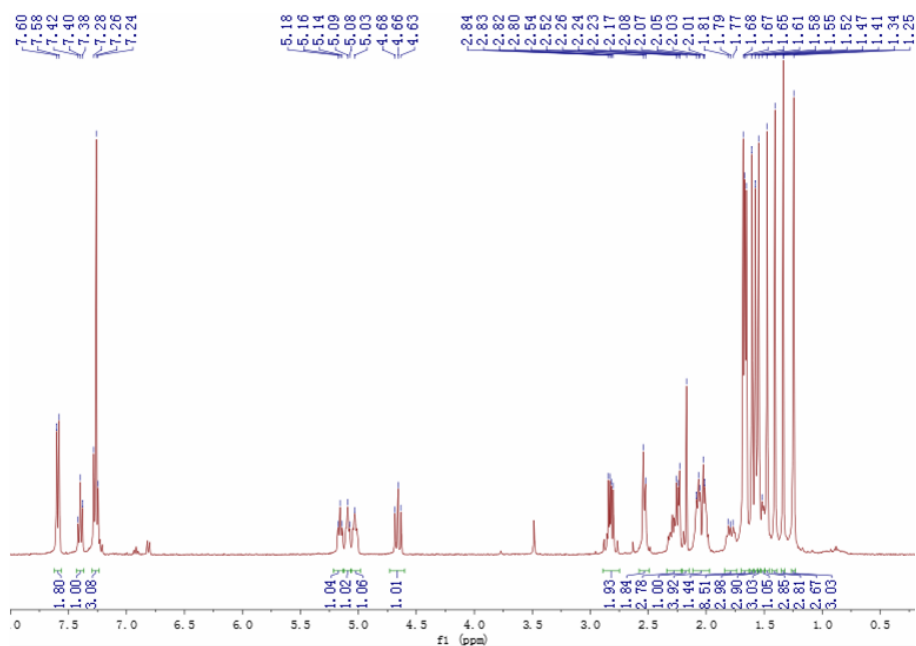


Figure S22. ^{13}C NMR spectrum (100 MHz) of compound **3** in CDCl_3

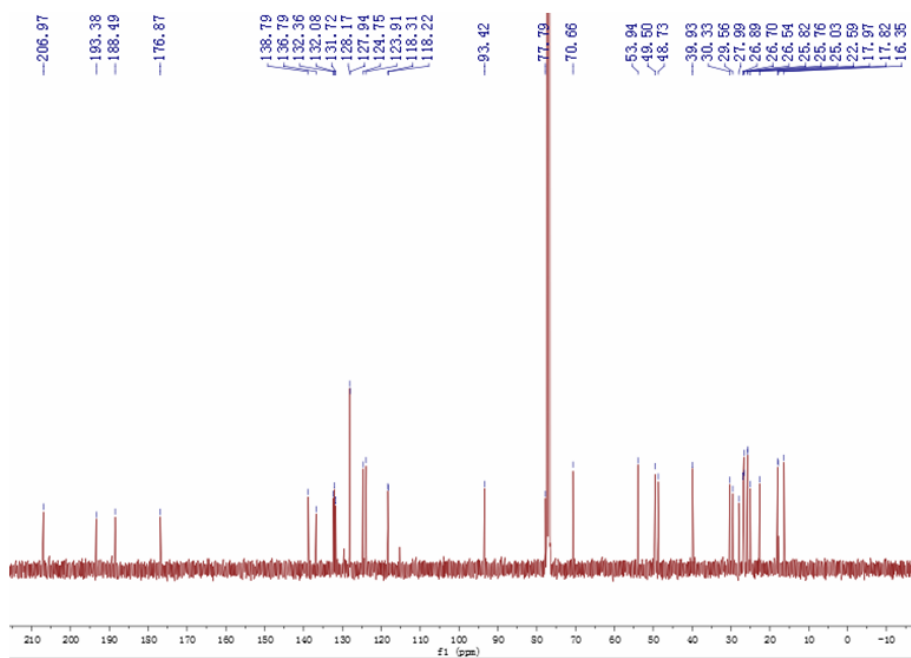


Figure S23. DEPT-135 spectrum (100 MHz) of compound **3** in CDCl₃

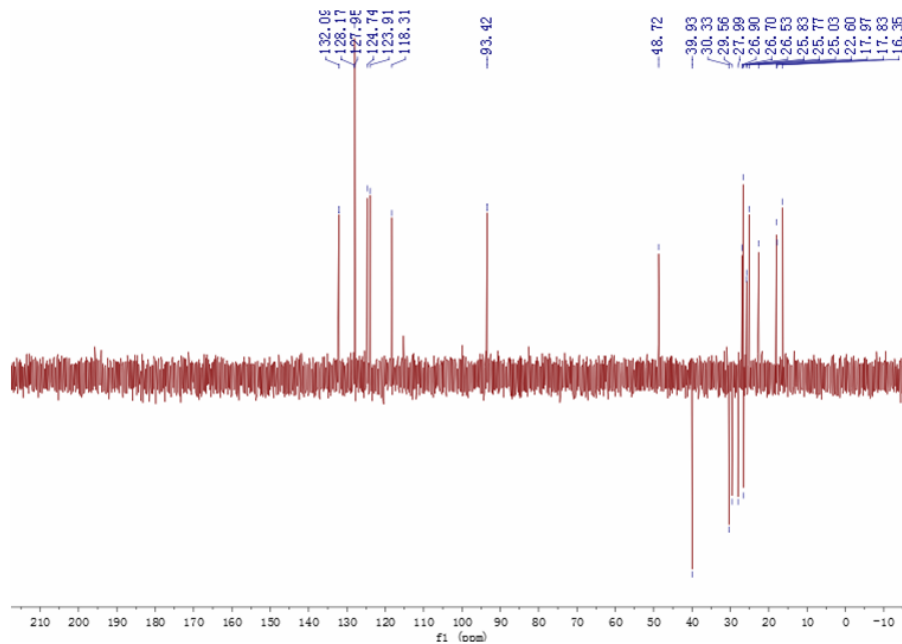


Figure S24. HSQC spectrum of compound **3** in CDCl₃

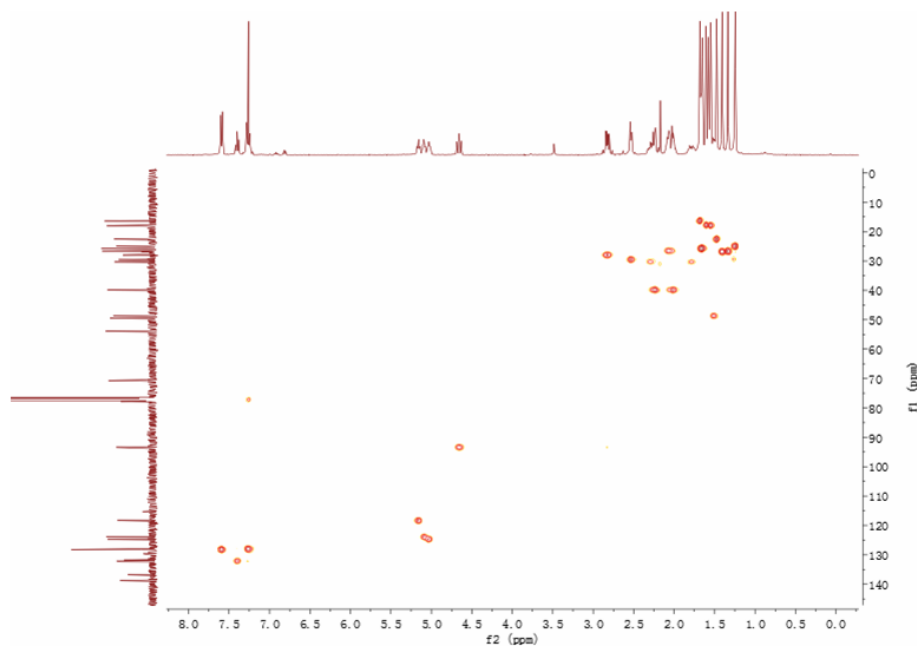


Figure S25. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3

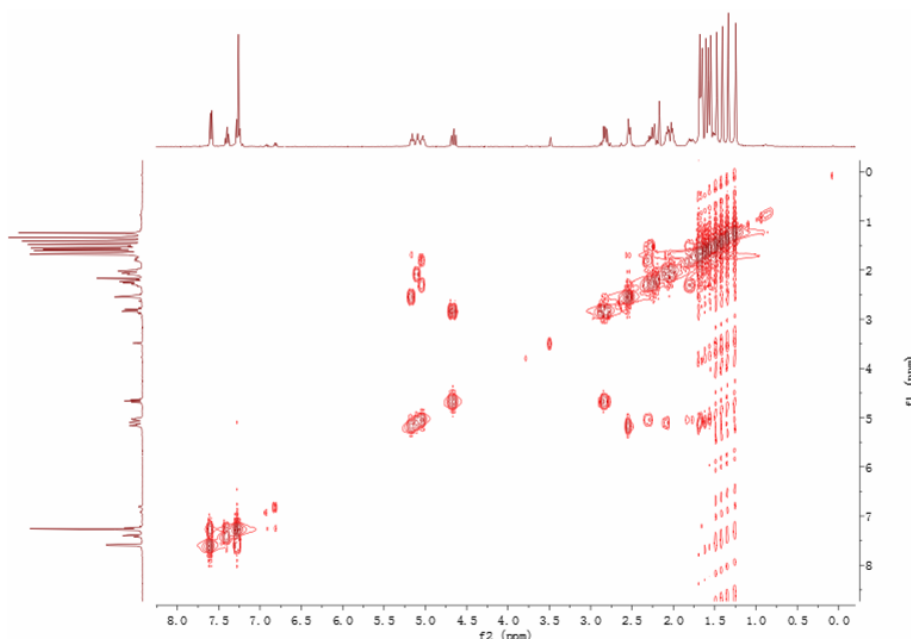


Figure S26. HMBC spectrum of compound **3** in CDCl_3

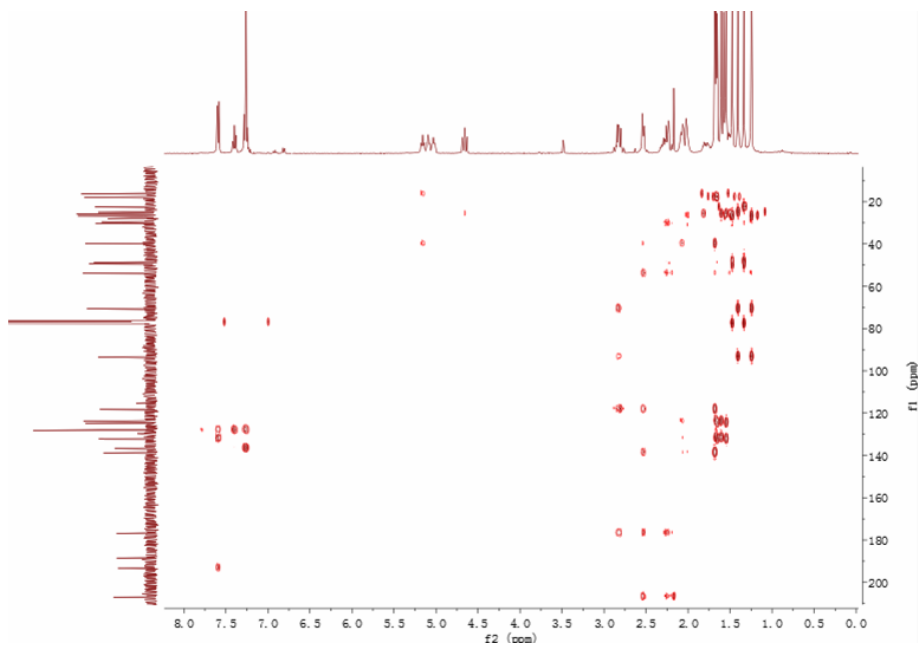


Figure S27. NOESY spectrum of compound **3** in CDCl₃

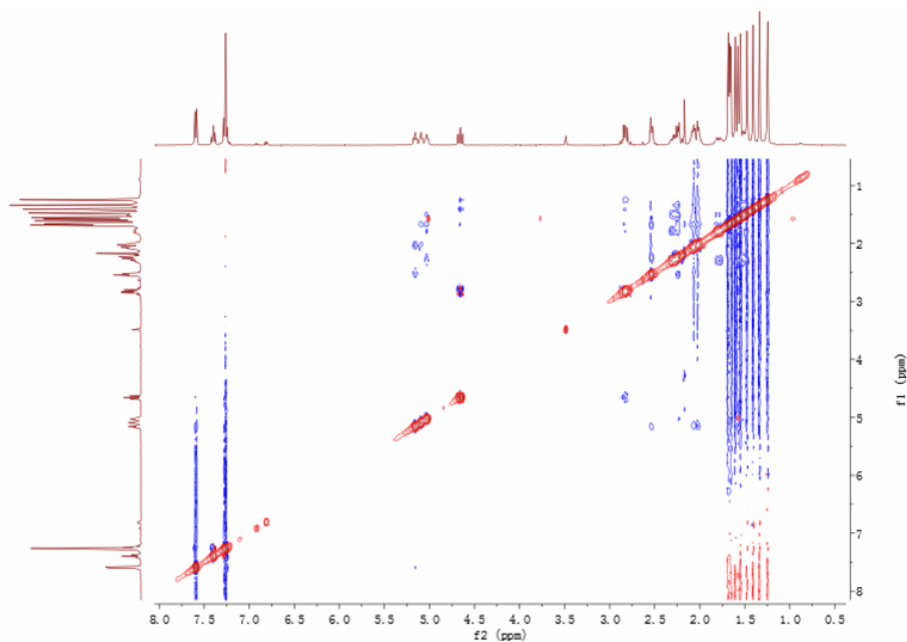


Figure S28. HRESIMS spectrum of compound **3**

ZH2-6-22 #22 RT: 0.30 AV: 1 NL: 2.06E7
T: FTMS + p ESI Full ms [50.00-1000.00]

