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Supporting Information

Crotonols A and B, Two Rare Tigliane Diterpenoid Derivatives

Against K562 cells from *Croton tiglium*

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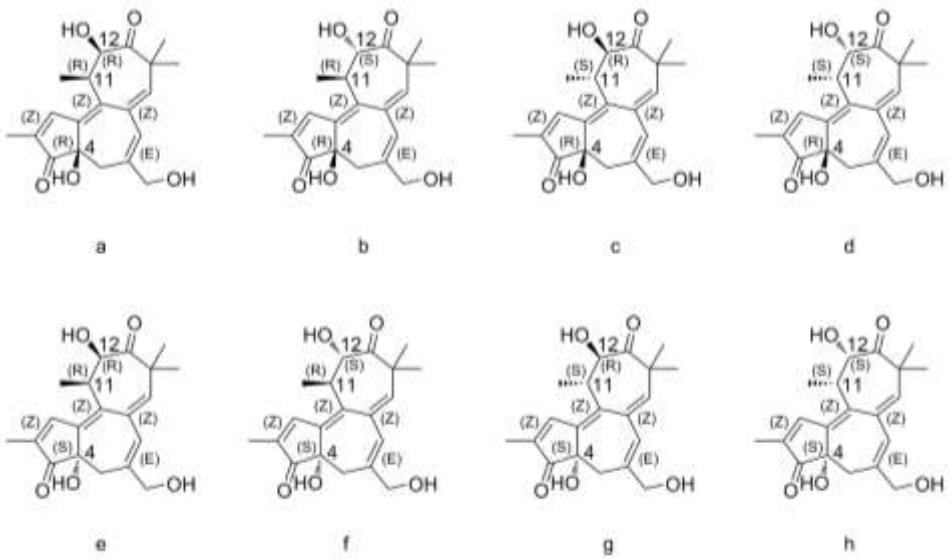


Figure S1. Chemical structures of all possible configurations of compound **2**.

Energies and Coordinates

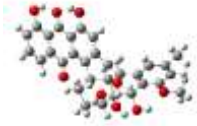
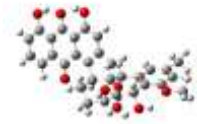
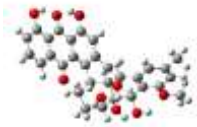
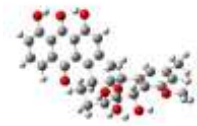
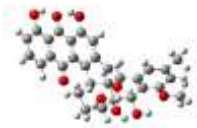
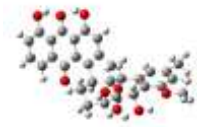
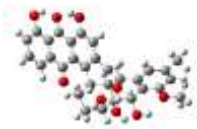
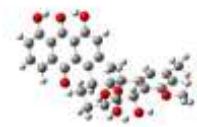
Energies at MMFF94 force field. Systematic conformational search was performed by Confab program at MMFF94 force field. Conformers for each configuration were obtained with filtration by RMSD threshold of 0.5 Å.

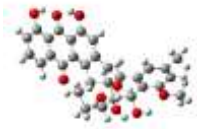
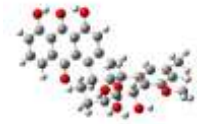
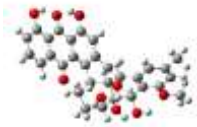
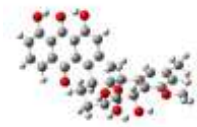
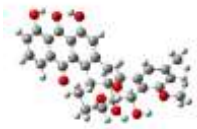
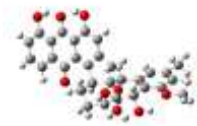
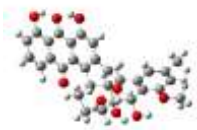
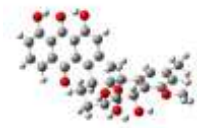
Table S1. Energies of dominative conformers at MMFF94 force field.

