

**Eutypellazines A–M, thiodiketopiperazine-type alkaloids from deep
sea derived fungus *Eutypella* sp. MCCC 3A00281**

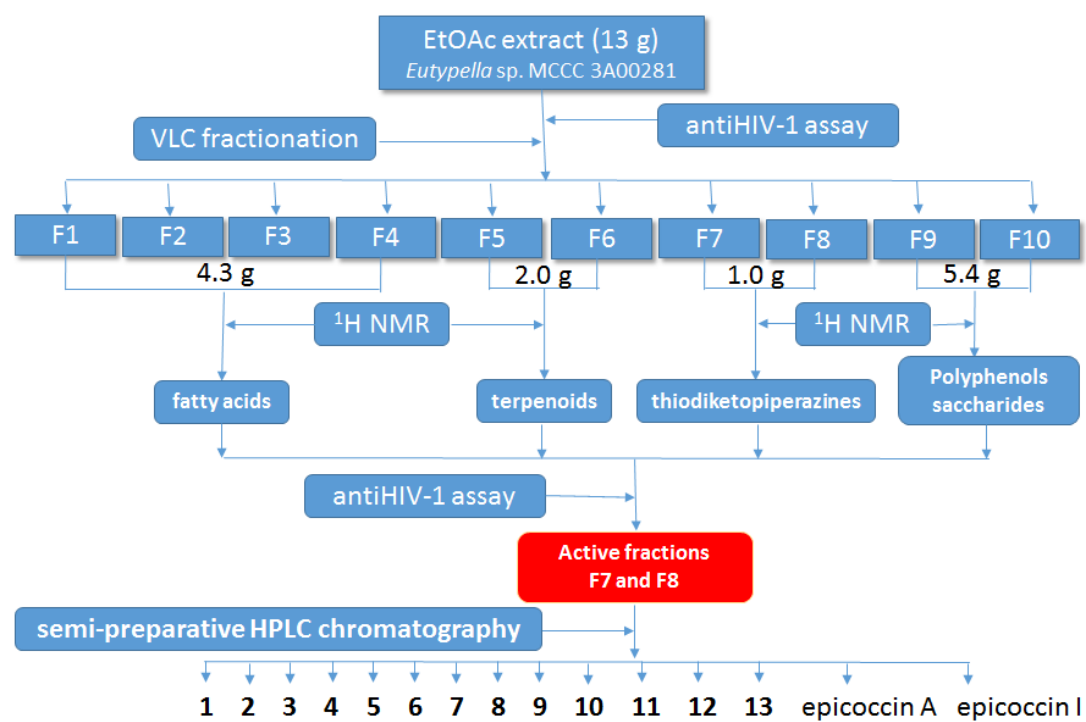
Supporting Information

List of contents

no	Contents
1	Scheme 1. Protocol for the isolation of compounds
2	Fig S1-1 IR Spectrum of Compound 1
3	Fig S1-2 The HRESIMS Data of Compound 1
4	Fig S1-3 The ¹ H NMR Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (400 MHz)
5	Fig S1-4 The APT Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (100 MHz)
6	Fig S1-5 The HSQC Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
7	Fig S1-6 The ¹ H- ¹ H COSY Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (400 MHz)
8	Fig S1-7 The HMBC Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
9	Fig S1-8 The NOESY Spectrum of Compound 1 in DMSO- <i>d</i> ₆ (400 MHz)
10	Fig S1-9 The CD curves of Compounds 1–3
11	Fig S2-1 IR Spectrum of Compound 2
12	Fig S2-2 The HRESIMS Data of Compound 2
13	Fig S2-3 The ¹ H NMR Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (400 MHz)
14	Fig S2-4 The APT Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (100 MHz)
15	Fig S2-5 The HSQC Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
16	Fig S2-6 The ¹ H- ¹ H COSY Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (400 MHz)
17	Fig S2-7 The HMBC Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
18	Fig S2-8 The NOESY Spectrum of Compound 2 in DMSO- <i>d</i> ₆ (400 MHz)
19	Fig S3-1 IR Spectrum of Compound 3
20	Fig S3-2 The HRESIMS Data of Compound 3
21	Fig S3-3 The ¹ H NMR Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (400 MHz)
22	Fig S3-4 The APT Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (100 MHz)
23	Fig S3-5 The HSQC Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
24	Fig S3-6 The ¹ H- ¹ H COSY Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (400 MHz)
25	Fig S3-7 The HMBC Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
26	Fig S3-8 The NOESY Spectrum of Compound 3 in DMSO- <i>d</i> ₆ (400 MHz)
27	Fig S3-9 The CD Spectrum of 3 in methanol
28	Fig S4-1 IR Spectrum of Compound 4
29	Fig S4-2 The HRESIMS Data of Compound 4
30	Fig S4-3 The ¹ H NMR Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (400 MHz)
31	Fig S4-4 The APT Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (100 MHz)
32	Fig S4-5 The HSQC Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
33	Fig S4-6 The ¹ H- ¹ H COSY Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (400 MHz)
34	Fig S4-7 The HMBC Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (400 MHz for ¹ H)
35	Fig S4-8 The NOESY Spectrum of Compound 4 in DMSO- <i>d</i> ₆ (400 MHz)
36	Fig S4-9 ¹ H NMR Spectrum of (<i>R</i>)-MPA ester of 4 (4a) in CDCl ₃ (400 MHz)
37	Fig S4-10 ¹ H NMR Spectrum of (<i>S</i>)-MPA ester of 4 (4b) in CDCl ₃ (400 MHz)
38	Fig S4-11 The CD spectrum of Compound 4
39	Fig S5-1 IR Spectrum of Compound 5
40	Fig S5-2 The HRESIMS Data of Compound 5

41	Fig S5-3 The ^1H NMR Spectrum of Compound 5 in $\text{DMSO}-d_6$ (400 MHz)
42	Fig S5-4 The APT Spectrum of Compound 5 in $\text{DMSO}-d_6$ (100 MHz)
43	Fig S5-5 The HSQC Spectrum of Compound 5 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
44	Fig S5-6 The ^1H - ^1H COSY Spectrum of Compound 5 in $\text{DMSO}-d_6$ (400 MHz)
45	Fig S5-7 The HMBC Spectrum of Compound 5 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
46	Fig S5-8 The NOESY Spectrum of Compound 5 in $\text{DMSO}-d_6$ (400 MHz)
47	Fig S5-9 The CD Spectrum of 5 in methanol
48	Fig S6-1 IR Spectrum of Compound 6
49	Fig S6-2 The HRESIMS Data of Compound 6
50	Fig S6-3 The ^1H NMR Spectrum of Compound 6 in $\text{DMSO}-d_6$ (400 MHz)
51	Fig S6-4 The APT Spectrum of Compound 6 in $\text{DMSO}-d_6$ (100 MHz)
52	Fig S6-5 The HSQC Spectrum of Compound 6 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
53	Fig S6-6 The ^1H - ^1H COSY Spectrum of Compound 6 in $\text{DMSO}-d_6$ (400 MHz)
54	Fig S6-7 The HMBC Spectrum of Compound 6 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
55	Fig S6-8 The NOESY Spectrum of Compound 6 in $\text{DMSO}-d_6$ (400 MHz)
56	Fig S7-1 IR Spectrum of Compound 7
57	Fig S7-2 The HRESIMS Data of Compound 7
58	Fig S7-3 The ^1H NMR Spectrum of Compound 7 in $\text{DMSO}-d_6$ (400 MHz)
59	Fig S7-4 The APT Spectrum of Compound 7 in $\text{DMSO}-d_6$ (100 MHz)
60	Fig S7-5 The HSQC Spectrum of Compound 7 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
61	Fig S7-6 The ^1H - ^1H COSY Spectrum of Compound 7 in $\text{DMSO}-d_6$ (400 MHz)
62	Fig S7-7 The HMBC Spectrum of Compound 7 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
63	Fig S7-8 The NOESY Spectrum of Compound 7 in $\text{DMSO}-d_6$ (400 MHz)
64	Fig S8-1 IR Spectrum of Compound 8
65	Fig S8-2 The HRESIMS Data of Compound 8
66	Fig S8-3 The ^1H NMR Spectrum of Compound 8 in $\text{DMSO}-d_6$ (400 MHz)
67	Fig S8-4 The APT Spectrum of Compound 8 in $\text{DMSO}-d_6$ (100 MHz)
68	Fig S8-5 The HSQC Spectrum of Compound 8 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
69	Fig S8-6 The ^1H - ^1H COSY Spectrum of Compound 8 in $\text{DMSO}-d_6$ (400 MHz)
70	Fig S8-7 The HMBC Spectrum of Compound 8 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
71	Fig S8-8 The NOESY Spectrum of Compound 8 in $\text{DMSO}-d_6$ (400 MHz)
72	Fig S9-1 IR Spectrum of Compound 9
73	Fig S9-2 The HRESIMS Data of Compound 9
74	Fig S9-3 The ^1H NMR Spectrum of Compound 9 in $\text{DMSO}-d_6$ (400 MHz)
75	Fig S9-4 The APT Spectrum of Compound 9 in $\text{DMSO}-d_6$ (100 MHz)
76	Fig S9-5 The HSQC Spectrum of Compound 9 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
77	Fig S9-6 The ^1H - ^1H COSY Spectrum of Compound 9 in $\text{DMSO}-d_6$ (400 MHz)
78	Fig S9-7 The HMBC Spectrum of Compound 9 in $\text{DMSO}-d_6$ (400 MHz for ^1H)
79	Fig S10-1 IR Spectrum of Compound 10
80	Fig S10-2 The HRESIMS Data of Compound 10
81	Fig S10-3 The ^1H NMR Spectrum of Compound 10 in $\text{DMSO}-d_6$ (400 MHz)
82	Fig S10-4 The APT Spectrum of Compound 10 in $\text{DMSO}-d_6$ (100 MHz)
83	Fig S10-5 The HSQC Spectrum of Compound 10 in $\text{DMSO}-d_6$ (400 MHz for ^1H)

84	Fig S10-6 The ^1H - ^1H COSY Spectrum of Compound 10 in DMSO- d_6 (400 MHz)
85	Fig S10-7 The HMBC Spectrum of Compound 10 in DMSO- d_6 (400 MHz for ^1H)
86	Fig S11-1 IR Spectrum of Compound 11
87	Fig S11-2 The HRESIMS Data of Compound 11
88	Fig S11-3 The ^1H NMR Spectrum of Compound 11 in DMSO- d_6 (400 MHz)
89	Fig S11-4 The APT Spectrum of Compound 11 in DMSO- d_6 (100 MHz)
90	Fig S11-5 The HSQC Spectrum of Compound 11 in DMSO- d_6 (400 MHz for ^1H)
91	Fig S11-6 The ^1H - ^1H COSY Spectrum of Compound 11 in DMSO- d_6 (400 MHz)
92	Fig S11-7 The HMBC Spectrum of Compound 11 in DMSO- d_6 (400 MHz for ^1H)
93	Fig S12-1 IR Spectrum of Compound 12
94	Fig S12-2 The HRESIMS Data of Compound 12
95	Fig S12-3 The ^1H NMR Spectrum of Compound 12 in DMSO- d_6 (400 MHz)
96	Fig S12-4 The APT Spectrum of Compound 12 in DMSO- d_6 (100 MHz)
97	Fig S12-5 The HSQC Spectrum of Compound 12 in DMSO- d_6 (400 MHz for ^1H)
98	Fig S12-6 The ^1H - ^1H COSY Spectrum of Compound 12 in DMSO- d_6 (400 MHz)
99	Fig S12-7 The HMBC Spectrum of Compound 12 in DMSO- d_6 (400 MHz for ^1H)
100	Fig S13-1 IR Spectrum of Compound 13
101	Fig S13-2 The HRESIMS Data of Compound 13
102	Fig S13-3 The ^1H NMR Spectrum of Compound 13 in DMSO- d_6 (400 MHz)
103	Fig S13-4 The APT Spectrum of Compound 13 in DMSO- d_6 (100 MHz)
104	Fig S13-5 The HSQC Spectrum of Compound 13 in DMSO- d_6 (400 MHz for ^1H)
105	Fig S13-6 The ^1H - ^1H COSY Spectrum of Compound 13 in DMSO- d_6 (400 MHz)
106	Fig S13-7 The HMBC Spectrum of Compound 13 in DMSO- d_6 (400 MHz for ^1H)