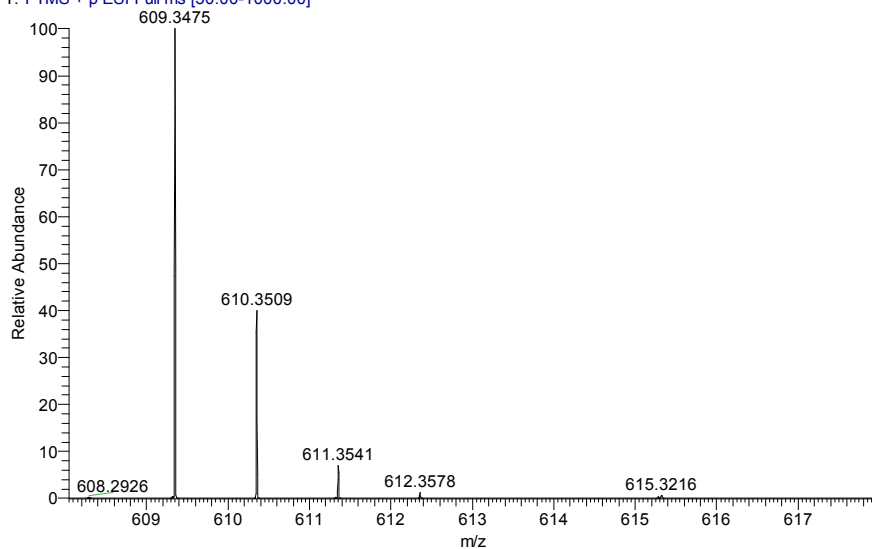


Figure S29. UV spectrum of compound **3**

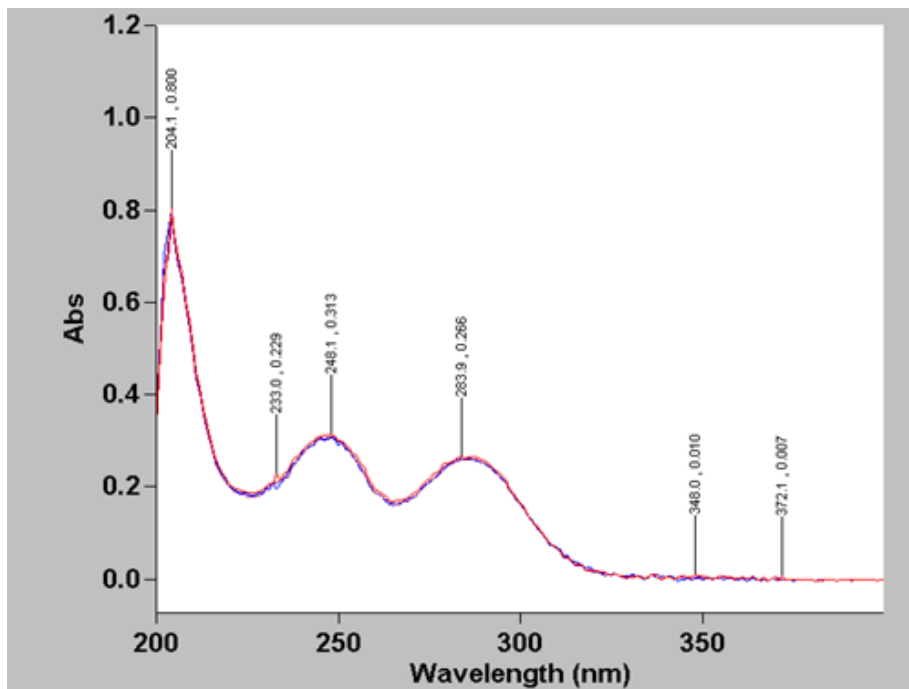


Figure S30. IR (KBr) spectrum of compound **3**

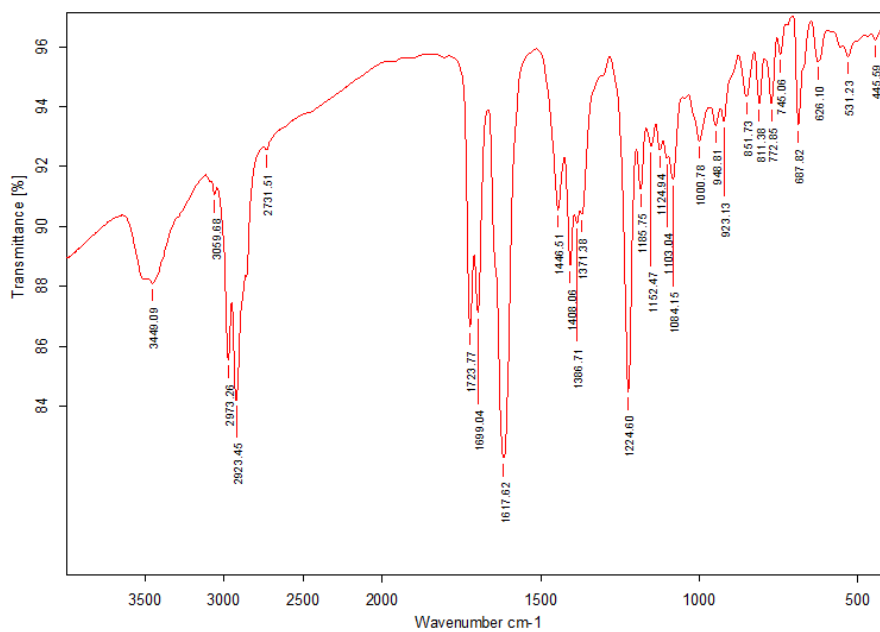


Figure S31. ^1H NMR spectrum (400 MHz) of compound **4** in CDCl_3

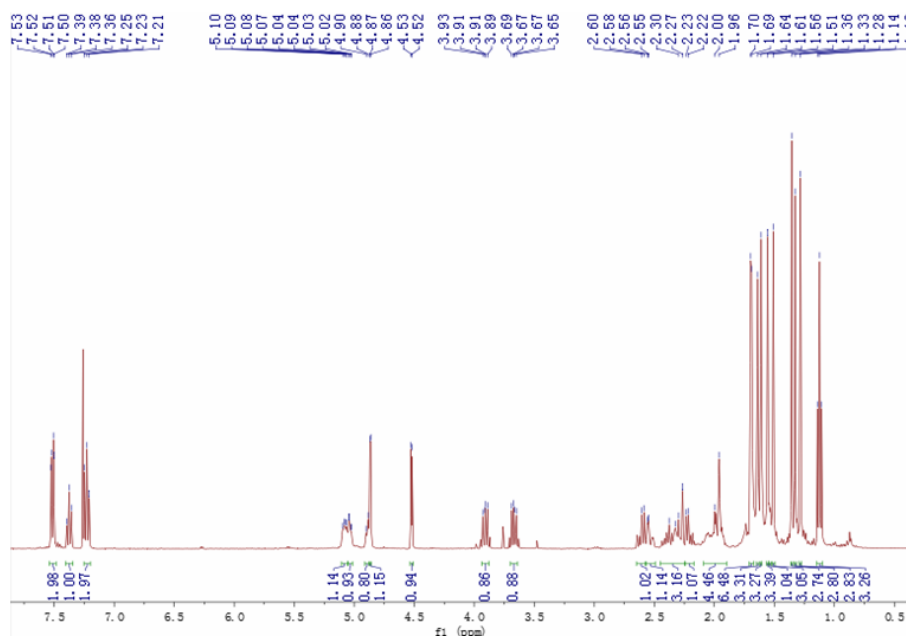


Figure S32. ^{13}C NMR spectrum (100 MHz) of compound **4** in CDCl_3

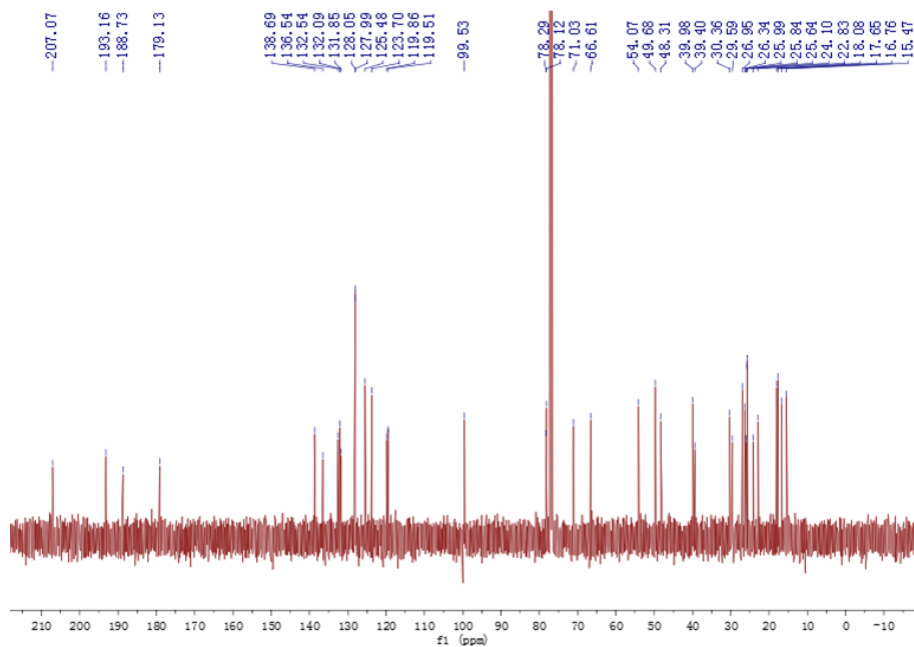


Figure S33. DEPT-135 spectrum (100 MHz) of compound **4** in CDCl₃

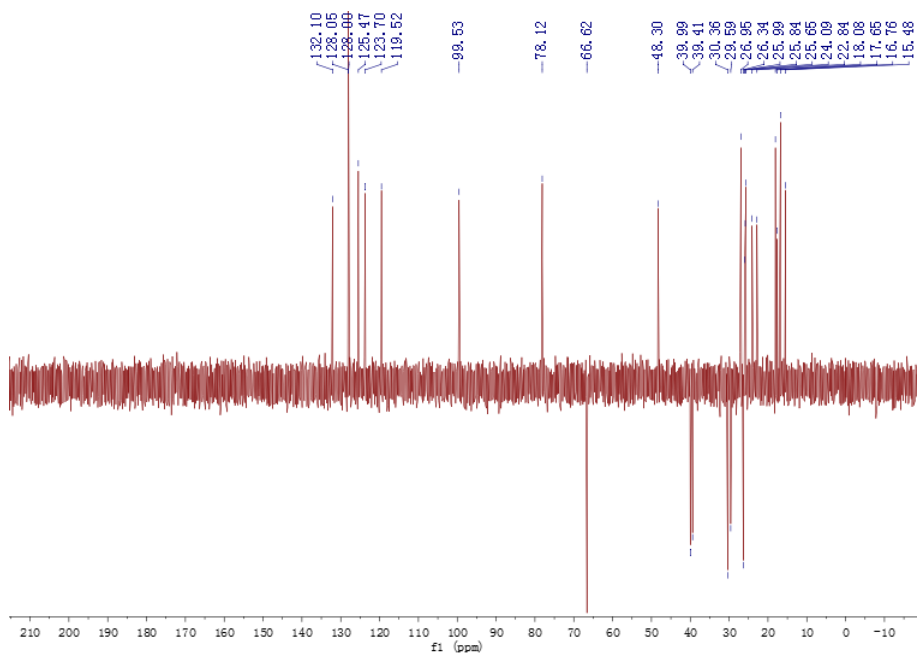


Figure S34. HSQC spectrum of compound **4** in CDCl₃

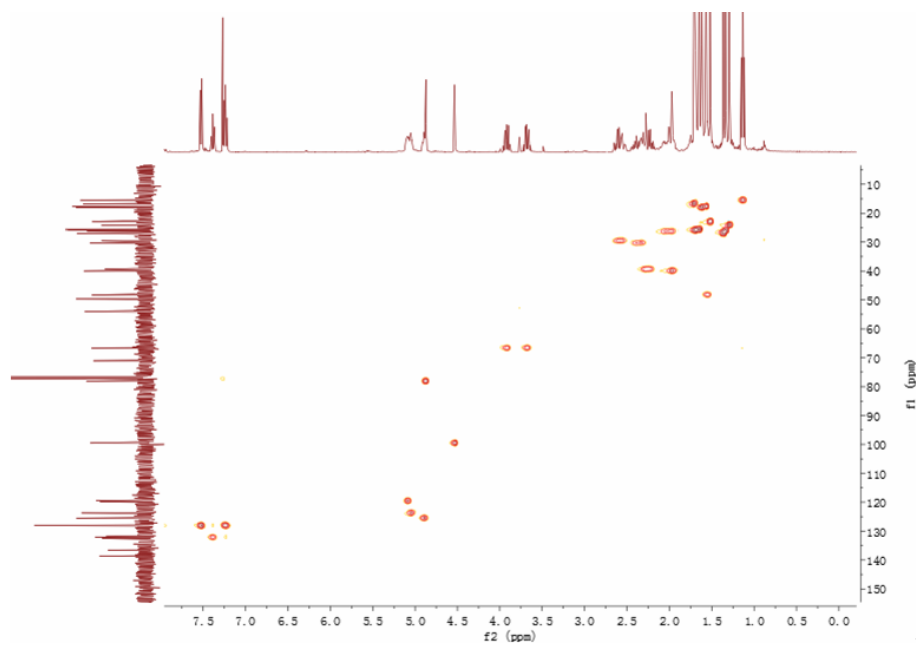


Figure S35. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3

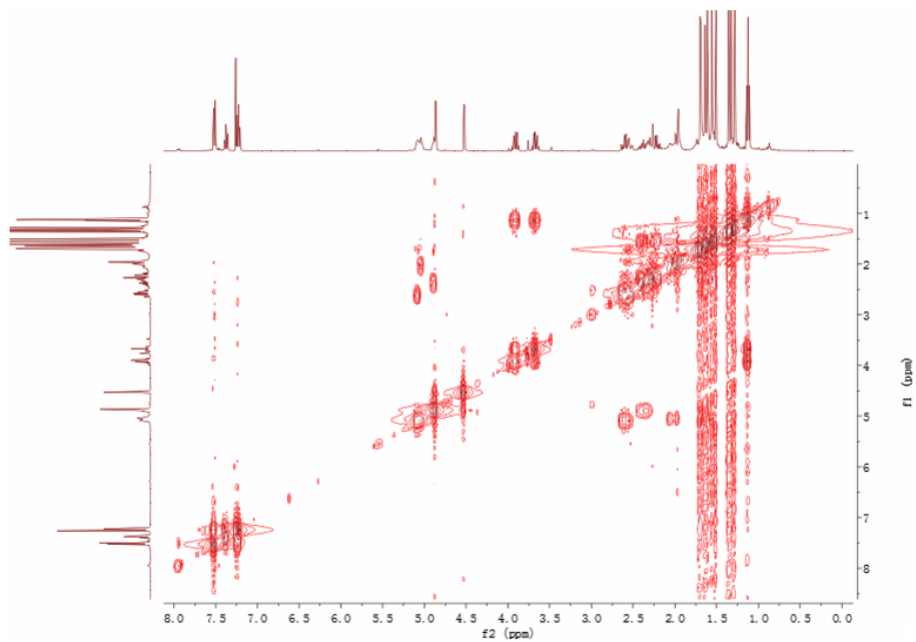


Figure S36. HMBC spectrum of compound **4** in CDCl_3

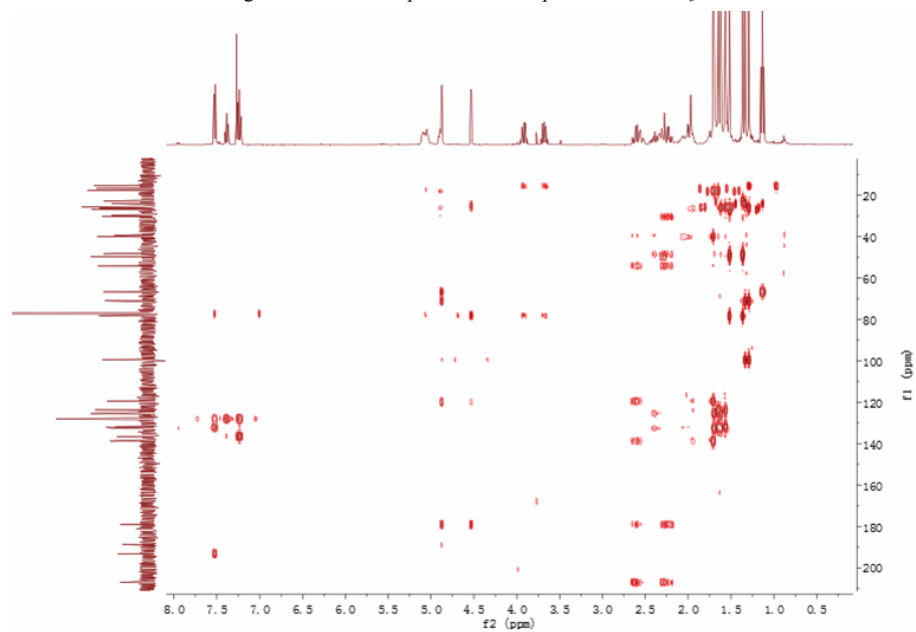


Figure S37. NOESY spectrum of compound **4** in CDCl₃

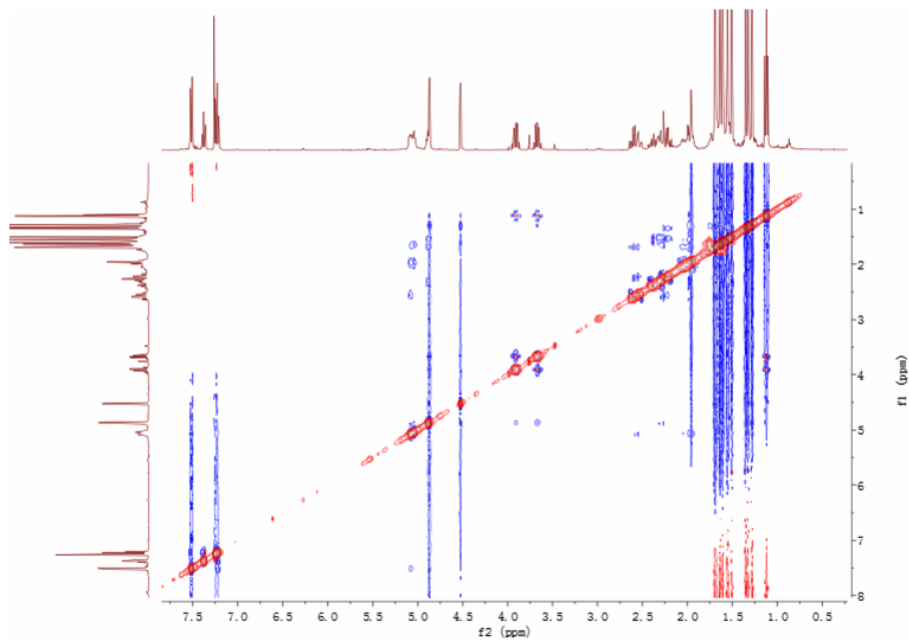


Figure S38. HRESIMS spectrum of compound **4**

Idy1-48-11 #25 RT: 0.35 AV: 1 NL: 4.20E6
T: FTMS + p ESI Full ms [50.00-1500.00]

