Supporting information

Novel phenylpropanoid-amino acid adducts from *Ligusticum chuanxiong*

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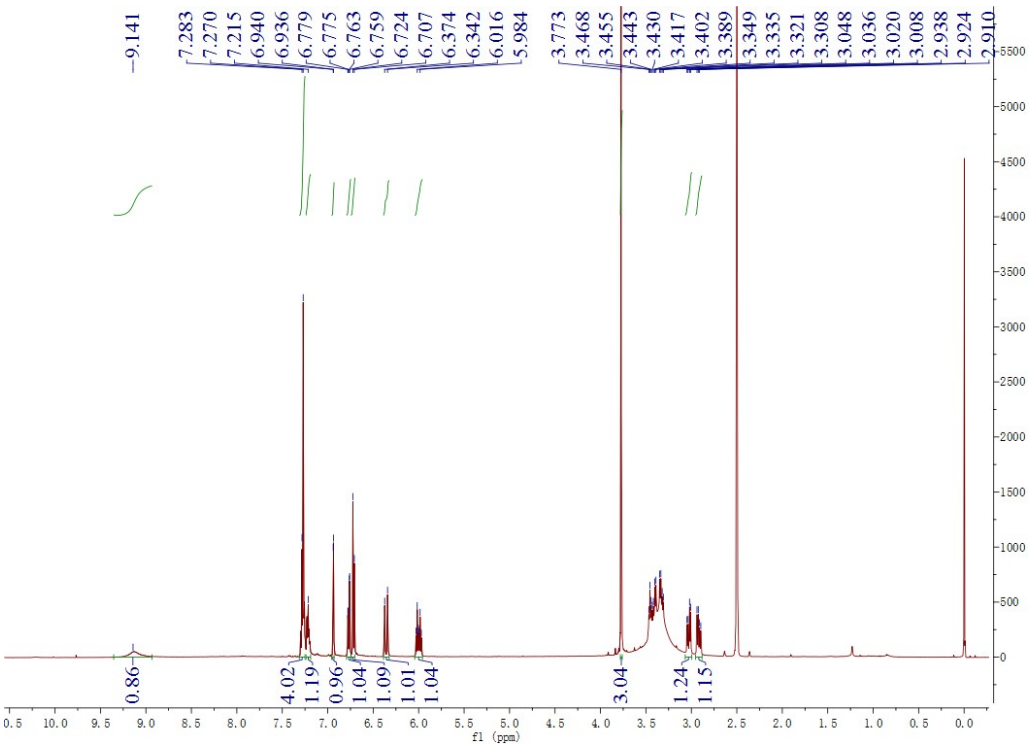


Figure S1. The ^{1}H NMR spectrum of compound **1** in DMSO-d_6

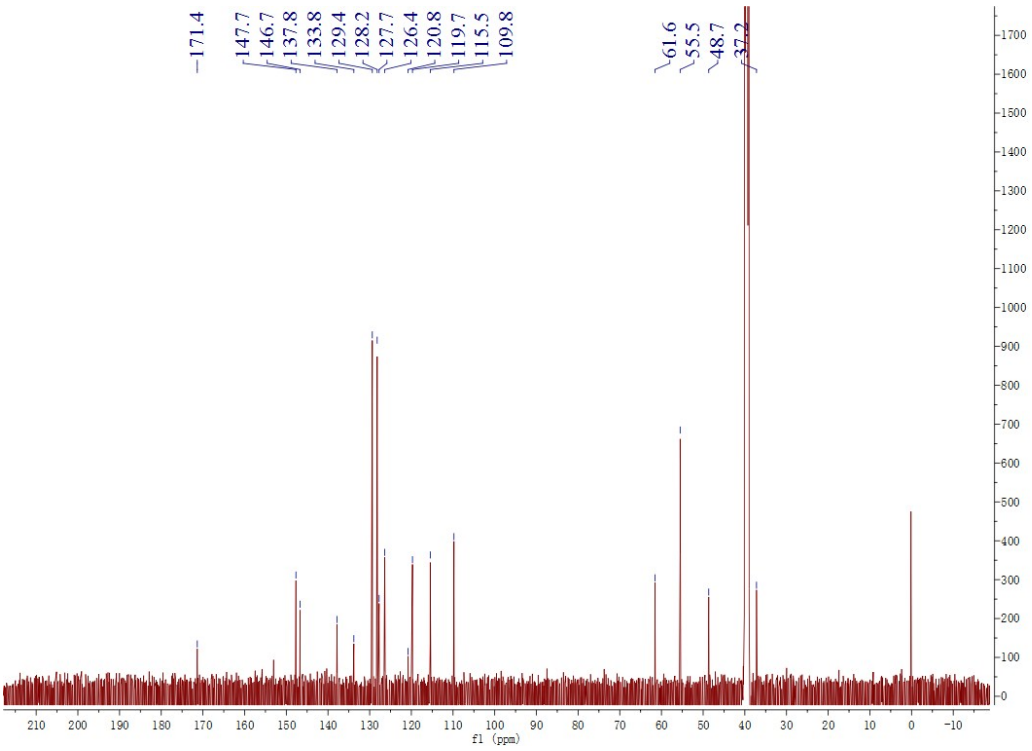


Figure S2. The ^{13}C NMR spectrum of compound **1** in DMSO-d_6

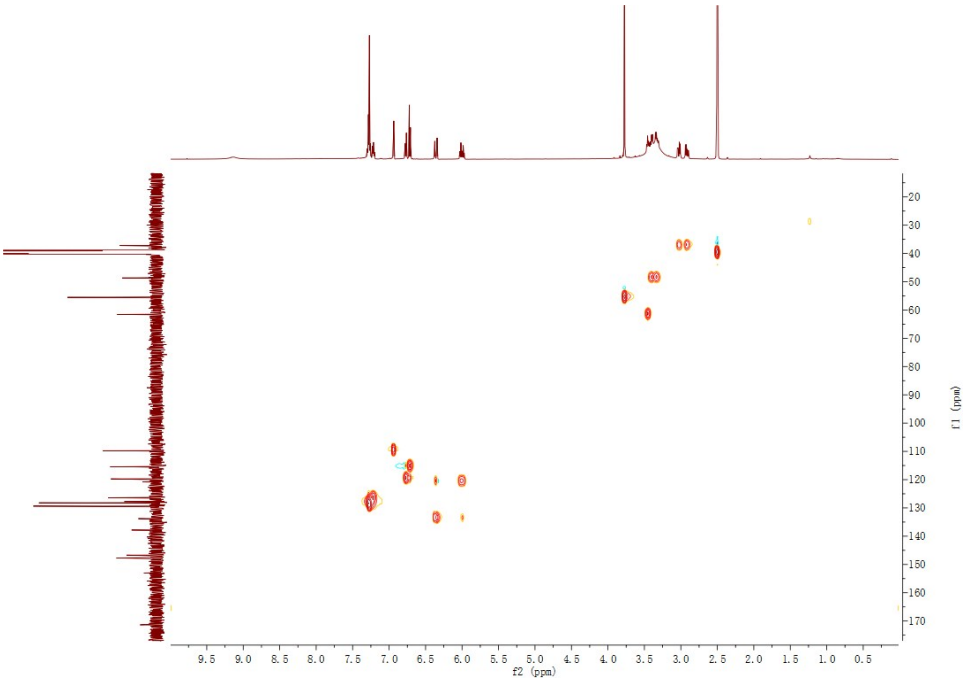


Figure S3. The HSQC spectrum of compound **1** in DMSO-d_6

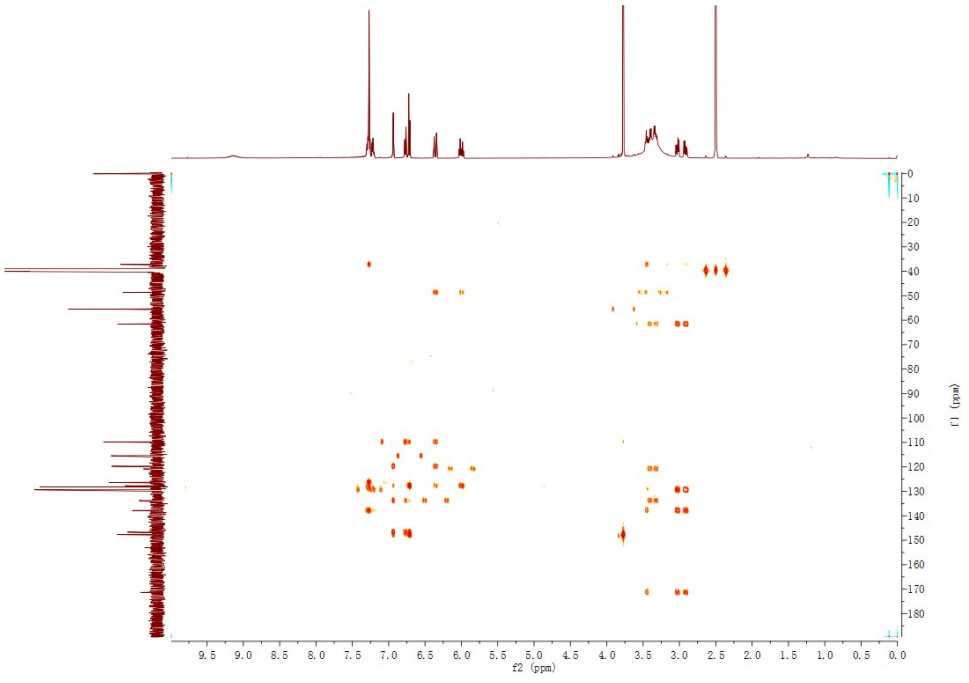


Figure S4. The HMBC spectrum of compound **1** in DMSO-d_6

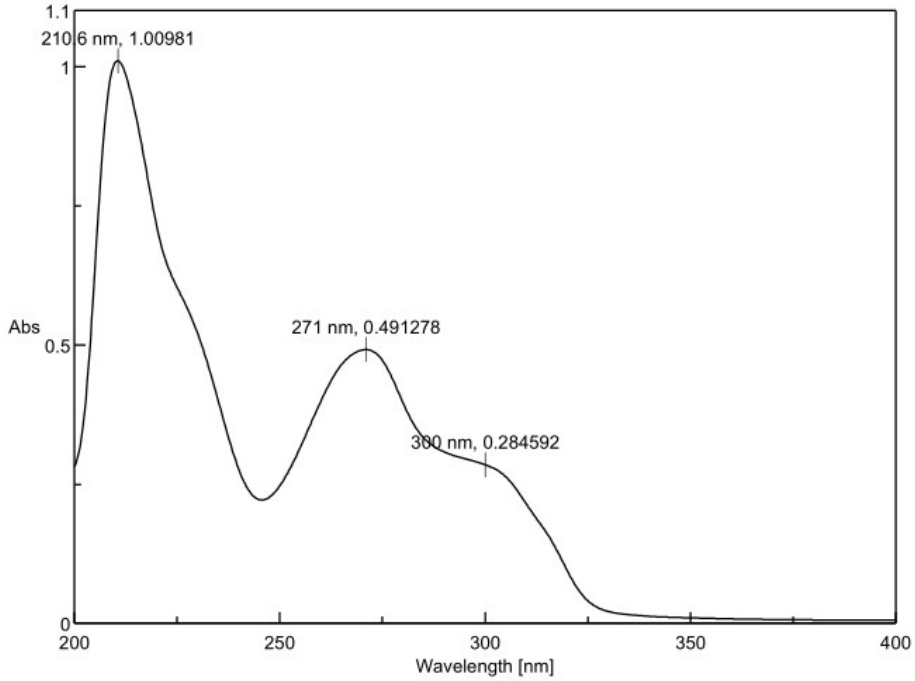


Figure S5. The UV spectrum of compound **1** in MeOH

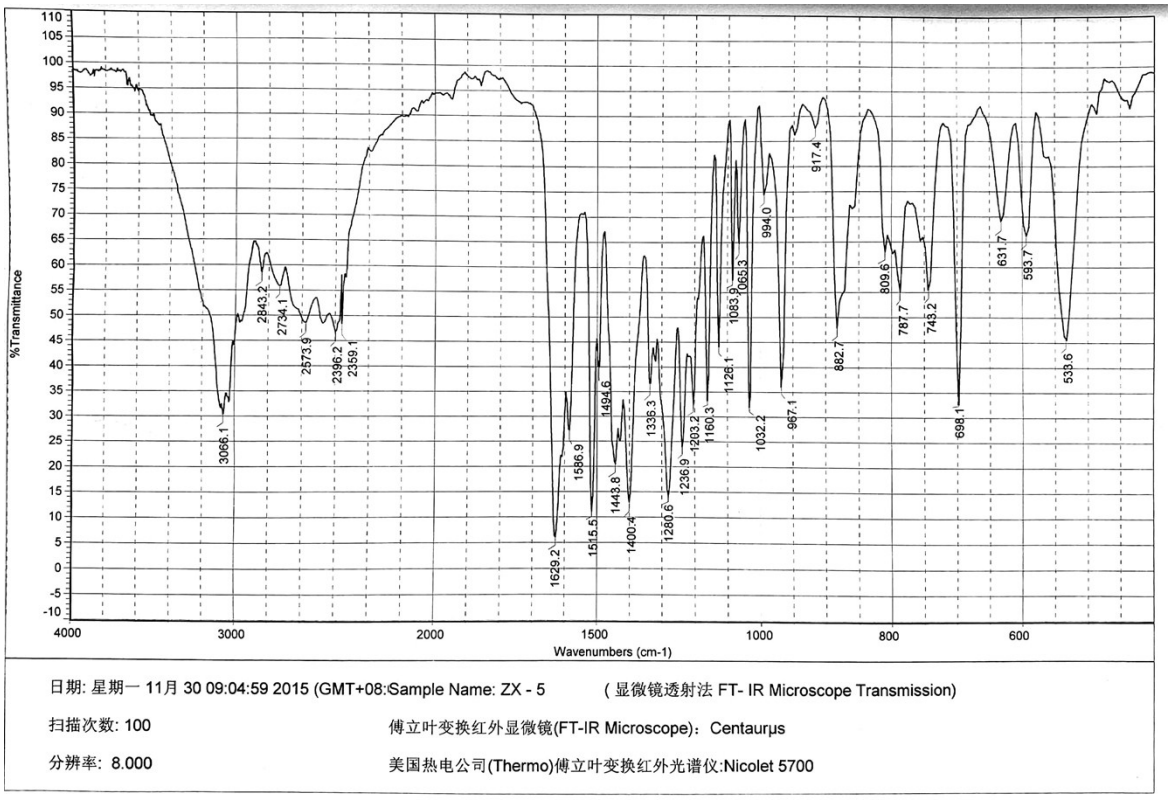
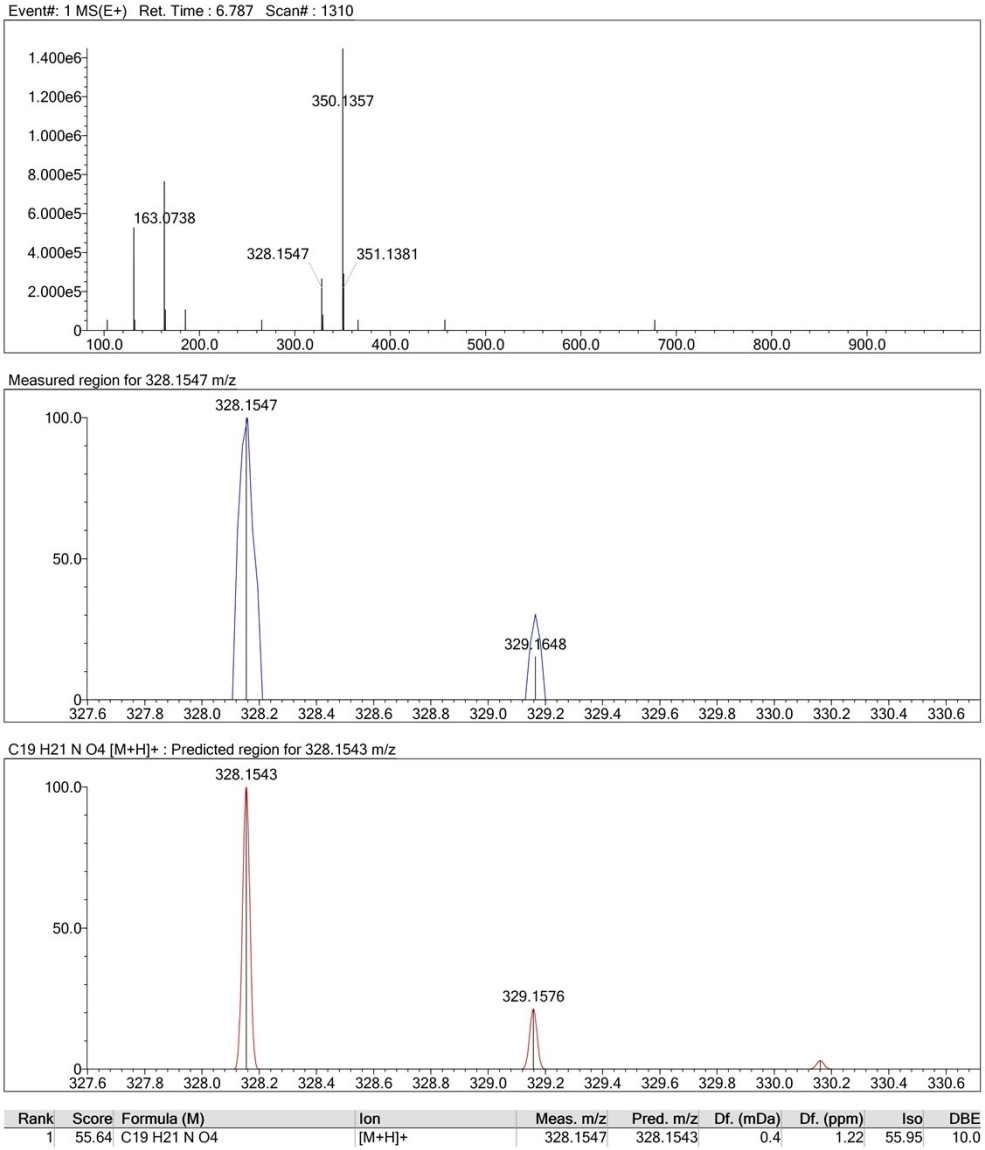


Figure S6. The IR spectrum of compound **1**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	55.64	C19 H21 N O4	[M+H]+	328.1547	328.1543	0.4	1.22	55.95	10.0