Scheme 1. Protocol for the isolation of compounds

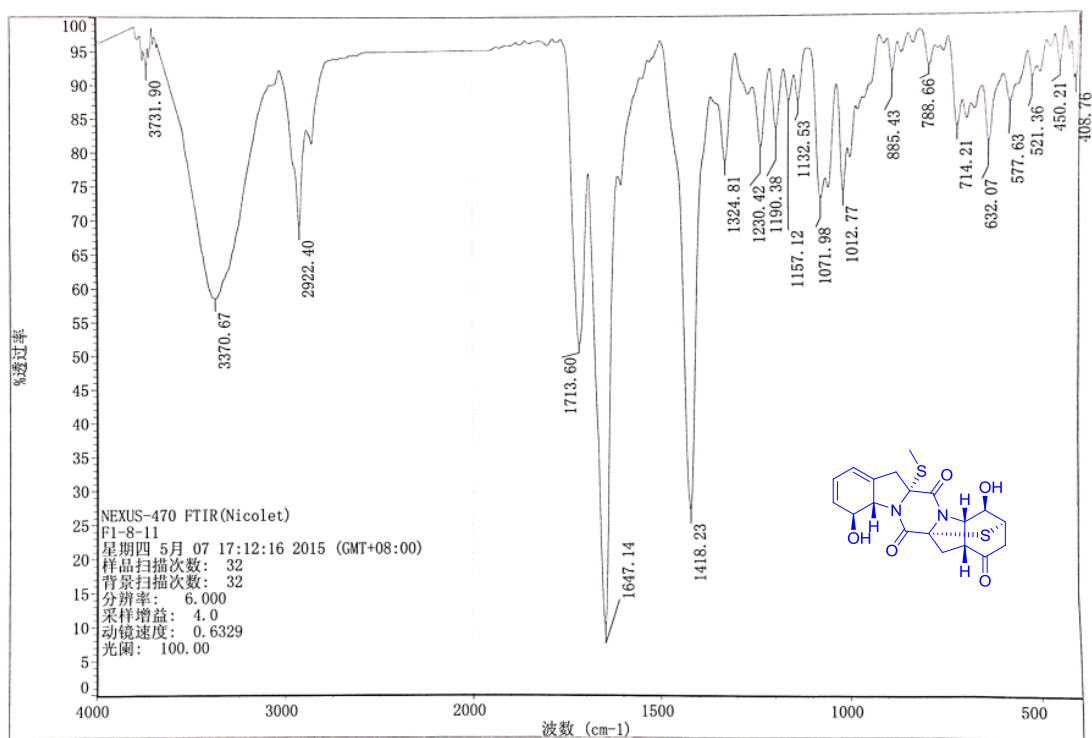


Fig S1-1 IR Spectrum of Compound 1

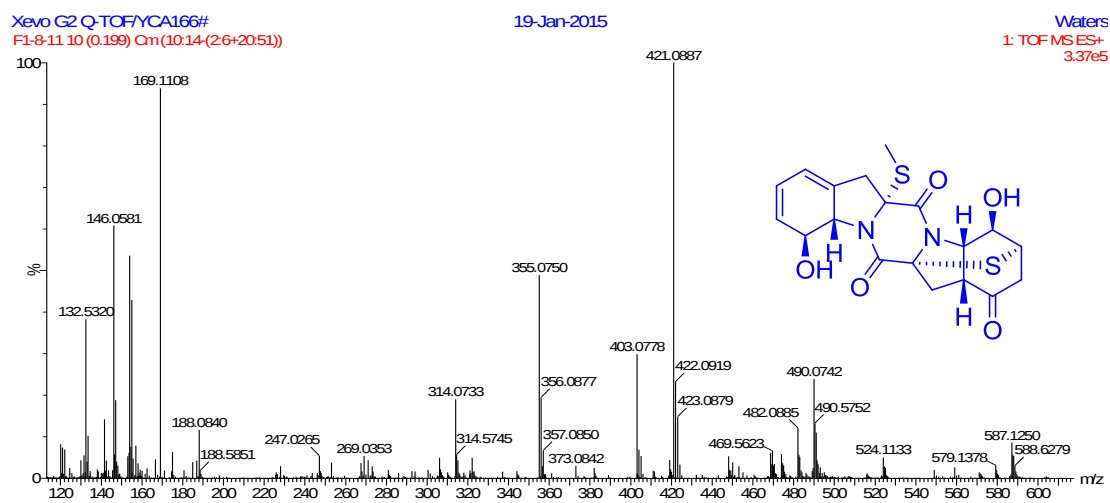


Fig S1-2 HRESIMS Data of Compound 1

F1-8-11 1H DMSO 400 MHz

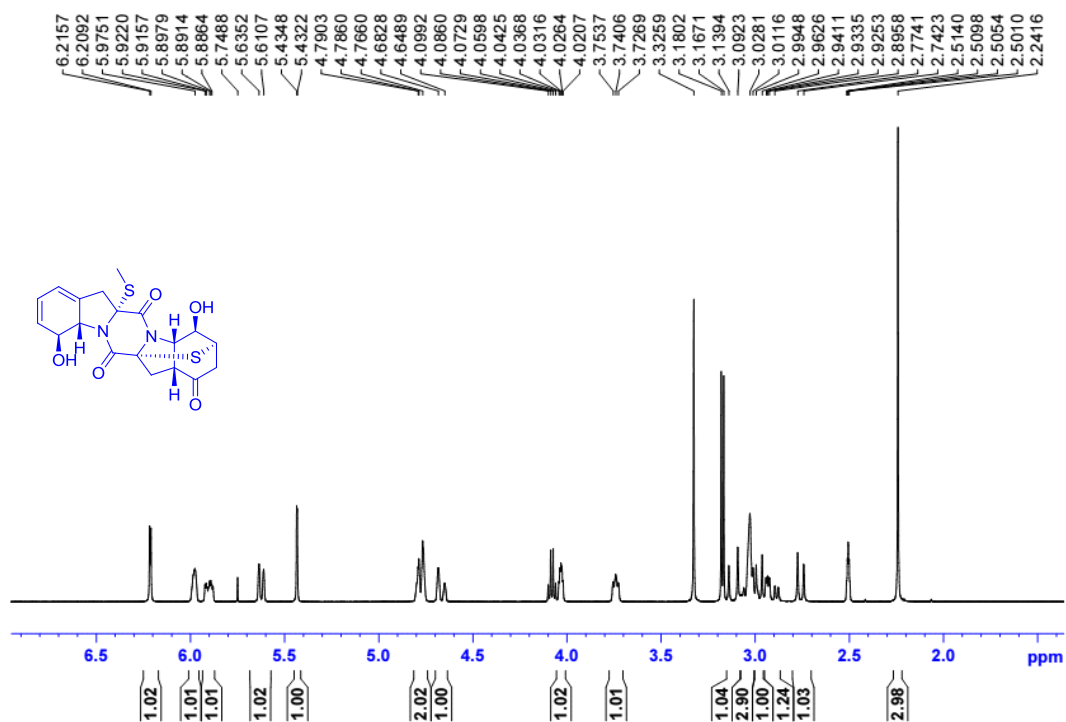


Fig S1-3 The ¹H NMR Spectrum of Compound 1

F1-8-11 APT DMSO 100 MHz

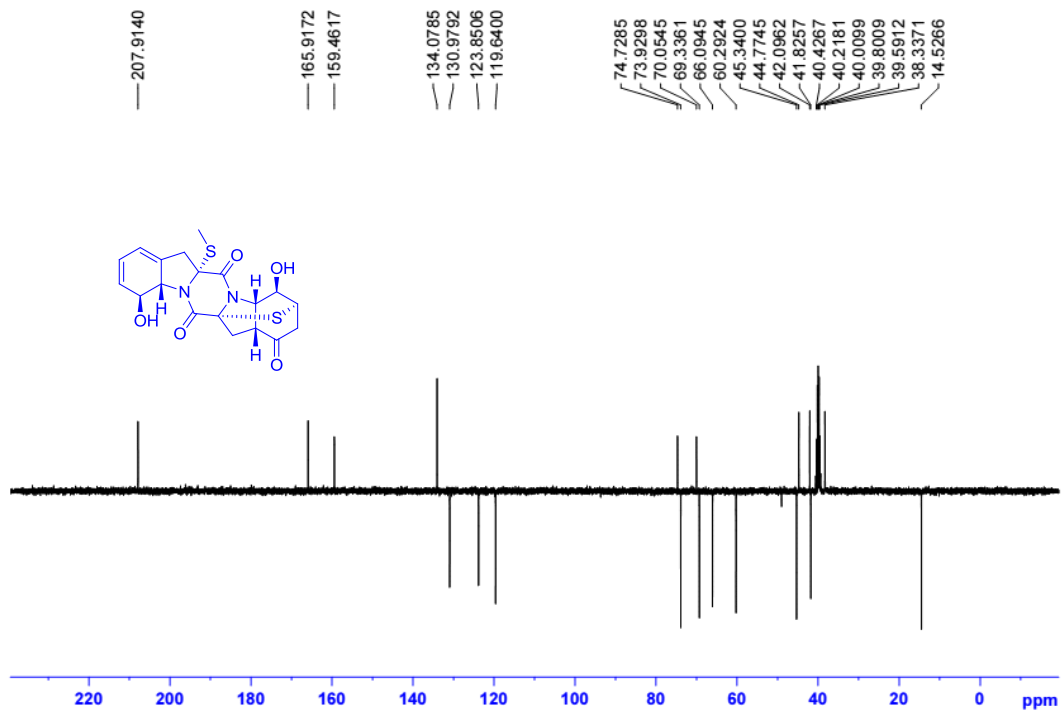


Fig S1-4 The APT Spectrum of Compound 1

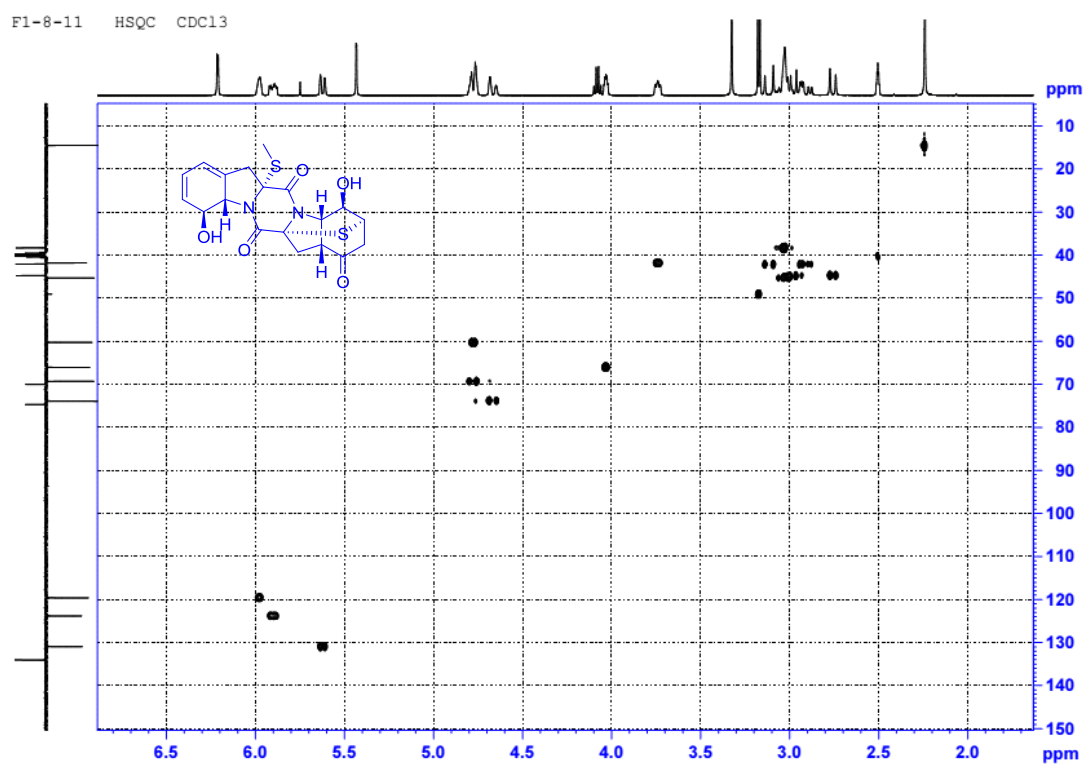


Fig S1-5 The HSQC Spectrum of Compound 1

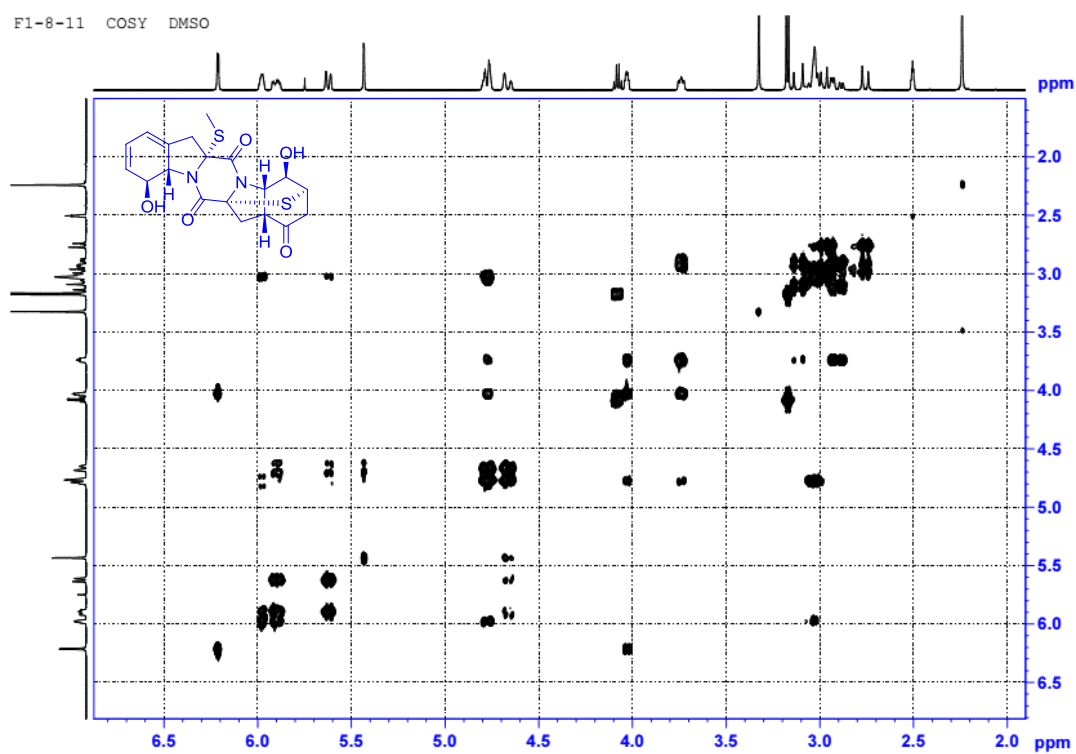


Fig S1-6 The ^1H - ^1H COSY Spectrum of Compound 1

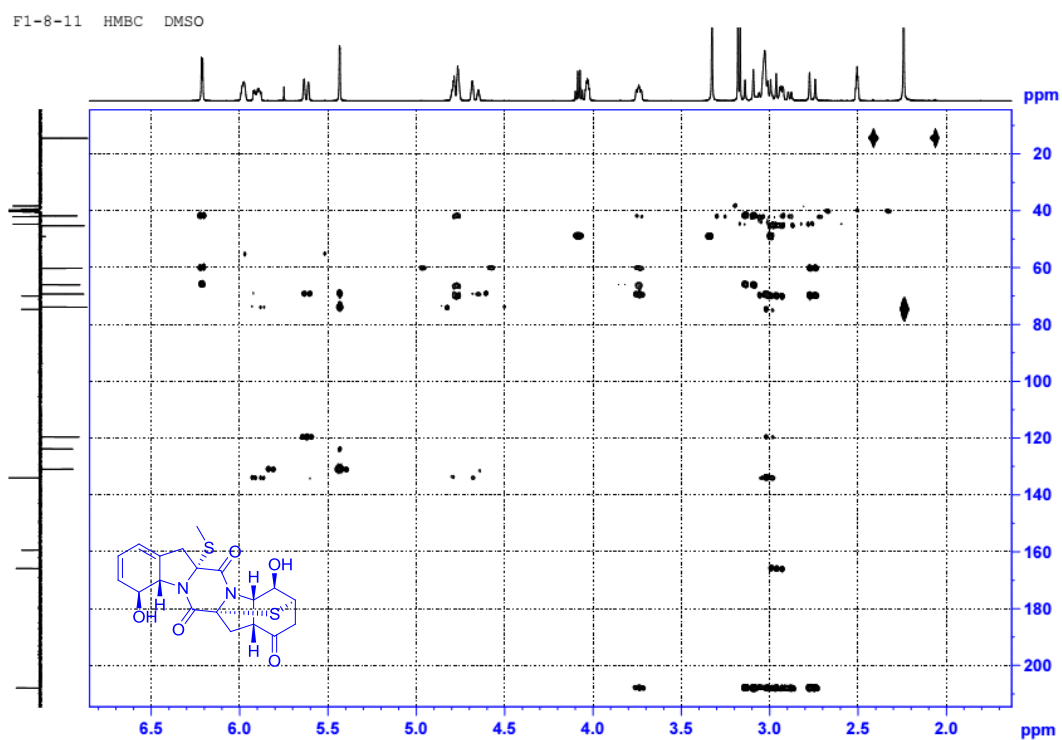


Fig S1-7 The HMBC Spectrum of Compound 1

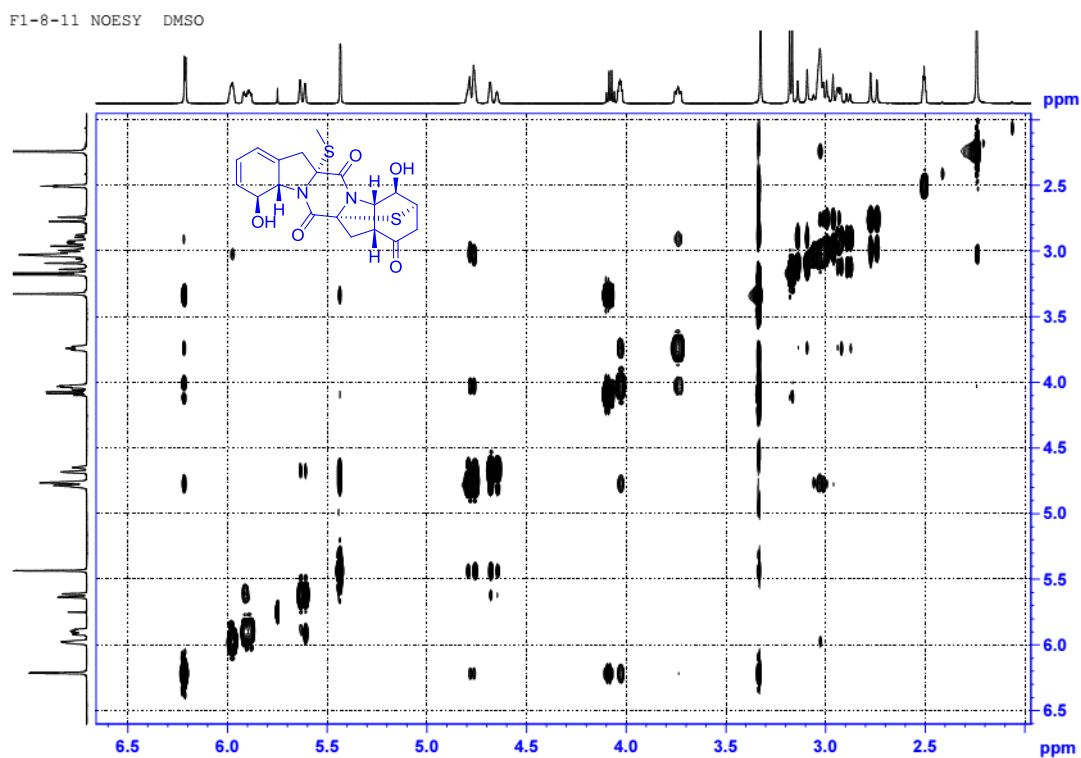


Fig S1-8 The NOESY Spectrum of Compound 1

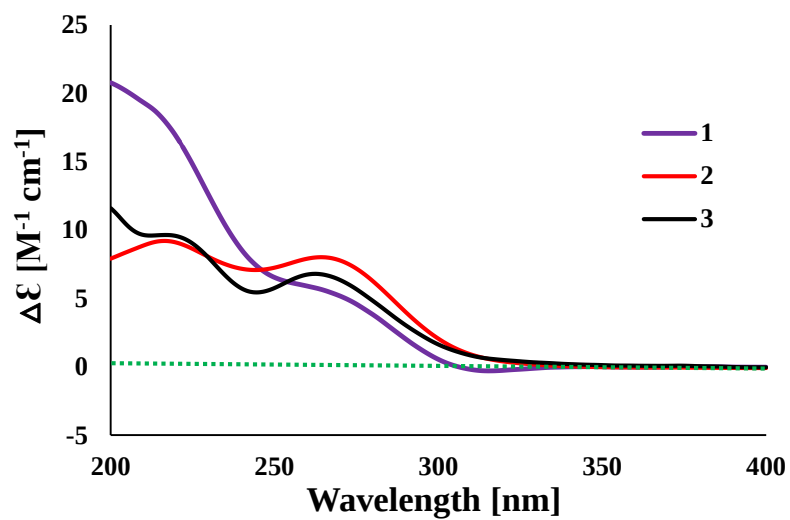


Fig S1-9 CD curves of Compounds 1–3

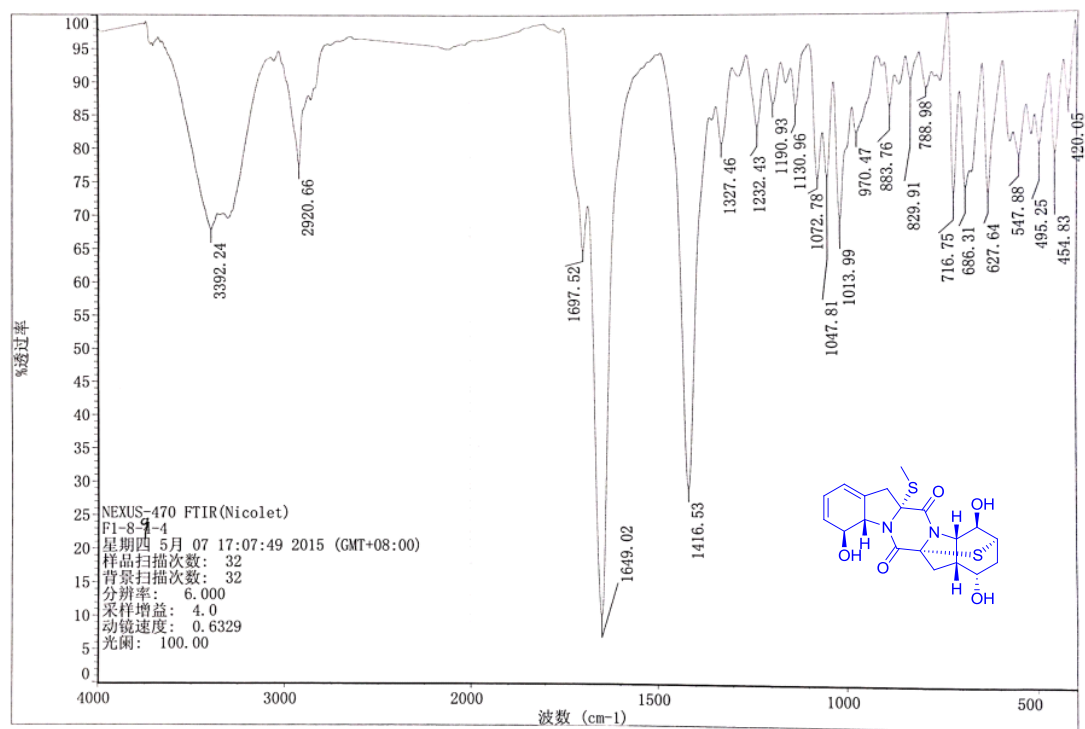


Fig S2-1 IR Spectrum of Compound 2

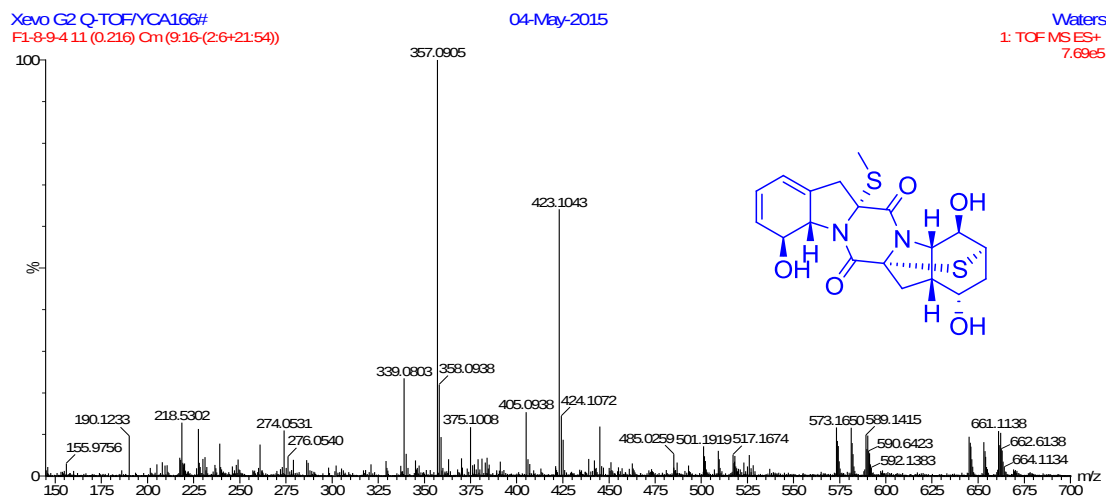


Fig S2-2 HRESIMS Data of Compound 2

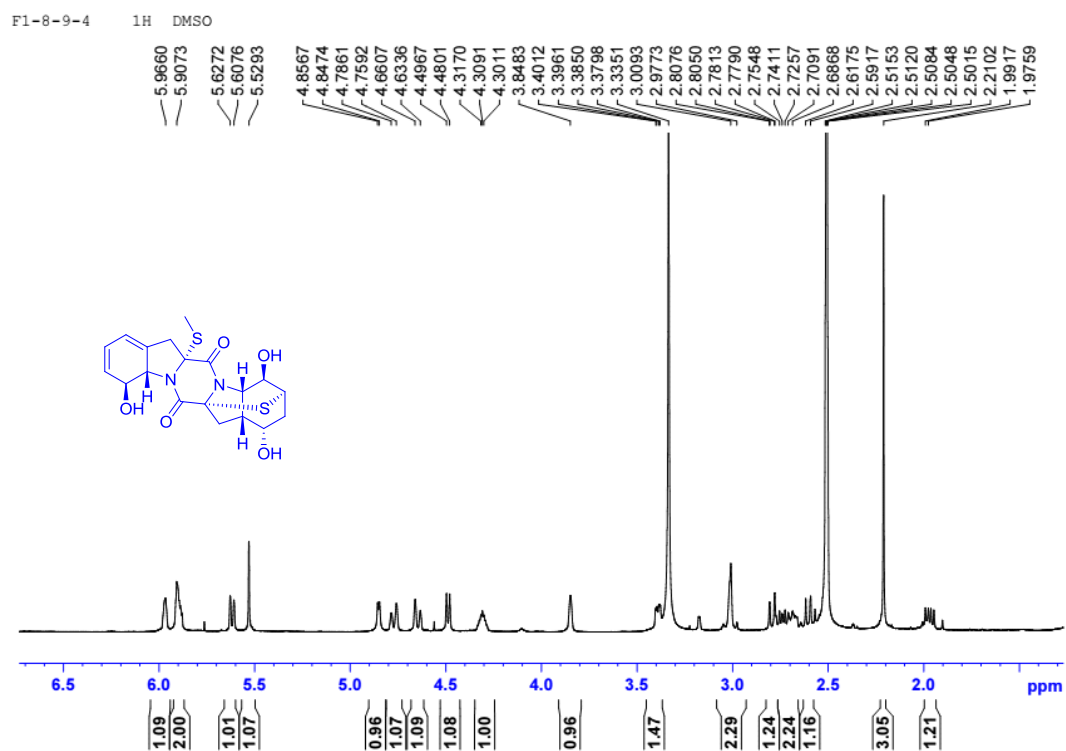


Fig S2-3 The ^1H NMR Spectrum of Compound 2

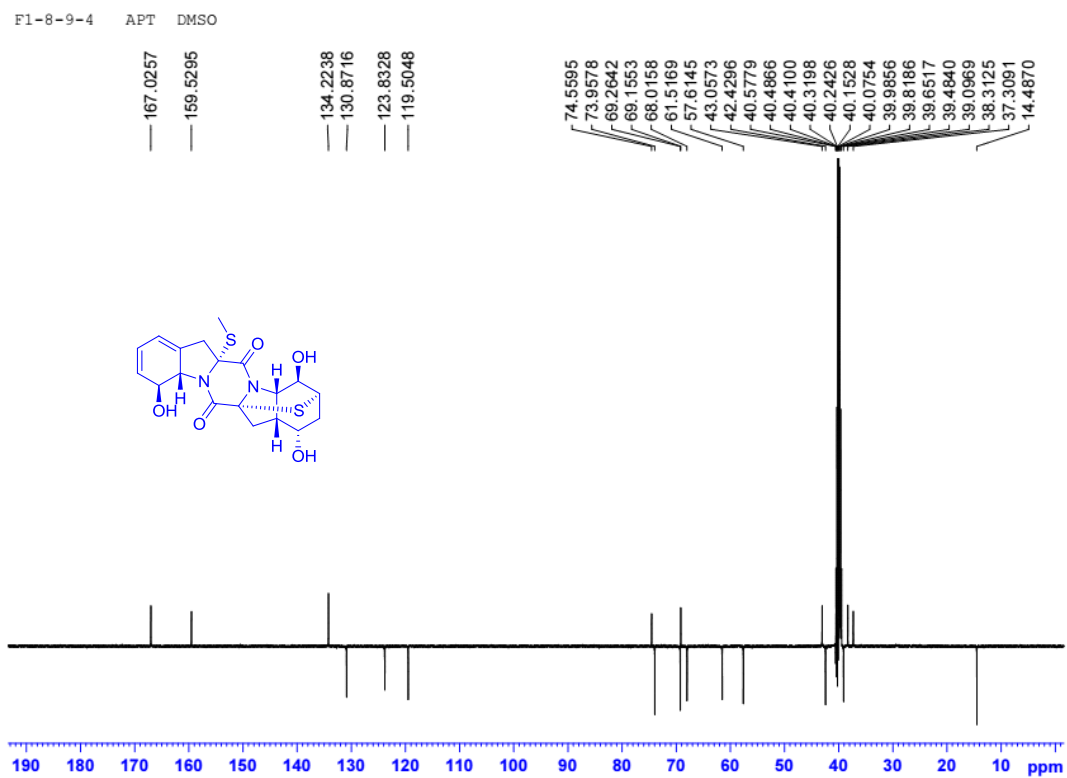


Fig S2-4 The APT Spectrum of Compound 2

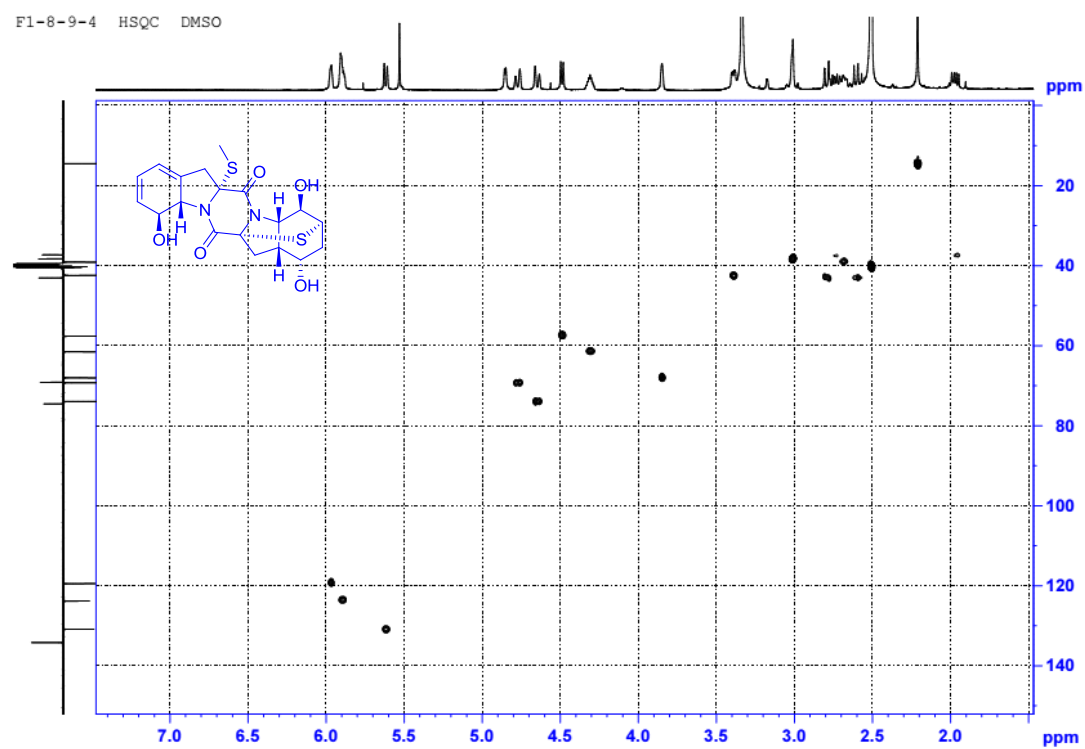


Fig S2-5 The HSQC Spectrum of Compound 2

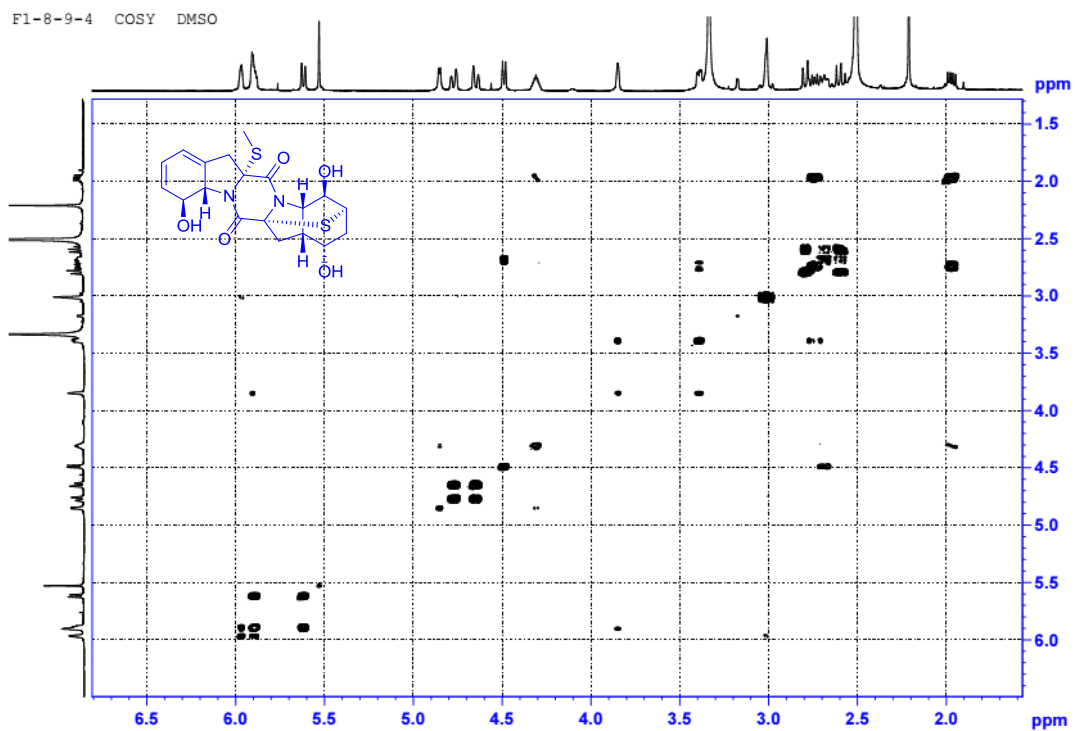


Fig S2-6 The ^1H - ^1H COSY Spectrum of Compound 2

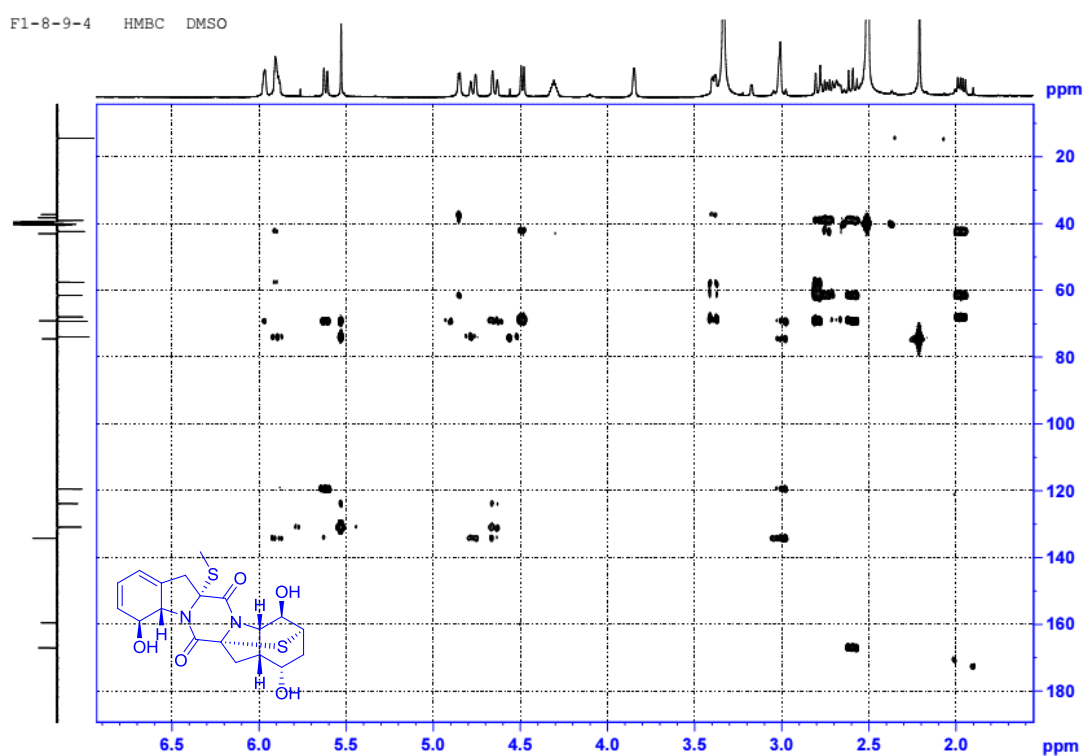