Compound	Conformer	Energy (kcal/mol)
a	1	121.0342
a	2	124.4055
b	1	130.0022
b	2	133.0971
c	**1**	**119.5838**
c	**2**	**122.8469**
d	1	125.5501
d	2	128.6177
e	1	129.0301
e	2	131.8892
f	1	137.5435
f	2	141.1494
g	1	128.3384
g	2	132.1104
h	1	138.9677
h	2	142.5042

Energies at B3LYP theory level. Structures for ECD calculations were optimized at B3LYP/6-311G(d,p) in methanol (**Table S2**).

Table S2. Energies of dominative conformers at B3LYP/6-311G(d,p) in methanol.

Configuration	Conformer	Structure	E (Hartree)	E (kcal/mol)	Population (%)
a	1		-1152.926111	-723472.052	5.72
a	2		-1152.928758	-723473.7125	94.28
b	1		-1152.937779	-723479.3738	60.86
b	2		-1152.937363	-723479.1123	39.14
c	**1**		**-1152.954372**	**-723489.7858**	**33.83**
c	**2**		**-1152.955005**	**-723490.1832**	**66.17**
d	1		-1152.953997	-723489.5503	43.37
d	2		-1152.954249	-723489.7083	56.63

e	1		-1152.953997	-723489.5503	43.37
e	2		-1152.954249	-723489.7083	56.63
f	1		-1152.954372	-723489.7858	33.83
f	2		-1152.955005	-723490.1832	66.17
g	1		-1152.937779	-723479.3738	60.86
g	2		-1152.937363	-723479.1123	39.14
h	1		-1152.926111	-723472.052	5.72
h	2		-1152.928758	-723473.7125	94.28

Coordinates at B3LYP theory level

Table S3. Standard orientations of configurations at B3LYP/6-311G(d,p) level in methanol.

Conformer a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.335800	-2.258582	0.415766
2	1	0	0.668274	-3.019320	0.798823
3	6	0	2.523529	-2.554890	-0.168118
4	6	0	3.147068	-1.297690	-0.604297
5	6	0	2.288243	-0.133746	-0.052662
6	6	0	1.006514	-0.835717	0.375027
7	6	0	2.150817	1.066597	-0.978713
8	1	0	1.514075	0.807931	-1.831656
9	1	0	3.141324	1.301769	-1.381901
10	6	0	1.582702	2.242302	-0.217986
11	6	0	0.371808	2.209934	0.339186
12	1	0	0.009196	3.105933	0.833839
13	6	0	-0.609078	1.092235	0.230509
14	6	0	-0.231733	-0.307011	0.573678
15	6	0	-1.835999	1.472839	-0.197005
16	1	0	-1.956628	2.545084	-0.340925
17	6	0	-2.772558	-0.766351	-0.908017
18	6	0	-2.362138	-1.692521	0.255427
19	1	0	-1.916944	-2.546959	-0.256906
20	6	0	-1.306379	-1.158271	1.256286
21	1	0	-0.823675	-2.058989	1.633133
22	6	0	3.153967	-3.889645	-0.385034
23	1	0	3.358687	-4.052132	-1.447729
24	1	0	4.116962	-3.950610	0.132303
25	1	0	2.515919	-4.697941	-0.025597
26	8	0	4.195458	-1.150164	-1.205859
27	8	0	2.964242	0.249877	1.171576
28	1	0	3.881889	0.444485	0.938497
29	6	0	2.489131	3.445454	-0.101142
30	1	0	3.466409	3.107934	0.274089
31	1	0	2.666475	3.864332	-1.098051
32	8	0	1.982541	4.510955	0.688620
33	1	0	1.933253	4.201513	1.600254
34	6	0	-3.066031	0.723840	-0.686298
35	6	0	-3.464536	1.356134	-2.039674
36	1	0	-2.661791	1.260712	-2.772080
37	1	0	-4.352500	0.867105	-2.443492
38	1	0	-3.685112	2.416761	-1.899862

