SIX NEW TRITERPENOIDS WITH F WITH ANTI-INFLAMMATORY ACTIVITY FROM *GYPSOPHILA OLDHAMIANA*

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Supporting Information

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Chart S1. Chart of extraction and isolation

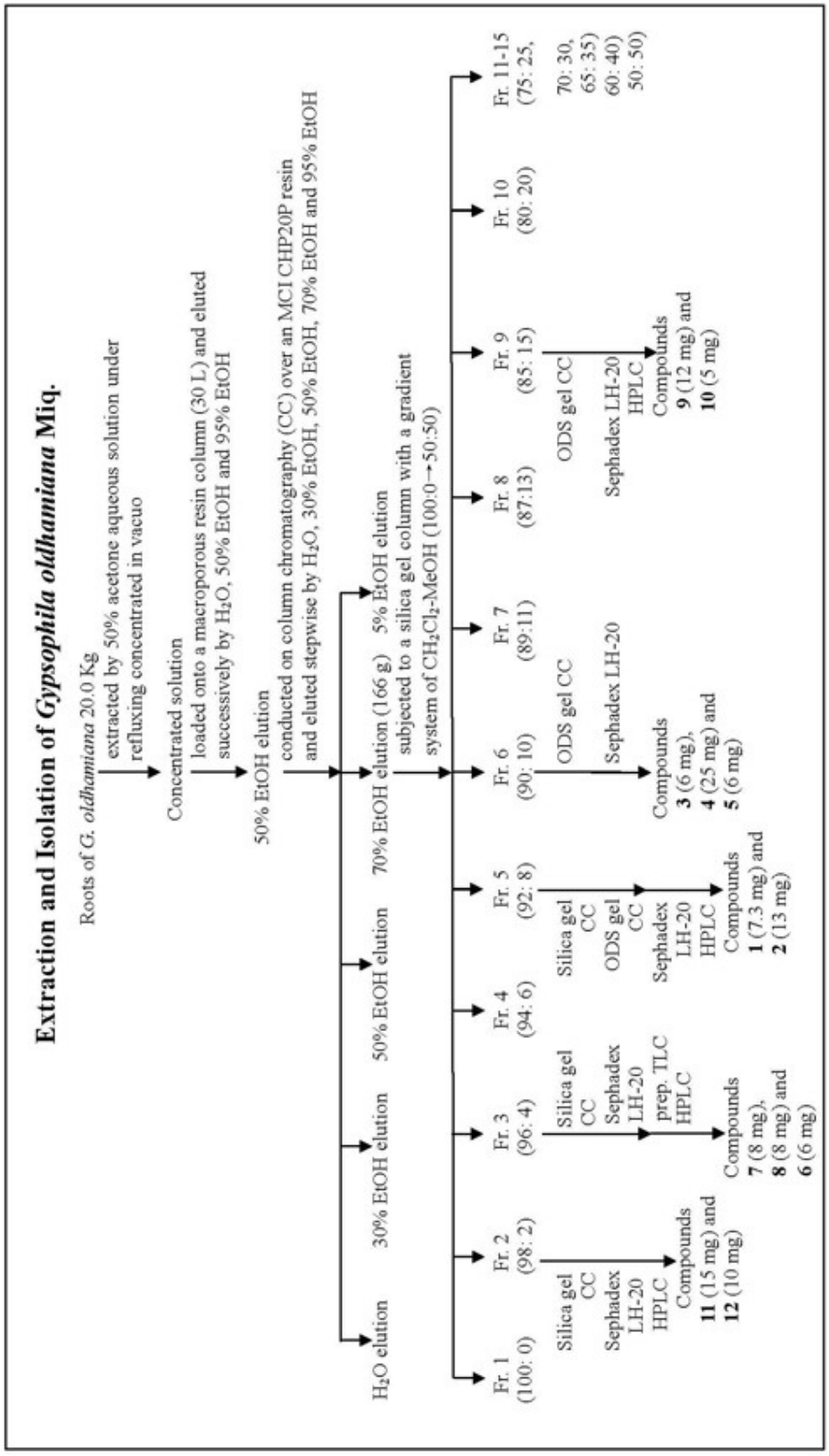


Table S1. Crystal data and structure refinement for compound **6**.

Identification code	cu_2019112001 (CCDC number: 2169252)	
Empirical formula	$C_{30}H_{46}O_4$	
Formula weight	470.67	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.4419(7) Å	□= 90°.
	b = 11.3693(11) Å	□= 94°.
	c = 14.9985(14) Å	□ = 90°.
Volume	1266.6(2) $Å^3$	
Z	2	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.623 mm^{-1}	
F(000)	516	
Theta range for data collection	4.9 to 66.6°.	
Index ranges	-8<=h<=8, -13<=k<=13, -16<=l<=17	
Reflections collected	9188	
Independent reflections	4042 [R(int) = 0.199]	
Completeness to theta = 66.59°	96.1 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.836 and 0.780	
Refinement method	Refinement on F^2	
Data / restraints / parameters	4042 / 1 / 315	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.1099, wR2 = 0.2523	
R indices (all data)	R1 = 0.1795, wR2 = 0.3047	
Absolute structure parameter	-0.9(6)	
Largest diff. peak and hole	0.45 and -0.65 $e.Å^{-3}$	

Table S2 *In vitro* inflammatory activity of compounds **1**-**12**.

compound	IC_{50}[a] (μM)	compound	IC_{50}[a] (μM)
	RAW264.7		RAW264.7
1	29.31±0.86 μM	7	8.61±0.32 μM
2	2.55±0.49 μM	8	5.51±0.63 μM
3	0.93±0.21 μM	9	11.26±0.58 μM
4	37.61±0.74 μM	10	21.47±0.54 μM
5	29.35±0.67 μM	11	1.71±0.35 μM
6	18.73±0.68 μM	12	46.3±0.81 μM
Dexamethasone[b]	0.86 ±0.08 μM		

[a] Means ± S.D. From three independent experiments (n=3)

[b] Positive control

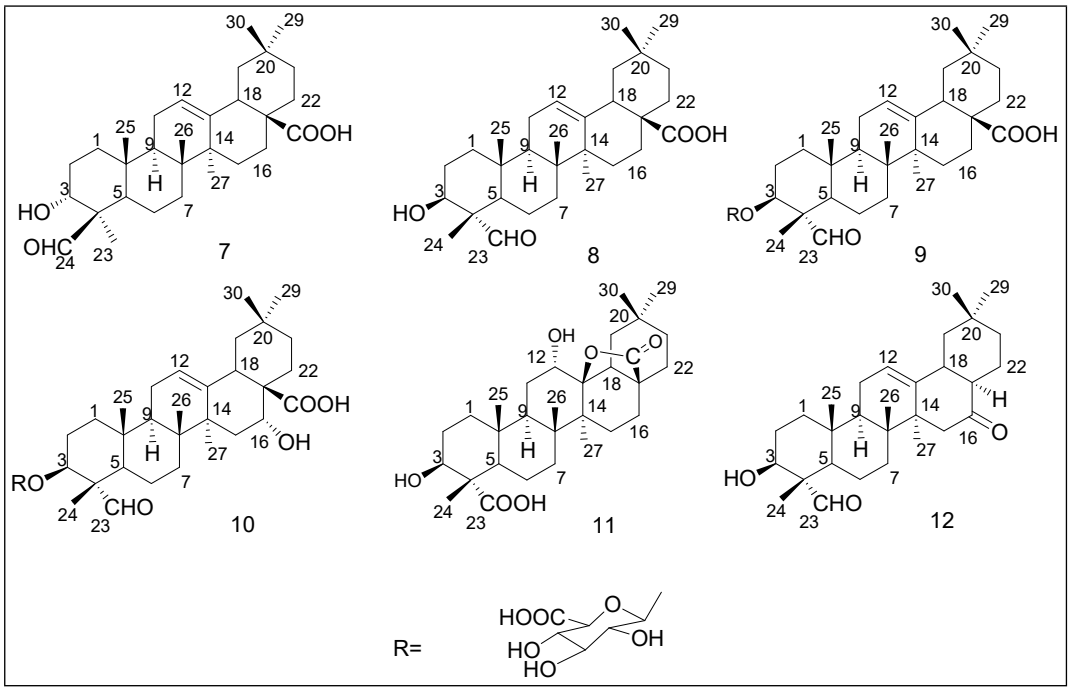


Figure S1. Structures of compounds **7**-**12**

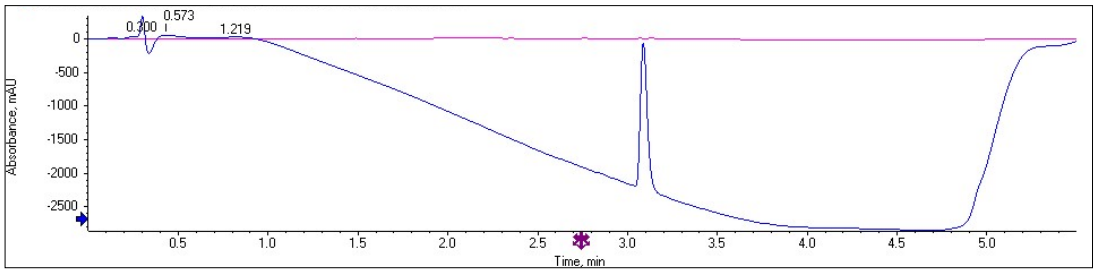


Figure S2. HPLC spectrum of compound **1**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm and 254nm.

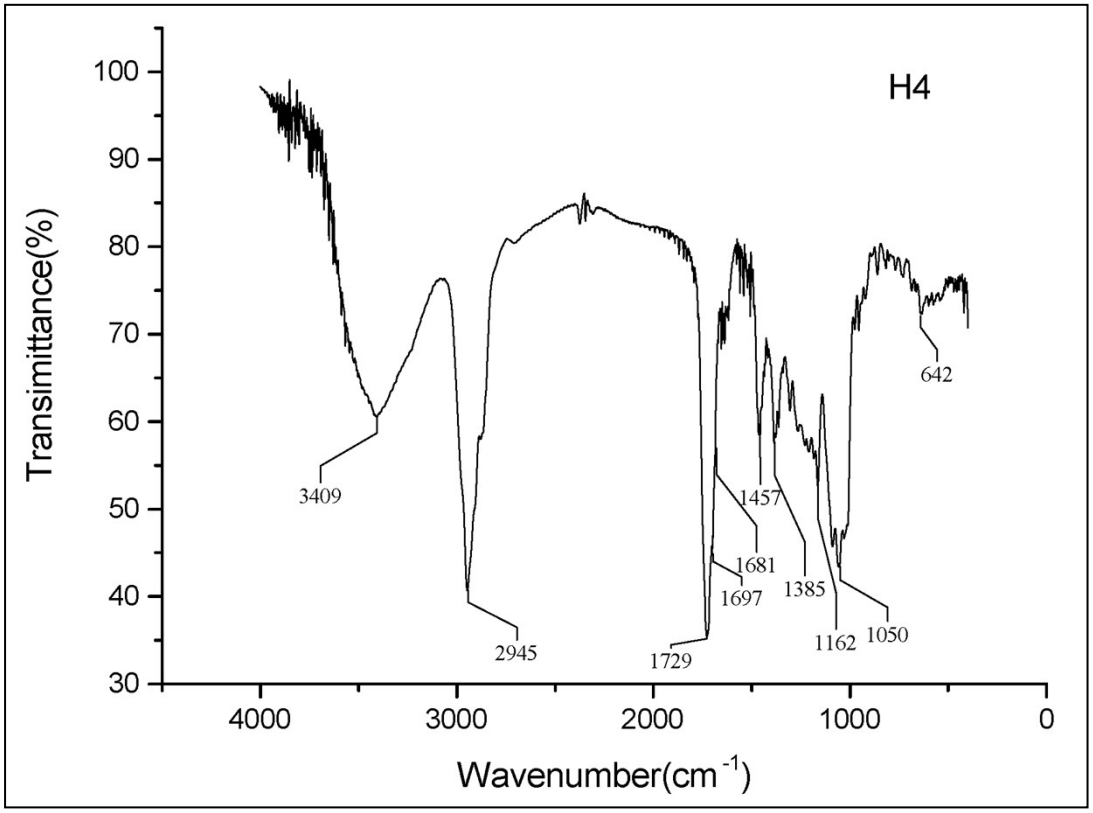


Figure S3. IR spectrum of compound **1**

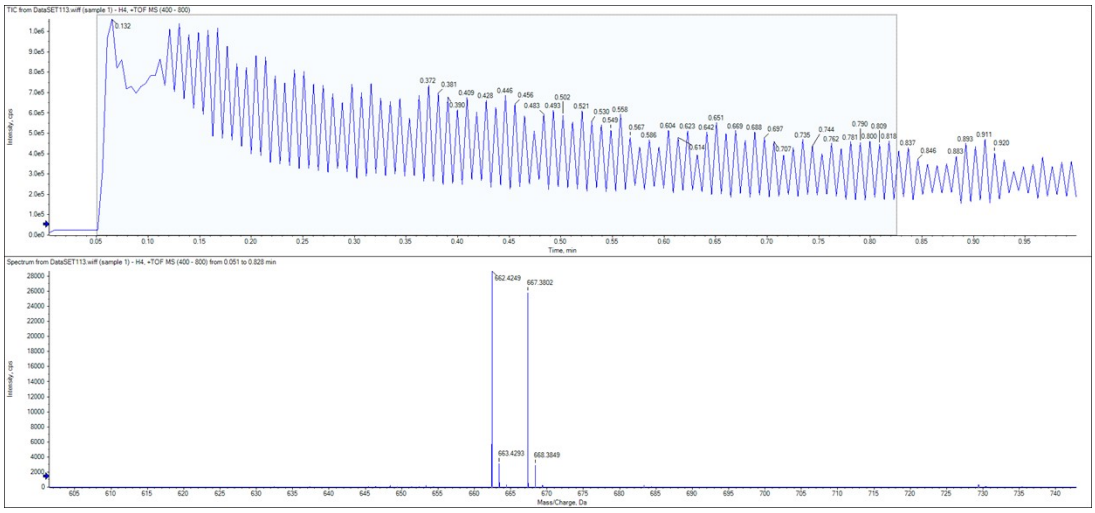


Figure S4. HR-ESI-MS spectrum ofcompound **1**

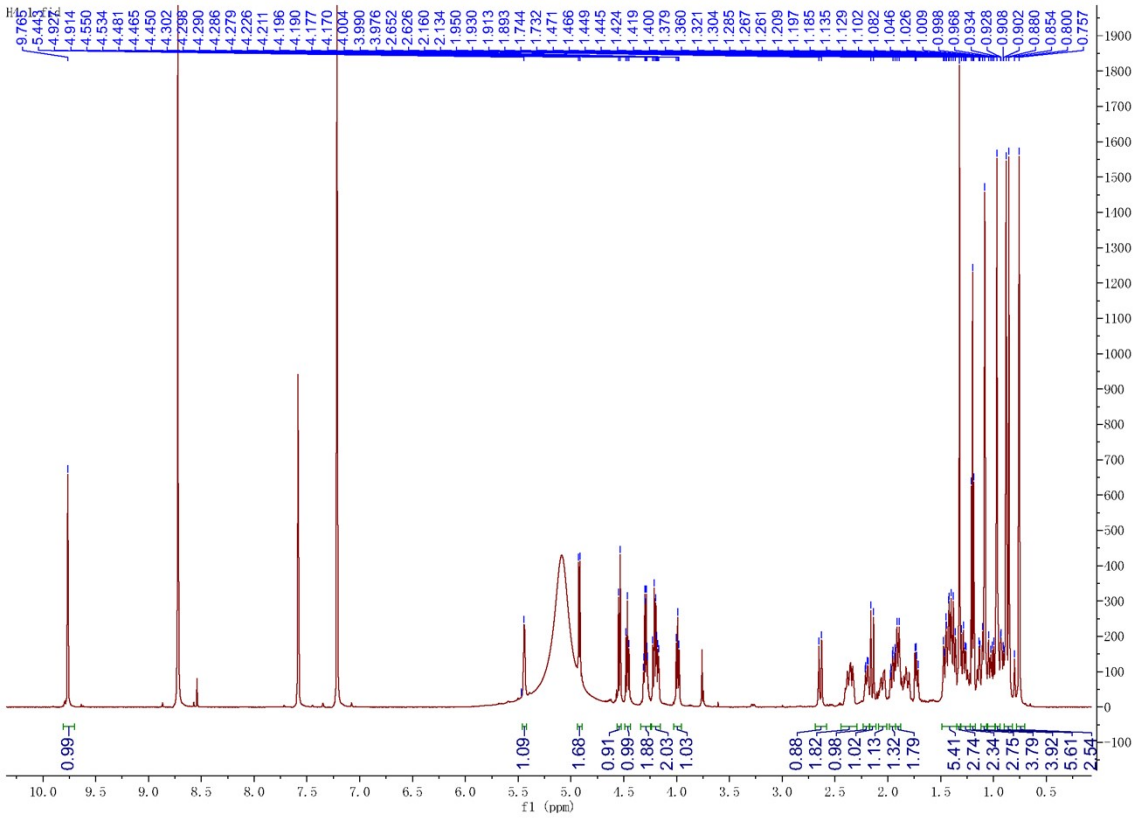


Figure S5. ^{1}H-NMR spectrum of compound **1** in C_5D_5N (600 MHz)

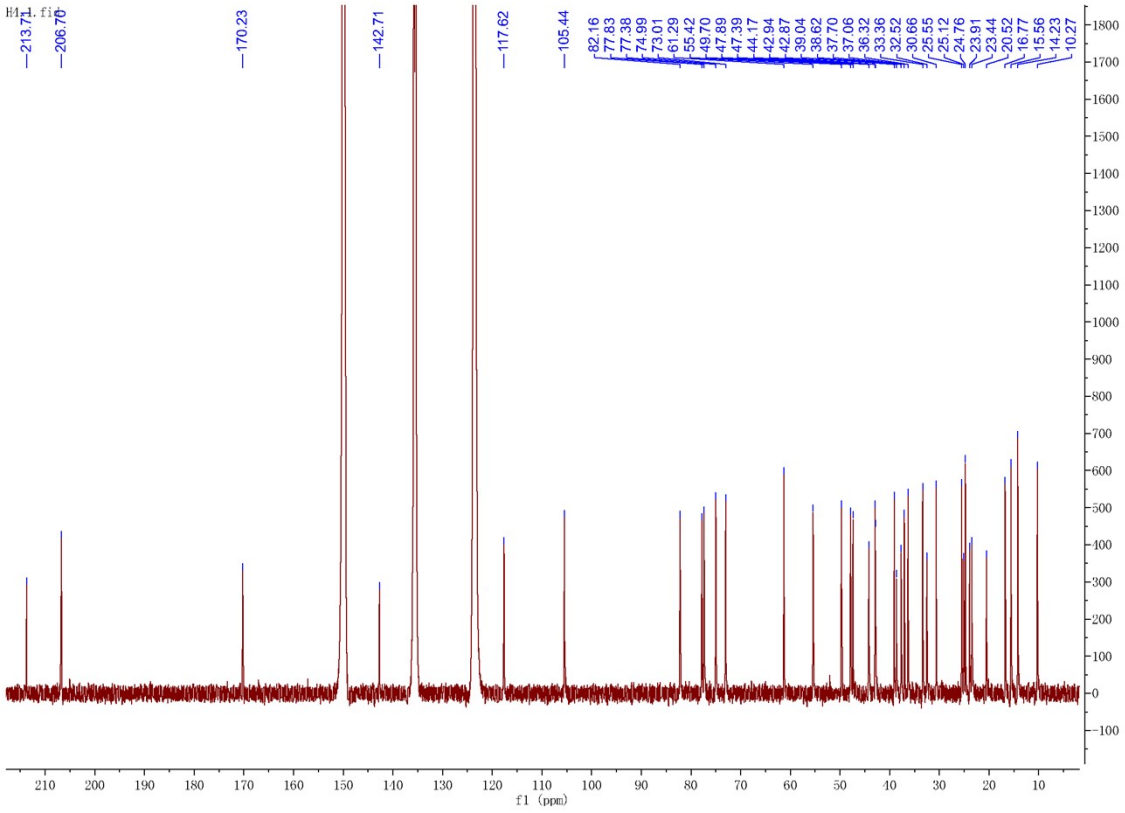


Figure S6. ^{13}C-NMR spectrum of compound **1** in C_5D_5N (150 MHz)