Fig S2-7 The HMBC Spectrum of Compound 2

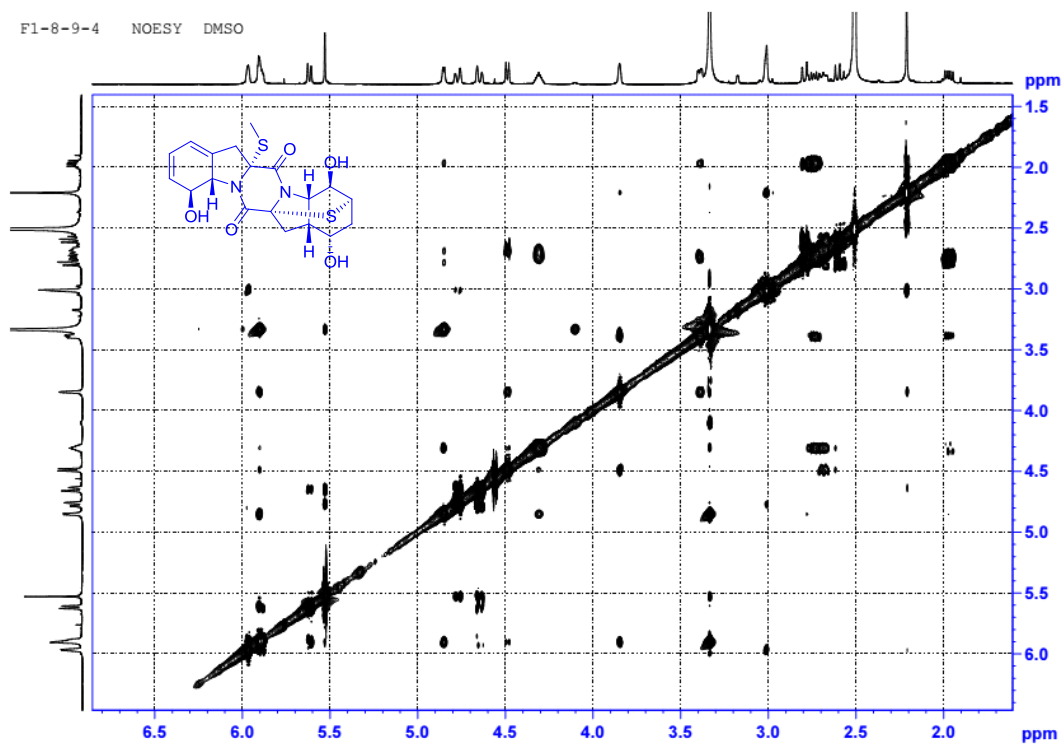


Fig S2-8 The NOESY Spectrum of Compound 2

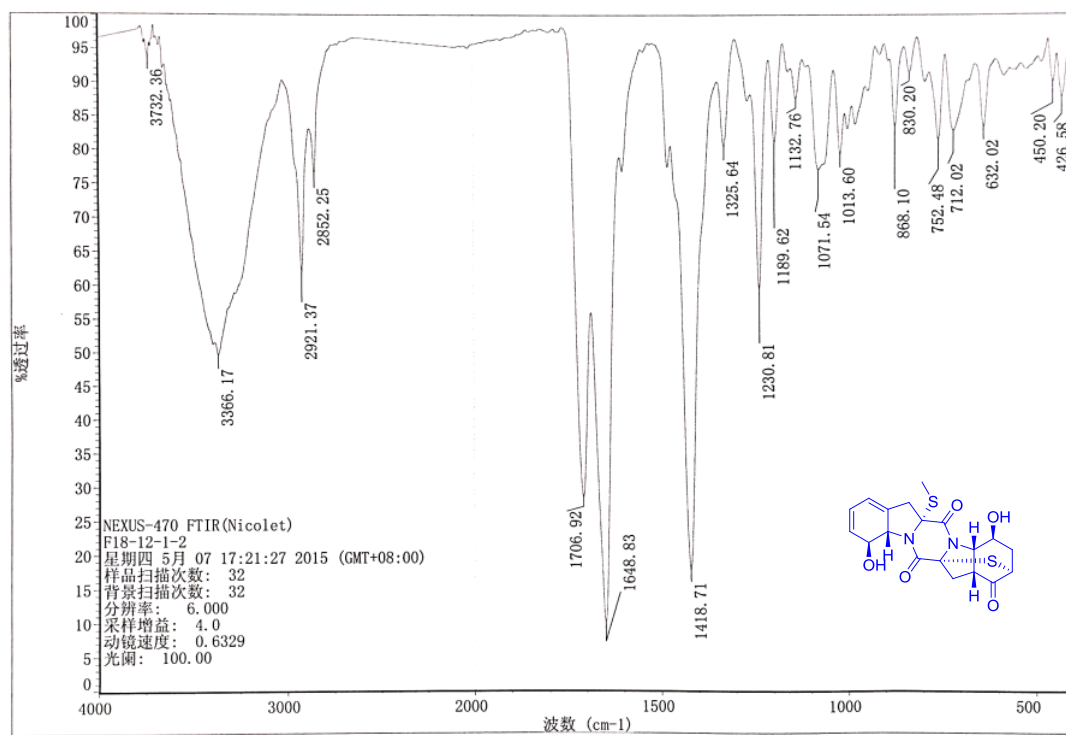


Fig S3-1 IR Spectrum of Compound 3

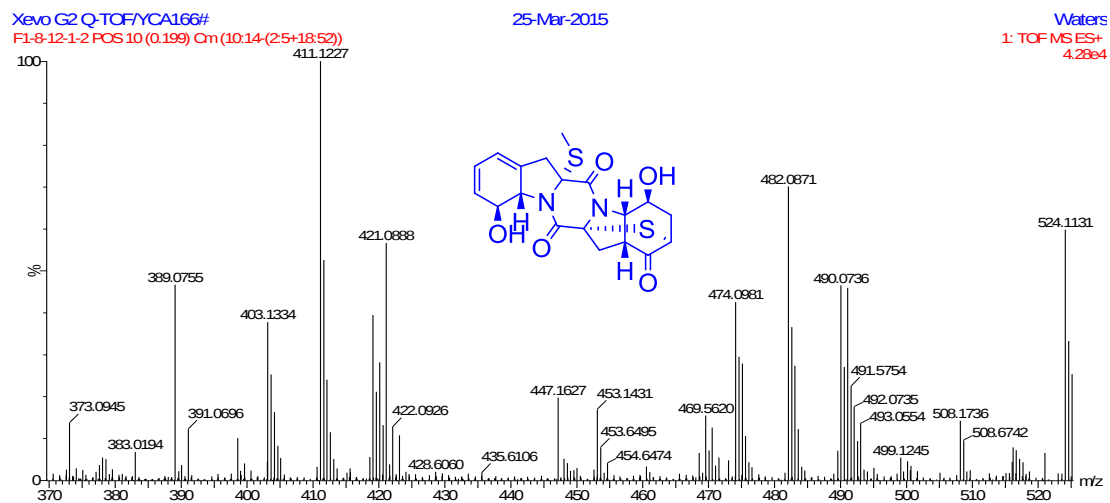


Fig S3-2 HRESIMS Data of Compound 3

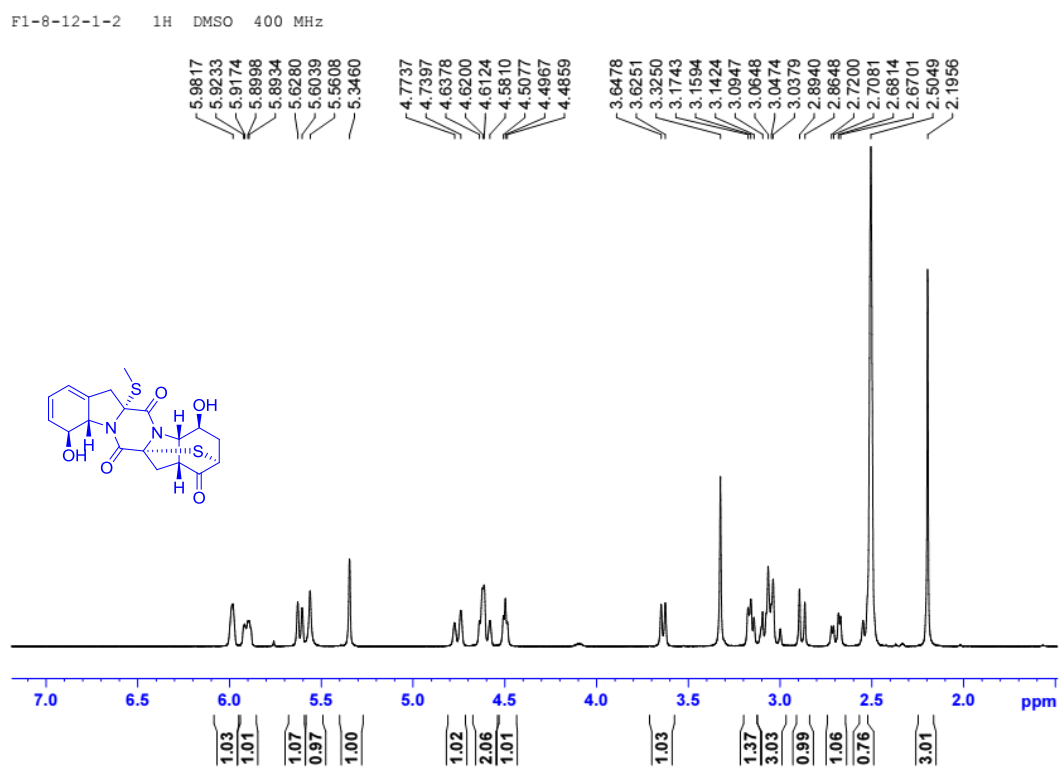


Fig S3-3 The ^1H NMR Spectrum of Compound 3

F1-8-12-1-2 APT DMSO 100 MHz

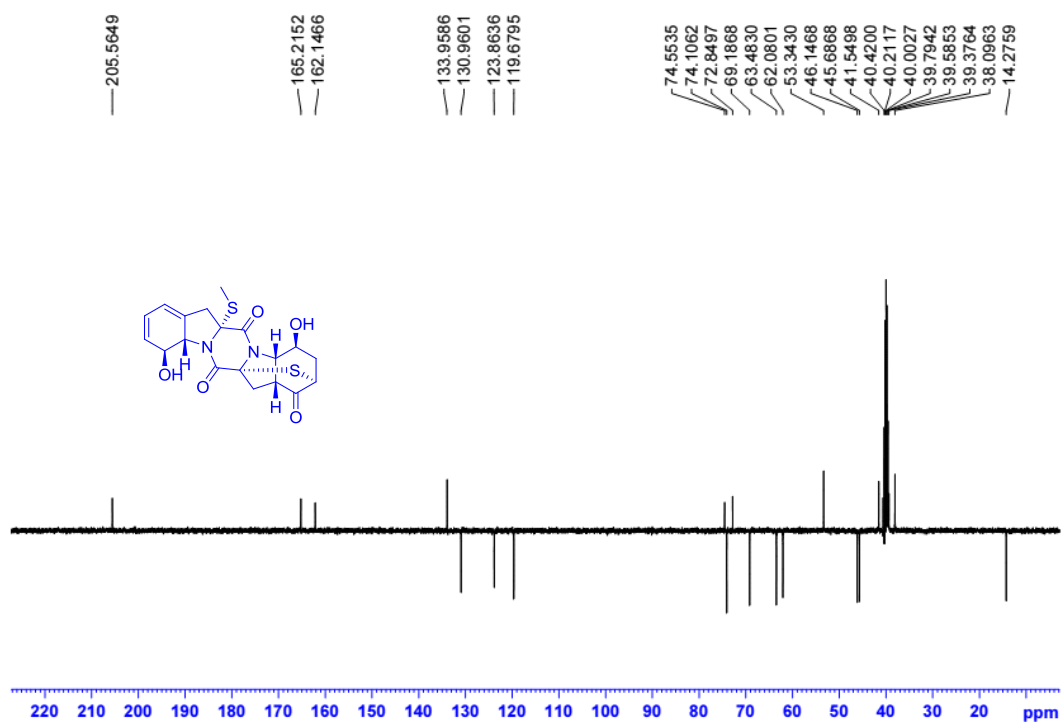


Fig S3-4 The APT Spectrum of Compound 3

F1-8-12-1-2 HSQC DMSO

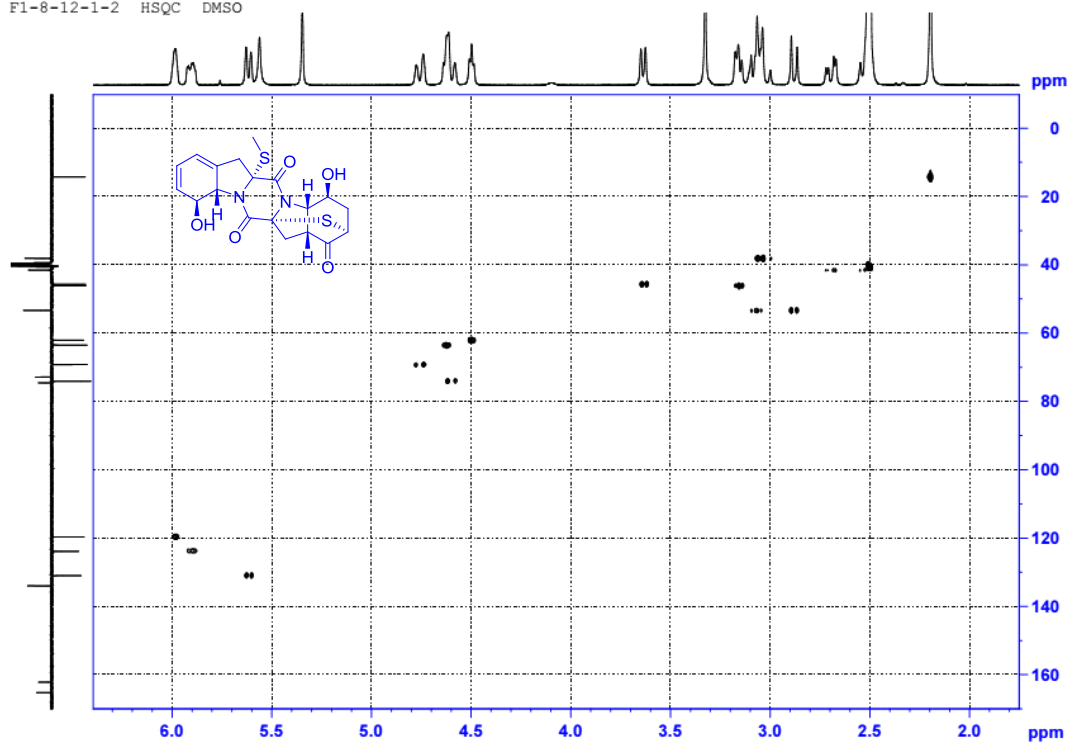


Fig S3-5 The HSQC Spectrum of Compound 3

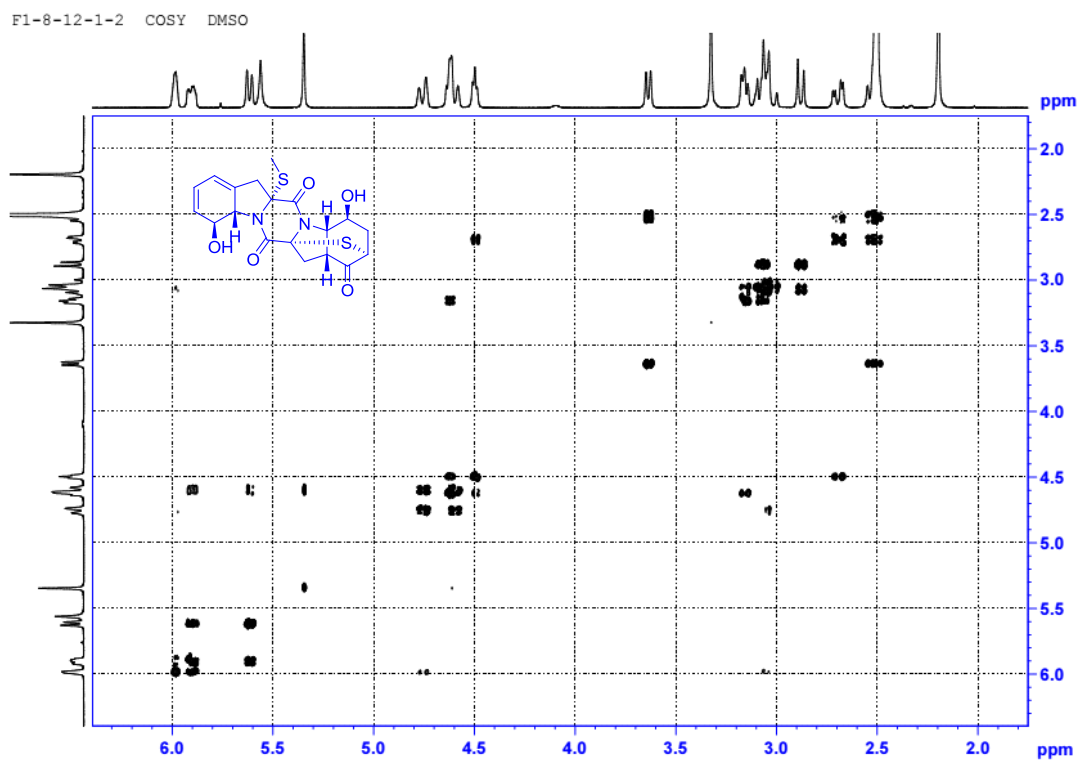


Fig S3-6 The ^1H - ^1H COSY Spectrum of Compound 3

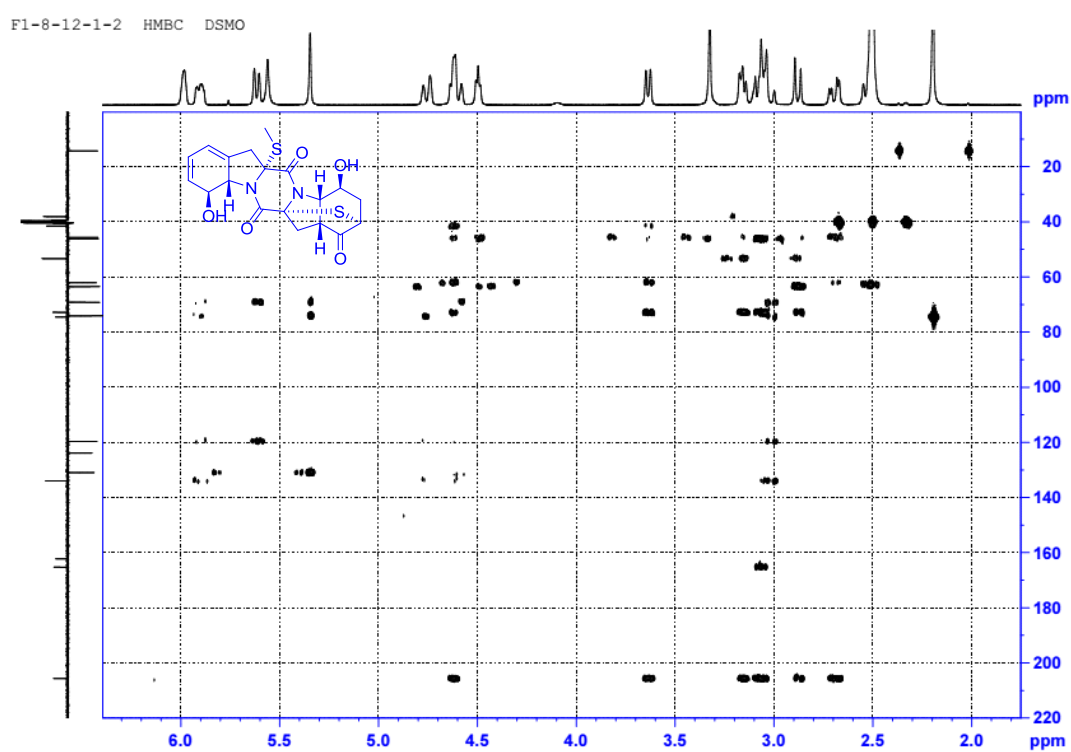


Fig S3-7 The HMBC Spectrum of Compound 3

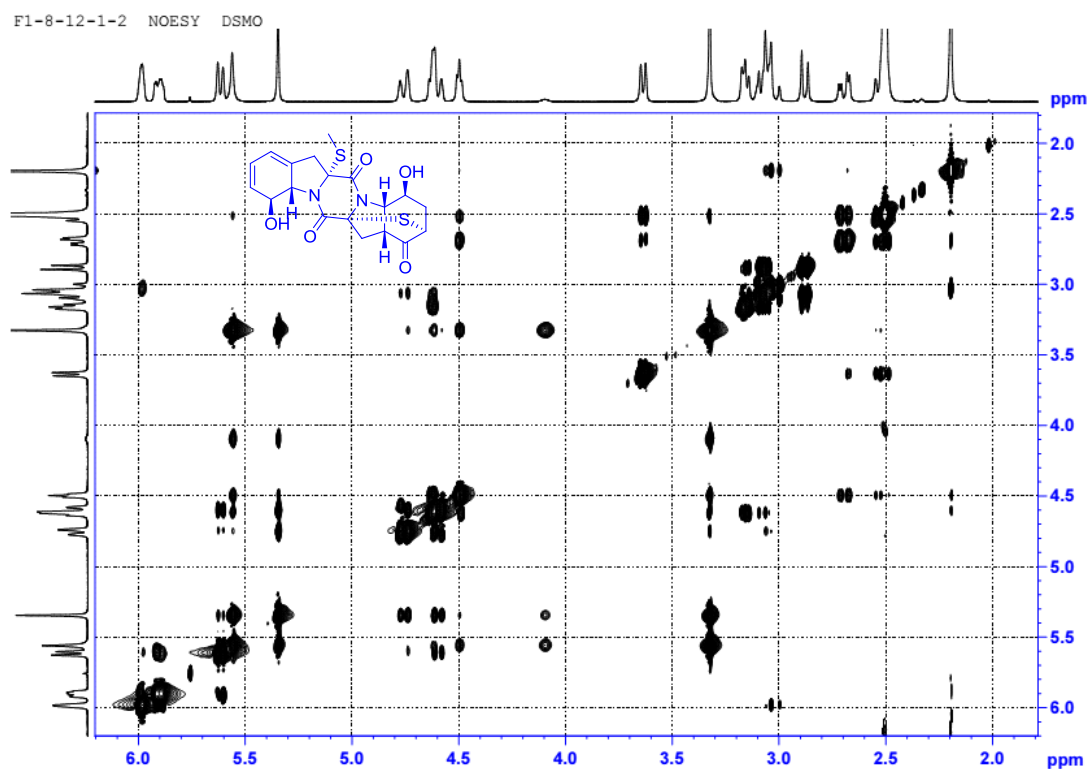


Fig S3-8 The NOESY Spectrum of Compound 3

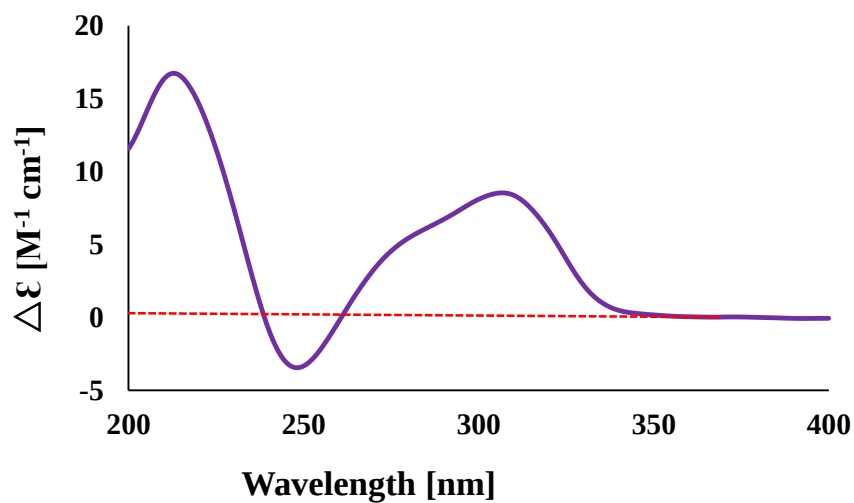


Fig S3-9 ECD Spectrum of 3 in methanol

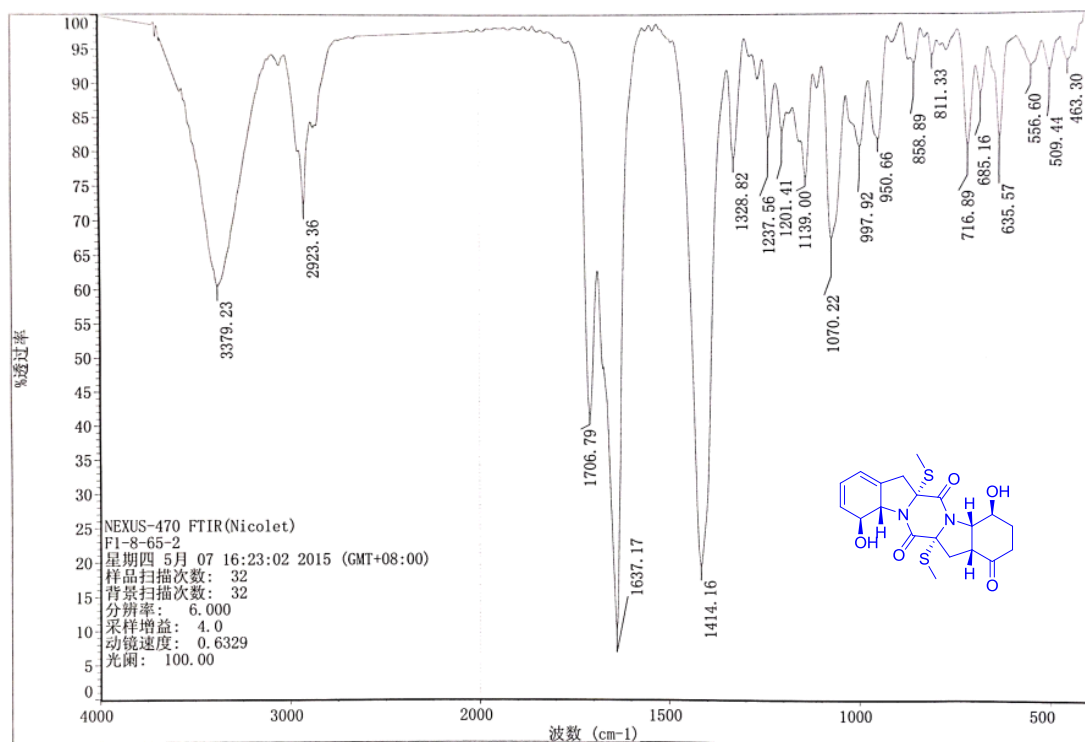


Fig S4-1 IR Spectrum of Compound 4

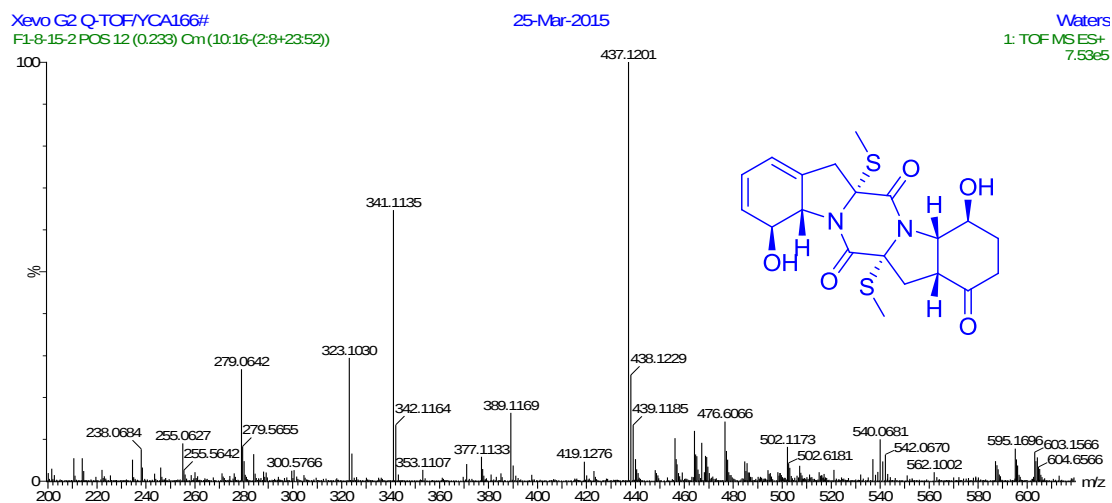


Fig S4-2 HRESIMS Data of Compound 4

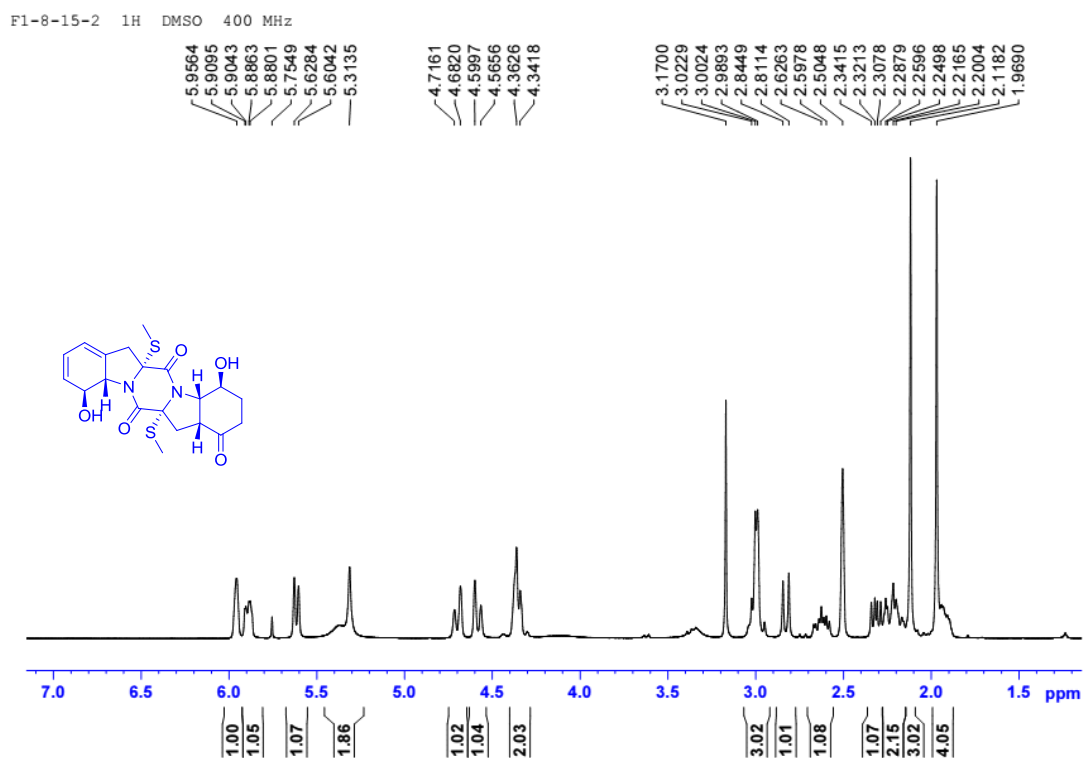


Fig S4-3 The ^1H NMR Spectrum of Compound **4**

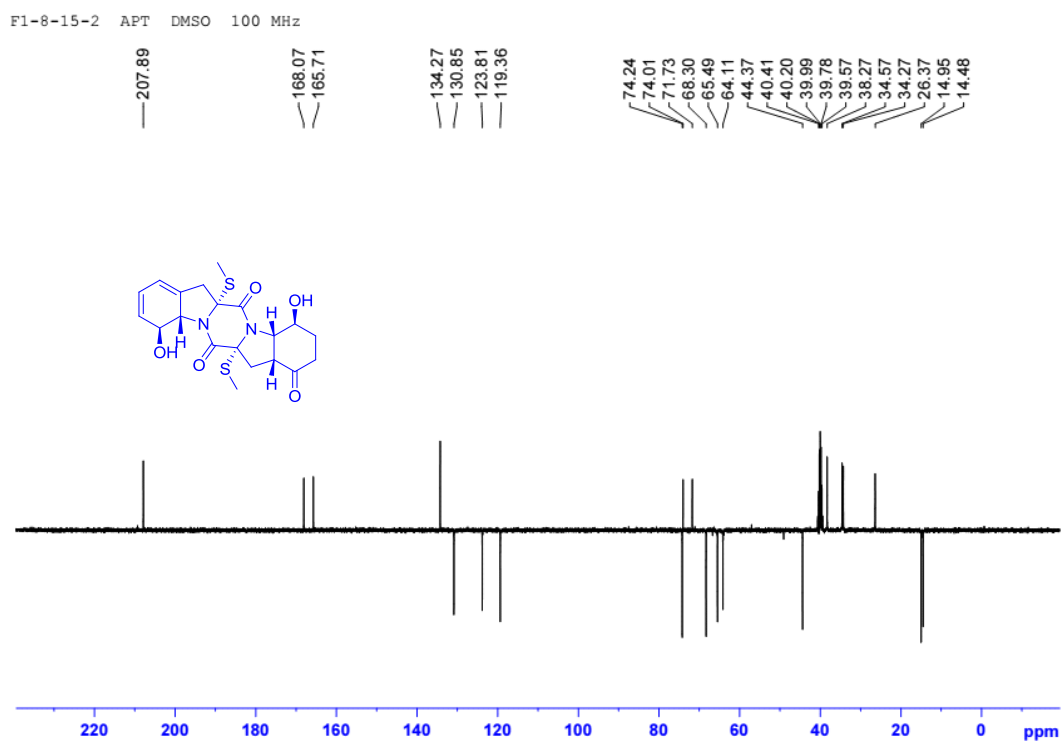


Fig S4-4 The APT Spectrum of Compound **4**

F1-8-15-2 HSQC DMSO

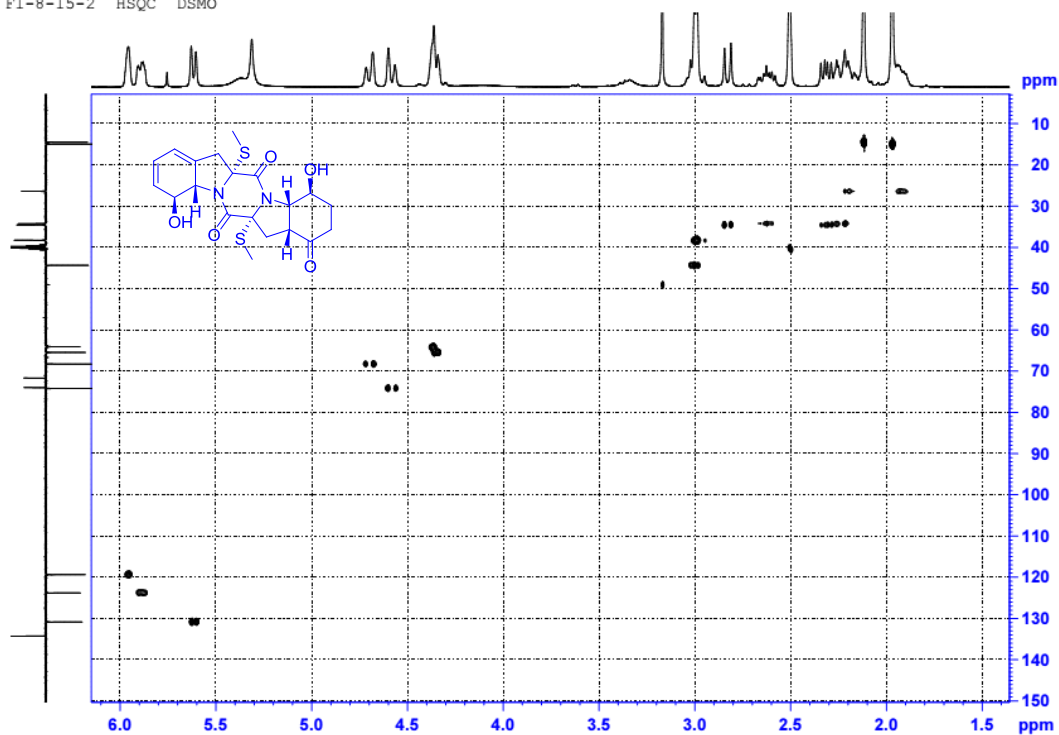


Fig S4-5 The HSQC Spectrum of Compound 4

