

Supplementary Information

Zephycandidine A, the First Naturally Occurring Imidazo[1,2-*f*]phenanthridine Alkaloid from *Zephyranthes candida*, Exhibits Significant Anti-tumor and Anti-acetylcholinesterase Activities

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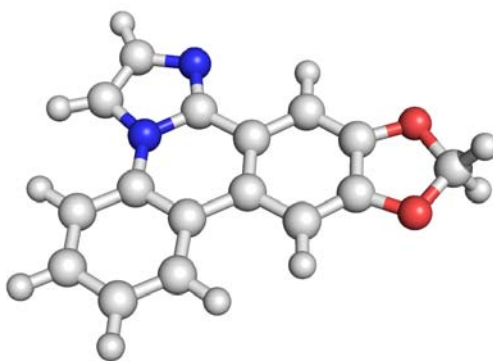
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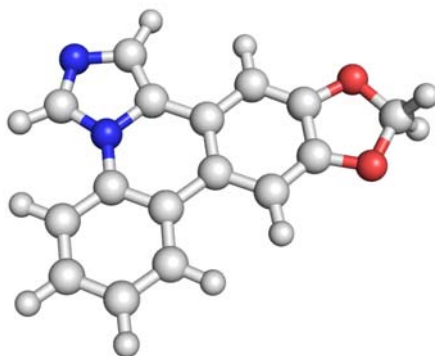
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Table S1. The optimized structure in methanol of compound **1a** at B3LYP/6-31G*

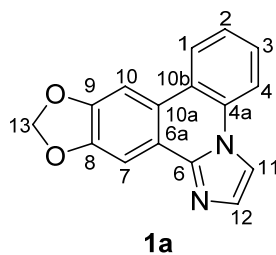
	x	y	z
C	1.381400	-1.441116	-0.000004
C	2.619630	-0.850787	-0.000013
C	2.788710	0.540815	-0.000030
C	1.717087	1.394627	-0.000038
C	0.424531	0.810093	-0.000026
C	0.237742	-0.595503	-0.000012
C	-0.733288	1.667865	-0.000016
N	-2.005026	1.119254	0.000014
C	-2.244044	-0.264140	0.000012
C	-1.125989	-1.136943	-0.000005
C	-3.555565	-0.761770	0.000021
C	-3.780210	-2.130653	0.000012
C	-2.693679	-3.015487	-0.000011
C	-1.397716	-2.522341	-0.000020
O	3.844678	-1.461911	-0.000031
C	4.824684	-0.410928	0.000122
O	4.122504	0.843427	-0.000058
N	-0.774249	2.995295	-0.000024
C	-2.110542	3.311144	0.000029
C	-2.893456	2.183970	0.000026
H	1.299687	-2.520322	0.000012
H	1.829065	2.471930	-0.000050
H	-4.396348	-0.077667	0.000035
H	-4.798007	-2.508633	0.000021
H	-2.861926	-4.088156	-0.000023
H	-0.575490	-3.228570	-0.000043
H	5.437445	-0.484498	0.903506
H	5.437788	-0.484561	-0.903019
H	-2.447592	4.339642	0.000047
H	-3.962925	2.053791	0.000035

HF=-875.689933532

Table S2. The optimized structure in methanol of compound **1b** at B3LYP/6-31G*

	x	y	z
C	2.633564	-0.841085	-0.000068
C	2.799041	0.548547	0.000047
C	1.724615	1.401139	0.000098
C	0.429420	0.821441	0.000037
C	0.250696	-0.585558	-0.000052
C	1.394329	-1.429766	-0.000117
C	-0.734902	1.673823	0.000035
N	-2.011865	1.111321	-0.000012
C	-2.238246	-0.278476	0.000010
C	-1.112678	-1.138773	-0.000038
C	-3.544372	-0.786679	0.000091
C	-3.757623	-2.158482	0.000094
C	-2.663750	-3.031898	0.000028
C	-1.371684	-2.525694	-0.000029
C	-0.944705	3.040808	-0.000010
N	-2.287336	3.324119	-0.000086
C	-2.902641	2.157282	-0.000086
O	3.860816	-1.450528	-0.000129
C	4.837294	-0.396853	0.000081
O	4.131190	0.856334	0.000071
H	1.858746	2.476581	0.000181
H	1.312791	-2.508951	-0.000205
H	-4.392624	-0.111870	0.000159
H	-4.772154	-2.544961	0.000156
H	-2.820899	-4.106251	0.000033
H	-0.543892	-3.225179	-0.000059
H	-0.202511	3.827434	-0.000003
H	-3.972475	2.015283	-0.000150
H	5.450738	-0.467572	-0.903097
H	5.450491	-0.467698	0.903421

HF=-875.684718638

Table S3. DFT Calculation Result for δ_{H} shifts of **1a**

Carbon Number	Chemical Shift	Calculated Shift	Corrected	difference	difference
1	8.47	8.63	8.61	0.14	0.14
2	7.58	7.97	7.73	0.15	0.15
3	7.67	8.06	7.85	0.18	0.18
4	8.14	8.31	8.18	0.04	0.04
7	7.88	8.15	7.97	0.09	0.09
10	7.99	7.88	7.61	-0.38	0.38
11	7.52	7.79	7.49	-0.03	0.03
12	8.32	8.31	8.18	-0.14	0.14
OCH ₂ O	6.16	6.75	6.11	-0.05	0.05
				average	0.13
				max	0.38

