

Supporting information

Phthalide Derivatives 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

Table of Contents

No.	Contents	Compounds	Page
1	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S5
2	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S5
3	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S6
4	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S6
5	The ¹ H- ¹ H COSY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S7
6	The ROESY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	1	S7
7	The [Mo ₂ (AcO) ₄] induced ECD spectrum in DMSO	1	S8
8	The ECD spectrum in MeOH	1	S8
9	The UV spectrum in MeOH	1	S9
10	The IR spectrum (KBr)	1	S9
11	The HR-ESI-MS data	1	S10
12	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S11
13	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S11
14	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S12
15	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S12
16	The ¹ H- ¹ H COSY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S13
17	The ROESY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	2	S13
18	The [Mo ₂ (AcO) ₄] induced ECD spectrum in DMSO	2	S14
19	The ECD spectrum in MeOH	2	S14
20	The UV spectrum in MeOH	2	S15
21	The IR spectrum (KBr)	2	S15
22	The HR-ESI-MS data	2	S16
23	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	3	S17

24	The ^{13}C NMR spectrum in DMSO- d_6 (500 MHz)	3	S17
25	The HSQC spectrum in DMSO- d_6 (500 MHz)	3	S18
26	The HMBC spectrum in DMSO- d_6 (500 MHz)	3	S18
27	The ^1H - ^1H COSY spectrum in DMSO- d_6 (500 MHz)	3	S19
28	The ROESY spectrum in DMSO- d_6 (500 MHz)	3	S19
29	The ECD spectrum in MeOH	3a	S20
30	The UV spectrum in MeOH	3	S20
31	The IR spectrum (KBr)	3	S21
32	The HR-ESI-MS data	3	S22
33	The ^1H NMR spectrum in DMSO- d_6 (500 MHz)	4	S23
34	The ^{13}C NMR spectrum in DMSO- d_6 (500 MHz)	4	S23
35	The HSQC spectrum in DMSO- d_6 (500 MHz)	4	S24
36	The HMBC spectrum in DMSO- d_6 (500 MHz)	4	S24
37	The NOE spectrum in DMSO- d_6 (500 MHz)	4	S25
38	The UV spectrum in MeOH	4	S25
39	The IR spectrum (KBr)	4	S26
40	The HR-ESI-MS data	4	S27
41	The ^1H NMR spectrum in DMSO- d_6 (500 MHz)	5	S28
42	The ^{13}C NMR spectrum in DMSO- d_6 (500 MHz)	5	S28
43	The HSQC spectrum in DMSO- d_6 (500 MHz)	5	S29
44	The HMBC spectrum in DMSO- d_6 (500 MHz)	5	S29
45	The NOE spectrum in DMSO- d_6 (600 MHz)	5	S30
46	The UV spectrum in MeOH	5	S30
47	The IR spectrum (KBr)	5	S31
48	The HR-ESI-MS data	5	S32
49	The ^1H NMR spectrum in DMSO- d_6 (600 MHz)	6	S33
50	The ^{13}C NMR spectrum in DMSO- d_6 (600 MHz)	6	S33
51	The HSQC spectrum in DMSO- d_6 (600 MHz)	6	S34
52	The HMBC spectrum in DMSO- d_6 (600 MHz)	6	S34
53	The TOCSY spectrum in DMSO- d_6 (500 MHz)	6	S35
54	The UV spectrum in MeOH	6	S35
55	The IR spectrum (KBr)	6	S36
56	The HR-ESI-MS data	6	S37
57	The ^1H NMR spectrum in DMSO- d_6 (600 MHz)	7	S38
58	The ^{13}C NMR spectrum in DMSO- d_6 (600 MHz)	7	S38
59	The HSQC spectrum in DMSO- d_6 (600 MHz)	7	S39
60	The HMBC spectrum in DMSO- d_6 (600 MHz)	7	S39

61	The TOCSY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	7	S40
62	The UV spectrum in MeOH	7	S40
63	The IR spectrum (KBr)	7	S41
64	The HR-ESI-MS data	7	S42
65	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	8	S43
66	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	8	S43
67	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	8	S44
68	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	8	S44
69	The TOCSY spectrum in DMSO- <i>d</i> ₆ (500 MHz)	8	S45
70	The UV spectrum in MeOH	8	S45
71	The IR spectrum (KBr)	8	S46
72	The HR-ESI-MS data	8	S47
73	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (600 MHz)	9	S48
74	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (600 MHz)	9	S48
75	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	9	S49
76	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	9	S49
77	The NOE spectrum in DMSO- <i>d</i> ₆ (600 MHz)	9	S50
78	The UV spectrum in MeOH	9	S50
79	The IR spectrum (KBr)	9	S51
80	The HR-ESI-MS data	9	S52
81	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	10	S53
82	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	10	S53
83	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	10	S54
84	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	10	S54
85	The IR spectrum (KBr)	10	S55
86	The HR-ESI-MS data	10	S56
87	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	11	S57
88	The ¹³ C NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	11	S57
89	The HSQC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	11	S58
90	The HMBC spectrum in DMSO- <i>d</i> ₆ (500 MHz)	11	S58
91	The IR spectrum (KBr)	11	S59
92	The HR-ESI-MS data	11	S60
93	The Gas Chromatographic separation of D-Glc		S61
94	The Gas Chromatographic separation of D-Api		S61
95	The Gas Chromatographic analyses of sugar moieties	4, 10	S61
96	The Gas Chromatographic analyses of sugar moieties	3, 5-9, 11	S61
97	The ¹ H NMR spectrum in DMSO- <i>d</i> ₆ (500 MHz)	3a	S62

98	The ^{13}C NMR spectrum in DMSO- d_6 (500 MHz)	3a	S62
99	The HSQC spectrum in DMSO- d_6 (500 MHz)	3a	S63
100	The HMBC spectrum in DMSO- d_6 (500 MHz)	3a	S63
101	The ^1H - ^1H COSY spectrum in DMSO- d_6 (500 MHz)	3a	S64
102	The ROESY spectrum in DMSO- d_6 (500 MHz)	3a	S64

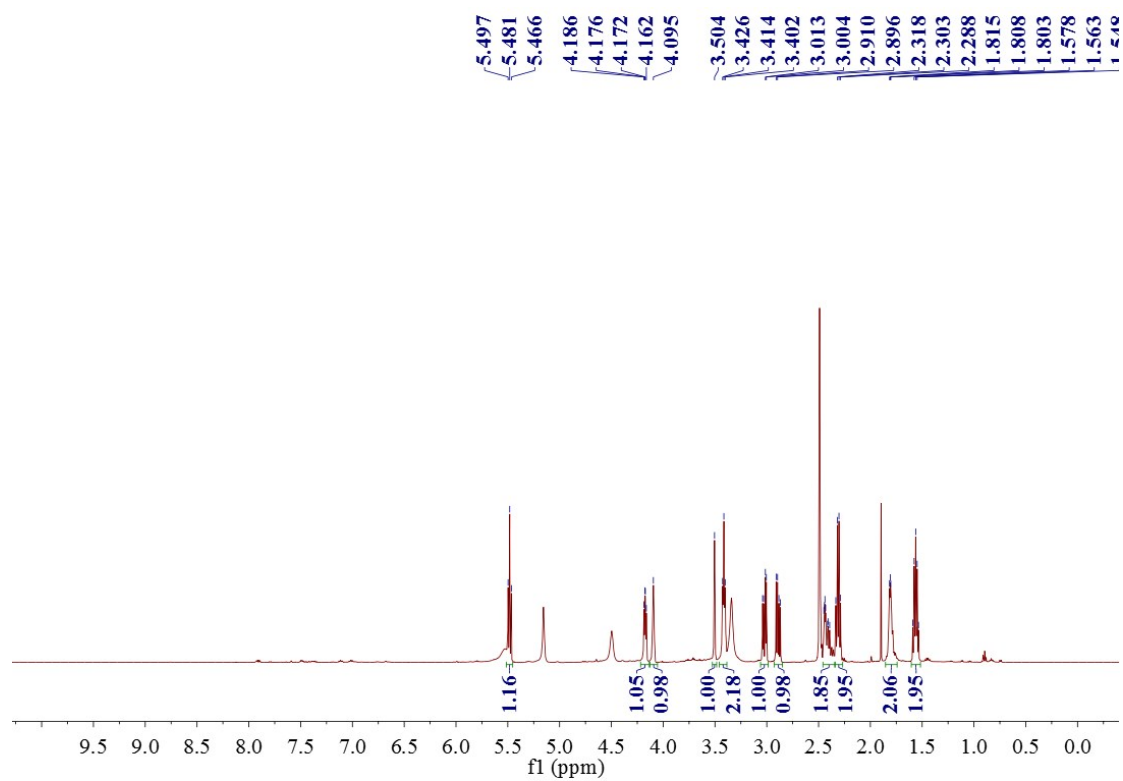


Figure S1. The ^1H NMR spectrum of compound **1** in $\text{DMSO}-d_6$

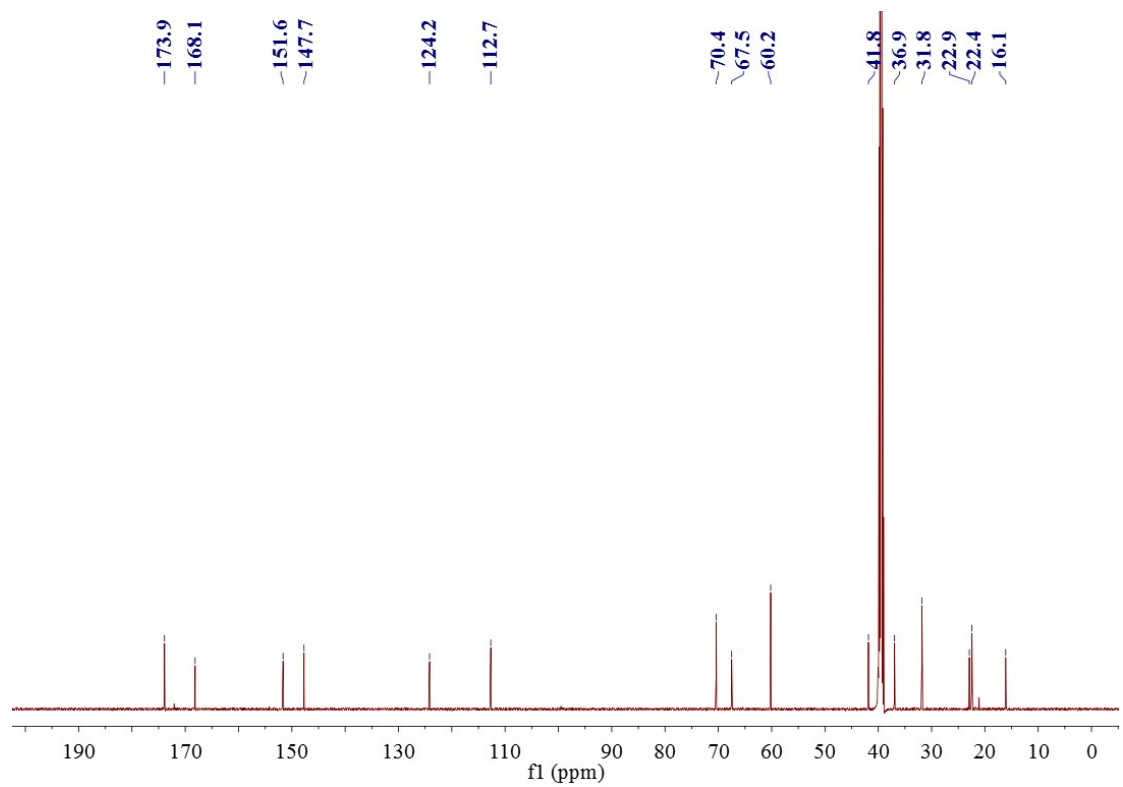


Figure S2. The ^{13}C NMR spectrum of compound **1** in $\text{DMSO}-d_6$

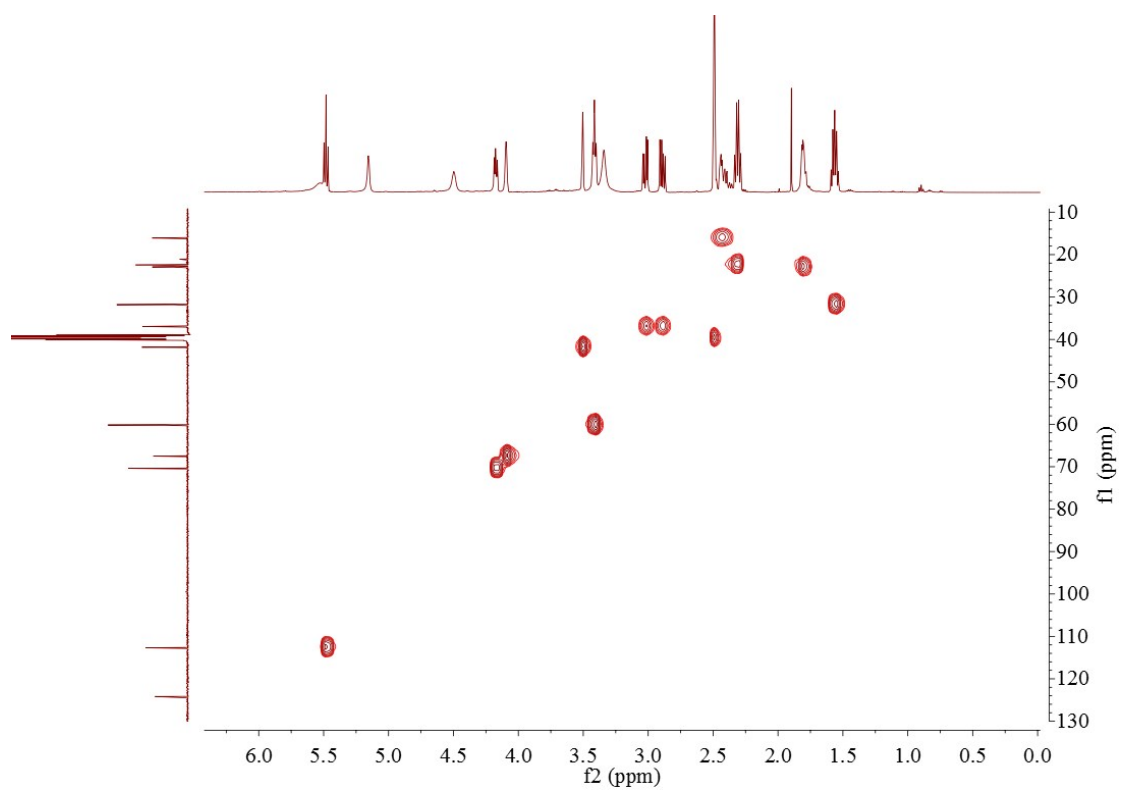


Figure S3. The HSQC spectrum of compound **1** in DMSO- d_6

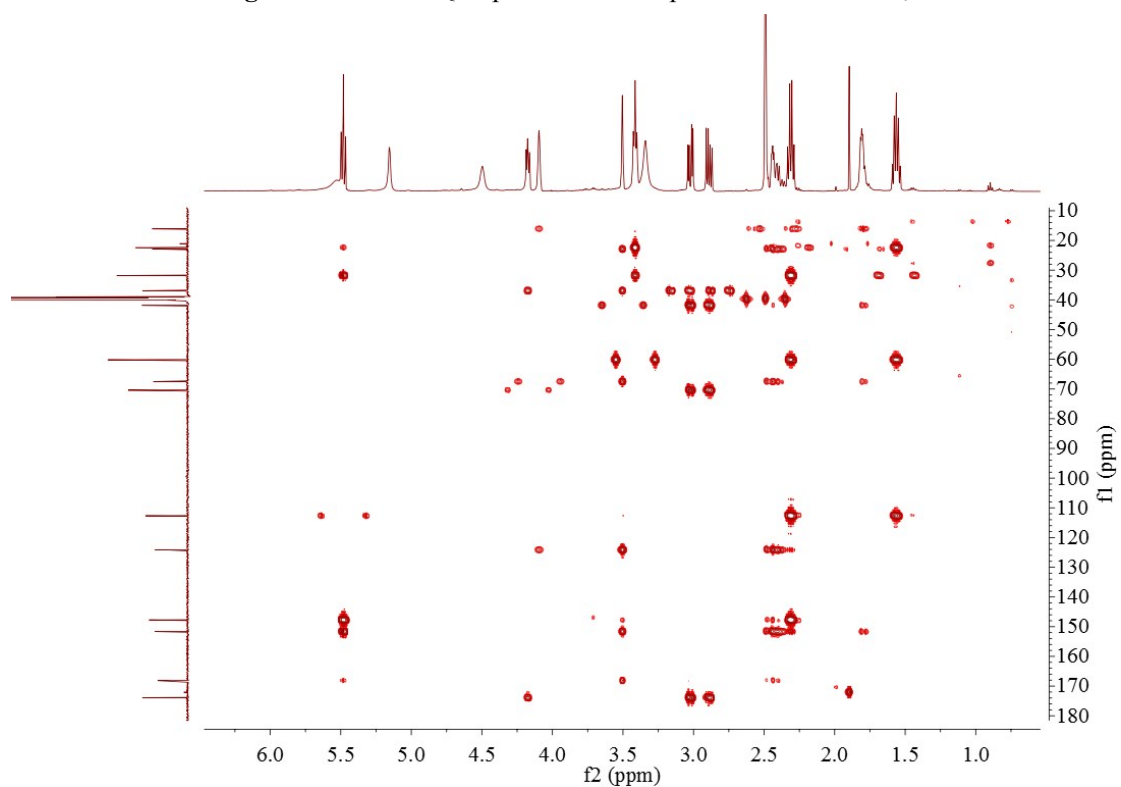


Figure S4. The HMBC spectrum of compound **1** in DMSO- d_6

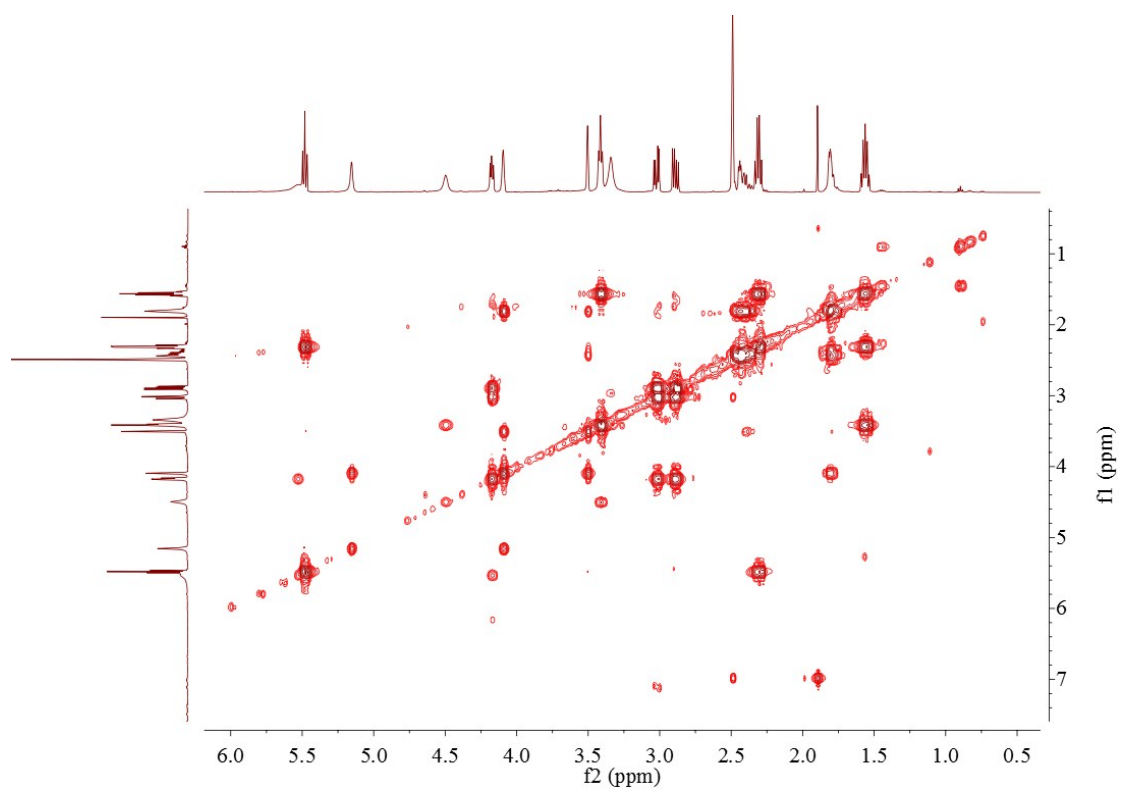


Figure S5. The ^1H - ^1H COSY spectrum of compound **1** in $\text{DMSO}-d_6$

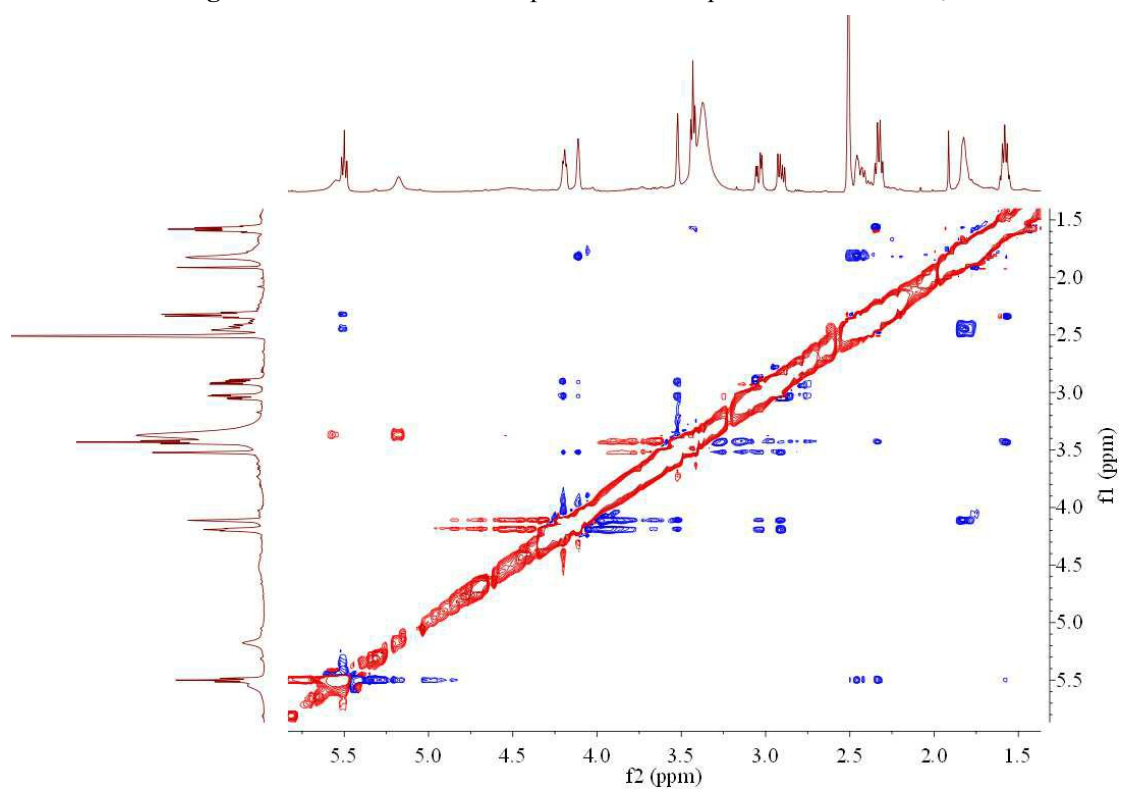


Figure S6. The ROESY spectrum of compound **1** in $\text{DMSO}-d_6$

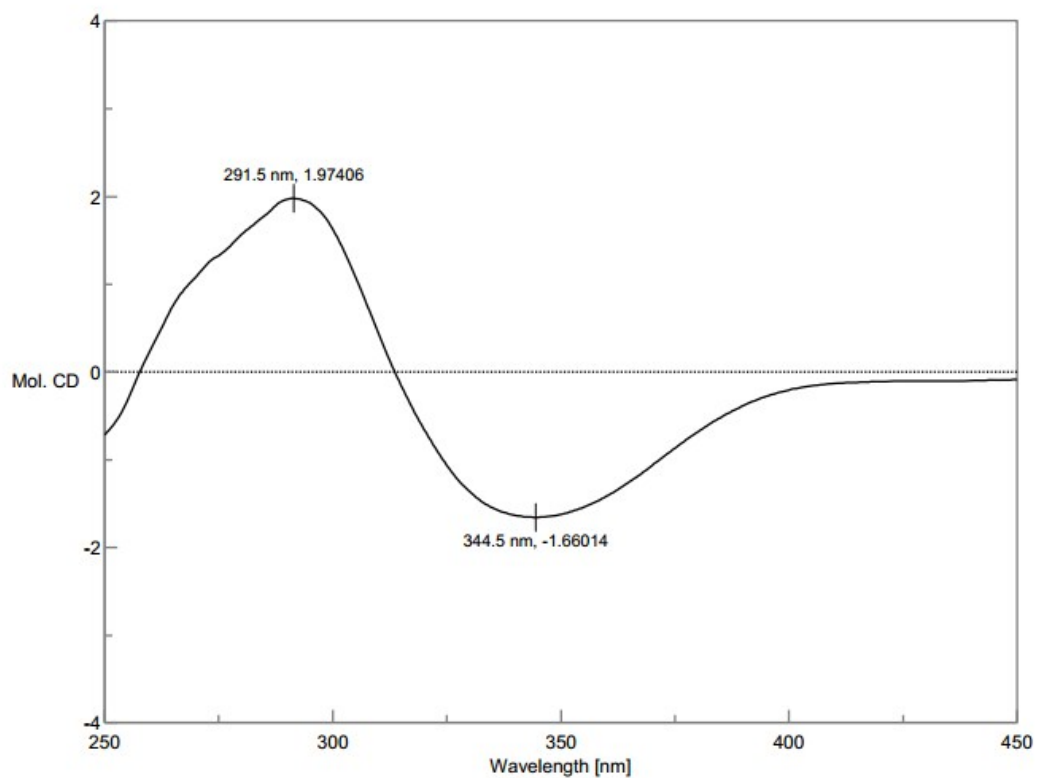


Figure S7. The $[\text{Mo}_2(\text{AcO})_4]$ induced ECD spectrum of compound **1** in DMSO

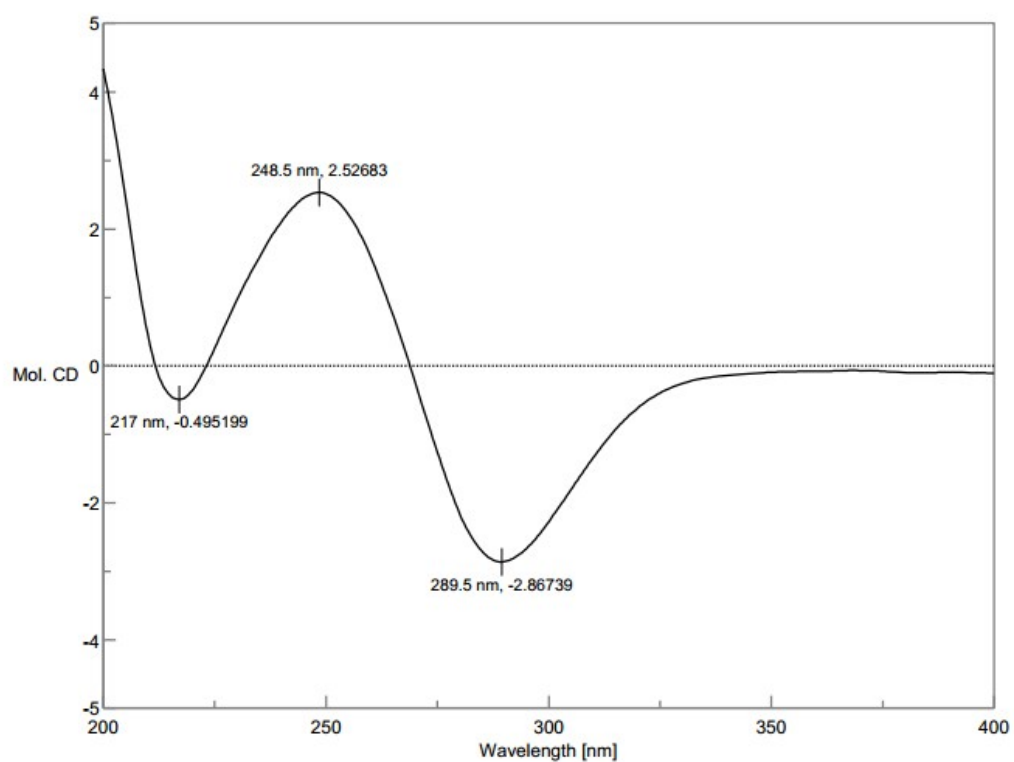


Figure S8. The ECD spectrum of compound **1** in MeOH

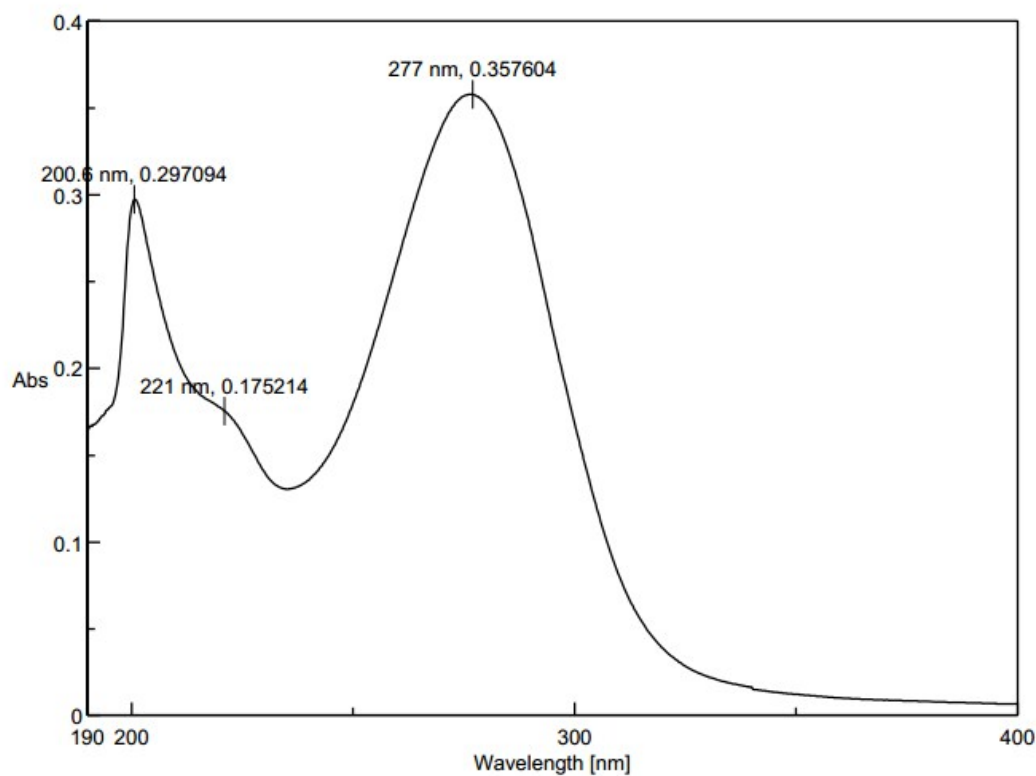


Figure S9. The UV spectrum of compound **1** in MeOH

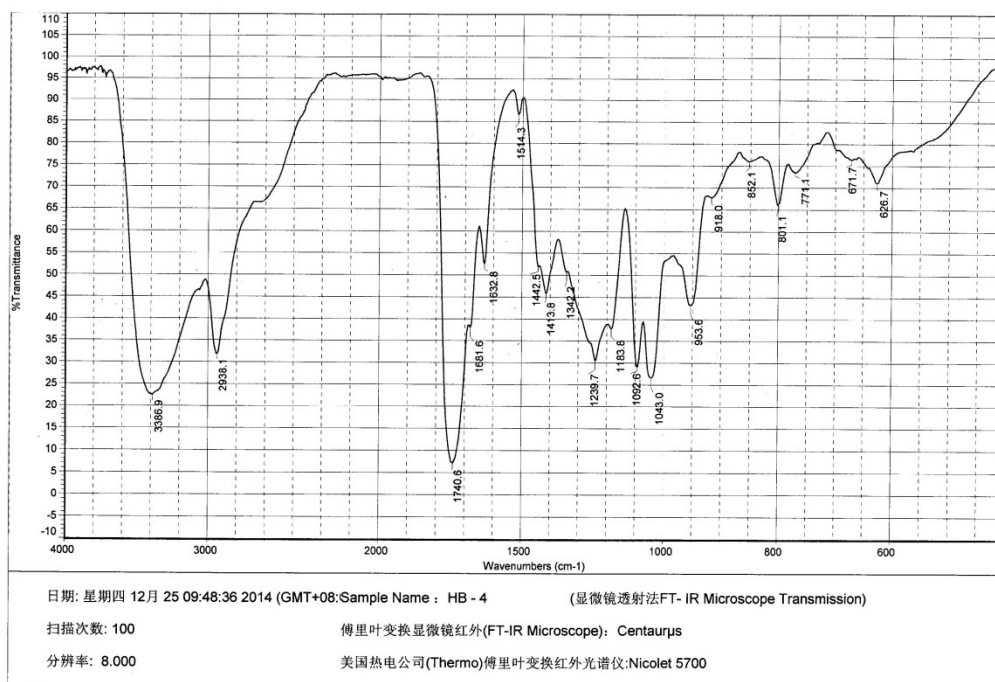
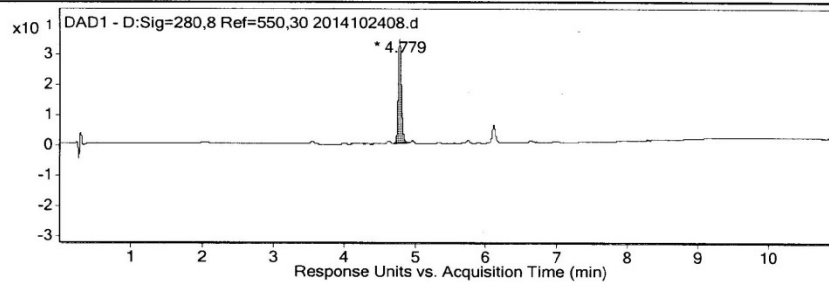


Figure S10. The IR spectrum (KBr) of compound **1**

Qualitative Analysis Report

Data Filename	2014102408.d	Sample Name	HB-4
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

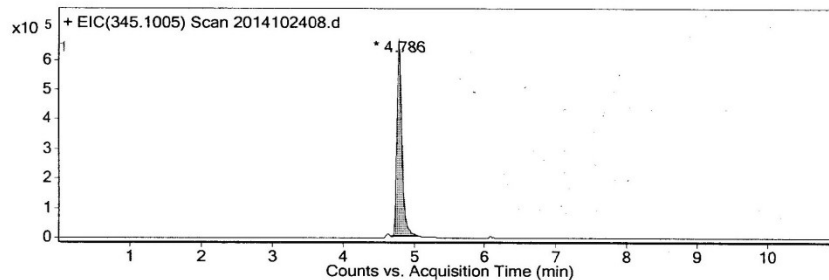
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.692	4.779	4.917	34.31	107.5	100

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.674	4.786	5.06	665326	3193955	100

