

Supporting information

Novel phenylpropanoid-amino acid adducts from
Ligusticum chuanxiong

Xu Zhang, Bing Han, Zi-Ming Feng, Ya-Nan Yang, Jian-Shuang Jiang, and Pei-Cheng Zhang*

State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, People's Republic of China

Corresponding author. Tel: +86-10-63165231. Fax: +86-10-63017757.

E-mail: pczhang@imm.ac.cn

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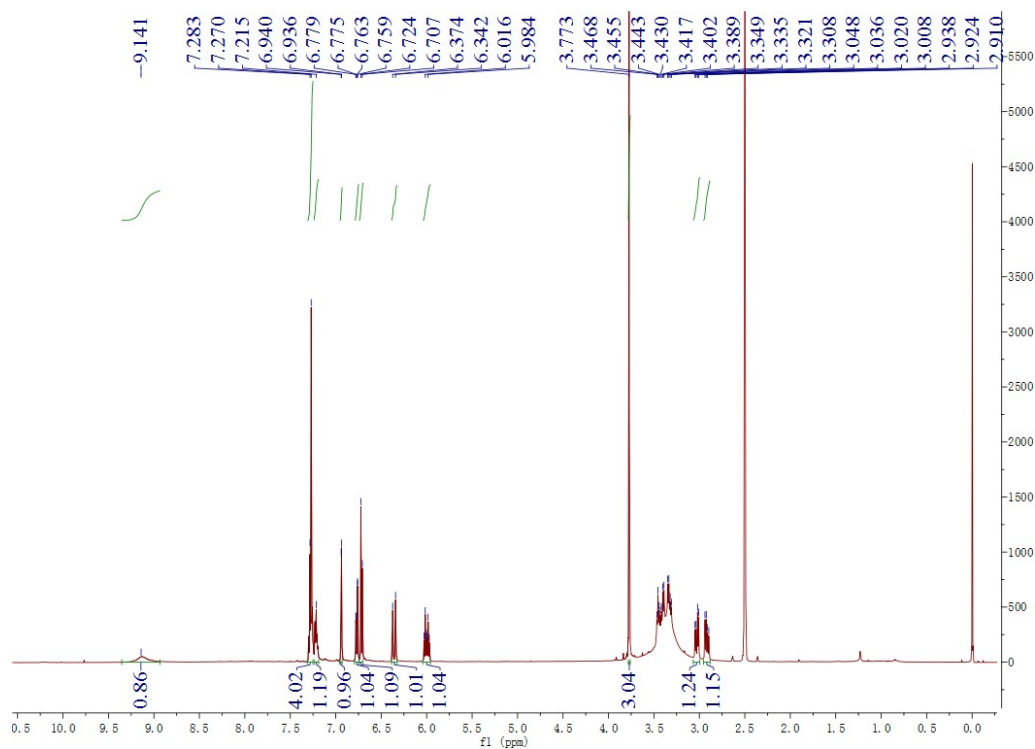


Figure S1. The ^1H NMR spectrum of compound **1** in $\text{DMSO-}d_6$

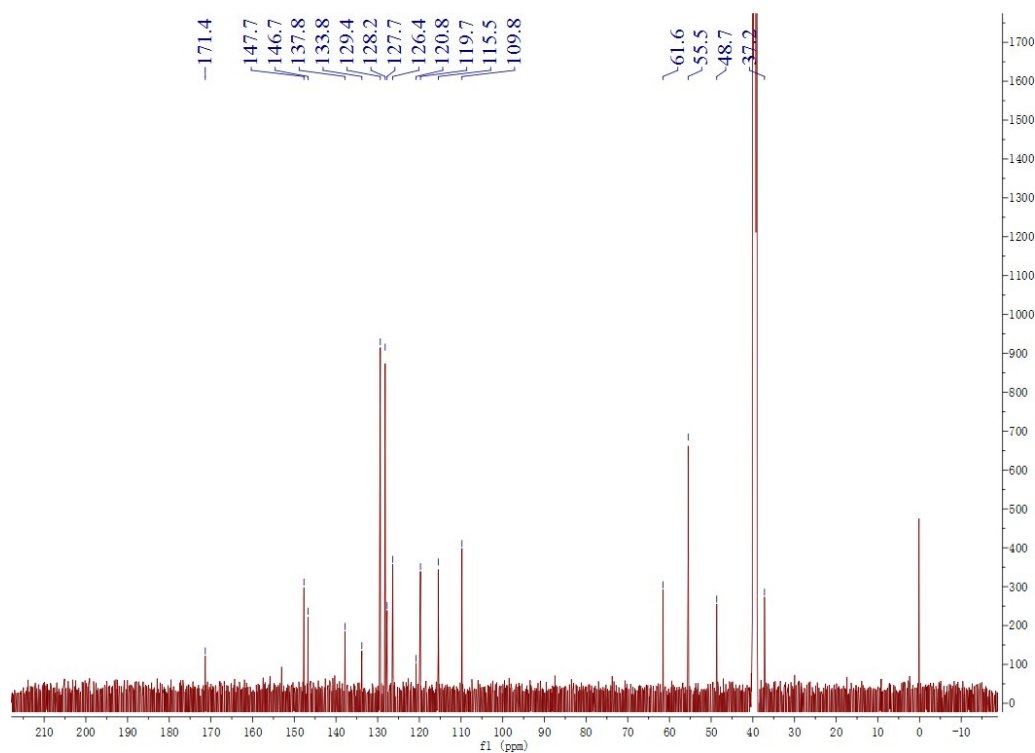


Figure S2. The ^{13}C NMR spectrum of compound **1** in $\text{DMSO-}d_6$

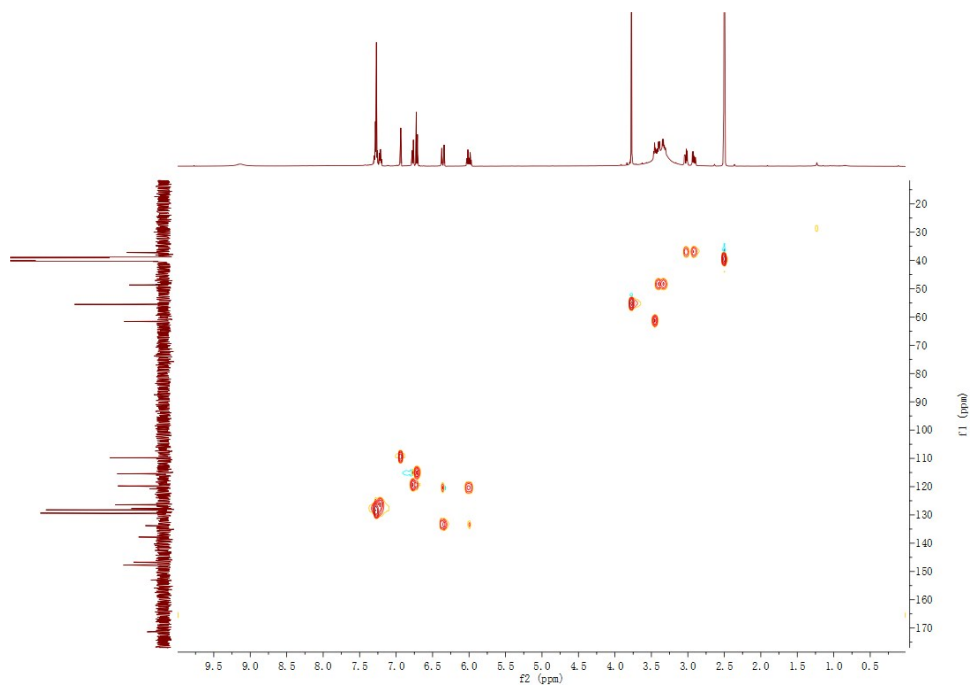


Figure S3. The HSQC spectrum of compound **1** in DMSO- d_6

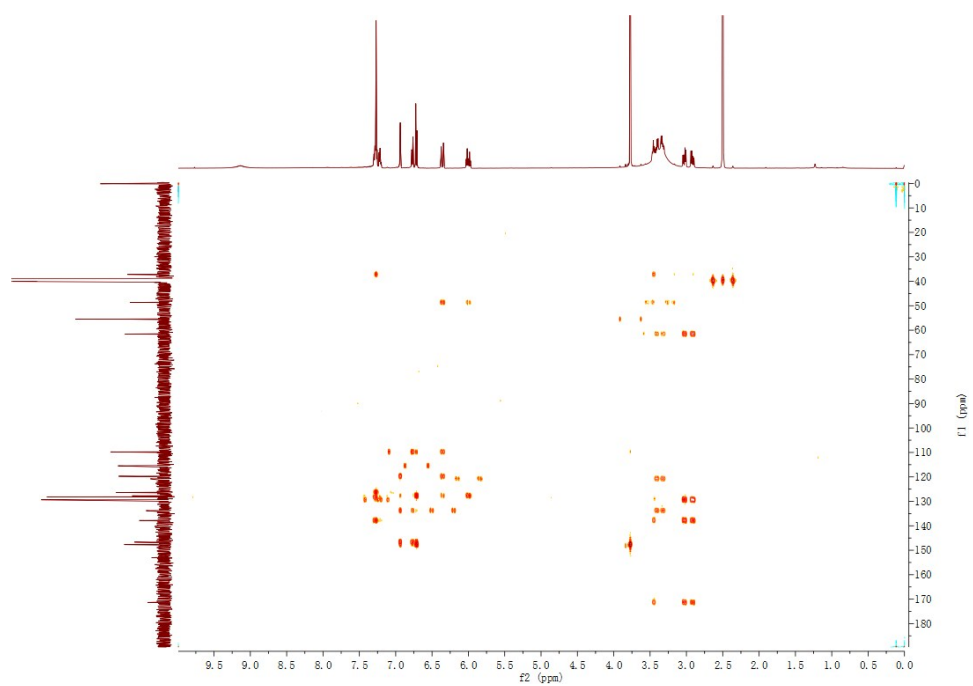


Figure S4. The HMBC spectrum of compound **1** in DMSO- d_6

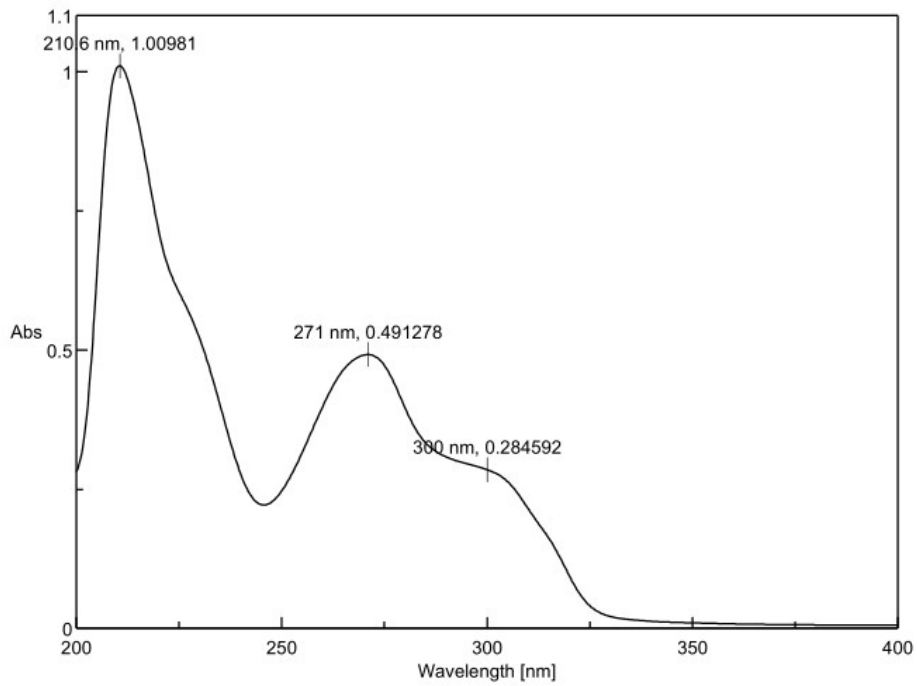


Figure S5. The UV spectrum of compound **1** in MeOH

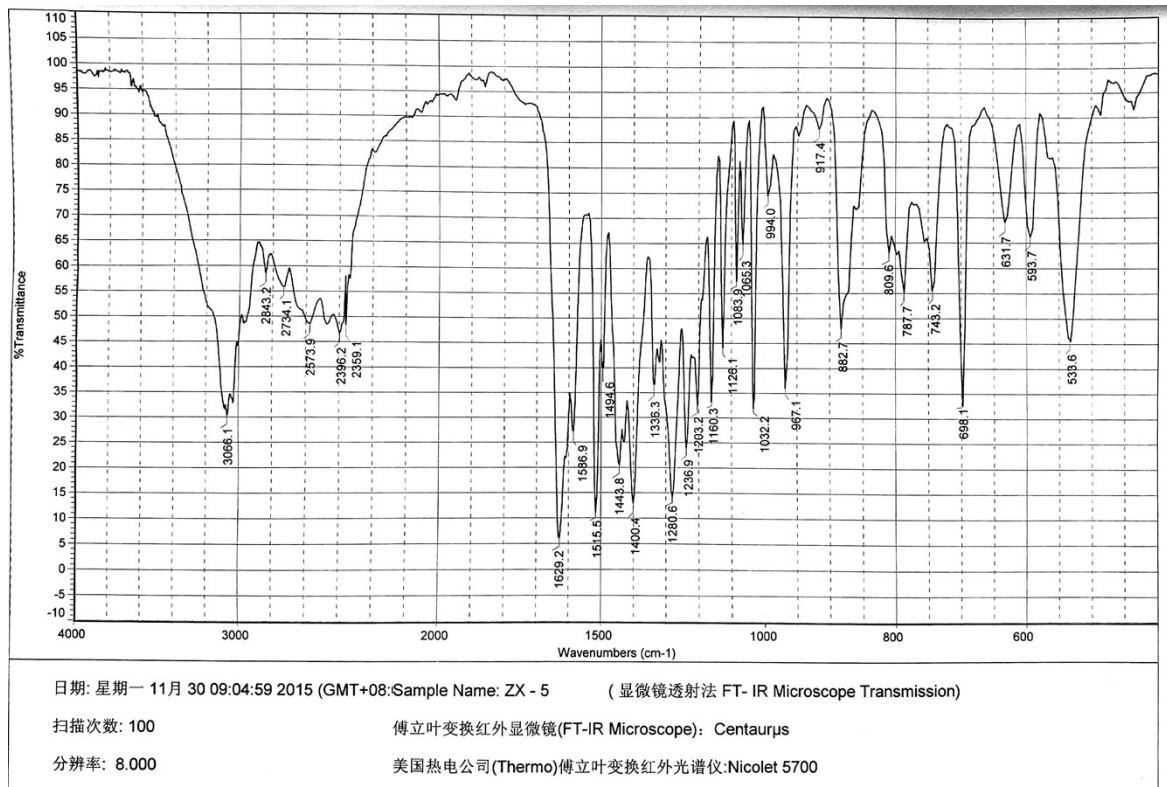
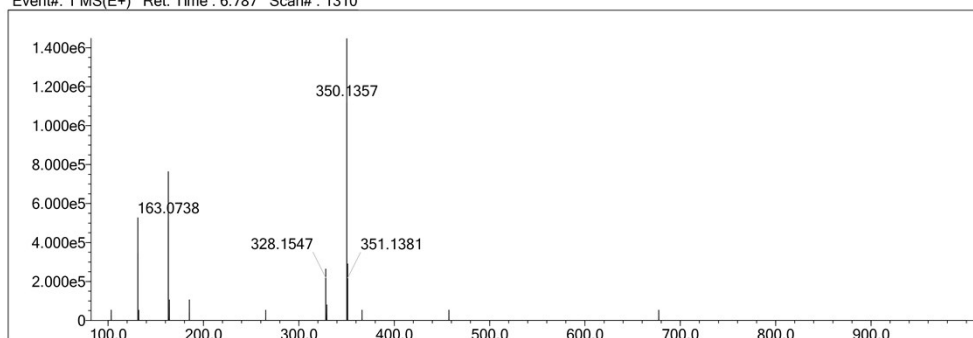
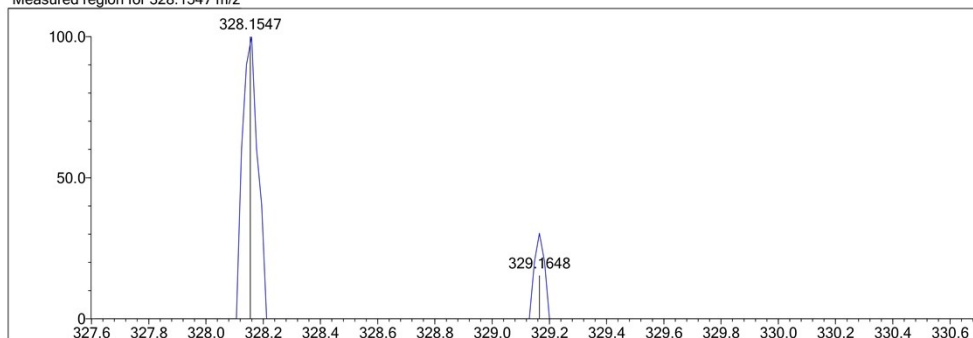


Figure S6. The IR spectrum of compound **1**

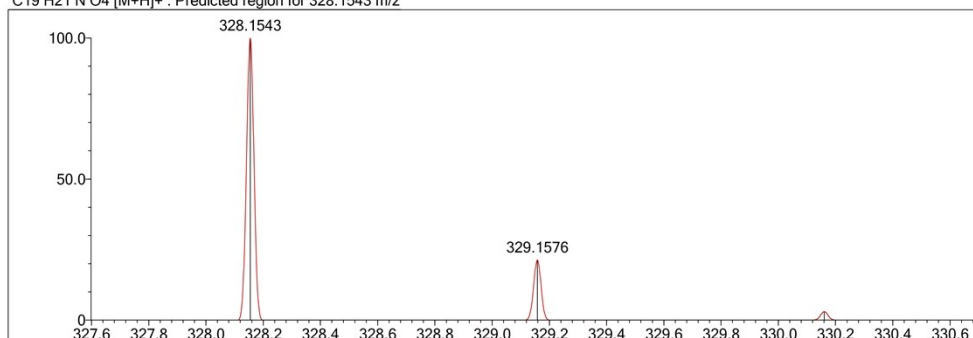
Event#: 1 MS(E+) Ret. Time : 6.787 Scan#: 1310