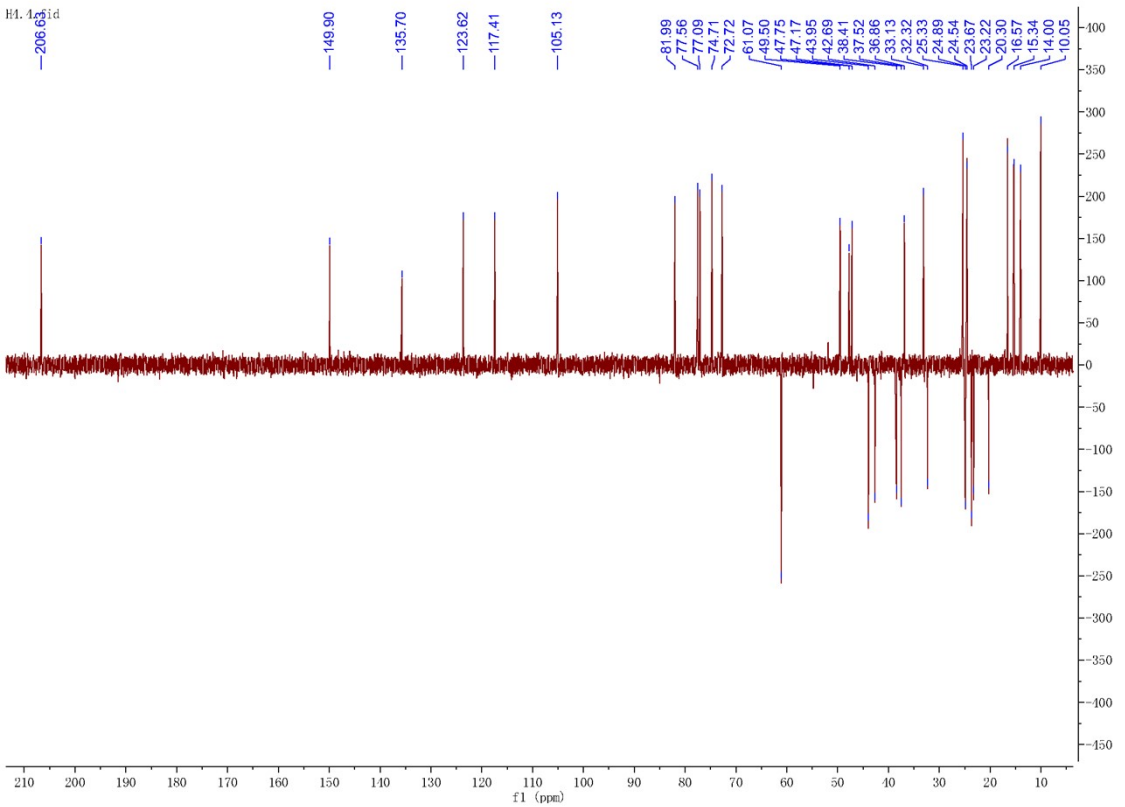


Figure S7. DEPT spectrum of compound **1** in C_5D_5N

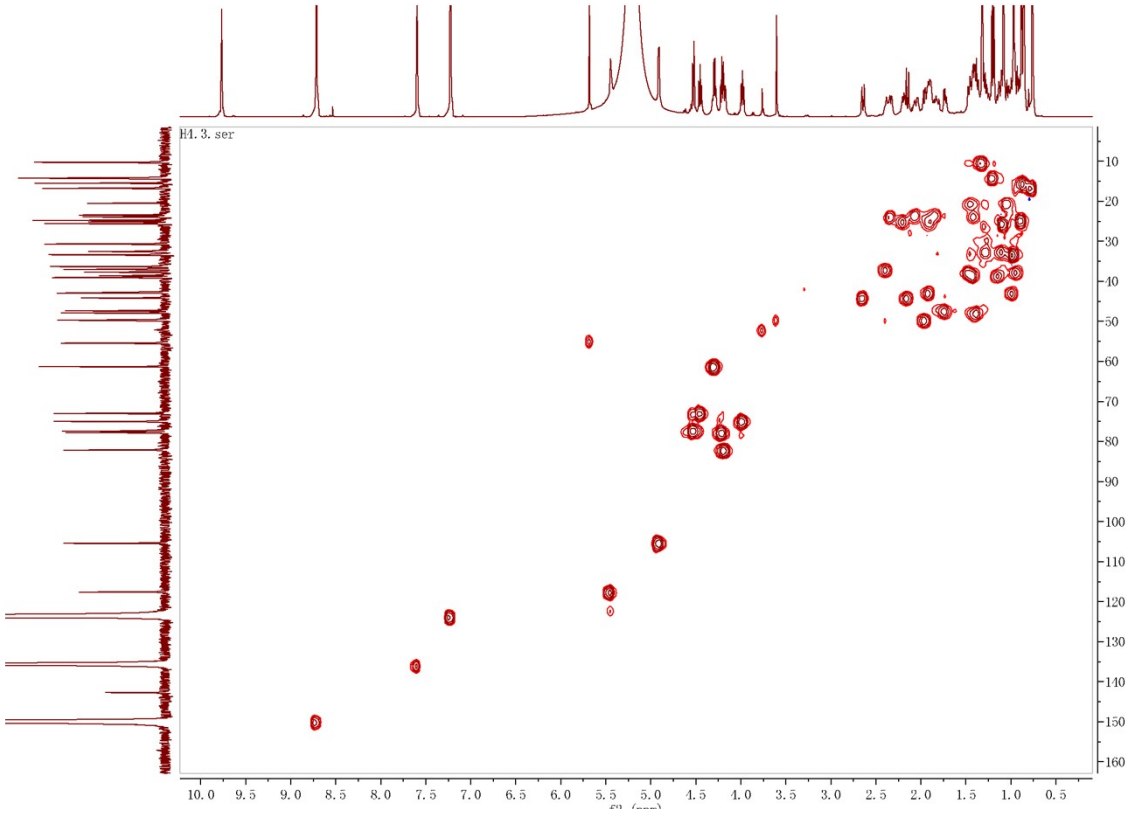


Figure S8. HSQC spectrum of compound **1** in C_5D_5N

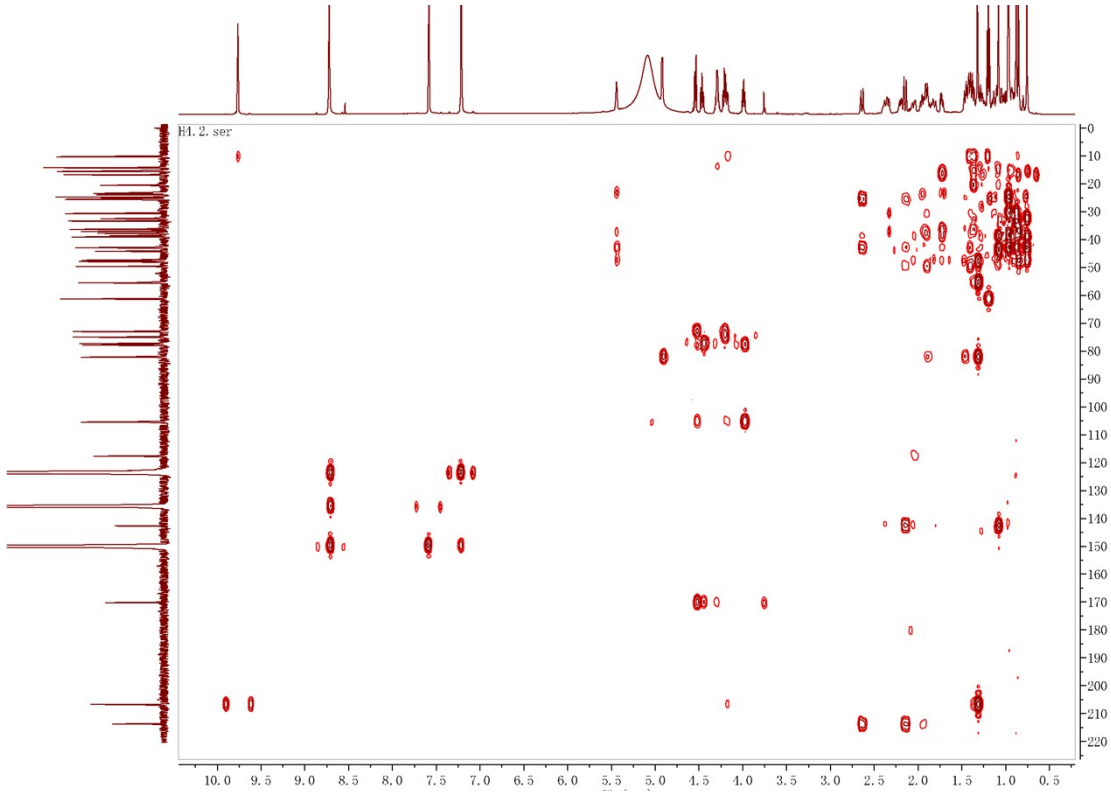


Figure S9. HMBC spectrum of compound **1** in C_5D_5N

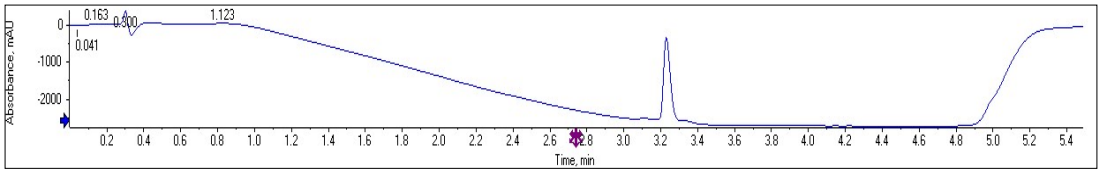
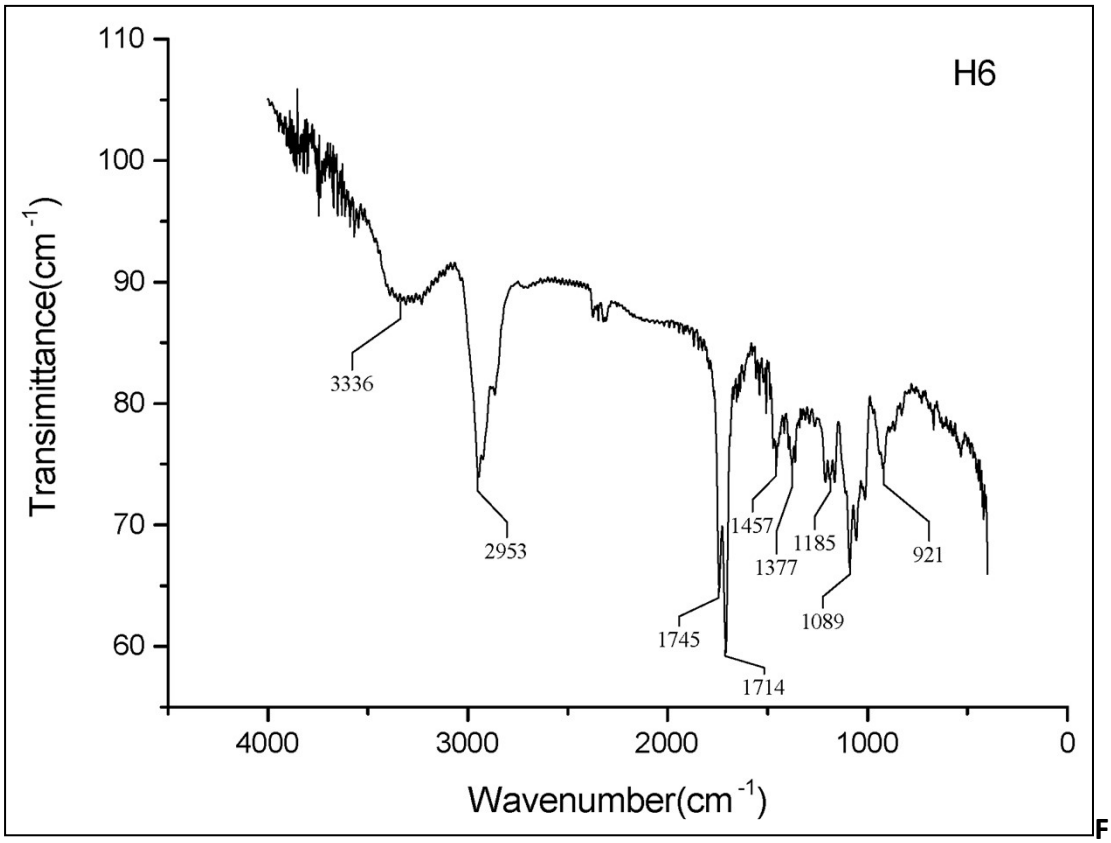


Figure S10. HPLC spectrum of compound **2**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.



igure S11. IR spectrum of compound **2**

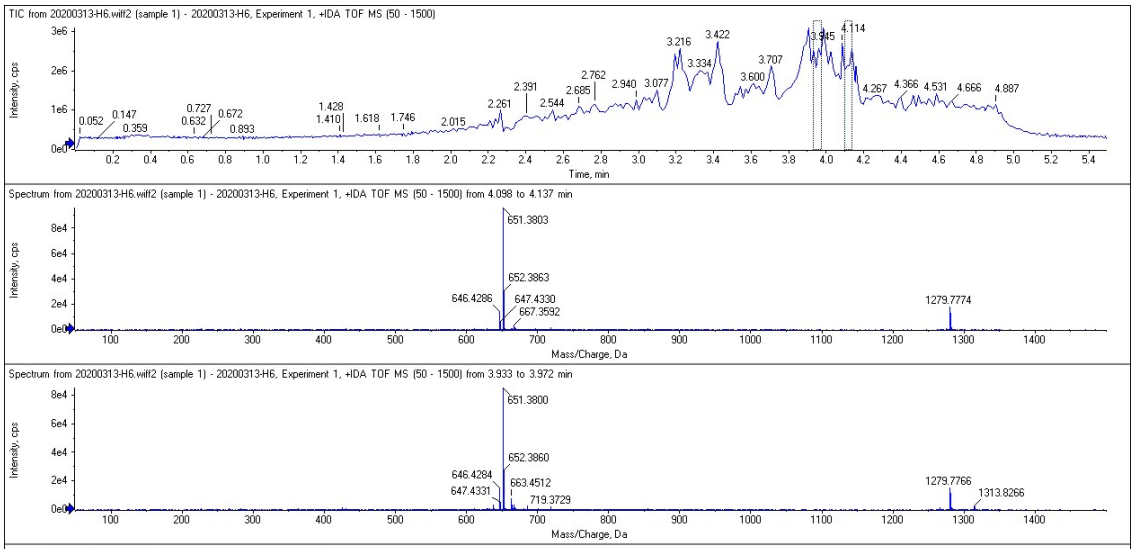


Figure S12. HR-ESI-MS spectrum ofcompound **2**

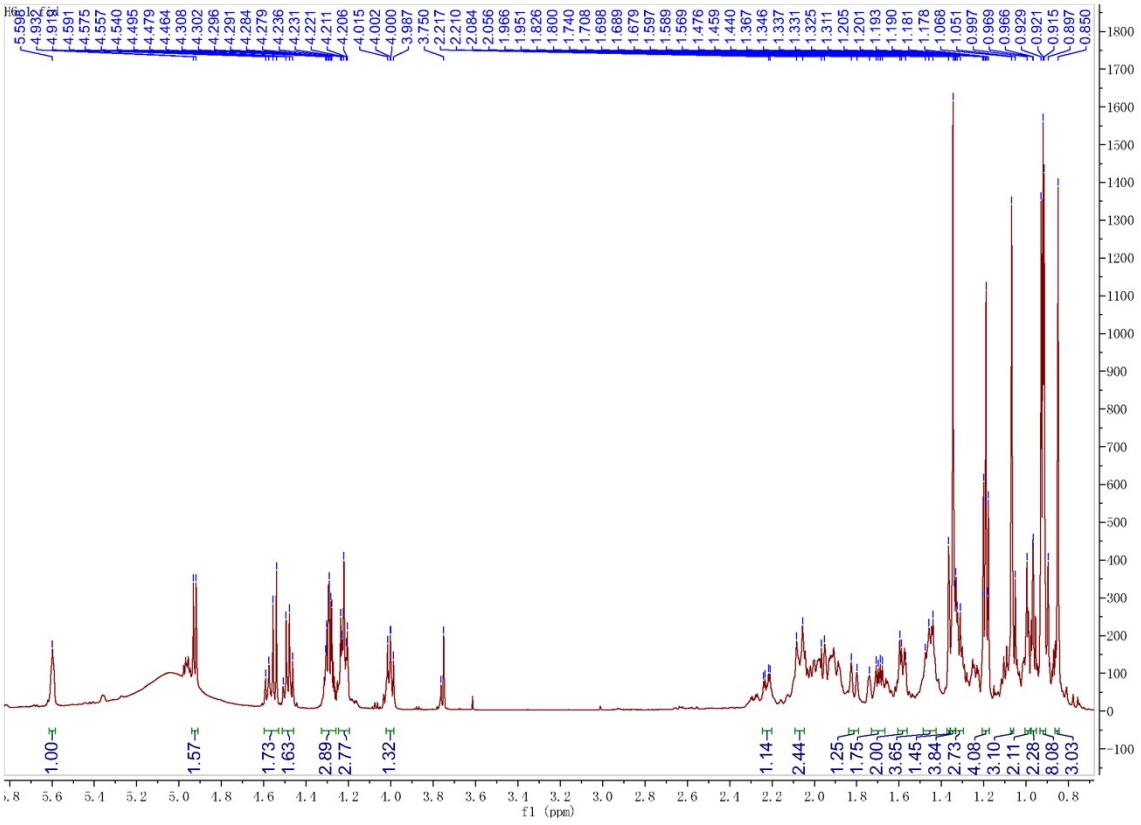


Figure S13. ^{1}H-NMR spectrum of compound **2** in C_5D_5N (600 MHz)

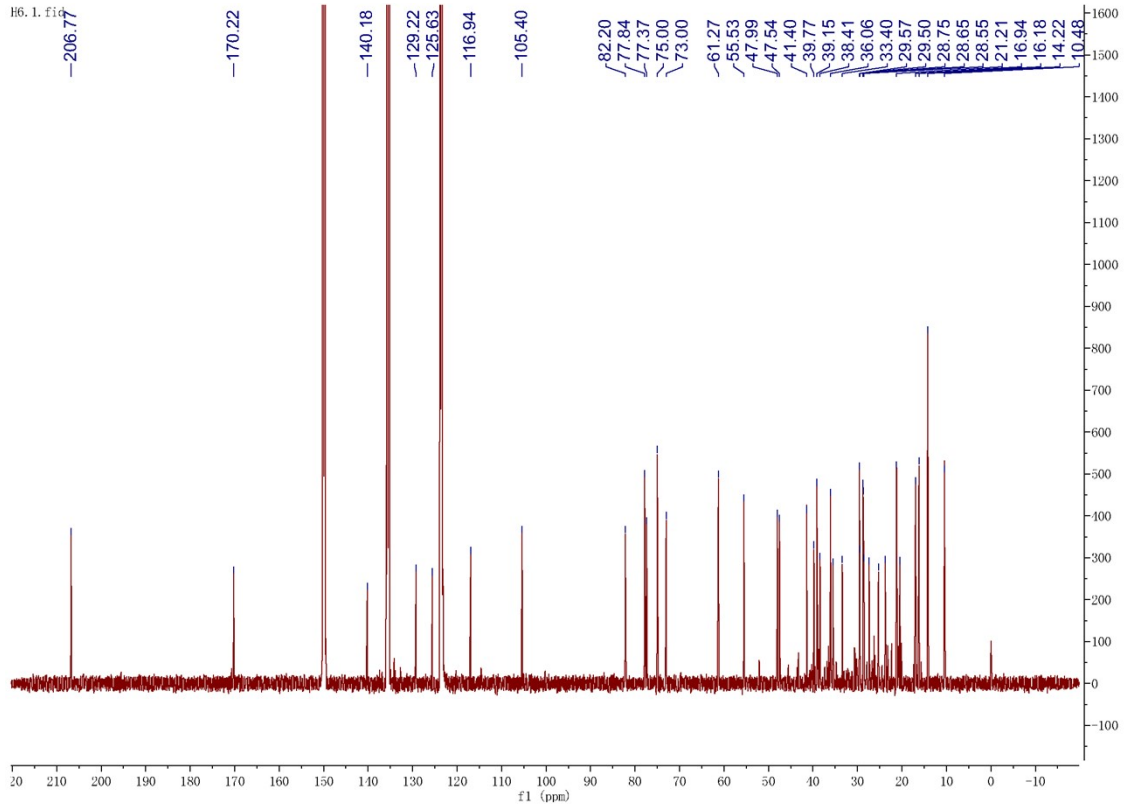


Figure S14. ^{13}C-NMR spectrum of compound **2** in C_5D_5N (150 MHz)