User Spectra

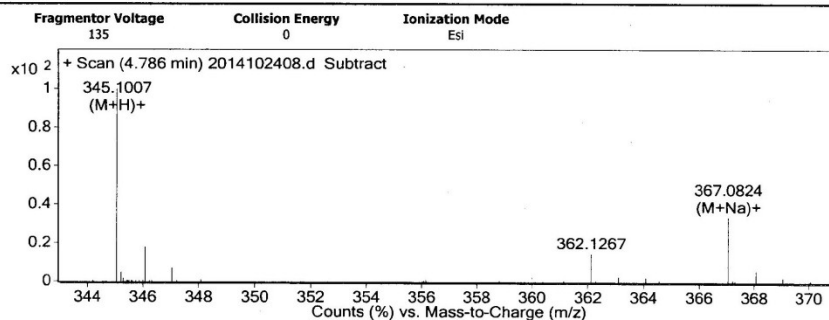


Figure S11. The HR-ESI-MS data of compound 1

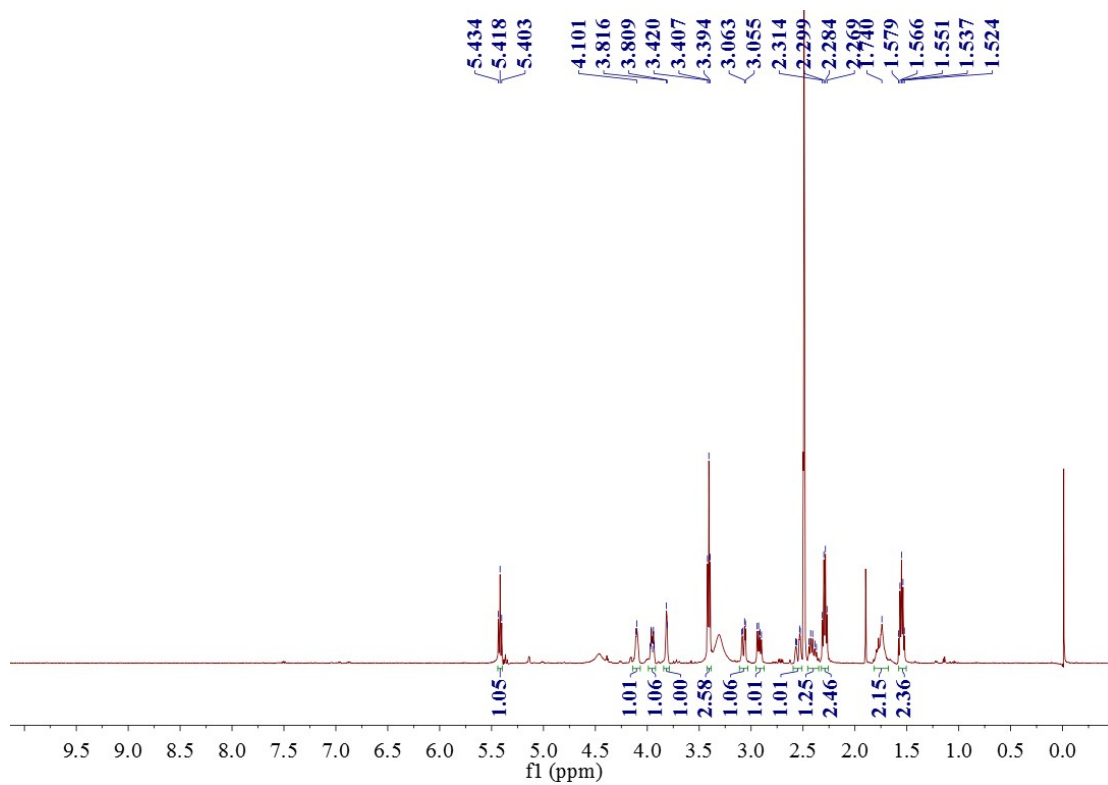


Figure S12. The ^1H NMR spectrum of compound **2** in $\text{DMSO-}d_6$

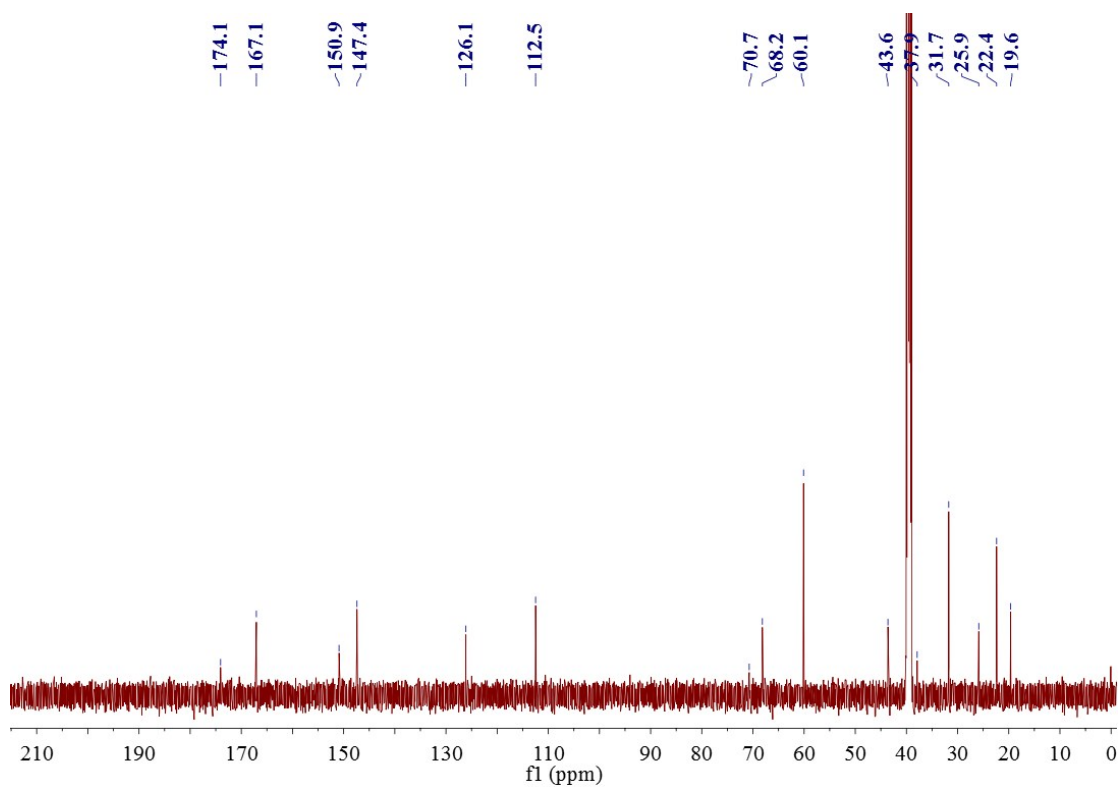


Figure S13. The ^{13}C NMR spectrum of compound **2** in $\text{DMSO-}d_6$

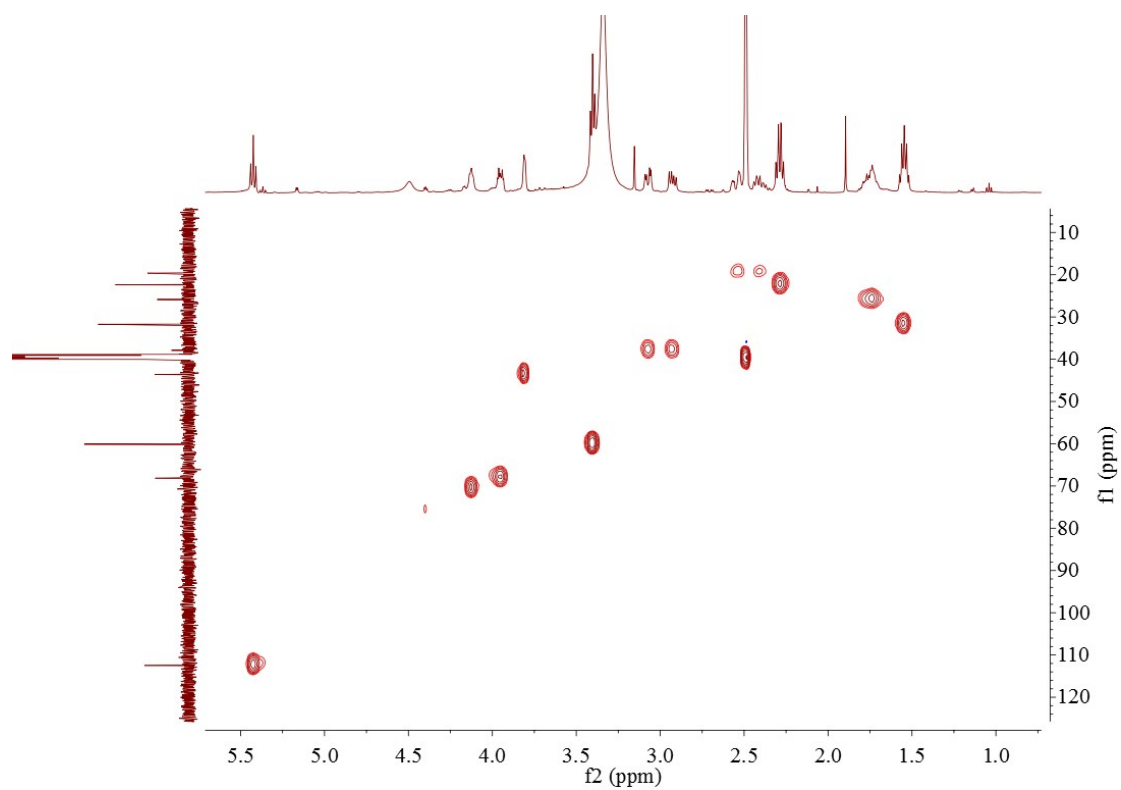


Figure S14. The HSQC spectrum of compound **2** in DMSO- d_6

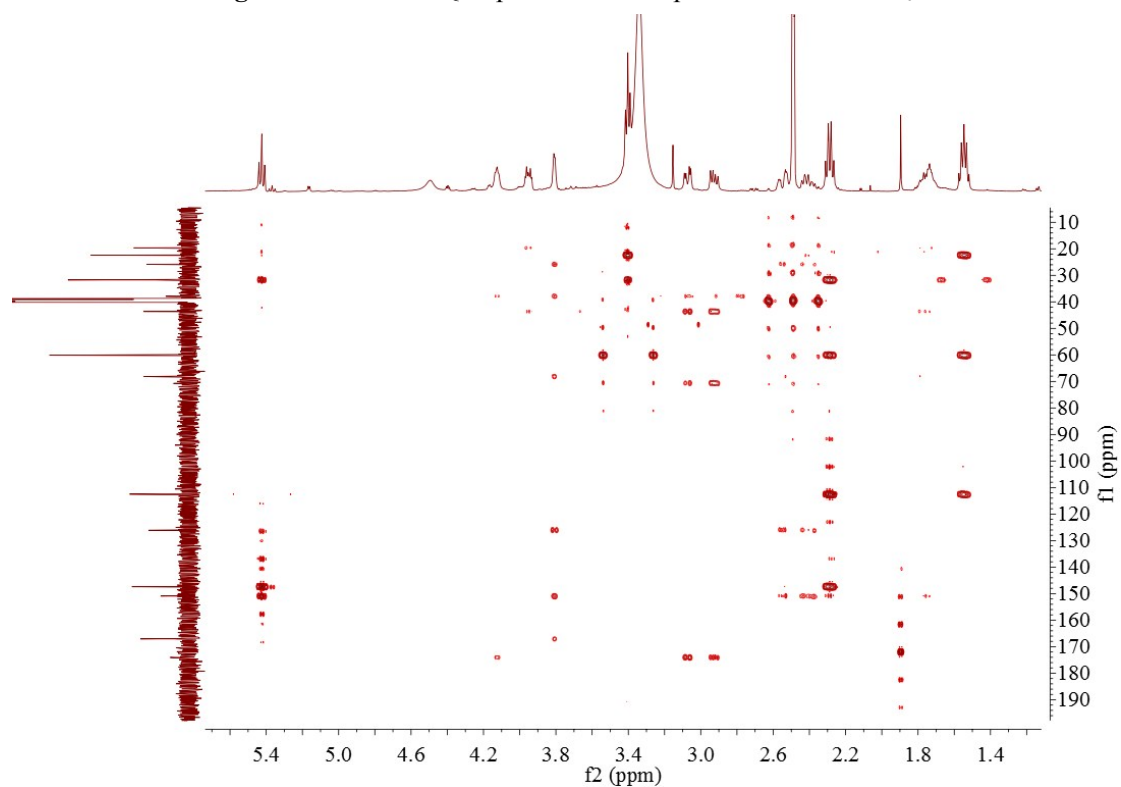


Figure S15. The HMBC spectrum of compound **2** in DMSO- d_6

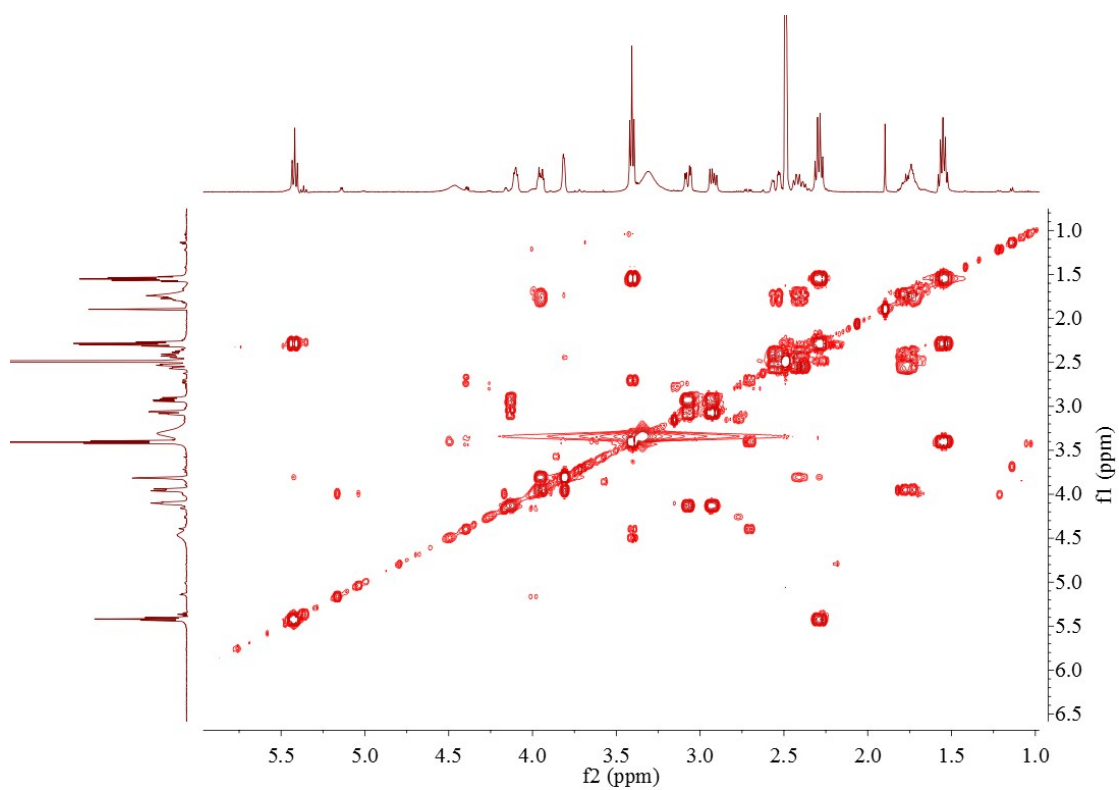


Figure S16. The ^1H - ^1H COSY spectrum of compound **2** in $\text{DMSO-}d_6$

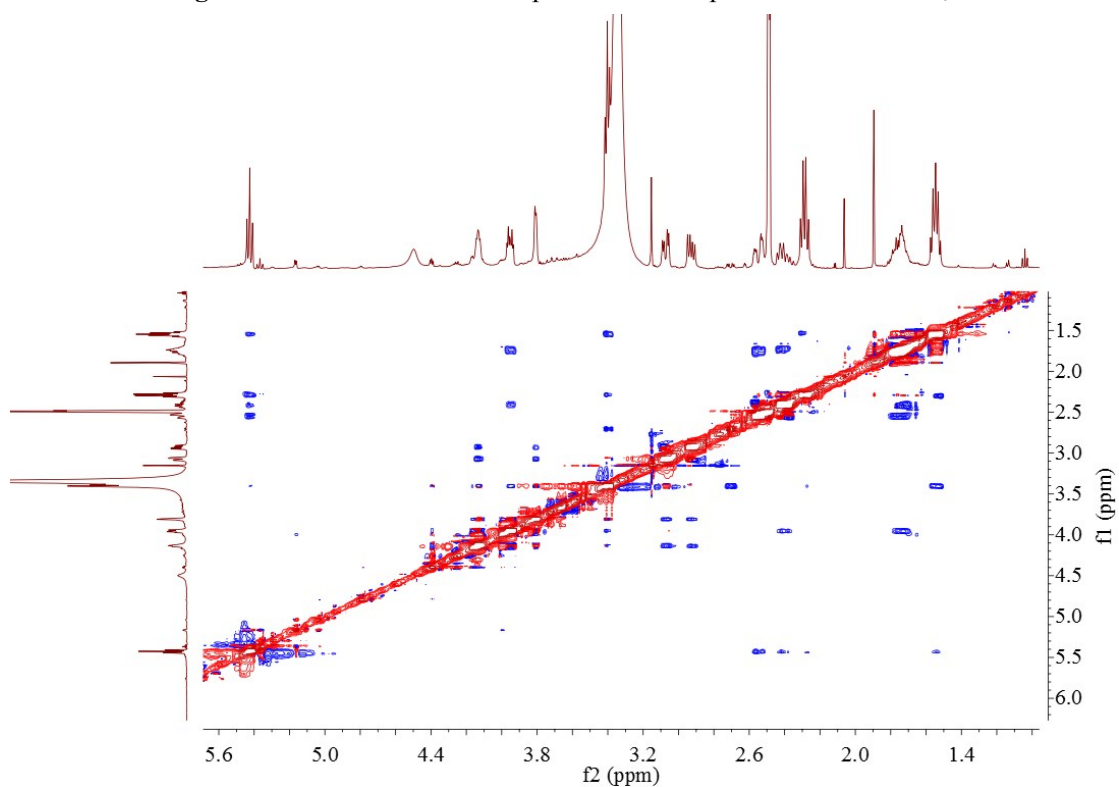


Figure S17. The ROESY spectrum of compound **2** in $\text{DMSO-}d_6$

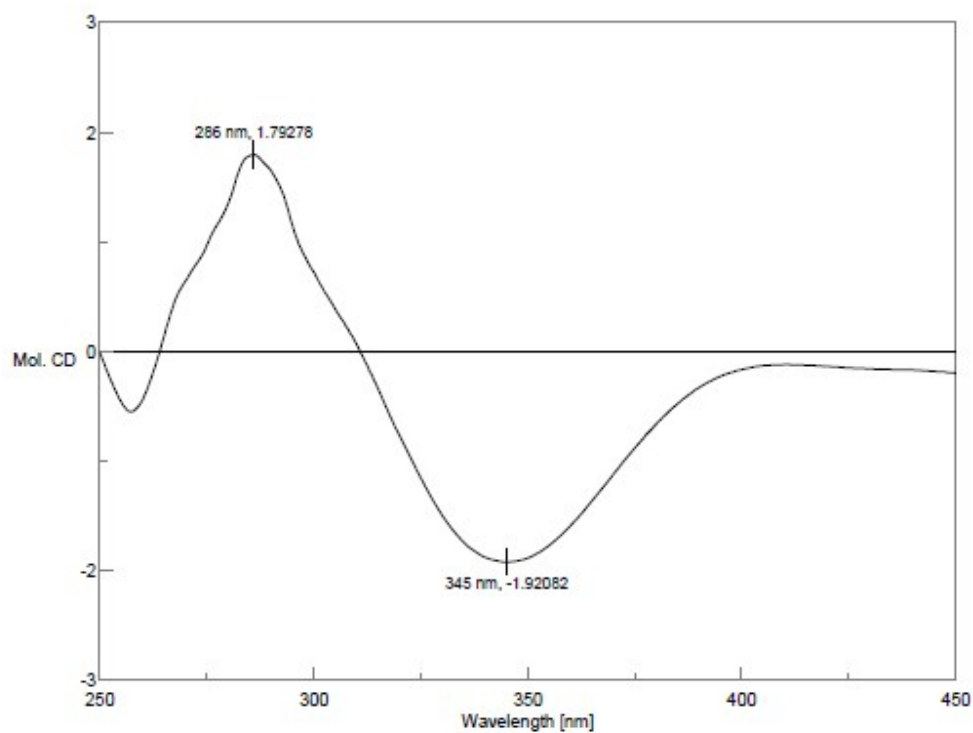


Figure S18. The $[\text{Mo}_2(\text{AcO})_4]$ induced ECD spectrum of compound **2** in DMSO

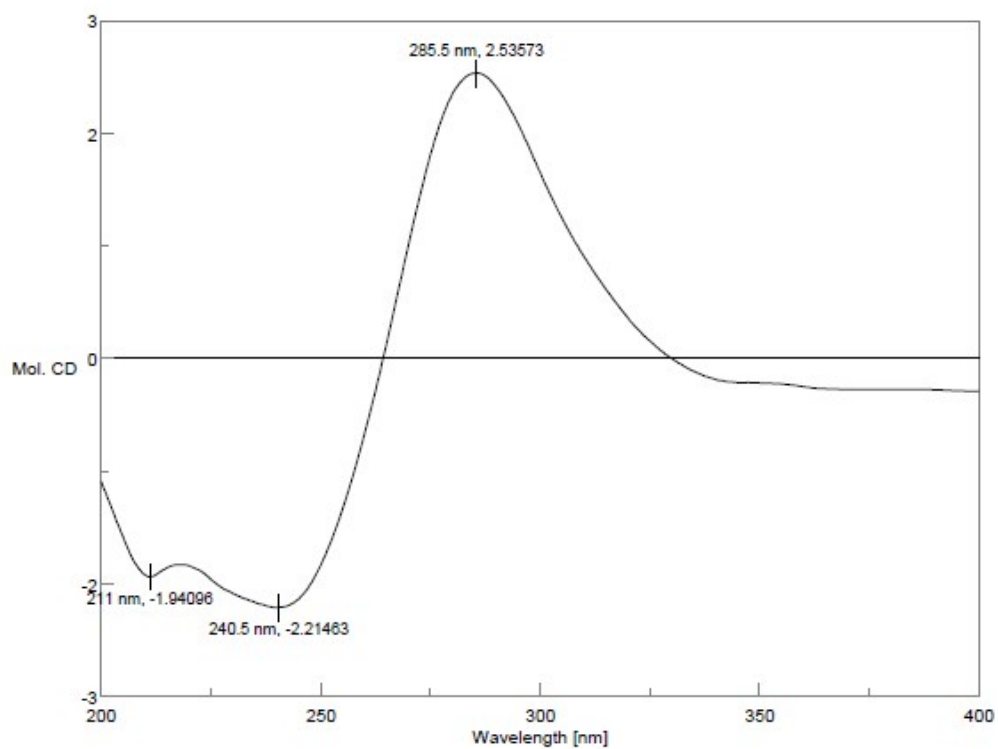


Figure S19. The ECD spectrum of compound **2** in MeOH

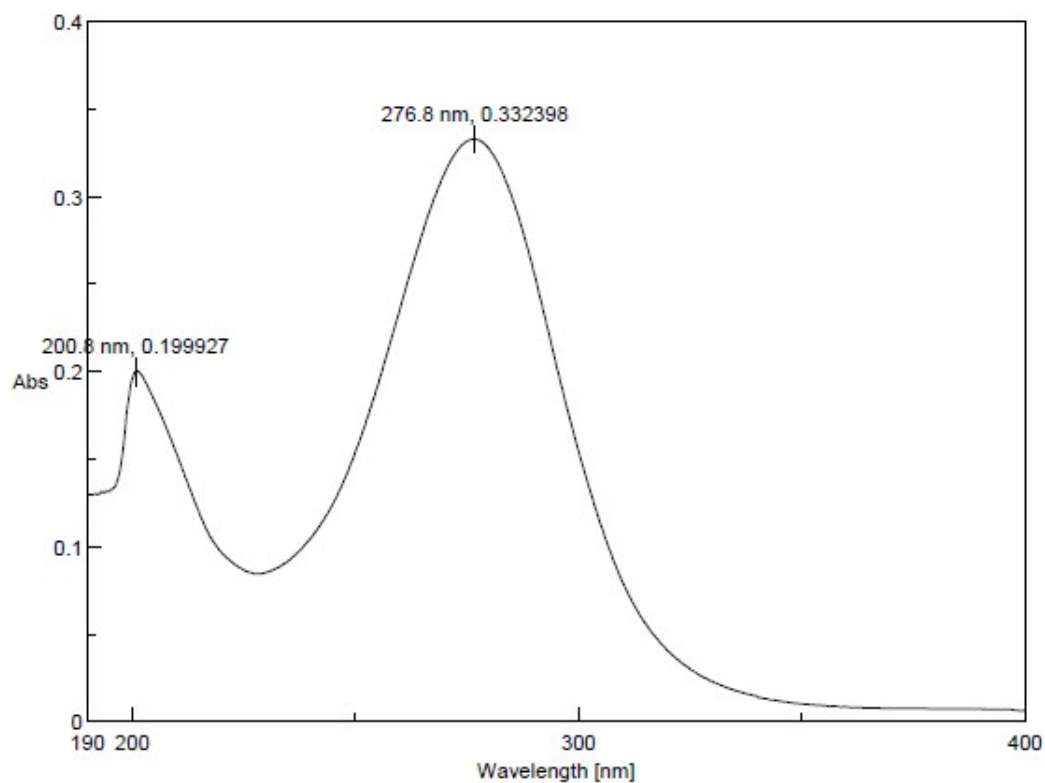


Figure S20. The UV spectrum of compound 2 in MeOH

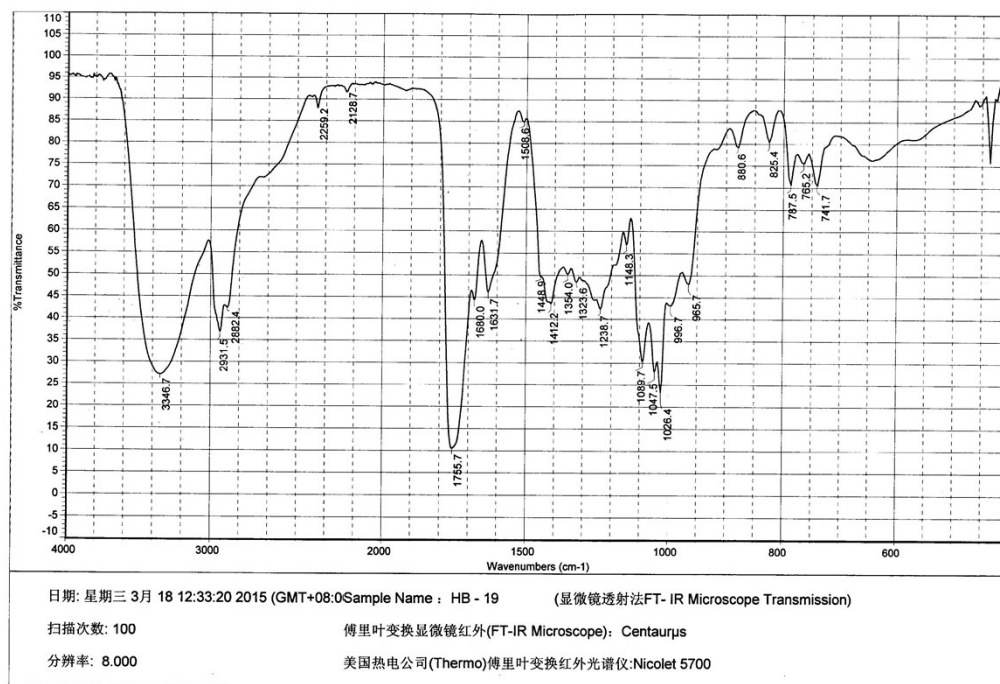
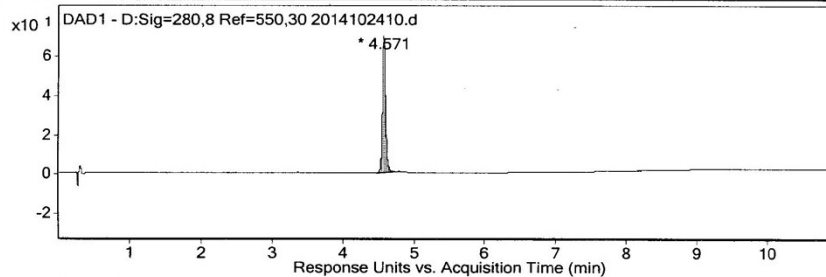


Figure S21. The IR spectrum (KBr) of compound 2

Qualitative Analysis Report

Data Filename	2014102410.d	Sample Name	HB-19
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	
DA Method	TEST LCMS.m	Comment	

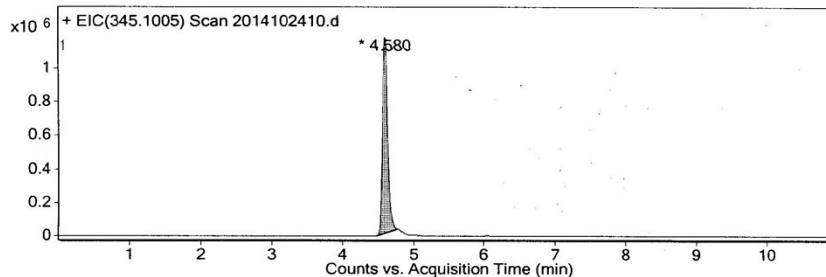
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.458	4.571	4.73	69.51	227.14	100

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.467	4.58	4.773	1171353	6283228	100