F1-8-15-2 COSY DMSO

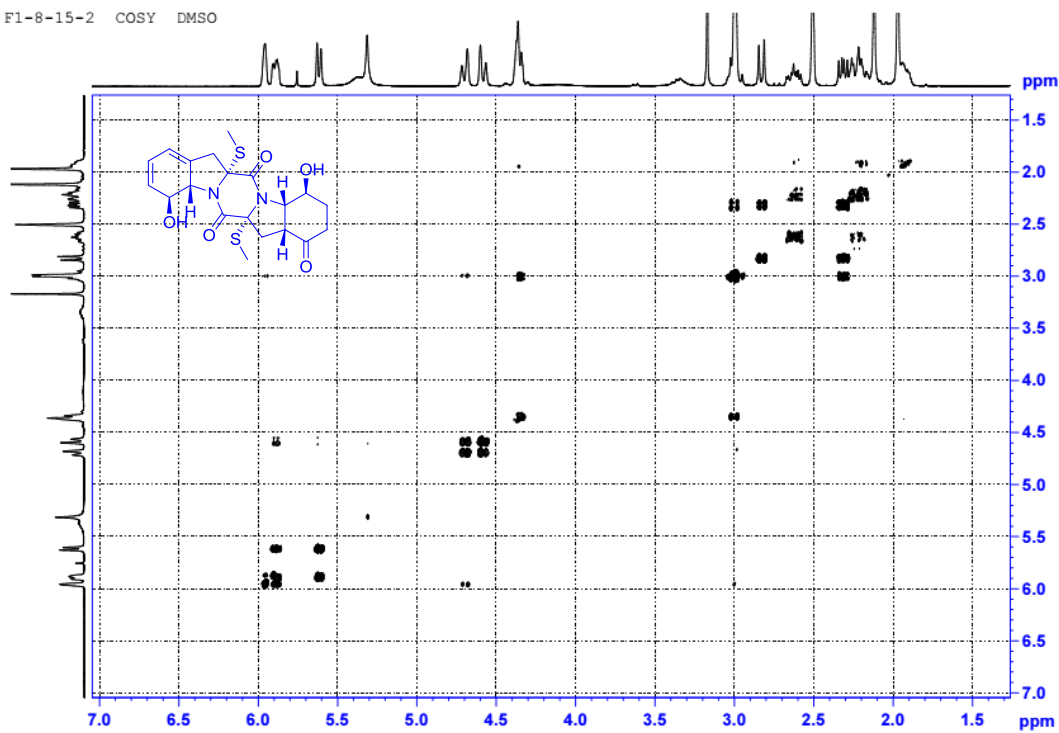


Fig S4-6 The ^1H - ^1H COSY Spectrum of Compound 4

F1-8-15-2 HMBC DMSO

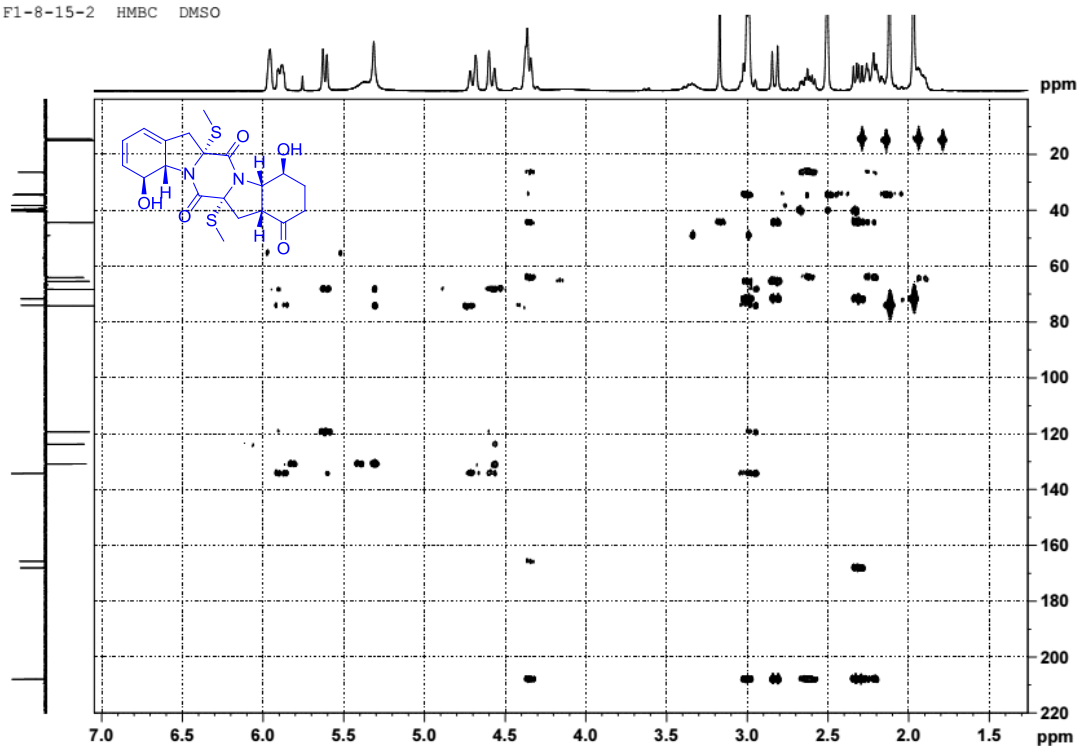


Fig S4-7 The HMBC Spectrum of Compound 4

F1-8-15-2 NOESY DMSO

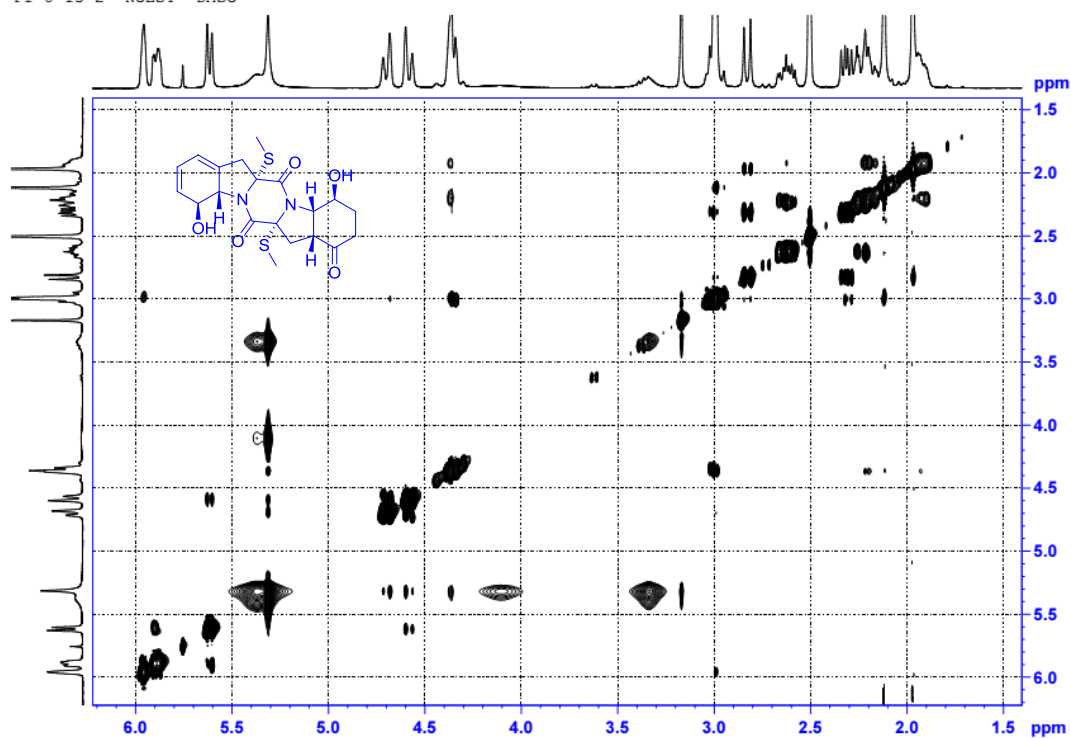


Fig S4-8 The NOESY Spectrum of Compound 4

F1-8-15-2-R 1H CDCl3 400 MHz

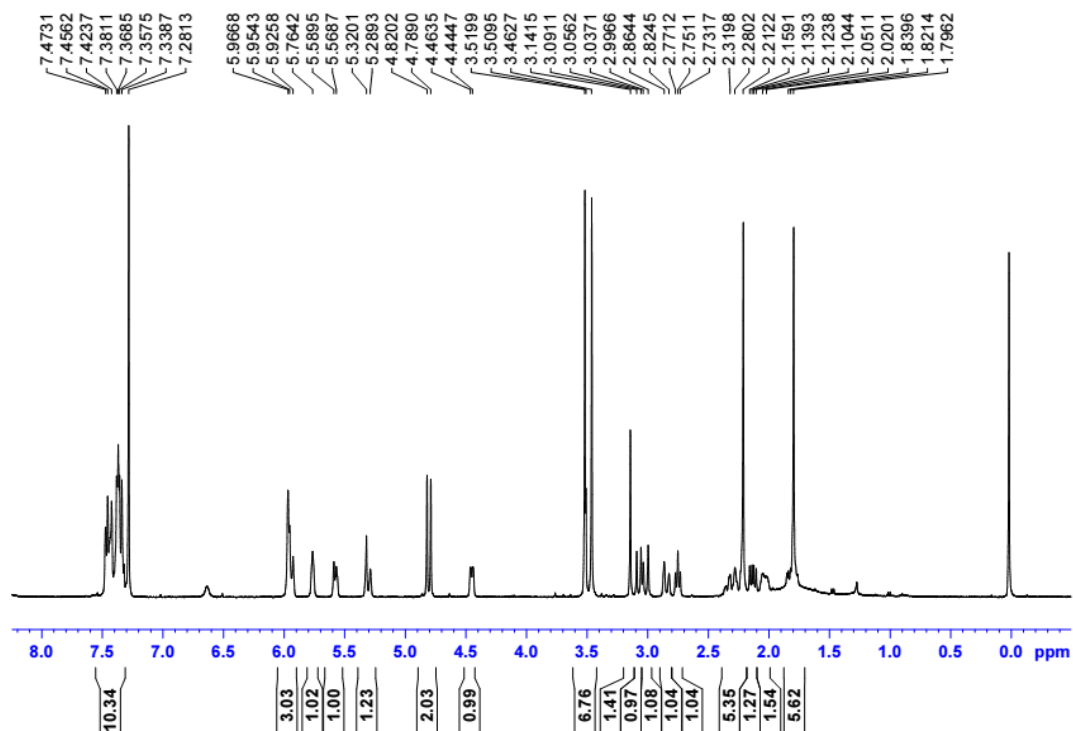


Fig S4-9 ^1H NMR Spectrum of (*R*)-MPA ester of **4a**

F1-8-15-2-S 1H CDCl3 400 MHz

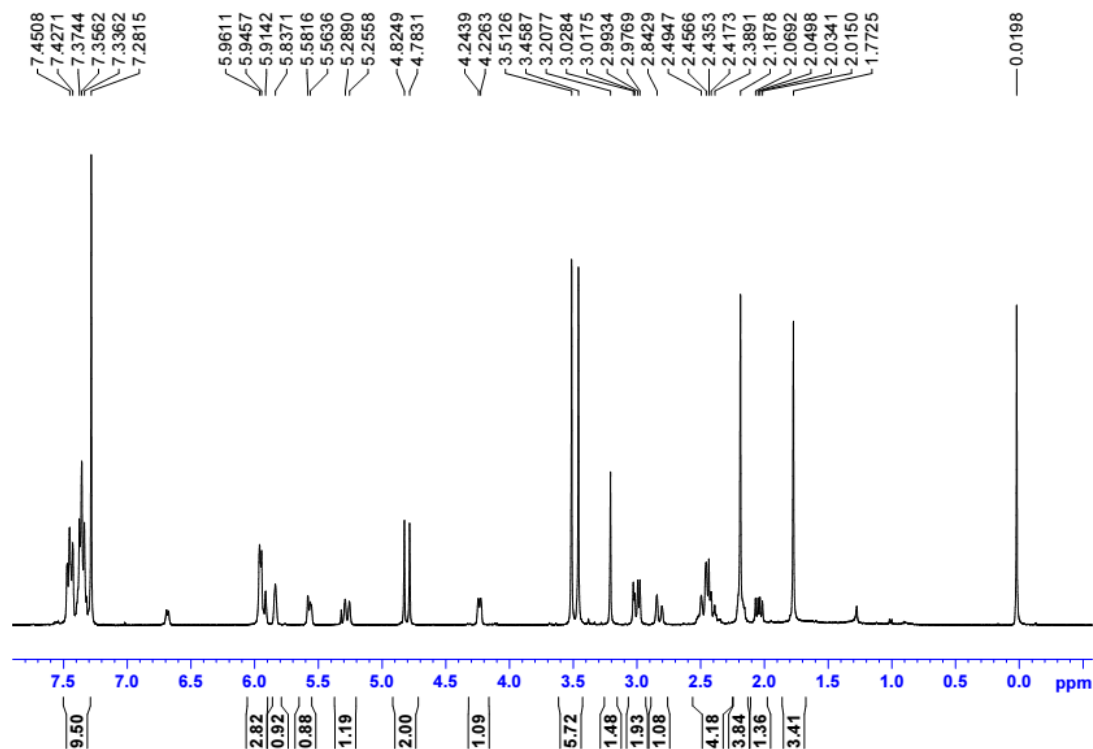


Fig S4-10 ^1H NMR Spectrum of (*S*)-MPA ester of **4b**

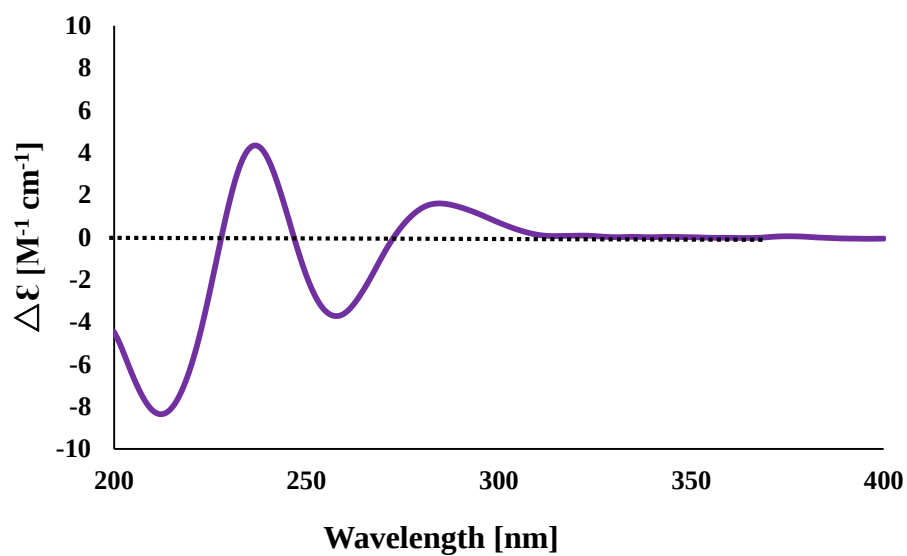


Fig S4-11 The CD Curve of Compound 4

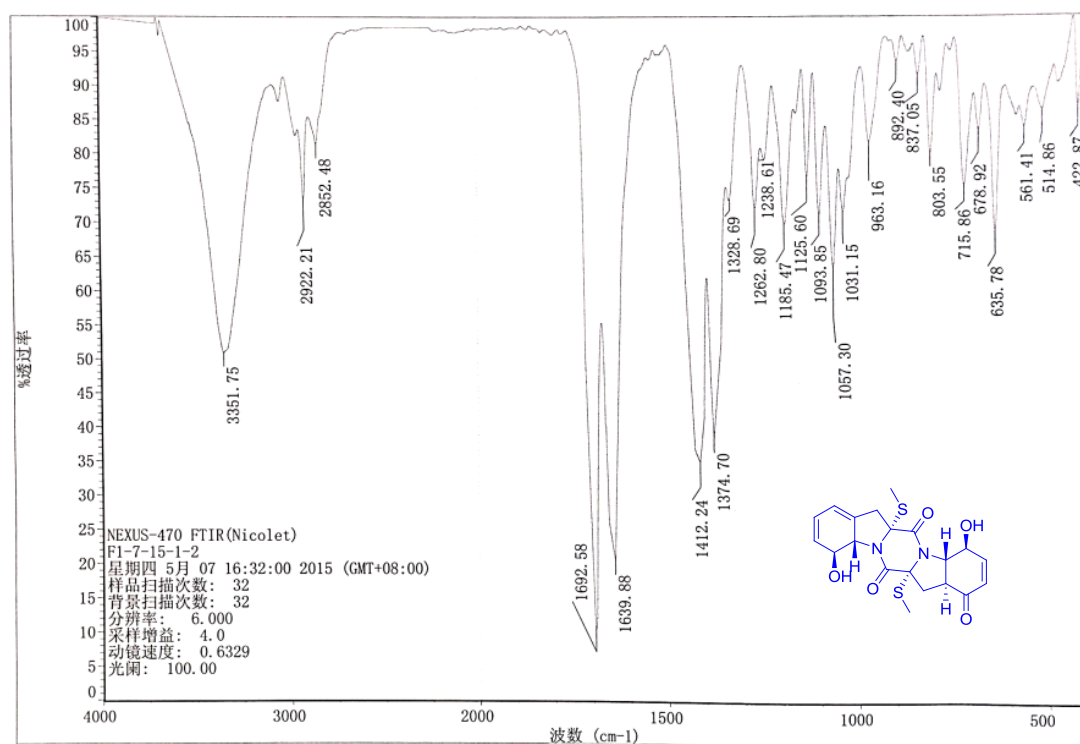


Fig S5-1 IR Spectrum of Compound 5

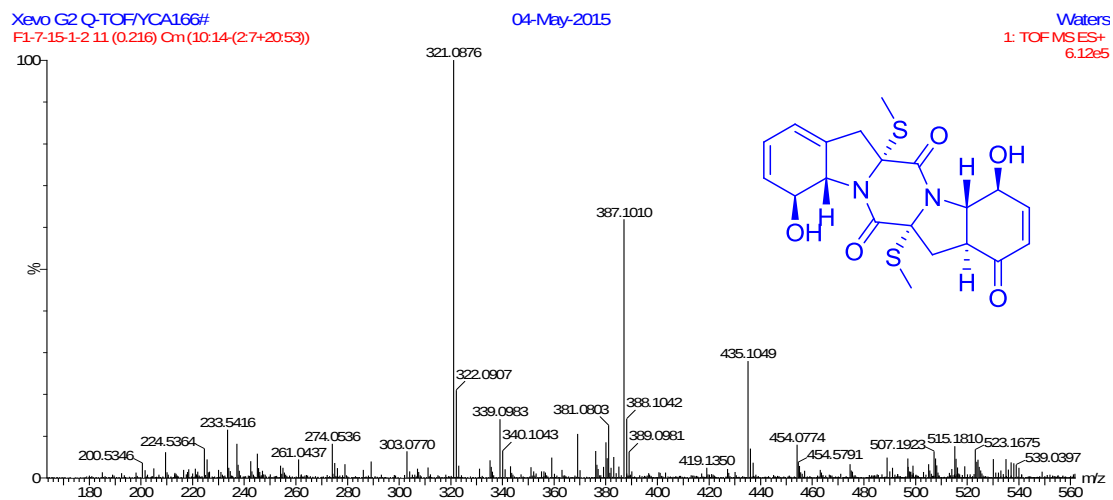


Fig S5-2 HRESIMS Data of Compound 5

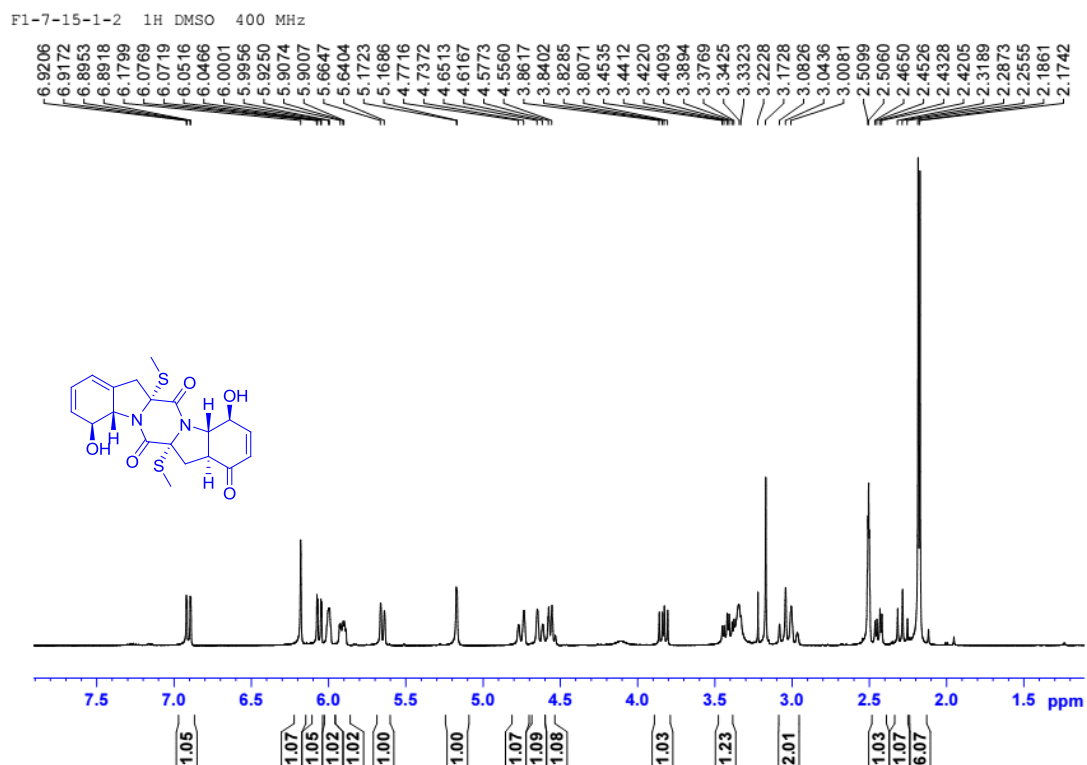


Fig S5-3 The ^1H NMR Spectrum of Compound 5

F1-7-15-1-2 APT DMSO 100 MHz

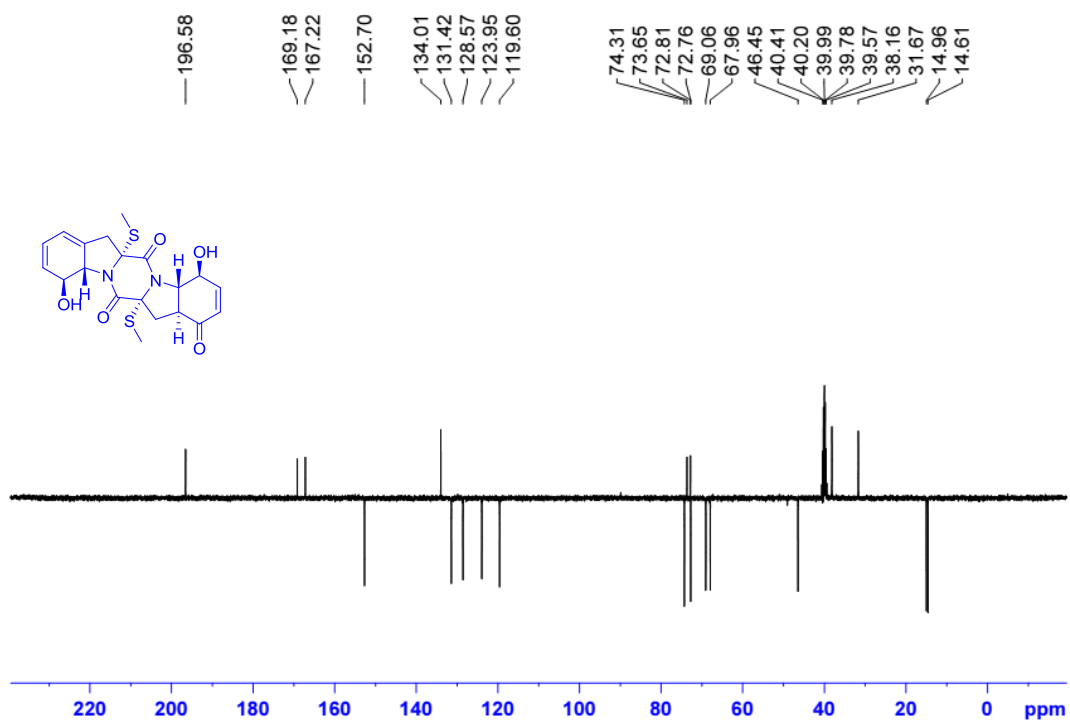


Fig S5-4 The APT Spectrum of Compound 5

F1-7-15-1-2 HSQC DMSO

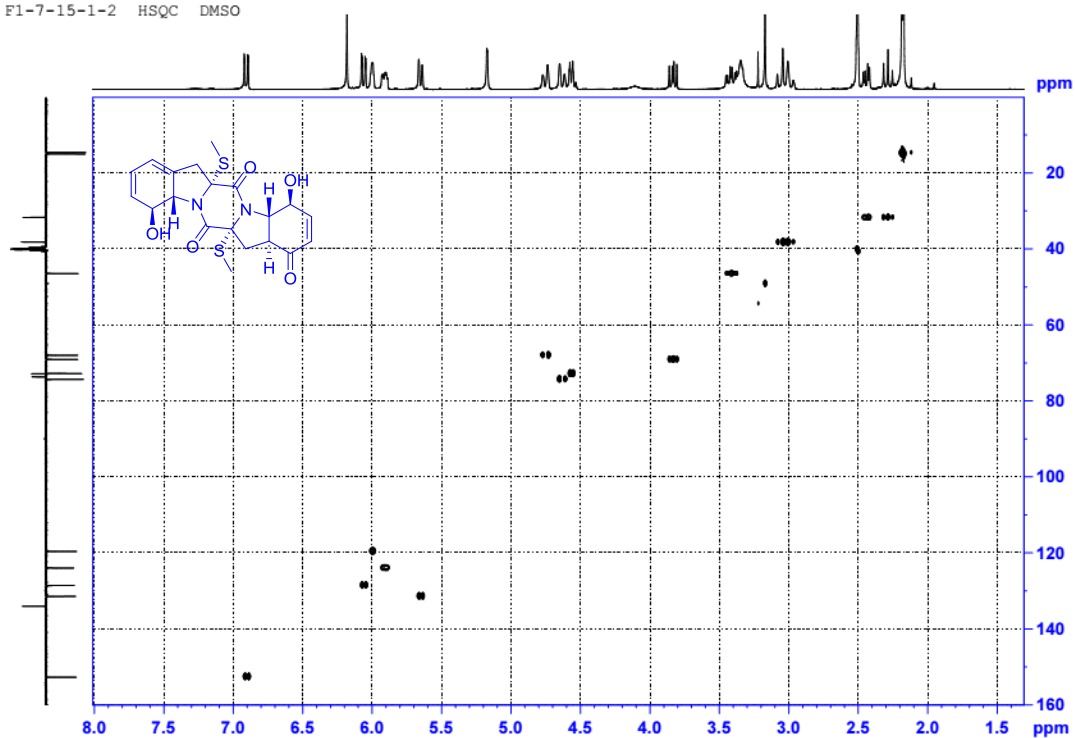


Fig S5-5 The HSQC Spectrum of Compound 5

F1-7-15-1-2 COSY DMSO

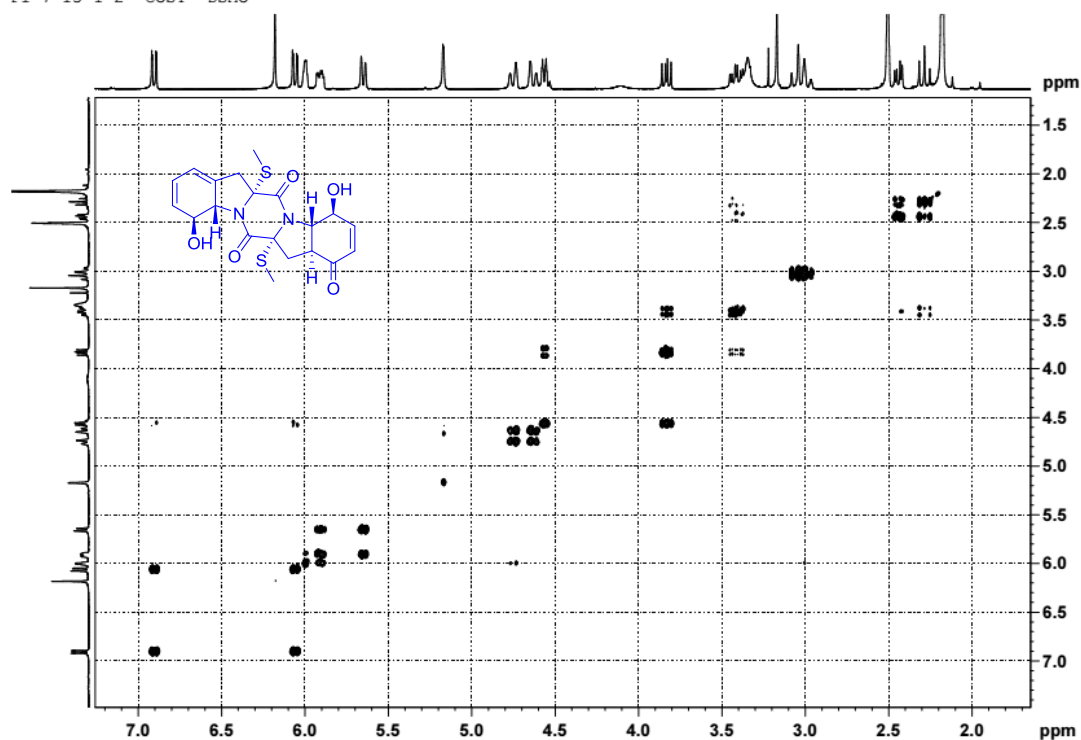


Fig S5-6 The ¹H-¹H COSY Spectrum of Compound 5

F1-7-15-1-2 HMBC DMSO

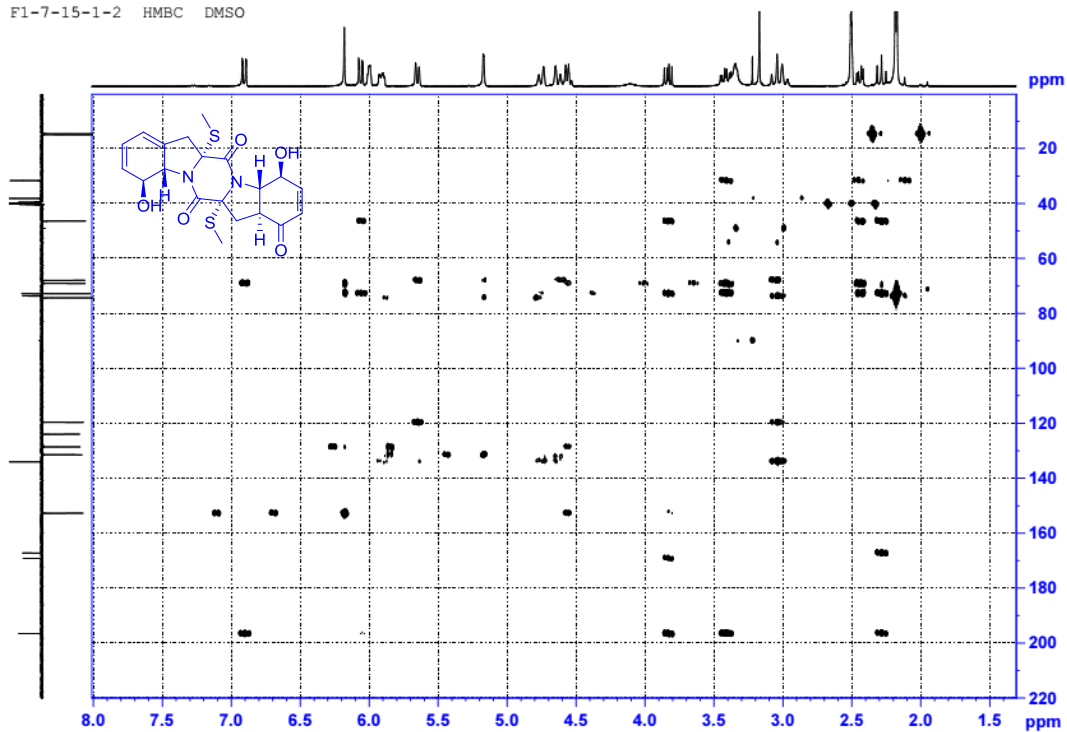


Fig S5-7 The HMBC Spectrum of Compound 5

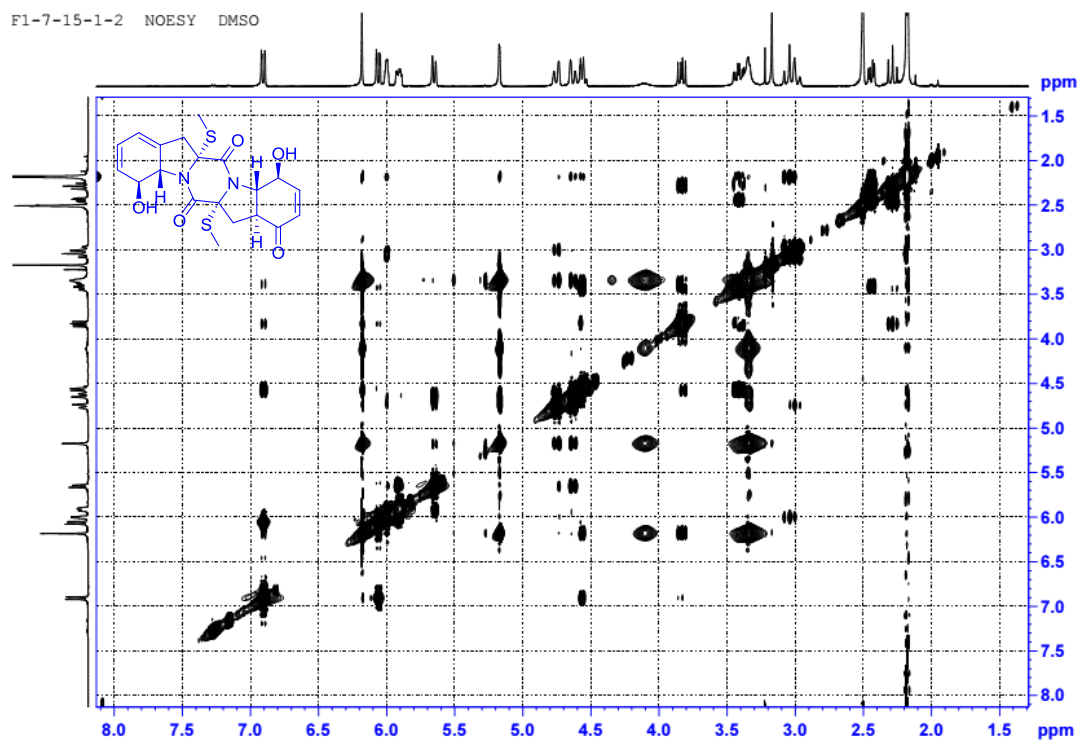


