Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Diketopiperazine Alkaloids from a Mangrove Rhizosphere Soil Derived Fungus *Aspergillus effuses* H1-1

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List of Supporting Information

Figure S1. The HR-ESI-MS spectrum of **1**

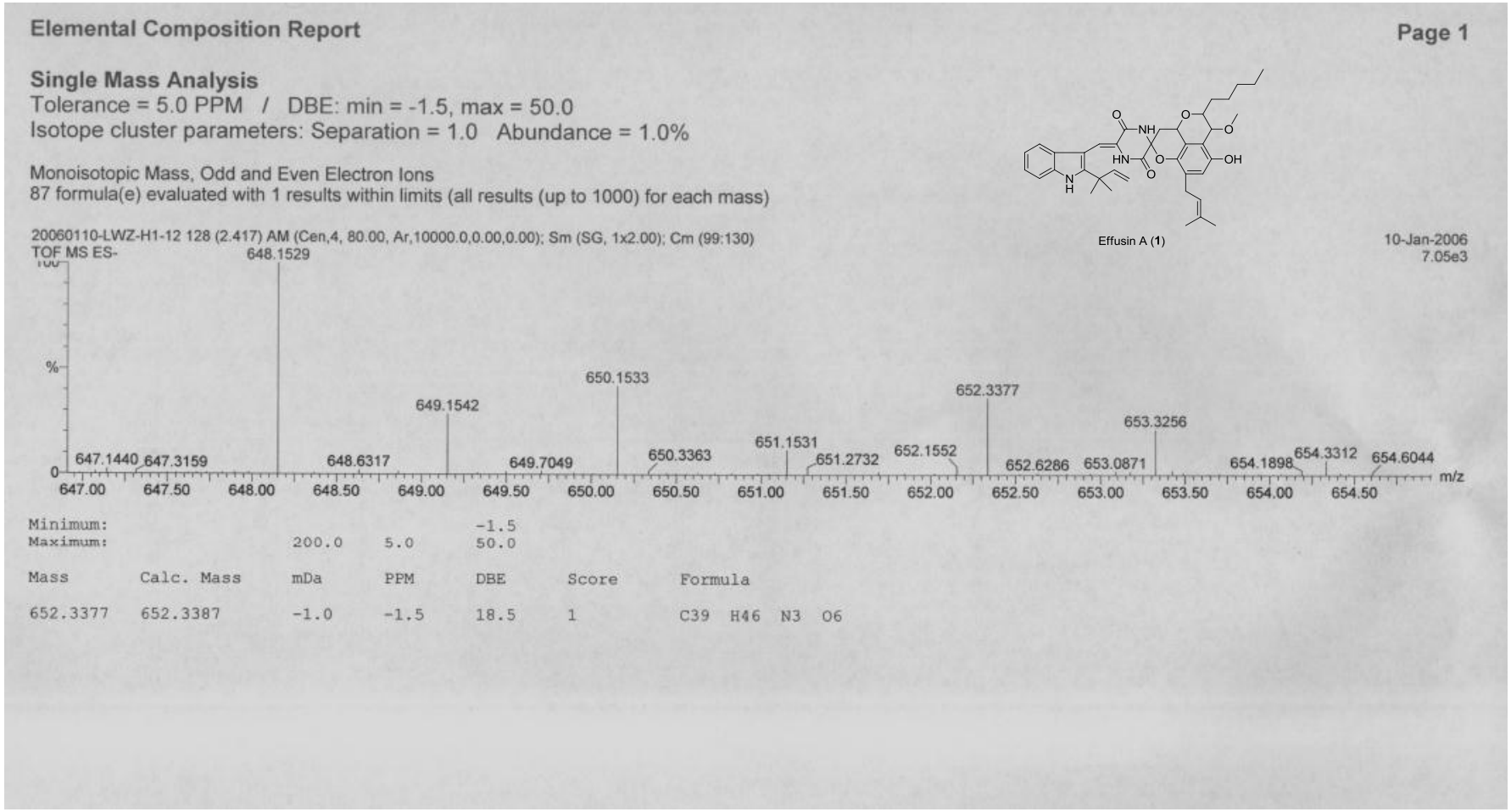