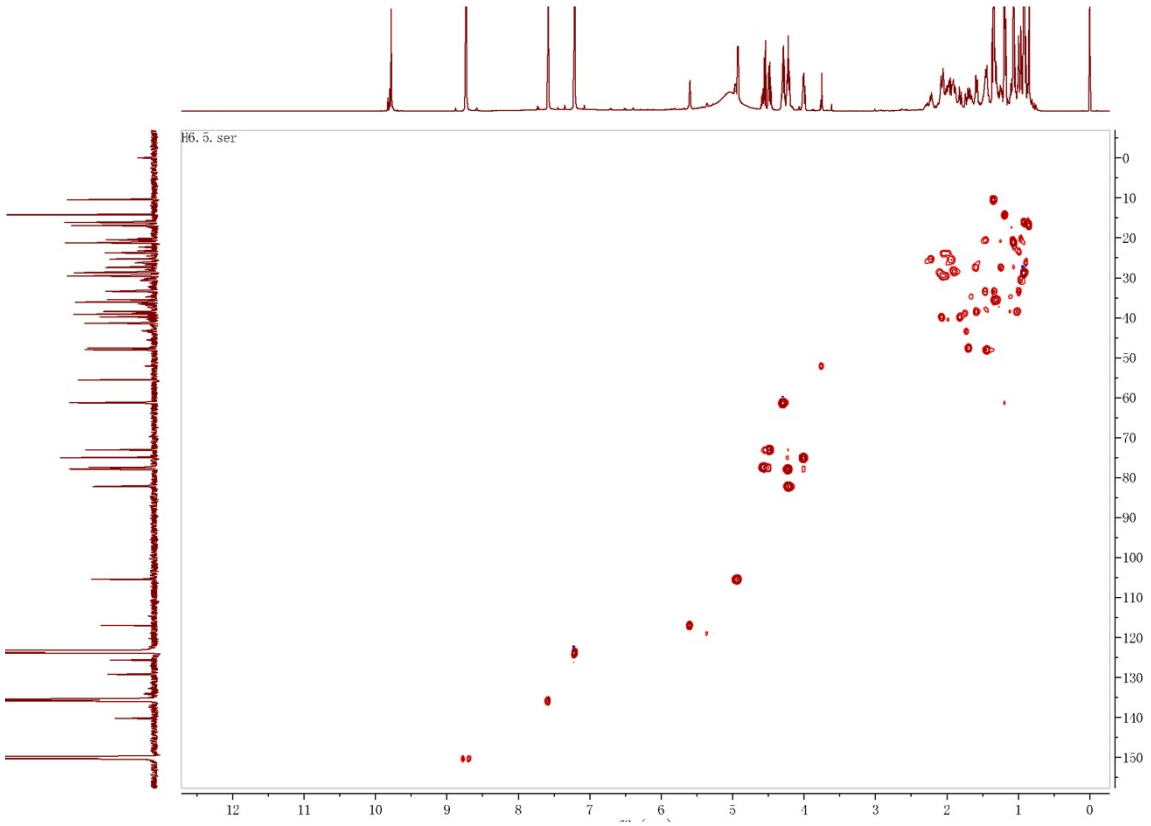


Figure S15. HSQC spectrum of compound **2** in C_5D_5N

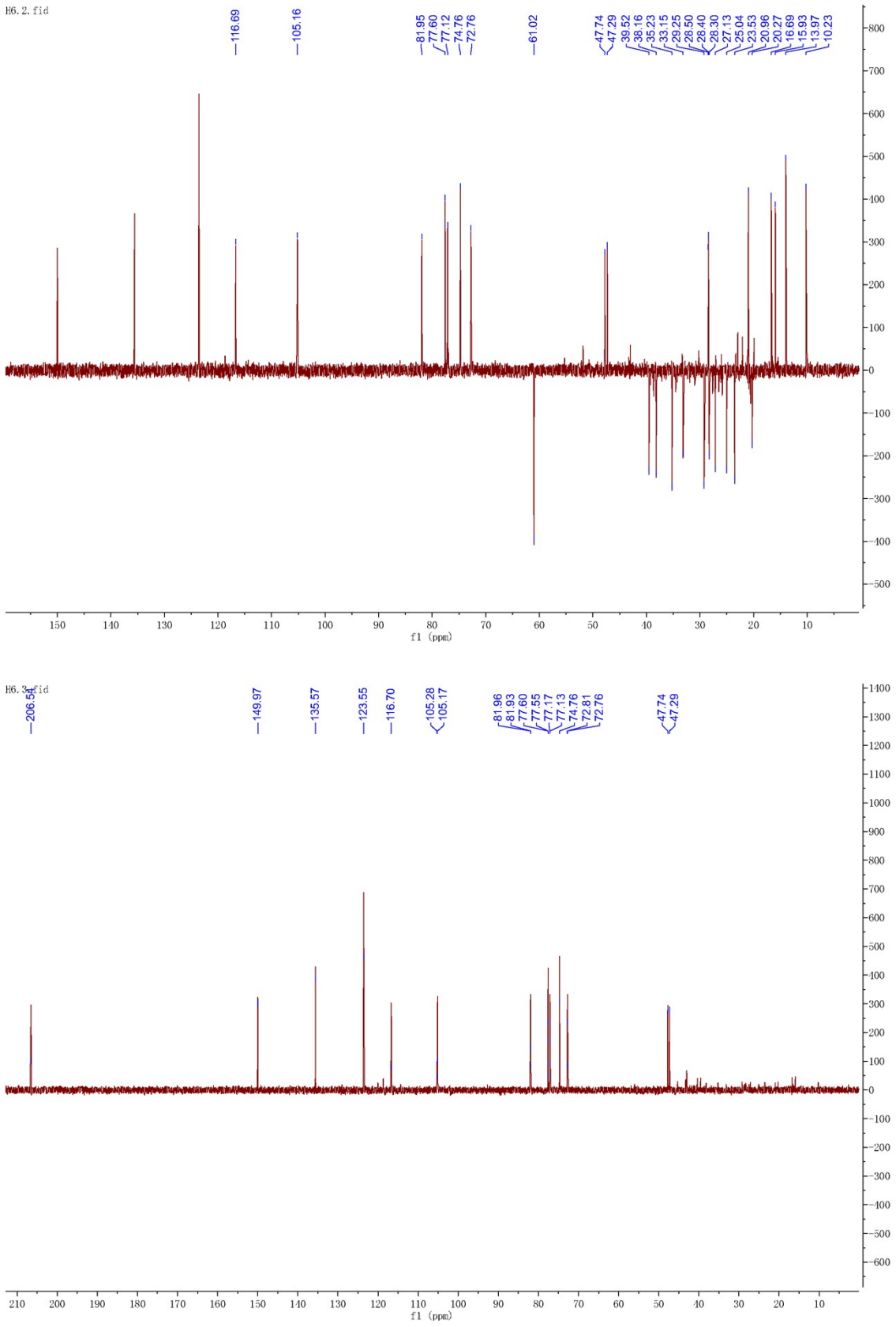


Figure S16. DEPT spectrum of compound **2** in C_5D_5N

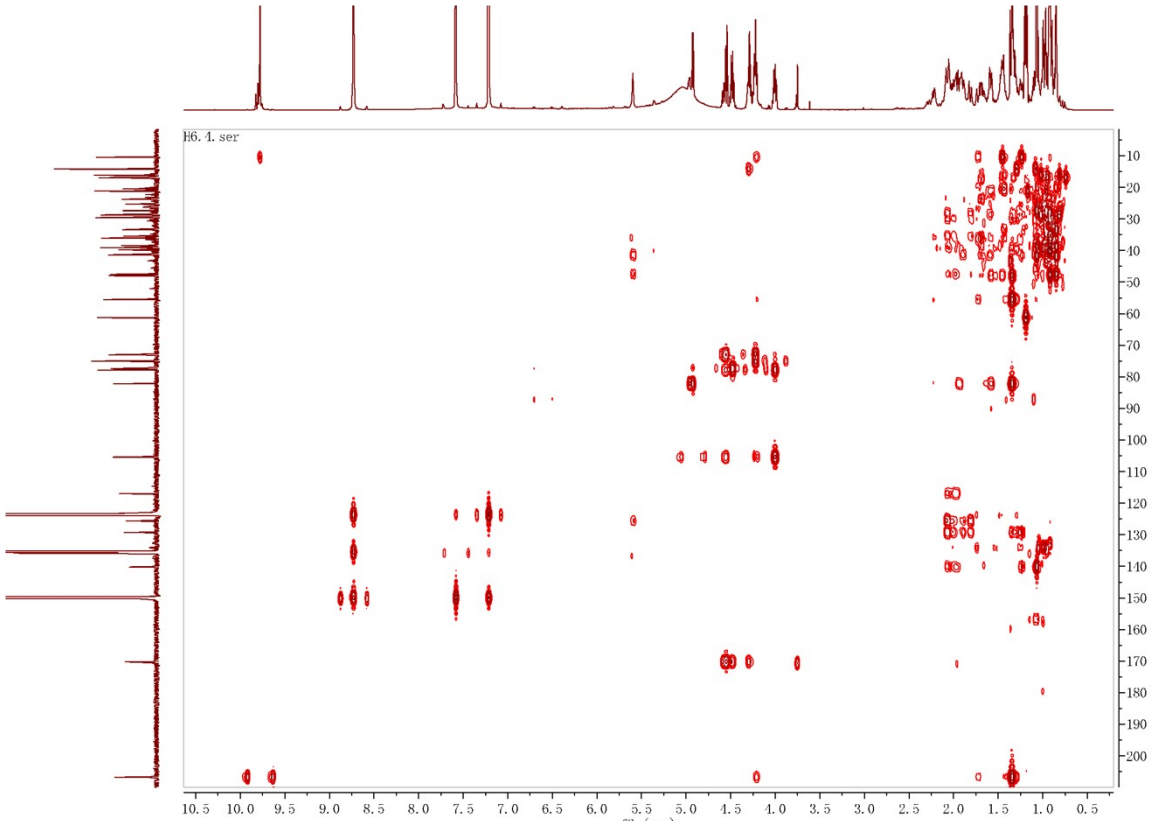


Figure S17. HMBC spectrum of compound **2** in C_5D_5N

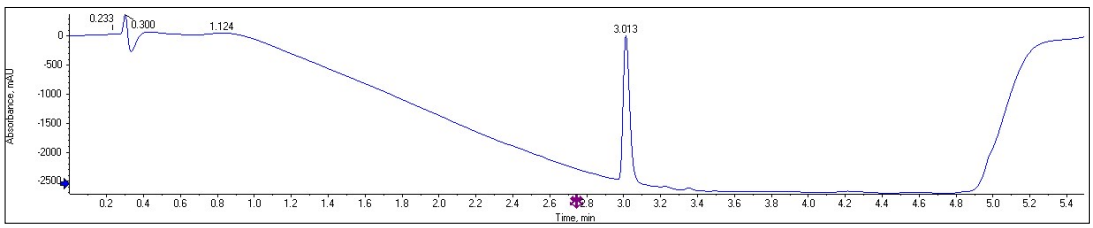


Figure S18. HPLC spectrum of compound **3**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

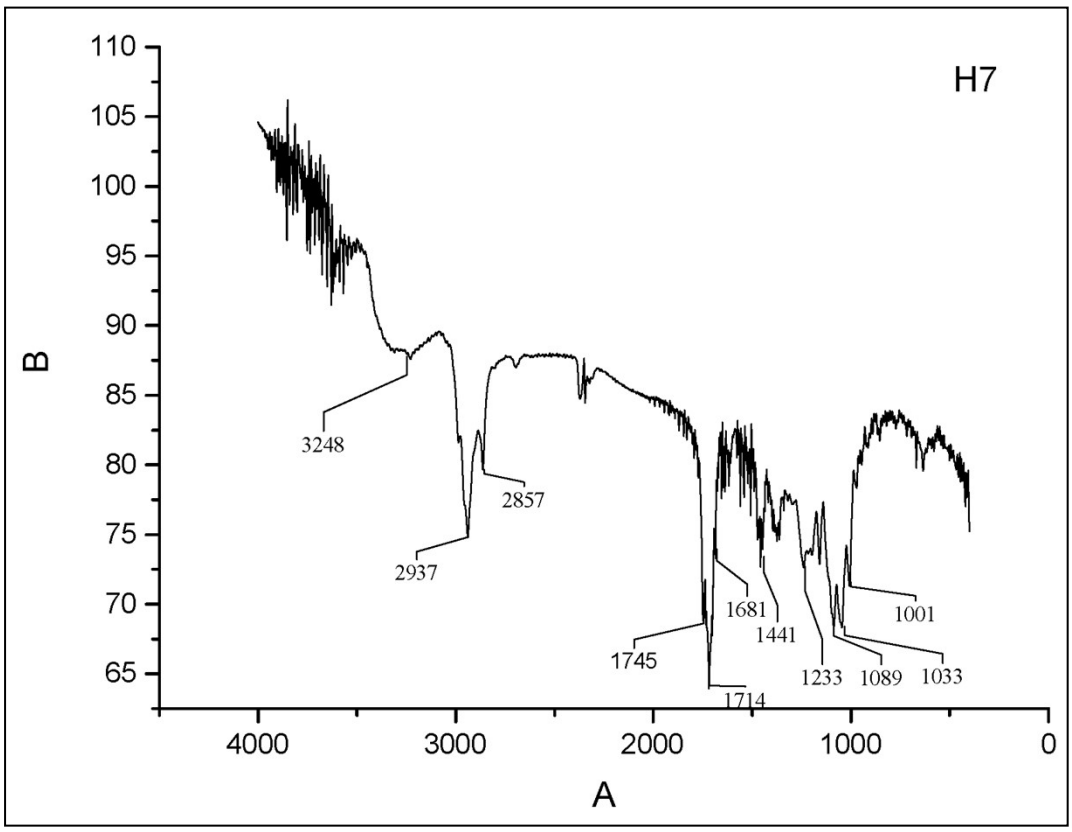


Figure S19. IR spectrum of compound **3**

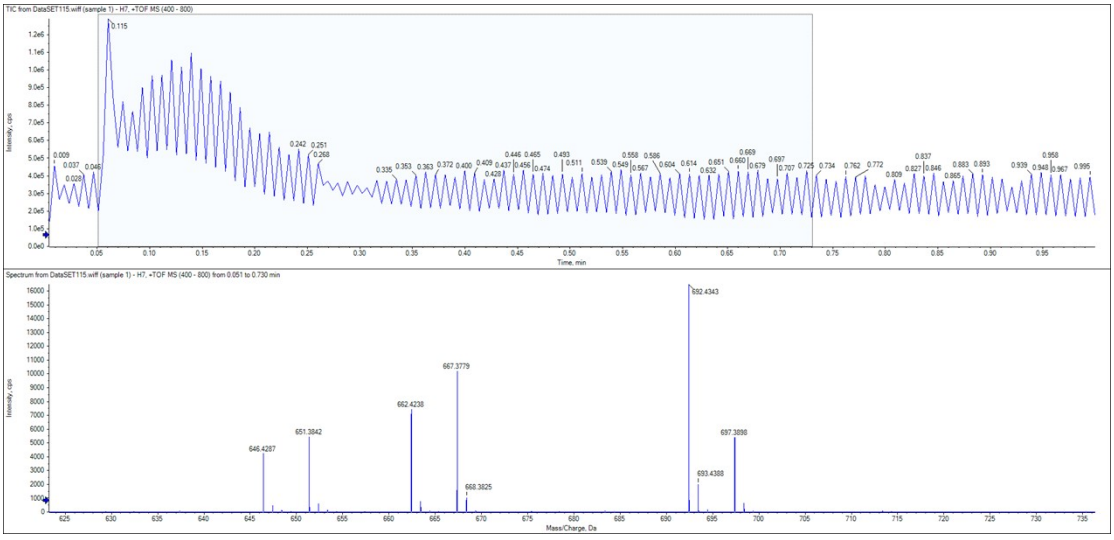


Figure S20. HR-ESI-MS spectrum ofcompound **3**

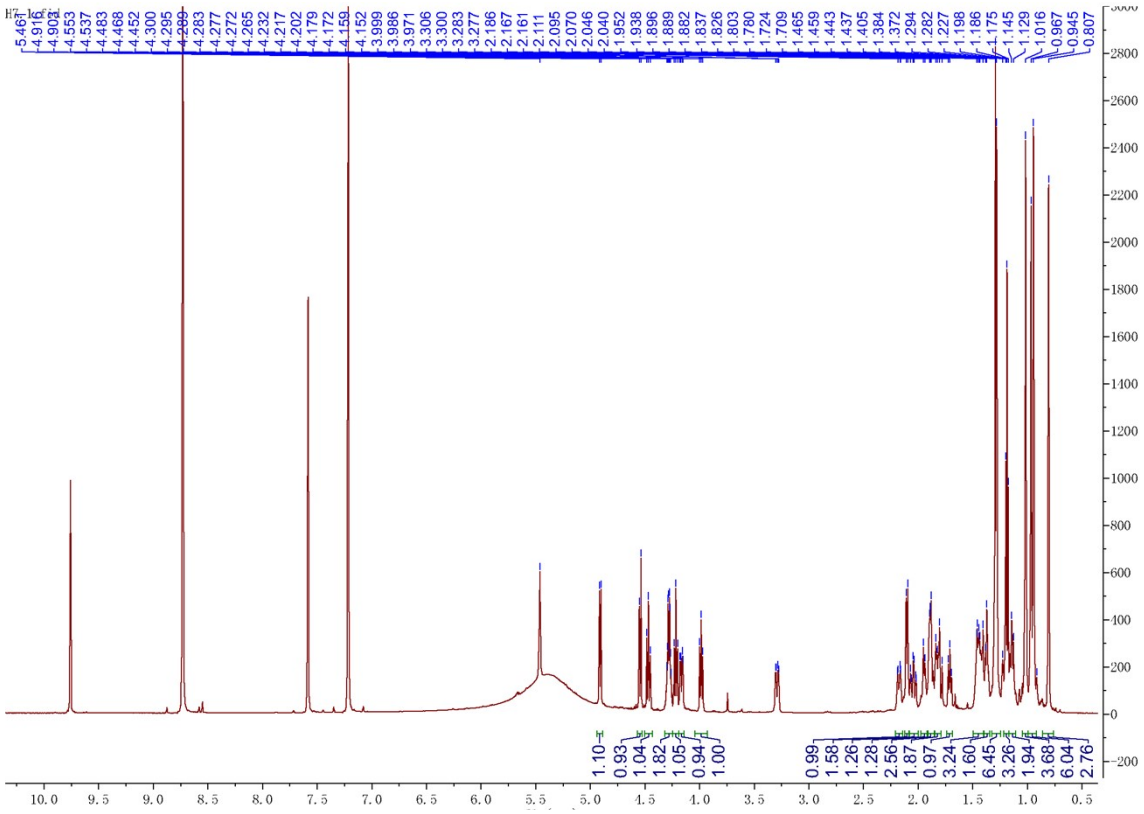


Figure S21. ^{1}H-NMR spectrum of compound **3** in C_5D_5N (600 MHz)

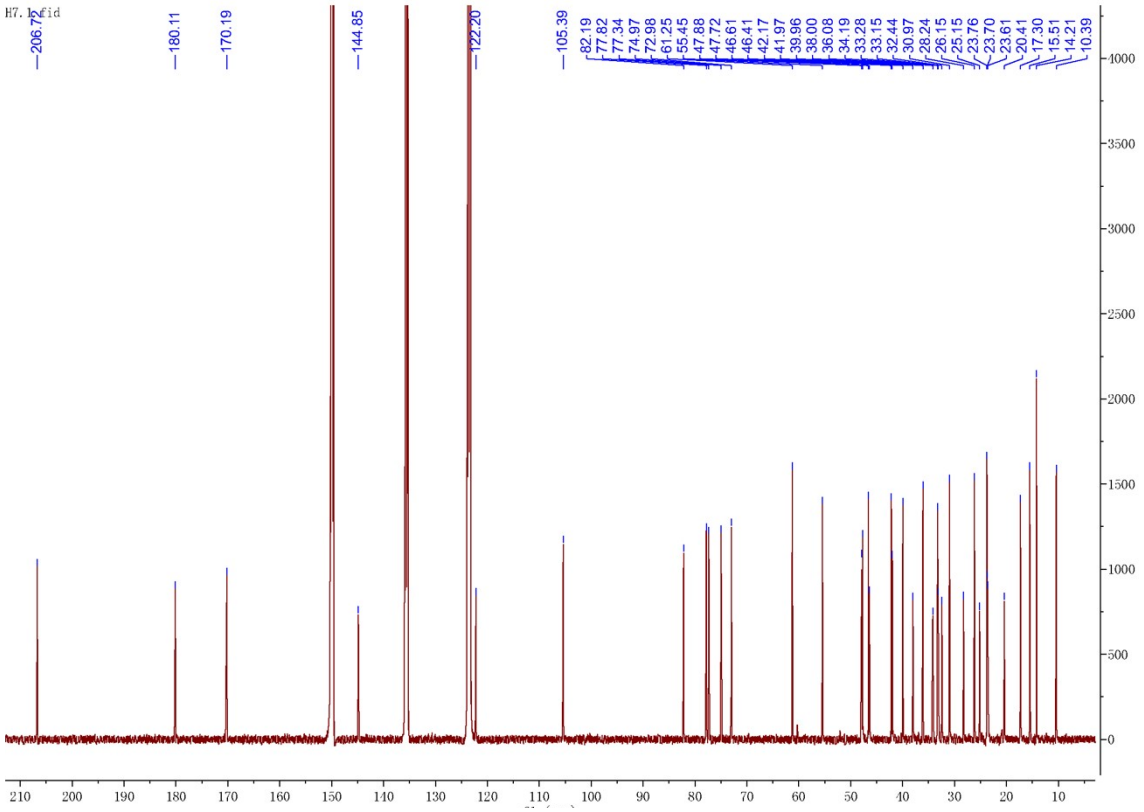


Figure S22. ^{13}C-NMR spectrum of compound **3** in C_5D_5N (150 MHz)