Measured region for 328.1547 m/z



C19 H21 N O4 [M+H]⁺ : Predicted region for 328.1543 m/z



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**

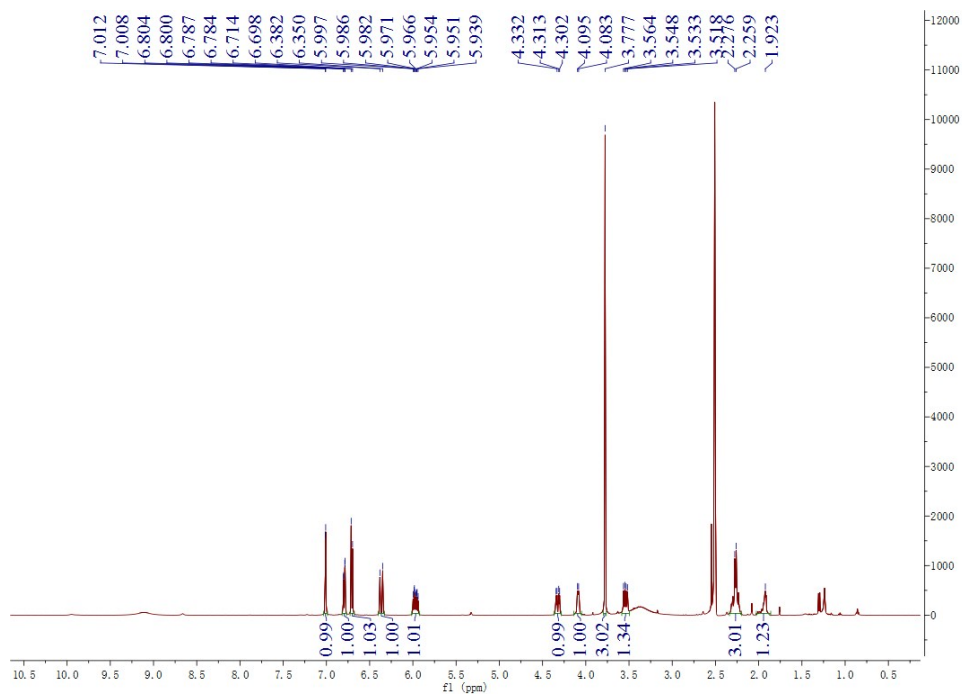


Figure S8. The ^1H NMR spectrum of compound **2** in $\text{DMSO-}d_6$

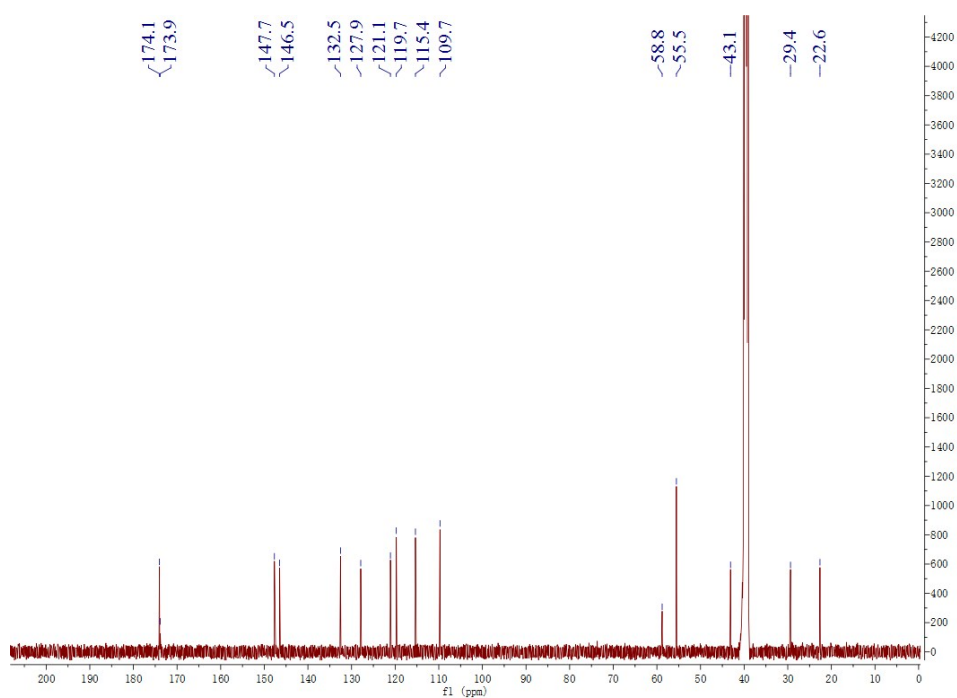


Figure S9. The ^{13}C NMR spectrum of compound **2** in $\text{DMSO-}d_6$

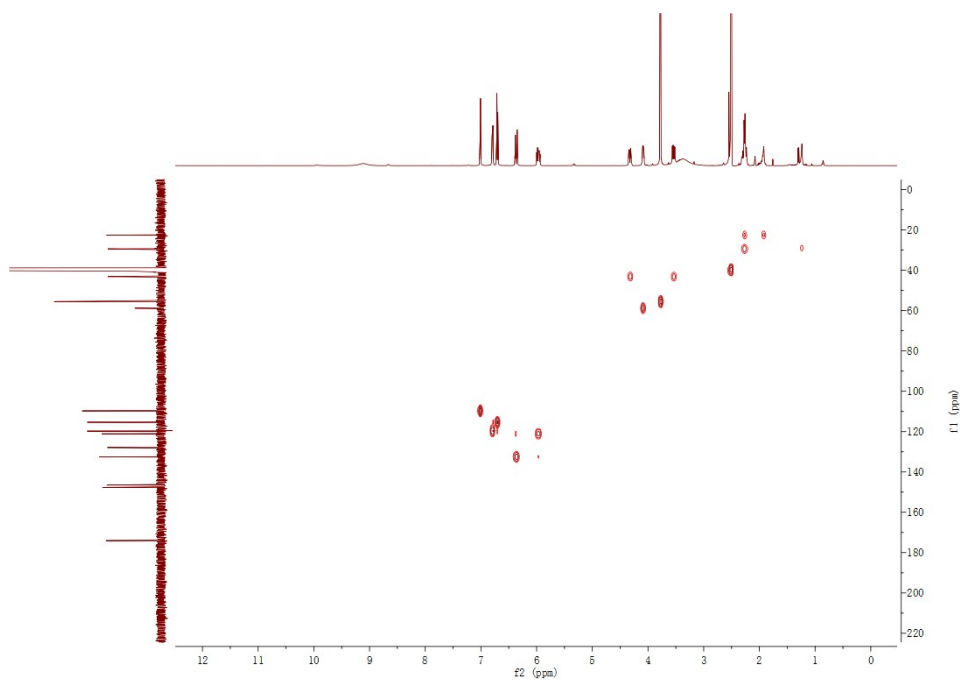


Figure S10. The HSQC spectrum of compound **2** in DMSO- d_6

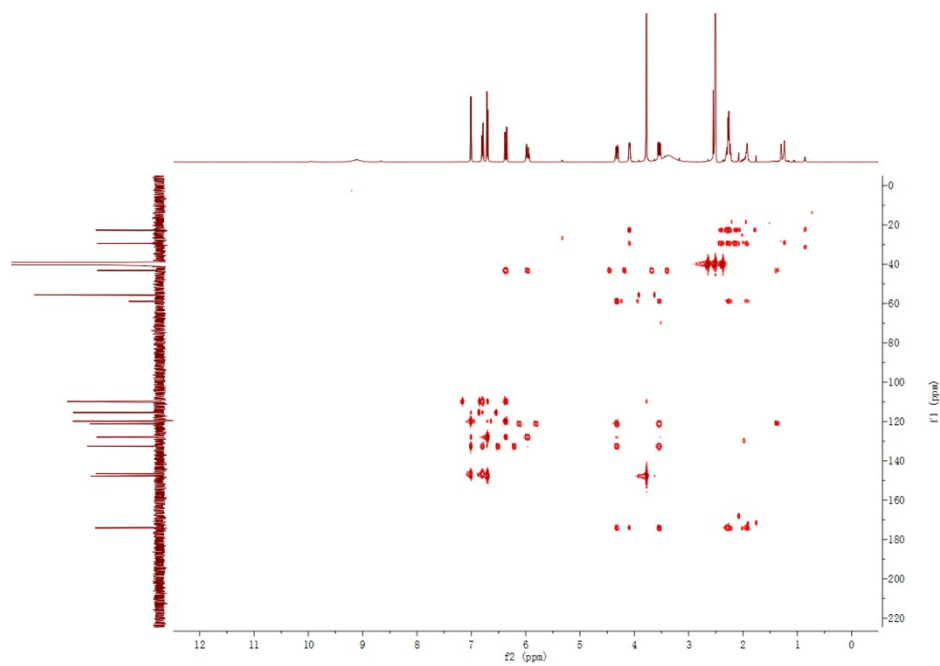


Figure S11. The HMBC spectrum of compound **2** in DMSO- d_6

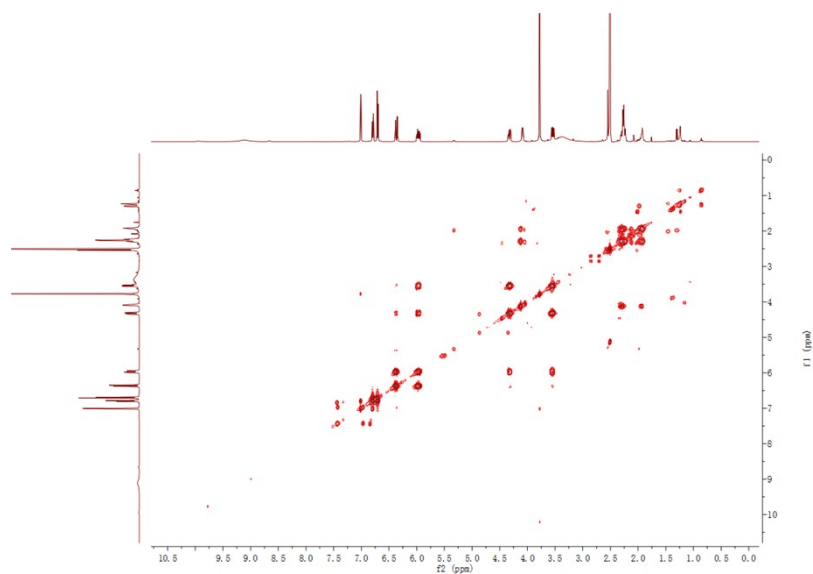


Figure S12. The ^1H - ^1H COSY spectrum in $\text{DMSO-}d_6$

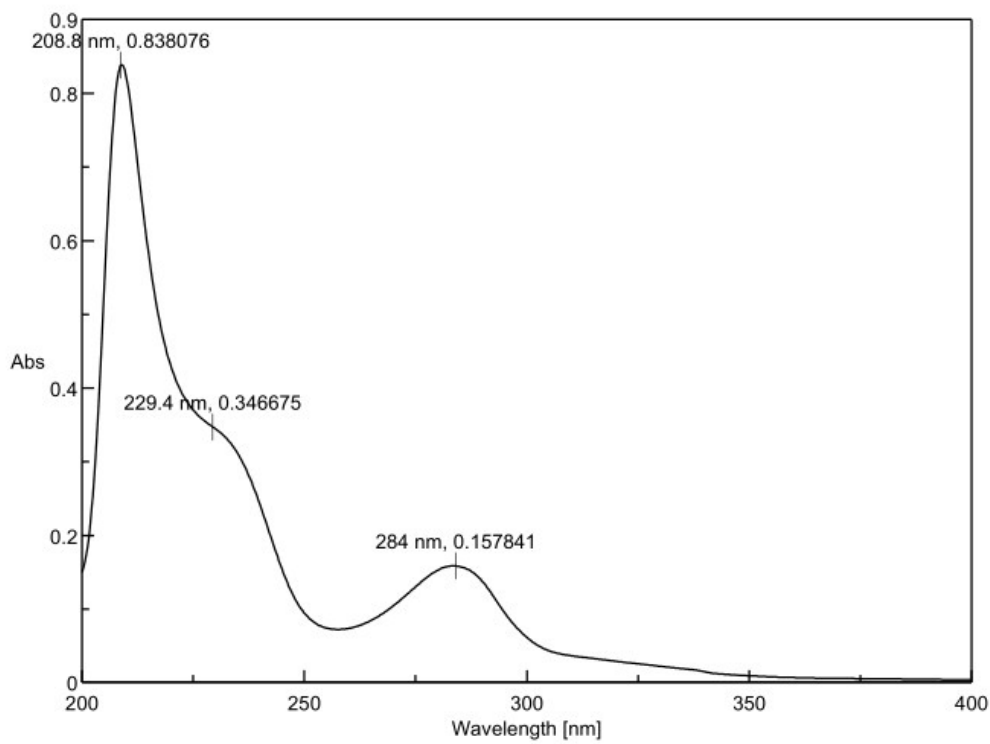


Figure S13. The UV spectrum of compound **2** in MeOH

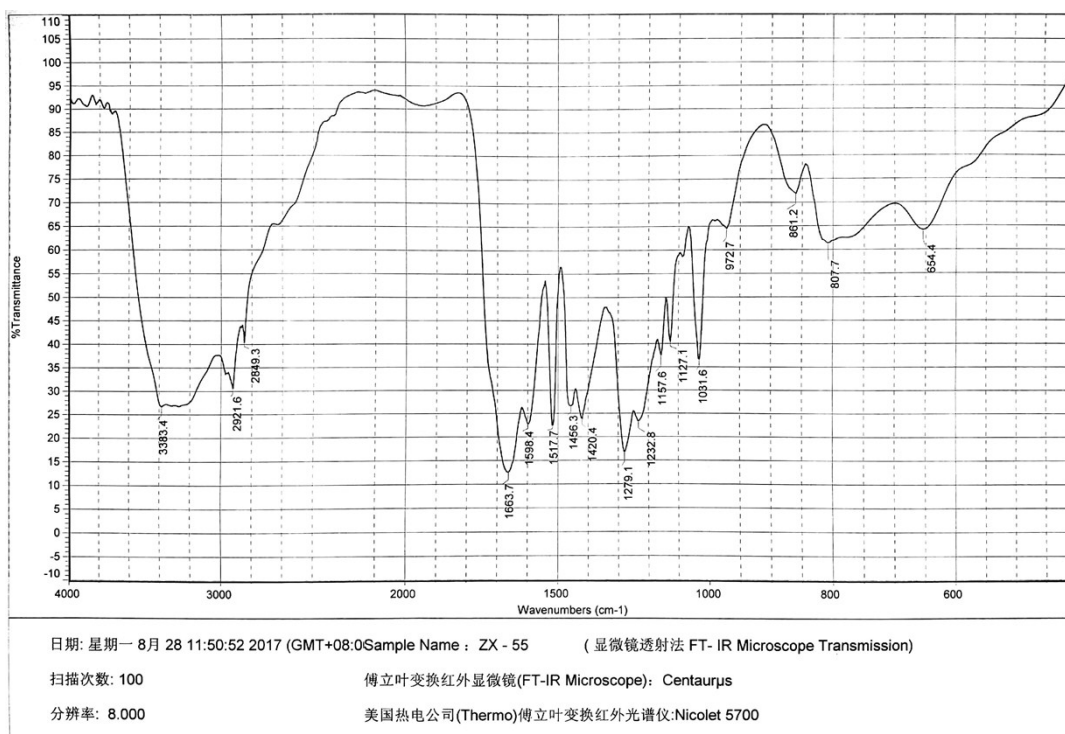
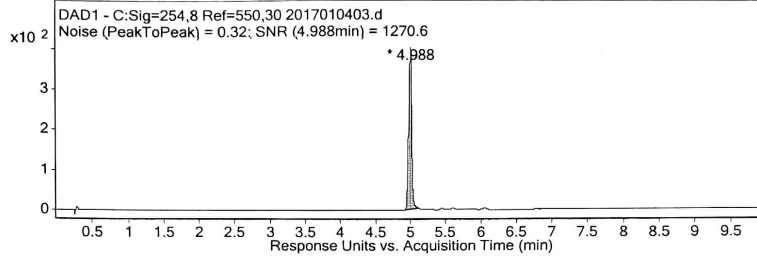


Figure S14. The IR spectrum of compound 2

Qualitative Analysis Report

Data Filename 2017010403.d	Sample Name ZX-55
Sample Type Sample	Position P1-C3
Instrument Name Instrument 1	User Name
Acq Method	IRM Calibration Status Some Ions Missed
DA Method TEST LCMS.m	Comment

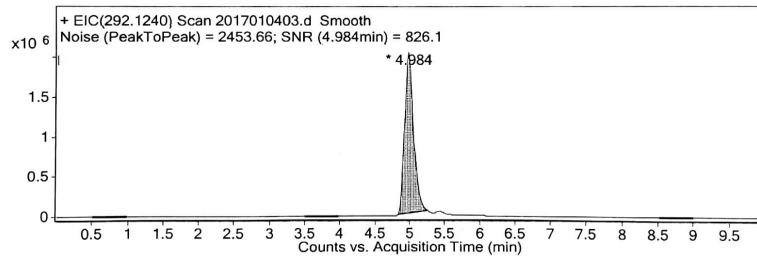
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
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Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
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User Spectra

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

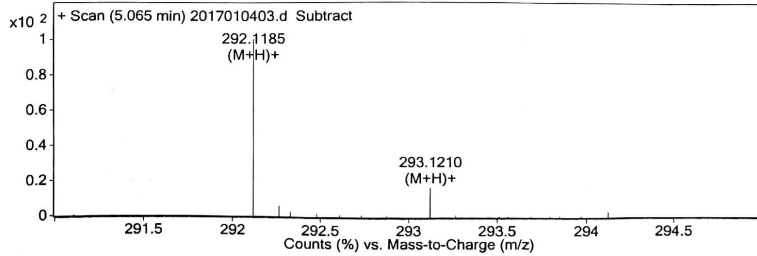


Figure S15. The HR-ESI-MS data of compound 2

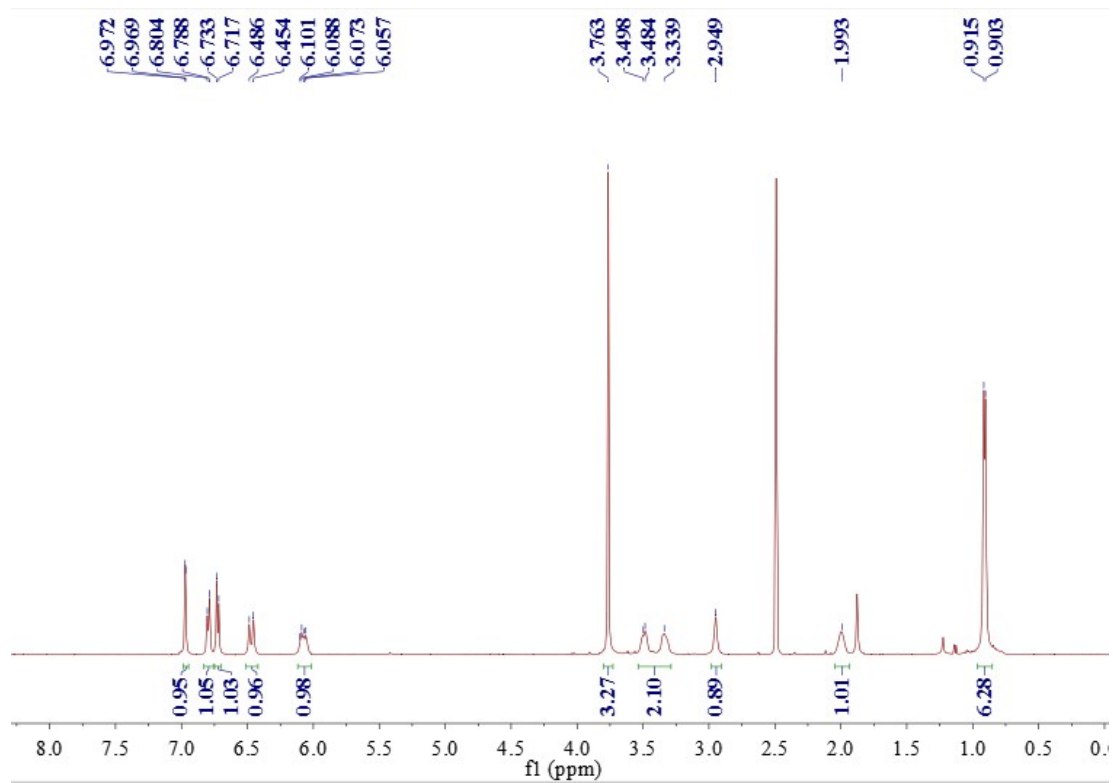


Figure S16. The ^1H NMR spectrum of compound **3** in $\text{DMSO-}d_6$

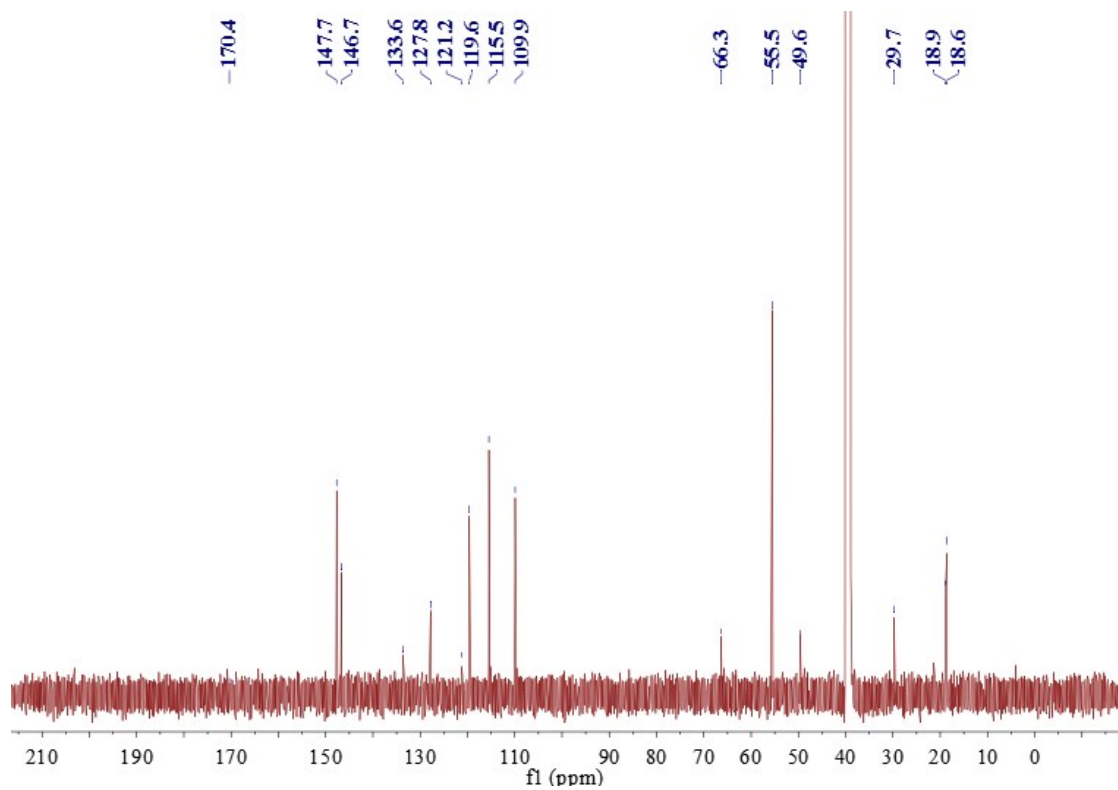


Figure S17. The ^{13}C NMR spectrum of compound **3** in $\text{DMSO-}d_6$

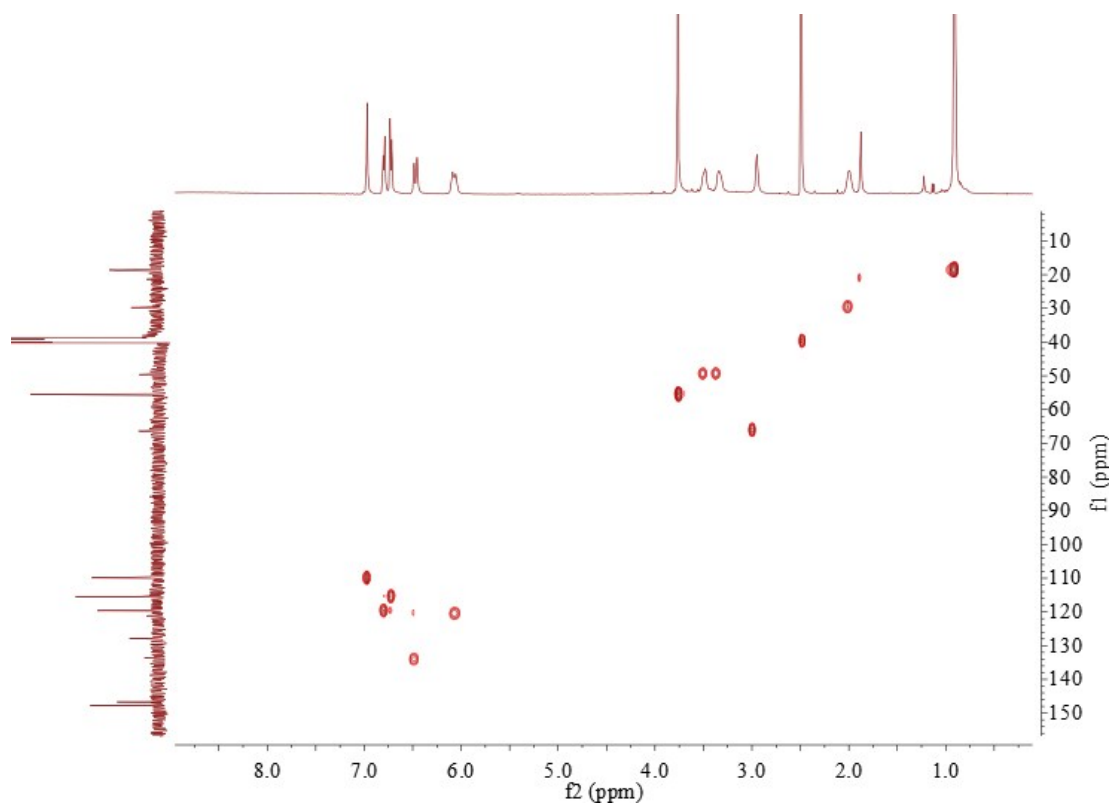


Figure S18. The HSQC spectrum of compound **3** in DMSO- d_6

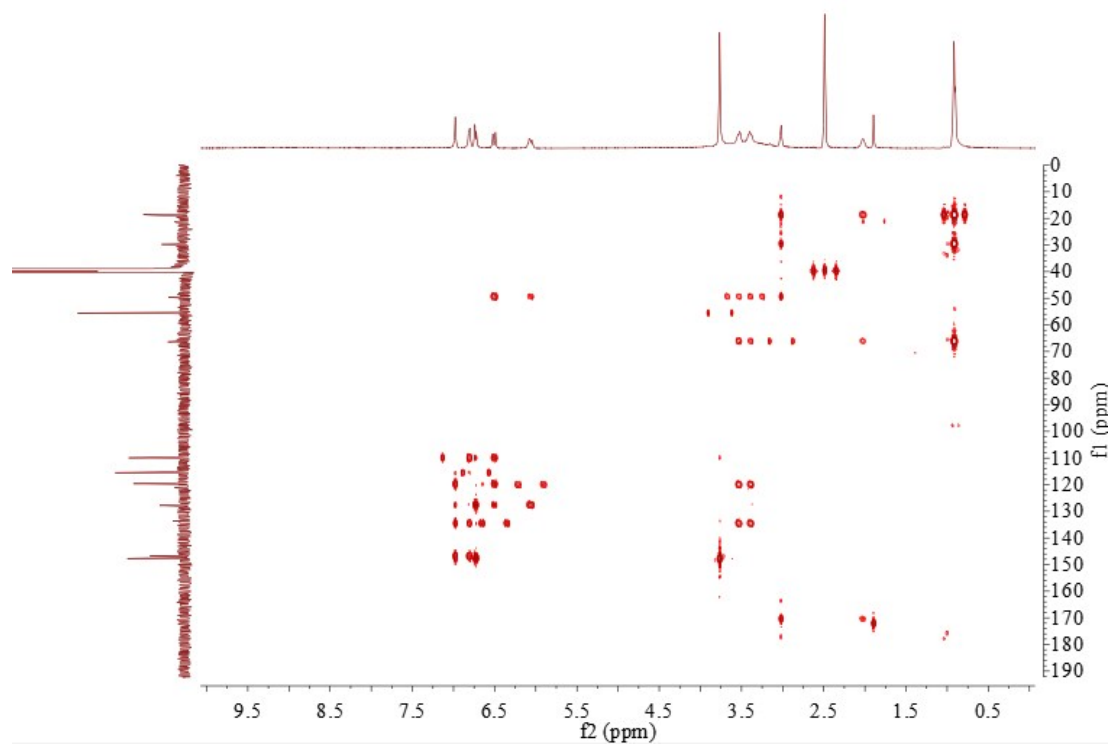


Figure S19. The HMBC spectrum of compound **3** in DMSO- d_6

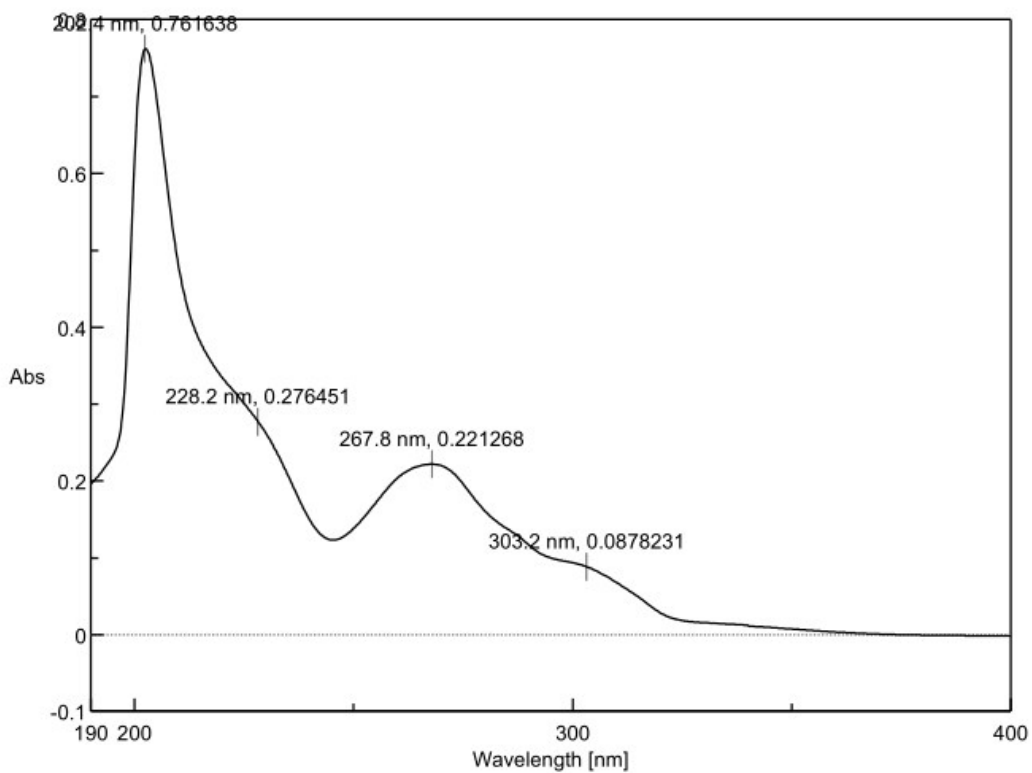


Figure S20. The UV spectrum of compound 3 in MeOH

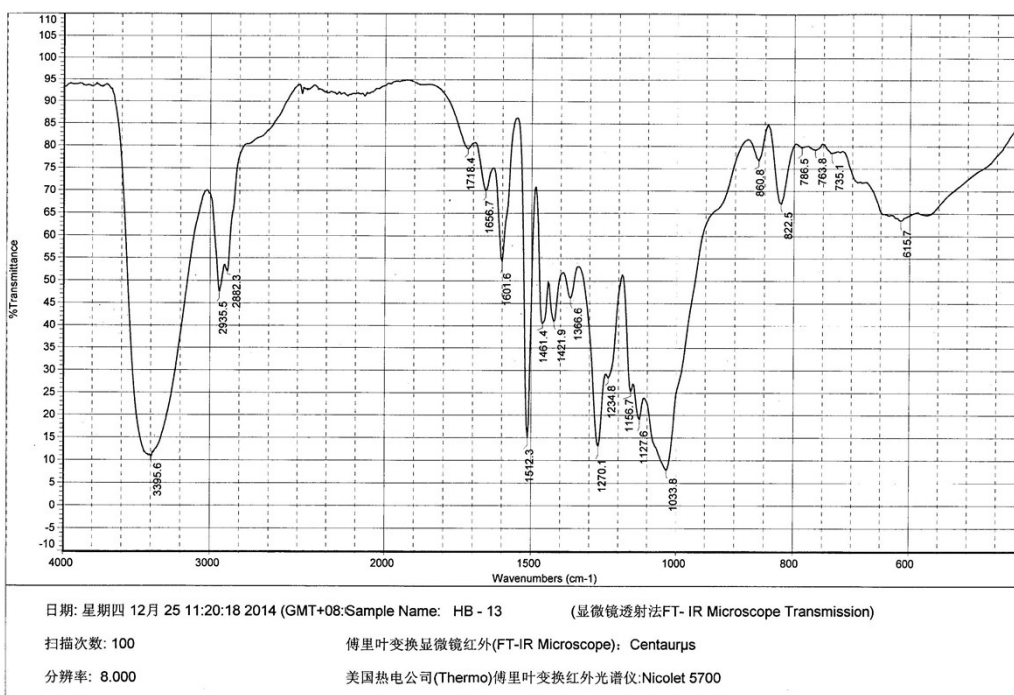
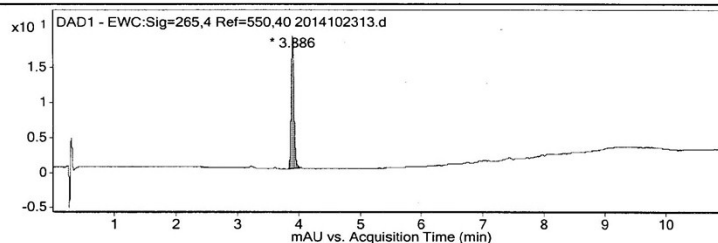


Figure S21. The IR spectrum of compound 3

Qualitative Analysis Report

Data Filename	2014102313.d	Sample Name	HB-13
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	██████████
DA Method	TEST LCMS.m	Comment	