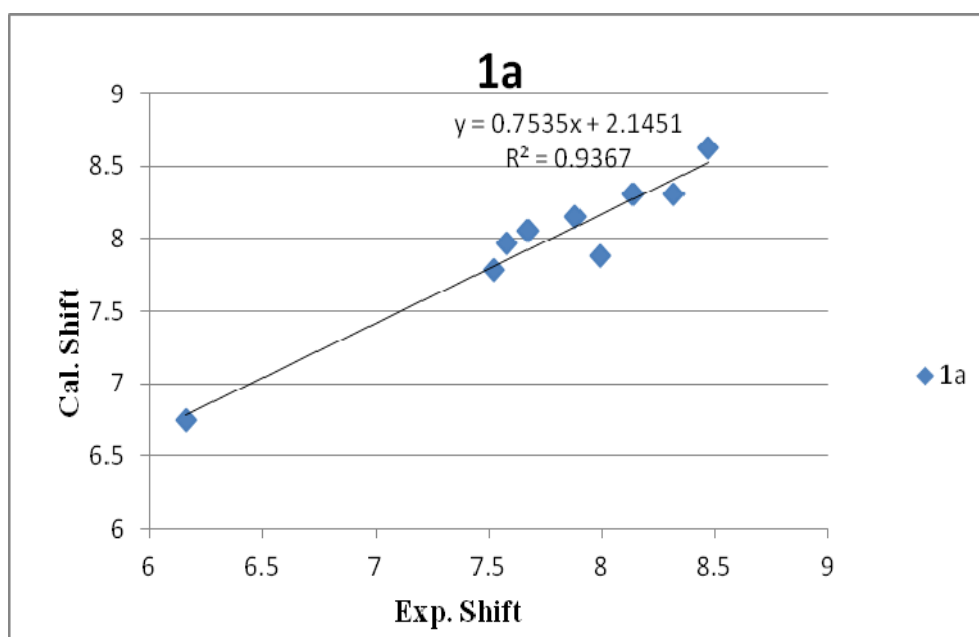
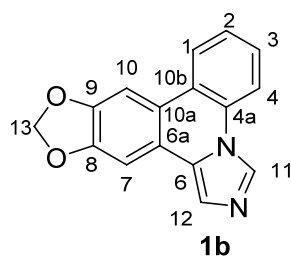
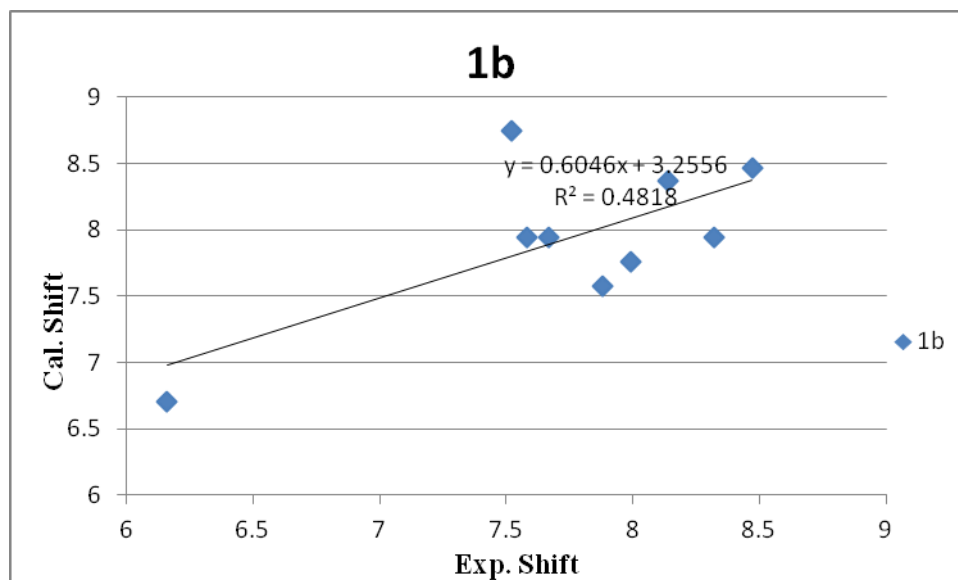
**Figure S1.** The ¹H NMR correlation of experimental data and calculated data about **1a**

Table S4. DFT Calculation Result for δ_{H} shifts of **1b**

Carbon Number	Chemical Shift	Calculated Shift	Corrected	difference	difference
1	8.47	8.47	8.43	-0.04	0.04
2	7.58	7.94	7.75	0.17	0.17
3	7.67	7.94	7.75	0.08	0.08
4	8.14	8.37	8.30	0.16	0.16
7	7.88	7.58	7.29	-0.59	0.59
10	7.99	7.76	7.52	-0.47	0.47
11	7.52	8.75	8.79	1.27	1.27
12	8.32	7.94	7.75	-0.57	0.57
OCH ₂ O	6.16	6.71	6.17	0.01	0.01
				average	0.37
				max	1.27

**Figure S2.** The ¹H NMR correlation of experimental data and calculated data about **1b**

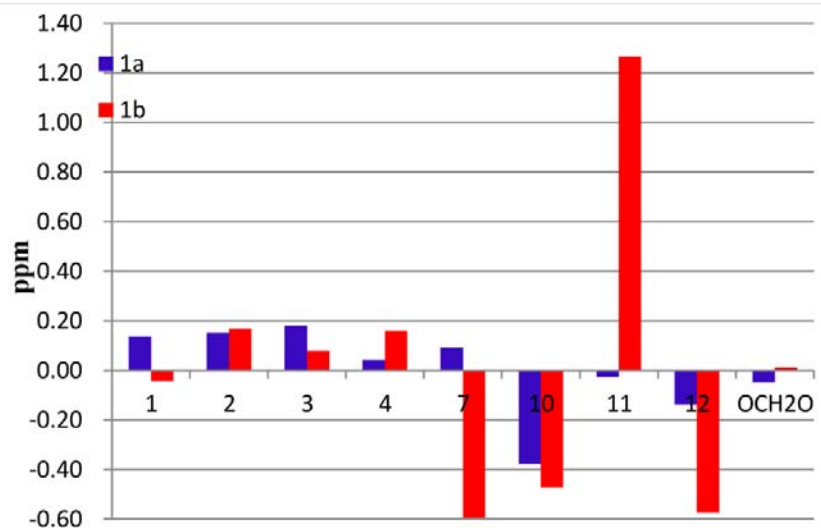
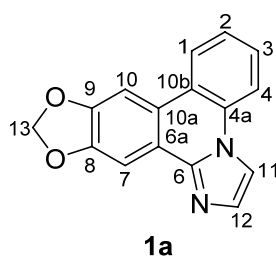


Figure S3. Comparing DFT calculated vs. experimental ^1H δ values for two possible structures.

Table S5. DFT Calculation Result for C shifts of **1a**



Carbon Number	Chemical Shift	Calculated Shift	Corrected	difference	difference
1	125.4	128.6	125.4	0.0	0.0
2	126.9	129.1	125.9	-1.0	1.0
3	129.8	131.8	128.9	-0.9	0.9
4	117.5	120.9	116.9	-0.6	0.6
4a	132.3	135.4	132.9	0.6	0.6
6	143.8	145.5	144.0	0.2	0.2
6a	119.8	125.0	121.4	1.6	1.6
7	103.2	107.8	102.5	-0.7	0.7
8	150.7	151.8	150.9	0.2	0.2
9	151.6	152.3	151.4	-0.2	0.2
10	103.1	106.8	101.4	-1.7	1.7
10a	125.5	128.1	124.8	-0.7	0.7
10b	123.1	127.3	123.9	0.8	0.8
11	113.8	116.8	112.4	-1.4	1.4
12	131.5	134.7	132.1	0.6	0.6
13	103.7	111.8	106.9	3.2	3.2
				average	0.9
				max	3.2

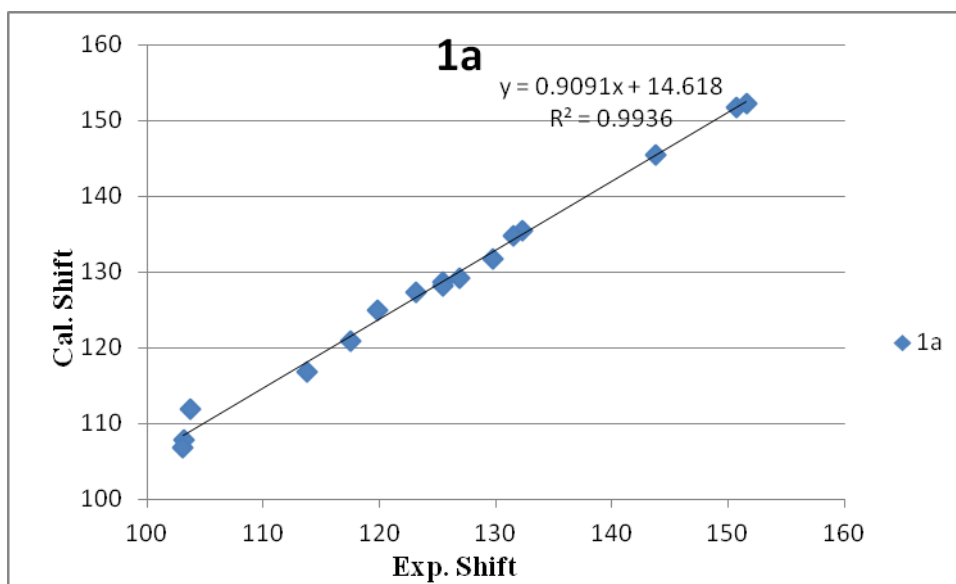
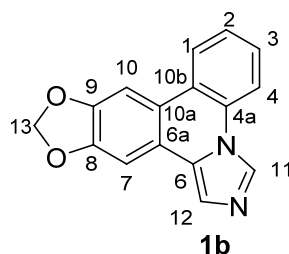