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

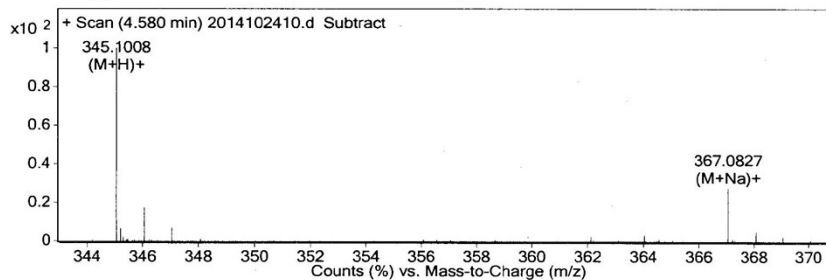


Figure S22. The HR-ESI-MS data of compound **2**

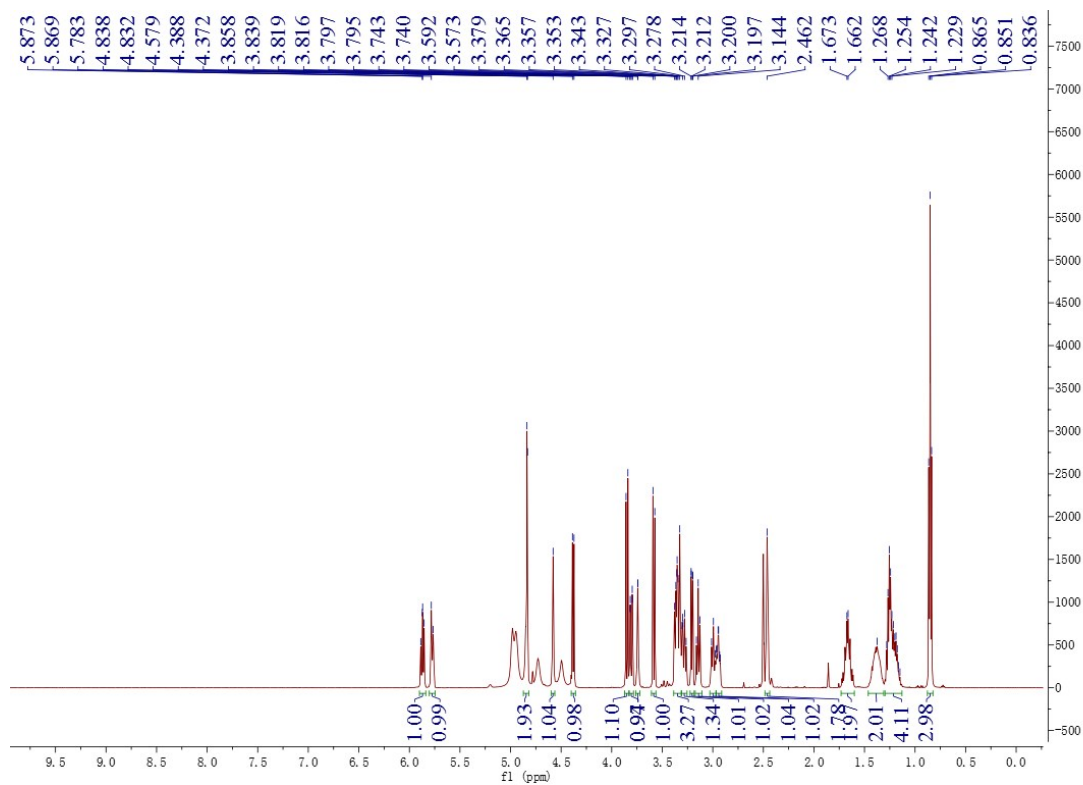


Figure S23. The ^1H NMR spectrum of compound **3** in $\text{DMSO}-d_6$

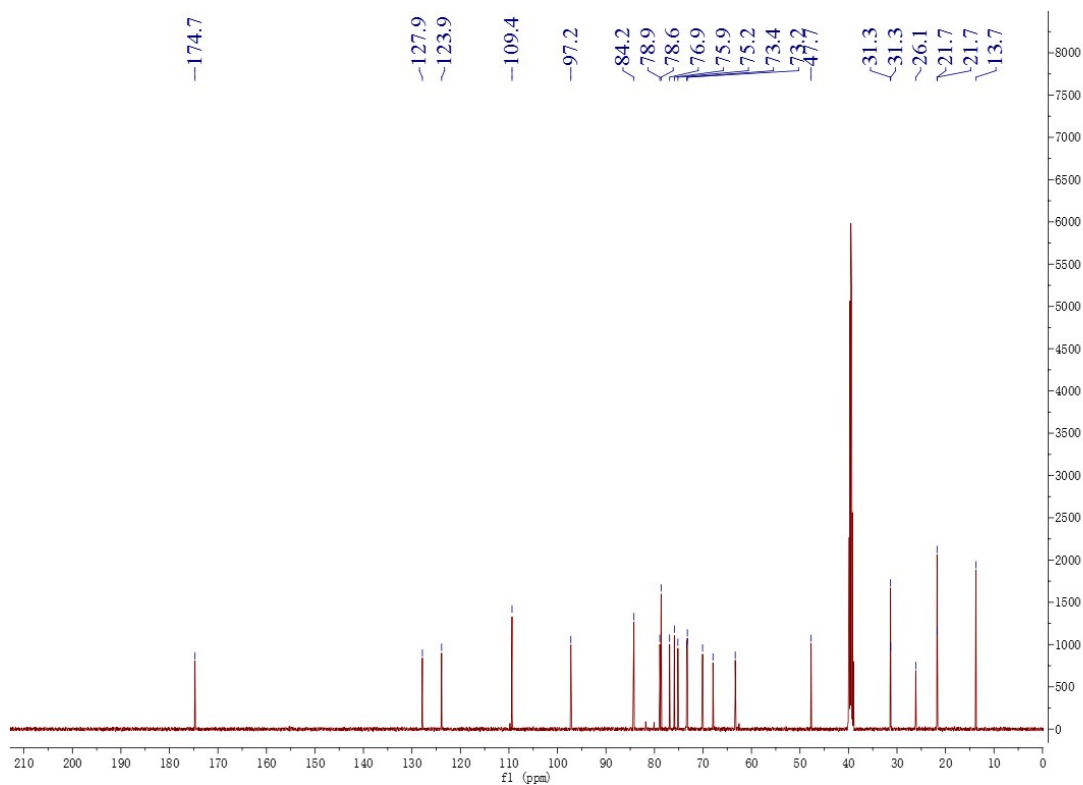


Figure S24. The ^{13}C NMR spectrum of compound **3** in $\text{DMSO}-d_6$

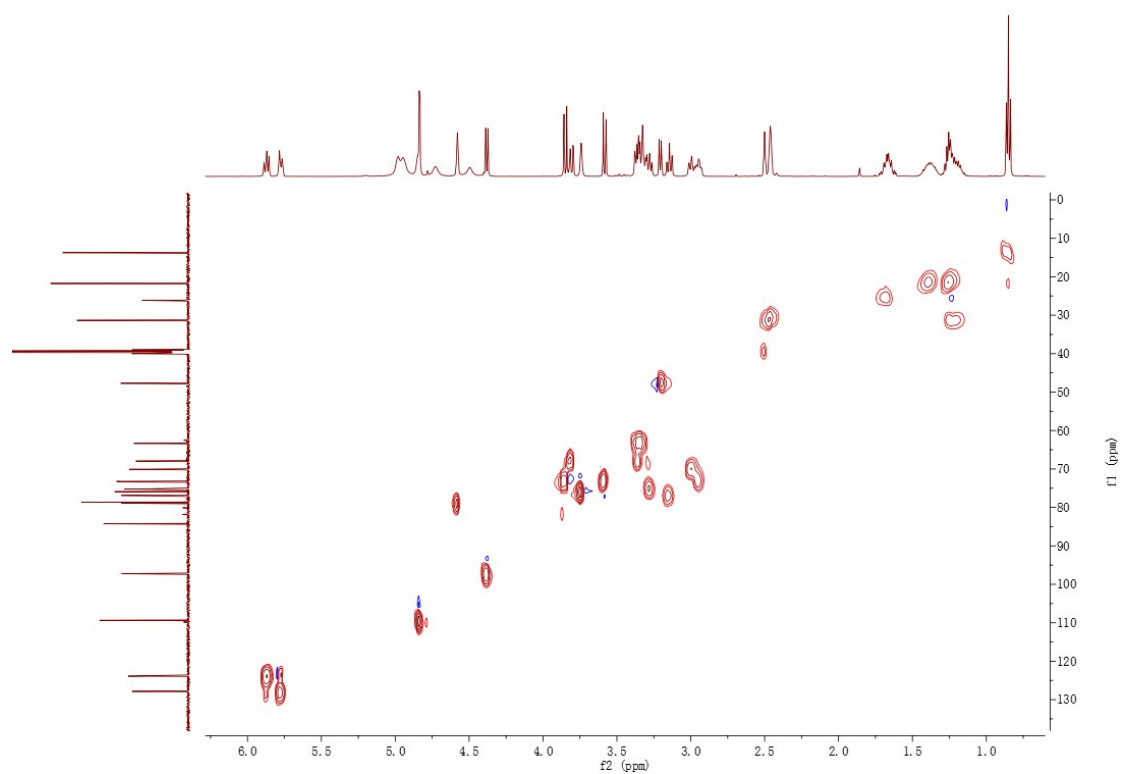


Figure S25. The HSQC spectrum of compound **3** in DMSO- d_6

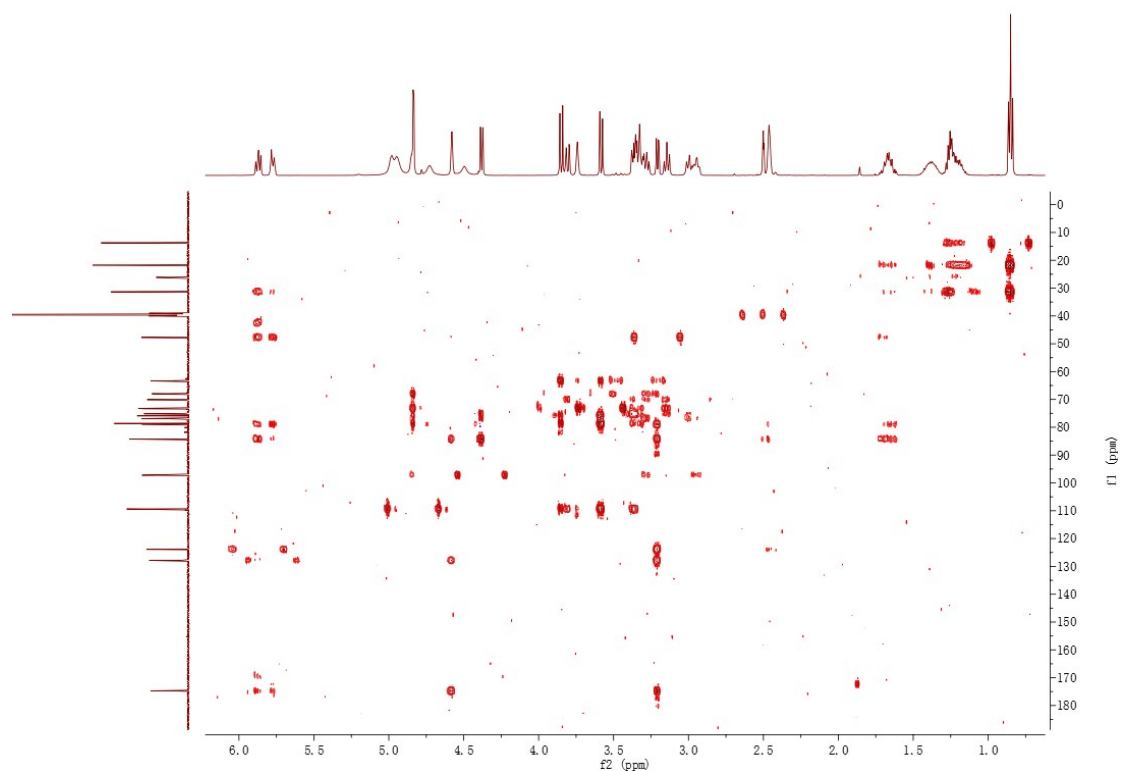


Figure S26. The HMBC spectrum of compound **3** in DMSO- d_6

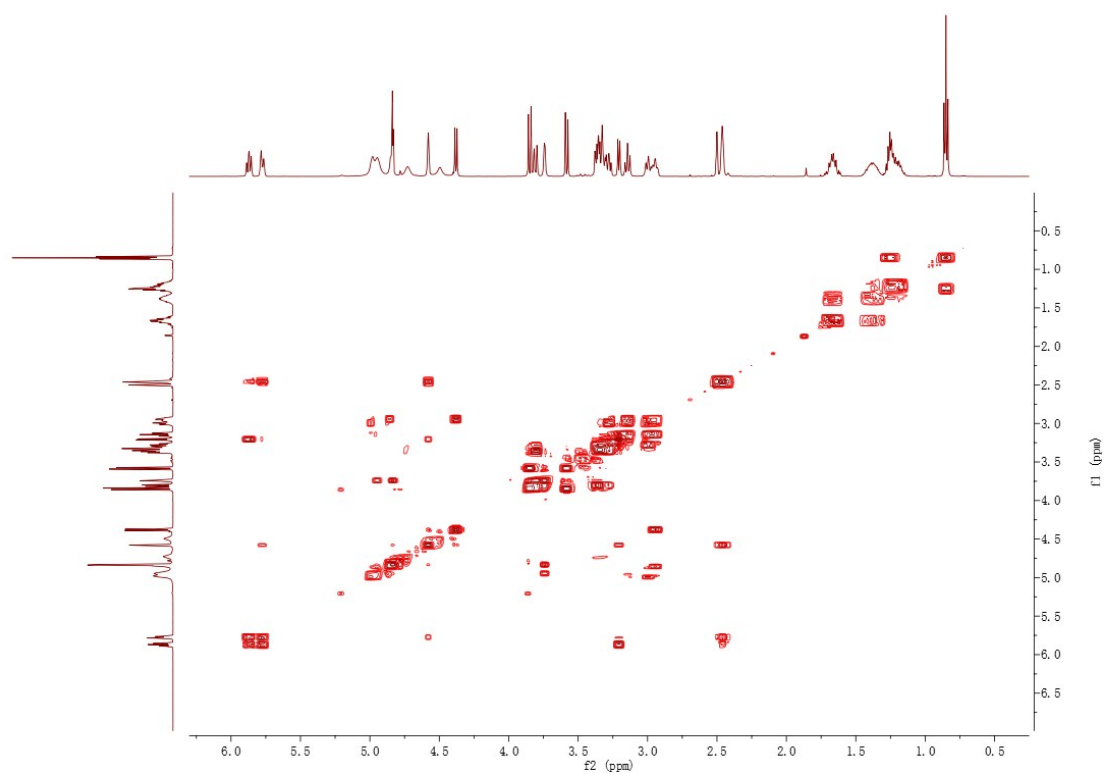


Figure S27. The ^1H - ^1H COSY spectrum of compound **3** in $\text{DMSO-}d_6$

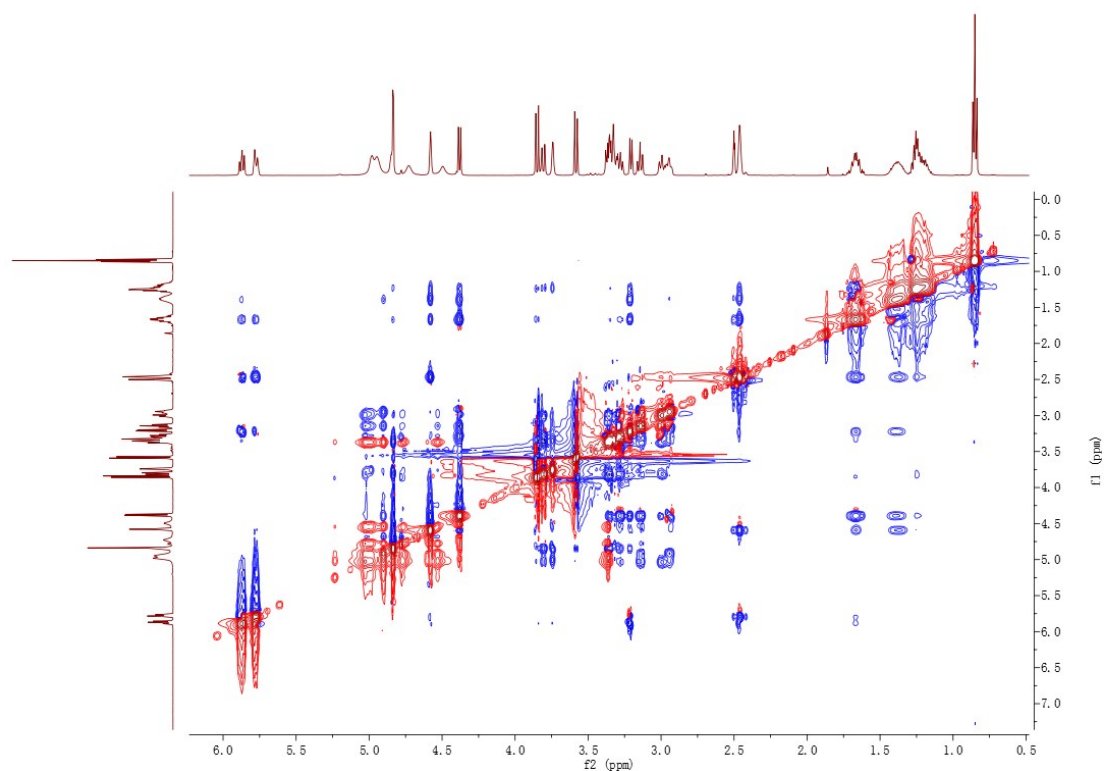


Figure S28. The ROESY spectrum of compound **3** in $\text{DMSO-}d_6$

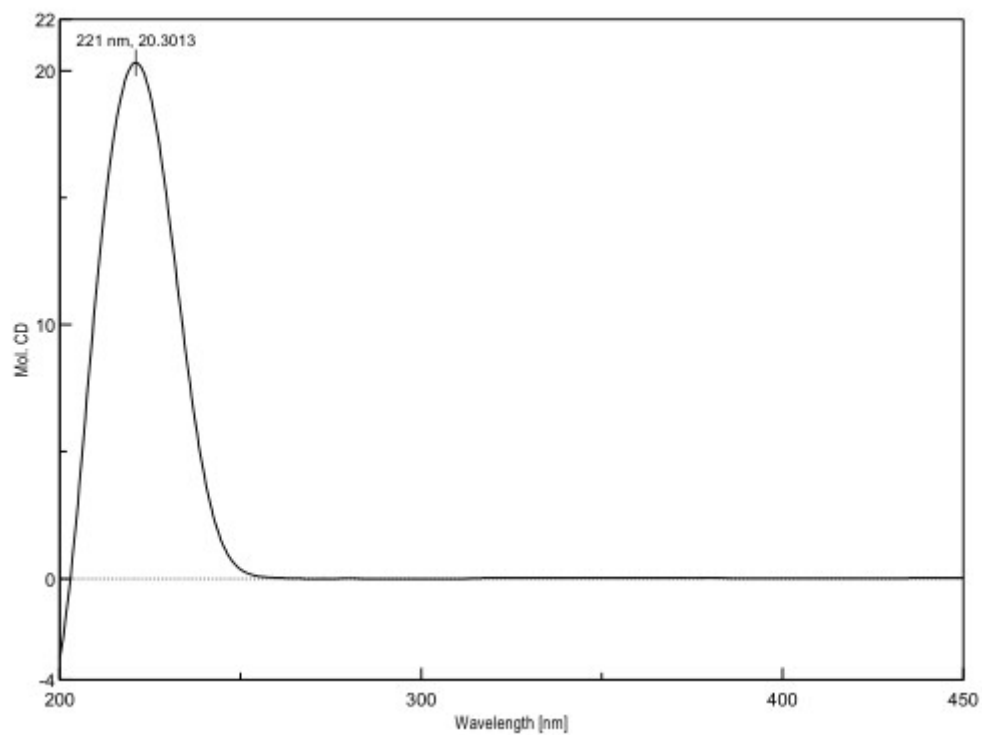


Figure S29. The ECD spectrum of compound **3a** in MeOH

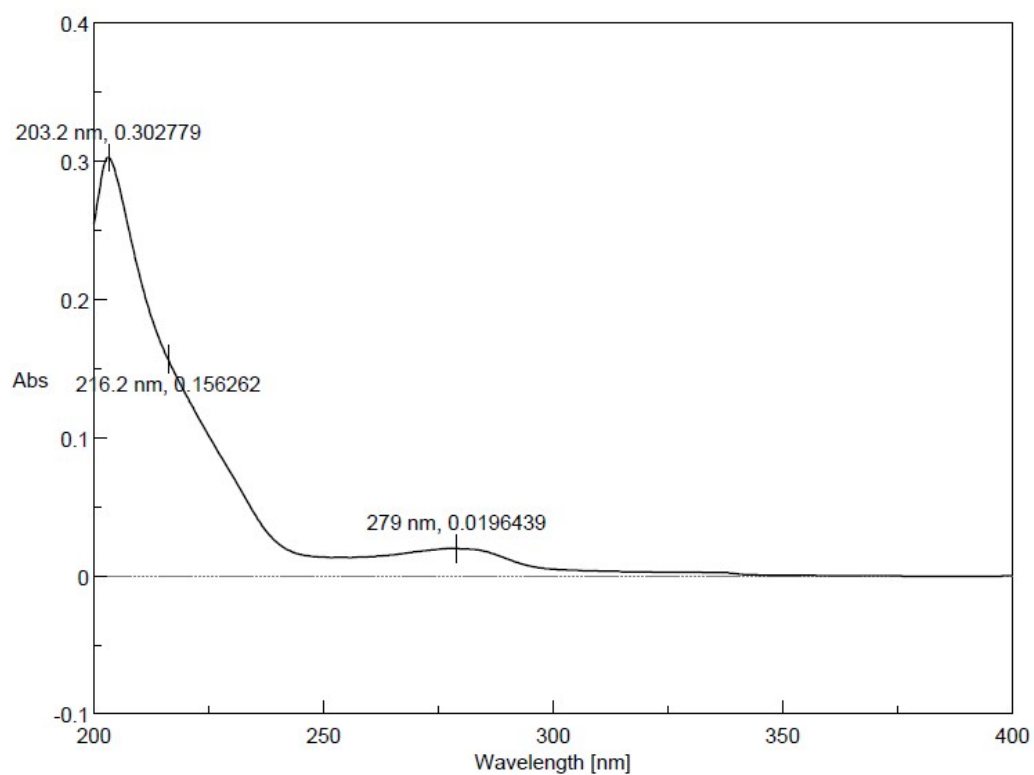


Figure S30. The UV spectrum of compound **3** in MeOH

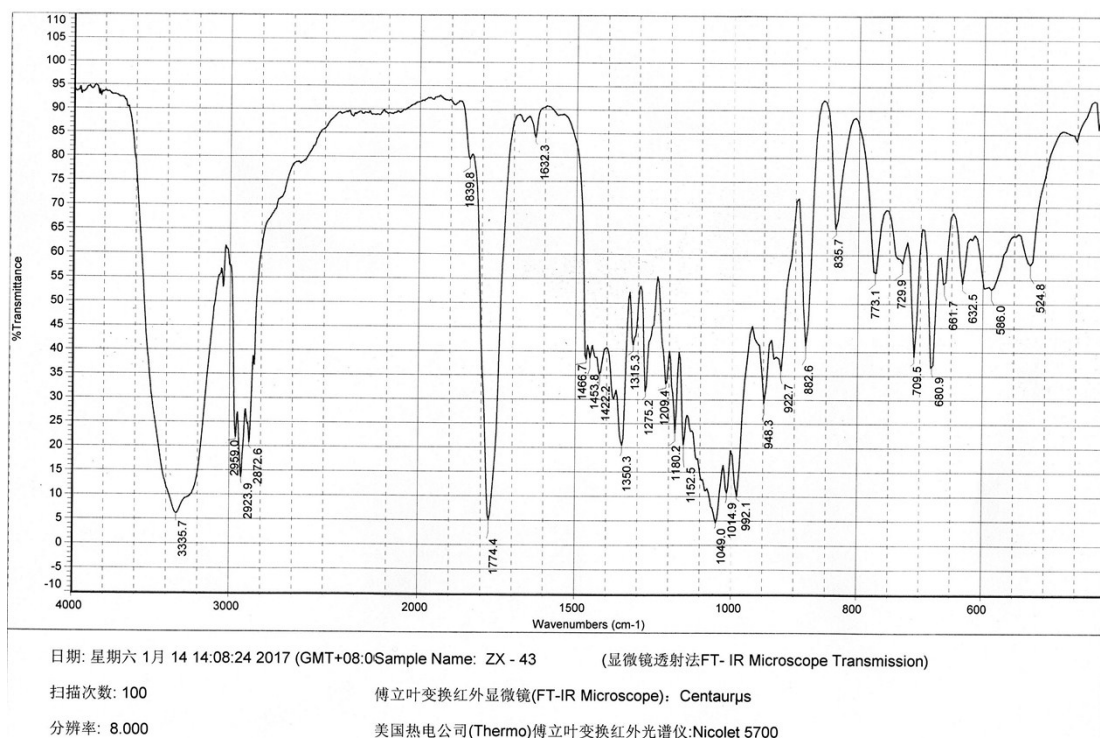


Figure S31. The IR spectrum (KBr) of compound **3**

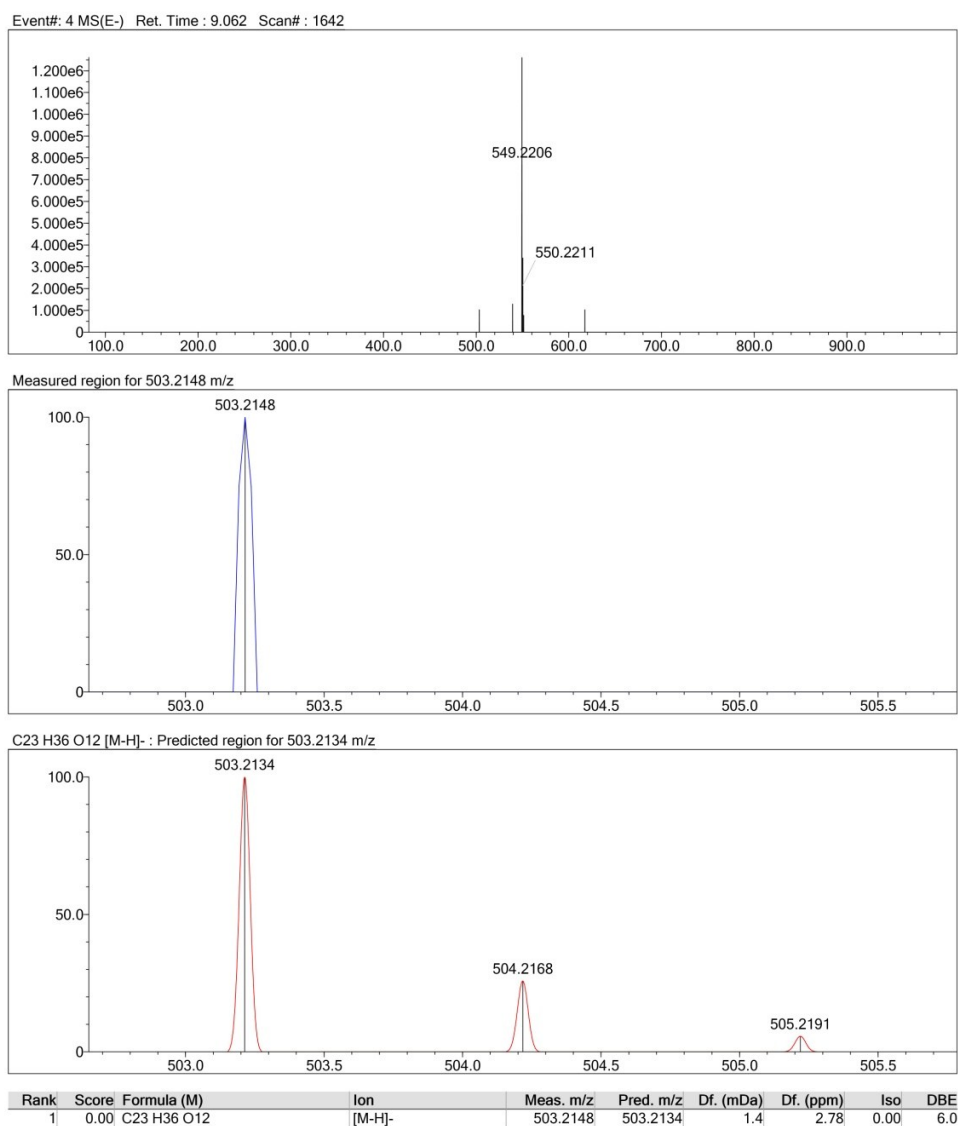


Figure S32. The HR-ESI-MS data of compound **3**

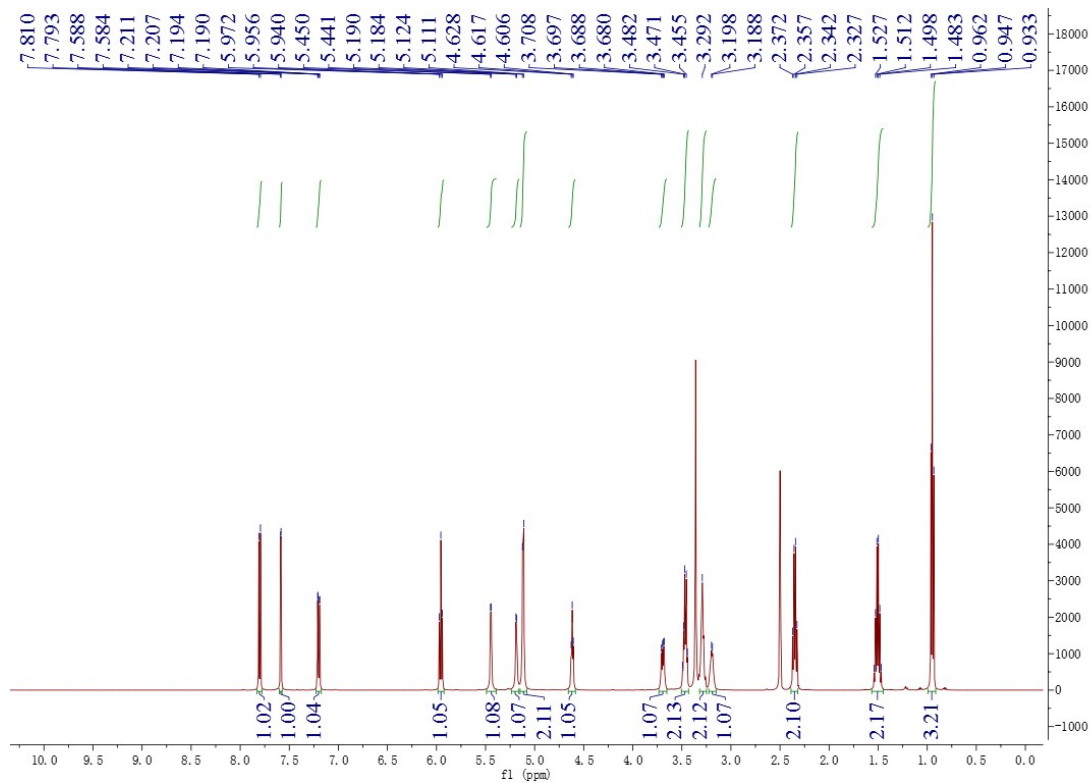


Figure S33. The ^1H NMR spectrum of compound **4** in $\text{DMSO-}d_6$

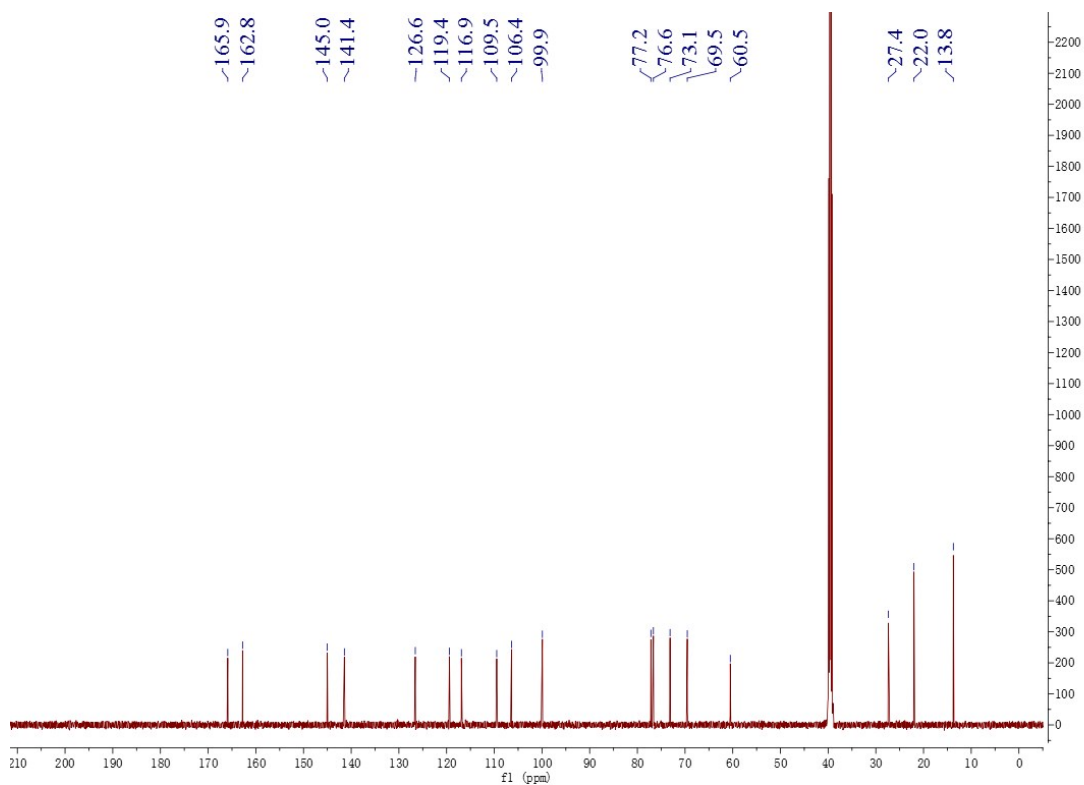


Figure S34. The ^{13}C NMR spectrum of compound **4** in $\text{DMSO-}d_6$

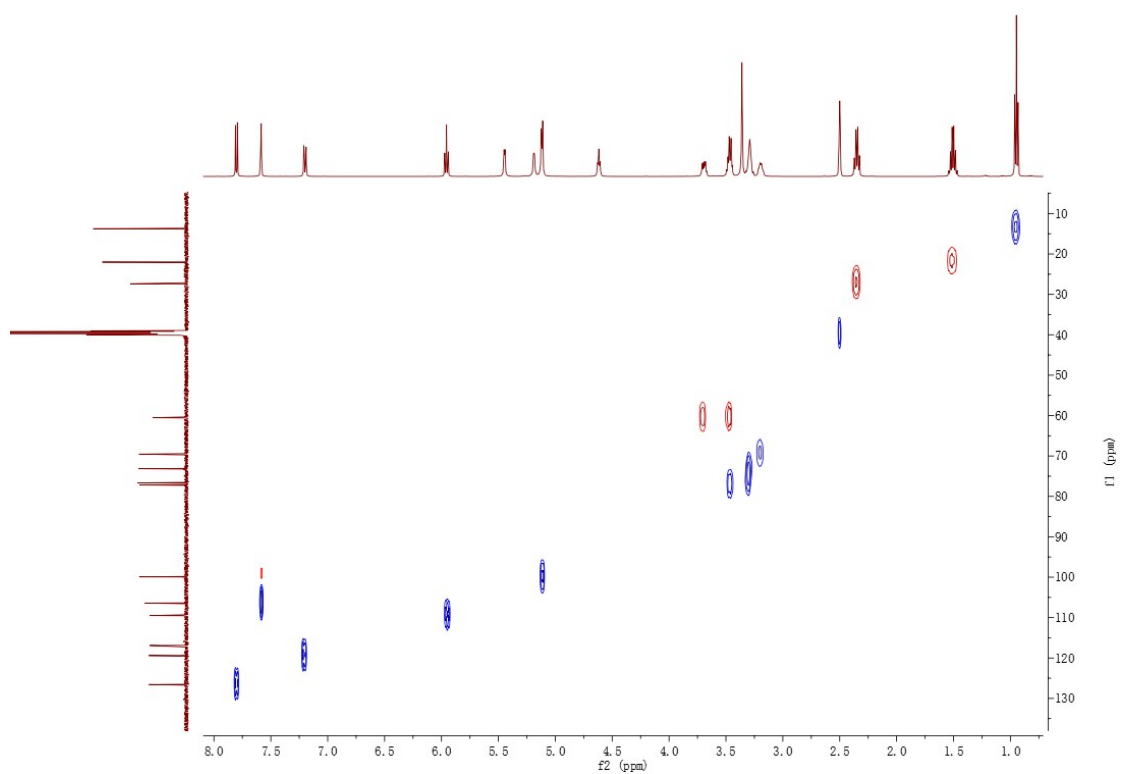


Figure S35. The HSQC spectrum of compound **4** in DMSO- d_6

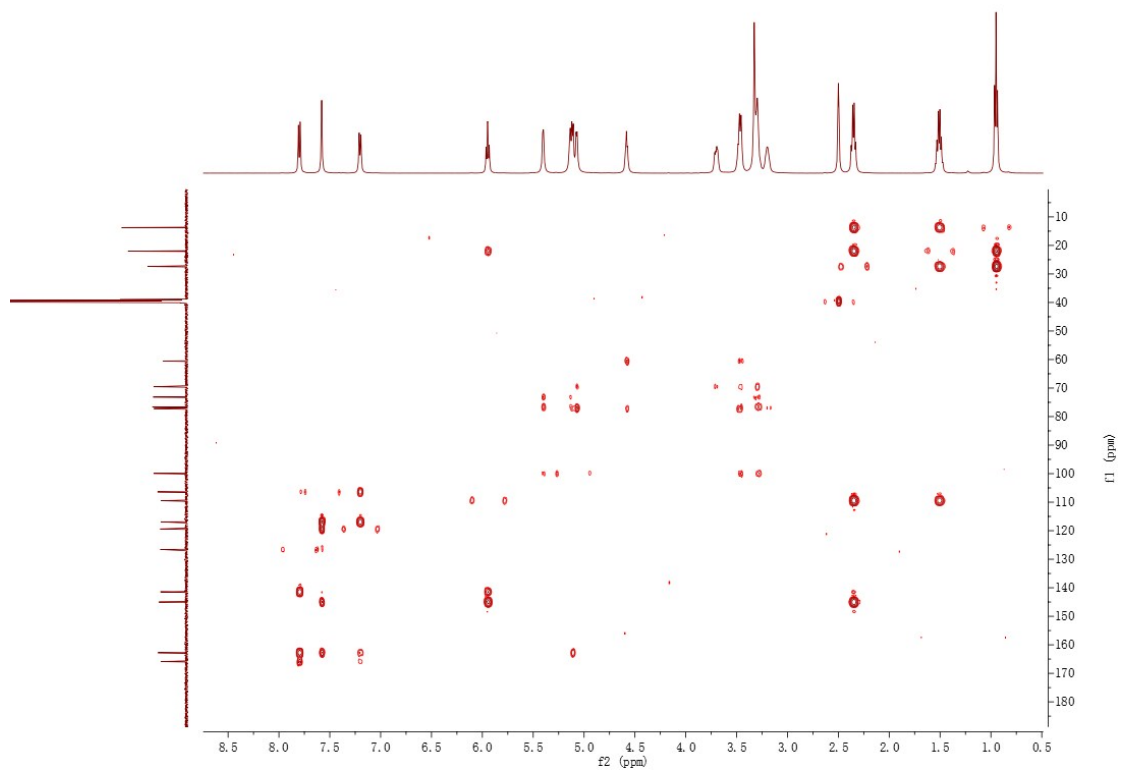


Figure S36. The HMBC spectrum of compound **4** in DMSO- d_6

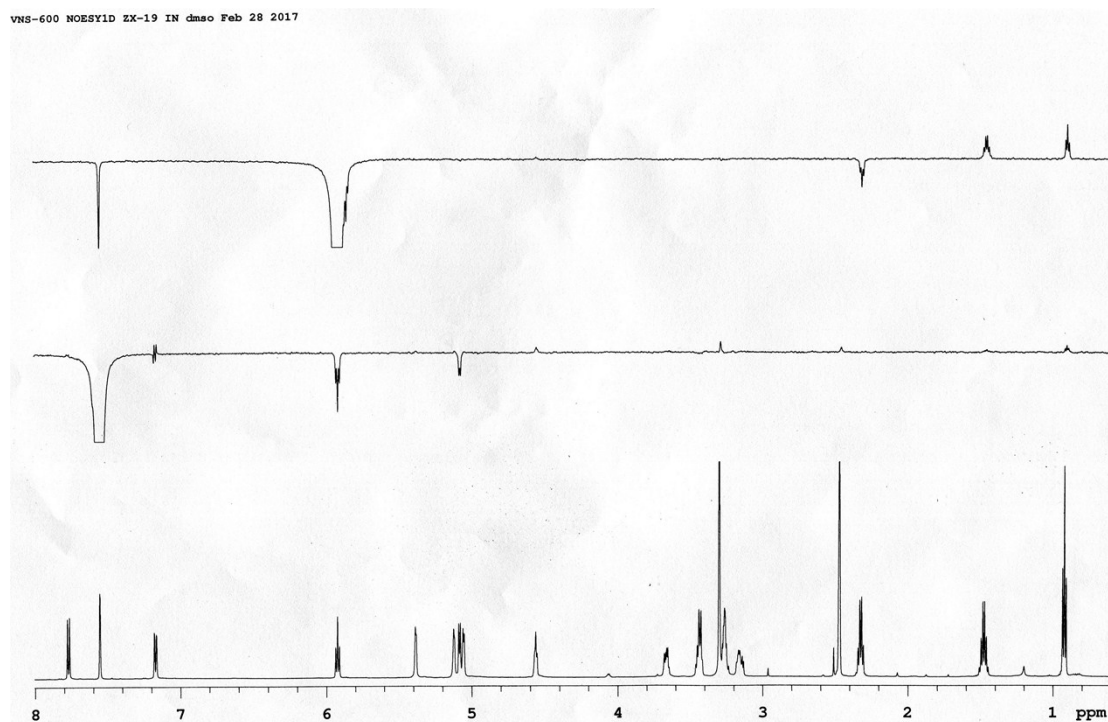