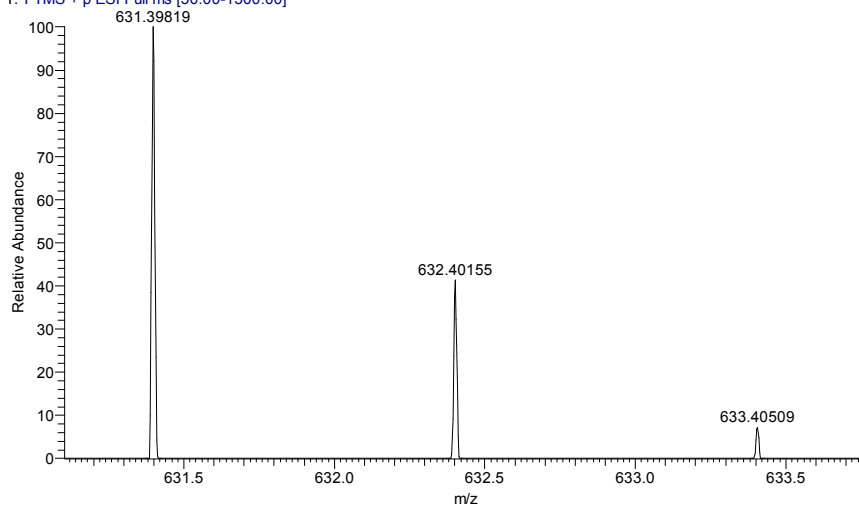


Figure S39. UV spectrum of compound 4

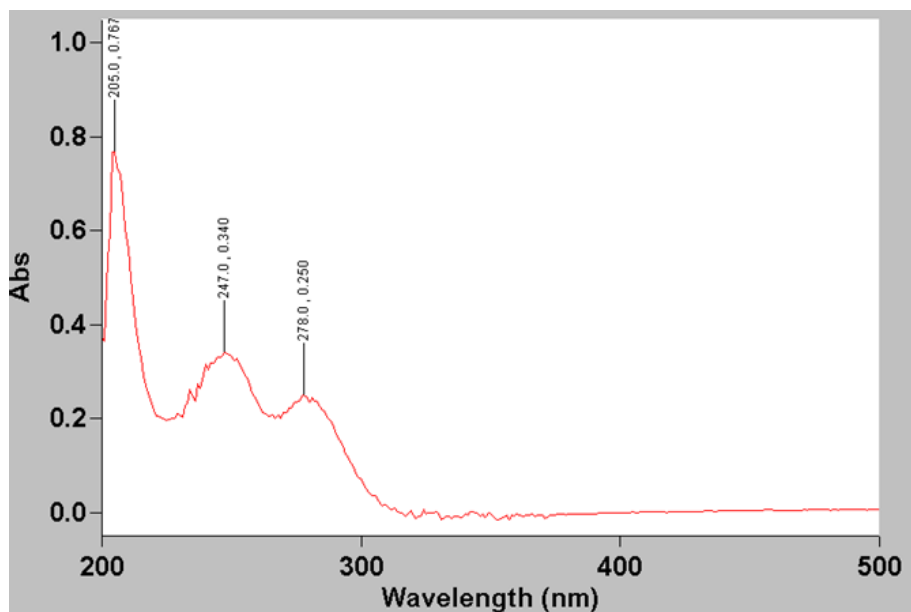


Figure S40. IR (KBr) spectrum of compound 4

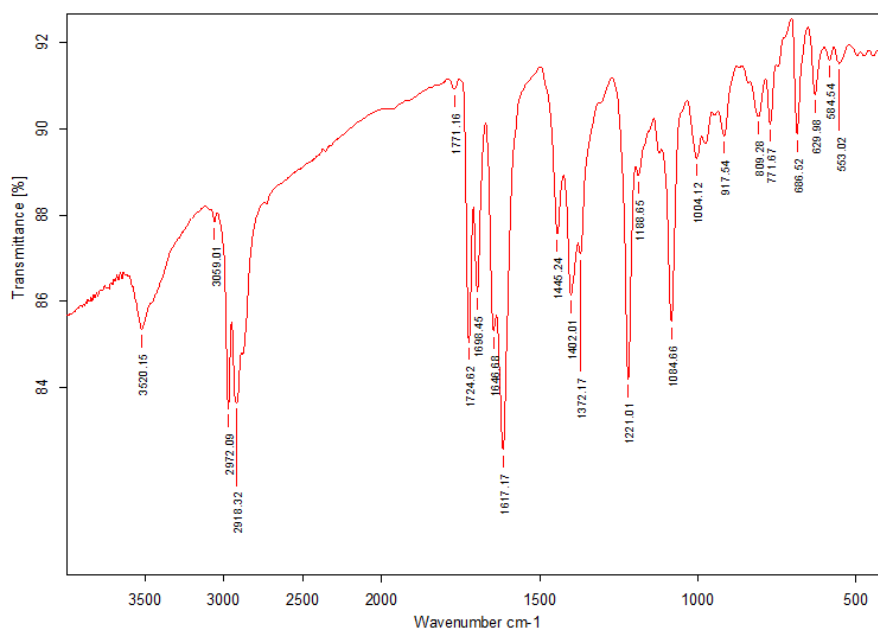


Figure S41. ^1H NMR spectrum (400 MHz) of compound **5** in CDCl_3

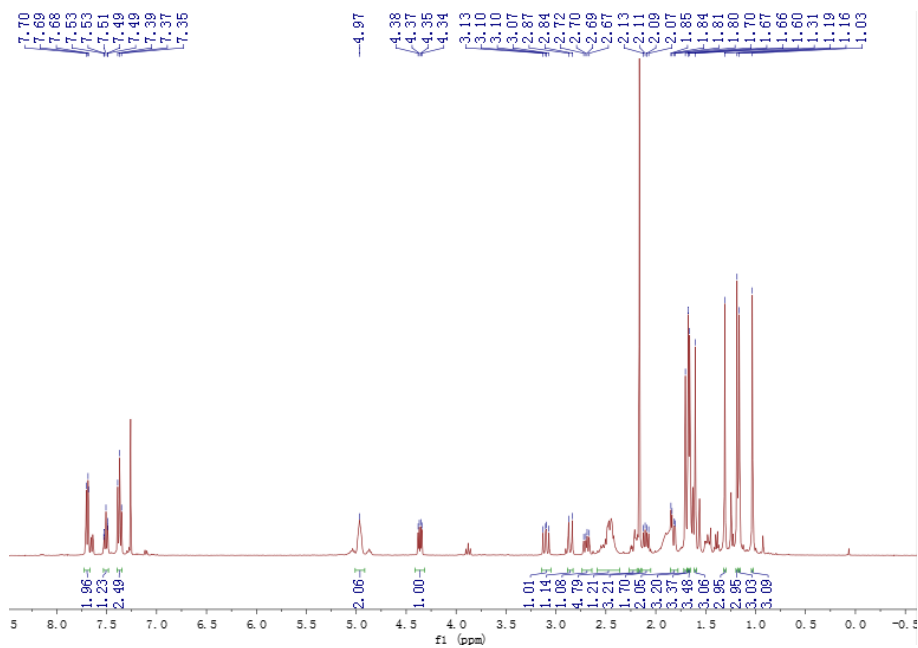


Figure S42. ^{13}C NMR spectrum (100 MHz) of compound **5** in CDCl_3

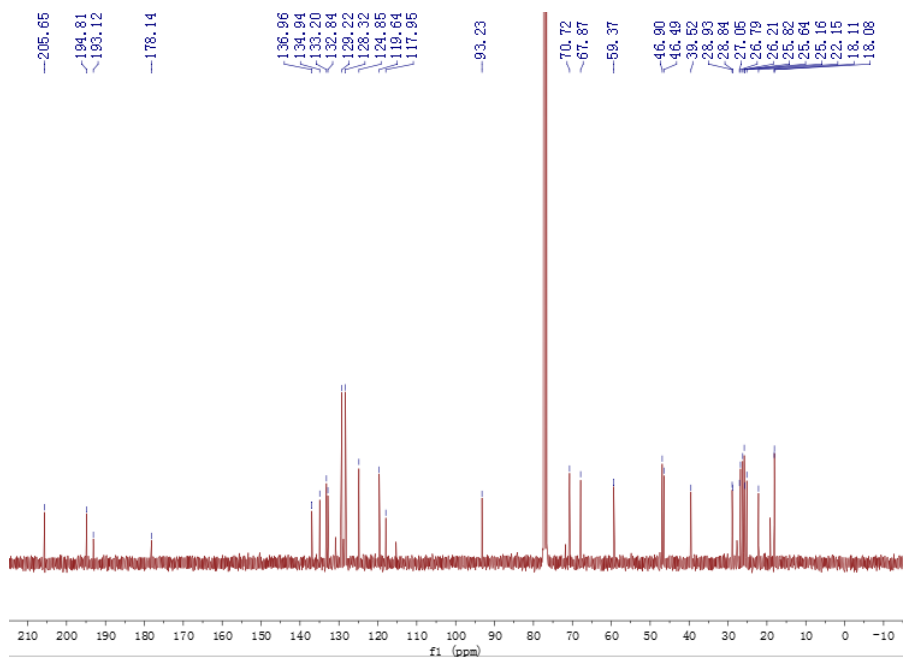


Figure S43. DEPT-135 spectrum (100 MHz) of compound **5** in CDCl₃

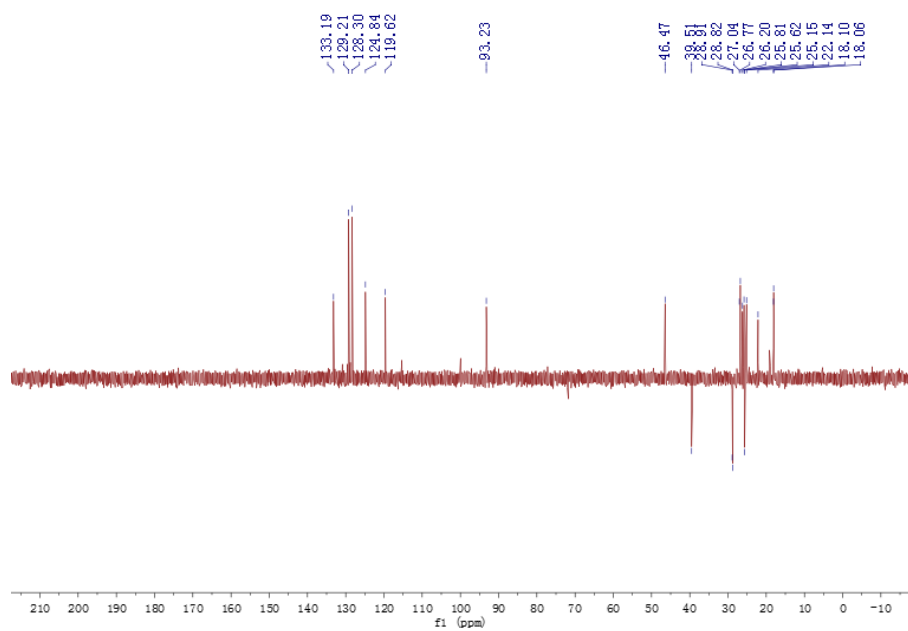


Figure S44. HSQC spectrum of compound **5** in CDCl₃

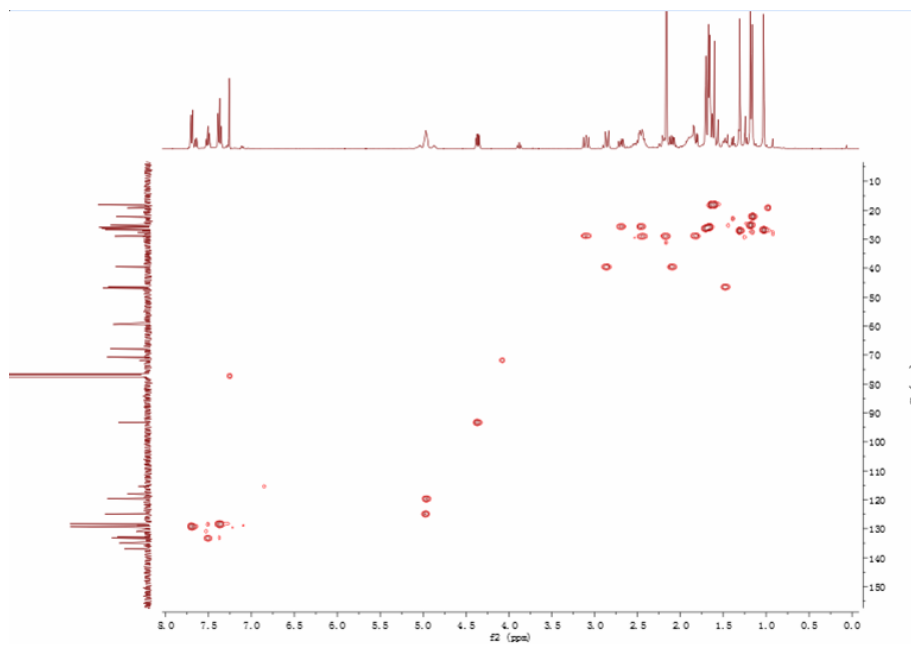


Figure S45. ^1H - ^1H COSY spectrum of compound **5** in CDCl_3

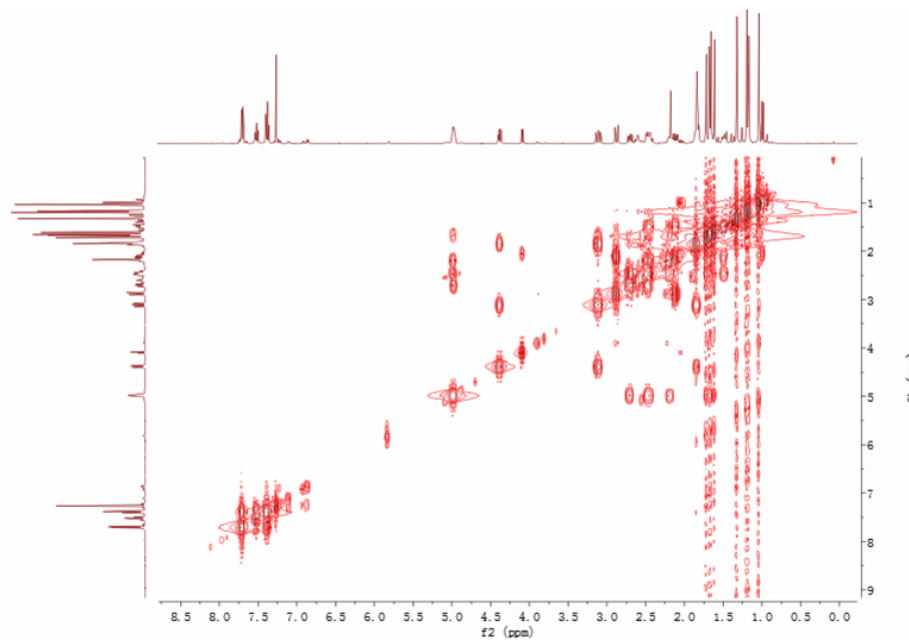


Figure S46. HMBC spectrum of compound **5** in CDCl_3

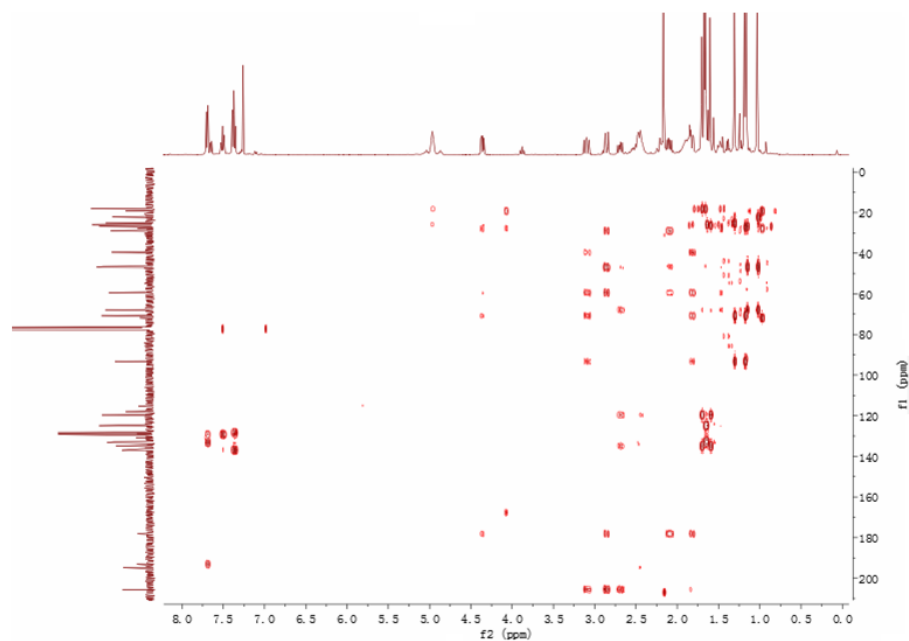


Figure S47. NOESY spectrum of compound **5** in CDCl₃

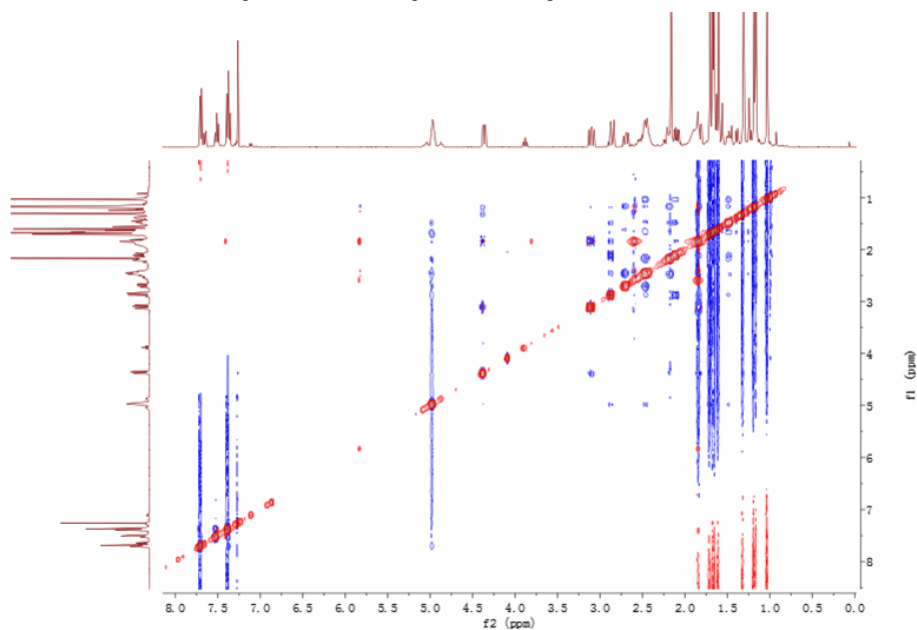


Figure S48. HRESIMS spectrum of compound **5**

zh1-89-6 #13 RT: 0.19 AV: 1 NL: 3.06E7
T: FTMS + p ESI Full ms [50.00-1000.00]