Figure S7. The HR-ESI-MS data of compound **1**

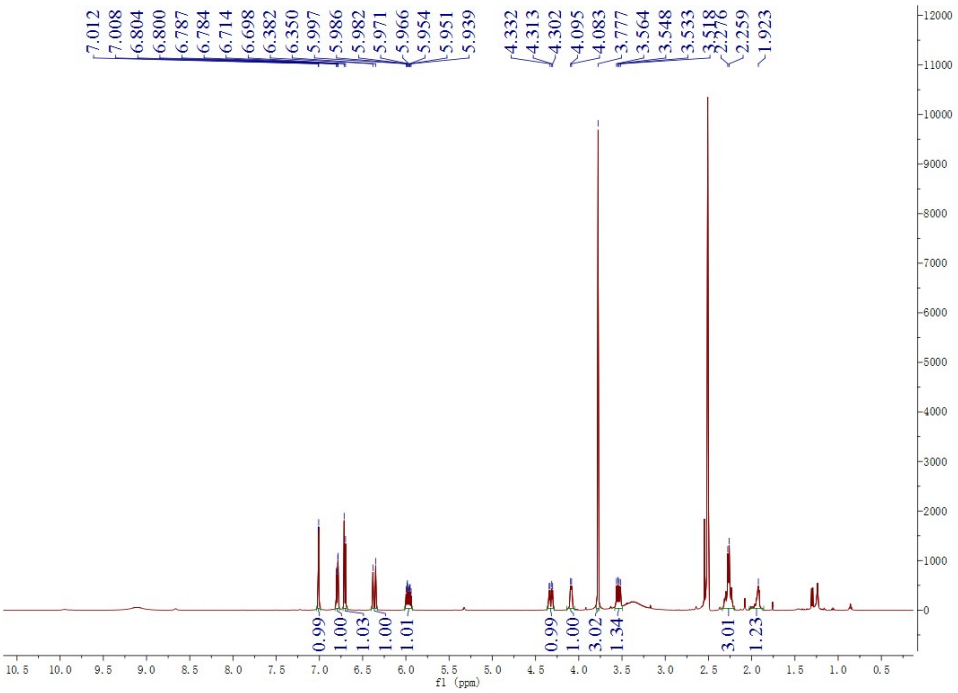


Figure S8. The ^{1}H NMR spectrum of compound **2** in DMSO-d_6

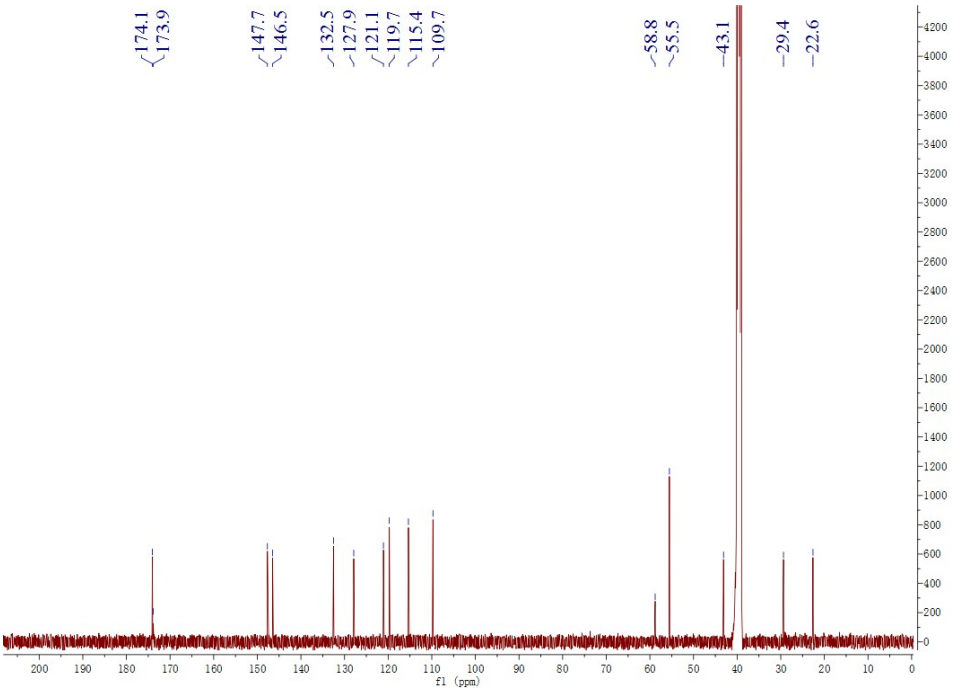


Figure S9. The ^{13}C NMR spectrum of compound **2** in DMSO-d_6

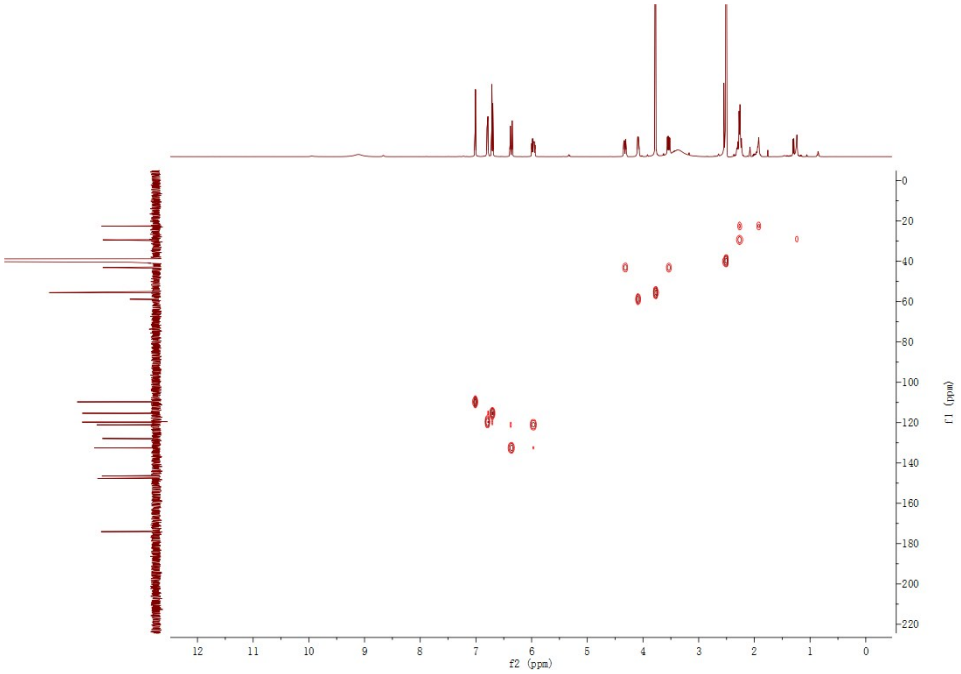


Figure S10. The HSQC spectrum of compound **2** in DMSO-d_6

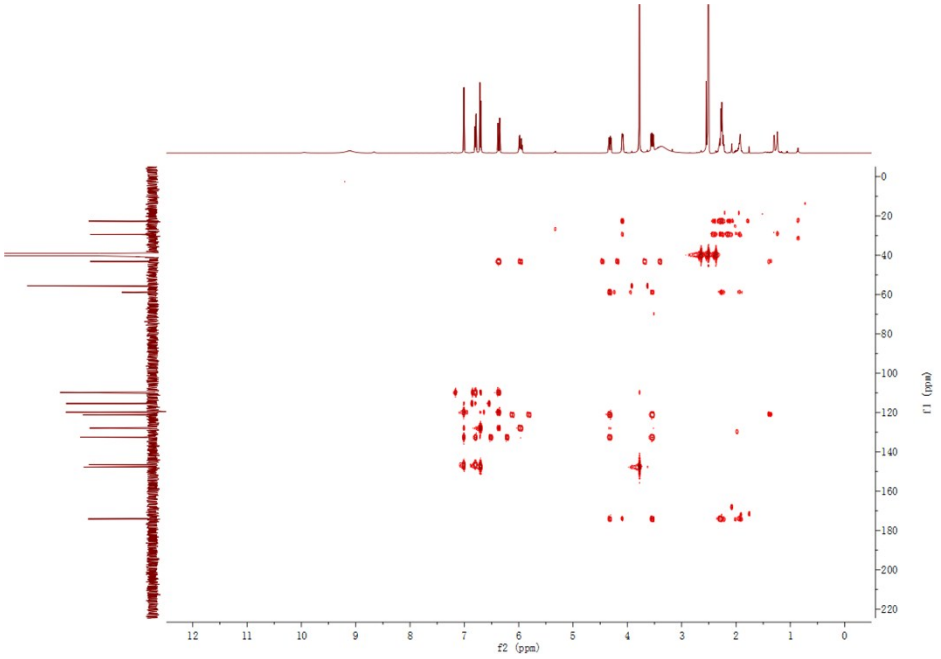


Figure S11. The HMBC spectrum of compound **2** in DMSO-d_6

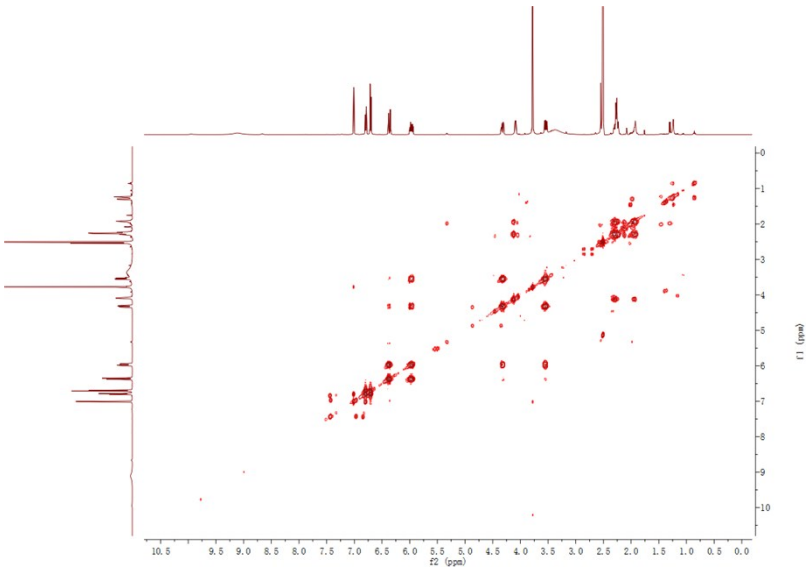


Figure S12. The ^{1}H-^{1}H COSY spectrum in DMSO-d_6

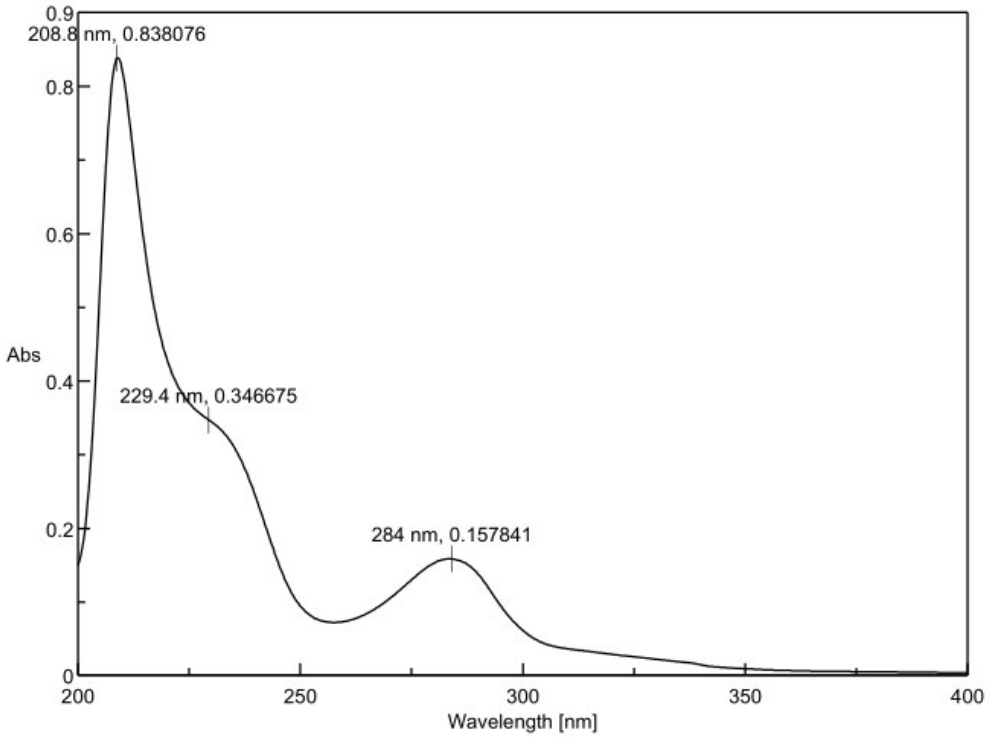


Figure S13. The UV spectrum of compound **2** in MeOH

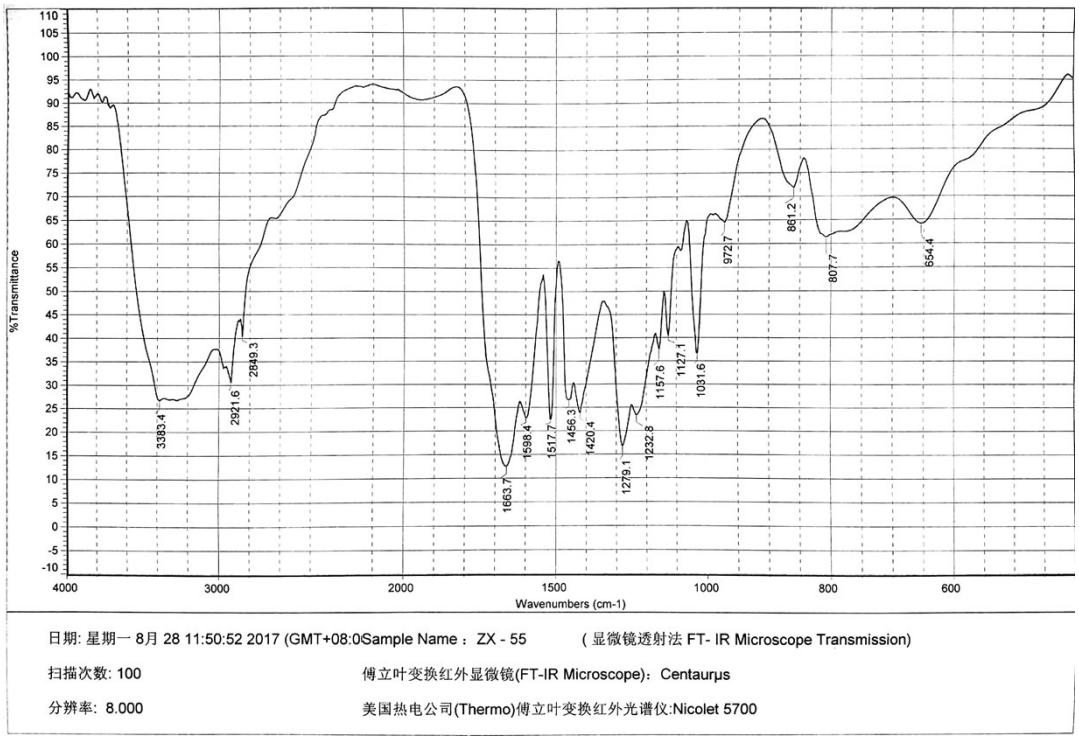


Figure S14. The IR spectrum of compound **2**

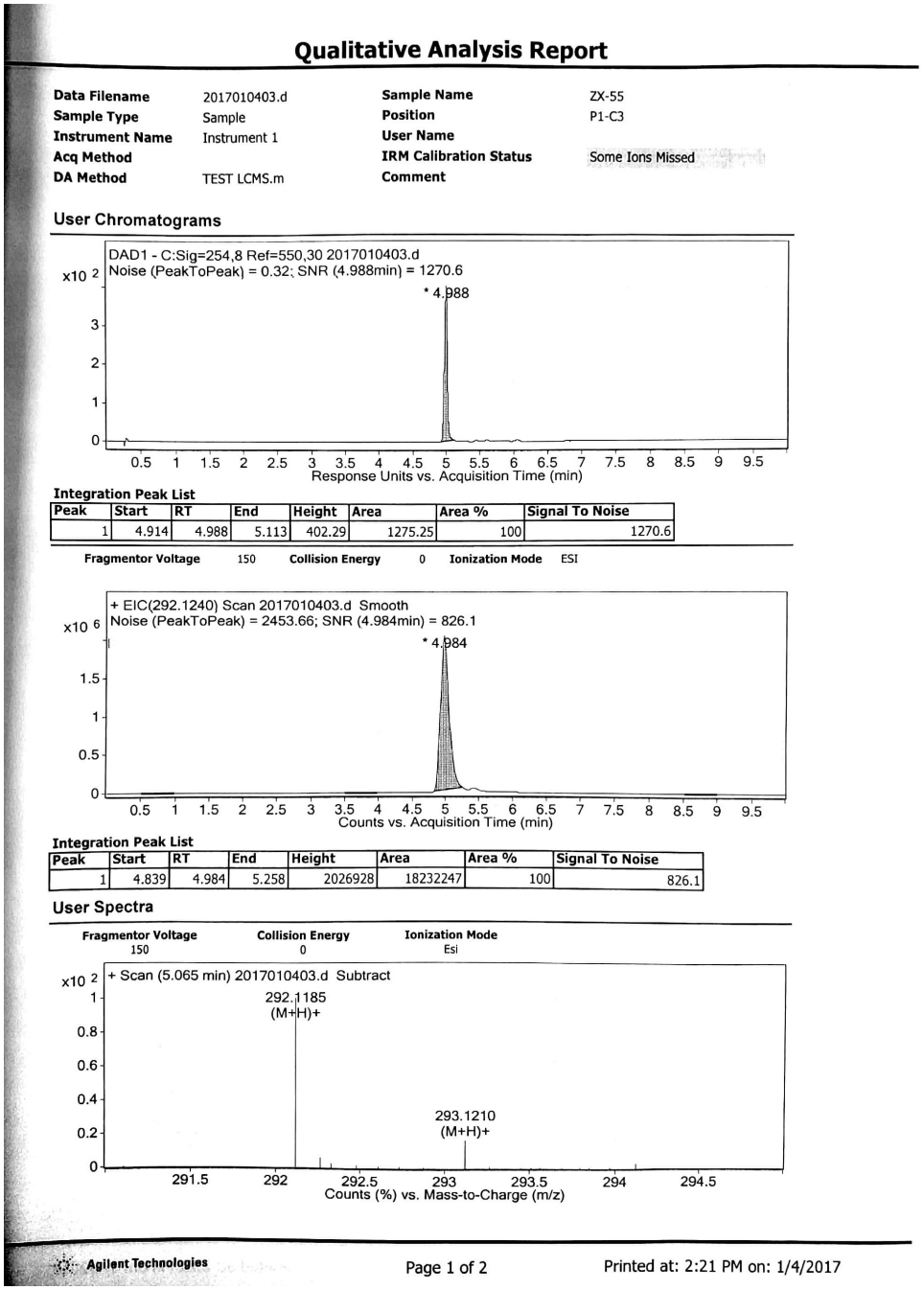


Figure S15. The HR-ESI-MS data of compound **2**

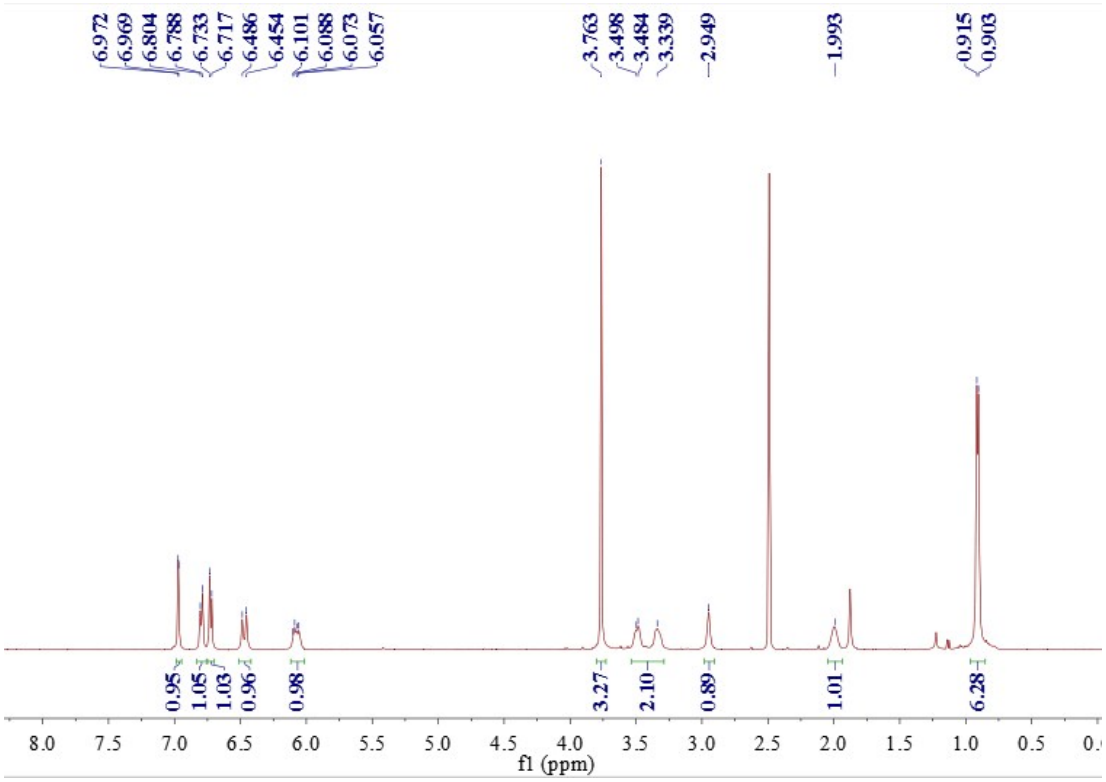


Figure S16. The ^{1}H NMR spectrum of compound **3** in DMSO-d_6

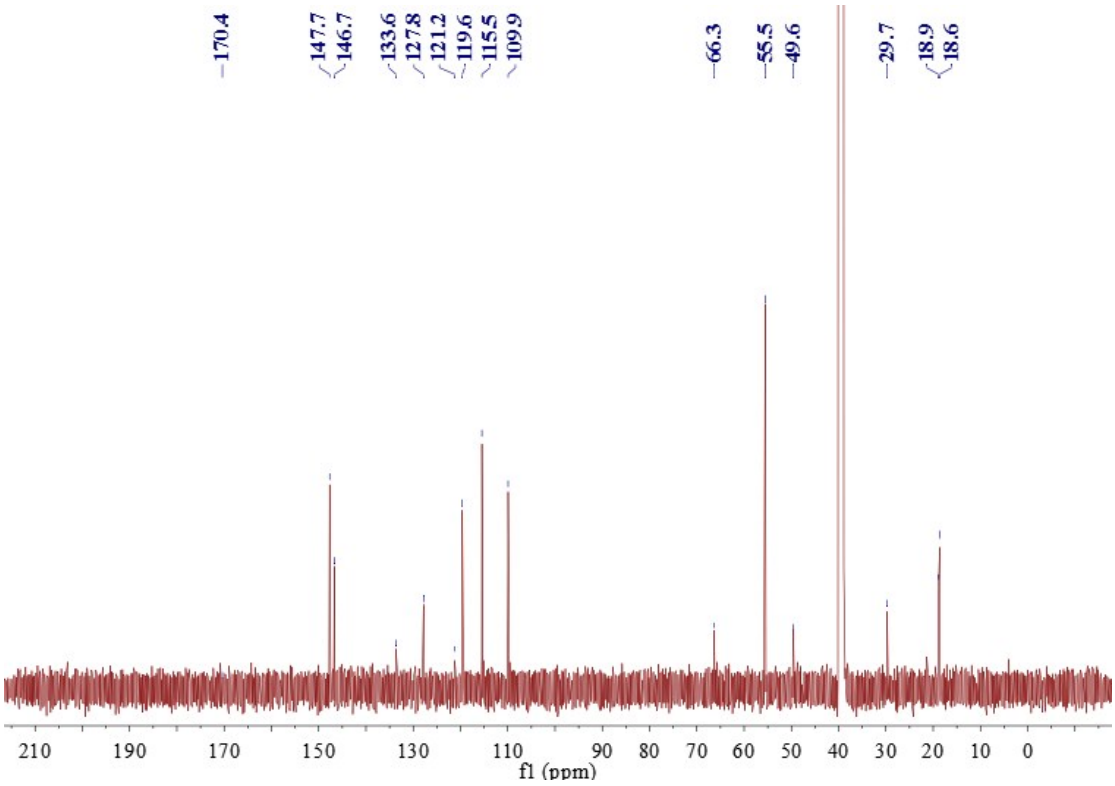


Figure S17. The ^{13}C NMR spectrum of compound **3** in DMSO-d_6

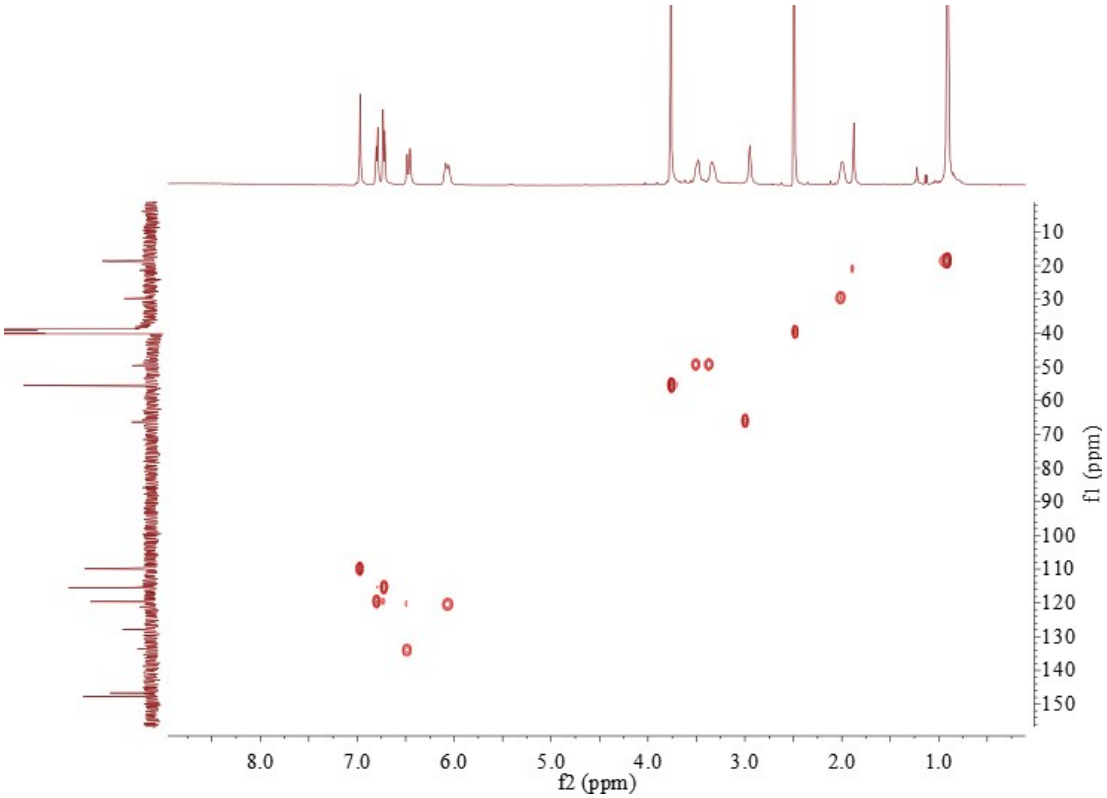


Figure S18. The HSQC spectrum of compound **3** in DMSO-d_6

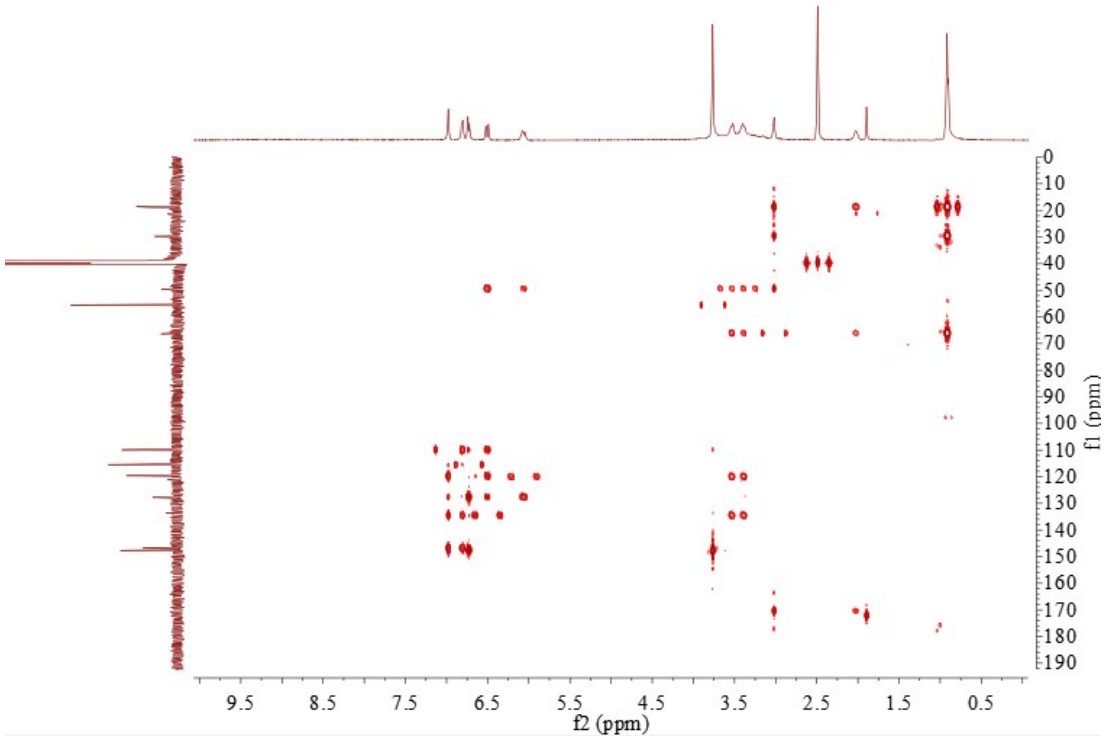