Figure S2. The ^{1}H-NMR spectrum of **1** in DMSO-d_6

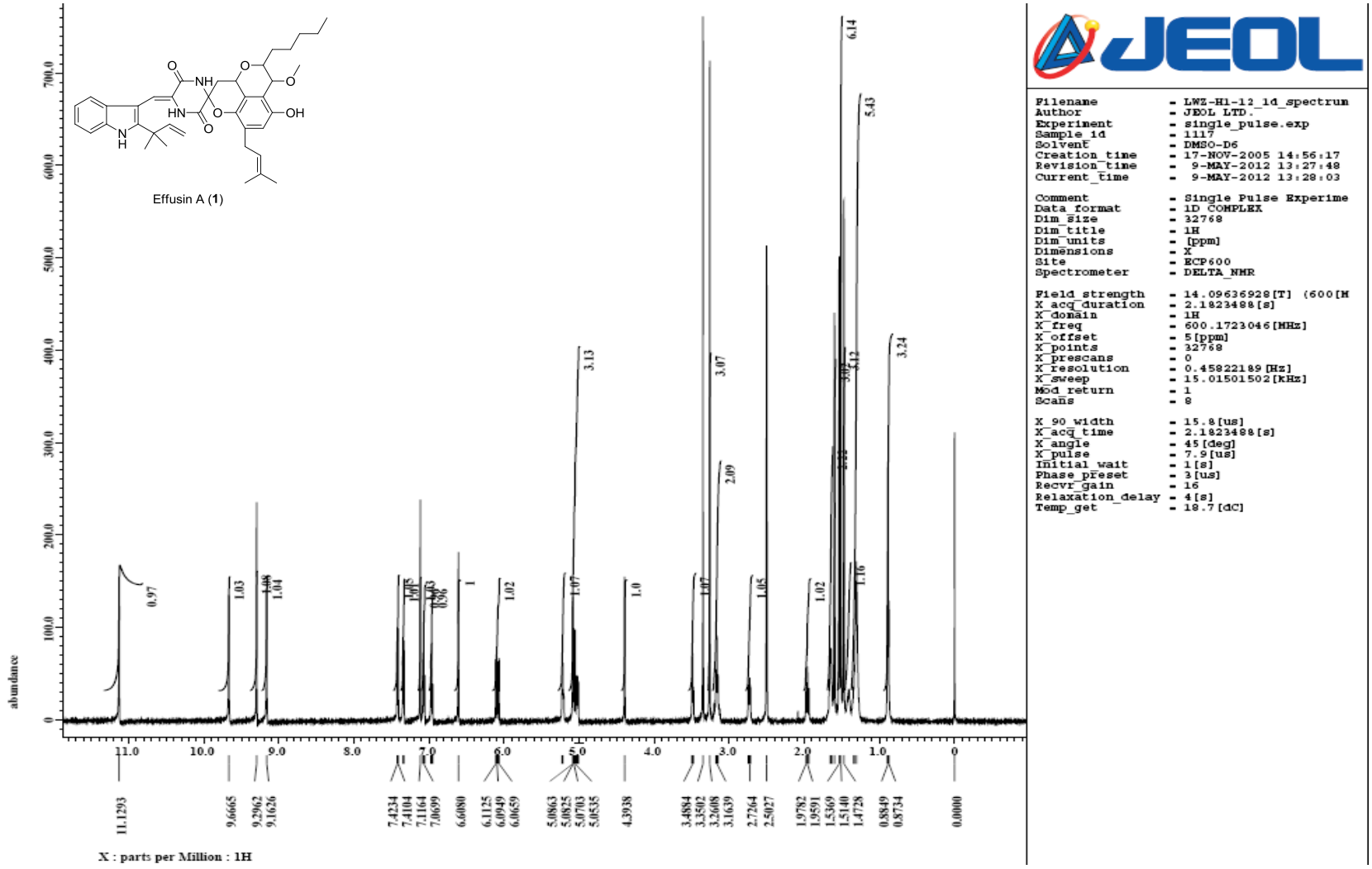


Figure S3. The ^{13}C-NMR spectrum of **1** in DMSO-d_6

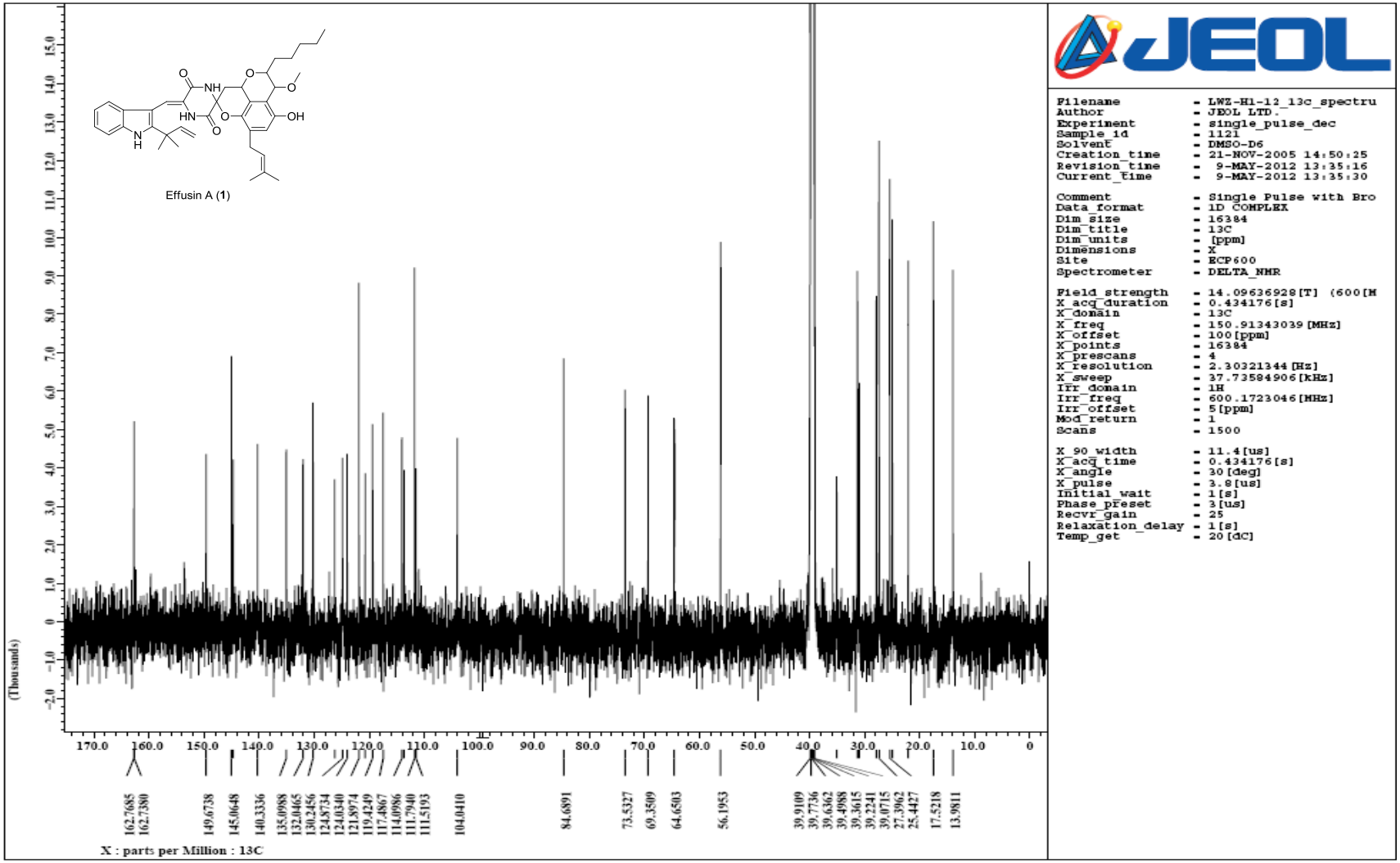


Figure S4. The DEPT spectrum of **1** in DMSO-d_6

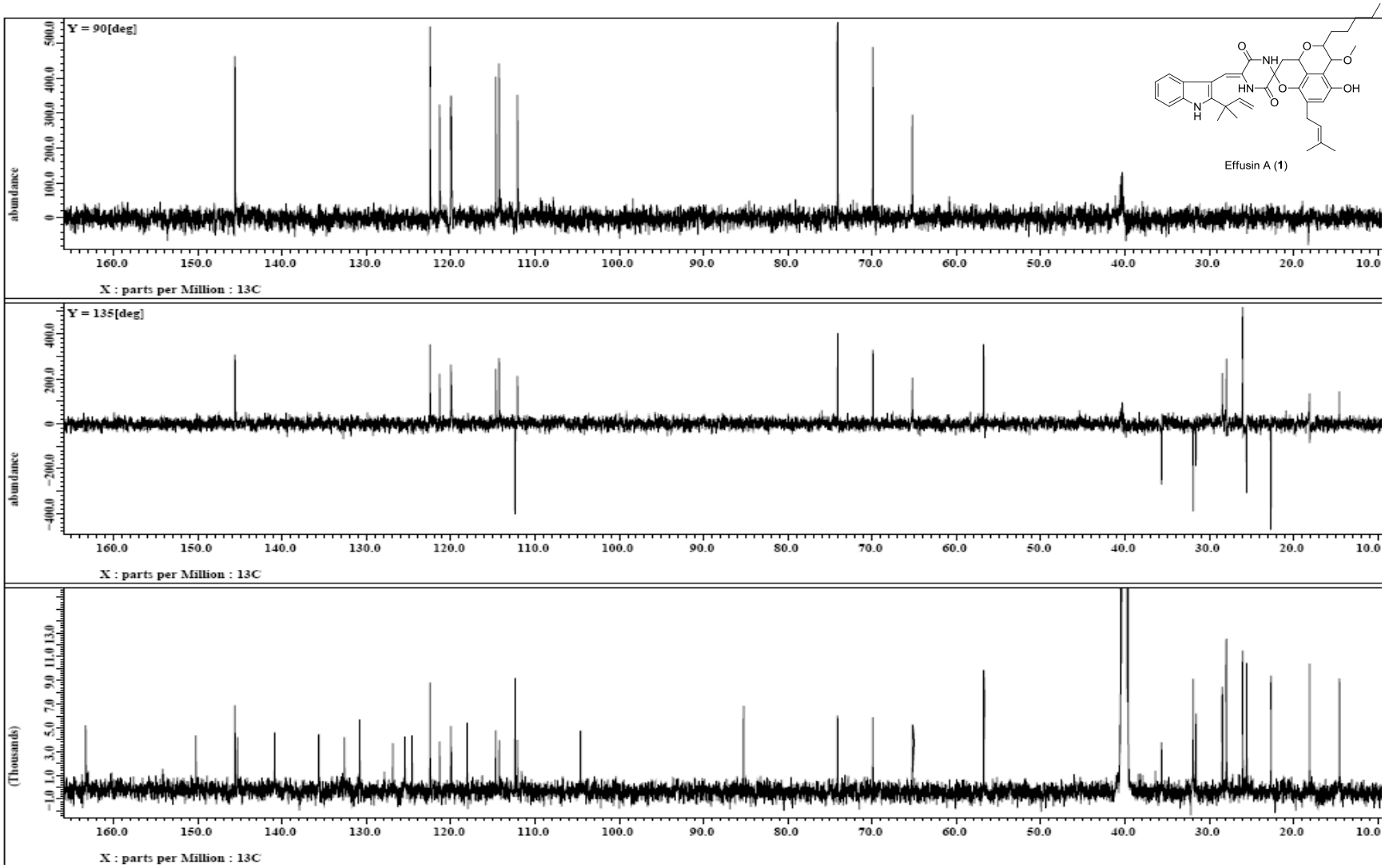


Figure S5. The HMQC spectrum of **1** in DMSO-d_6

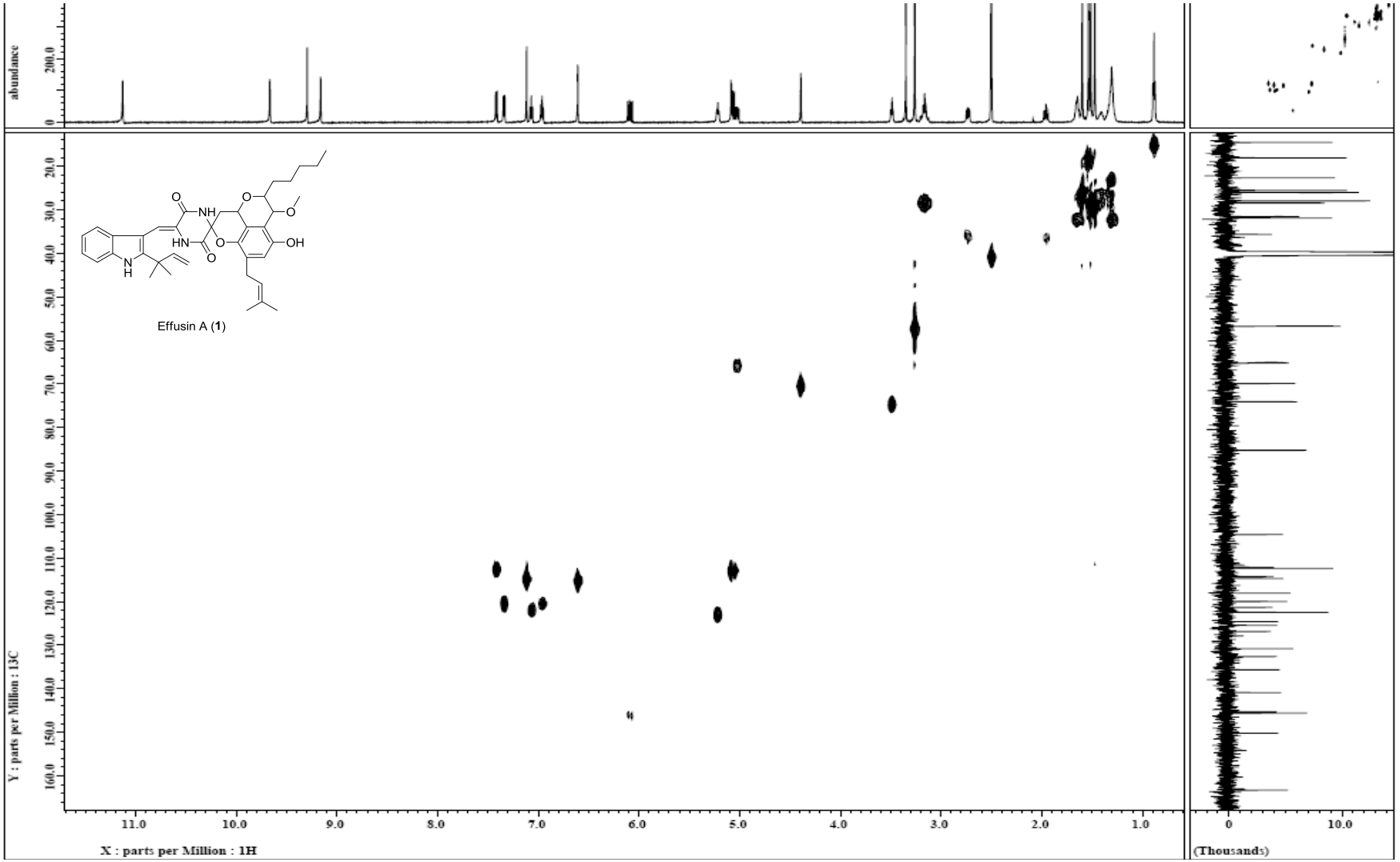