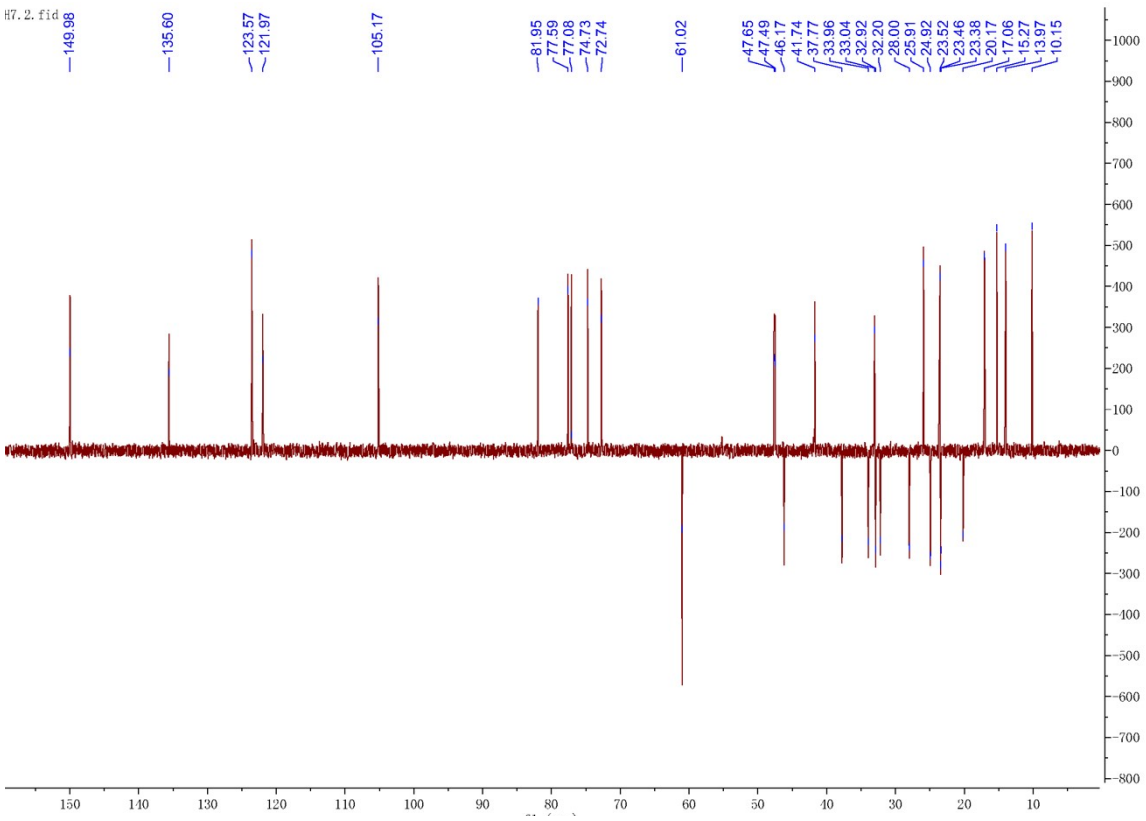


Figure S23. DEPT spectrum of compound **3** in C_5D_5N

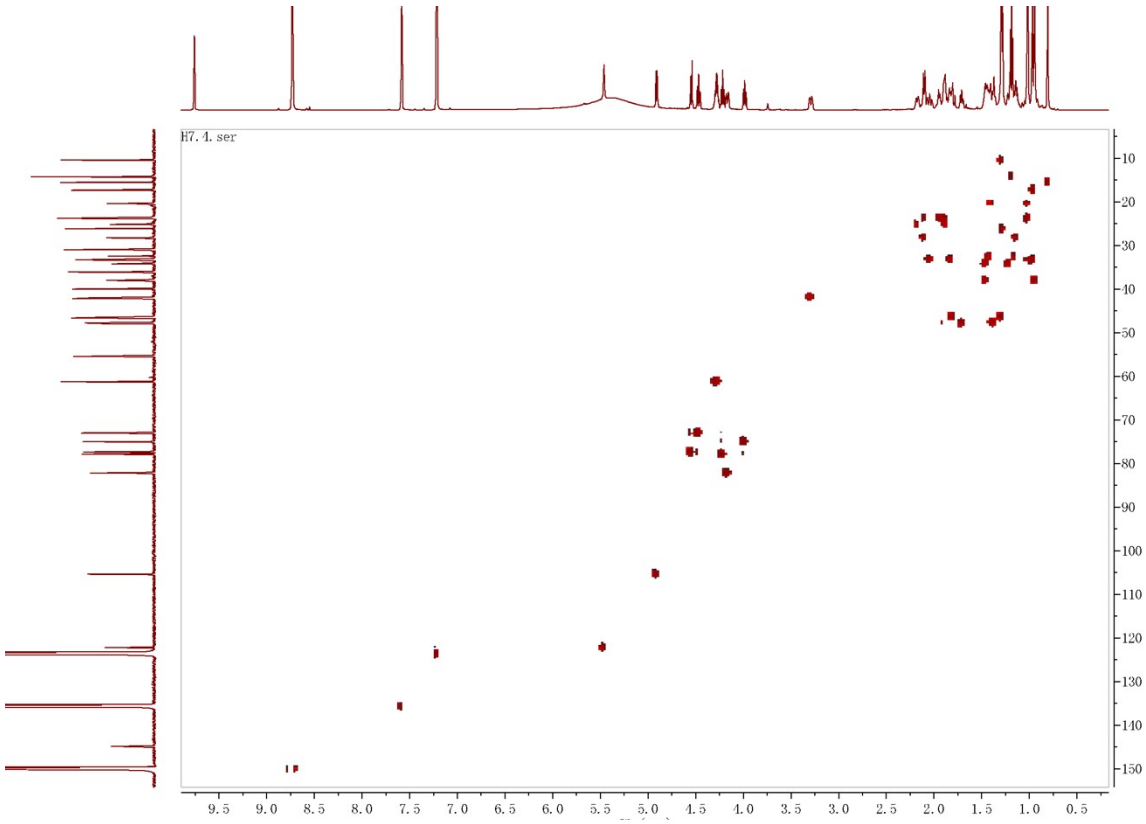


Figure S24. HSQC spectrum of compound **3** in C_5D_5N

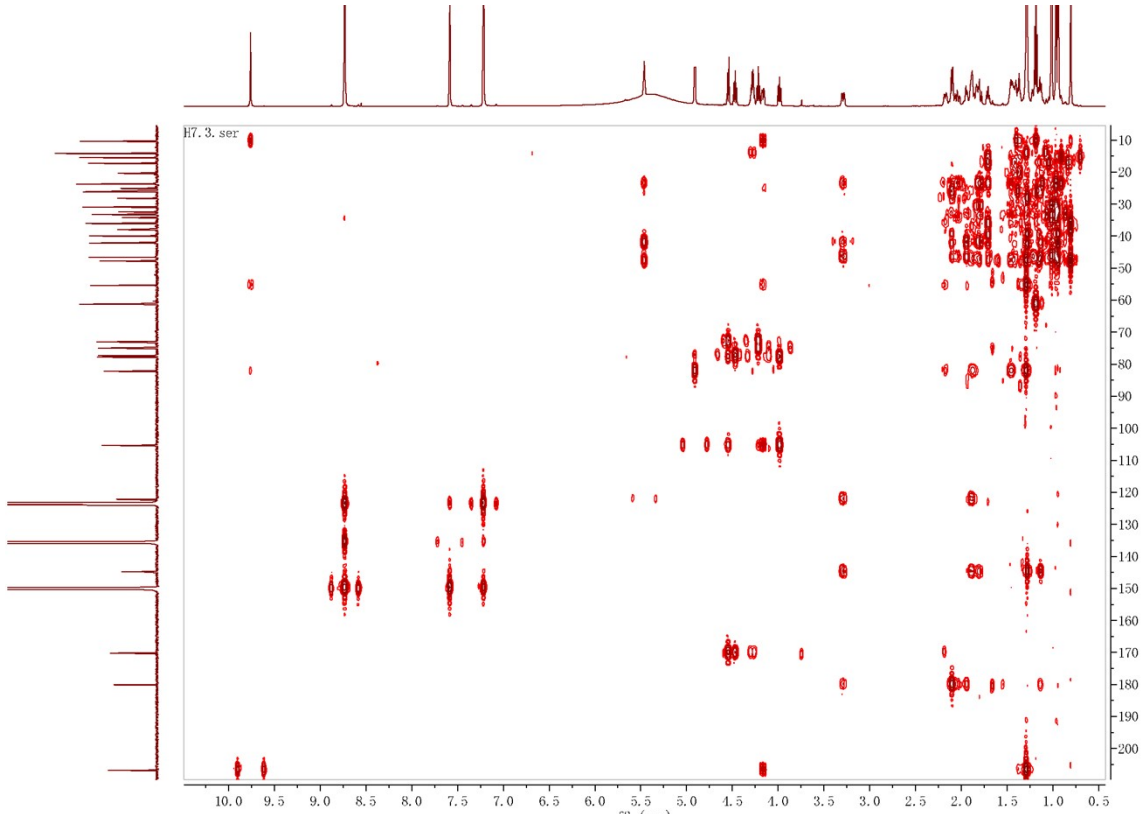


Figure S25. HMBC spectrum of compound **3** in C_5D_5N

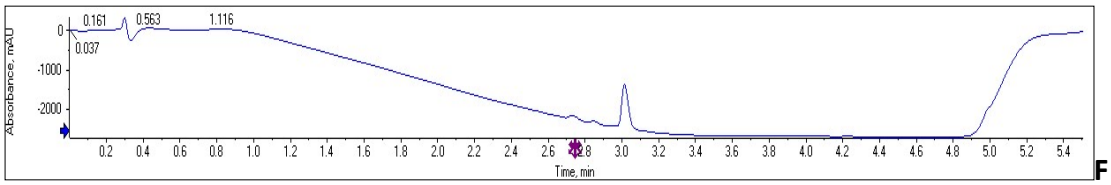


Figure S26. HPLC spectrum of compound **4**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

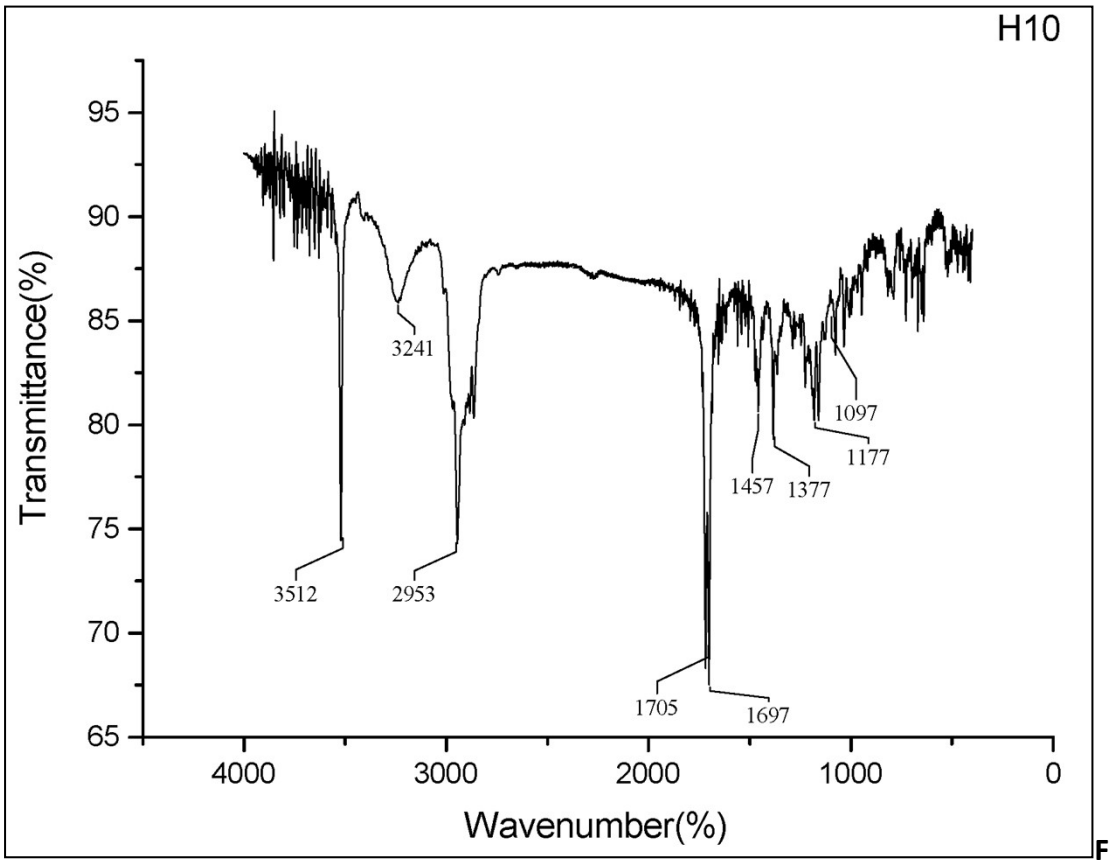


Figure S27. IR spectrum of compound **4**

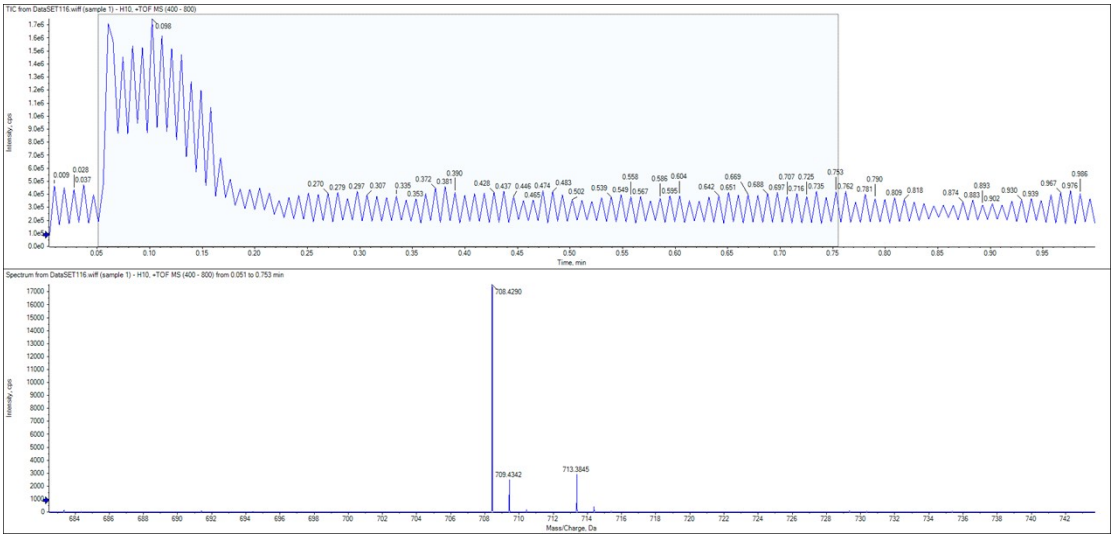


Figure S28. HR-ESI-MS spectrum ofcompound **4**

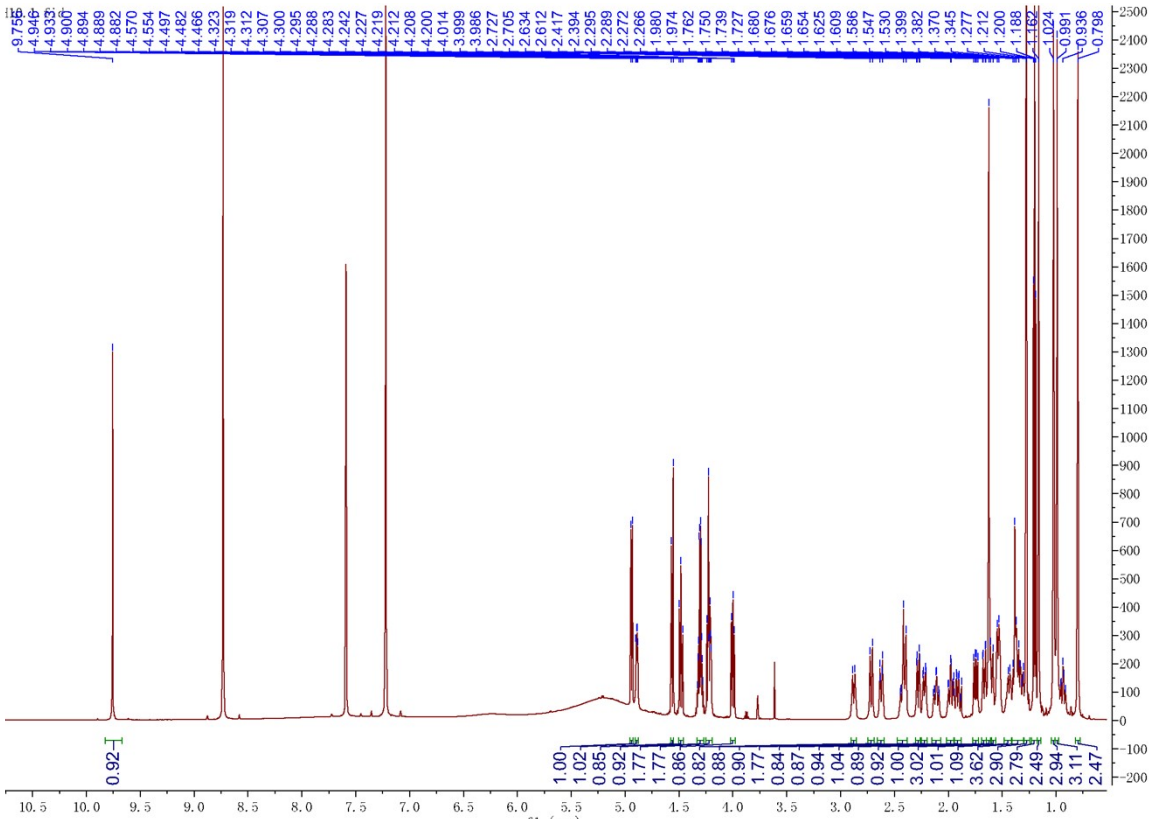


Figure S29. ^{1}H-NMR spectrum of compound **4** in C_5D_5N (600 MHz)

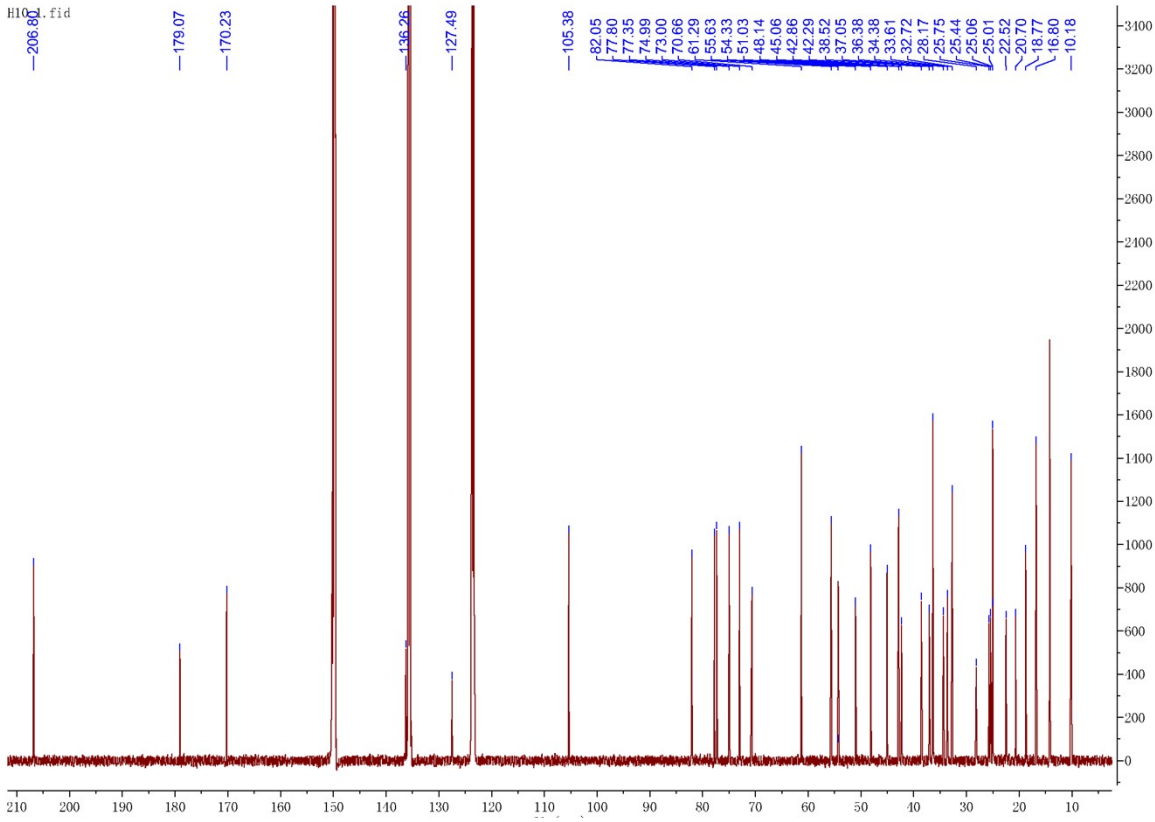


Figure S30. ^{13}C-NMR spectrum of compound **4** in C_5D_5N (150 MHz)