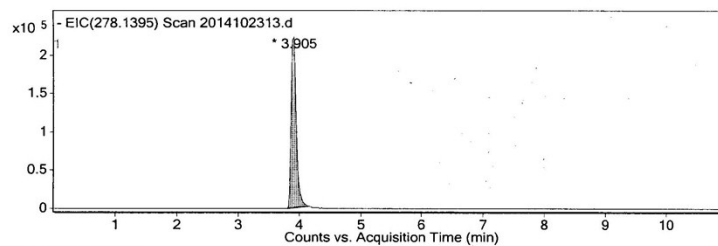
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.809	3.886	4.021	18.89	64.801	100

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.792	3.905	4.147	223433	1179188	100

User Spectra

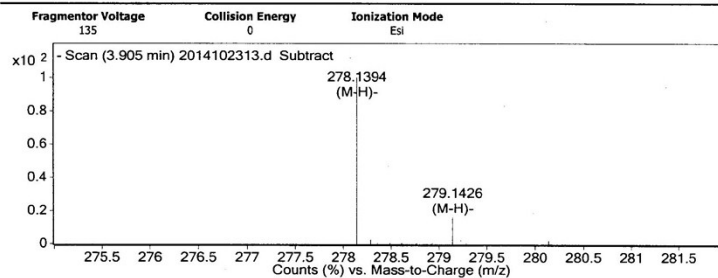


Figure S22. The HR-ESI-MS data of compound **3**

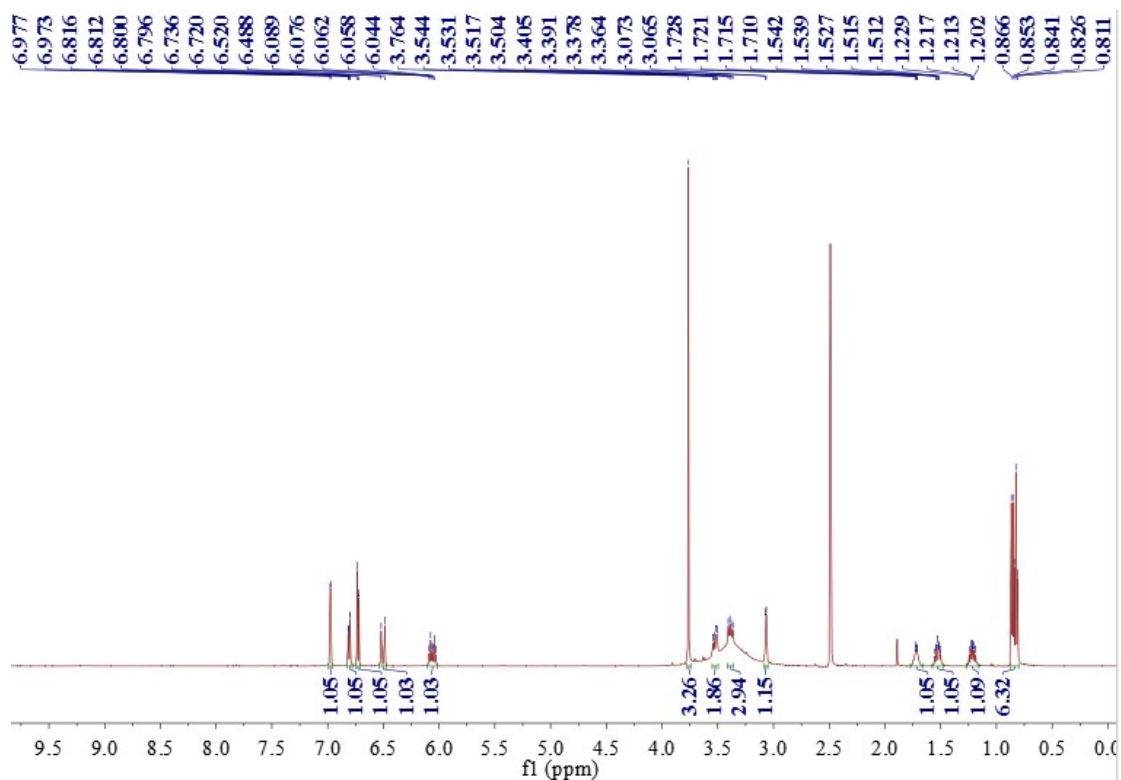


Figure S23. The ^1H NMR spectrum of compound **4** in $\text{DMSO-}d_6$

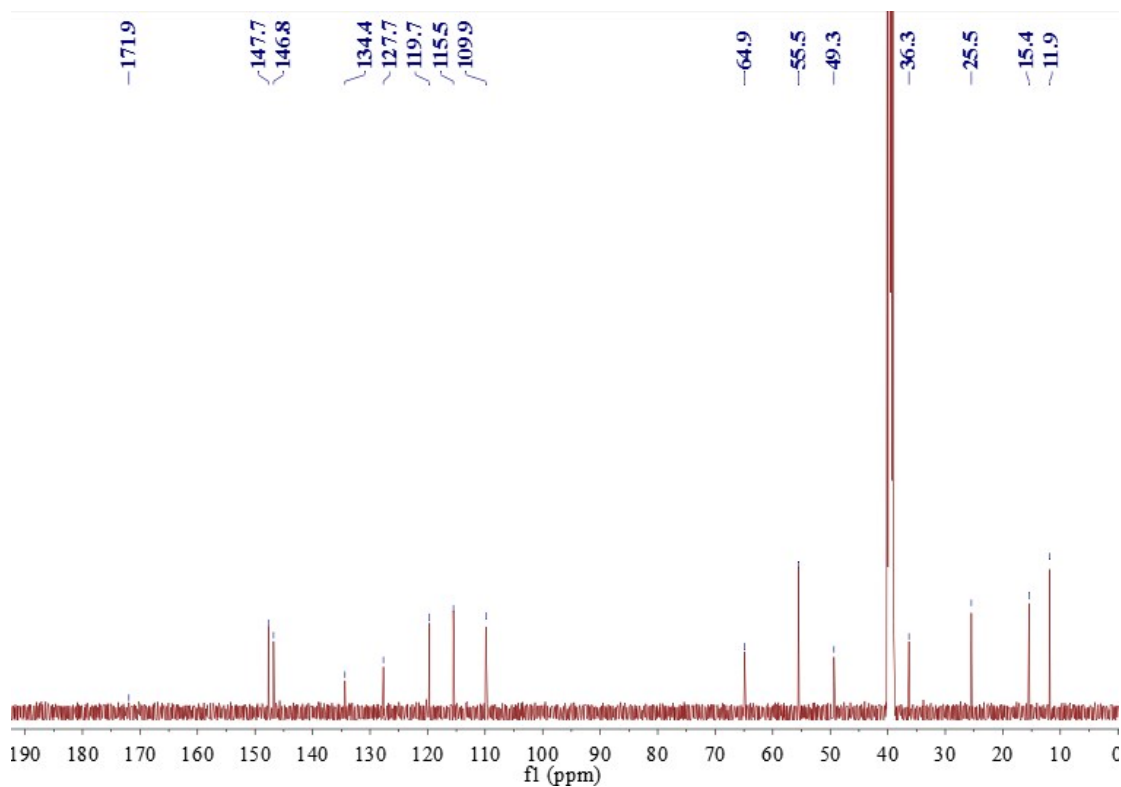


Figure S24. The ^{13}C NMR spectrum of compound **4** in $\text{DMSO-}d_6$

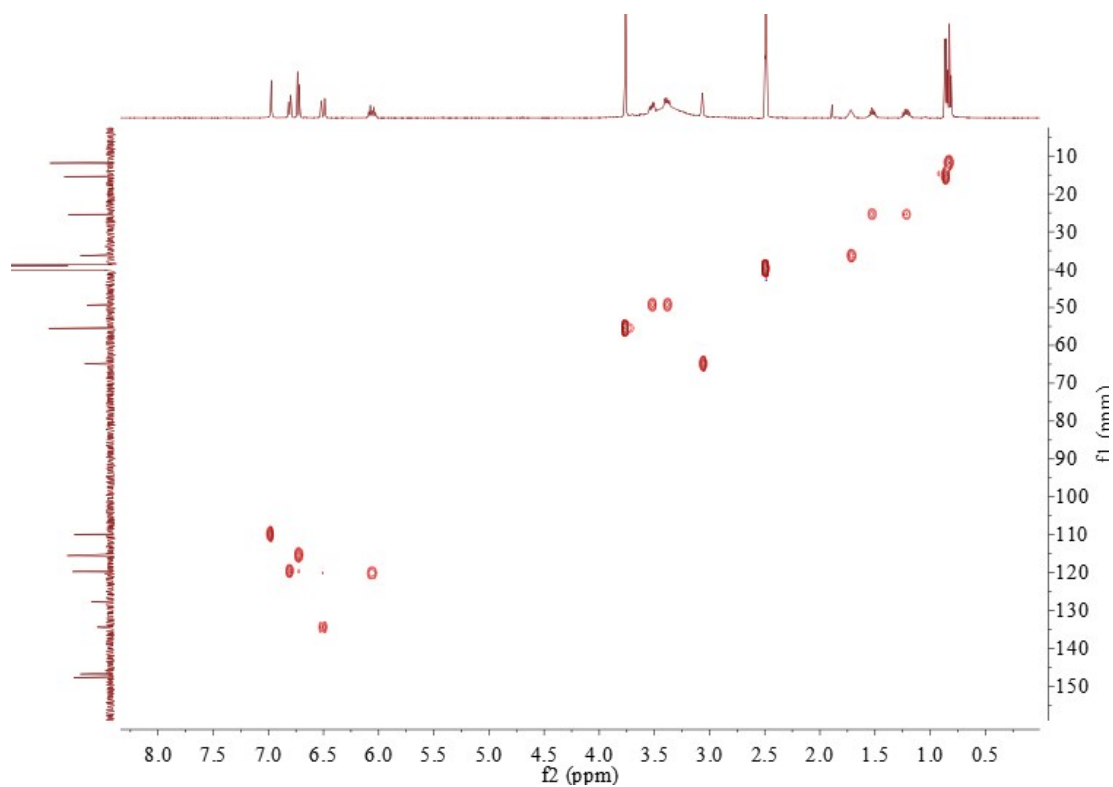


Figure S25. The HSQC spectrum of compound **4** in DMSO- d_6

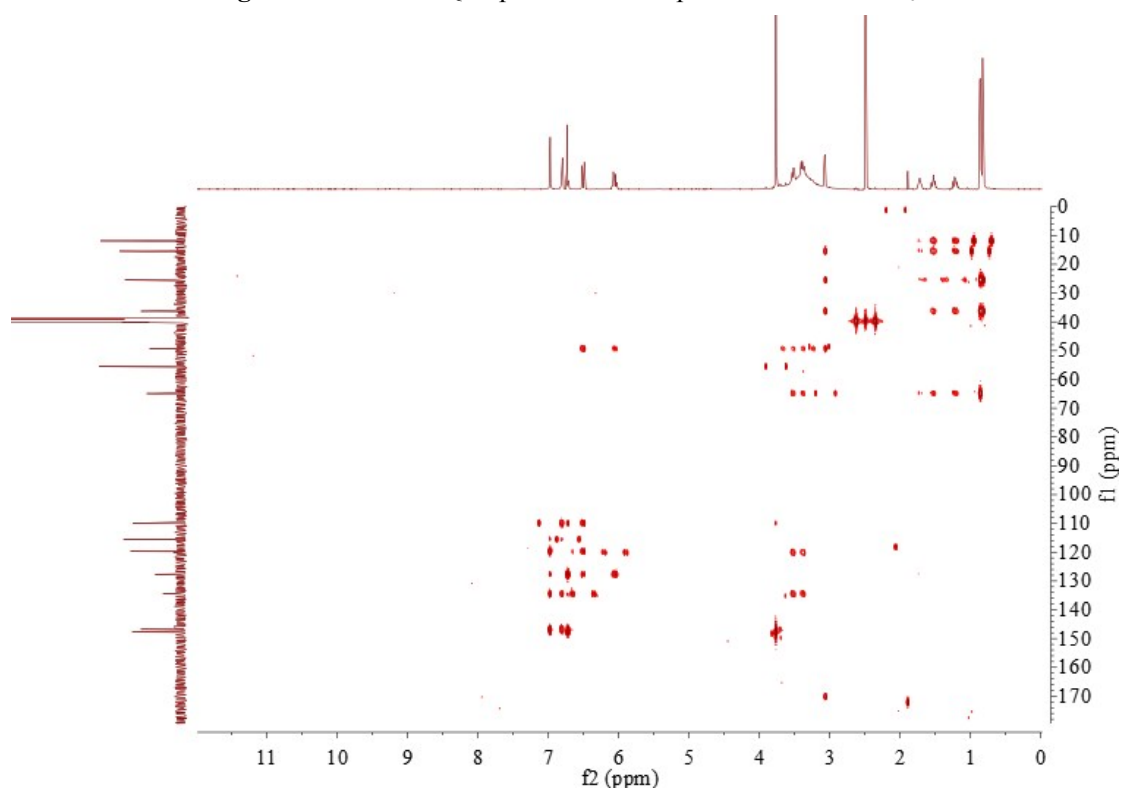


Figure S26. The HMBC spectrum of compound **4** in DMSO- d_6

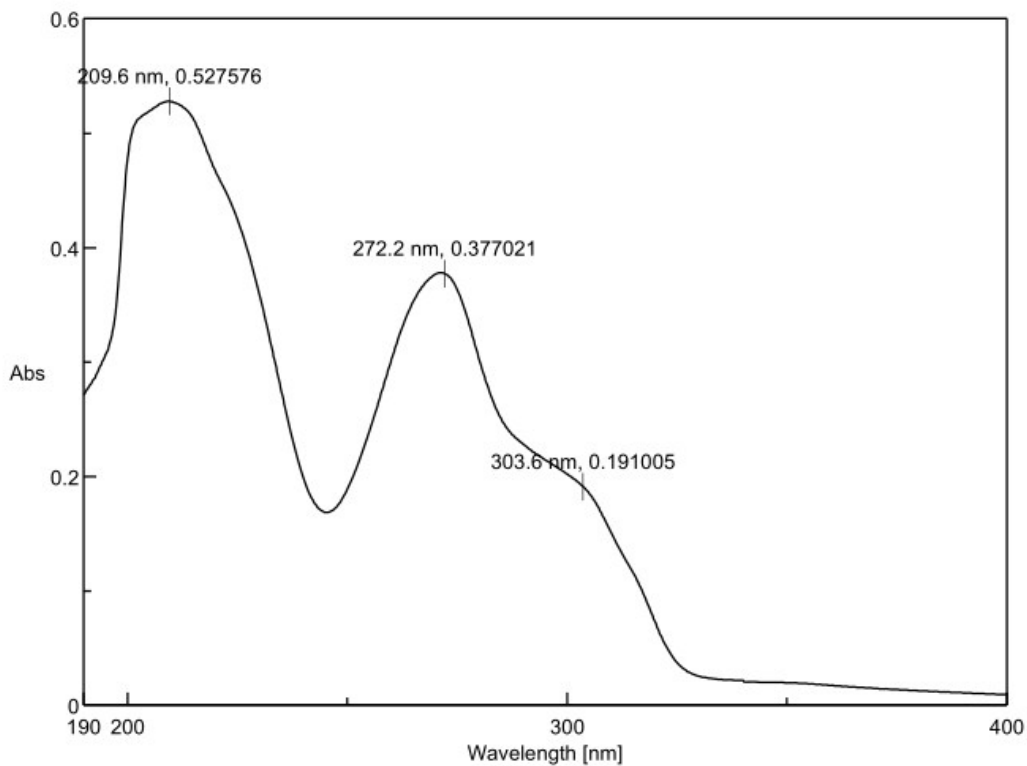


Figure S27. The UV spectrum of compound 4 in MeOH

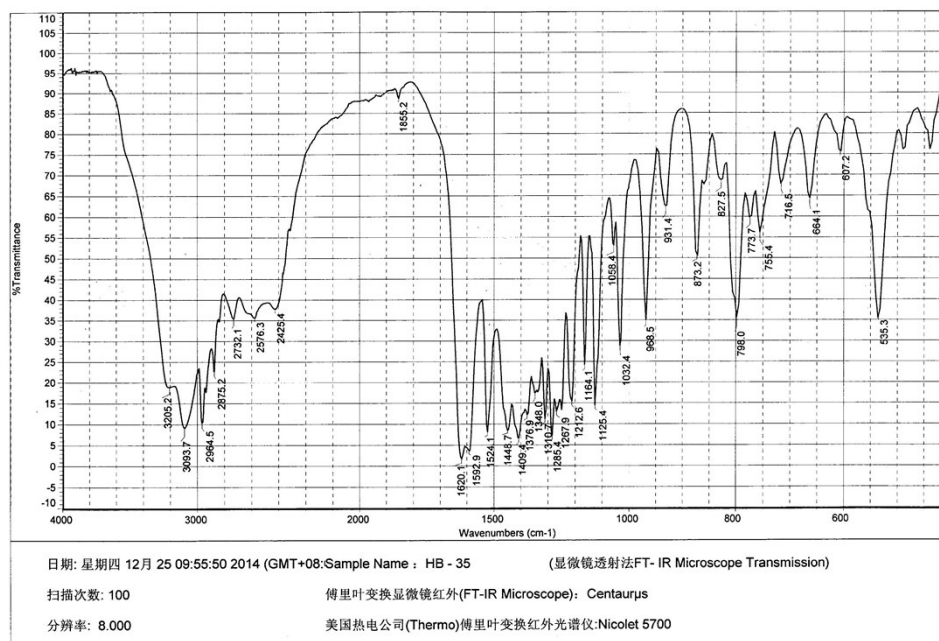
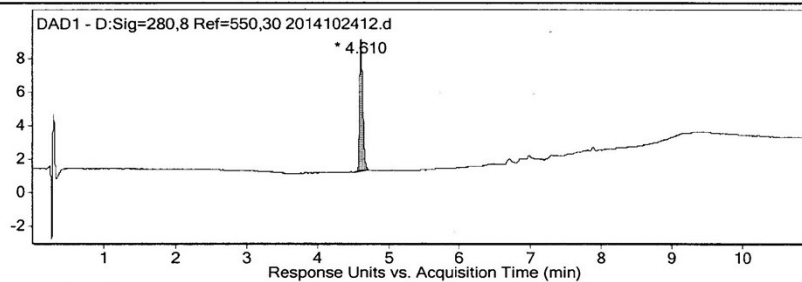


Figure S28. The IR spectrum of compound 4

Qualitative Analysis Report

Data Filename	2014102412.d	Sample Name	HB-35
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	XXXXXXXXXX
DA Method	TEST LCMS.m	Comment	

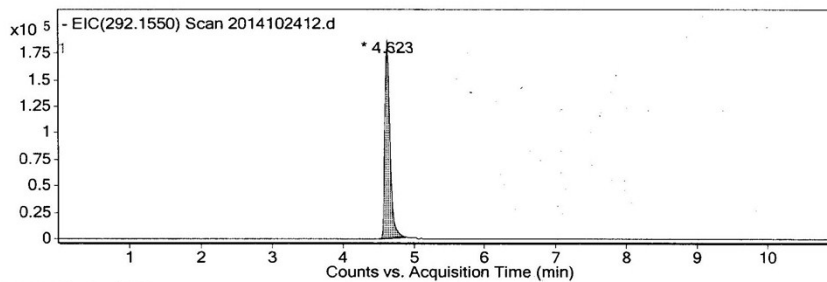
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
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Fragmentor Voltage: 135 Collision Energy: 0 Ionization Mode: ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.495	4.623	4.881	187387	969022	100