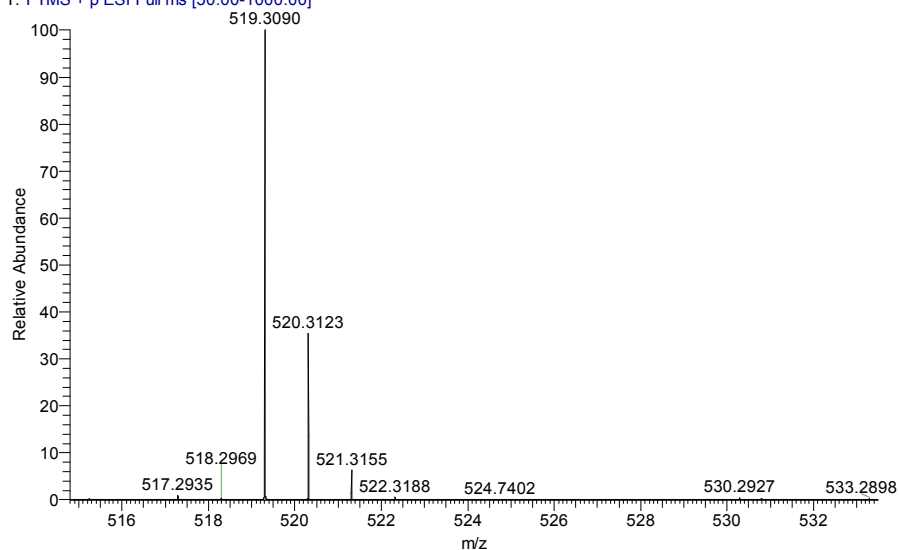


Figure S49. UV spectrum of compound **5**

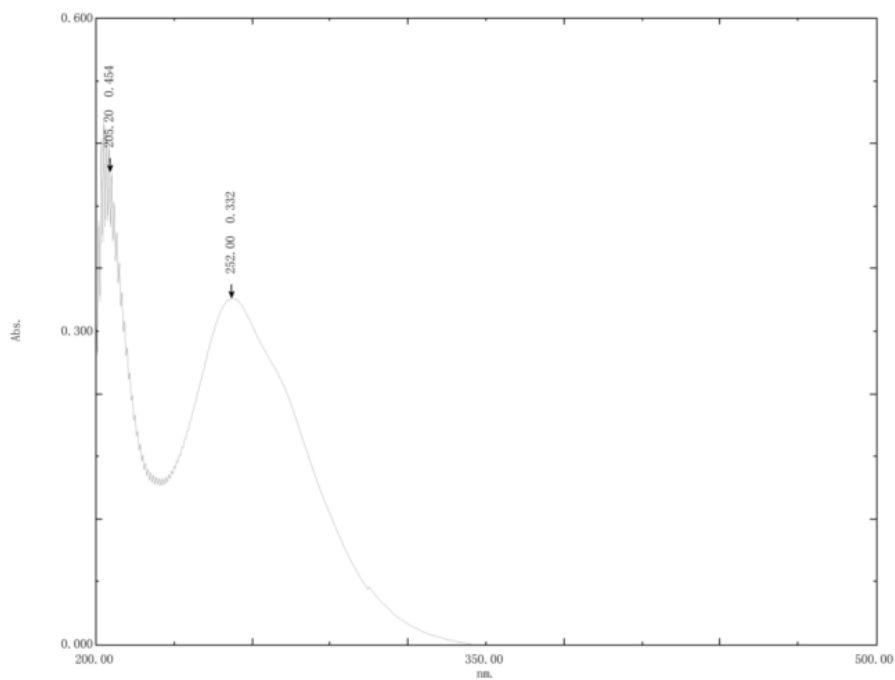


Figure S50. IR (KBr) spectrum of compound **5**

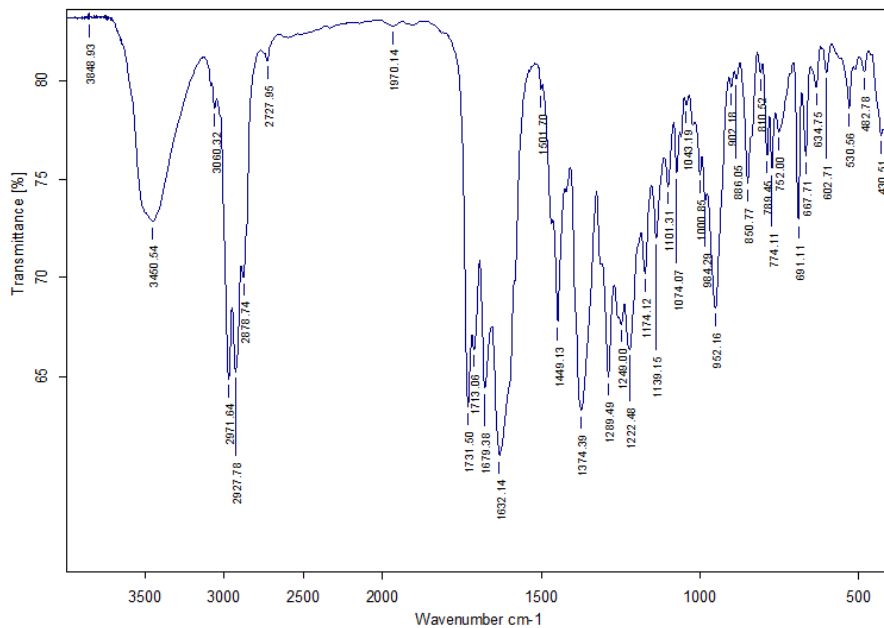


Figure S51. ^1H NMR spectrum (400 MHz) of compound **6** in CDCl_3

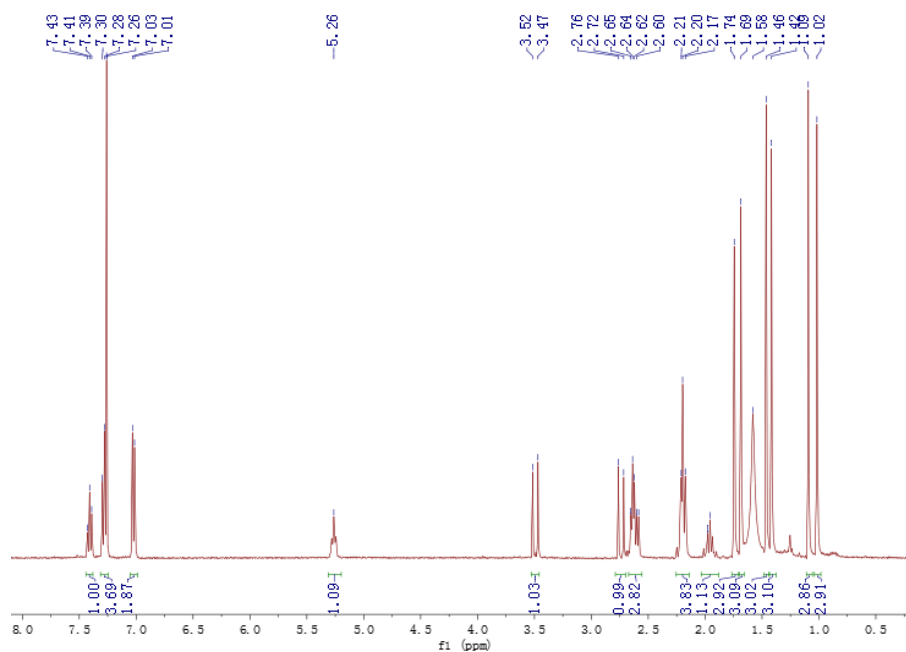


Figure S52. ^{13}C NMR spectrum (100 MHz) of compound **6** in CDCl_3

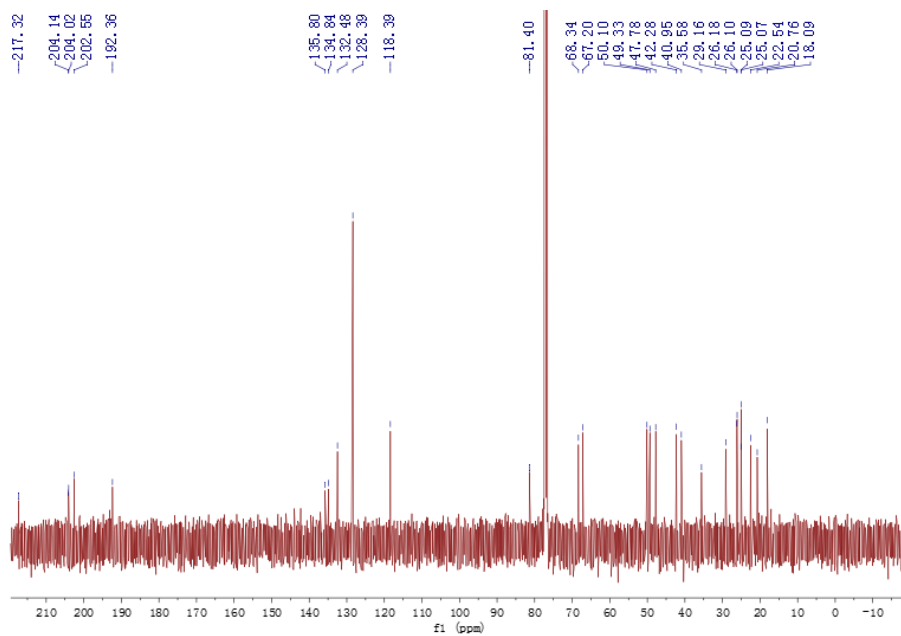


Figure S53. DEPT-135 spectrum (100 MHz) of compound **6** in CDCl₃

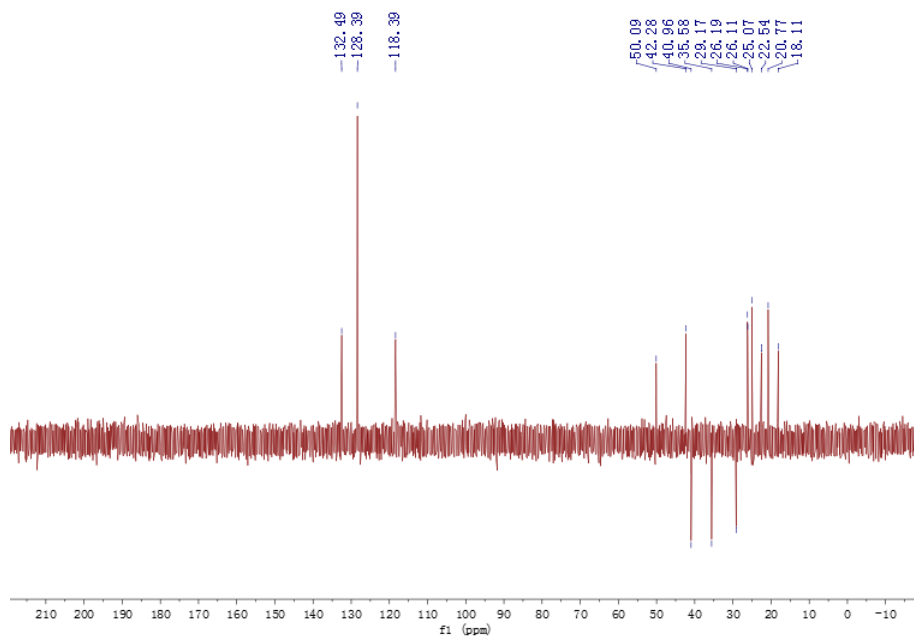


Figure S54. HSQC spectrum of compound **6** in CDCl₃

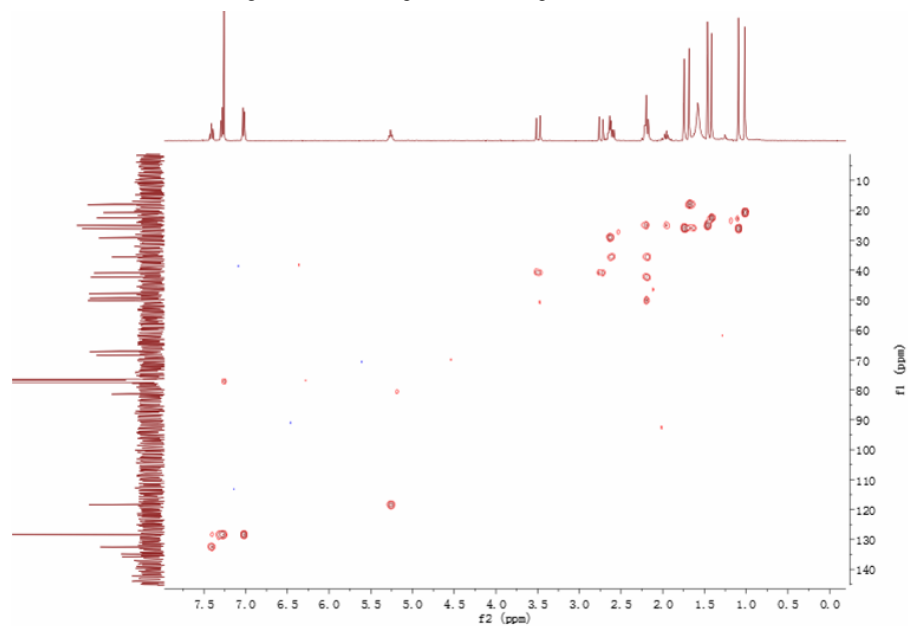


Figure S55. ^1H - ^1H COSY spectrum of compound **6** in CDCl_3

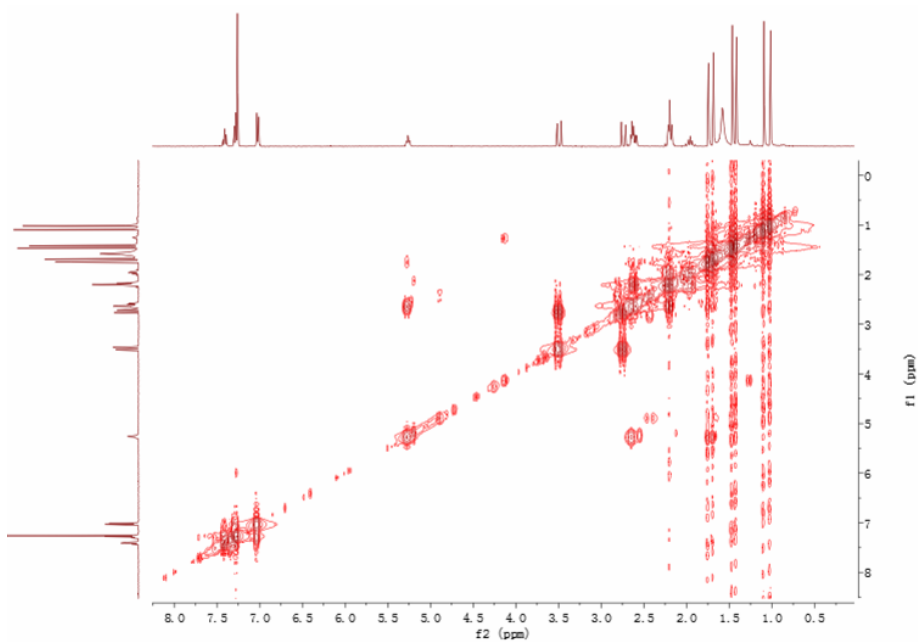


Figure S56. HMBC spectrum of compound **6** in CDCl_3

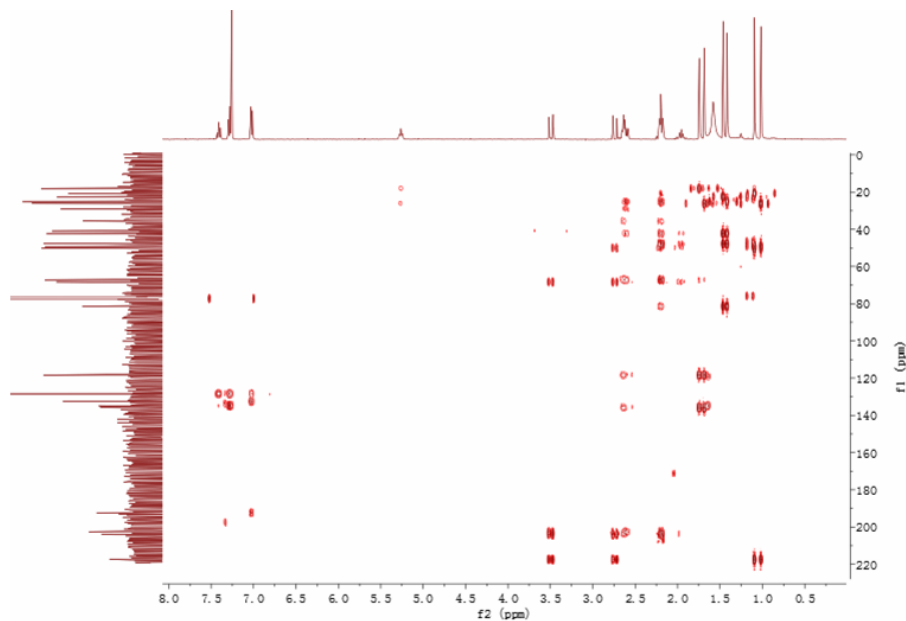


Figure S57. NOESY spectrum of compound **6** in CDCl₃

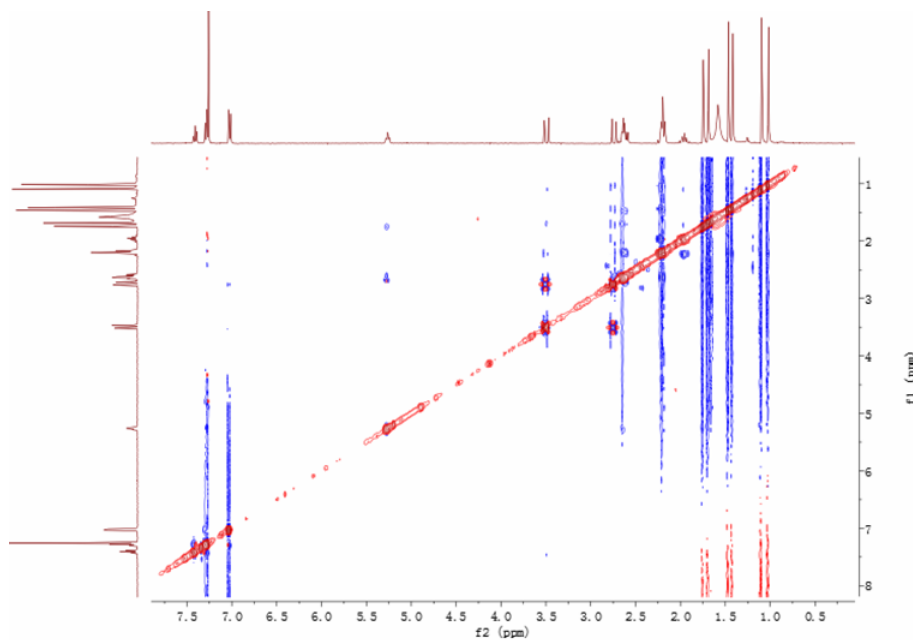


Figure S58. HRESIMS spectrum of compound **6**

LDY1-44-2 #23 RT: 0.32 AV: 1 NL: 1.94E7
T: FTMS + p ESI Full ms [50.00-1500.00]

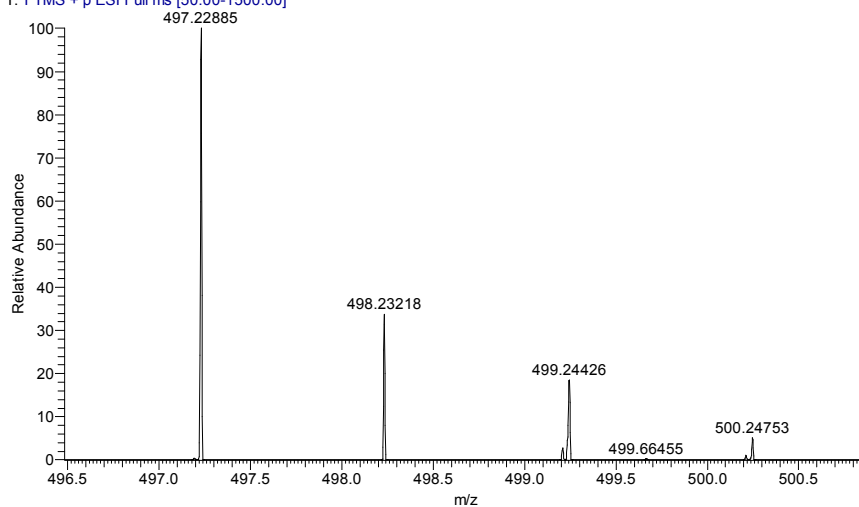


Figure S59. UV spectrum of compound 6

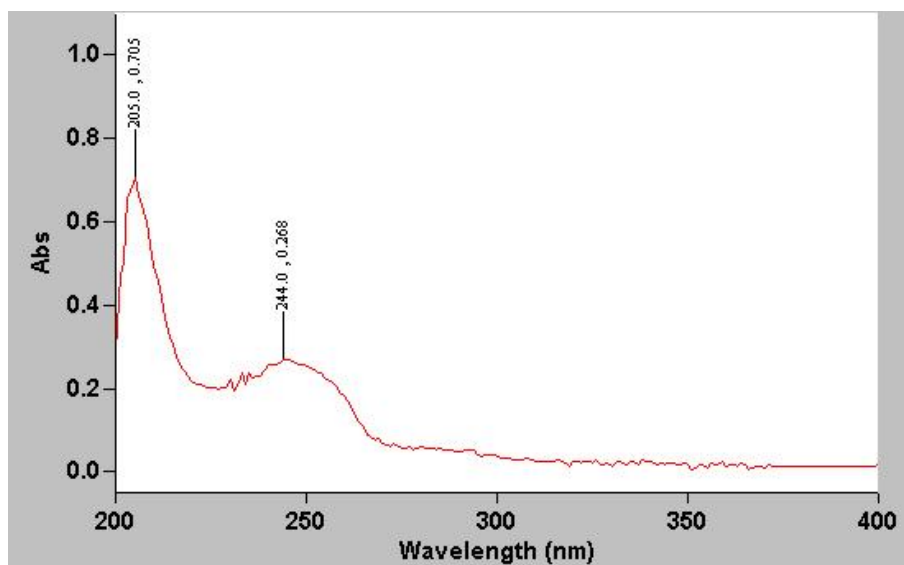


Figure S60. IR (KBr) spectrum of compound 6

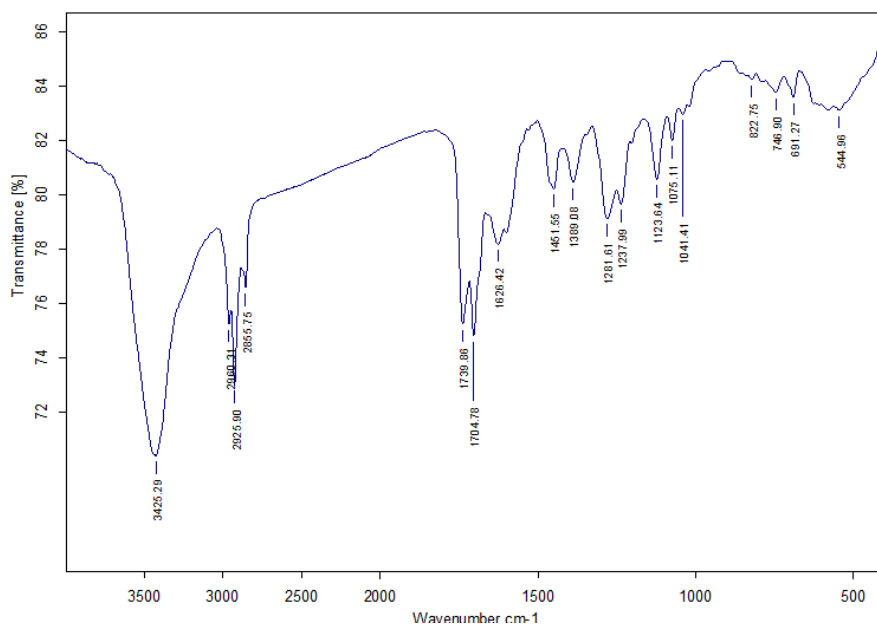


Figure S61. ^1H NMR spectrum (400 MHz) of compound **7** in CDCl_3

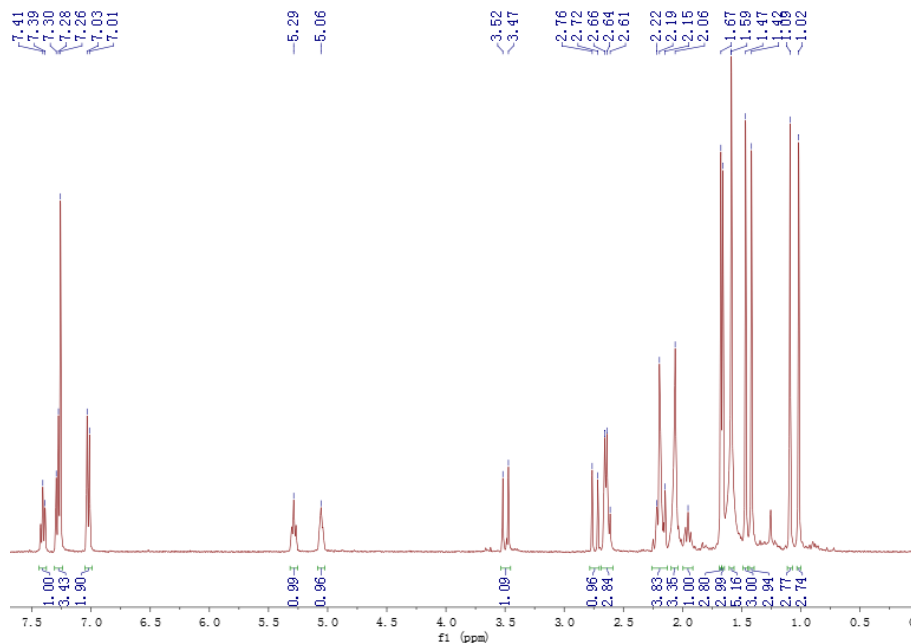


Figure S62. ^{13}C NMR spectrum (100 MHz) of compound **7** in CDCl_3

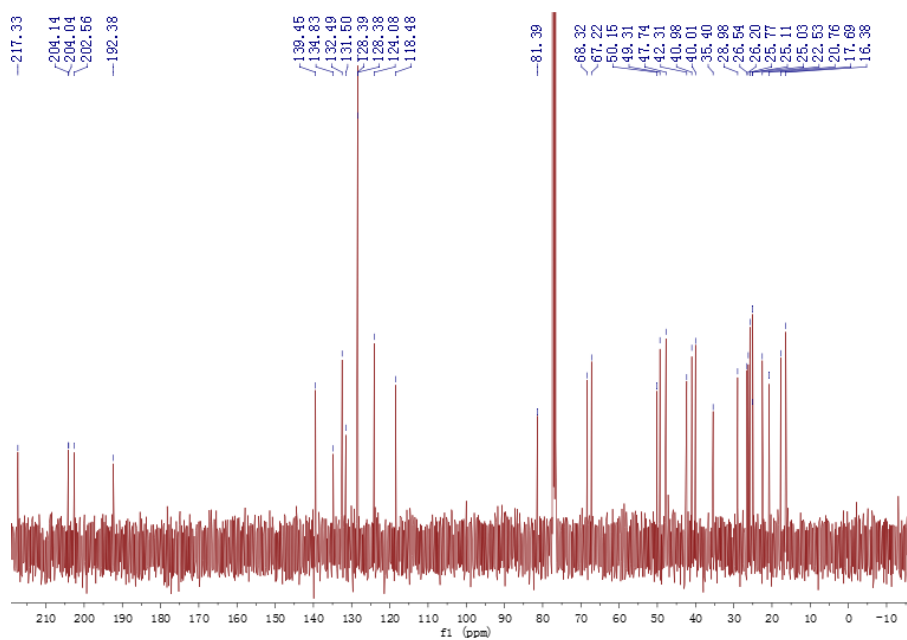


Figure S63. DEPT-135 spectrum (100 MHz) of compound **7** in CDCl₃

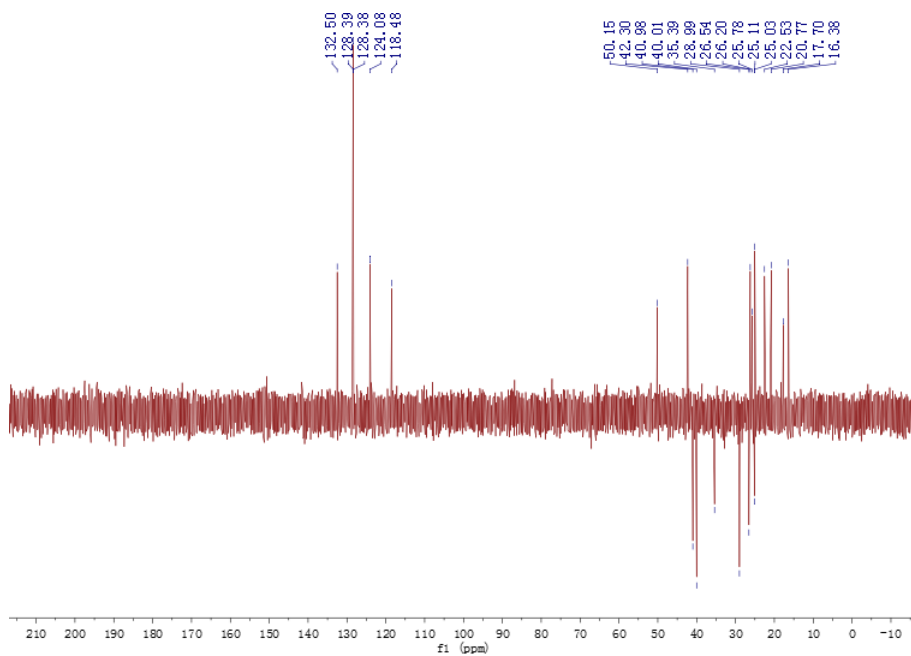


Figure S64. HSQC spectrum of compound **7** in CDCl₃

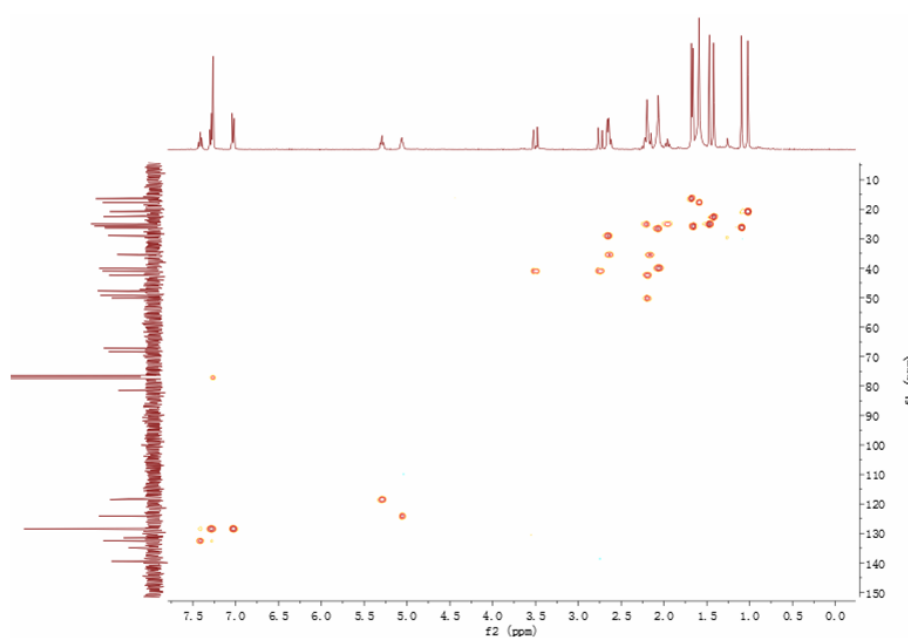


Figure S65. ^1H - ^1H COSY spectrum of compound 7 in CDCl_3

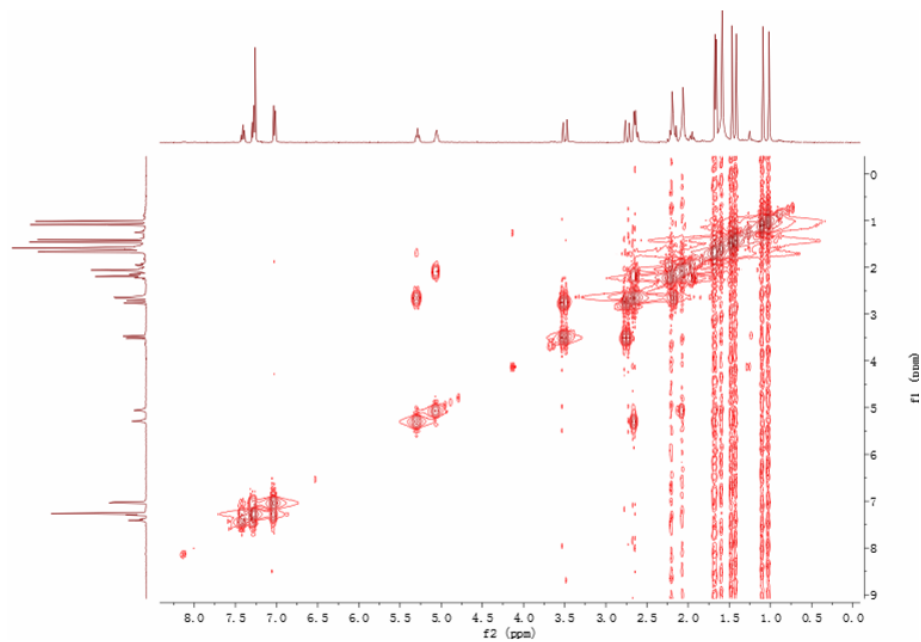


Figure S66. HMBC spectrum of compound 7 in CDCl_3

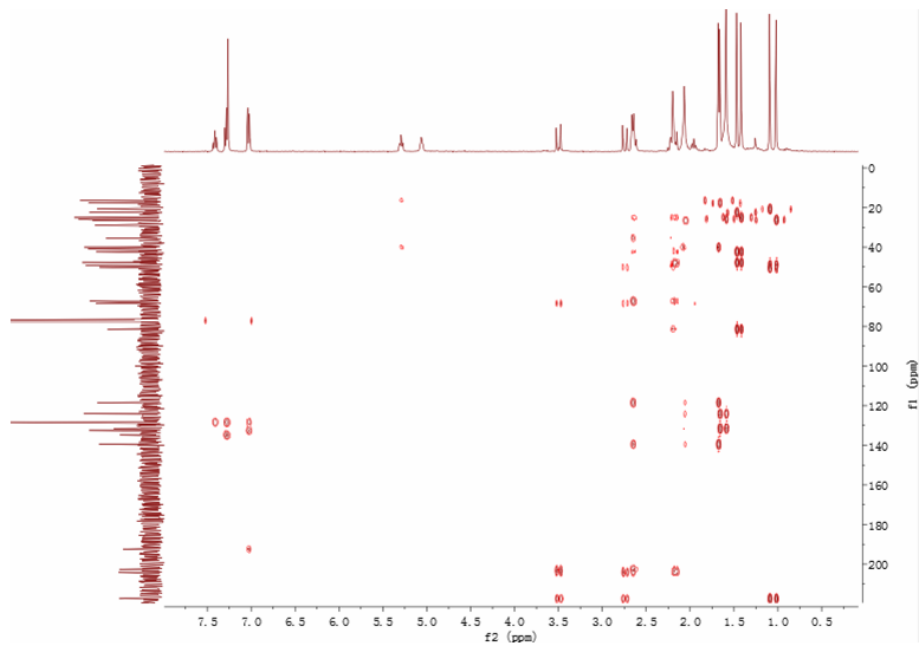


Figure S67. NOESY spectrum of compound **7** in CDCl₃

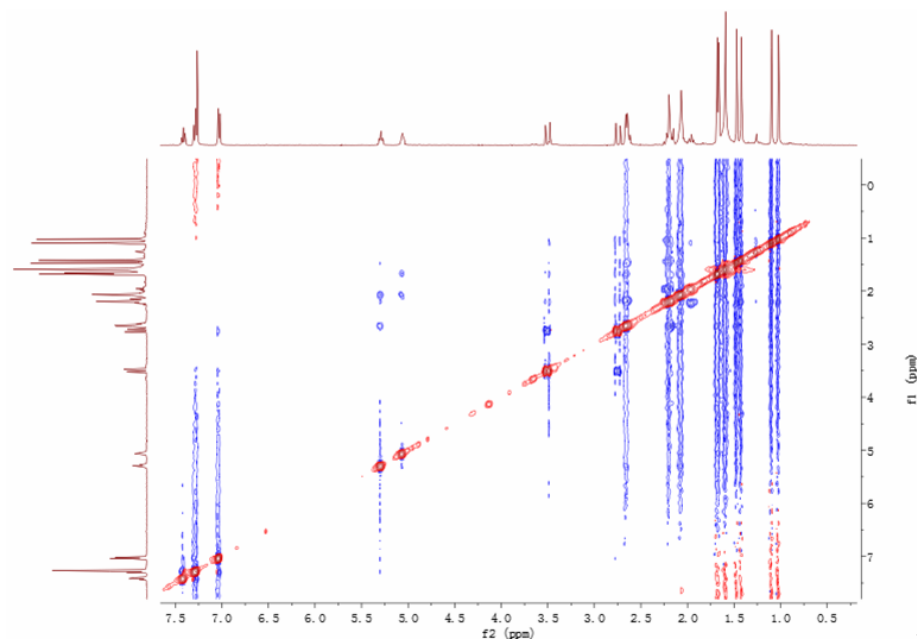


Figure S68. HRESIMS spectrum of compound **7**

LDY1-42-7 #29 RT: 0.41 AV: 1 NL: 4.49E6
T: FTMS + p ESI Full ms [50.00-1500.00]