Fig S5-8 The NOESY Spectrum of Compound 5

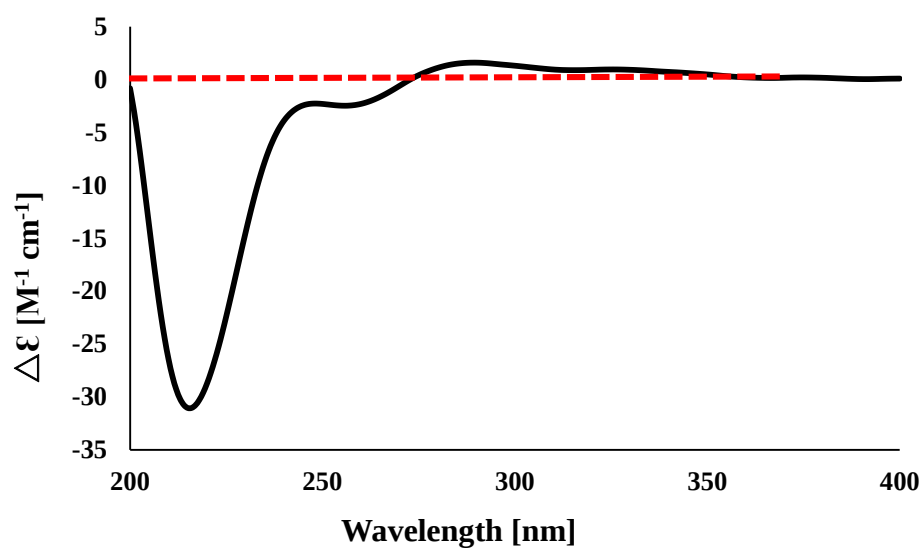


Fig S5-9 The CD Spectrum of 5 in methanol

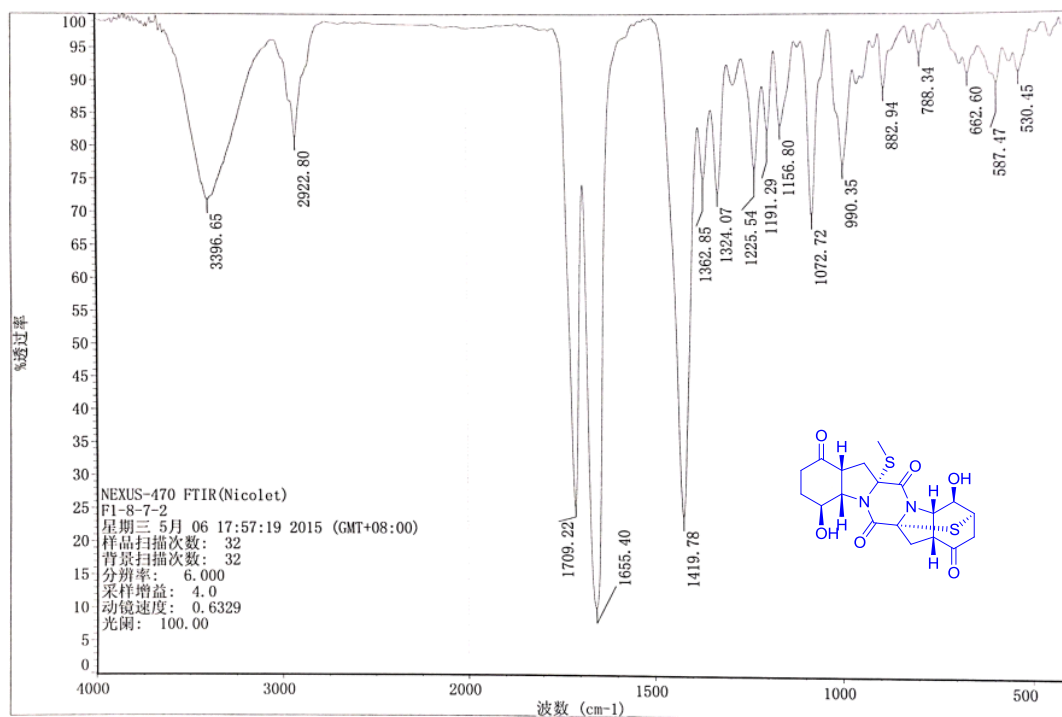


Fig S6-1 IR Spectrum of Compound 6

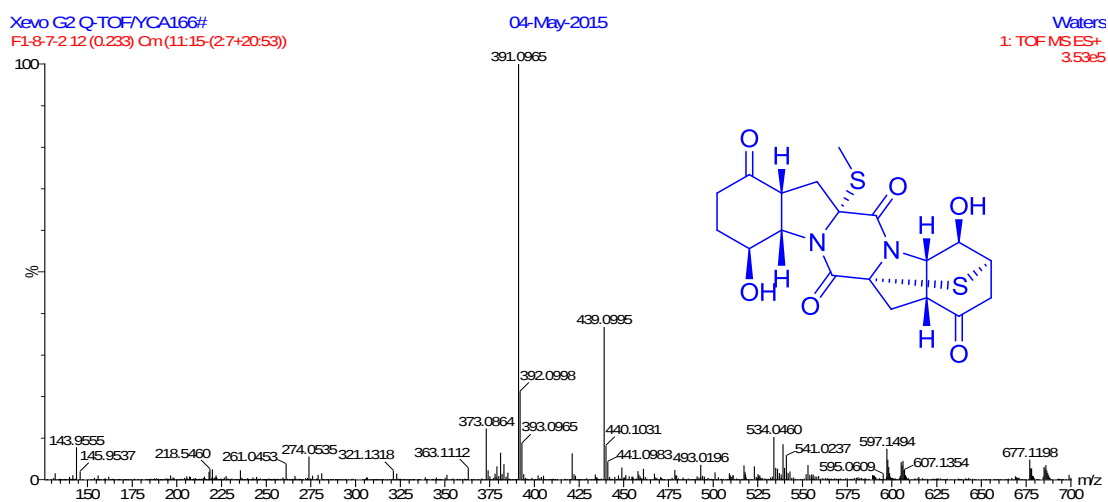


Fig S6-2 HRESIMS Data of Compound 6

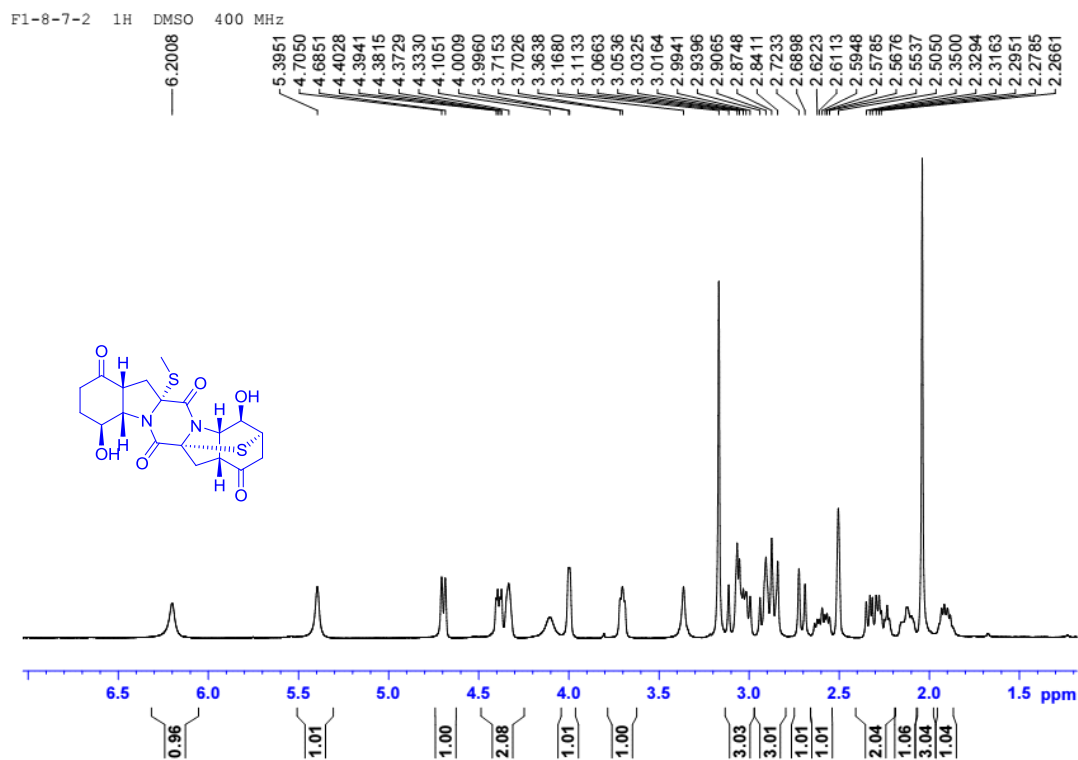


Fig S6-3 The ^1H NMR Spectrum of Compound 6

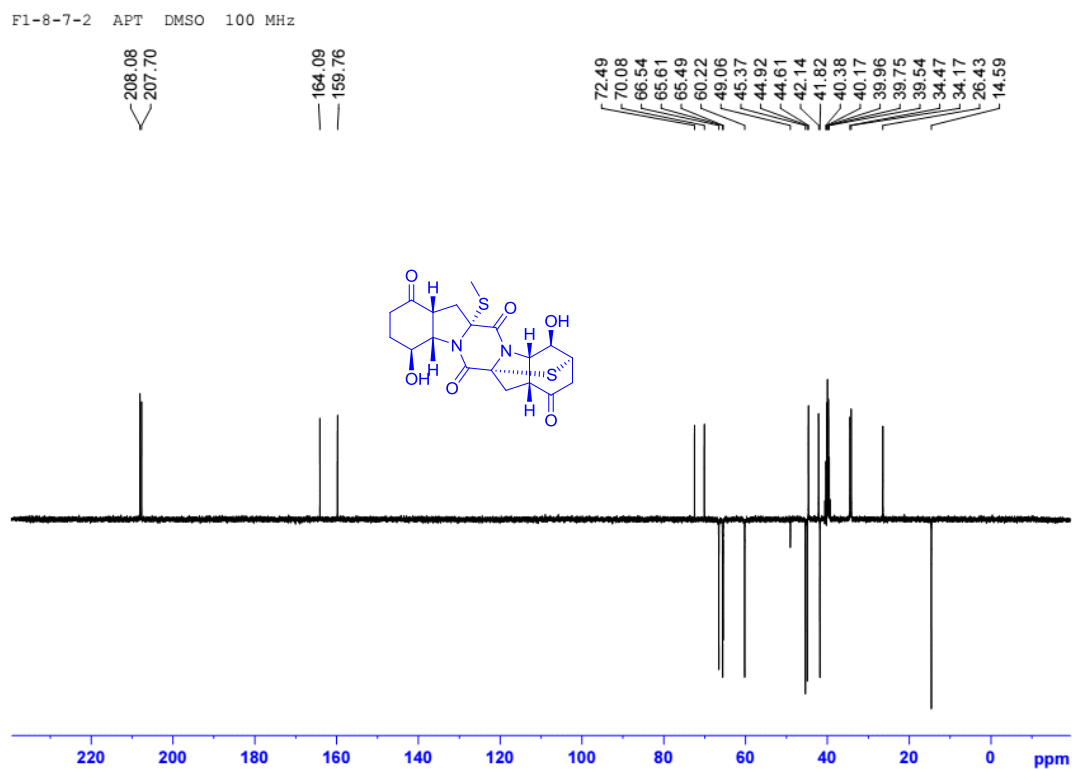


Fig S6-4 The APT Spectrum of Compound 6

F1-8-7-2 HSQC DMSO

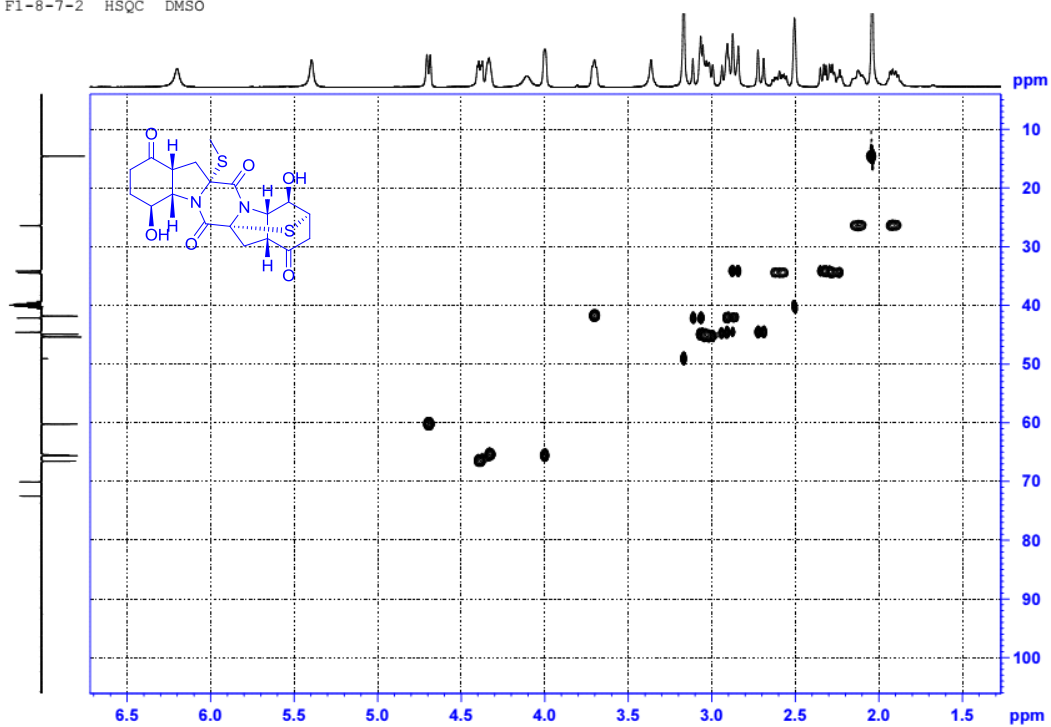


Fig S6-5 The HSQC Spectrum of Compound 6

F1-8-7-2 COSY DMSO

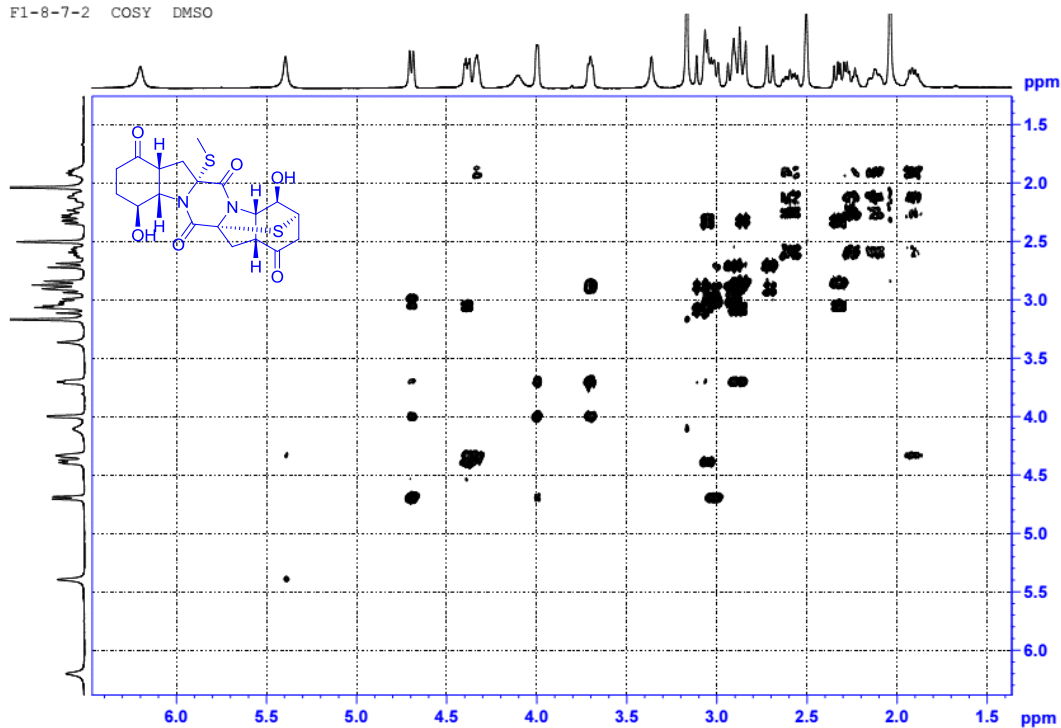


Fig S6-6 The ^1H - ^1H COSY Spectrum of Compound 6

F1-8-7-2 HMBC DMSO

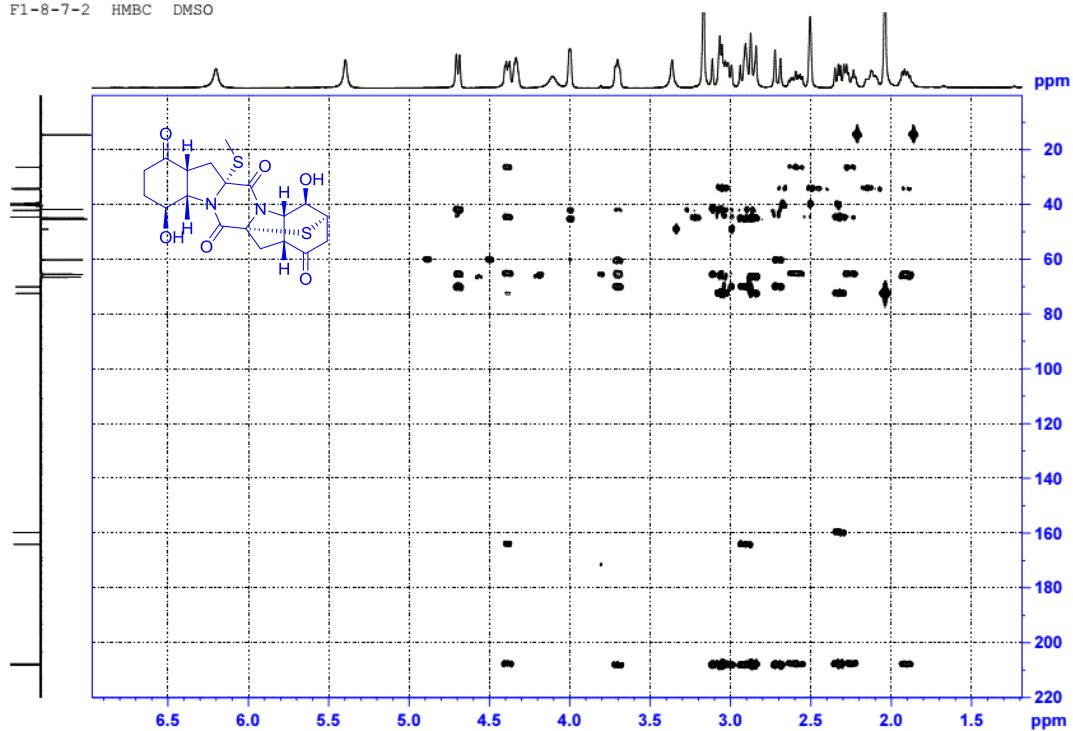


Fig S6-7 The HMBC Spectrum of Compound 6

F1-8-7-2 NOESY DMSO

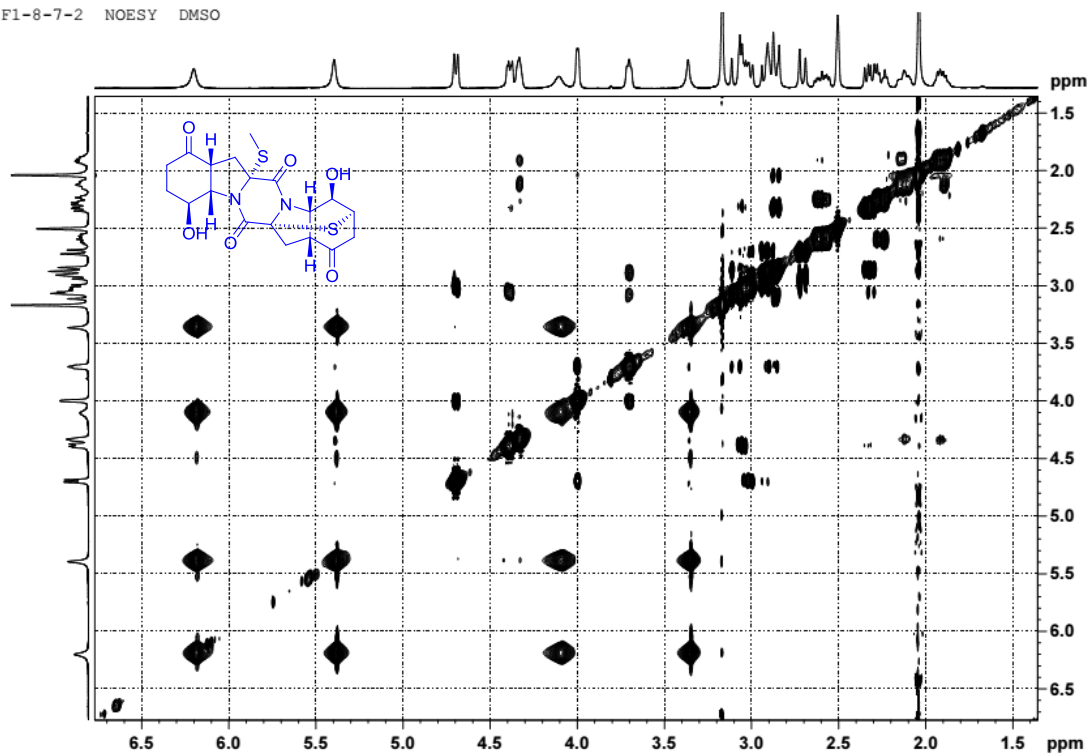


Fig S6-8 The NOESY Spectrum of Compound 6

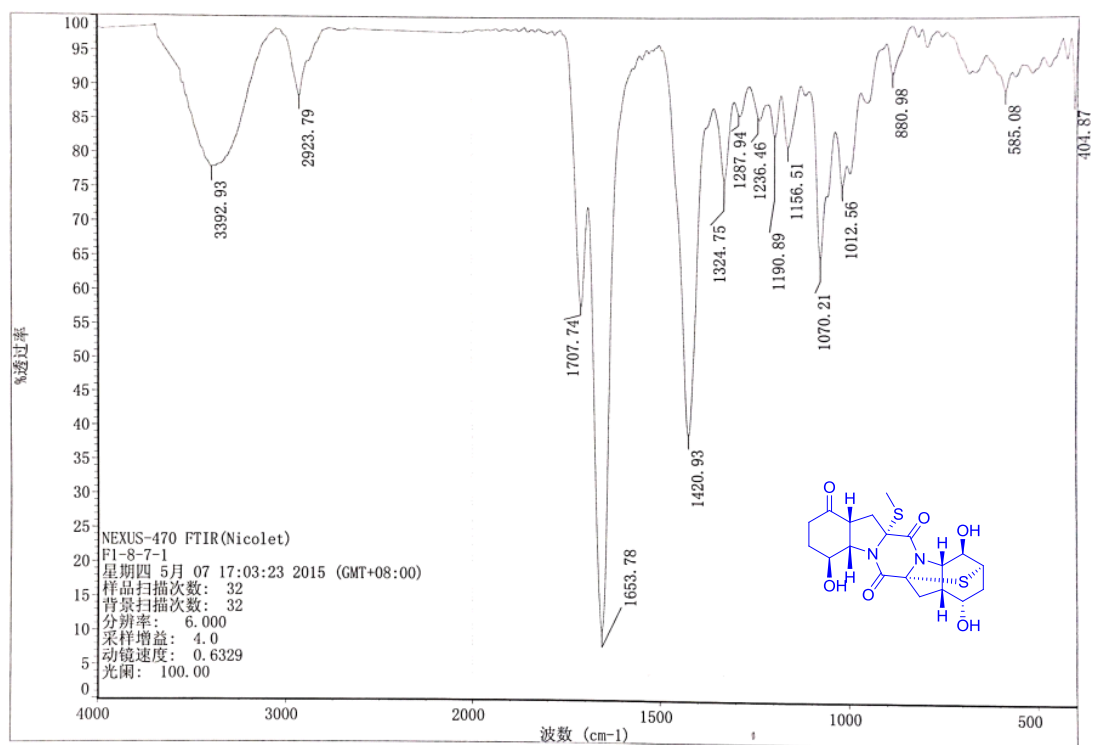


Fig S7-1 IR Spectrum of Compound 7

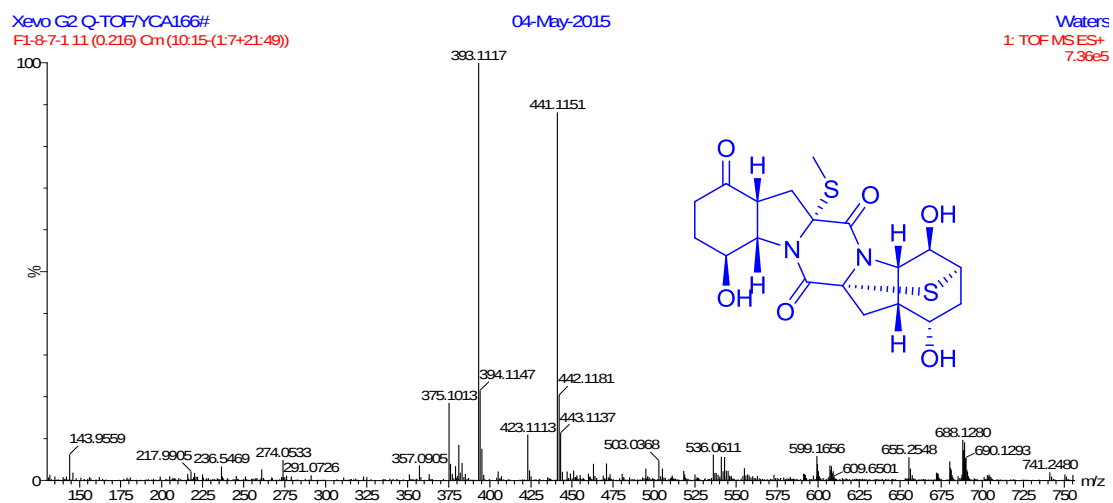


Fig S7-2 HRESIMS Data of Compound 7

F1-8-7-1 1H DMSO 400 MHz

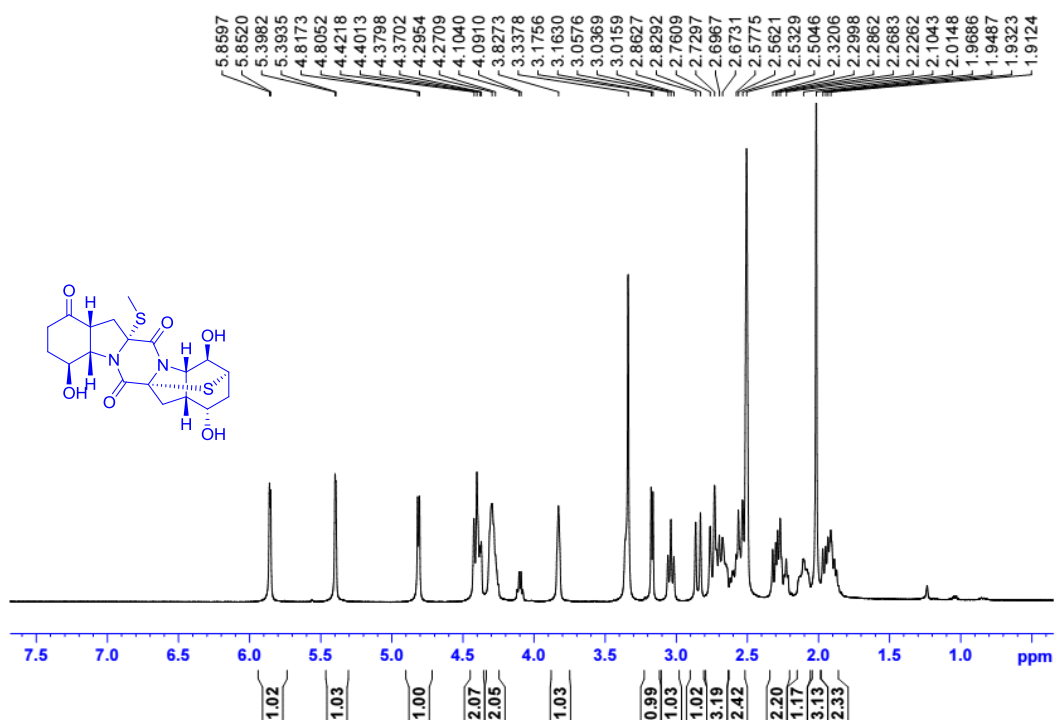


Fig S7-3 The ^1H NMR Spectrum of Compound 7

F1-8-7-1 APT DMSO 100 MHz

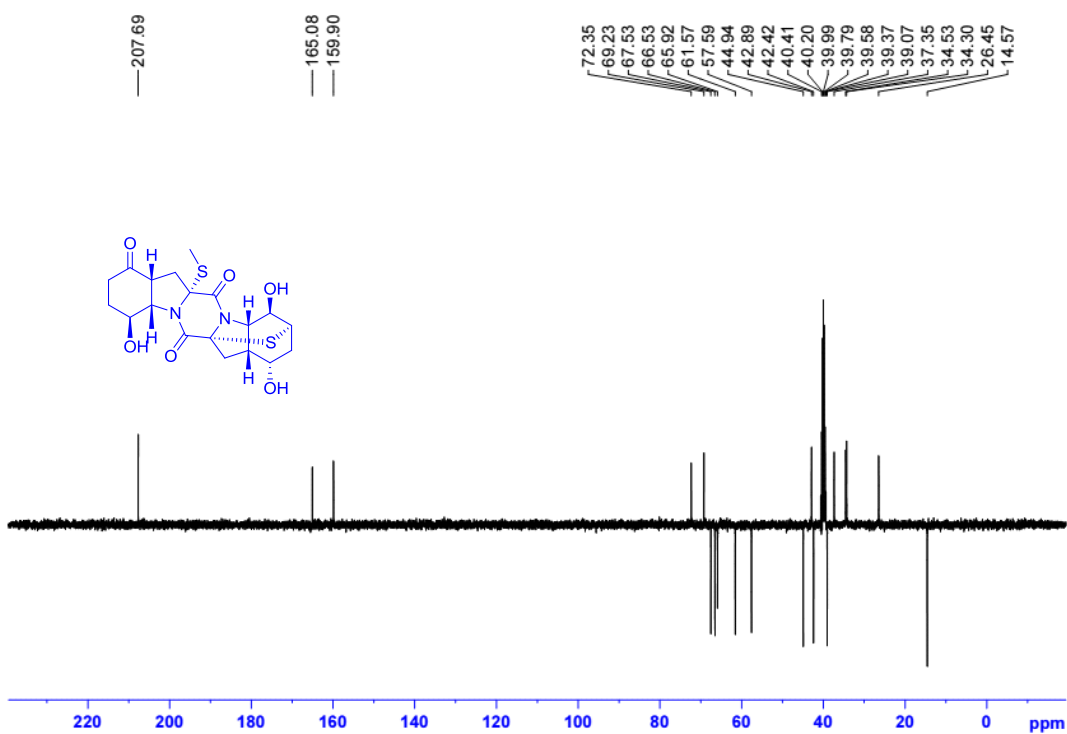


Fig S7-4 The APT Spectrum of Compound 7

F1-8-7-1 HSQC DMSO

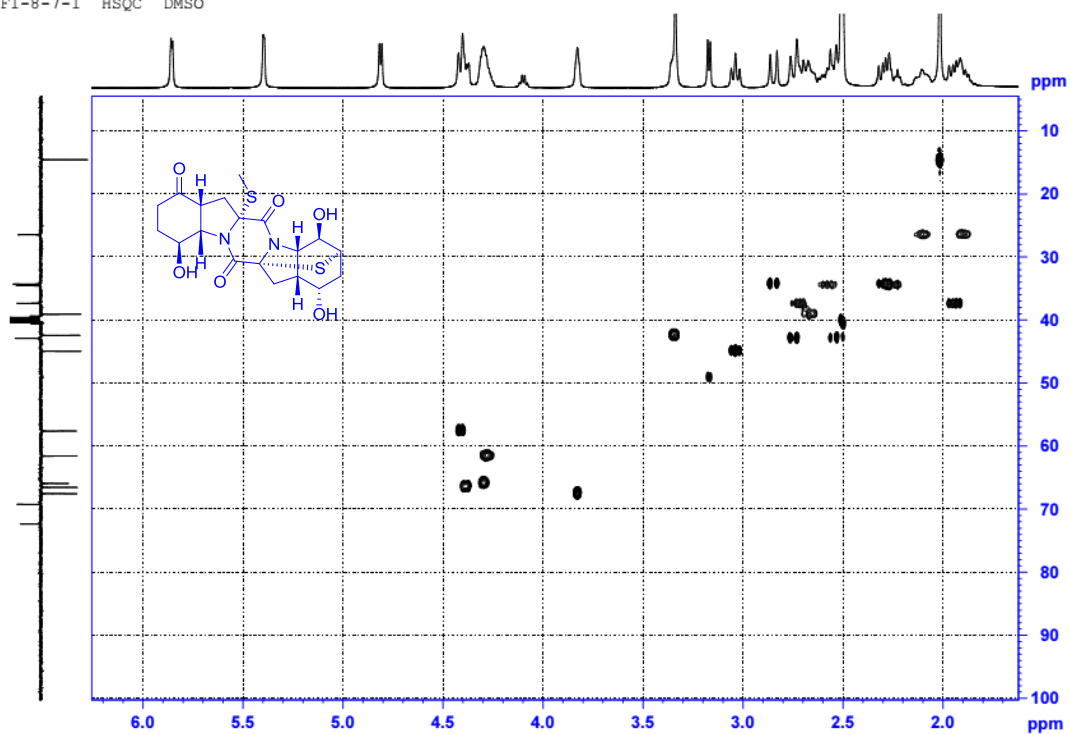


Fig S7-5 The HSQC Spectrum of Compound 7

F1-8-7-1 COSY DMSO