Figure S4. The ^{13}C NMR correlation of experimental data and calculated data about **1a**

Table S6. DFT Calculation Result for C shifts of **1b**



Carbon Number	Chemical Shift	Calculated Shift	Corrected	difference	difference
1	125.4	128.6	126.2	0.8	0.8
2	126.9	129.8	127.7	0.8	0.8
3	129.8	131.9	130.3	0.5	0.5
4	117.5	120.3	115.8	-1.7	1.7
4a	132.3	134.4	133.5	1.2	1.2
6	143.8	132.8	131.5	-12.3	12.3
6a	119.8	125.2	121.9	2.1	2.1
7	103.2	107.3	99.5	-3.7	3.7
8	150.7	151.9	155.4	4.7	4.7
9	151.6	151.3	154.6	3.0	3.0
10	103.1	107.4	99.6	-3.5	3.5
10a	125.5	126.1	123.1	-2.4	2.4
10b	123.1	127.9	125.3	2.2	2.2
11	113.8	131.5	129.8	16.0	16.0
12	131.5	125.3	122.1	-9.4	9.4
13	103.7	111.8	105.2	1.5	1.5
				average	4.1
				max	16.0

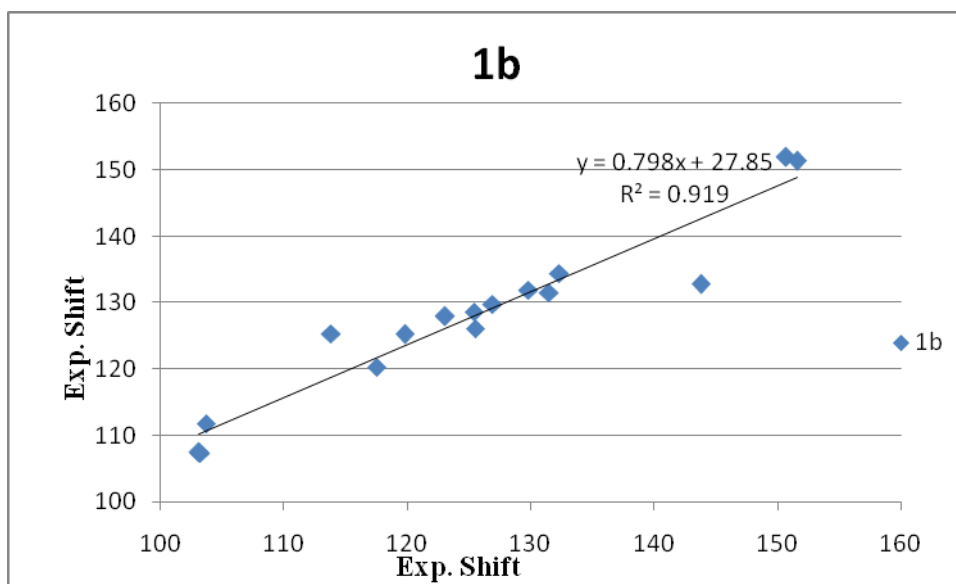


Figure S5. The ^{13}C NMR correlation of experimental data and calculated data about **1b**

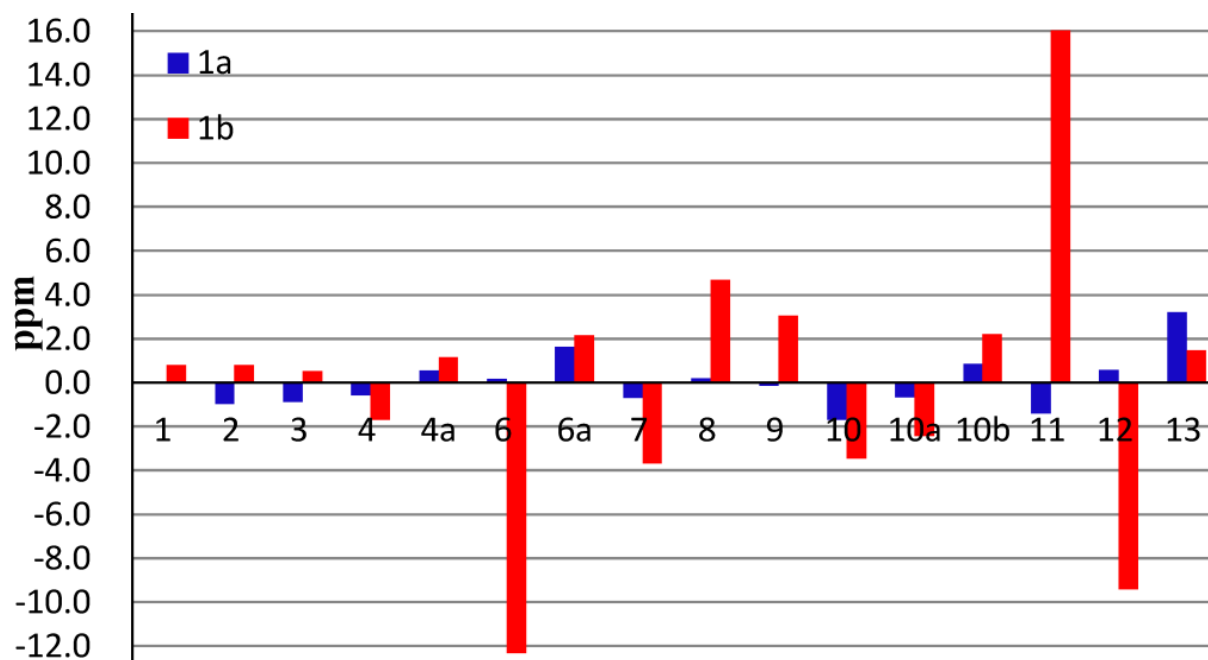


Figure S6. Comparing DFT calculated vs. experimental ^{13}C δ values for two possible structures.