User Spectra

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

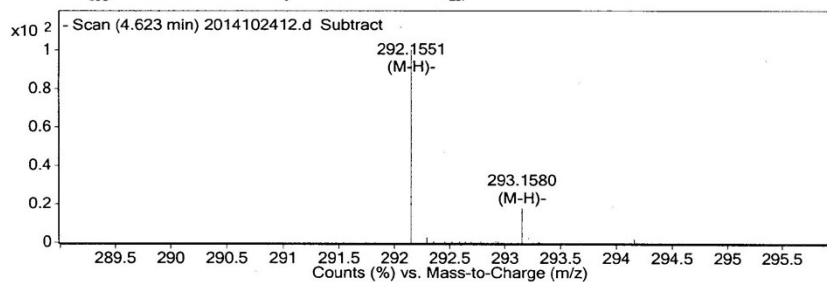


Figure S29. The HR-ESI-MS data of compound 4

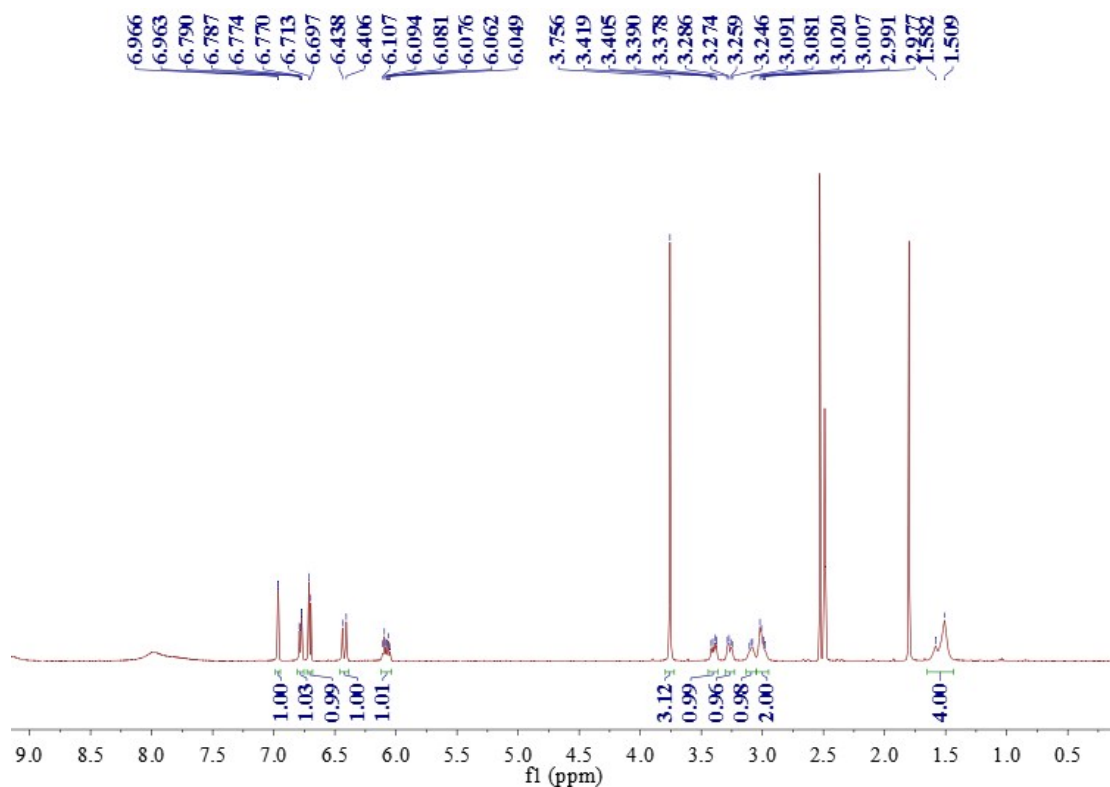


Figure S30. The ^1H NMR spectrum of compound **5** in $\text{DMSO-}d_6$

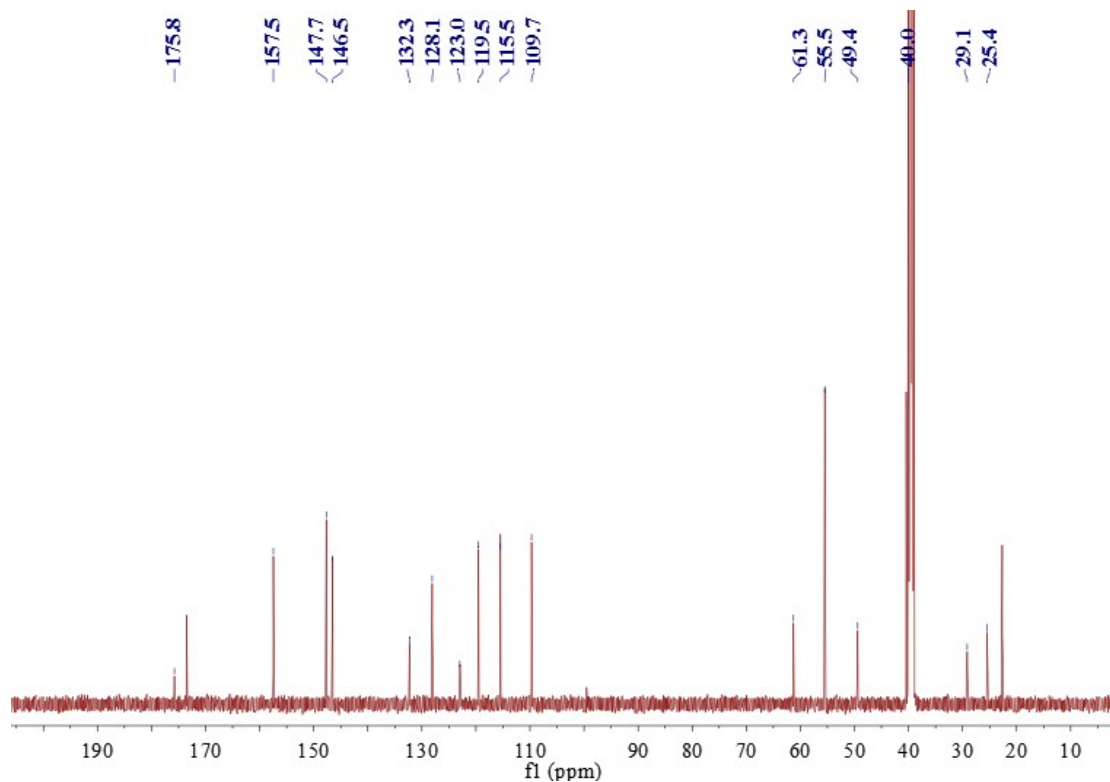


Figure S31. The ^{13}C NMR spectrum of compound **5** in $\text{DMSO-}d_6$

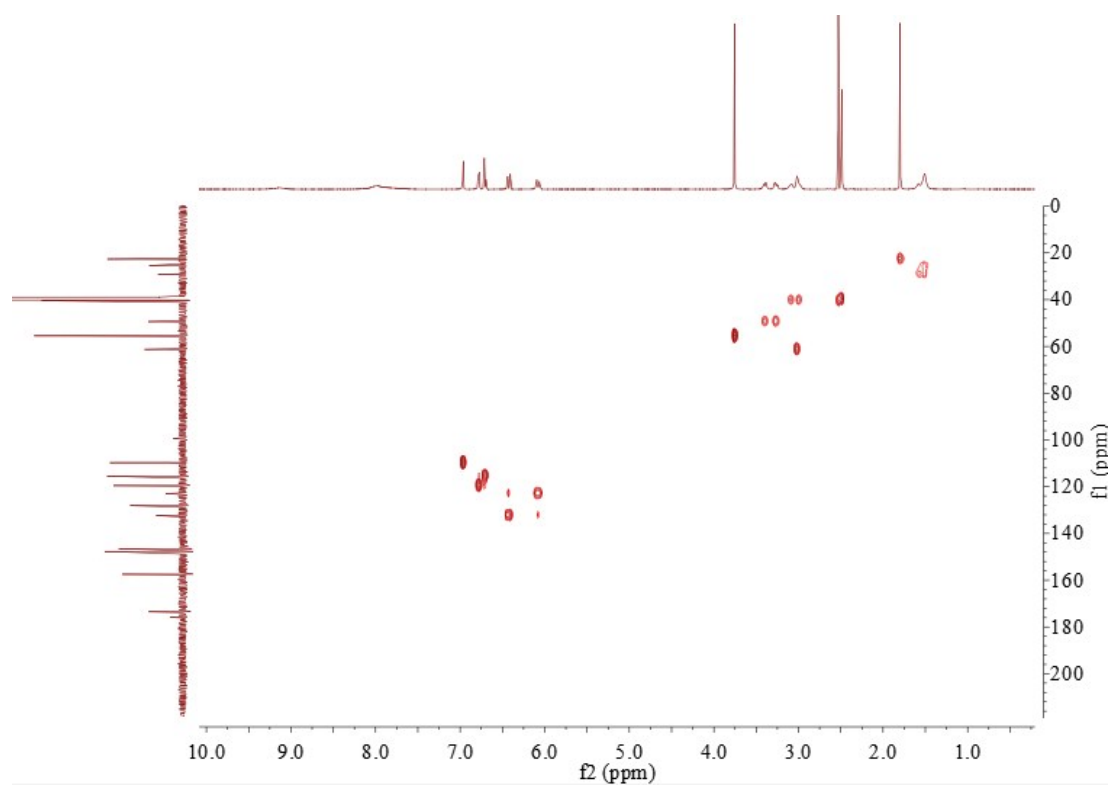


Figure S32. The HSQC spectrum of compound **5** in DMSO- d_6

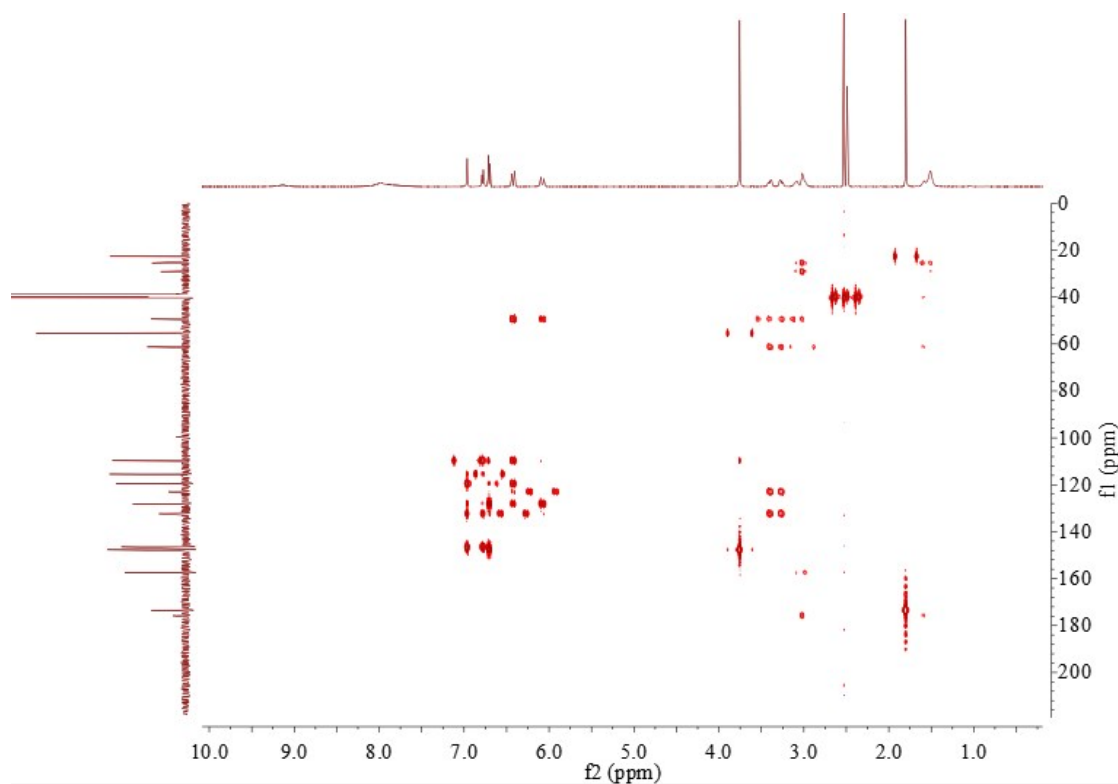


Figure S33. The HMBC spectrum of compound **5** in DMSO- d_6

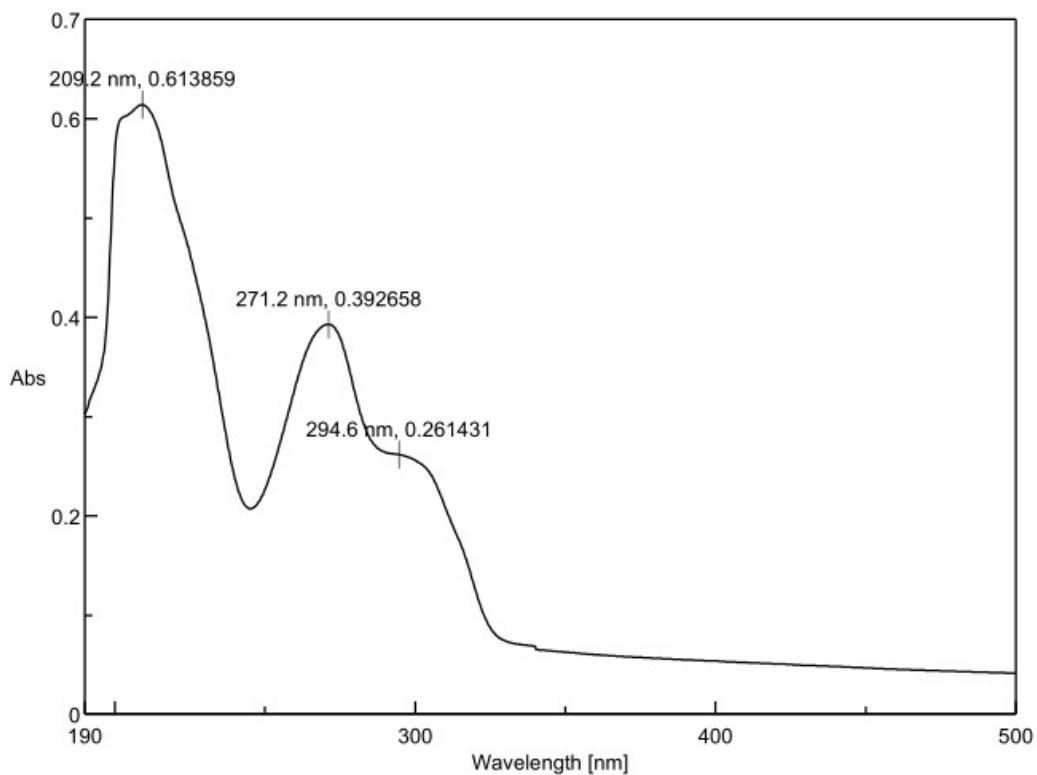


Figure S34. The UV spectrum of compound 5 in MeOH

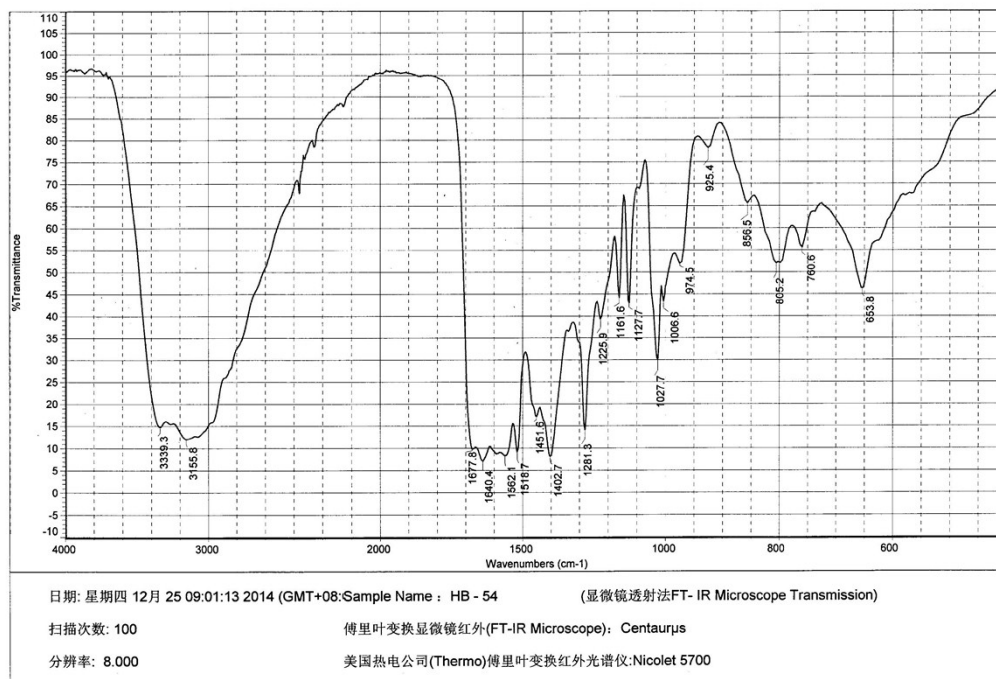


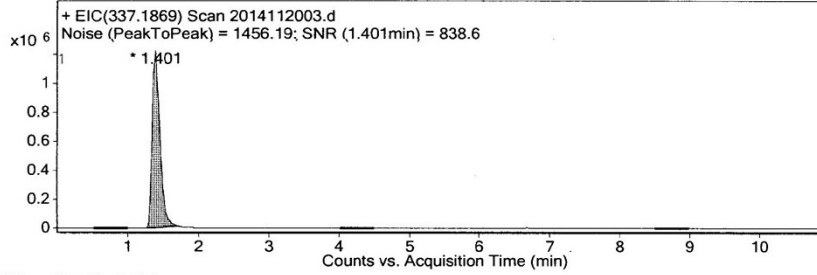
Figure S35. The IR spectrum of compound 5

Qualitative Analysis Report

Data Filename 2014112003.d	Sample Name HB-54
Sample Type Sample	Position P1-C3
Instrument Name Instrument 1	User Name
Acq Method TEST LCMS.m	IRM Calibration Status XXXXXXXXXX
DA Method TEST LCMS.m	Comment

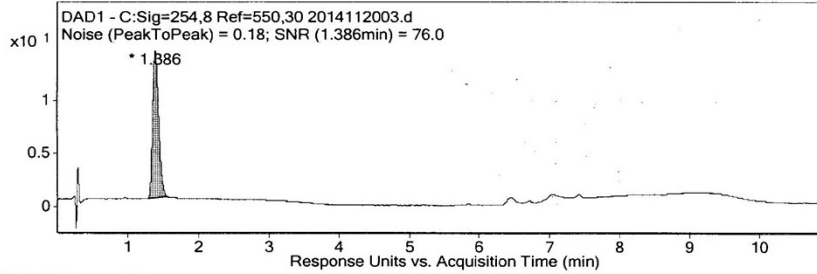
User Chromatograms

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.272	1.401	1.723	1221116	9277301	100	838.6



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.284	1.386	1.568	13.84	82.63	100	76