39	6	0	-4.261080	0.911545	0.288780
40	1	0	-4.483585	1.977121	0.382009
41	1	0	-5.152100	0.412982	-0.100681
42	1	0	-4.061342	0.539103	1.292424
43	8	0	-2.879030	-1.266963	-2.008368
44	8	0	-3.532642	-2.228076	0.878248
45	1	0	-3.953289	-1.545453	1.411629
46	6	0	-1.840667	-0.461640	2.524516
47	1	0	-2.293672	0.509907	2.335693
48	1	0	-2.563771	-1.101253	3.036060
49	1	0	-1.008895	-0.303940	3.214999

Conformer a-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.233997	2.245313	0.345811
2	1	0	-0.566689	3.015663	0.709480
3	6	0	-2.424388	2.521425	-0.240423
4	6	0	-3.039379	1.251455	-0.664133
5	6	0	-2.184133	0.105622	-0.068949
6	6	0	-0.905391	0.820310	0.344588
7	6	0	-2.036011	-1.126969	-0.950691
8	1	0	-1.339625	-0.920264	-1.769459
9	1	0	-3.011758	-1.353346	-1.383433
10	6	0	-1.550549	-2.272067	-0.089166
11	6	0	-0.361350	-2.222907	0.518213
12	1	0	-0.054818	-3.054190	1.148612
13	6	0	0.660240	-1.150297	0.320698
14	6	0	0.321485	0.277622	0.577927
15	6	0	1.870386	-1.596606	-0.084957
16	1	0	1.960302	-2.679150	-0.156462
17	6	0	2.865710	0.569809	-0.932873
18	6	0	2.481942	1.578316	0.171346
19	1	0	2.056518	2.409018	-0.393823
20	6	0	1.417305	1.138751	1.208846
21	1	0	0.960195	2.074770	1.527433
22	6	0	-3.059918	3.847093	-0.491534
23	1	0	-3.282543	3.971188	-1.555665
24	1	0	-4.014573	3.923916	0.039037
25	1	0	-2.417760	4.667876	-0.169957
26	8	0	-4.050283	1.094908	-1.317695
27	8	0	-2.951400	-0.245723	1.126242
28	1	0	-2.320268	-0.414941	1.836274
29	6	0	-2.511429	-3.412682	0.136295
30	1	0	-2.614457	-4.004543	-0.780878

31	1	0	-2.120978	-4.075041	0.918657
32	8	0	-3.827967	-2.955180	0.463713
33	1	0	-3.730873	-2.101900	0.914825
34	6	0	3.117286	-0.913496	-0.623726
35	6	0	3.490275	-1.636692	-1.938502
36	1	0	2.687691	-1.561189	-2.673423
37	1	0	4.390330	-1.198768	-2.372777
38	1	0	3.680590	-2.693142	-1.736327
39	6	0	4.311976	-1.077849	0.356636
40	1	0	4.508371	-2.141986	0.506984
41	1	0	5.212846	-0.624681	-0.064255
42	1	0	4.128458	-0.646331	1.339728
43	8	0	2.988901	1.000412	-2.060388
44	8	0	3.667867	2.121082	0.755937
45	1	0	4.076254	1.460005	1.324753
46	6	0	1.941597	0.508873	2.515248
47	1	0	2.365346	-0.485006	2.384202
48	1	0	2.687847	1.158075	2.978868
49	1	0	1.112698	0.419799	3.221225

Conformer b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.240941	-2.194196	0.470726
2	1	0	0.544175	-2.938949	0.830959
3	6	0	2.424416	-2.507234	-0.115584
4	6	0	3.062542	-1.262307	-0.559686
5	6	0	2.207977	-0.081224	-0.038174
6	6	0	0.932708	-0.768775	0.426673
7	6	0	2.054484	1.081813	-1.009480
8	1	0	1.408764	0.786327	-1.843719
9	1	0	3.039419	1.302889	-1.433902
10	6	0	1.491941	2.289911	-0.295895
11	6	0	0.291932	2.282238	0.285971
12	1	0	-0.067073	3.202327	0.737177
13	6	0	-0.682440	1.155503	0.255530
14	6	0	-0.294781	-0.226495	0.650920
15	6	0	-1.920997	1.493722	-0.171706
16	1	0	-2.071966	2.552191	-0.374589
17	6	0	-2.781399	-0.803457	-0.719620
18	6	0	-2.485788	-1.626028	0.534109
19	1	0	-3.406206	-1.662550	1.131926
20	6	0	-1.343277	-1.037676	1.413311
21	1	0	-0.858040	-1.934921	1.790957
22	6	0	3.034169	-3.852033	-0.332746