Figure S37. The NOE spectrum of compound **4** in DMSO- d_6

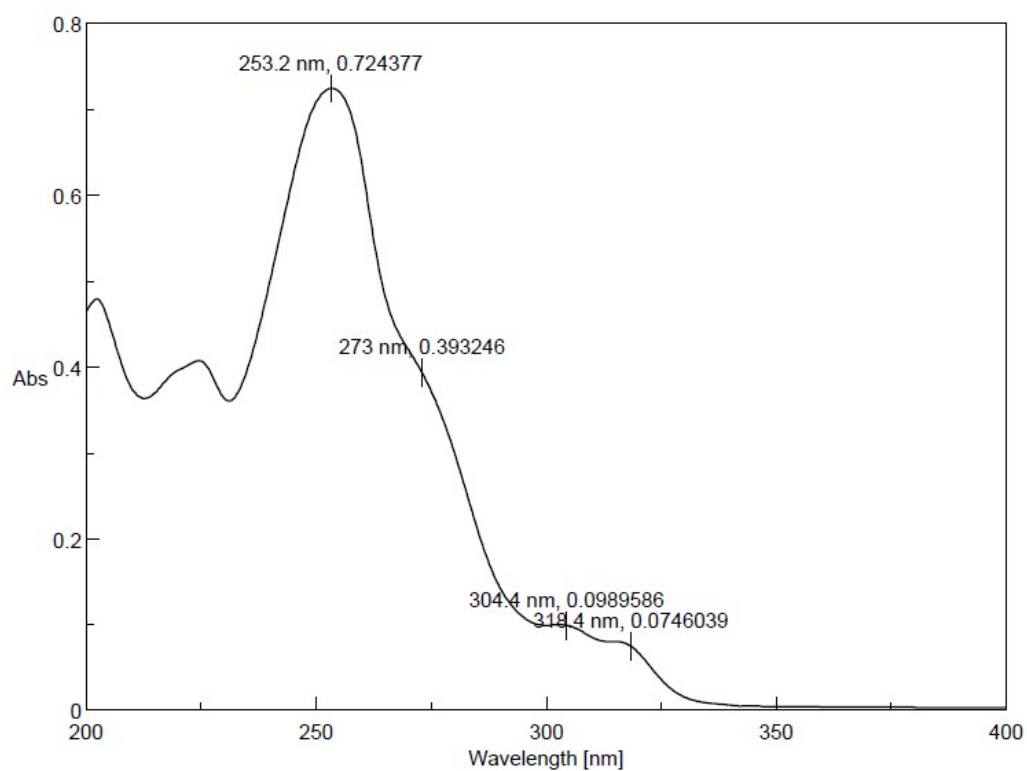


Figure S38. The UV spectrum of compound **4** in MeOH

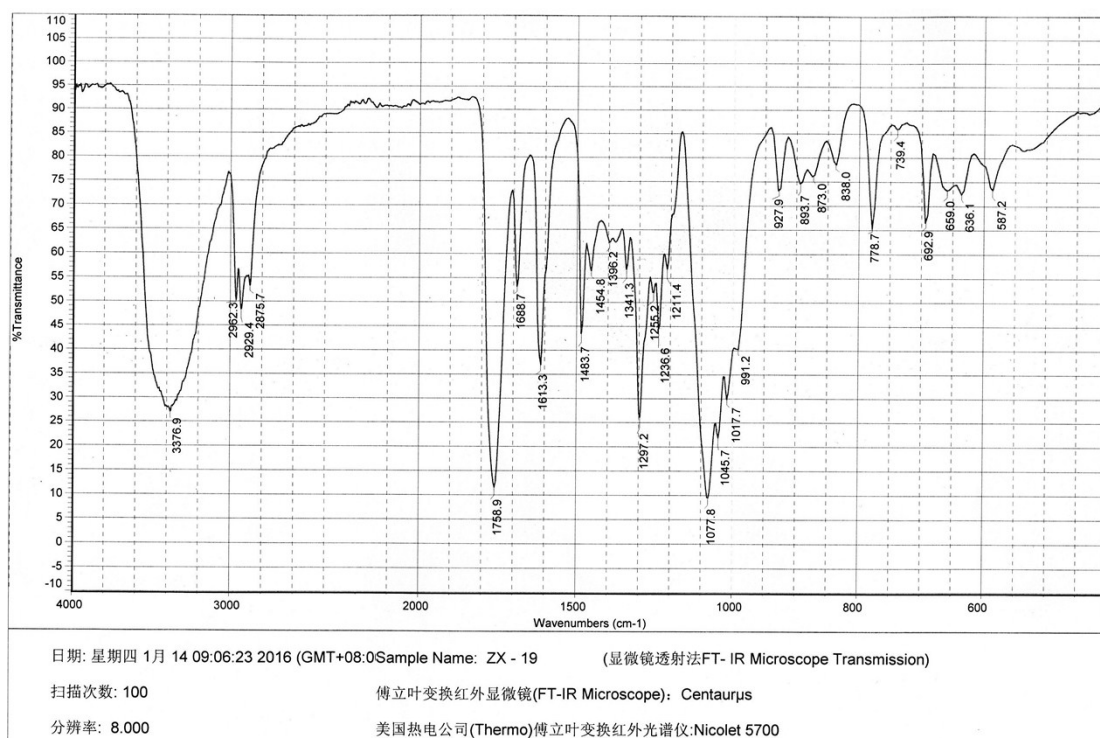


Figure S39. The IR spectrum (KBr) of compound **4**

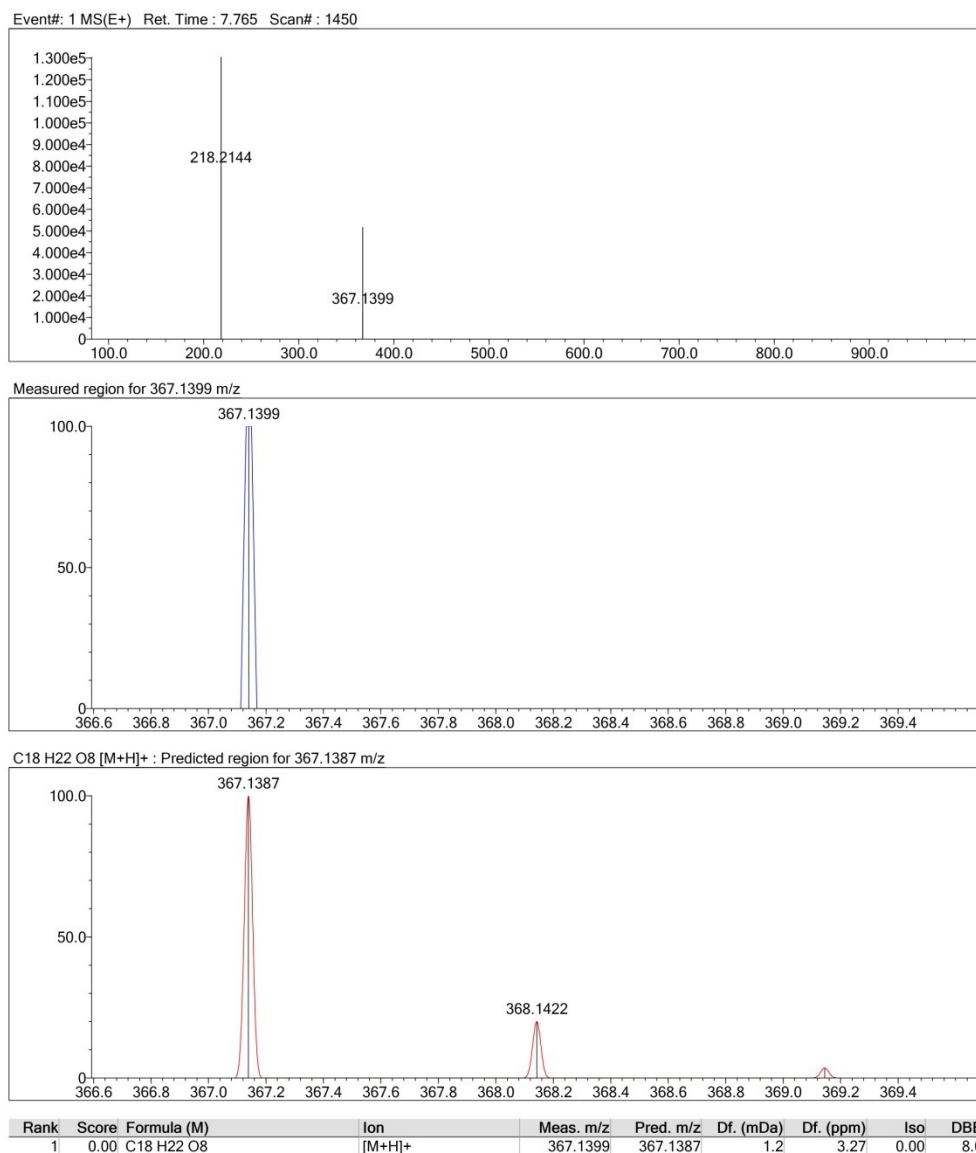


Figure S40. The HR-ESI-MS data of compound **4**

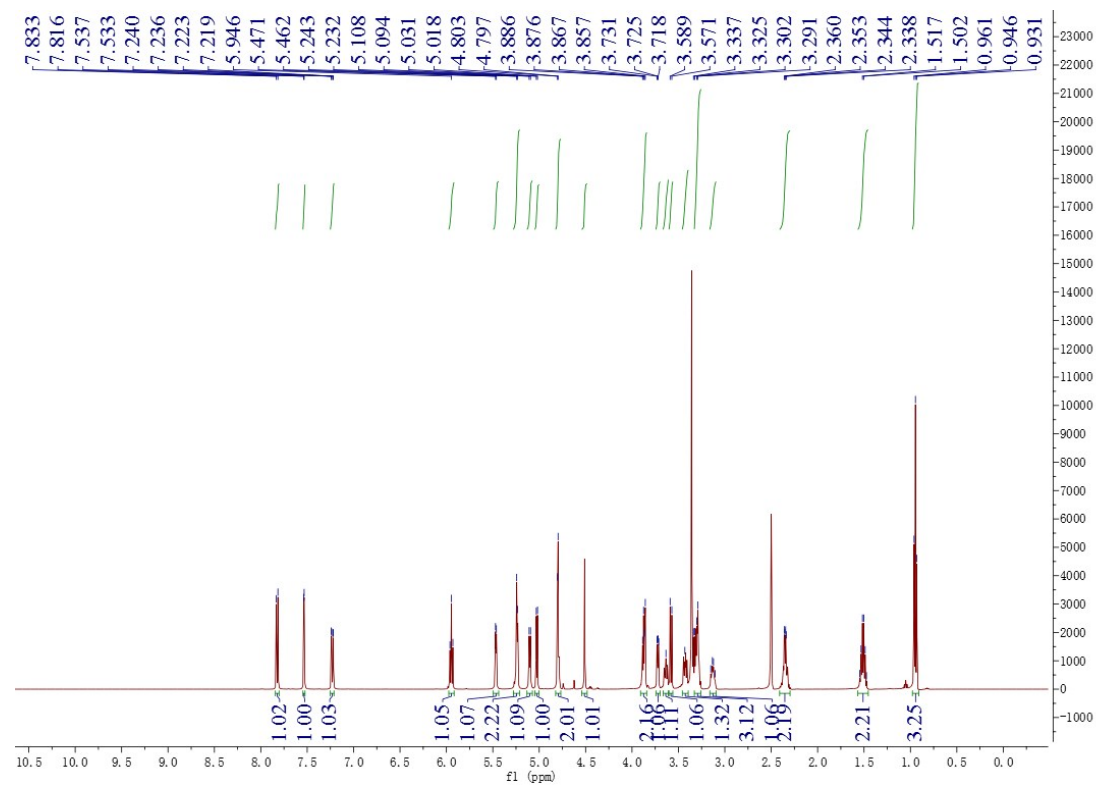


Figure S41. The ^1H NMR spectrum of compound **5** in $\text{DMSO-}d_6$

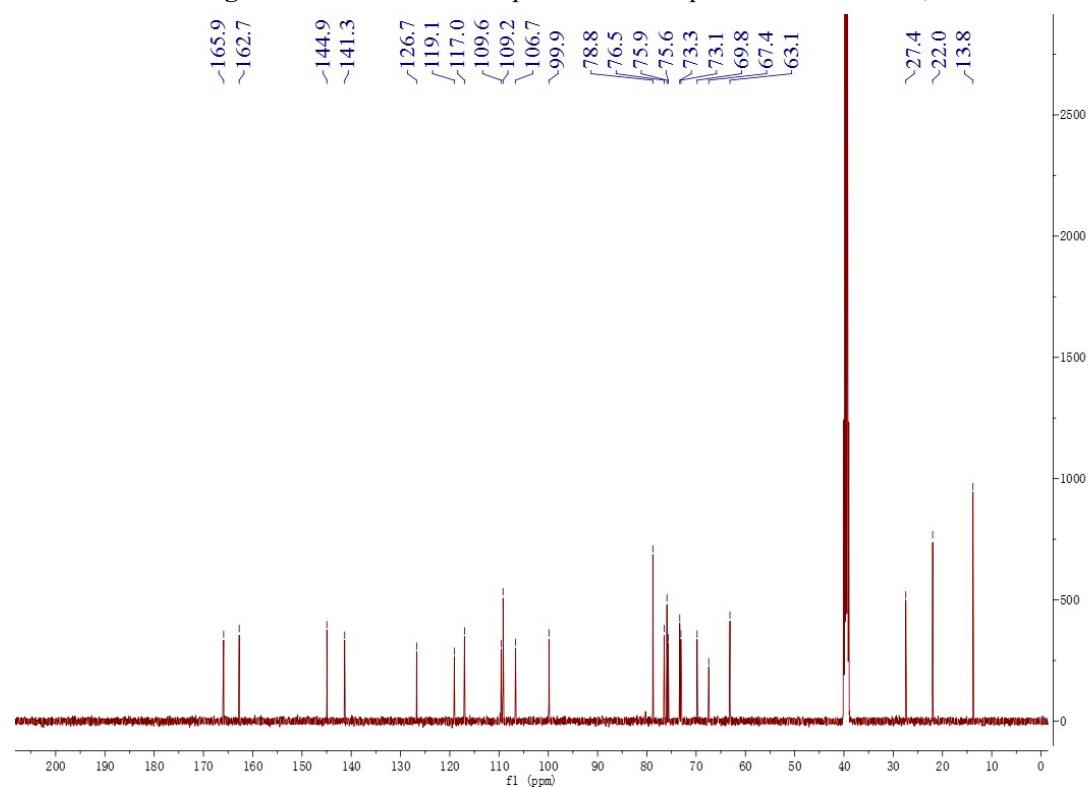


Figure S42. The ^{13}C NMR spectrum of compound **5** in $\text{DMSO-}d_6$

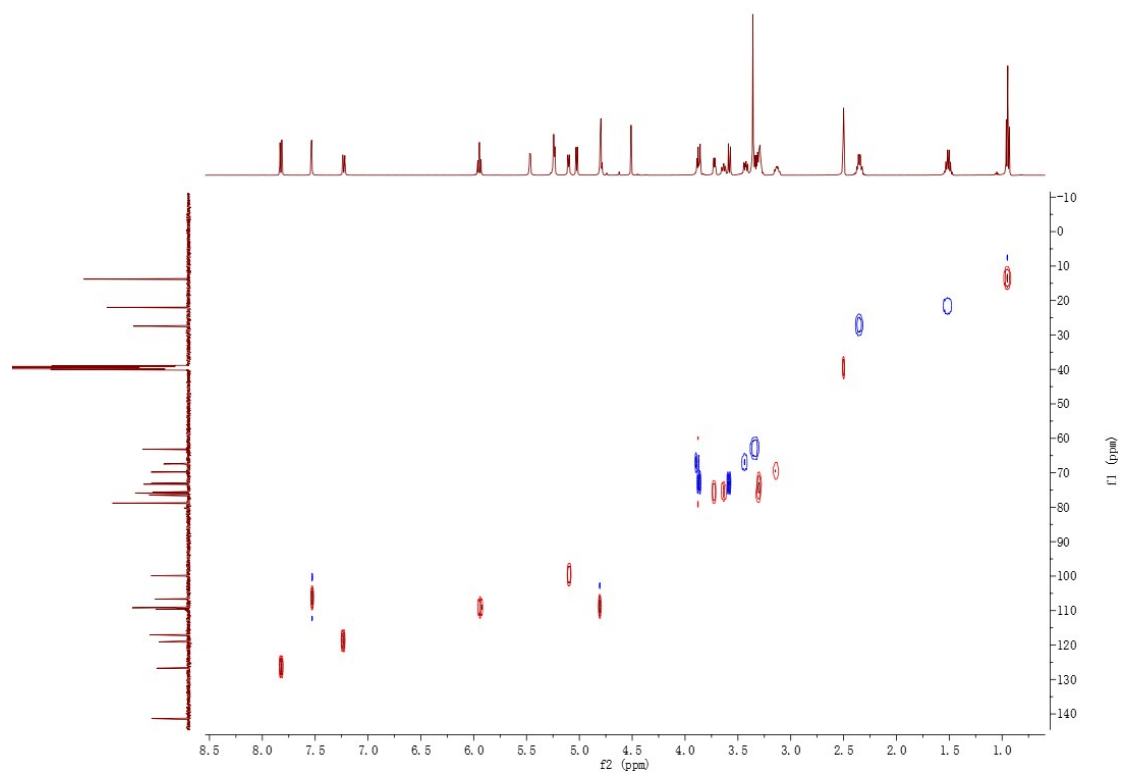


Figure S43. The HSQC spectrum of compound **5** in DMSO- d_6

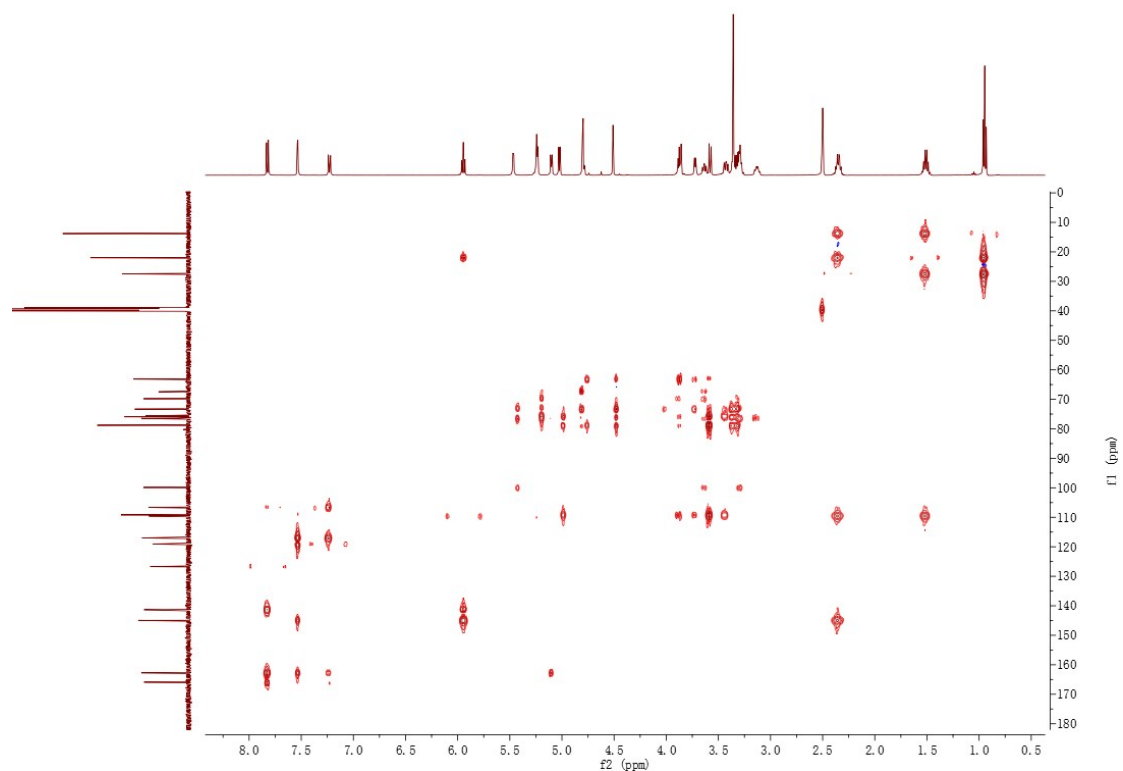


Figure S44. The HMBC spectrum of compound **5** in DMSO- d_6

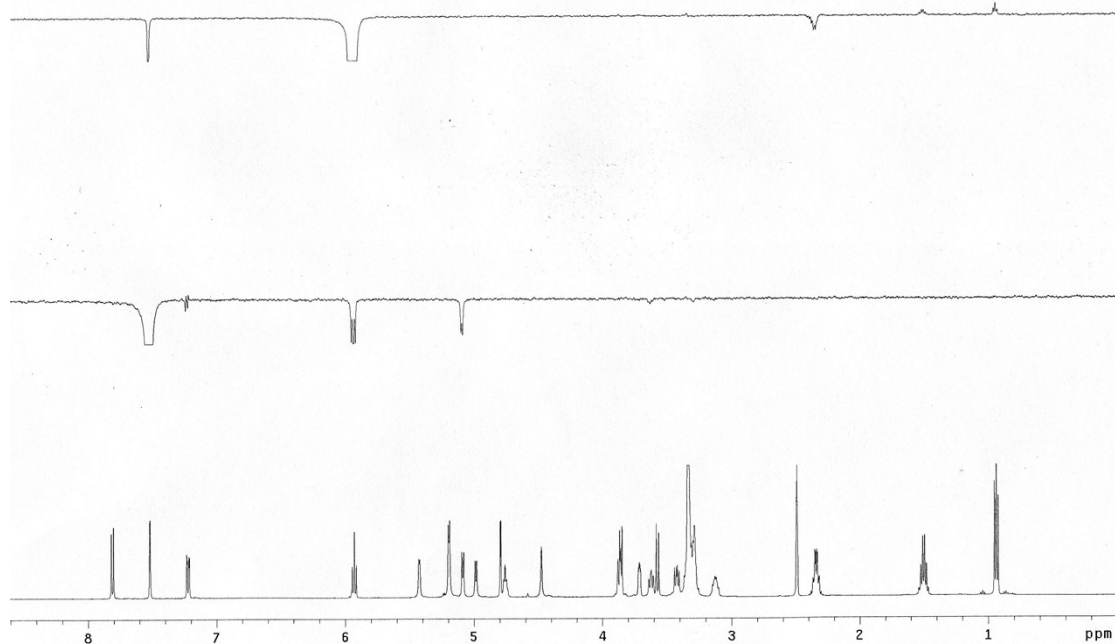


Figure S45. The NOE spectrum of compound **5** in DMSO- d_6

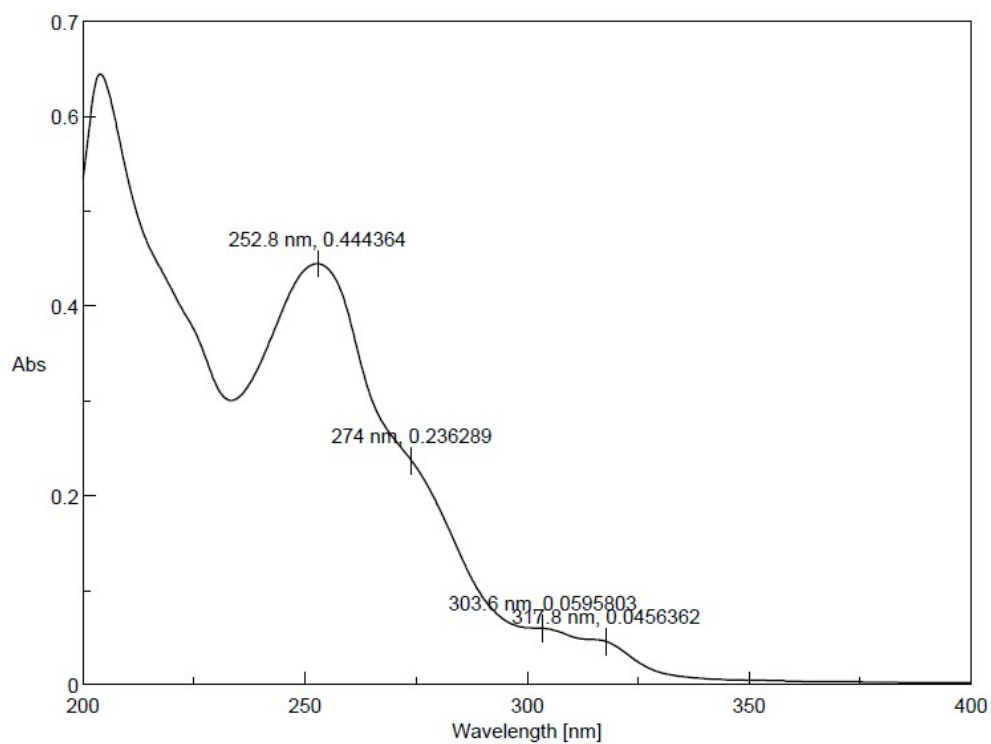


Figure S46. The UV spectrum of compound **5** in MeOH

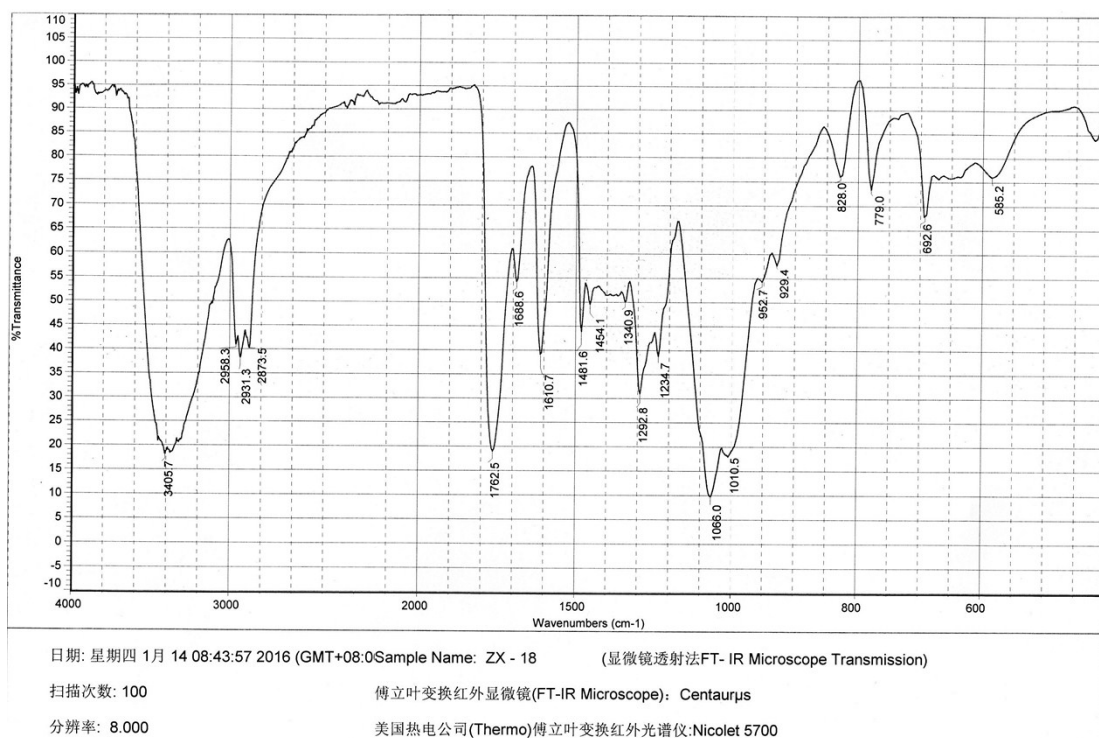


Figure S47. The IR spectrum (KBr) of compound **5**

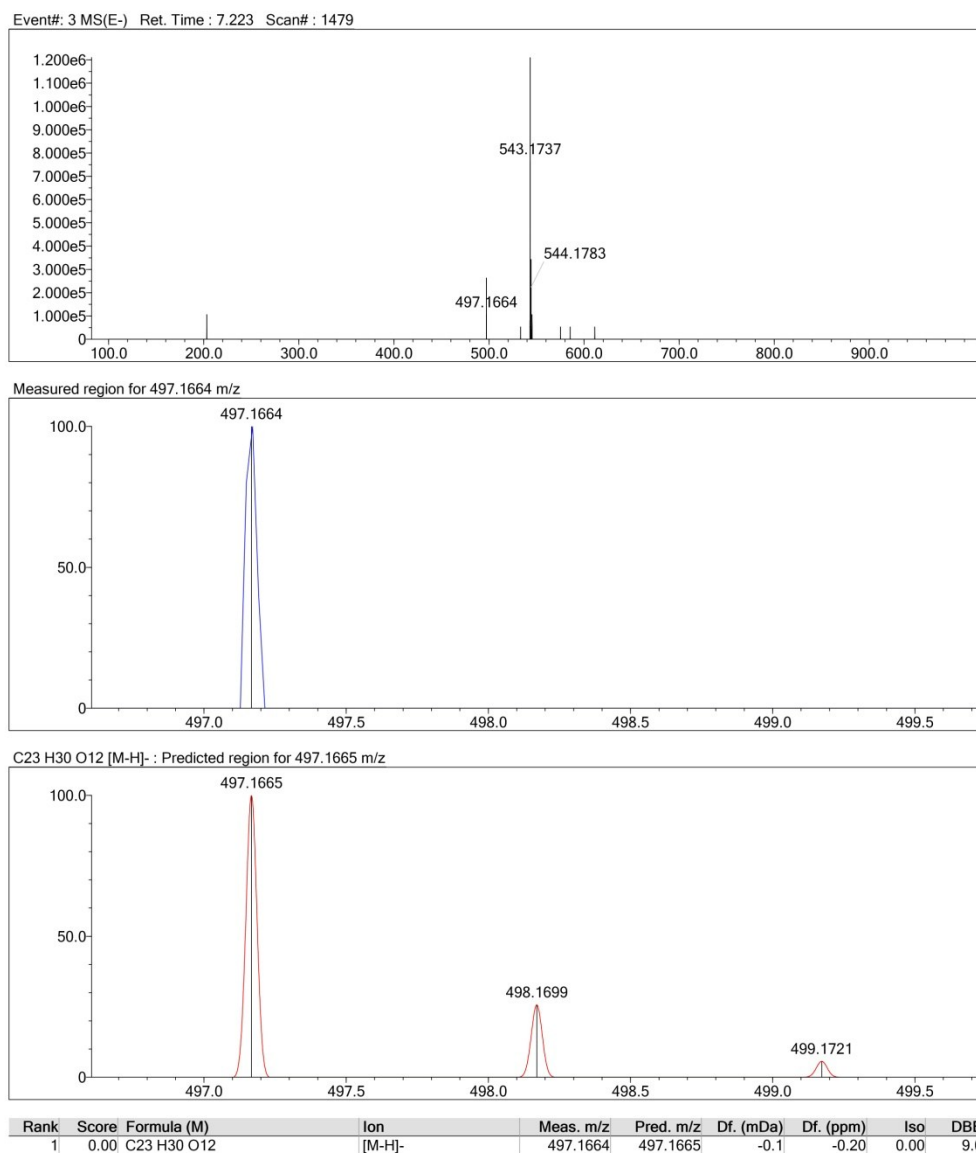


Figure S48. The HR-ESI-MS data of compound **5**

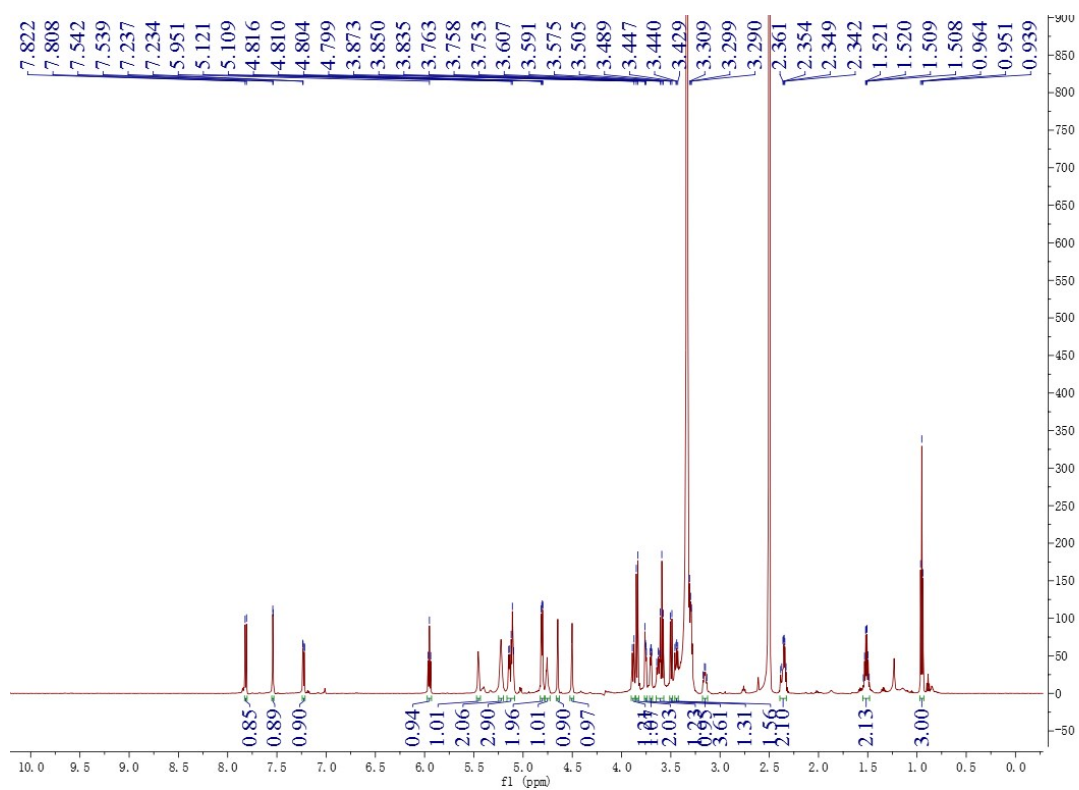


Figure S49. The ^1H NMR spectrum of compound **6** in $\text{DMSO}-d_6$

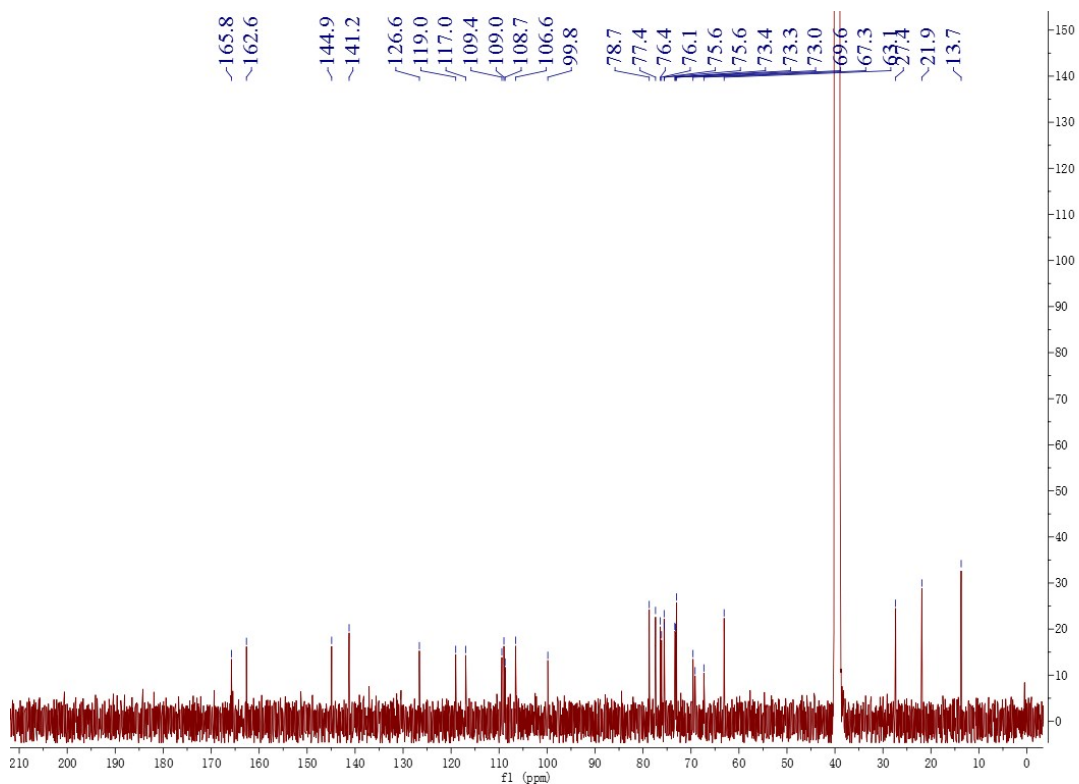


Figure S50. The ^{13}C NMR spectrum of compound **6** in $\text{DMSO}-d_6$

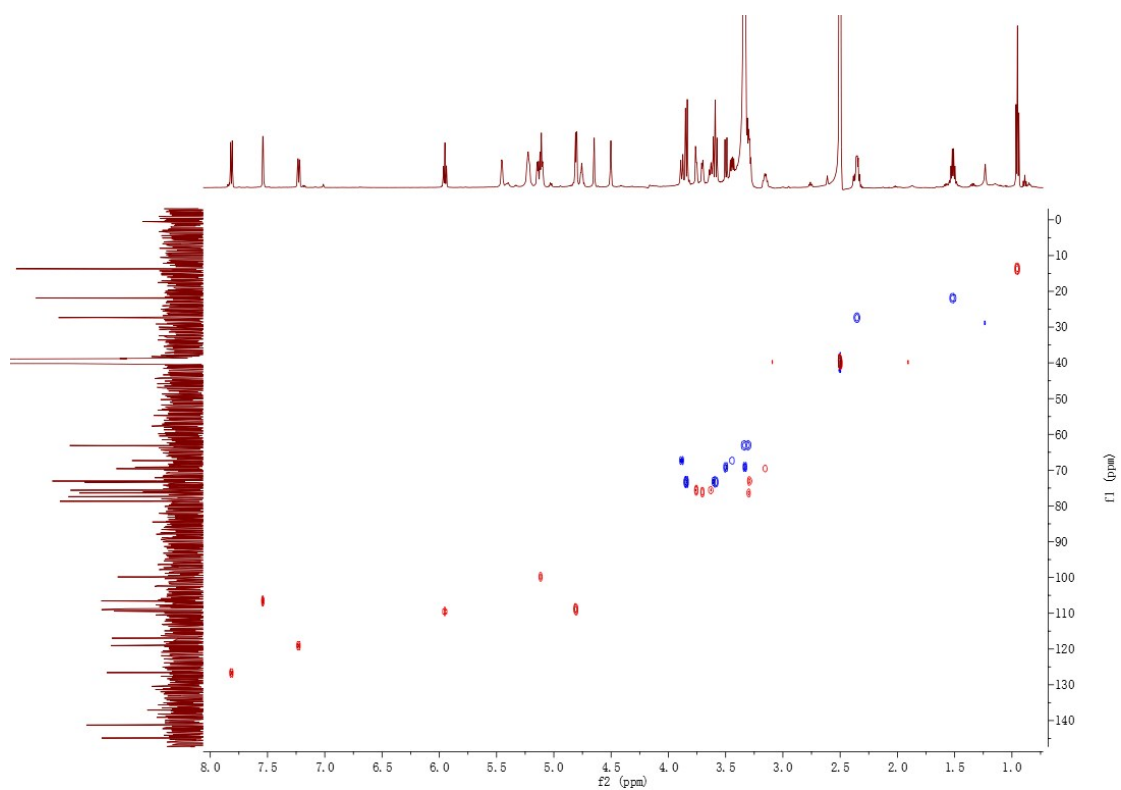


Figure S51. The HSQC spectrum of compound **6** in DMSO- d_6

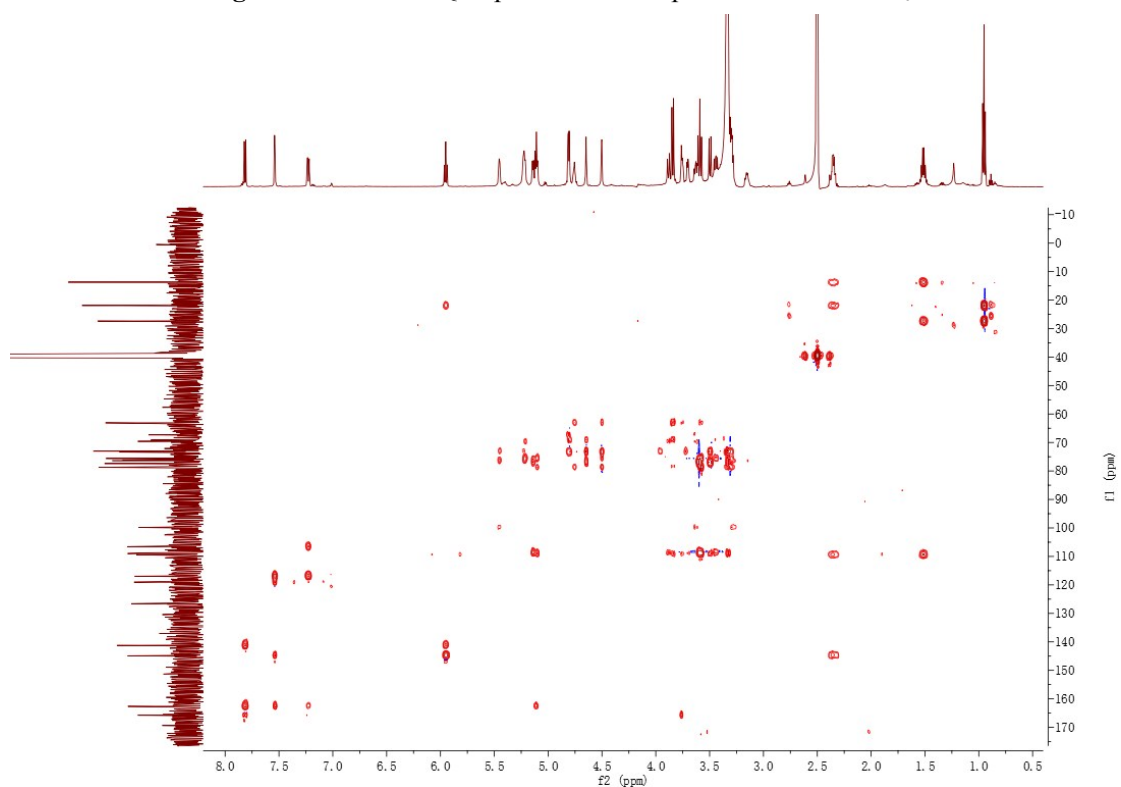


Figure S52. The HMBC spectrum of compound **6** in DMSO- d_6

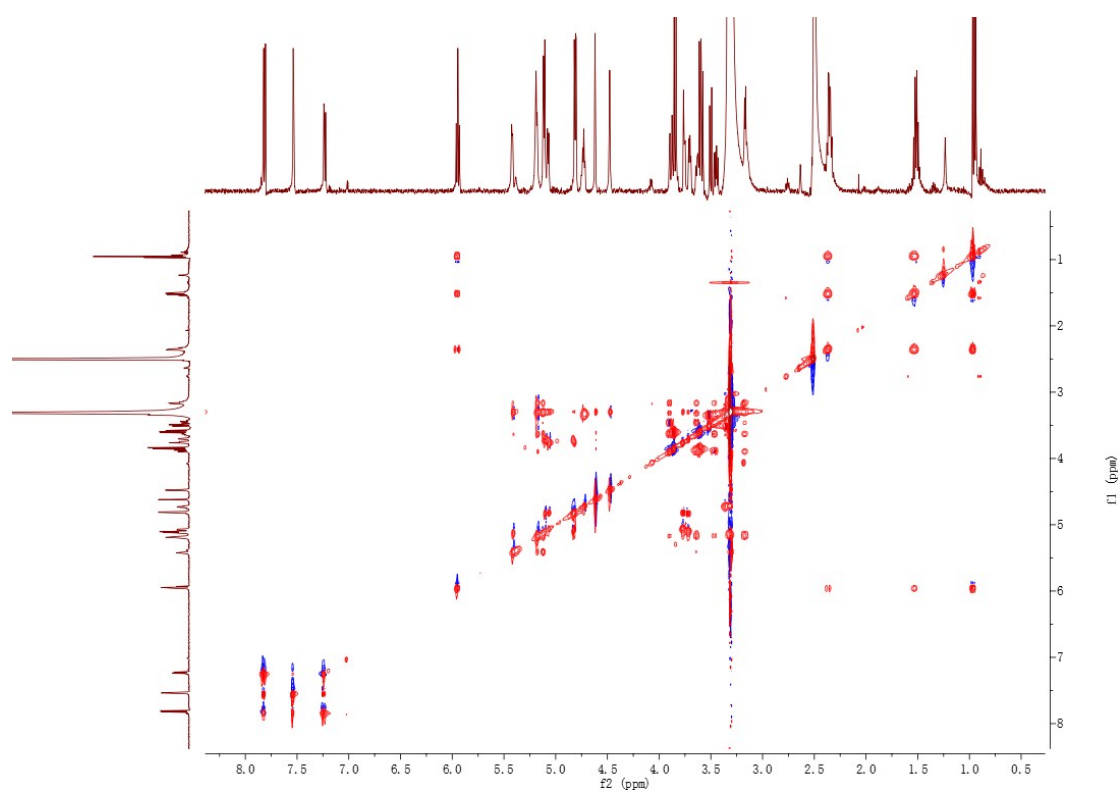


Figure S53. The TOCSY spectrum of compound **6** in DMSO- d_6