Figure S6. The ^{1}H-^{1}H COSY spectrum of **1** in DMSO-d_6

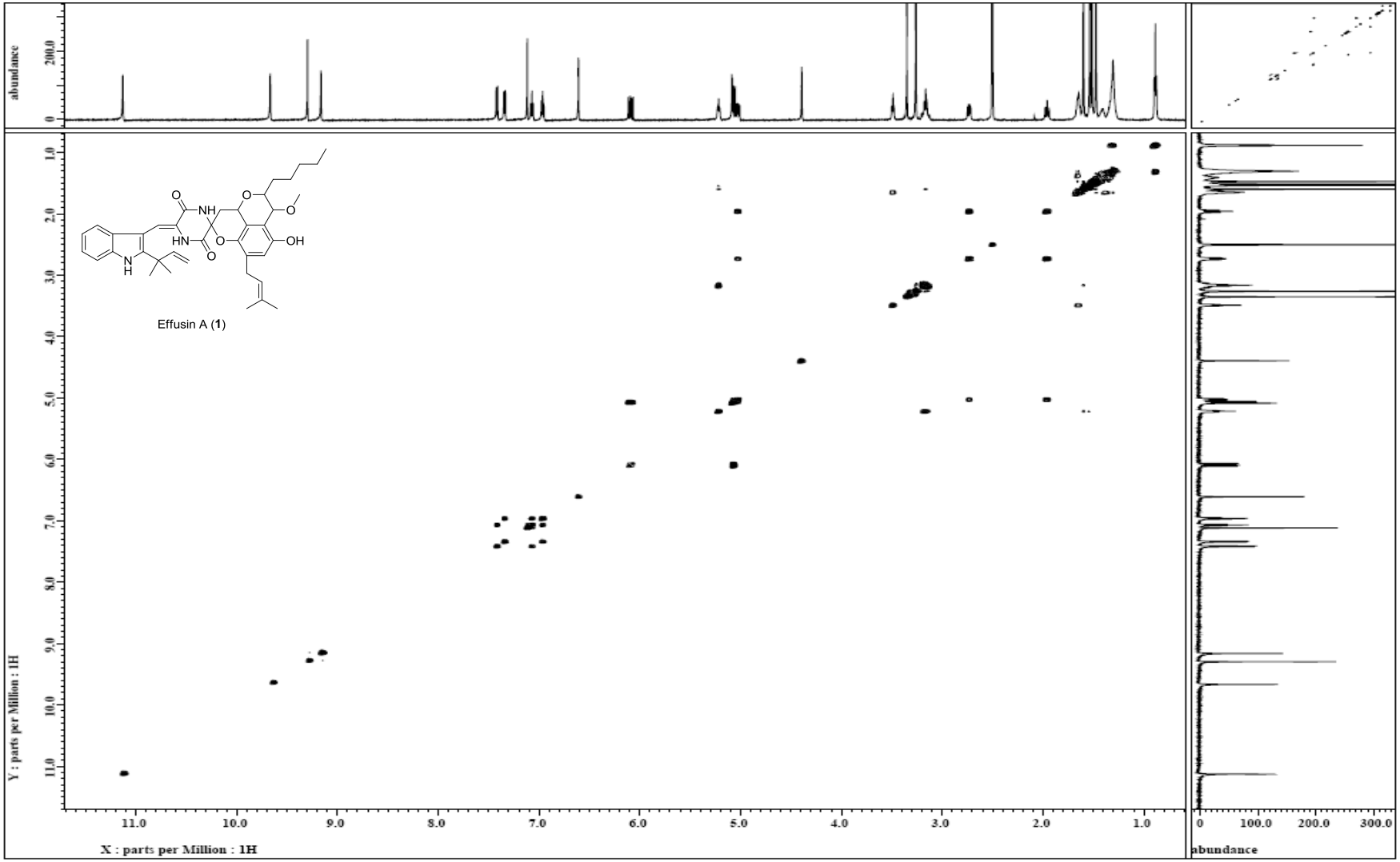


Figure S7. The HMBC spectrum of **1** in DMSO-d_6

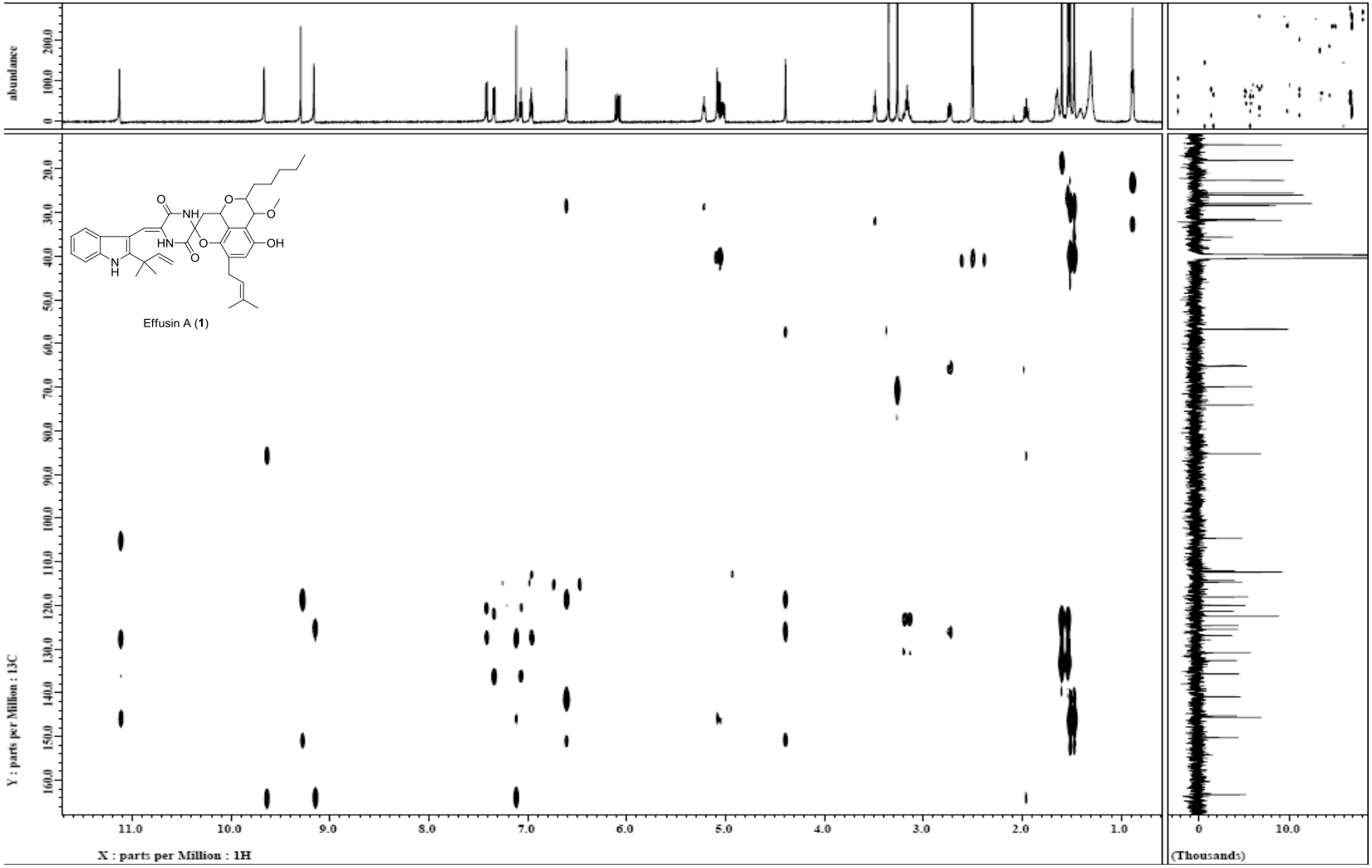


Figure S8. The NOE spectrum of **1** in DMSO-d_6

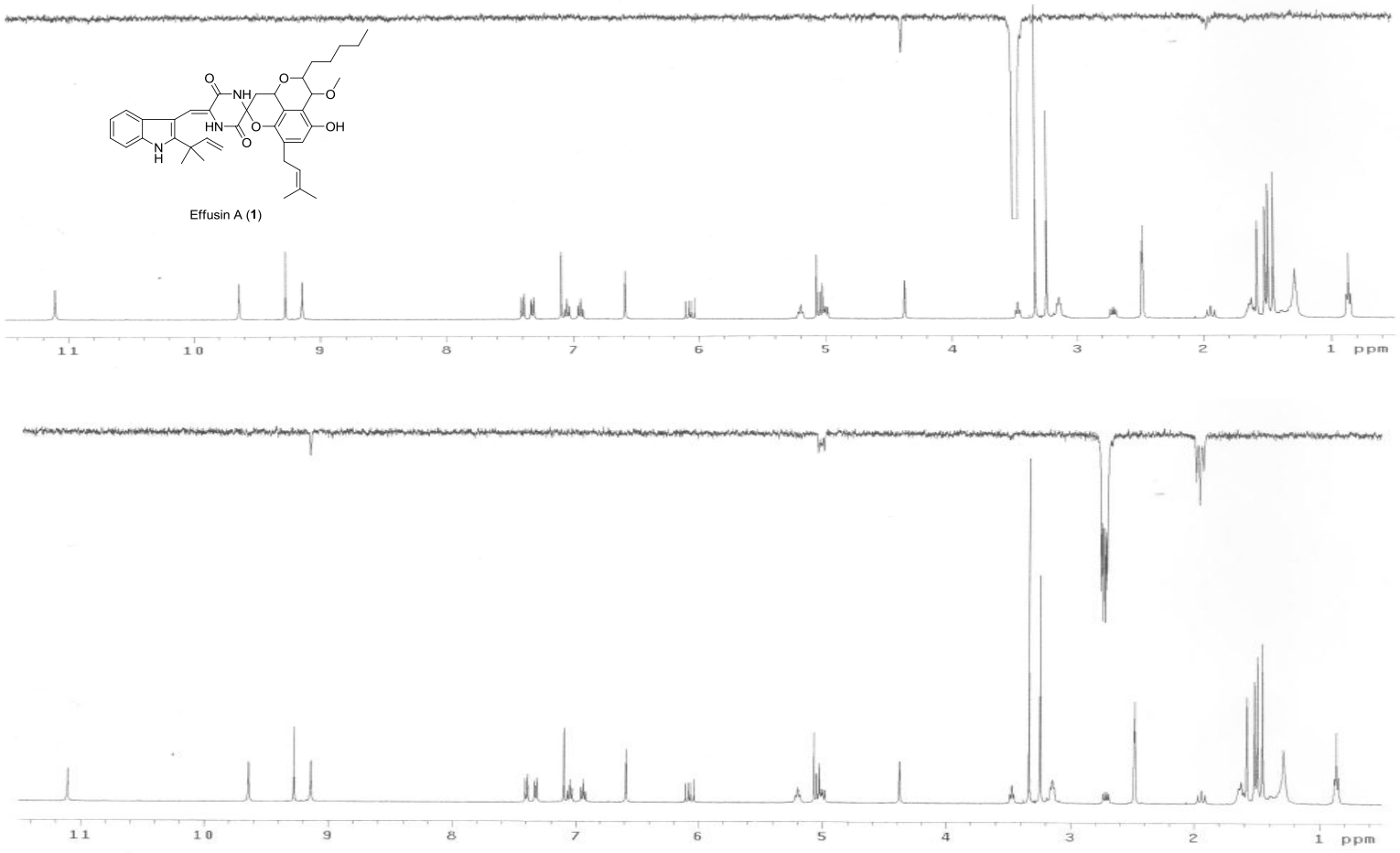
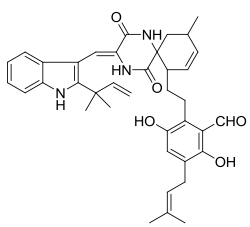