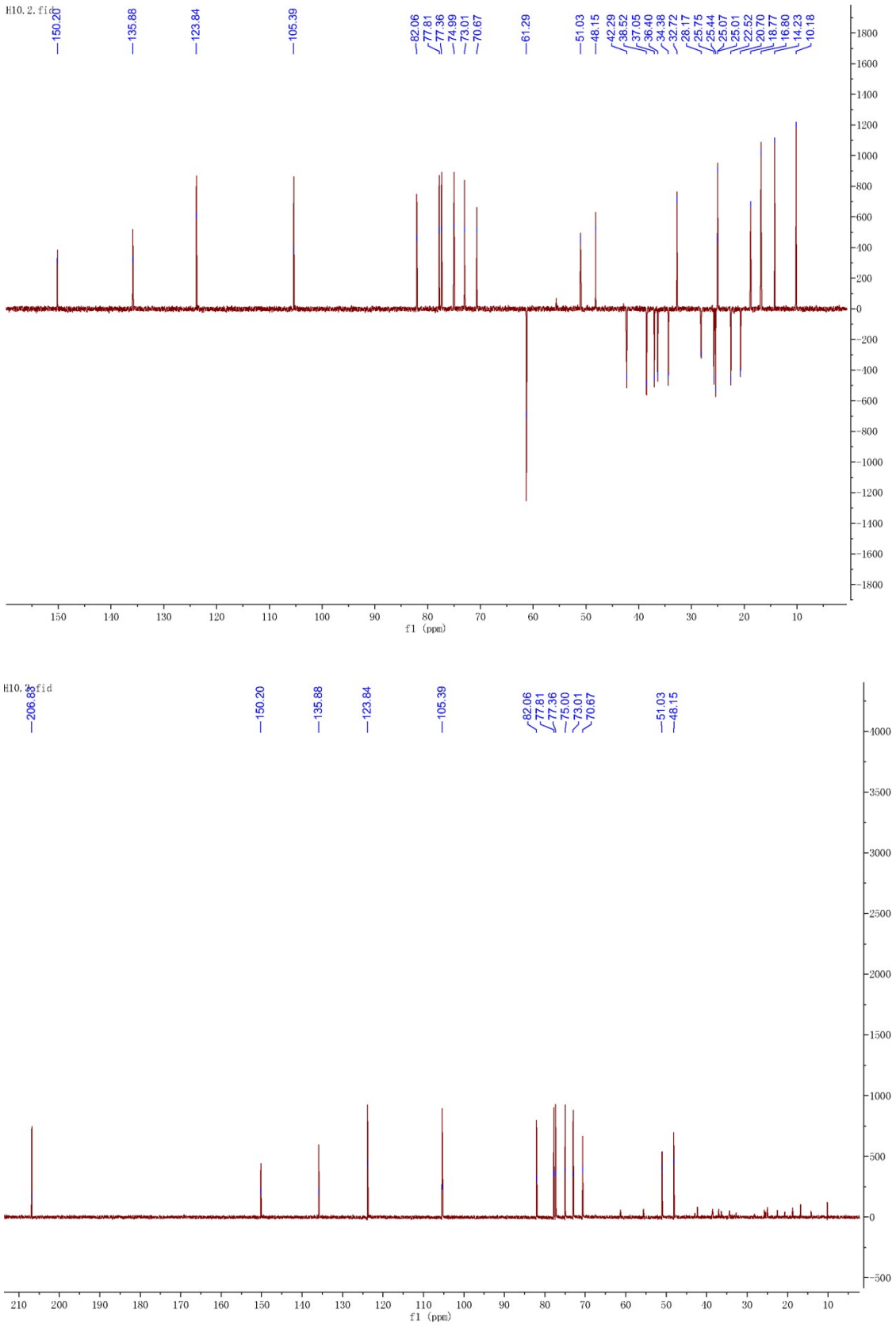


Figure S31. DEPT spectrum of compound **4** in C_5D_5N

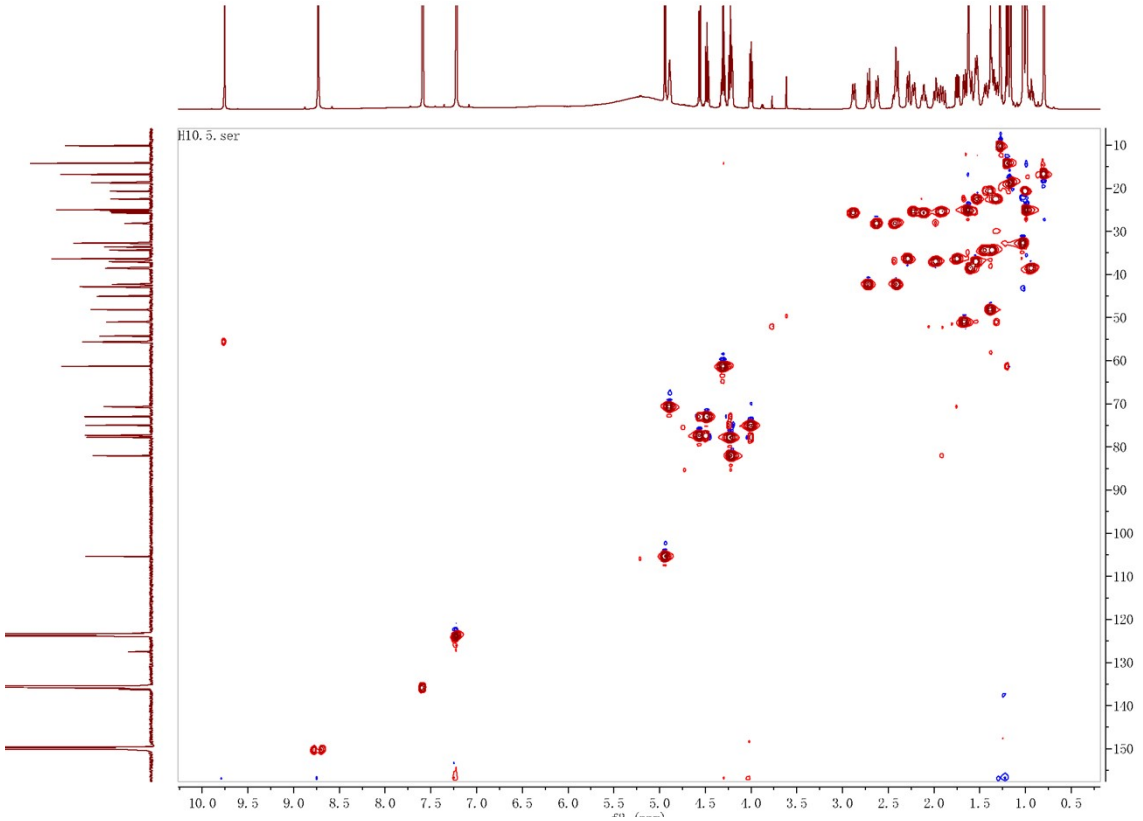


Figure S32. HSQC spectrum of compound **4** in C_5D_5N

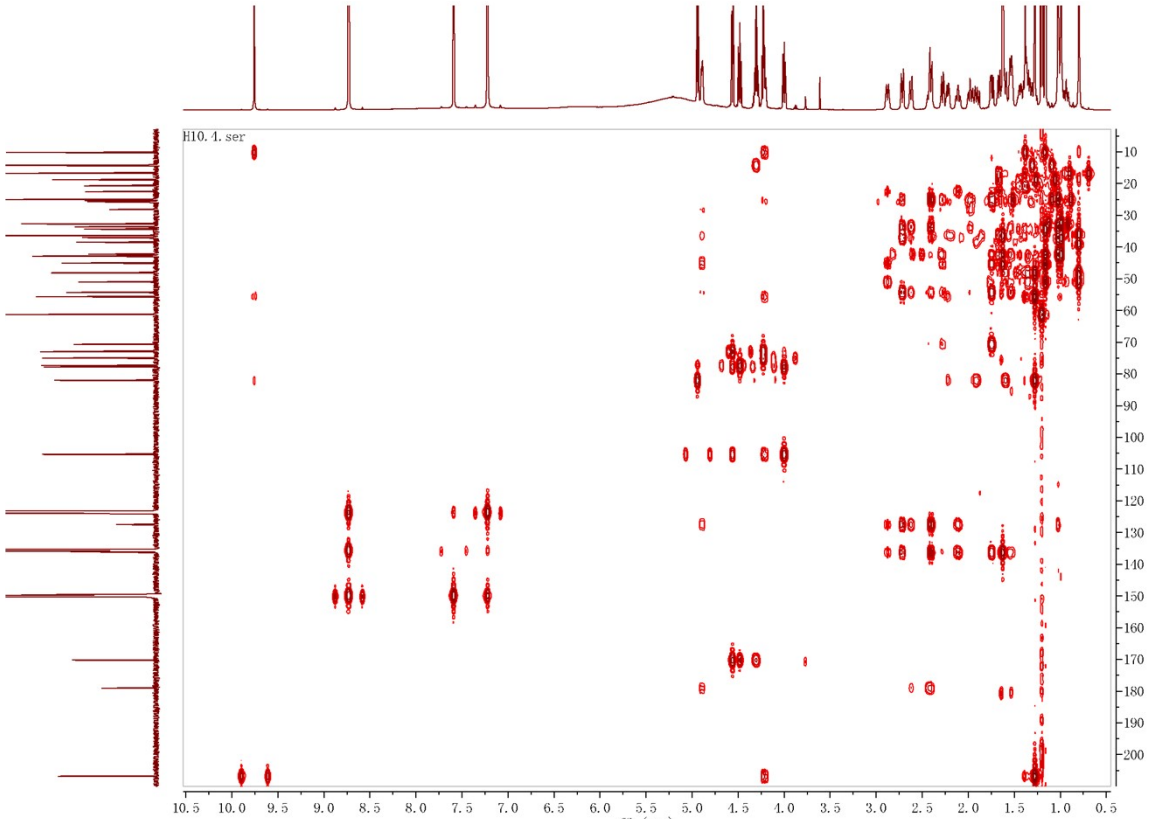


Figure S33. HMBC spectrum of compound **4** in C_5D_5N

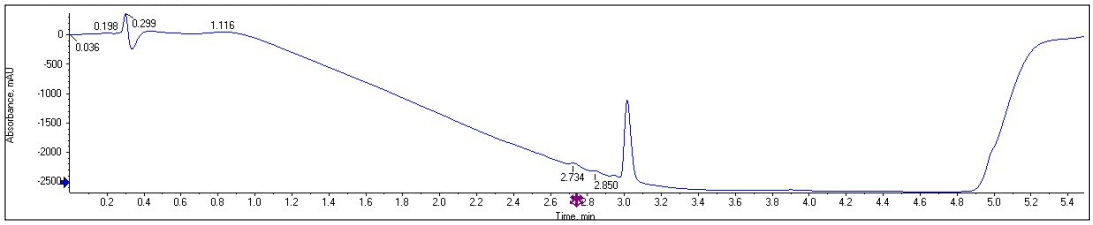


Figure S34. HPLC spectrum of compound **5**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

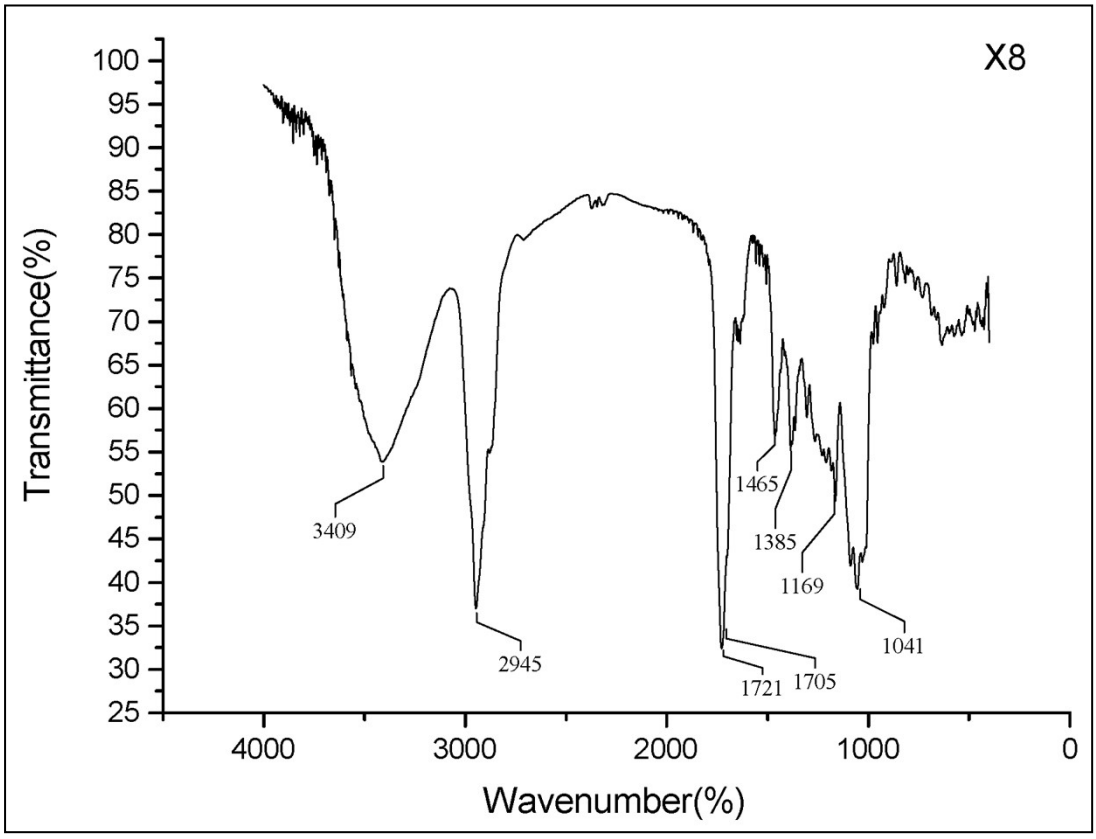


Figure S35. IR spectrum of compound **5**

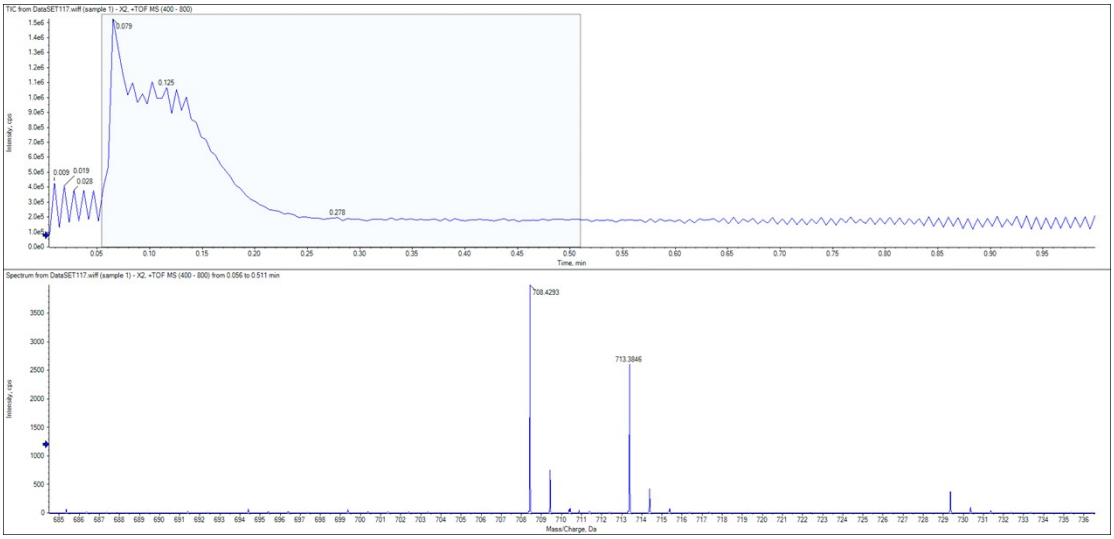


Figure S36. HR-ESI-MS spectrum ofcompound **5**

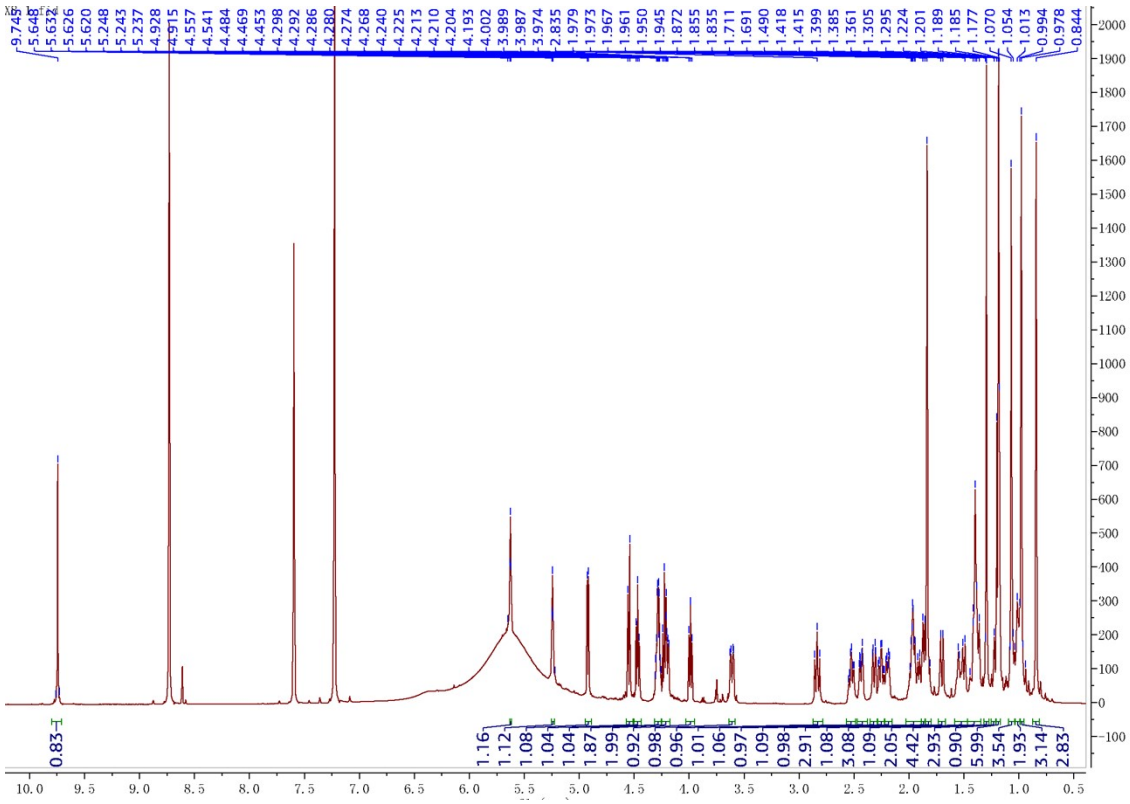


Figure S37. ^{1}H-NMR spectrum of compound **5** in C_5D_5N (600 MHz)

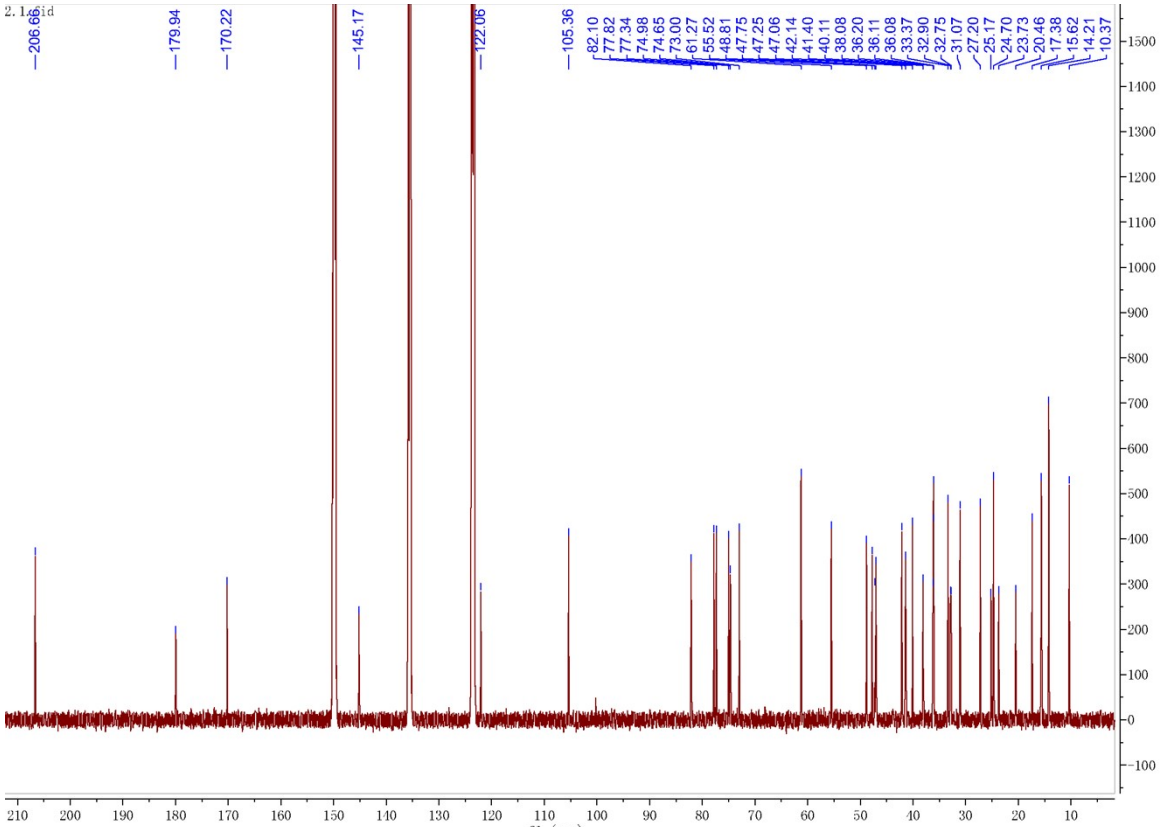


Figure S38. ^{13}C-NMR spectrum of compound **5** in C_5D_5N (150 MHz)

