Supporting Information

***Rec. Nat. Prod*. 16:4 (2022) 382-386**

Fissistigmol A: A New Polyacetylene alcohol from *Fissistigma minuticalyx*

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[1] These authors contributed equally to this paper.

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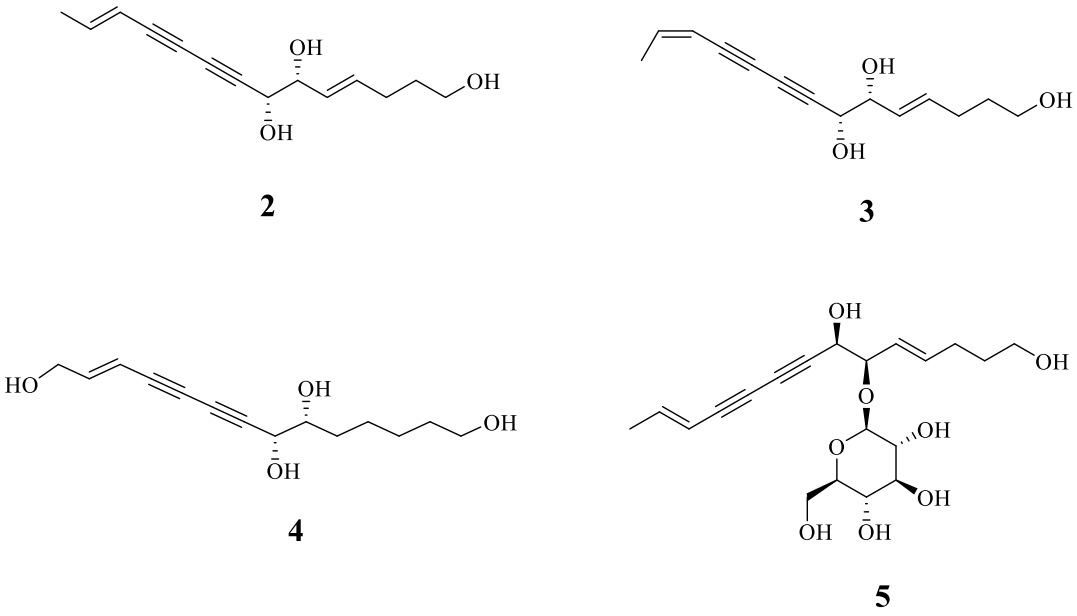
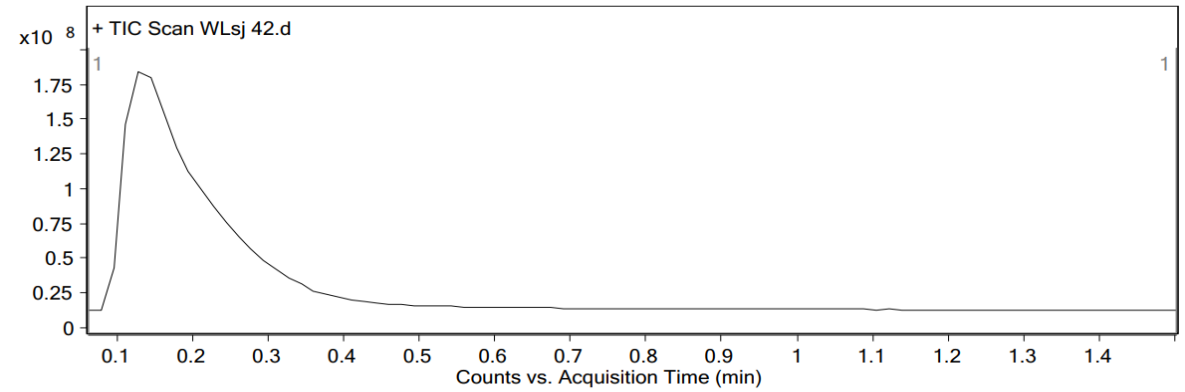


Figure S1: The structures of **2-5**

Qualitative Analysis Report

Data File	WLsj 42.d	**Sample Name**	WLsj 42
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	20200905-HRMS(+).m	**Acquired Time**	9/16/2020 5:02:38 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