ZGQ2-43-5 #32 RT: 0.46 AV: 1 NL: 1.02E8
T: FTMS + p ESI Full ms [50.00-1500.00]

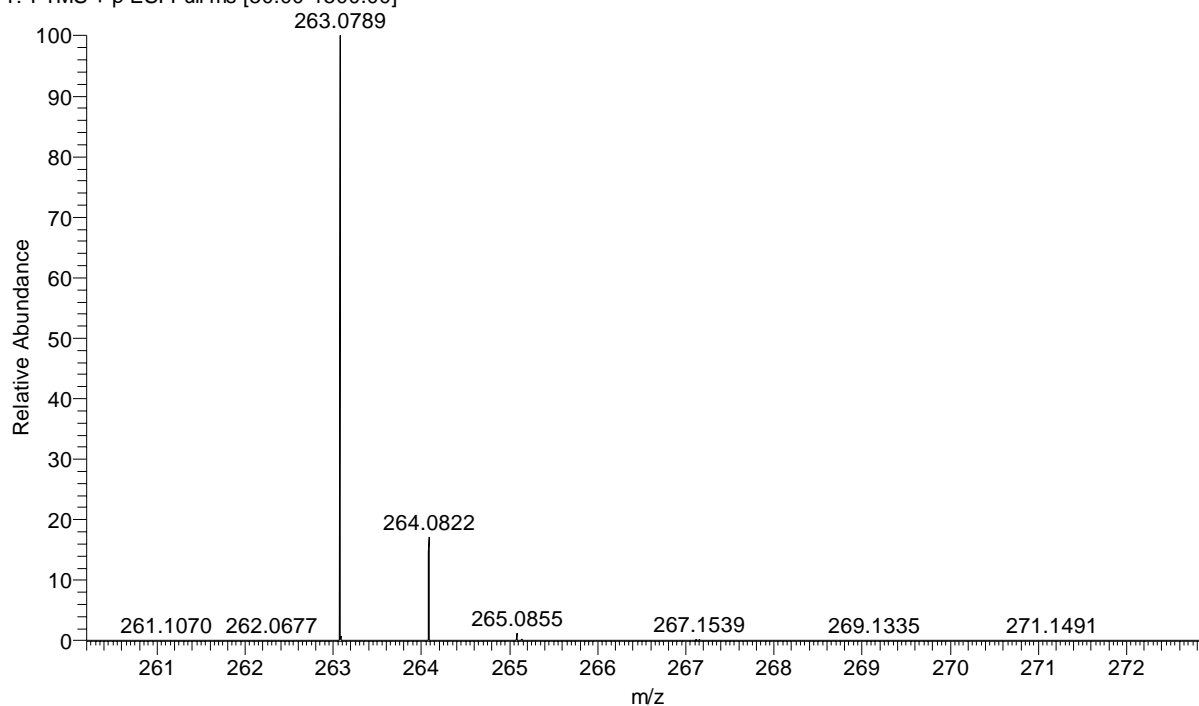


Figure S7. (+)-HRESI-MS spectrum of **1**

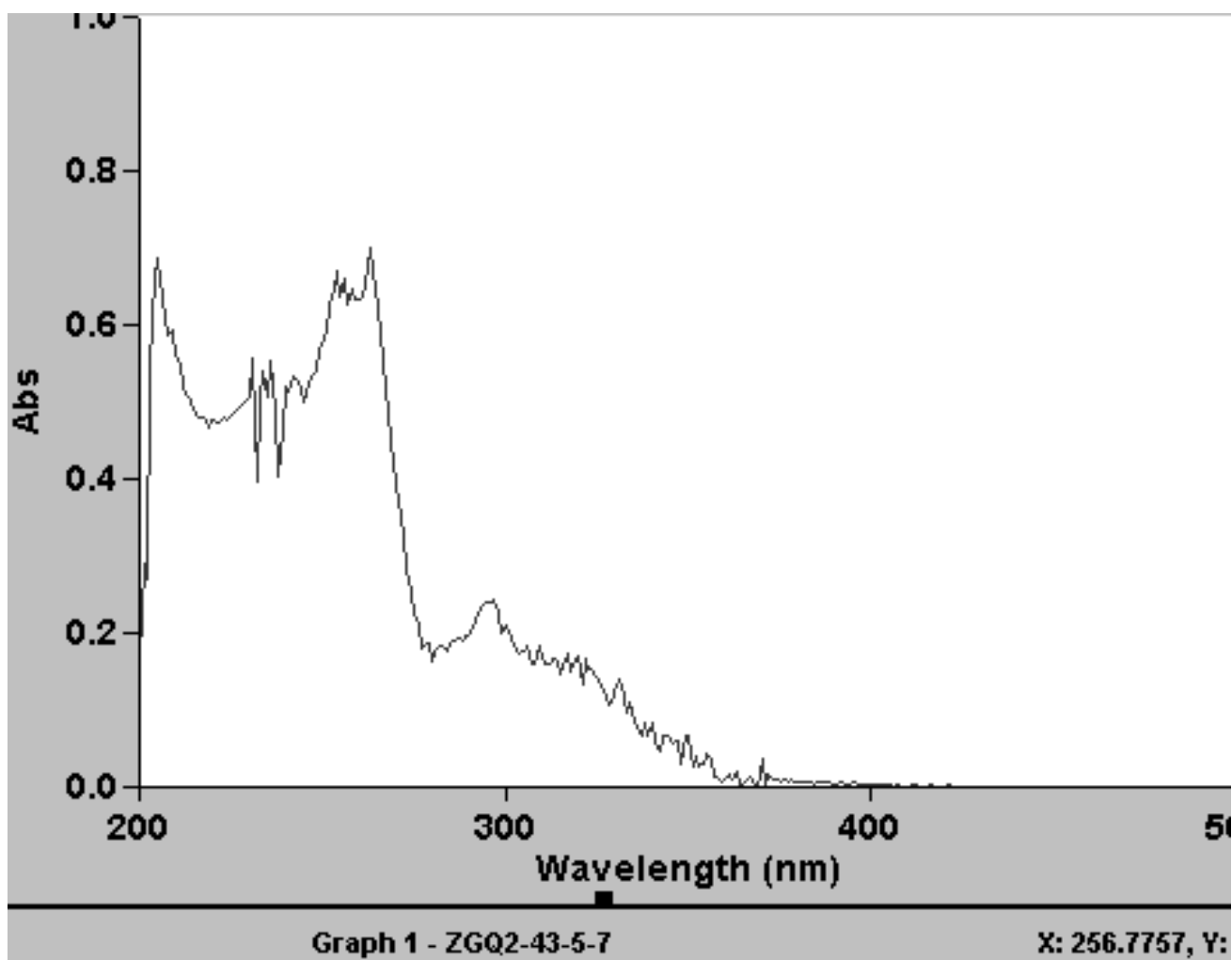


Figure S8. UV spectrum of **1** (MeOH)