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

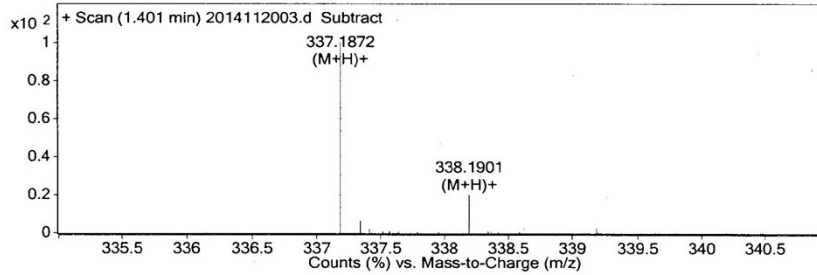


Figure S36. The HR-ESI-MS data of compound 5

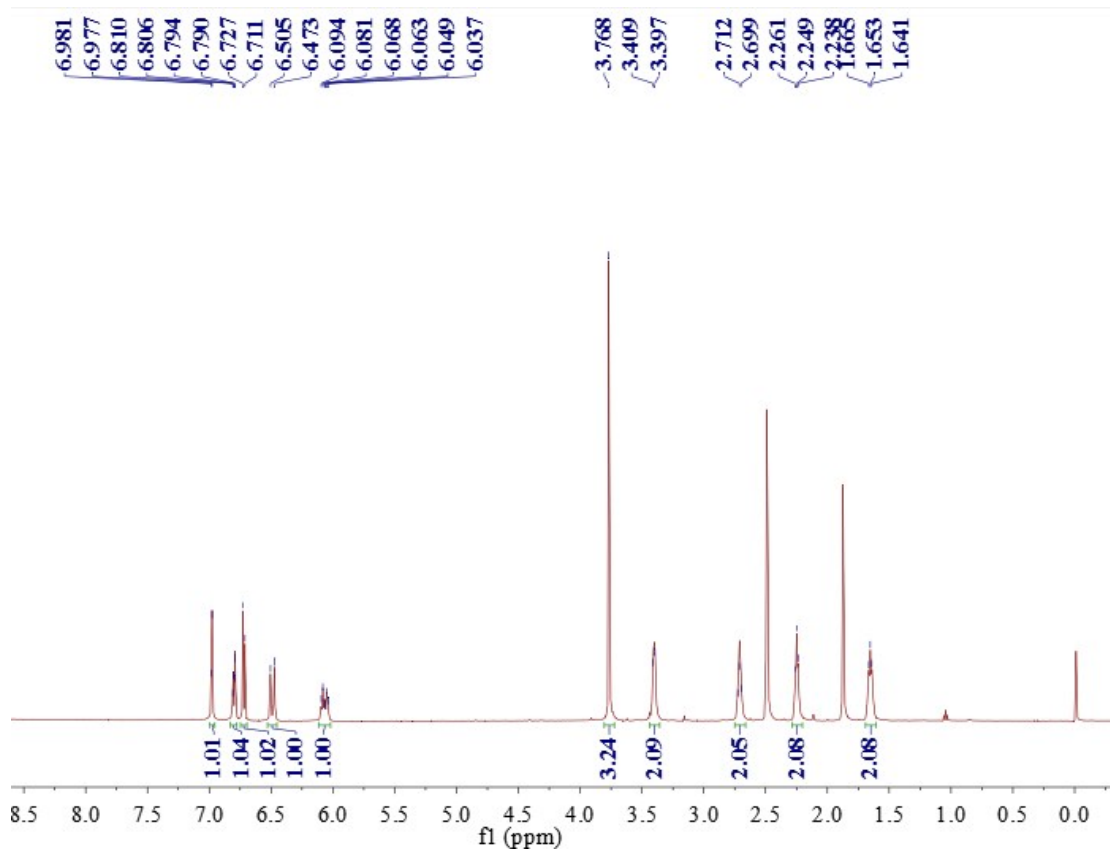


Figure S37. The ^1H NMR spectrum of compound **6** in $\text{DMSO-}d_6$

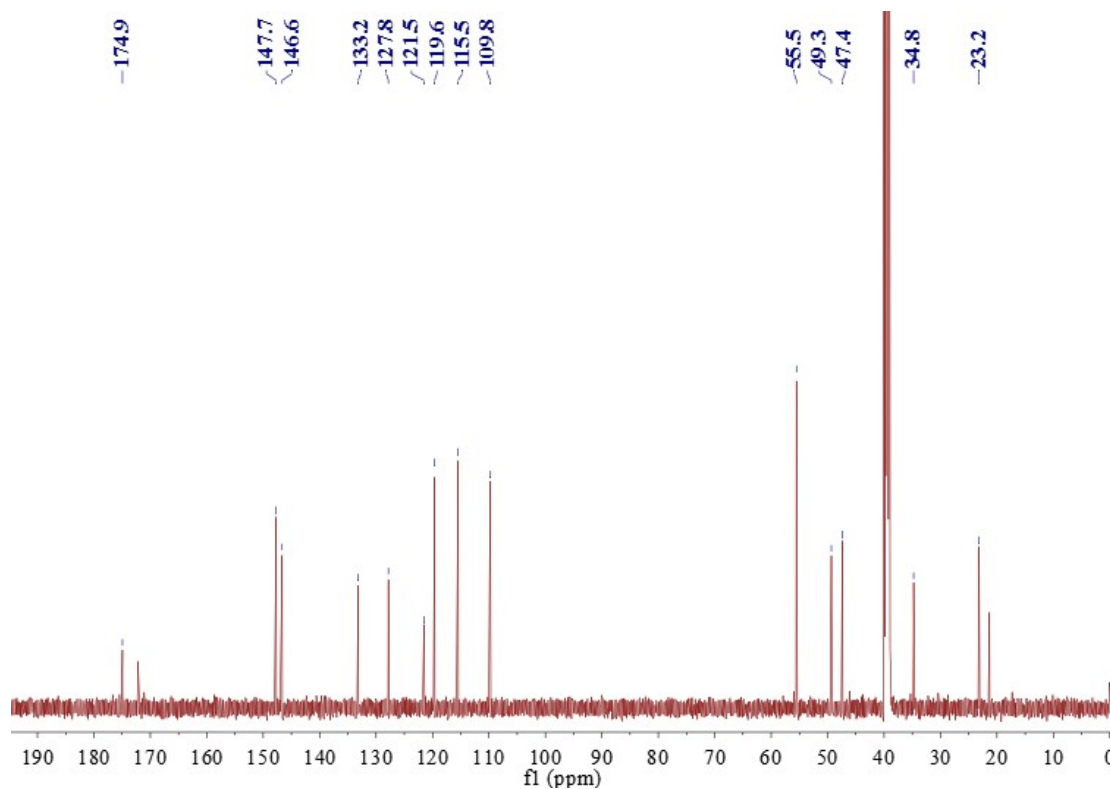


Figure S38. The ^{13}C NMR spectrum of compound **6** in $\text{DMSO-}d_6$

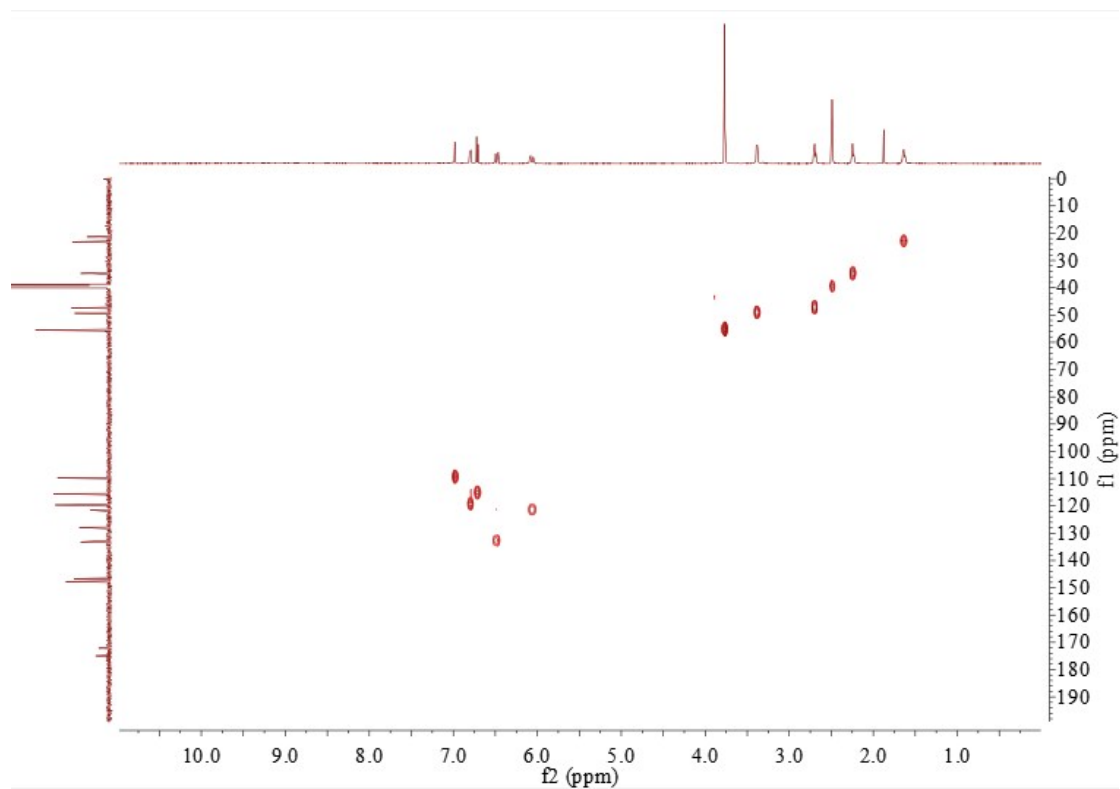


Figure S39. The HSQC spectrum of compound **6** in DMSO- d_6

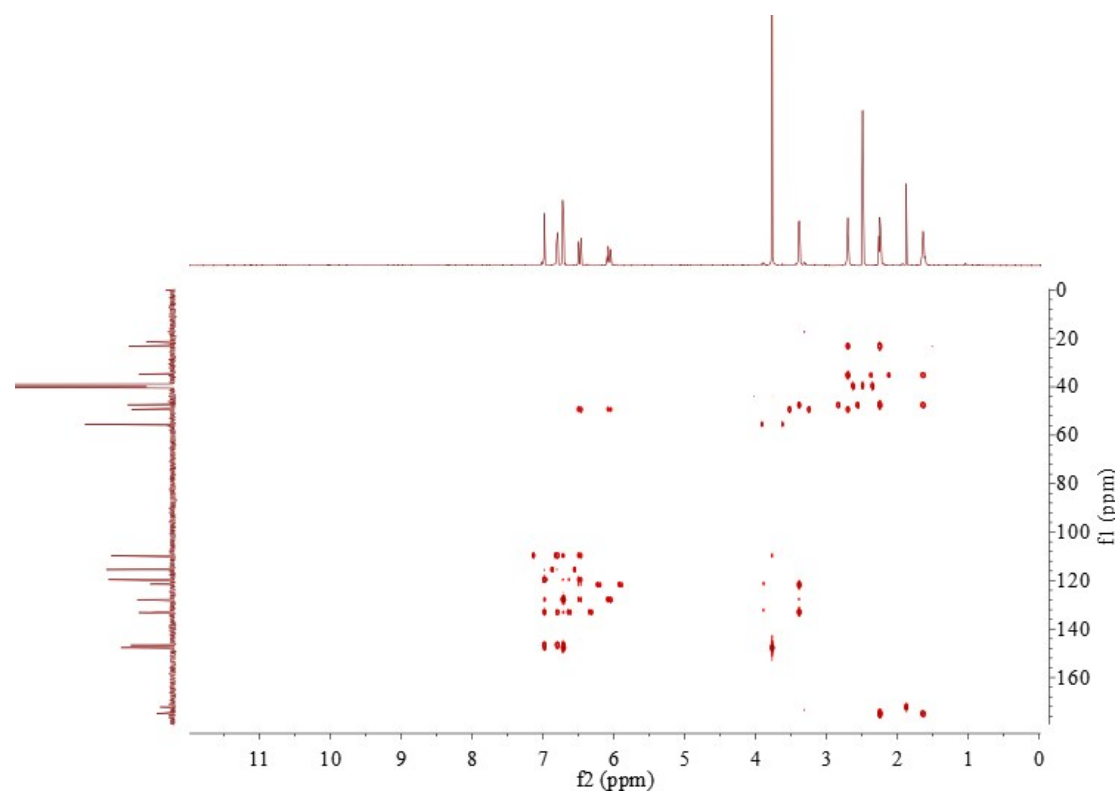


Figure S40. The HMBC spectrum of compound **6** in DMSO- d_6

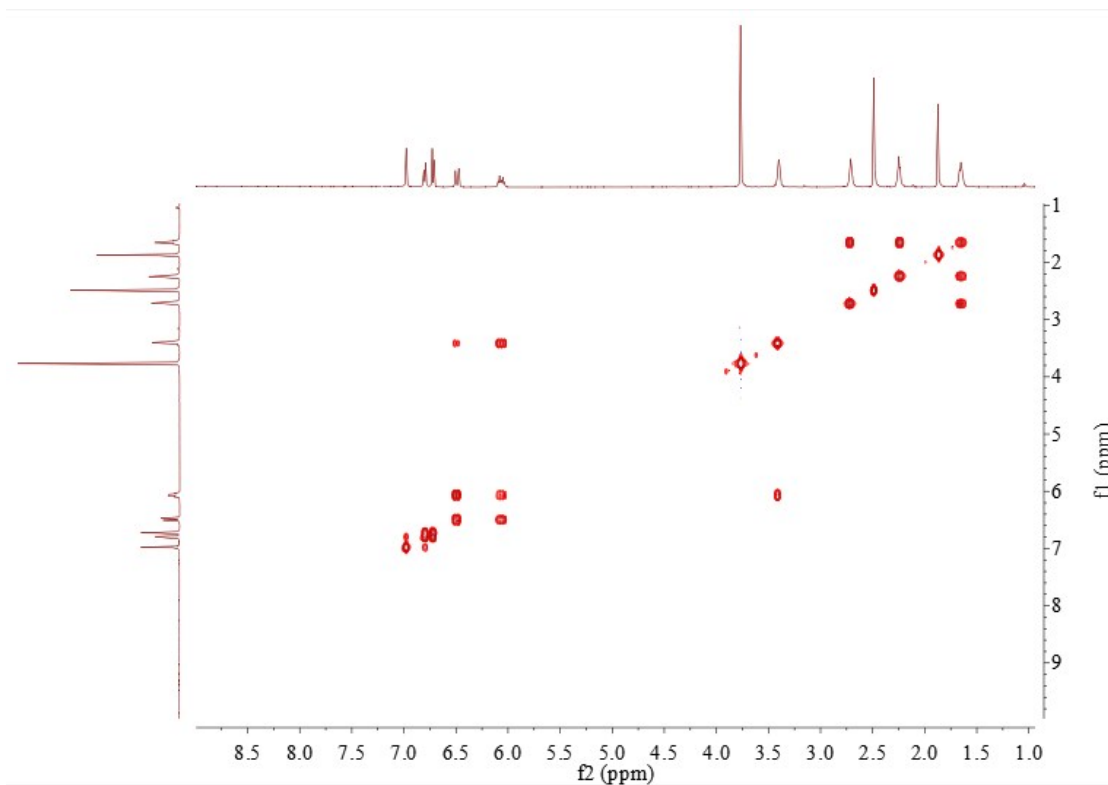


Figure S41. The ^1H - ^1H COSY spectrum of compound **6** in $\text{DMSO-}d_6$

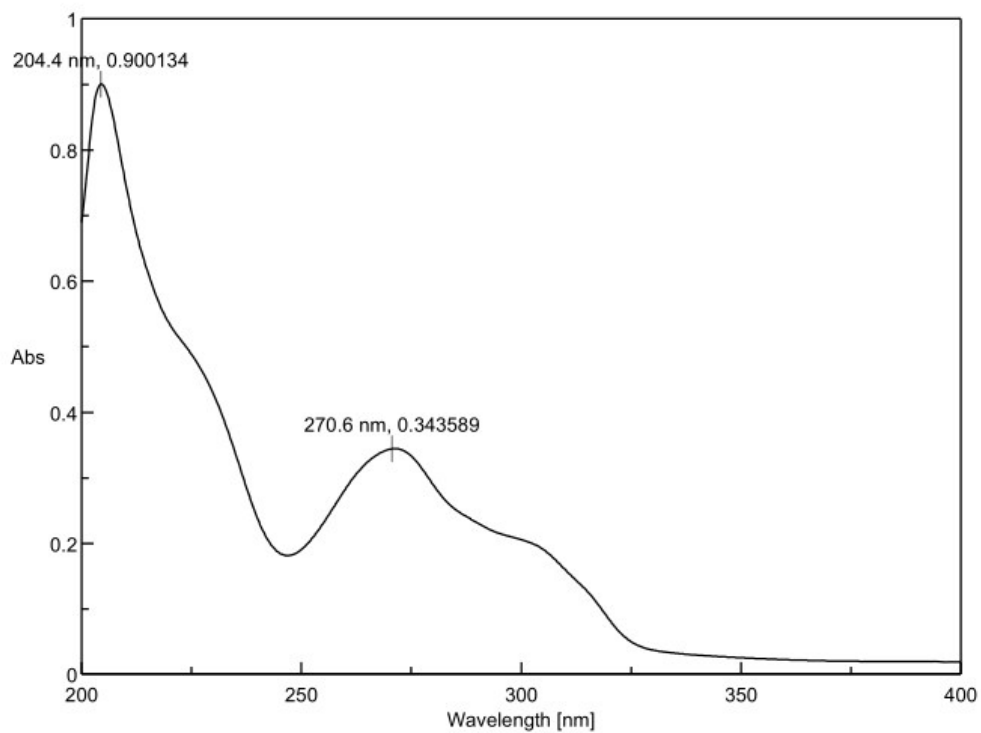


Figure S42. The UV spectrum of compound **6** in MeOH

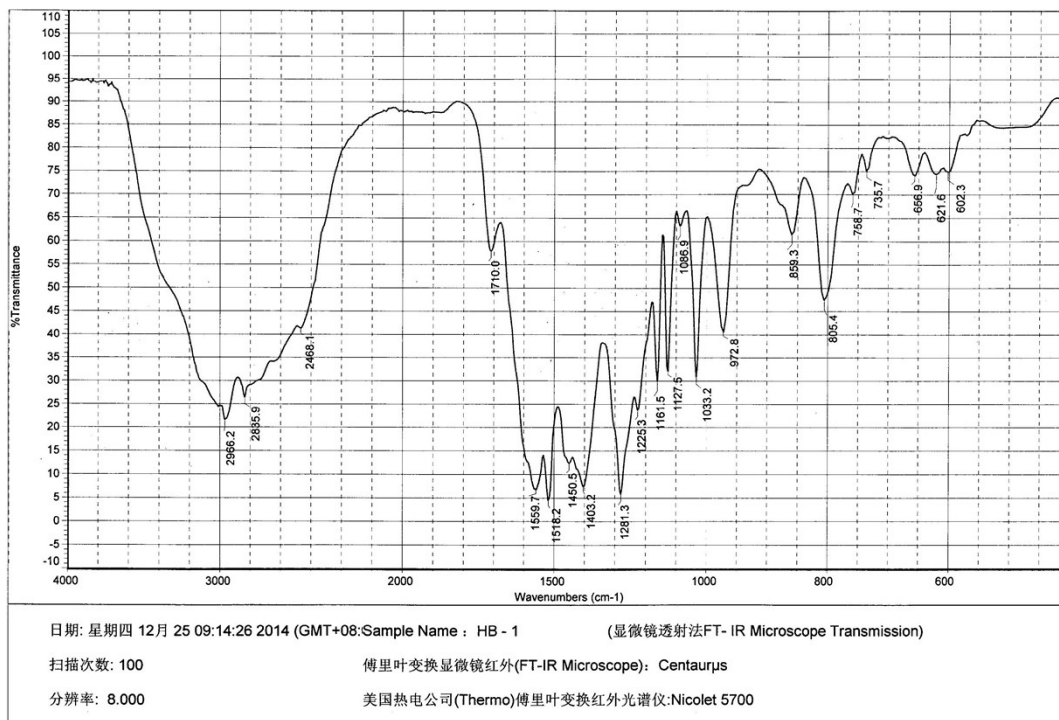
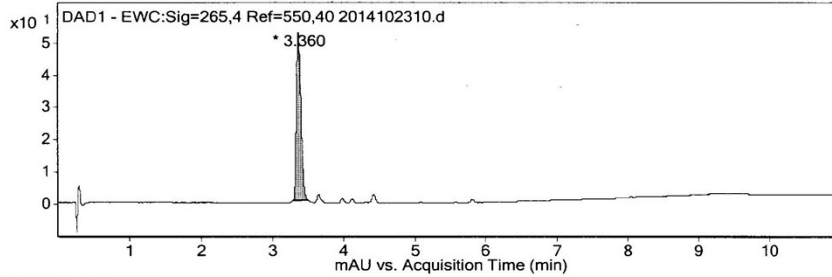


Figure S43. The IR spectrum of compound 6

Qualitative Analysis Report

Data Filename	2014102310.d	Sample Name	HB-1
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	XXXXXXXXXX
DA Method	TEST LCMS.m	Comment	

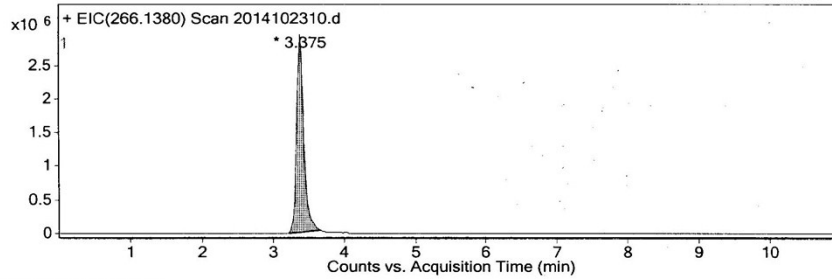
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.279	3.36	3.491	52.18	226.169	100

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



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.214	3.375	3.665	2939277	19639135	100

User Spectra

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

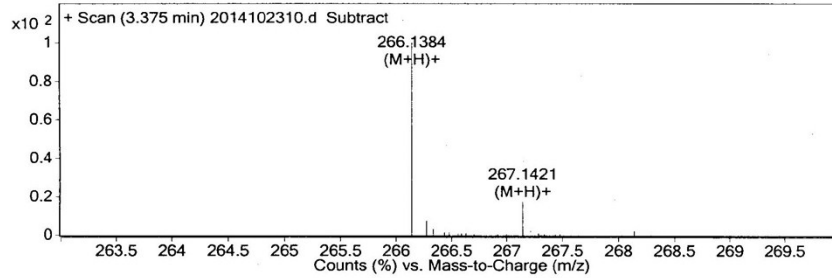


Figure S44. The HR-ESI-MS data of compound 6

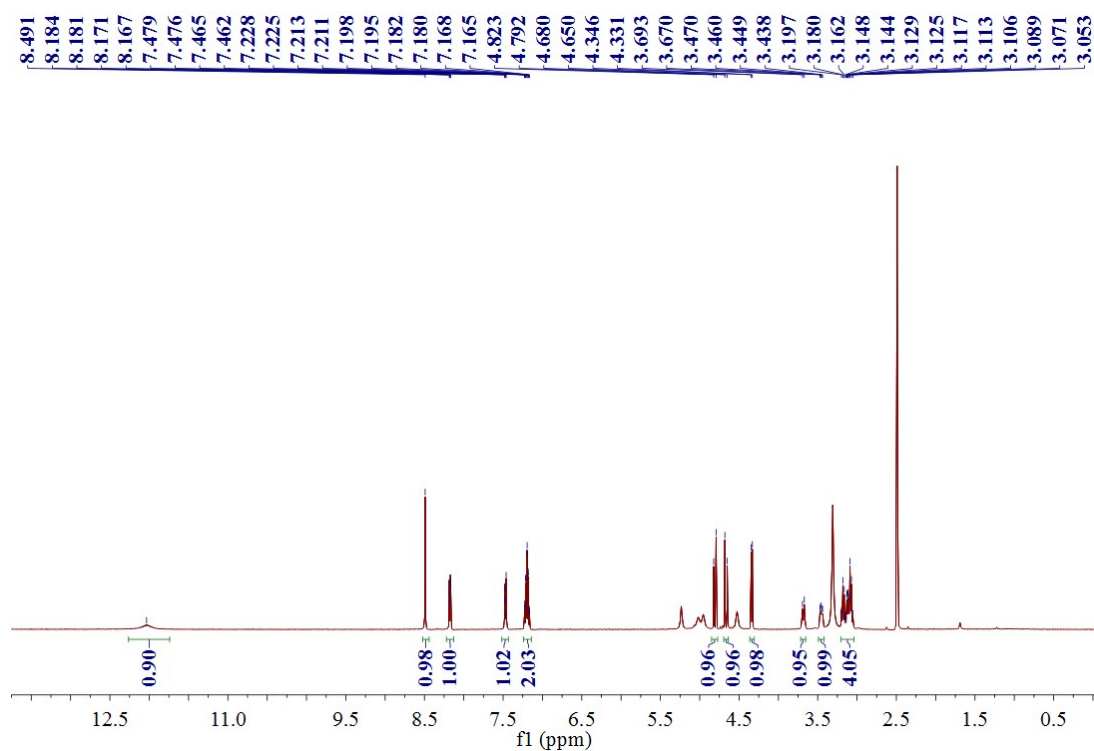


Figure S45. The ^1H NMR spectrum of compound **7** in $\text{DMSO-}d_6$

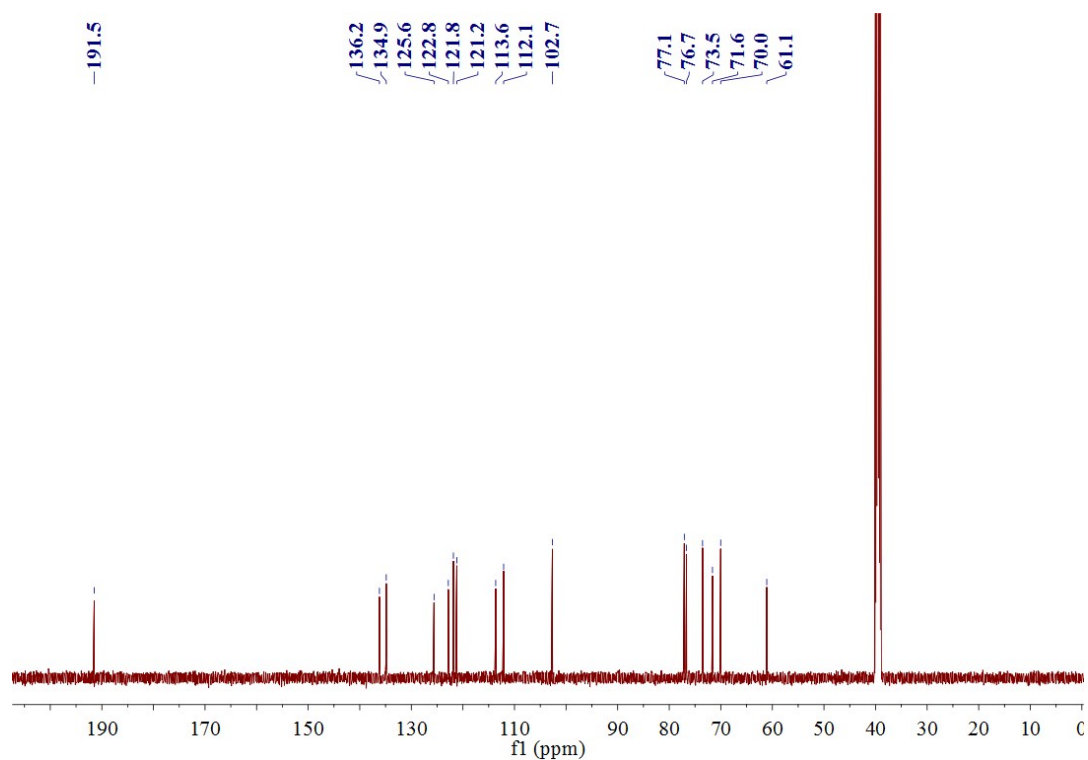


Figure S46. The ^{13}C NMR spectrum of compound **7** in $\text{DMSO-}d_6$

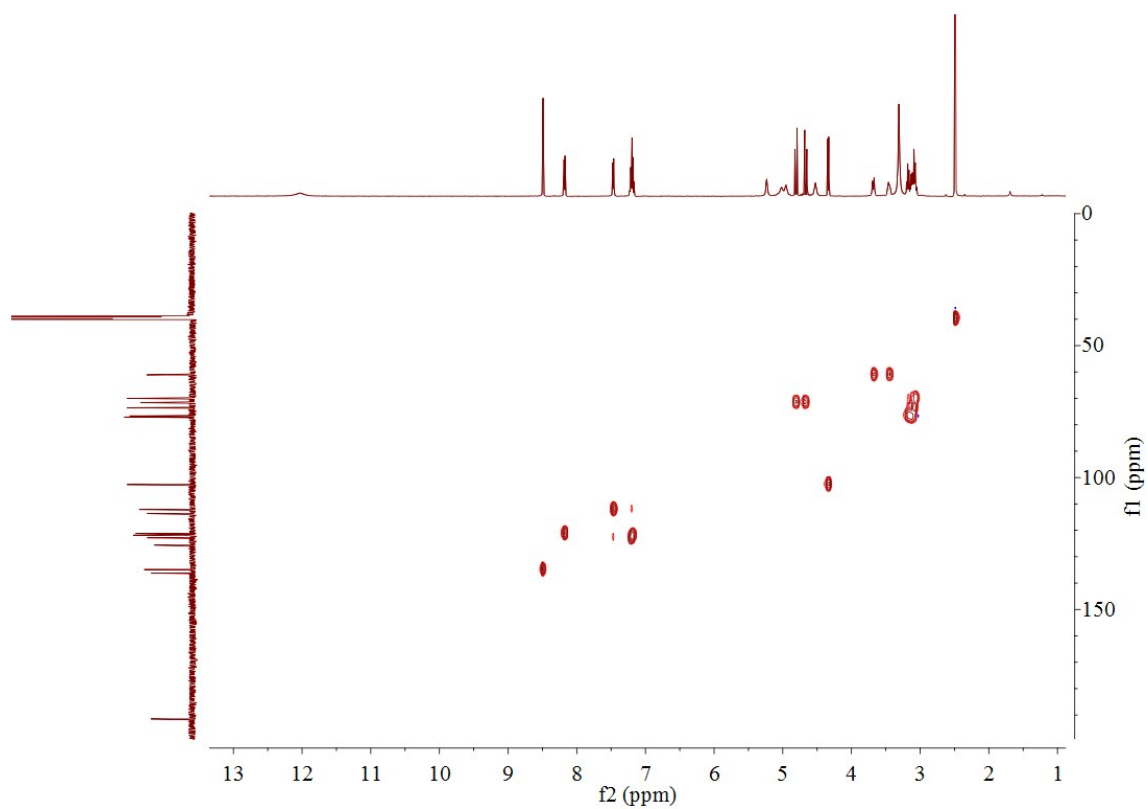


Figure S47. The HSQC spectrum of compound **7** in DMSO-*d*₆

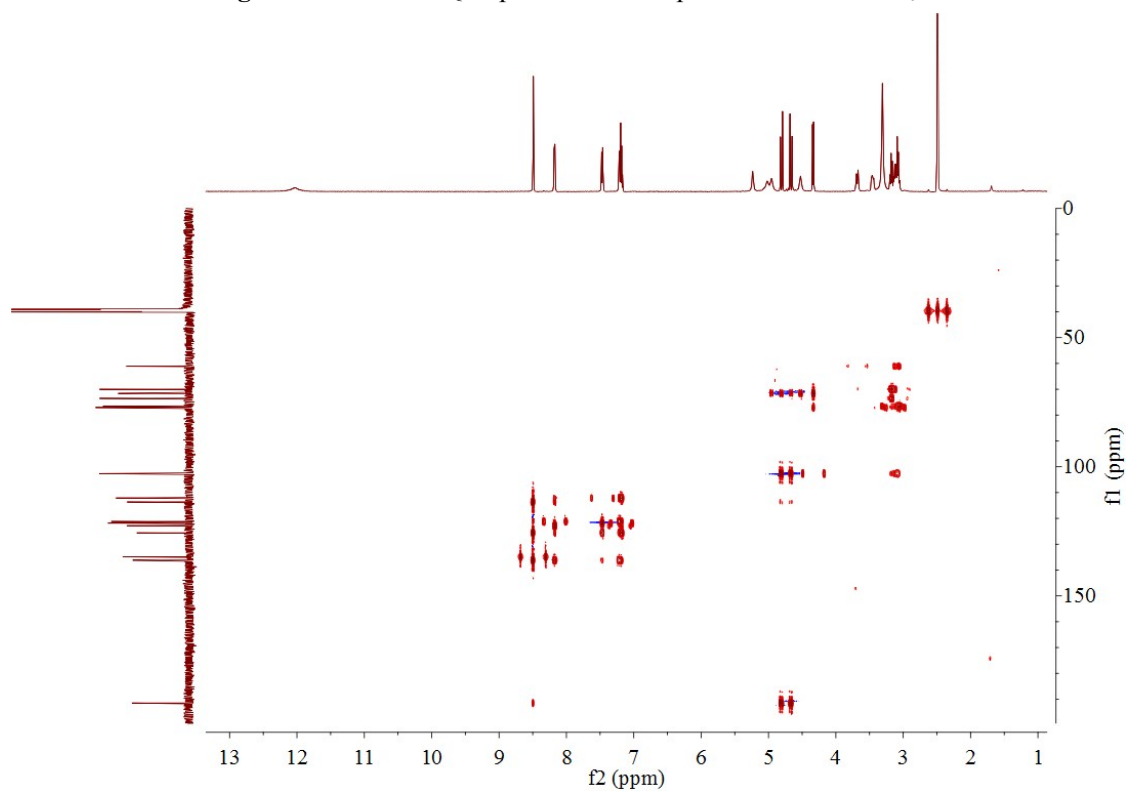


Figure S48. The HMBC spectrum of compound **7** in DMSO-*d*₆

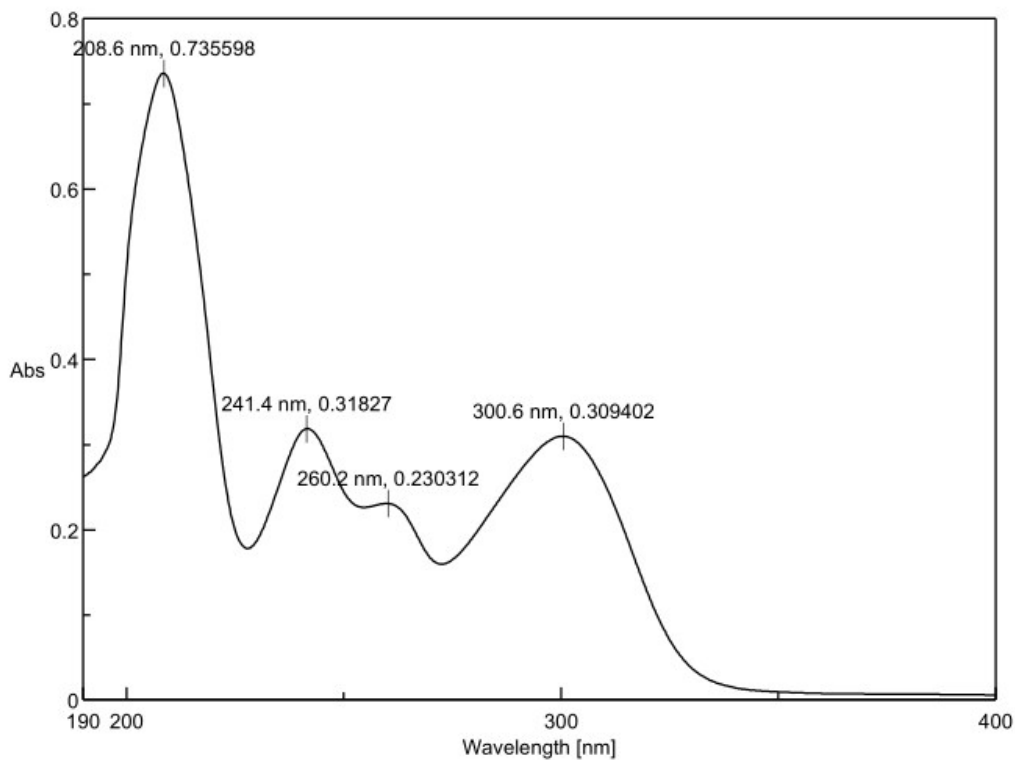


Figure S49. The UV spectrum of compound 7 in MeOH

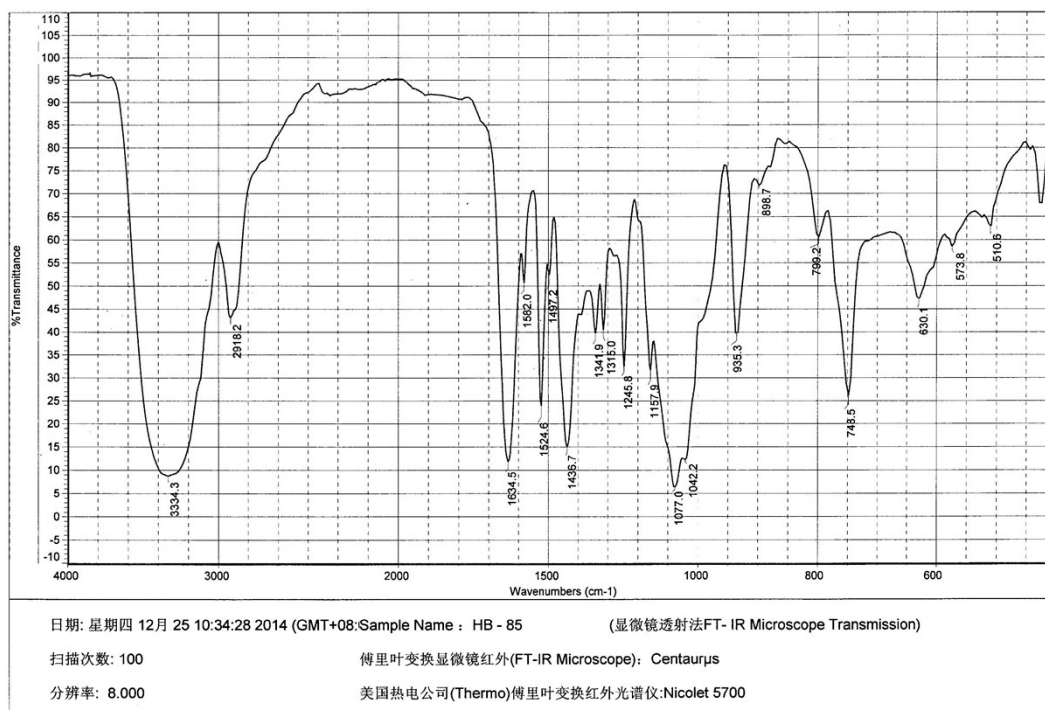


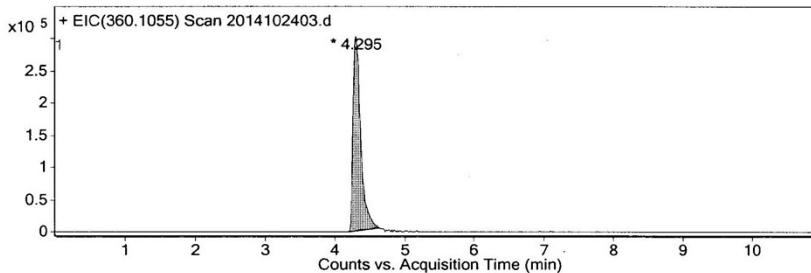
Figure S50. The IR spectrum of compound 7

Qualitative Analysis Report

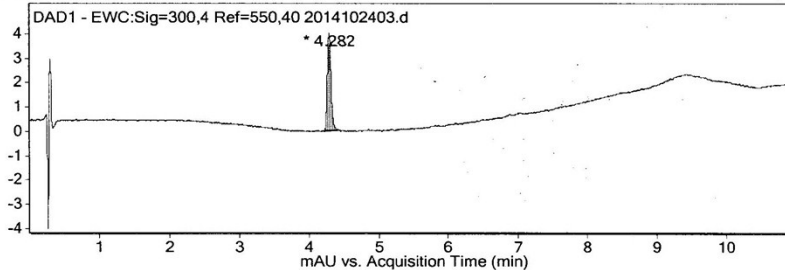
Data Filename	2014102403.d	Sample Name	HB-85
Sample Type	Sample	Position	P1-C3
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	XXXXXXXXXX
DA Method	TEST LCMS.m	Comment	

