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Supporting Information

Racemic Alkaloids from *Macleaya cordata*: Structural Elucidation, Chiral Resolution, and Cytotoxic, Antibacterial Activities

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1 Computational methods for ECD of compounds 1 and 2

Computational methods

The Spartan 14.0 (Wavefunction Inc., Irvine, CA, USA) searches using molecular mechanics MMFF were performed for (*SS*)-**1** and (*R*)-**2**, which gave 100 conformers and 21 conformers, respectively. The low-energy conformers of (*SS*)-**1** and (*R*)-**2** separately accounting for more than 3% and 5% Boltzmann distribution was further optimized successively in the gas phase by semi-empirical method and the Hartree-Fork (HF) method at the 6-31G (d) level in Gaussian 09 program package,[1] which was reoptimized and analysed frequency, orderly, using the density functional theory (DFT) at the B3LYP/6-31G (d, p) level and the same way in the methanol, resulted in no imaginary frequencies. Solvent effects were taken into consideration by using the conductor polarizable continuum model (CPCM). The conformers of (*SS*)-**1** and (*R*)-**2** were calculated electronic circular dichroism (ECD) by the time-dependent density functional theory (TD-DFT) method at the B3LYP/6-31+G (d, p) level with the CPCM model in methanol solution. The overall calculated ECD curves of the **1** and **2** were generated severally by Boltzmann weighting of their selected low-energy conformers using SpecDis 1.51 [2] with σ = 0.30eV at 0 nm shift, together with σ = 0.30eV at -19 nm shift .

Table S1 Energy analysis of compound (*S*,*S*)-**1**

Label	MMFF	
	rel. E (Kal/mol)	Boltzmann Dist.
1-1	0.00	0.295
1-2	0.71	0.222
1-3	1.65	0.152
1-4	2.48	0.109

1-5	4.09	0.057
1-6	4.55	0.047

Table S2 Energy analysis of compound (*R*)-**2**

Label	MMFF	
	rel. E (Kal/mol)	Boltzmann Dist.
2-1	0.00	0.467
2-2	1.44	0.261
2-3	2.56	0.166
2-4	4.94	0.064

Table S3 Computational methods for ECD of compound **1**

Standard orientation of **1-1**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.422109	1.333070	1.117146
2	6	0	-5.564239	0.223638	0.283124
3	6	0	-4.432750	-0.294720	-0.375028
4	6	0	-3.169628	0.266629	-0.152435
5	6	0	-3.030072	1.386911	0.694987
6	6	0	-4.174119	1.918345	1.310953
7	6	0	-1.924159	-0.274271	-0.830421
8	7	0	-1.007727	0.819173	-1.203929
9	6	0	-0.722387	1.721194	-0.134139
10	6	0	-1.691377	1.993772	0.837088
11	6	0	0.565993	2.336359	-0.078916
12	6	0	0.844193	3.272606	0.974301
13	6	0	-0.152102	3.513367	1.955689
14	6	0	-1.371839	2.882571	1.897779
15	6	0	1.581334	2.021246	-1.038596
16	6	0	2.778309	2.666349	-0.927443
17	6	0	3.042875	3.606204	0.092988
18	6	0	2.118328	3.919392	1.046414
19	8	0	3.886915	2.539928	-1.723780
20	6	0	4.910944	3.353488	-1.132905

21	8	0	4.315826	4.089643	-0.052870
22	1	0	-2.206405	-0.781950	-1.753753
23	6	0	-1.143367	-1.309153	0.029338
24	6	0	-2.016028	-2.491703	0.502275
25	8	0	-1.339422	-3.325243	1.442162
26	6	0	0.020262	-1.842773	-0.820417
27	6	0	1.392146	-1.936418	-0.253610
28	1	0	-0.770915	-0.801275	0.922065
29	8	0	-0.206604	-2.217593	-1.970292
30	6	0	2.453574	-2.185298	-1.149295
31	6	0	3.749599	-2.285770	-0.671240
32	6	0	4.018178	-2.155355	0.711444
33	6	0	2.959851	-1.942584	1.603997
34	6	0	1.656788	-1.825340	1.118539
35	8	0	5.291963	-2.230396	1.168234
36	8	0	3.193709	-1.779069	2.949520
37	6	0	3.623750	-2.960230	3.645978
38	8	0	4.876687	-2.497188	-1.414999
39	6	0	4.738592	-2.627215	-2.831048
40	6	0	-1.373355	1.484501	-2.464677
41	8	0	-6.820312	-0.308880	0.088840
42	6	0	-7.020136	-1.614788	0.656043
43	8	0	-4.532247	-1.398788	-1.197601
44	6	0	-5.253289	-1.182528	-2.424489
45	1	0	-6.307768	1.731057	1.602086
46	1	0	-4.099410	2.802585	1.934231
47	1	0	0.069602	4.197587	2.769814
48	1	0	-2.102796	3.068695	2.677695
49	1	0	1.400142	1.277189	-1.802746
50	1	0	2.333173	4.627150	1.839373
51	1	0	5.708206	2.711512	-0.741462
52	1	0	5.297503	4.052170	-1.879451
53	1	0	-2.893195	-2.106410	1.026217
54	1	0	-2.366290	-3.064669	-0.365196
55	1	0	-0.692621	-3.861490	0.964056
56	1	0	2.227387	-2.286751	-2.202782
57	1	0	0.862688	-1.683426	1.840618
58	1	0	5.864293	-2.391040	0.398506
59	1	0	2.871812	-3.753517	3.564181
60	1	0	4.582141	-3.322456	3.263744
61	1	0	3.733614	-2.672281	4.692734
62	1	0	5.745806	-2.779431	-3.217585
63	1	0	4.112361	-3.488543	-3.086518
64	1	0	4.309390	-1.719335	-3.267991

65	1	0	-0.627576	2.244725	-2.704424
66	1	0	-1.382632	0.745638	-3.271078
67	1	0	-2.358997	1.972773	-2.423226
68	1	0	-6.880128	-1.587649	1.742785
69	1	0	-8.051269	-1.891096	0.430060
70	1	0	-6.337155	-2.346717	0.216270
71	1	0	-4.760249	-0.413839	-3.029821
72	1	0	-5.234502	-2.133430	-2.958921
73	1	0	-6.286818	-0.888270	-2.226220

Standard orientation of **1-2**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.461302	1.053395	1.085661
2	6	0	-5.549234	-0.074230	0.264318
3	6	0	-4.381880	-0.550570	-0.374696
4	6	0	-3.153101	0.075059	-0.162414
5	6	0	-3.065600	1.214476	0.669689
6	6	0	-4.234792	1.690509	1.274961
7	6	0	-1.881064	-0.419097	-0.826694
8	7	0	-1.015426	0.710036	-1.216230
9	6	0	-0.774238	1.642115	-0.160183
10	6	0	-1.758313	1.886370	0.803397
11	6	0	0.485019	2.315425	-0.112162
12	6	0	0.717941	3.279954	0.926637
13	6	0	-0.291968	3.492067	1.900610
14	6	0	-1.482185	2.806500	1.849622
15	6	0	1.516737	2.032287	-1.064602
16	6	0	2.683598	2.731478	-0.959816
17	6	0	2.903035	3.697203	0.046881
18	6	0	1.962066	3.983472	0.992545
19	8	0	3.799299	2.643066	-1.751956
20	6	0	4.784935	3.507951	-1.168904
21	8	0	4.153788	4.235401	-0.103789
22	1	0	-2.134758	-0.955523	-1.741987
23	6	0	-1.052568	-1.399124	0.052264
24	6	0	-1.866678	-2.611113	0.554701
25	8	0	-1.149144	-3.388388	1.512587
26	6	0	0.133104	-1.895997	-0.788939

27	6	0	1.508055	-1.921890	-0.221538
28	1	0	-0.701415	-0.855713	0.932541
29	8	0	-0.076566	-2.300762	-1.931898
30	6	0	2.578161	-2.145866	-1.113456
31	6	0	3.877419	-2.185471	-0.635308
32	6	0	4.141334	-2.018982	0.744358
33	6	0	3.075905	-1.829877	1.633738
34	6	0	1.768949	-1.772940	1.147759
35	8	0	5.417196	-2.037417	1.201321
36	8	0	3.303932	-1.632748	2.975862
37	6	0	3.777046	-2.784787	3.692835
38	8	0	5.011528	-2.366355	-1.376543
39	6	0	4.877757	-2.527524	-2.789758
40	6	0	-1.410539	1.338805	-2.486627
41	8	0	-6.691730	-0.780166	0.029423
42	6	0	-7.895574	-0.338875	0.655925
43	8	0	-4.427702	-1.691082	-1.150266
44	6	0	-5.098668	-1.550573	-2.413618
45	1	0	-6.343469	1.445606	1.576508
46	1	0	-4.207845	2.584499	1.888492
47	1	0	-0.104193	4.198861	2.704021
48	1	0	-2.223554	2.972896	2.624313
49	1	0	1.371721	1.270236	-1.818760
50	1	0	2.142244	4.712354	1.774995
51	1	0	5.606333	2.906053	-0.763607
52	1	0	5.146251	4.210357	-1.924541
53	1	0	-2.761200	-2.256043	1.070386
54	1	0	-2.189632	-3.221013	-0.297916
55	1	0	-0.476724	-3.902577	1.045614
56	1	0	2.355520	-2.277470	-2.164372
57	1	0	0.970612	-1.647395	1.868159
58	1	0	5.994889	-2.191827	0.434329
59	1	0	3.875632	-2.474908	4.734441
60	1	0	3.055070	-3.606681	3.624711
61	1	0	4.748375	-3.117822	3.316676
62	1	0	5.889968	-2.646501	-3.174915
63	1	0	4.286137	-3.417573	-3.028808
64	1	0	4.412454	-1.645513	-3.242443
65	1	0	-0.698643	2.126919	-2.739341
66	1	0	-1.388044	0.587770	-3.281586
67	1	0	-2.416608	1.784380	-2.452503
68	1	0	-8.670069	-1.036676	0.337380
69	1	0	-7.809573	-0.364750	1.748041
70	1	0	-8.164953	0.674258	0.336924

71	1	0	-6.153243	-1.299408	-2.274920
72	1	0	-4.614268	-0.782486	-3.027443
73	1	0	-5.013991	-2.517863	-2.911829

Standard orientation of **1-3**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.302558	1.514637	1.192548
2	6	0	-5.532239	0.486356	0.277875
3	6	0	-4.445815	-0.068015	-0.425313
4	6	0	-3.142550	0.375636	-0.171135
5	6	0	-2.914506	1.414178	0.757732
6	6	0	-4.012213	1.983875	1.421697
7	6	0	-1.943529	-0.203223	-0.899482
8	7	0	-0.953280	0.847115	-1.201751
9	6	0	-0.593967	1.640359	-0.069935
10	6	0	-1.532900	1.905662	0.932264
11	6	0	0.736693	2.153675	0.016083
12	6	0	1.092371	2.977892	1.137289
13	6	0	0.124117	3.211669	2.148193
14	6	0	-1.139879	2.679792	2.056308
15	6	0	1.716498	1.847650	-0.982490
16	6	0	2.956905	2.396409	-0.839434
17	6	0	3.299789	3.227497	0.249870
18	6	0	2.410327	3.524516	1.241320
19	8	0	4.058978	2.227394	-1.640676
20	6	0	5.064394	3.118439	-1.133868
21	8	0	4.613753	3.599824	0.141320
22	1	0	-2.265266	-0.620573	-1.854734
23	6	0	-1.236820	-1.350663	-0.122481
24	6	0	-2.184752	-2.510841	0.244593
25	8	0	-1.569051	-3.457255	1.119367
26	6	0	-0.091812	-1.873893	-1.004764
27	6	0	1.272319	-2.051125	-0.437478
28	1	0	-0.845669	-0.939571	0.811362
29	8	0	-0.323305	-2.150601	-2.180166
30	6	0	1.499515	-2.167121	0.948609
31	6	0	2.794627	-2.354680	1.415654
32	6	0	3.884314	-2.406620	0.520611