Fragmentor Voltage 175 **Collision Energy** 0 **Ionization Mode** ESI



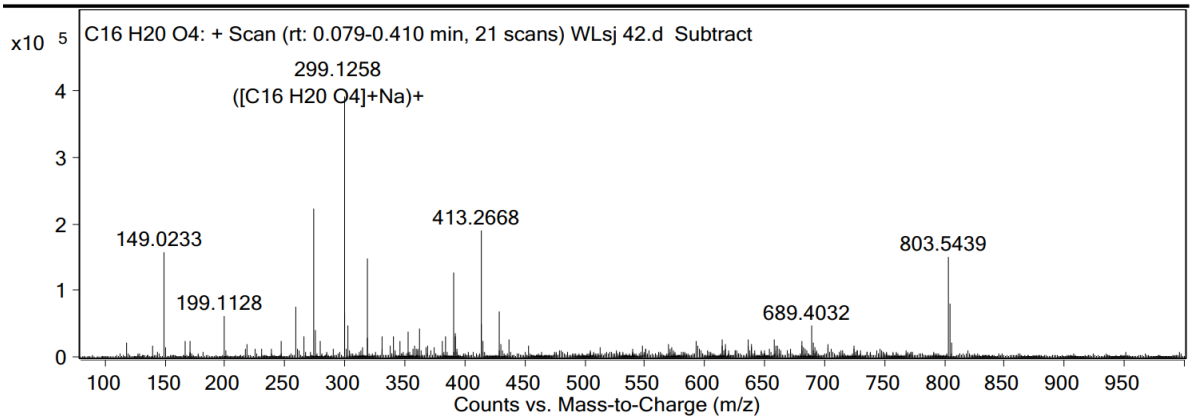


Figure S2: HR-ESI-MS spectrum of **1**

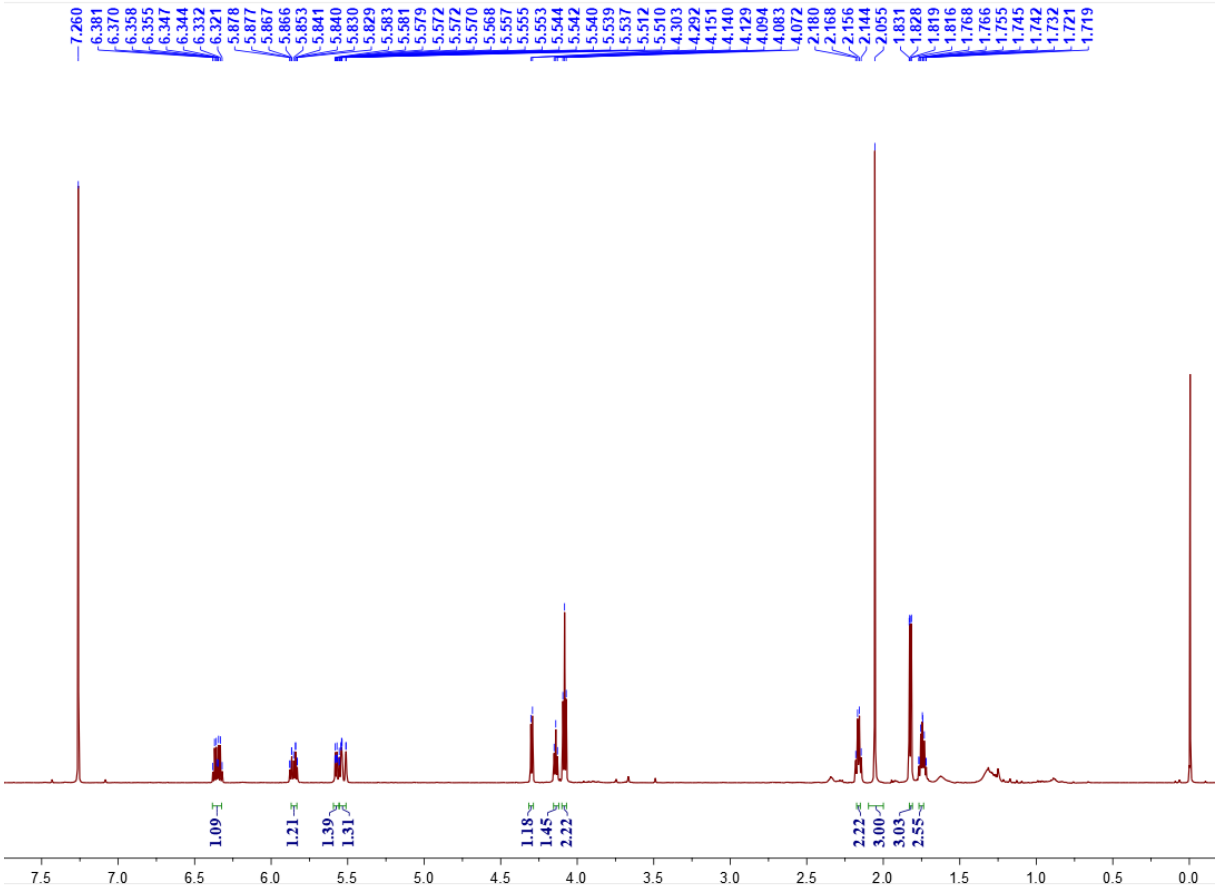


Figure S3: ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of **1**

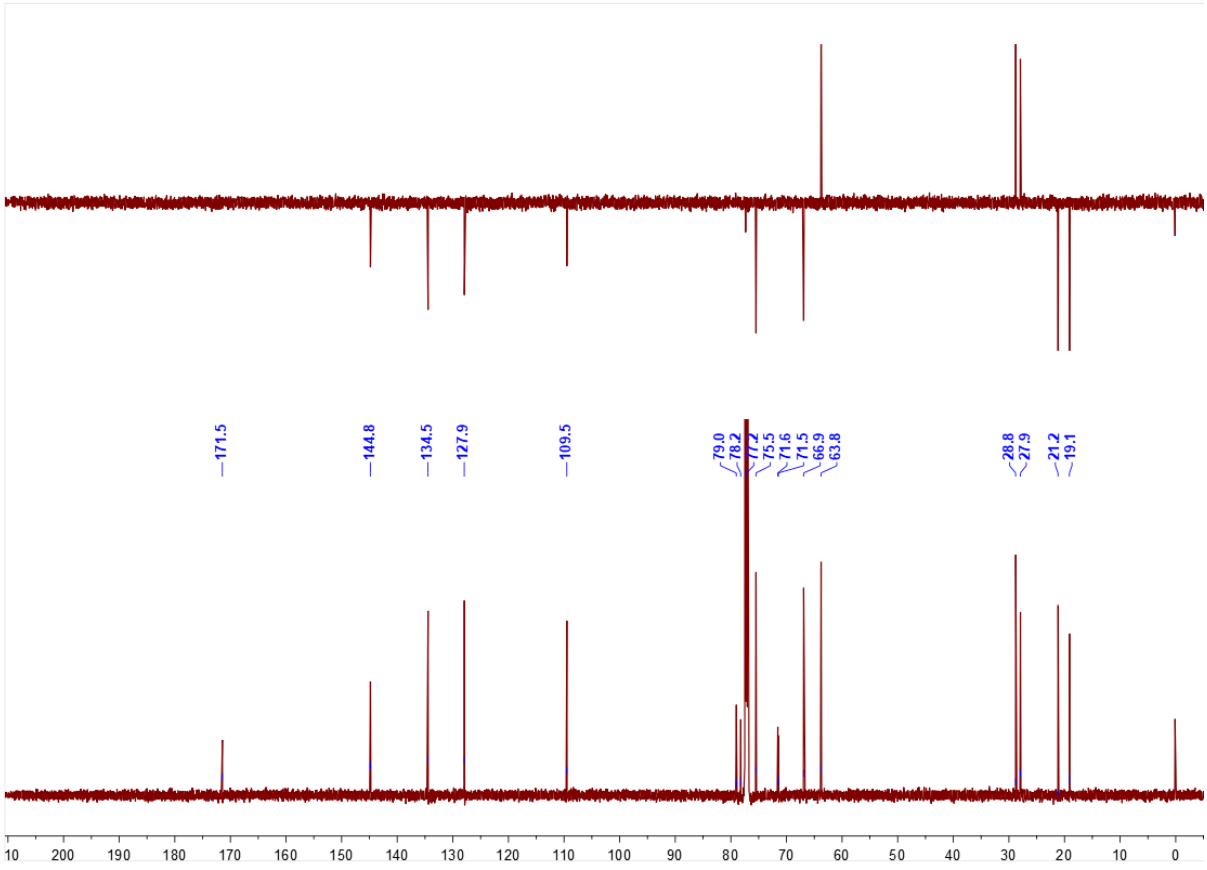


Figure S4: ^{13}C-NMR (150 MHz, $CDCl_3$) spectrum of **1**

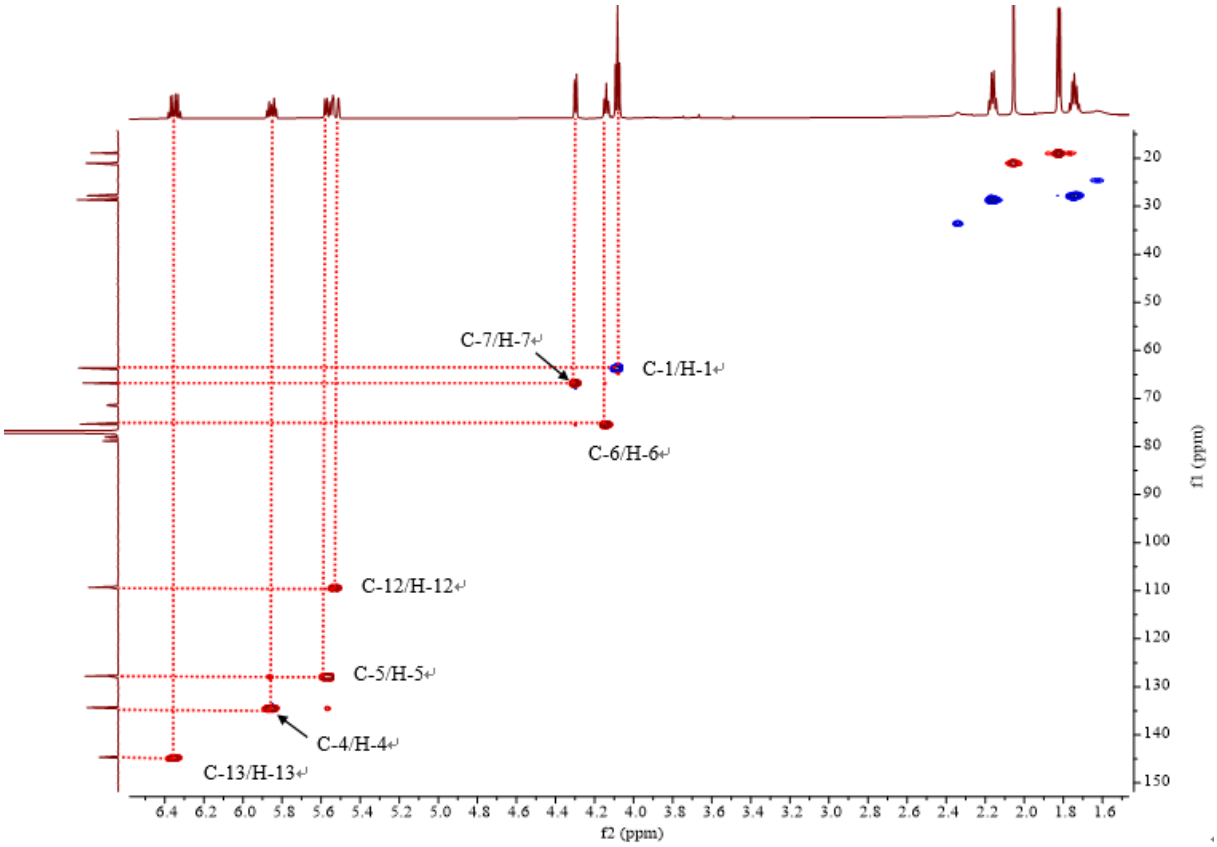


Figure S5: HSQC spectrum of **1**

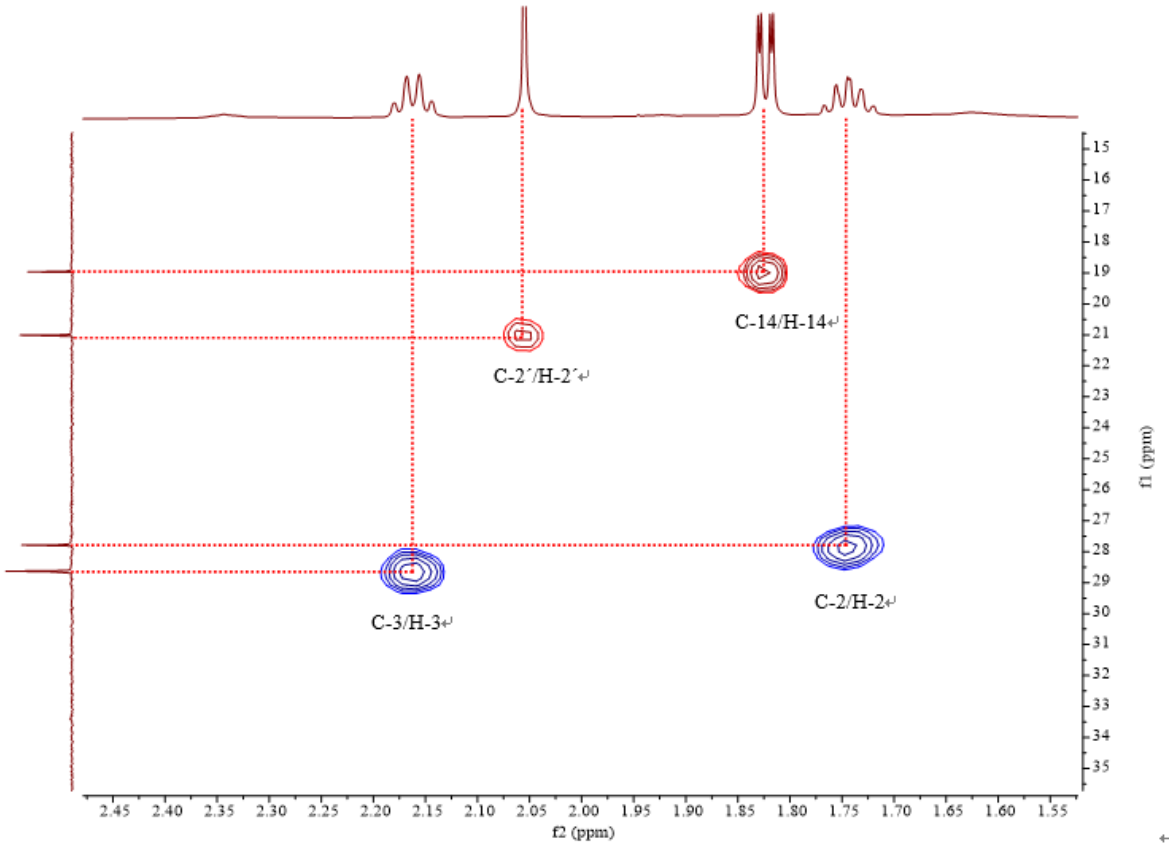


Figure S6: Enlarged HSQC spectrum of **1** (From δ_C15 ppm to δ_C 35 ppm)