Figure S9. The HR-ESI-MS spectrum of **2**

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

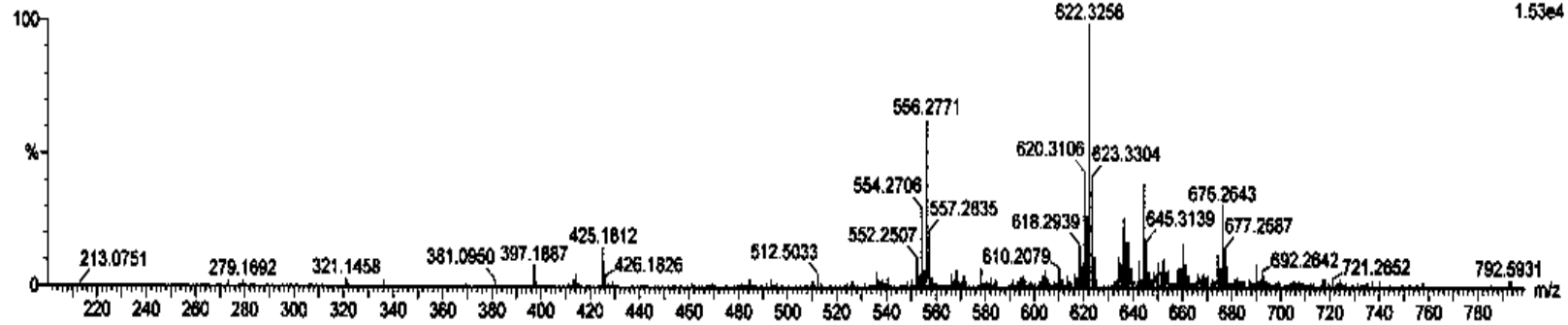
Monoisotopic Mass, Odd and Even Electron Ions
1190 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Dihydrocryptoechinulin D (**2**)

LWZ-H1-16
20060110-LWZ-H1-16 113 (2.138) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Sm (SG, 1x2.00); Cm (95:120)

10-Jan-2006
TOF MS ES+
1.53e4



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
622.3256	622.3281	-2.5	-4.0	18.5	1	C38 H44 N3 O5