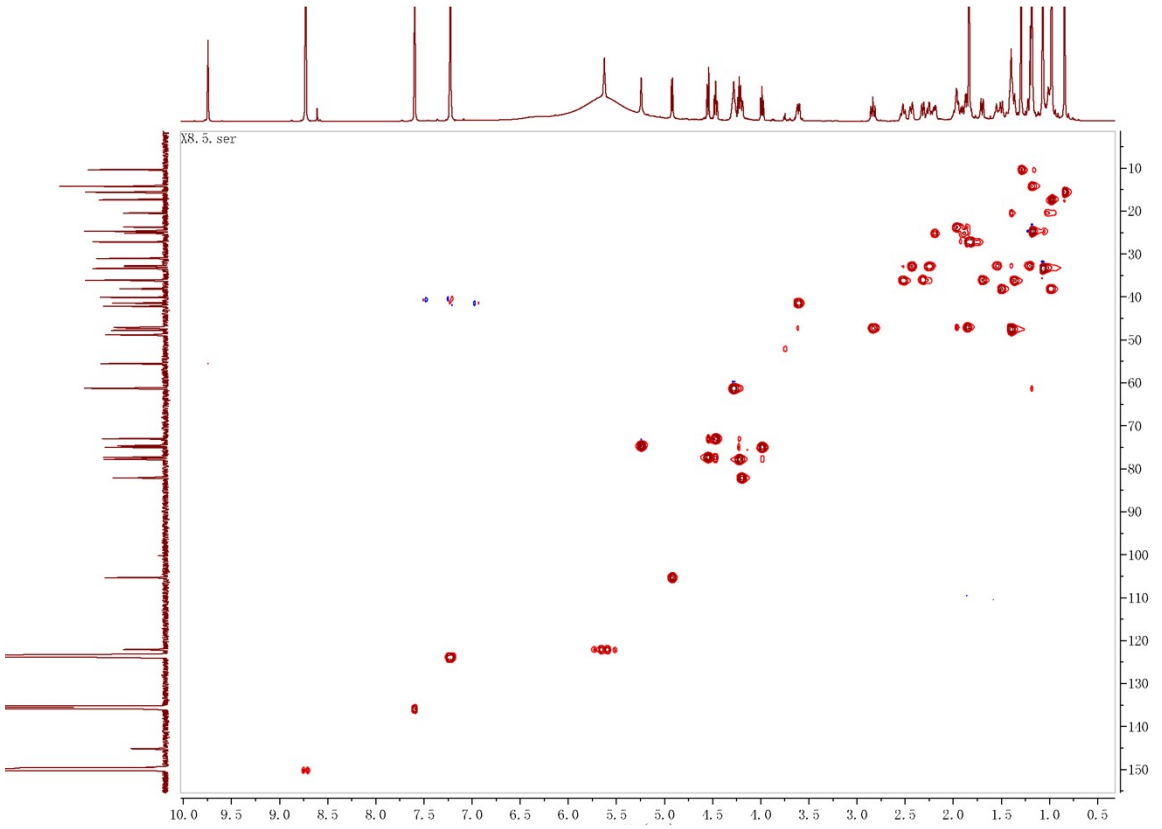


Figure S39. HSQC spectrum of compound **5** in C_5D_5N

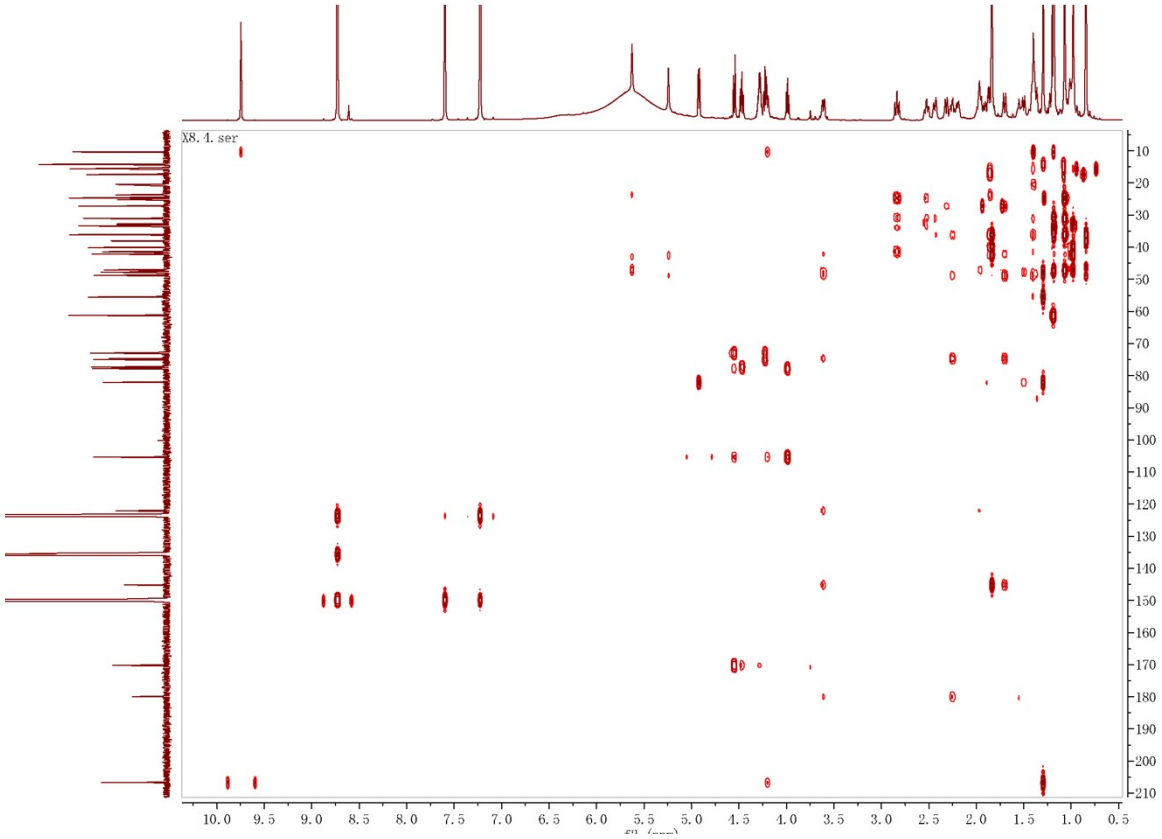


Figure S40. HMBC spectrum of compound **5** in C_5D_5N

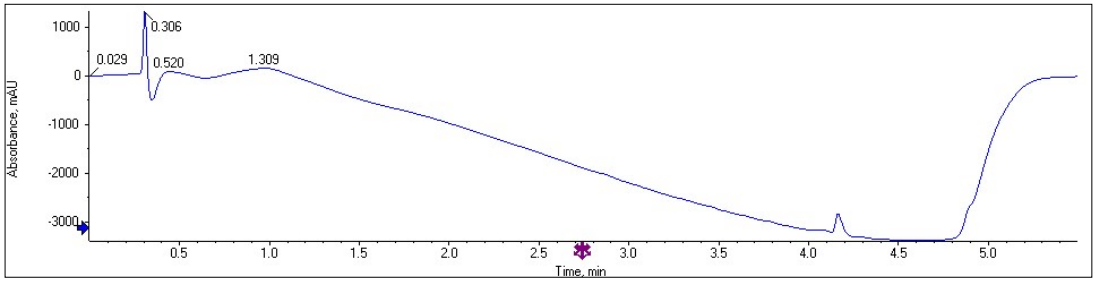
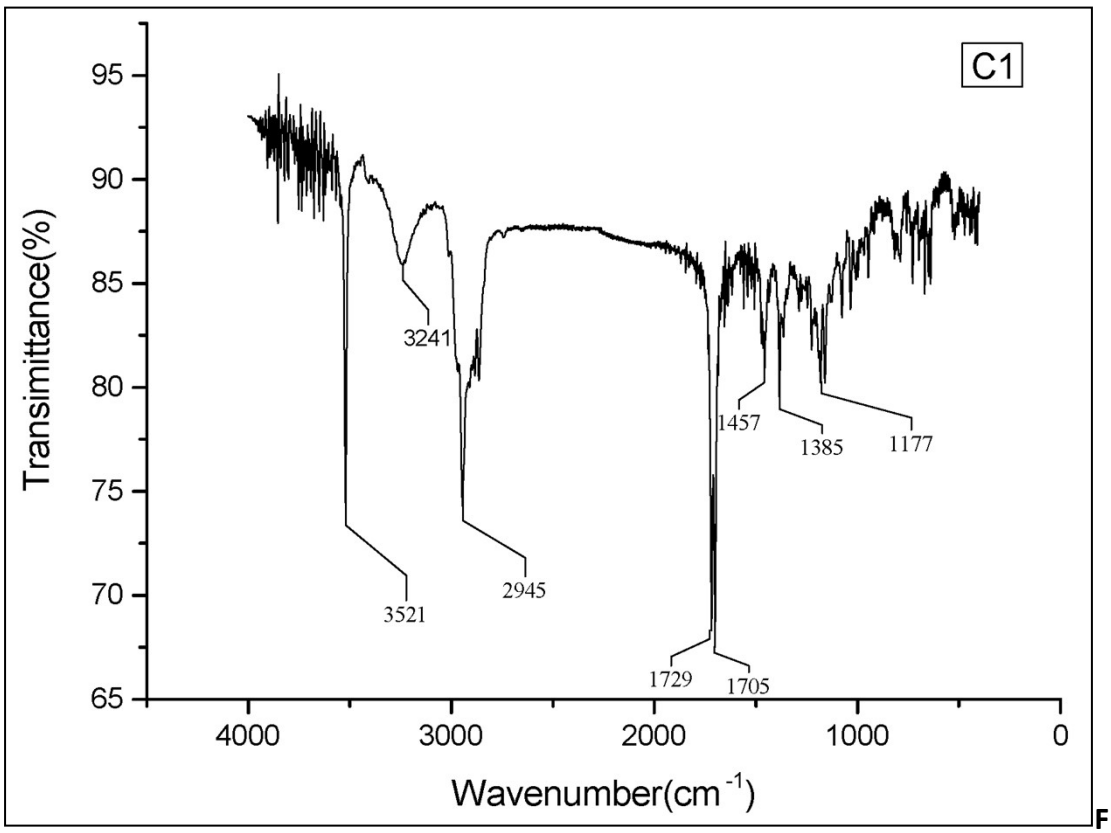


Figure S41. HPLC spectrum of compound **6**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.



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igure S42. IR spectrum of compound **6**

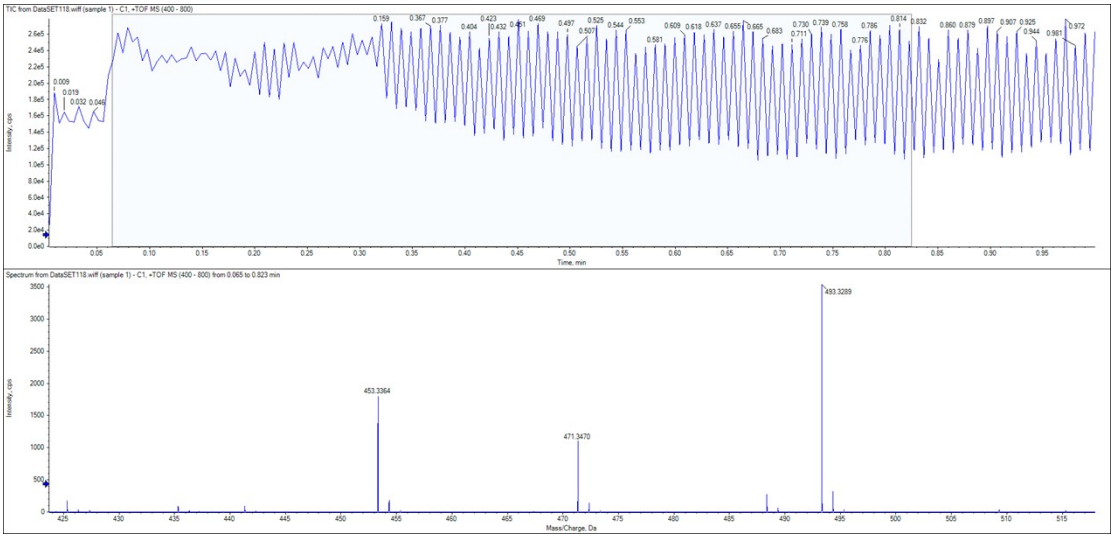

Figure S43. HR-ESI-MS spectrum ofcompound **6**

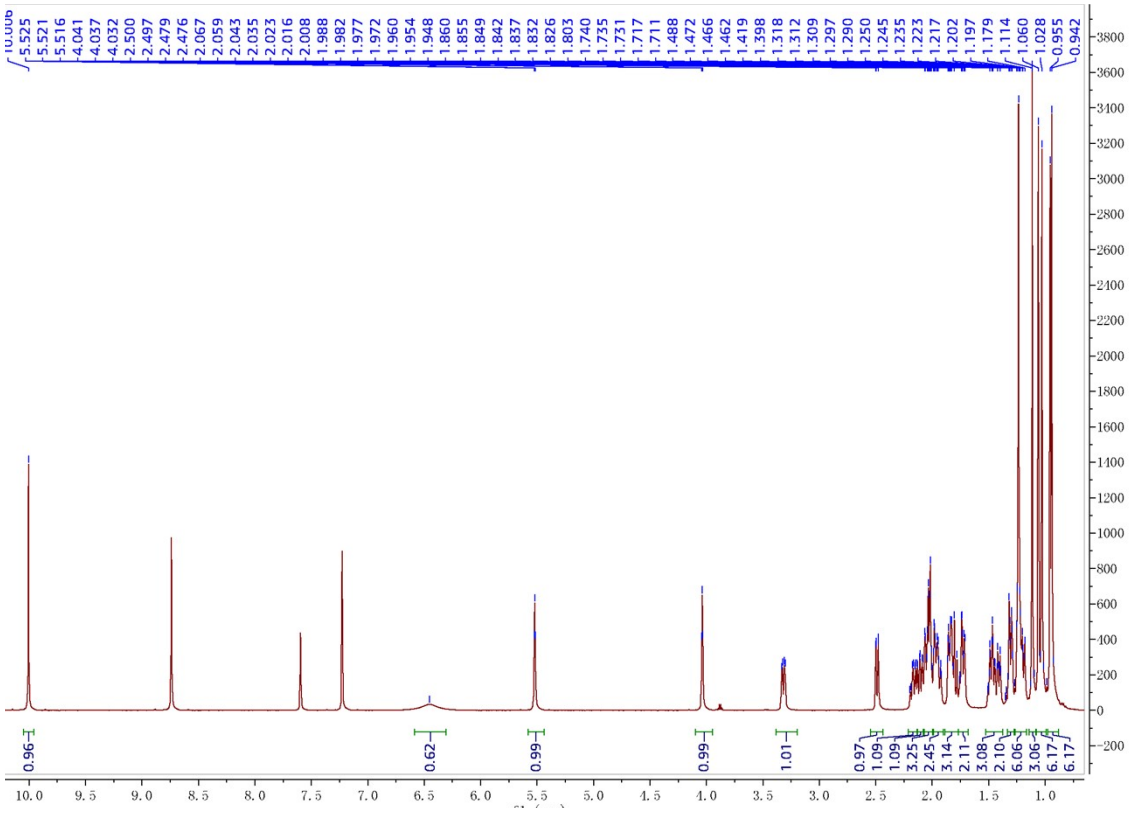

Figure S44. ^{1}H-NMR spectrum of compound **6** in C_5D_5N (600 MHz)

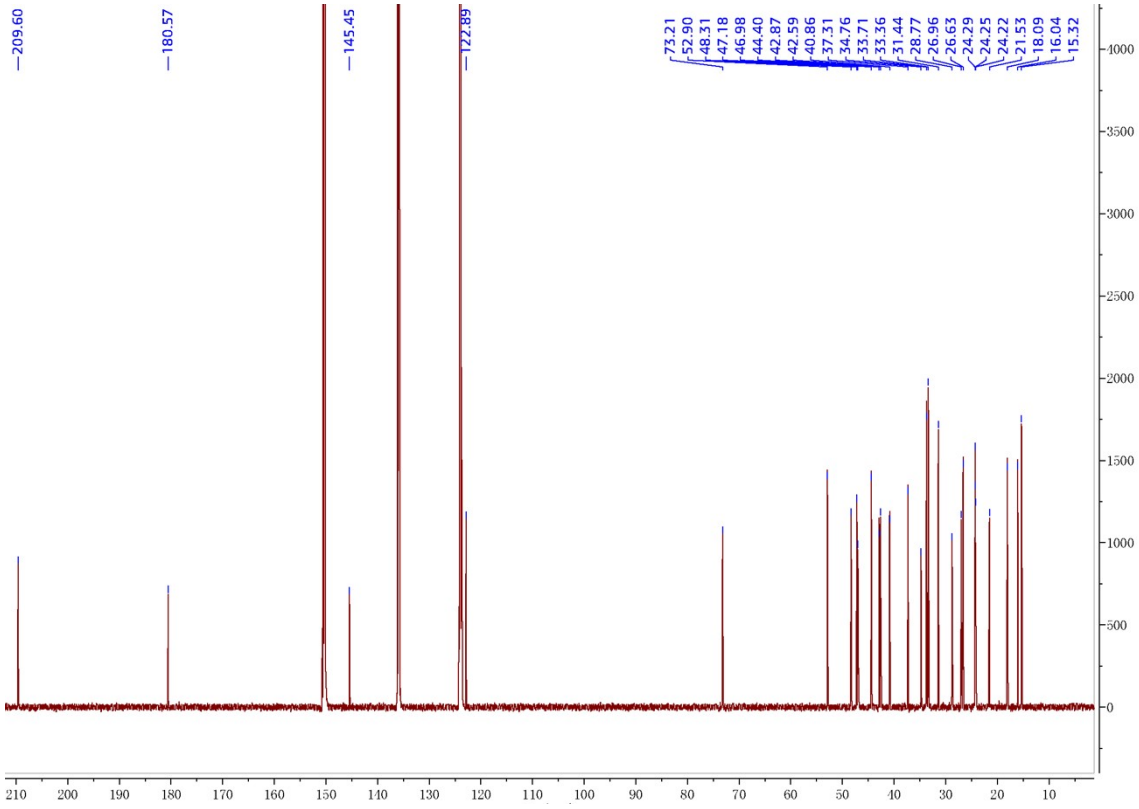

Figure S45. ^{13}C-NMR spectrum of compound **6** in C_5D_5N (150 MHz)