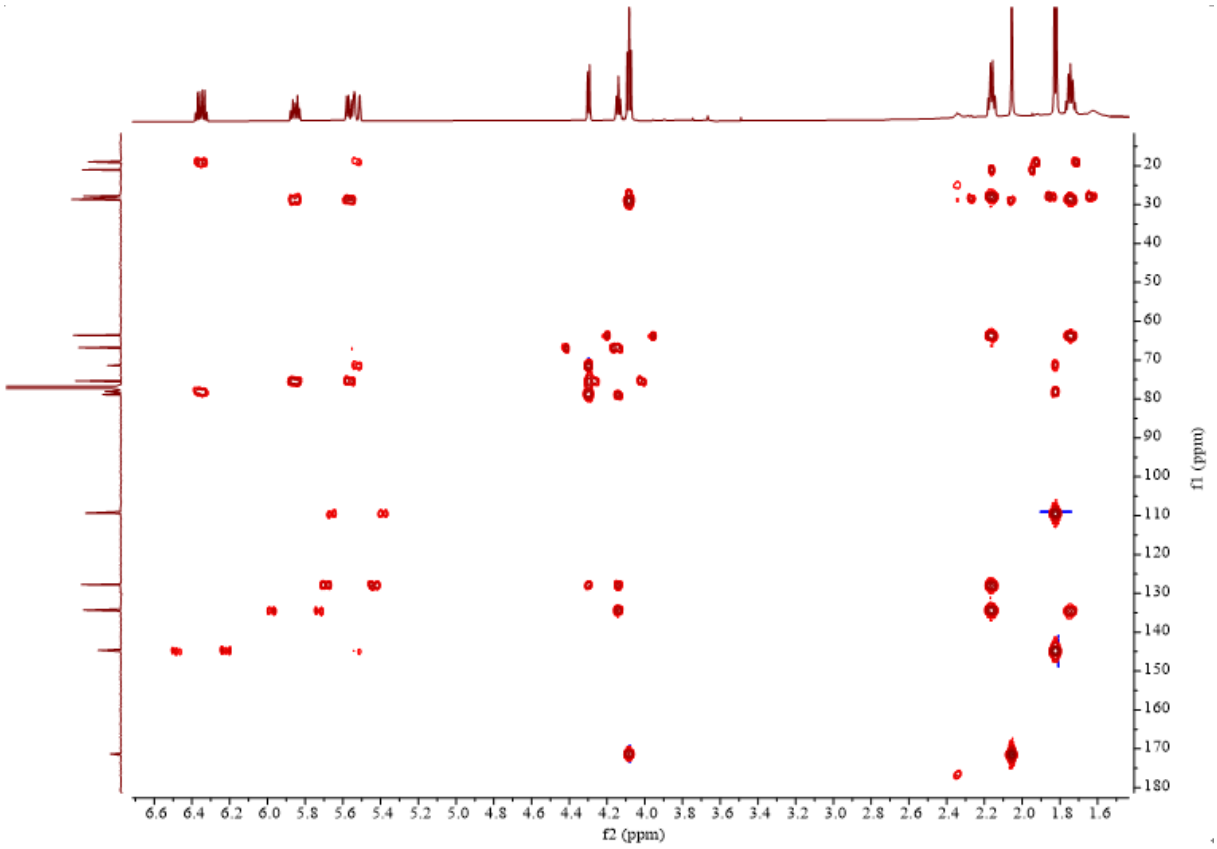


Figure S7: HMBC spectrum of **1**

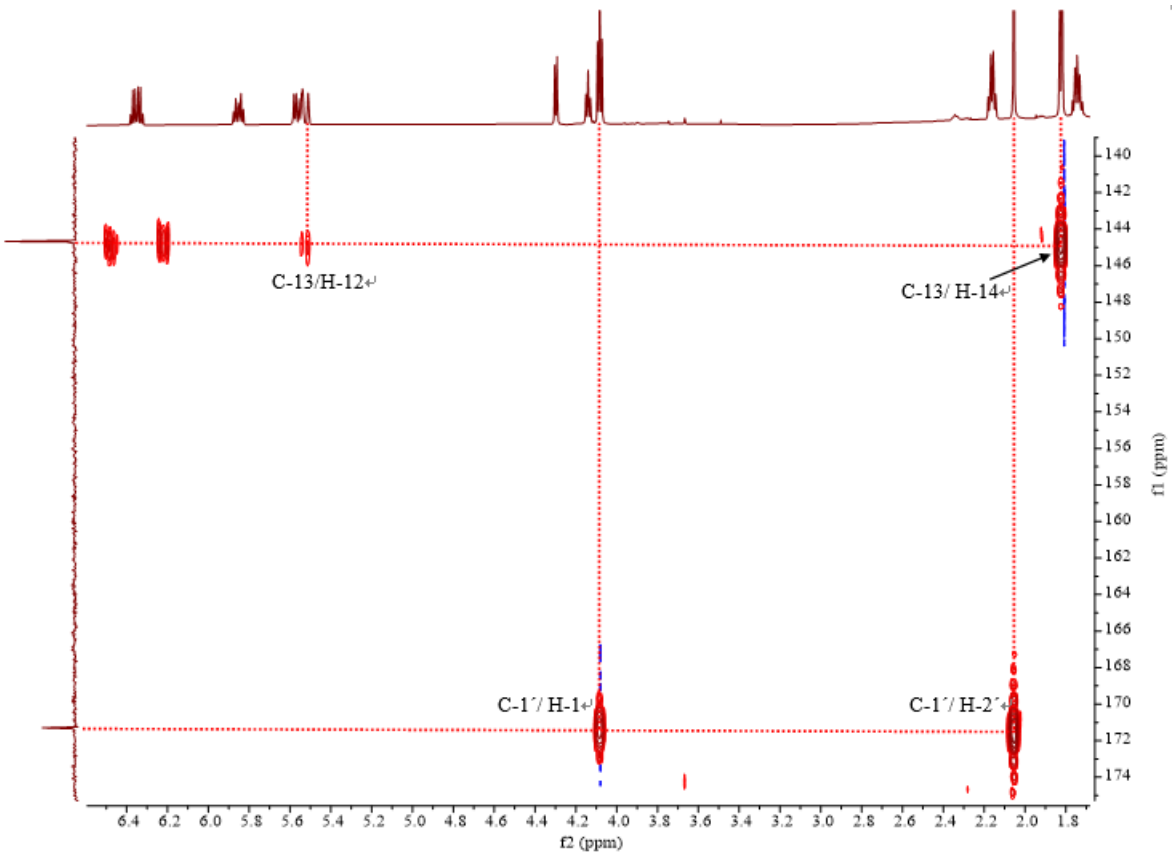


Figure S8: Enlarged HMBC spectrum of **1** (From δ_C 140 ppm to δ_C 175 ppm)

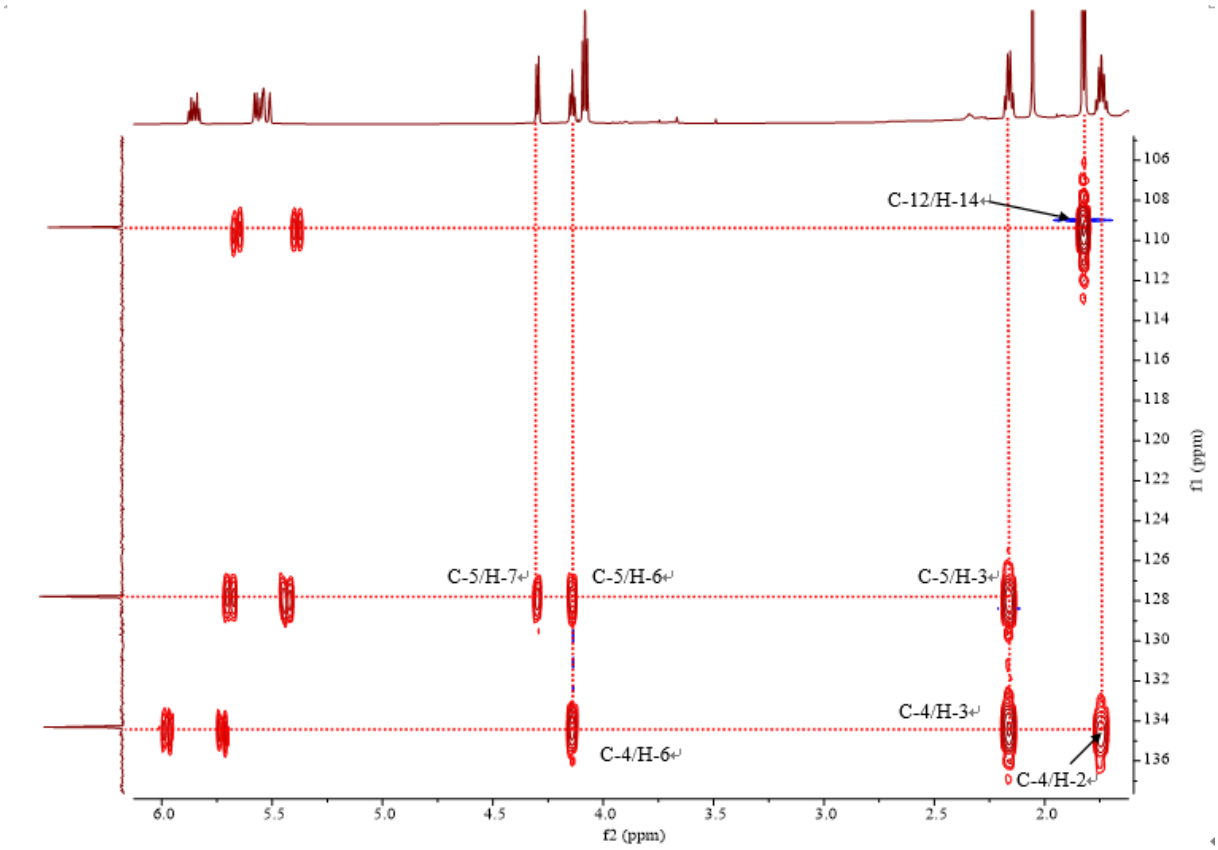


Figure S9: Enlarged HMBC spectrum of **1** (From δ_C 105 ppm to δ_C 140 ppm)

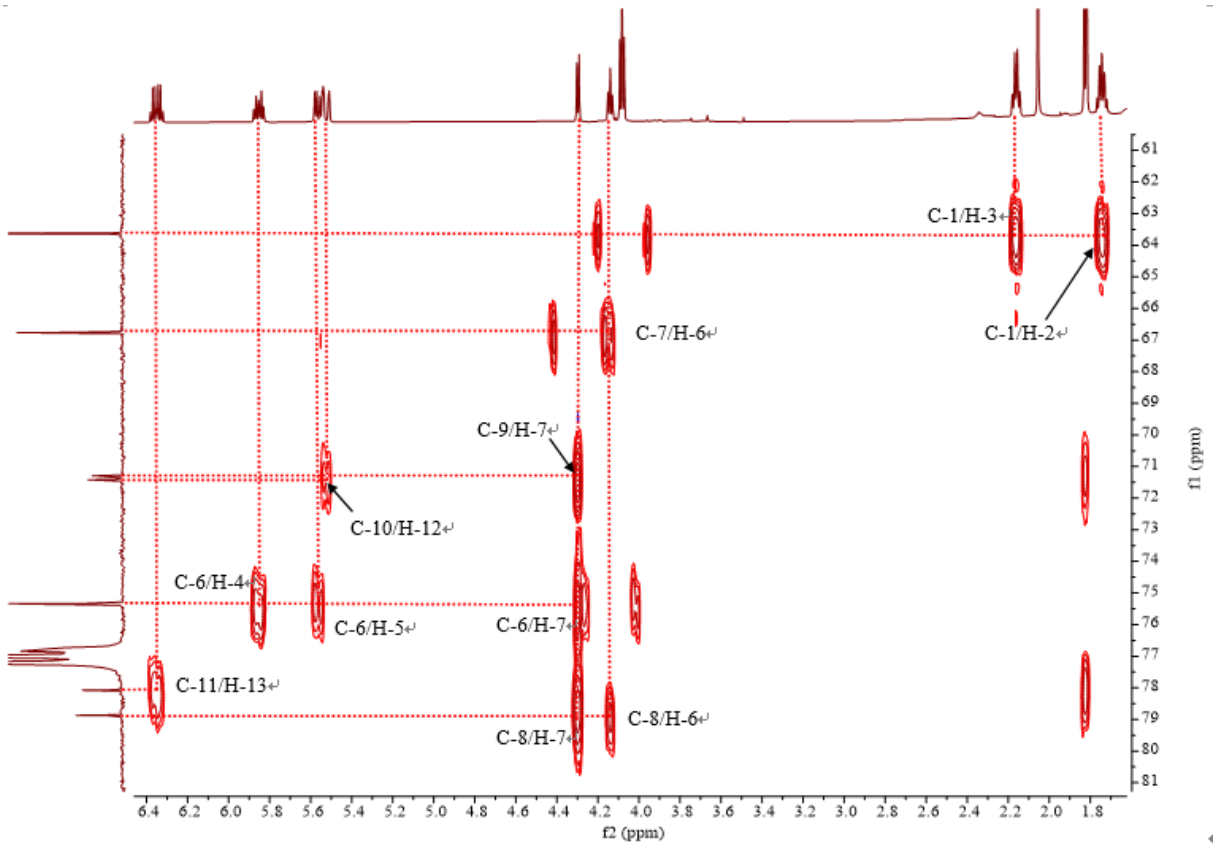


Figure S10: Enlarged HMBC spectrum of **1** (From δ_C 60 ppm to δ_C 80 ppm)