Figure S19. The HMBC spectrum of compound **3** in DMSO-d_6

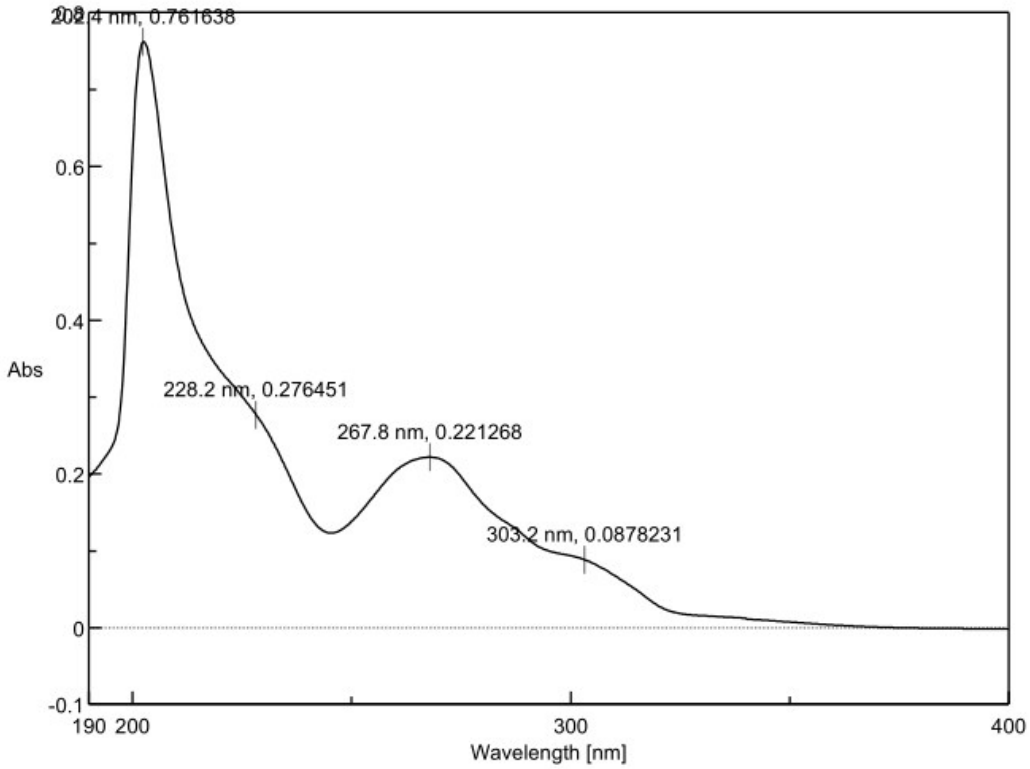


Figure S20. The UV spectrum of compound **3** in MeOH

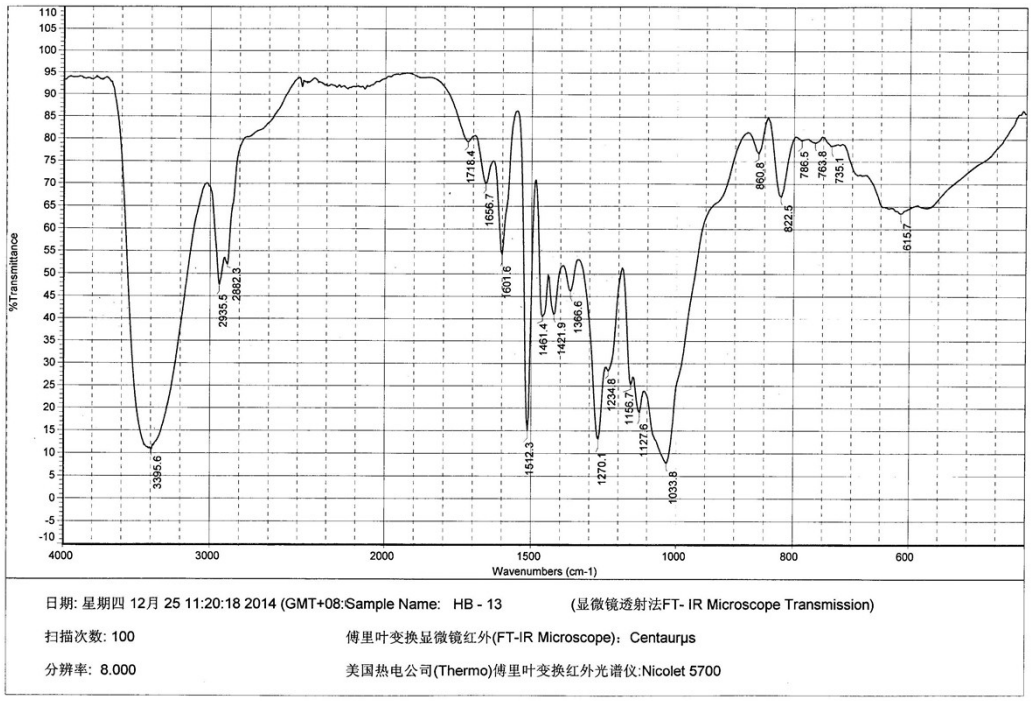


Figure S21. The IR spectrum of compound **3**

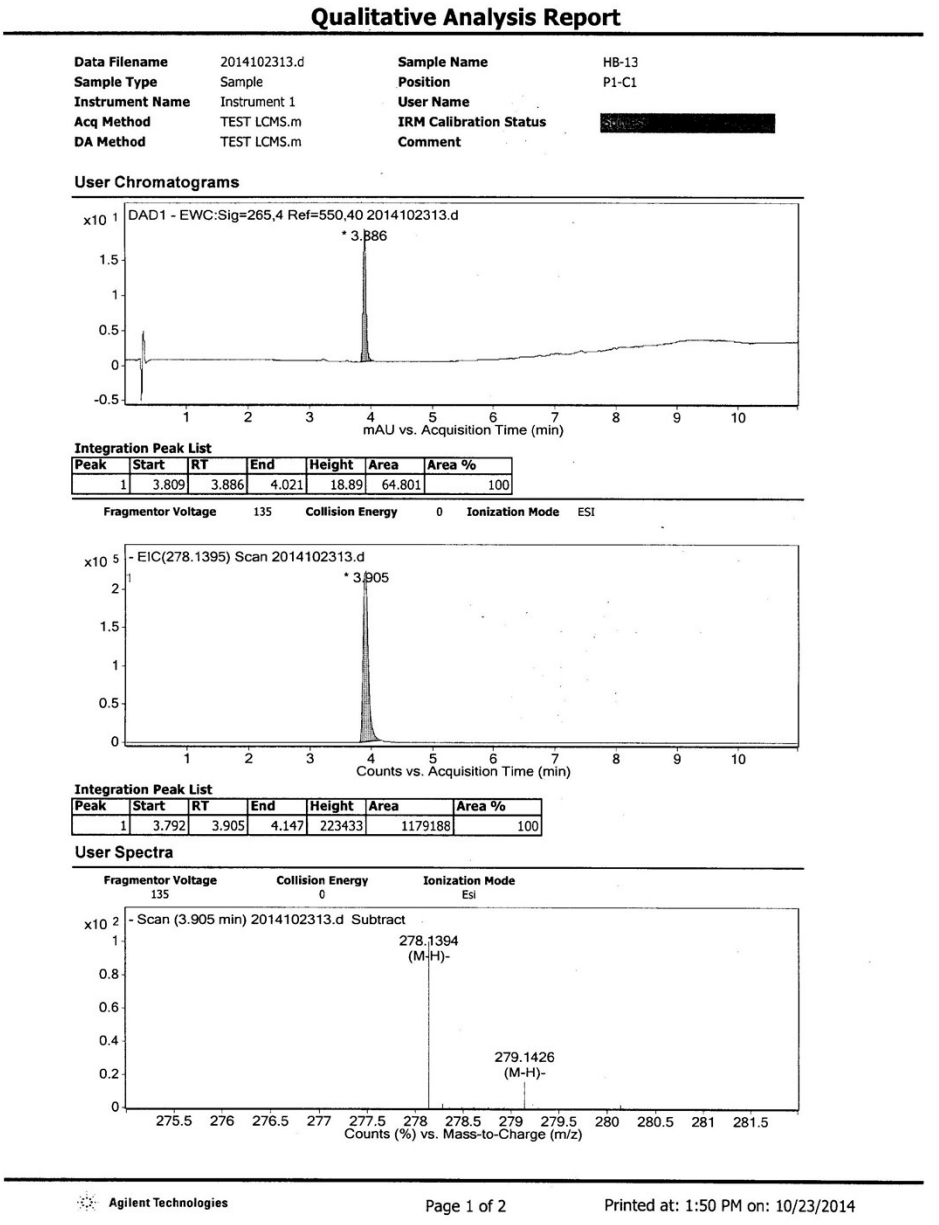


Figure S22. The HR-ESI-MS data of compound **3**

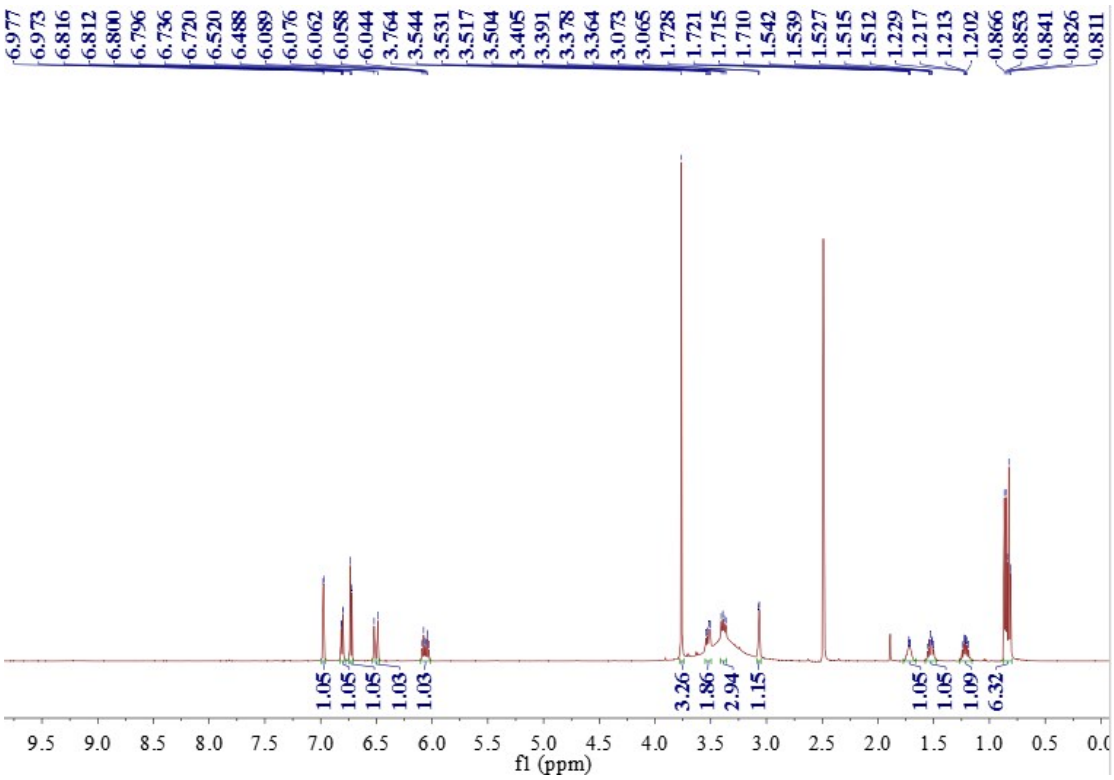


Figure S23. The ^{1}H NMR spectrum of compound **4** in DMSO-d_6

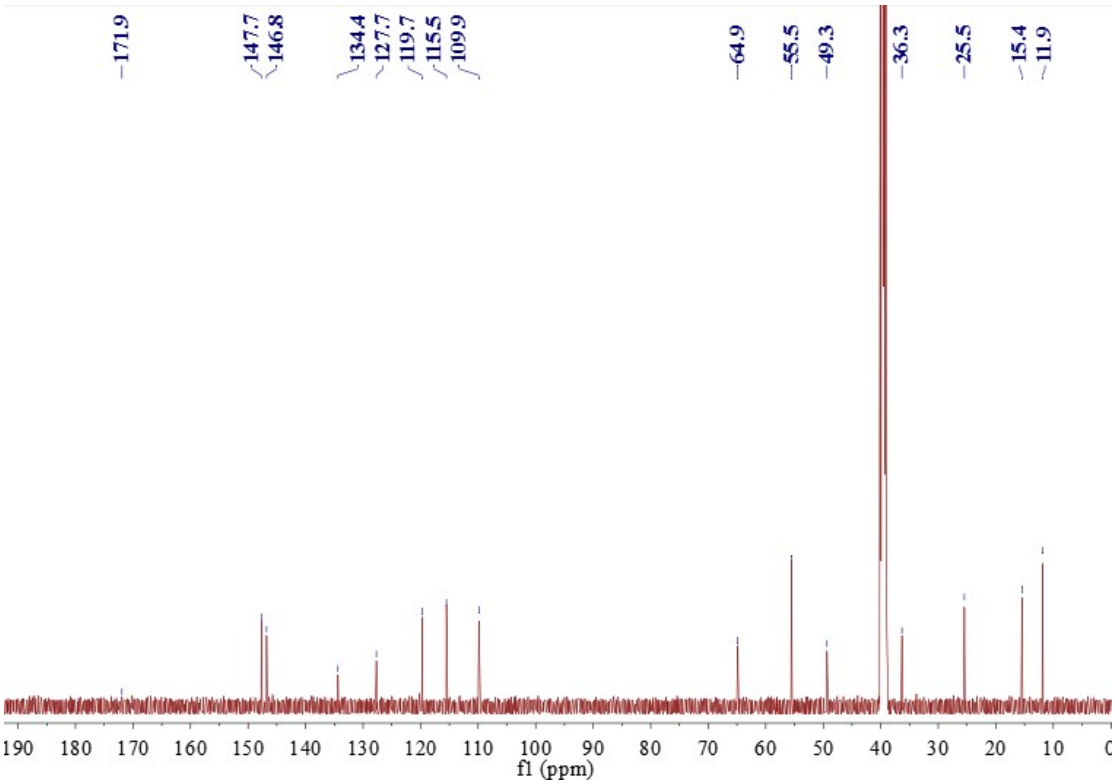


Figure S24. The ^{13}C NMR spectrum of compound **4** in DMSO-d_6

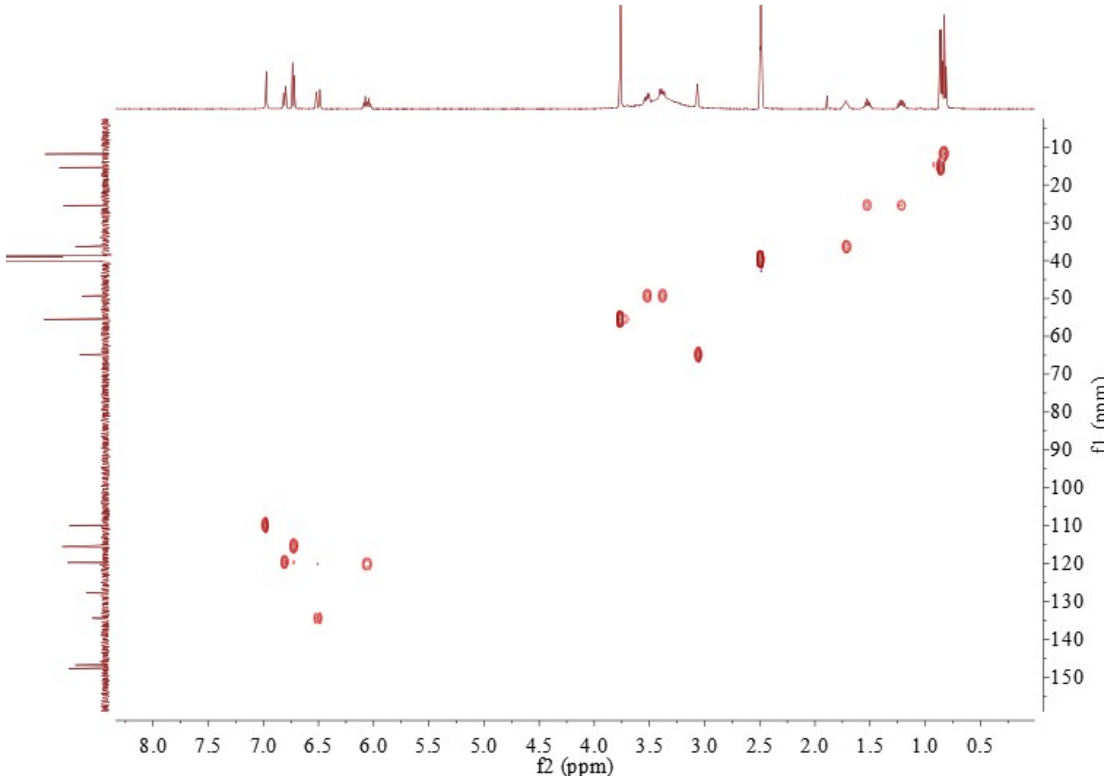


Figure S25. The HSQC spectrum of compound **4** in DMSO-d_6

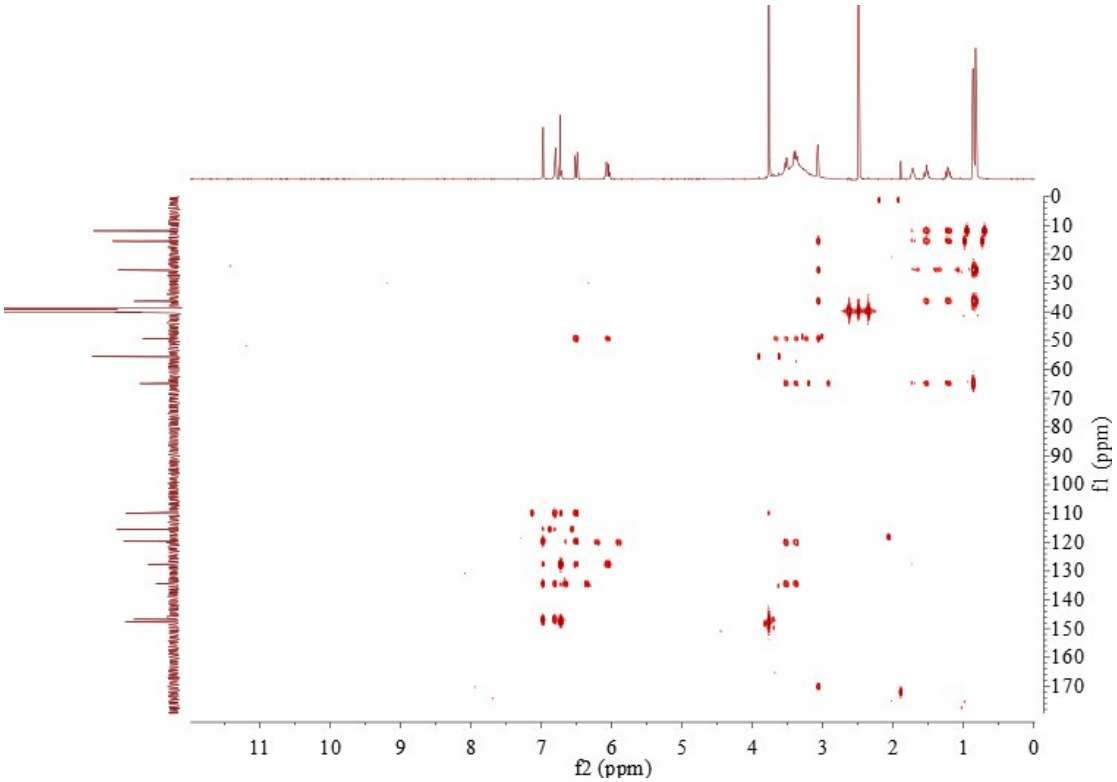


Figure S26. The HMBC spectrum of compound **4** in DMSO-d_6

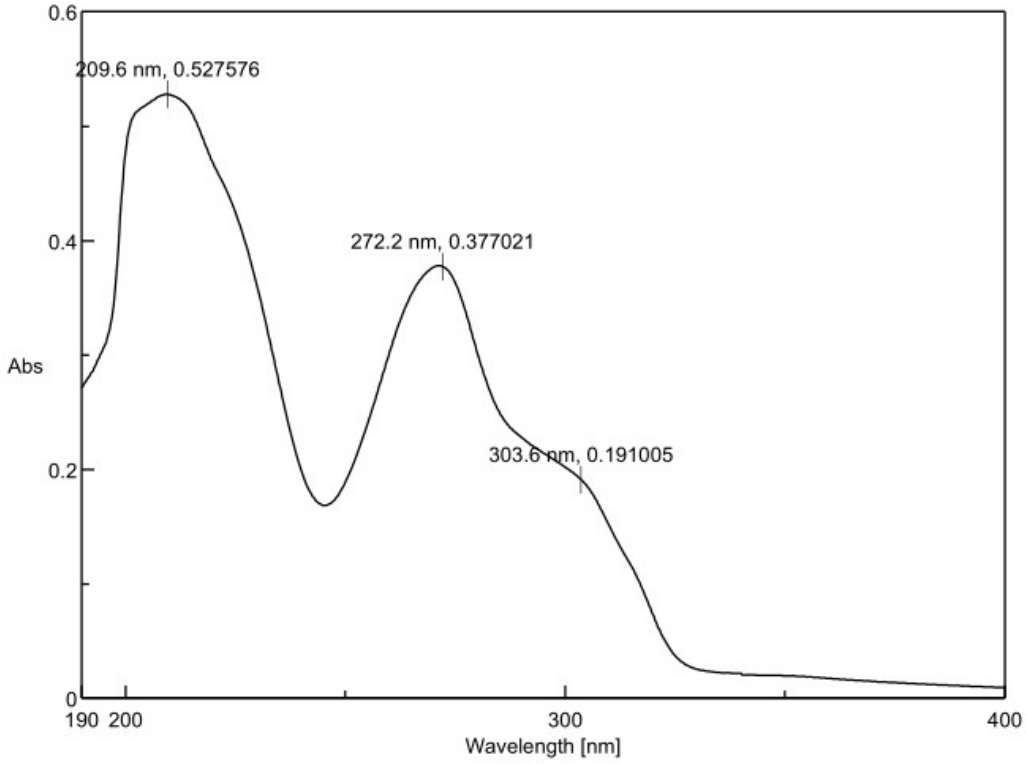


Figure S27. The UV spectrum of compound **4** in MeOH

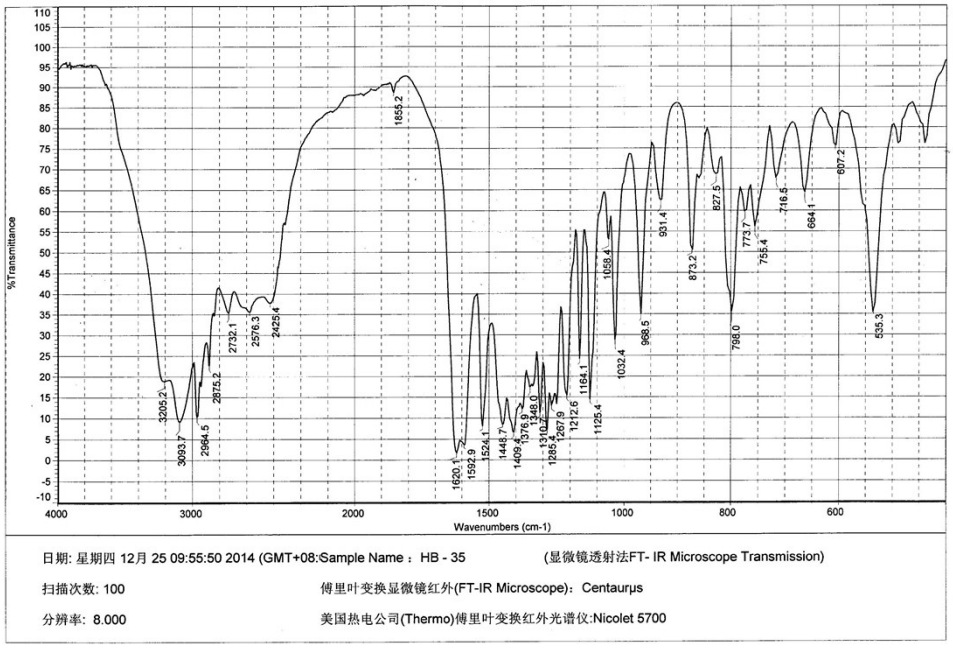


Figure S28. The IR spectrum of compound **4**

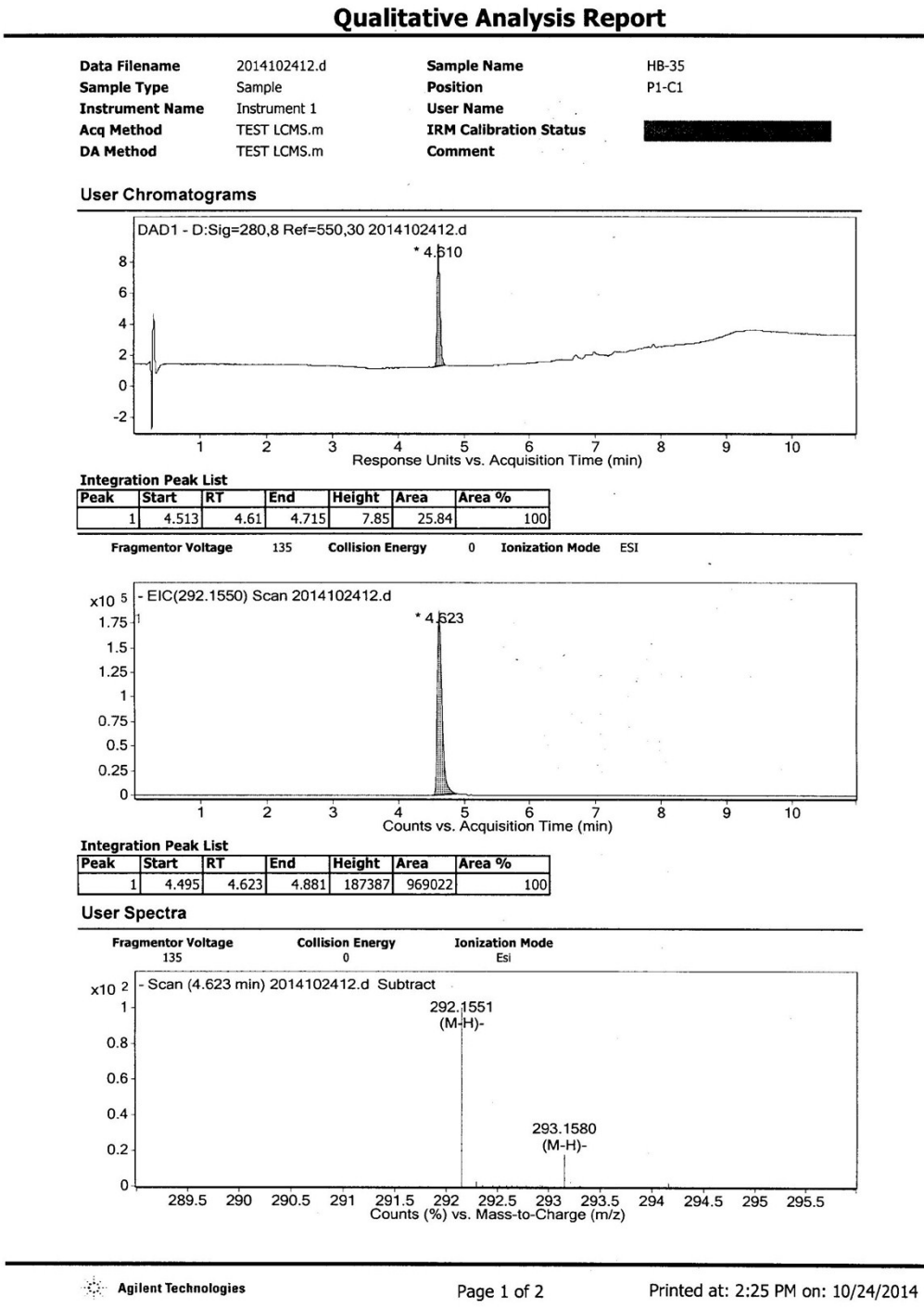


Figure S29. The HR-ESI-MS data of compound **4**

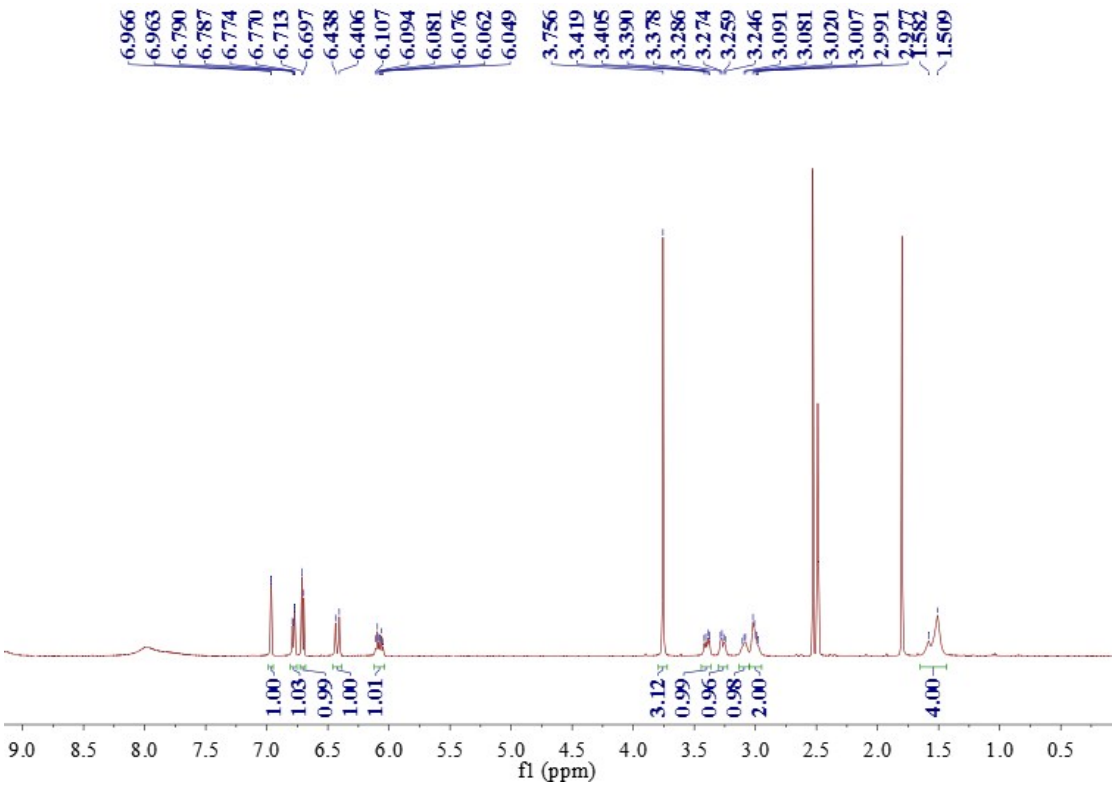


Figure S30. The ^{1}H NMR spectrum of compound **5** in DMSO-d_6

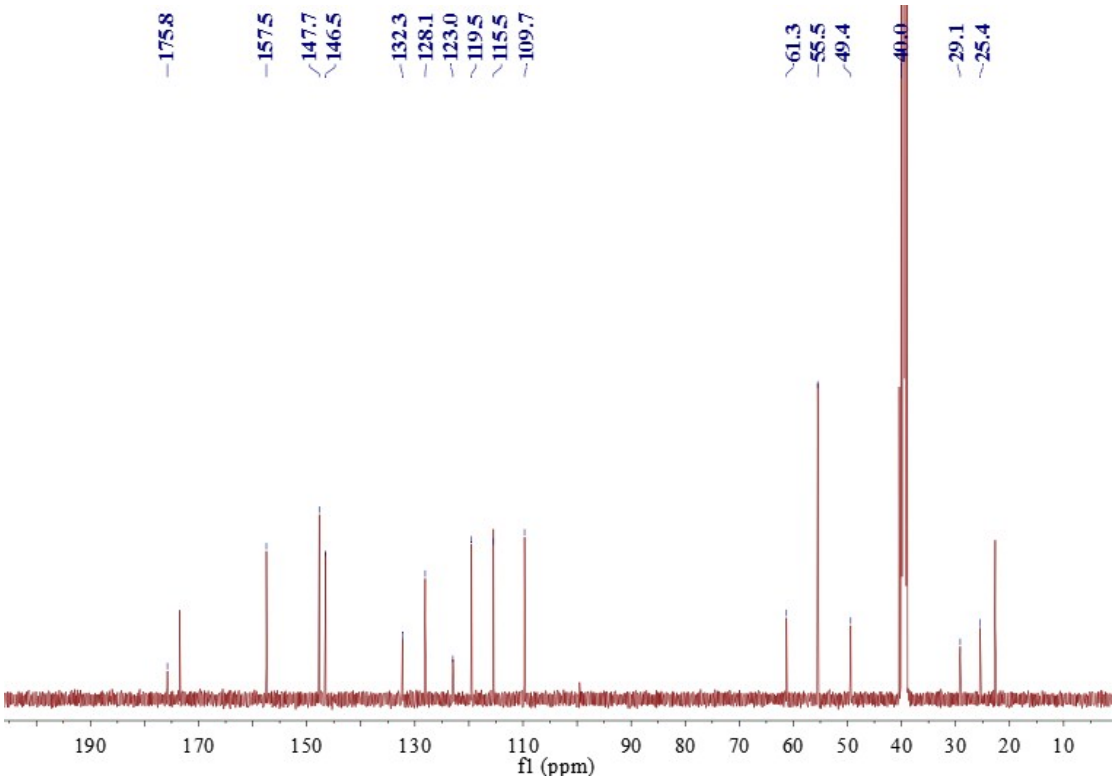