33	6	0	3.656213	-2.272540	-0.858020
34	6	0	2.354829	-2.114945	-1.326108
35	8	0	5.143077	-2.595191	0.988644
36	8	0	4.694006	-2.353885	-1.756164
37	6	0	5.618960	-1.252792	-1.723055
38	8	0	3.167477	-2.514950	2.721844
39	6	0	2.154982	-2.471555	3.728424
40	6	0	-1.281599	1.632900	-2.402239
41	8	0	-6.826339	0.070076	0.051885
42	6	0	-7.130068	-1.251246	0.530122
43	8	0	-4.632352	-1.096442	-1.326908
44	6	0	-5.336496	-0.733833	-2.528929
45	1	0	-6.153743	1.943086	1.712068
46	1	0	-3.867352	2.809618	2.109463
47	1	0	0.402605	3.809800	3.011198
48	1	0	-1.849329	2.855973	2.858123
49	1	0	1.475564	1.181012	-1.799459
50	1	0	2.684606	4.144452	2.087696
51	1	0	6.002033	2.573647	-1.006318
52	1	0	5.184536	3.963412	-1.822261
53	1	0	-3.044562	-2.116926	0.790443
54	1	0	-2.556312	-2.991939	-0.668177
55	1	0	-0.980012	-4.017279	0.596010
56	1	0	0.666860	-2.168578	1.638784
57	1	0	2.183057	-2.030172	-2.392736
58	1	0	5.083046	-2.650972	1.957682
59	1	0	5.096529	-0.302851	-1.883048
60	1	0	6.160912	-1.217920	-0.773731
61	1	0	6.322998	-1.424701	-2.538970
62	1	0	2.670761	-2.610419	4.678080
63	1	0	1.640836	-1.504399	3.727400
64	1	0	1.424657	-3.275430	3.586722
65	1	0	-0.486111	2.355552	-2.593373
66	1	0	-1.350711	0.961871	-3.263181
67	1	0	-2.229515	2.184416	-2.308509
68	1	0	-6.987628	-1.309658	1.615311
69	1	0	-8.180151	-1.428169	0.292086
70	1	0	-6.508301	-2.003920	0.037526
71	1	0	-4.786792	0.038584	-3.078099
72	1	0	-5.391307	-1.640334	-3.133458
73	1	0	-6.344137	-0.377460	-2.301575

Standard orientation of **1-4**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.366374	1.259973	1.109747
2	6	0	-5.537473	0.184736	0.233110
3	6	0	-4.408951	-0.342246	-0.435349
4	6	0	-3.137540	0.180443	-0.197853
5	6	0	-2.965927	1.267515	0.689723
6	6	0	-4.096399	1.795952	1.324307
7	6	0	-1.905038	-0.371432	-0.890659
8	7	0	-0.961664	0.710789	-1.230192
9	6	0	-0.651401	1.569577	-0.130692
10	6	0	-1.613231	1.836123	0.849165
11	6	0	0.653554	2.146289	-0.056225
12	6	0	0.957633	3.040295	1.026203
13	6	0	-0.032610	3.277247	2.014602
14	6	0	-1.268928	2.681428	1.937519
15	6	0	1.660173	1.834579	-1.026203
16	6	0	2.875213	2.440183	-0.893281
17	6	0	3.165918	3.339187	0.155794
18	6	0	2.249367	3.648540	1.118286
19	8	0	3.983589	2.303271	-1.691093
20	6	0	5.025600	3.084067	-1.084427
21	8	0	4.453503	3.788911	0.027585
22	1	0	-2.196531	-0.845018	-1.829200
23	6	0	-1.149740	-1.449718	-0.061586
24	6	0	-2.046565	-2.628867	0.367351
25	8	0	-1.383143	-3.511304	1.274046
26	6	0	0.011544	-1.968020	-0.925480
27	6	0	1.386531	-2.056192	-0.363578
28	1	0	-0.771214	-0.977709	0.848559
29	8	0	-0.215189	-2.316112	-2.082837
30	6	0	1.630822	-2.089883	1.023983
31	6	0	2.937038	-2.196596	1.485673
32	6	0	4.019963	-2.247670	0.582340
33	6	0	3.773753	-2.196127	-0.798658
34	6	0	2.462854	-2.119151	-1.259737
35	8	0	5.290141	-2.356549	1.045002
36	8	0	4.806601	-2.280317	-1.702538
37	6	0	5.675920	-1.135421	-1.744771
38	8	0	3.328094	-2.272072	2.794195

39	6	0	2.323057	-2.223186	3.807992
40	6	0	-1.317262	1.429607	-2.464015
41	8	0	-6.728623	-0.423511	-0.031345
42	6	0	-7.895968	0.069700	0.624848
43	8	0	-4.540321	-1.434309	-1.268918
44	6	0	-5.199327	-1.177144	-2.520129
45	1	0	-6.216900	1.690095	1.624119
46	1	0	-4.003396	2.653633	1.981688
47	1	0	0.207038	3.929284	2.849867
48	1	0	-1.994838	2.862477	2.723470
49	1	0	1.458077	1.120880	-1.813489
50	1	0	2.483511	4.324565	1.933215
51	1	0	5.818746	2.418650	-0.726590
52	1	0	5.411375	3.803252	-1.812008
53	1	0	-2.914828	-2.244915	0.906721
54	1	0	-2.409704	-3.163323	-0.518505
55	1	0	-0.781790	-4.072800	0.766588
56	1	0	0.804679	-2.091029	1.721964
57	1	0	2.278002	-2.097650	-2.327318
58	1	0	5.241486	-2.365259	2.016227
59	1	0	5.105662	-0.223384	-1.954291
60	1	0	6.223777	-1.017897	-0.805405
61	1	0	6.380705	-1.320120	-2.557233
62	1	0	2.852506	-2.289428	4.757967
63	1	0	1.764955	-1.281819	3.763100
64	1	0	1.629346	-3.065665	3.715096
65	1	0	-0.552486	2.177446	-2.682348
66	1	0	-1.351845	0.720374	-3.295999
67	1	0	-2.288977	1.942620	-2.398331
68	1	0	-8.093769	1.114118	0.358748
69	1	0	-8.719162	-0.554570	0.277182
70	1	0	-7.808163	-0.017296	1.713645
71	1	0	-6.229891	-0.848969	-2.363059
72	1	0	-4.655265	-0.420869	-3.097497
73	1	0	-5.193921	-2.121960	-3.066304

Standard orientation of **1-5**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.431098	1.307627	0.937195

2	6	0	-5.565893	0.086345	0.270609
3	6	0	-4.420076	-0.515616	-0.297430
4	6	0	-3.167024	0.082935	-0.164948
5	6	0	-3.031810	1.317478	0.510446
6	6	0	-4.179579	1.914683	1.045230
7	6	0	-1.916571	-0.544231	-0.753077
8	7	0	-1.010528	0.489193	-1.289287
9	6	0	-0.727124	1.539313	-0.361423
10	6	0	-1.697658	1.946999	0.559852
11	6	0	0.560526	2.156955	-0.393963
12	6	0	0.839461	3.230308	0.518949
13	6	0	-0.158930	3.610181	1.452913
14	6	0	-1.379613	2.978950	1.482467
15	6	0	1.576085	1.711028	-1.300243
16	6	0	2.775055	2.361453	-1.276181
17	6	0	3.041726	3.431464	-0.393836
18	6	0	2.116149	3.876497	0.504721
19	8	0	3.883498	2.126567	-2.048587
20	6	0	4.914636	2.994934	-1.556746
21	8	0	4.315894	3.888367	-0.605249
22	1	0	-2.191296	-1.190390	-1.587907
23	6	0	-1.123043	-1.422655	0.255271
24	6	0	-1.970307	-2.539894	0.900428
25	8	0	-1.275780	-3.202442	1.956477
26	6	0	0.054056	-2.058068	-0.499618
27	6	0	1.430872	-2.020763	0.062318
28	1	0	-0.768590	-0.777427	1.061839
29	8	0	-0.168486	-2.630942	-1.565939
30	6	0	2.485112	-2.459149	-0.767117
31	6	0	3.786126	-2.451609	-0.292847
32	6	0	4.067956	-2.023771	1.025629
33	6	0	3.021525	-1.591723	1.850021
34	6	0	1.712869	-1.589153	1.365841
35	8	0	5.340505	-2.041228	1.490536
36	8	0	3.258972	-1.224733	3.154646
37	6	0	3.956123	0.021241	3.319381
38	8	0	4.903839	-2.839717	-0.977208
39	6	0	4.746647	-3.316950	-2.314592
40	6	0	-1.392413	0.966384	-2.627919
41	8	0	-6.736101	-0.598372	0.126883
42	6	0	-7.919583	-0.031231	0.687387
43	8	0	-4.514589	-1.744261	-0.918930
44	6	0	-5.176744	-1.737936	-2.194612
45	1	0	-6.295914	1.795839	1.369396

46	1	0	-4.115498	2.879515	1.536560
47	1	0	0.062432	4.403168	2.161725
48	1	0	-2.112253	3.274220	2.226375
49	1	0	1.393663	0.869776	-1.955463
50	1	0	2.330594	4.687806	1.191638
51	1	0	5.689653	2.399089	-1.060686
52	1	0	5.330843	3.572532	-2.385833
53	1	0	-2.860554	-2.103220	1.357675
54	1	0	-2.299432	-3.247182	0.129213
55	1	0	-0.607351	-3.780077	1.564104
56	1	0	2.246802	-2.795200	-1.767918
57	1	0	0.930277	-1.278208	2.045787
58	1	0	5.905868	-2.364382	0.768166
59	1	0	4.024037	0.191765	4.395048
60	1	0	4.961982	-0.025761	2.892430
61	1	0	3.398233	0.842565	2.854914
62	1	0	4.316670	-2.542977	-2.959084
63	1	0	5.747984	-3.568680	-2.662503
64	1	0	4.112552	-4.209505	-2.340271
65	1	0	-0.649685	1.682947	-2.984131
66	1	0	-1.412073	0.119313	-3.319763
67	1	0	-2.377554	1.457367	-2.645903
68	1	0	-8.721332	-0.735722	0.465803
69	1	0	-7.829010	0.087576	1.772897
70	1	0	-8.151904	0.938959	0.234098
71	1	0	-5.142746	-2.765748	-2.560000
72	1	0	-6.216845	-1.416447	-2.097877
73	1	0	-4.652649	-1.083957	-2.900996

Standard orientation of **1-6**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.461351	1.053209	1.085719
2	6	0	-5.549262	-0.074419	0.264380
3	6	0	-4.381884	-0.550764	-0.374593
4	6	0	-3.153139	0.074925	-0.162367
5	6	0	-3.065650	1.214345	0.669735
6	6	0	-4.234850	1.690345	1.275020
7	6	0	-1.881084	-0.419133	-0.826685

8	7	0	-1.015613	0.710101	-1.216320
9	6	0	-0.774372	1.642150	-0.160249
10	6	0	-1.758387	1.886276	0.803433
11	6	0	0.484851	2.315523	-0.112259
12	6	0	0.717819	3.279906	0.926667
13	6	0	-0.292021	3.491863	1.900750
14	6	0	-1.482227	2.806282	1.849757
15	6	0	1.516531	2.032579	-1.064794
16	6	0	2.683385	2.731777	-0.959954
17	6	0	2.902864	3.697351	0.046876
18	6	0	1.961924	3.983454	0.992620
19	8	0	3.799047	2.643492	-1.752167
20	6	0	4.784673	3.508392	-1.169113
21	8	0	4.153601	4.235593	-0.103778
22	1	0	-2.134756	-0.955626	-1.741942
23	6	0	-1.052417	-1.399042	0.052230
24	6	0	-1.866459	-2.611093	0.554766
25	8	0	-1.148857	-3.388358	1.512553
26	6	0	0.133231	-1.895871	-0.788982
27	6	0	1.508169	-1.921886	-0.221552
28	1	0	-0.701282	-0.855581	0.932481
29	8	0	-0.076410	-2.300492	-1.932004
30	6	0	1.769075	-1.772889	1.147733
31	6	0	3.076035	-1.829789	1.633730
32	6	0	4.141461	-2.018974	0.744372
33	6	0	3.877527	-2.185579	-0.635290
34	6	0	2.578281	-2.145949	-1.113448
35	8	0	5.417323	-2.037419	1.201316
36	8	0	5.011643	-2.366506	-1.376504
37	6	0	4.877861	-2.528119	-2.789671
38	8	0	3.304009	-1.632562	2.975839
39	6	0	3.777490	-2.784415	3.692878
40	6	0	-1.410992	1.338911	-2.486616
41	8	0	-6.691743	-0.780365	0.029451
42	6	0	-7.895612	-0.339069	0.655905
43	8	0	-4.427721	-1.691316	-1.150122
44	6	0	-5.098475	-1.550746	-2.413578
45	1	0	-6.343524	1.445403	1.576573
46	1	0	-4.207910	2.584319	1.888577
47	1	0	-0.104179	4.198537	2.704252
48	1	0	-2.223558	2.972532	2.624516
49	1	0	1.371548	1.270690	-1.819121
50	1	0	2.142110	4.712212	1.775184
51	1	0	5.606182	2.906503	-0.764033