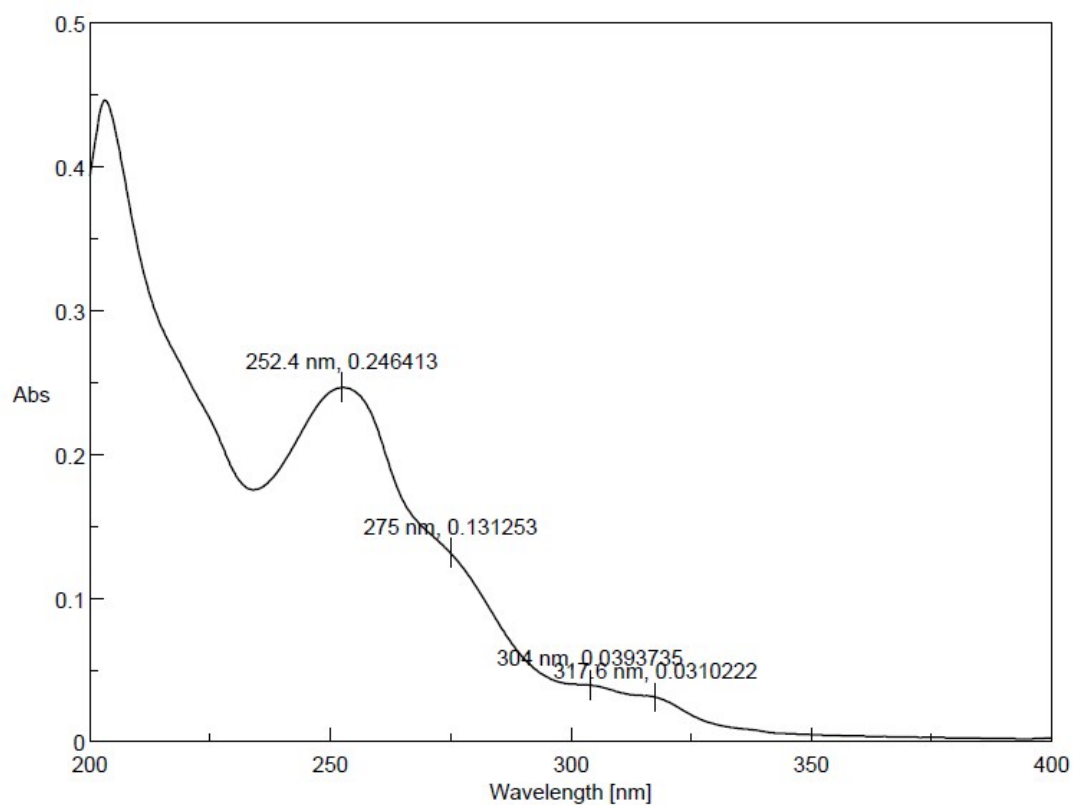
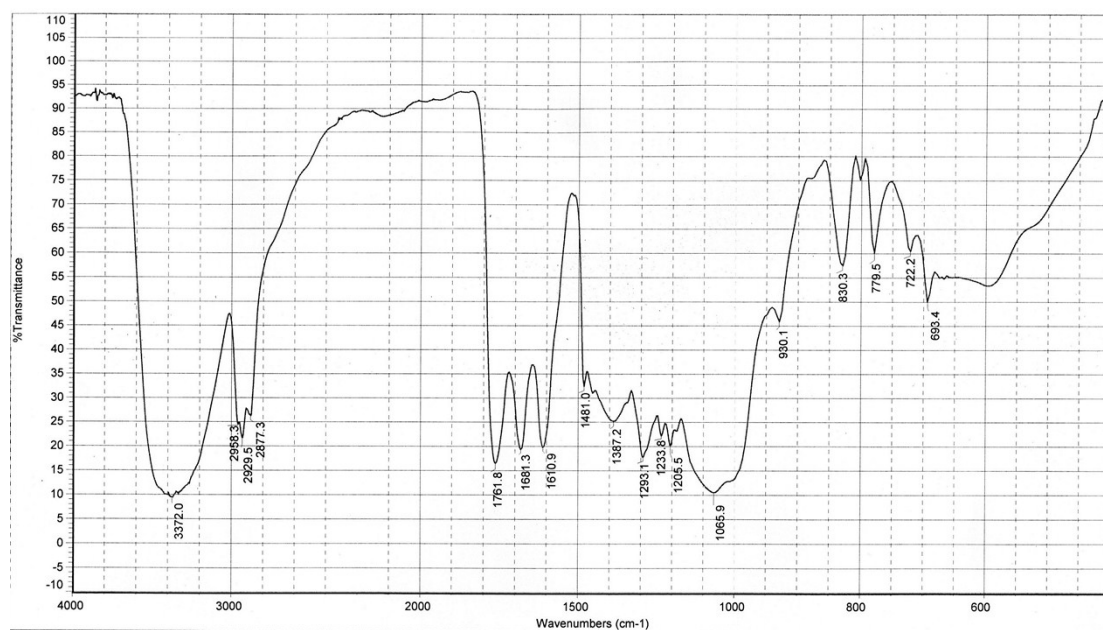


Figure S54. The UV spectrum of compound **6** in MeOH



日期: 星期四 1月 14 09:37:18 2016 (GMT+08:00) Sample Name: ZX - 21 (显微镜透射法FT- IR Microscope Transmission)

扫描次数: 100

傅立叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

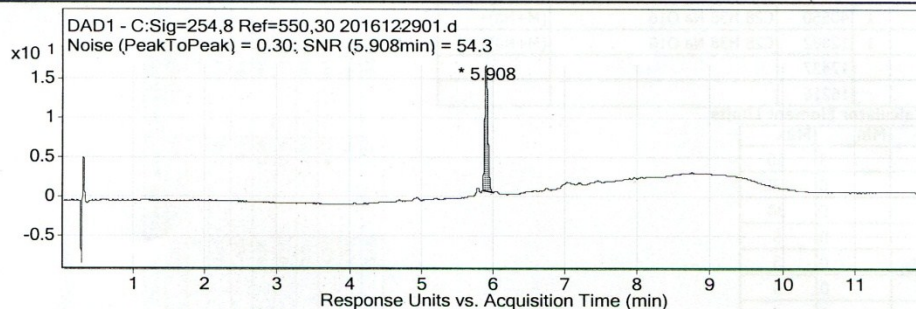
美国热电公司(Thermo)傅立叶变换红外光谱仪:Nicolet 5700

Figure S55. The IR spectrum (KBr) of compound **6**

Qualitative Analysis Report

Data Filename	2016122901.d	Sample Name	ZX-21
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

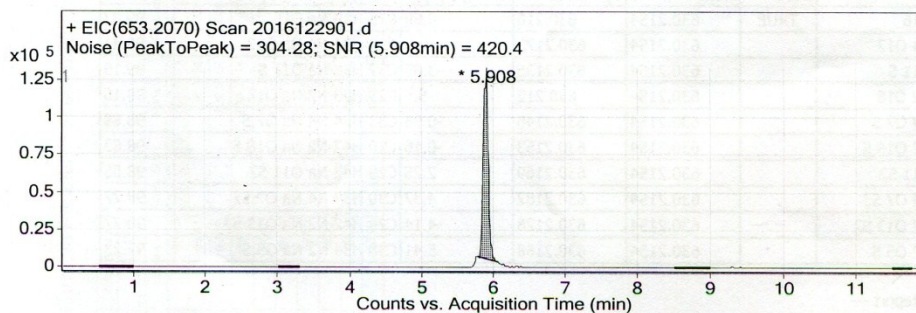
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.853	5.908	6.005	16.06	50.67	100	54.3

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.779	5.908	6.069	127927	622179	100	420.4

User Spectra

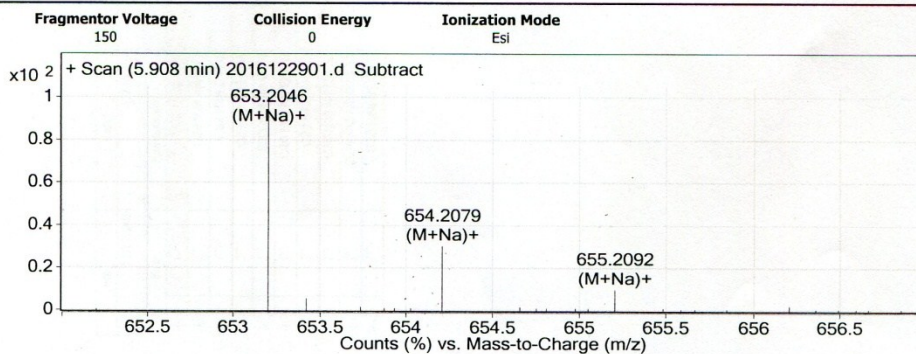


Figure S56. The HR-ESI-MS data of compound **6**

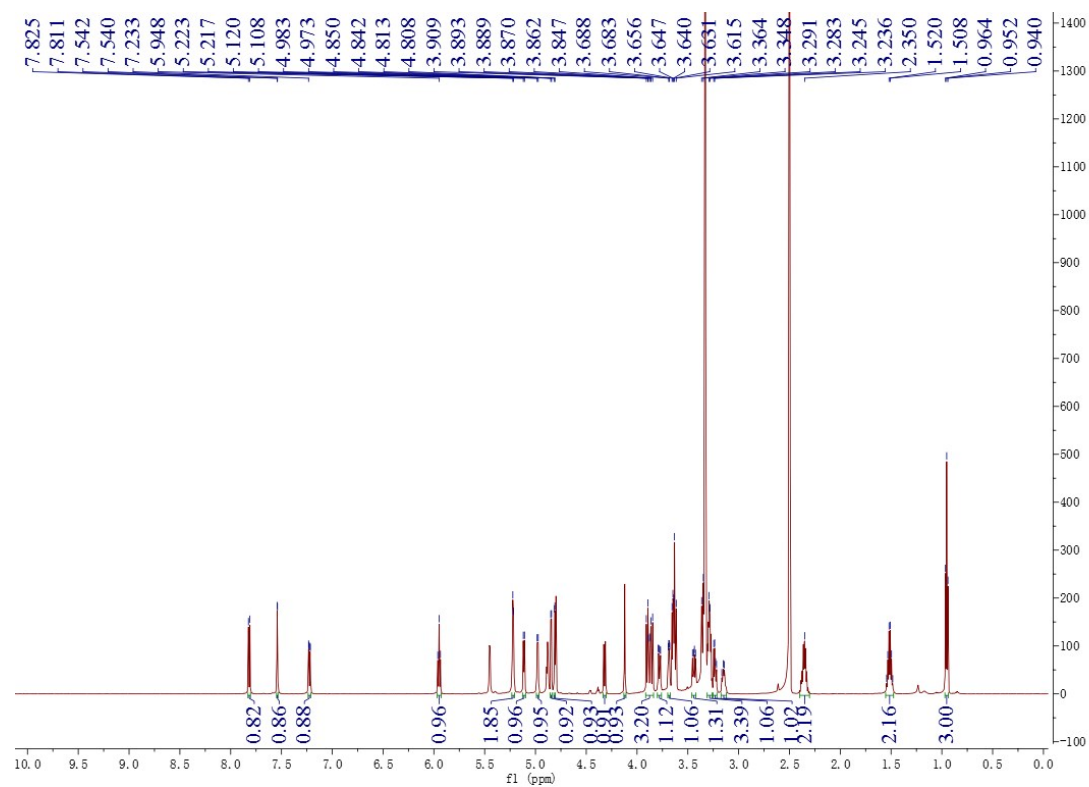


Figure S57. The ¹H NMR spectrum of compound **7** in DMSO-*d*₆

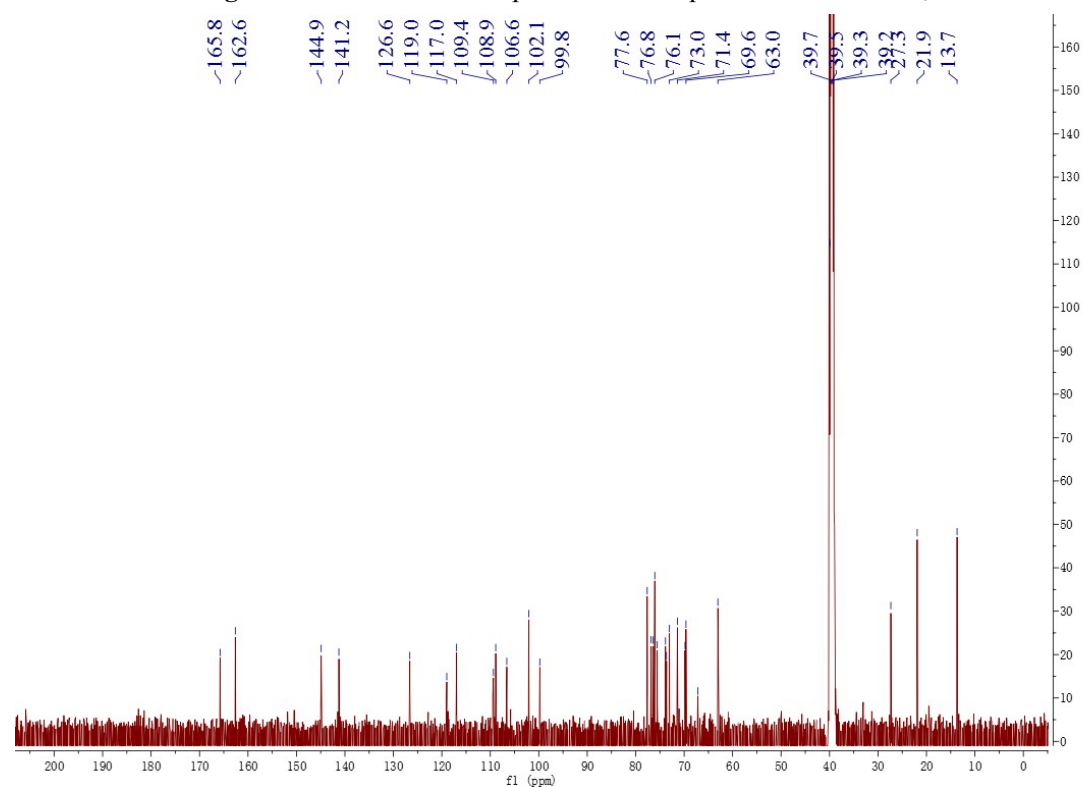


Figure S58. The ¹³C NMR spectrum of compound **7** in DMSO-*d*₆

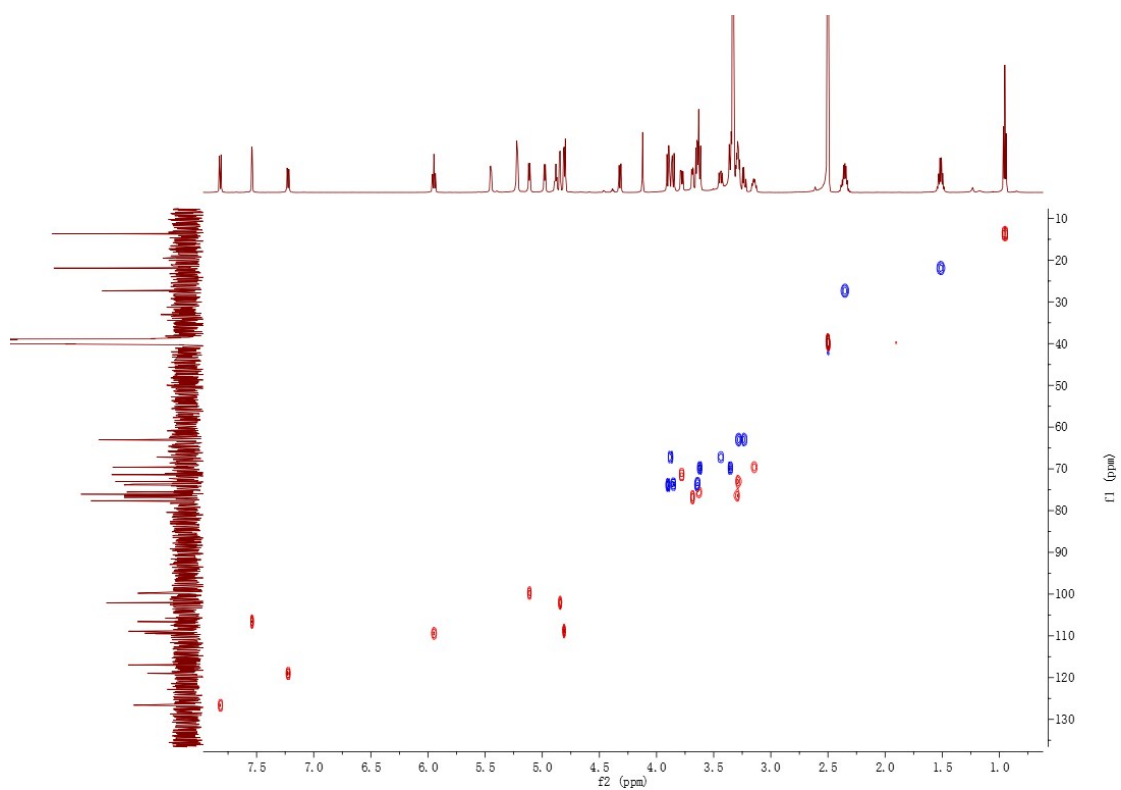


Figure S59. The HSQC spectrum of compound **7** in DMSO- d_6

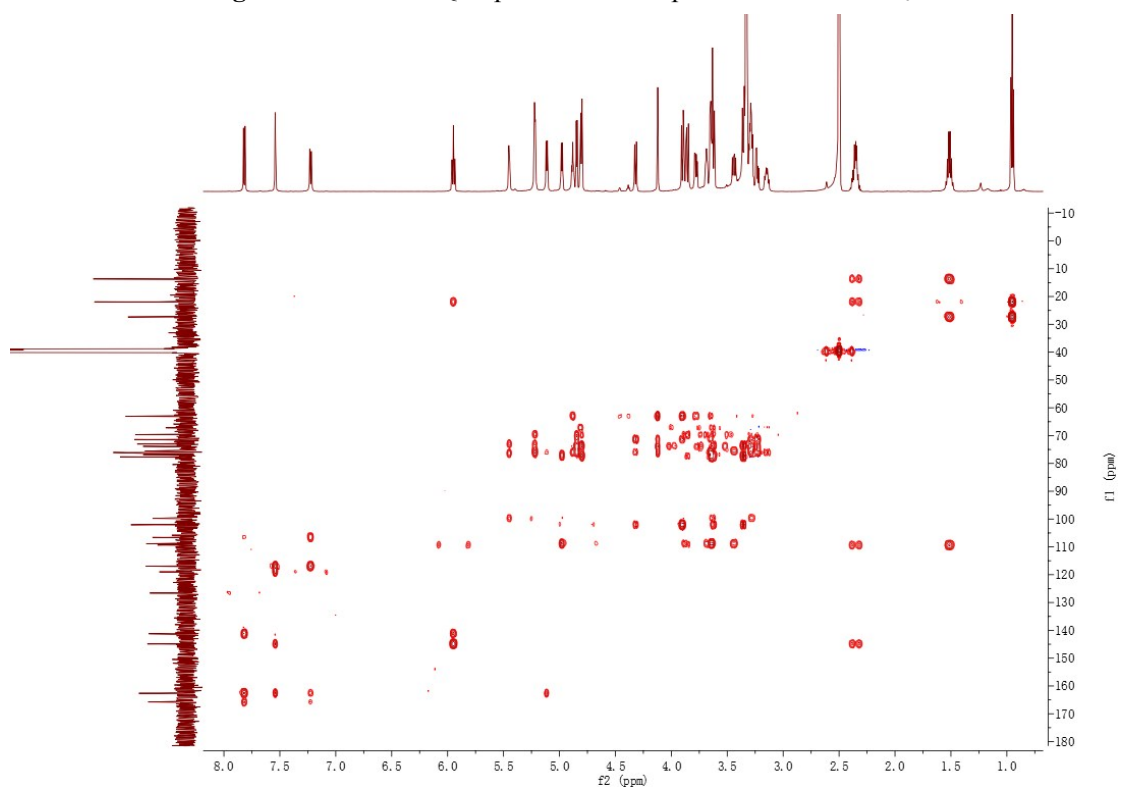


Figure S60. The HMBC spectrum of compound **7** in DMSO- d_6

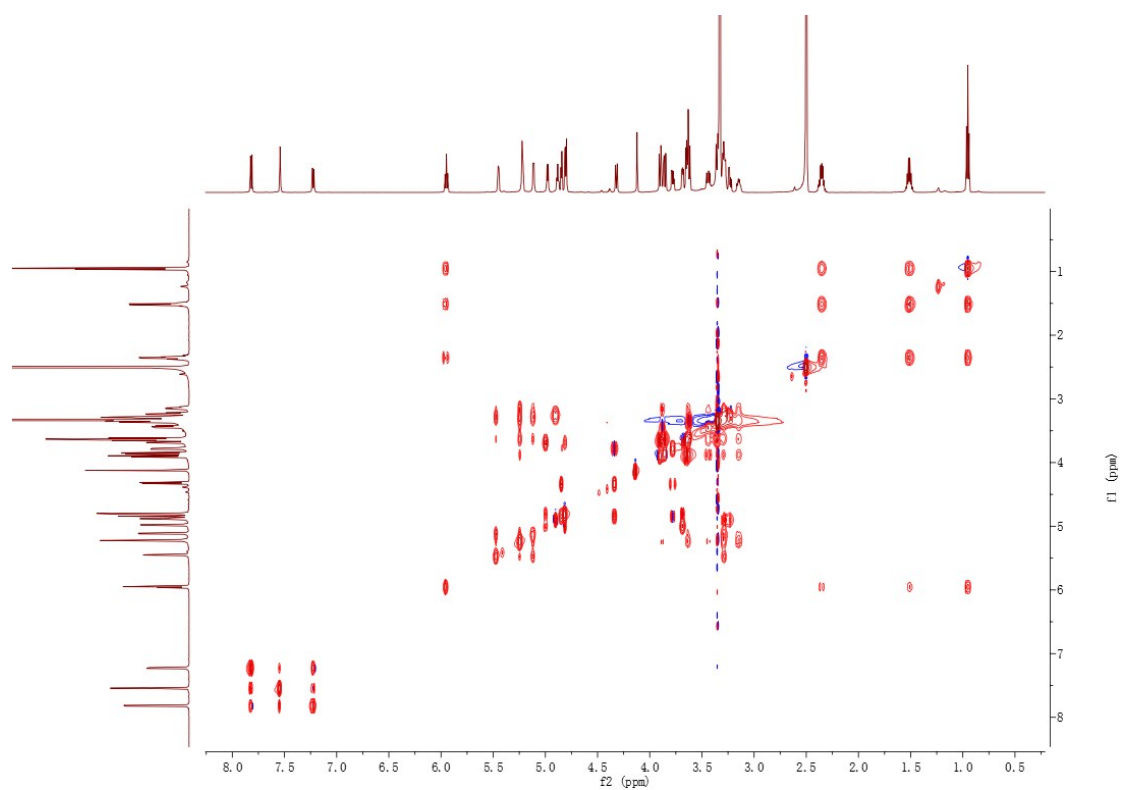


Figure S61. The TOCSY spectrum of compound **7** in DMSO- d_6

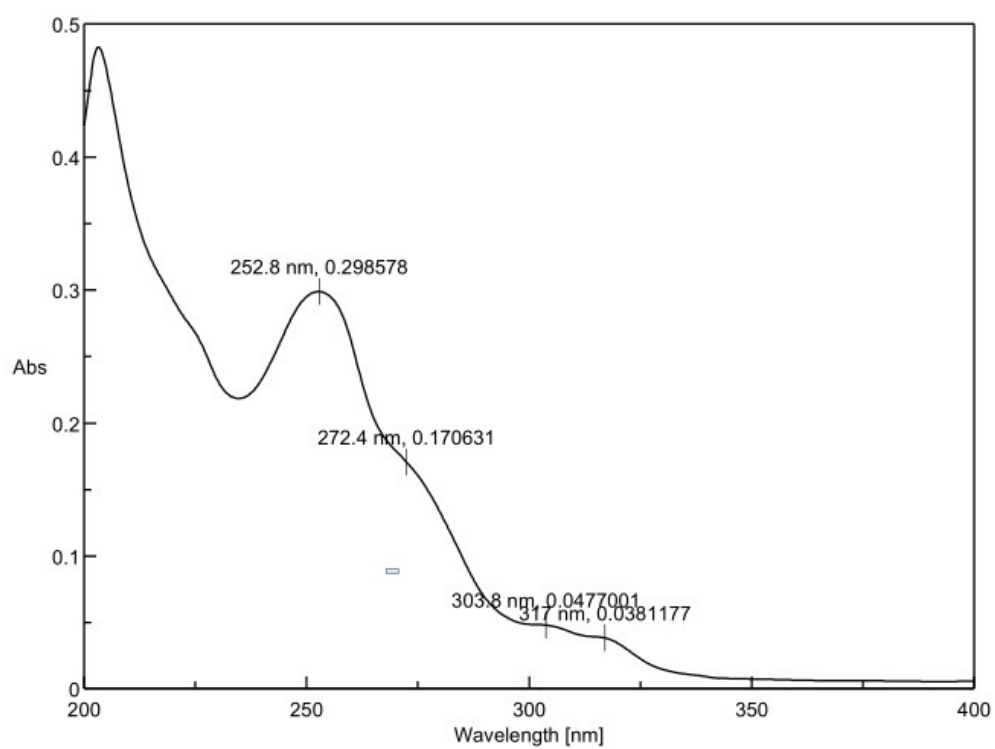


Figure S62. The UV spectrum of compound **7** in MeOH

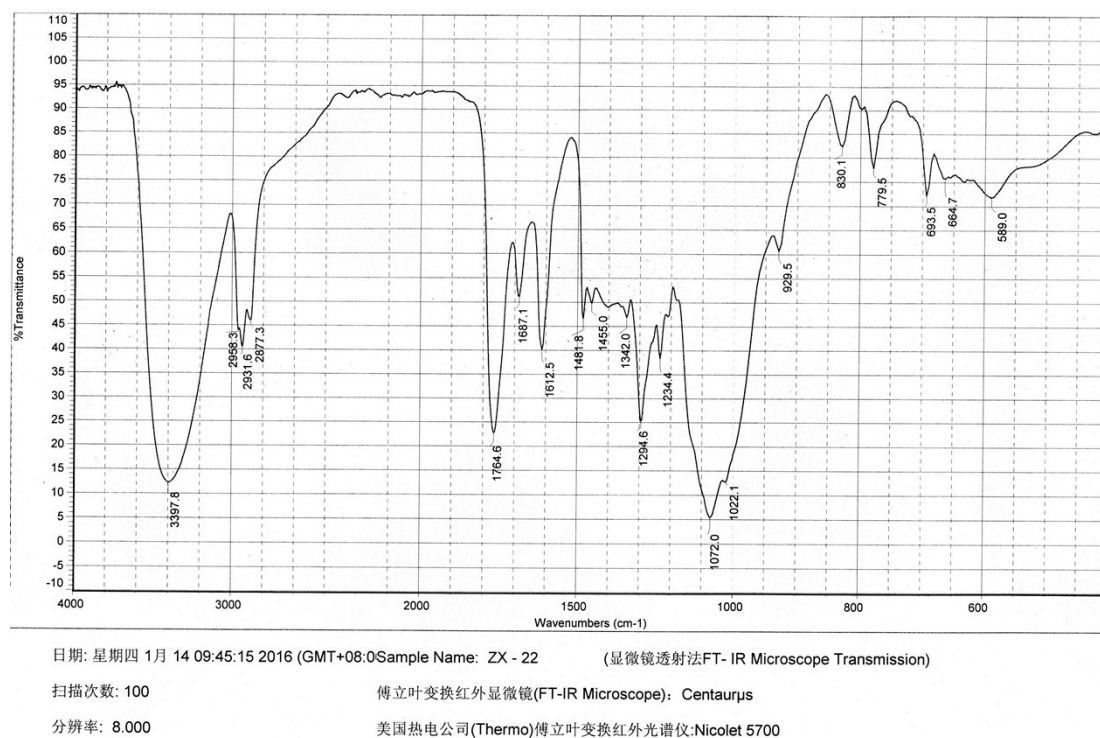


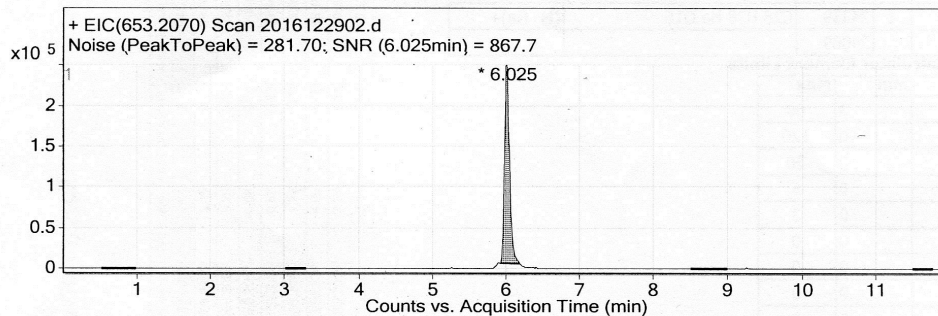
Figure S63. The IR spectrum (KBr) of compound **7**