Figure S31. The ^{13}C NMR spectrum of compound **5** in DMSO-d_6

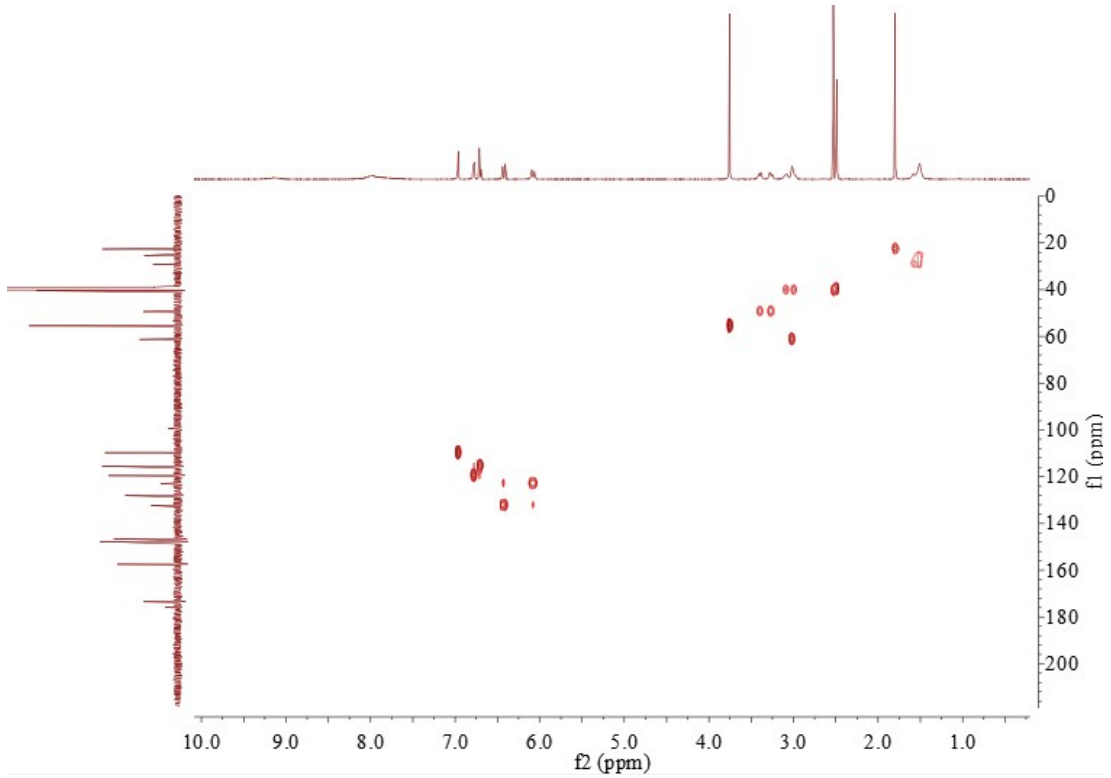


Figure S32. The HSQC spectrum of compound **5** in DMSO-d_6

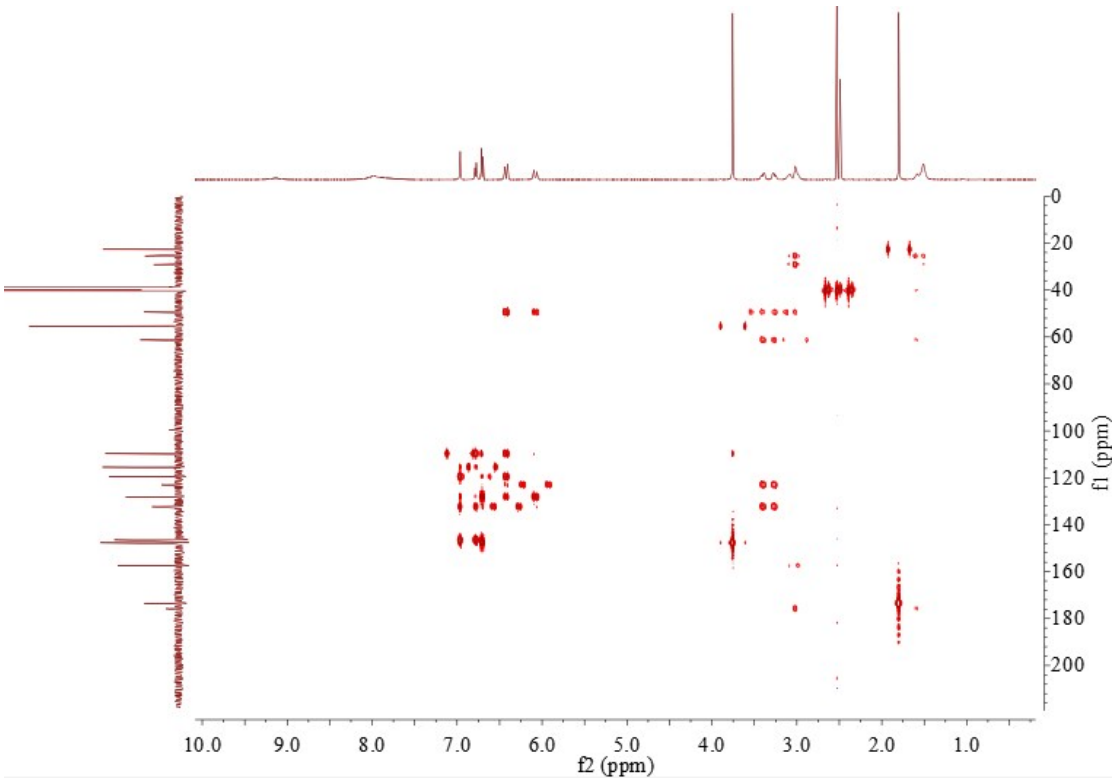


Figure S33. The HMBC spectrum of compound **5** in DMSO-d_6

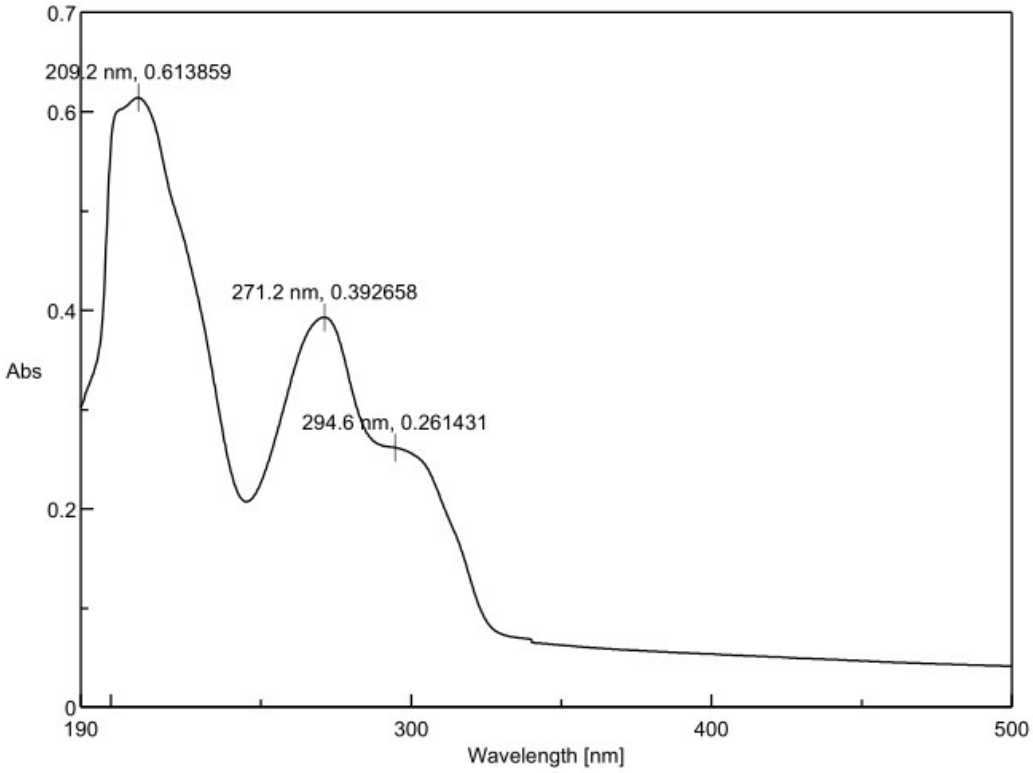


Figure S34. The UV spectrum of compound **5** in MeOH

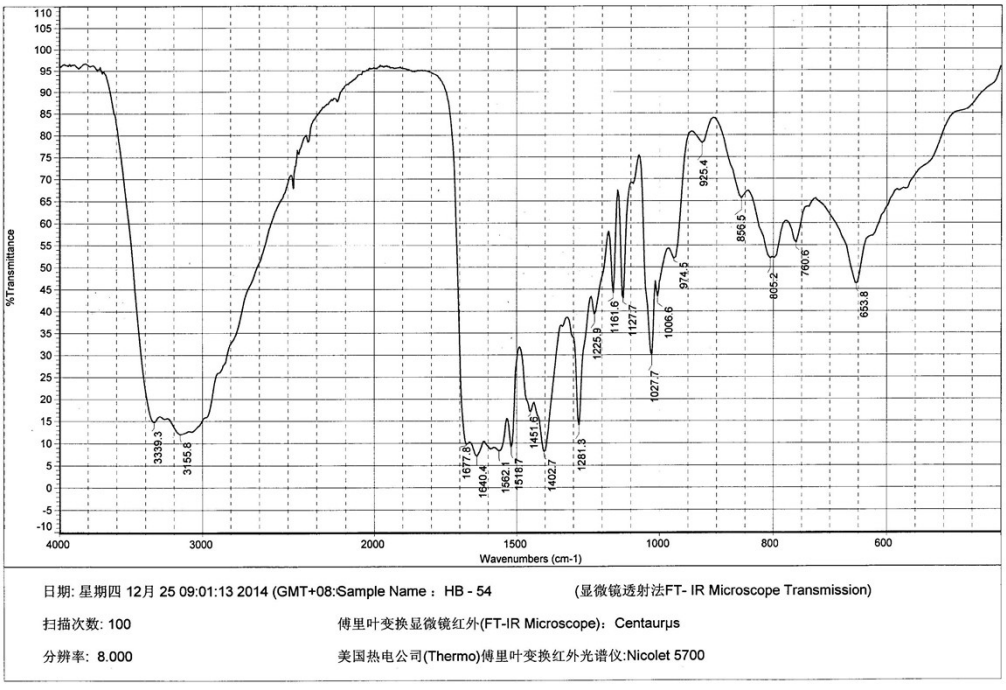


Figure S35. The IR spectrum of compound **5**

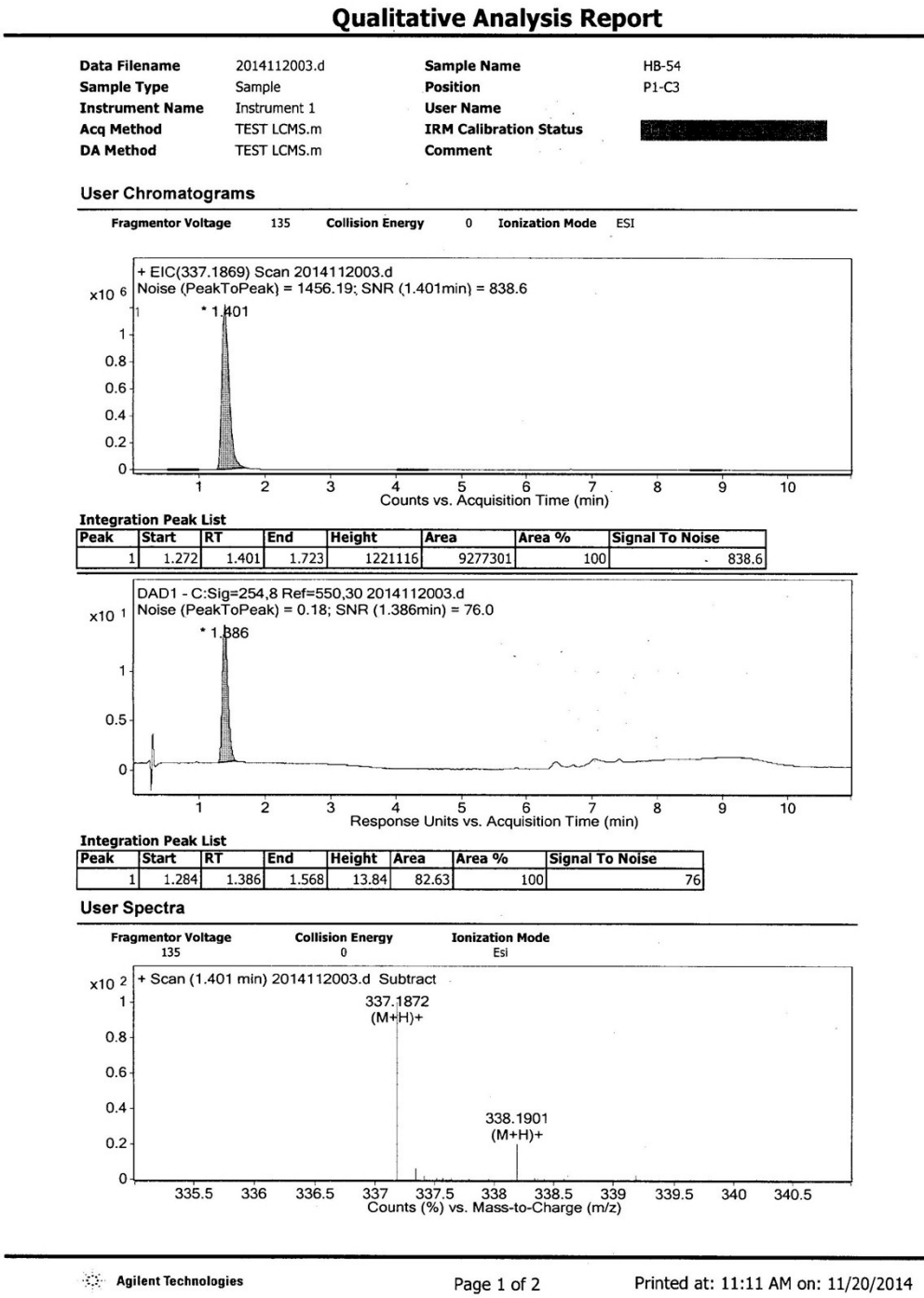


Figure S36. The HR-ESI-MS data of compound **5**

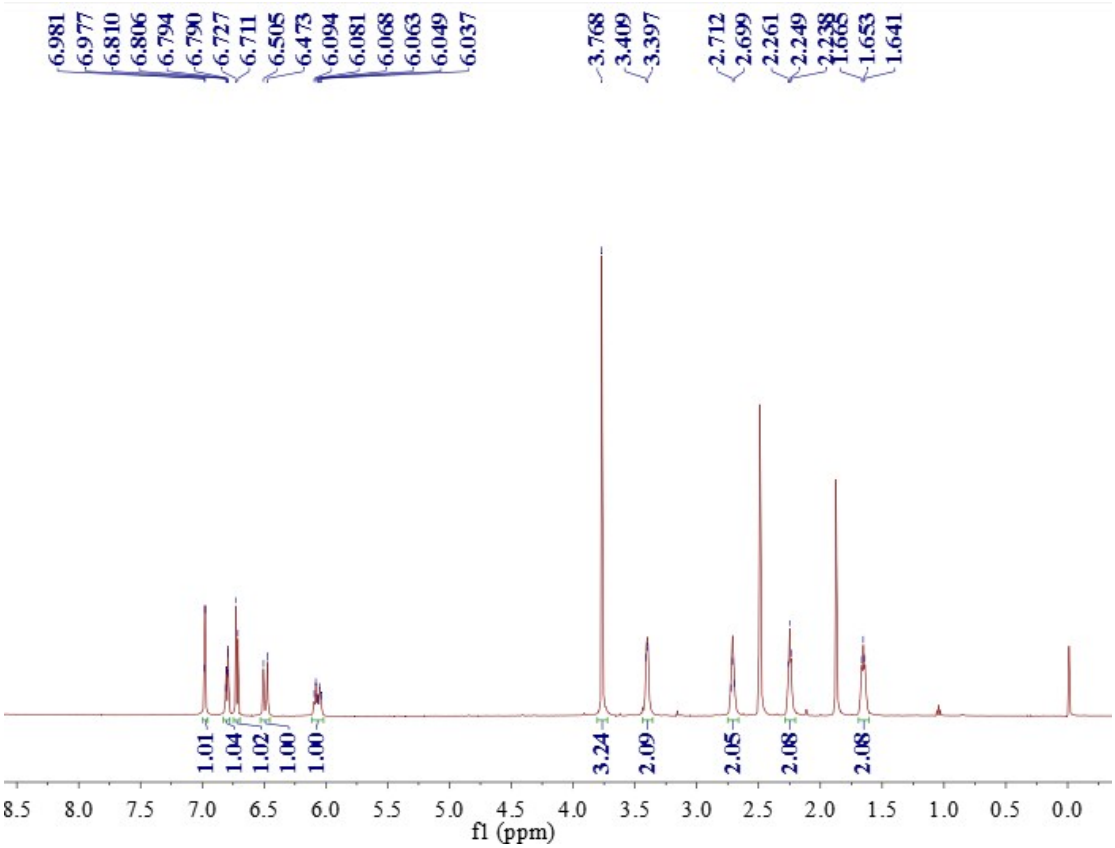


Figure S37. The ^{1}H NMR spectrum of compound **6** in DMSO-d_6

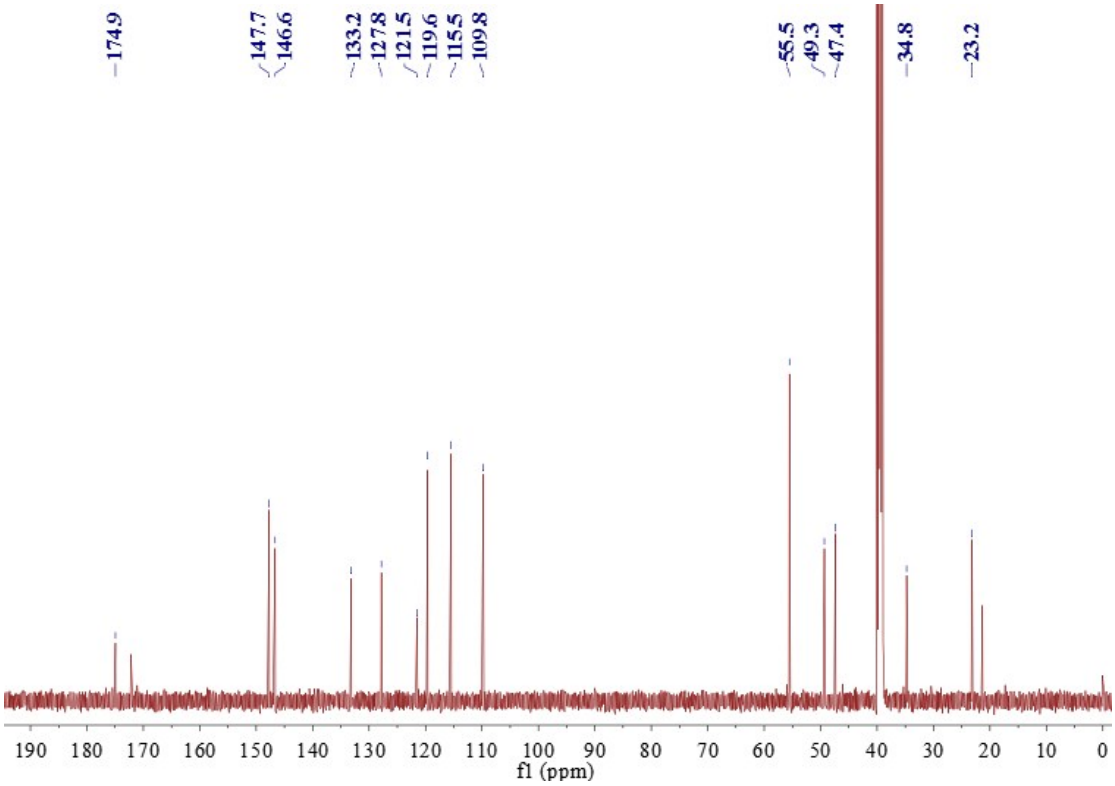


Figure S38. The ^{13}C NMR spectrum of compound **6** in DMSO-d_6

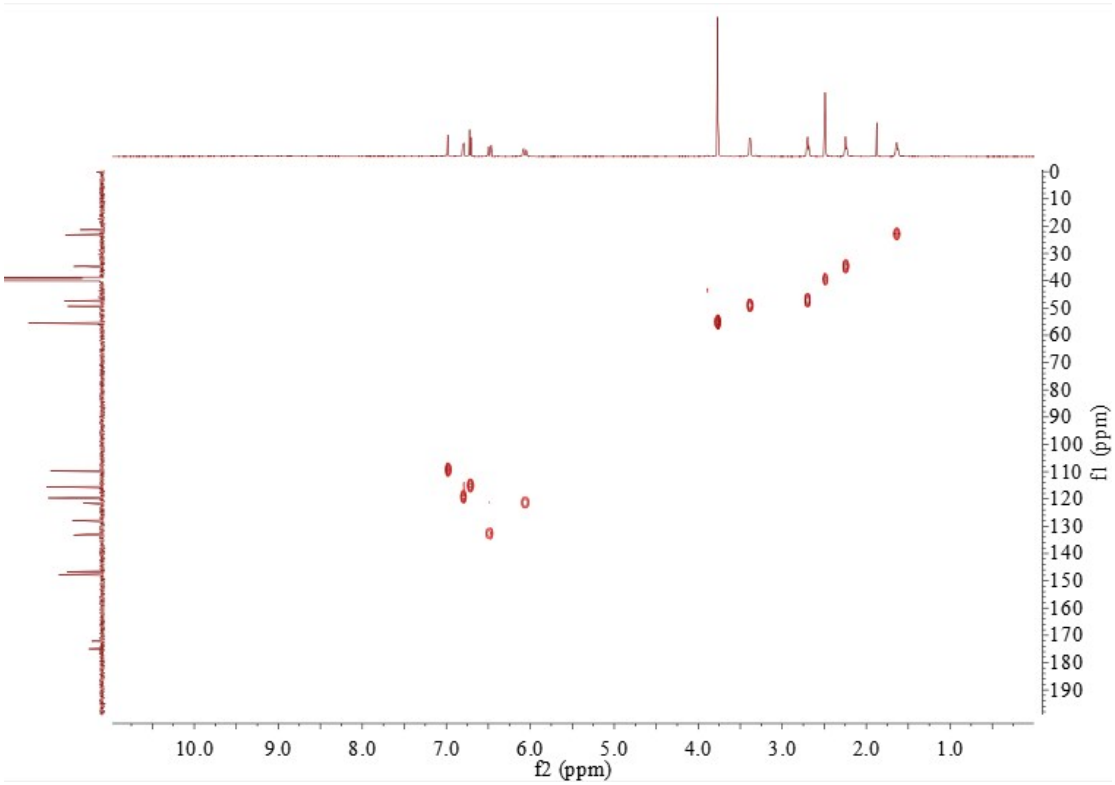


Figure S39. The HSQC spectrum of compound **6** in DMSO-d_6

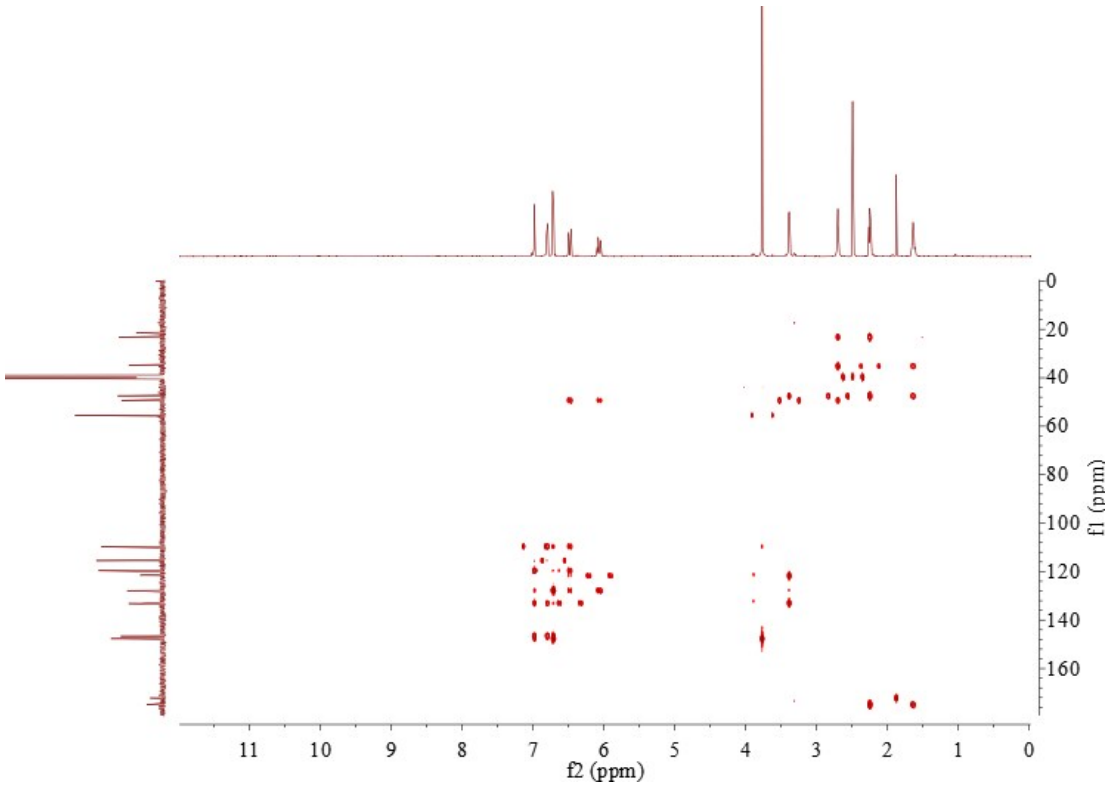


Figure S40. The HMBC spectrum of compound **6** in DMSO-d_6

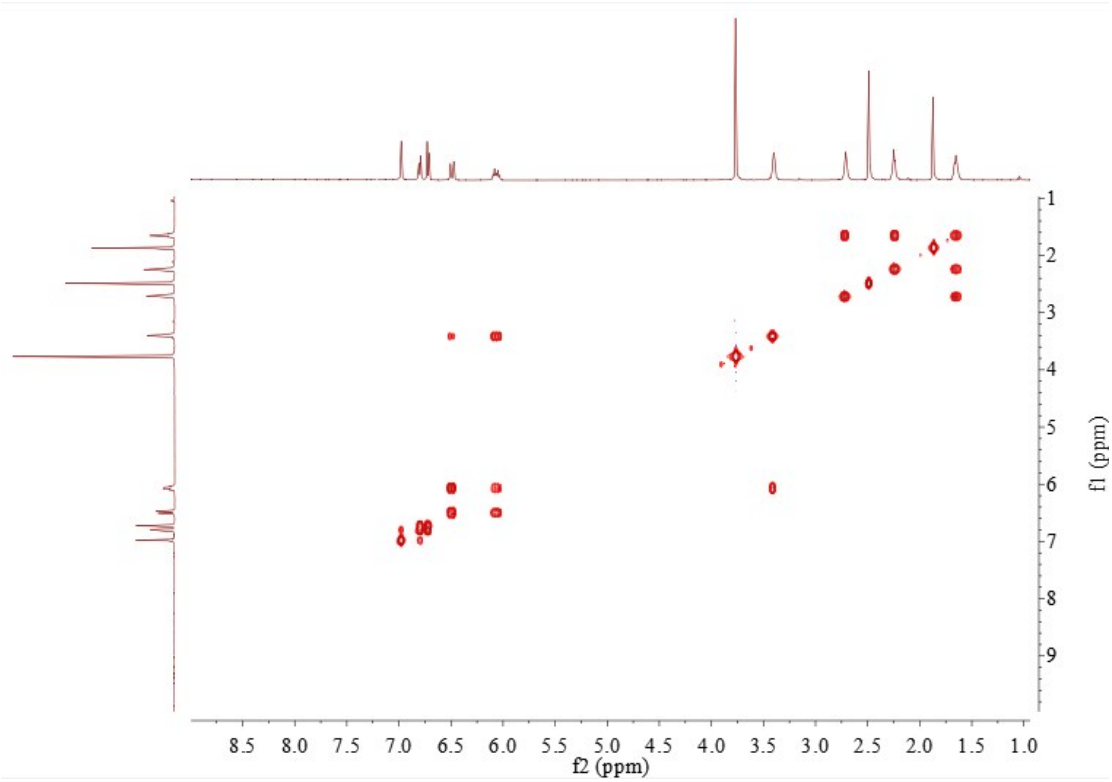


Figure S41. The ^{1}H-^{1}H COSY spectrum of compound **6** in DMSO-d_6

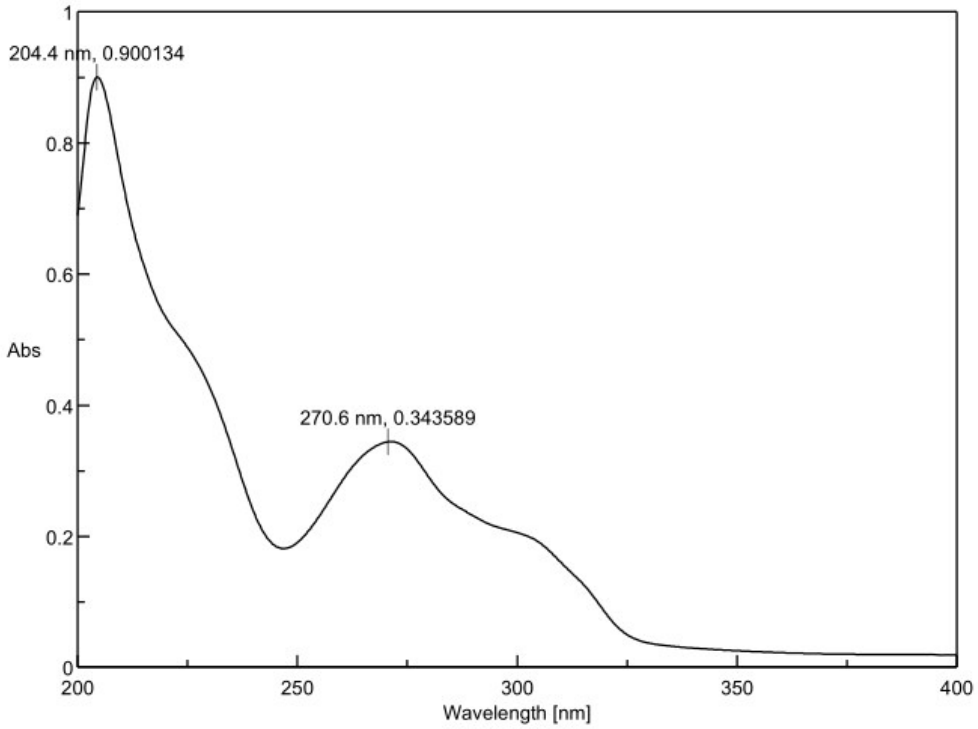


Figure S42. The UV spectrum of compound **6** in MeOH

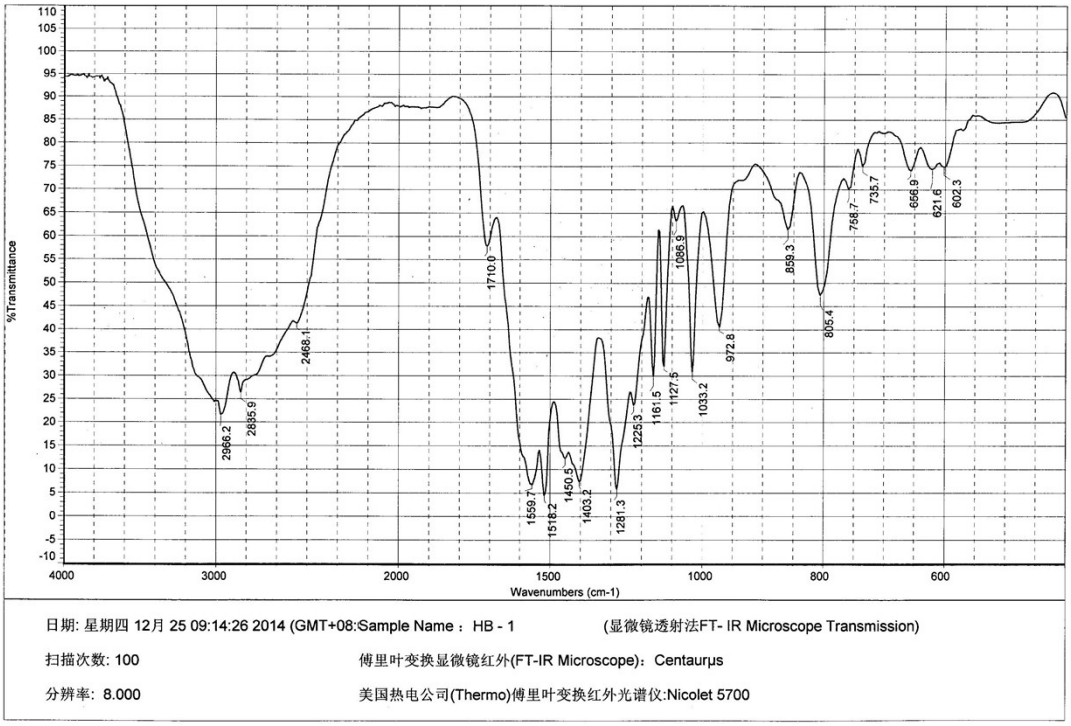