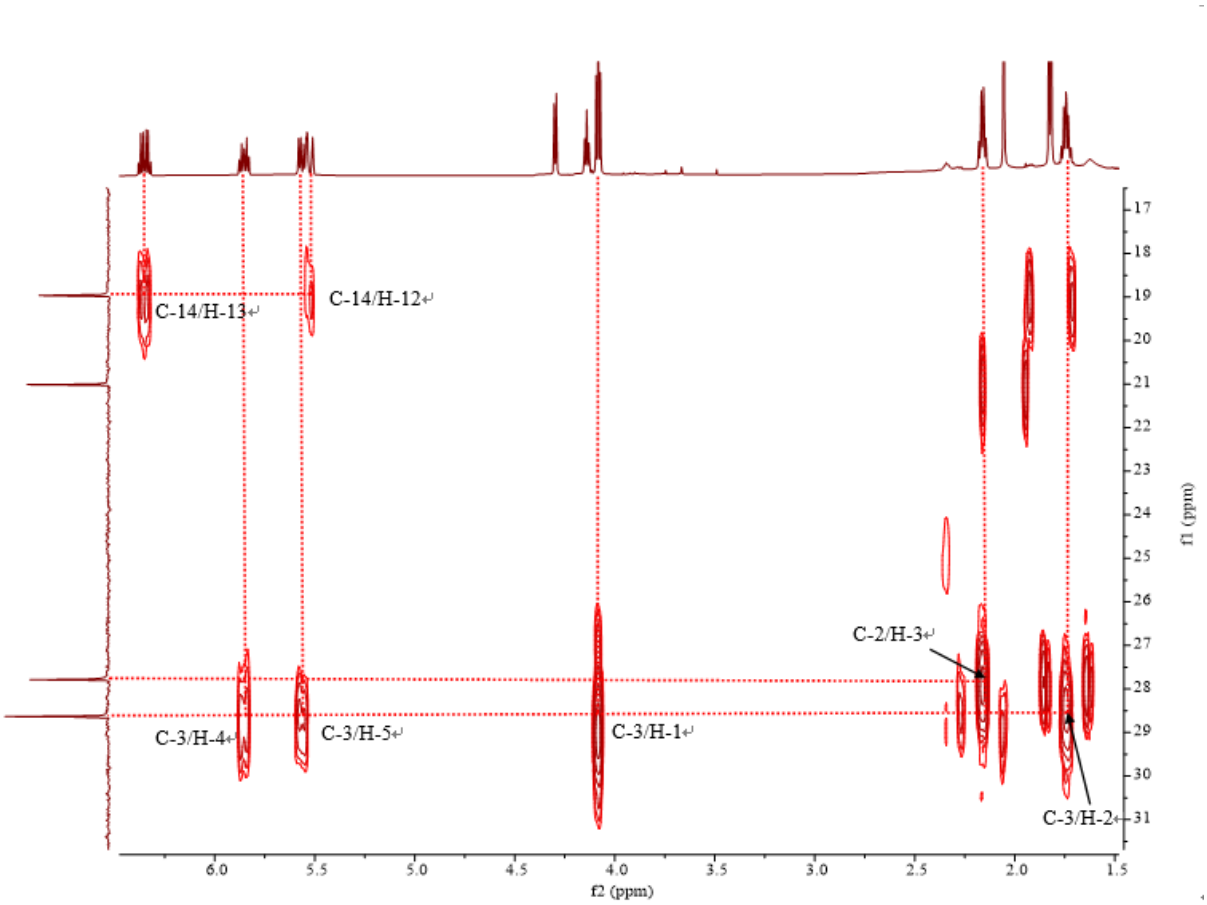


Figure S11: Enlarged HMBC spectrum of **1** (From δ_C 15 ppm to δ_C 30 ppm)

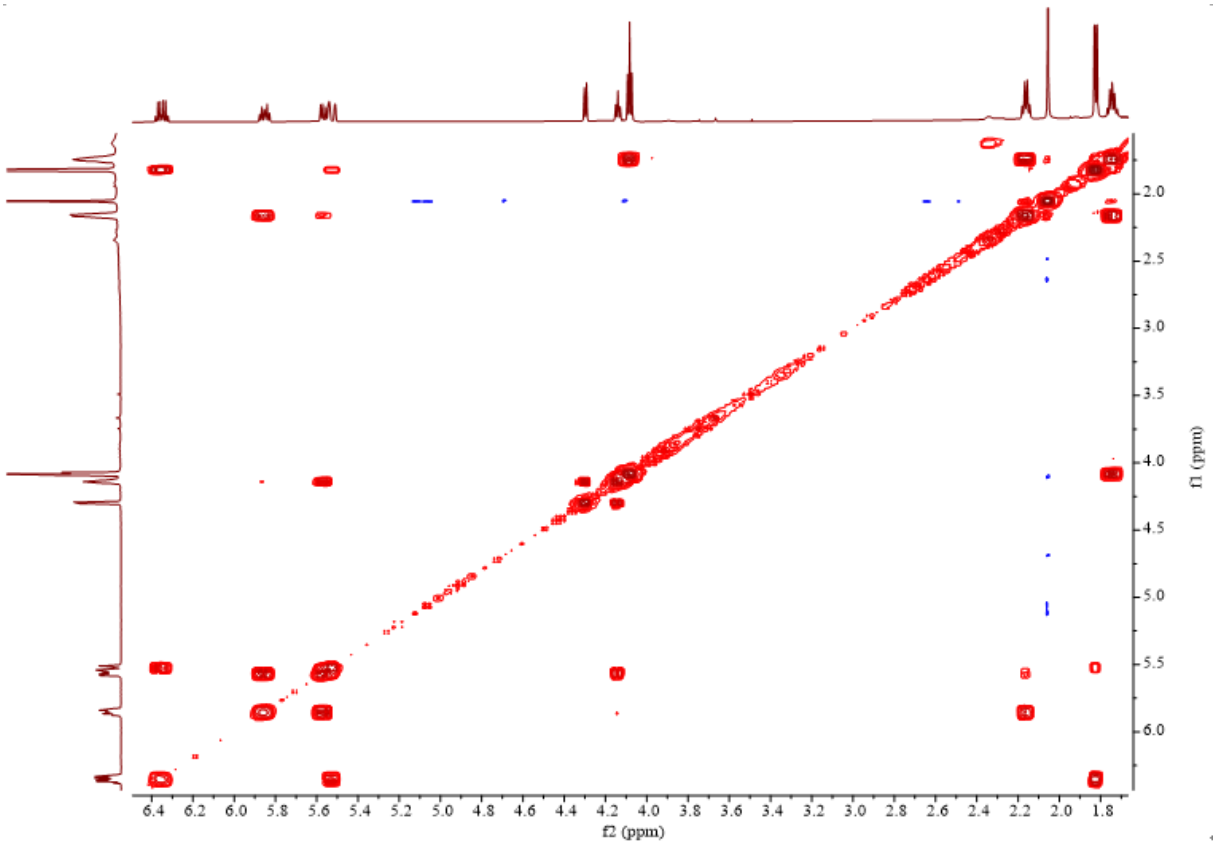


Figure S12: ^{1}H-^{1}H COSY spectrum of **1**

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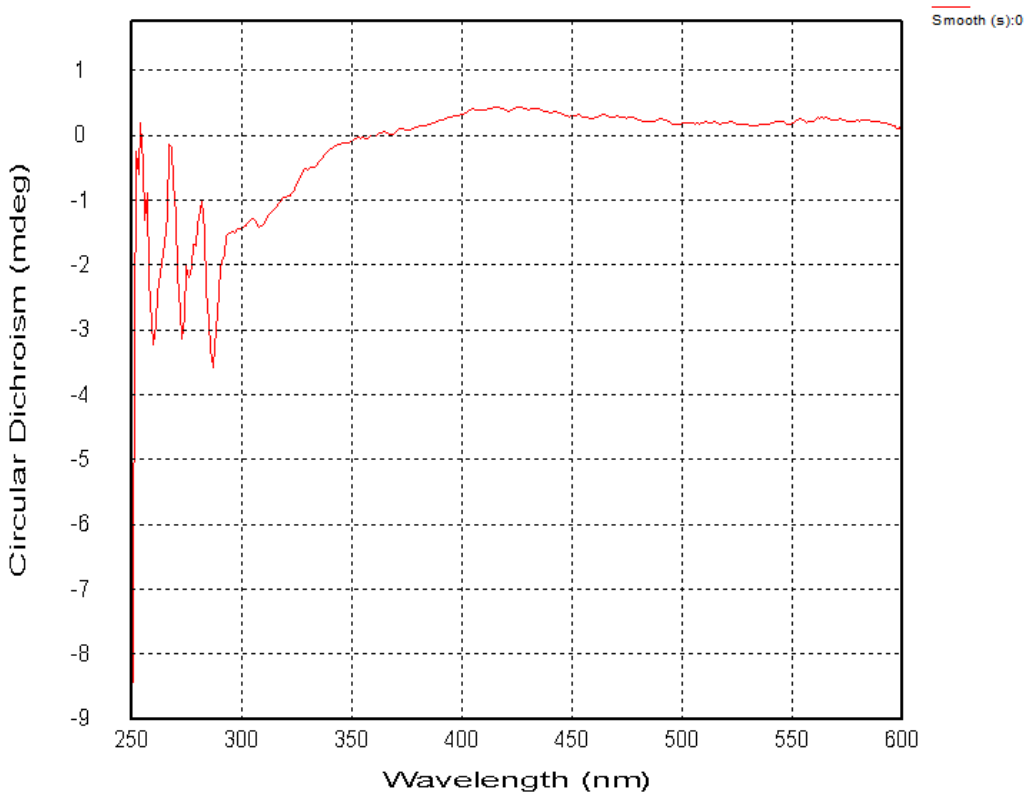

Figure S13: ICD spectrum of **1** (Fissistigmol A)

Computional Methods

MMFF94S conformational searches generated low-energy conformers of model compound **1** within 5 kcal/mol energy window were performed with CONFLEX.[1,2] Selected total distribution over 90% conformers in Gibb's free energy of each model compound (**1a** to **1r,** total 18 conformers) were further optimized by the density functional theory method at the B3LYP/6-31g(d) level. The specific optical rotation (589.3 nm) calculations were using DFT-B3LYP/6-311+g(d,p) of theory on optimized geometries through the IEFPCM model (in MeOH). All the above calculations were carried out with the *Gaussian* 09 package of programs.[3] As result, the calculated specific optical rotation of compound **1** at 589.3 nm is +93.63 degrees based on Boltzmann Method.

References

(1) Goto H, Osawa E. J. Am. Chem. Soc., 1989, 111, 8950–8951.

(2) Goto, H, Osawa E, J. Chem. Soc., Perkin Trans. 2, 1993, 187–198.

(3) Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Keith T, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg, JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ. Gaussian 09, revision C.01. Gaussian, Inc., Wallingford CT, 2010.

The different conformations and its coordinate for the specific optical rotation calculation :

1a Distribution in Gibb's free eneygy: 15.11%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.513178	-0.951858	-1.362116
2	6	0	-2.024048	-1.383288	-1.021588
3	6	0	-1.191386	-1.506560	0.017378
4	6	0	0.173758	-0.881893	0.065842
5	6	0	1.275765	-1.917101	0.413178
6	6	0	2.622408	-1.346861	0.238133
7	6	0	3.742328	-0.885324	0.103036
8	6	0	4.994986	-0.369056	-0.051426
9	6	0	6.112220	0.107902	-0.187948
10	6	0	7.427844	0.606939	-0.355104
11	6	0	-4.688378	0.004663	-0.192546
12	8	0	-5.766158	0.911063	-0.530502
13	6	0	7.753882	1.913802	-0.293413
14	6	0	-6.071315	1.850650	0.386430

15	6	0	-7.208102	2.723589	-0.087010
16	8	0	-5.493532	1.961061	1.451092
17	6	0	9.139617	2.448546	-0.469451
18	6	0	-3.398454	-1.988986	-1.113548
19	8	0	0.267995	0.090062	1.122846
20	8	0	1.079056	-2.402447	1.738934
21	1	0	-4.290198	-0.375802	-2.269242
22	1	0	-5.459256	-1.476308	-1.540132
23	1	0	-1.702263	-0.802979	-1.889488
24	1	0	-1.483426	-2.077664	0.898135
25	1	0	0.411459	-0.418390	-0.901442
26	1	0	1.163863	-2.779392	-0.253726
27	1	0	8.208802	-0.130610	-0.544792
28	1	0	-3.782606	0.587189	0.000097
29	1	0	-4.948713	-0.527642	0.728649
30	1	0	6.966348	2.641877	-0.103358
31	1	0	-6.944619	3.204136	-1.034668
32	1	0	-8.099940	2.113898	-0.265091
33	1	0	-7.425969	3.483303	0.664250
34	1	0	9.863405	1.649286	-0.656368
35	1	0	9.179489	3.157536	-1.307272
36	1	0	9.457908	3.005253	0.422165
37	1	0	-3.416327	-2.702875	-1.948930
38	1	0	-3.616584	-2.563559	-0.204294
39	1	0	-0.566650	0.585178	1.140856
40	1	0	0.898701	-1.601335	2.266612