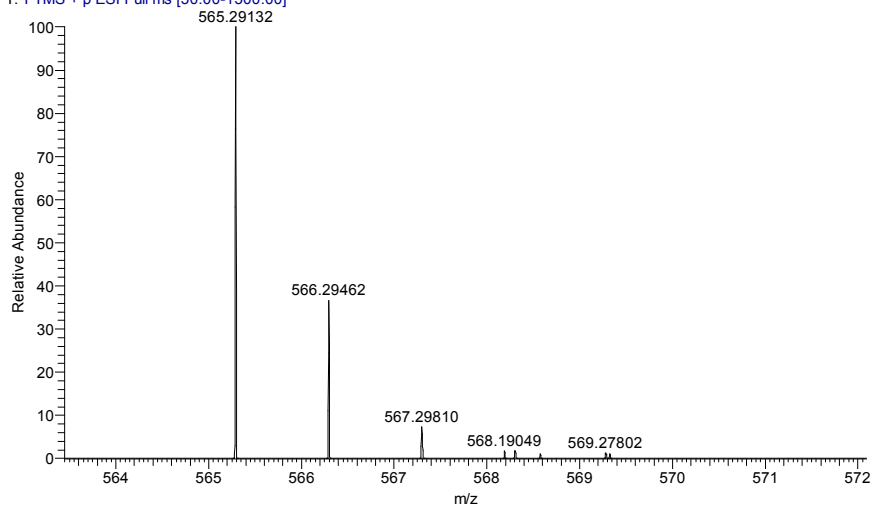


Figure S69. UV spectrum of compound 7

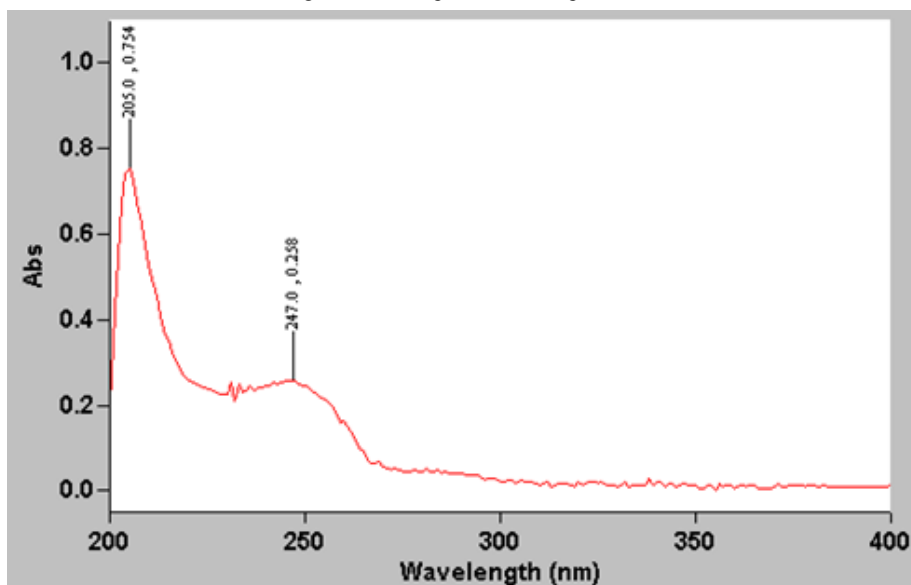


Figure S70. IR (KBr) spectrum of compound 7

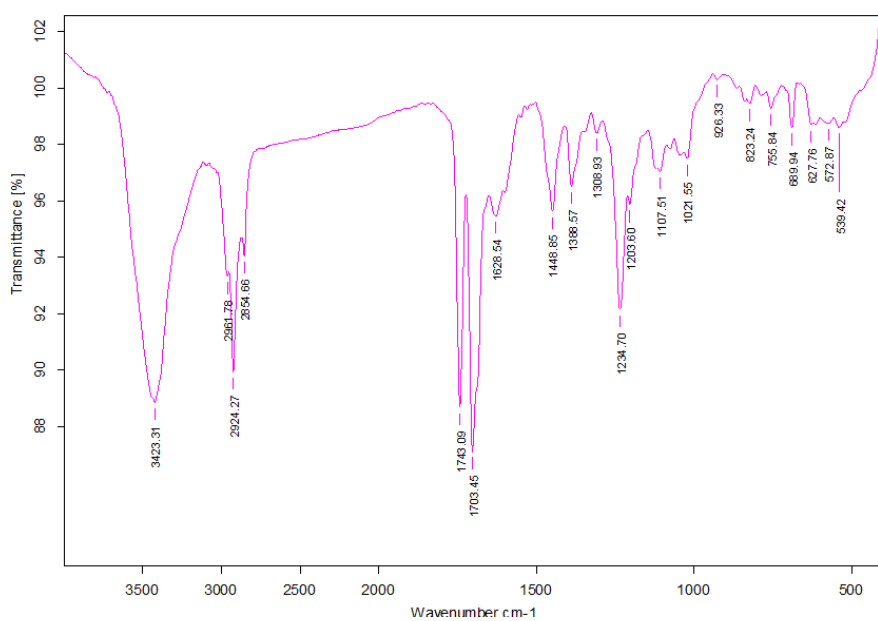


Figure S71. ^1H NMR spectrum (400 MHz) of compound **8** in CDCl_3

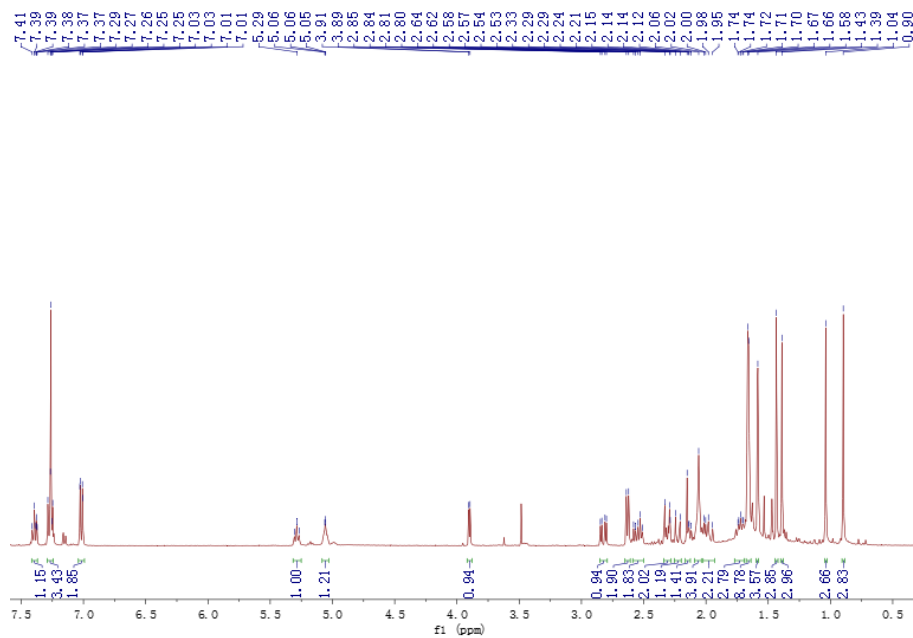


Figure S72. ^{13}C NMR spectrum (100 MHz) of compound **8** in CDCl_3

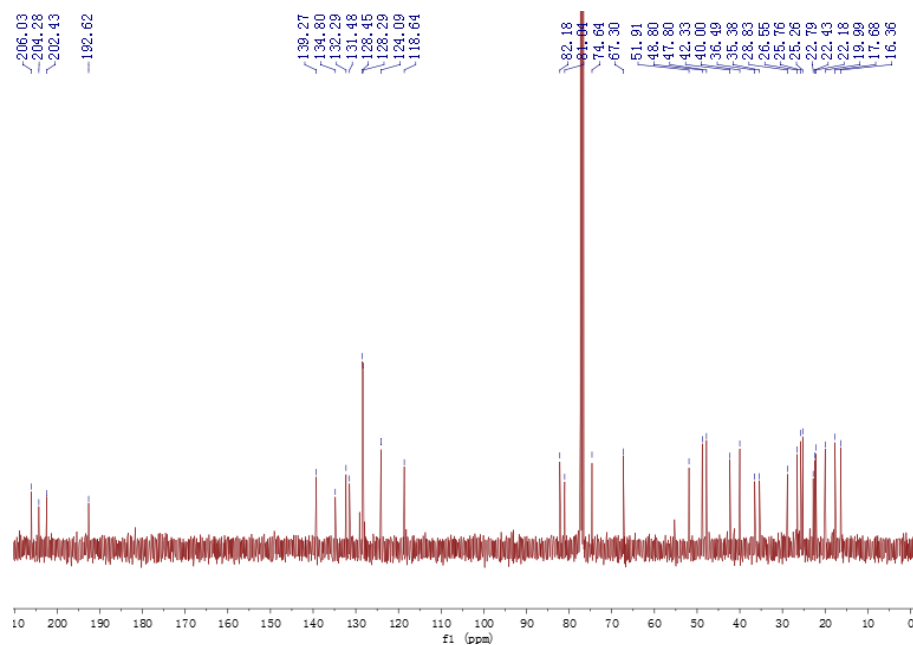


Figure S73. DEPT-135 spectrum (100 MHz) of compound **8** in CDCl₃

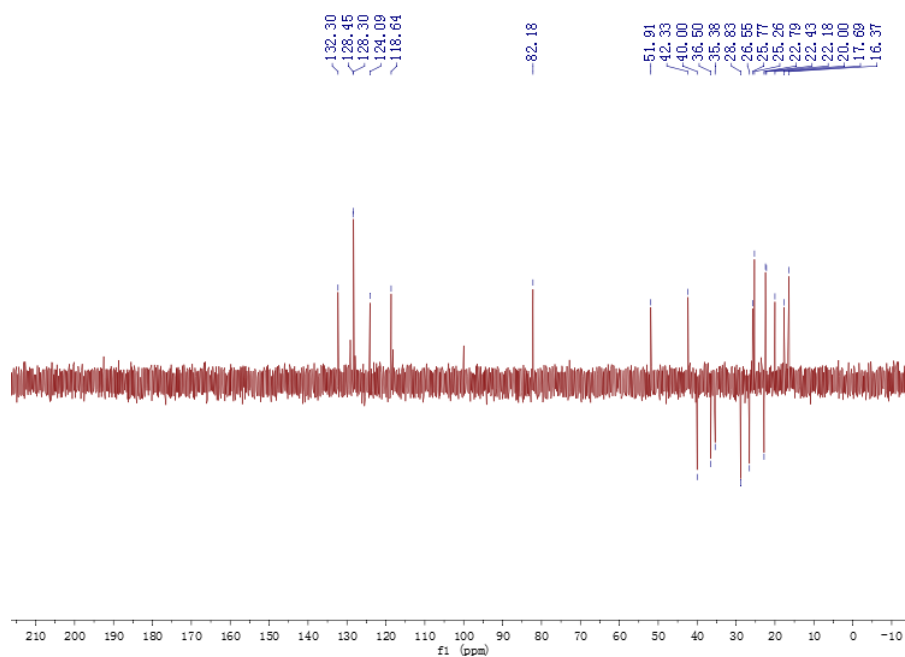


Figure S74. HSQC spectrum of compound **8** in CDCl₃

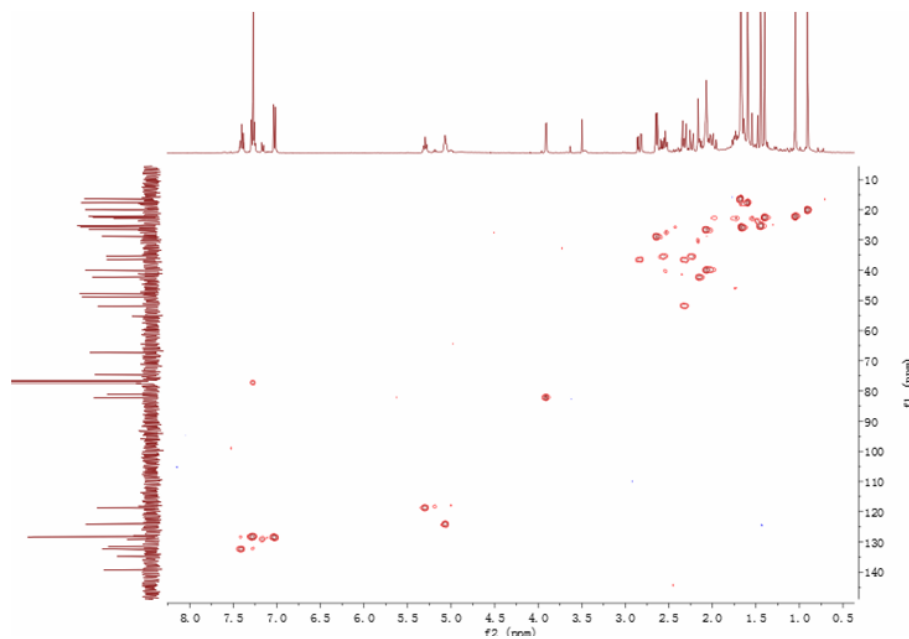


Figure S75. ^1H - ^1H COSY spectrum of compound **8** in CDCl_3

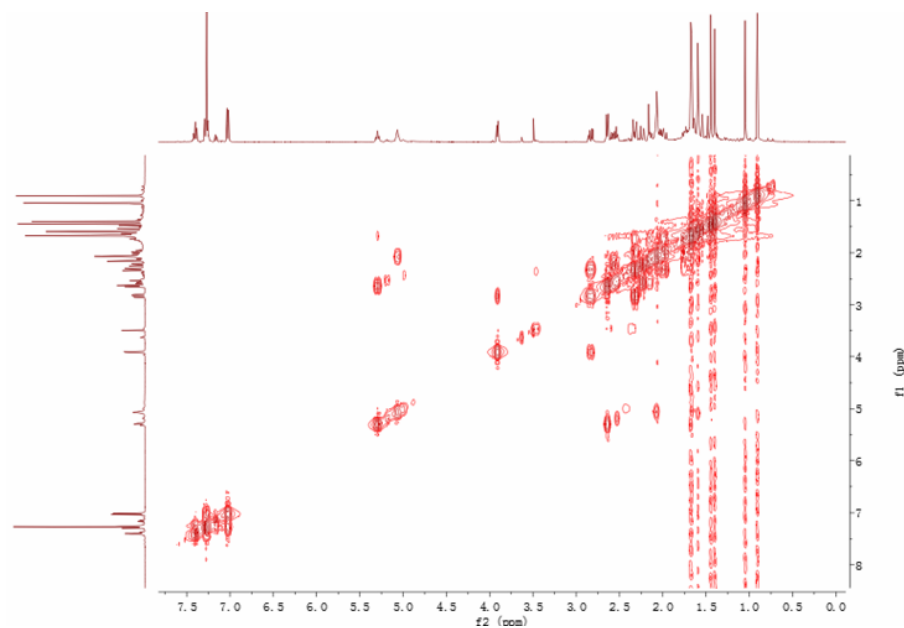


Figure S76. HMBC spectrum of compound **8** in CDCl_3

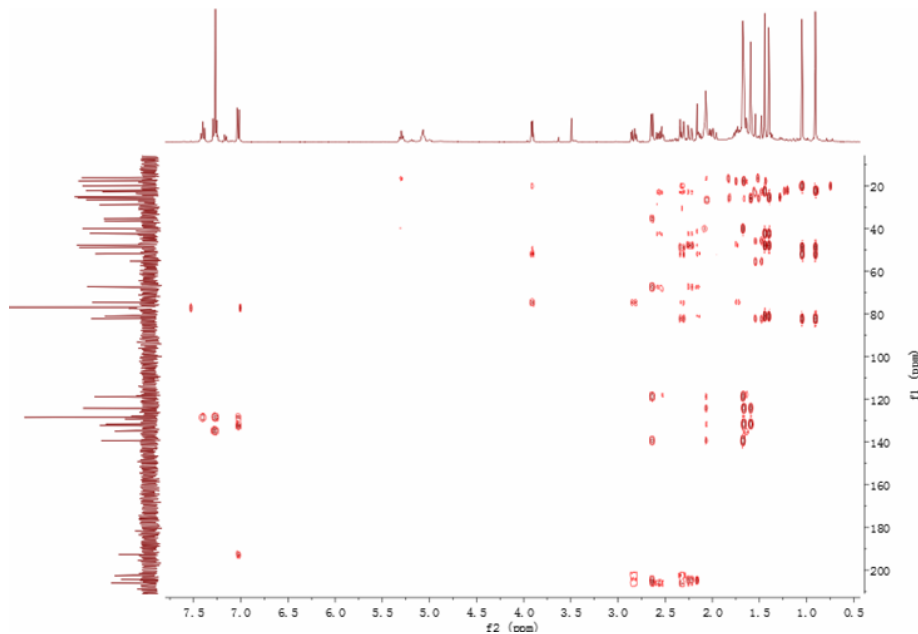


Figure S77. NOESY spectrum of compound **8** in CDCl₃

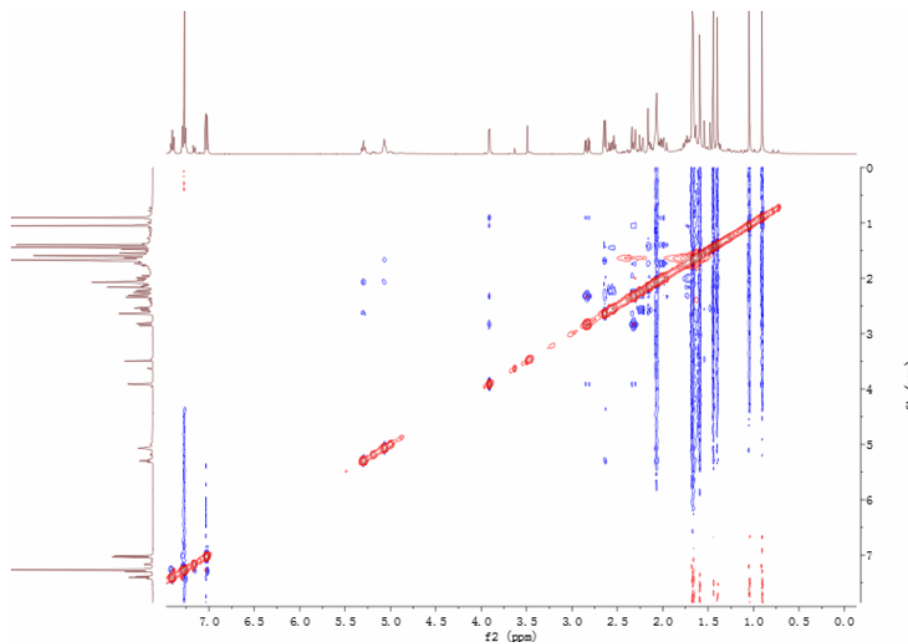


Figure S78. HRESIMS spectrum of compound **8**

LDY1-49-2 #26 RT: 0.37 AV: 1 NL: 1.27E7
T: FTMS + p ESI Full ms [50.00-1500.00]