Figure S43. The IR spectrum of compound **6**

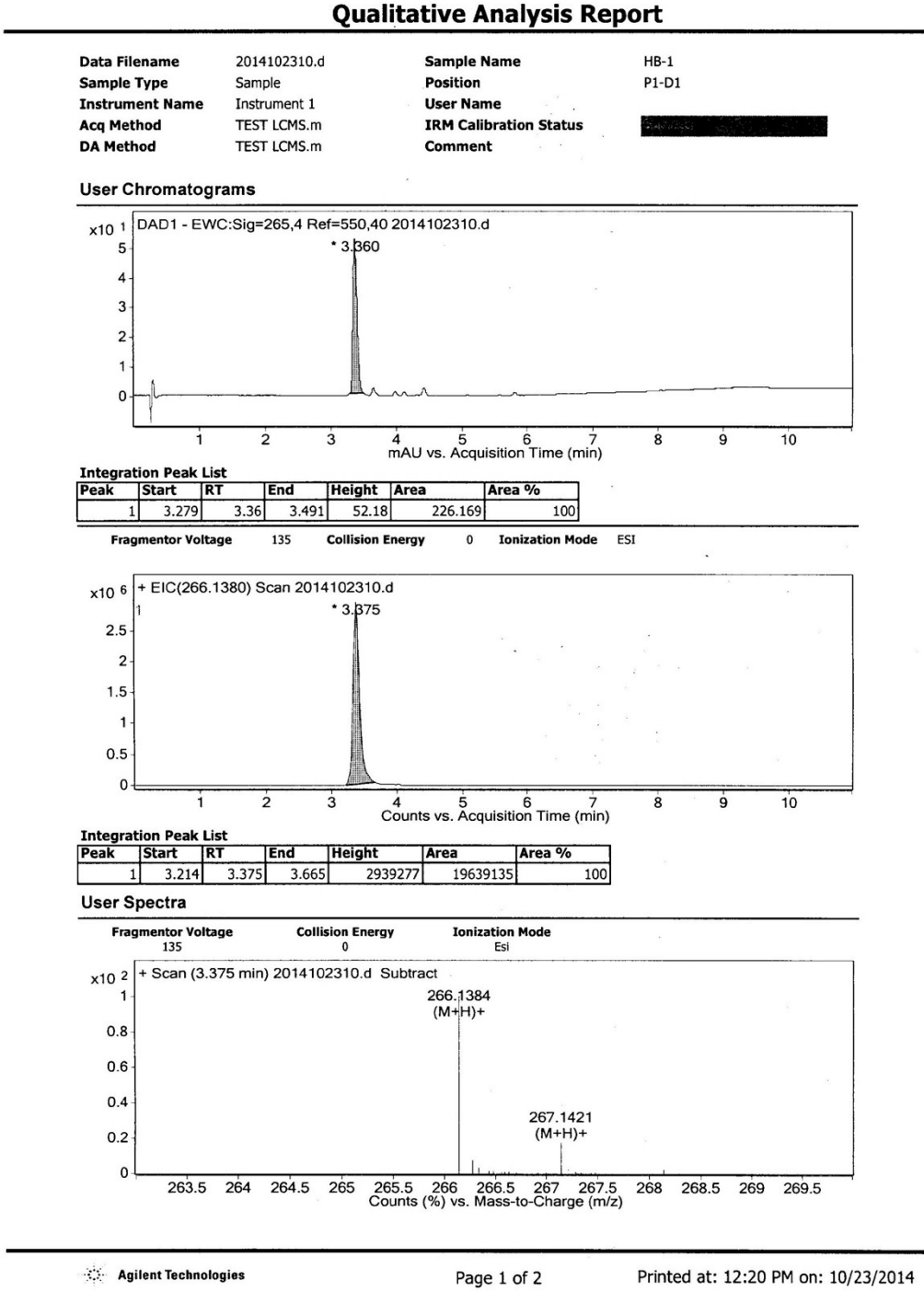


Figure S44. The HR-ESI-MS data of compound **6**

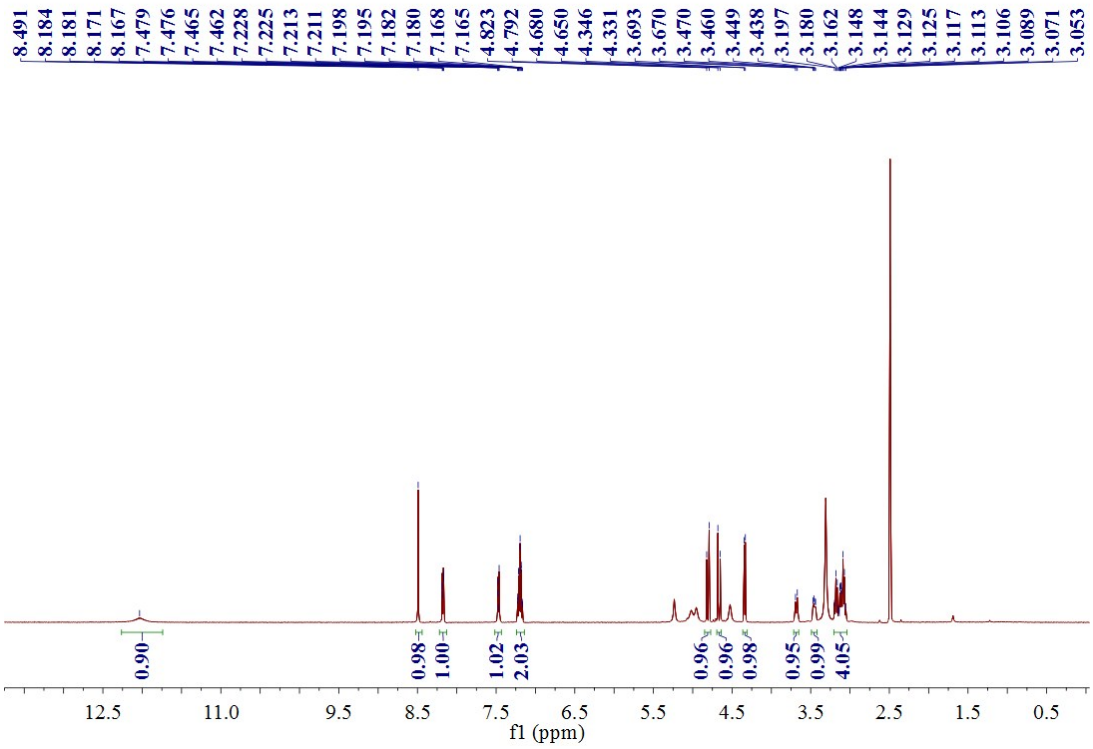


Figure S45. The ^{1}H NMR spectrum of compound **7** in DMSO-d_6

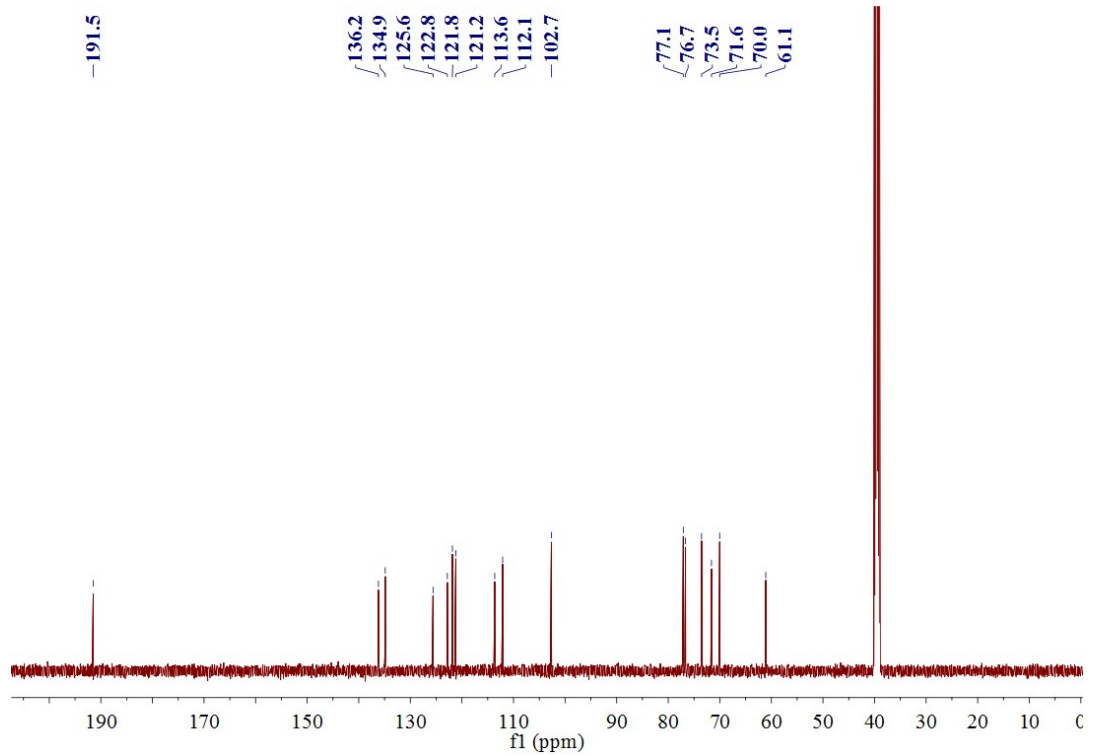


Figure S46. The ^{13}C NMR spectrum of compound **7** in DMSO-d_6

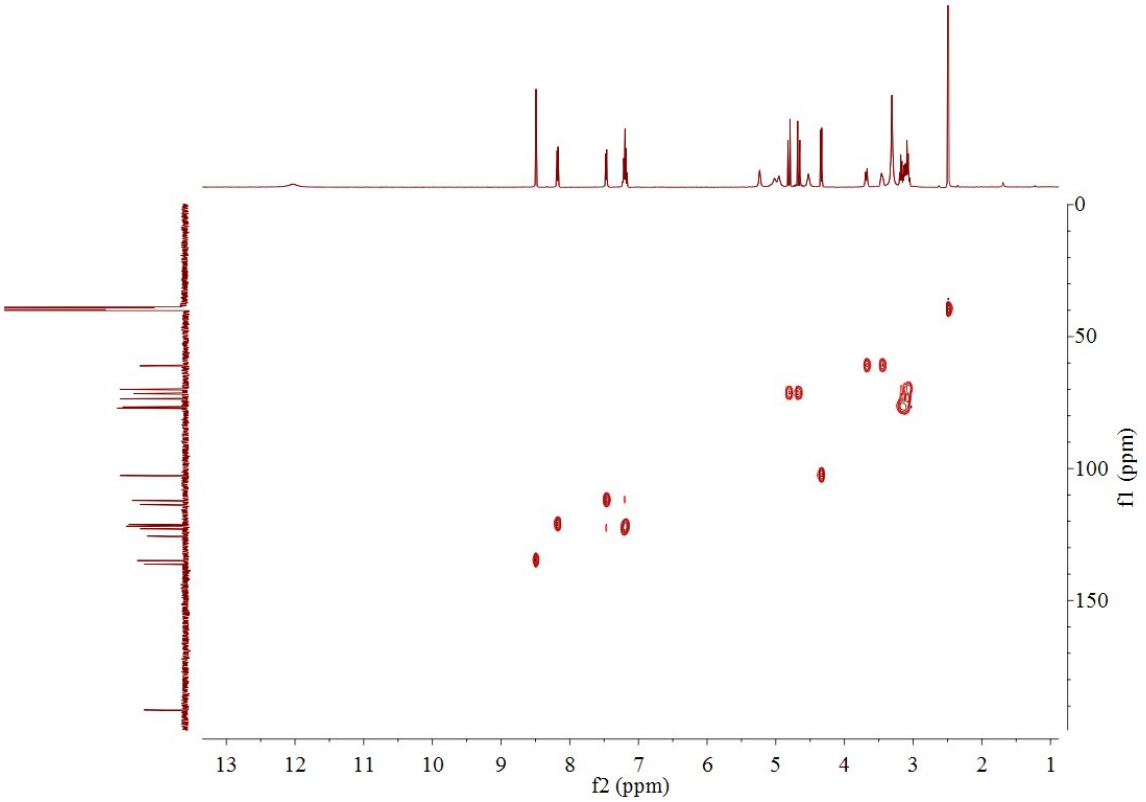


Figure S47. The HSQC spectrum of compound **7** in DMSO-d_6

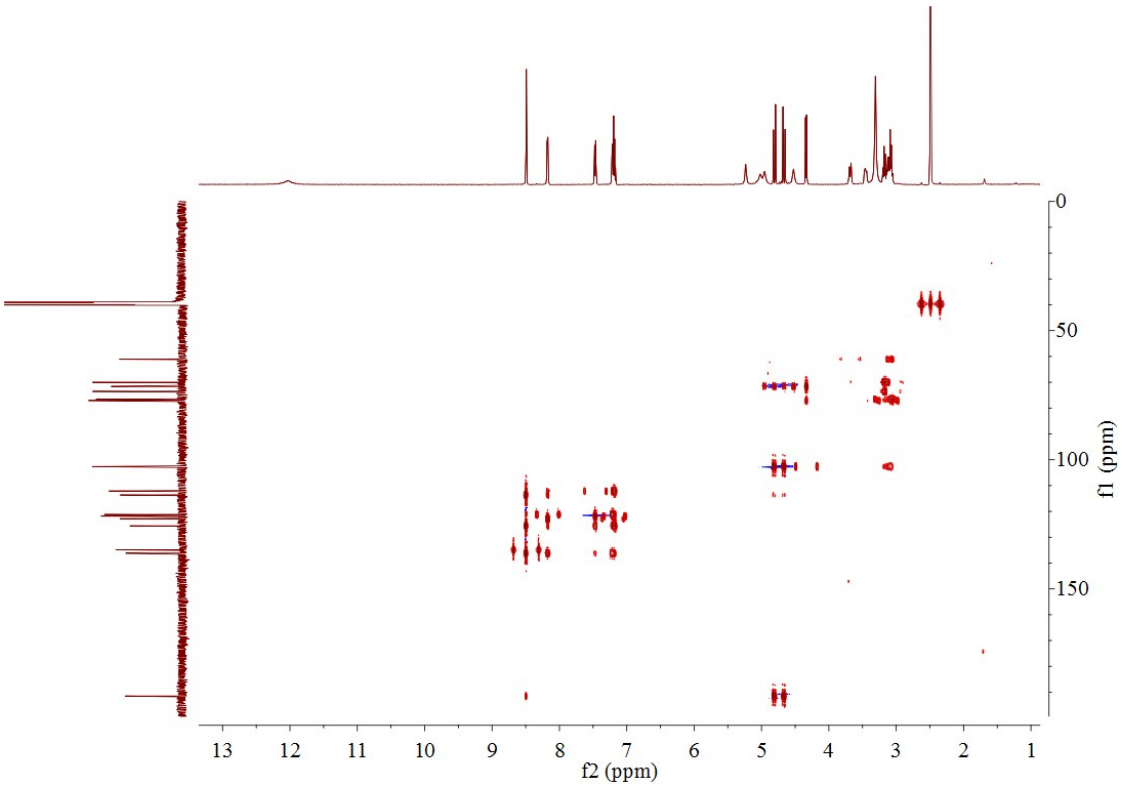


Figure S48. The HMBC spectrum of compound **7** in DMSO-d_6

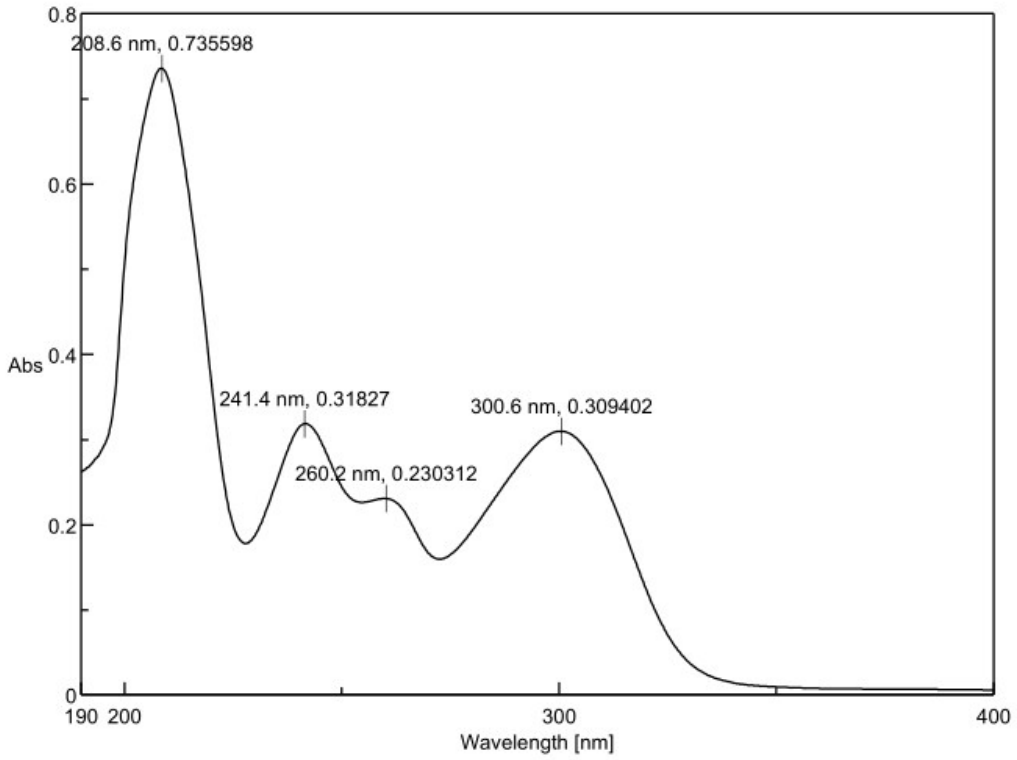


Figure S49. The UV spectrum of compound **7** in MeOH

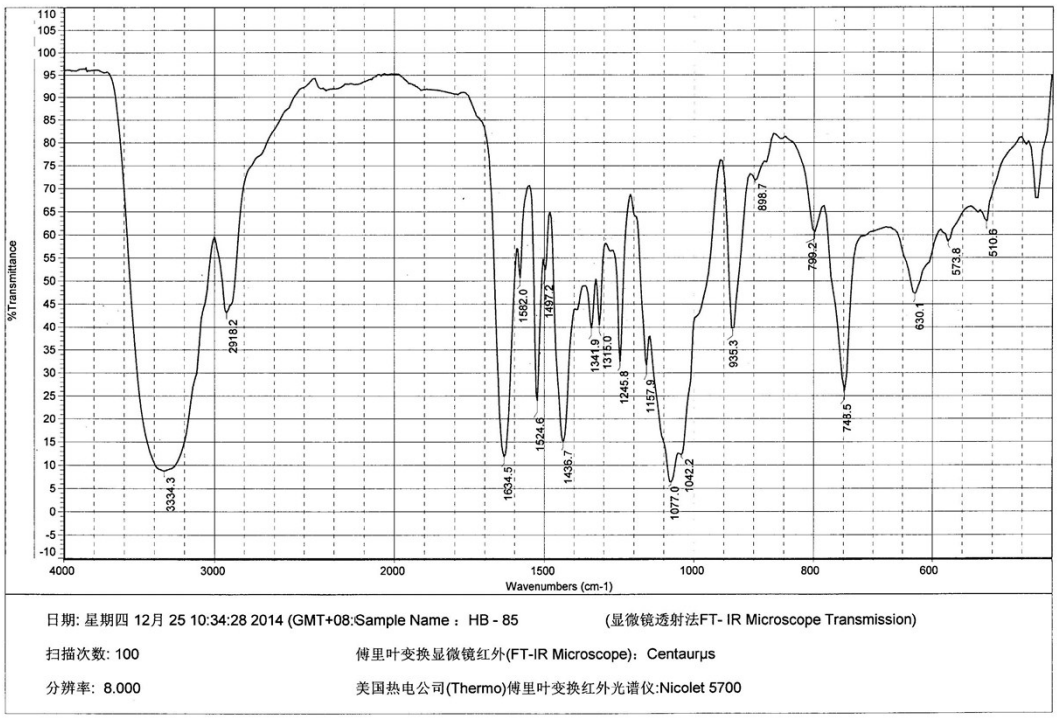


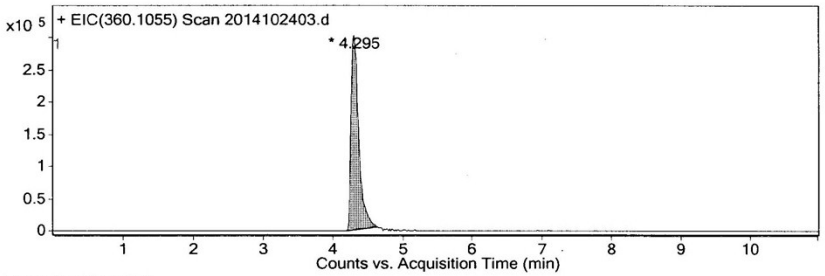
Figure S50. The IR spectrum of compound **7**

Qualitative Analysis Report

Data Filename	2014102403.d	**Sample Name**	HB-85
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST LCMS.m	**IRM Calibration Status**	[redacted]
DA Method	TEST LCMS.m	**Comment**	

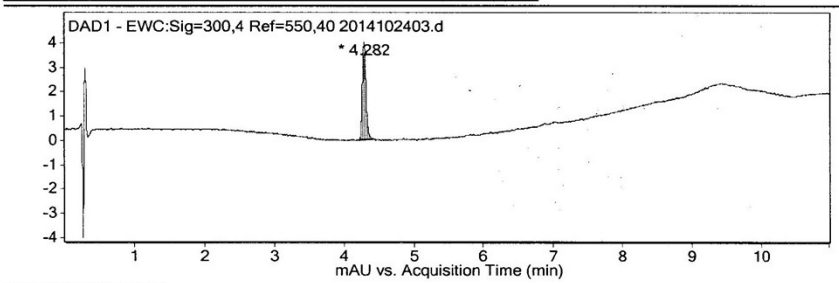
User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.182	4.295	4.633	301897	2357883	100



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.202	4.282	4.427	4.01	14.569	100