1b Distribution in Gibb's free eneygy: 11.44%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.964898	0.142364	-0.413832
2	6	0	1.786457	-1.052668	-0.878650
3	6	0	0.832566	-1.593715	-0.114365
4	6	0	-0.636562	-1.416868	-0.372022
5	6	0	-1.392975	-0.924604	0.889775
6	6	0	-2.776909	-0.534766	0.570165
7	6	0	-3.925380	-0.210713	0.322117
8	6	0	-5.209005	0.154395	0.041810
9	6	0	-6.358654	0.493798	-0.197924
10	6	0	-7.692906	0.847900	-0.517690
11	6	0	5.467544	-0.023873	-0.248634
12	8	0	6.028929	1.292346	-0.025609
13	6	0	-8.384965	1.824398	0.103200
14	6	0	7.363860	1.354899	0.150840
15	6	0	7.817295	2.777627	0.370978
16	8	0	8.089043	0.378733	0.130066
17	6	0	-9.792812	2.205182	-0.228761
18	6	0	3.265686	-1.208997	-0.659533

19	8	0	-1.268898	-2.670958	-0.686586
20	8	0	-1.349842	-1.930316	1.899098
21	1	0	3.768942	0.821526	-1.253099
22	1	0	3.550994	0.614418	0.485279
23	1	0	1.493915	-0.434811	-1.730314
24	1	0	1.093094	-2.212699	0.743635
25	1	0	-0.792948	-0.695966	-1.186121
26	1	0	-0.862558	-0.054826	1.293675
27	1	0	-8.168921	0.281896	-1.319497
28	1	0	5.928733	-0.458940	-1.141529
29	1	0	5.715161	-0.663484	0.604897
30	1	0	-7.900026	2.383274	0.902537
31	1	0	7.552831	3.393871	-0.494481
32	1	0	7.311598	3.203230	1.243645
33	1	0	8.896898	2.799982	0.522557
34	1	0	-10.199148	1.593777	-1.040371
35	1	0	-10.442989	2.094981	0.649481
36	1	0	-9.850474	3.261000	-0.525645
37	1	0	3.448449	-1.883952	0.185886
38	1	0	3.712639	-1.680851	-1.547377
39	1	0	-0.663127	-3.168501	-1.258994
40	1	0	-1.555741	-2.758527	1.425247

1c Distribution in Gibb's free eneygy: 11.22%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.093867	-0.343475	-0.234549
2	6	0	1.687869	0.334562	-0.612673
3	6	0	0.765104	0.979362	0.108098
4	6	0	-0.660977	0.523522	0.228316
5	6	0	-1.665852	1.657004	-0.106264
6	6	0	-3.042526	1.142898	-0.204945
7	6	0	-4.187123	0.731367	-0.282679
8	6	0	-5.467074	0.269529	-0.372106
9	6	0	-6.611529	-0.154581	-0.440671
10	6	0	-7.948719	-0.607322	-0.562430
11	6	0	5.547237	0.063277	-0.421502
12	8	0	6.370461	-1.016510	0.082050
13	6	0	-8.482409	-1.596164	0.182818
14	6	0	7.704846	-0.838551	0.011043
15	6	0	8.443099	-2.031782	0.567259
16	8	0	8.224077	0.161861	-0.445916
17	6	0	-9.892775	-2.079440	0.062092
18	6	0	3.128367	0.744737	-0.743264
19	8	0	-0.983321	0.165768	1.584694
20	8	0	-1.561230	2.694710	0.865454
21	1	0	3.905117	-0.537490	0.828186
22	1	0	3.911996	-1.283524	-0.770580

23	1	0	1.399101	-0.569109	-1.153631
24	1	0	1.023139	1.882435	0.660452
25	1	0	-0.843835	-0.325836	-0.444087
26	1	0	-1.380930	2.100099	-1.067160
27	1	0	-8.565684	-0.109475	-1.311658
28	1	0	5.787760	0.978218	0.129725
29	1	0	5.789339	0.231025	-1.476231
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35	1	0	-9.917488	-3.149575	-0.183691
36	1	0	-10.424710	-1.969051	1.016605
37	1	0	3.349900	0.945510	-1.802254
38	1	0	3.300278	1.682213	-0.199757
39	1	0	-0.217707	-0.303676	1.952942
40	1	0	-1.533519	2.224598	1.720451

1d Distribution in Gibb's free eneygy: 6.92%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.668602	-0.752623	1.011089
2	6	0	2.161016	-1.208751	0.955315
3	6	0	1.260606	-1.587950	0.042371
4	6	0	-0.103768	-0.972370	-0.083418
5	6	0	-1.228452	-2.040708	-0.066079
6	6	0	-2.559115	-1.418123	0.038481
7	6	0	-3.666669	-0.915906	0.119566
8	6	0	-4.905168	-0.353000	0.213396
9	6	0	-6.009915	0.164532	0.290995
10	6	0	-7.309893	0.716300	0.407083
11	6	0	4.773416	-0.148651	-0.385772
12	8	0	5.909784	0.745986	-0.484620
13	6	0	-7.648093	1.949602	-0.020226
14	6	0	5.715235	2.034356	-0.131674
15	6	0	6.988316	2.831127	-0.281911
16	8	0	4.650303	2.479000	0.252346
17	6	0	-9.017274	2.539894	0.098736
18	6	0	3.536856	-1.795841	1.118942
19	8	0	-0.268849	-0.318680	-1.354663
20	8	0	-1.124837	-2.867792	-1.222523
21	1	0	4.503344	0.051427	1.738343
22	1	0	5.622938	-1.228915	1.264495
23	1	0	1.899212	-0.411306	1.654589
24	1	0	1.491830	-2.379110	-0.670252
25	1	0	-0.274276	-0.261593	0.736712
26	1	0	-1.071662	-2.694632	0.799150

27	1	0	-8.067362	0.085720	0.874481
28	1	0	3.867043	0.396529	-0.656911
29	1	0	4.966228	-0.920807	-1.135114
30	1	0	-6.883763	2.570594	-0.485631
31	1	0	7.765176	2.420252	0.371228
32	1	0	7.356067	2.764813	-1.310738
33	1	0	6.802603	3.873477	-0.021079
34	1	0	-9.718174	1.849075	0.577433
35	1	0	-8.990609	3.469460	0.683028
36	1	0	-9.412761	2.807562	-0.890284
37	1	0	3.607402	-2.262602	2.111526
38	1	0	3.692872	-2.595887	0.383829
39	1	0	0.558585	0.148192	-1.553329
40	1	0	-0.980110	-2.241690	-1.957169

1e Distribution in Gibb's free eneygy: 5.89%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.221223	-0.336317	1.128176
2	6	0	-1.865101	-0.084612	0.239989
3	6	0	-0.910861	-0.936590	-0.148743
4	6	0	0.532571	-0.801325	0.243514
5	6	0	1.477311	-0.847616	-0.985989
6	6	0	2.857654	-0.489743	-0.617418
7	6	0	4.005546	-0.201324	-0.326393
8	6	0	5.288837	0.123899	0.000678
9	6	0	6.442151	0.419149	0.278263
10	6	0	7.768238	0.746818	0.655126
11	6	0	-5.704177	-0.401601	0.798396
12	8	0	-6.087606	0.866689	0.210426
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14	6	0	-7.369346	0.983440	-0.190406
15	6	0	-7.631258	2.345237	-0.786251
16	8	0	-8.190500	0.093560	-0.076468
17	6	0	10.106708	1.553629	0.189663
18	6	0	-3.321364	-0.192016	-0.114683
19	8	0	0.963042	-1.912492	1.051188
20	8	0	1.413517	-2.135791	-1.593150
21	1	0	-3.960325	-1.255693	1.667211
22	1	0	-4.043549	0.497092	1.819884
23	1	0	-1.589513	0.762222	0.872490
24	1	0	-1.153739	-1.792420	-0.777943
25	1	0	0.690905	0.144098	0.780268
26	1	0	1.110535	-0.133335	-1.731743
27	1	0	8.024305	0.609774	1.706568
28	1	0	-6.306963	-0.568041	1.696476
29	1	0	-5.927904	-1.202045	0.085522
30	1	0	8.438021	1.339497	-1.246784

31	1	0	-7.406995	3.126429	-0.052804
32	1	0	-6.978688	2.509004	-1.649990
33	1	0	-8.674815	2.417019	-1.094257
34	1	0	10.285757	1.389557	1.256740
35	1	0	10.828296	0.953577	-0.380816
36	1	0	10.325989	2.604378	-0.042851
37	1	0	-3.628312	0.709952	-0.661771
38	1	0	-3.481785	-1.044234	-0.787363
39	1	0	0.238615	-2.128761	1.659930
40	1	0	1.460291	-2.759544	-0.843751

1f Distribution in Gibb's free eneygy: 5.67%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.146202	-1.474427	0.357558
2	6	0	1.787164	-0.851560	-0.312158
3	6	0	0.981932	0.173841	-0.016353
4	6	0	-0.468281	0.015033	0.340857
5	6	0	-1.386486	0.904675	-0.537592
6	6	0	-2.808055	0.579645	-0.330102
7	6	0	-3.999855	0.323895	-0.162968
8	6	0	-5.320768	0.037583	0.021696
9	6	0	-6.502868	-0.211224	0.171883
10	6	0	-7.866402	-0.522351	0.398735
11	6	0	5.624974	-1.417813	0.009335
12	8	0	6.048296	-0.032819	0.077868
13	6	0	-8.855343	-0.272217	-0.483090
14	6	0	7.362886	0.205380	-0.100736
15	6	0	7.671180	1.677833	0.021917
16	8	0	8.178095	-0.669303	-0.323619
17	6	0	-10.297232	-0.594546	-0.250165
18	6	0	3.246348	-0.736959	-0.653736
19	8	0	-0.729939	0.467109	1.681955
20	8	0	-1.118985	2.280071	-0.274888
21	1	0	3.994988	-1.059430	1.361674
22	1	0	3.860520	-2.533334	0.406332
23	1	0	1.377086	-1.863911	-0.300975
24	1	0	1.361643	1.195186	-0.016381
25	1	0	-0.772500	-1.034407	0.225549
26	1	0	-1.131241	0.733372	-1.589408
27	1	0	-8.107319	-0.991472	1.353594
28	1	0	5.817406	-1.792112	-1.002146
29	1	0	6.226426	-2.004995	0.709223
30	1	0	-8.603636	0.196556	-1.433522
31	1	0	7.042448	2.256106	-0.662080
32	1	0	7.451685	2.020239	1.038829
33	1	0	8.723861	1.852742	-0.202542
34	1	0	-10.454844	-1.076682	0.719557

35	1	0	-10.910420	0.315875	-0.289651
36	1	0	-10.679456	-1.259149	-1.036414
37	1	0	3.418961	-1.169648	-1.650844
38	1	0	3.538739	0.317499	-0.707826
39	1	0	0.011743	0.178206	2.237484
40	1	0	-1.078205	2.338159	0.698540