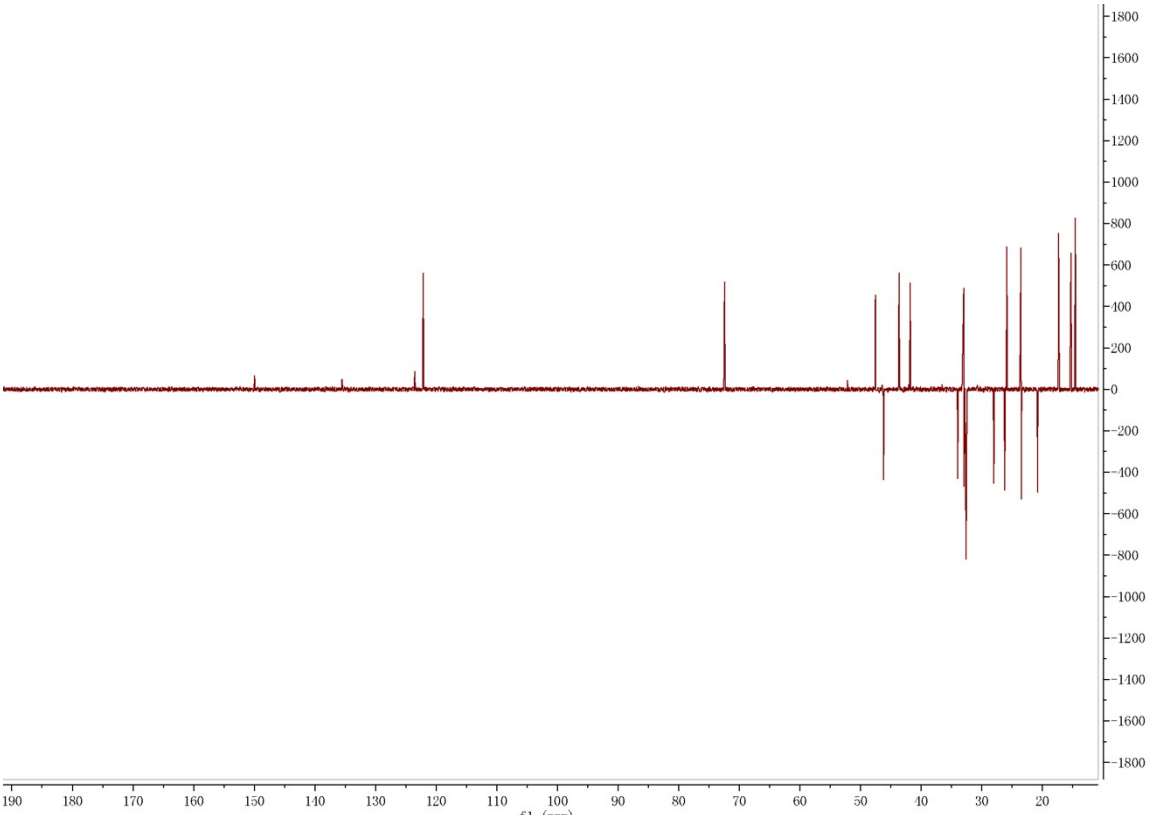

Figure S46. DEPT spectrum of compound **6** in C_5D_5N

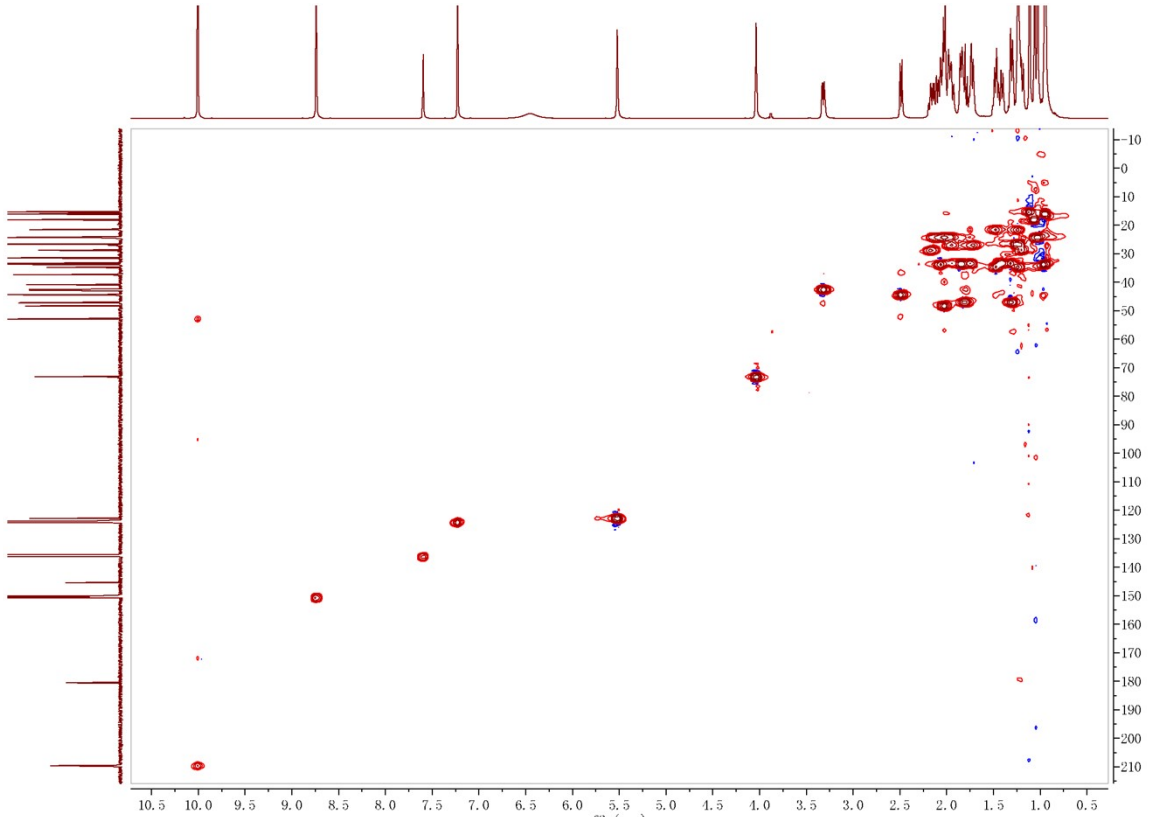

Figure S47. HSQC spectrum of compound **6** in C_5D_5N

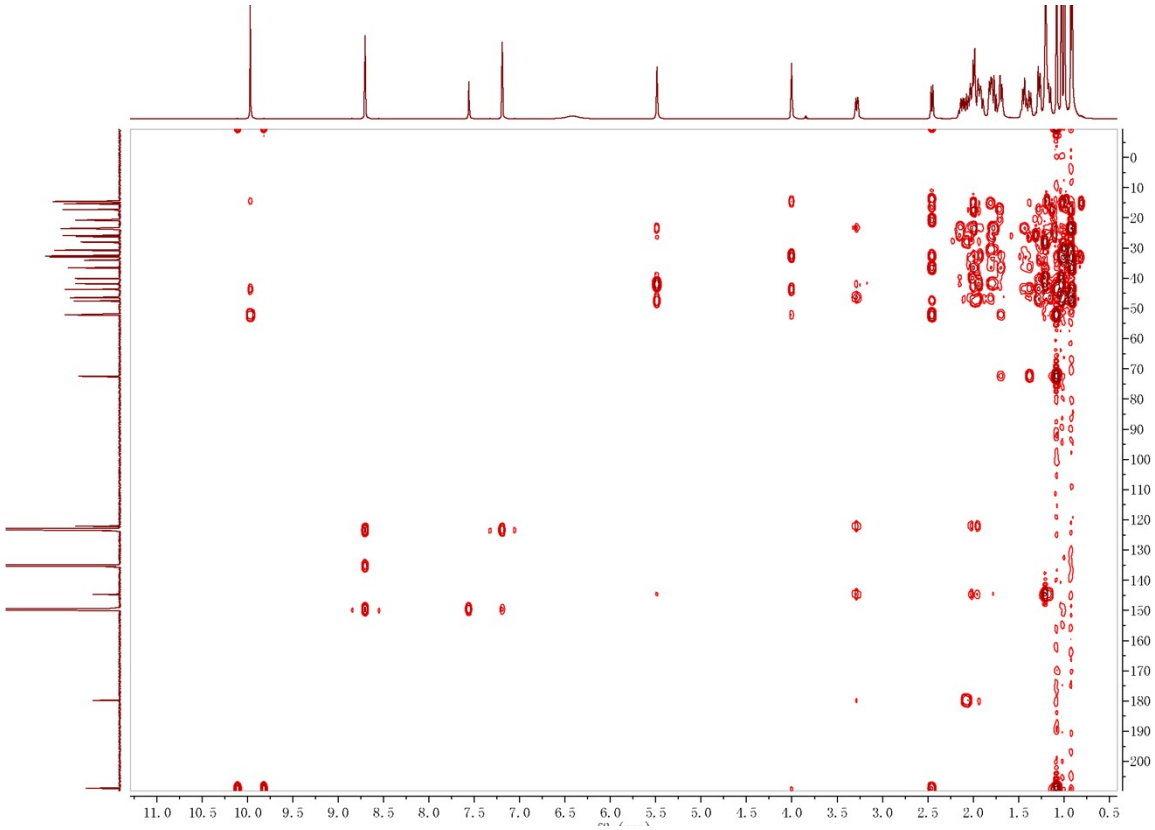

Figure S48. HMBC spectrum of compound**6** in C_5D_5N

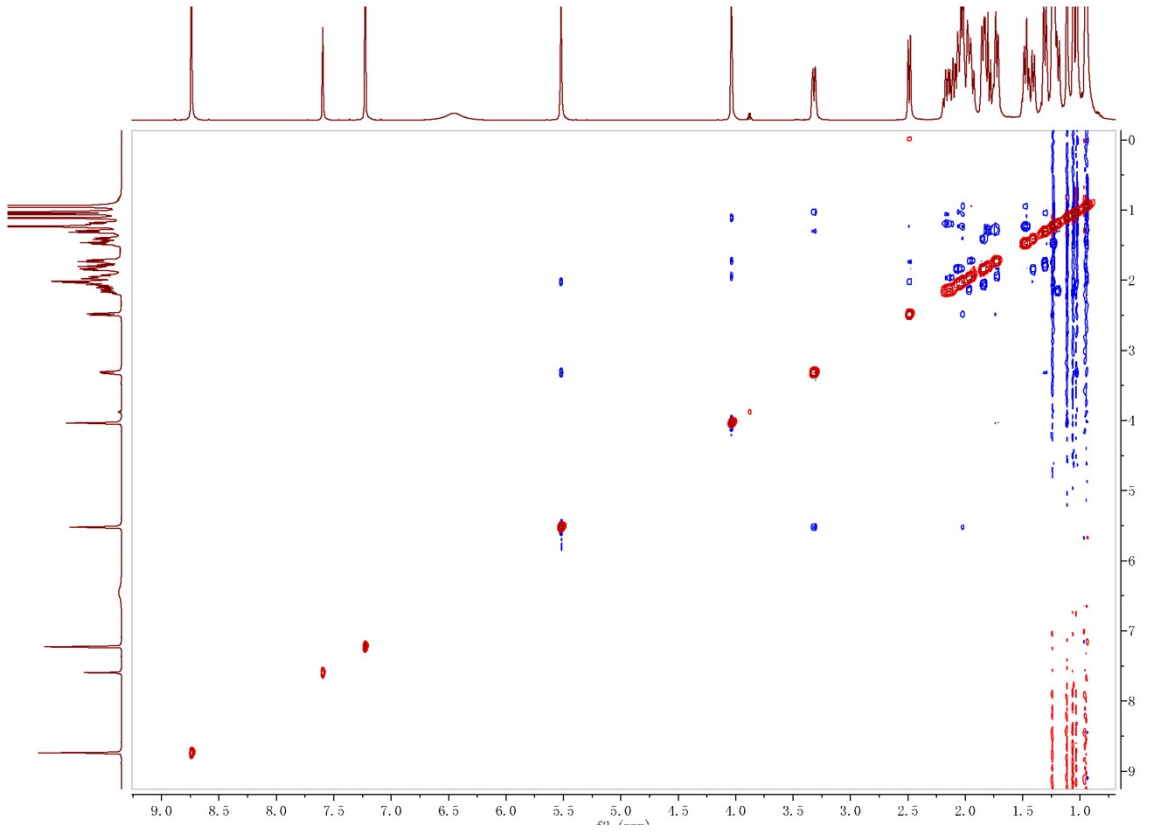

Figure S49. NOESY spectrum of compound **6** in C_5D_5N

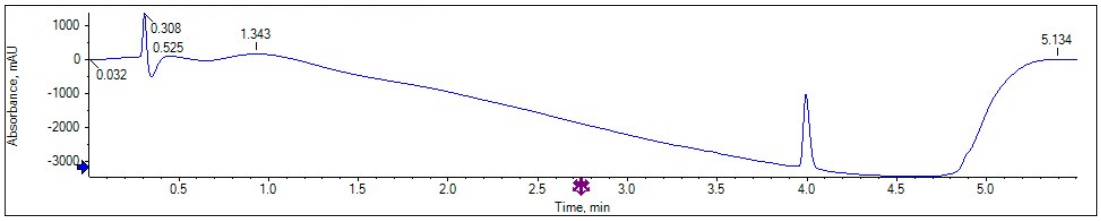

Figure S53. HPLC spectrum of compound **7**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

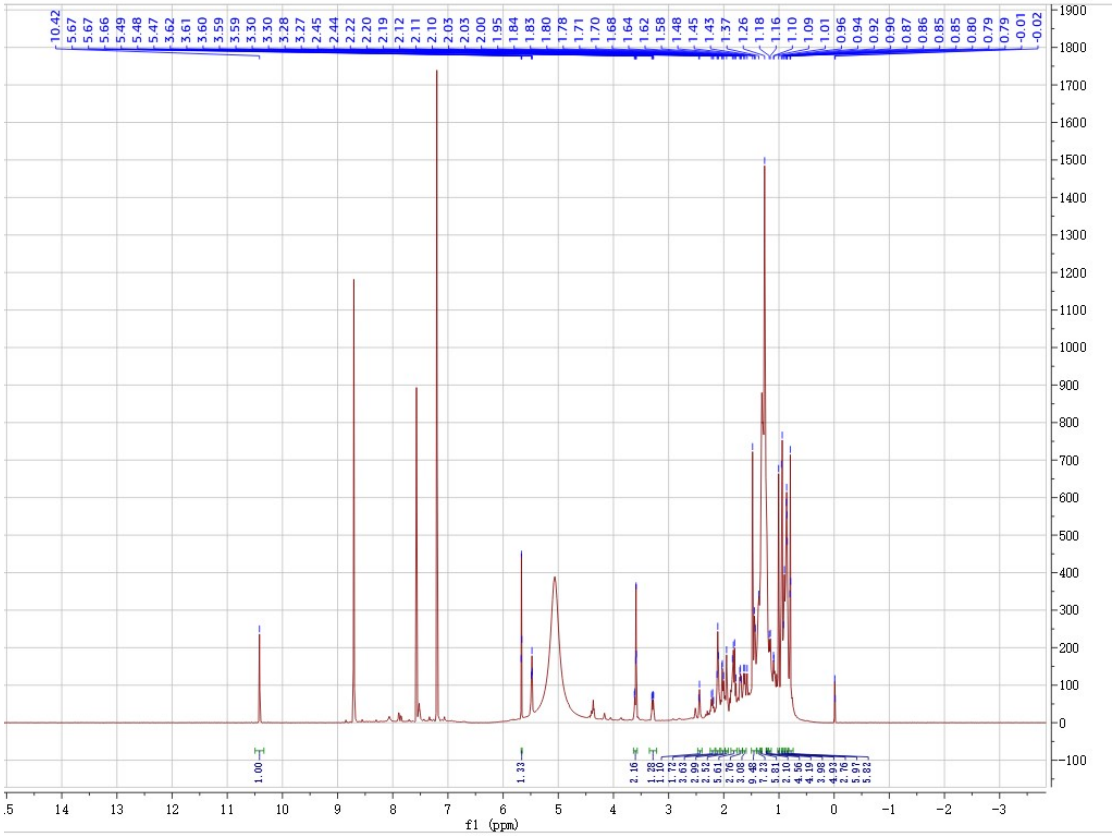

Figure S54. 1H-NMR spectrum of compound **7** in C_5D_5N (600 MHz)

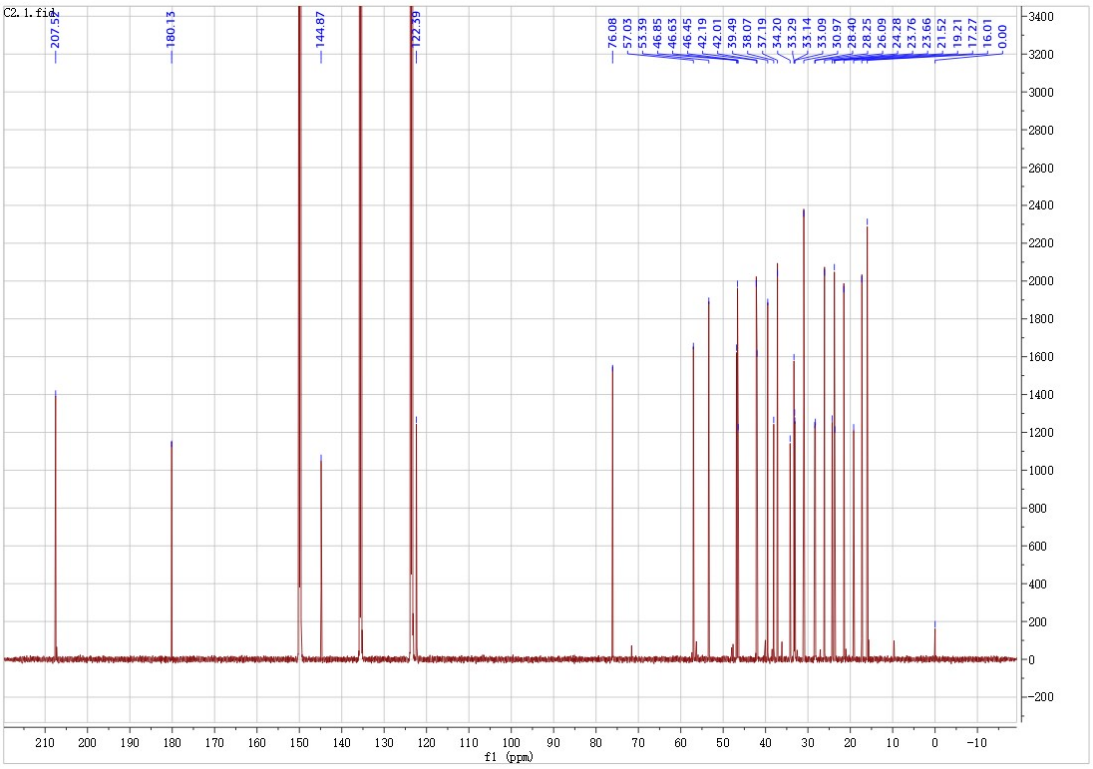

Figure S55. 13C-NMR spectrum of compound **7** in C_5D_5N (150 MHz)

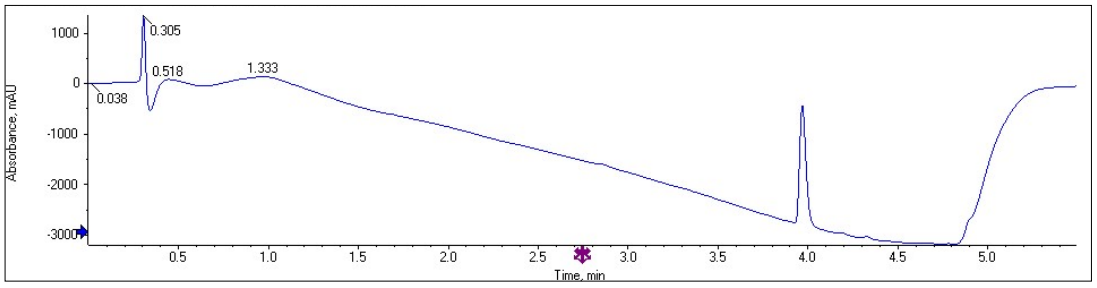

Figure S50. HPLC spectrum of compound **8**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

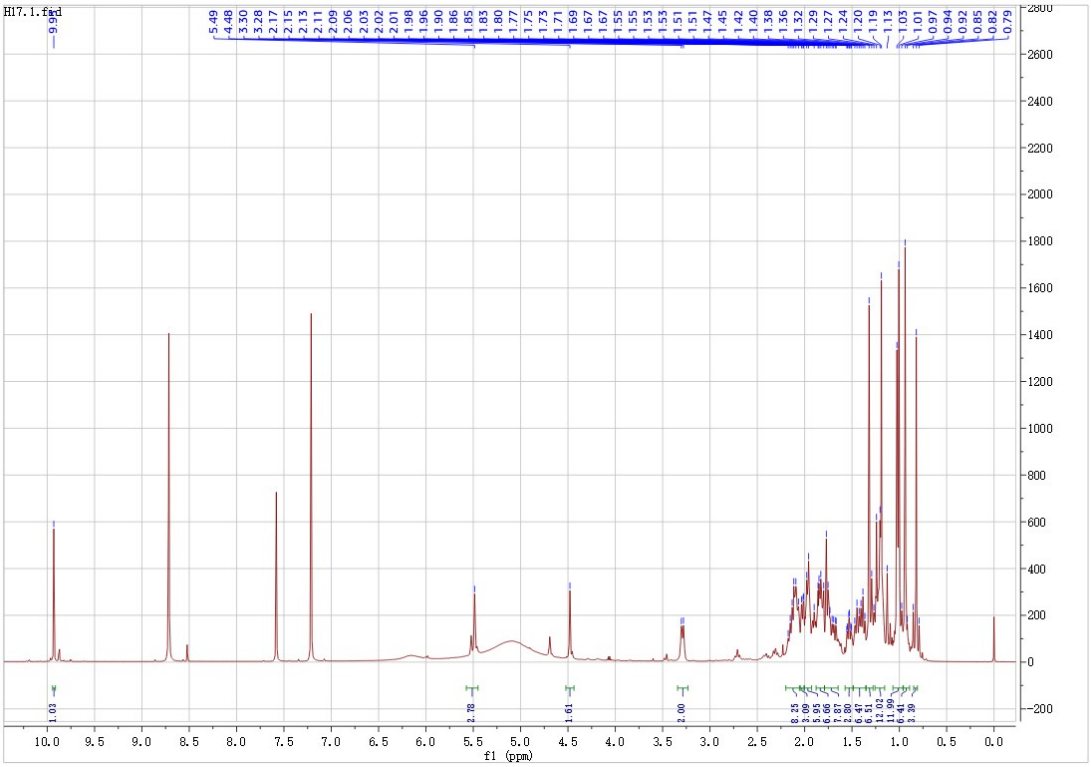

Figure S51. 1H-NMR spectrum of compound **8** in C_5D_5N (600 MHz)

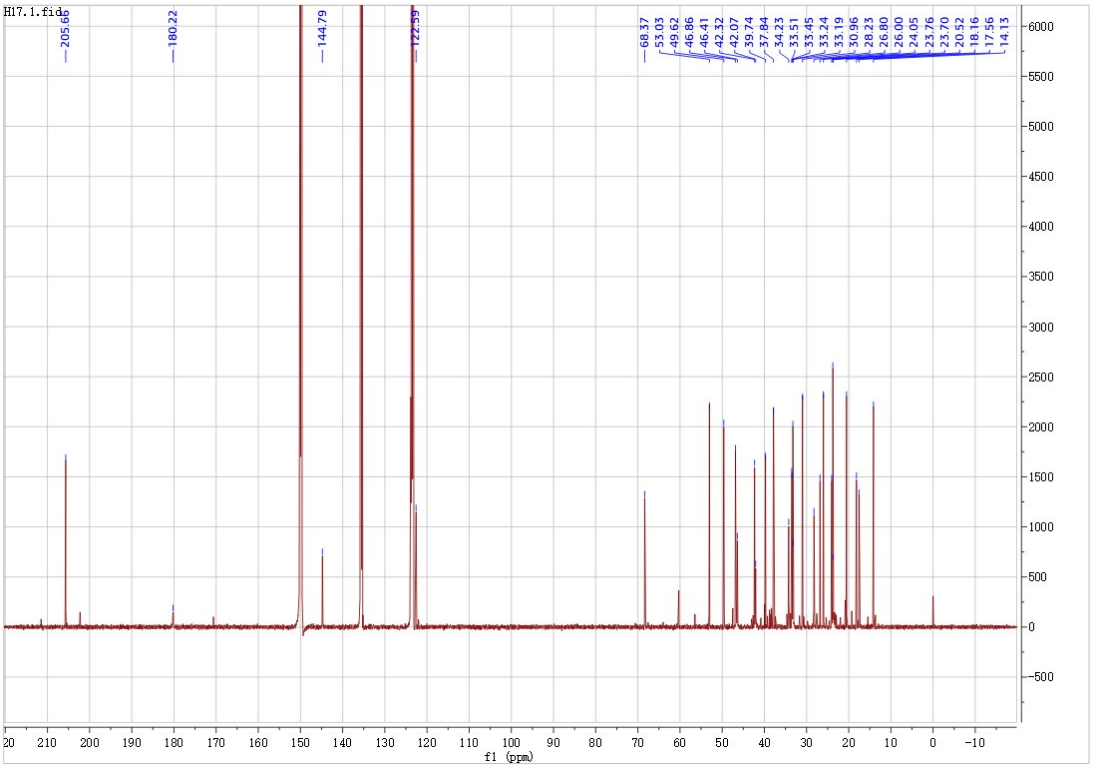

Figure S52. 13C-NMR spectrum of compound **8** in C_5D_5N (150 MHz)

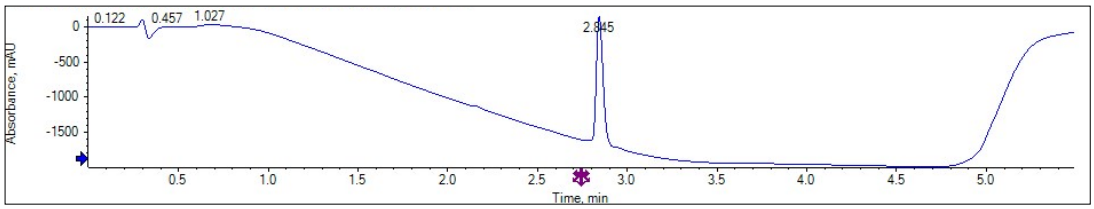

Figure S56. HPLC spectrum of compound **9**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

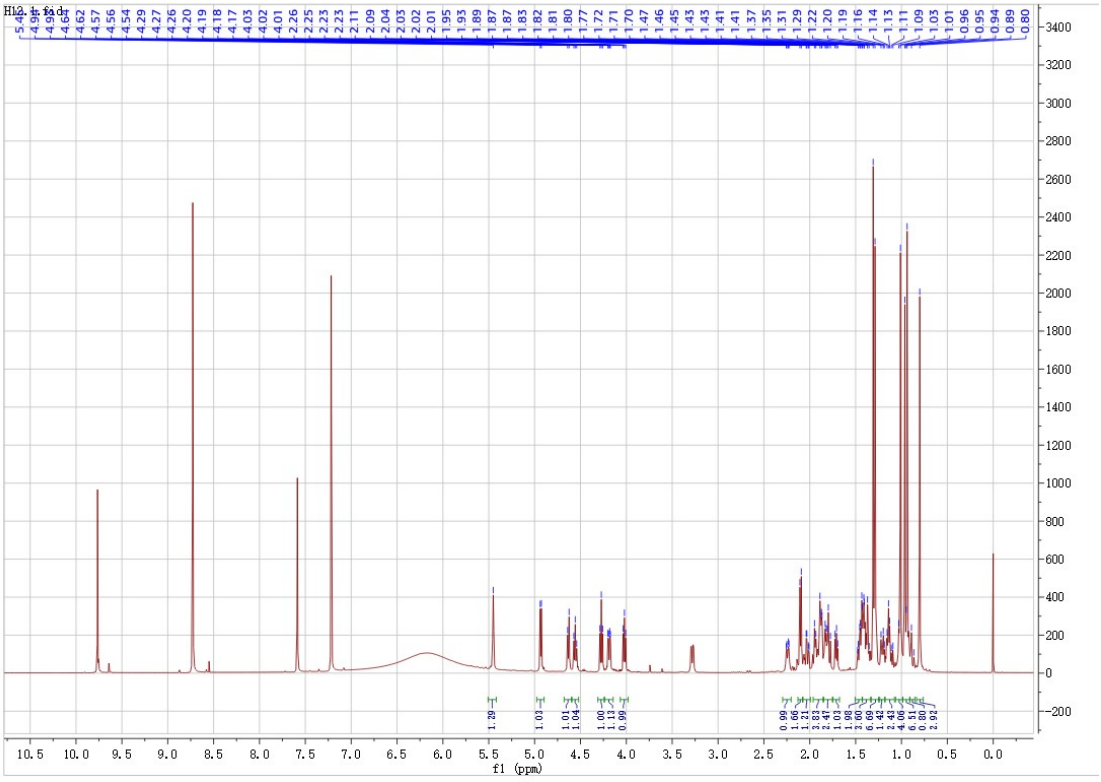

Figure S57. 1H-NMR spectrum of compound **9** in C_5D_5N (600 MHz)