User Chromatograms

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



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



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

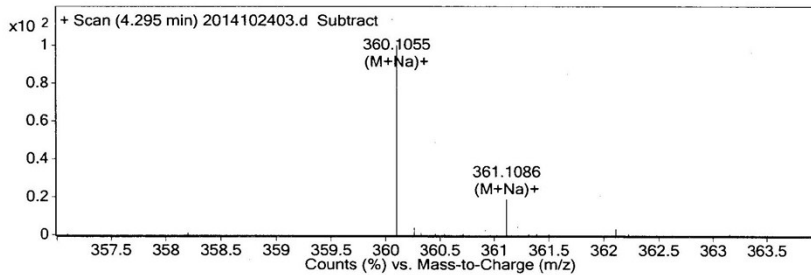


Figure S51. The HR-ESI-MS data of compound 7

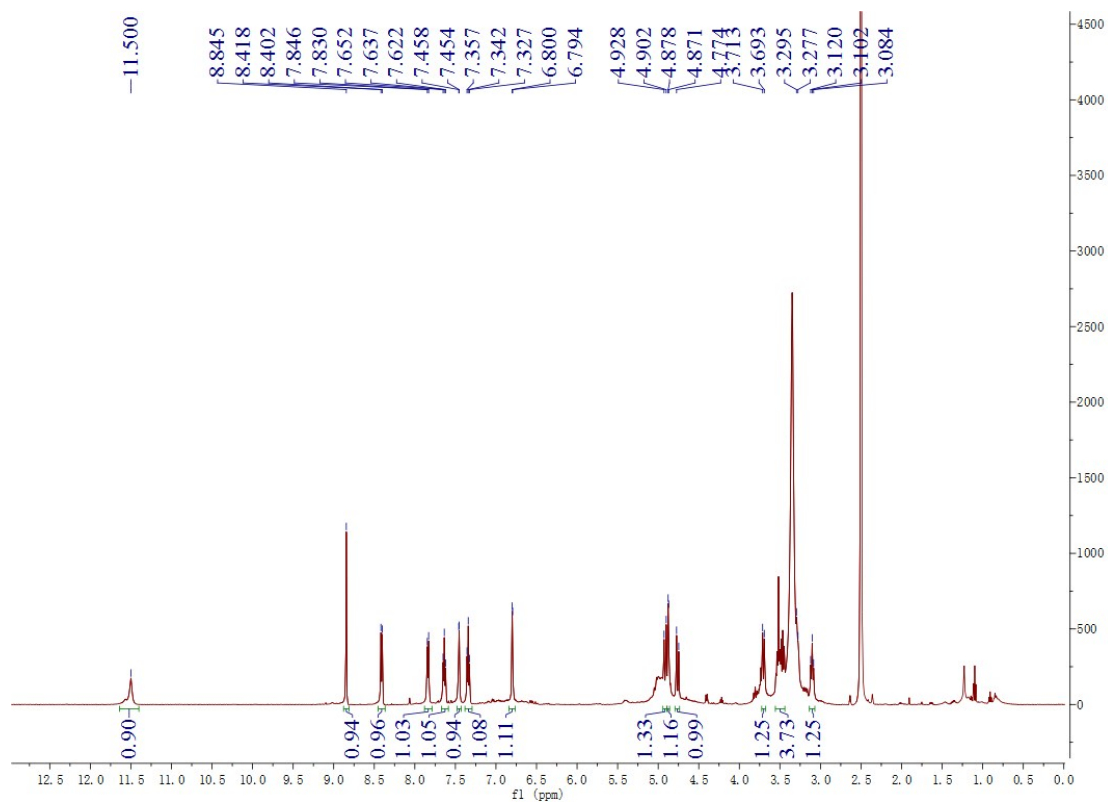


Figure S52. The ^1H NMR spectrum of compound **8** in $\text{DMSO-}d_6$

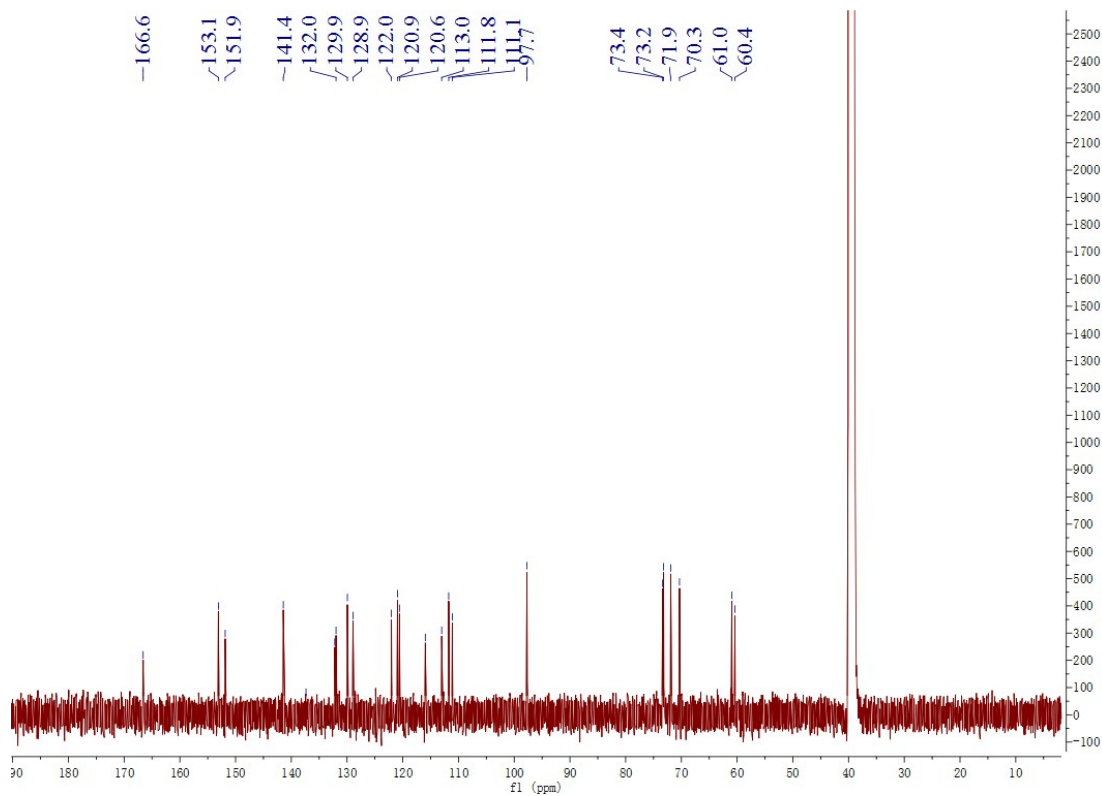


Figure S53. The ^{13}C NMR spectrum of compound **8** in $\text{DMSO-}d_6$

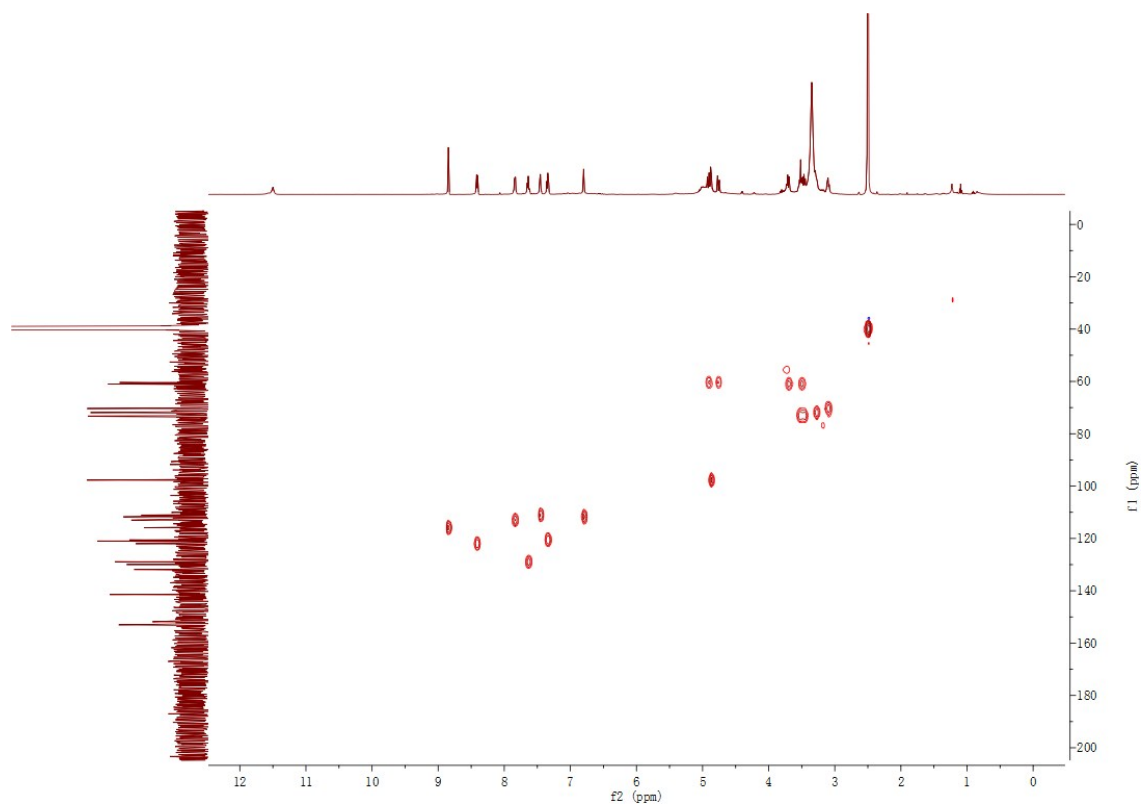


Figure S54. The HSQC spectrum of compound **8** in DMSO- d_6

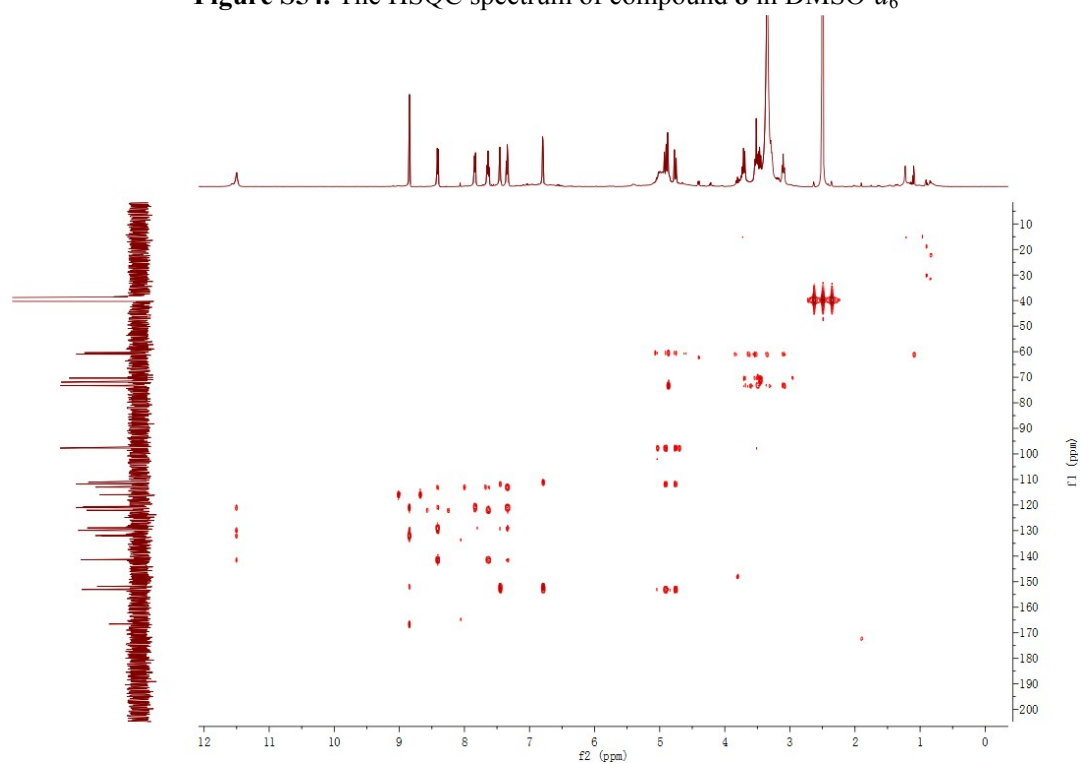


Figure S55. The HMBC spectrum of compound **8** in DMSO- d_6

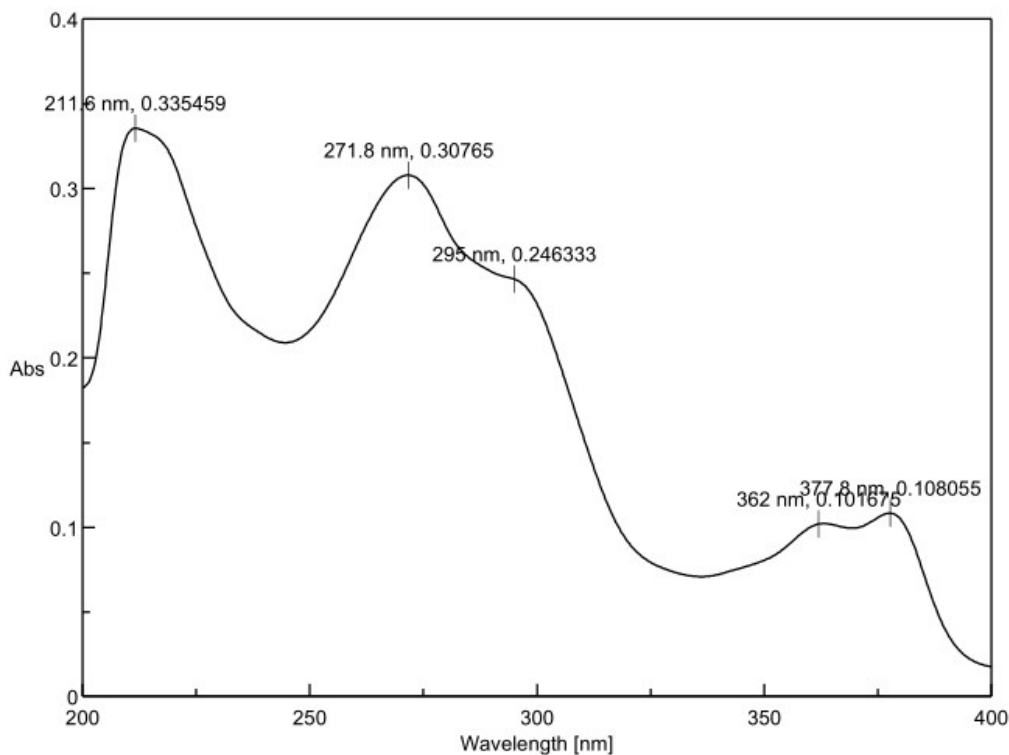


Figure S56. The UV spectrum of compound 8 in MeOH

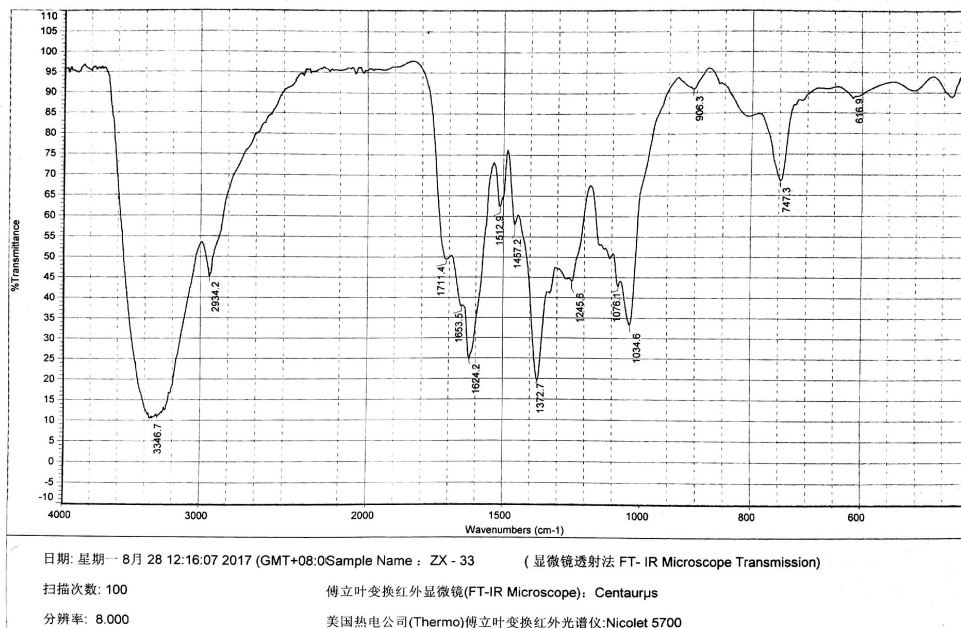
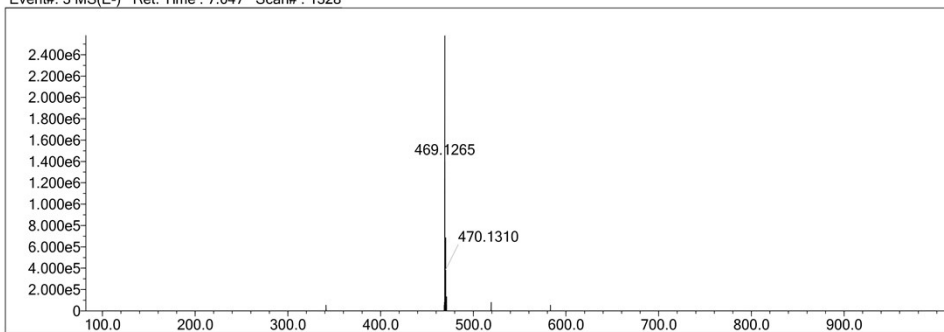
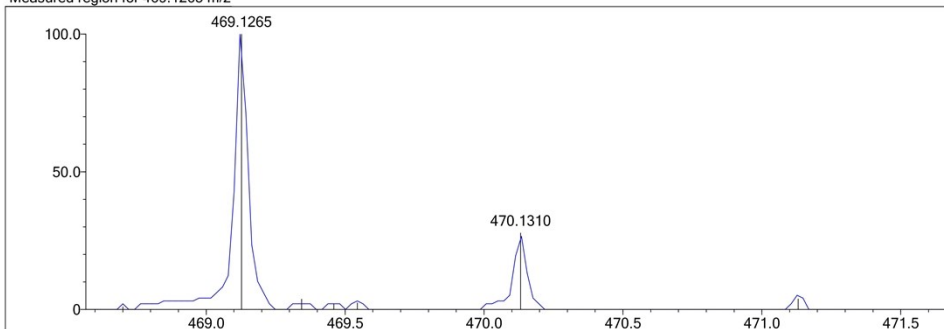


Figure S57. The IR spectrum of compound 8

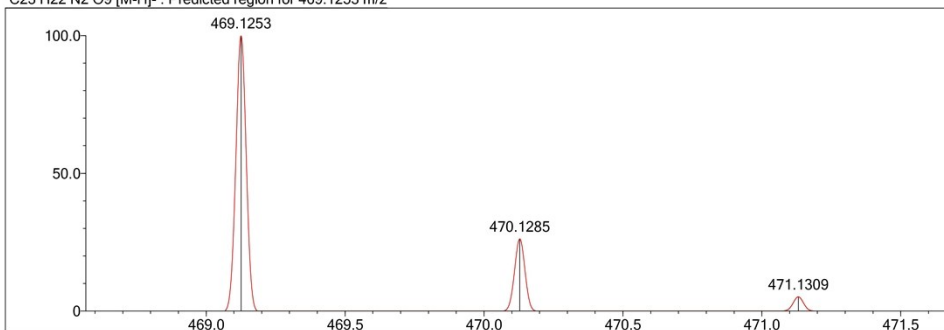
Event#: 3 MS(E-) Ret. Time : 7.047 Scan#: 1328



Measured region for 469.1265 m/z



C23 H22 N2 O9 [M-H]- : Predicted region for 469.1253 m/z



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

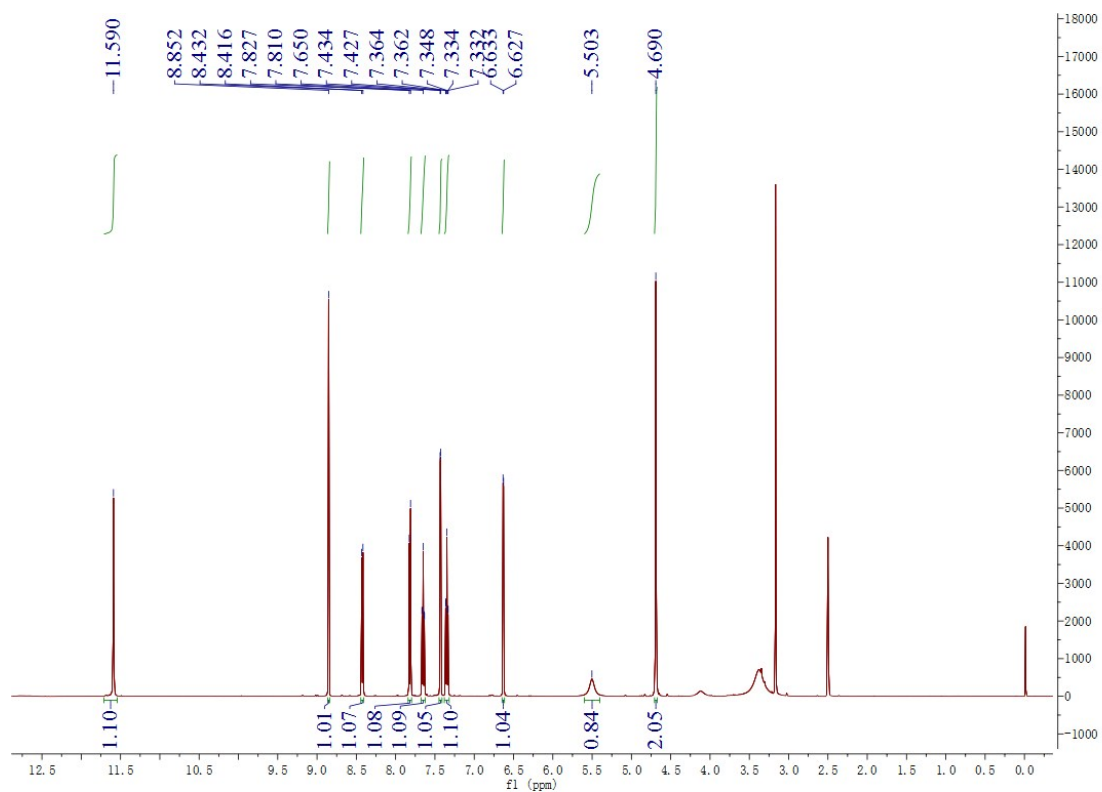


Figure S59. The ^1H NMR spectrum of compound **9** in $\text{DMSO-}d_6$

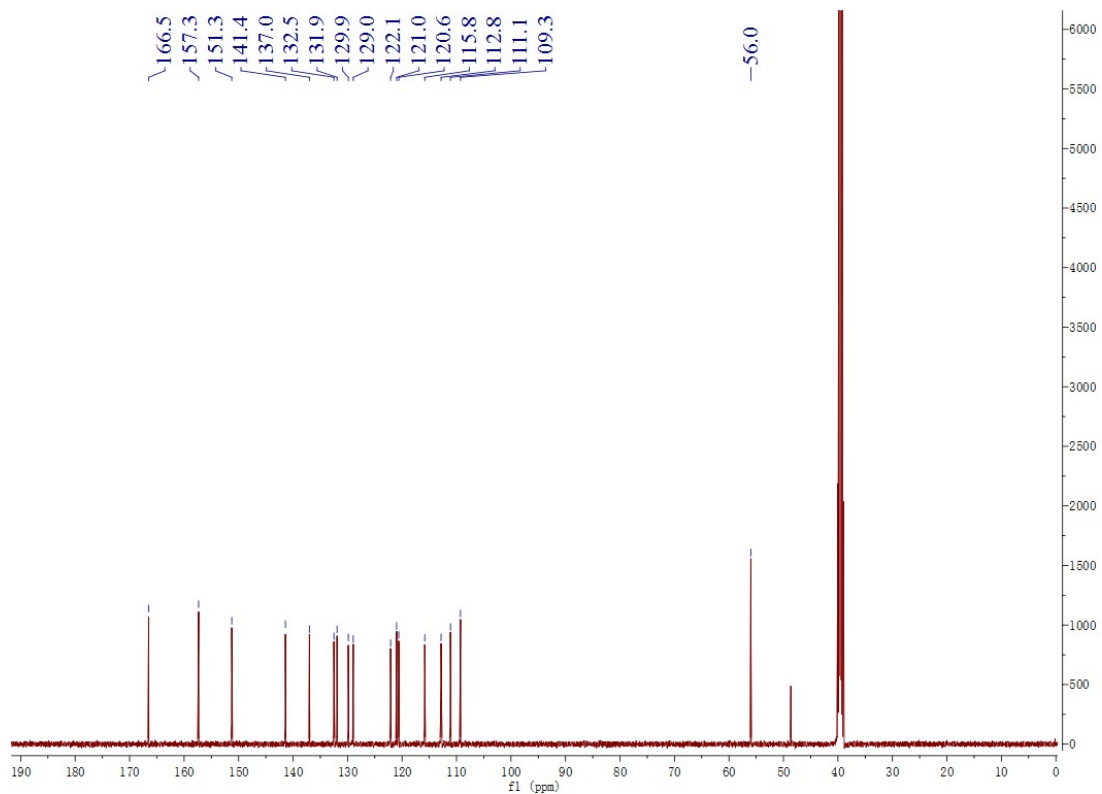
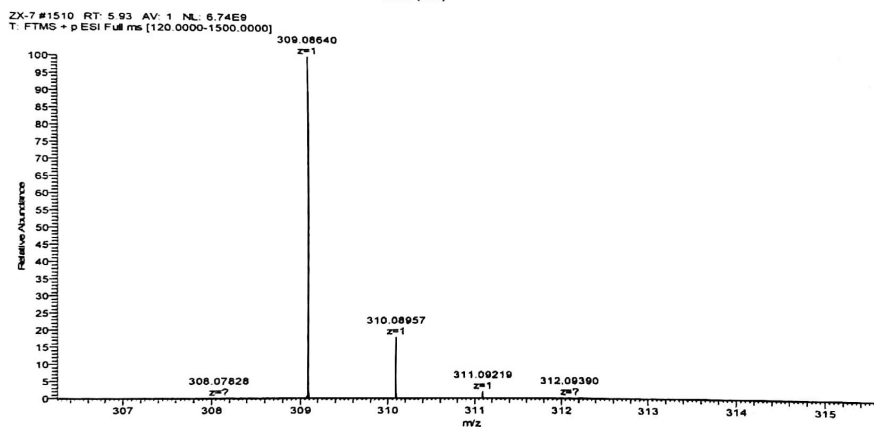
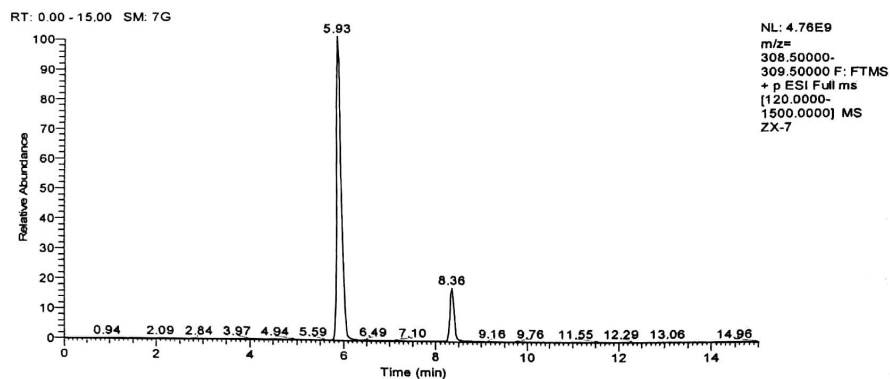