User Spectra

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** Esi

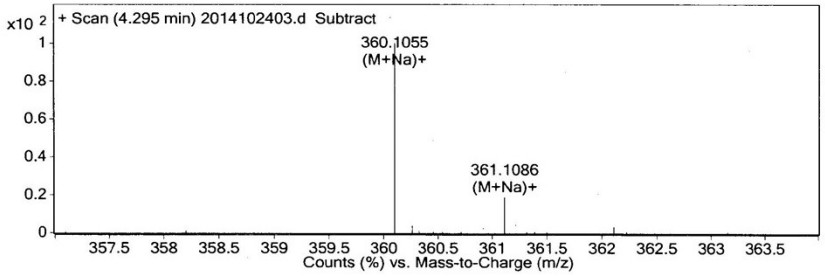


Figure S51. The HR-ESI-MS data of compound **7**

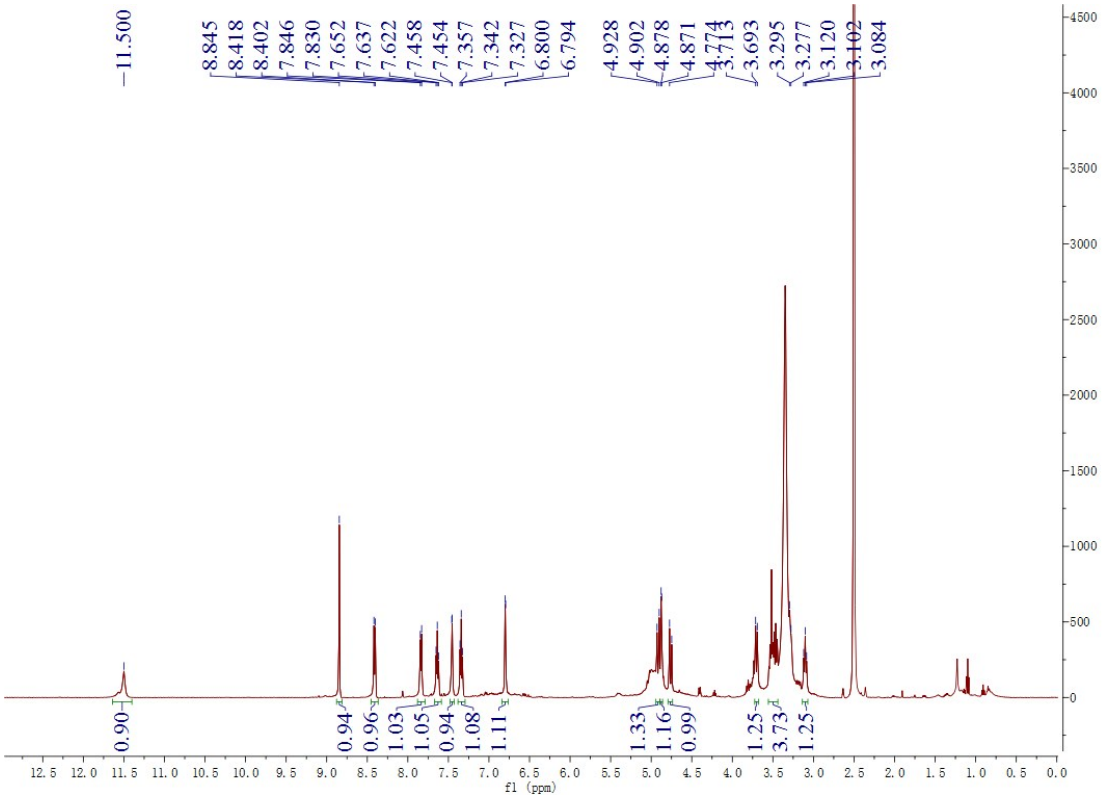


Figure S52. The ^{1}H NMR spectrum of compound **8** in DMSO-d_6

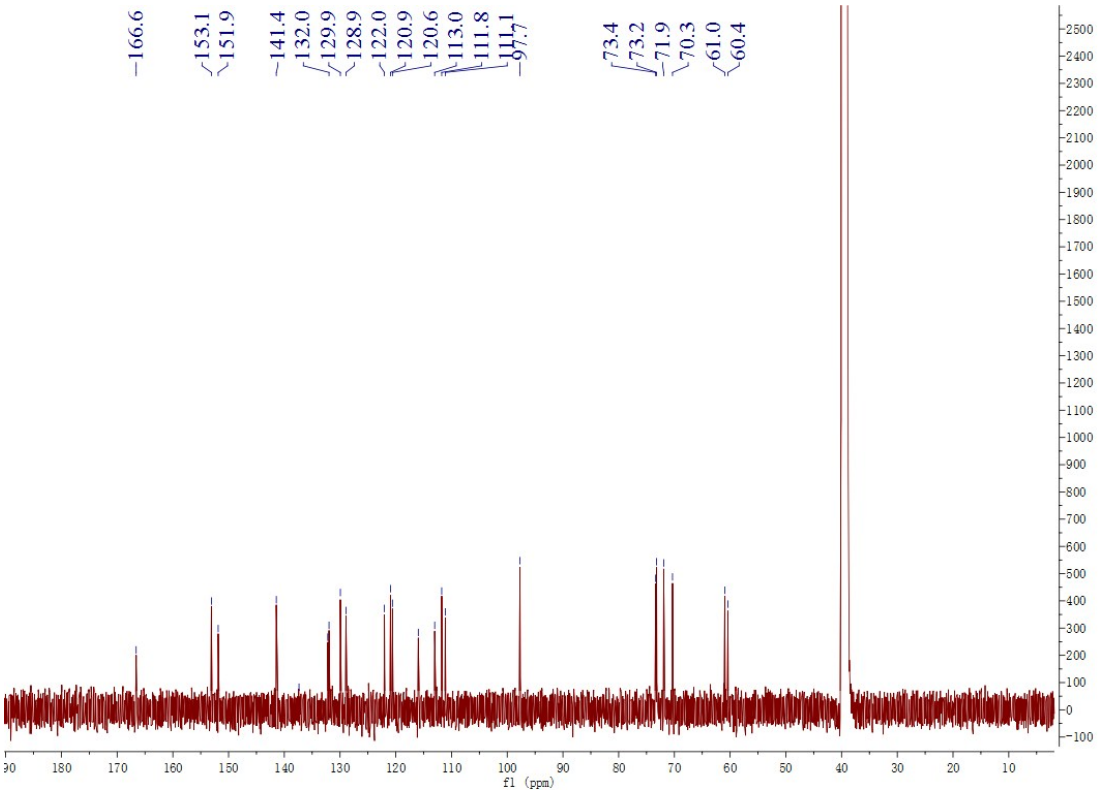


Figure S53. The ^{13}C NMR spectrum of compound **8** in DMSO-d_6

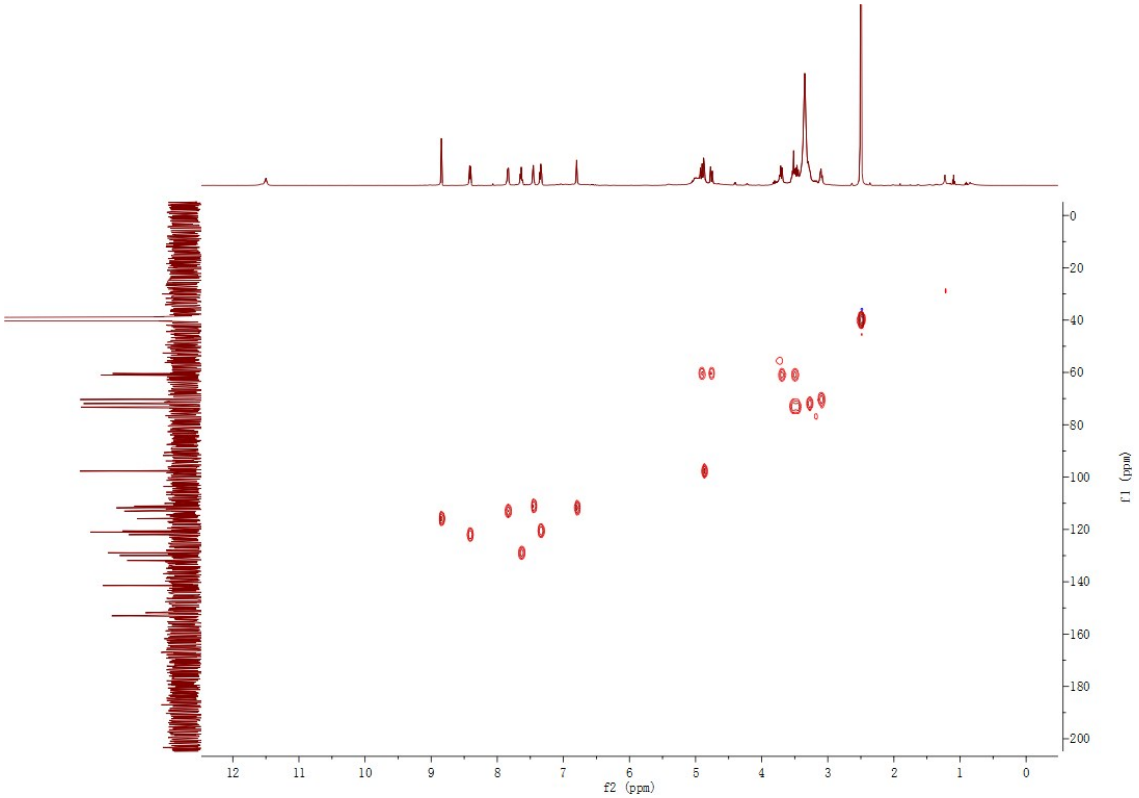


Figure S54. The HSQC spectrum of compound **8** in DMSO-d_6

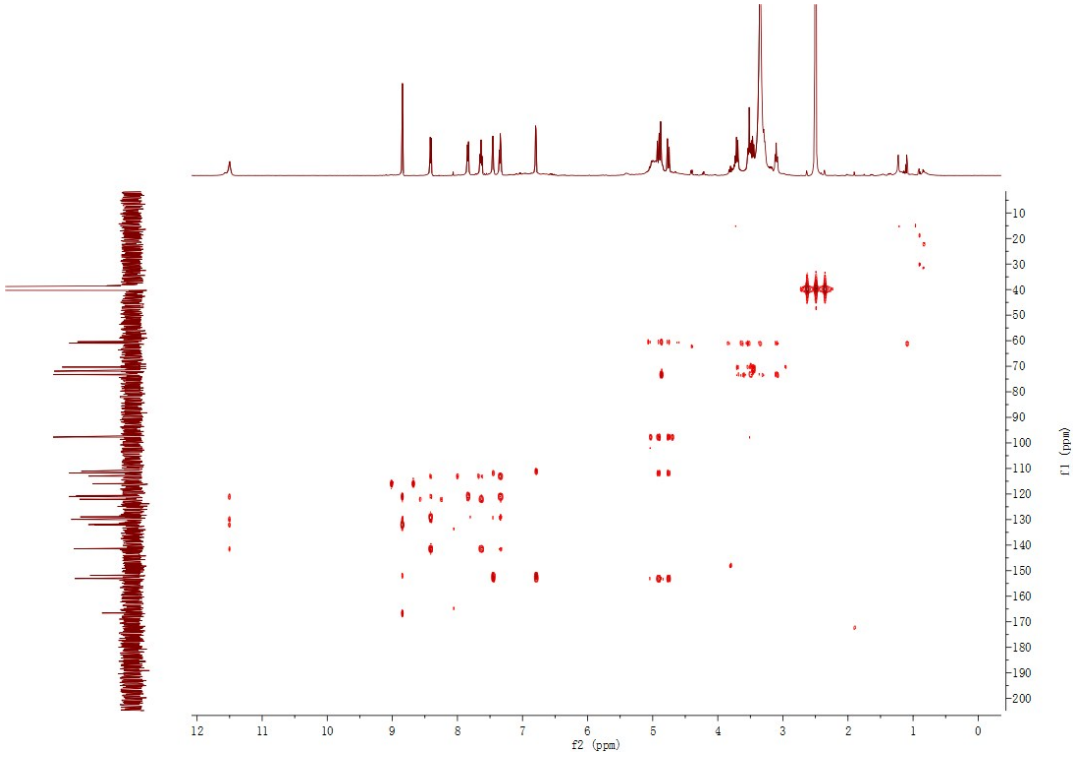


Figure S55. The HMBC spectrum of compound **8** in DMSO-d_6

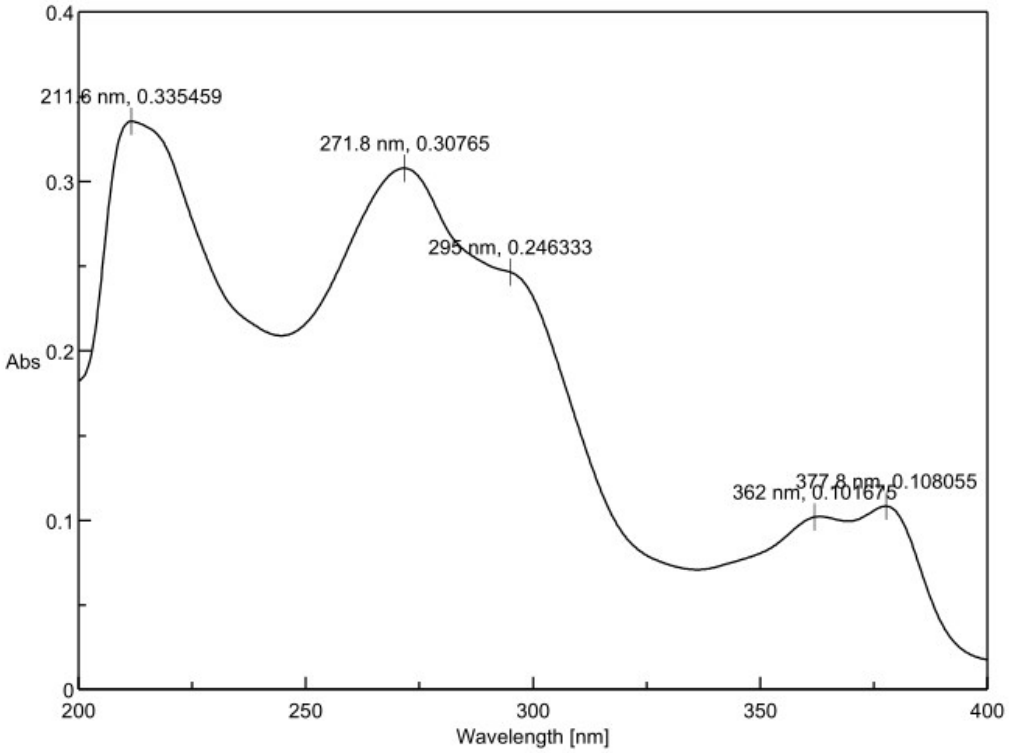


Figure S56. The UV spectrum of compound **8** in MeOH

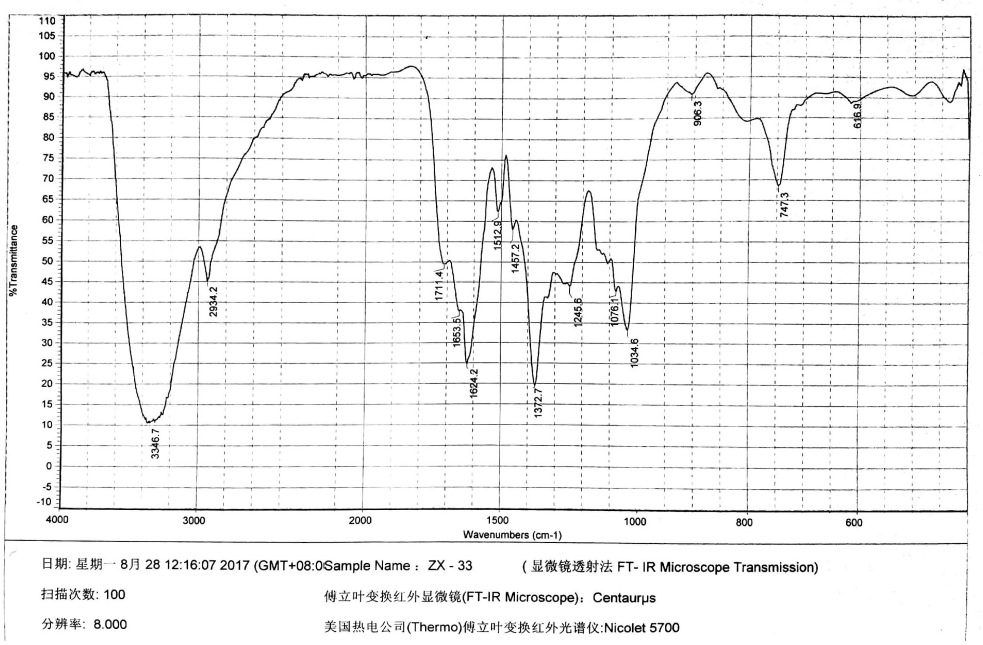
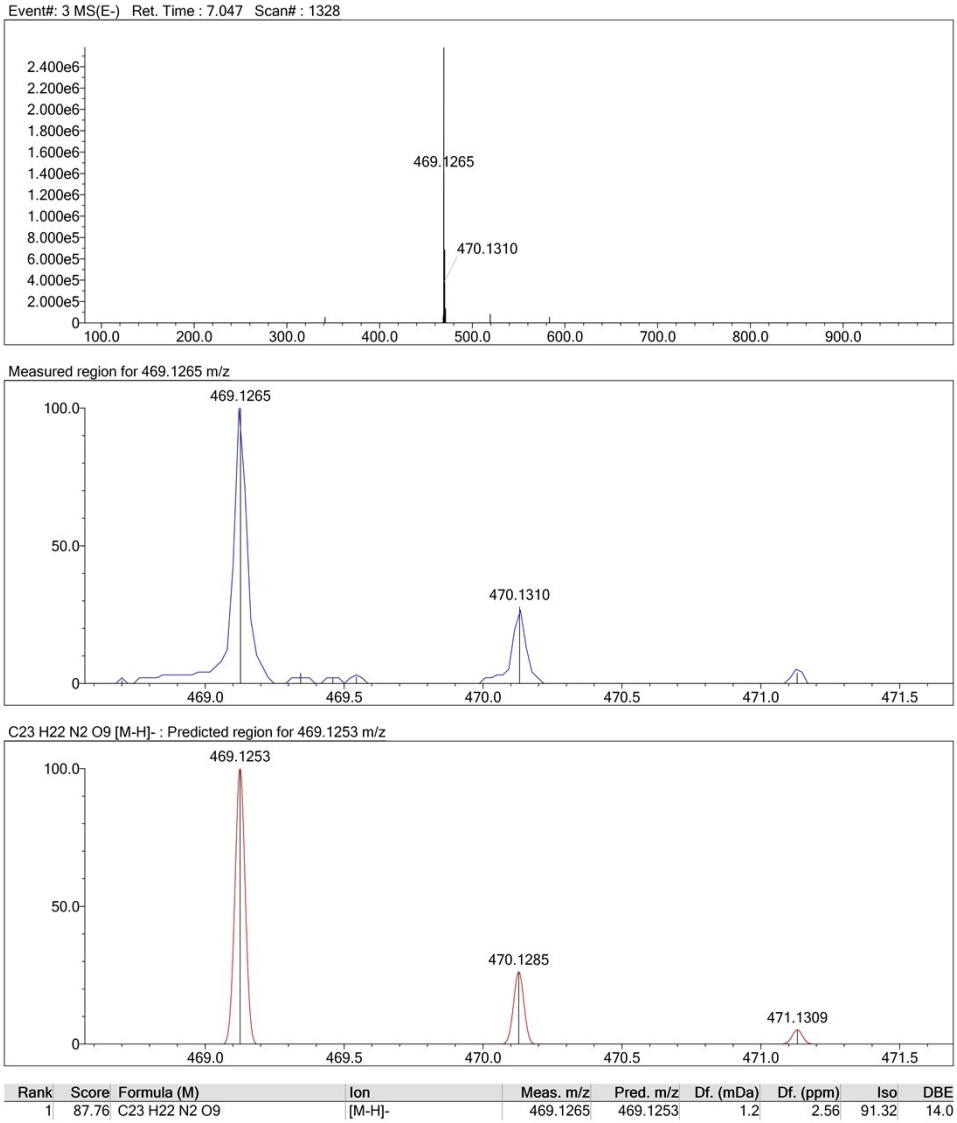


Figure S57. The IR spectrum of compound **8**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.76	C23 H22 N2 O9	[M-H]-	469.1265	469.1253	1.2	2.56	91.32	14.0

Figure S58. The HR-ESI-MS data of compound **8**

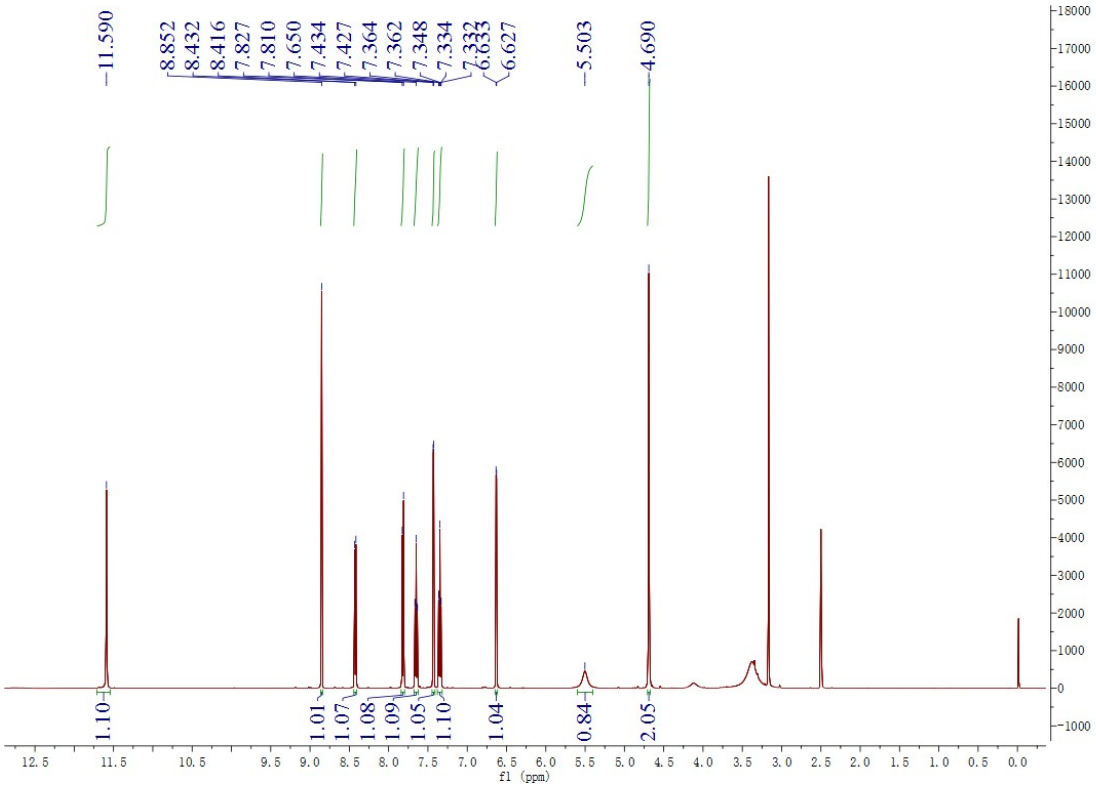


Figure S59. The ^{1}H NMR spectrum of compound **9** in DMSO-d_6

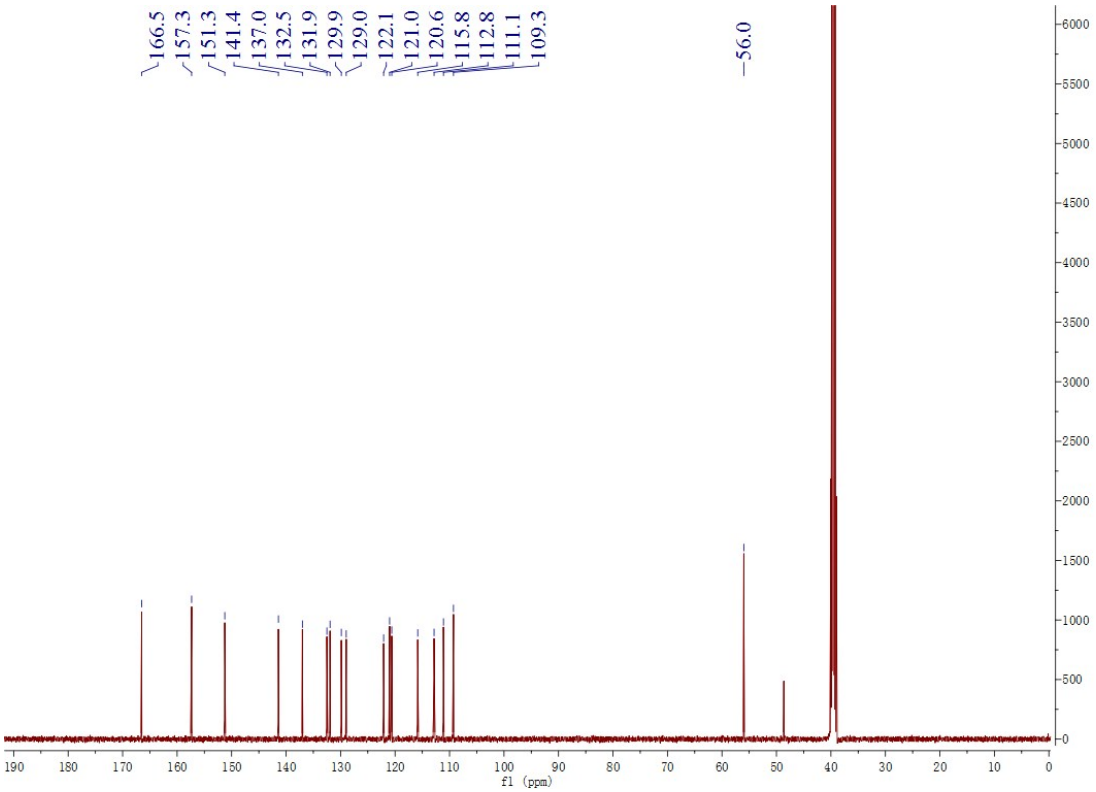
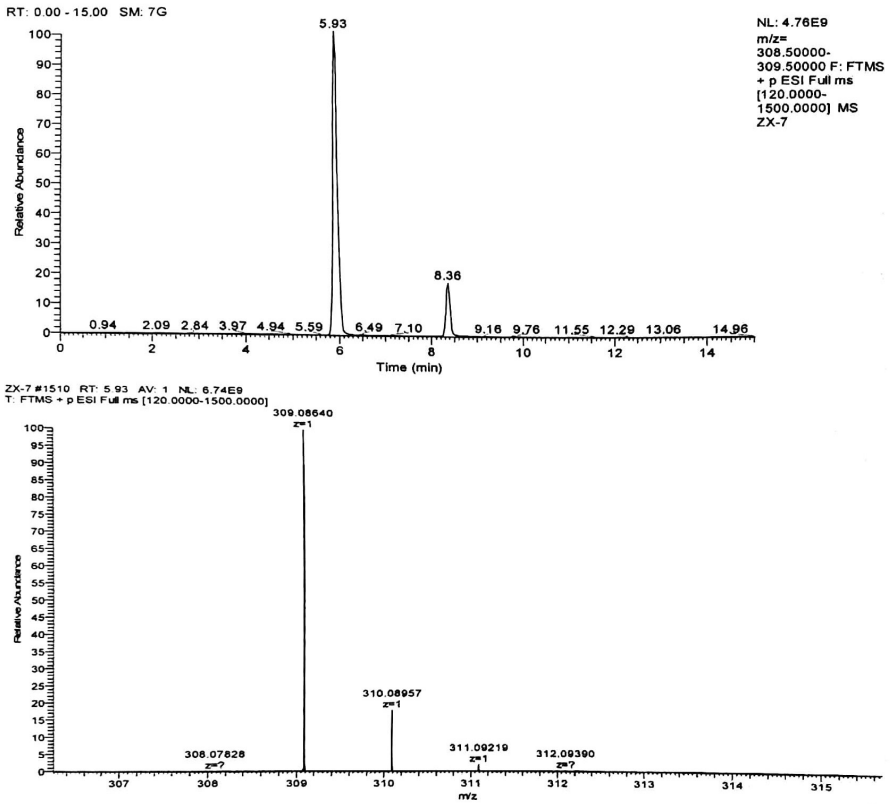