52	1	0	5.145799	4.210972	-1.924679
53	1	0	-2.760919	-2.255994	1.070532
54	1	0	-2.189499	-3.220943	-0.297864
55	1	0	-0.476388	-3.902464	1.045564
56	1	0	0.970760	-1.647293	1.868147
57	1	0	2.355646	-2.277588	-2.164362
58	1	0	5.995017	-2.191814	0.434321
59	1	0	4.286136	-3.418174	-3.028431
60	1	0	4.412667	-1.646201	-3.242653
61	1	0	5.890059	-2.647346	-3.174782
62	1	0	3.875806	-2.474495	4.734496
63	1	0	3.055856	-3.606599	3.624656
64	1	0	4.749003	-3.117056	3.316849
65	1	0	-0.699083	2.126956	-2.739511
66	1	0	-1.388767	0.587869	-3.281573
67	1	0	-2.417007	1.784578	-2.452229
68	1	0	-8.164972	0.674067	0.336897
69	1	0	-8.670101	-1.036863	0.337329
70	1	0	-7.809662	-0.364942	1.748026
71	1	0	-6.153059	-1.299514	-2.275040
72	1	0	-4.613943	-0.782675	-3.027320
73	1	0	-5.013793	-2.518027	-2.911807

Table S4 Computational methods for ECD of compound **2**

Standard orientation of **2-1**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.792178	-2.356213	-0.291838
2	6	0	4.344518	-1.110133	0.008628
3	6	0	3.499396	0.009143	0.130017
4	6	0	2.114397	-0.138776	-0.011816
5	6	0	1.558061	-1.402689	-0.299902
6	6	0	2.417028	-2.504157	-0.445339
7	6	0	1.168022	1.038412	0.146154
8	7	0	-0.103910	0.631756	0.766570
9	6	0	-0.707199	-0.502835	0.142382
10	6	0	0.089133	-1.510630	-0.411768
11	6	0	-2.132656	-0.585706	0.099638

12	6	0	-2.744421	-1.743371	-0.490666
13	6	0	-1.910793	-2.741748	-1.057873
14	6	0	-0.541931	-2.620380	-1.034605
15	6	0	-2.953496	0.468035	0.616600
16	6	0	-4.306369	0.302150	0.557971
17	6	0	-4.907432	-0.848064	0.000636
18	6	0	-4.169260	-1.865427	-0.530536
19	8	0	-5.285648	1.171134	0.964543
20	6	0	-6.537442	0.498008	0.766628
21	8	0	-6.269925	-0.722861	0.059028
22	6	0	0.894217	1.749478	-1.193617
23	6	0	0.117445	3.043885	-0.969582
24	7	0	-0.953833	3.237751	-1.776467
25	8	0	0.463888	3.868391	-0.122105
26	1	0	1.621422	1.779815	0.805830
27	8	0	5.712533	-1.002701	0.140858
28	6	0	6.169727	-0.736744	1.477465
29	6	0	-0.033182	0.529747	2.233298
30	8	0	3.999361	1.257778	0.437415
31	6	0	4.856212	1.849117	-0.555186
32	1	0	4.459615	-3.207153	-0.383720
33	1	0	2.014143	-3.491442	-0.642331
34	1	0	-2.373680	-3.603719	-1.530022
35	1	0	0.065708	-3.387546	-1.502973
36	1	0	-2.503147	1.367735	1.014424
37	1	0	-4.635411	-2.736609	-0.977366
38	1	0	-6.986805	0.265639	1.738887
39	1	0	-7.198906	1.128171	0.166577
40	1	0	1.851163	2.018839	-1.653887
41	1	0	0.377892	1.079909	-1.887611
42	1	0	-1.494697	4.084781	-1.678601
43	1	0	-1.254713	2.550396	-2.448855
44	1	0	5.779277	0.214955	1.848982
45	1	0	5.870167	-1.545139	2.154243
46	1	0	7.258709	-0.692097	1.424874
47	1	0	-1.021003	0.287083	2.630028
48	1	0	0.672996	-0.241681	2.576965
49	1	0	0.275248	1.494429	2.646308
50	1	0	4.333445	1.940357	-1.513869
51	1	0	5.106760	2.843903	-0.183890
52	1	0	5.767434	1.262283	-0.692742

Standard orientation of **2-2**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.865944	-2.172453	-0.101502
2	6	0	4.365535	-0.902047	0.201057
3	6	0	3.468031	0.186263	0.289770
4	6	0	2.099542	-0.011918	0.102481
5	6	0	1.593559	-1.298801	-0.187090
6	6	0	2.497011	-2.364021	-0.287484
7	6	0	1.107388	1.131472	0.221650
8	7	0	-0.166934	0.686150	0.810460
9	6	0	-0.713070	-0.475375	0.181313
10	6	0	0.133724	-1.460454	-0.337800
11	6	0	-2.132976	-0.608197	0.098900
12	6	0	-2.687161	-1.793491	-0.493836
13	6	0	-1.803337	-2.768376	-1.024585
14	6	0	-0.440678	-2.598472	-0.964547
15	6	0	-3.004952	0.420767	0.581159
16	6	0	-4.348994	0.205827	0.487818
17	6	0	-4.893432	-0.970977	-0.072068
18	6	0	-4.105228	-1.966712	-0.571166
19	8	0	-5.369953	1.044410	0.855577
20	6	0	-6.588621	0.315100	0.650805
21	8	0	-6.261252	-0.892500	-0.053781
22	6	0	0.845511	1.817345	-1.133631
23	6	0	0.017395	3.085454	-0.946780
24	7	0	-1.035998	3.233135	-1.786391
25	8	0	0.309477	3.930686	-0.099159
26	1	0	1.515815	1.895746	0.884468
27	8	0	5.678389	-0.619428	0.439720
28	6	0	6.623175	-1.685542	0.357292
29	6	0	-0.131803	0.597452	2.279087
30	8	0	3.916379	1.445217	0.630607
31	6	0	4.749955	2.104274	-0.336095
32	1	0	4.533978	-3.021922	-0.172553
33	1	0	2.139251	-3.369179	-0.482481
34	1	0	-2.222358	-3.651703	-1.498379
35	1	0	0.206941	-3.349236	-1.405373
36	1	0	-2.597744	1.339826	0.981410
37	1	0	-4.527493	-2.858952	-1.020196
38	1	0	-7.032922	0.063232	1.620905

39	1	0	-7.274070	0.914013	0.046181
40	1	0	1.804496	2.115569	-1.571206
41	1	0	0.372960	1.121719	-1.833264
42	1	0	-1.608471	4.061681	-1.713656
43	1	0	-1.293185	2.528897	-2.459412
44	1	0	6.407702	-2.467759	1.093821
45	1	0	6.642952	-2.126847	-0.645532
46	1	0	7.593902	-1.240507	0.576125
47	1	0	-1.121212	0.324344	2.651492
48	1	0	0.590664	-0.146797	2.648174
49	1	0	0.132697	1.575028	2.692421
50	1	0	4.924225	3.109855	0.050650
51	1	0	5.703486	1.584947	-0.457504
52	1	0	4.245493	2.173260	-1.306776

Standard orientation of **2-3**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.787262	-2.384739	0.013789
2	6	0	4.341215	-1.112510	0.163584
3	6	0	3.491154	0.007950	0.217899
4	6	0	2.108293	-0.151999	0.078126
5	6	0	1.553115	-1.436494	-0.099894
6	6	0	2.410270	-2.548770	-0.107202
7	6	0	1.167558	1.038283	0.109584
8	7	0	-0.125633	0.697541	0.724710
9	6	0	-0.718073	-0.490540	0.197936
10	6	0	0.086365	-1.551639	-0.231121
11	6	0	-2.142617	-0.573254	0.125565
12	6	0	-2.745188	-1.782913	-0.360931
13	6	0	-1.902888	-2.836139	-0.801962
14	6	0	-0.534512	-2.716856	-0.754961
15	6	0	-2.971111	0.528889	0.513296
16	6	0	-4.322907	0.361162	0.437014
17	6	0	-4.915451	-0.837673	-0.017596
18	6	0	-4.169121	-1.904863	-0.425148
19	8	0	-5.308146	1.268978	0.728582
20	6	0	-6.556472	0.576879	0.580760
21	8	0	-6.278410	-0.703455	-0.007450
22	6	0	0.951282	1.632345	-1.296251

23	6	0	0.180903	2.946932	-1.218460
24	7	0	-0.844870	3.083890	-2.093384
25	8	0	0.493805	3.835052	-0.423723
26	1	0	1.607555	1.832481	0.715007
27	8	0	5.707688	-0.990243	0.298563
28	6	0	6.371737	-0.372694	-0.816902
29	6	0	-0.101499	0.741151	2.195826
30	8	0	3.997427	1.286071	0.341129
31	6	0	4.617196	1.579468	1.606445
32	1	0	4.455772	-3.239610	-0.004962
33	1	0	2.006684	-3.551249	-0.197226
34	1	0	-2.358176	-3.740021	-1.196757
35	1	0	0.081237	-3.528706	-1.127510
36	1	0	-2.526553	1.462495	0.831777
37	1	0	-4.628119	-2.815363	-0.794266
38	1	0	-7.015926	0.434305	1.565736
39	1	0	-7.212427	1.146412	-0.082271
40	1	0	1.931313	1.852884	-1.734126
41	1	0	0.456750	0.907804	-1.949859
42	1	0	-1.375530	3.942917	-2.096689
43	1	0	-1.117002	2.348527	-2.726037
44	1	0	6.223704	-0.963682	-1.728086
45	1	0	6.010142	0.646641	-0.978294
46	1	0	7.433715	-0.351461	-0.566970
47	1	0	-1.100934	0.533741	2.583088
48	1	0	0.594701	0.010543	2.635842
49	1	0	0.192006	1.743259	2.521496
50	1	0	5.474262	0.925671	1.785538
51	1	0	4.947945	2.617586	1.549170
52	1	0	3.894435	1.471746	2.422932

Standard orientation of **2-4**:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.865941	-2.172457	-0.101484
2	6	0	4.365533	-0.902050	0.201070
3	6	0	3.468030	0.186261	0.289774
4	6	0	2.099541	-0.011917	0.102482
5	6	0	1.593557	-1.298800	-0.187084

6	6	0	2.497007	-2.364022	-0.287469
7	6	0	1.107389	1.131475	0.221644
8	7	0	-0.166934	0.686157	0.810453
9	6	0	-0.713071	-0.475369	0.181305
10	6	0	0.133723	-1.460452	-0.337799
11	6	0	-2.132977	-0.608183	0.098880
12	6	0	-2.687162	-1.793477	-0.493860
13	6	0	-1.803338	-2.768369	-1.024595
14	6	0	-0.440679	-2.598471	-0.964545
15	6	0	-3.004951	0.420785	0.581131
16	6	0	-4.348994	0.205850	0.487782
17	6	0	-4.893432	-0.970954	-0.072110
18	6	0	-4.105229	-1.966692	-0.571202
19	8	0	-5.369964	1.044461	0.855467
20	6	0	-6.588576	0.314958	0.651074
21	8	0	-6.261256	-0.892430	-0.053894
22	6	0	0.845511	1.817344	-1.133641
23	6	0	0.017392	3.085451	-0.946784
24	7	0	-1.036039	3.233105	-1.786351
25	8	0	0.309492	3.930691	-0.099178
26	1	0	1.515815	1.895753	0.884456
27	8	0	5.678387	-0.619432	0.439731
28	6	0	6.623172	-1.685548	0.357311
29	6	0	-0.131802	0.597449	2.279081
30	8	0	3.916382	1.445216	0.630608
31	6	0	4.749950	2.104267	-0.336107
32	1	0	4.533972	-3.021929	-0.172529
33	1	0	2.139245	-3.369181	-0.482461
34	1	0	-2.222359	-3.651697	-1.498388
35	1	0	0.206940	-3.349239	-1.405364
36	1	0	-2.597741	1.339844	0.981380
37	1	0	-4.527494	-2.858927	-1.020241
38	1	0	-7.032409	0.062800	1.621320
39	1	0	-7.274395	0.913852	0.046864
40	1	0	1.804495	2.115574	-1.571216
41	1	0	0.372964	1.121716	-1.833273
42	1	0	-1.608463	4.061689	-1.713667
43	1	0	-1.293168	2.528915	-2.459443
44	1	0	6.407696	-2.467759	1.093846
45	1	0	6.642947	-2.126860	-0.645510
46	1	0	7.593899	-1.240512	0.576141
47	1	0	-1.121216	0.324358	2.651484
48	1	0	0.590652	-0.146816	2.648161
49	1	0	0.132717	1.575018	2.692418

50	1	0	4.245475	2.173253	−1.306782
51	1	0	4.924227	3.109849	0.050633
52	1	0	5.703477	1.584936	−0.457525

References

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Mo ro ku ma , K . ; Z a kr ze w sk i, V. G .; Vo th, G. A.; Sa lv a d or , P .; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.;Farkas, O; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision C1; Gaussian, Inc.: Wallingford, CT, 2010. [4]. Bruhn, T.; Hemberger, Y.; Schaumlöffel, A.; Bringmann, G. *Spec Dis*, version 1.51, University of Würzburg, Germany, 2010.