Qualitative Analysis Report

Data Filename	2016122902.d	Sample Name	ZX-22
Sample Type	Sample	Position	P1-C2
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	Some Ions Missed
DA Method	TEST LCMS.m	Comment	

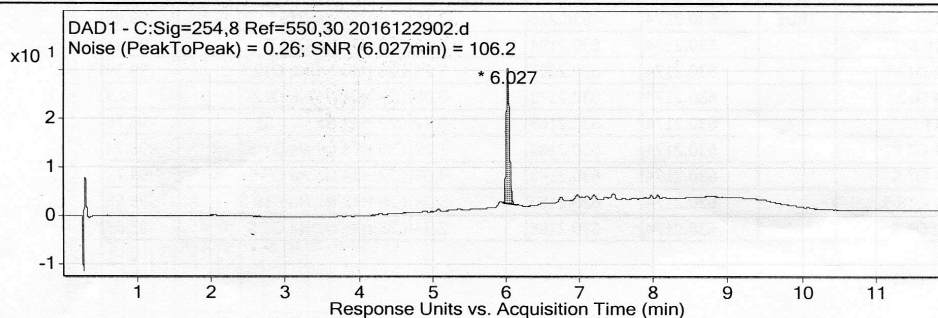
User Chromatograms

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.928	6.025	6.186	244423	1274728	100	867.7



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.961	6.027	6.148	27.94	89.19	100	106.2

User Spectra

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

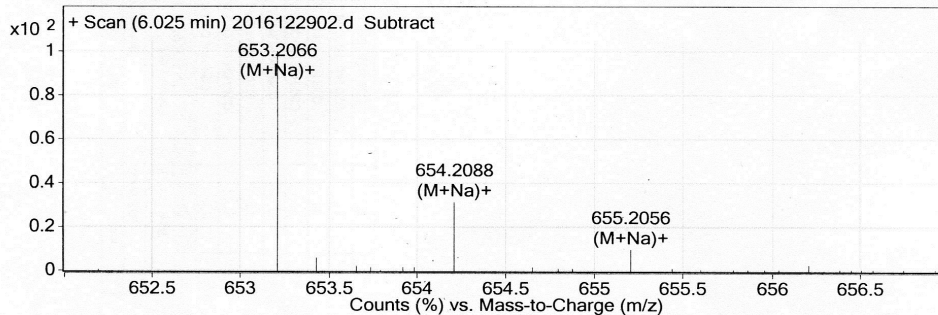


Figure S64. The HR-ESI-MS data of compound 7

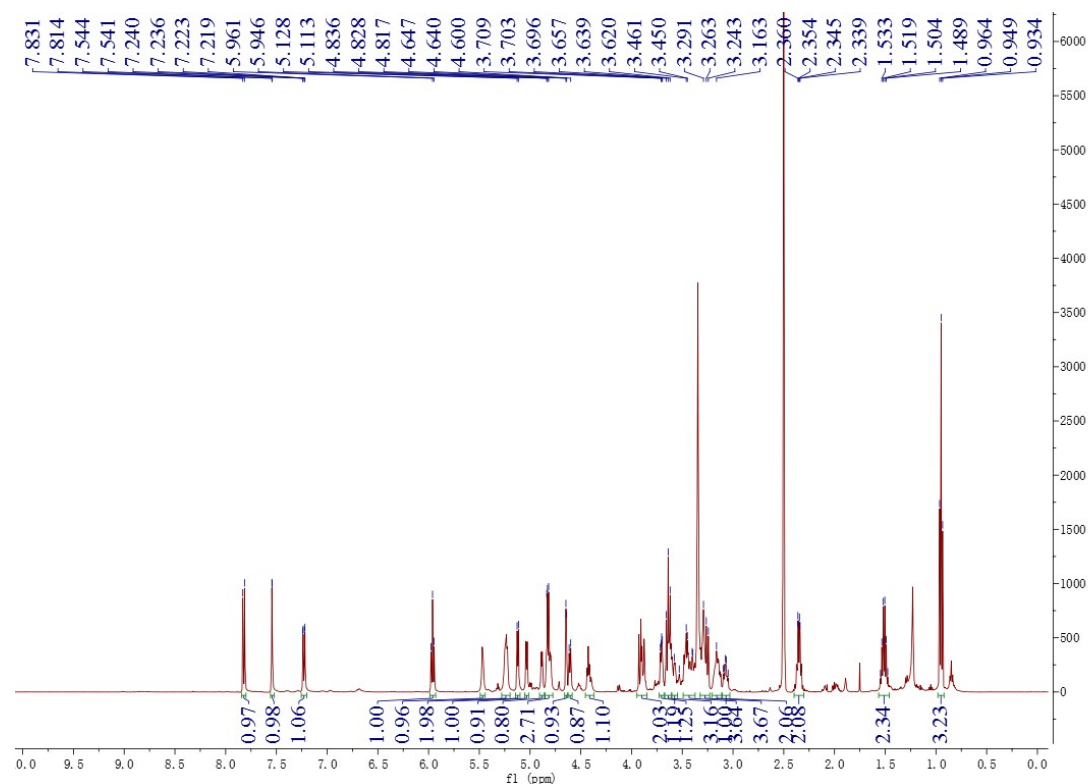


Figure S65. The ^1H NMR spectrum of compound **8** in $\text{DMSO}-d_6$

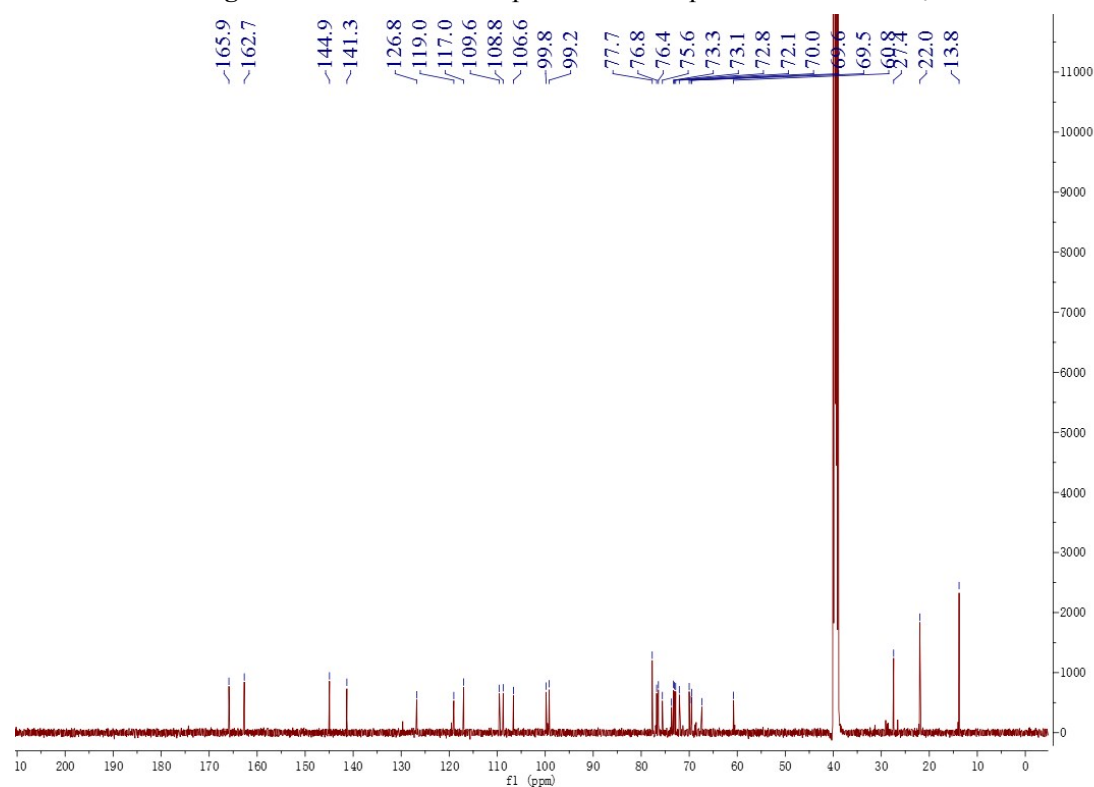


Figure S66. The ^{13}C NMR spectrum of compound **8** in $\text{DMSO}-d_6$

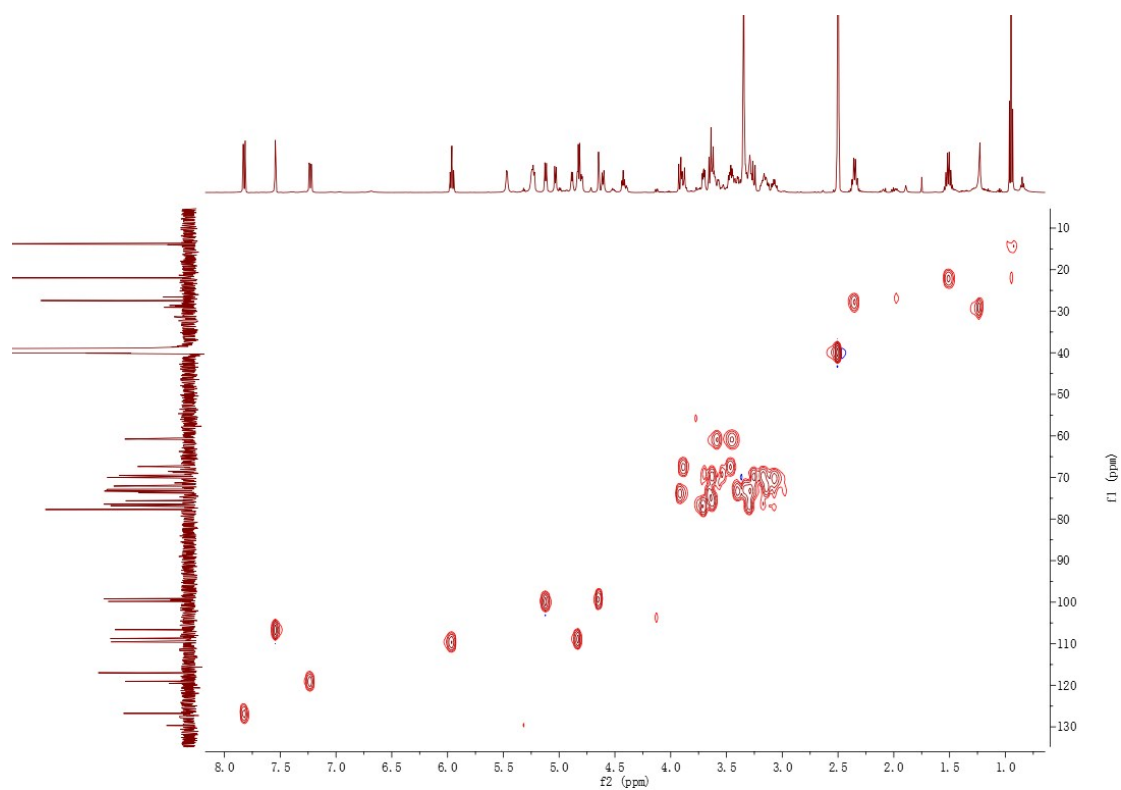


Figure S67. The HSQC spectrum of compound **8** in DMSO- d_6

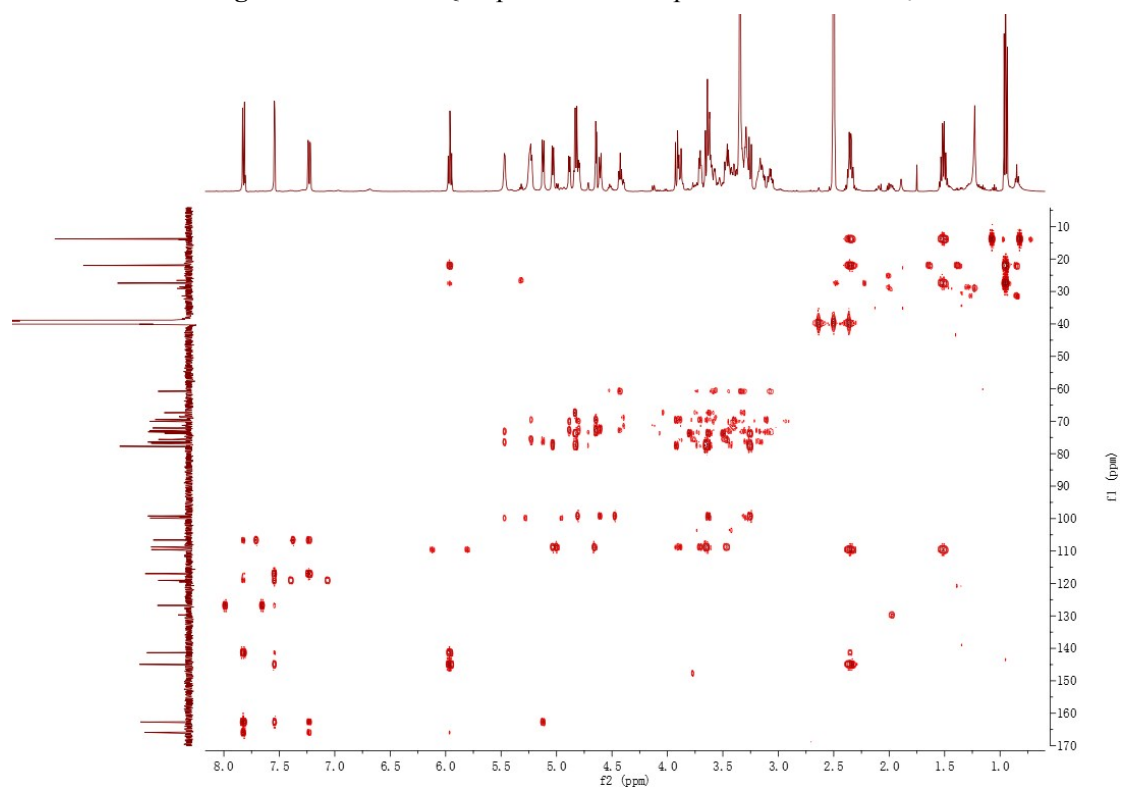


Figure S68. The HMBC spectrum of compound **8** in DMSO- d_6

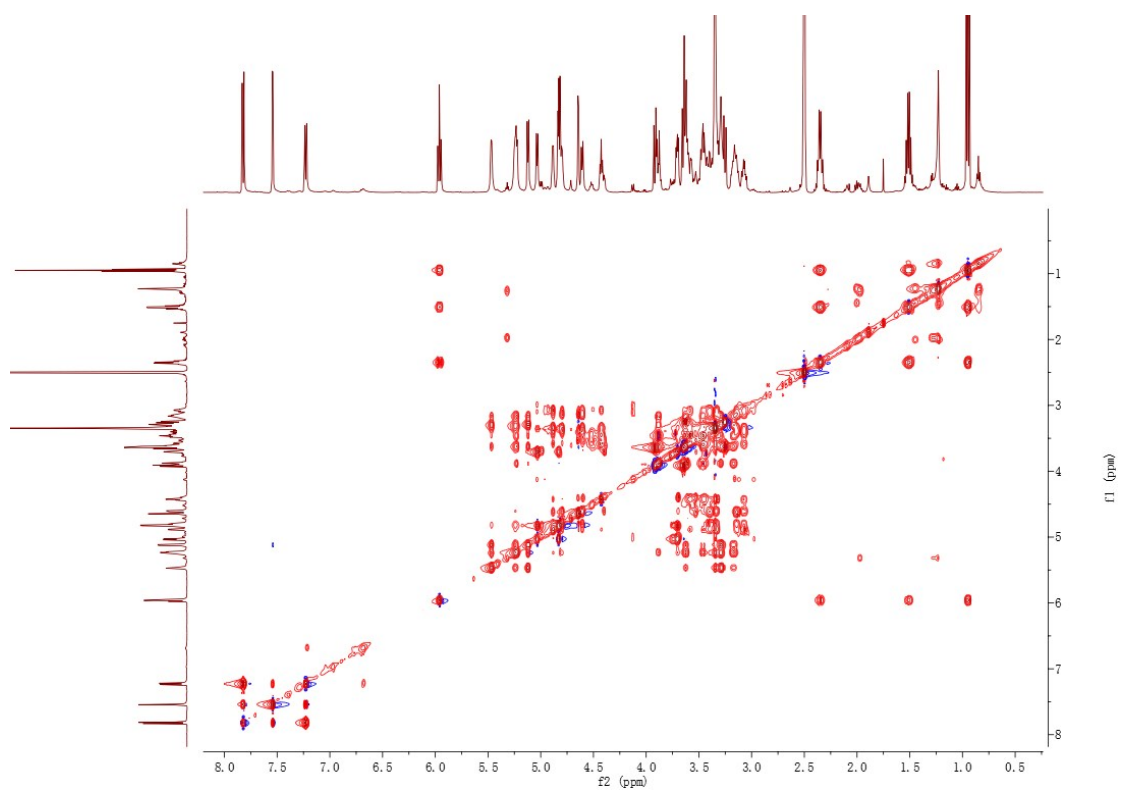


Figure S69. The TOCSY spectrum of compound **8** in DMSO- d_6

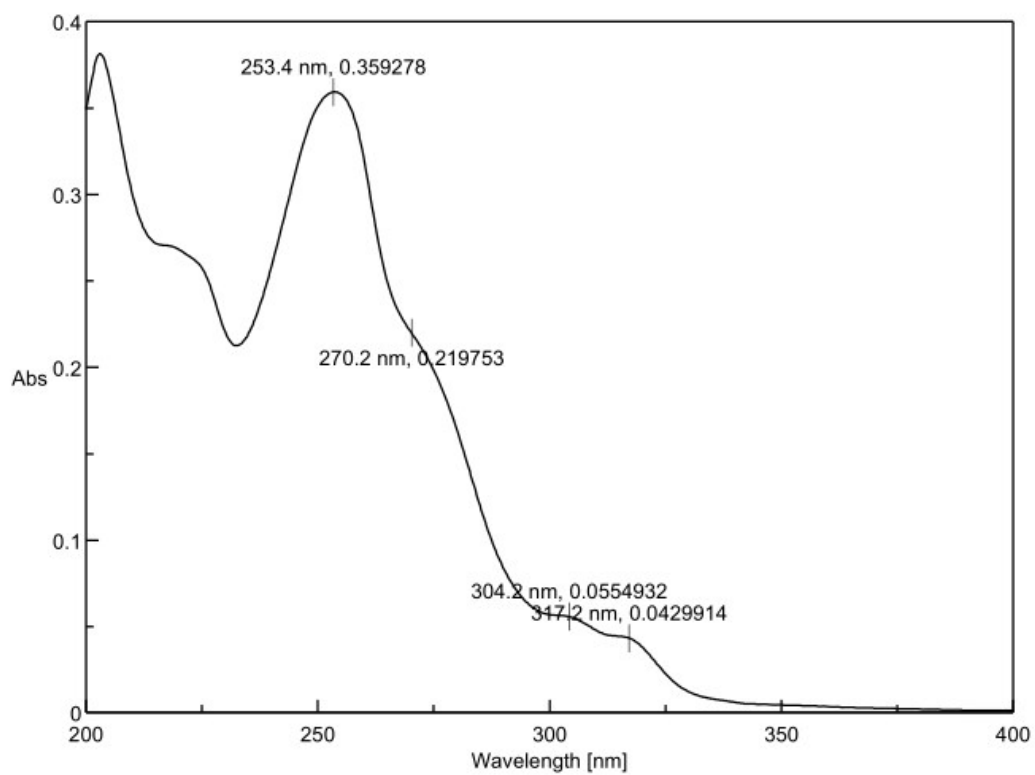


Figure S70. The UV spectrum of compound **8** in MeOH

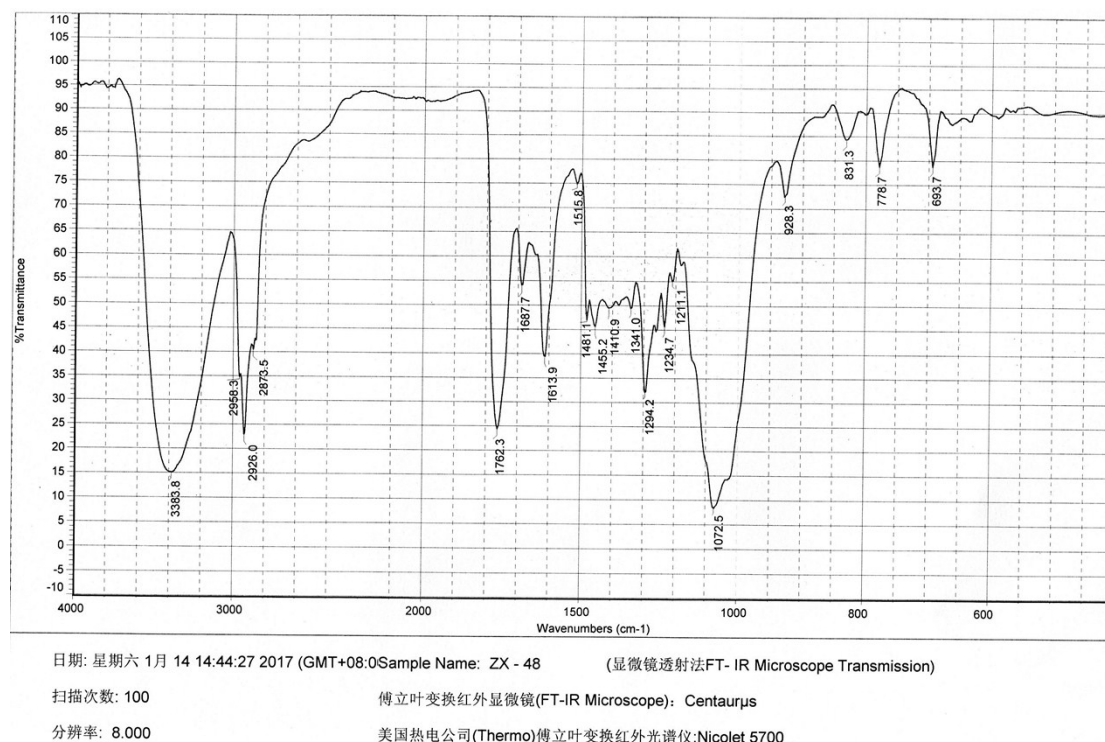


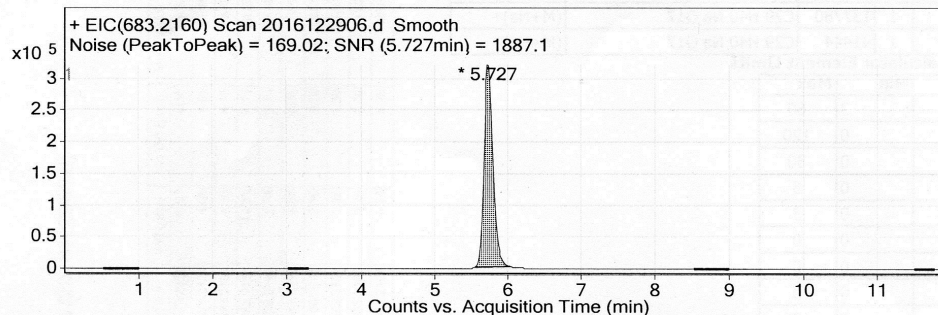
Figure S71. The IR spectrum (KBr) of compound **8**

Qualitative Analysis Report

Data Filename	2016122906.d	Sample Name	ZX-48
Sample Type	Sample	Position	P1-C6
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

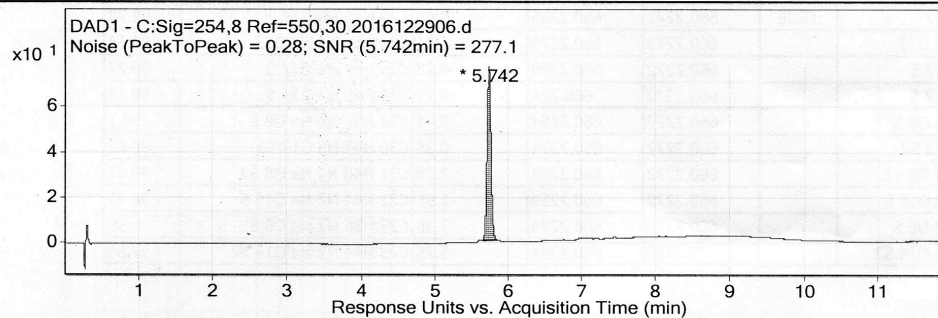
User Chromatograms

Fragmentor Voltage: 150 Collision Energy: 0 Ionization Mode: ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.55	5.727	6.033	318944	2749856	100	1887.1



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.653	5.742	5.851	76.51	277.61	100	277.1