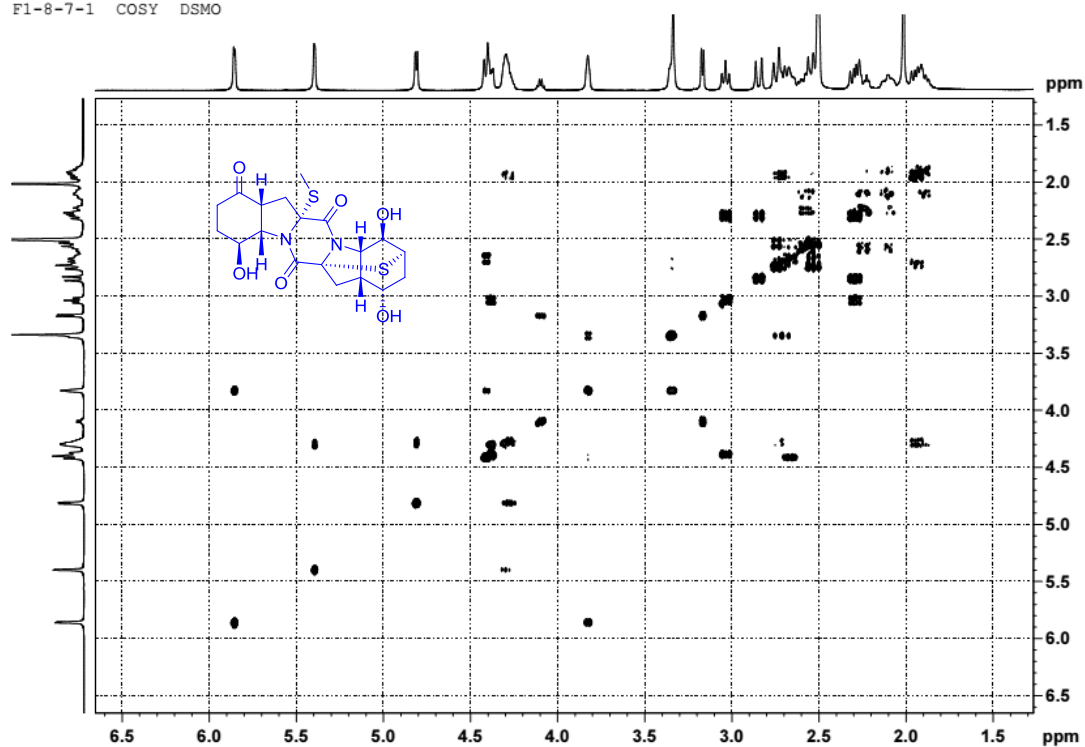


Fig S7-6 The ^1H - ^1H COSY Spectrum of Compound 7

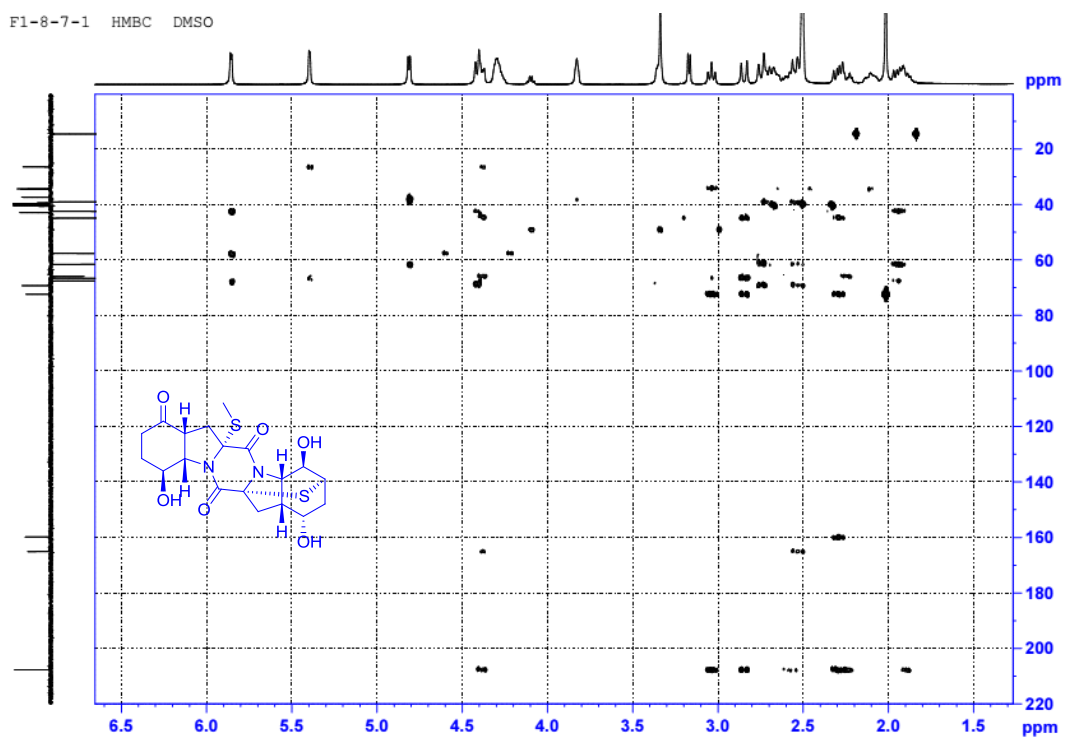


Fig S7-7 The HMBC Spectrum of Compound 7

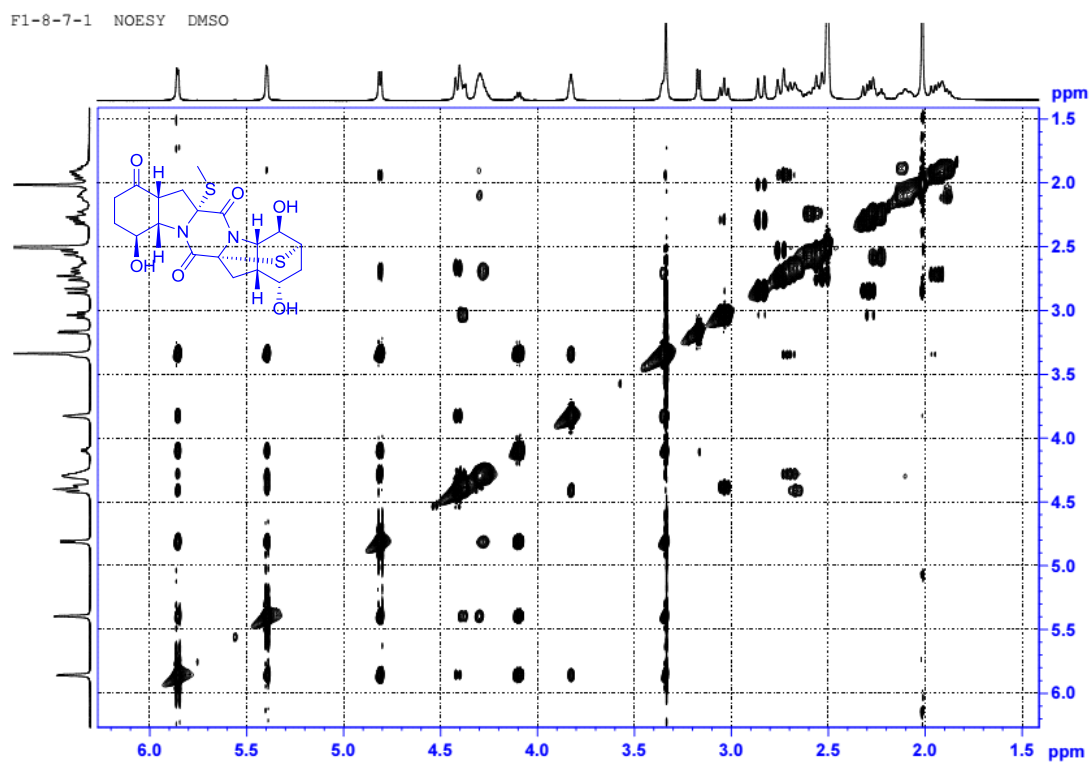


Fig S7-8 The NOESY Spectrum of Compound 7

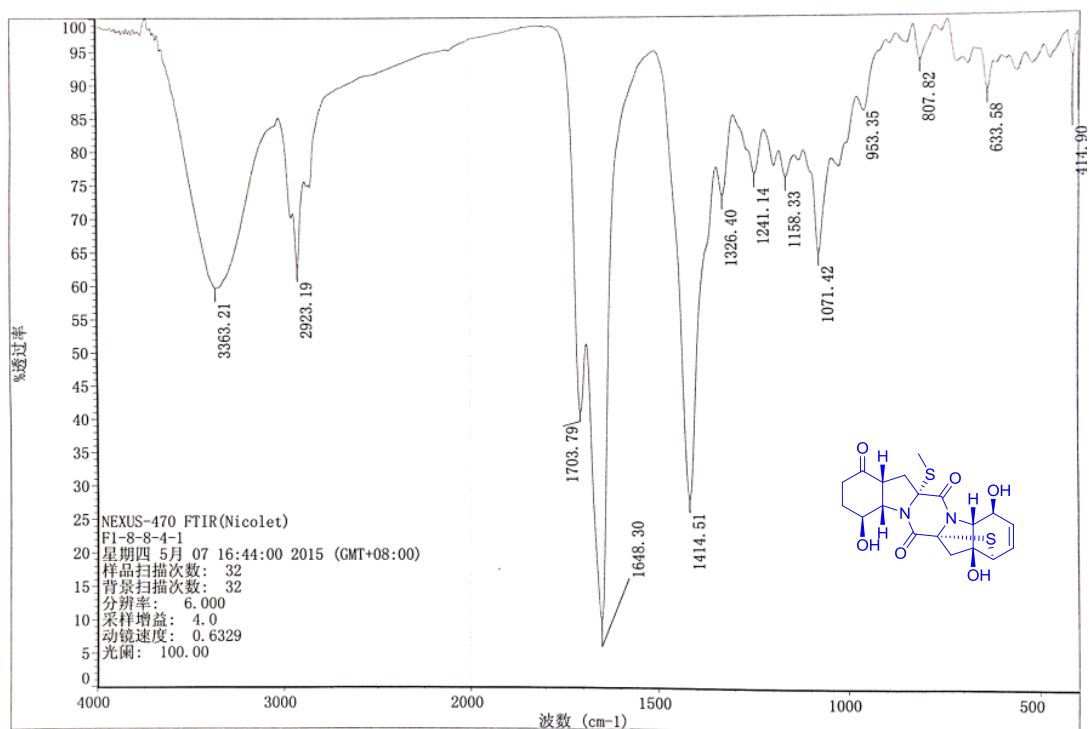


Fig S8-1 IR Spectrum of Compound 8

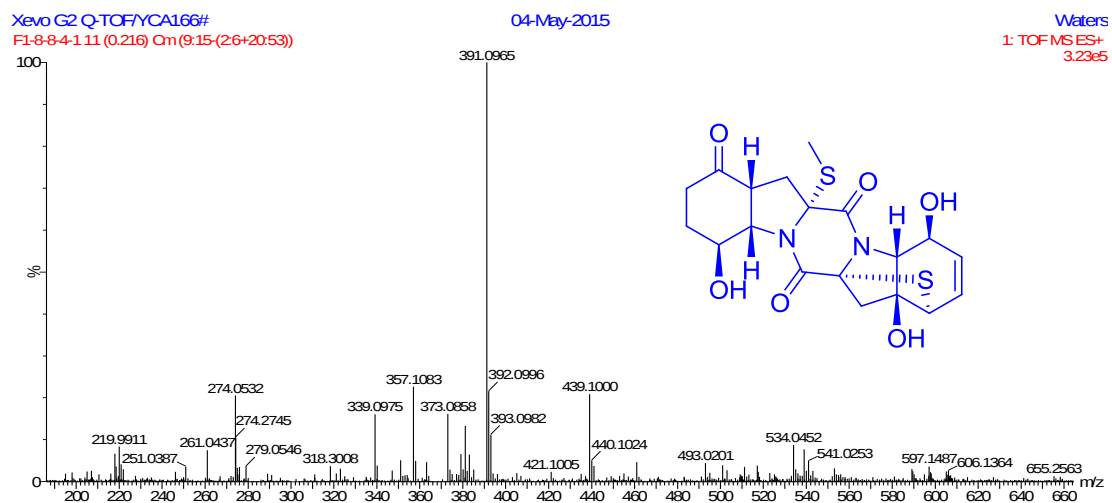


Fig S8-2 HRESIMS Data of Compound 8

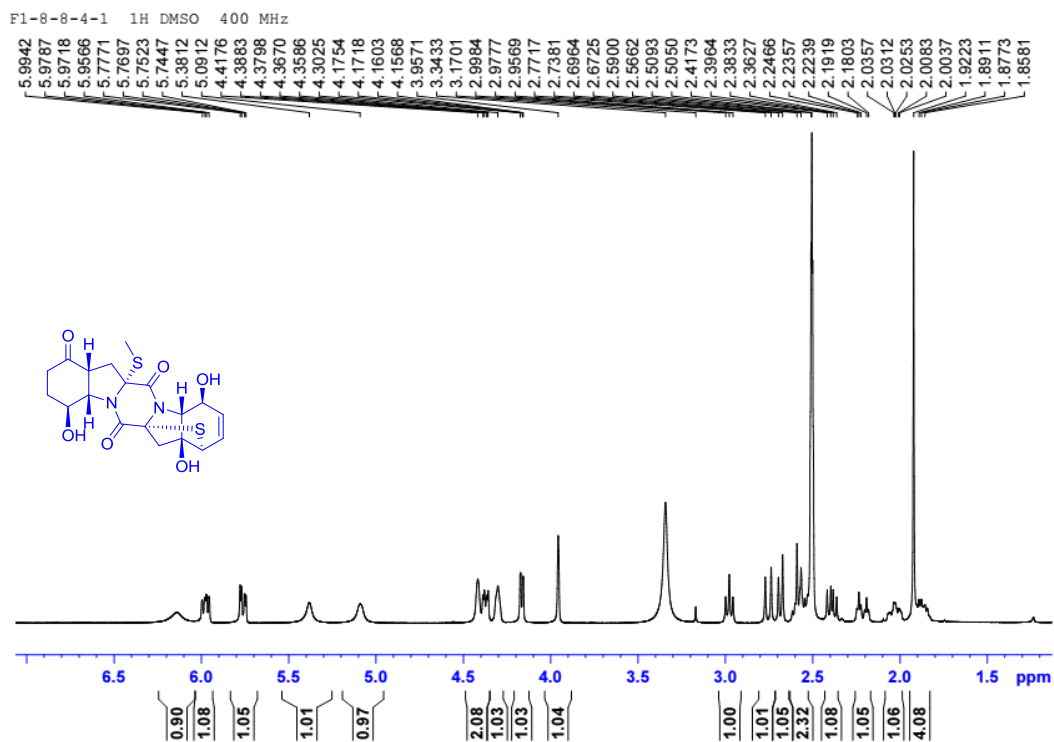


Fig S8-3 The ^1H NMR Spectrum of Compound **8**

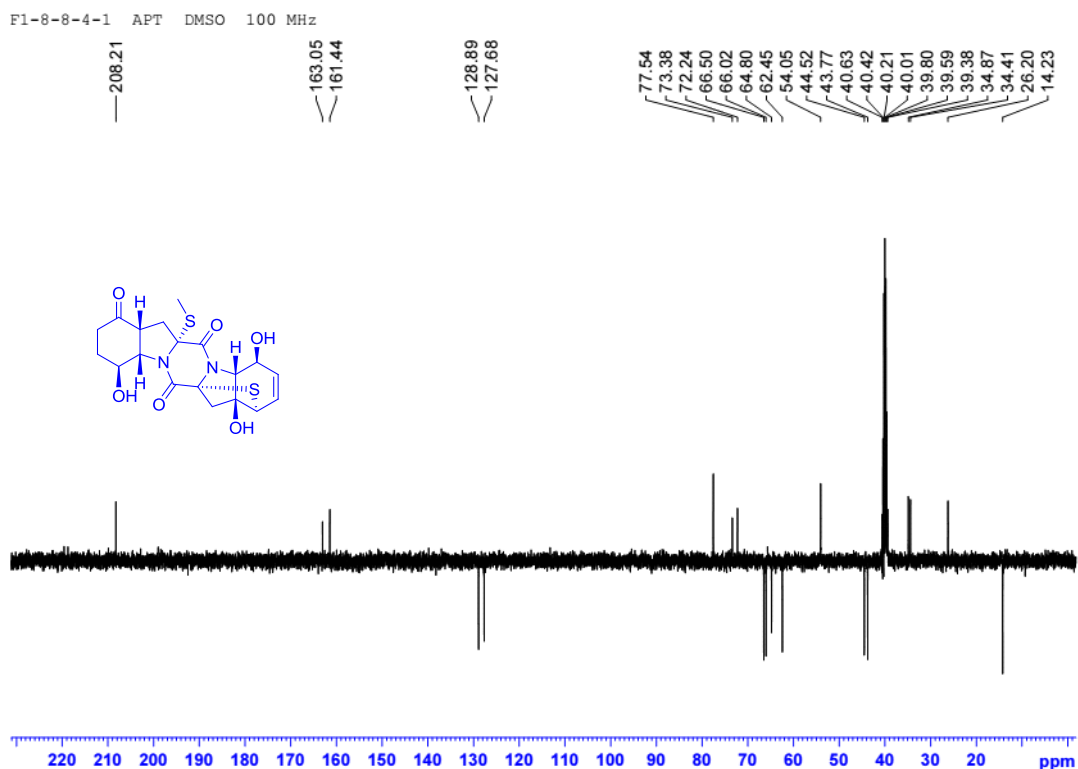


Fig S8-4 The APT Spectrum of Compound **8**

F1-8-8-4-1 HSQC DMSO

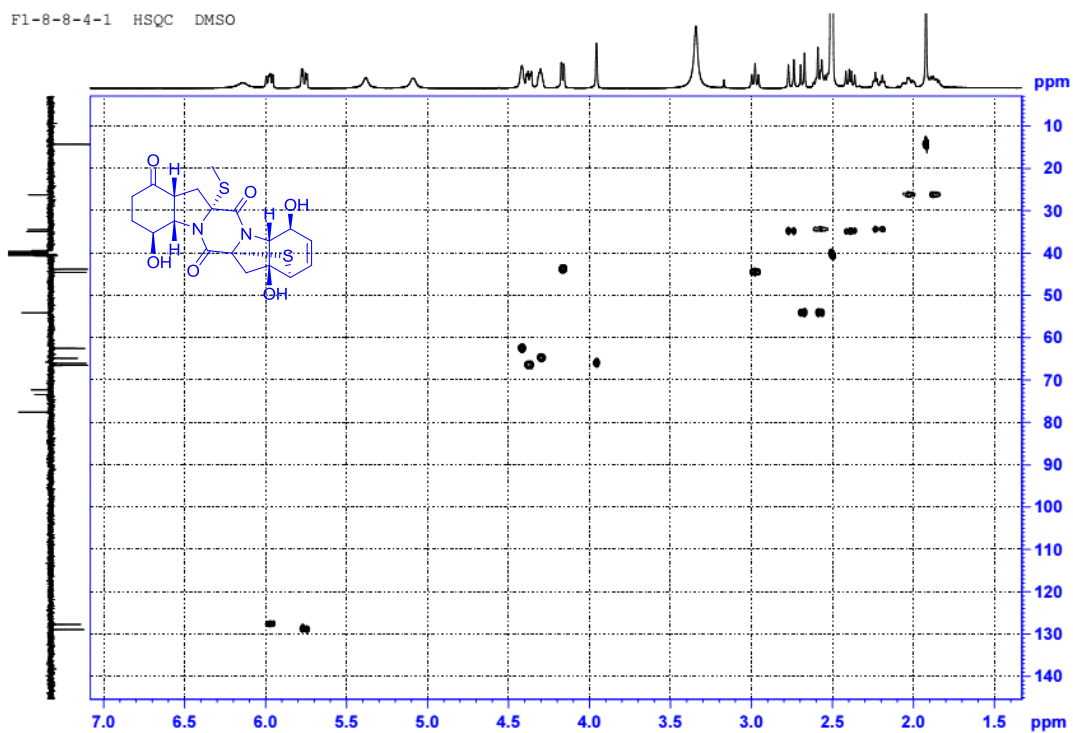


Fig S8-5 The HSQC Spectrum of Compound **8**

F1-8-8-4-1 COSY DMSO

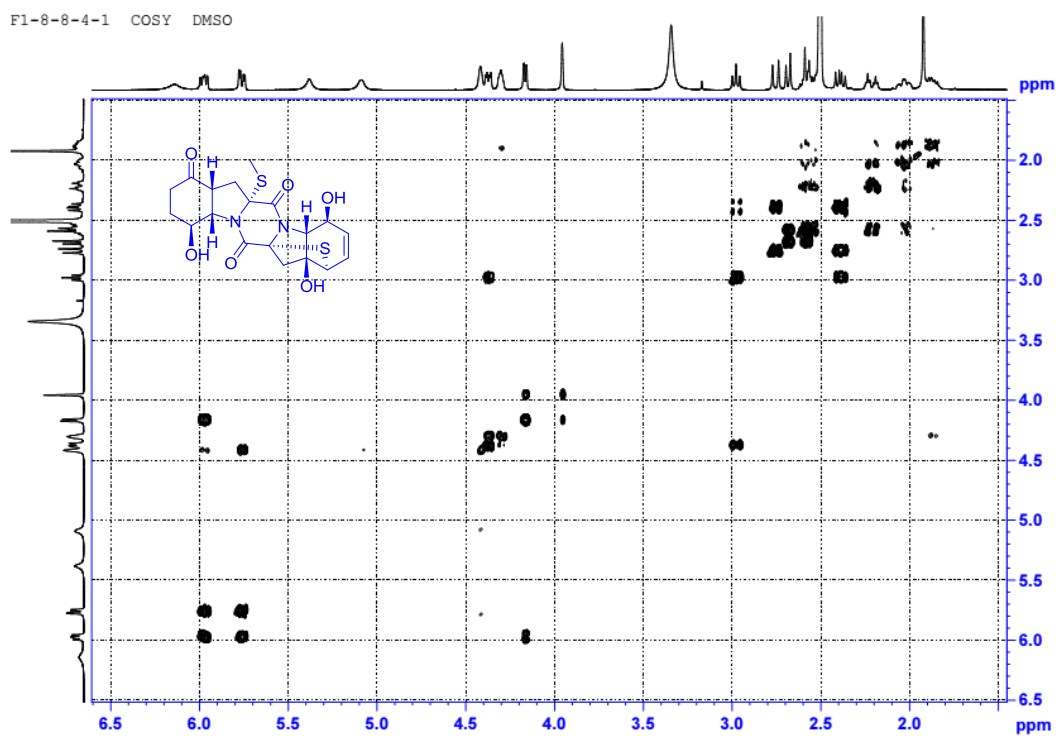


Fig S8-6 The ^1H - ^1H COSY Spectrum of Compound **8**

F1-8-8-4-1 HMBC DMSO

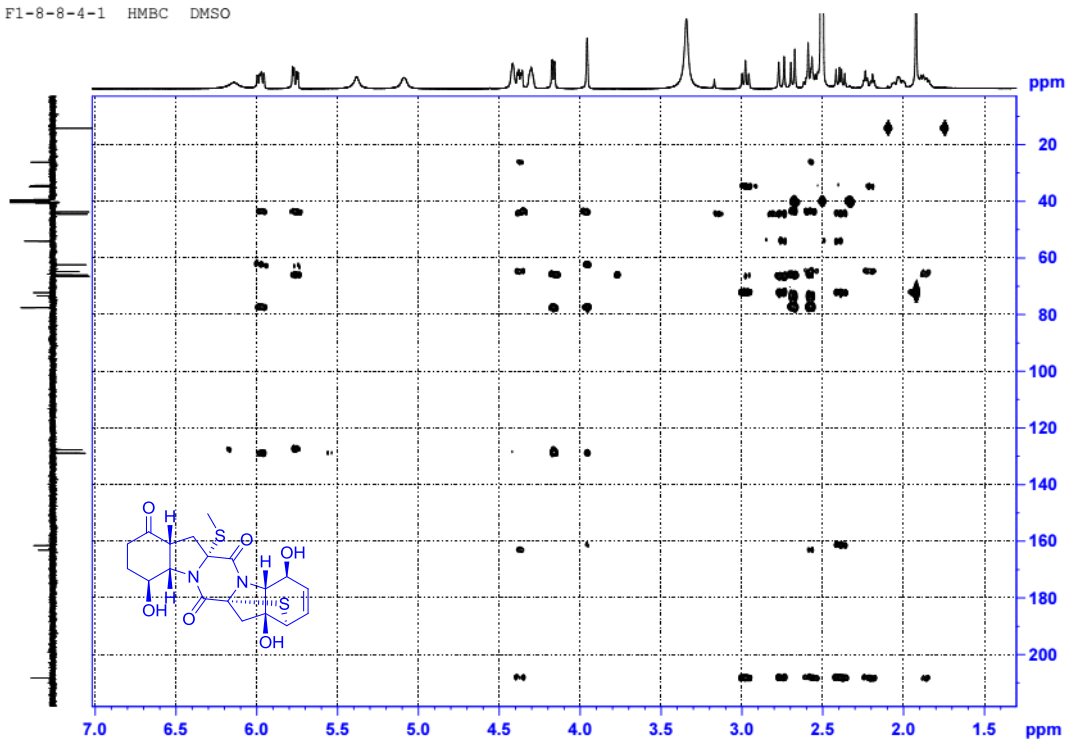


Fig S8-7 The HMBC Spectrum of Compound 8

F1-8-8-4-1 NOESY DMSO

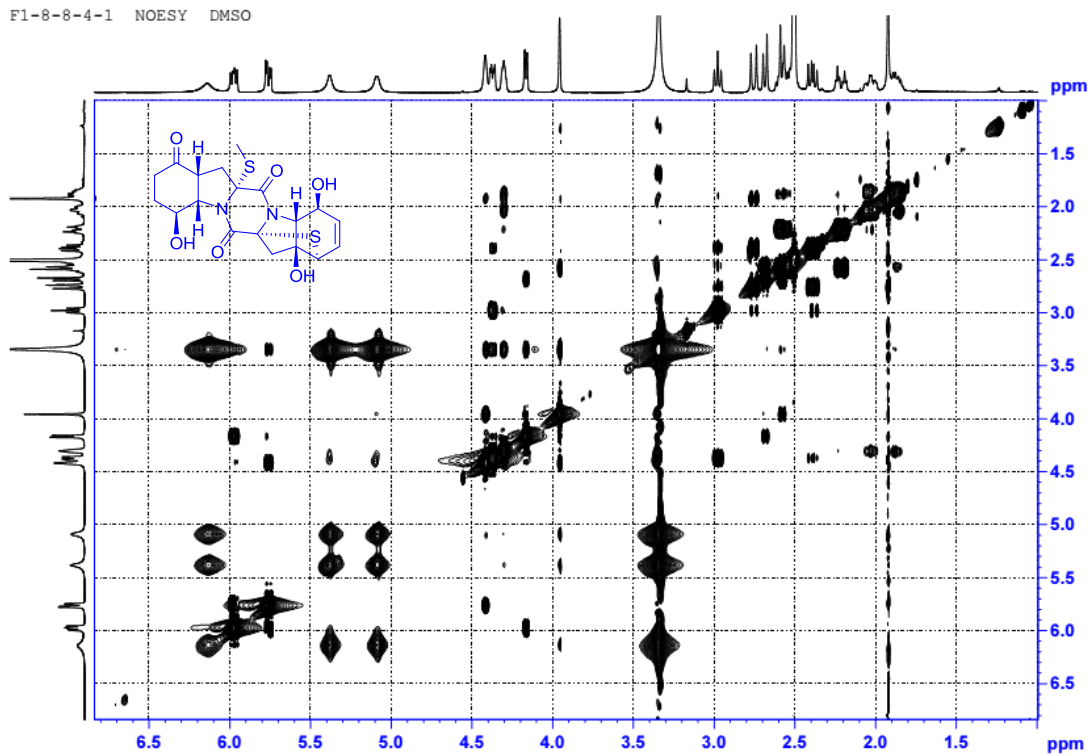


Fig S8-8 The NOESY Spectrum of Compound 8

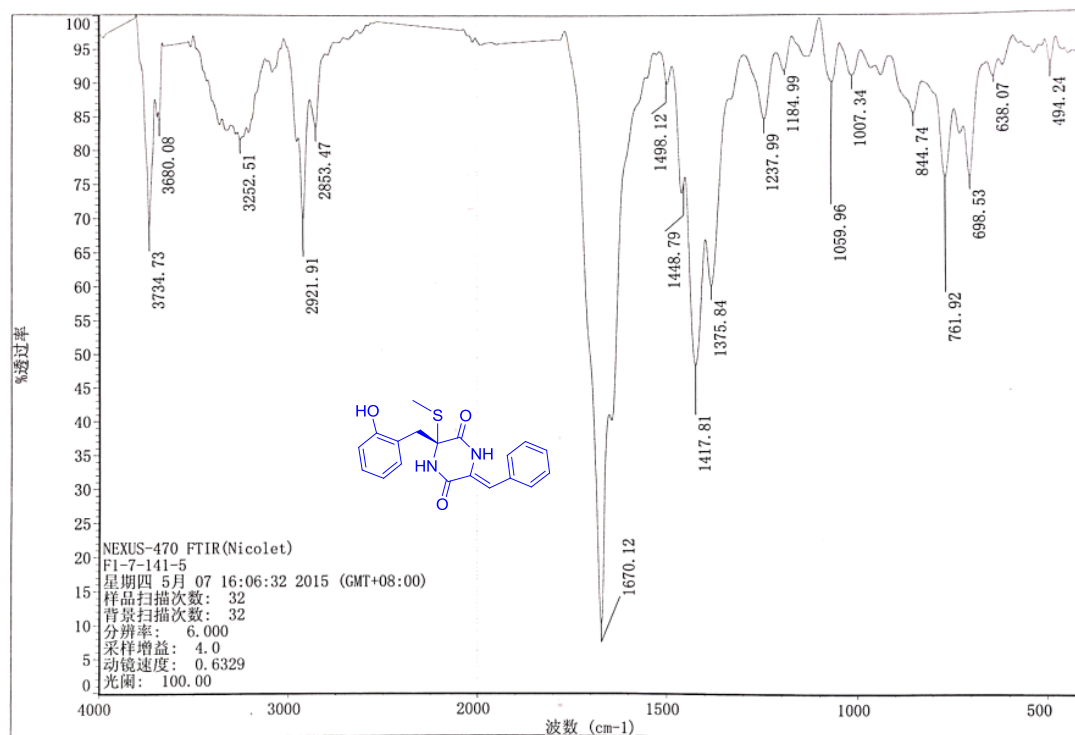


Fig S9-1 IR Spectrum of Compound 9

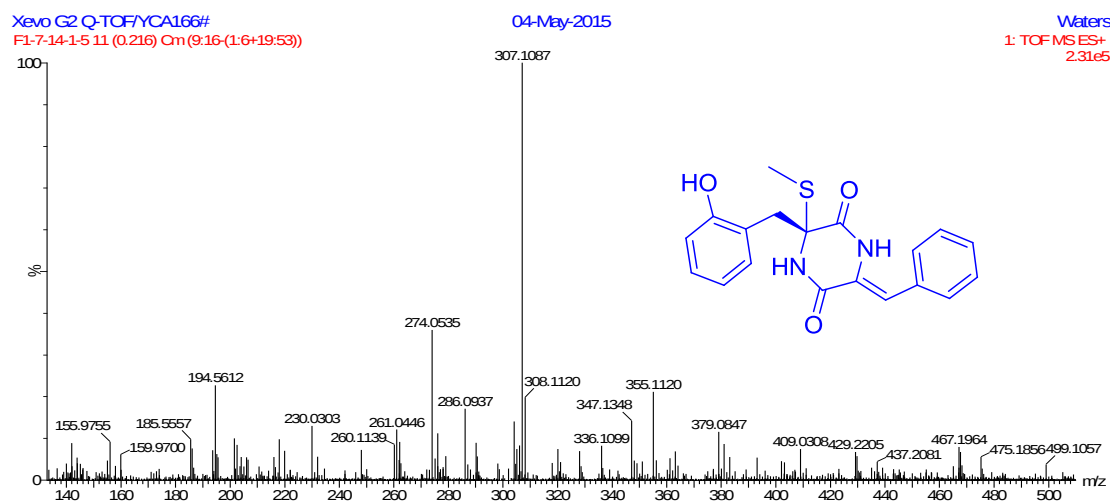


Fig S9-2 HRESIMS Data of Compound 9

F1-7-14-1-5 1H DMSO 400 MHz

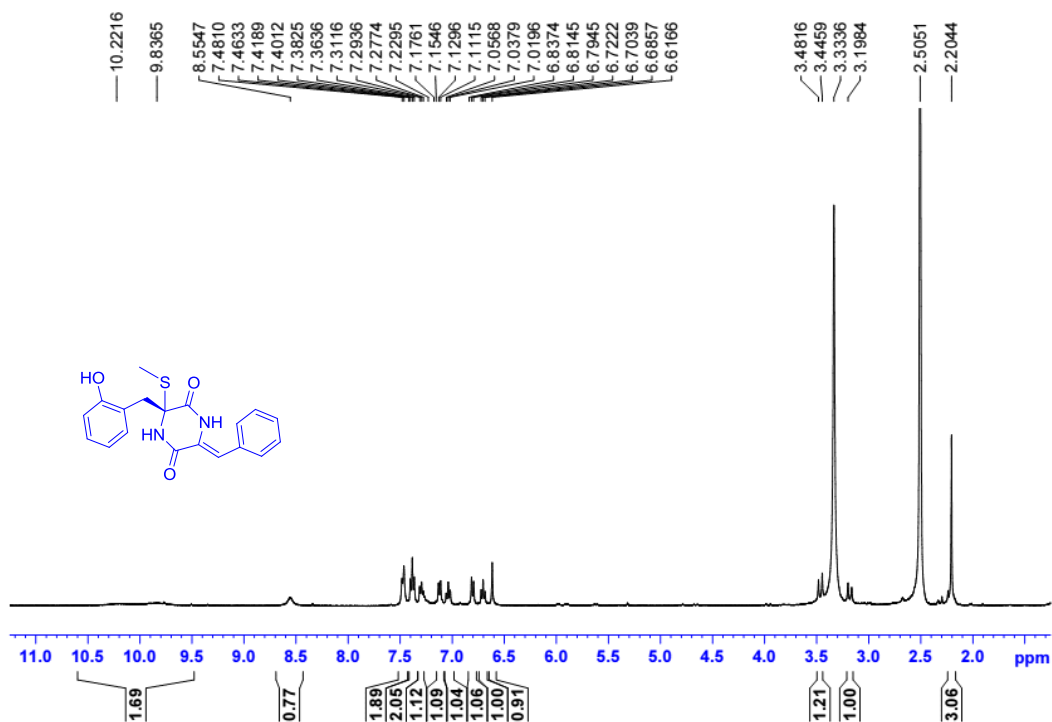


Fig S9-3 The ^1H NMR Spectrum of Compound 9

F1-7-14-1-5 APT DMSO 100 MHz

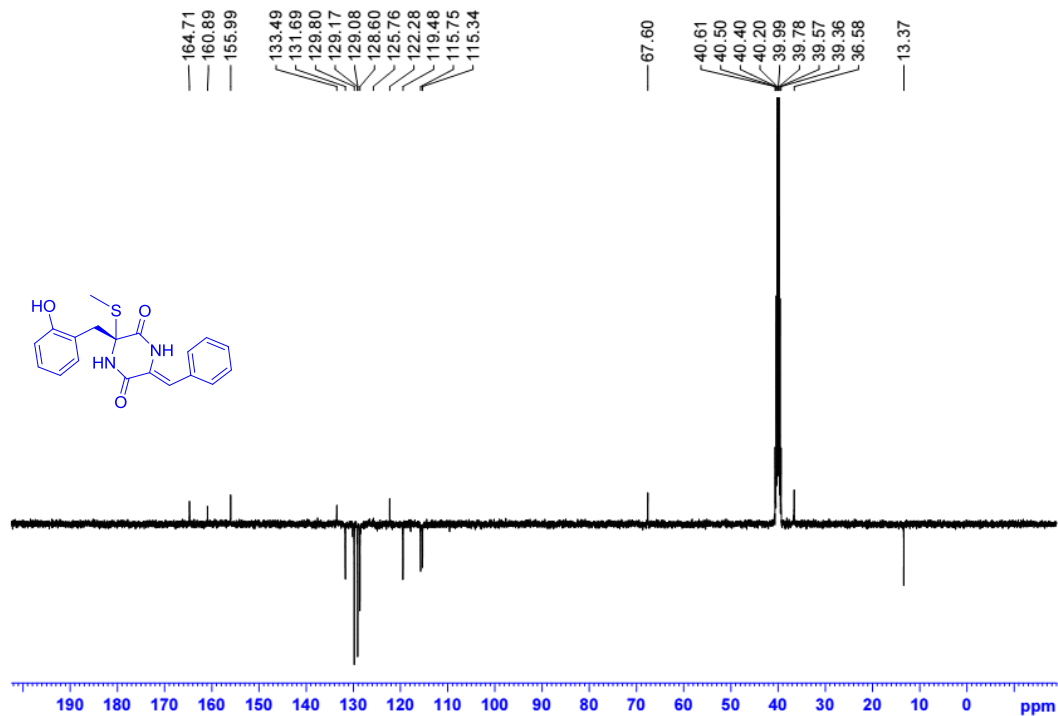