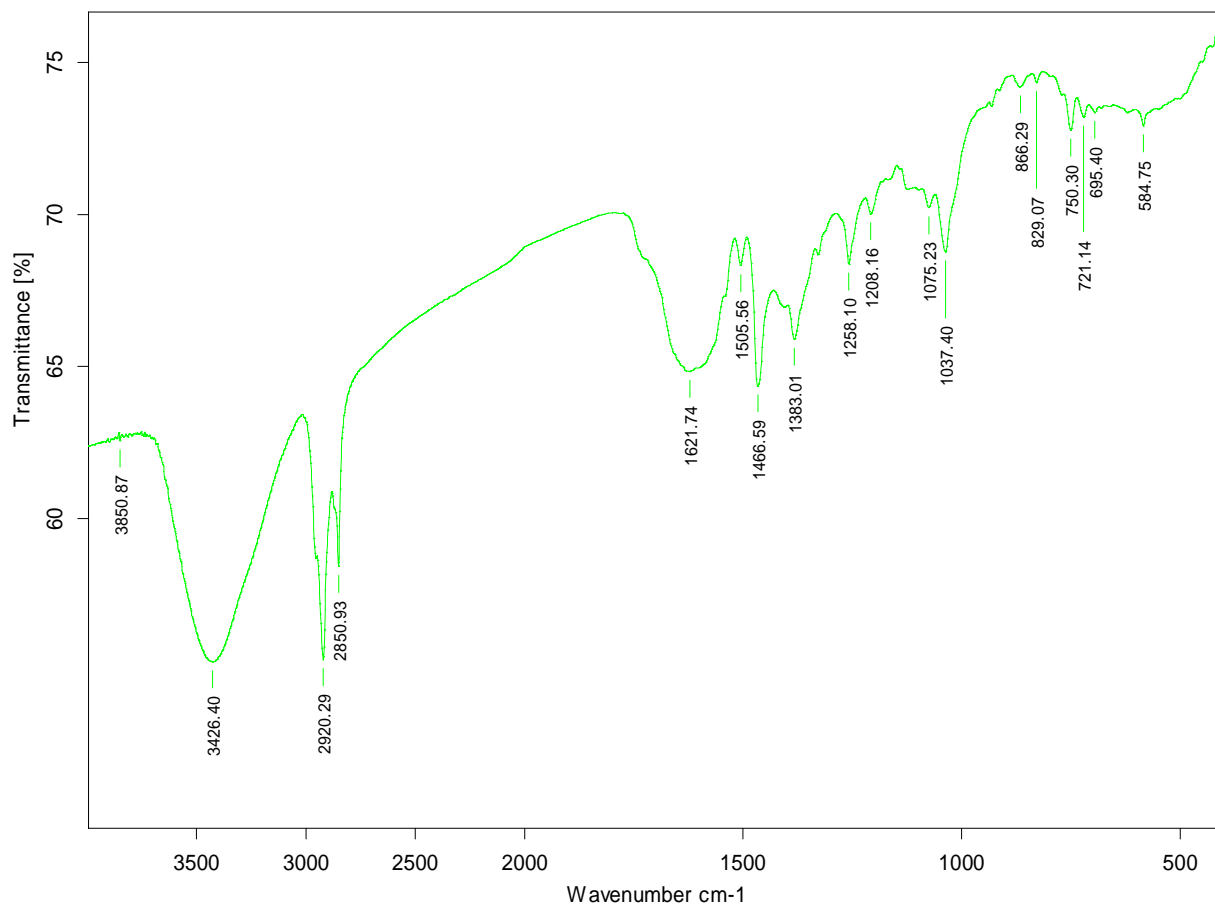


Figure S9. IR spectrum of **1** (KBr disc)

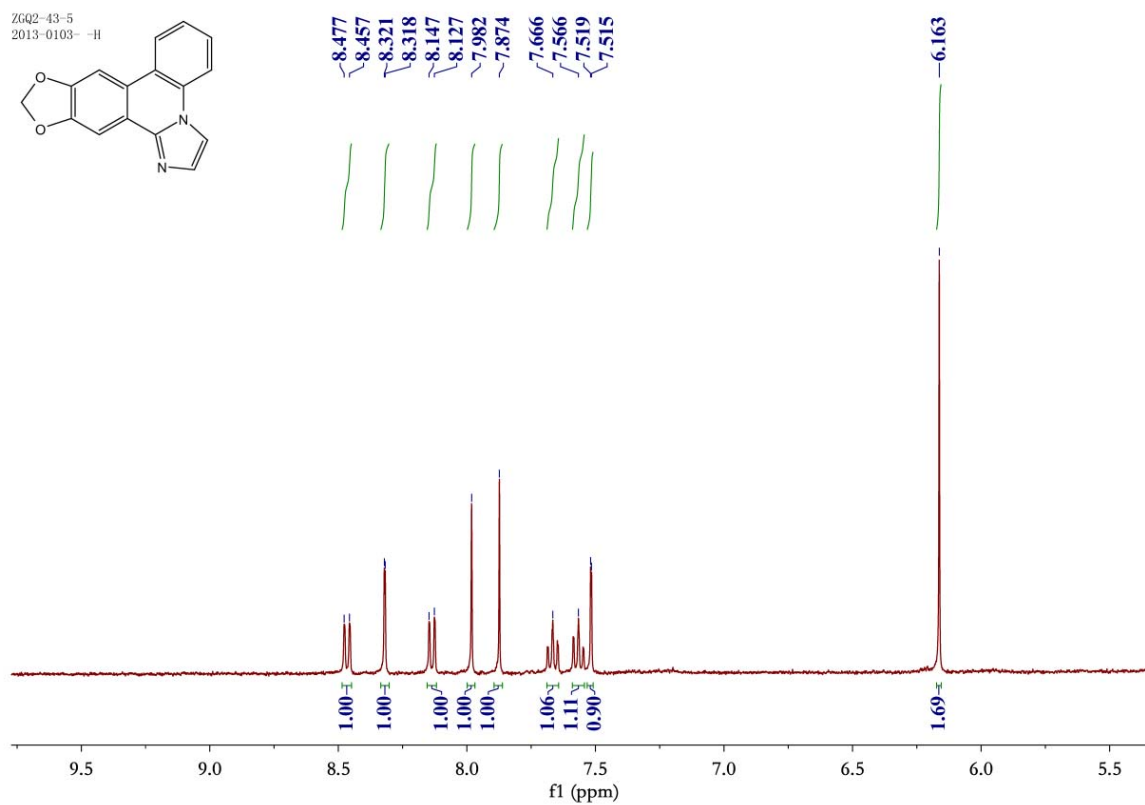
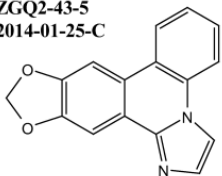


Figure S10. ^1H NMR spectrum of **1** (CD_3OD , 400 MHz)