1g Distribution in Gibb's free eneygy: 5.52%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.517934	-1.108666	1.344999
2	6	0	2.009271	-1.355166	0.964595
3	6	0	1.181953	-1.385669	-0.085435
4	6	0	-0.136653	-0.667286	-0.124620
5	6	0	-1.304117	-1.612951	-0.511173
6	6	0	-2.609622	-0.955638	-0.330204
7	6	0	-3.696278	-0.420954	-0.193159
8	6	0	-4.910940	0.178951	-0.037468
9	6	0	-6.006383	0.702901	0.103300
10	6	0	-7.250714	1.362836	0.258080
11	6	0	4.770839	-0.123022	0.214461
12	8	0	5.904315	0.693792	0.596120
13	6	0	-8.417292	0.730294	0.496768
14	6	0	6.281688	1.645720	-0.280315
15	6	0	7.469211	2.421083	0.236408
16	8	0	5.723851	1.836619	-1.344198
17	6	0	-9.734641	1.419600	0.660047
18	6	0	3.337812	-2.056872	1.047890
19	8	0	-0.154121	0.340083	-1.152050
20	8	0	-1.128766	-2.072289	-1.849178
21	1	0	4.324993	-0.553044	2.271573
22	1	0	5.423968	-1.703159	1.510823
23	1	0	1.718069	-0.783711	1.848987
24	1	0	1.444324	-1.945510	-0.982601
25	1	0	-0.350927	-0.217876	0.854770
26	1	0	-1.258774	-2.499894	0.130748
27	1	0	-7.239532	2.450350	0.174178
28	1	0	3.909051	0.527100	0.037101
29	1	0	5.004191	-0.636492	-0.724505
30	1	0	-8.417260	-0.355861	0.578629
31	1	0	7.226241	2.885602	1.197480
32	1	0	8.314757	1.745754	0.402807
33	1	0	7.748482	3.189723	-0.484879
34	1	0	-9.640618	2.505482	0.561640
35	1	0	-10.455420	1.063201	-0.088054
36	1	0	-10.171963	1.195367	1.642224
37	1	0	3.296613	-2.799661	1.856850
38	1	0	3.527106	-2.612348	0.120518

39	1	0	0.711555	0.779047	-1.146866
40	1	0	-0.889492	-1.270667	-2.352015

1h Distribution in Gibb's free eneygy: 4.72%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.315322	-0.100255	-0.078608
2	6	0	-1.849513	-0.388074	-0.559282
3	6	0	-0.886204	-1.185348	-0.086650
4	6	0	0.488527	-0.700300	0.274776
5	6	0	1.600759	-1.540610	-0.405703
6	6	0	2.925725	-0.922870	-0.226918
7	6	0	4.028441	-0.424598	-0.081216
8	6	0	5.260707	0.136268	0.081538
9	6	0	6.369486	0.633769	0.213575
10	6	0	7.637476	1.231997	0.418854
11	6	0	-5.724087	-0.513159	-0.492233
12	8	0	-6.724526	0.104344	0.355234
13	6	0	8.653752	1.171978	-0.465217
14	6	0	-7.157044	1.334730	0.005318
15	6	0	-8.188116	1.840398	0.984600
16	8	0	-6.761246	1.939569	-0.972700
17	6	0	9.994316	1.801561	-0.255969
18	6	0	-3.242864	-0.827278	-0.913712
19	8	0	0.747285	-0.859956	1.681699
20	8	0	1.570919	-2.874404	0.096468
21	1	0	-4.171014	-0.324203	0.985191
22	1	0	-4.210148	0.984210	-0.201260
23	1	0	-1.634757	0.673267	-0.701041
24	1	0	-1.070652	-2.248068	0.067714
25	1	0	0.606567	0.352077	-0.017654
26	1	0	1.379292	-1.606002	-1.476924
27	1	0	7.776669	1.769574	1.357744
28	1	0	-5.877672	-1.586853	-0.358600
29	1	0	-5.926238	-0.246840	-1.532712
30	1	0	8.504261	0.632529	-1.399605
31	1	0	-9.032905	1.146036	1.034198
32	1	0	-7.753411	1.900186	1.987699
33	1	0	-8.536902	2.826133	0.675288
34	1	0	10.054441	2.320318	0.705762
35	1	0	10.789627	1.045103	-0.294078
36	1	0	10.214566	2.522345	-1.054823
37	1	0	-3.424649	-0.618809	-1.978773
38	1	0	-3.337521	-1.912476	-0.781786
39	1	0	-0.066444	-0.626366	2.156548
40	1	0	1.481203	-2.767855	1.062594

1i Distribution in Gibb's free eneygy: 3.56%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.914480	-0.498504	-0.071594
2	6	0	1.626602	-1.678131	-0.039112
3	6	0	0.953306	-0.597718	0.369535
4	6	0	-0.528357	-0.601833	0.617257
5	6	0	-1.247592	0.548660	-0.135056
6	6	0	-2.711497	0.397795	-0.075732
7	6	0	-3.924340	0.285598	-0.031272
8	6	0	-5.280930	0.155829	0.017691
9	6	0	-6.498001	0.045112	0.046797
10	6	0	-7.903948	-0.108650	0.133644
11	6	0	5.389903	-0.712807	-0.371565
12	8	0	6.071649	0.540673	-0.124481
13	6	0	-8.766185	0.262713	-0.834142
14	6	0	7.401650	0.554407	-0.343655
15	6	0	7.987254	1.914156	-0.049789
16	8	0	8.027467	-0.415030	-0.728243
17	6	0	-10.251022	0.102672	-0.750853
18	6	0	3.105408	-1.779075	-0.304176
19	8	0	-0.830206	-0.349802	2.002023
20	8	0	-0.826520	1.804530	0.392023
21	1	0	3.533880	0.309000	-0.708751
22	1	0	3.805229	-0.166860	0.968142
23	1	0	1.070536	-2.601795	-0.209899
24	1	0	1.456540	0.348947	0.554529
25	1	0	-0.961571	-1.560734	0.301336
26	1	0	-0.929703	0.528403	-1.183566
27	1	0	-8.289381	-0.558321	1.049660
28	1	0	5.555095	-1.005474	-1.413670
29	1	0	5.827835	-1.485372	0.269076
30	1	0	-8.370420	0.710876	-1.744617
31	1	0	7.514301	2.671851	-0.682879
32	1	0	7.793561	2.189588	0.991945
33	1	0	9.062012	1.899080	-0.233373
34	1	0	-10.558834	-0.354714	0.194522
35	1	0	-10.752994	1.074760	-0.847199
36	1	0	-10.621961	-0.520035	-1.575996
37	1	0	3.510724	-2.591643	0.318102
38	1	0	3.244438	-2.121739	-1.341084
39	1	0	-0.177528	-0.831340	2.535205
40	1	0	-0.851255	1.681206	1.360074

1j Distribution in Gibb's free eneygy: 3.09%
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	4.937199	1.928806	-0.751804
2	6	0	2.562409	1.788885	0.128710
3	6	0	1.837254	0.827342	0.707477
4	6	0	0.465617	0.417714	0.253889
5	6	0	-0.559292	0.388501	1.420749
6	6	0	-1.936929	0.233545	0.922542
7	6	0	-3.080265	0.101221	0.521146
8	6	0	-4.359073	-0.044228	0.070279
9	6	0	-5.510487	-0.164332	-0.322431
10	6	0	-6.825928	-0.339478	-0.819387
11	6	0	4.792895	0.606451	-1.496606
12	8	0	5.078402	-0.502897	-0.600154
13	6	0	-7.916176	0.261104	-0.301120
14	6	0	4.198755	-1.513187	-0.518502
15	6	0	4.634729	-2.537240	0.498248
16	8	0	3.167743	-1.582112	-1.171134
17	6	0	-9.307419	0.082015	-0.820528
18	6	0	3.996677	2.091586	0.464150
19	8	0	0.481119	-0.931427	-0.239296
20	8	0	-0.210203	-0.653604	2.327613
21	1	0	4.737978	2.721624	-1.485163
22	1	0	5.974750	2.059194	-0.422254
23	1	0	2.122654	2.366305	-0.687654
24	1	0	2.257835	0.236046	1.521013
25	1	0	0.103501	1.106035	-0.522325
26	1	0	-0.485643	1.330627	1.976067
27	1	0	-6.938976	-1.005948	-1.675501
28	1	0	5.519198	0.538512	-2.311675
29	1	0	3.789765	0.473590	-1.901759
30	1	0	-7.792235	0.924780	0.553647
31	1	0	5.708399	-2.727078	0.424242
32	1	0	4.432818	-2.151469	1.504286
33	1	0	4.073344	-3.461067	0.354041
34	1	0	-9.337652	-0.599705	-1.676110
35	1	0	-9.967389	-0.313379	-0.036745
36	1	0	-9.735214	1.045727	-1.127920
37	1	0	4.095201	3.123867	0.827579
38	1	0	4.328745	1.435154	1.276555
39	1	0	1.367938	-1.116774	-0.607787
40	1	0	0.028708	-1.397954	1.740362

1k Distribution in Gibb's free eneygy: 2.78%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.558079	-1.107198	0.044550
2	6	0	-2.074947	-1.231385	-0.572055

3	6	0	-1.042448	-1.804358	0.055239
4	6	0	0.303643	-1.154775	0.204907
5	6	0	1.453892	-2.080997	-0.269668
6	6	0	2.736021	-1.358501	-0.326264
7	6	0	3.803997	-0.772773	-0.369054
8	6	0	4.997903	-0.115731	-0.418474
9	6	0	6.064303	0.481098	-0.448956
10	6	0	7.314340	1.143205	-0.531807
11	6	0	-4.816913	0.296792	-0.482198
12	8	0	-5.924671	0.841048	0.276035
13	6	0	7.738191	2.070441	0.350562
14	6	0	-6.304747	2.097308	-0.031849
15	6	0	-7.463285	2.540939	0.827891
16	8	0	-5.769654	2.766983	-0.894668
17	6	0	9.056669	2.772312	0.271731
18	6	0	-3.439433	-1.850719	-0.718778
19	8	0	0.611440	-0.902632	1.587896
20	8	0	1.532458	-3.224317	0.578190
21	1	0	-5.485455	-1.686725	-0.037472
22	1	0	-4.303557	-1.053298	1.109980
23	1	0	-1.933194	-0.243978	-1.014771
24	1	0	-1.145312	-2.791869	0.504368
25	1	0	0.337813	-0.219633	-0.370674
26	1	0	1.208922	-2.452290	-1.271142
27	1	0	7.957090	0.868534	-1.369231
28	1	0	-5.085547	0.287186	-1.544097
29	1	0	-3.952769	0.956133	-0.358477
30	1	0	7.088392	2.337092	1.183093
31	1	0	-8.316887	1.870953	0.682409
32	1	0	-7.186206	2.494427	1.885977
33	1	0	-7.746509	3.560610	0.565093
34	1	0	9.641846	2.443264	-0.592530
35	1	0	8.915198	3.859283	0.203280
36	1	0	9.647173	2.593951	1.180420
37	1	0	-3.707047	-1.890419	-1.784962
38	1	0	-3.408919	-2.886813	-0.362994
39	1	0	-0.200782	-0.586915	2.015449
40	1	0	1.464523	-2.862092	1.481989

1l Distribution in Gibb's free eneygy: 2.75%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.271494	-0.272320	-0.757668
2	6	0	1.806338	0.266853	-0.920845
3	6	0	0.932643	0.901695	-0.133048
4	6	0	-0.447384	0.386258	0.159447
5	6	0	-1.538222	1.455676	-0.110535
6	6	0	-2.889753	0.875024	-0.036990