Figure S60. The ^{13}C NMR spectrum of compound **9** in DMSO-d_6

Thermo Qexactive Focus Report

compound NO. : ZX-7

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
309.08640	309.08592	0.48	14.5	C16 H10 N6 Na	
	309.08698	-0.58	12.5	C17 H13 O4 N2	M+H
	309.08726	-0.86	14	C18 H12 O N3 Na	

Figure S61. The HR-ESI-MS data of compound **9**

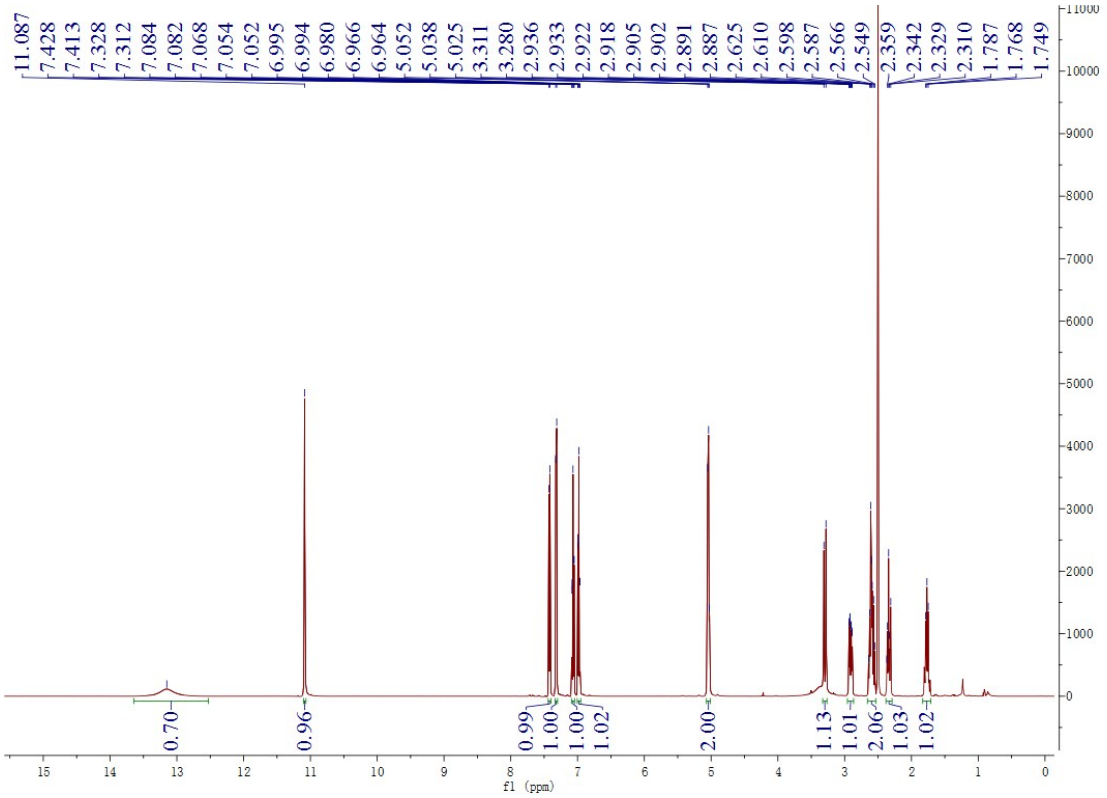


Figure S62. The ^{1}H NMR spectrum of compound **10** in DMSO-d_6

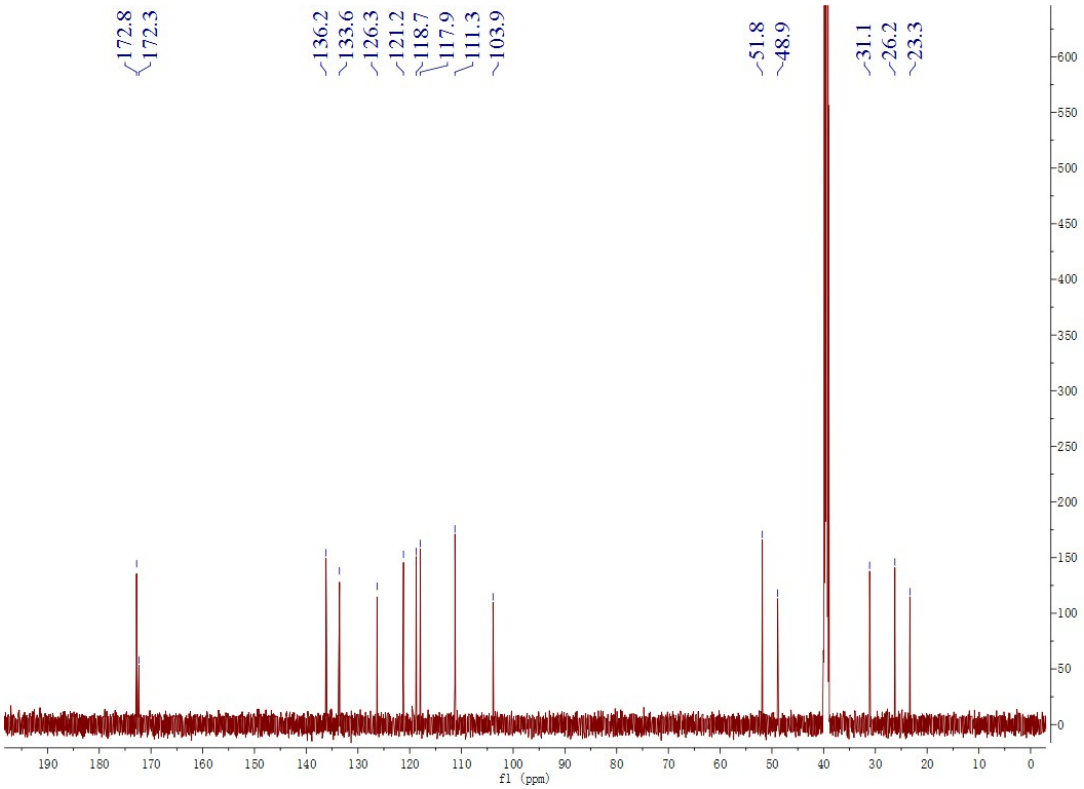
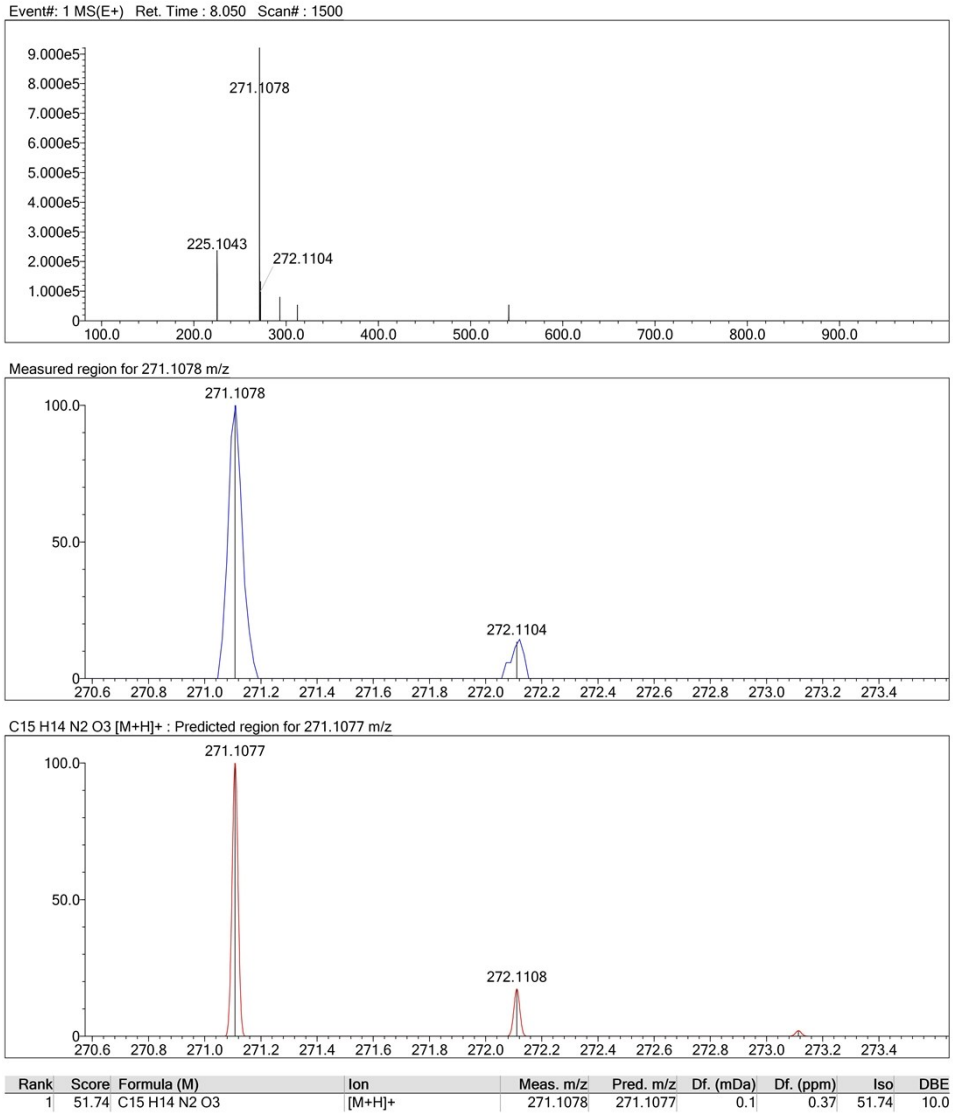


Figure S63. The ^{13}C NMR spectrum of compound **10** in DMSO-d_6



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.74	C15 H14 N2 O3	[M+H]+	271.1078	271.1077	0.1	0.37	51.74	10.0

Figure S64. The HR-ESI-MS data of compound **10**

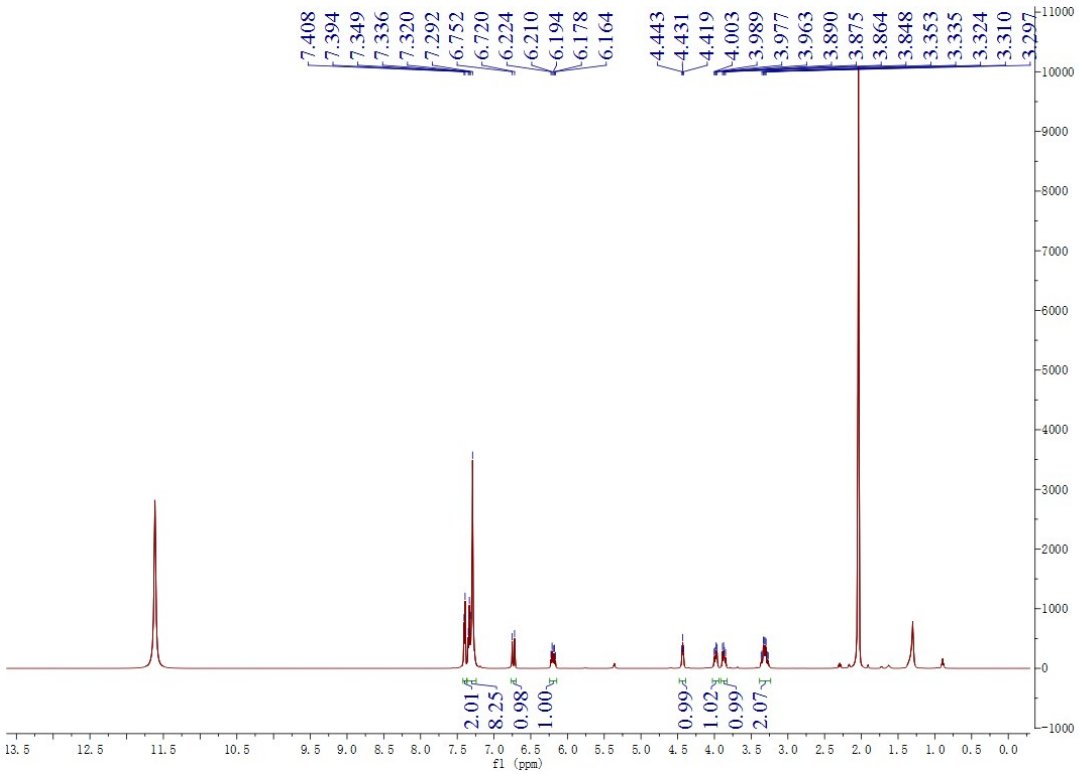


Figure S65. The ^{1}H NMR spectrum of compound **1b** in acetic acid-d_4

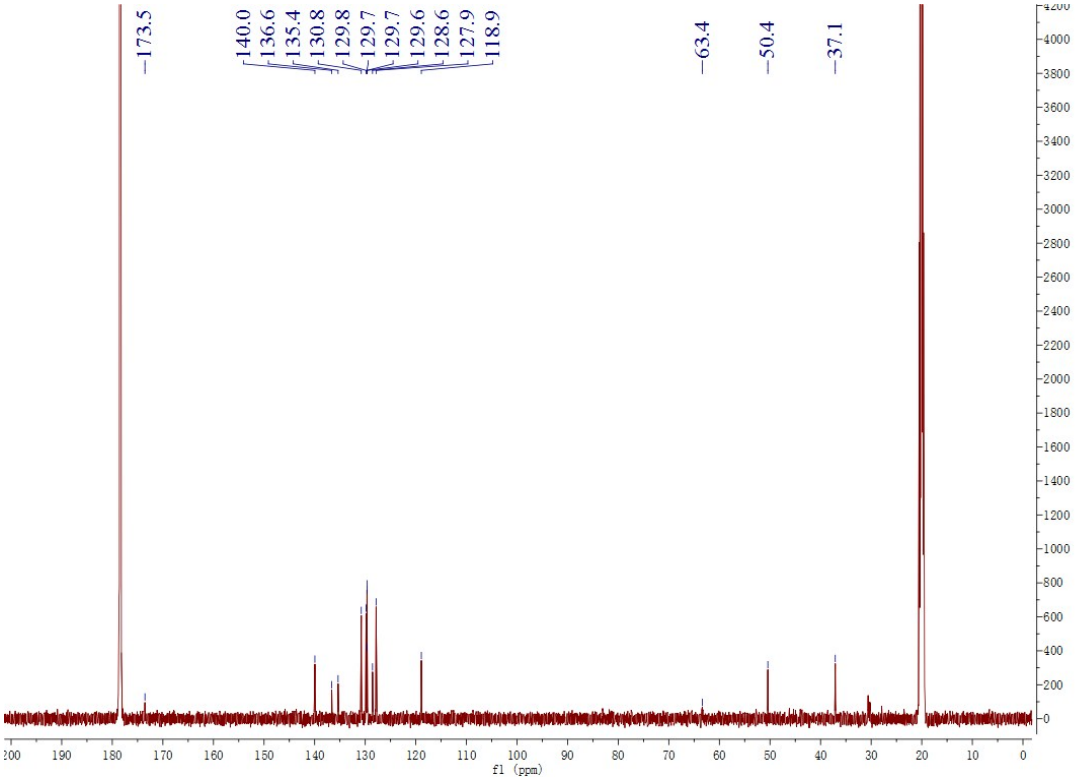
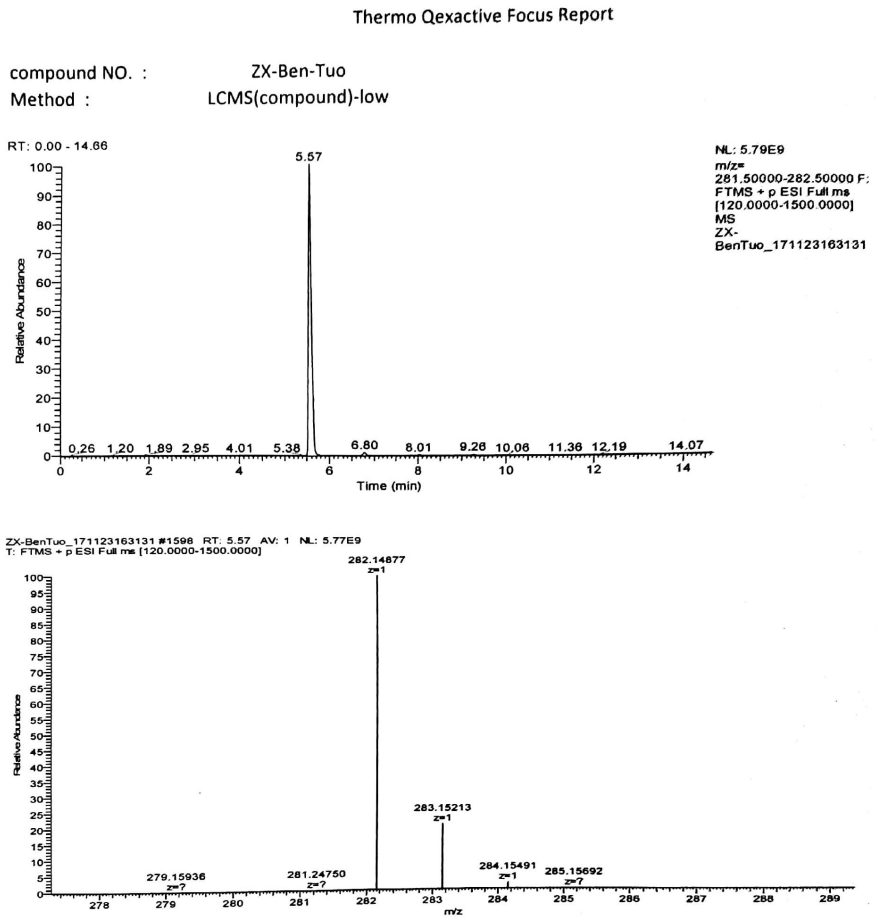


Figure S66. The ^{13}C NMR spectrum of compound **1b** in acetic acid-d_4



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
282.14877	282.14886	-0.09	9.5	C18 H20 O2 N	M+H
	282.14645	2.32	6.5	C16 H21 O2 N Na	
	282.14618	2.59	5	C15 H22 O5	
	282.14377	5	2	C13 H23 O5 Na	

Figure S67. The HR-ESI-MS data of compound **1b**

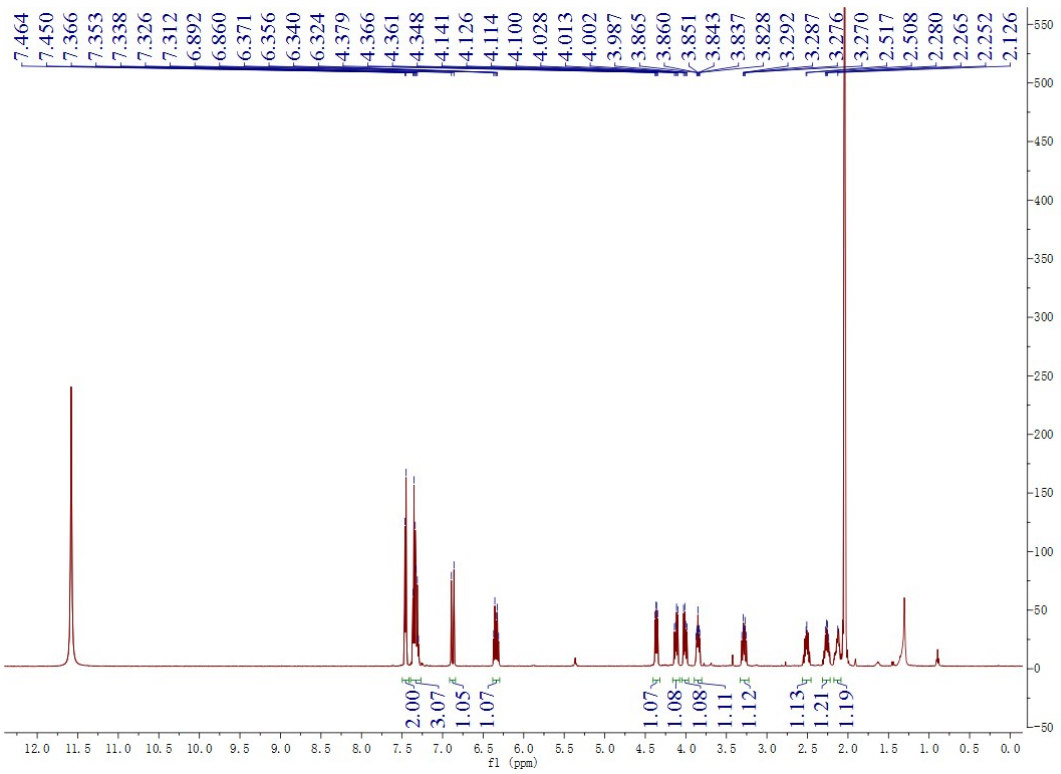


Figure S68. The ^{1}H NMR spectrum of compound **2b** in acetic acid-d_4

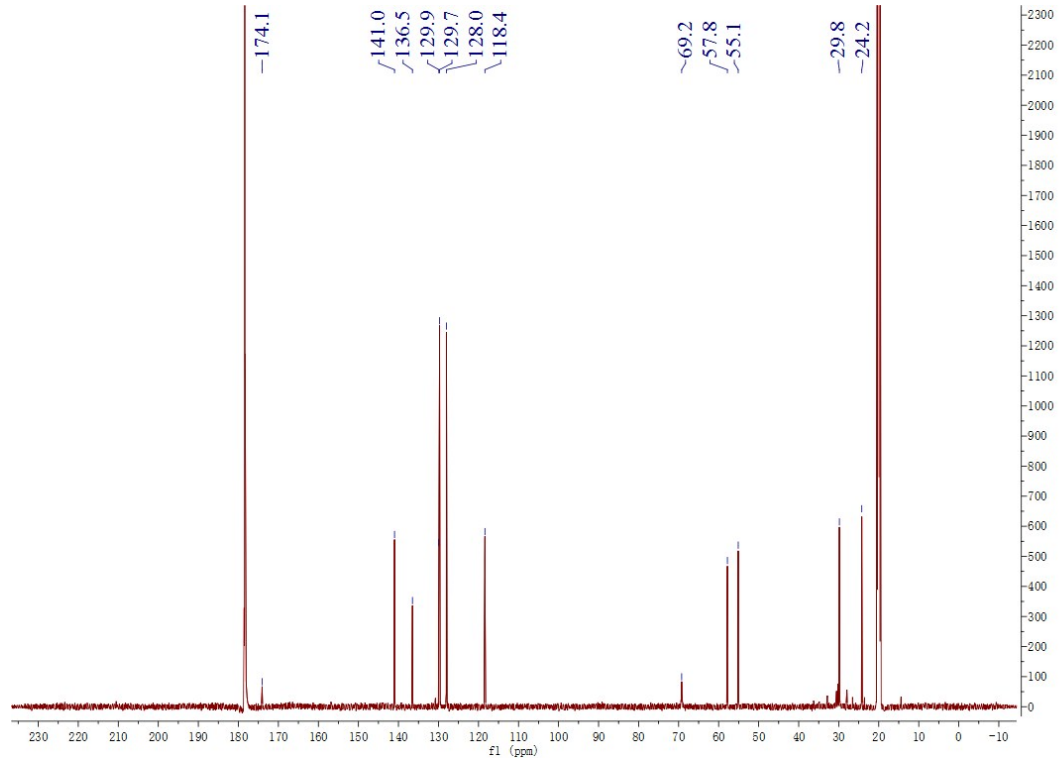
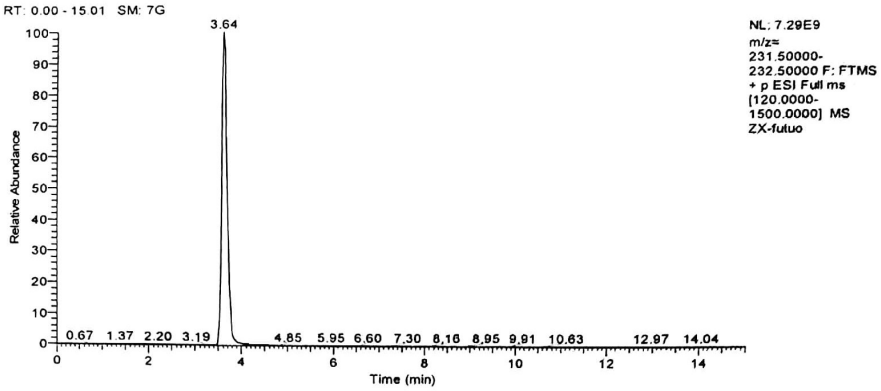
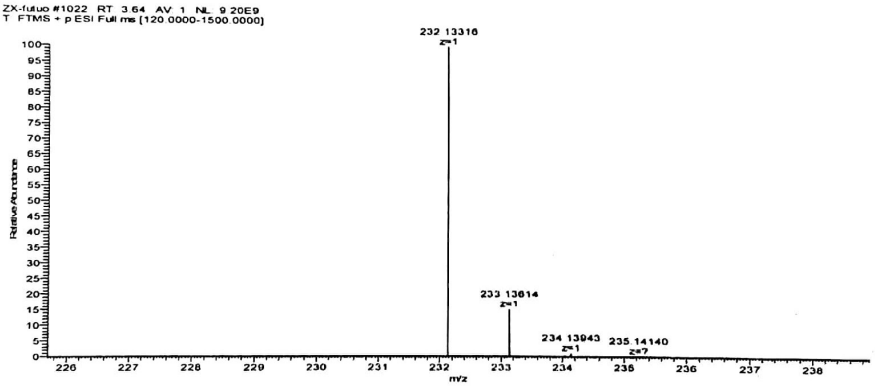


Figure S69. The ^{13}C NMR spectrum of compound **2b** in acetic acid-d_4

Thermo Qexactive Focus Report

compound NO. : ZX-FuTuo
Method : LCMS(compound)-low





m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
232.13316	232.13321	-0.05	6.5	C14 H18 O2 N	M+H