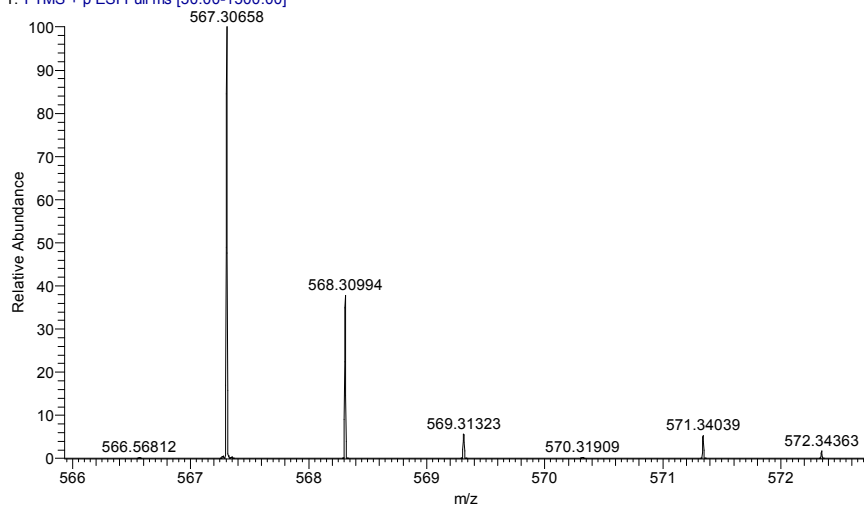


Figure S79. UV spectrum of compound **8**

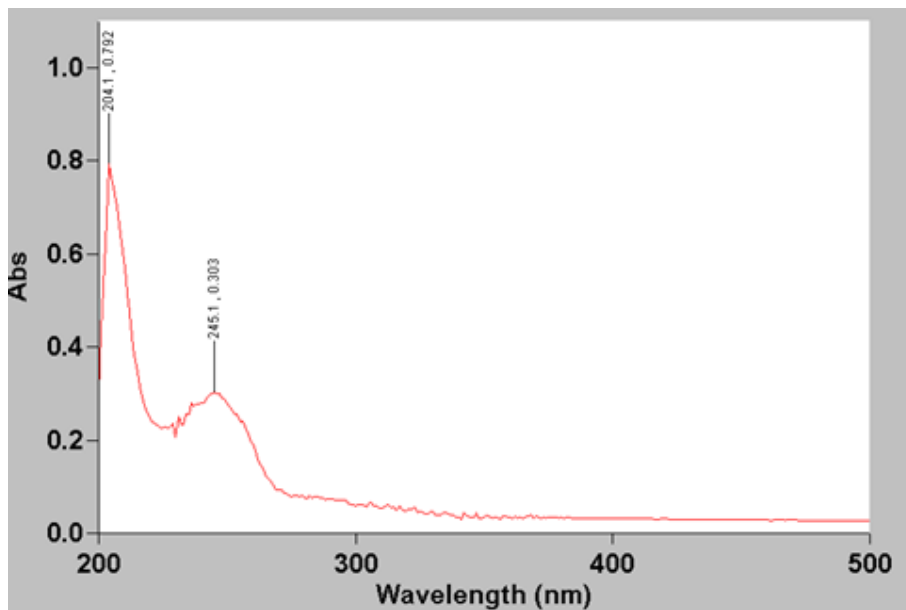


Figure S80. IR (KBr) spectrum of compound **8**

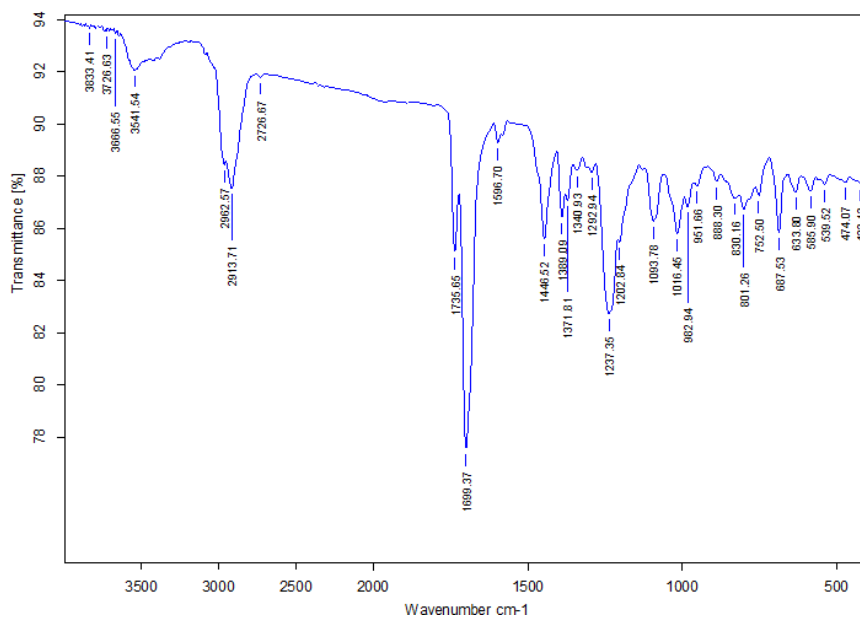


Figure S81. ^1H NMR spectrum (400 MHz) of compound **9** in CDCl_3

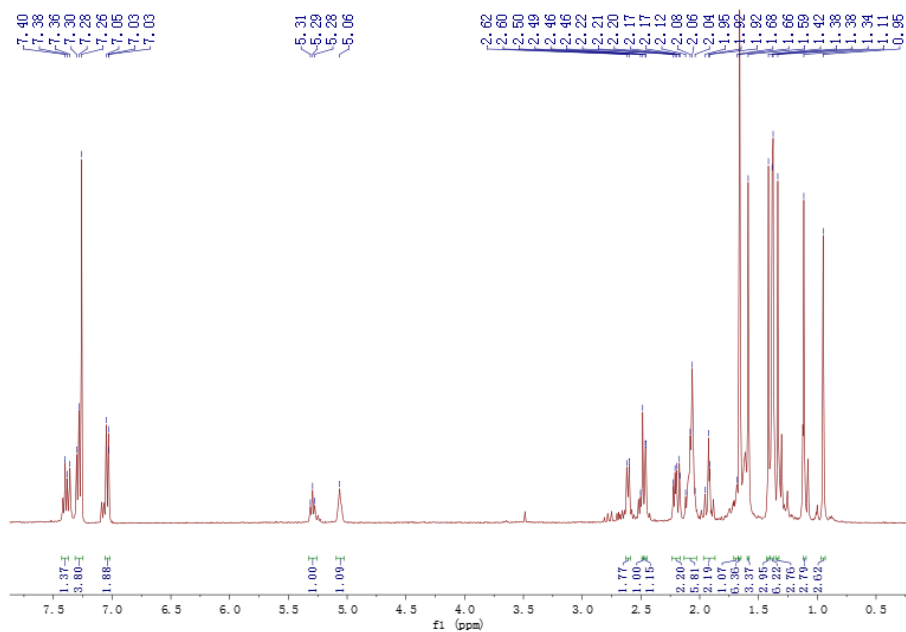


Figure S82. ^{13}C NMR spectrum (100 MHz) of compound **9** in CDCl_3

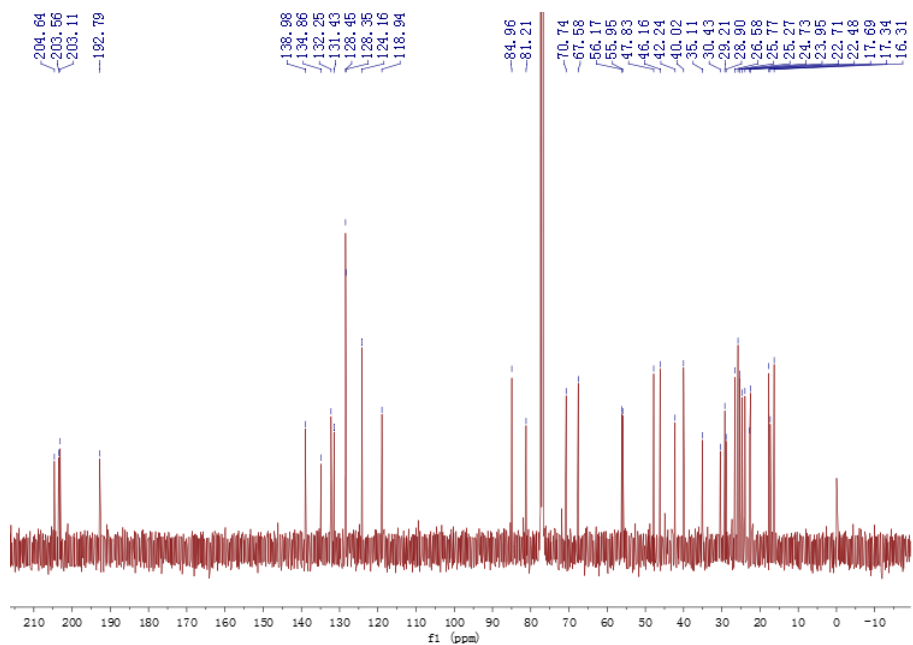


Figure S83. DEPT-135 spectrum (100 MHz) of compound **9** in CDCl₃

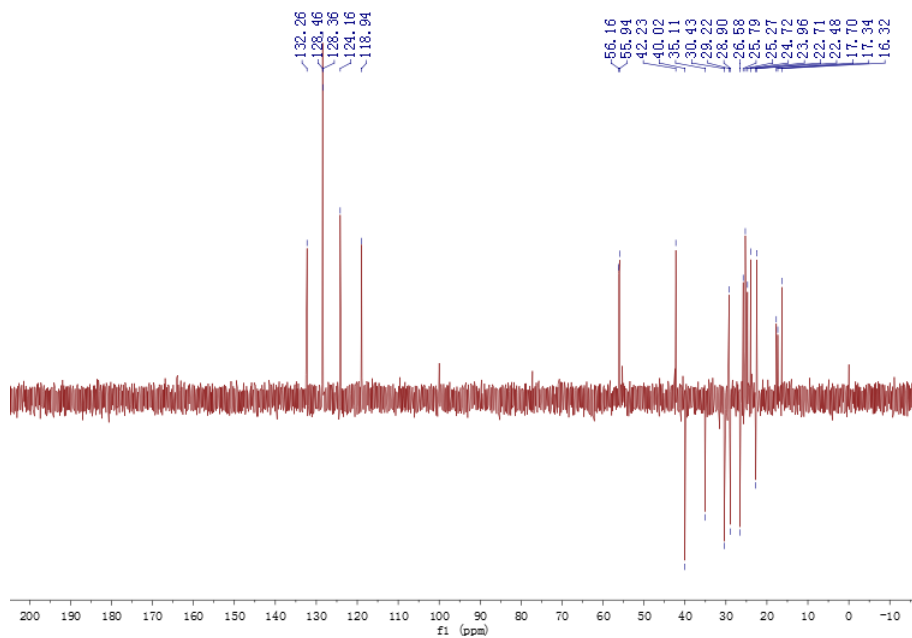


Figure S84. HSQC spectrum of compound **9** in CDCl₃

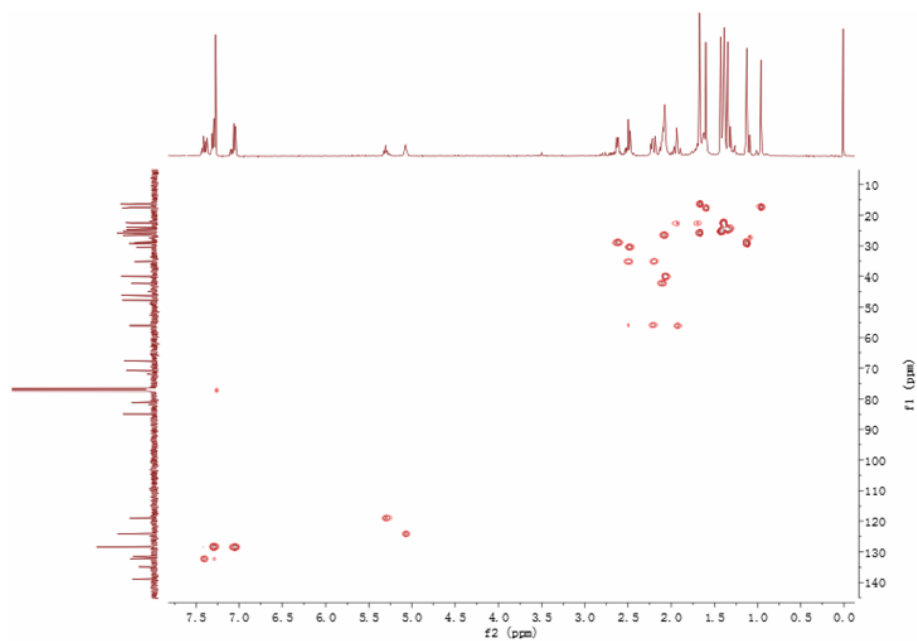


Figure S85. ^1H - ^1H COSY spectrum of compound **9** in CDCl_3

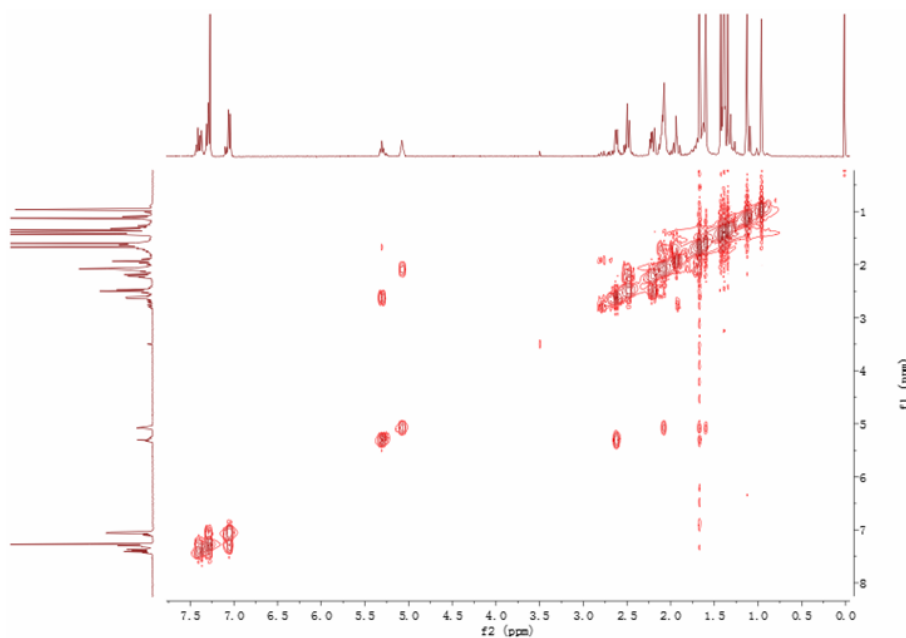


Figure S86. HMBC spectrum of compound **9** in CDCl_3

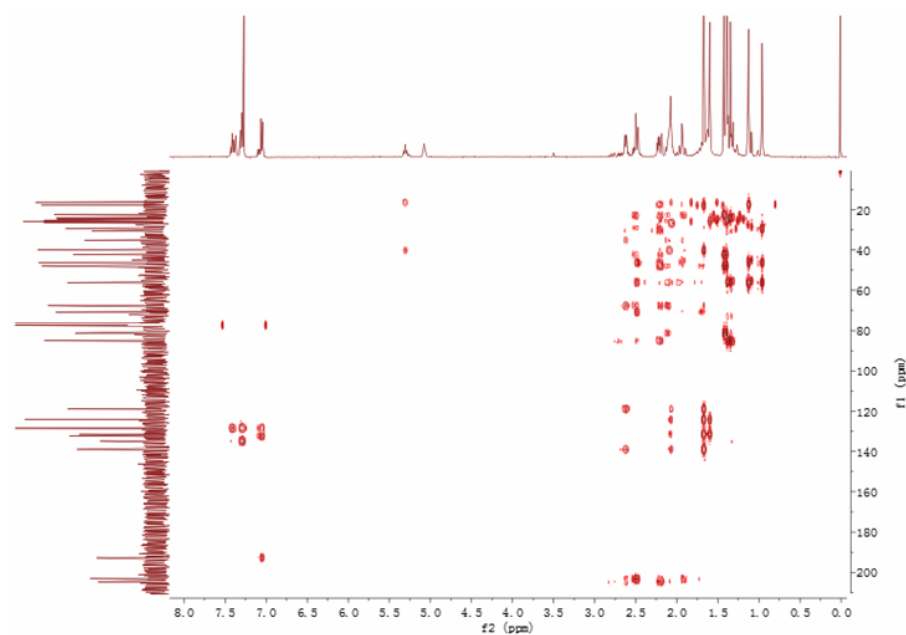


Figure S87. NOESY spectrum of compound **9** in CDCl₃

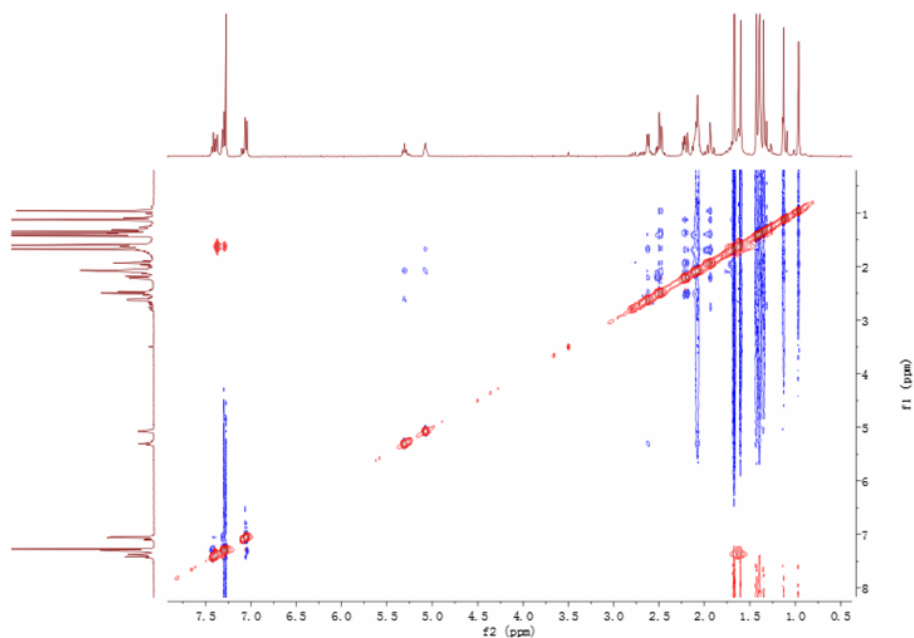


Figure S88. HRESIMS spectrum of compound **9**

LDY2-3-1 #15 RT: 0.23 AV: 1 NL: 5.08E5
T: FTMS + p ESI Full ms [50.00-1500.00]