User Spectra

Fragmentor Voltage: 150 Collision Energy: 0 Ionization Mode: Esi

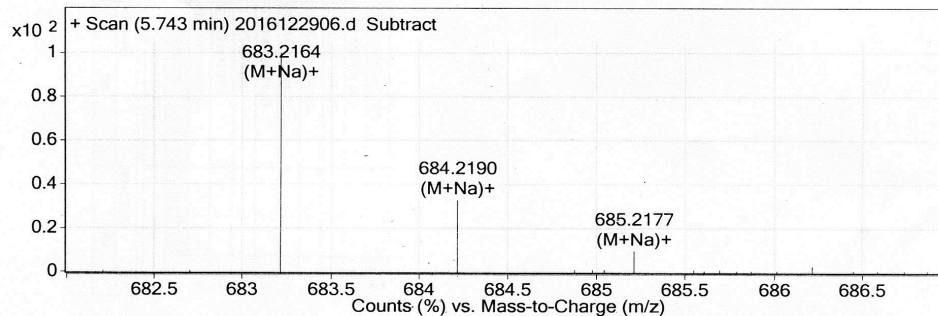


Figure S72. The HR-ESI-MS data of compound **8**

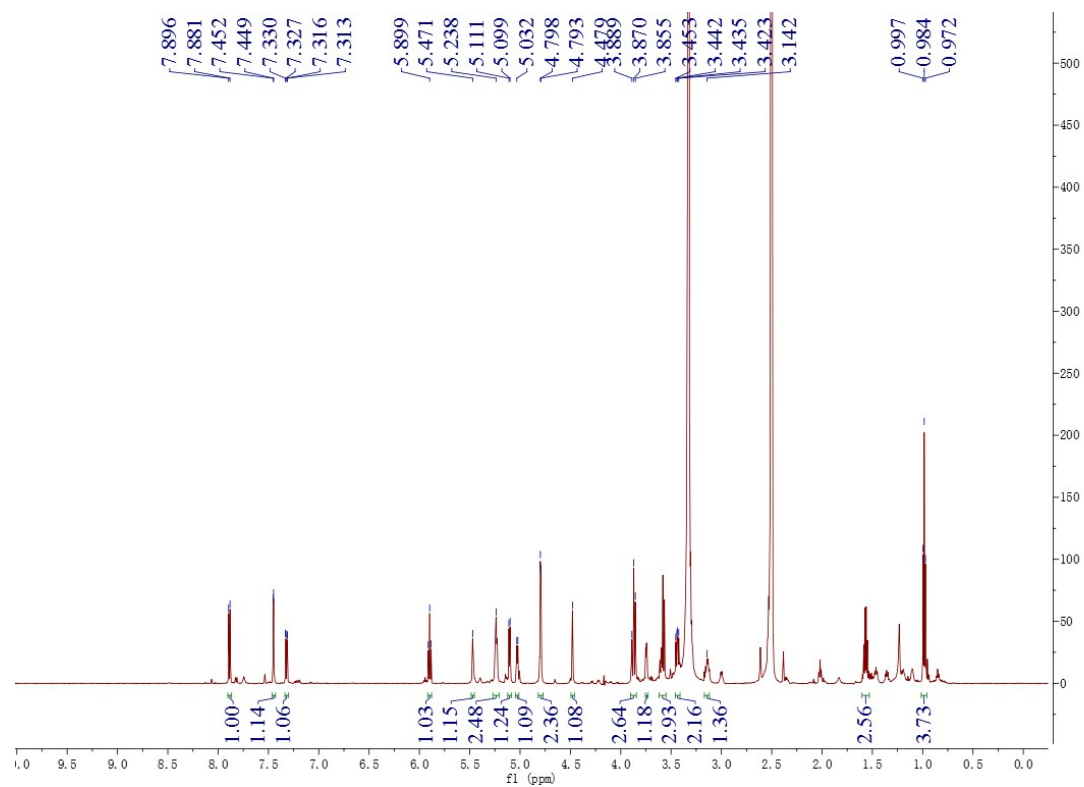


Figure S73. The ¹H NMR spectrum of compound **9** in DMSO-*d*₆

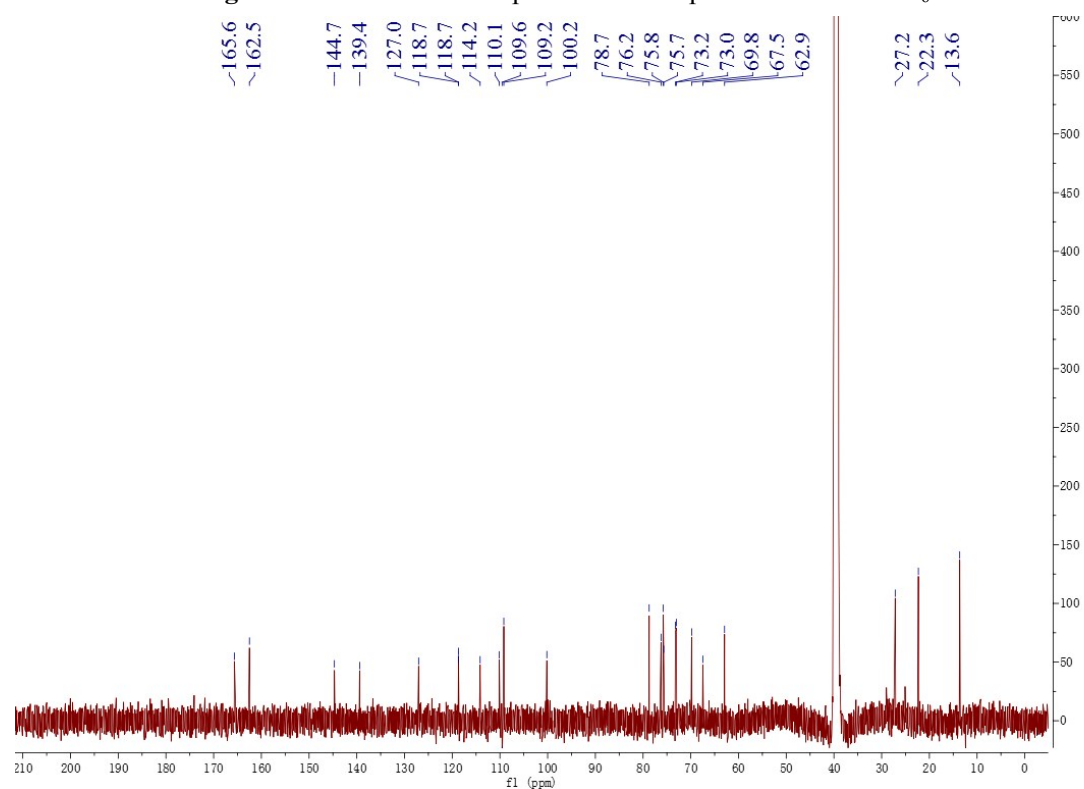


Figure S74. The ¹³C NMR spectrum of compound **9** in DMSO-*d*₆

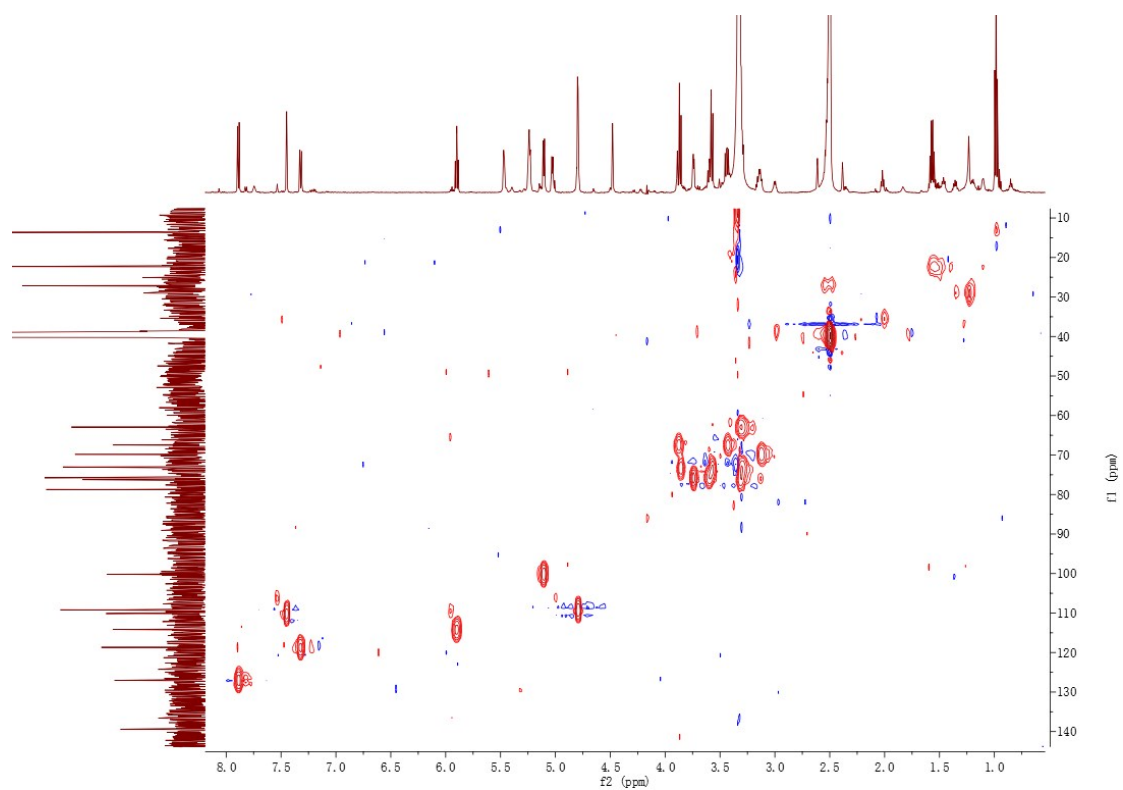


Figure S75. The HSQC spectrum of compound **9** in DMSO- d_6

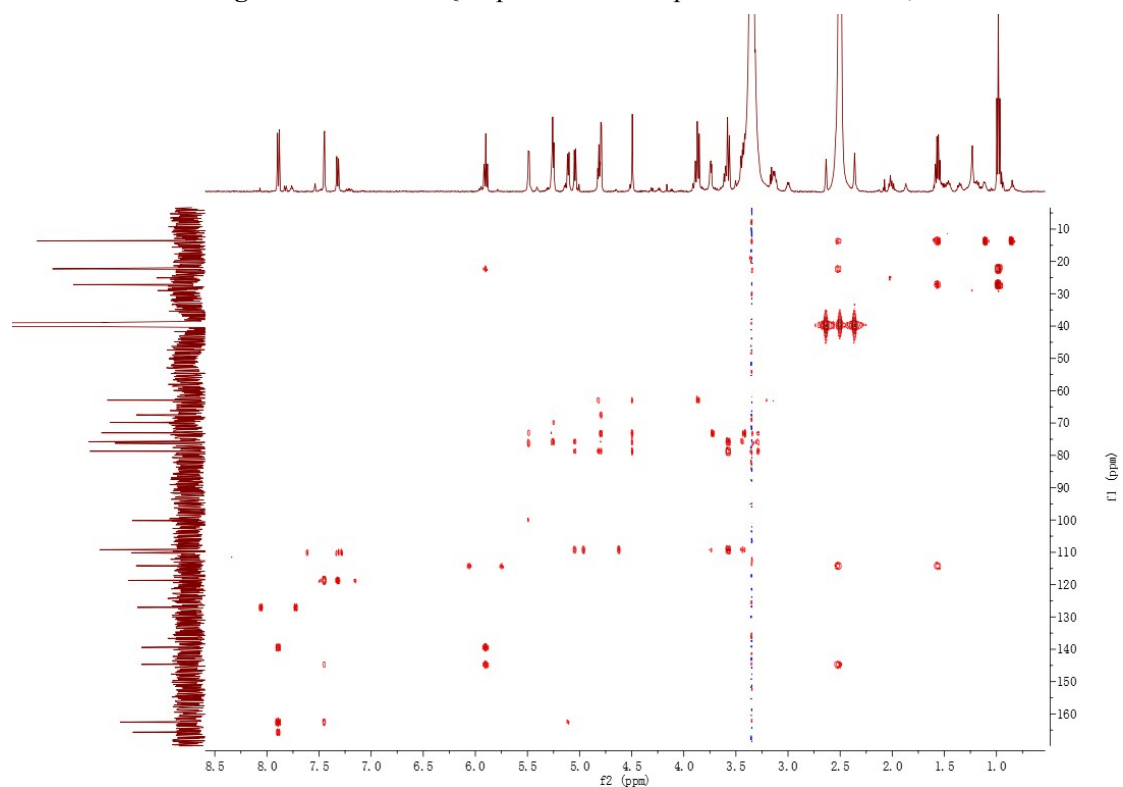


Figure S76. The HMBC spectrum of compound **9** in DMSO- d_6

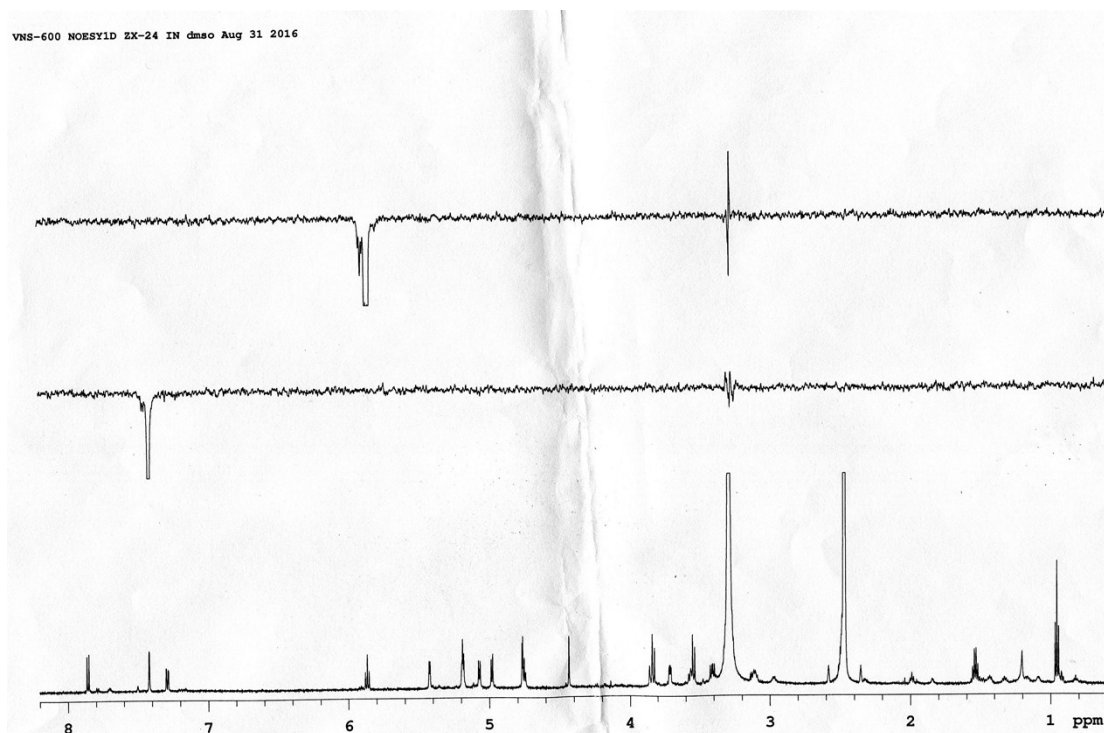


Figure S77. The NOE spectrum of compound **9** in DMSO- d_6

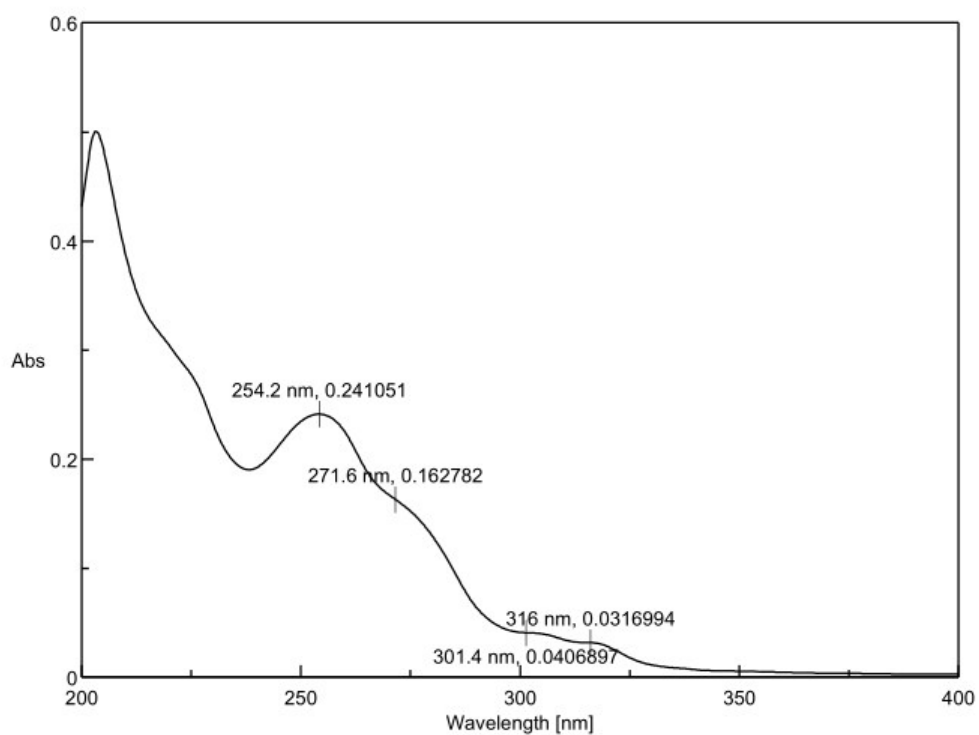


Figure S78. The UV spectrum of compound **9** in MeOH

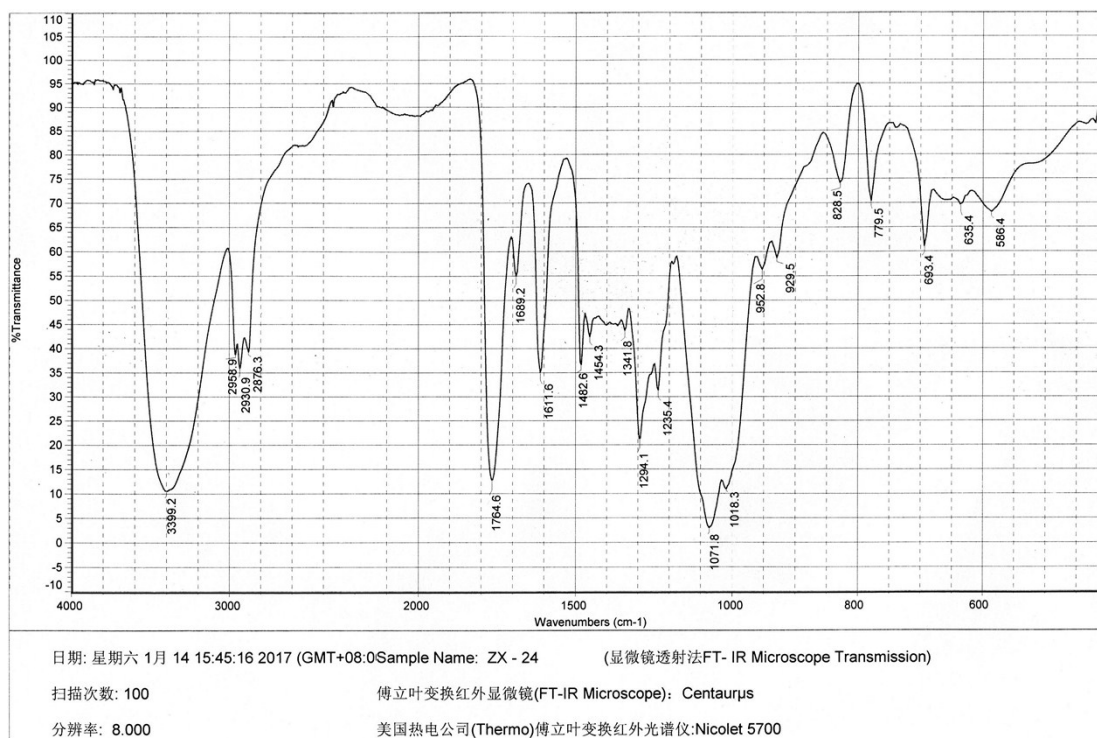
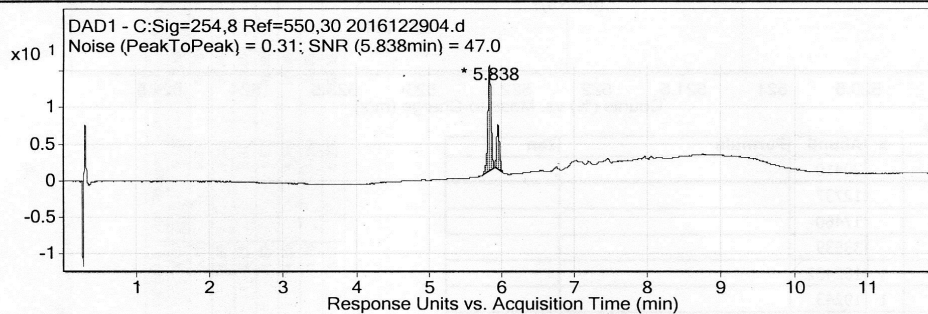


Figure S79. The IR spectrum (KBr) of compound **9**

Qualitative Analysis Report

Data Filename	2016122904.d	Sample Name	ZX-24
Sample Type	Sample	Position	P1-C4
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	Success
DA Method	TEST LCMS.m	Comment	

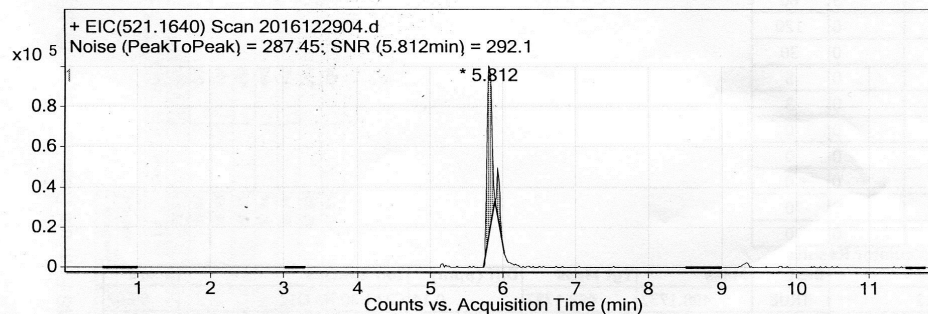
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.748	5.838	5.901	14.43	46.33	100	47
2	5.913	5.955	6.018	6.06	17.44	37.65	19.7

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.732	5.812	5.893	83969	373682	100	292.1
2	5.893	5.925	6.022	22748	67003	17.93	79.1

User Spectra

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

Figure S80. The HR-ESI-MS data of compound **9**

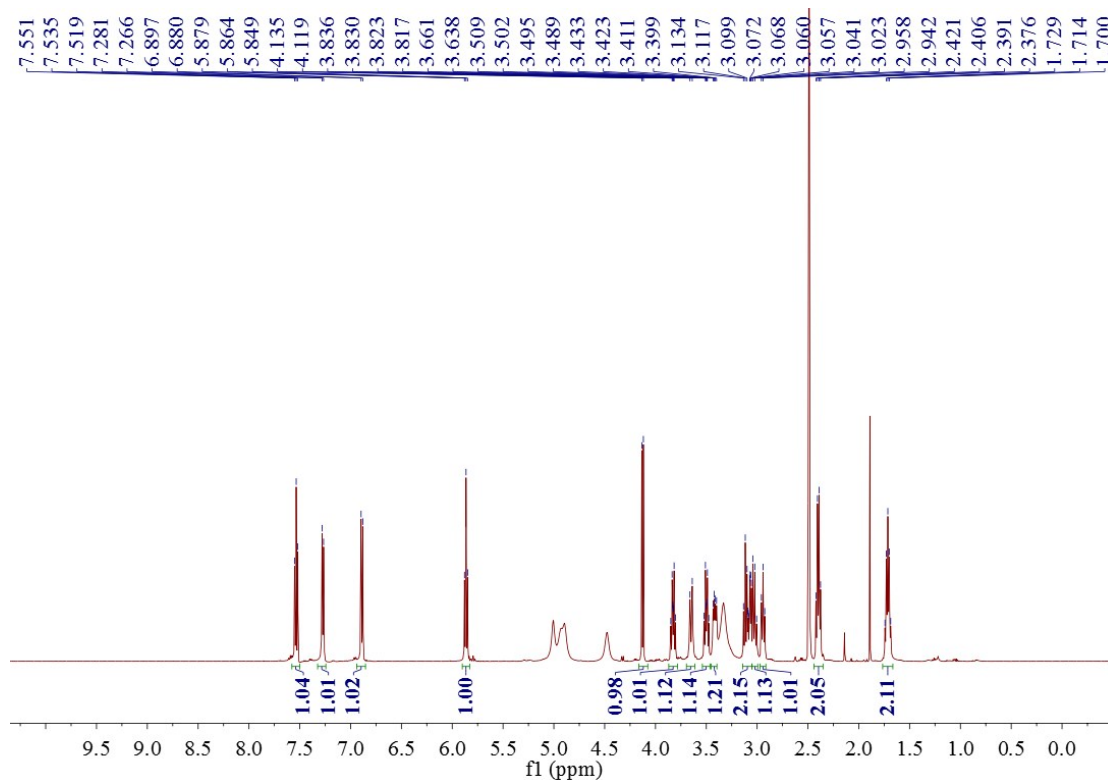


Figure S81. The ^1H NMR spectrum of compound **10** in $\text{DMSO}-d_6$

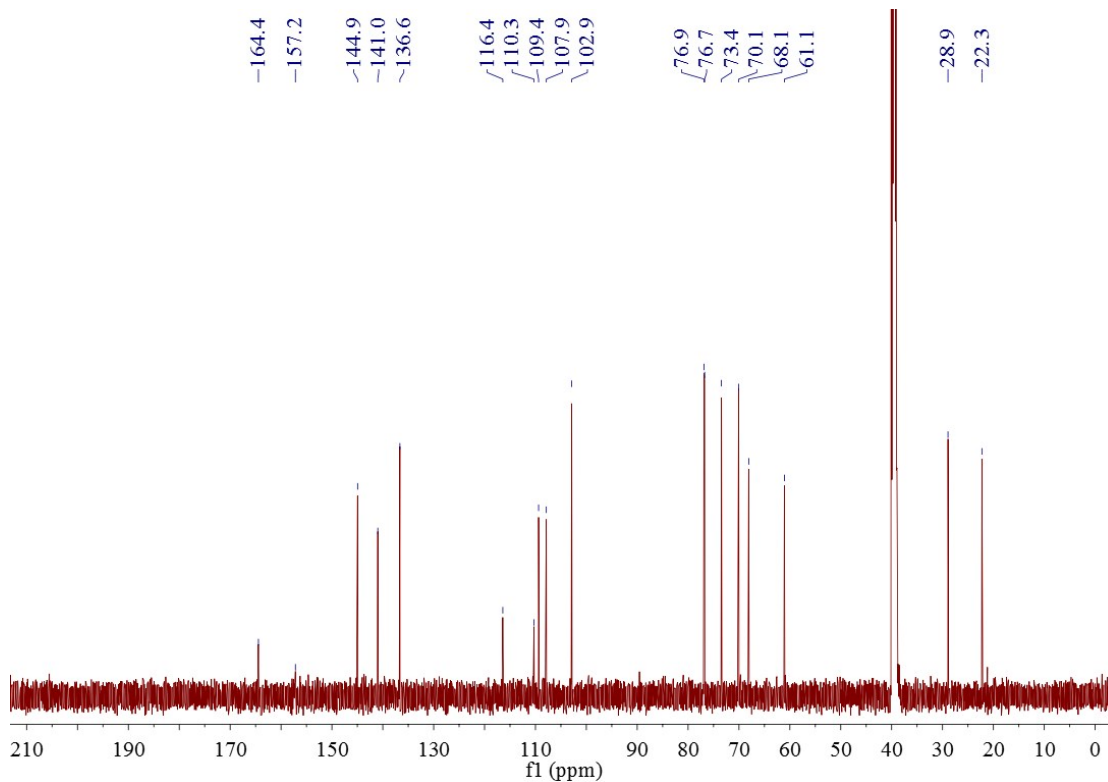


Figure S82. The ^{13}C NMR spectrum of compound **10** in $\text{DMSO}-d_6$

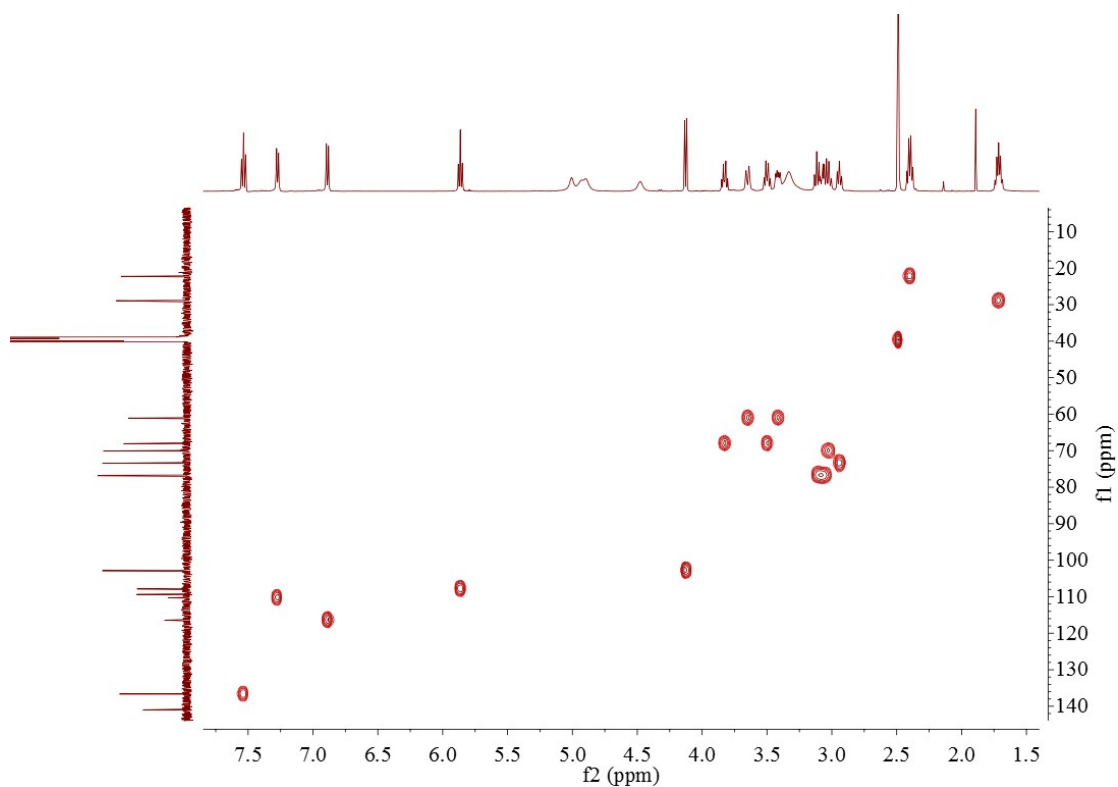


Figure S83. The HSQC spectrum of compound **10** in DMSO- d_6

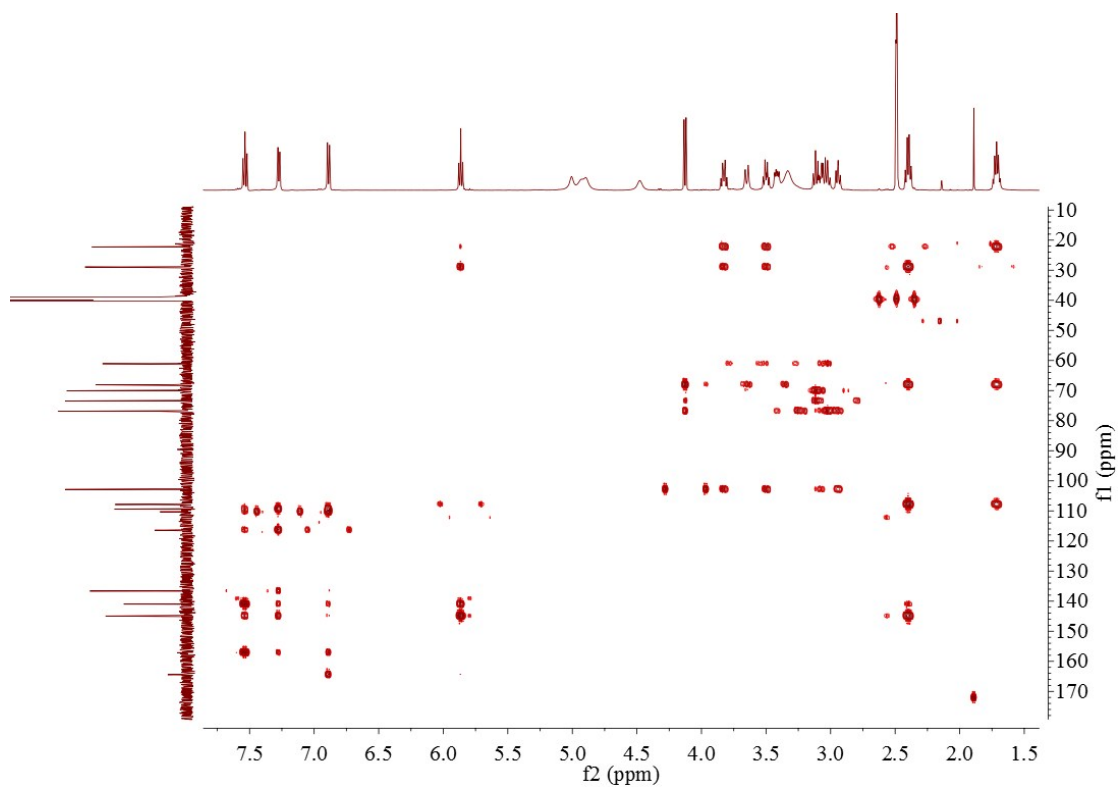


Figure S84. The HMBC spectrum of compound **10** in DMSO- d_6

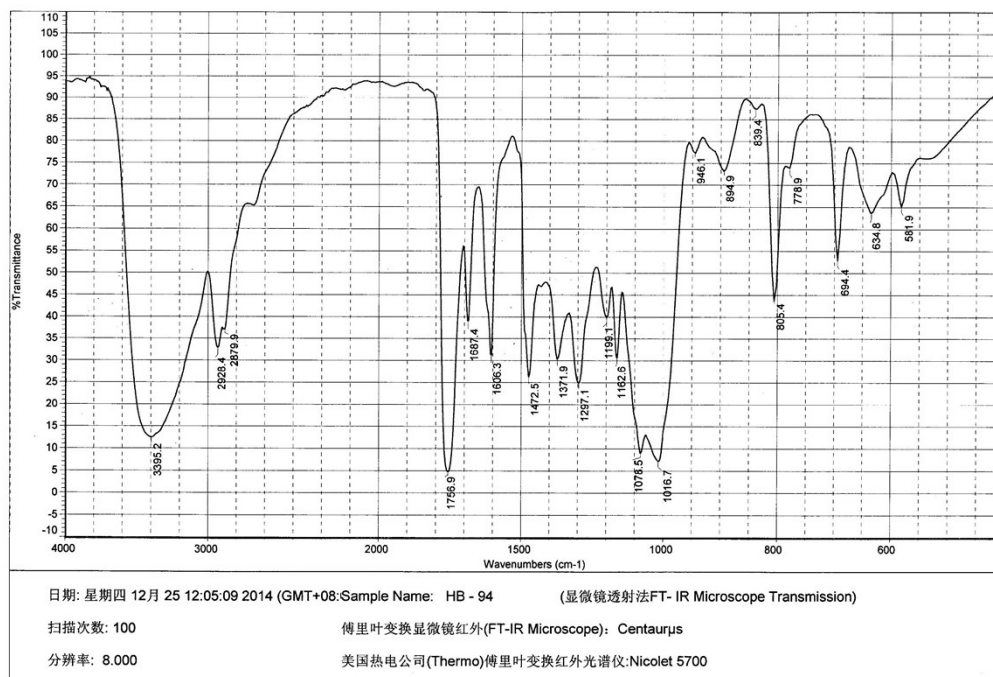


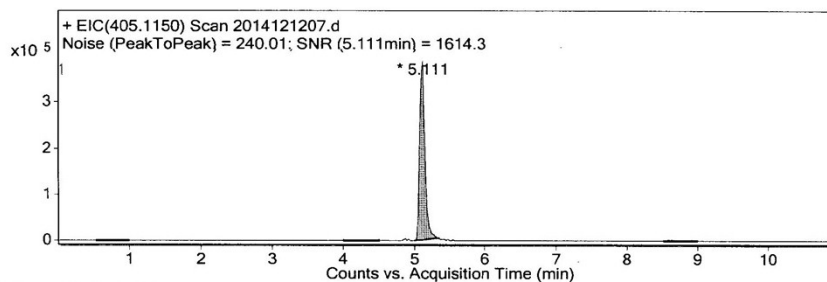
Figure S85. The IR spectrum (KBr) of compound **10**

Qualitative Analysis Report

Data Filename	2014121207.d	Sample Name	HB-94
Sample Type	Sample	Position	P1-C7
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	
DA Method	TEST LCMS.m	Comment	

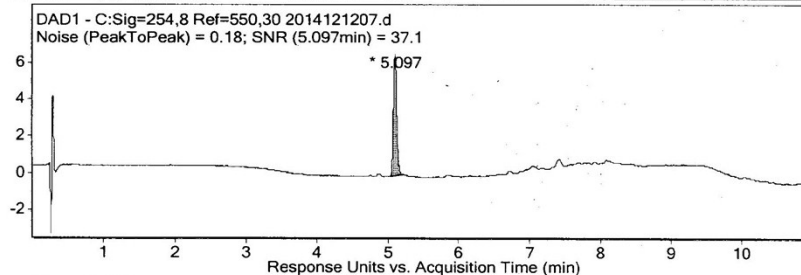
User Chromatograms

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	4.999	5.111	5.353	387449	2018348	100	1614.3



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.027	5.097	5.204	6.61	21.42	100	37.1