Figure S70. The HR-ESI-MS data of compound **2b**

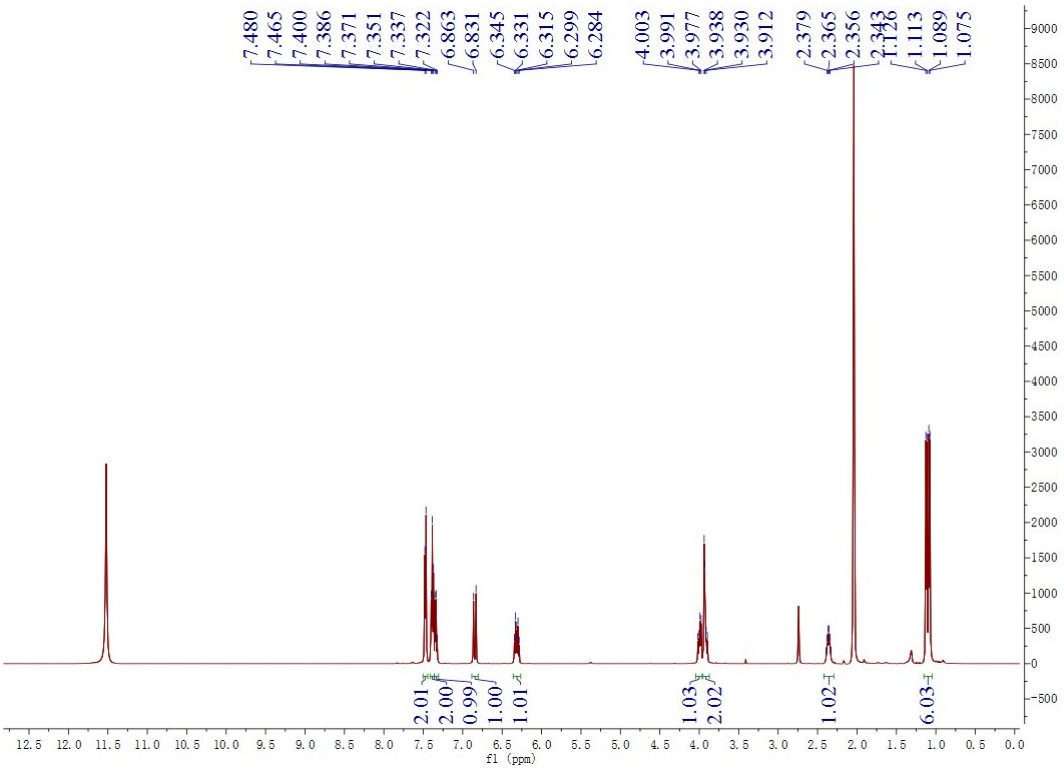


Figure S71. The ^{1}H NMR spectrum of compound **3b** in acetic acid-d_4

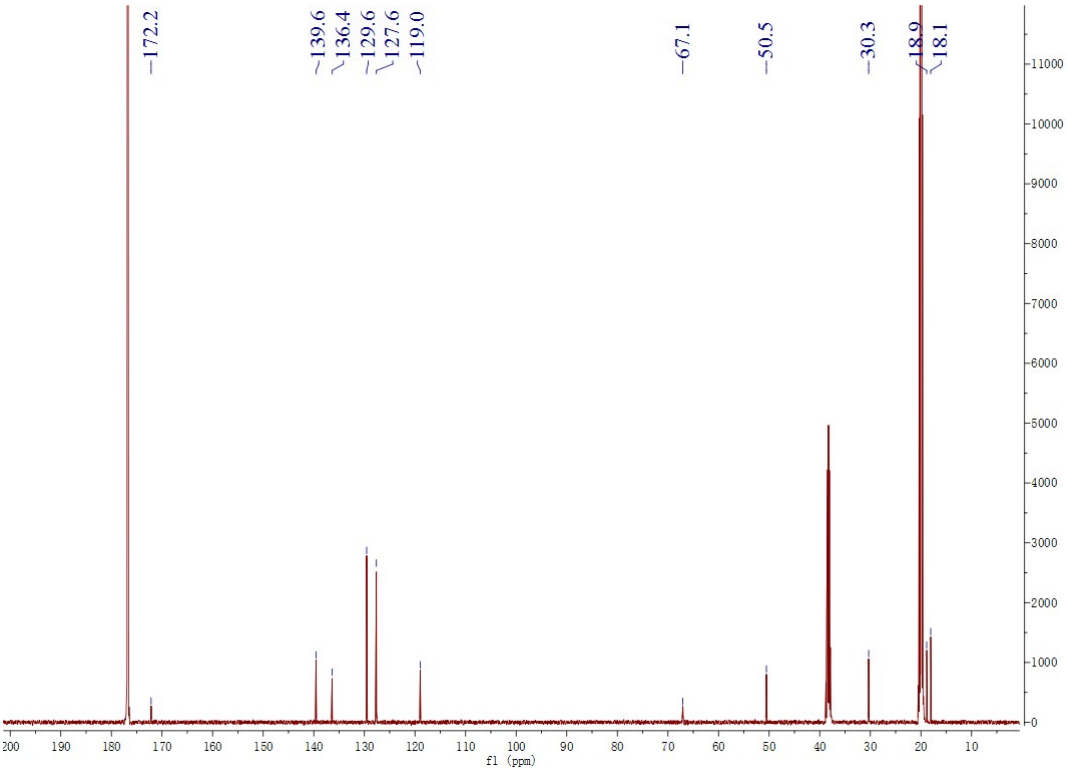
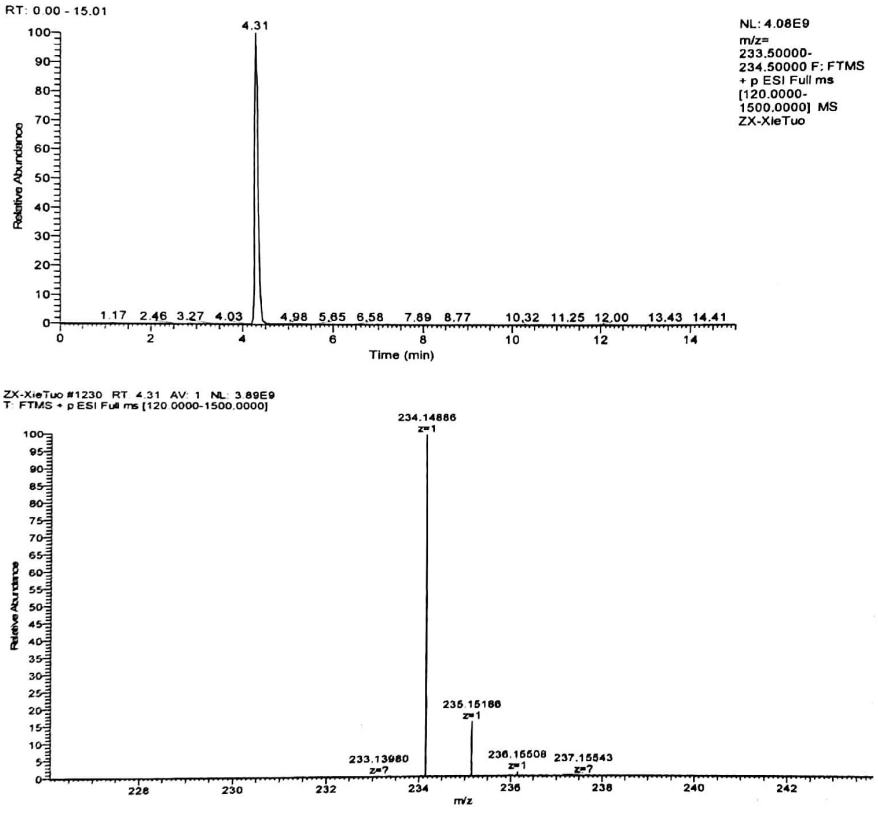


Figure S72. The ^{13}C NMR spectrum of compound **3b** in acetic acid-d_4

Thermo Qexactive Focus Report

compound NO. : ZX-Xie-Tuo

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
234.14886	234.14886	0	5.5	C14 H20 O2 N	M+H
	234.14645	2.41	2.5	C12 H21 O2 N Na	
	234.14618	2.68	1	C11 H22 O5	

Figure S73. The HR-ESI-MS data of compound **3b**

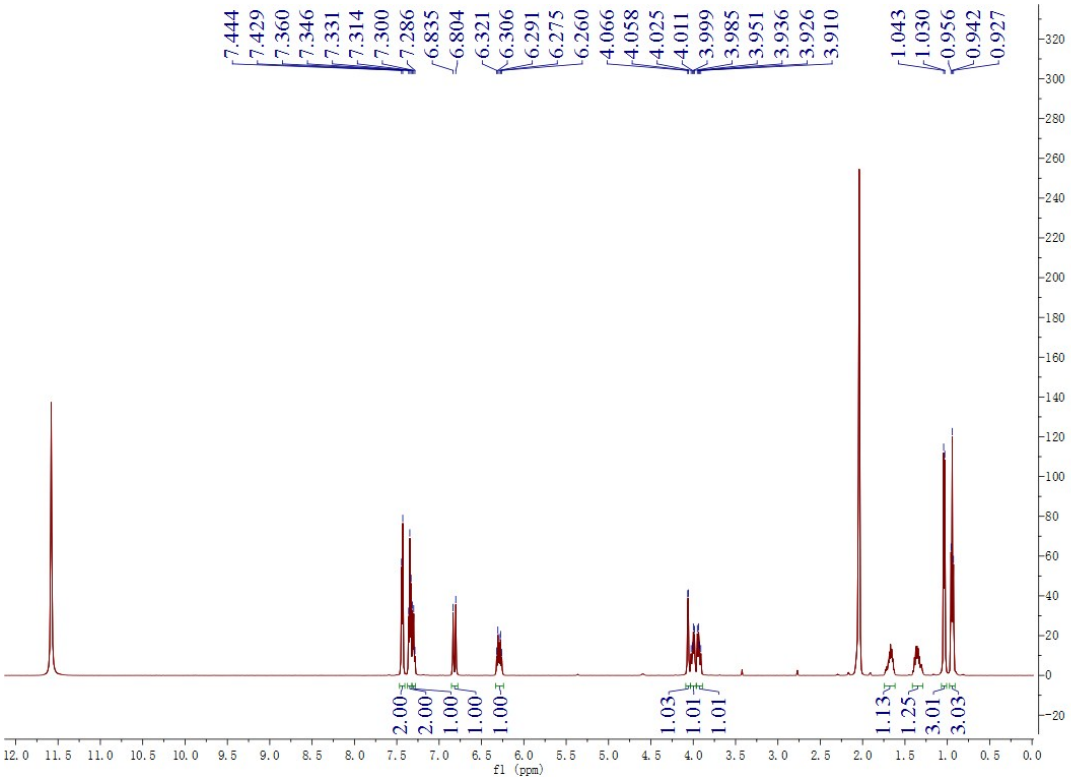


Figure S74. The ^{1}H NMR spectrum of compound **4b** in acetic acid-d_4

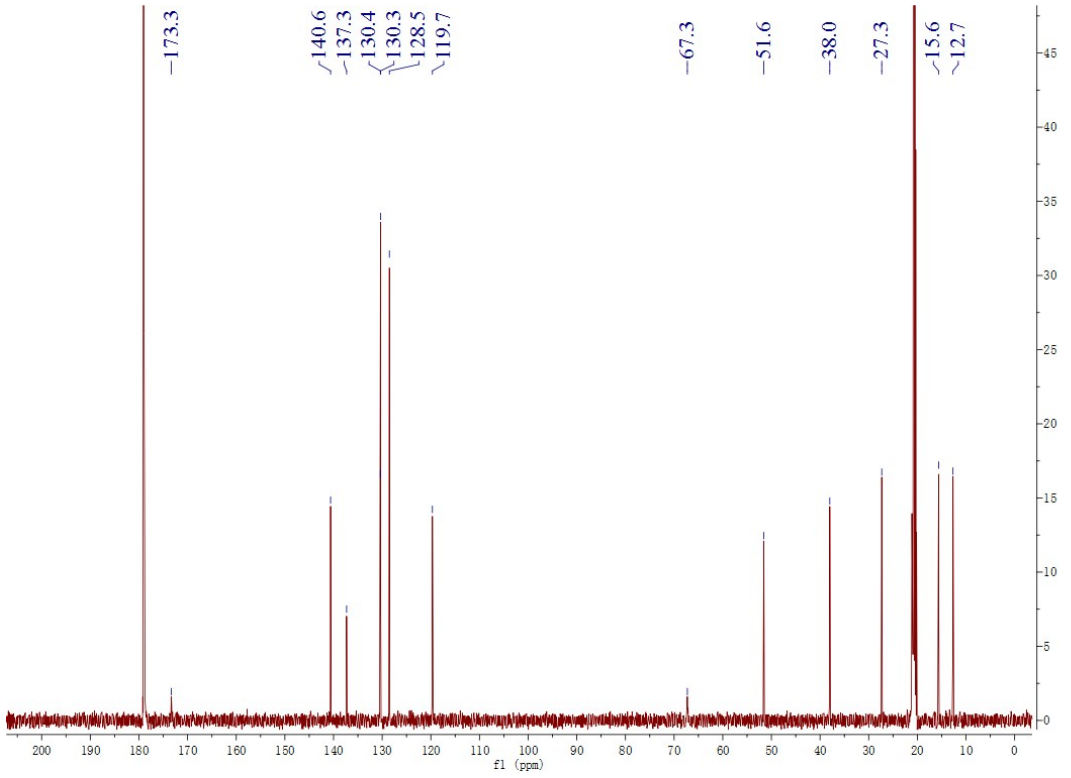
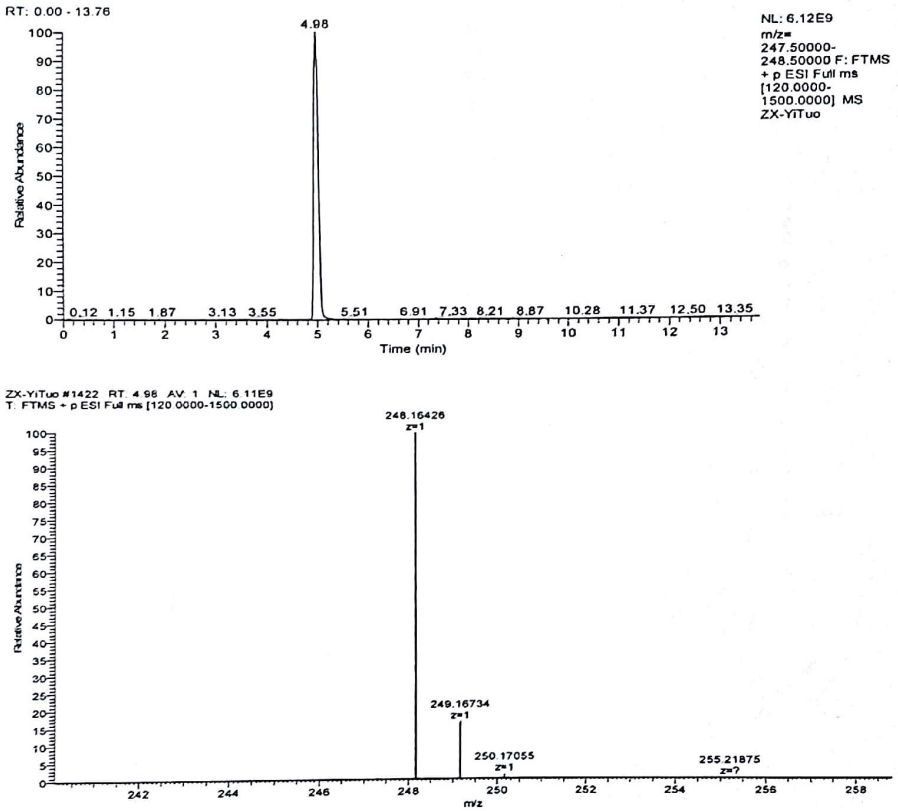


Figure S75. The ^{13}C NMR spectrum of compound **4b** in acetic acid-d_4

Thermo Qexactive Focus Report

compound NO. : ZX-Yi-Tuo

Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
248.16426	248.16451	-0.25	5.5	C15 H22 O2 N	M+H
	248.16210	2.16	2.5	C13 H23 O2 N Na	
	248.16183	2.43	1	C12 H24 O5	

Figure S76. The HR-ESI-MS data of compound **4b**

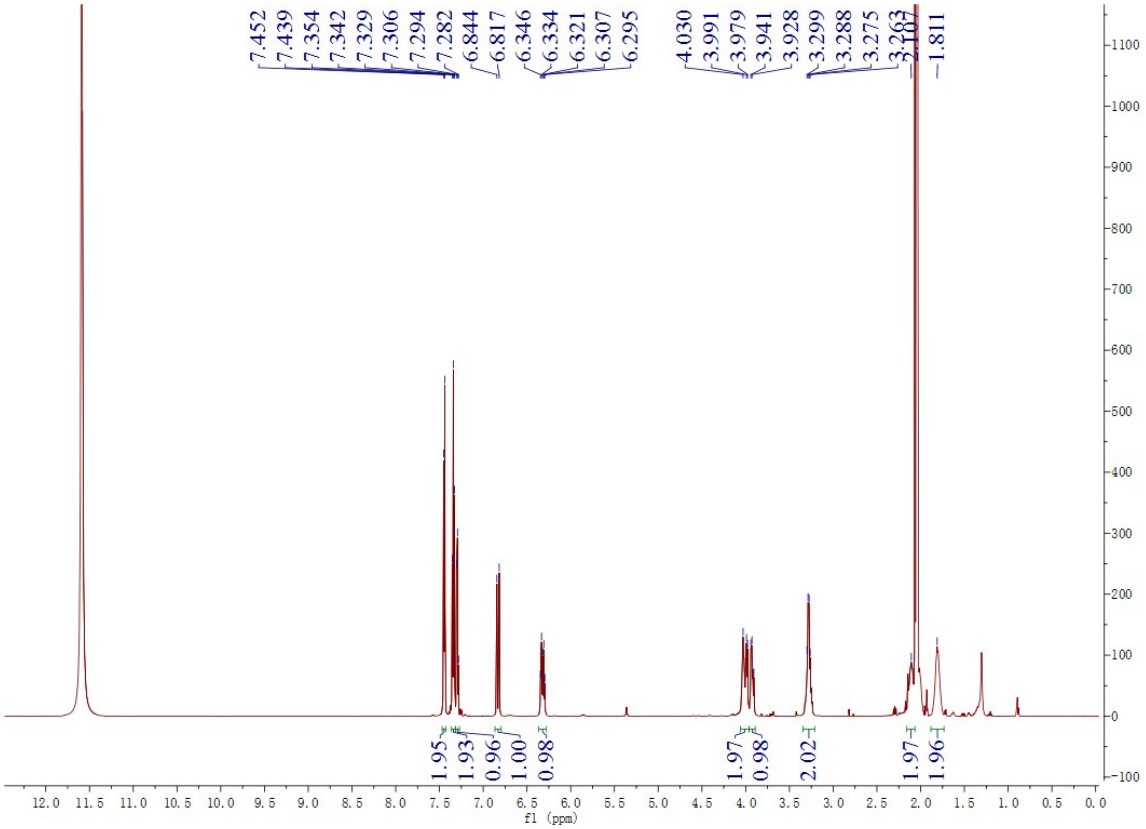


Figure S77. The ^{1}H NMR spectrum of compound **5b** in acetic acid-d_4

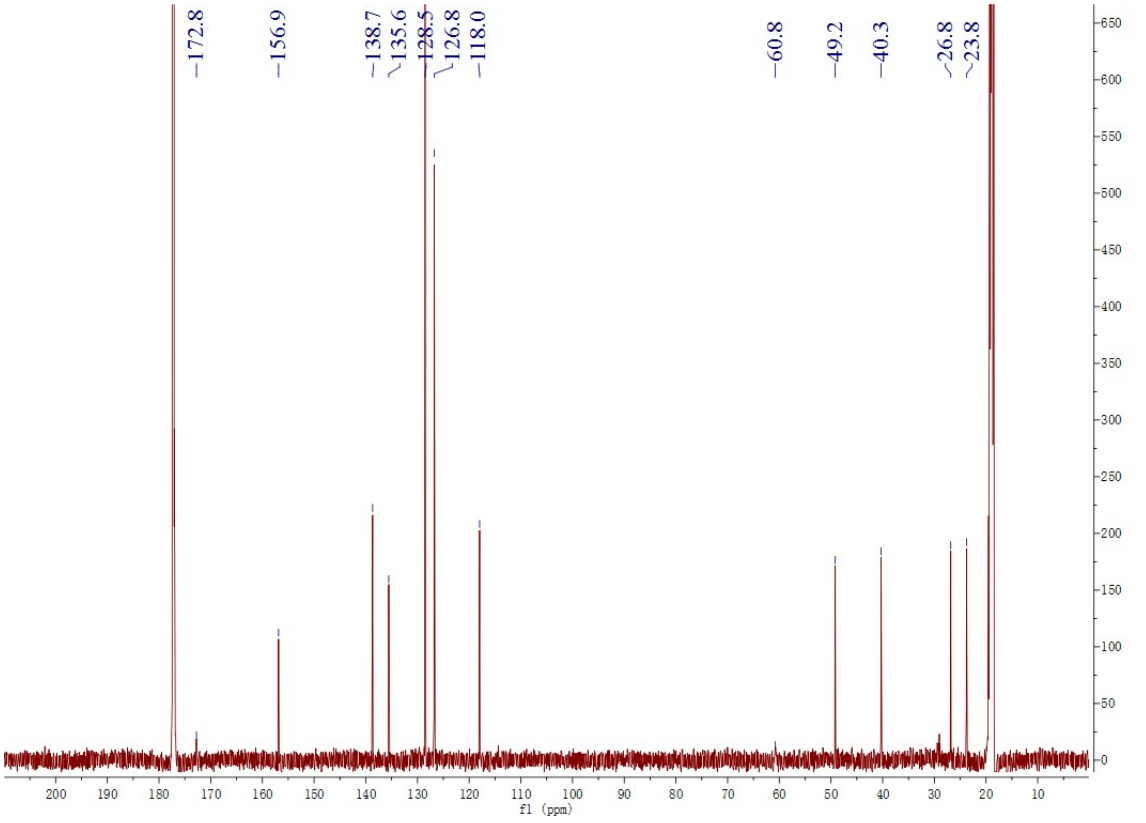
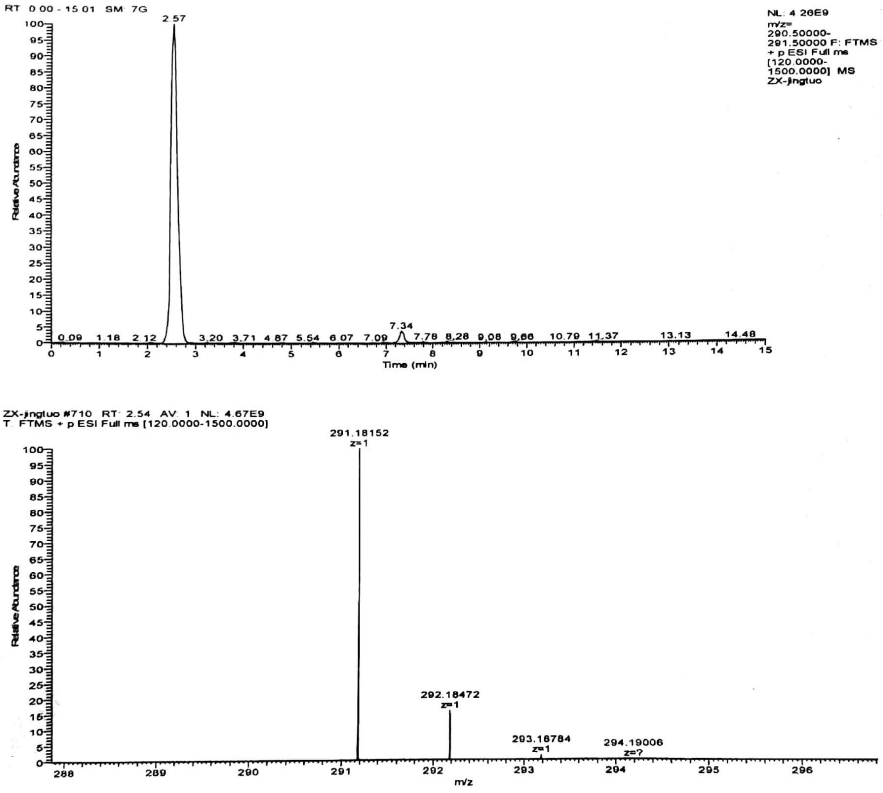


Figure S78. The ^{13}C NMR spectrum of compound **5b** in acetic acid-d_4

Thermo Qexactive Focus Report

compound NO. : ZX-JingTuo
Method : LCMS(compound)-low



m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition	
291.18152	291.18155	-0.03	6.5	C15 H23 O2 N4	M+H
	291.18049	1.03	3	C15 H26 O3 N Na	
	291.18022	1.3	1.5	C14 H27 O6	
	291.18021	1.31	7	C13 H21 O N7	
	291.1829	-1.38	6	C17 H25 O3 N	

Figure S79. The HR-ESI-MS data of compound **5b**

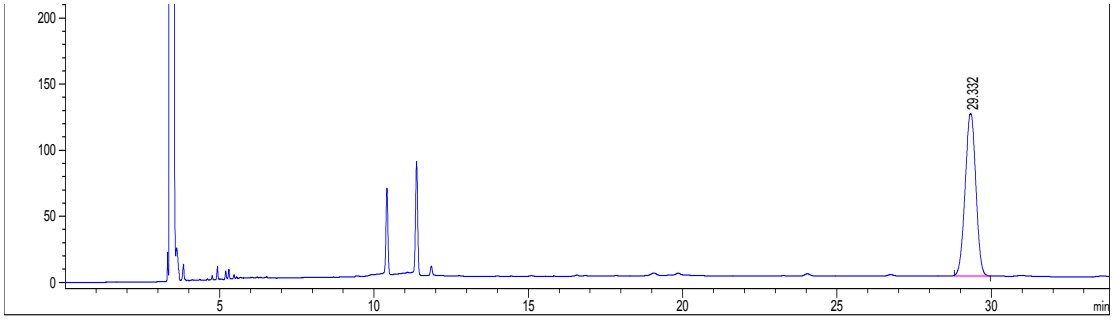


Figure S80. The Gas Chromatographic separation of D-Glc

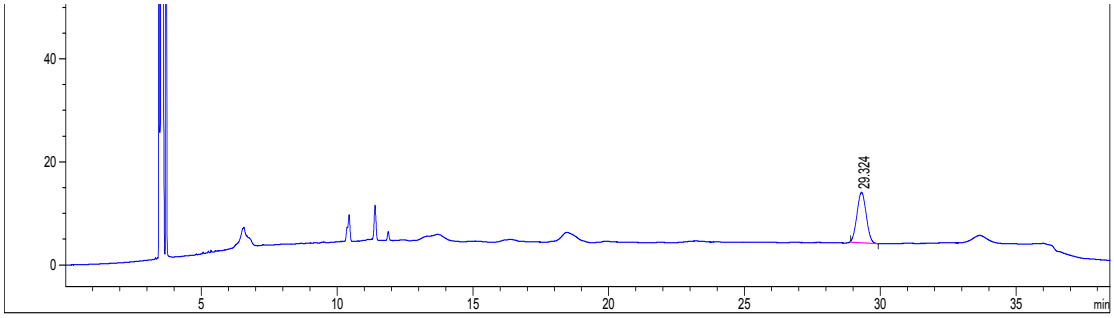


Figure S81. The Gas Chromatographic analyses of sugar moeities of compounds **7-8**

Table S82. The neuroprotective effects of **1-10**

	Concentration	cell viability rate (%)			increase the cell viability rate	P
		1	2	3		
Control		100%	100%	100%		
H_2O_2	0.0034%	69.39%	69.39%	68.04%		2.68265E-07
edaravone	10μM	81.97%	93.96%	89.42%	24.16%	0.042695737
1	10μM	59.46%	63.56%	60.38%	-11.32%	0.004108491
2	10μM	68.89%	72.38%	72.86%	3.55%	0.141597005
3	10μM	71.40%	77.91%	70.80%	6.41%	0.12862467
4	10μM	68.71%	69.25%	67.53%	-0.65%	0.547273969
5	10μM	67.82%	72.88%	66.29%	0.06%	0.9806331
6	10μM	70.32%	72.02%	69.02%	2.19%	0.198582198
7	10μM	56.97%	60.50%	55.61%	-16.33%	0.001803455
8	10μM	68.69%	67.36%	66.90%	-1.87%	0.139812224
9	10μM	92.83%	96.89%	93.55%	32.55%	0.008953877
10	10μM	70.32%	72.02%	69.02%	2.19%	0.198582198