Figure S10. The ^{1}H-NMR spectrum of **2** in DMSO-d_6

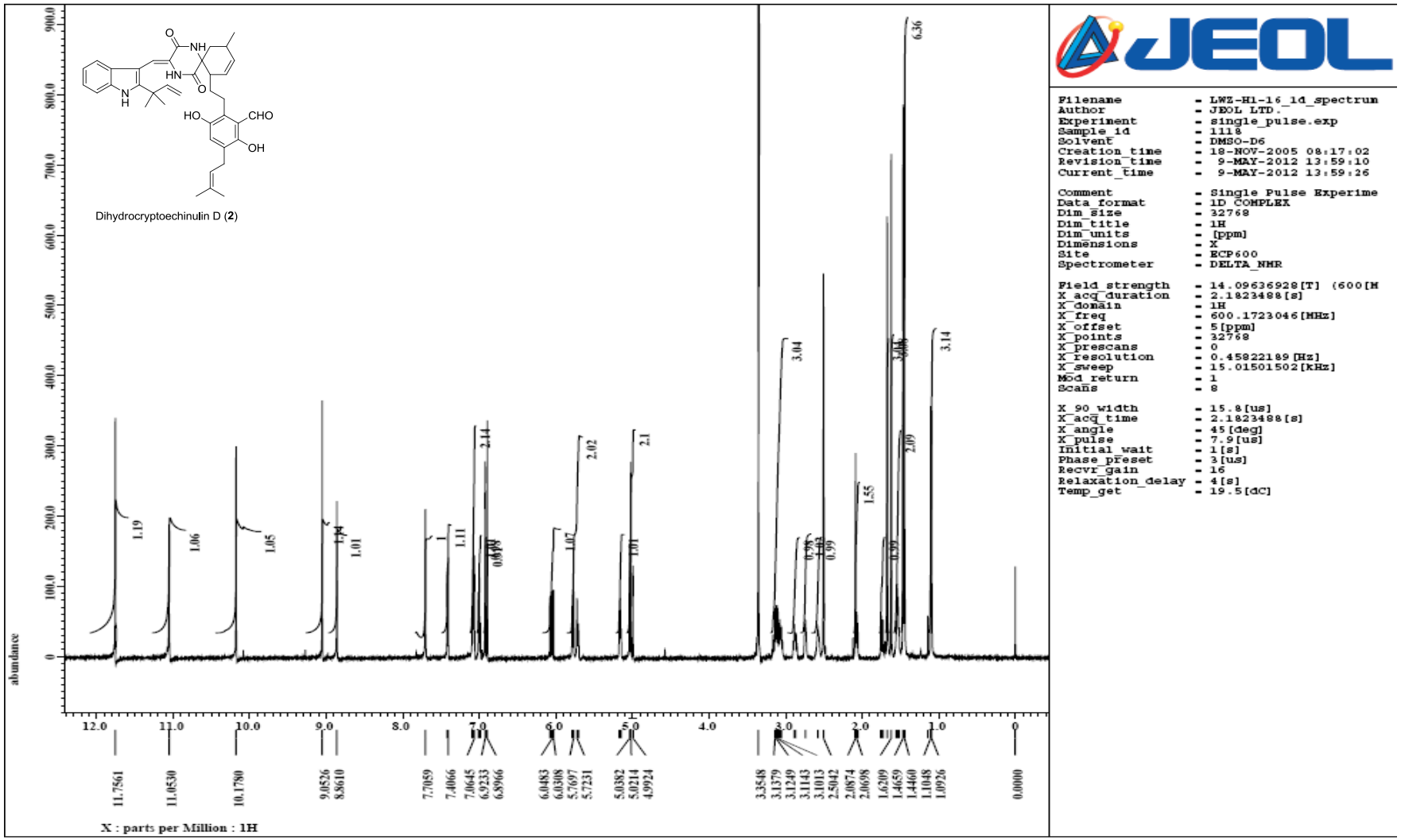


Figure S11. The ^{13}C-NMR spectrum of **2** in DMSO-d_6

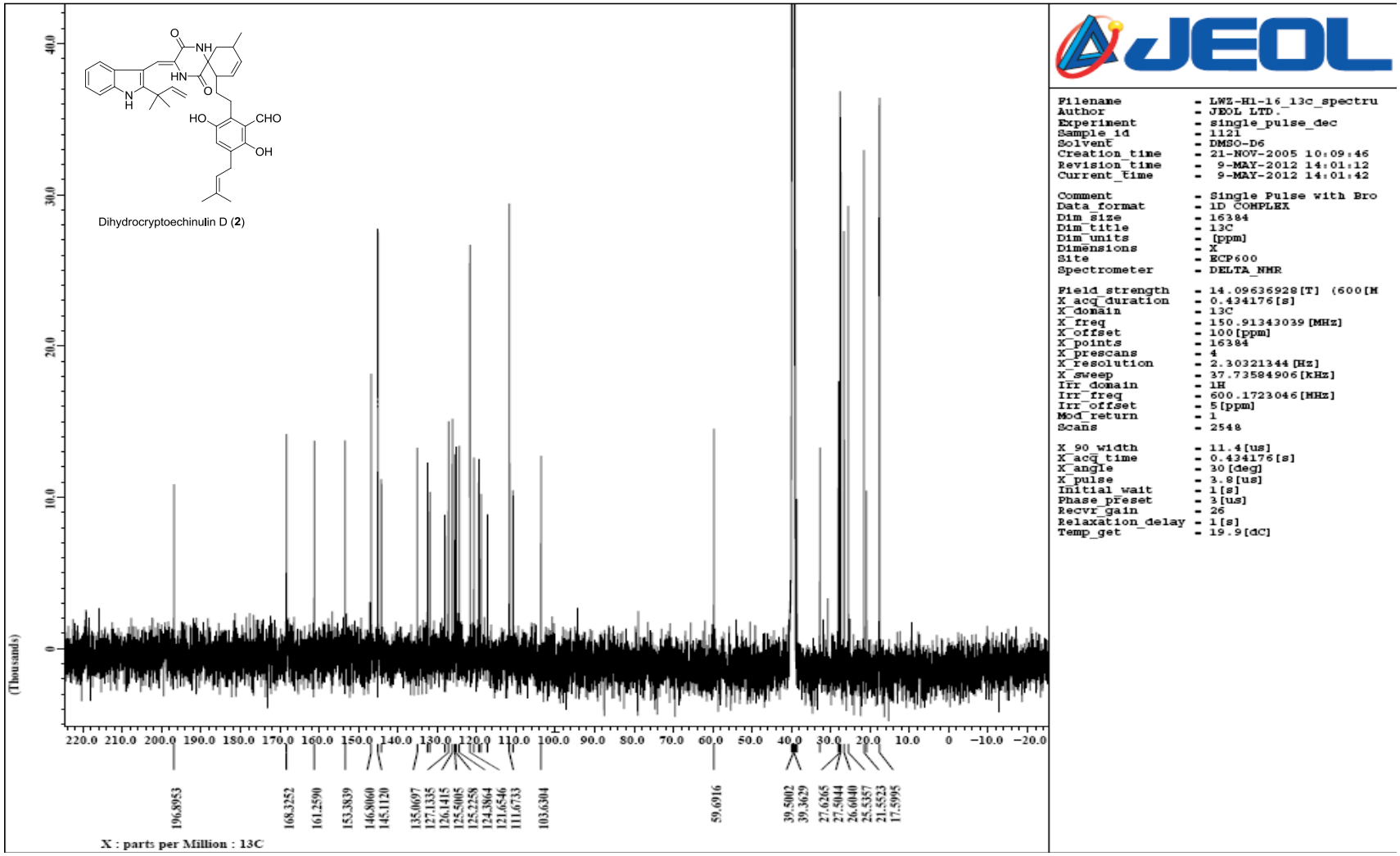


Figure S12. The DEPT spectrum of **2** in DMSO-d_6

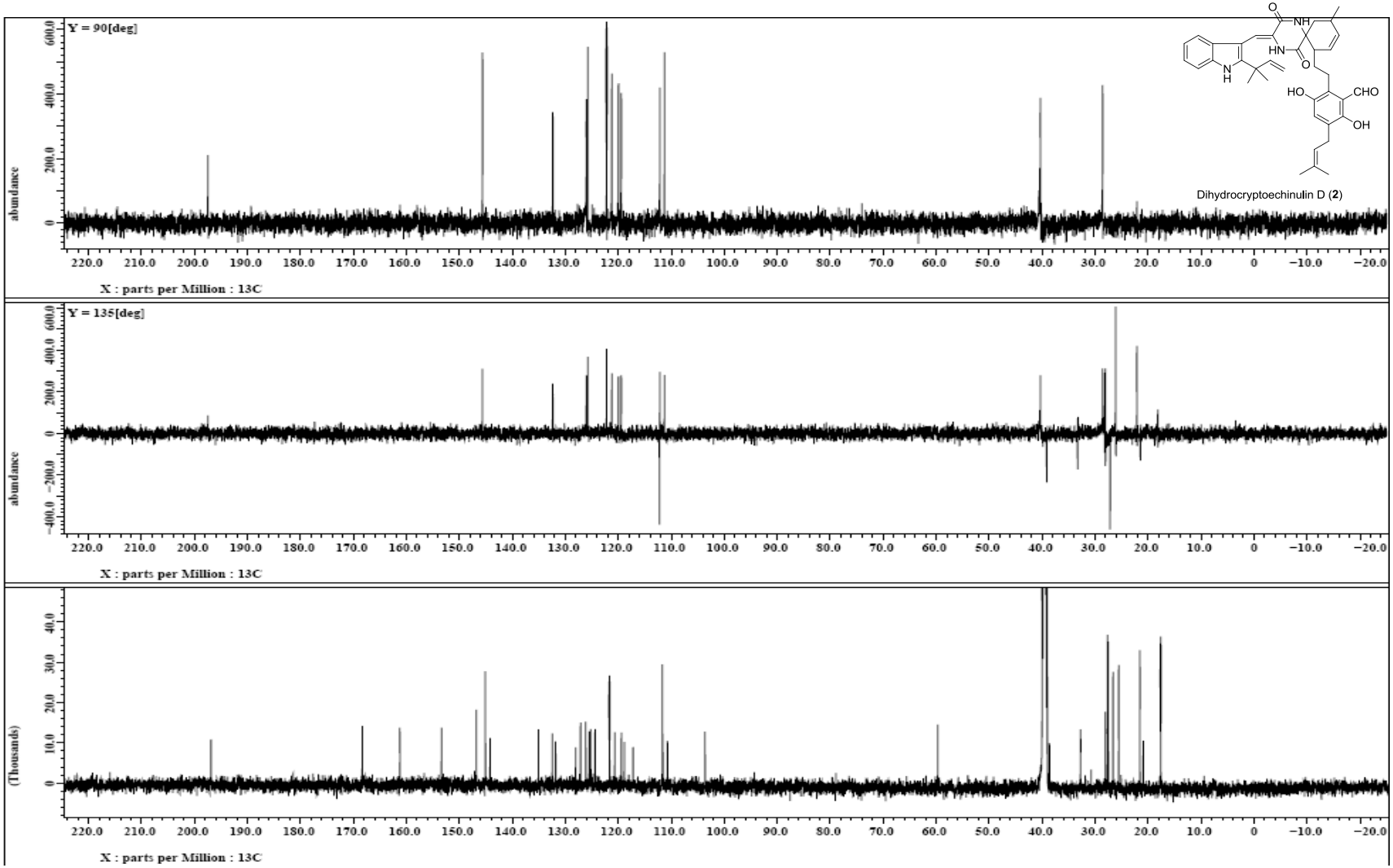


Figure S13. The HMQC spectrum of **2** in DMSO-d_6