[2] Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. Quantifying the Comparison of Calculated and Experimental Electronic Circular Dichroism Spectra, Chirality 2013, 25, 243–249.

Table S5. 2D Structures of **1** and **2**.

label	structure

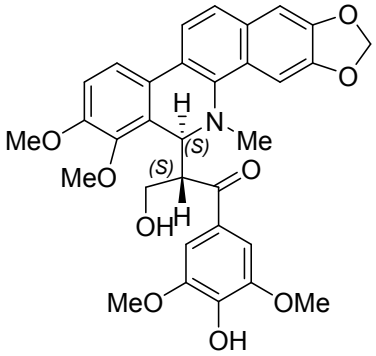
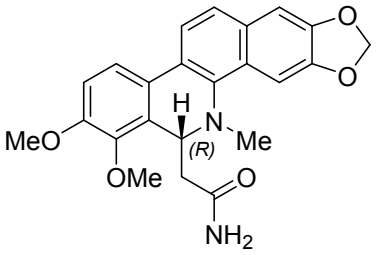
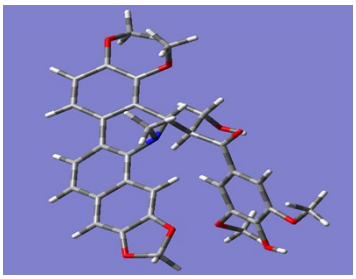
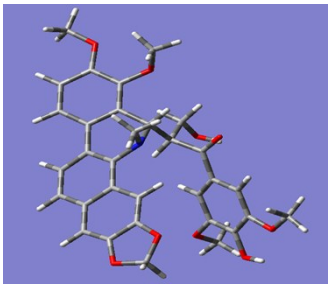
1	
2	

Table S6 B3LYP/6-31++G (d, p) optimized lowest energy 3D conformers of (*S*,*S*)-**1**.

label	conformer	Boltzmann weighting factors
1-1		0.44
1-2		27.45

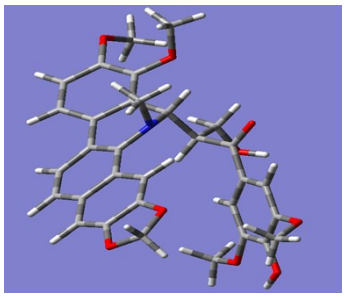
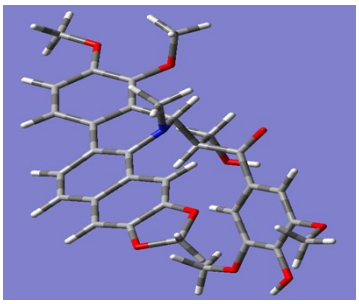
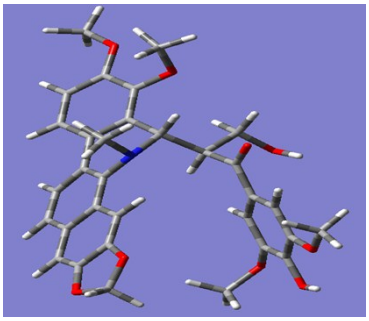
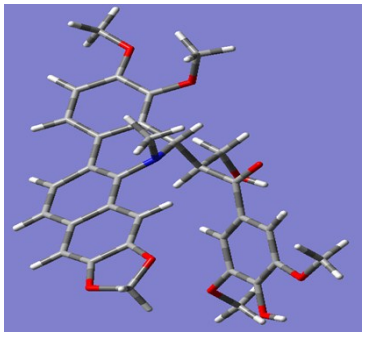
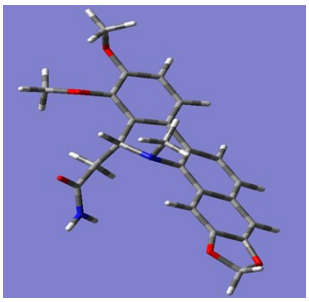
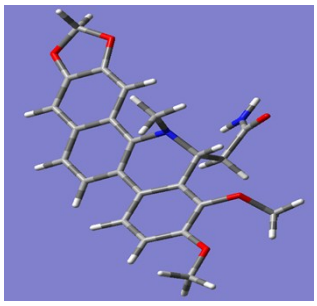
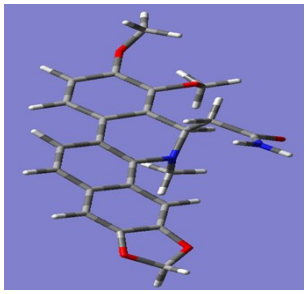
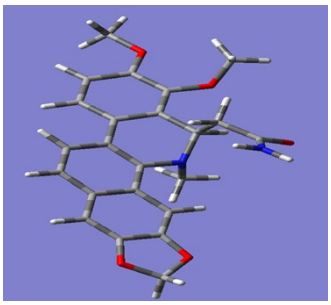
1-3		0.17
1-4		9.37
1-5		35.14
1-6		27.43

Table S7 B3LYP/6-31++G (d, p) optimized lowest energy 3D conformers of (*R*)- **2**.