23	1	0	3.231016	-4.021842	-1.395842
24	1	0	3.998765	-3.926251	0.179996
25	1	0	2.386222	-4.649586	0.033099
26	8	0	4.118998	-1.129858	-1.152495
27	8	0	2.896552	0.352892	1.161150
28	1	0	3.813172	0.529379	0.909962
29	6	0	2.390719	3.504070	-0.267103
30	1	0	3.375545	3.197886	0.115334
31	1	0	2.551643	3.858828	-1.291322
32	8	0	1.886805	4.615033	0.459325
33	1	0	1.862632	4.369586	1.391176
34	6	0	-3.132258	0.678741	-0.604331
35	6	0	-3.547867	1.200393	-1.999421
36	1	0	-2.738260	1.087539	-2.721181
37	1	0	-4.415342	0.650943	-2.370258
38	1	0	-3.811100	2.258194	-1.931835
39	6	0	-4.328394	0.882743	0.364403
40	1	0	-4.572500	1.946314	0.412600
41	1	0	-5.208856	0.349884	-0.004700
42	1	0	-4.120125	0.541089	1.376450
43	8	0	-2.722795	-1.368393	-1.795448
44	8	0	-2.137664	-2.942492	0.145161
45	1	0	-2.238365	-2.961029	-0.821728
46	6	0	-1.822271	-0.283606	2.669448
47	1	0	-2.299278	0.669668	2.446521
48	1	0	-2.526765	-0.904093	3.229849
49	1	0	-0.966788	-0.077900	3.317459

Conformer b-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.068276	-2.282904	0.308112
2	1	0	0.316655	-3.027810	0.532546
3	6	0	2.262318	-2.579272	-0.264928
4	6	0	2.982659	-1.322662	-0.508057
5	6	0	2.161531	-0.176007	0.131254
6	6	0	0.833936	-0.849635	0.445719
7	6	0	2.114676	1.111910	-0.679199
8	1	0	1.496617	0.962905	-1.571420
9	1	0	3.123204	1.344968	-1.029713
10	6	0	1.578483	2.245130	0.167320
11	6	0	0.347732	2.225266	0.687178
12	1	0	0.008651	3.088349	1.255270
13	6	0	-0.676420	1.164181	0.472927
14	6	0	-0.373556	-0.275673	0.696184

15	6	0	-1.875793	1.620207	0.044350
16	1	0	-1.970558	2.702573	-0.019451
17	6	0	-2.819848	-0.545807	-0.825384
18	6	0	-2.626107	-1.528706	0.329457
19	1	0	-3.571807	-1.579763	0.885137
20	6	0	-1.491053	-1.118659	1.312559
21	1	0	-1.064714	-2.080205	1.590580
22	6	0	2.814486	-3.914232	-0.639285
23	1	0	3.055967	-3.949046	-1.706176
24	1	0	3.747328	-4.111553	-0.100913
25	1	0	2.110190	-4.716410	-0.415178
26	8	0	4.071682	-1.172910	-1.033330
27	8	0	2.806236	0.053714	1.409703
28	1	0	3.737444	0.236773	1.225740
29	6	0	2.509459	3.399418	0.431670
30	1	0	2.012754	4.152397	1.054852
31	1	0	3.392876	3.045118	0.971545
32	8	0	3.020858	3.982258	-0.773883
33	1	0	2.265182	4.303975	-1.278810
34	6	0	-3.097451	0.930910	-0.546081
35	6	0	-3.406422	1.640120	-1.885462
36	1	0	-2.566059	1.565545	-2.576507
37	1	0	-4.281006	1.192924	-2.361823
38	1	0	-3.614730	2.696149	-1.701038
39	6	0	-4.335063	1.084186	0.379163
40	1	0	-4.532882	2.146157	0.540537
41	1	0	-5.216816	0.644726	-0.094807
42	1	0	-4.199895	0.617183	1.353024
43	8	0	-2.744539	-0.981179	-1.958663
44	8	0	-2.337470	-2.808446	-0.203710
45	1	0	-2.396240	-2.705990	-1.168806
46	6	0	-1.986009	-0.501359	2.635427
47	1	0	-2.416509	0.491445	2.513869
48	1	0	-2.735904	-1.153356	3.090990
49	1	0	-1.148890	-0.413028	3.332070