Figure S60. The ^{13}C NMR spectrum of compound **9** in $\text{DMSO-}d_6$

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

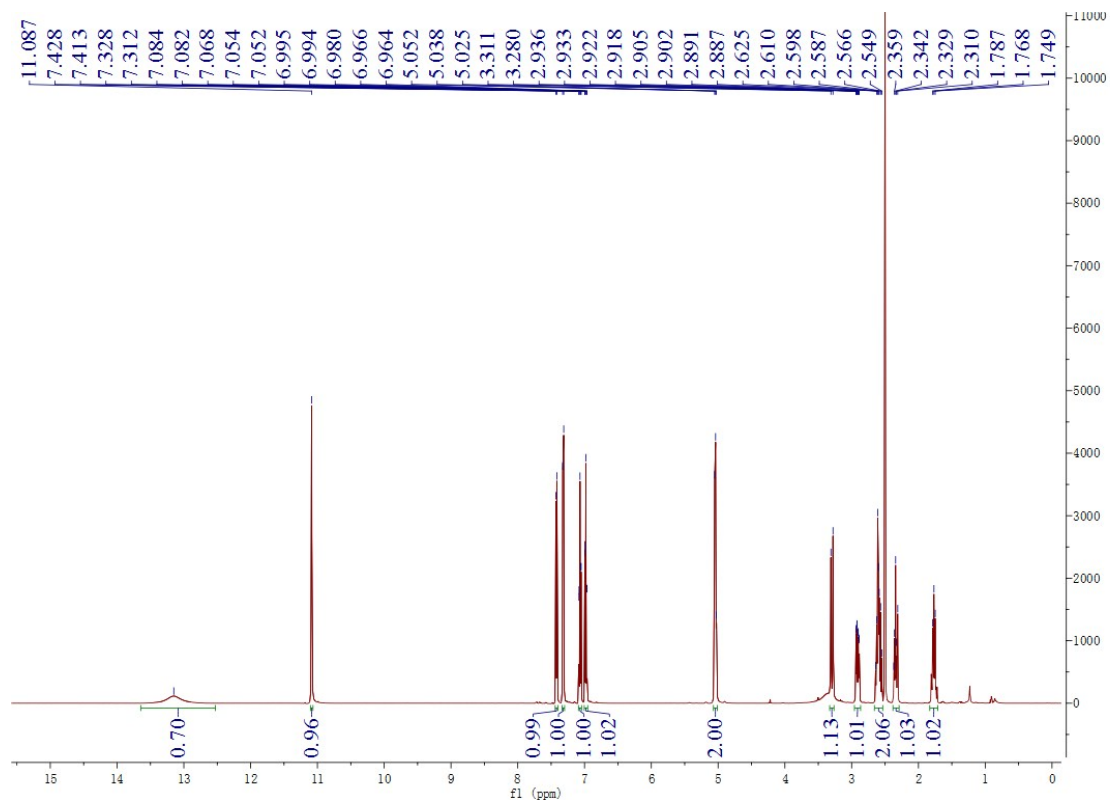


Figure S62. The ^1H NMR spectrum of compound **10** in $\text{DMSO-}d_6$

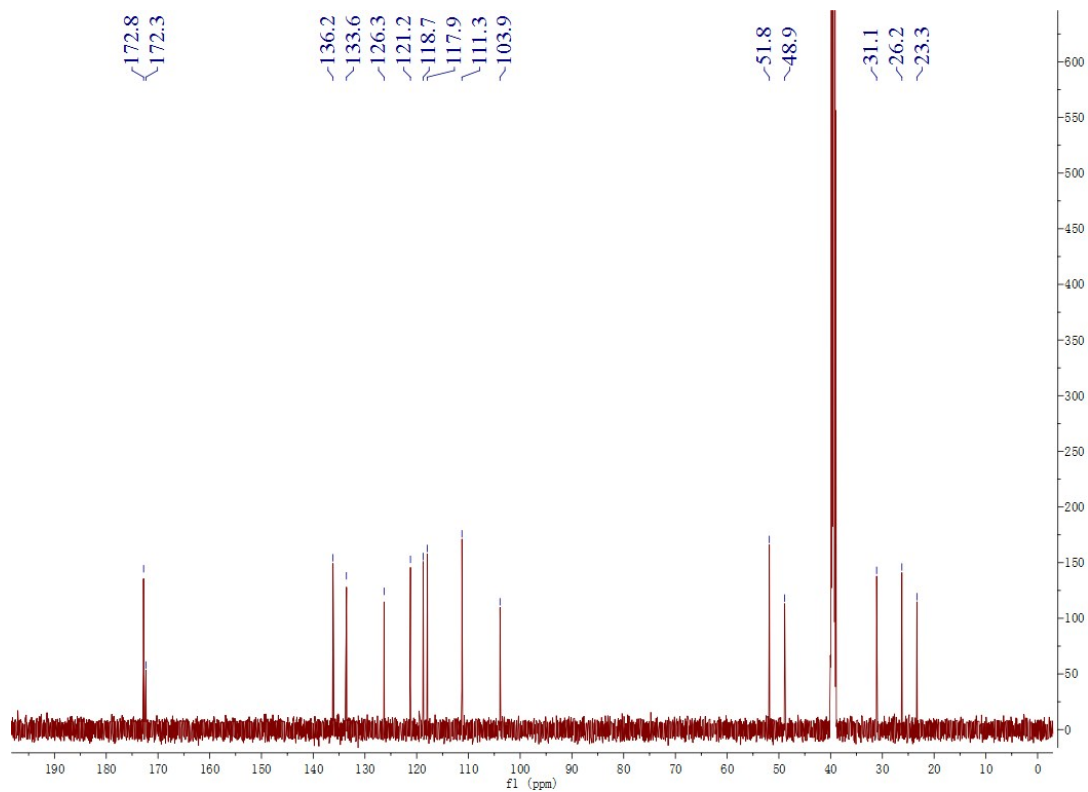


Figure S63. The ^{13}C NMR spectrum of compound **10** in $\text{DMSO-}d_6$

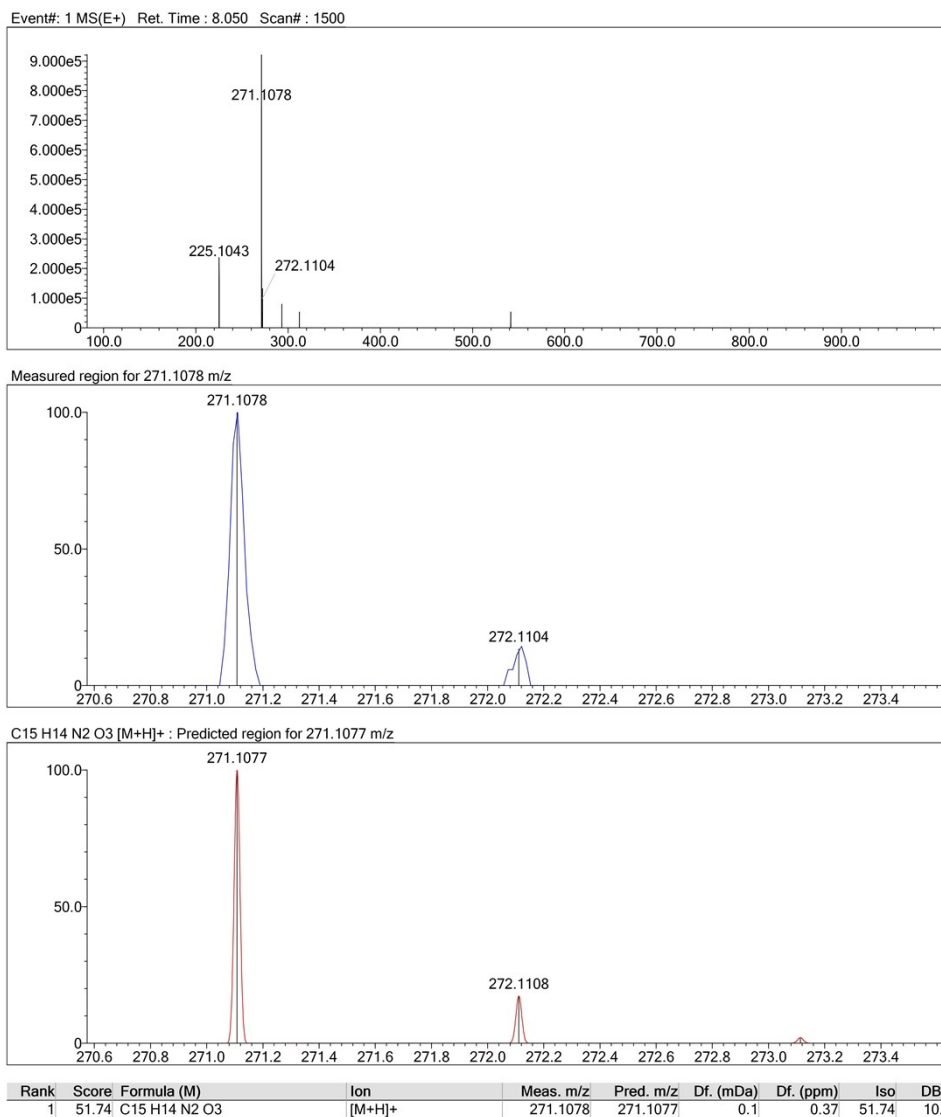


Figure S64. The HR-ESI-MS data of compound **10**

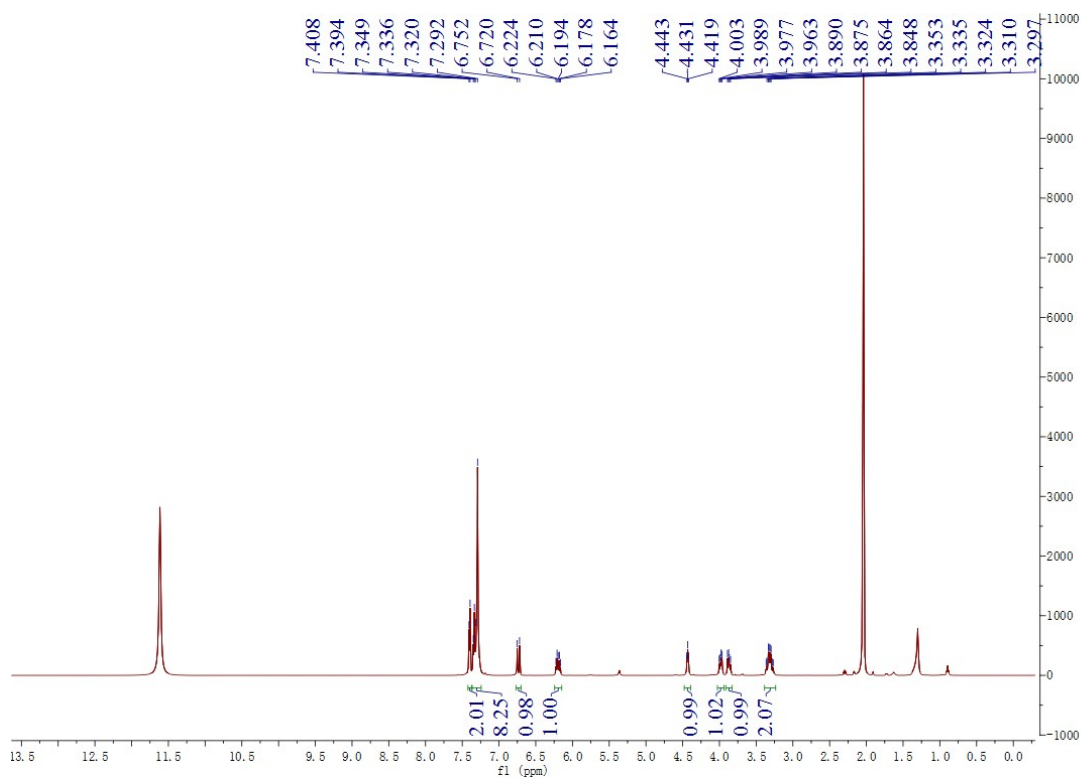


Figure S65. The ^1H NMR spectrum of compound **1b** in acetic acid- d_4

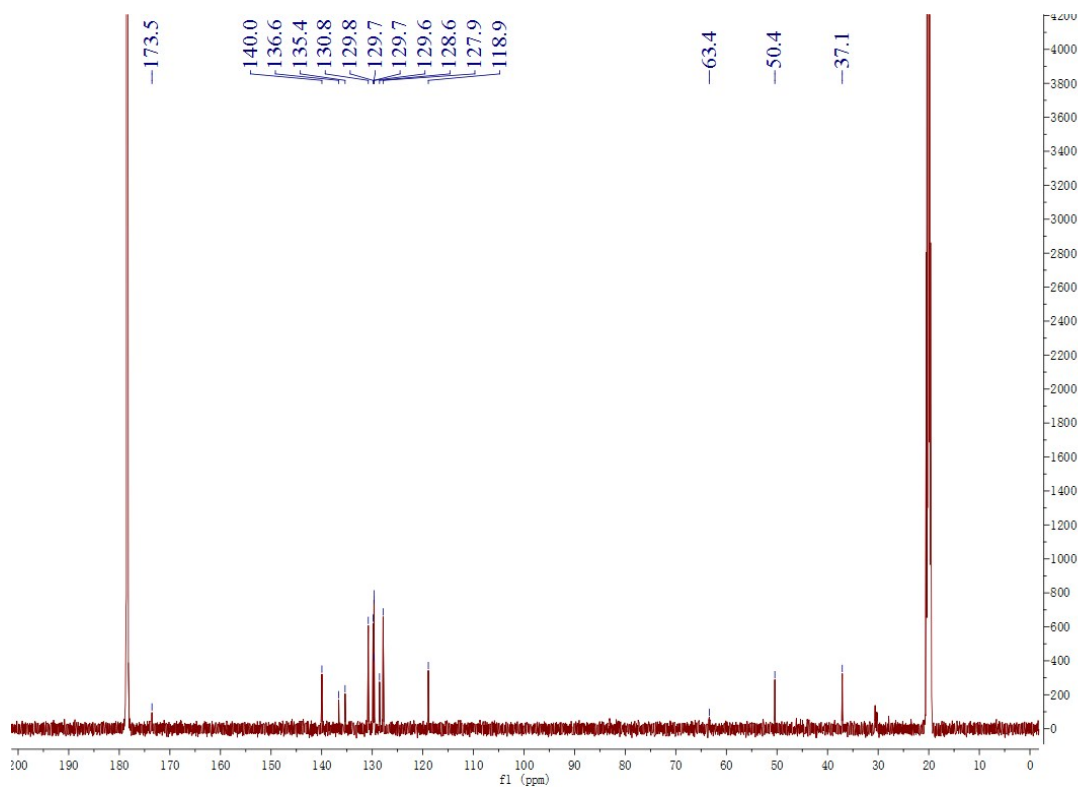
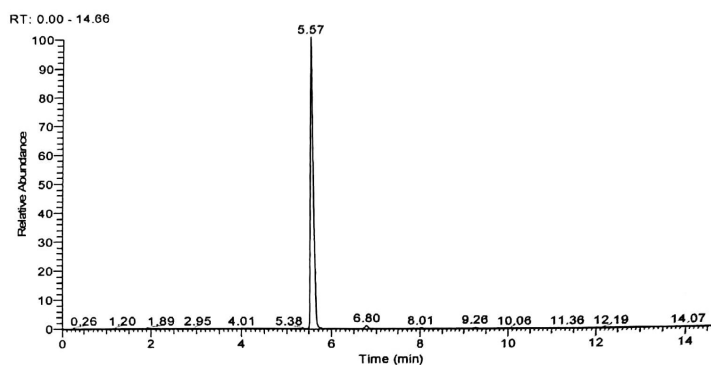


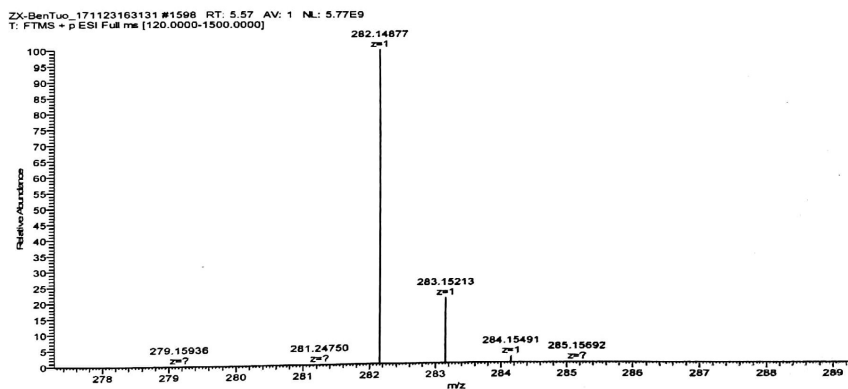
Figure S66. The ^{13}C NMR spectrum of compound **1b** in acetic acid- d_4

Thermo Qexactive Focus Report

compound NO. : ZX-Ben-Tuo
 Method : LCMS(compound)-low



NL: 5.79E9
 m/z= 281.50000-282.50000 F:
 FTMS + p ESI Full ms
 [120.0000-1500.0000]
 MS
 ZX-
 BenTuo_171123163131



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

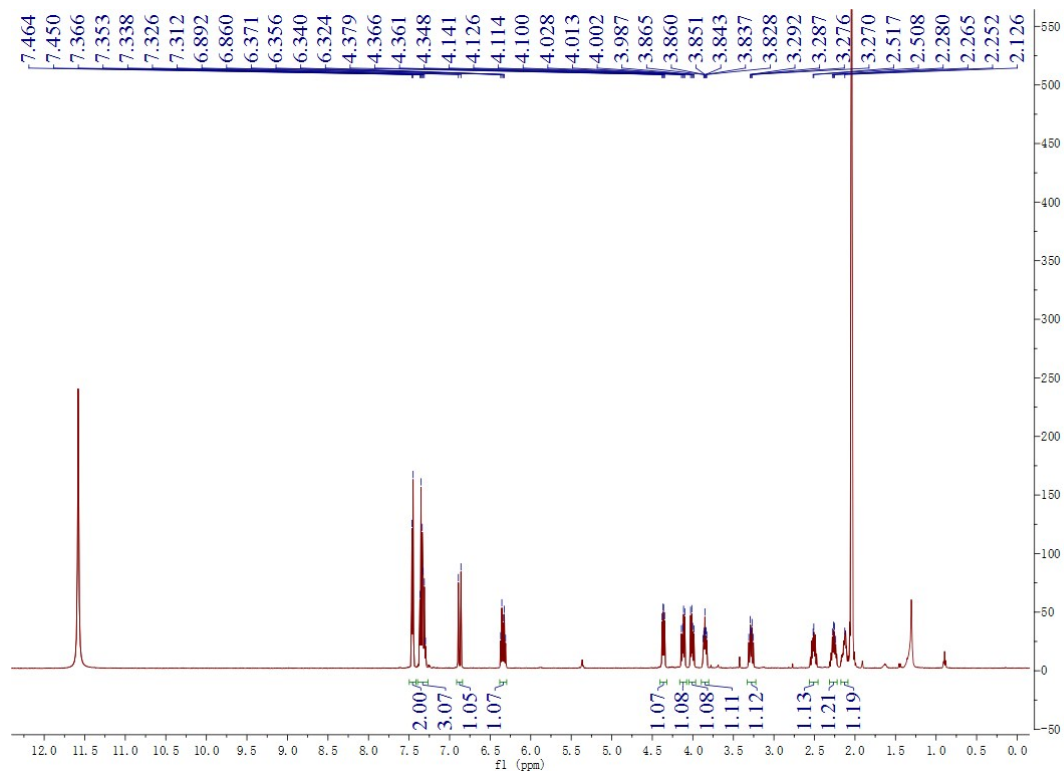


Figure S68. The ^1H NMR spectrum of compound **2b** in acetic acid- d_4

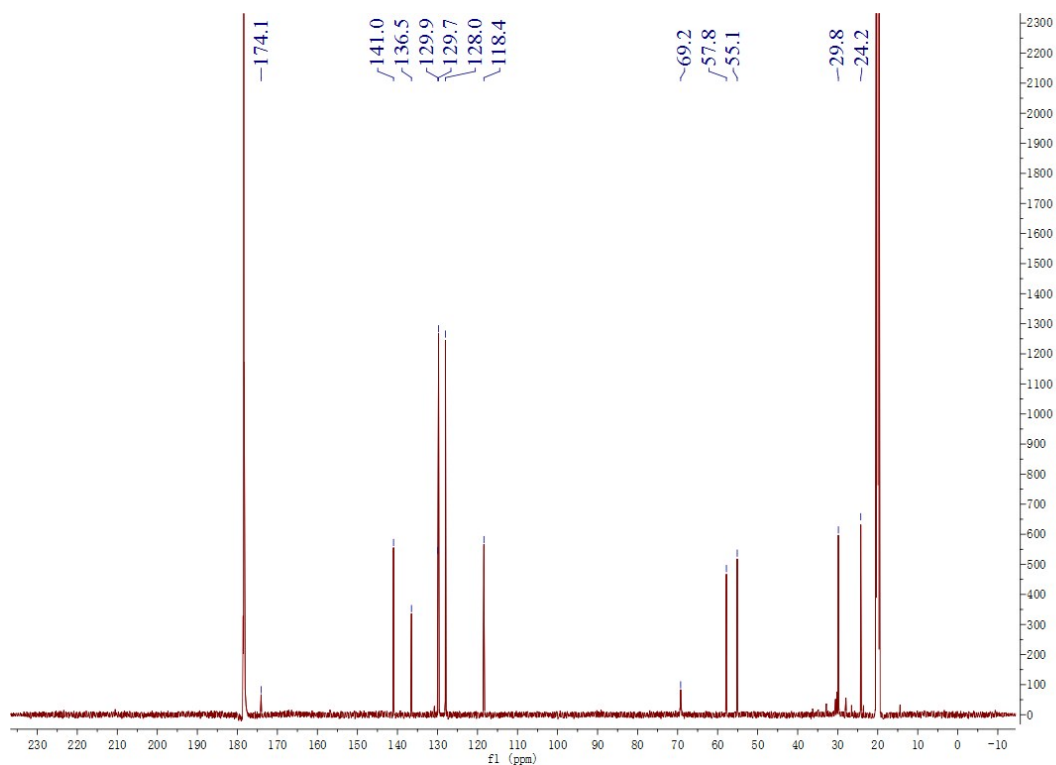
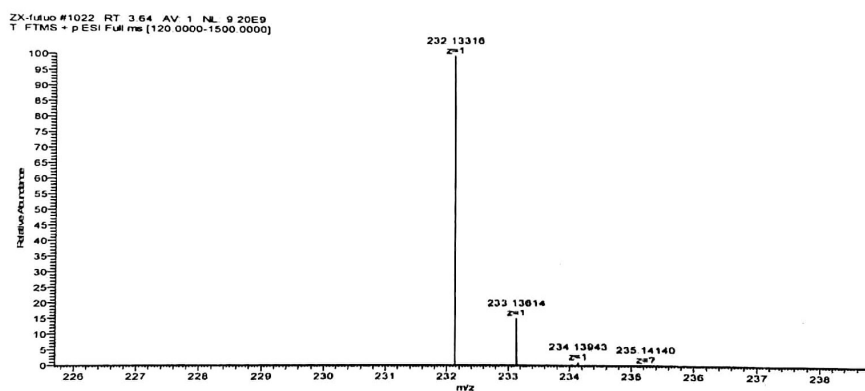
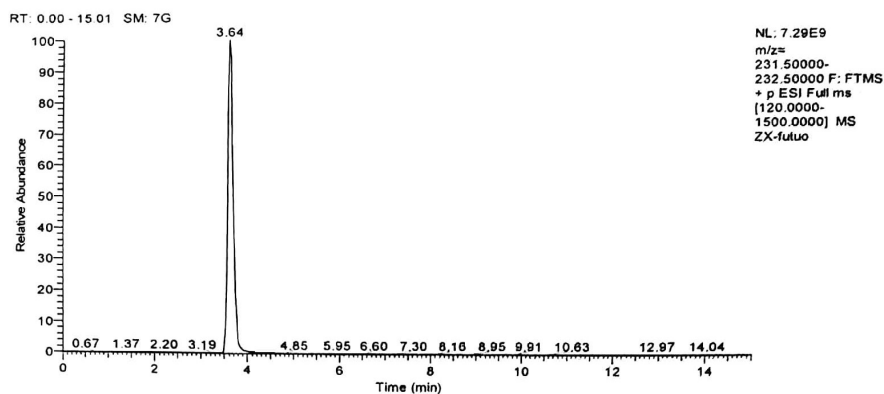