label	conformer	Boltzmann weighting factors

2-1		25.6
2-2		25.93
2-3		22.87
2-4		25.60

2 The 1D and 2D NMR spectra of compounds 1-3

Fig. 1 ^{1}H NMR spectrum of compound 1 in DMSO-d_6

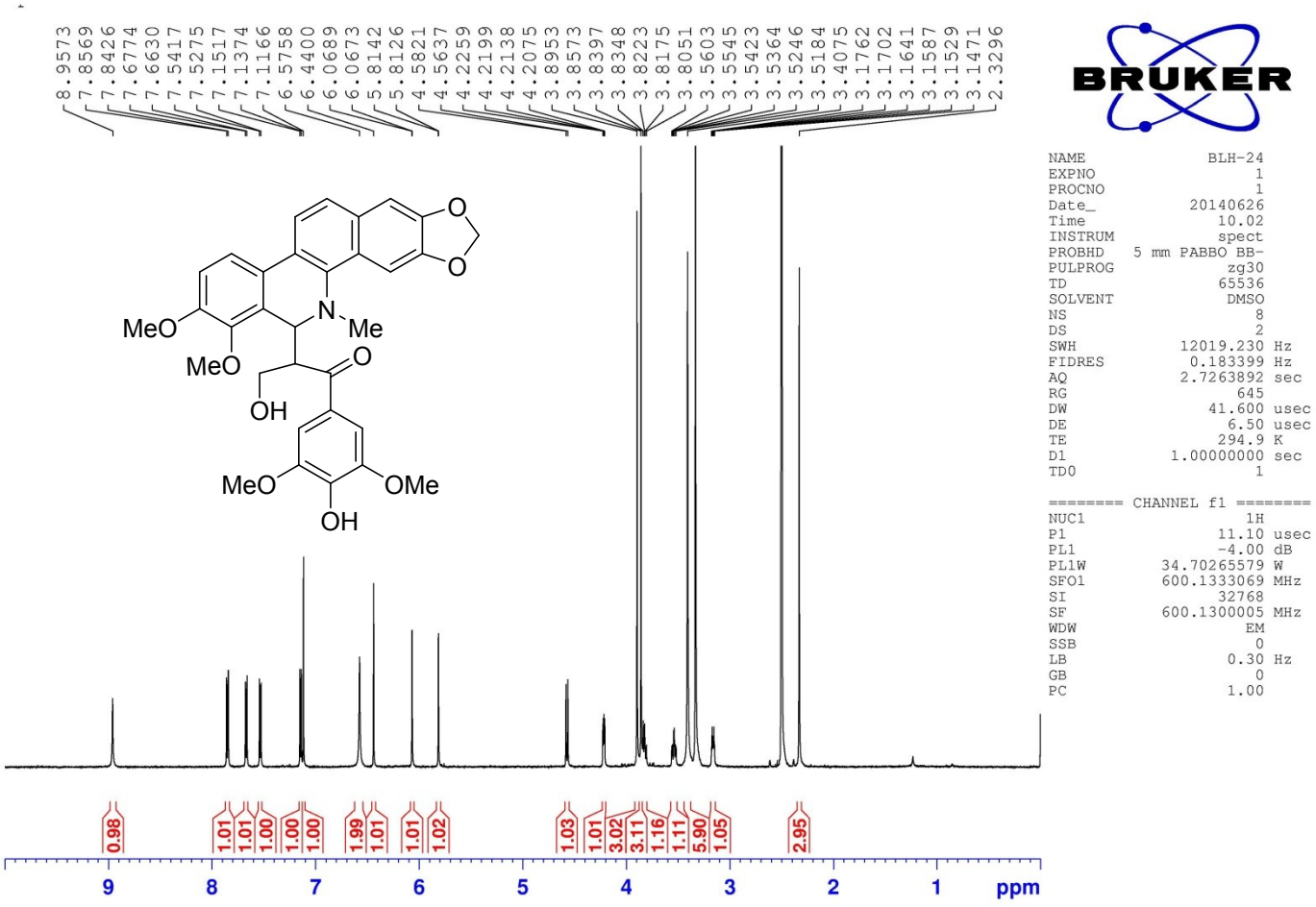


Fig. 2 ^{13}C NMR spectrum of compound 1 in DMSO-d_6

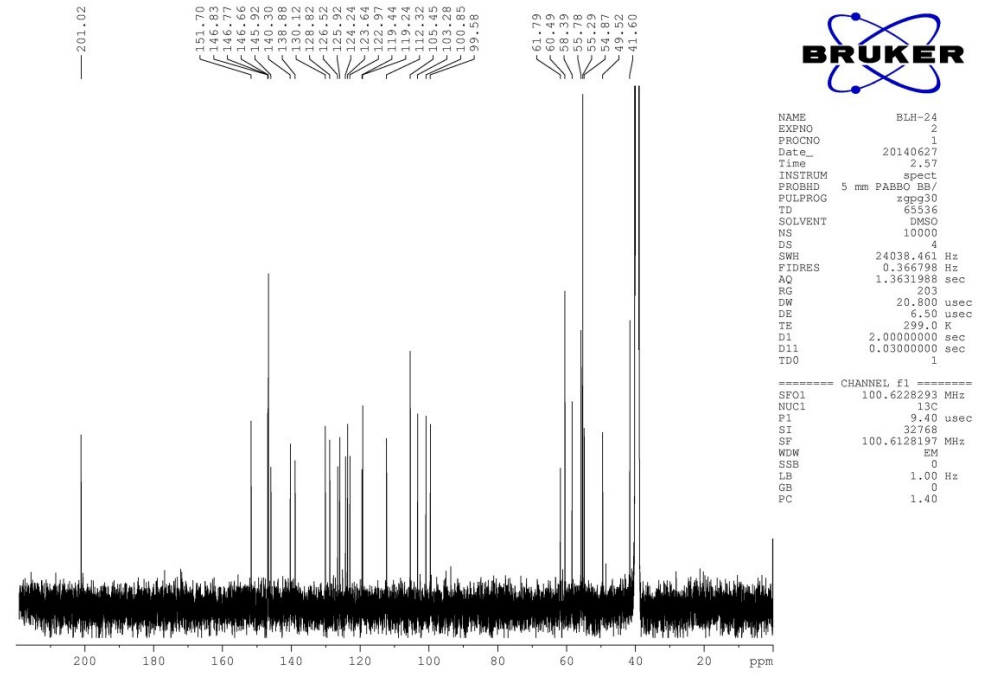


Fig. 3 HSQC spectrum of compound 1 in DMSO-d_6

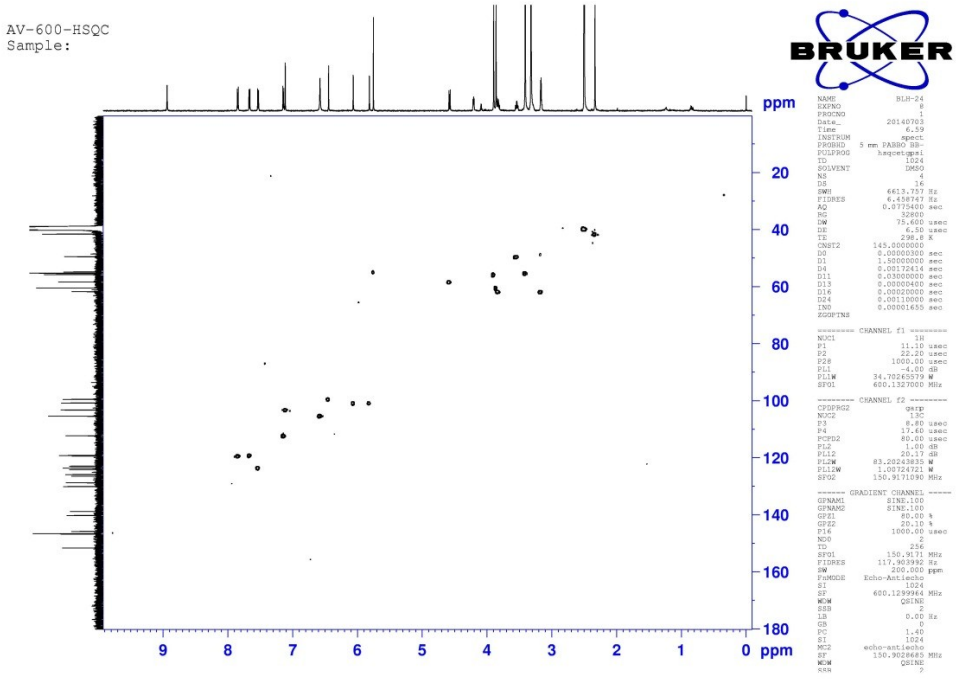


Fig. 4 HMBC spectrum of compound 1 in DMSO-d_6

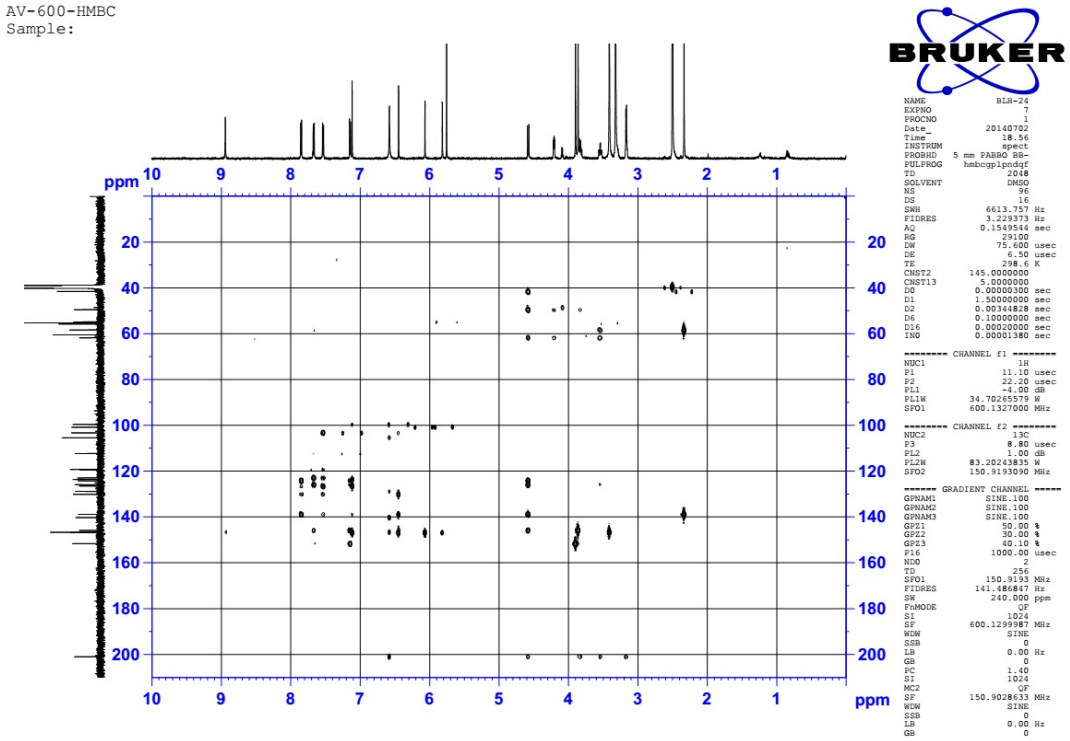


Fig. 5 ^{1}H-^{1}H COSY spectrum of compound 1 in DMSO-d_6

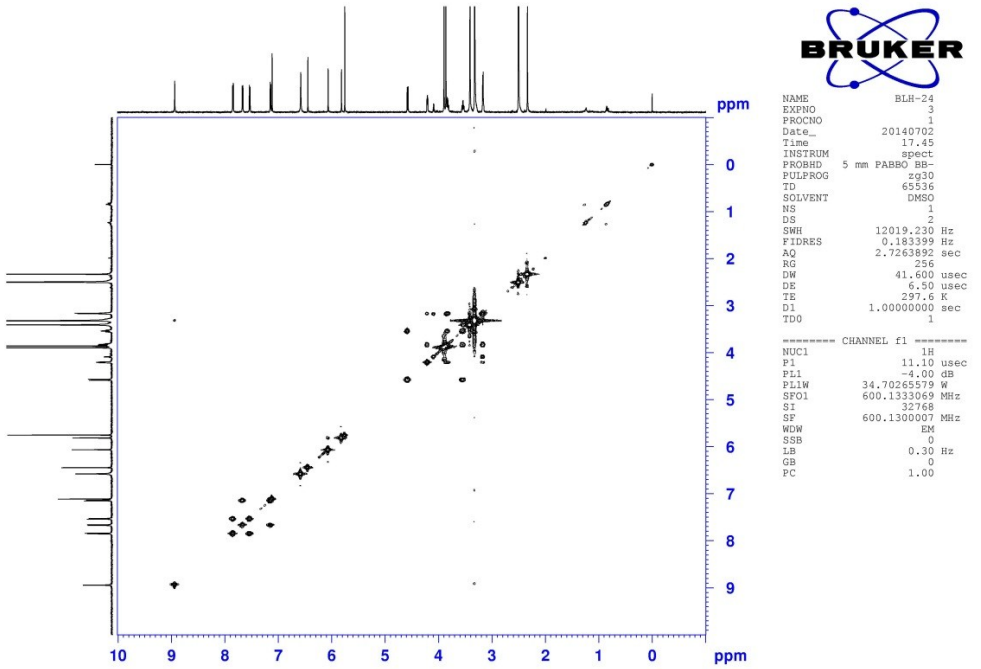


Fig. 6 NOESY spectrum of compound 1 in DMSO-d_6

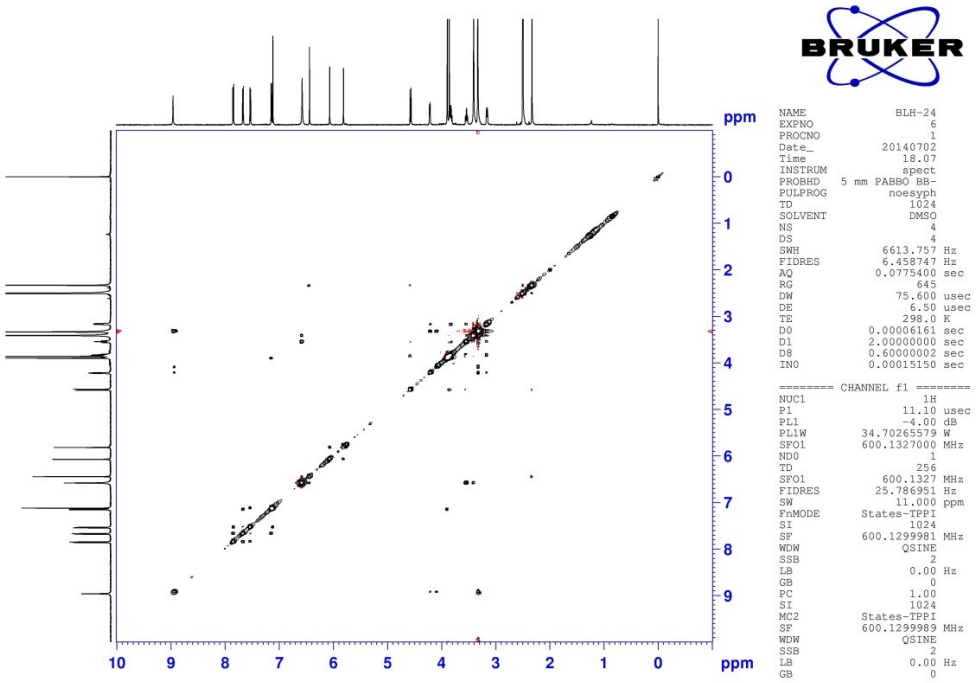
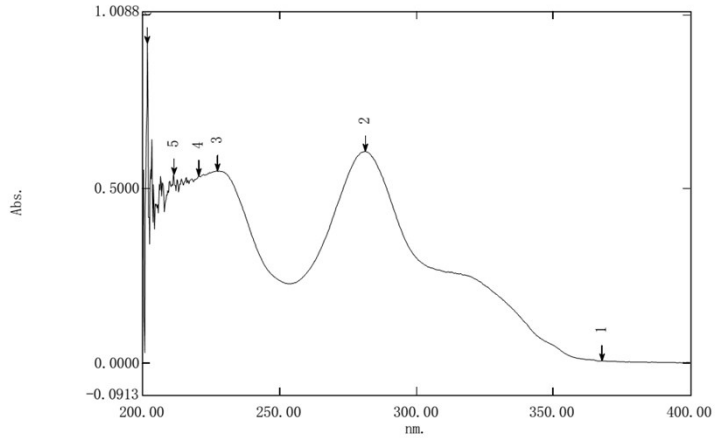


Fig. 7 UV spectrum of compound 1 in MeOH



测定属性
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扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 自动

试样准备属性
重量:
体积 :
稀释:
光程长:
附加信息:

仪器属性
仪器类型: UV-1700
测定方式: 吸收值
狭缝宽: 1.0 nm
光源改变波长: 340.8 nm
S/R 转换: 标准

附件属性
附件: 无

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2	↑	281.20	.6079	
3	↑	227.40	.5514	
4	↑	220.40	.5367	
5	↑	211.40	.5420	
6	↑	201.80	.9171	
7	↓	366.40	.0057	
8	↓	253.60	.2274	
9	↓	221.20	.5341	
10	↓	215.00	.5104	
11	↓	208.00	.4338	