Conformer c-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.211900	-2.171010	0.529607
2	6	0	-2.407679	-2.534825	-0.002404
3	6	0	-2.884026	-1.432918	-0.847476
4	6	0	-1.897341	-0.251307	-0.716590
5	6	0	-0.785118	-0.839766	0.129913
6	6	0	-2.595449	0.917775	-0.004475

7	6	0	-1.761385	2.158592	0.216025
8	6	0	-0.421986	2.246345	0.201883
9	6	0	0.599058	1.196960	-0.006079
10	6	0	0.349888	-0.192920	0.471679
11	6	0	1.742920	1.556878	-0.622323
12	6	0	3.145641	-0.540147	-0.259634
13	6	0	2.830657	-0.450208	1.225285
14	6	0	1.334681	-0.809298	1.456623
15	6	0	-3.152187	-3.818190	0.155495
16	8	0	-3.860823	-1.409428	-1.576756
17	8	0	-1.431462	0.112637	-2.014943
18	6	0	-2.574352	3.412154	0.446281
19	8	0	-3.454819	3.291729	1.572680
20	6	0	2.868420	0.680921	-1.132722
21	6	0	4.194615	1.494050	-1.107813
22	6	0	2.560104	0.248712	-2.583530
23	8	0	3.653217	-1.557546	-0.692220
24	8	0	3.657680	-1.337965	1.955504
25	6	0	0.949091	-0.447351	2.904291
26	1	0	-0.633101	-2.809757	1.184974
27	1	0	-3.472759	1.193679	-0.603986
28	1	0	-3.000483	0.567833	0.952486
29	1	0	0.000248	3.242903	0.312981
30	1	0	1.835688	2.599862	-0.917384
31	1	0	3.025232	0.563627	1.584102
32	1	0	1.300526	-1.896467	1.350557
33	1	0	-2.603844	-4.526786	0.777405
34	1	0	-4.133251	-3.644226	0.608958
35	1	0	-3.335707	-4.277979	-0.820536
36	1	0	-2.216927	0.188421	-2.574406
37	1	0	-3.234799	3.596107	-0.406779
38	1	0	-1.913300	4.279023	0.557172
39	1	0	-2.903541	3.152384	2.351326
40	1	0	4.076625	2.390378	-1.721422
41	1	0	4.460219	1.808708	-0.095718
42	1	0	5.014857	0.900382	-1.515621
43	1	0	2.454581	1.130650	-3.219385
44	1	0	1.628761	-0.318480	-2.629087
45	1	0	3.369955	-0.369956	-2.973647
46	1	0	3.899881	-2.037498	1.328658
47	1	0	0.935739	0.637265	3.043326
48	1	0	-0.041627	-0.834721	3.150260
49	1	0	1.674770	-0.877437	3.597431
	Conformer c-2				