Fig S9-4 The APT Spectrum of Compound 9

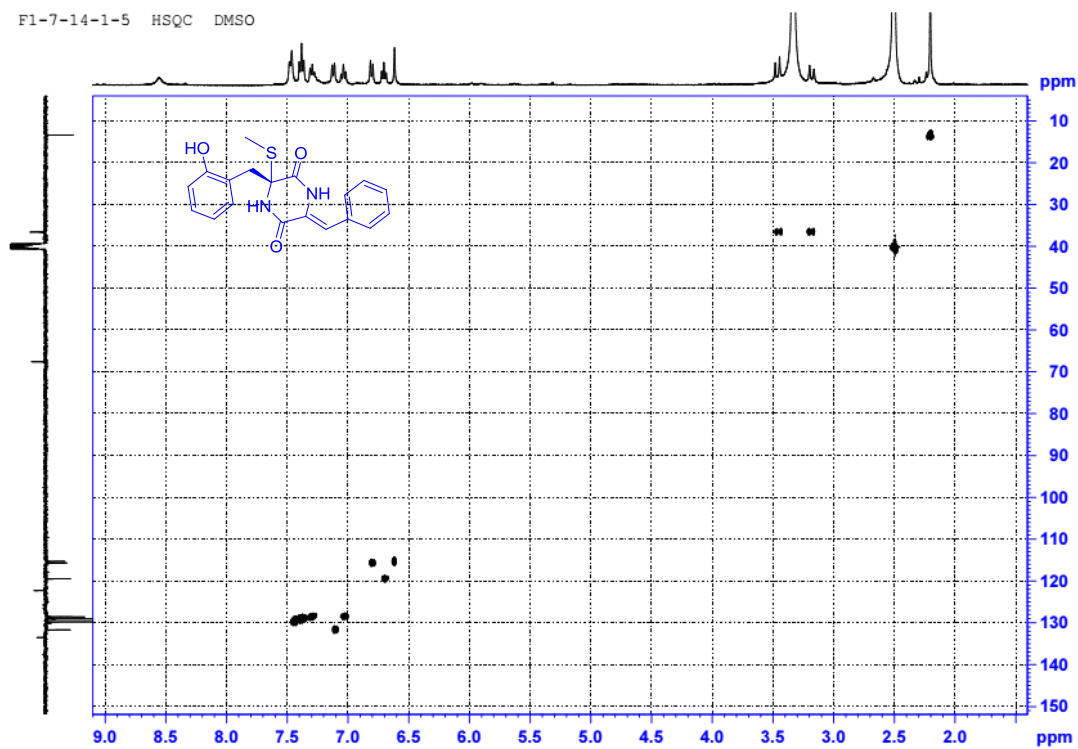


Fig S9-5 The HSQC Spectrum of Compound 9

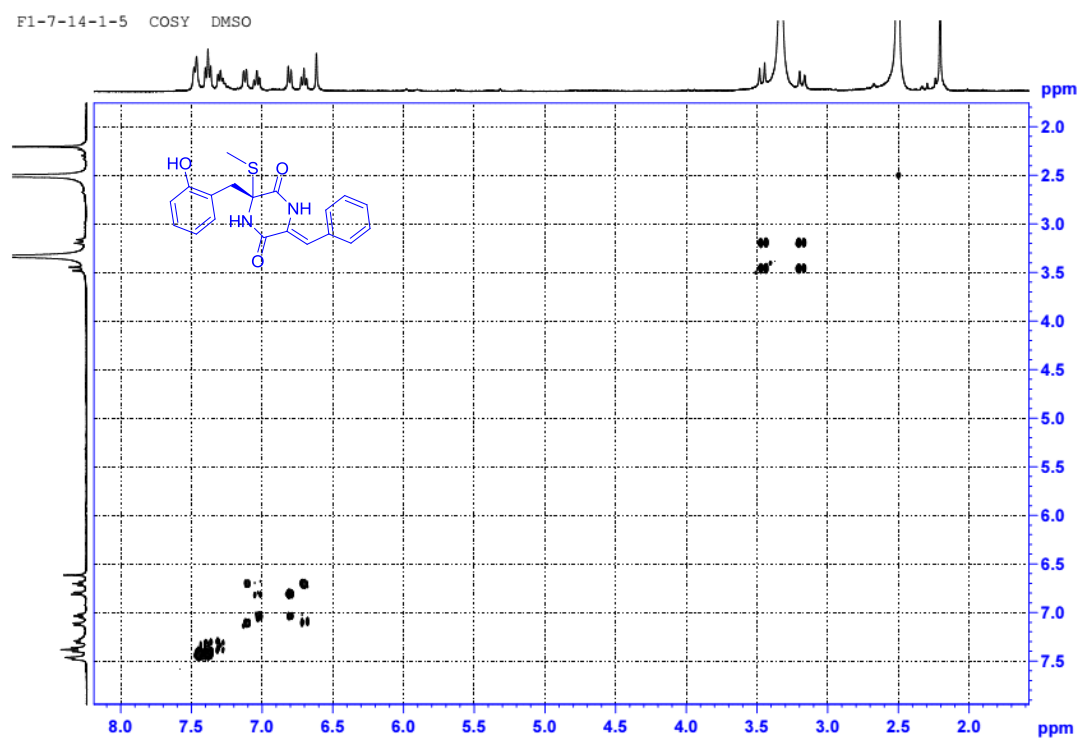


Fig S9-6 The ^1H - ^1H COSY Spectrum of Compound 9

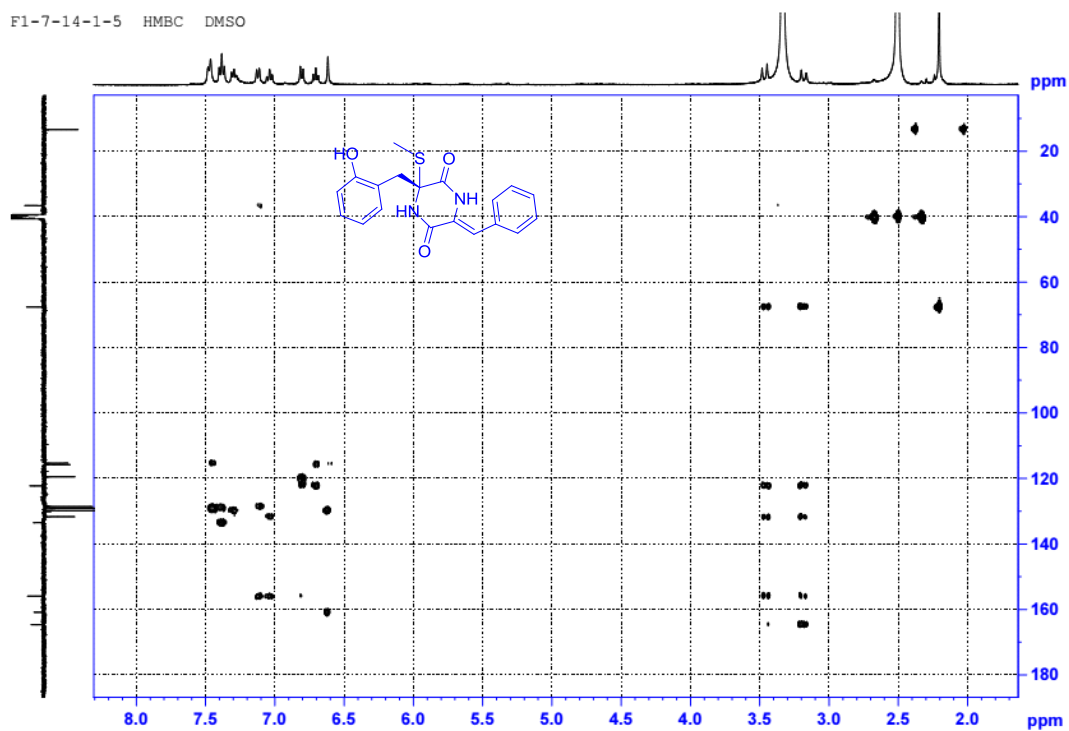


Fig S9-7 The HMBC Spectrum of Compound 9

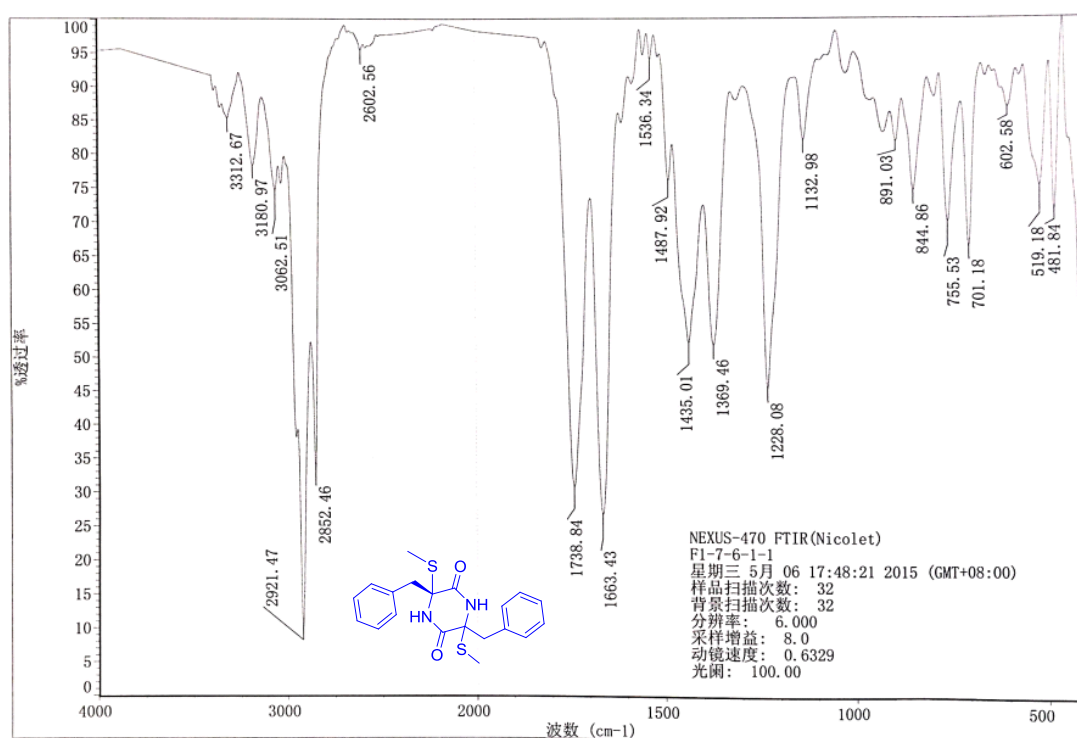


Fig S10-1 IR Spectrum of Compound 10

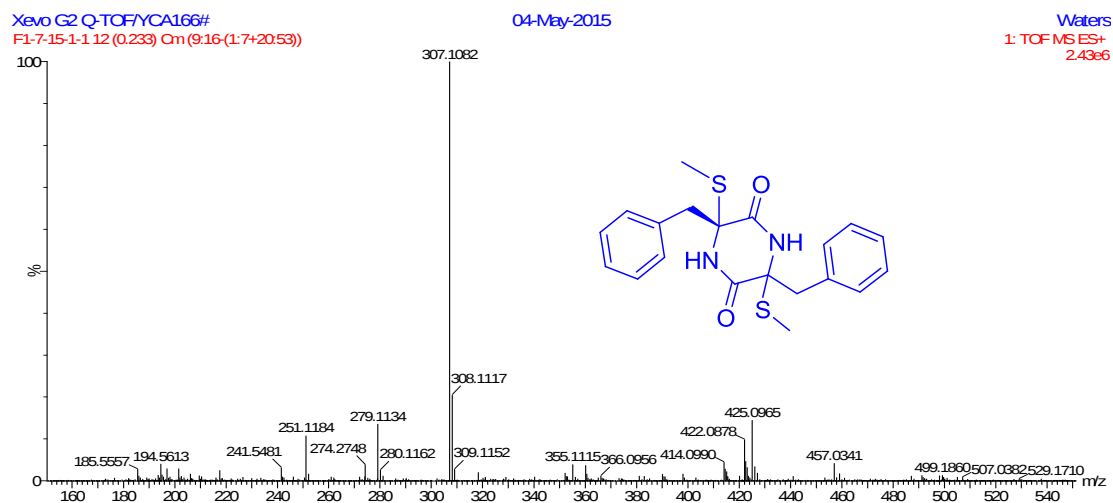


Fig S10-2 HRESIMS Data of Compound 10

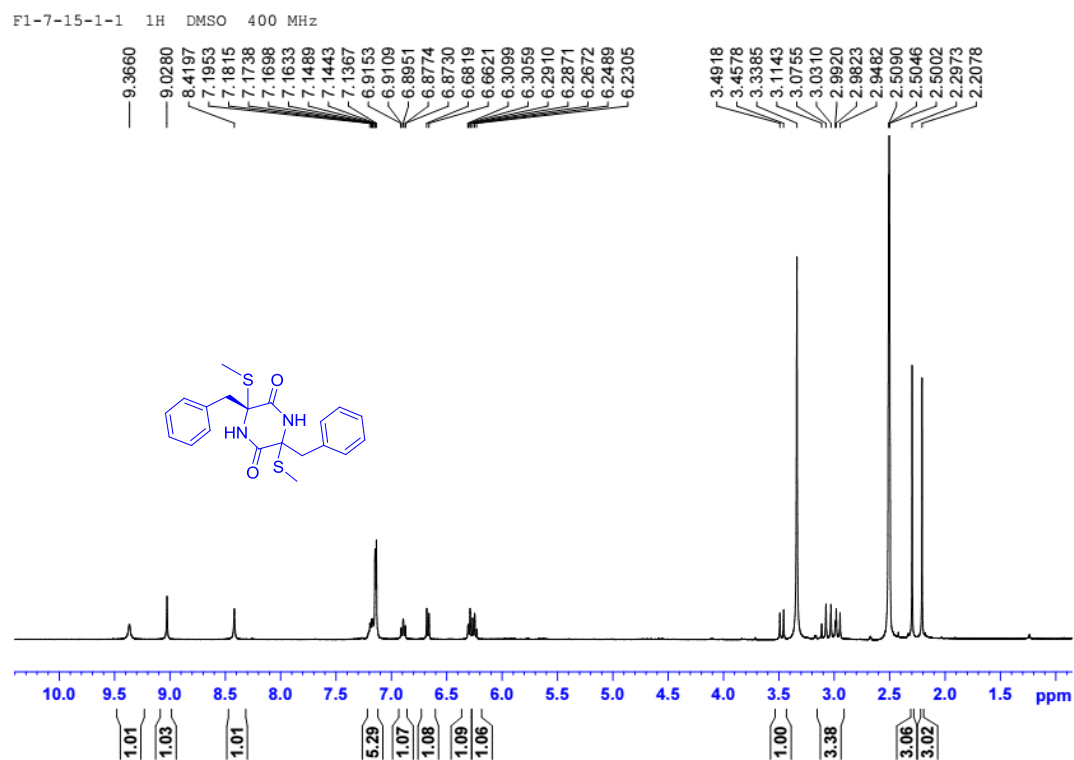


Fig S10-3 The ^1H NMR Spectrum of Compound 10

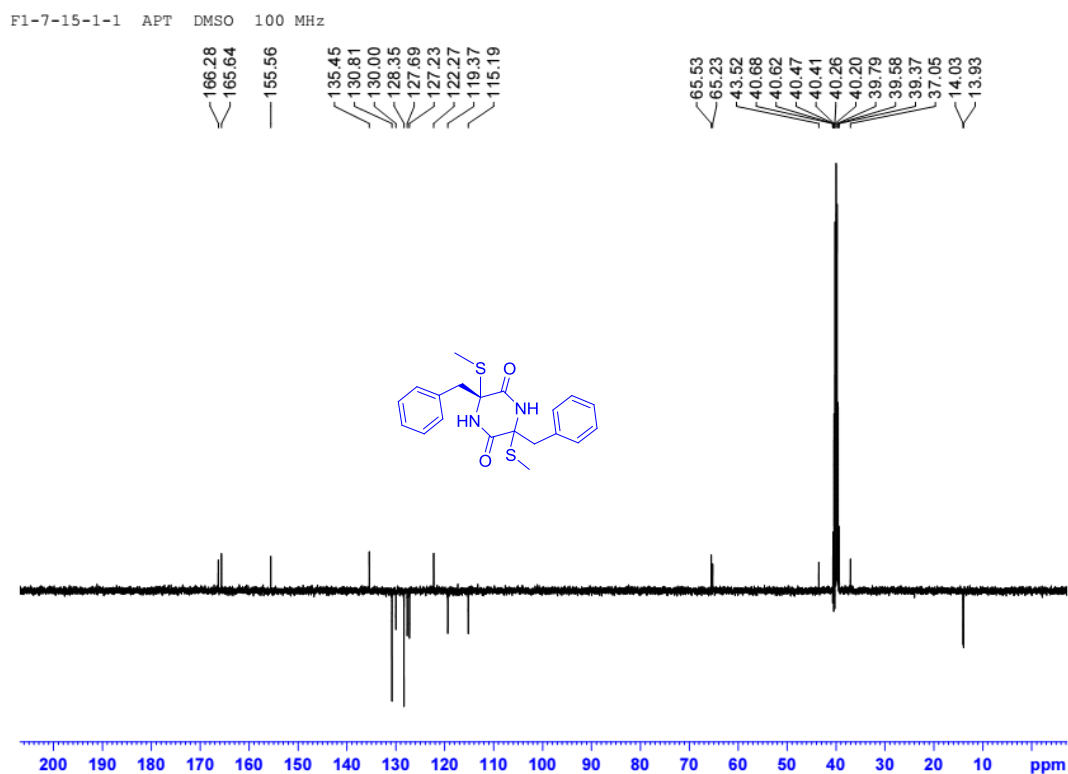


Fig S10-4 The APT Spectrum of Compound 10

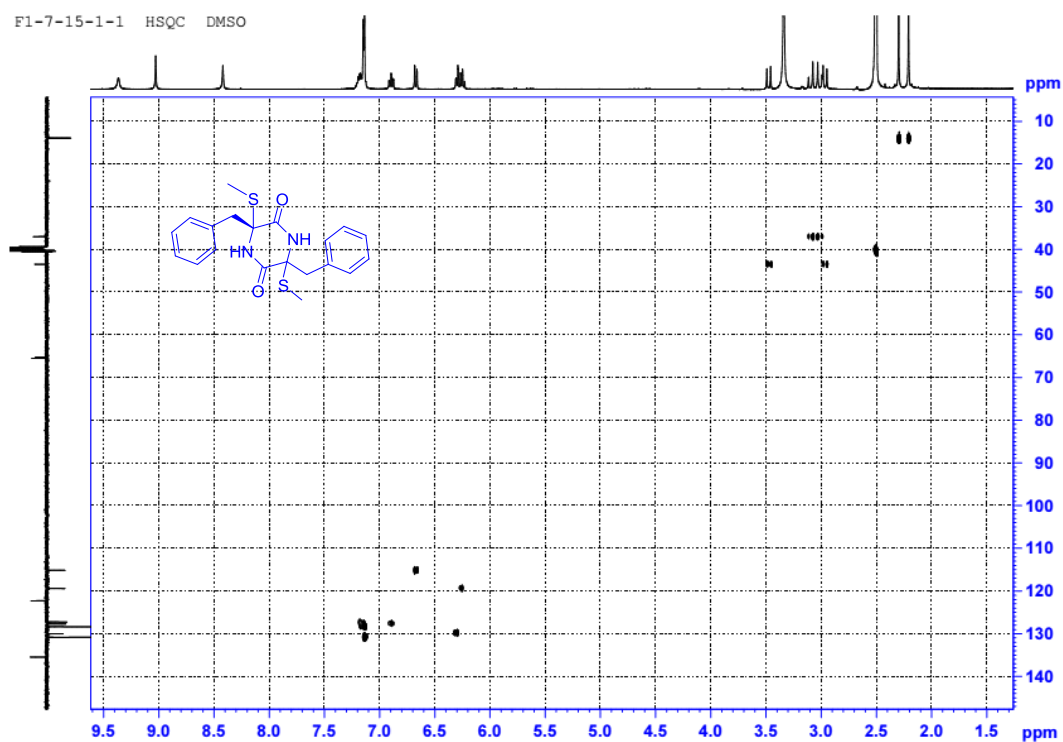


Fig S10-5 The HSQC Spectrum of Compound 10

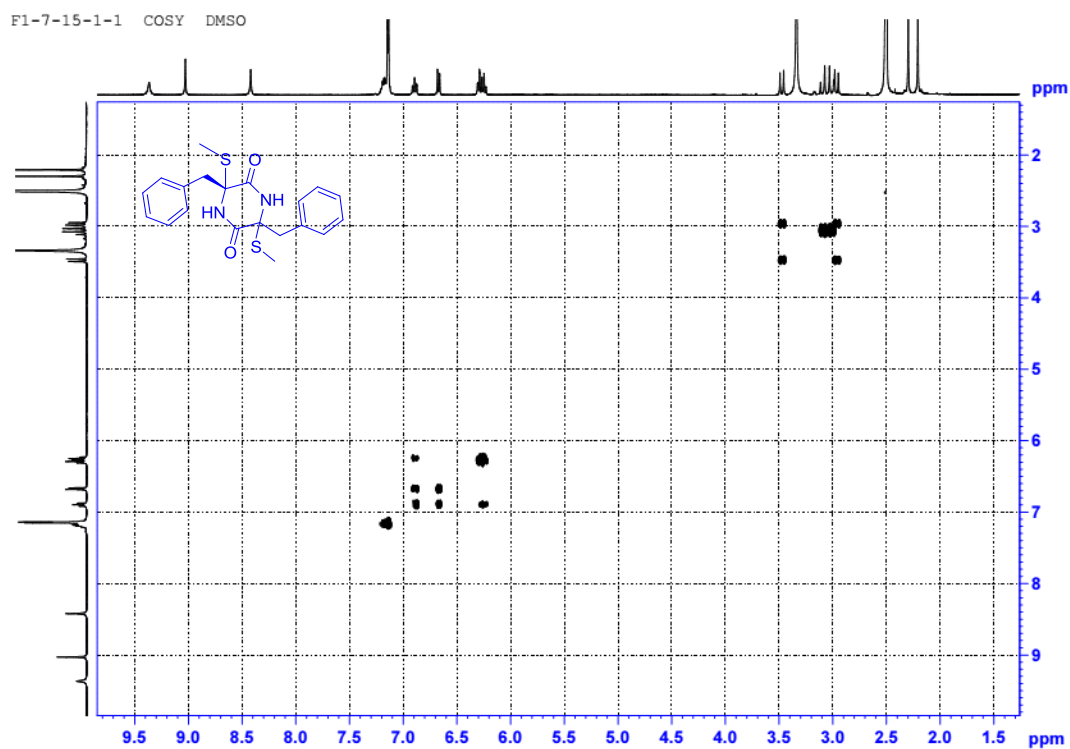


Fig S10-6 The ^1H - ^1H COSY Spectrum of Compound 10

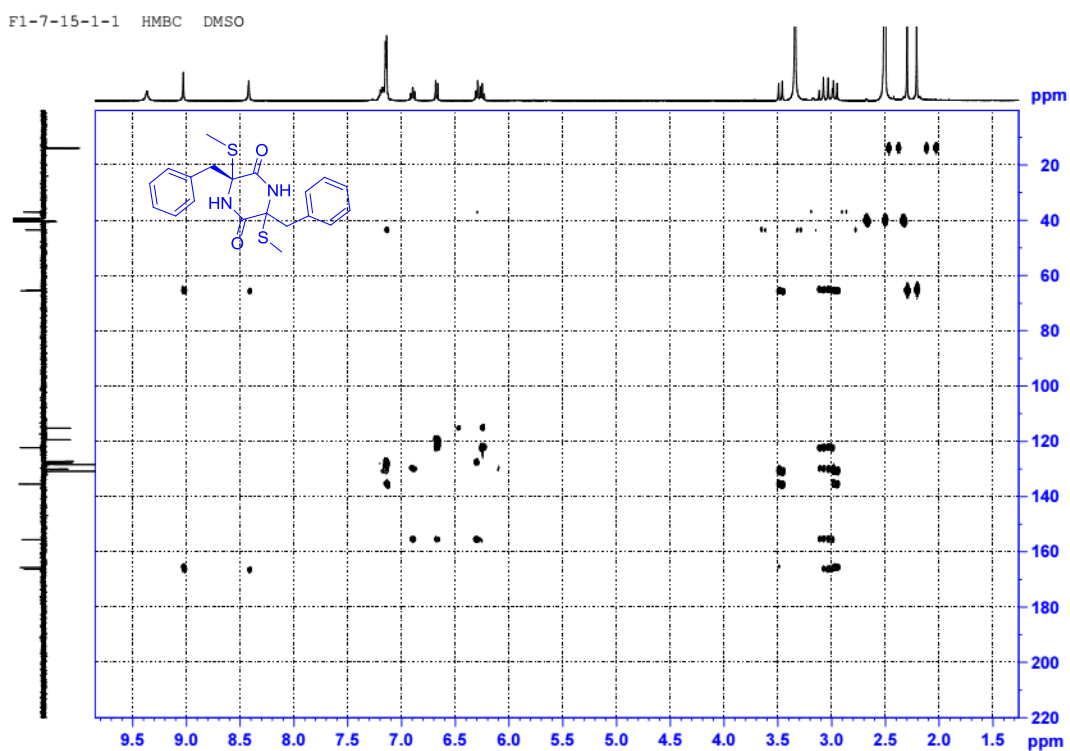


Fig S10-7 The HMBC Spectrum of Compound 10

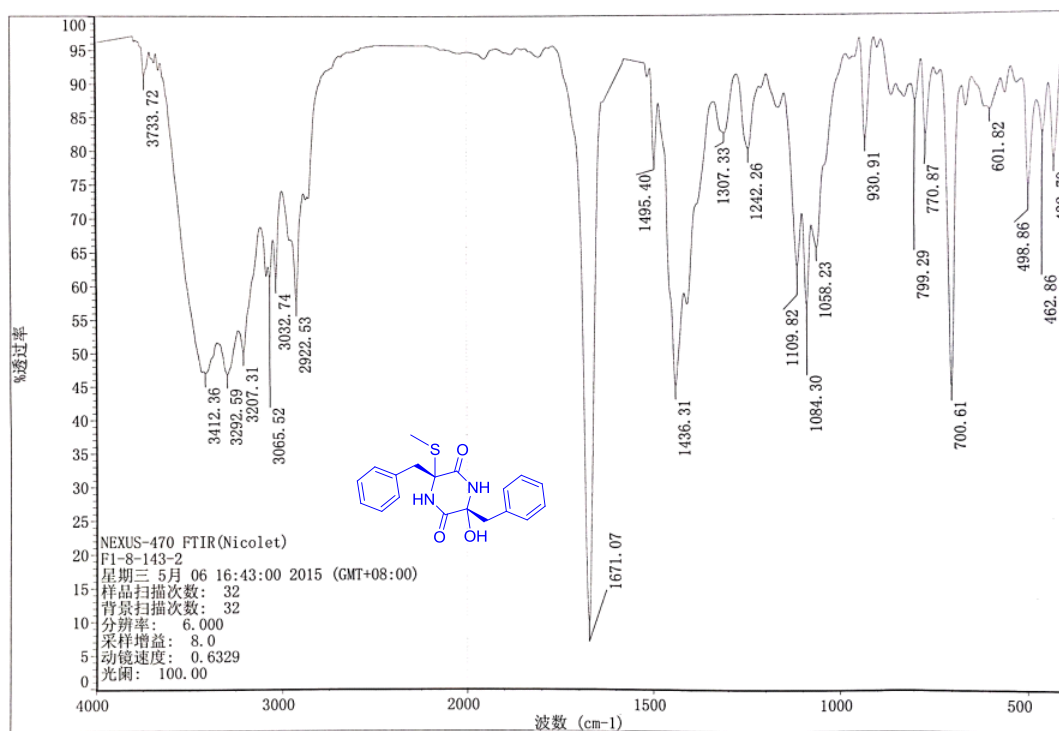


Fig S11-1 IR Spectrum of Compound **11**

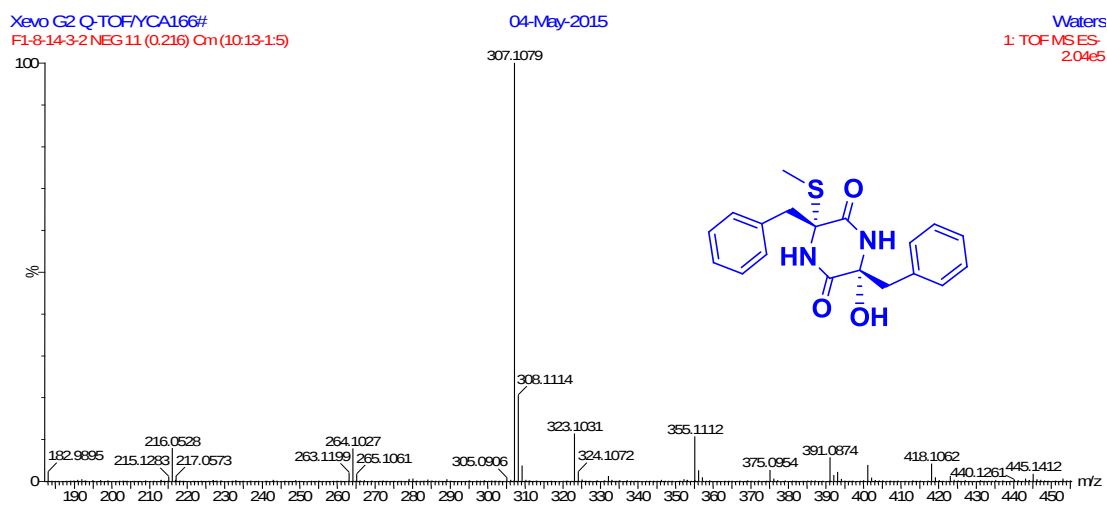


Fig S11-2 HRESIMS Data of Compound **11**

F1-8-14-3-2 1H DMSO 400 MHz

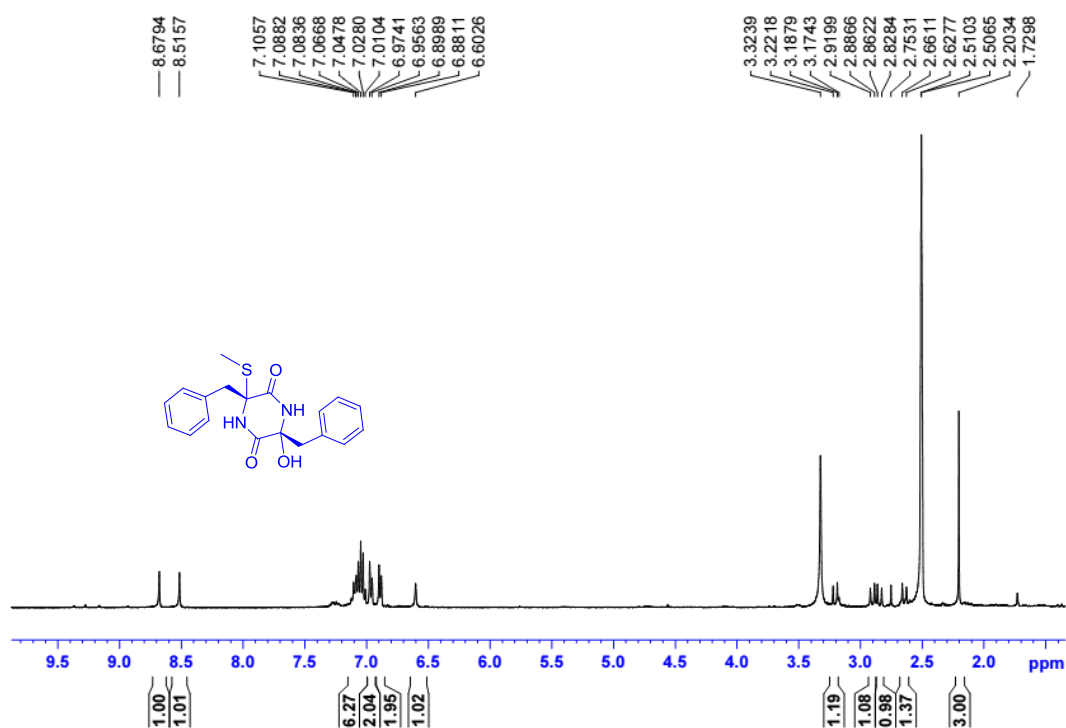


Fig S11-3 The ^1H NMR Spectrum of Compound **11**

F1-8-14-3-2 APT DMSO 100 MHz

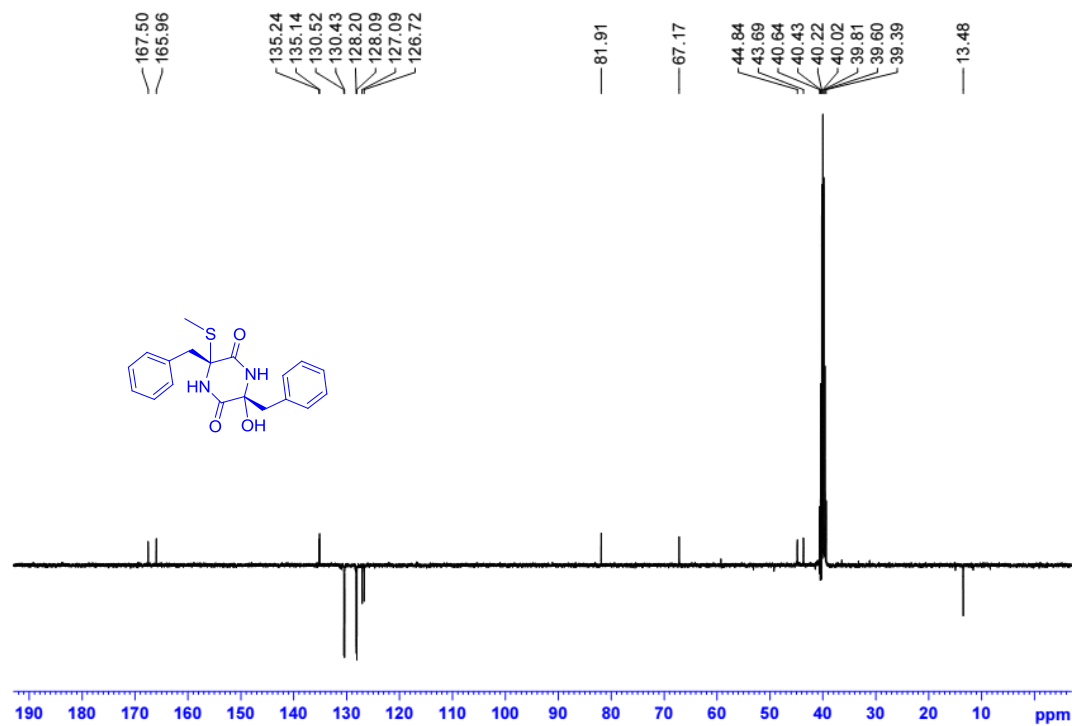


Fig S11-4 The APT Spectrum of Compound **11**

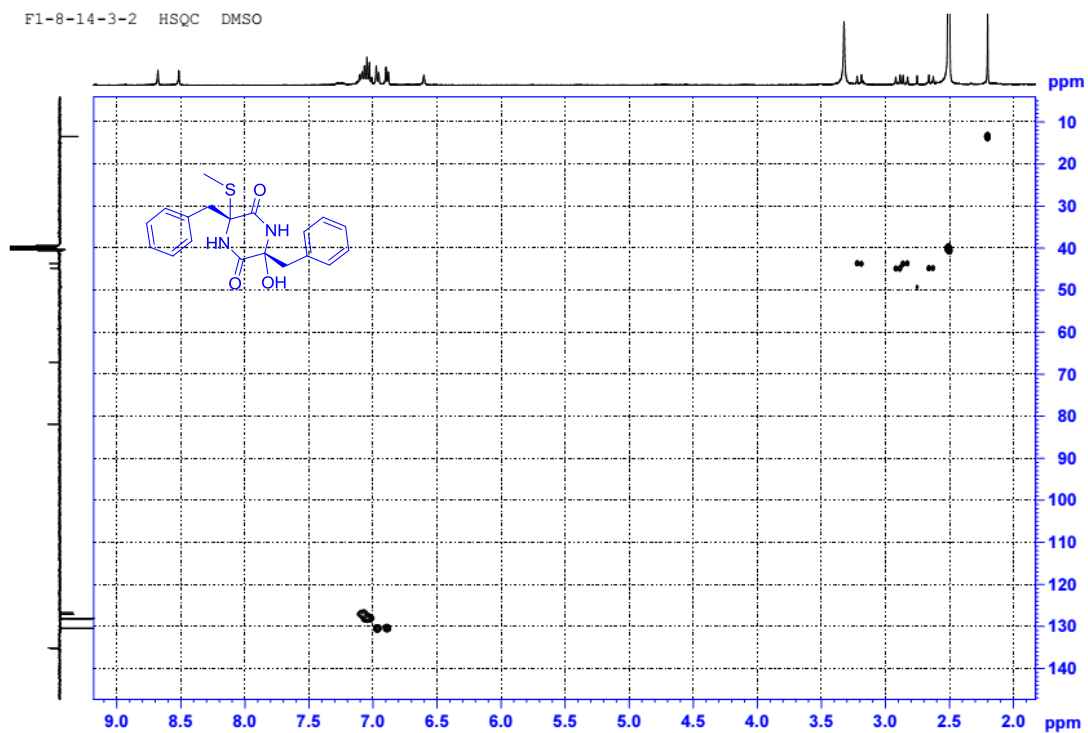


Fig S11-5 The HSQC Spectrum of Compound **11**