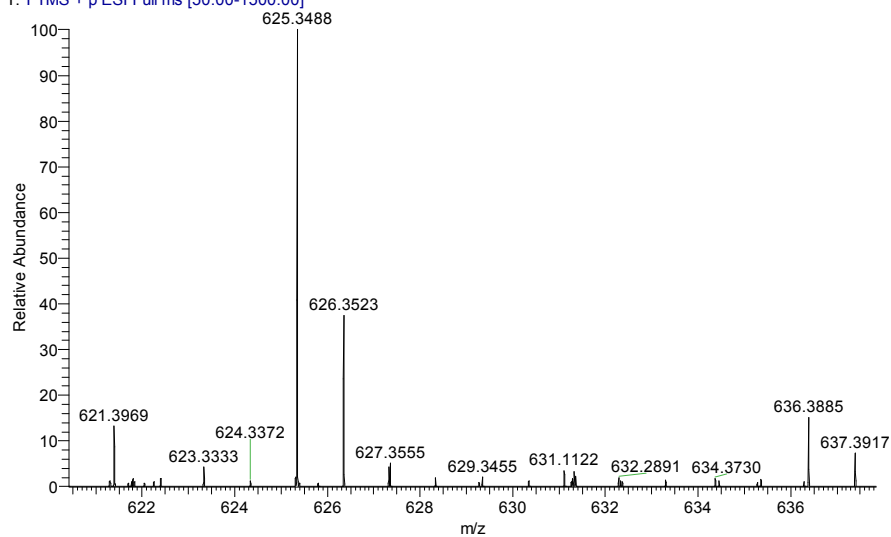


Figure S89. UV spectrum of compound **9**

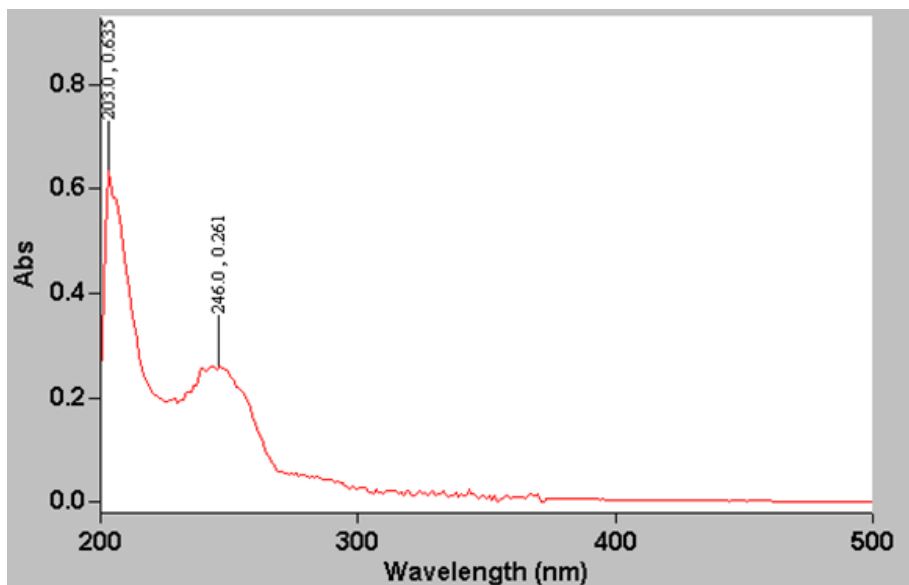


Figure S90. IR (KBr) spectrum of compound **9**

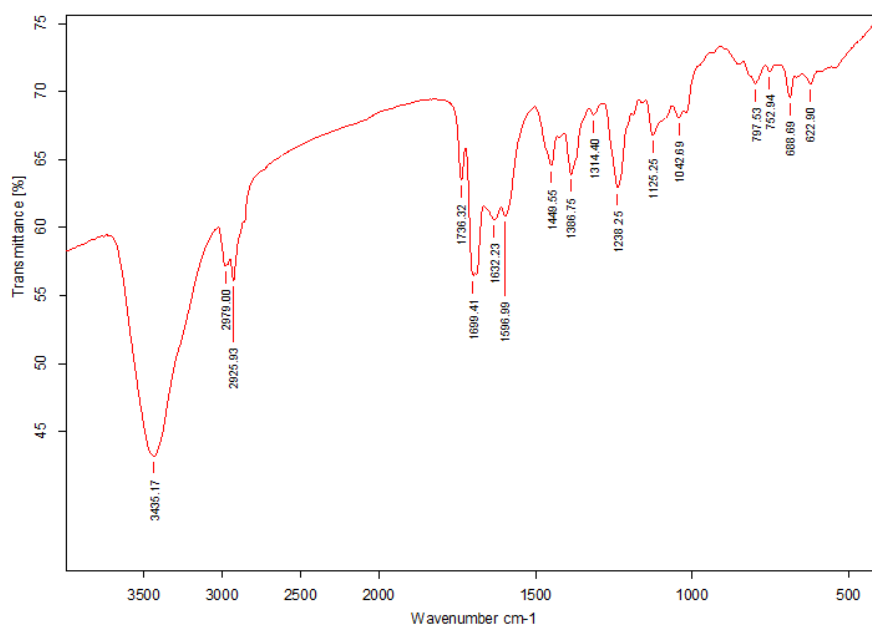


Figure S91. ^1H NMR spectrum (400 MHz) of compound **6** in pyridine- d_5

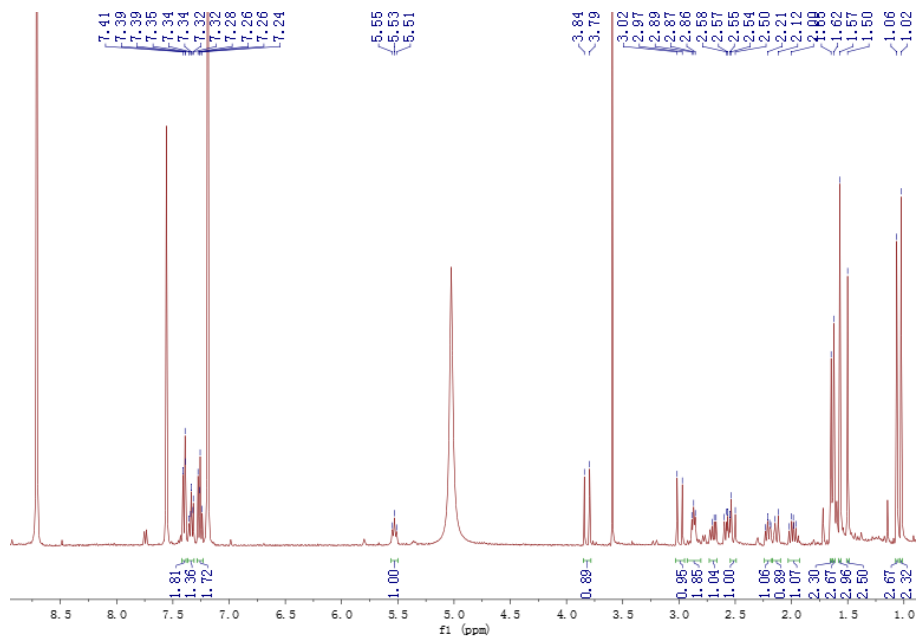


Figure S92. ^{13}C NMR spectrum (100 MHz) of compound **6** in pyridine- d_5

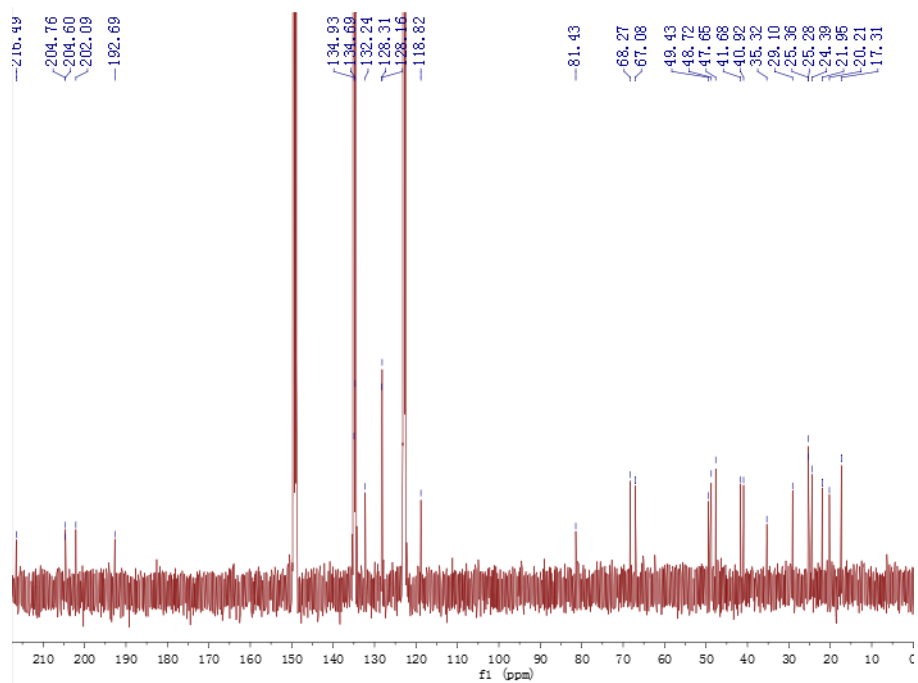


Figure S93. DEPT-135 spectrum (100 MHz) of compound **6** in pyridine-*d*₅

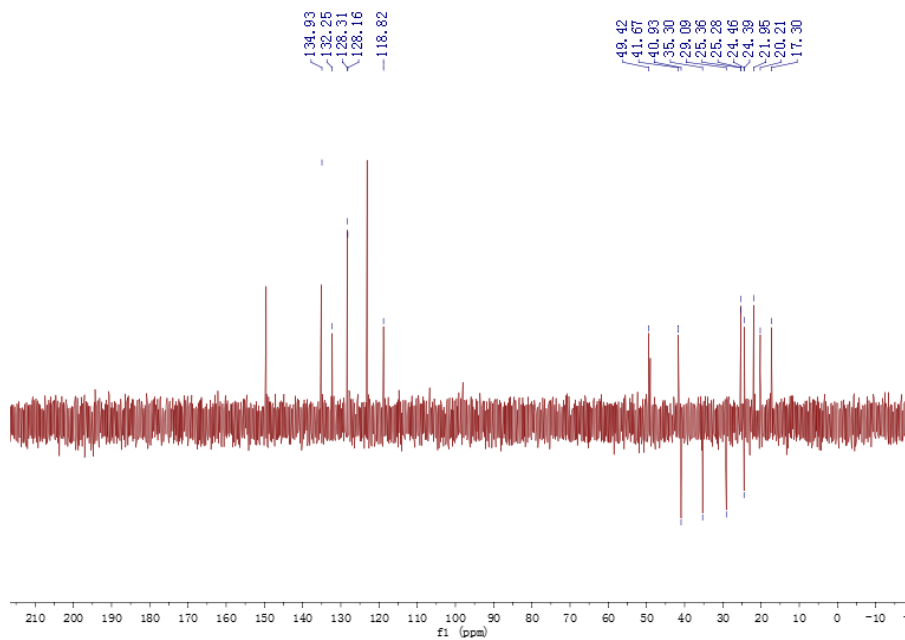


Figure S94. HSQC spectrum of compound **6** in pyridine-*d*₅

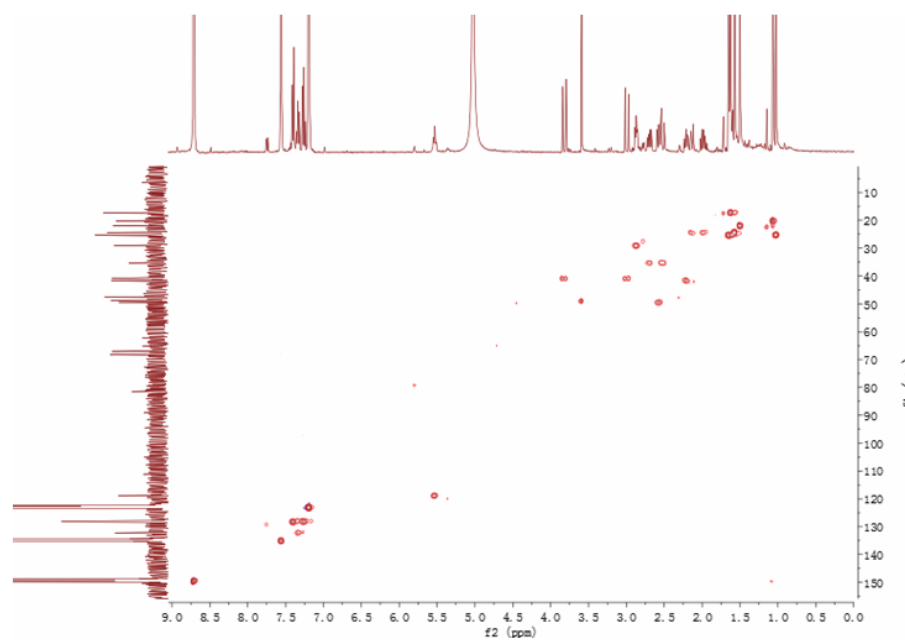


Figure S95. ^1H - ^1H COSY spectrum of compound **6** in pyridine- d_5

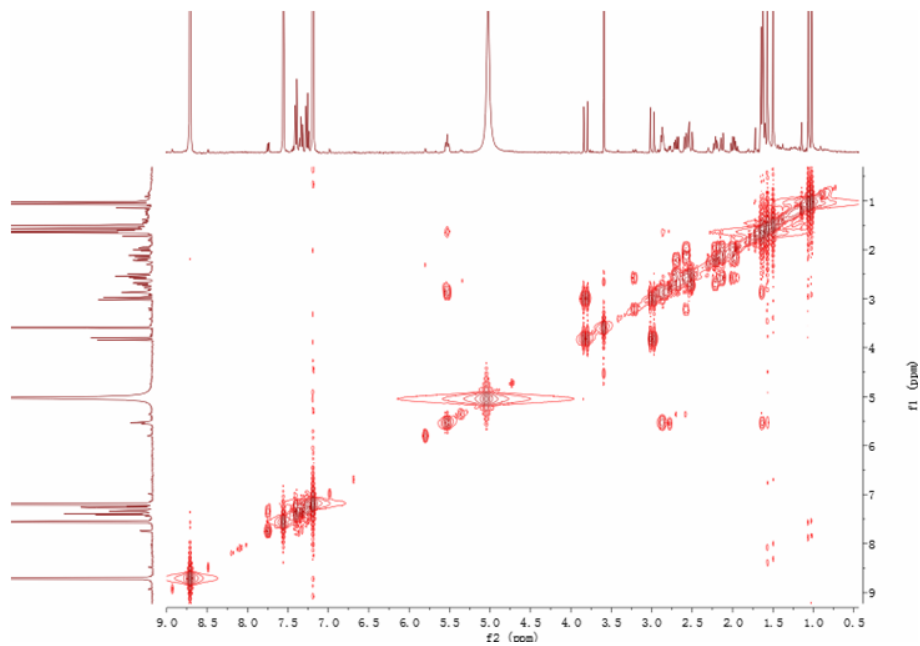


Figure S96. HMBC spectrum of compound **6** in pyridine- d_5

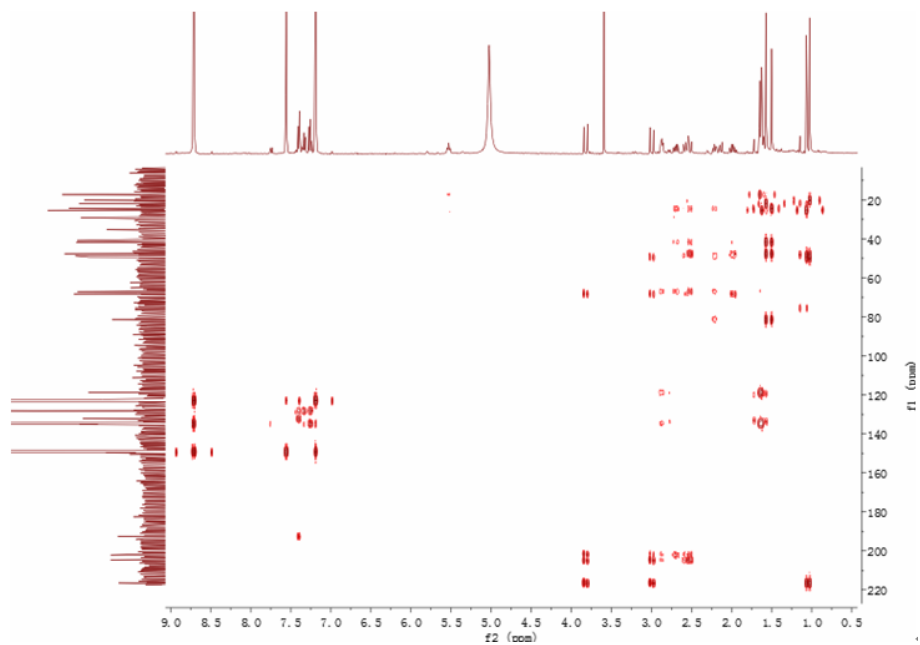


Figure S97. NOESY spectrum of compound **6** in pyridine-*d*₅

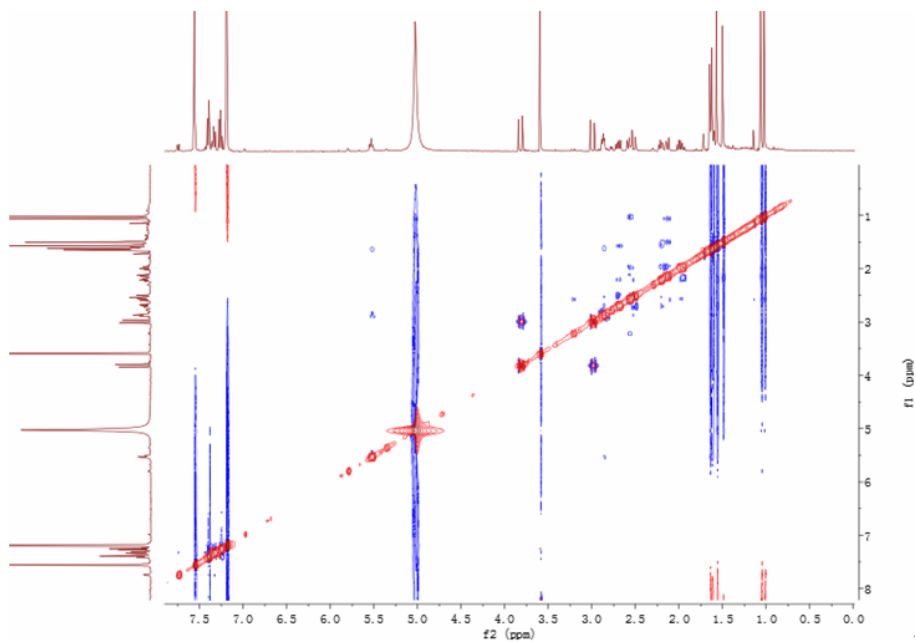


Figure S98. ¹H NMR spectrum (400 MHz) of compound **7** in pyridine-*d*₅

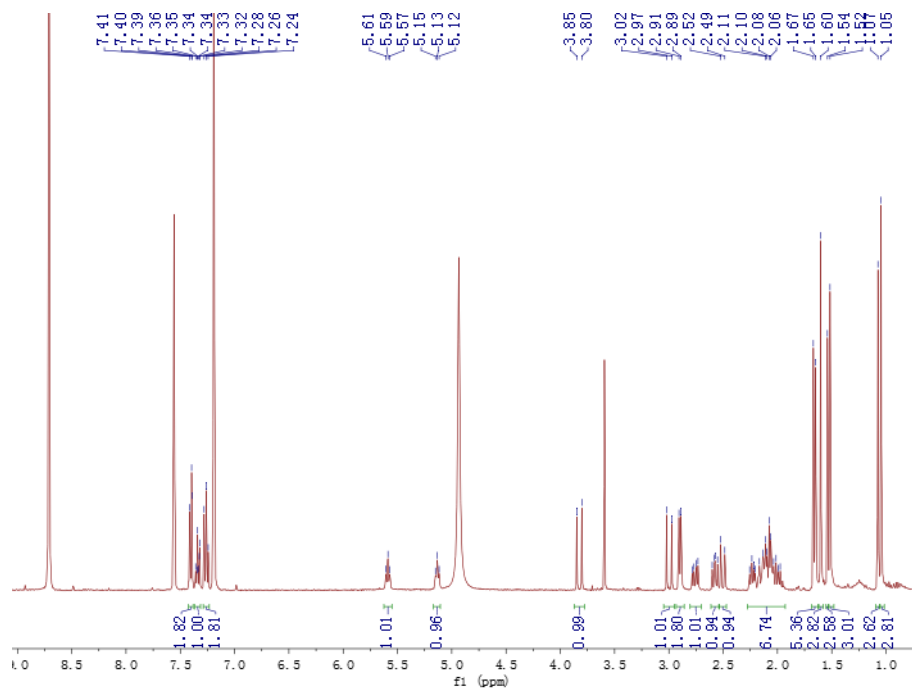


Figure S99. ^{13}C NMR spectrum (100 MHz) of compound **7** in pyridine- d_5

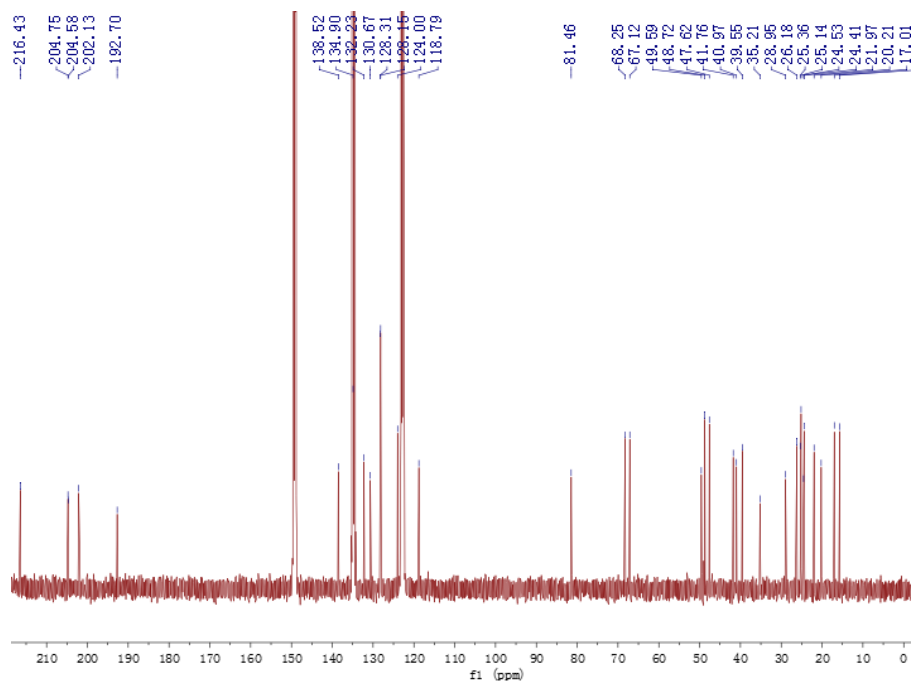


Figure S100. DEPT-135 spectrum (100 MHz) of compound **7** in pyridine- d_5

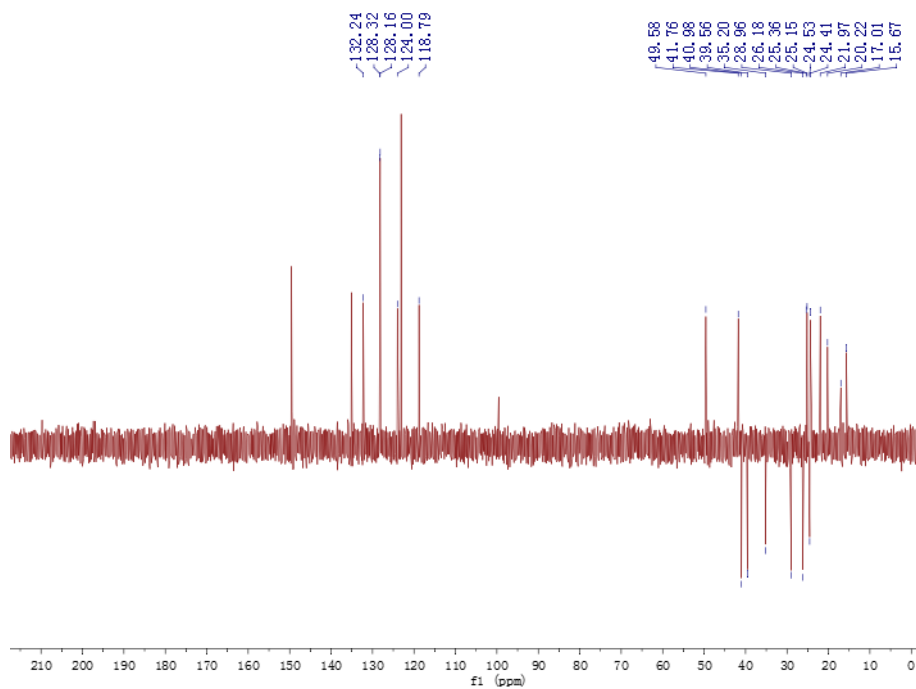


Figure S101. HSQC spectrum of compound **7** in pyridine- d_5

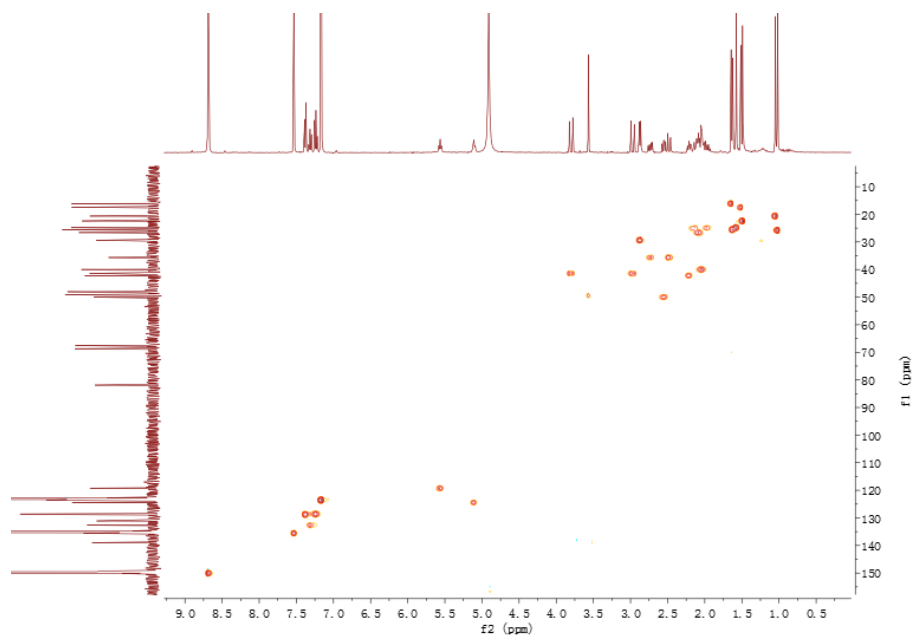


Figure S102. ^1H - ^1H COSY spectrum of compound **7** in pyridine- d_5

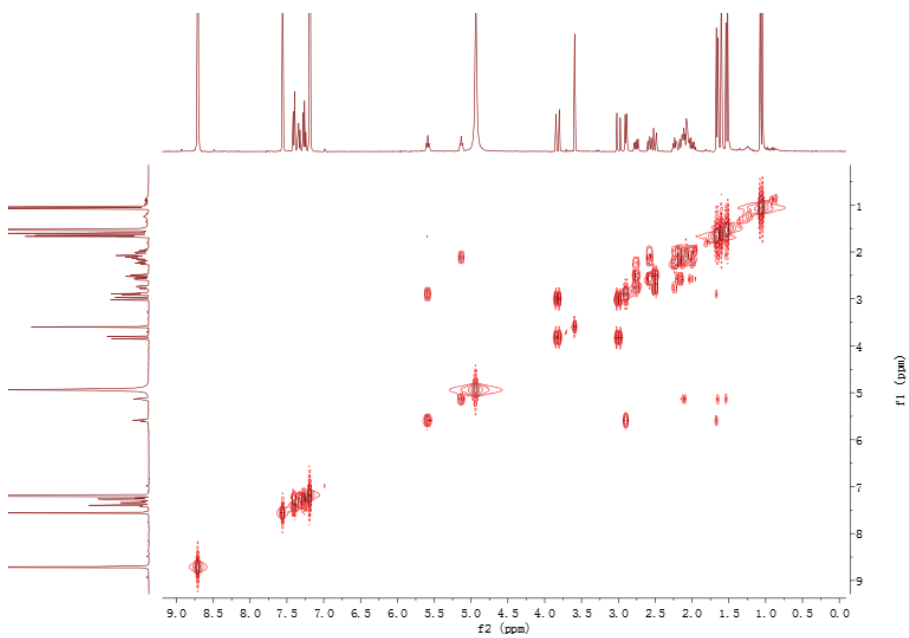


Figure S103. HMBC spectrum of compound **7** in pyridine- d_5

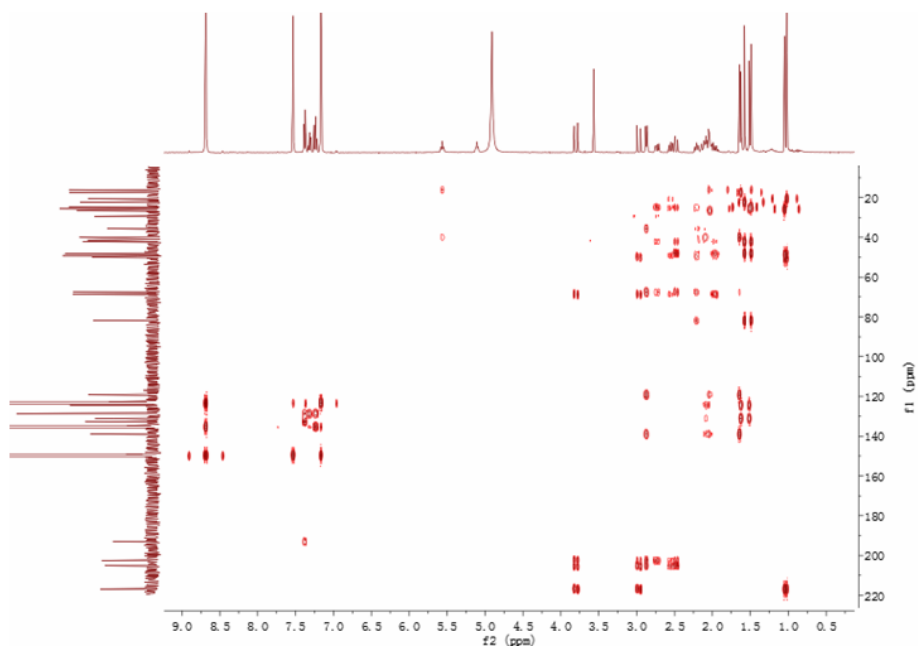


Figure S104. NOESY spectrum of compound **2** in pyridine- d_5

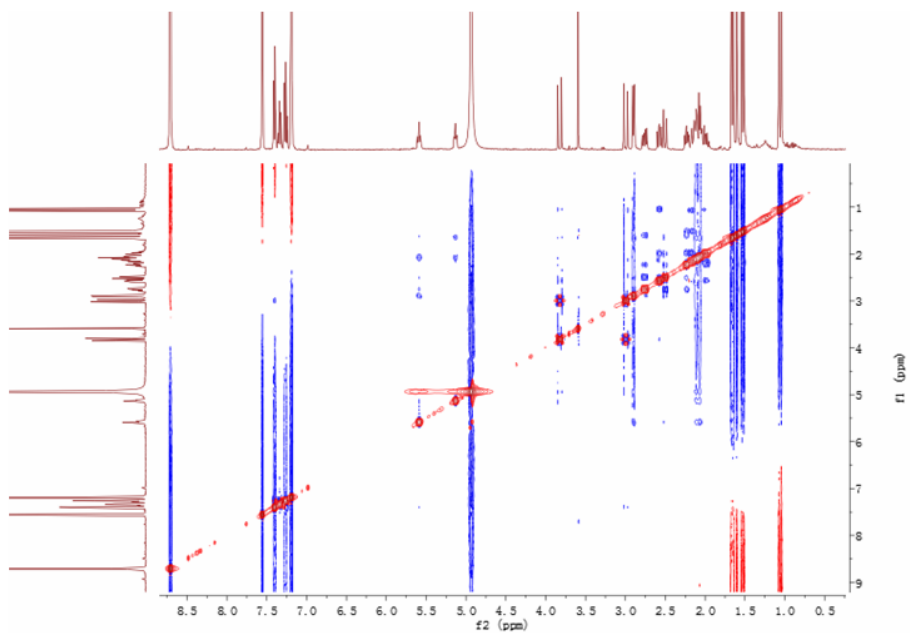


Figure S105. CD spectrum of compound **5**

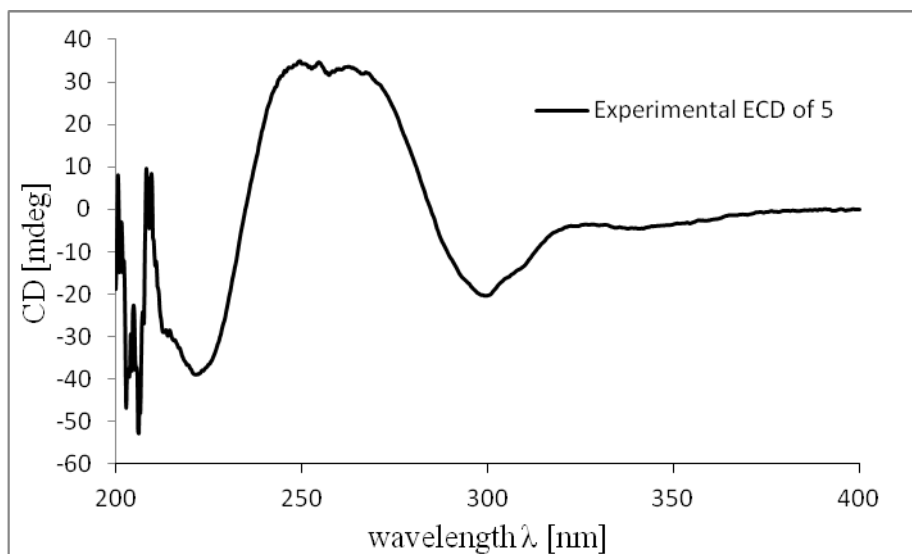
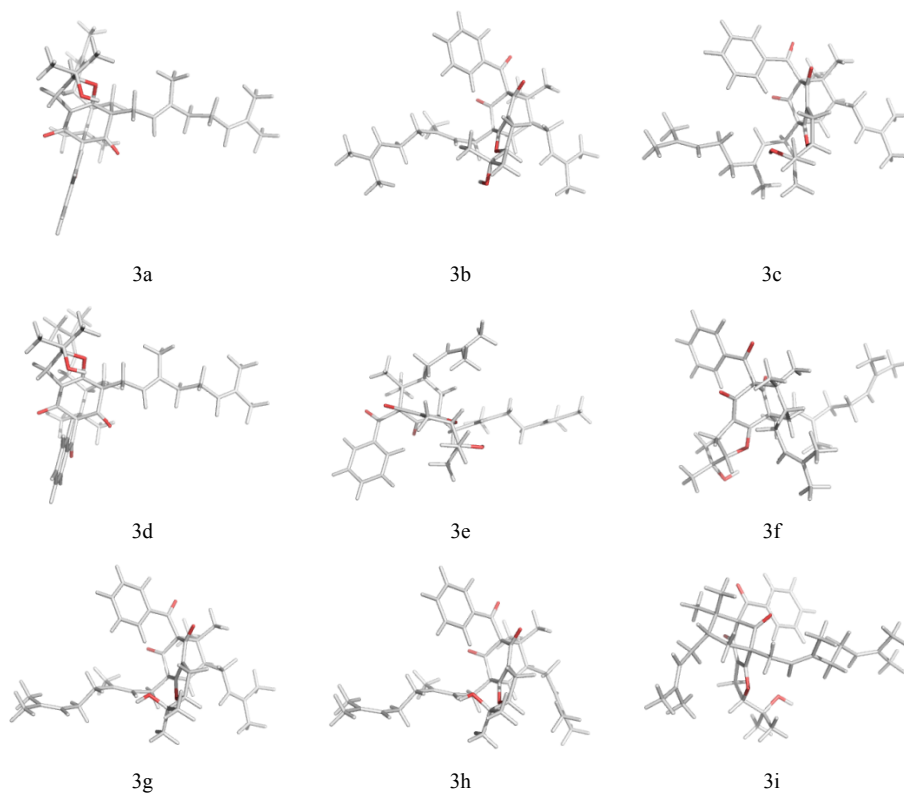
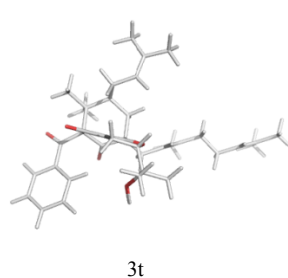
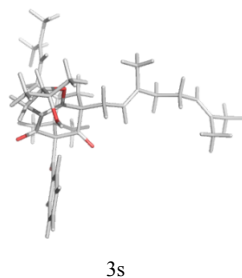
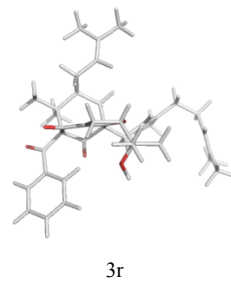
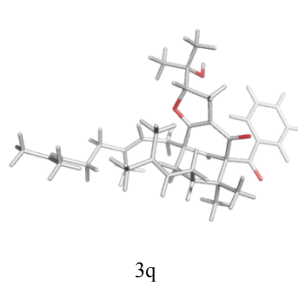
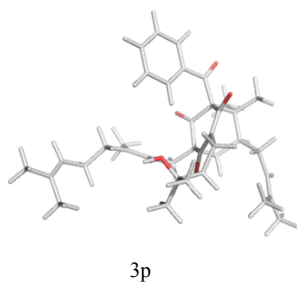
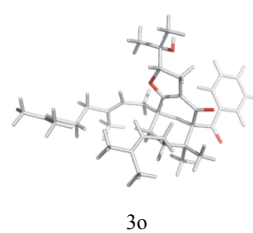
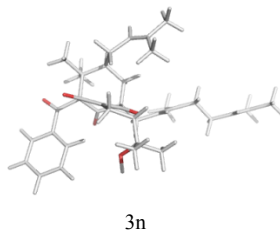
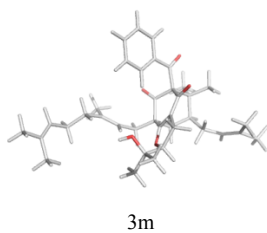
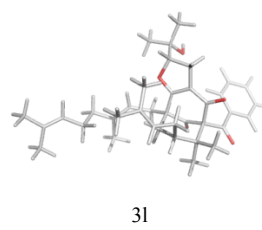
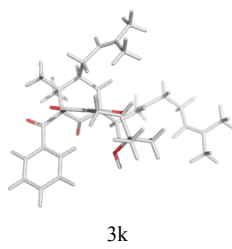
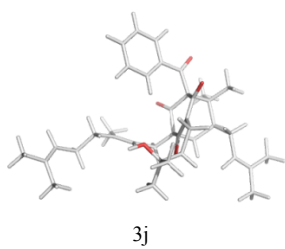
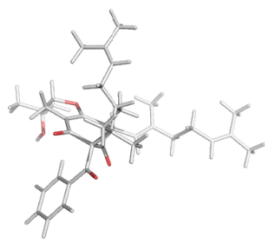


Figure S106. Twenty lowest energy conformers of the 1*S*,6*S*,8*S*,10*S* isomer and fourteen lowest energy conformers of the 1*R*,6*R*,8*R*,10*R* isomer of compound **3**.

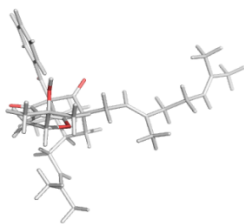