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.098812	-2.319068	0.291802
2	6	0	-2.321245	-2.628107	-0.213153
3	6	0	-2.894712	-1.408606	-0.795257
4	6	0	-1.933562	-0.231955	-0.515987
5	6	0	-0.742141	-0.919475	0.122716
6	6	0	-2.602407	0.754214	0.455078
7	6	0	-1.789817	1.967751	0.836355
8	6	0	-0.459679	2.117719	0.735939
9	6	0	0.573299	1.162682	0.281449
10	6	0	0.395787	-0.300807	0.505301
11	6	0	1.661242	1.674848	-0.329423
12	6	0	3.135992	-0.398200	-0.464431
13	6	0	2.930642	-0.598568	1.029033
14	6	0	1.465116	-1.049361	1.290493
15	6	0	-3.013253	-3.949445	-0.250847
16	8	0	-3.927925	-1.290311	-1.431652
17	8	0	-1.584423	0.387432	-1.752900
18	6	0	-2.621351	3.132264	1.327825
19	8	0	-3.566790	3.588670	0.350279
20	6	0	2.771541	0.955574	-1.066580
21	6	0	2.378230	0.800227	-2.552551
22	6	0	4.075926	1.797771	-0.965733
23	8	0	3.629137	-1.298991	-1.116484
24	8	0	3.830480	-1.575553	1.519881
25	6	0	1.177834	-0.975164	2.803071
26	1	0	-0.452919	-3.044159	0.770749
27	1	0	-2.907893	0.214804	1.362011
28	1	0	-3.530251	1.105579	-0.010078
29	1	0	-0.061935	3.100960	0.978077
30	1	0	1.704530	2.757284	-0.429439
31	1	0	3.128580	0.336869	1.558607
32	1	0	1.450532	-2.099217	0.987184
33	1	0	-3.244330	-4.232111	-1.282635
34	1	0	-3.968276	-3.902754	0.282086
35	1	0	-2.404029	-4.735201	0.197521
36	1	0	-2.414947	0.534971	-2.226361
37	1	0	-3.229506	2.827654	2.185343
38	1	0	-1.968034	3.950319	1.651214
39	1	0	-3.063296	3.865860	-0.424039
40	1	0	2.215027	1.784176	-2.997849
41	1	0	3.173282	0.294153	-3.102624
42	1	0	1.457196	0.223119	-2.651840

43	1	0	3.893623	2.790852	-1.383627
44	1	0	4.403028	1.920486	0.069500
45	1	0	4.880520	1.325628	-1.532632
46	1	0	4.035026	-2.142198	0.759648
47	1	0	1.145128	0.063896	3.142336
48	1	0	1.964281	-1.495856	3.353208
49	1	0	0.219047	-1.440850	3.040049

Conformer d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.522517	-2.162746	-0.573557
2	1	0	0.969755	-2.878737	-1.168006
3	6	0	2.777110	-2.397416	-0.109175
4	6	0	3.202228	-1.226048	0.665150
5	6	0	2.106435	-0.143495	0.556588
6	6	0	0.997441	-0.861100	-0.190149
7	6	0	2.645232	1.048647	-0.249693
8	1	0	3.537234	1.422800	0.270716
9	1	0	3.004409	0.691017	-1.223864
10	6	0	1.684626	2.194547	-0.448338
11	6	0	0.350854	2.169722	-0.326547
12	1	0	-0.150036	3.129294	-0.420179
13	6	0	-0.562702	1.049673	-0.017679
14	6	0	-0.220799	-0.336583	-0.449873
15	6	0	-1.718738	1.368439	0.602794
16	1	0	-1.883447	2.423480	0.804792
17	6	0	-3.335689	-0.477927	0.102780
18	6	0	-2.461508	-1.609725	-0.436725
19	1	0	-2.065290	-2.183022	0.406865
20	6	0	-1.251147	-1.091799	-1.272703
21	1	0	-0.791198	-2.012411	-1.632897
22	6	0	3.625227	-3.613569	-0.276198
23	1	0	4.559068	-3.367277	-0.791503
24	1	0	3.109191	-4.387952	-0.845041
25	1	0	3.904519	-4.023460	0.699352
26	8	0	4.216198	-1.084960	1.327355
27	8	0	1.694702	0.235754	1.867700
28	1	0	2.504533	0.391909	2.373216
29	6	0	2.398262	3.495193	-0.769598
30	1	0	3.134722	3.305604	-1.564603
31	1	0	2.967943	3.816306	0.109468
32	8	0	1.557847	4.588235	-1.108918
33	1	0	1.125531	4.378788	-1.944730
34	6	0	-2.800801	0.465311	1.187133