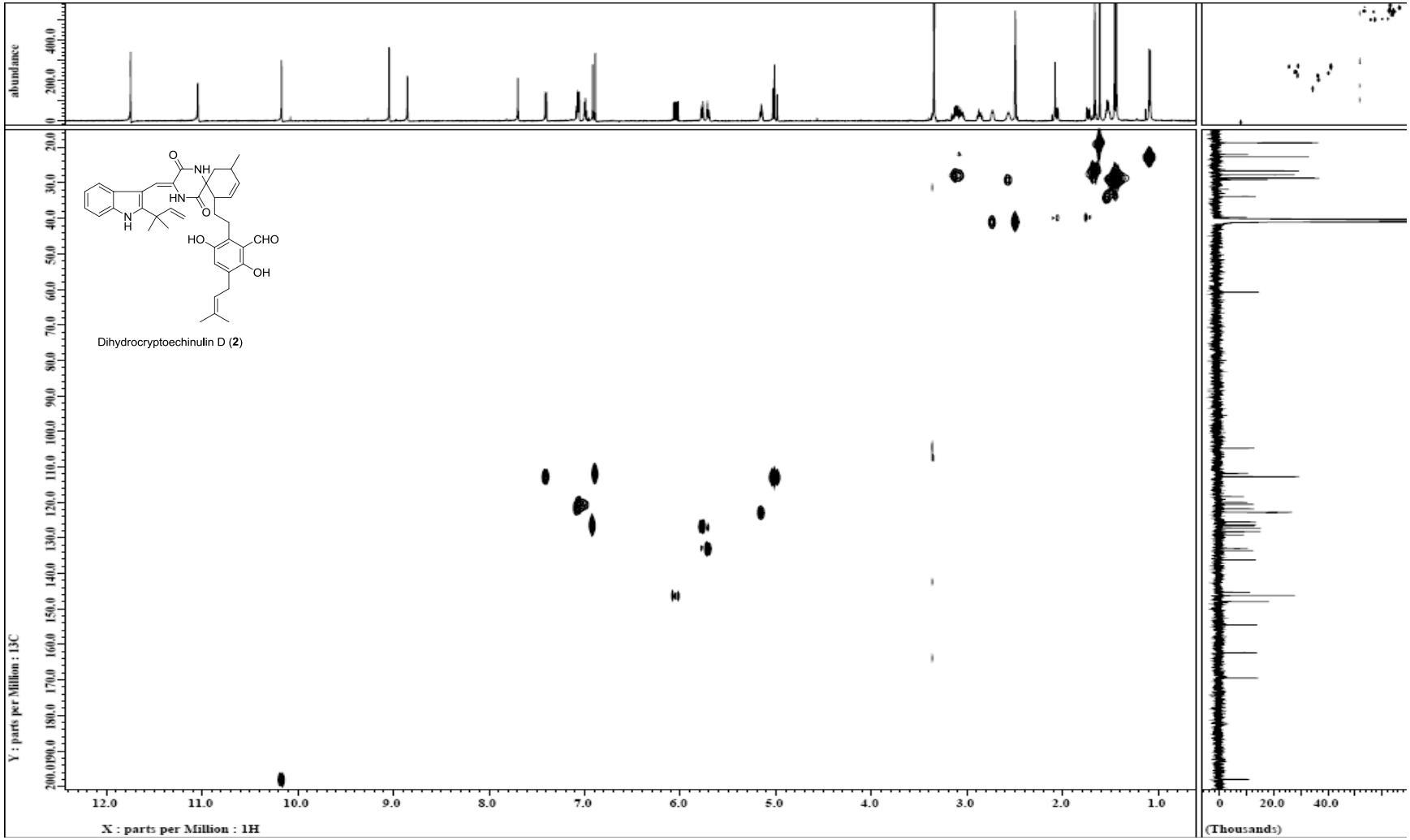


Figure S14. The ^{1}H-^{1}H COSY spectrum of **2** in DMSO-d_6

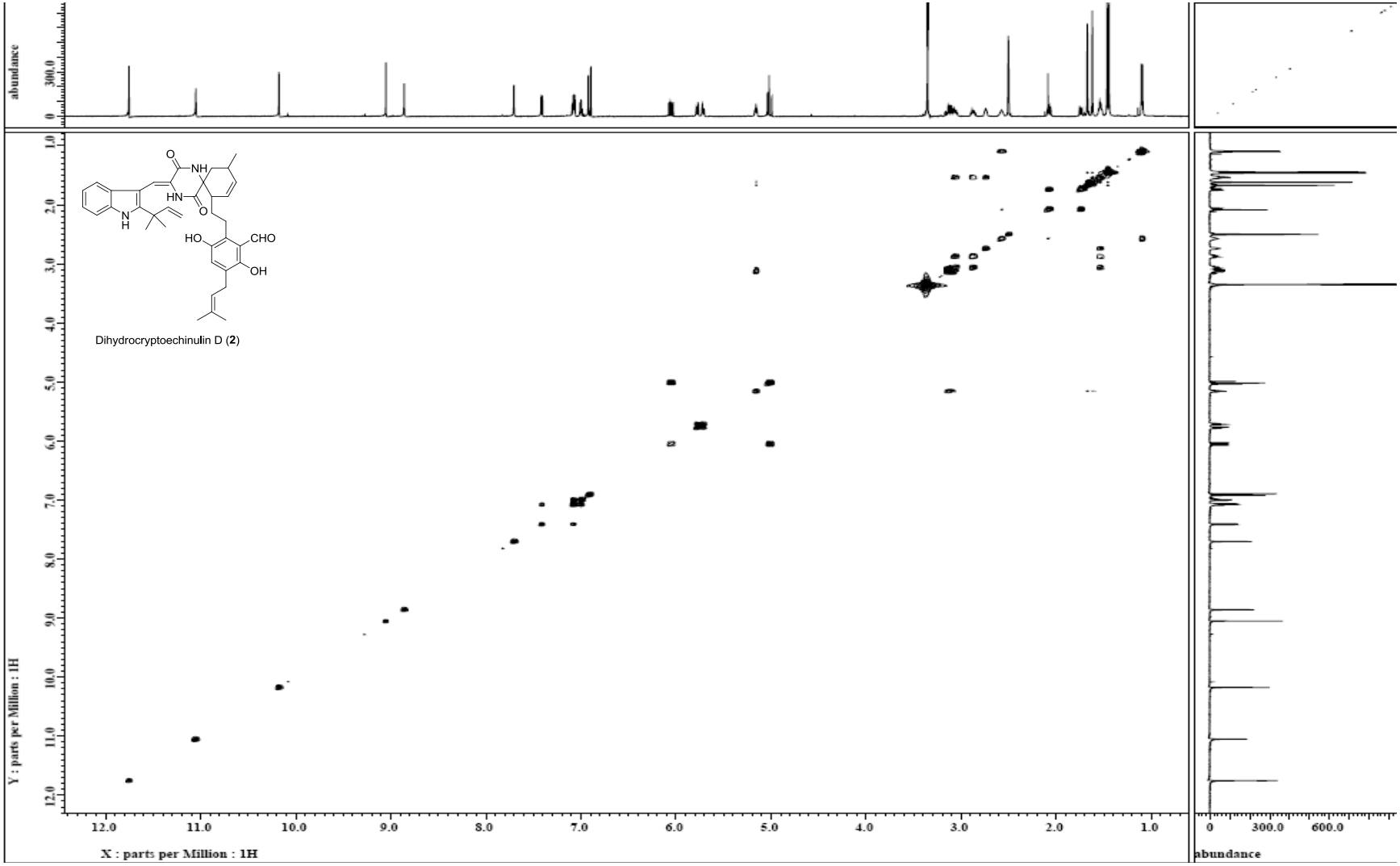


Figure S15. The HMBC spectrum of **2** in DMSO-d_6

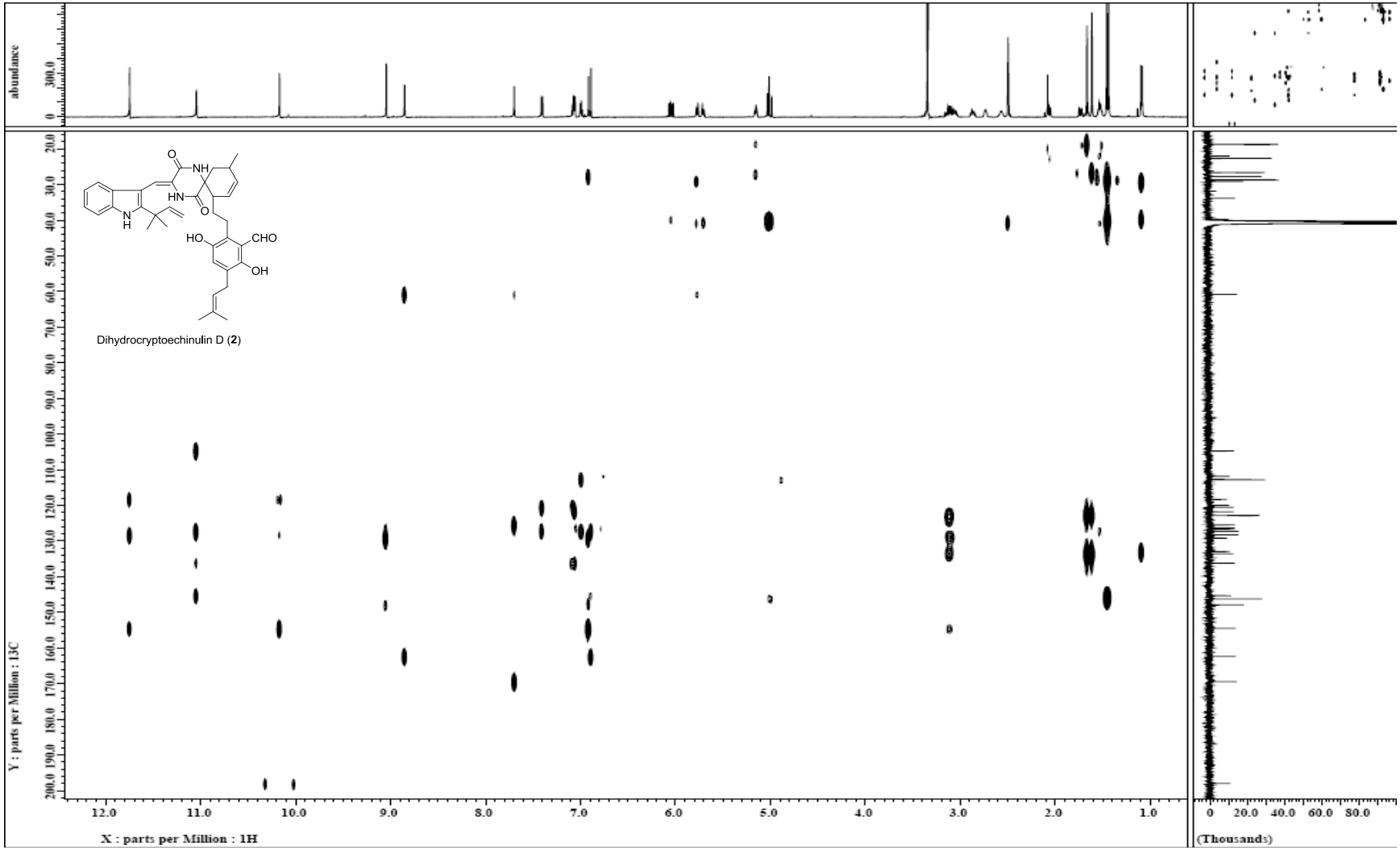
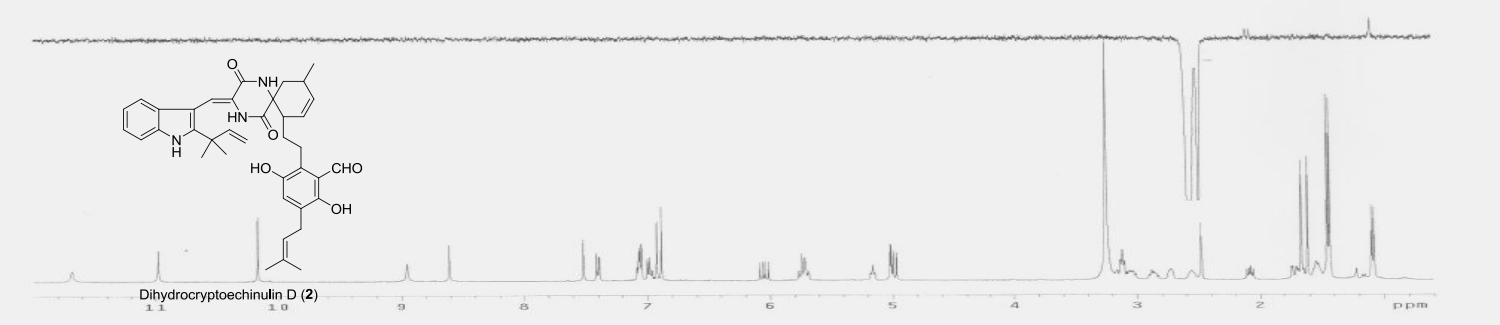
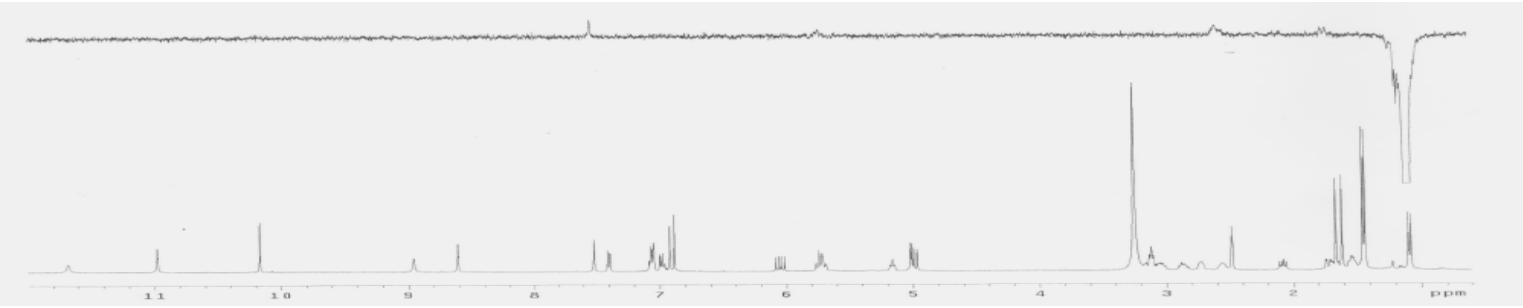