ZGQ2-43-5
2014-01-25-C



151.610
150.695

143.777

132.309
131.449
129.822
126.865
125.478
125.444
123.105
119.751
117.479
113.862

103.704
103.143
103.088

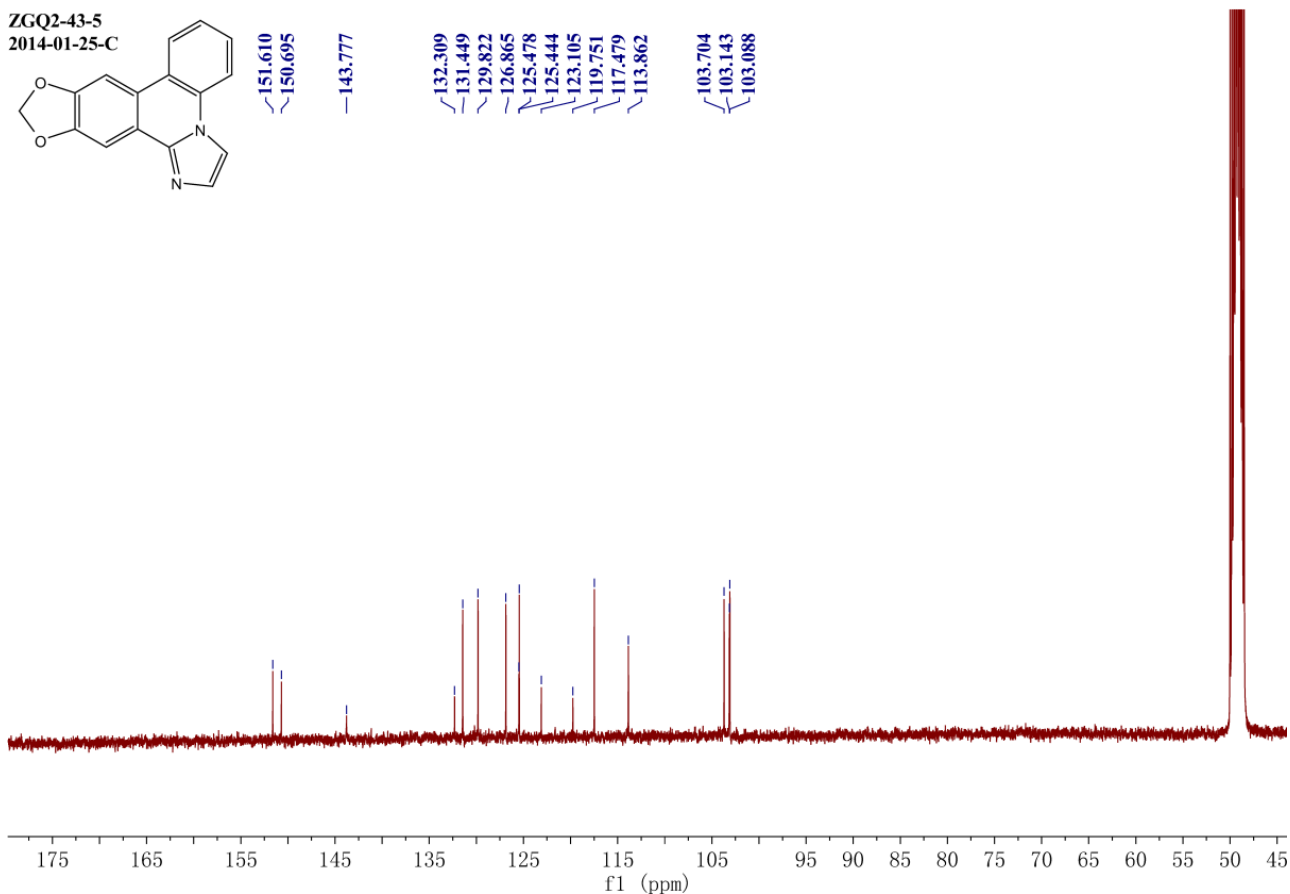
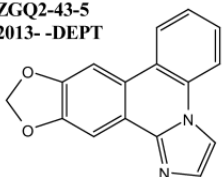


Figure S11. ^{13}C NMR spectrum of **1** (CD_3OD , 100 MHz)

ZGQ2-43-5
2013- -DEPT



131.473
129.823
126.864
125.445

117.480
113.858

103.701
103.172
103.088

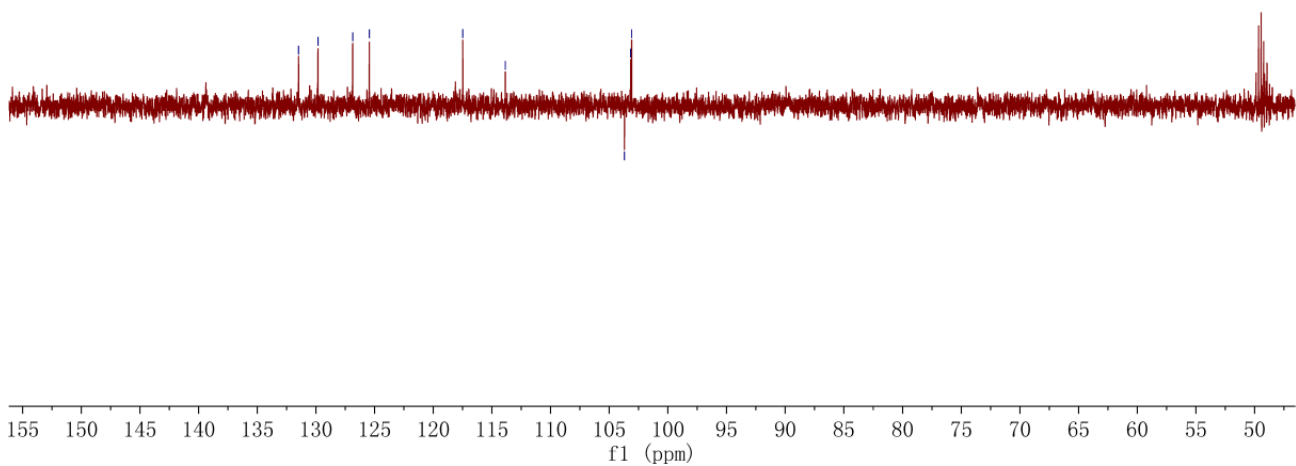


Figure S12. DEPT spectrum of **1** (CD_3OD , 100 MHz)

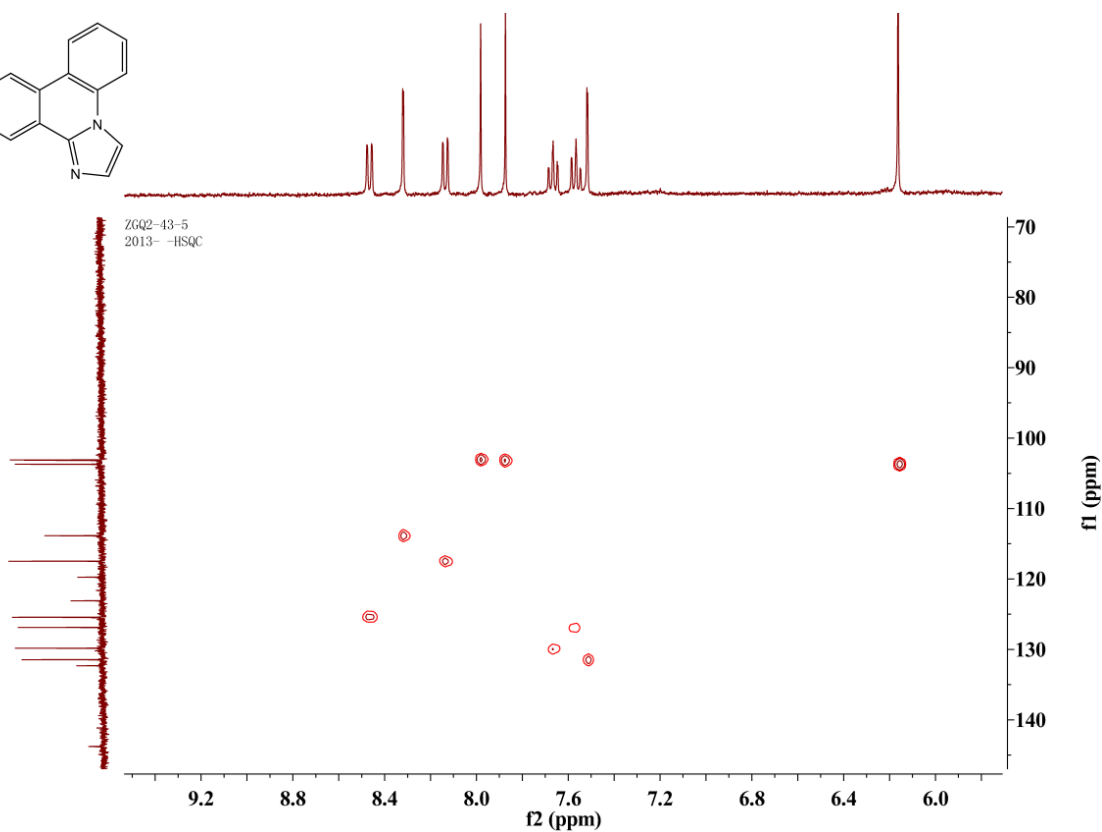
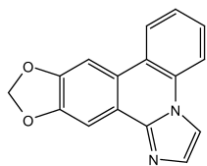