7	6	0	-4.014021	0.408946	0.028635
8	6	0	-5.270737	-0.115422	0.101073
9	6	0	-6.402229	-0.574788	0.156334
10	6	0	-7.694090	-1.147690	0.259797
11	6	0	5.678072	0.190913	-1.122723
12	8	0	6.669476	-0.802342	-0.760941
13	6	0	-8.772044	-0.710177	-0.421755
14	6	0	7.159650	-0.757517	0.496540
15	6	0	8.173109	-1.853861	0.717318
16	8	0	6.822075	0.064414	1.326821
17	6	0	-10.138521	-1.309459	-0.317416
18	6	0	3.202388	0.736554	-1.221911
19	8	0	-0.605493	0.076768	1.556275
20	8	0	-1.383122	2.541321	0.800181
21	1	0	4.205526	-0.405387	0.328030
22	1	0	4.087077	-1.250944	-1.218482
23	1	0	1.509249	-0.674431	-1.388157
24	1	0	1.200723	1.841252	0.349169
25	1	0	-0.657068	-0.500804	-0.453887
26	1	0	-1.380208	1.866109	-1.114231
27	1	0	-7.798756	-1.994294	0.939612
28	1	0	5.926315	1.135413	-0.632311
29	1	0	5.788222	0.306511	-2.203933
30	1	0	-8.656547	0.135921	-1.097921
31	1	0	7.706367	-2.831846	0.561090
32	1	0	8.990800	-1.761636	-0.004640
33	1	0	8.566872	-1.791786	1.732243
34	1	0	-10.161559	-2.150798	0.382088
35	1	0	-10.867865	-0.559143	0.016180
36	1	0	-10.484525	-1.662352	-1.298213
37	1	0	3.305180	0.884937	-2.307471
38	1	0	3.377774	1.711398	-0.749999
39	1	0	0.218885	-0.336756	1.858936
40	1	0	-1.240097	2.113236	1.665697

1m Distribution in Gibb's free eneygy: 2.70%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.920915	-1.168224	-1.628881
2	6	0	-2.609719	-1.631134	-0.691140
3	6	0	-1.872321	-1.096120	0.286250
4	6	0	-0.450927	-0.642245	0.117324
5	6	0	0.487684	-1.221584	1.210989
6	6	0	1.904196	-0.976026	0.889680
7	6	0	3.079230	-0.772995	0.636841
8	6	0	4.393901	-0.548735	0.352057
9	6	0	5.568516	-0.335371	0.089021
10	6	0	6.944401	-0.136937	-0.185955

11	6	0	-4.649424	0.330549	-1.695604
12	8	0	-4.932316	0.945189	-0.407998
13	6	0	7.429733	0.888910	-0.914000
14	6	0	-4.002913	1.734900	0.152076
15	6	0	-4.451064	2.233261	1.502386
16	8	0	-2.925210	1.999016	-0.360196
17	6	0	8.880252	1.104965	-1.208493
18	6	0	-4.078820	-1.932709	-0.581955
19	8	0	-0.354437	0.781516	0.283188
20	8	0	0.134164	-0.668233	2.475627
21	1	0	-4.717008	-1.565559	-2.632173
22	1	0	-5.984765	-1.345214	-1.431381
23	1	0	-2.147897	-1.814750	-1.663918
24	1	0	-2.313198	-0.900432	1.263834
25	1	0	-0.074321	-0.939845	-0.871150
26	1	0	0.320531	-2.302665	1.279855
27	1	0	7.635322	-0.872864	0.227536
28	1	0	-5.312671	0.813157	-2.419252
29	1	0	-3.614813	0.546947	-1.961870
30	1	0	6.731239	1.618218	-1.322238
31	1	0	-5.498869	2.542801	1.474262
32	1	0	-4.363589	1.419990	2.232137
33	1	0	-3.817259	3.062888	1.817506
34	1	0	9.506516	0.326883	-0.761211
35	1	0	9.059856	1.116478	-2.291925
36	1	0	9.213154	2.080536	-0.829440
37	1	0	-4.260581	-3.006734	-0.726444
38	1	0	-4.429770	-1.683823	0.426047
39	1	0	-1.200787	1.184264	0.003704
40	1	0	-0.019556	0.276807	2.277570

1n Distribution in Gibb's free eneygy: 2.51%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.358591	0.032683	1.317185
2	6	0	-1.881741	0.620184	1.171133
3	6	0	-1.067680	1.172046	0.265081
4	6	0	0.307781	0.651854	-0.041307
5	6	0	1.385783	1.763375	0.055772
6	6	0	2.745523	1.202702	-0.027627
7	6	0	3.875315	0.752001	-0.102656
8	6	0	5.139201	0.246395	-0.186279
9	6	0	6.269602	-0.214473	-0.248556
10	6	0	7.587362	-0.720927	-0.371208
11	6	0	-4.538299	-0.358824	-0.146124
12	8	0	-5.509552	-1.425336	-0.288687
13	6	0	8.165143	-1.553636	0.517766
14	6	0	-6.808087	-1.070401	-0.390327

15	6	0	-7.688898	-2.288256	-0.529072
16	8	0	-7.199642	0.080960	-0.374659
17	6	0	9.555404	-2.091508	0.392095
18	6	0	-3.265362	1.104785	1.510212
19	8	0	0.404243	0.195761	-1.402640
20	8	0	1.161411	2.741761	-0.955787
21	1	0	-4.109509	-0.863152	1.900132
22	1	0	-5.309474	0.416961	1.701972
23	1	0	-1.535701	-0.254303	1.727106
24	1	0	-1.383681	2.043905	-0.306923
25	1	0	0.568109	-0.158952	0.652842
26	1	0	1.268351	2.276011	1.017231
27	1	0	8.149806	-0.402540	-1.249919
28	1	0	-3.617346	-0.769008	-0.565702
29	1	0	-4.857792	0.496021	-0.747705
30	1	0	7.594591	-1.865459	1.391654
31	1	0	-7.390909	-2.870437	-1.406934
32	1	0	-7.574550	-2.934551	0.347257
33	1	0	-8.730330	-1.979946	-0.625730
34	1	0	10.052580	-1.726562	-0.511992
35	1	0	10.162875	-1.807658	1.261943
36	1	0	9.547215	-3.189451	0.365526
37	1	0	-3.284237	1.413473	2.564868
38	1	0	-3.506197	1.996609	0.917656
39	1	0	-0.417822	-0.275698	-1.612460
40	1	0	0.987593	2.221555	-1.763181

1o Distribution in Gibb's free eneygy: 2.39%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.123371	-0.341159	-0.204420
2	6	0	1.704707	0.321236	-0.539293
3	6	0	0.779609	0.921553	0.214275
4	6	0	-0.649225	0.450860	0.323082
5	6	0	-1.645157	1.537607	-0.164281
6	6	0	-3.018372	1.031666	-0.251572
7	6	0	-4.167045	0.633809	-0.341613
8	6	0	-5.450262	0.185073	-0.440843
9	6	0	-6.599570	-0.224846	-0.514686
10	6	0	-7.936515	-0.673306	-0.650212
11	6	0	5.570411	0.090036	-0.384940
12	8	0	6.410817	-0.999826	0.066734
13	6	0	-8.569142	-1.442701	0.258714
14	6	0	7.742222	-0.805633	-0.012746
15	6	0	8.498668	-2.012051	0.488044
16	8	0	8.246502	0.217003	-0.436245
17	6	0	-9.980067	-1.920604	0.126776
18	6	0	3.140355	0.754284	-0.661042

19	8	0	-0.984046	0.085834	1.662628
20	8	0	-1.531264	2.598833	0.796182
21	1	0	3.944920	-0.581315	0.850646
22	1	0	3.948759	-1.260720	-0.777306
23	1	0	1.424444	-0.562204	-1.117363
24	1	0	1.037420	1.802503	0.802310
25	1	0	-0.791273	-0.444324	-0.290223
26	1	0	-1.326789	1.885799	-1.157805
27	1	0	-8.466042	-0.364196	-1.552229
28	1	0	5.805070	0.984021	0.202182
29	1	0	5.802311	0.304468	-1.433501
30	1	0	-8.029651	-1.744717	1.155427
31	1	0	8.230986	-2.217669	1.529514
32	1	0	8.229768	-2.895279	-0.100312
33	1	0	9.571293	-1.831045	0.412042
34	1	0	-10.443215	-1.571759	-0.801306
35	1	0	-10.021841	-3.017872	0.146381
36	1	0	-10.588575	-1.572881	0.972336
37	1	0	3.355002	1.004164	-1.711135
38	1	0	3.303951	1.669773	-0.078452
39	1	0	-1.141068	0.927440	2.127855
40	1	0	-2.245482	3.236116	0.635096

1p Distribution in Gibb's free eneygy: 1.83%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.464880	-0.957539	0.213904
2	6	0	2.184132	-1.528589	-0.803272
3	6	0	1.140930	-2.196899	-0.300330
4	6	0	-0.287513	-1.772618	-0.489013
5	6	0	-1.053417	-1.694359	0.857871
6	6	0	-2.375278	-1.066387	0.689067
7	6	0	-3.473015	-0.552628	0.561772
8	6	0	-4.700690	0.023768	0.418323
9	6	0	-5.794027	0.553533	0.284009
10	6	0	-7.085781	1.120450	0.149661
11	6	0	4.621531	0.414114	-0.426105
12	8	0	5.485725	1.193801	0.436042
13	6	0	-7.324828	2.353823	-0.339379
14	6	0	5.732246	2.462224	0.051583
15	6	0	6.642187	3.160572	1.032626
16	8	0	5.271123	2.957878	-0.958870
17	6	0	-8.686339	2.956859	-0.482779
18	6	0	3.624060	-1.935783	-0.636575
19	8	0	-1.026662	-2.744838	-1.250158
20	8	0	-1.162035	-2.996649	1.425960
21	1	0	4.009346	-0.845536	1.205196
22	1	0	5.462139	-1.388676	0.362900

23	1	0	1.993680	-0.619457	-1.376265
24	1	0	1.292193	-3.112102	0.271580
25	1	0	-0.328445	-0.791106	-0.980849
26	1	0	-0.460228	-1.096526	1.559167
27	1	0	-7.923997	0.499944	0.469340
28	1	0	3.667430	0.939026	-0.529627
29	1	0	5.079768	0.346481	-1.418737
30	1	0	-6.480643	2.965131	-0.655735
31	1	0	6.187301	3.167503	2.028372
32	1	0	7.593309	2.623910	1.110051
33	1	0	6.822516	4.184013	0.702348
34	1	0	-9.471261	2.274768	-0.141618
35	1	0	-8.761724	3.889503	0.092301
36	1	0	-8.886518	3.221874	-1.529651
37	1	0	3.670193	-2.926068	-0.169386
38	1	0	4.091520	-2.030980	-1.627742
39	1	0	-0.448086	-3.060337	-1.962818
40	1	0	-1.428169	-3.566148	0.679193