Fig. 8 IR spectrum of compound 1

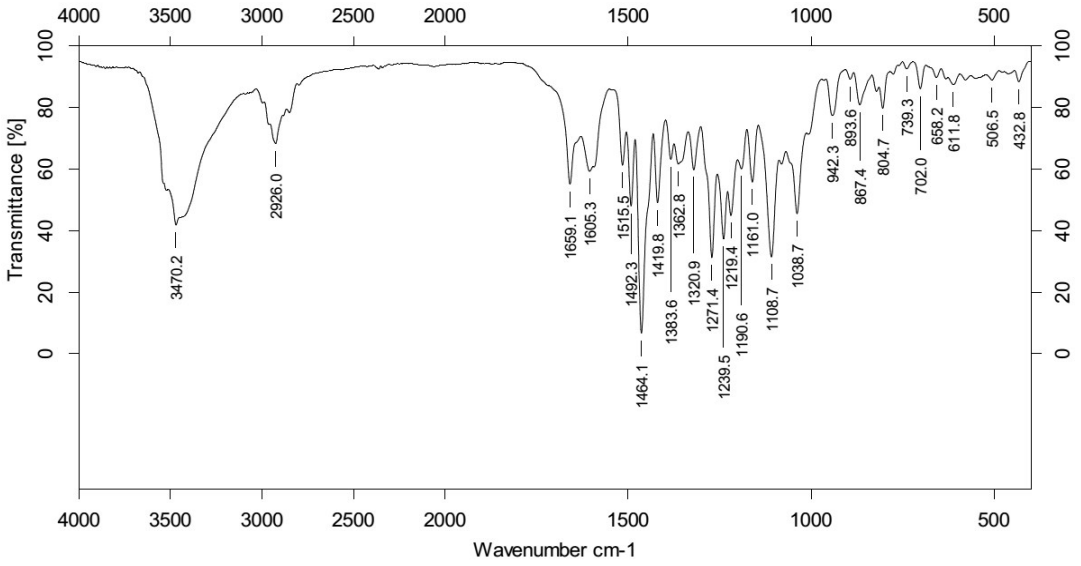

Fig. 9 ECD spectra of compound 1a and 1b

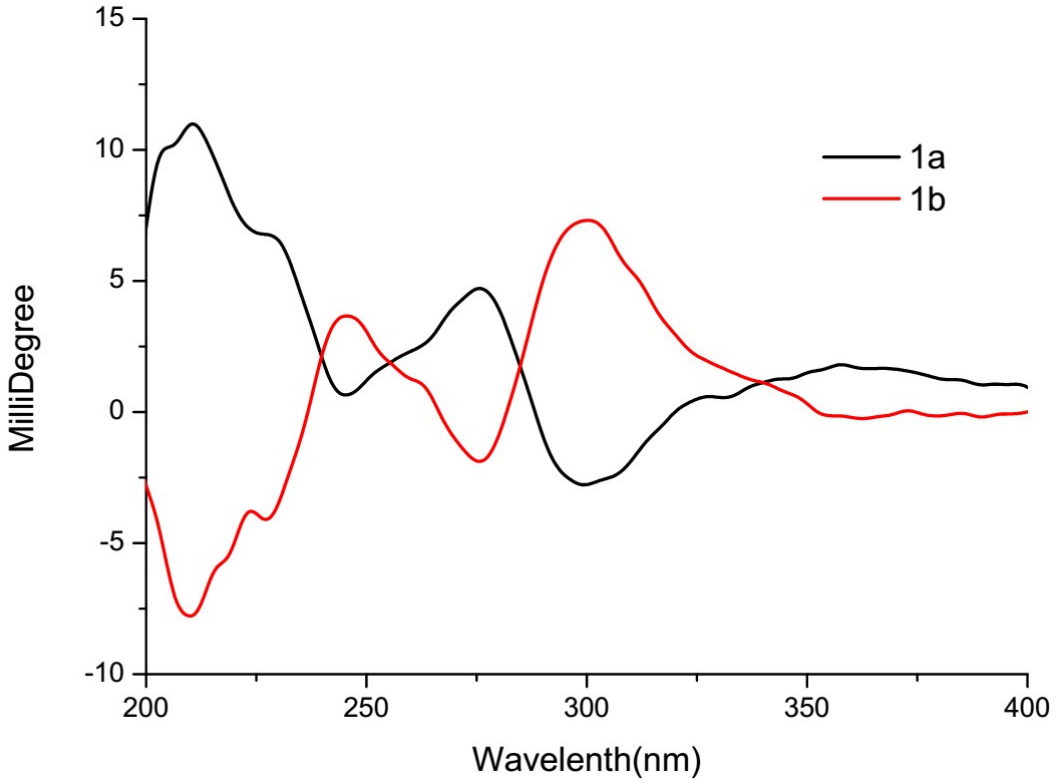

Fig. 10 HRESIMS of compound 1

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name	D:\Data\20140915CEYANG\BLH-24_1-B,9_01_3751.d	Acquisition Date	9/16/2014 4:13:58 PM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	BLH-24	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C32H31N1O9Na						
Formula, max.							
Measured m/z	596.189	Tolerance	5	ppm	Charge	1	
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Nirogen Rule	no	Electron Configuration	both				
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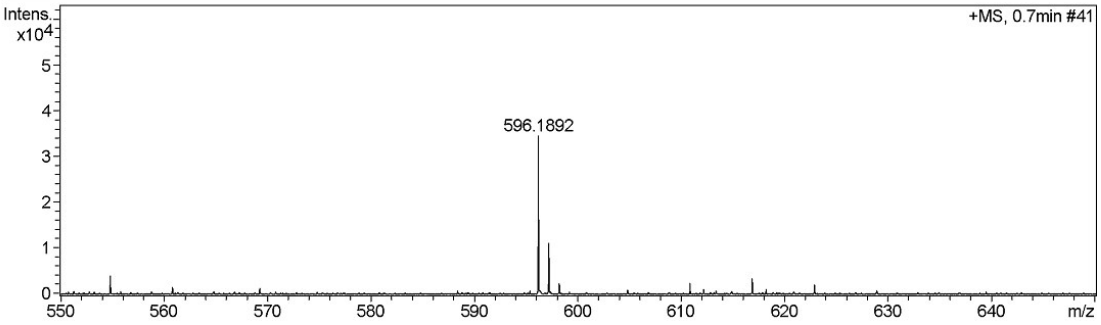
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 32 H 31 N 1 Na 1 O 9	0.020	596.1891	-0.12	0.68	-0.07	17.50	ok	even

Fig. 11 ^{1}H NMR spectrum of compound 2 in DMSO-d_6

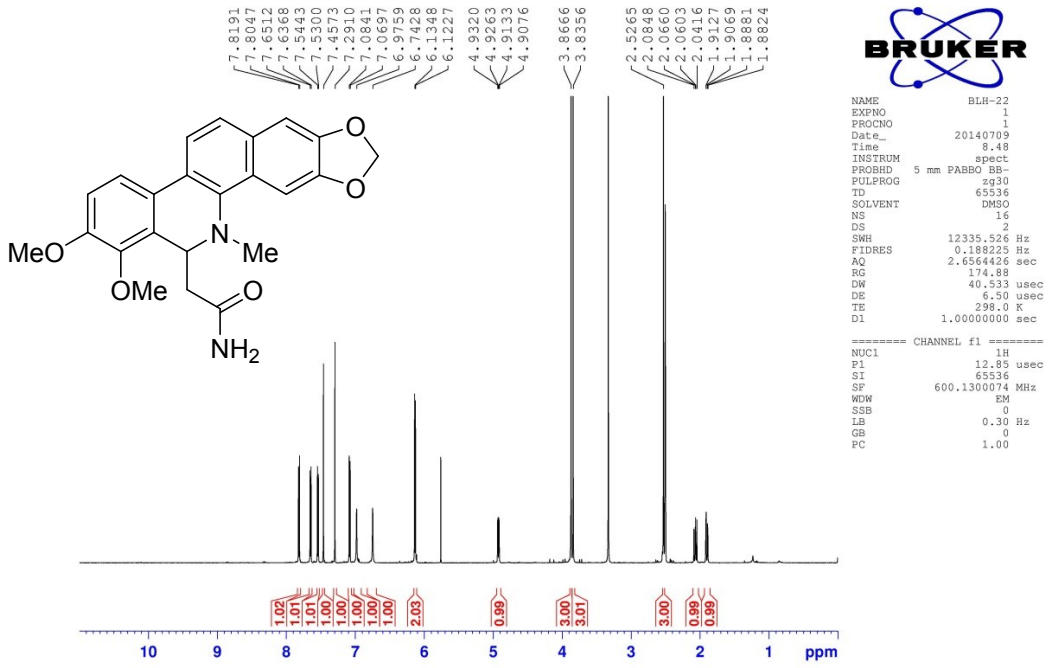


Fig. 12 ^{13}C NMR spectrum of compound 2 in DMSO-d_6

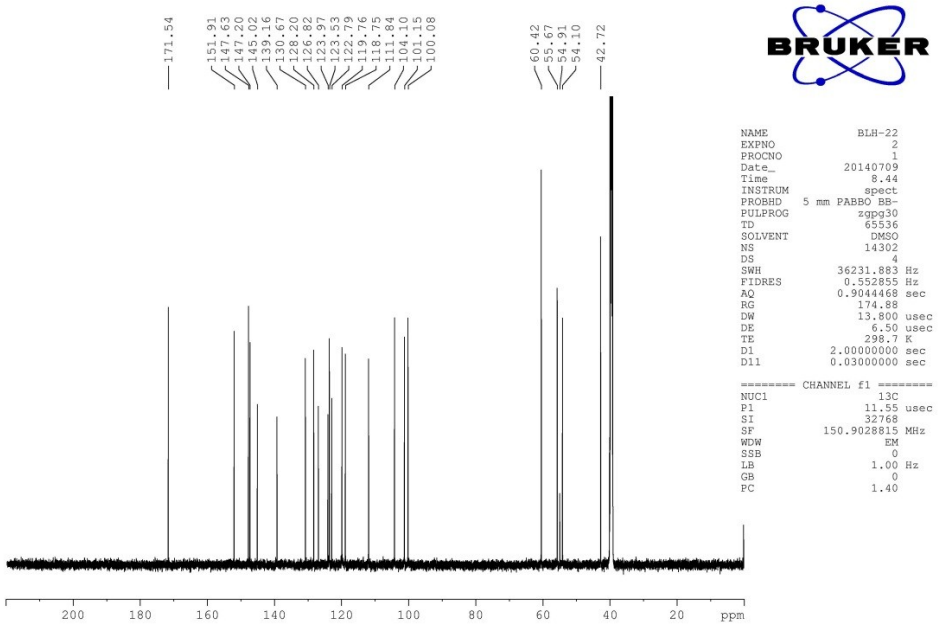


Fig. 13 HSQC spectrum of compound 2 in DMSO-d_6

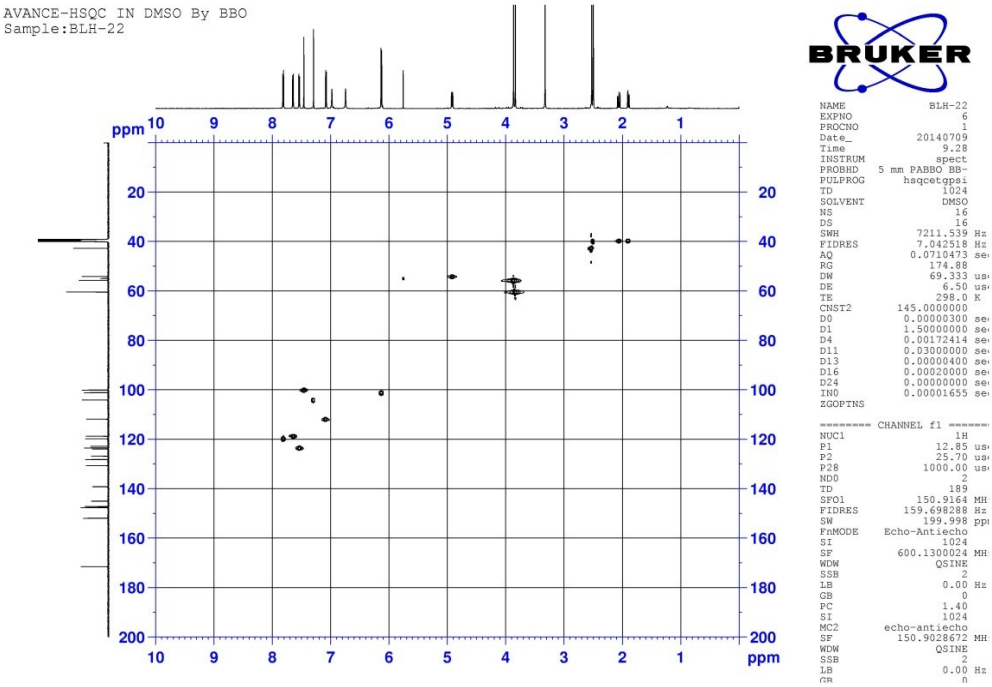


Fig. 14 HMBC spectrum of compound 2 in DMSO-d_6

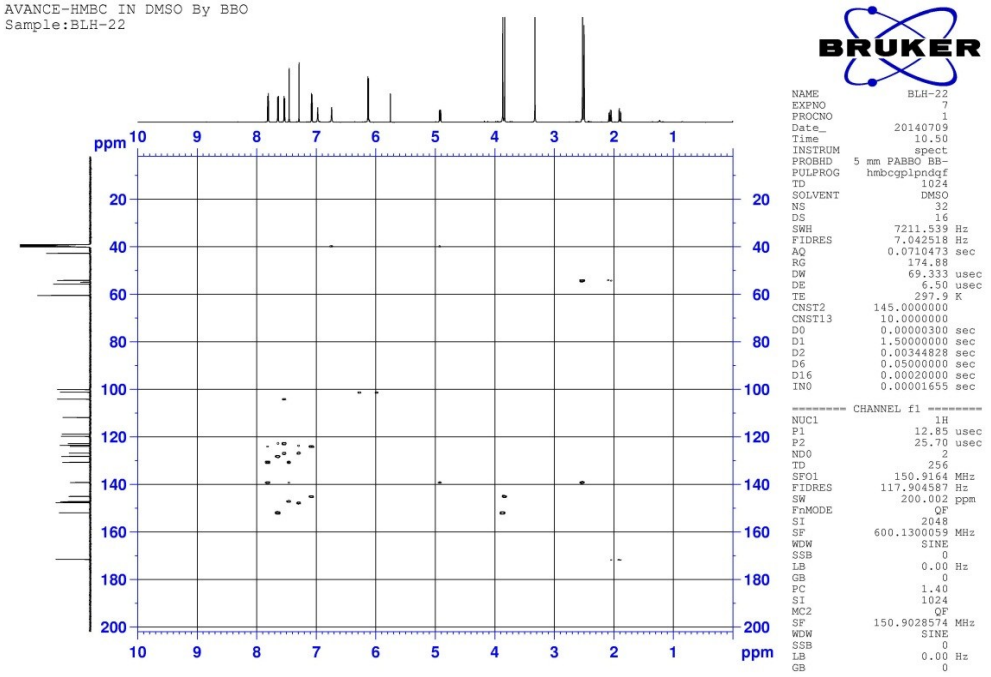
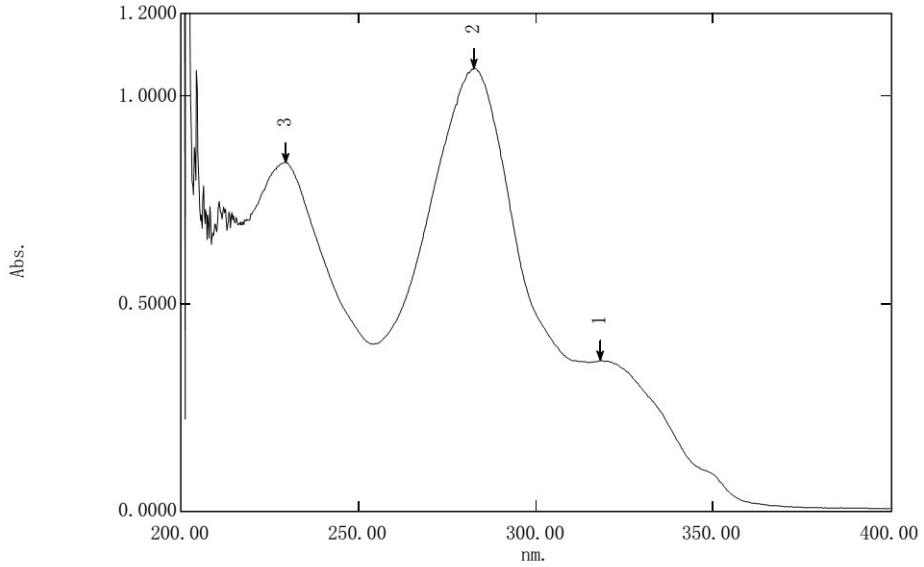