Figure S13. HSQC spectrum of **1** (CD₃OD)

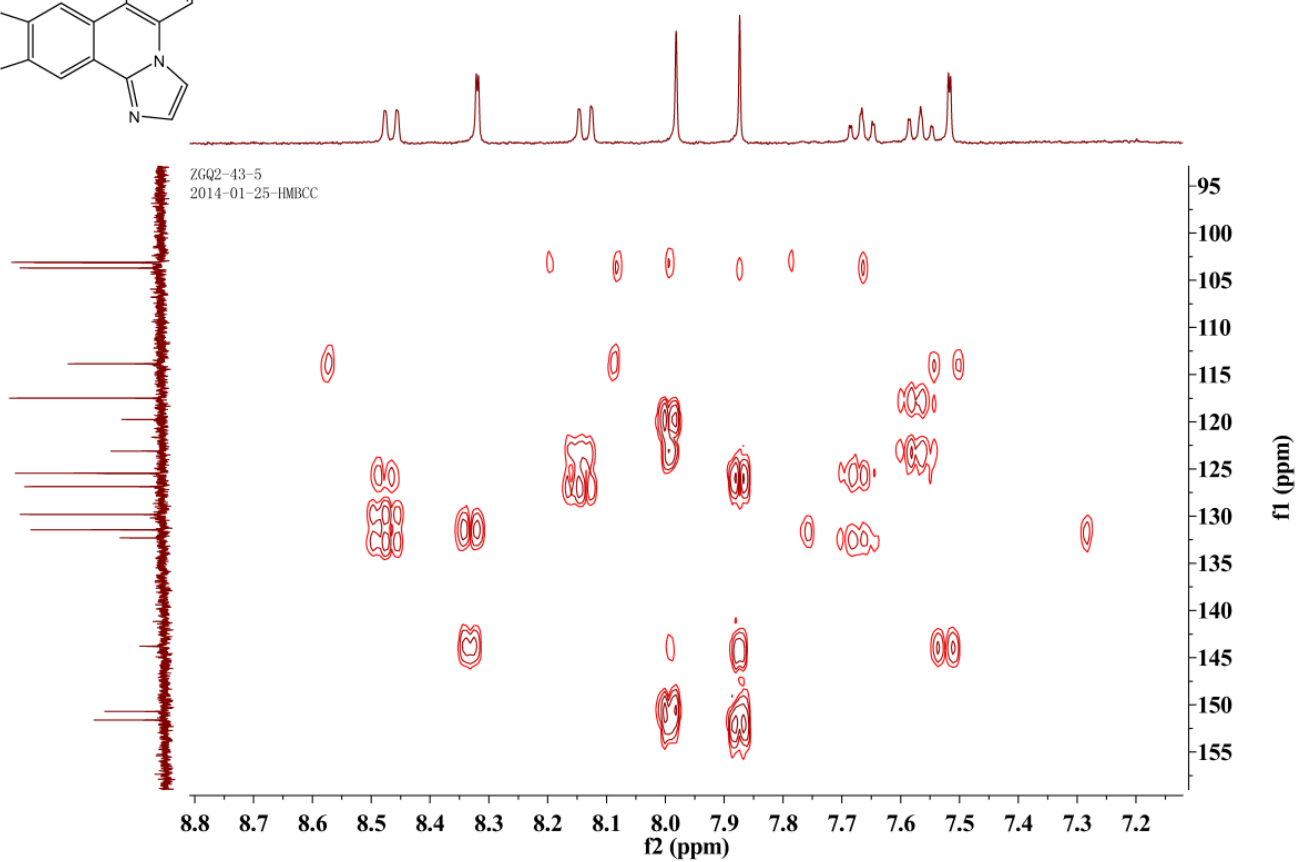
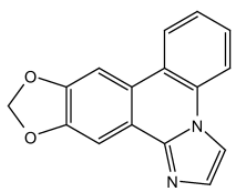


Figure S14. HMBC spectrum of **1** (CD₃OD)

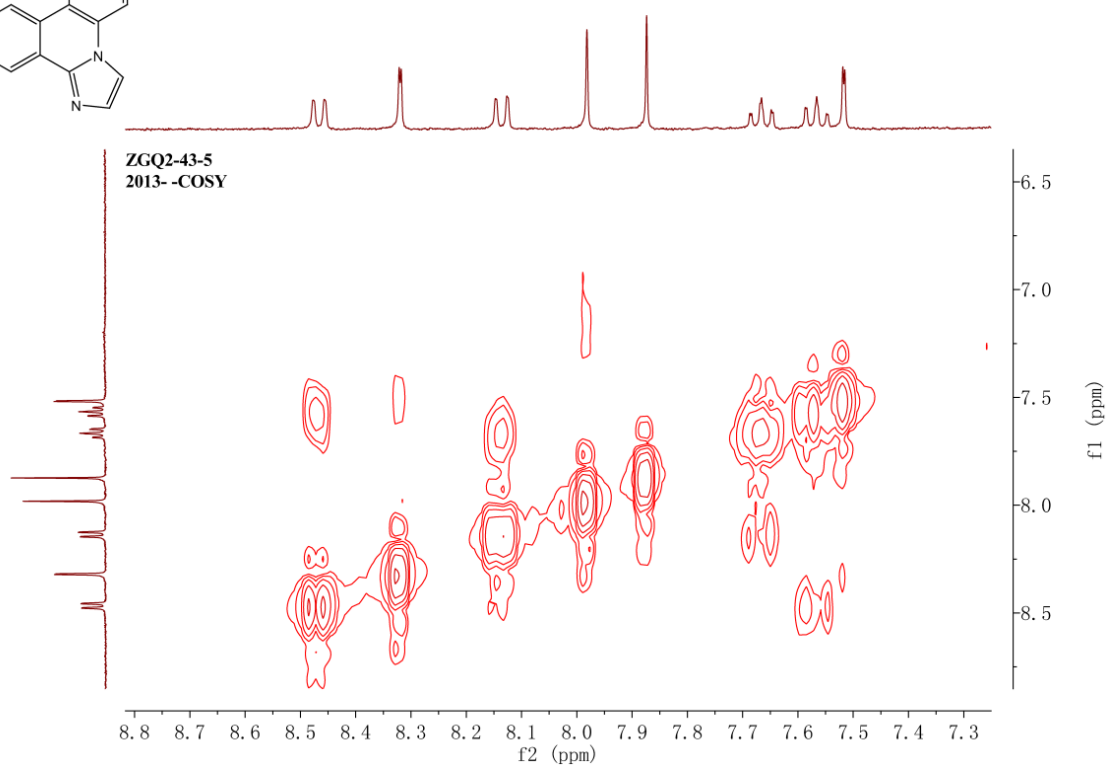
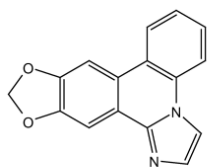