Figure S69. The ^{13}C NMR spectrum of compound **2b** in acetic acid- d_4

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

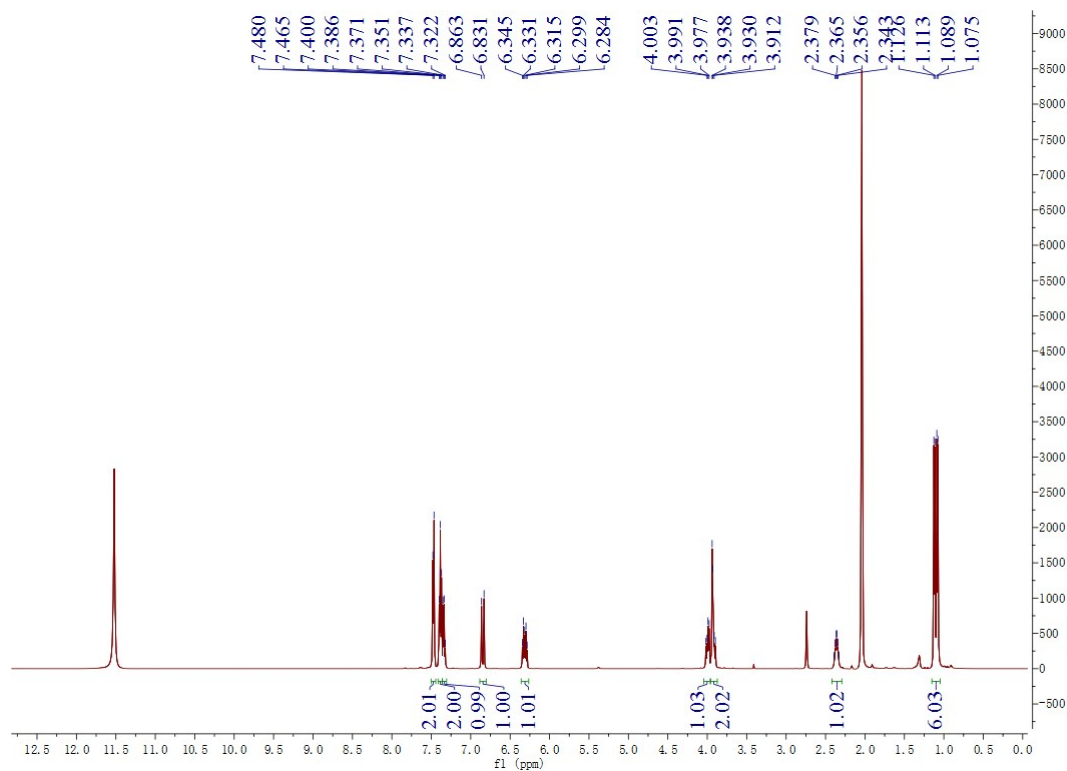


Figure S71. The ^1H NMR spectrum of compound **3b** in acetic acid- d_4

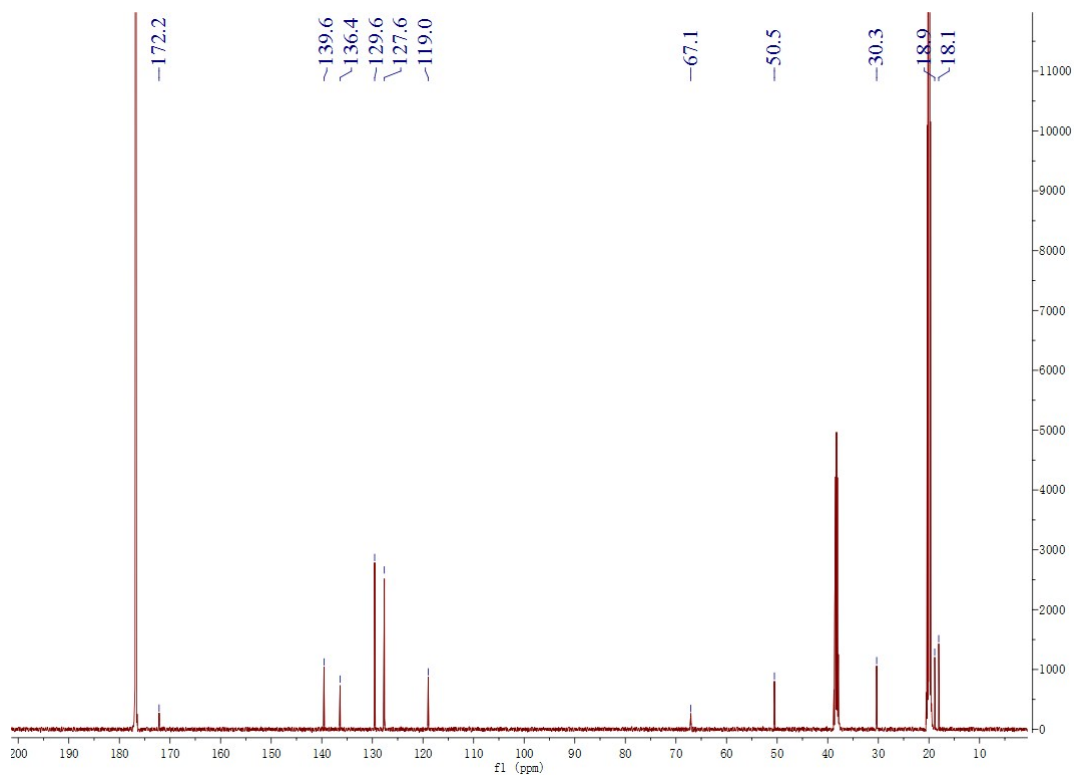
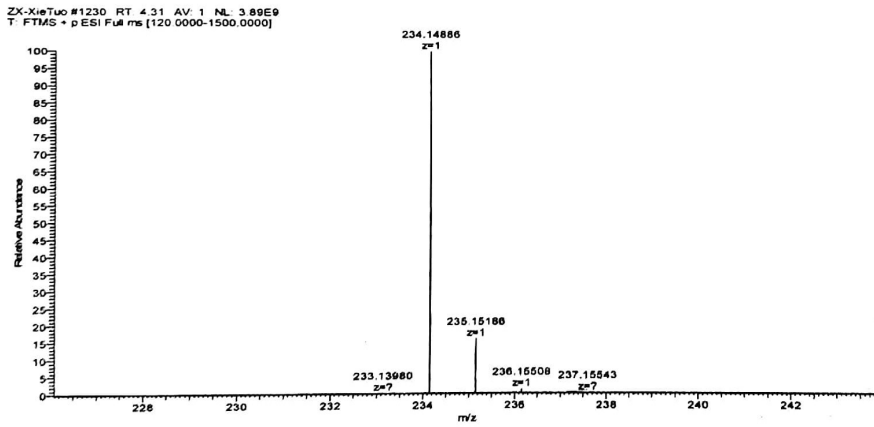
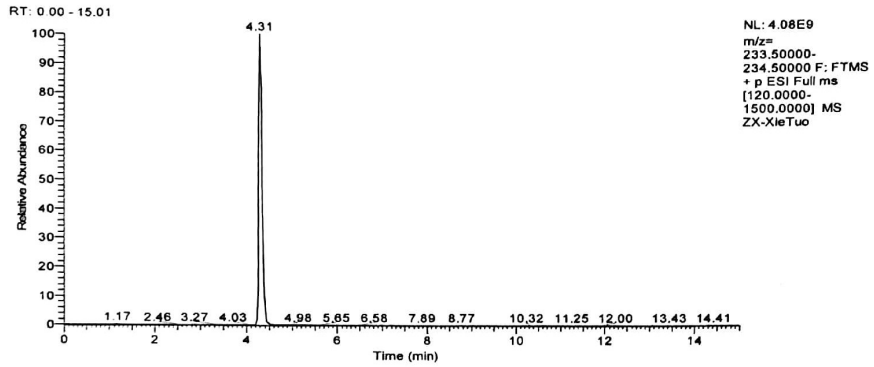


Figure S72. The ^{13}C NMR spectrum of compound **3b** in acetic acid- d_4

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

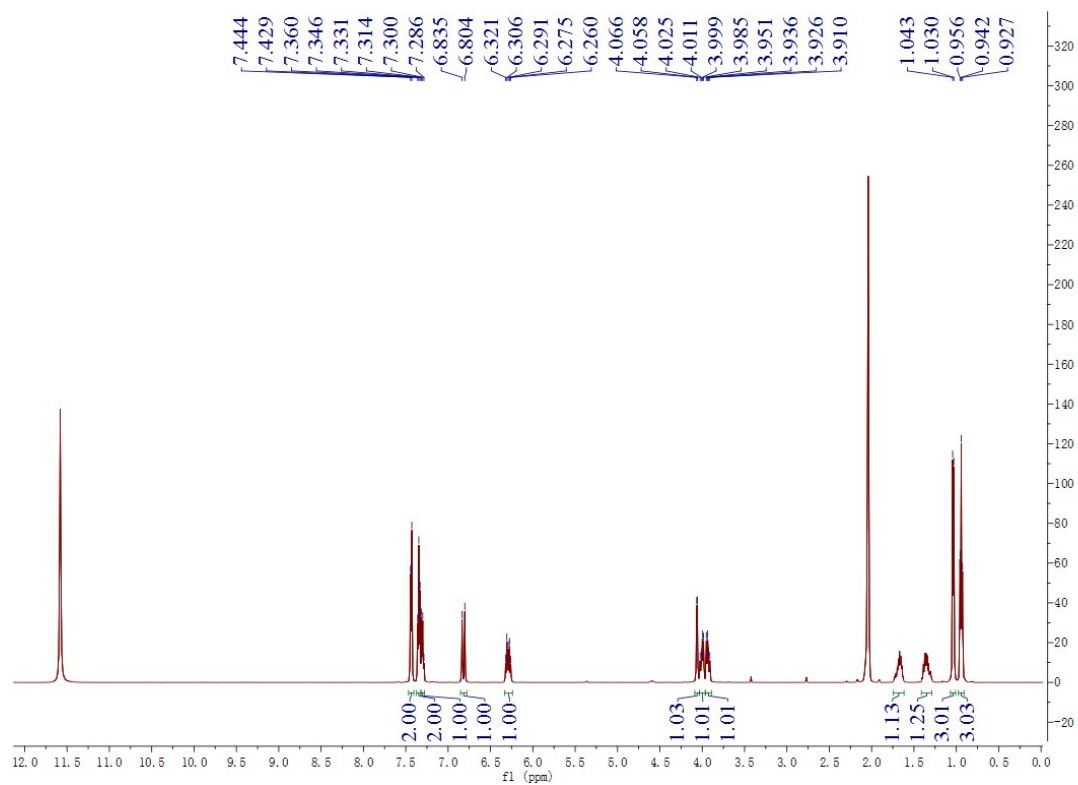


Figure S74. The ^1H NMR spectrum of compound **4b** in acetic acid- d_4

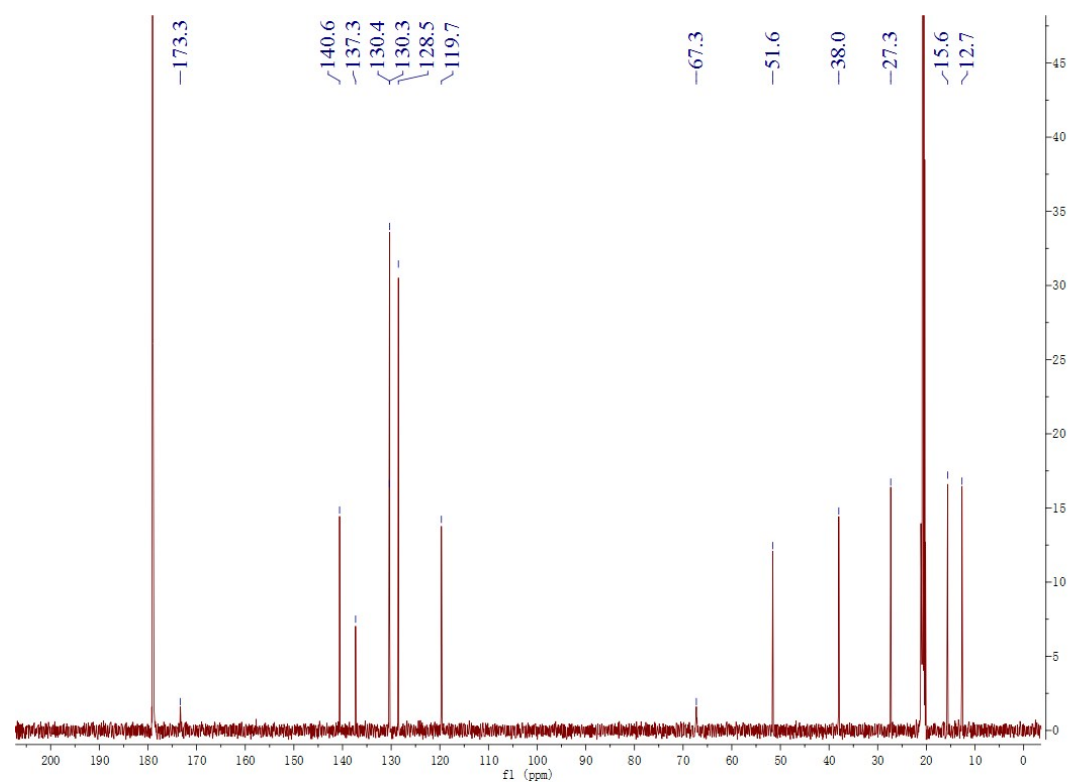
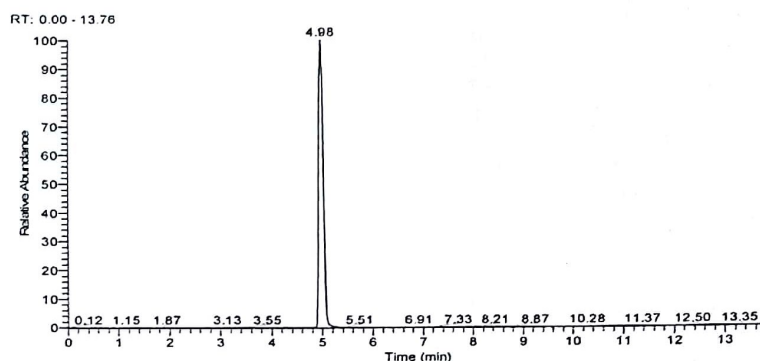


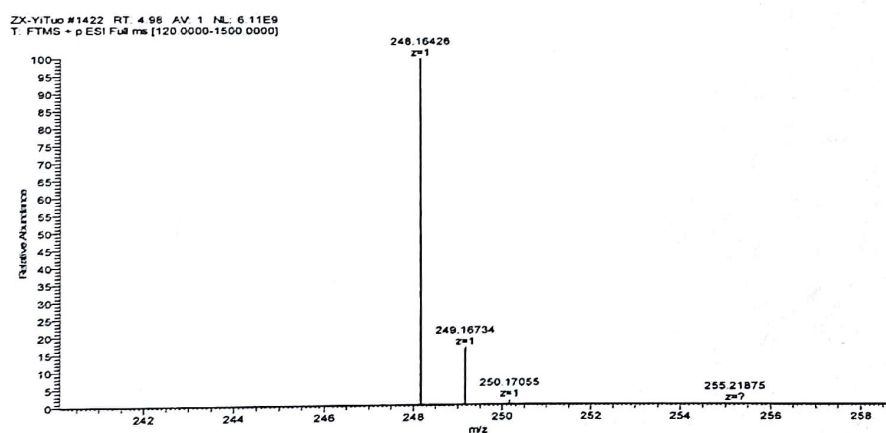
Figure S75. The ^{13}C NMR spectrum of compound **4b** in acetic acid- d_4

Thermo Qexactive Focus Report

compound NO. : ZX-Yi-Tuo
 Method : LCMS(compound)-low



NL: 6.12E9
 m/z=
 247.50000-
 248.50000 F: FTMS
 + p ESI Full ms
 [120.0000-
 1500.0000] MS
 ZX-YiTuo



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

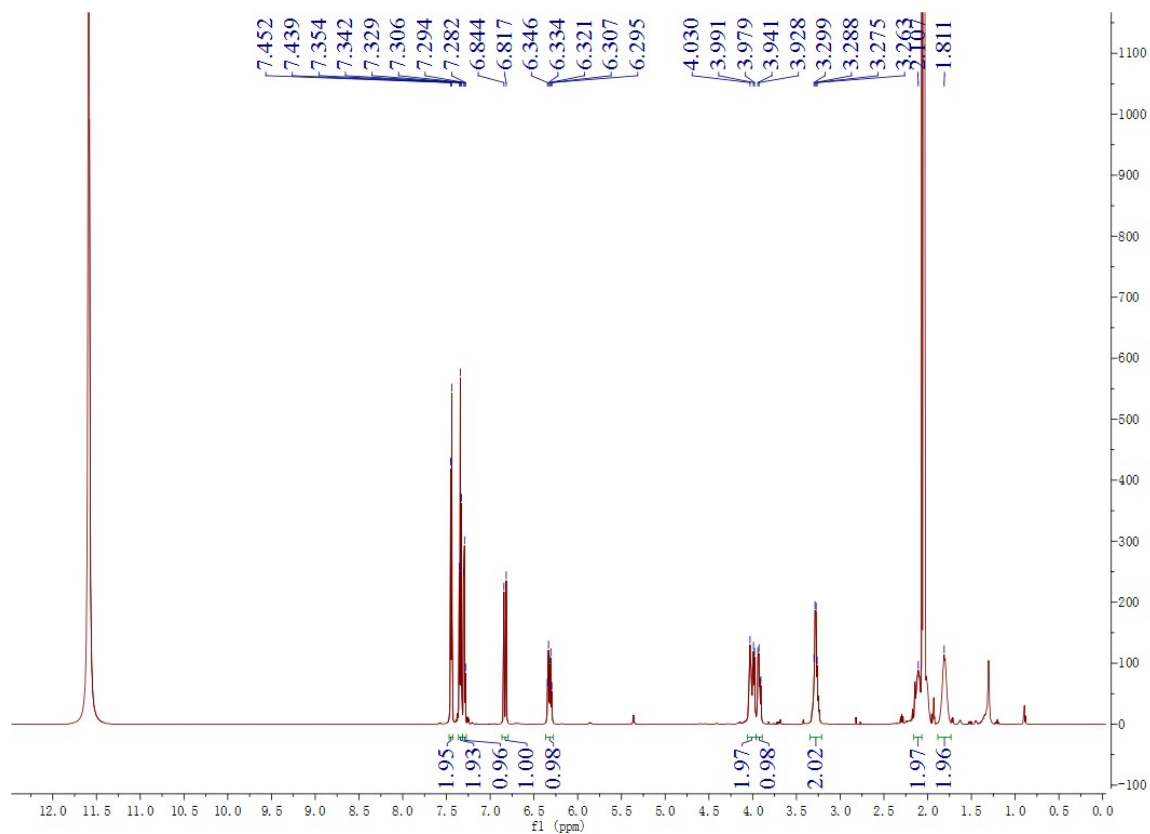


Figure S77. The ^1H NMR spectrum of compound **5b** in acetic acid- d_4

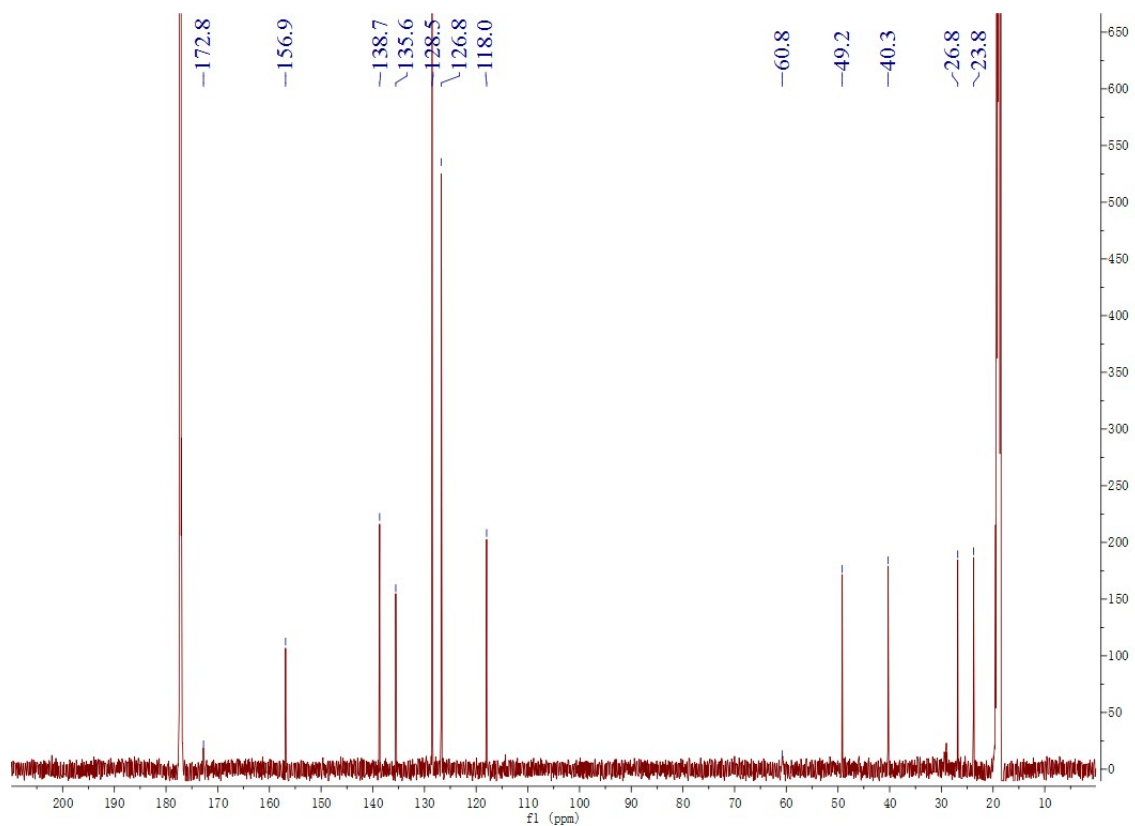
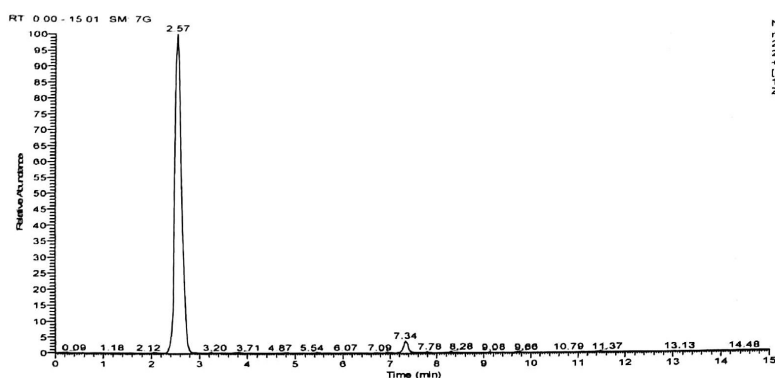


Figure S78. The ^{13}C NMR spectrum of compound **5b** in acetic acid- d_4

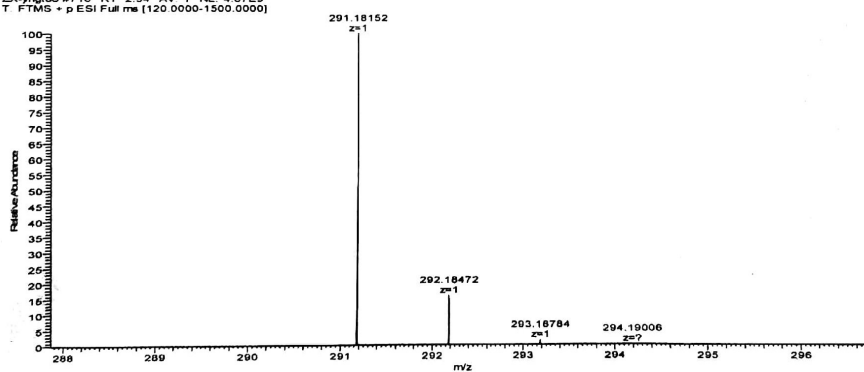
Thermo Qexactive Focus Report

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



NL: 4 26E9
 m/z: 290.50000
 291.50000 F: FTMS
 + p ESI Full ms
 [120.0000-
 1500.0000] MS
 ZX-jingtuo

ZX-jingtuo #710 RT: 2.54 AV: 1 NL: 4 67E9
 T: FTMS + p ESI Full ms [120.0000-1500.0000]



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

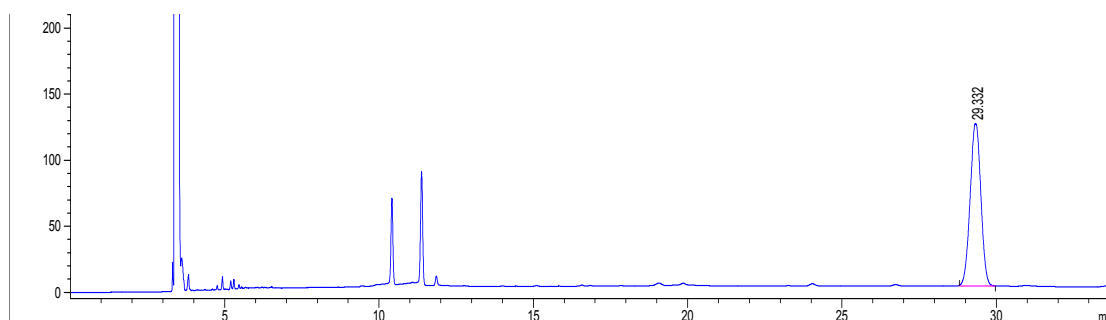


Figure S80. The Gas Chromatographic separation of D-Glc

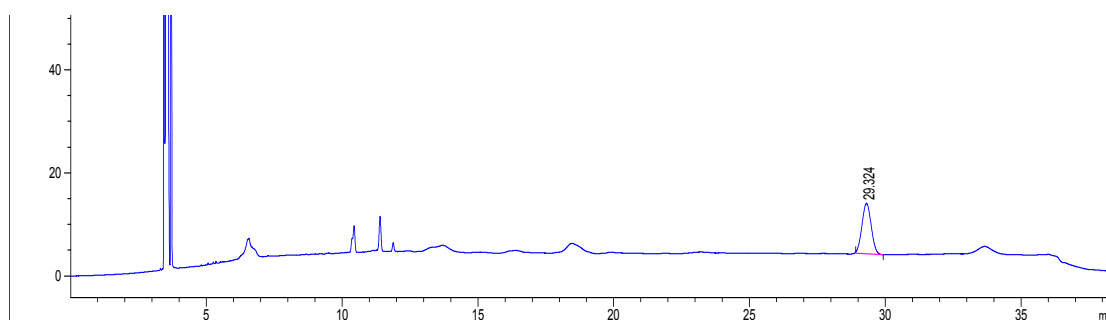


Figure S81. The Gas Chromatographic analyses of sugar moieties of compounds 7-8

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