35	6	0	-2.221337	-0.352317	2.373627
36	1	0	-1.326350	-0.906875	2.092638
37	1	0	-2.965675	-1.051328	2.766134
38	1	0	-1.945071	0.336879	3.174533
39	6	0	-3.958451	1.342484	1.695835
40	1	0	-3.588311	2.027281	2.462361
41	1	0	-4.748258	0.729304	2.133720
42	1	0	-4.395069	1.929429	0.886454
43	8	0	-4.456657	-0.361003	-0.357548
44	8	0	-3.248493	-2.474856	-1.230529
45	1	0	-4.086283	-2.003667	-1.371187
46	6	0	-1.702889	-0.303270	-2.514525
47	1	0	-2.165003	0.651427	-2.254990
48	1	0	-2.423941	-0.894378	-3.081392
49	1	0	-0.846964	-0.097904	-3.161212

Conformer d-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.270091	2.306578	-0.377069
2	1	0	-0.648911	3.049237	-0.860921
3	6	0	-2.515279	2.574565	0.093785
4	6	0	-3.048661	1.346797	0.695797
5	6	0	-2.034301	0.206450	0.462160
6	6	0	-0.855005	0.928470	-0.162636
7	6	0	-2.637124	-0.825938	-0.501490
8	1	0	-3.562319	-1.205200	-0.053225
9	1	0	-2.938467	-0.321613	-1.429719
10	6	0	-1.762060	-2.010657	-0.827189
11	6	0	-0.431158	-2.101568	-0.676079
12	1	0	0.011911	-3.072746	-0.885693
13	6	0	0.556203	-1.100402	-0.217461
14	6	0	0.327135	0.350481	-0.471449
15	6	0	1.670735	-1.585111	0.370415
16	1	0	1.748866	-2.667032	0.437538
17	6	0	3.432533	0.189985	0.142598
18	6	0	2.648908	1.442931	-0.248035
19	1	0	2.267074	1.918831	0.660226
20	6	0	1.431986	1.125361	-1.170113
21	1	0	1.047719	2.114790	-1.419249
22	6	0	-3.264799	3.864564	0.077666
23	1	0	-4.204626	3.759974	-0.473673
24	1	0	-2.680557	4.663182	-0.381103
25	1	0	-3.531051	4.166361	1.095445
26	8	0	-4.088776	1.199347	1.314272

27	8	0	-1.687086	-0.371860	1.719059
28	1	0	-2.520787	-0.543119	2.178703
29	6	0	-2.525277	-3.219690	-1.322055
30	1	0	-1.826949	-4.017028	-1.599787
31	1	0	-3.110337	-2.959790	-2.209826
32	8	0	-3.490021	-3.692536	-0.371640
33	1	0	-3.007492	-3.932310	0.428092
34	6	0	2.809019	-0.856102	1.077027
35	6	0	2.277203	-0.169813	2.365391
36	1	0	1.433536	0.489294	2.163034
37	1	0	3.068880	0.406056	2.853398
38	1	0	1.937554	-0.939971	3.061317
39	6	0	3.889443	-1.882378	1.461919
40	1	0	3.456068	-2.638750	2.120403
41	1	0	4.715161	-1.400006	1.988079
42	1	0	4.294689	-2.380274	0.579792
43	8	0	4.555333	0.060787	-0.308847
44	8	0	3.510996	2.353907	-0.899380
45	1	0	4.322719	1.853815	-1.085219
46	6	0	1.867614	0.468813	-2.491679
47	1	0	2.264792	-0.537229	-2.342417
48	1	0	2.638121	1.078128	-2.966770
49	1	0	1.018686	0.398217	-3.175165