Figure S16. The NOE spectrum of **2** in DMSO-d_6





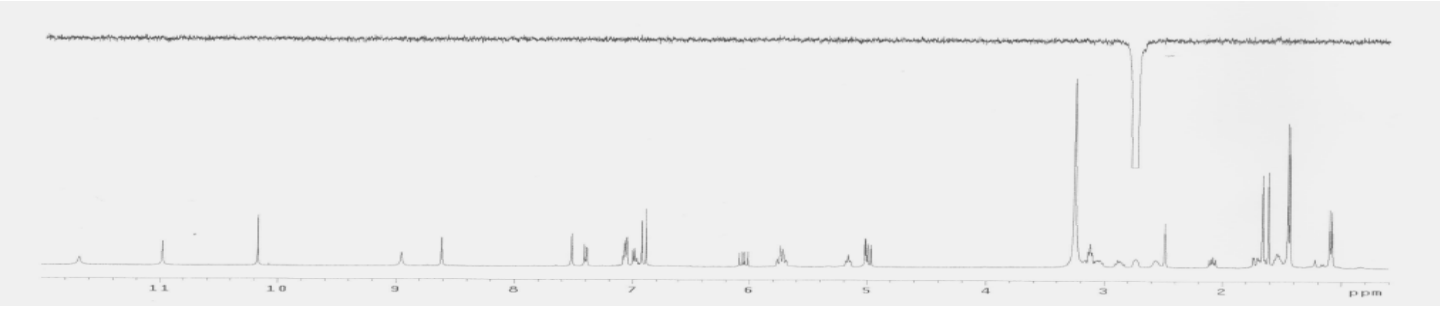


Table S1. Cartesian coordinates for the lowest energy reoptimized MMFF conformers calculated at B3LYP/6-31G(d) level of theory in vacuo.

Compound 1 Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-4.80692	-3.94023	-1.68618
2	C	-5.90454	-3.42417	-2.40263
3	C	-6.36015	-2.1298	-2.17881
4	C	-5.67737	-1.36026	-1.23306
5	C	-4.54796	-1.84317	-0.52118
6	C	-4.13263	-3.17021	-0.74536
7	N	-5.9223	-0.08253	-0.77915
8	C	-5.00486	0.277276	0.185791
9	C	-4.12154	-0.78365	0.374972
10	C	-5.12435	1.643974	0.859151
11	C	-3.02017	-0.8378	1.329105
12	C	-1.76203	-1.27898	1.103869
13	N	-1.29367	-1.72897	-0.14175
14	C	0.010471	-1.95215	-0.48839
15	C	1.048175	-1.56316	0.586688
16	N	0.486308	-1.71277	1.902906
17	C	-0.79101	-1.29412	2.234305
18	C	-5.891	2.580632	-0.06792
19	C	-7.10972	3.091356	0.119395
20	C	-3.73274	2.290358	1.080954
21	C	-5.83215	1.464726	2.221852
22	O	-1.09441	-1.01564	3.386519
23	O	0.339448	-2.35473	-1.59314
24	O	1.253815	-0.12714	0.366737
25	C	2.416716	0.316632	-0.24026
26	C	3.621901	-0.33328	0.013722
27	C	3.554428	-1.55939	0.882138
28	C	2.339053	-2.37837	0.439351
29	C	2.359952	1.446929	-1.06666
30	C	3.562264	1.90806	-1.60509
31	C	4.778273	1.251687	-1.38131
32	C	4.81628	0.101985	-0.56998
33	C	6.053074	-0.75893	-0.4074
34	C	5.945855	-1.6684	0.841226
35	O	4.706823	-2.38405	0.772317
36	O	5.889891	1.757014	-1.98743
37	C	1.042403	2.147249	-1.34943
38	C	0.582854	3.014206	-0.19853
39	C	0.365127	4.338127	-0.18942
40	C	-0.09344	5.030616	1.073251
41	C	0.543339	5.25918	-1.37207
42	O	7.220434	0.084375	-0.35494
43	C	6.148432	-0.92113	2.160559
44	C	8.446423	-0.59135	-0.61236
45	H	-4.48715	-4.96263	-1.86674
46	H	-6.41052	-4.05054	-3.13175
47	H	-7.22075	-1.73474	-2.71224
48	H	-3.31227	-3.59936	-0.17746
49	H	-6.65764	0.533343	-1.09572
50	H	-1.96482	-1.85778	-0.89189
51	H	1.134962	-1.61585	2.678602
52	H	-5.3463	2.852297	-0.97411
53	H	-7.54782	3.773124	-0.60492
54	H	-7.71005	2.872971	0.998151
55	H	-3.18507	2.392339	0.138052
56	H	-3.11507	1.702026	1.762749
57	H	-3.86007	3.289286	1.512302
58	H	-6.82129	1.010031	2.10455
59	H	-5.24309	0.812036	2.873143

60	H	-5.95051	2.430861	2.725114
61	H	3.427581	-1.25542	1.937264
62	H	2.249116	-3.29674	1.026982
63	H	2.460414	-2.65296	-0.61061
64	H	3.573895	2.790157	-2.23877
65	H	6.149418	-1.41404	-1.28961
66	H	6.698679	-2.46009	0.76695
67	H	6.659041	1.330678	-1.55679
68	H	1.142972	2.728207	-2.27025
69	H	0.2782	1.380982	-1.53734
70	H	0.422004	2.466457	0.729652
71	H	-1.05562	5.540345	0.920296
72	H	-0.20948	4.328788	1.904985
73	H	0.621967	5.806759	1.380738
74	H	1.279455	6.042638	-1.14351
75	H	-0.39695	5.778364	-1.60561
76	H	0.874229	4.746704	-2.27829
77	H	7.171331	-0.53875	2.224041
78	H	5.474785	-0.06425	2.258312
79	H	5.979566	-1.60308	3.00037
80	H	9.21978	0.177285	-0.67985
81	H	8.403559	-1.14922	-1.55882
82	H	8.707526	-1.28444	0.197464
83	H	-3.18898	-0.50116	2.348076

B3LYP Energy = -1972.78752512 a.u.; E+ZPVE = -1972.098226 a.u.

Compound 1 Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-4.33033	-4.20099	-1.14649
2	C	-5.52213	-4.03227	-1.87799
3	C	-6.22082	-2.83127	-1.8372
4	C	-5.68507	-1.79986	-1.06142
5	C	-4.46673	-1.92822	-0.3445
6	C	-3.80308	-3.1705	-0.37666
7	N	-6.17596	-0.53951	-0.79907
8	C	-5.33439	0.146153	0.049984
9	C	-4.24497	-0.67148	0.351907
10	C	-5.72707	1.54748	0.517337
11	C	-3.14436	-0.34977	1.250892
12	C	-1.8299	-0.62712	1.086677
13	N	-1.28641	-1.21993	-0.06384
14	C	0.033062	-1.4658	-0.32497
15	C	1.047376	-0.94435	0.715807
16	N	0.41989	-0.71575	1.991228
17	C	-0.88084	-0.29315	2.184702
18	C	-6.72	2.137488	-0.47844
19	C	-8.01354	2.397839	-0.27802
20	C	-4.50538	2.500829	0.531064
21	C	-6.3211	1.447534	1.941312
22	O	-1.22598	0.248381	3.22758
23	O	0.405235	-2.00519	-1.35563
24	O	1.449197	0.368629	0.207107
25	C	2.67036	0.509625	-0.43275
26	C	3.773359	-0.21014	0.021793
27	C	3.52818	-1.16786	1.154824
28	C	2.230381	-1.91872	0.84985
29	C	2.78709	1.415521	-1.49607
30	C	4.046575	1.56148	-2.08061
31	C	5.155765	0.820479	-1.658
32	C	5.024377	-0.08974	-0.59259
33	C	6.130809	-1.0336	-0.16611
34	C	5.885959	-1.57624	1.262692
35	O	4.565023	-2.12762	1.312095
36	O	6.332272	1.009334	-2.32007
37	C	1.607199	2.25194	-1.95587
38	C	1.522267	3.559787	-1.19872
39	C	0.563196	3.980554	-0.36082
40	C	0.670528	5.329638	0.311417
41	C	-0.67498	3.199096	0.001306
42	O	7.40145	-0.36145	-0.27135
43	C	6.162991	-0.55009	2.362662
44	C	8.526943	-1.23231	-0.29717
45	H	-3.81751	-5.15812	-1.17843
46	H	-5.90812	-4.85605	-2.47159
47	H	-7.1541	-2.7025	-2.3791
48	H	-2.90277	-3.33547	0.206857
49	H	-7.03575	-0.14759	-1.15604
50	H	-1.92161	-1.49794	-0.80506
51	H	1.038439	-0.4102	2.736562
52	H	-6.28698	2.371637	-1.45283
53	H	-8.62185	2.845508	-1.0596
54	H	-8.51353	2.197739	0.665206
55	H	-4.04227	2.56016	-0.45961
56	H	-3.7404	2.173724	1.238105
57	H	-4.82966	3.506811	0.819215
58	H	-7.18719	0.778192	1.96924
59	H	-5.57572	1.053414	2.638466
60	H	-6.63264	2.435285	2.298855
61	H	3.413929	-0.60205	2.097418
62	H	2.002862	-2.64592	1.634649

63	H	2.353548	-2.45315	-0.0944
64	H	4.188018	2.256292	-2.90387
65	H	6.147696	-1.89735	-0.852
66	H	6.529343	-2.44725	1.42521
67	H	7.0303	0.60326	-1.76627
68	H	1.734151	2.467558	-3.02558
69	H	0.686753	1.673539	-1.85322
70	H	2.376877	4.219063	-1.35838
71	H	0.673774	5.225635	1.405747
72	H	1.580911	5.862028	0.018288
73	H	-0.19083	5.966361	0.06347
74	H	-1.58002	3.758275	-0.27568
75	H	-0.72665	3.041858	1.08753
76	H	-0.72032	2.218137	-0.47432
77	H	7.225995	-0.29228	2.378752
78	H	5.60524	0.378989	2.210546
79	H	5.892408	-0.97129	3.336435
80	H	9.39888	-0.61106	-0.51448
81	H	8.421253	-1.99814	-1.07897
82	H	8.679769	-1.72946	0.669215
83	H	-3.36307	0.160071	2.184539

B3LYP Energy = -1972.78684810 a.u.; E+ZPVE = -1972.097518 a.u.