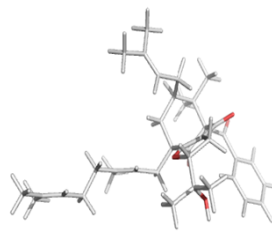
3a–3t: twenty lowest energy conformers of isomer 1*S*, 6*S*, 8*S*, 10*S* of compound **3**.



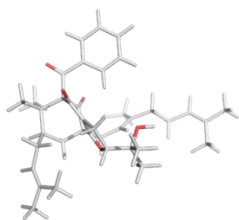
3a'



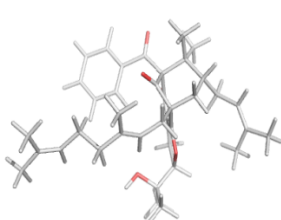
3b'



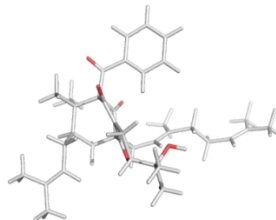
3c'



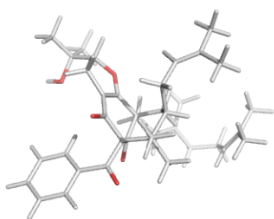
3d'



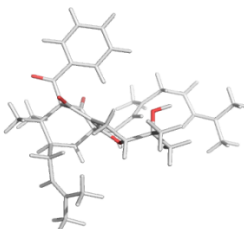
3e'



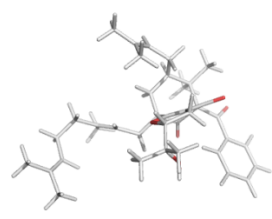
3f'



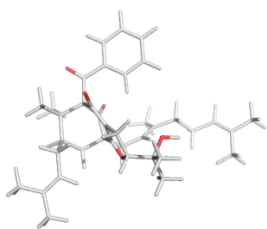
3g'



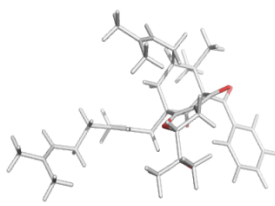
3h'



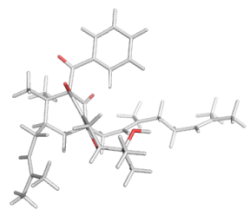
3i'



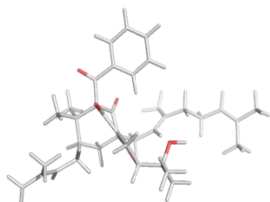
3j'



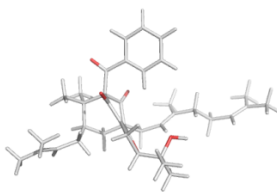
3k'



3l'



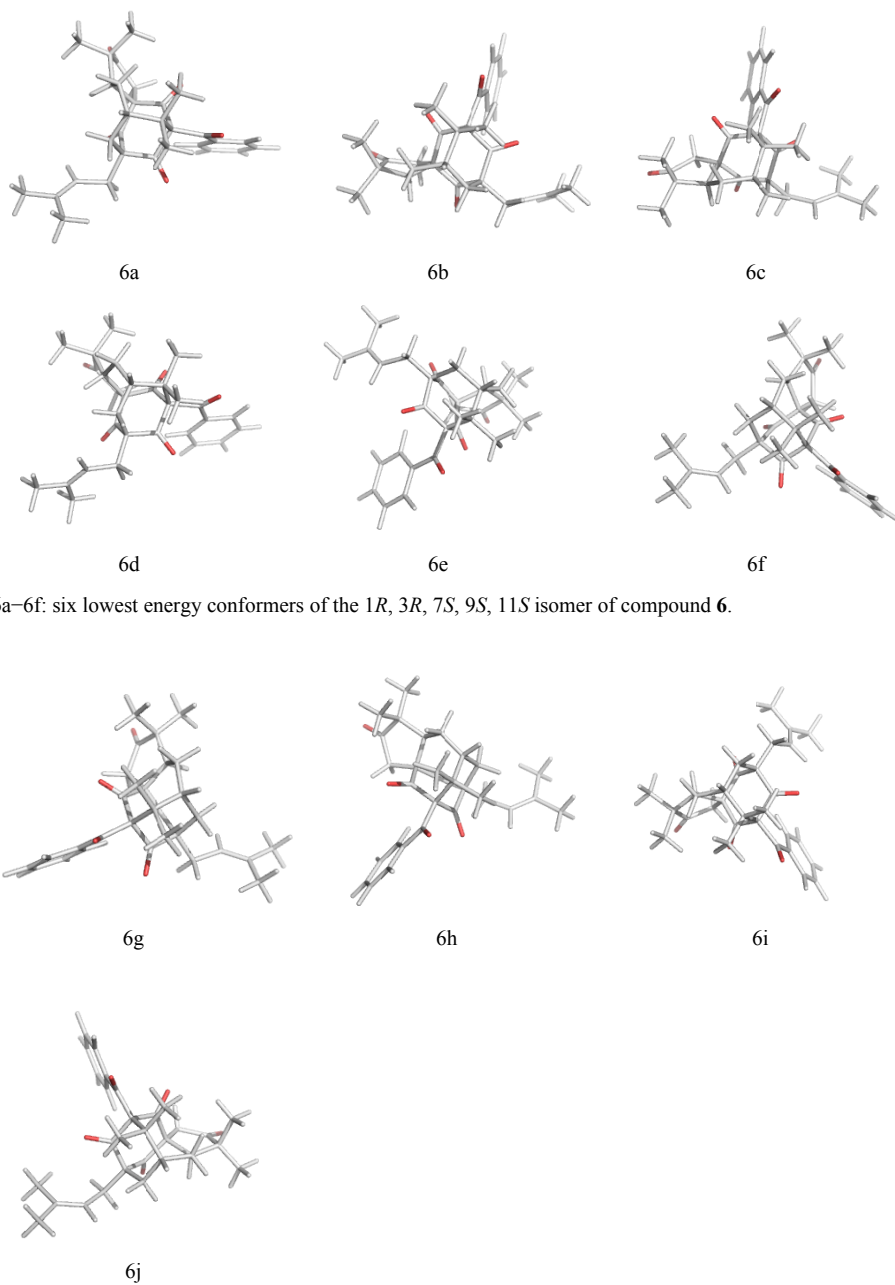
3m'



3n'

3a'–3n': fourteen lowest energy conformers of isomer 1*R*, 6*R*, 8*R*, 10*R* of compound **3**.

Figure S107. Six lowest energy conformers of the 1*R*,3*R*,7*S*,9*S*,11*S* isomer and four lowest energy conformers of the 1*S*,3*S*,7*R*,9*R*,11*R* isomer of compound **6**.



6a–6f: six lowest energy conformers of the 1*R*, 3*R*, 7*S*, 9*S*, 11*S* isomer of compound **6**.

6g–6j: four lowest energy conformers of the 1*S*, 3*S*, 7*R*, 9*R*, 11*R* isomer of compound **6**.

Table S1. Relative free energies (ΔG) and equilibrium populations (P) of the conformers of the 1*S*,6*S*,8*S*,10*S* and 1*R*,6*R*,8*R*,10*R* isomers of compound **3**

conformer	isomer 1 <i>S</i> ,6 <i>S</i> ,8 <i>S</i> ,10 <i>S</i>		conformer	Isomer 1 <i>R</i> ,6 <i>R</i> ,8 <i>R</i> ,10 <i>R</i>	
	ΔG (kcal/mol)	P (%)		ΔG (kcal/mol)	P (%)
3a	0.0000	12.33	3a'	1.5041	2.35
3b	0.1176	10.11	3b'	1.4098	2.75
3c	0.8617	2.88	3c'	0.9930	5.56
3d	0.6950	3.81	3d'	0.8784	6.74
3e	0.0851	10.68	3e'	1.8339	1.34
3f	0.4622	5.65	3f'	1.6874	1.72
3g	1.1178	1.87	3g'	1.2539	3.58
3h	0.2112	8.63	3h'	0.0042	29.47
3i	1.2372	1.53	3i'	1.0709	4.87
3j	0.8405	2.98	3j'	1.4295	2.66
3k	0.5325	5.02	3k'	1.5862	2.04
3l	1.1824	1.68	3l'	0.0000	29.68
3m	0.5025	5.28	3m'	1.0909	4.71
3n	0.9201	2.61	3n'	1.4589	2.53
3o	1.1612	1.74			
3p	0.2913	7.54			
3q	0.8675	2.85			
3r	0.9747	2.38			
3s	0.7919	3.24			
3t	0.4319	5.95			

Table S2. Relative free energies (ΔG) and equilibrium populations (P) of the conformers of the 1*R*,3*R*,7*S*,9*S*,11*S* and 1*S*,3*S*,7*R*,9*R*,11*R* isomers of compound **6**

conformer	isomer 1 <i>S</i> ,6 <i>S</i> ,8 <i>S</i> ,10 <i>S</i>		conformer	Isomer 1 <i>R</i> ,6 <i>R</i> ,8 <i>R</i> ,10 <i>R</i>	
	ΔG (kcal/mol)	P (%)		ΔG (kcal/mol)	P (%)
6a	0.0000	43.08	6g	0.0000	51.24
6b	1.2125	5.57	6h	0.1212	41.77
6c	1.5769	3.01	6i	1.5983	3.45
6d	0.8600	10.10	6j	1.5851	3.53
6e	1.5937	2.93			
6f	0.1179	35.31			