Figure S15. ^1H - ^1H COSY spectrum of **1** (CD_3OD)

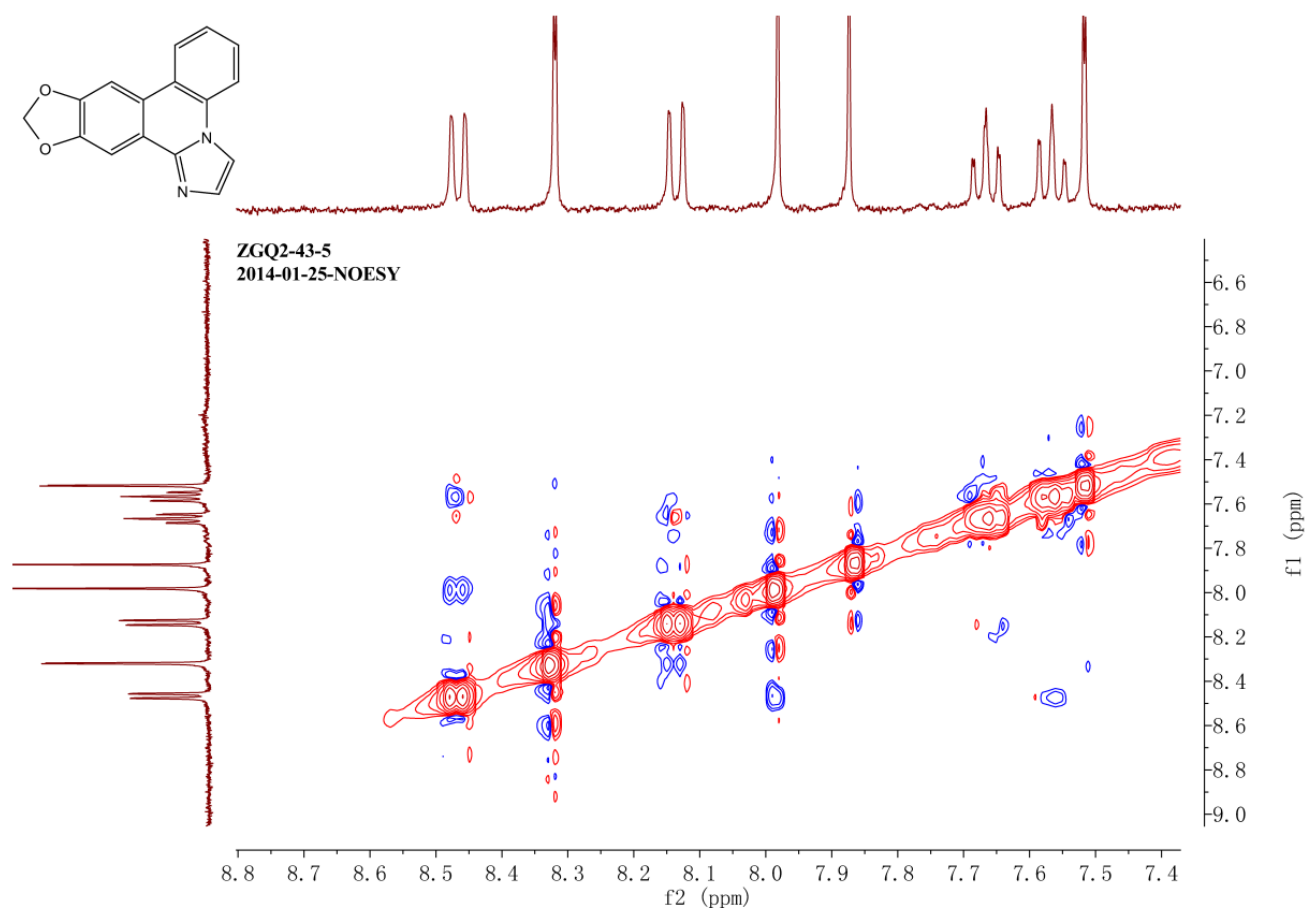
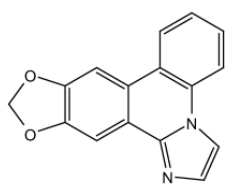


Figure S16. NOESY spectrum of **1** (CD_3OD)

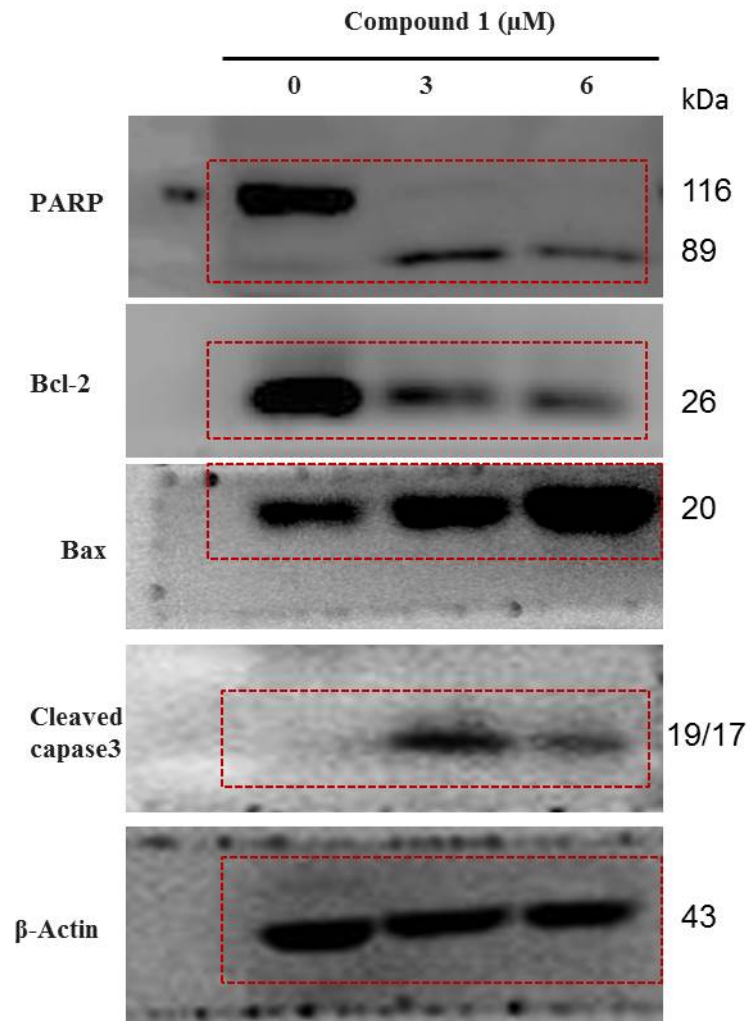


Figure S17. Original blots of Figure 5C.

After transfer the blots from the gels to the PVDF membrane, cut the membrane into different parts according the corresponding of the marker and the target proteins. In this case, we could incubate different antibodies with each part at the same time, and then a Bio-imaging System was used for the visualizing of the blots bands. The bands of β-Actin is not in linear is because the membrane was slanted when transferring the blots from the gel to it.