Compound 2 Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	4.300187	-3.83098	-1.37838
2	C	5.295196	-3.82587	-2.37594
3	C	6.138156	-2.73306	-2.54018
4	C	5.946331	-1.63843	-1.69234
5	C	4.936978	-1.60645	-0.6961
6	C	4.118948	-2.74118	-0.53524
7	N	6.641382	-0.45316	-1.59769
8	C	6.140561	0.331102	-0.57866
9	C	5.060951	-0.33689	0.000818
10	C	6.730779	1.730183	-0.4042
11	C	4.21522	0.139925	1.088082
12	C	2.867291	0.081518	1.166928
13	N	2.041369	-0.38569	0.125701
14	C	0.695664	-0.57142	0.165309
15	C	0.005896	-0.33783	1.5117
16	N	0.811627	0.576743	2.32682
17	C	2.178532	0.643775	2.364659
18	C	8.223905	1.647954	-0.70549
19	C	8.88077	2.224819	-1.71416
20	C	6.598838	2.260568	1.043343
21	C	5.991724	2.69601	-1.35993
22	O	2.782825	1.177827	3.29014
23	O	0.086339	-0.97426	-0.82922
24	C	-1.41168	0.273403	1.311316
25	C	-2.12472	0.283642	2.651301
26	C	-1.86351	-0.57071	3.646457
27	C	-0.83969	-1.67931	3.577245
28	C	-0.14591	-1.73211	2.192226
29	C	-1.39872	1.66464	0.620456
30	C	-1.79926	1.66491	-0.87678
31	C	-3.21798	1.201066	-1.15983
32	C	-3.47485	-0.1048	-1.58227
33	C	-4.79695	-0.51121	-1.86267
34	C	-5.89081	0.323913	-1.72842
35	C	-5.65775	1.642269	-1.28311
36	C	-4.33702	2.084637	-1.00321
37	C	-7.30369	-0.14756	-2.02455
38	C	-8.0825	-0.46573	-0.76767
39	C	-8.60346	-1.64227	-0.38802
40	C	-9.35741	-1.76009	0.916541
41	C	-8.51424	-2.92989	-1.17081
42	C	0.148772	-1.62727	4.76207
43	O	-6.72801	2.448798	-1.14684
44	O	-2.53789	-1.07668	-1.78241
45	C	-4.16104	3.462752	-0.57612
46	O	-5.08002	4.279856	-0.41332
47	H	3.667285	-4.70634	-1.26344
48	H	5.411568	-4.69254	-3.02033
49	H	6.919412	-2.73135	-3.29562
50	H	3.365016	-2.77425	0.245195
51	H	7.443567	-0.18626	-2.15105
52	H	2.481664	-0.63092	-0.75641
53	H	0.357517	0.940843	3.157415
54	H	8.787484	1.045848	0.009259
55	H	9.956884	2.112854	-1.81687
56	H	8.388546	2.842838	-2.45979
57	H	7.016151	1.555604	1.770457
58	H	5.557785	2.457762	1.310125
59	H	7.149311	3.203035	1.131055
60	H	4.928692	2.730754	-1.10342
61	H	6.398615	3.709859	-1.27492
62	H	6.074052	2.376183	-2.40389

63	H	-1.95234	-0.42527	0.663129
64	H	-2.90571	1.031414	2.777989
65	H	-2.42857	-0.49607	4.575108
66	H	-1.39247	-2.62518	3.684678
67	H	0.843718	-2.19517	2.289605
68	H	-0.7268	-2.35964	1.507305
69	H	-2.07818	2.33482	1.160369
70	H	-0.40172	2.111479	0.719257
71	H	-1.65563	2.680099	-1.26311
72	H	-1.09565	1.047929	-1.44163
73	H	-4.93413	-1.53587	-2.19799
74	H	-7.82821	0.649401	-2.56816
75	H	-7.25412	-1.01242	-2.69194
76	H	-8.21806	0.388986	-0.10606
77	H	-9.39943	-0.80593	1.450993
78	H	-10.3889	-2.10194	0.749604
79	H	-8.88889	-2.50168	1.579527
80	H	-8.02215	-3.7114	-0.57483
81	H	-9.51793	-3.30936	-1.40893
82	H	-7.96443	-2.83244	-2.10977
83	H	0.793661	-0.74341	4.732421
84	H	0.796487	-2.51158	4.759456
85	H	-0.39296	-1.61476	5.715063
86	H	-6.38692	3.330796	-0.83857
87	H	-1.65382	-0.86283	-1.42041
88	H	-3.13174	3.807326	-0.38554
89	H	4.673835	0.615103	1.947679

B3LYP Energy = -2014.30676863 a.u.; E+ZPVE = -2013.559702 a.u.

Compound 2 Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-0.40799	-3.50404	0.463066
2	C	-1.11584	-4.64738	0.043658
3	C	-2.48815	-4.59962	-0.17426
4	C	-3.12948	-3.37341	0.019932
5	C	-2.43698	-2.19674	0.408611
6	C	-1.05327	-2.28806	0.657296
7	N	-4.46395	-3.04226	-0.07576
8	C	-4.66088	-1.71345	0.232113
9	C	-3.42549	-1.139	0.528774
10	C	-6.08061	-1.14714	0.239502
11	C	-3.1893	0.238091	0.943464
12	C	-2.19783	1.064887	0.54434
13	N	-1.23764	0.724855	-0.42961
14	C	-0.29991	1.539689	-0.98058
15	C	-0.33291	3.016875	-0.57672
16	N	-1.04674	3.180745	0.692304
17	C	-2.08472	2.420219	1.157371
18	C	-6.97175	-2.04242	-0.61436
19	C	-7.96554	-2.83148	-0.20114
20	C	-6.12838	0.260622	-0.40796
21	C	-6.57308	-1.05949	1.702457
22	O	-2.83401	2.810452	2.048304
23	O	0.4903	1.109915	-1.82557
24	C	1.112573	3.554147	-0.42707
25	C	1.085163	5.063499	-0.3111
26	C	0.097476	5.834265	-0.77933
27	C	-1.10868	5.31603	-1.52704
28	C	-1.03362	3.783277	-1.73966
29	C	1.898255	2.89427	0.732353
30	C	3.436051	2.847341	0.470419
31	C	3.966405	1.445573	0.224392
32	C	3.826644	0.887277	-1.046
33	C	4.340414	-0.38934	-1.32648
34	C	4.975817	-1.17017	-0.37108
35	C	5.093688	-0.64142	0.929024
36	C	4.594563	0.658225	1.23697
37	C	5.518942	-2.55147	-0.69261
38	C	4.593296	-3.66086	-0.24597
39	C	4.001471	-4.60147	-0.99768
40	C	3.109881	-5.64319	-0.36172
41	C	4.144752	-4.7413	-2.49391
42	C	-2.43311	5.791274	-0.89153
43	O	5.693001	-1.40906	1.858366
44	O	3.24365	1.60436	-2.0745
45	C	4.719788	1.13001	2.606758
46	O	5.256387	0.497938	3.527637
47	H	0.660556	-3.57551	0.644167
48	H	-0.58426	-5.58434	-0.09623
49	H	-3.04318	-5.48492	-0.47329
50	H	-0.49493	-1.43124	1.022356
51	H	-5.21804	-3.66758	-0.32216
52	H	-1.22895	-0.22911	-0.77905
53	H	-0.98929	4.100403	1.115114
54	H	-6.75069	-2.00088	-1.68265
55	H	-8.55195	-3.41002	-0.91014
56	H	-8.24863	-2.92206	0.843605
57	H	-5.75221	0.233251	-1.43643
58	H	-5.53087	0.985341	0.149225
59	H	-7.16406	0.617047	-0.43114
60	H	-5.93437	-0.38448	2.279849
61	H	-7.59815	-0.67455	1.741686
62	H	-6.5496	-2.03787	2.193275

63	H	1.627586	3.286258	-1.3555
64	H	1.932608	5.526882	0.192462
65	H	0.149397	6.913936	-0.64112
66	H	-1.07616	5.769818	-2.52966
67	H	-2.04152	3.376224	-1.88633
68	H	-0.46387	3.563383	-2.64904
69	H	1.690583	3.428815	1.666766
70	H	1.532009	1.874082	0.889253
71	H	3.667227	3.442839	-0.41854
72	H	3.970422	3.320566	1.297018
73	H	4.230087	-0.76069	-2.34224
74	H	5.718001	-2.60962	-1.76643
75	H	6.482226	-2.67329	-0.18002
76	H	4.406447	-3.67378	0.82747
77	H	3.03655	-5.51168	0.722617
78	H	2.094225	-5.60334	-0.78196
79	H	3.484601	-6.65859	-0.55491
80	H	4.564803	-5.72335	-2.75329
81	H	3.162105	-4.68658	-2.98321
82	H	4.783339	-3.97802	-2.94441
83	H	-2.60284	5.361081	0.100574
84	H	-3.28327	5.510334	-1.52396
85	H	-2.44129	6.88274	-0.78867
86	H	5.693204	-0.89087	2.707759
87	H	2.284287	1.394736	-2.10626
88	H	4.292515	2.117896	2.843084
89	H	-3.85695	0.689645	1.672011

B3LYP Energy = -2014.30356824 a.u.; E+ZPVE = -2013.556933 a