1q Distribution in Gibb's free eneygy: 1.26%
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.004905	-0.274623	0.226608
2	6	0	1.694243	-1.301545	0.234476
3	6	0	0.675283	-1.318689	-0.628407
4	6	0	-0.776276	-1.127849	-0.265078
5	6	0	-1.288831	0.286263	-0.664049
6	6	0	-2.758145	0.360037	-0.587537
7	6	0	-3.971636	0.447046	-0.514924
8	6	0	-5.330227	0.537394	-0.439473
9	6	0	-6.548086	0.607657	-0.360505
10	6	0	-7.959048	0.728877	-0.311437
11	6	0	5.470402	-0.506039	-0.106864
12	8	0	6.198186	0.688169	0.269831
13	6	0	-8.750171	0.019340	0.518416
14	6	0	7.526701	0.680018	0.042323
15	6	0	8.160685	1.979196	0.476616
16	8	0	8.116777	-0.262638	-0.450276
17	6	0	-10.239836	0.141184	0.576279
18	6	0	3.139040	-1.496765	-0.135872
19	8	0	-1.031543	-1.211864	1.135811
20	8	0	-0.672260	1.279514	0.146603
21	1	0	3.643853	0.607808	-0.315203
22	1	0	3.910345	-0.055150	1.297626
23	1	0	1.492073	-1.127531	1.291822
24	1	0	0.863570	-1.481400	-1.690272
25	1	0	-1.381892	-1.867119	-0.810928
26	1	0	-0.977407	0.489441	-1.695146

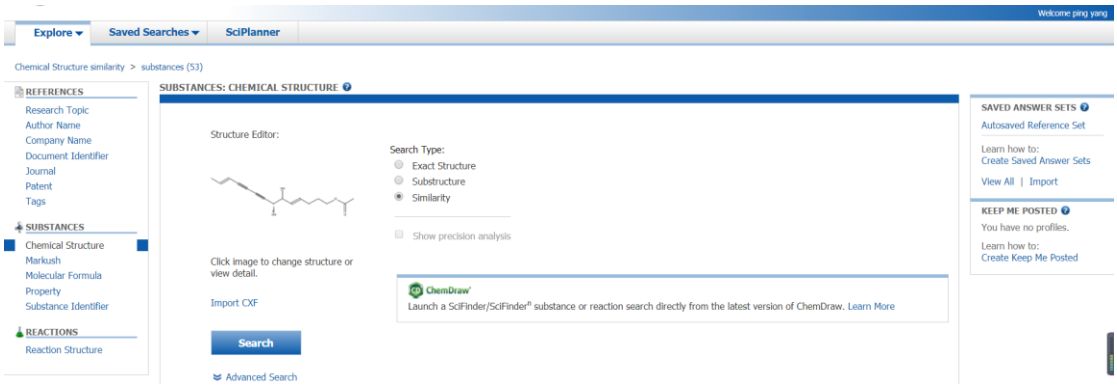
27	1	0	-8.410844	1.447196	-0.996817
28	1	0	5.620325	-0.689076	-1.175960
29	1	0	5.881979	-1.359367	0.442402
30	1	0	-8.288583	-0.695038	1.198881
31	1	0	7.713163	2.816320	-0.068876
32	1	0	7.979351	2.148141	1.542967
33	1	0	9.233770	1.946633	0.285692
34	1	0	-10.616027	0.878190	-0.139941
35	1	0	-10.717627	-0.824934	0.365229
36	1	0	-10.567333	0.434814	1.582637
37	1	0	3.533968	-2.376867	0.393669
38	1	0	3.224079	-1.708566	-1.209222
39	1	0	-0.611190	-2.021182	1.468754
40	1	0	-0.708864	0.923224	1.053492

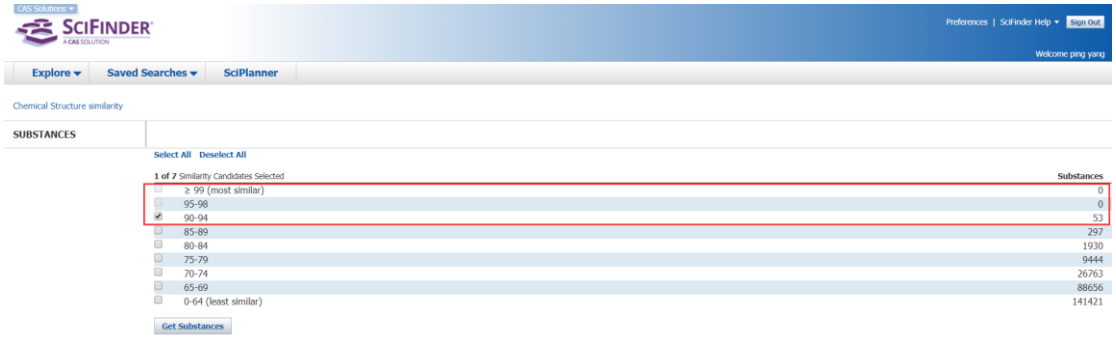
1r Distribution in Gibb's free eneygy: 1.14%
Standard orientation:

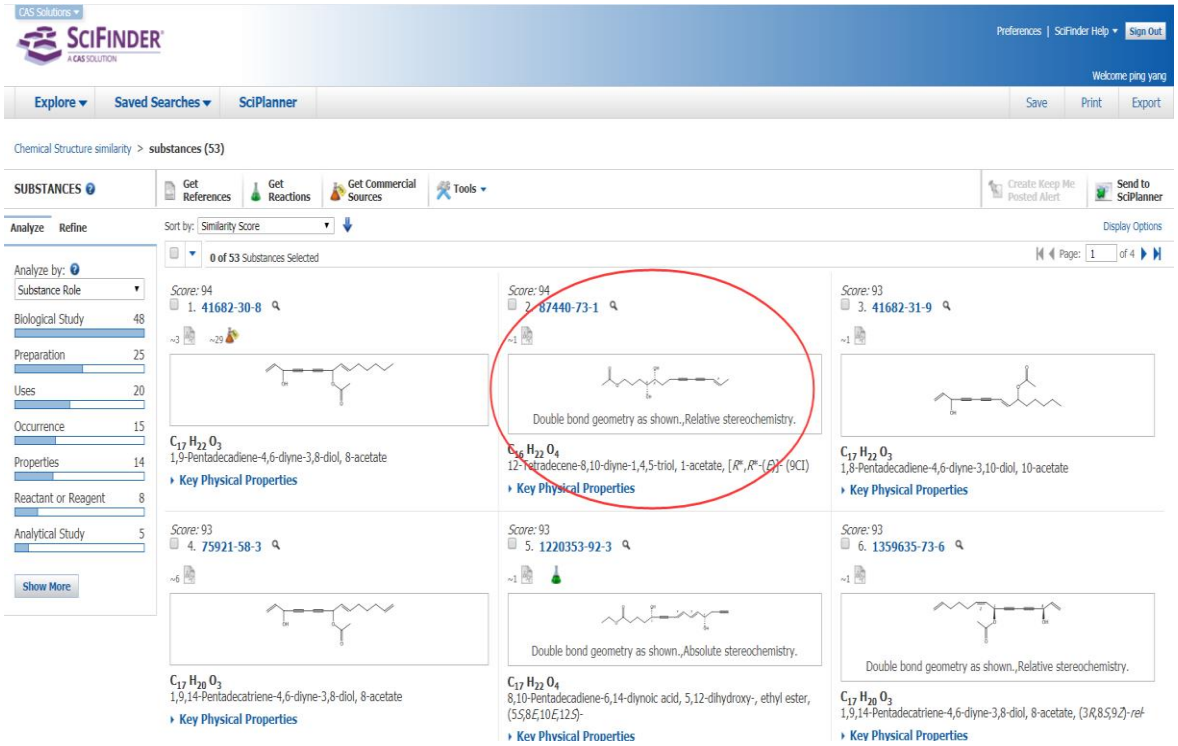
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.436624	-1.838359	0.364527
2	6	0	-2.019998	-1.183109	0.825247
3	6	0	-1.281984	-0.084058	0.635594
4	6	0	0.122958	-0.108278	0.104767
5	6	0	1.106820	0.661390	1.024954
6	6	0	2.505596	0.439914	0.620334
7	6	0	3.667431	0.270164	0.293461
8	6	0	4.966835	0.077151	-0.072384
9	6	0	6.136336	-0.092243	-0.385312
10	6	0	7.474613	-0.300306	-0.801954
11	6	0	-4.635651	-1.045551	-0.923087
12	8	0	-5.129518	0.293581	-0.657361
13	6	0	8.545230	-0.184376	0.009438
14	6	0	-6.466244	0.450758	-0.550602
15	6	0	-6.817380	1.889948	-0.261149
16	8	0	-7.267805	-0.455435	-0.674941
17	6	0	9.960861	-0.400814	-0.422257
18	6	0	-3.429730	-1.206151	1.348455
19	8	0	0.219730	0.580228	-1.155341
20	8	0	0.775006	2.047661	1.030907
21	1	0	-4.099154	-2.845148	0.082943
22	1	0	-5.405694	-1.959114	0.861394
23	1	0	-1.585314	-2.156350	0.585158
24	1	0	-1.686665	0.901688	0.863141
25	1	0	0.469262	-1.145668	0.000444
26	1	0	0.971815	0.304408	2.052152
27	1	0	7.623306	-0.569287	-1.848560
28	1	0	-5.334964	-1.553303	-1.590474
29	1	0	-3.688373	-0.884196	-1.442401
30	1	0	8.385205	0.084860	1.052672

31	1	0	-6.386098	2.192664	0.698841
32	1	0	-6.396433	2.544459	-1.030743
33	1	0	-7.901273	2.004597	-0.228192
34	1	0	10.027262	-0.665827	-1.481973
35	1	0	10.562087	0.502130	-0.250727
36	1	0	10.429214	-1.200684	0.166870
37	1	0	-3.454758	-1.792582	2.277742
38	1	0	-3.752172	-0.190584	1.605283
39	1	0	-0.571878	0.359008	-1.671503
40	1	0	0.620912	2.264173	0.091635

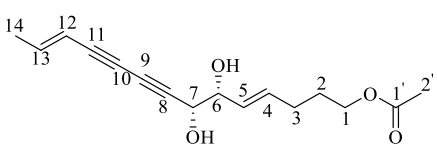
Scifinder search report



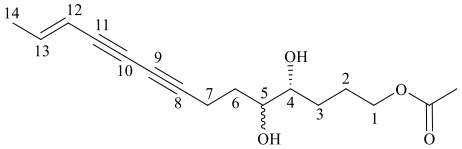




NMR comparison for the most simialr compound (Similarity :94%)



Fissistigmol A



12-Tetradecene-8, 10-diyne-1,4,5-triol, 1-acetate, [*R**, *R**-(*E*)] - (9CI)

Table 1. ^{1}H and ^{13}C NMR data for compounds in $CDCl_3$, δ (ppm)

Position	Fissistigmol A[a]		12-Tetradecene-8, 10-diyne-1,4,5-triol, 1-acetate, [*R**, *R**-(*E*)] - (9CI)[b]
	δC	**δH**	**δH**
1	63.8	4.08	4.11
2	28.0	1.74	1.71
3	28.8	2.16	1.55
4	134.5	5.85	3.59
5	127.9	5.57	3.46
6	75.5	4.14	1.71
7	66.9	4.30	2.50
8	79.0	/	/
9	71.6	/	/
10	71.5	/	/
11	78.2	/	/
12	109.5	5.53	5.50
13	144.8	6.35	6.29
14	19.1	1.82	1.79
1´	171.5	/	/
2´	21.2	2.05	2.04(H-A_C-Me)

a: Data were measured on δ_H 600 MHz and δ_C 150 MHz
b: Data were measured on δ_H 400 MHz
Reference: El-Masry Sawsan et al. An acetylenic triol from Hyoseris lucida[J]. 1983, 22(2):592-593.