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

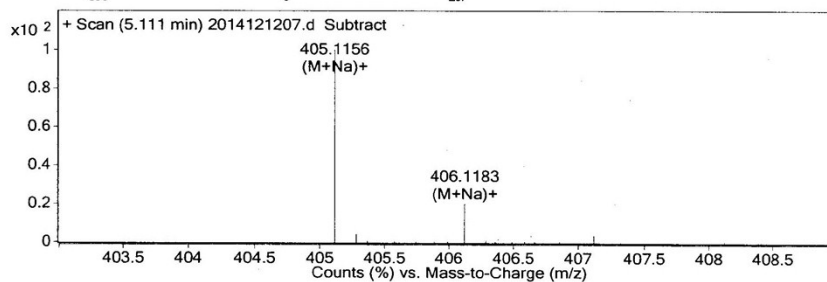


Figure S86. The HR-ESI-MS data of compound 10

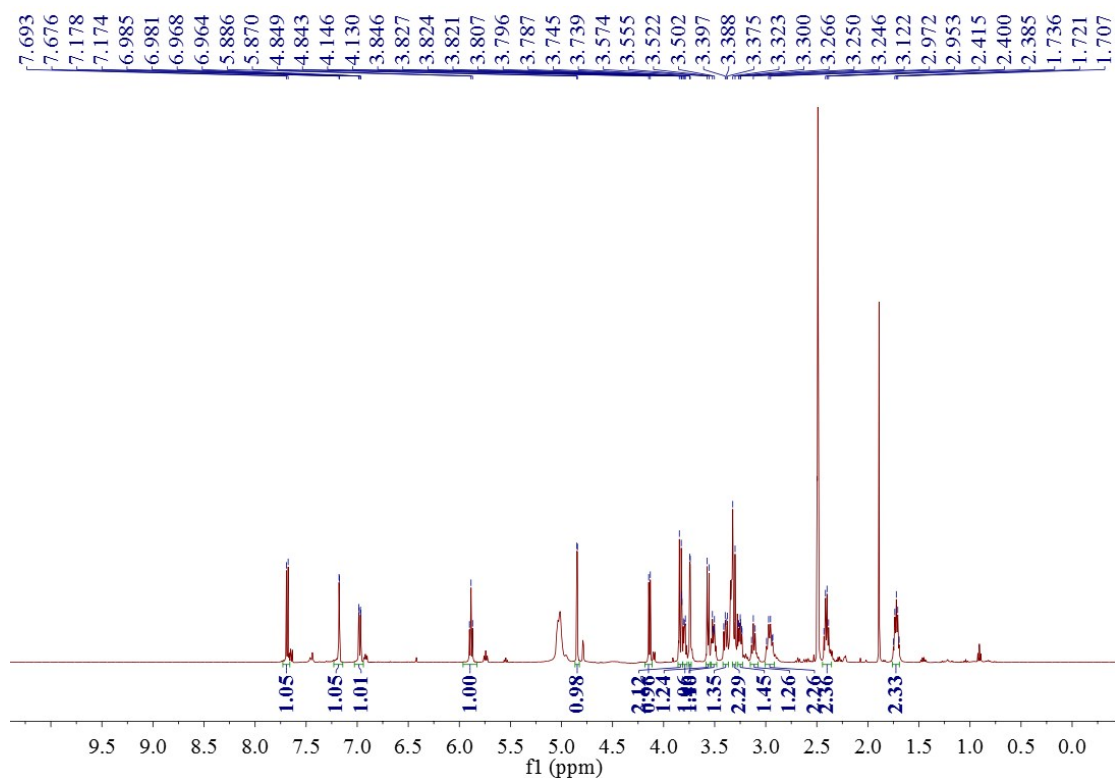


Figure S87. The ^1H NMR spectrum of compound **11** in $\text{DMSO}-d_6$

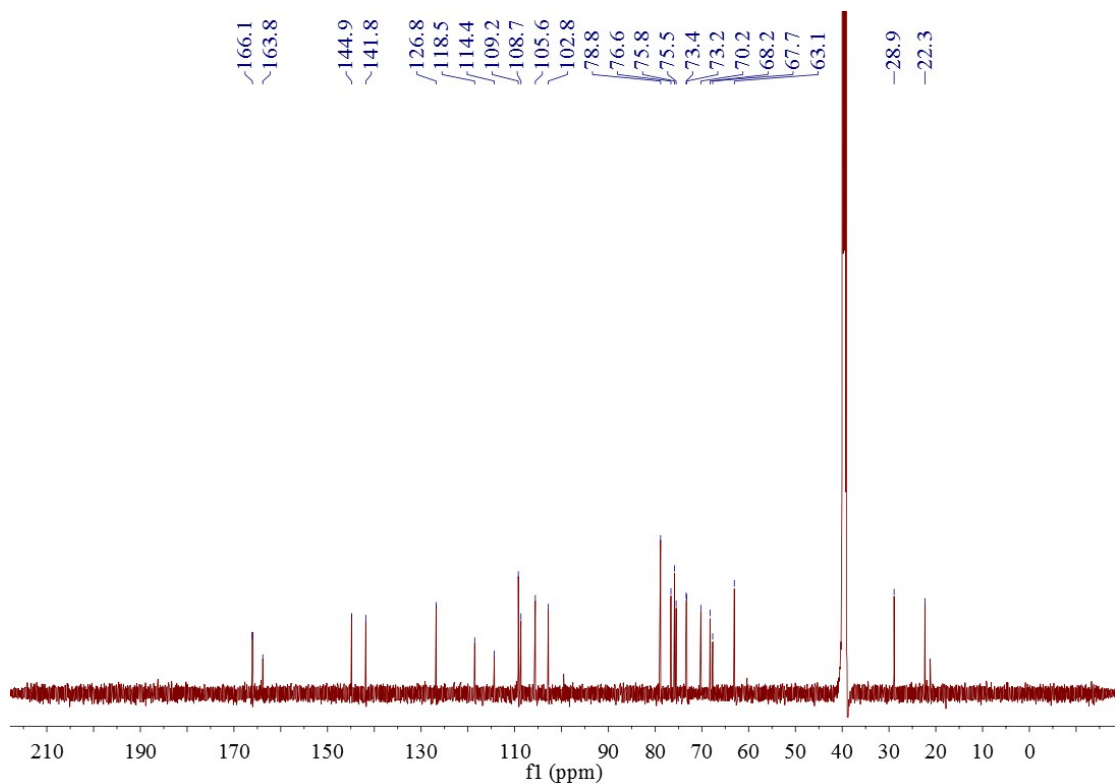


Figure S88. The ^{13}C NMR spectrum of compound **11** in $\text{DMSO}-d_6$

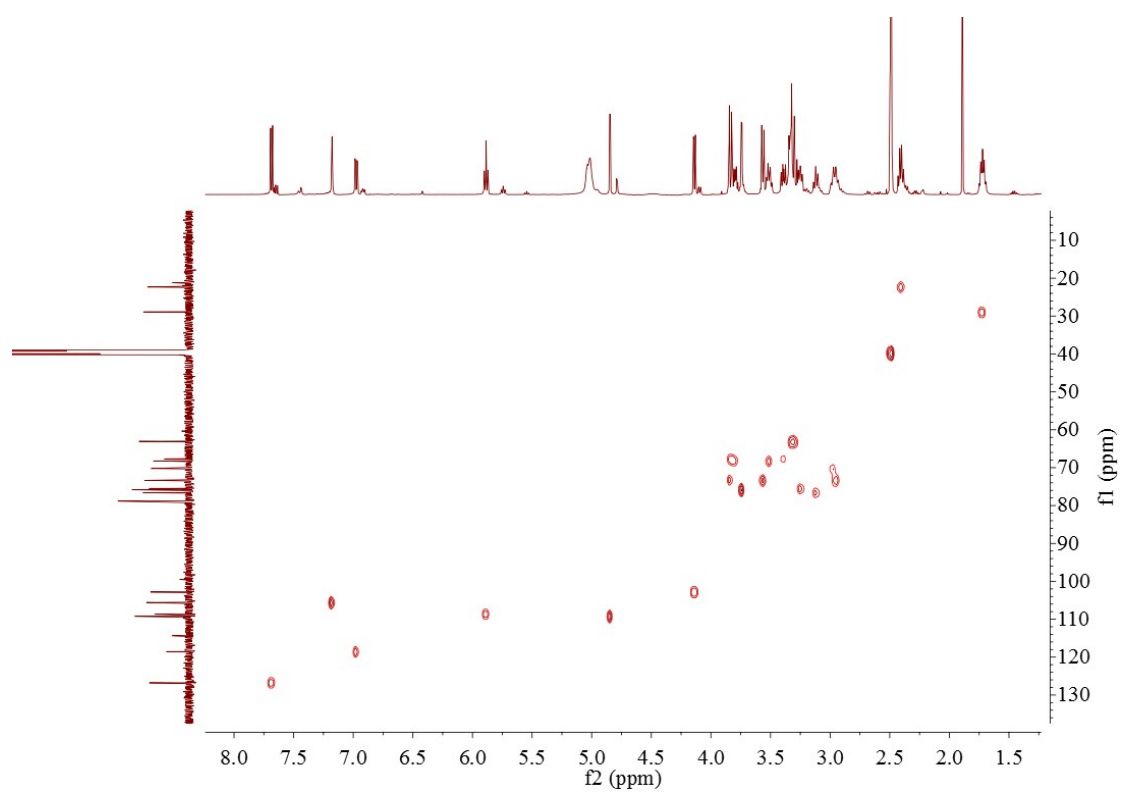


Figure S89. The HSQC spectrum of compound **11** in DMSO- d_6

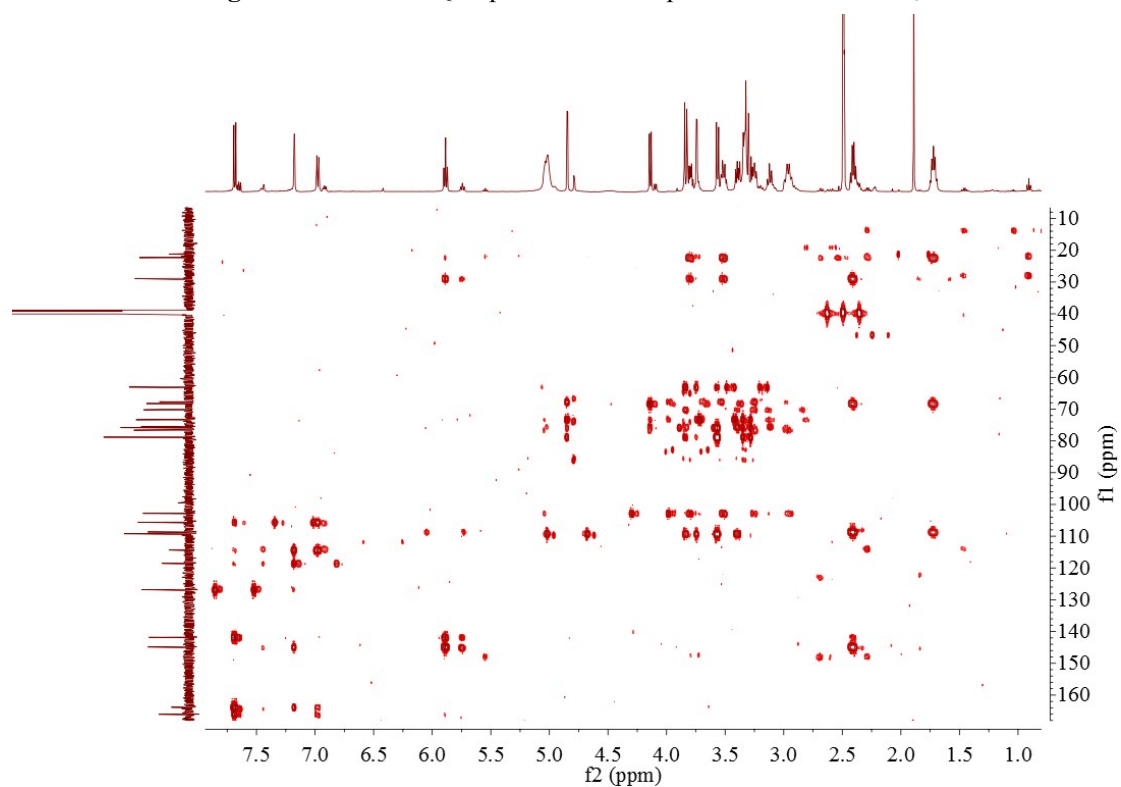


Figure S90. The HMBC spectrum of compound **11** in DMSO- d_6

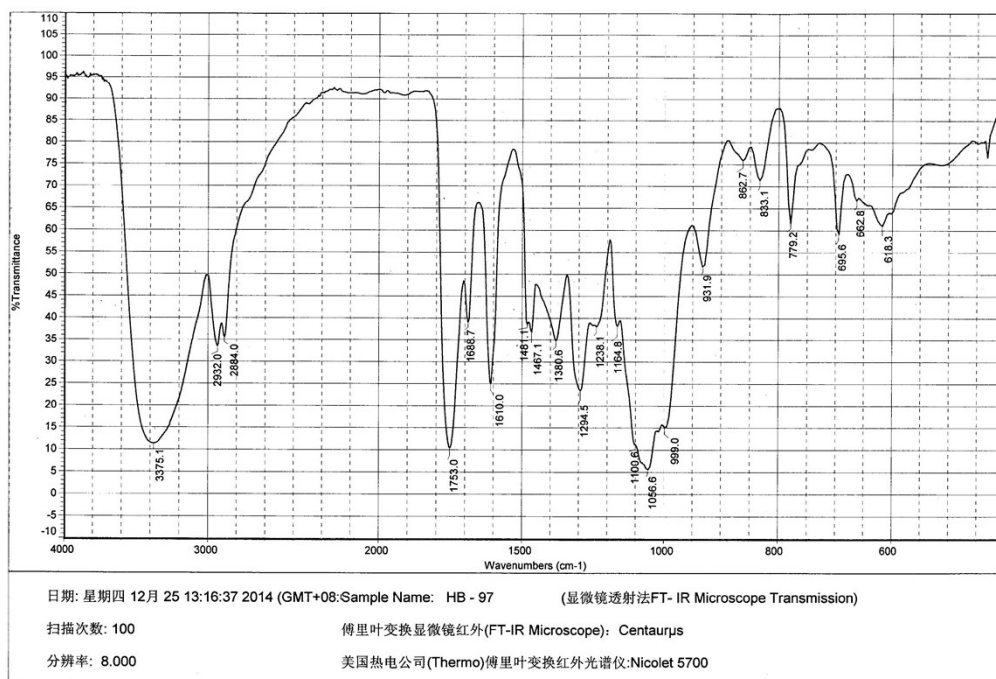
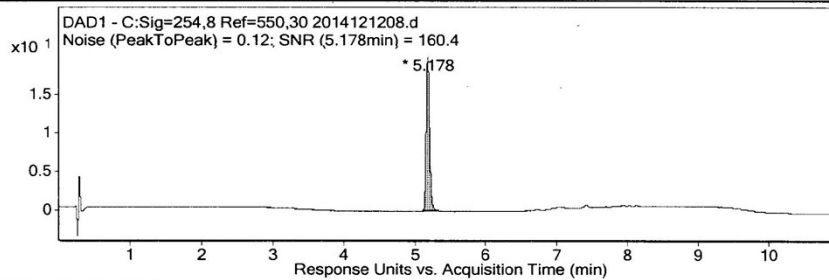


Figure S91. The IR spectrum (KBr) of compound **11**

Qualitative Analysis Report

Data Filename	2014121208.d	Sample Name	HB-97
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	TEST LCMS.m	IRM Calibration Status	
DA Method	TEST LCMS.m	Comment	

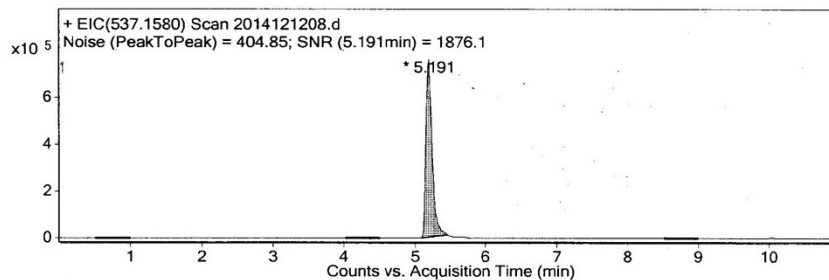
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.098	5.178	5.334	19.97	66.73	100	160.4

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	5.078	5.191	5.465	759520	4699563	100	1876.1

User Spectra

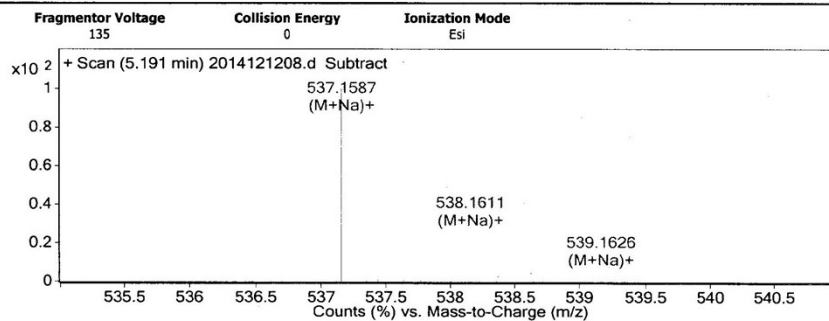


Figure S92. The HR-ESI-MS data of compound 11

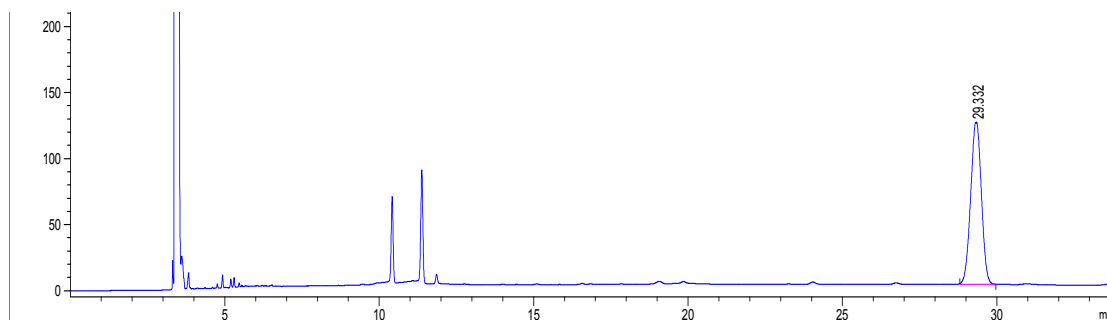


Figure S93. The Gas Chromatographic separation of D-Glc

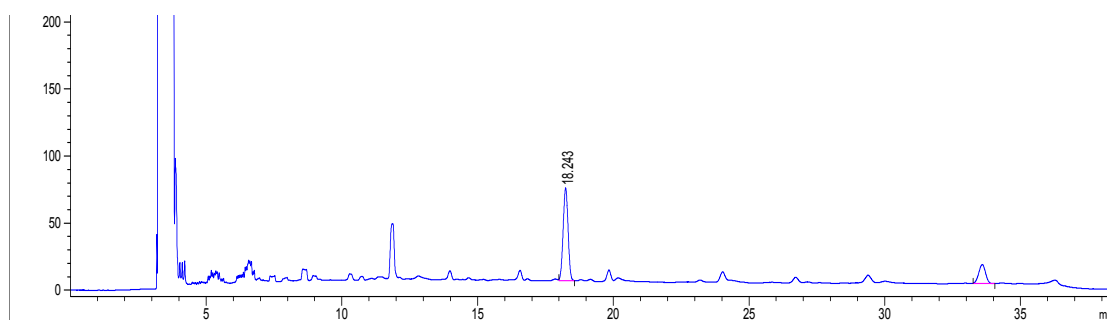


Figure S94. The Gas Chromatographic separation of D-Api

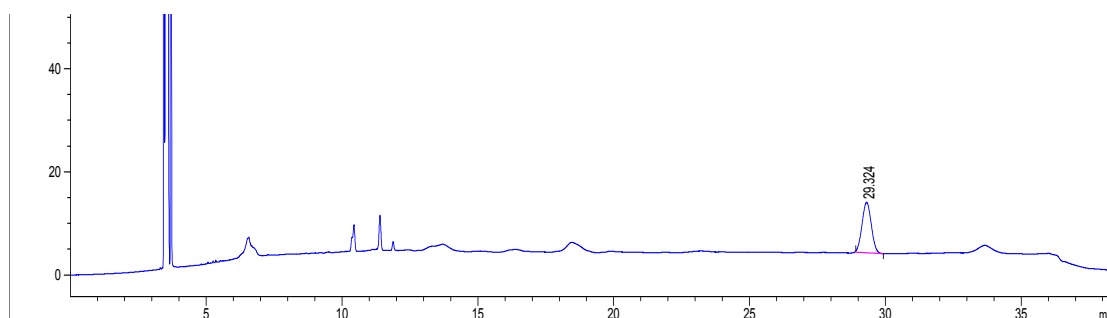


Figure S95. The Gas Chromatographic analyses of sugar moieties of compounds **4** and **10**

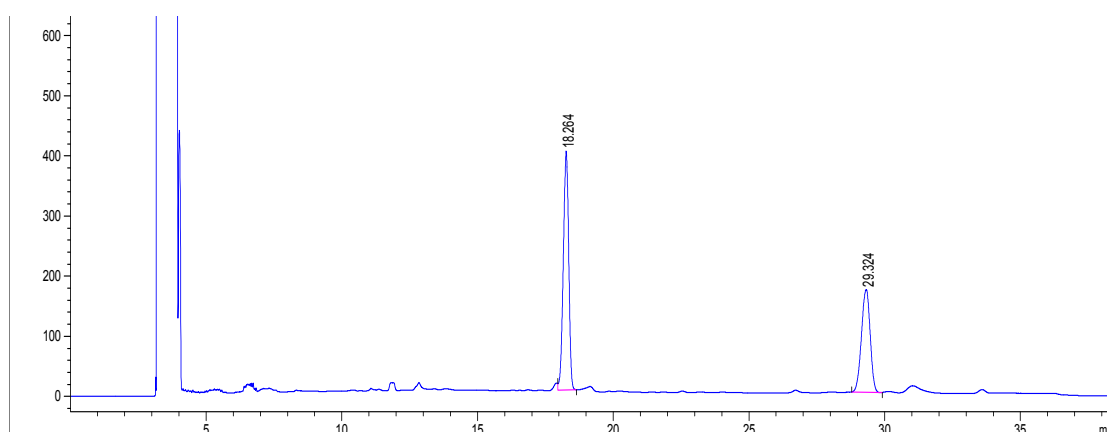


Figure S96. The Gas Chromatographic analyses of sugar moieties of compounds **3**, **5-9** and **11**

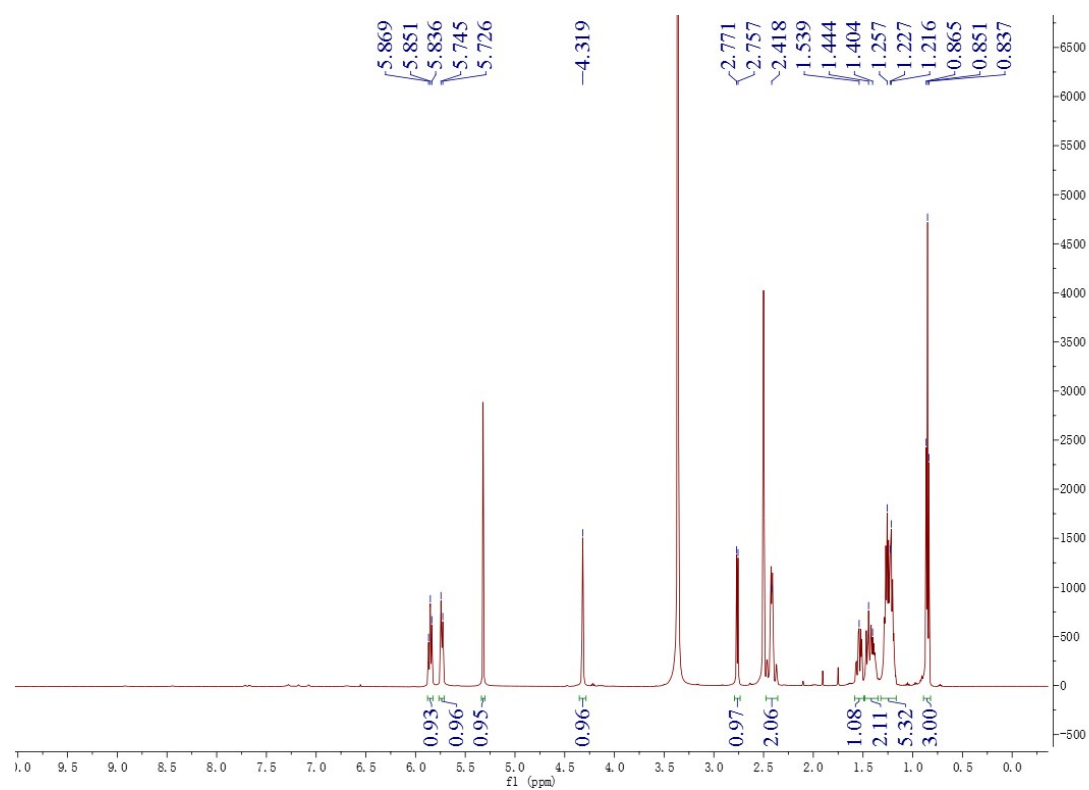


Figure S97. The ¹H NMR spectrum of compound **3a** in DMSO-*d*₆

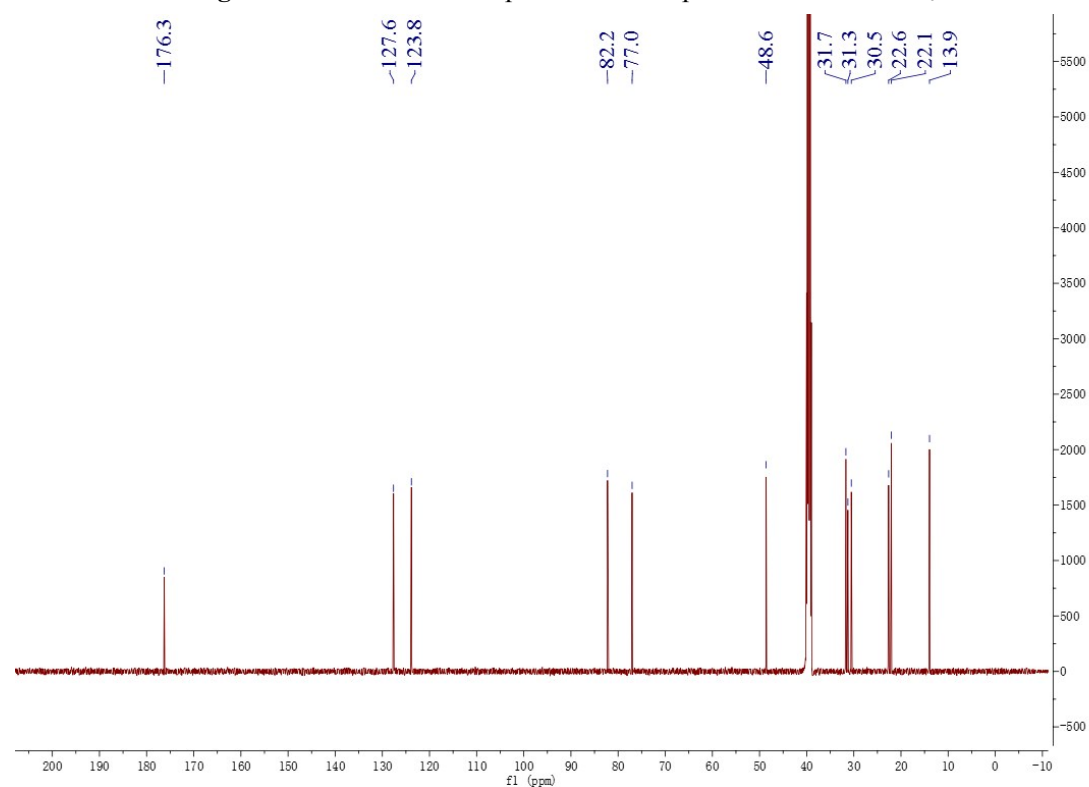


Figure S98. The ¹³C NMR spectrum of compound **3a** in DMSO-*d*₆

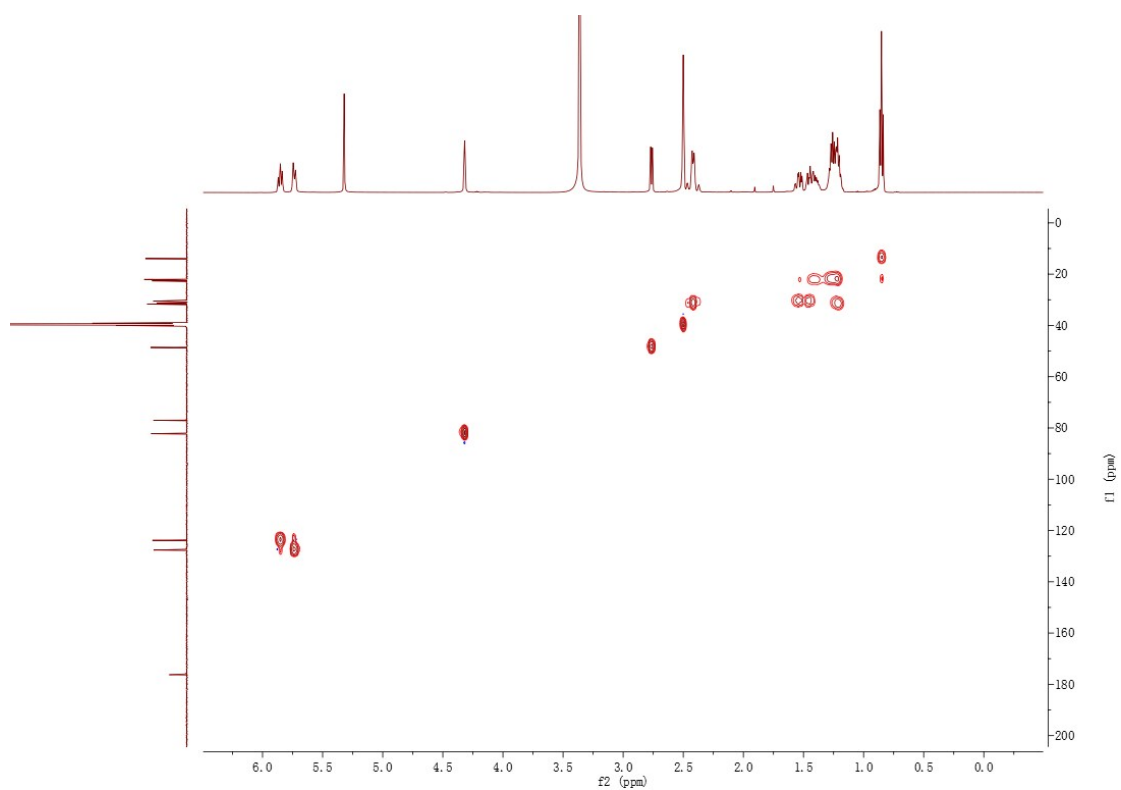


Figure S99. The HSQC spectrum of compound **3a** in DMSO-*d*₆

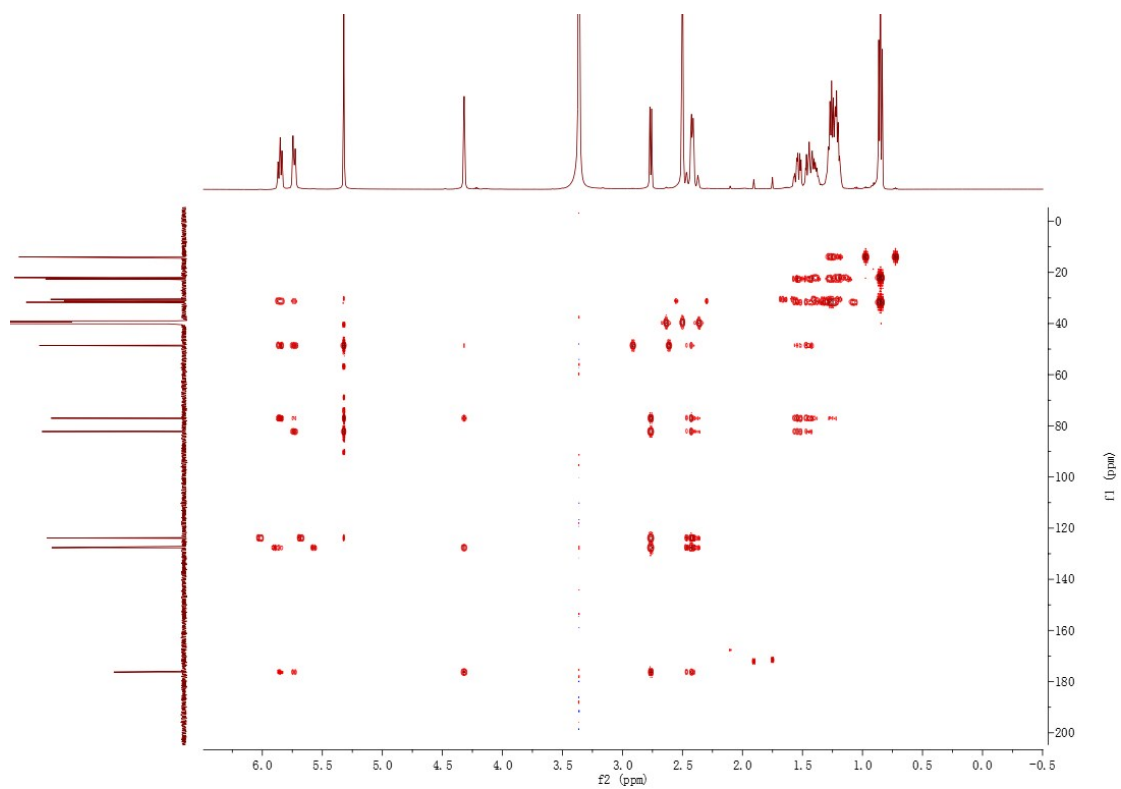


Figure S100. The HMBC spectrum of compound **3a** in DMSO-*d*₆

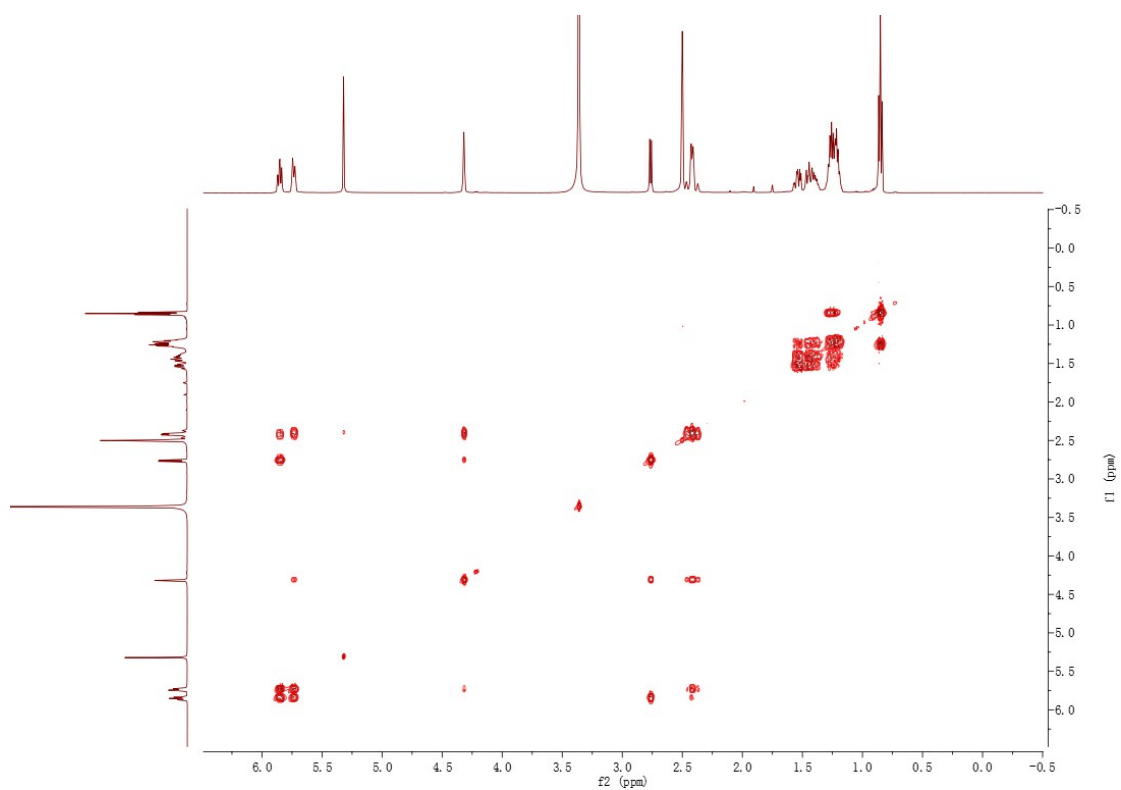


Figure S101. The ^1H - ^1H COSY spectrum of compound **3a** in $\text{DMSO-}d_6$

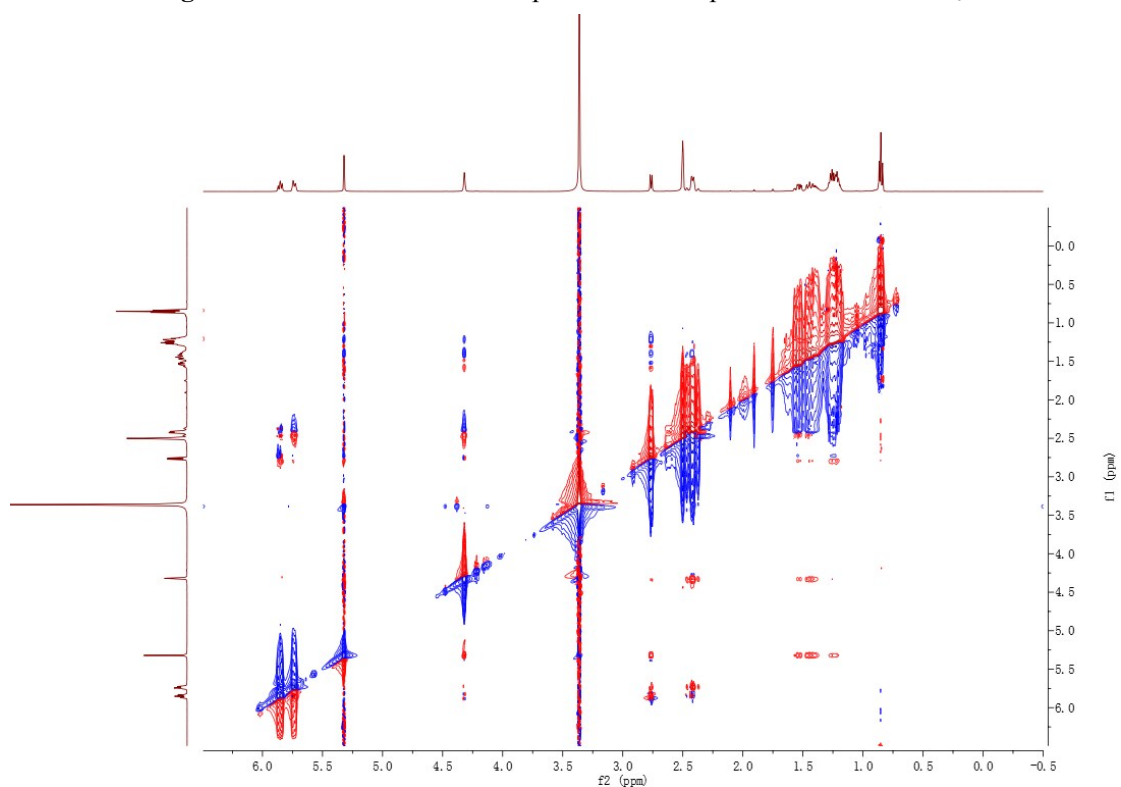


Figure S102. The ROESY spectrum of compound **3a** in $\text{DMSO-}d_6$