Fig. 15 UV spectrum of compound 2 in MeOH



测定属性
波长范围 (nm.): 200.00到400.00
扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 自动

试样准备属性
重量:
体积 :
稀释:
光程长:
附加信息:

仪器属性
仪器类型: UV-1700
测定方式: 吸收值
狭缝宽: 1.0 nm
光源改变波长: 340.8 nm
S/R 转换: 标准

No.	P/V	Wavelength	Abs.	描述
1	↑	318.40	.3618	
2	↑	282.80	1.0679	
3	↑	229.40	.8414	
4	↓	366.40	.0117	
5	↓	315.00	.3568	
6	↓	254.60	.4016	
7	↓	208.60	.6417	

Fig. 16 IR spectrum of compound 2

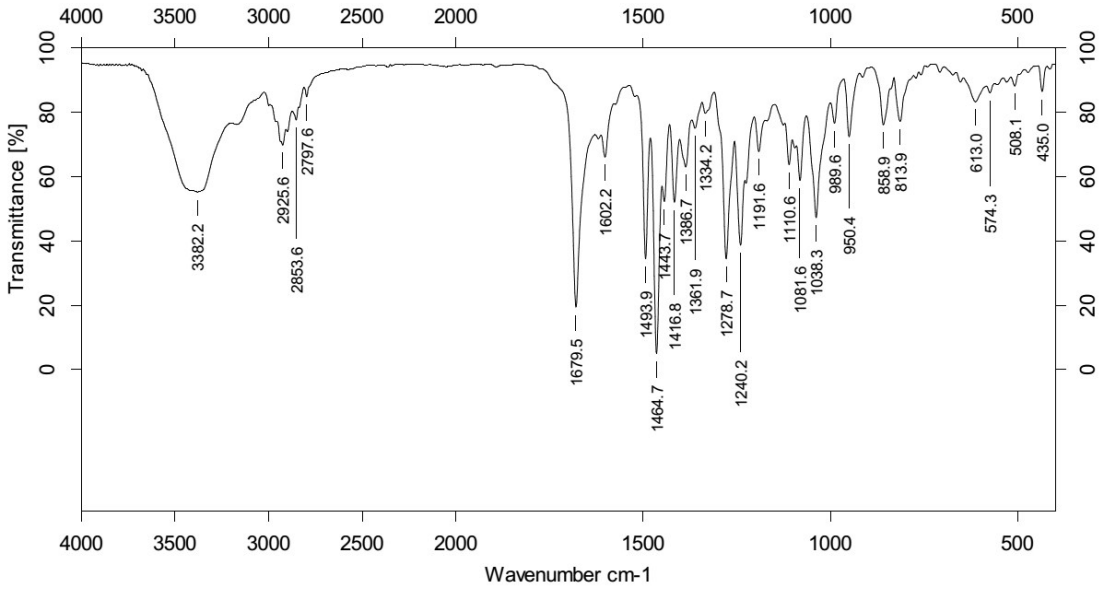


Fig. 17 ECD spectra of compound 2a and 2b

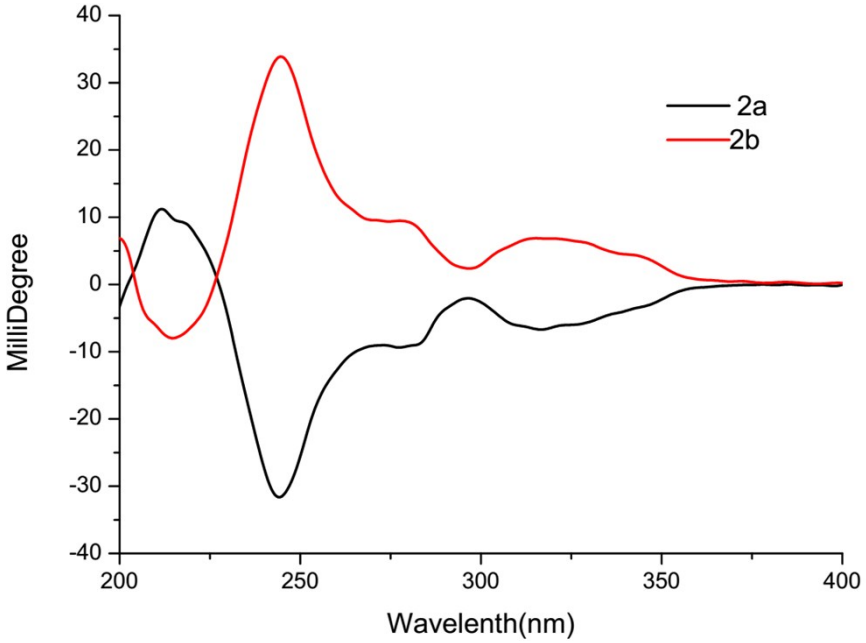


Fig. 18 HRESIMS of compound 2

Mass Spectrum Molecular Formula Report

Analysis Info

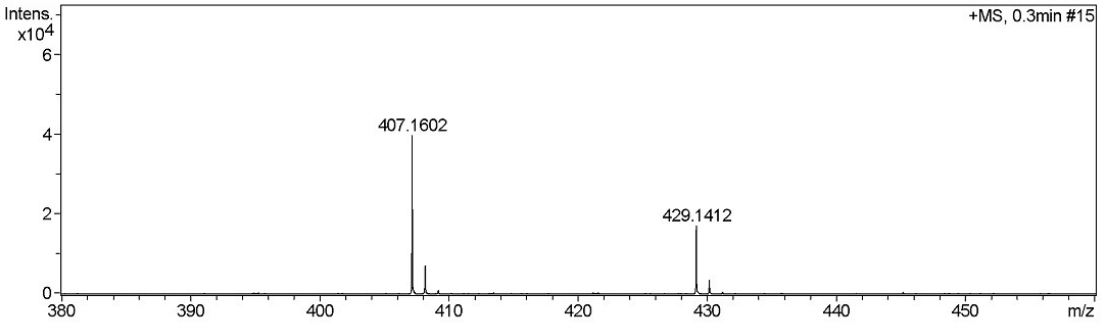
Analysis Name	D:\Data\20140710ceyang\BLH-22.d	Acquisition Date	7/10/2014 10:12:56 AM
Method	Liu_low_20131025.m	Operator	Bruker Customer
Sample Name	BLH-22	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C23H22N2O5H				
Formula, max.					
Measured m/z	407.16	Tolerance	5 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
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Fig. 19 ^{1}H NMR spectrum of compound 3 in DMSO-d_6