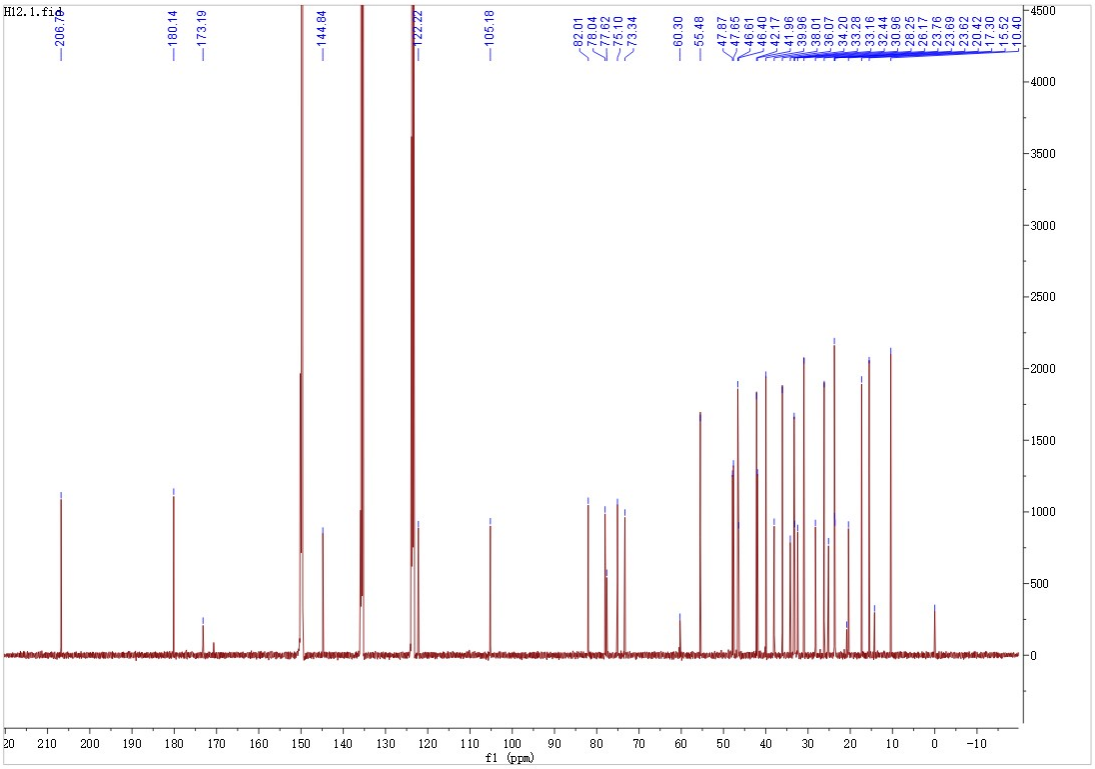

Figure S58. 13C-NMR spectrum of compound **9** in C_5D_5N (150 MHz)

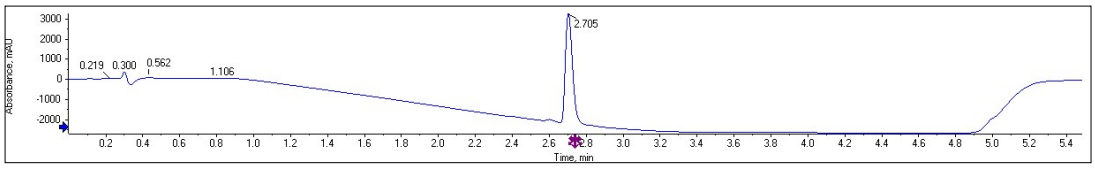

Figure S59. HPLC spectrum of compound **10**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

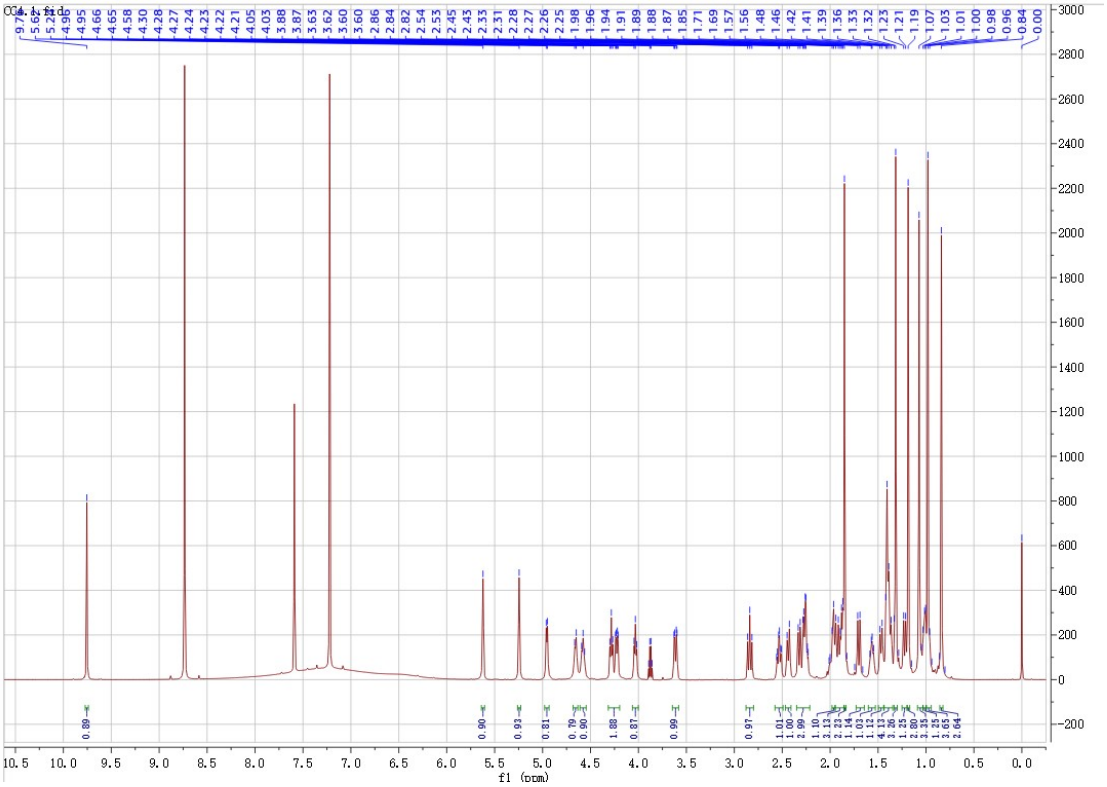

Figure S60. 1H-NMR spectrum of compound **10** in C_5D_5N (600 MHz)

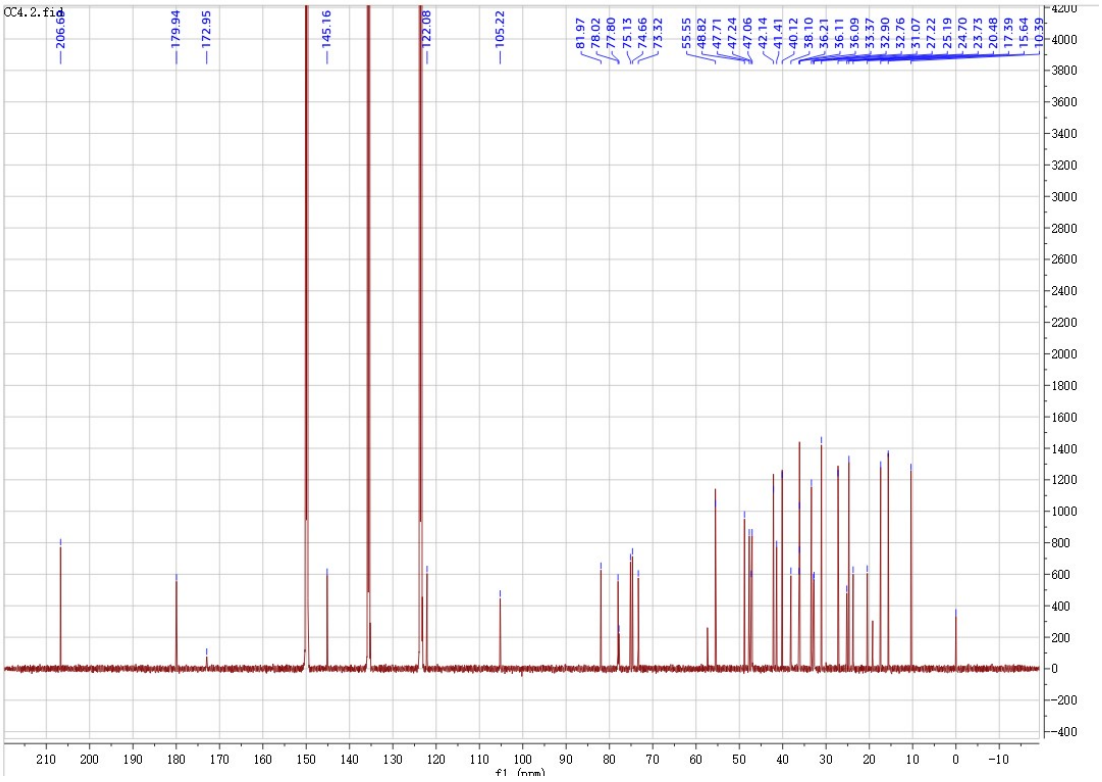

Figure S61. 13C-NMR spectrum of compound **10** in C_5D_5N (150 MHz)

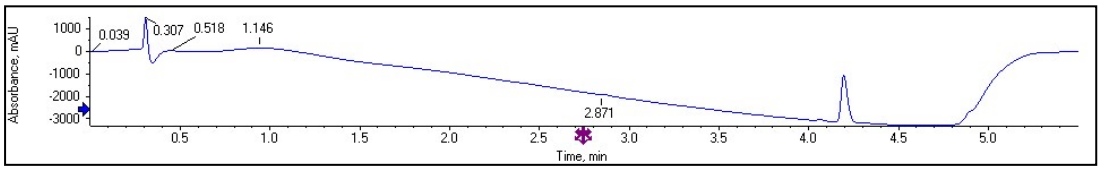

Figure S62. HPLC spectrum of compound **11**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm.

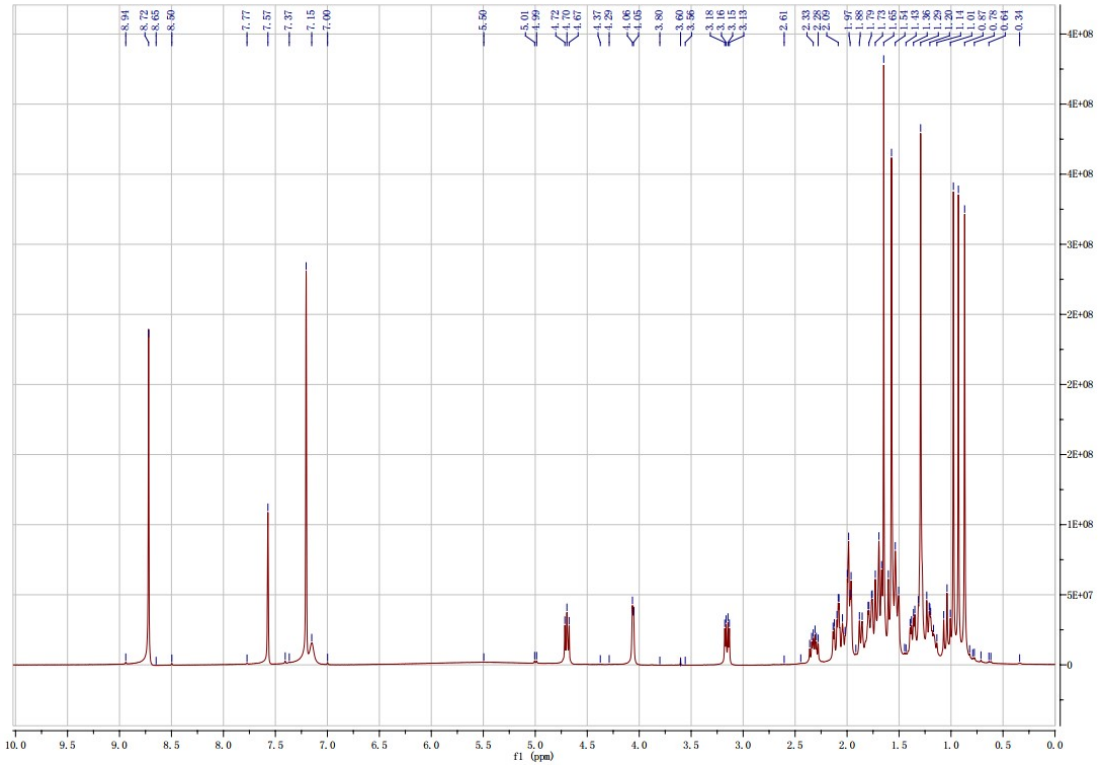

Figure S63. 1H-NMR spectrum of compound **11** in C_5D_5N (600 MHz)

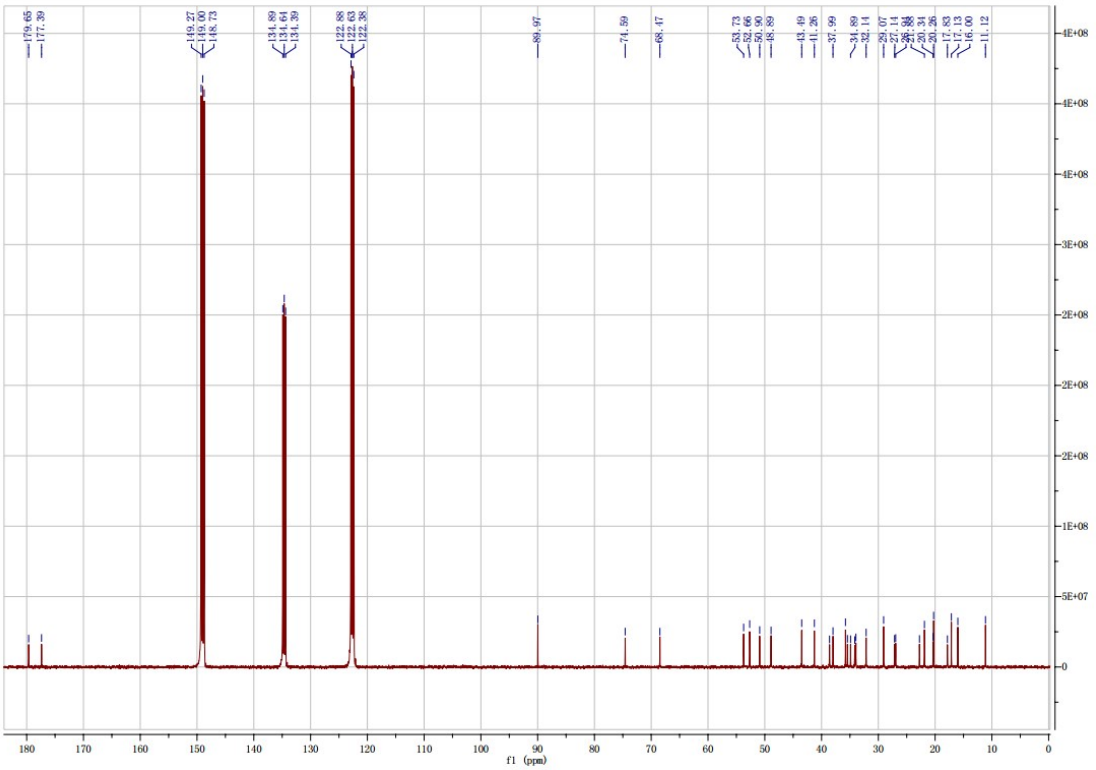

Figure S64. 13C-NMR spectrum of compound **11** in C_5D_5N (150 MHz)

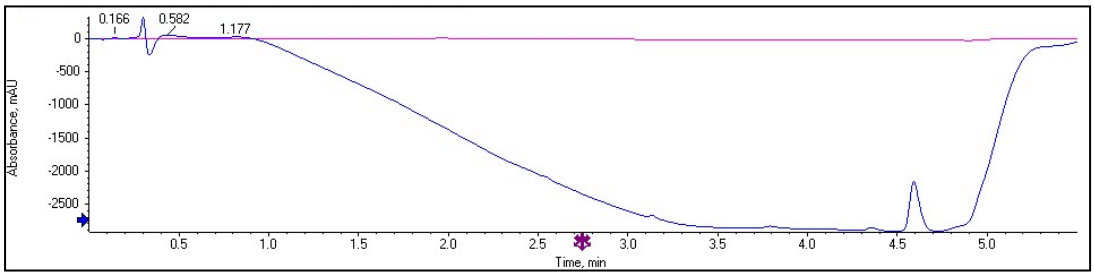

Figure S65. HPLC spectrum of compound **12**

The sample was separated on InertSustain® C18 column with water (A)- acetonitrile (B) as the mobile phase for gradient elution. The analysis was performed at a flowrate of 0.8 mL/min, column temperature of 45℃and the detection wavelength was set at 210 nm and 254nm.

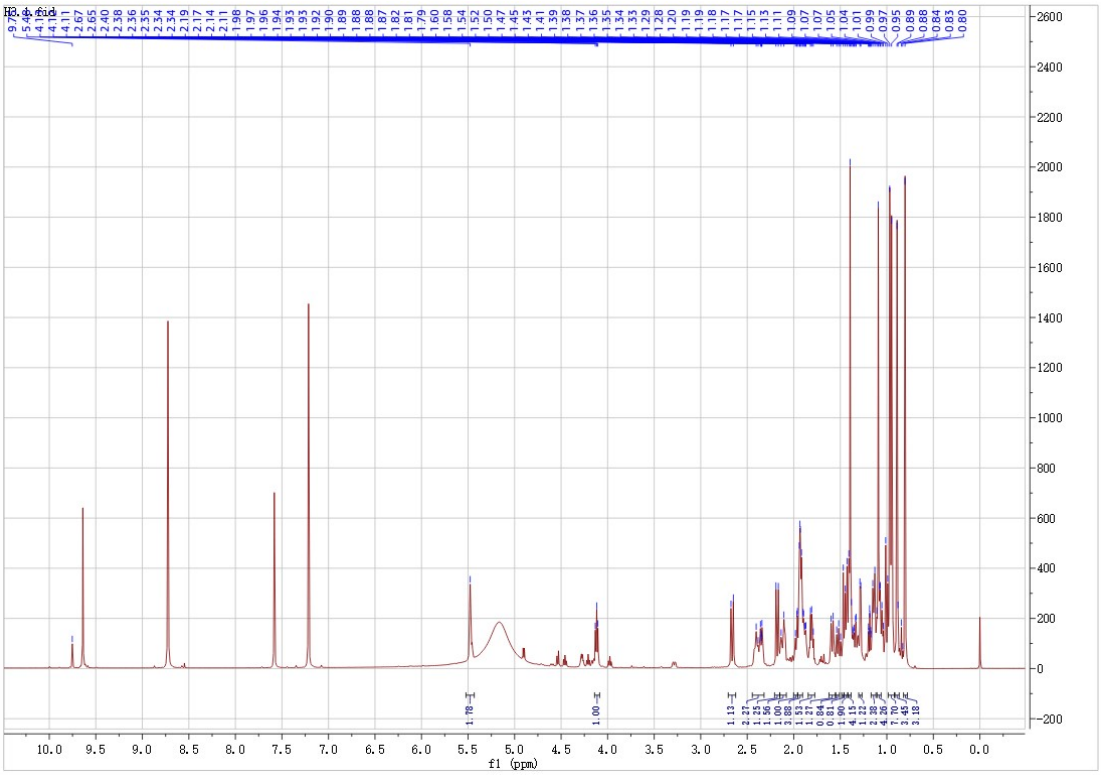

Figure S66. 1H-NMR spectrum of compound **12** in C_5D_5N (600 MHz)

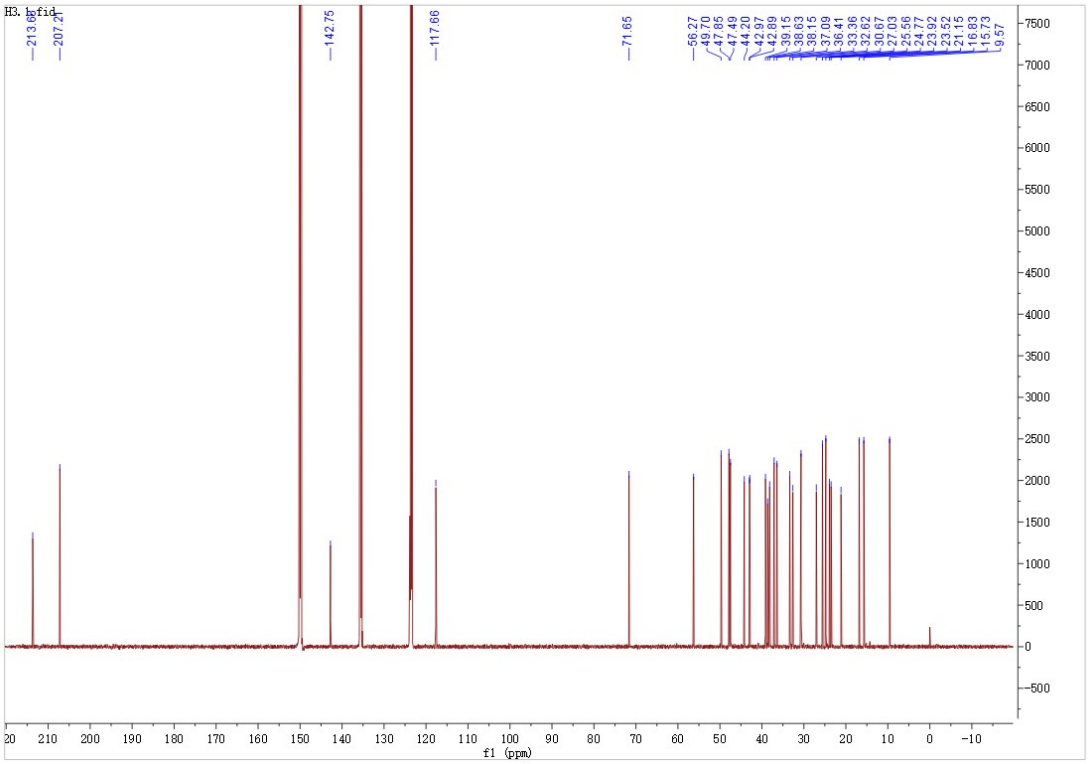

Figure S67. 13C-NMR spectrum of compound **12** in C_5D_5N (150 MHz)