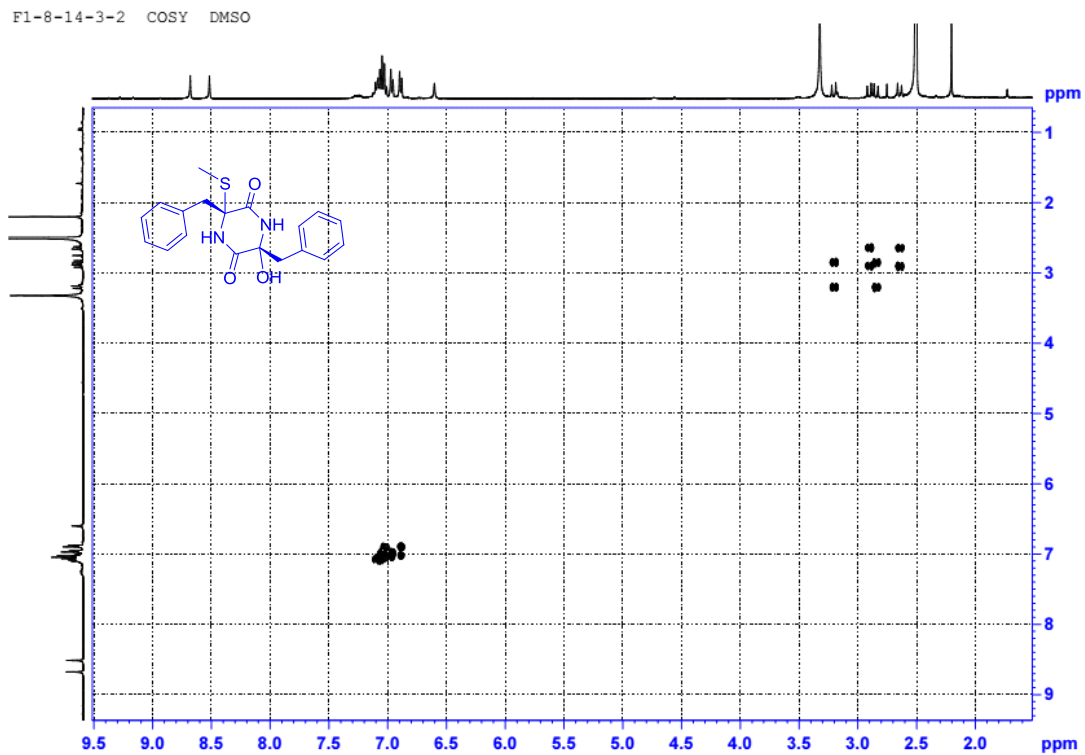


Fig S11-6 The ^1H - ^1H COSY Spectrum of Compound **11**

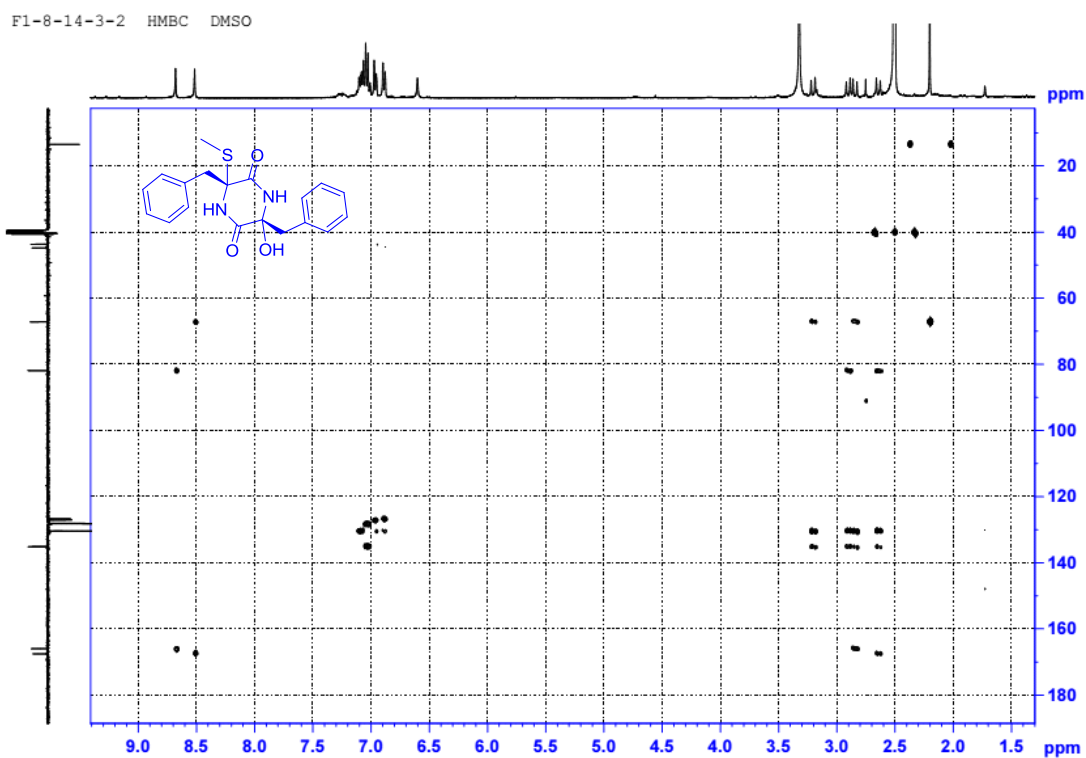


Fig S11-7 The HMBC Spectrum of Compound 11

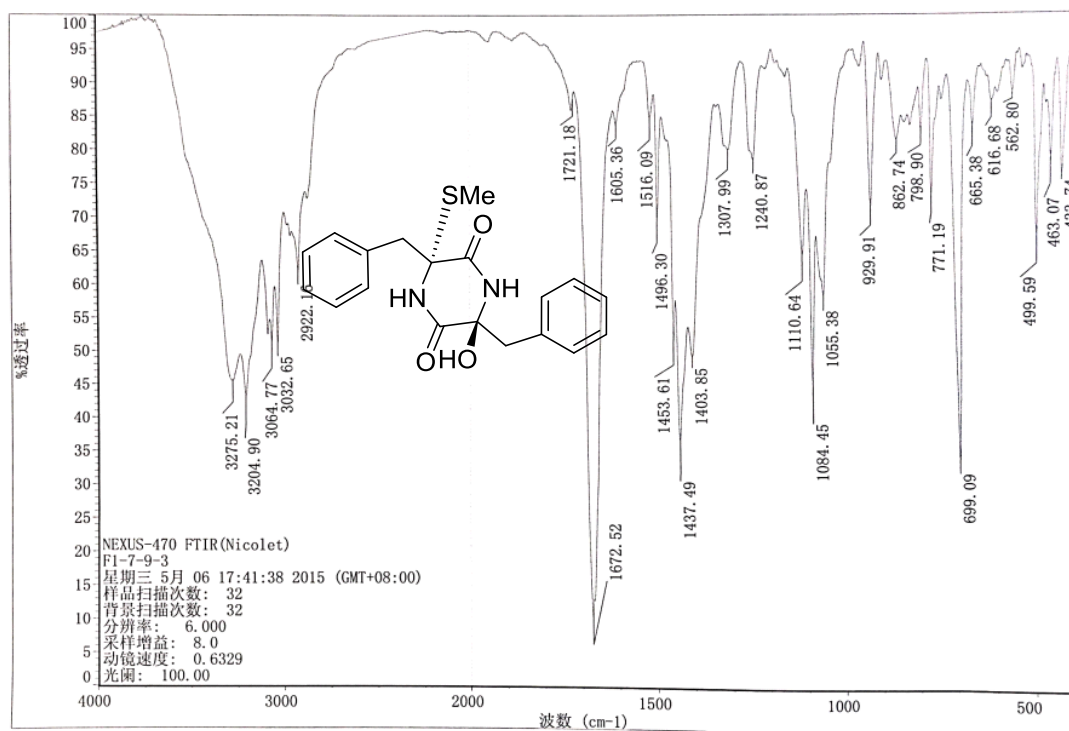


Fig S12-1 IR Spectrum of Compound 12

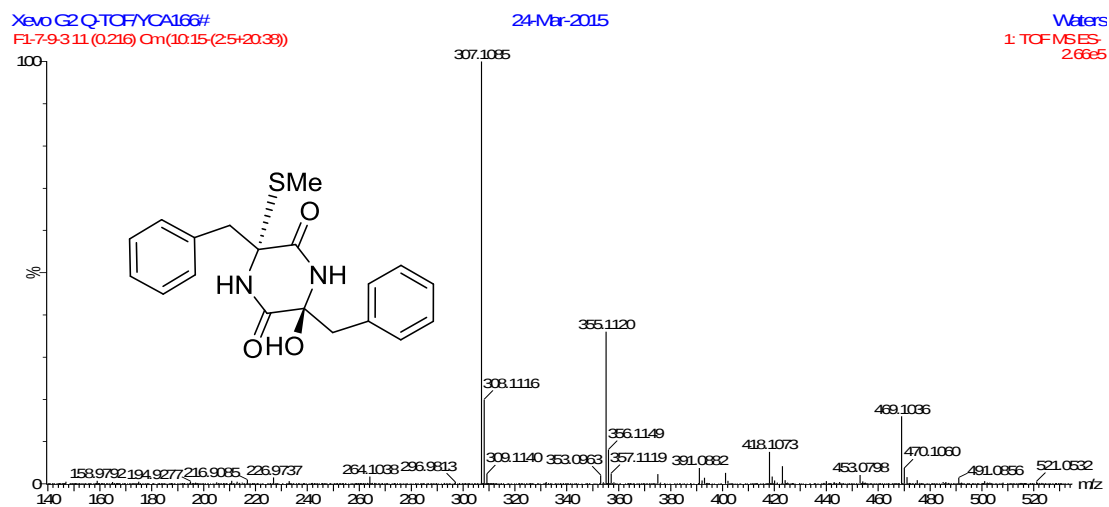


Fig S12-2 HRESIMS Data of Compound 12

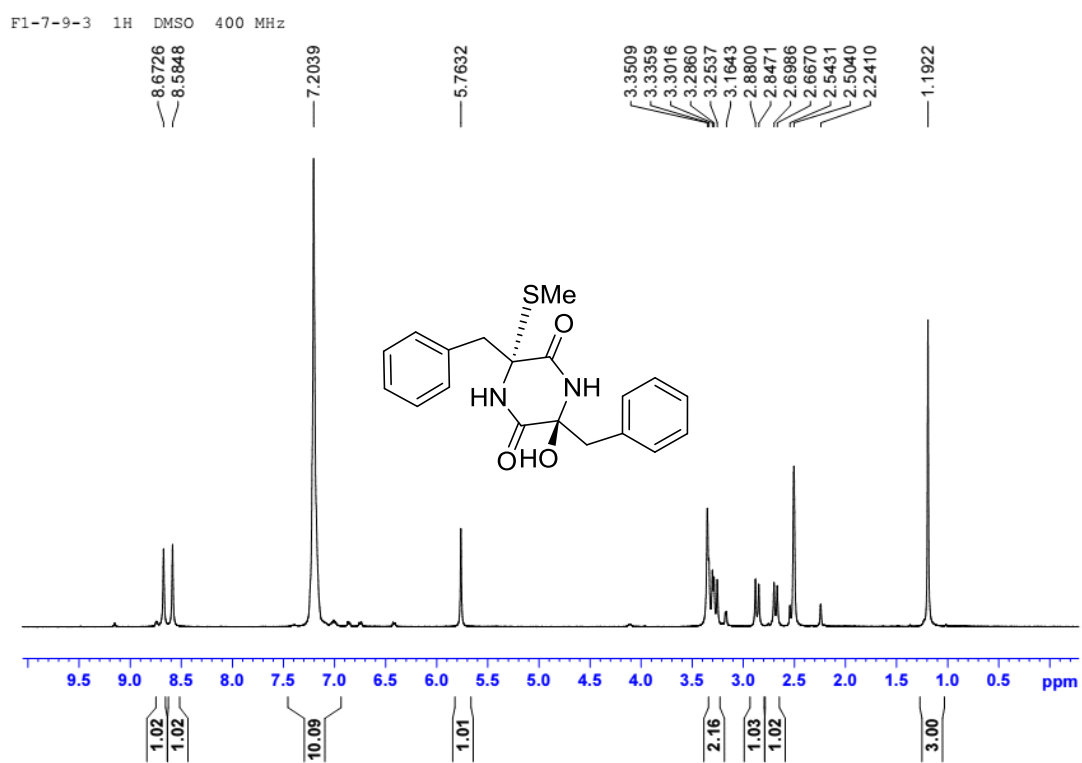


Fig S12-3 The ¹H NMR Spectrum of Compound 12

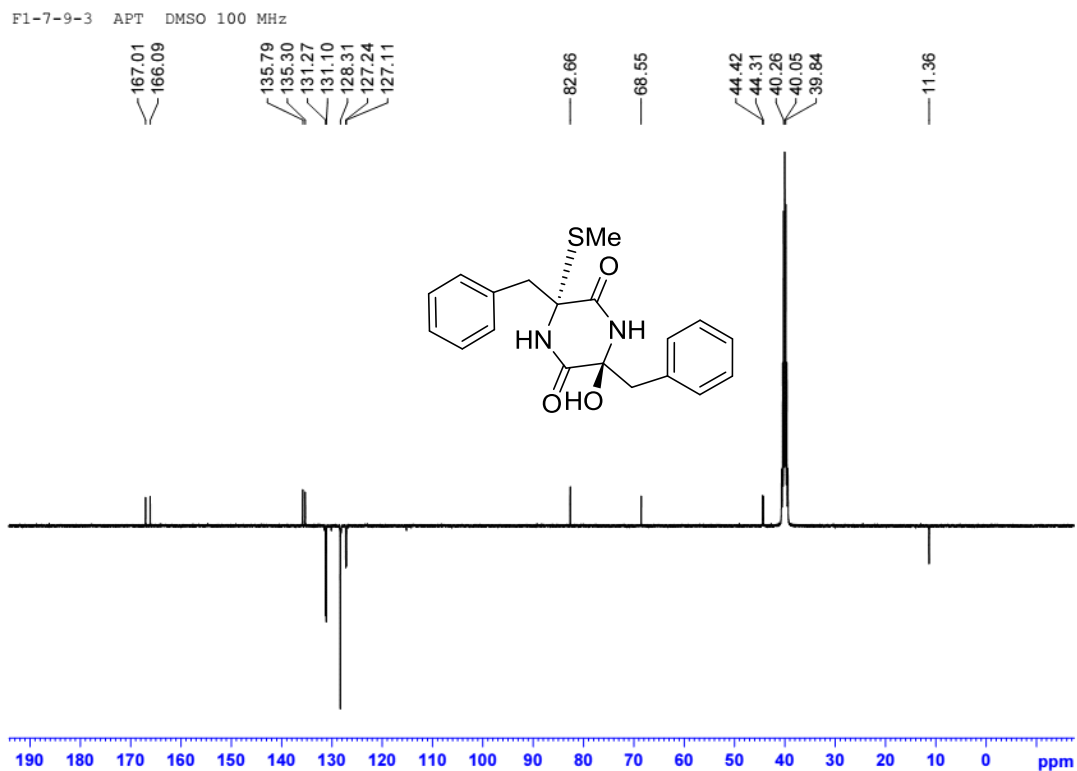


Fig S12-4 The APT Spectrum of Compound 12

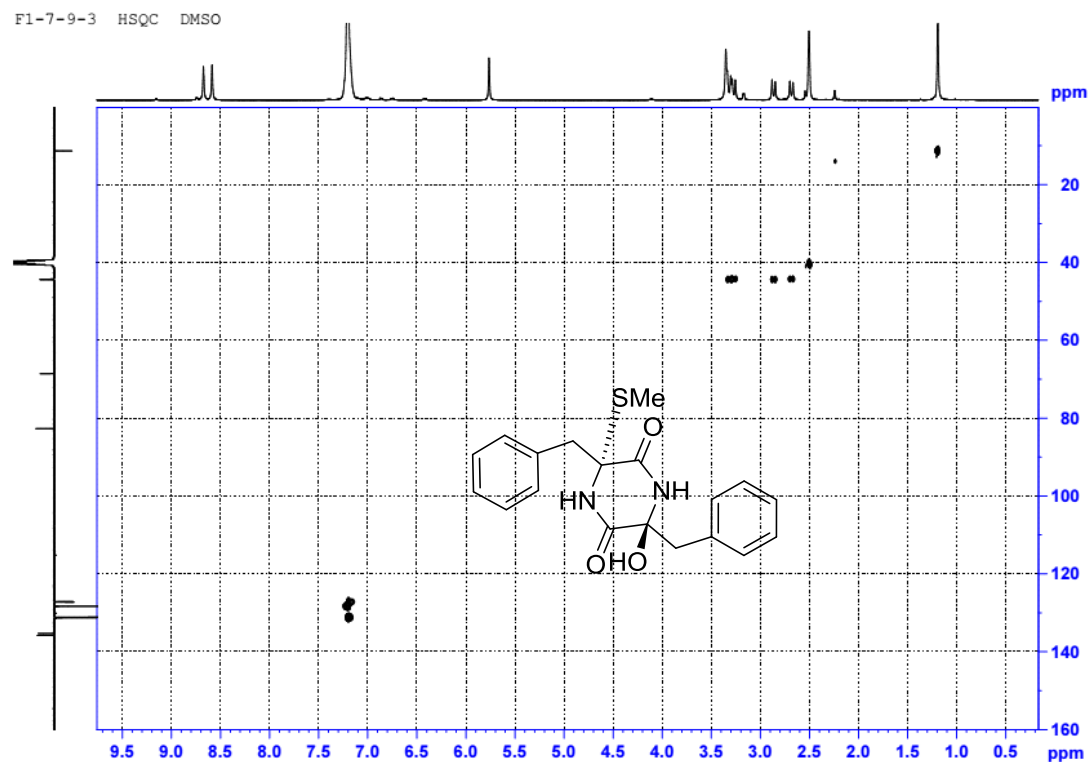


Fig S12-5 The HSQC Spectrum of Compound 12

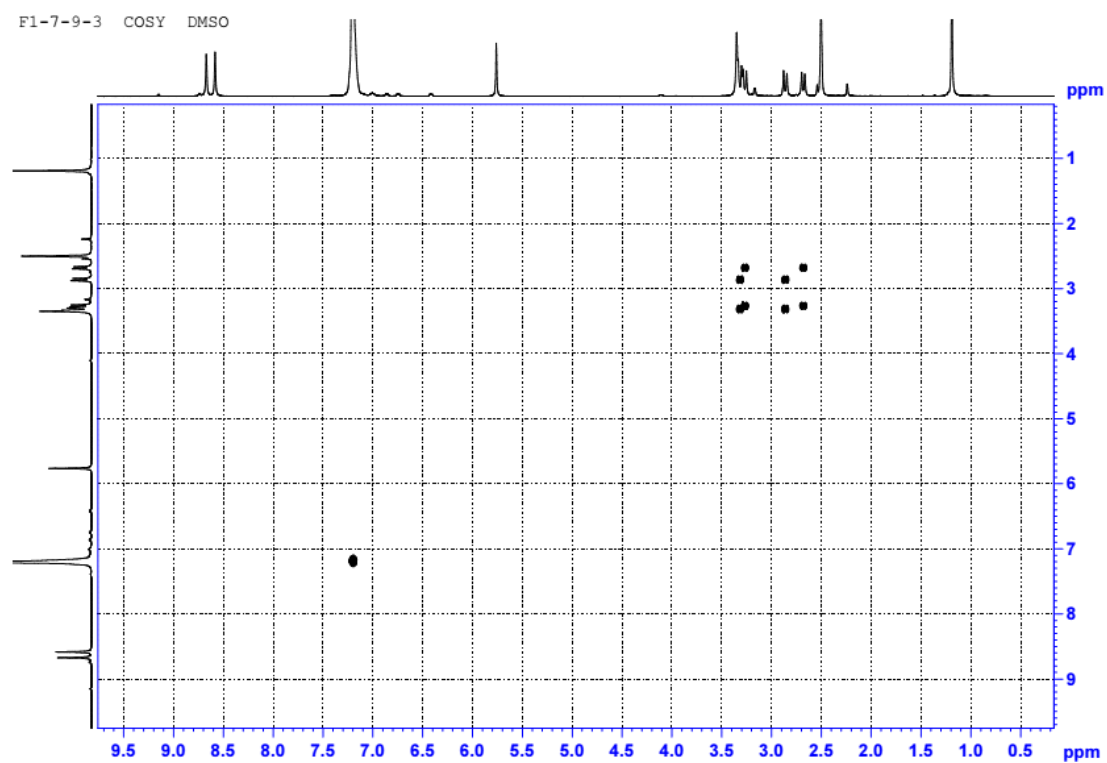


Fig S12-6 The ^1H - ^1H COSY Spectrum of Compound 12

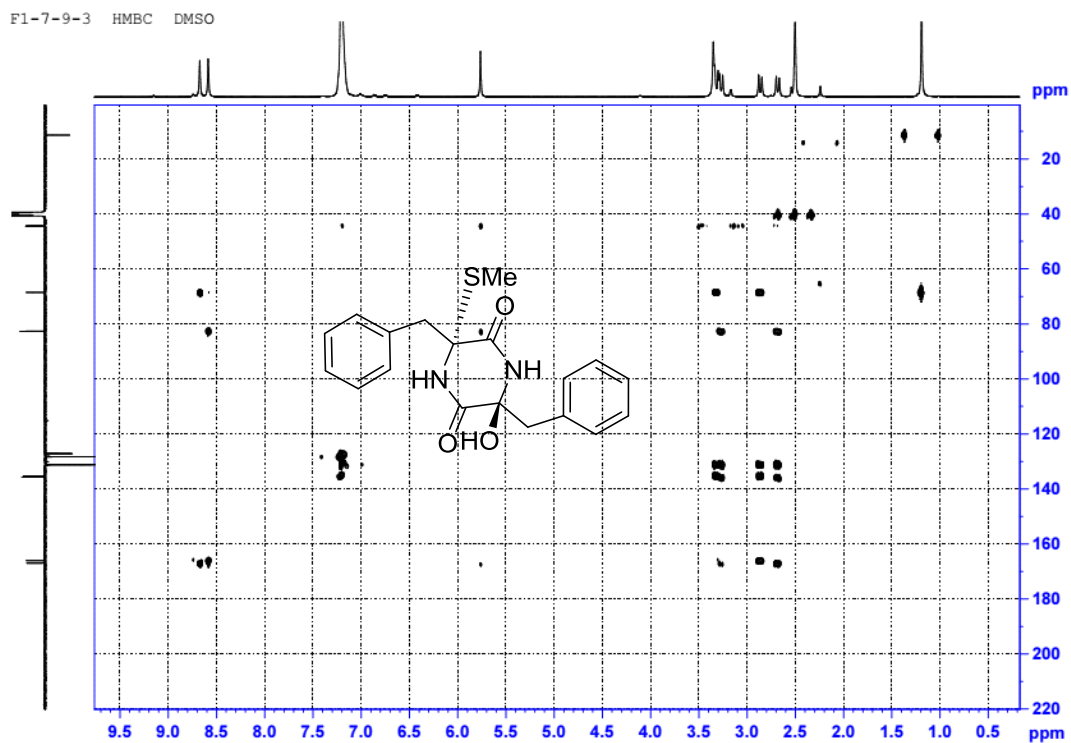


Fig S12-7 The HMBC Spectrum of Compound 12

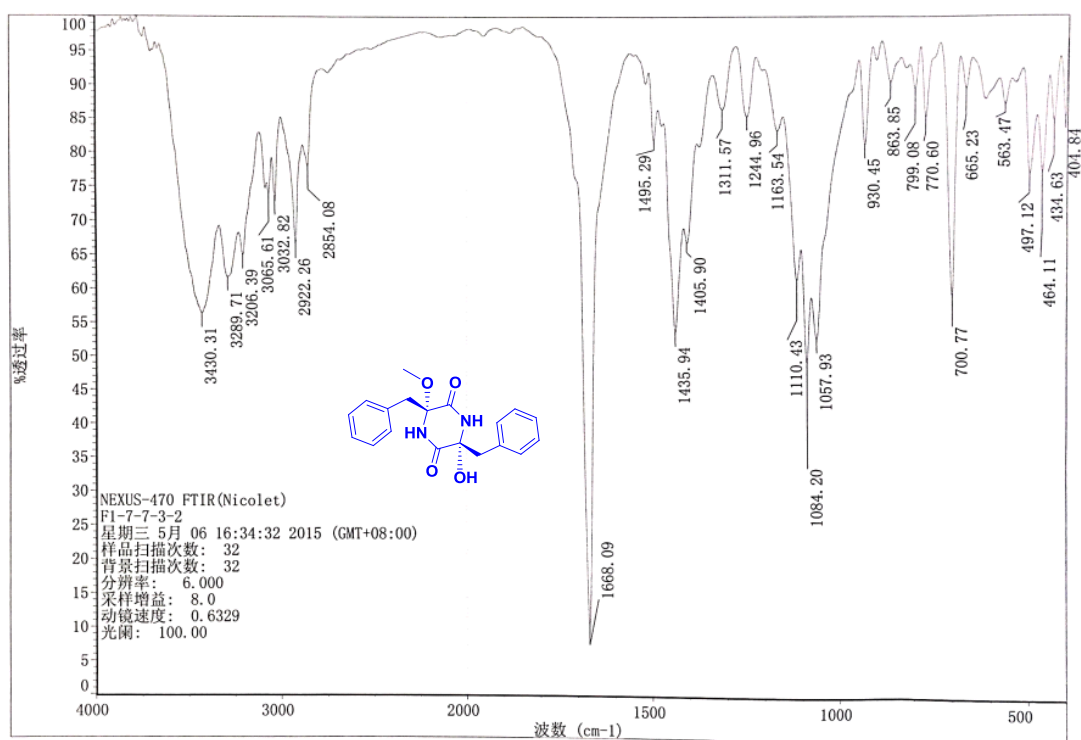


Fig S13-1 IR Spectrum of Compound 13

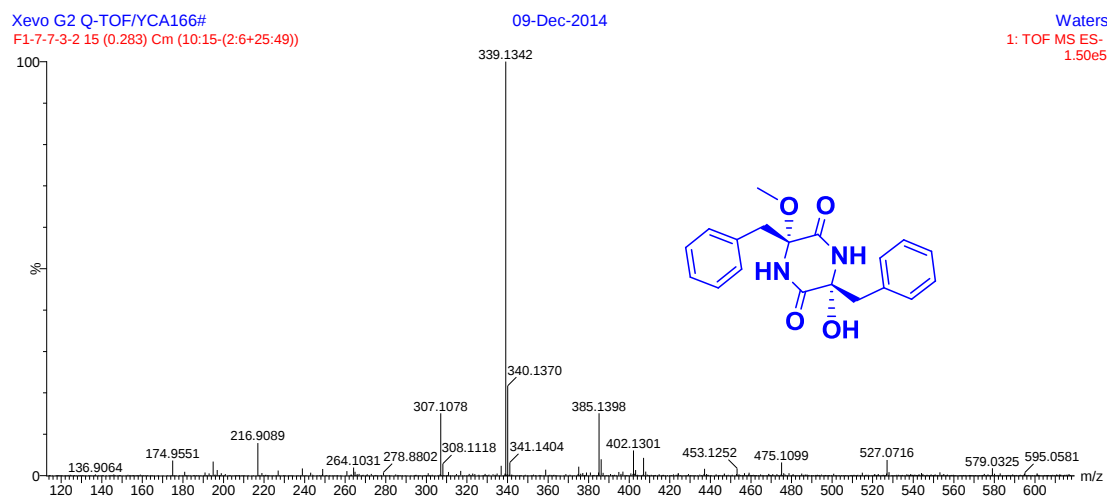


Fig S13-2 HRESIMS Data of Compound 13

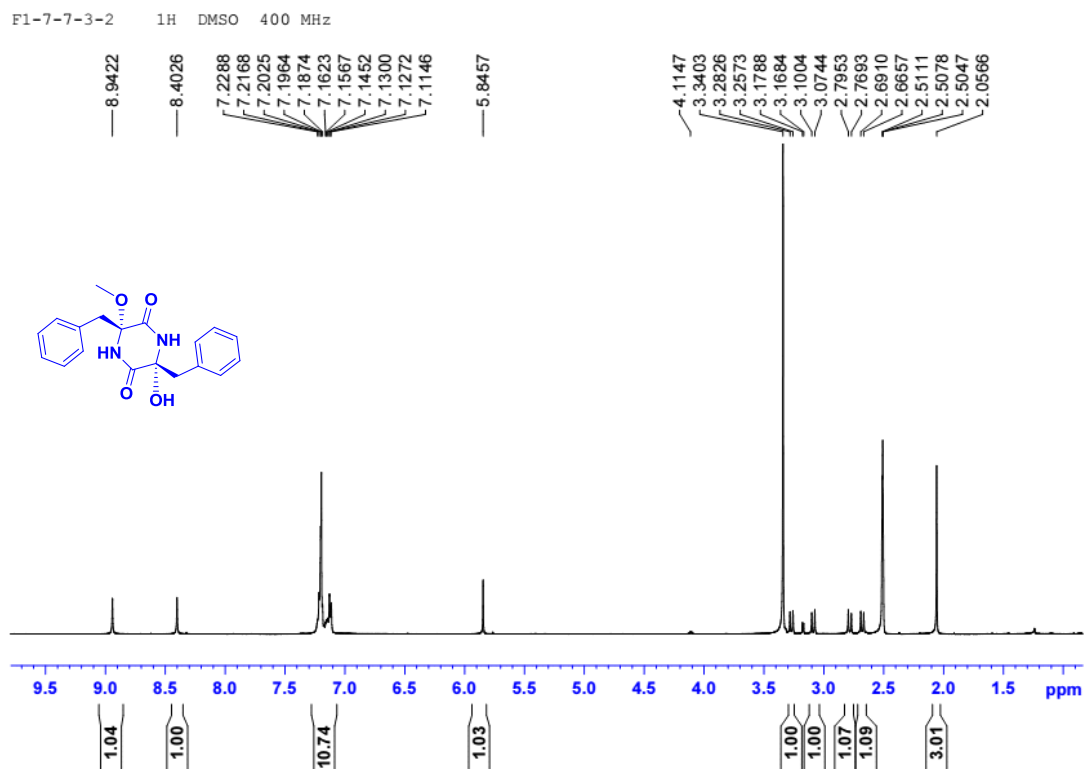


Fig S13-3 The ^1H NMR Spectrum of Compound 13

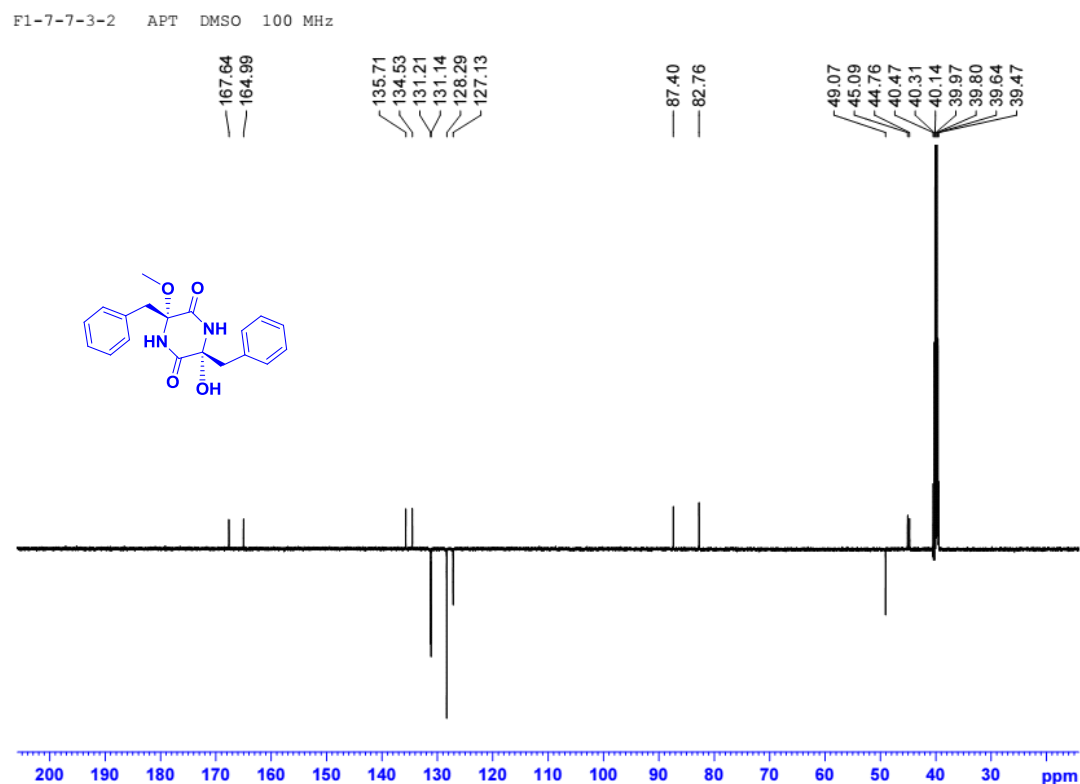


Fig S13-4 The APT Spectrum of Compound 13

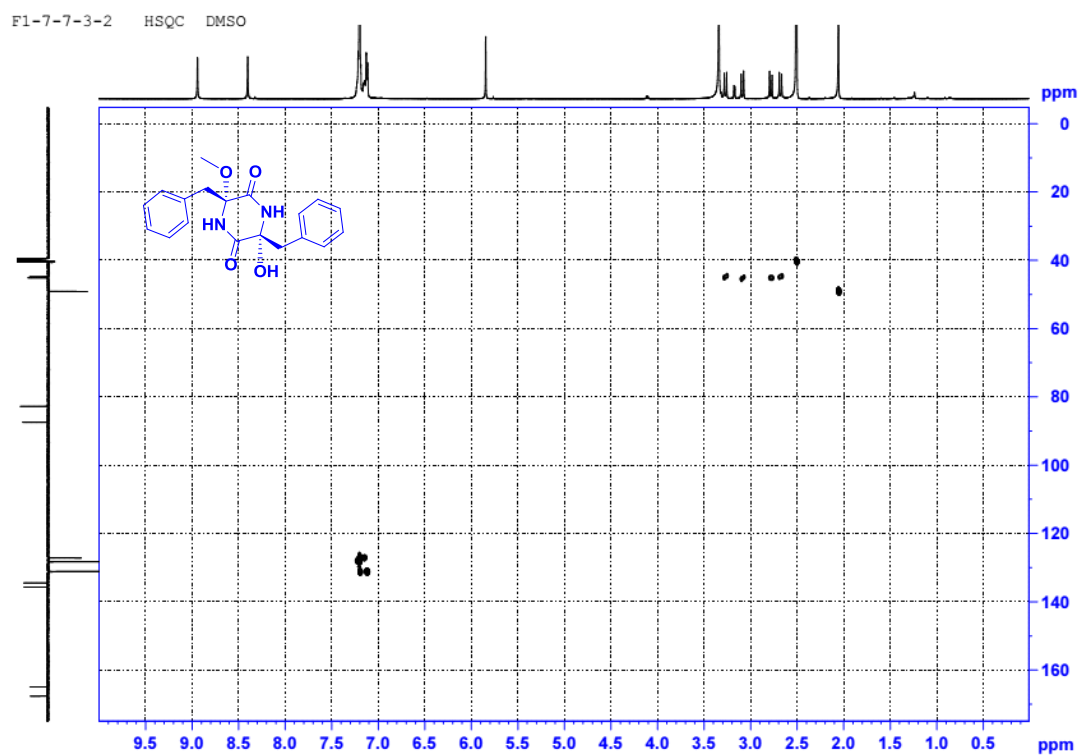


Fig S13-5 The HSQC Spectrum of Compound 13

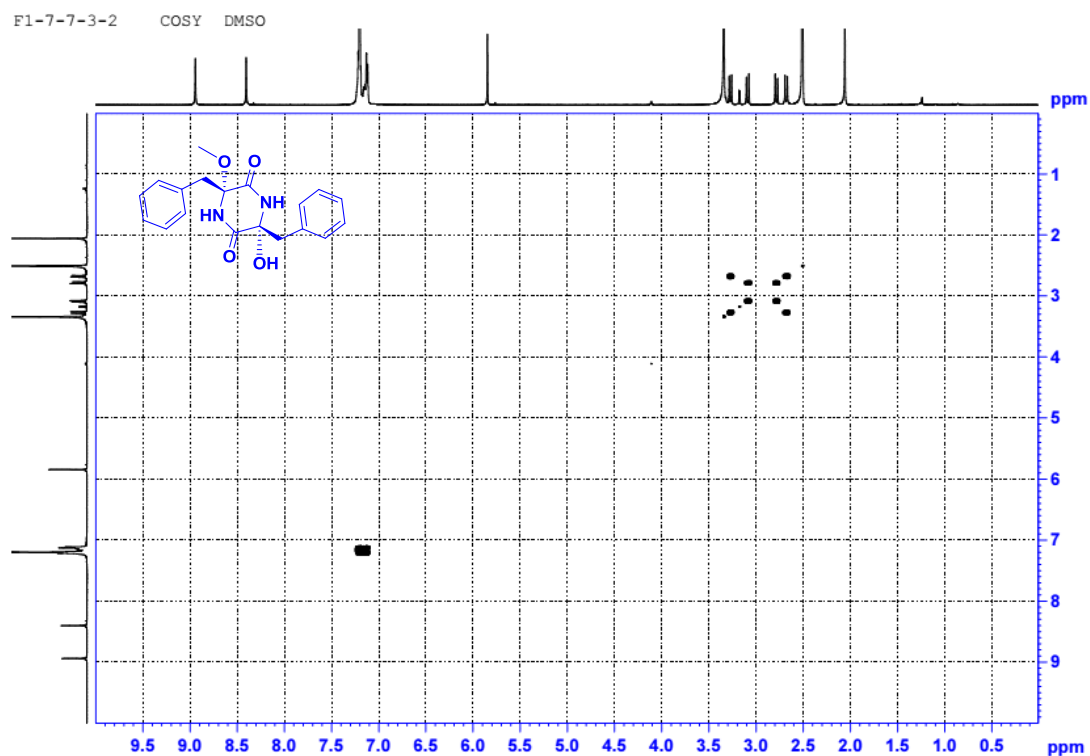


Fig S13-6 The ^1H - ^1H COSY Spectrum of Compound 13

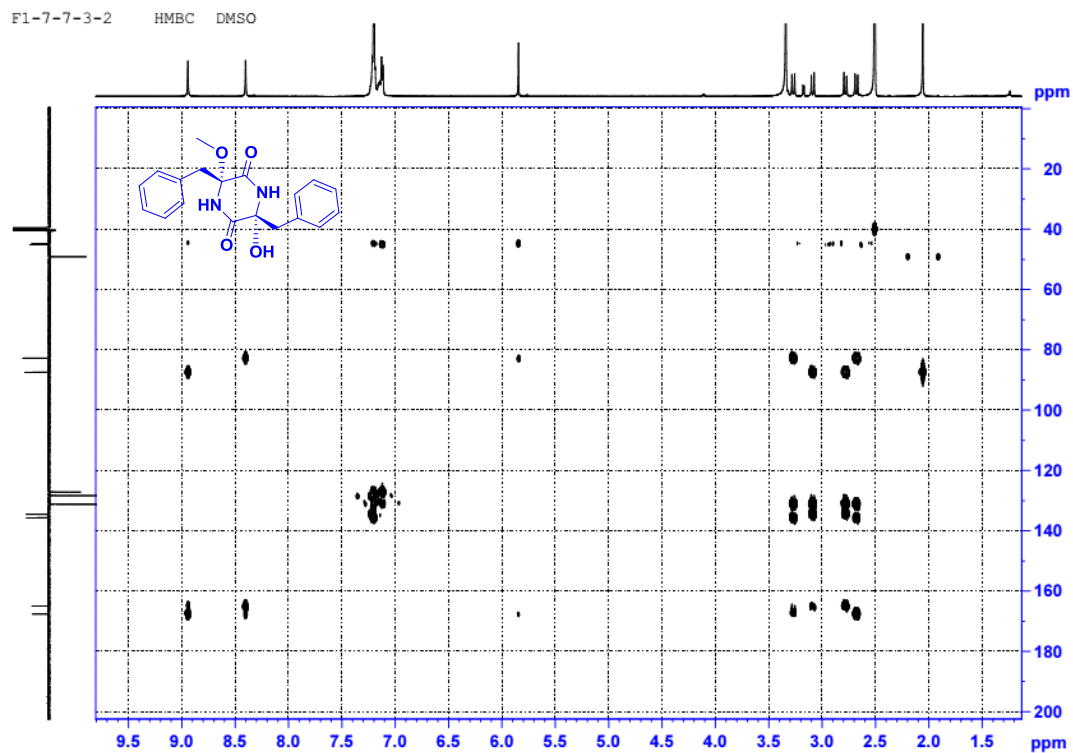


Fig S13-7 The HMBC Spectrum of Compound 13