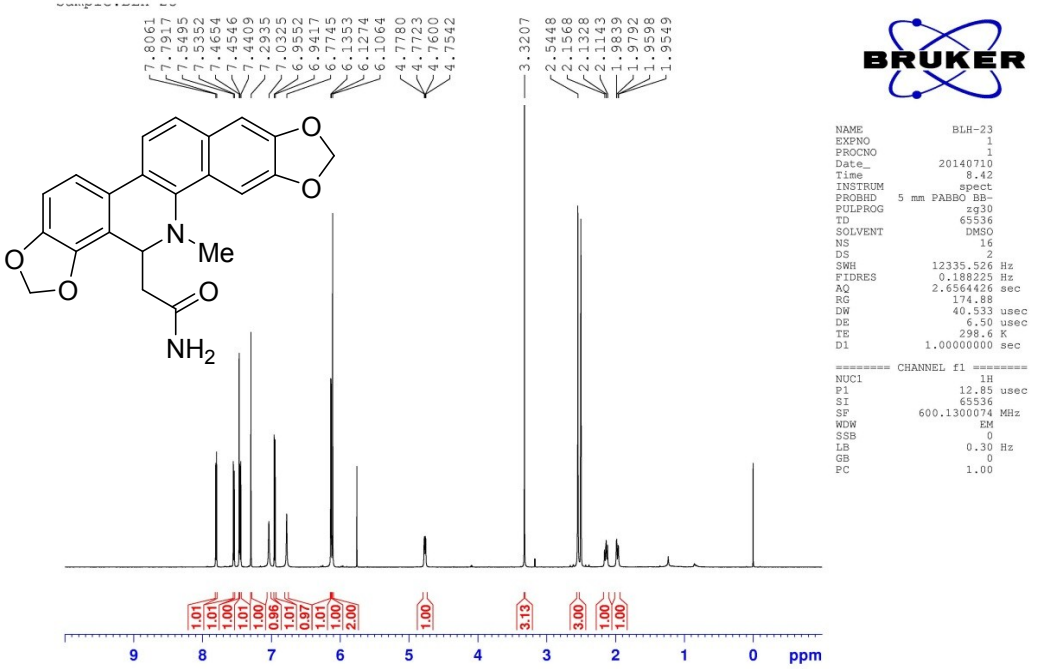


Fig. 20 ^{13}C NMR spectrum of compound 3 in DMSO-d_6

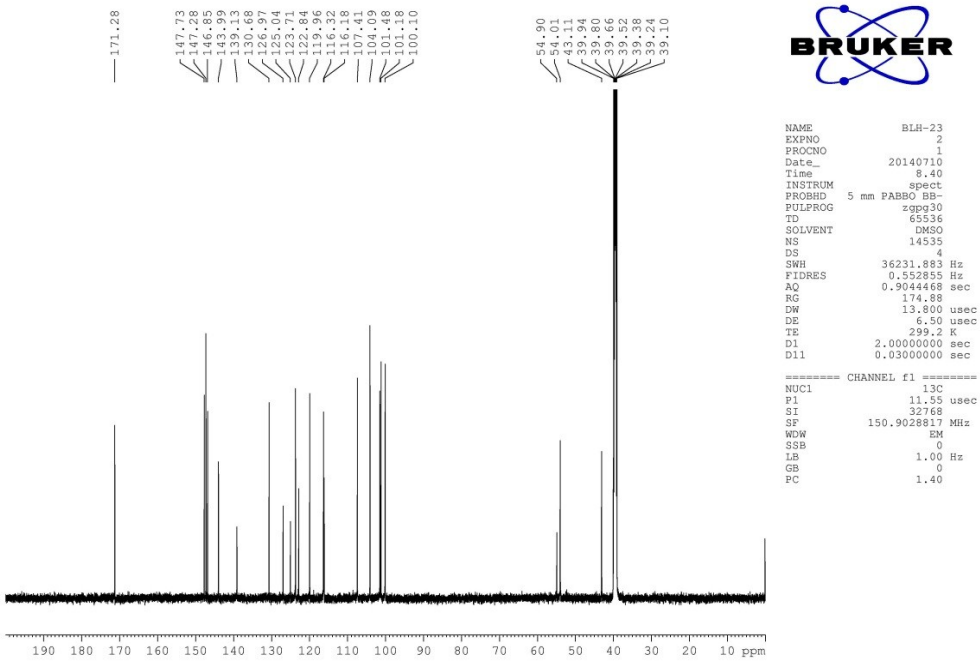


Fig. 21 HSQC spectrum of compound 3 in DMSO-d_6

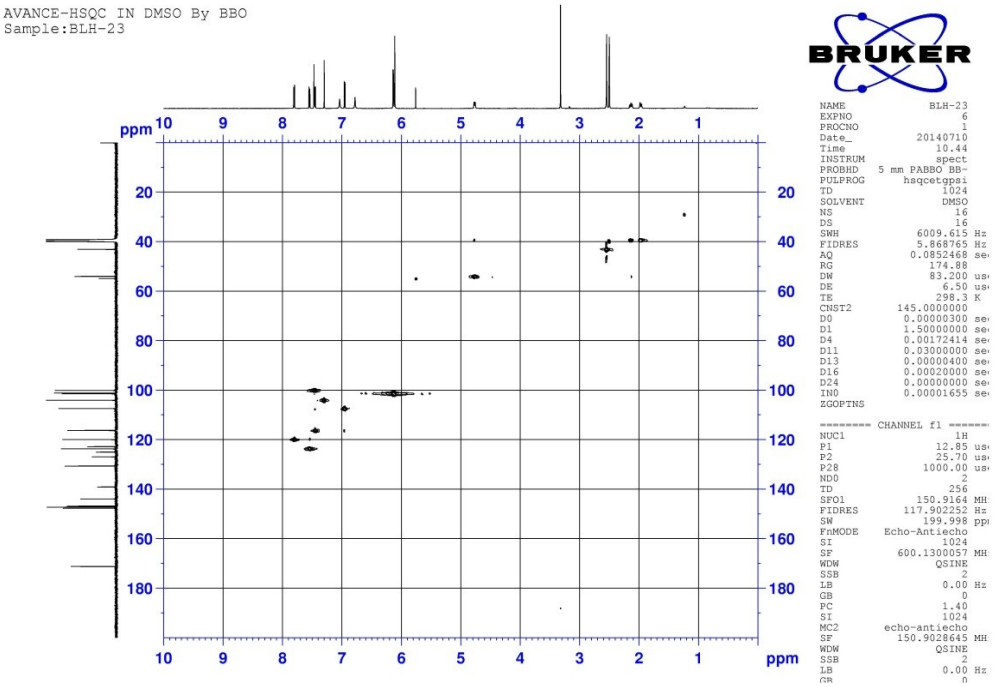


Fig. 22 HMBC spectrum of compound 3 in DMSO-d_6

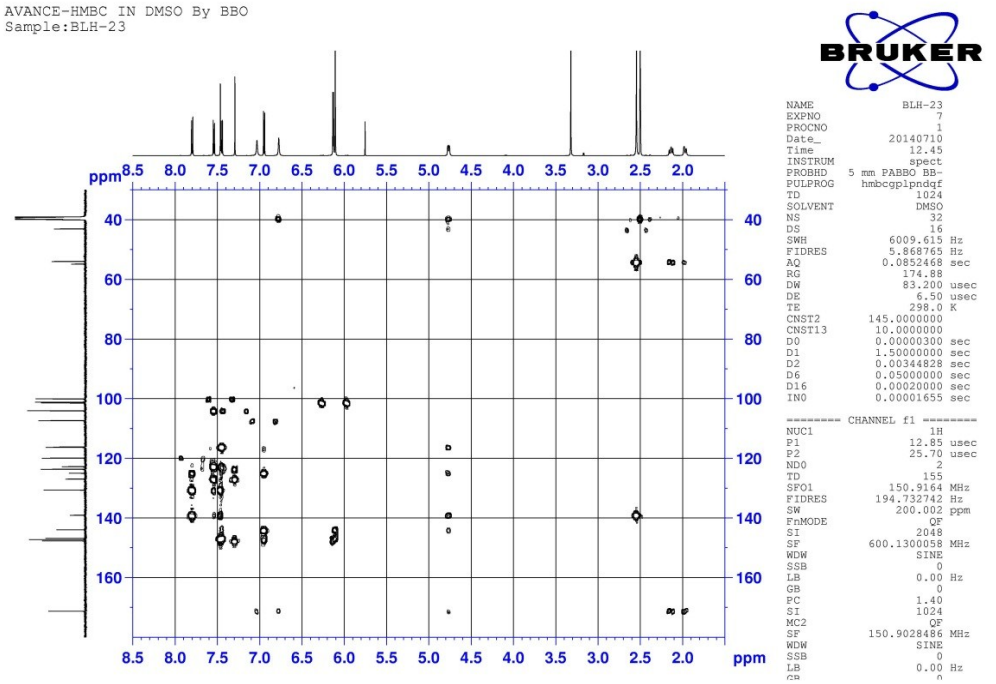
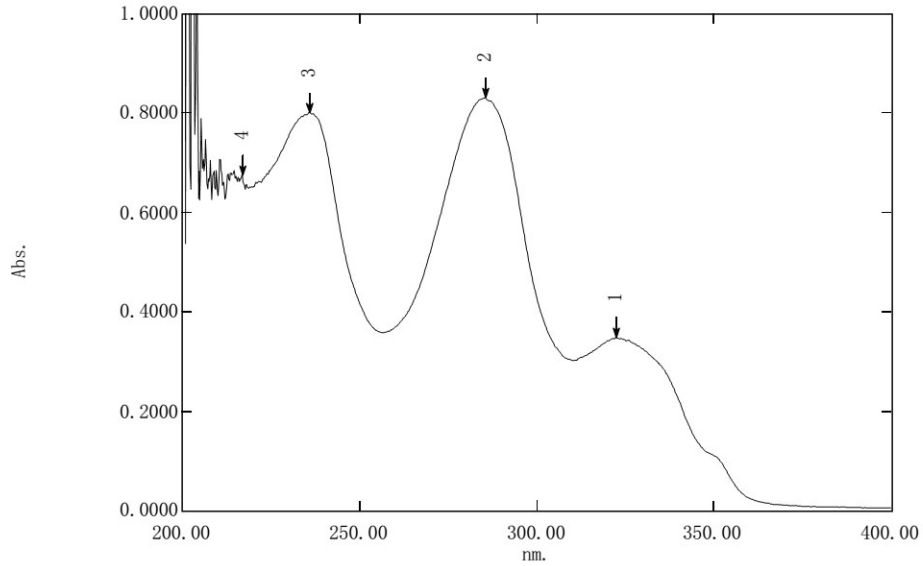


Fig. 23 UV spectrum of compound 3 in MeOH



测定属性
波长范围（nm.）: 200.00到400.00
扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 自动

试样准备属性
重量:
体积 :
稀释:
光程长:
附加信息:

仪器属性
仪器类型: UV-1700
测定方式: 吸收值
狭缝宽: 1.0 nm
光源改变波长: 340.8 nm
S/R 转换: 标准

No.	P/V	Wavelength	Abs.	描述
1	↑	322.60	.3480	
2	↑	285.60	.8322	
3	↑	235.80	.8019	
4	↑	217.00	.6768	
5	↑	203.20	2.5001	
6	↓	371.80	.0090	
7	↓	310.40	.3011	
8	↓	256.80	.3582	
9	↓	217.80	.6467	
10	↓	212.00	.6273	
11	↓	201.00	.5370	

Fig. 24 IR spectrum of compound 3

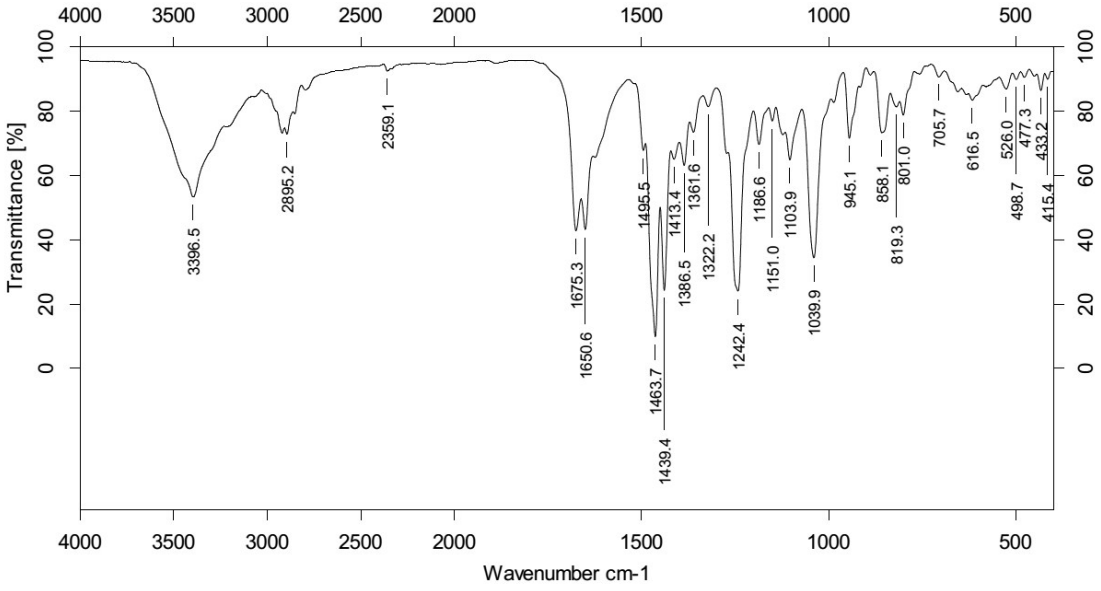


Fig. 25 ECD spectra of compound 3a and 3b

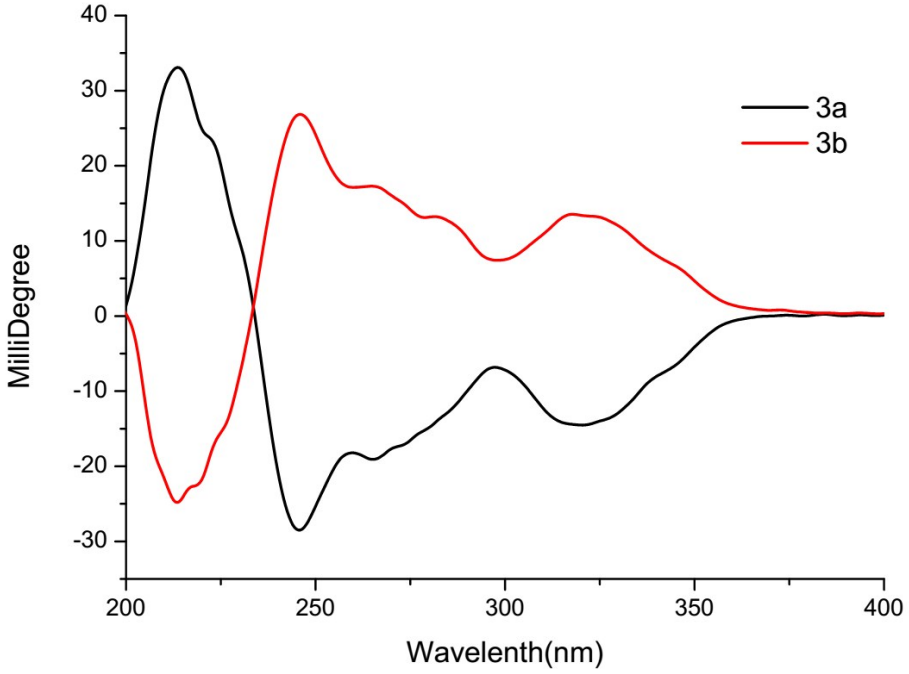


Fig. 26 HRESIMS of compound 3

Mass Spectrum Molecular Formula Report

Analysis Info

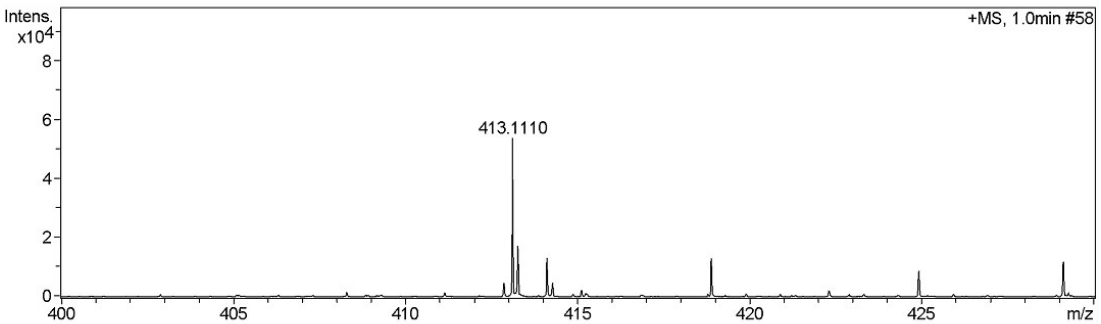
Analysis Name	D:\Data\20140915CEYANG\BLH-23_1-C,1_01_3752.d	Acquisition Date	9/16/2014 4:18:08 PM
Method	20131026_ceyang.m	Operator	Bruker Customer
Sample Name	BLH-23	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C22H18N2O5Na						
Formula, max.							
Measured m/z	413.111	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 22 H 18 N 2 Na 1 O 5	0.004	413.1108	-0.38	0.30	-0.16	14.50	ok	even