Conformer e-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.522517	-2.162746	-0.573557
2	1	0	-0.969755	-2.878737	-1.168006
3	6	0	-2.777110	-2.397416	-0.109175
4	6	0	-3.202228	-1.226048	0.665150
5	6	0	-2.106435	-0.143495	0.556588
6	6	0	-0.997441	-0.861100	-0.190149
7	6	0	-2.645232	1.048647	-0.249693
8	1	0	-3.537234	1.422800	0.270716
9	1	0	-3.004409	0.691017	-1.223864
10	6	0	-1.684626	2.194547	-0.448338
11	6	0	-0.350854	2.169722	-0.326547
12	1	0	0.150036	3.129294	-0.420179
13	6	0	0.562702	1.049673	-0.017679
14	6	0	0.220799	-0.336583	-0.449873
15	6	0	1.718738	1.368439	0.602794
16	1	0	1.883447	2.423480	0.804792
17	6	0	3.335689	-0.477927	0.102780
18	6	0	2.461508	-1.609725	-0.436725

19	1	0	2.065290	-2.183022	0.406865
20	6	0	1.251147	-1.091799	-1.272703
21	1	0	0.791198	-2.012411	-1.632897
22	6	0	-3.625227	-3.613569	-0.276198
23	1	0	-4.559068	-3.367277	-0.791503
24	1	0	-3.109191	-4.387952	-0.845041
25	1	0	-3.904519	-4.023460	0.699352
26	8	0	-4.216198	-1.084960	1.327355
27	8	0	-1.694702	0.235754	1.867700
28	1	0	-2.504533	0.391909	2.373216
29	6	0	-2.398262	3.495193	-0.769598
30	1	0	-3.134722	3.305604	-1.564603
31	1	0	-2.967943	3.816306	0.109468
32	8	0	-1.557847	4.588235	-1.108918
33	1	0	-1.125531	4.378788	-1.944730
34	6	0	2.800801	0.465311	1.187133
35	6	0	2.221337	-0.352317	2.373627
36	1	0	1.326350	-0.906875	2.092638
37	1	0	2.965675	-1.051328	2.766134
38	1	0	1.945071	0.336879	3.174533
39	6	0	3.958451	1.342484	1.695835
40	1	0	3.588311	2.027281	2.462361
41	1	0	4.748258	0.729304	2.133720
42	1	0	4.395069	1.929429	0.886454
43	8	0	4.456657	-0.361003	-0.357548
44	8	0	3.248493	-2.474856	-1.230529
45	1	0	4.086283	-2.003667	-1.371187
46	6	0	1.702889	-0.303270	-2.514525
47	1	0	2.165003	0.651427	-2.254990
48	1	0	2.423941	-0.894378	-3.081392
49	1	0	0.846964	-0.097904	-3.161212

Conformer e-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.270091	-2.306578	-0.377069
2	1	0	-0.648911	-3.049237	-0.860921
3	6	0	-2.515279	-2.574565	0.093785
4	6	0	-3.048661	-1.346797	0.695797
5	6	0	-2.034301	-0.206450	0.462160
6	6	0	-0.855005	-0.928470	-0.162636
7	6	0	-2.637124	0.825938	-0.501490
8	1	0	-3.562319	1.205200	-0.053225
9	1	0	-2.938467	0.321613	-1.429719
10	6	0	-1.762060	2.010657	-0.827189

11	6	0	-0.431158	2.101568	-0.676079
12	1	0	0.011911	3.072746	-0.885693
13	6	0	0.556203	1.100402	-0.217461
14	6	0	0.327135	-0.350481	-0.471449
15	6	0	1.670735	1.585111	0.370415
16	1	0	1.748866	2.667032	0.437538
17	6	0	3.432533	-0.189985	0.142598
18	6	0	2.648908	-1.442931	-0.248035
19	1	0	2.267074	-1.918831	0.660226
20	6	0	1.431986	-1.125361	-1.170113
21	1	0	1.047719	-2.114790	-1.419249
22	6	0	-3.264799	-3.864564	0.077666
23	1	0	-4.204626	-3.759974	-0.473673
24	1	0	-2.680557	-4.663182	-0.381103
25	1	0	-3.531051	-4.166361	1.095445
26	8	0	-4.088776	-1.199347	1.314272
27	8	0	-1.687086	0.371860	1.719059
28	1	0	-2.520787	0.543119	2.178703
29	6	0	-2.525277	3.219690	-1.322055
30	1	0	-1.826949	4.017028	-1.599787
31	1	0	-3.110337	2.959790	-2.209826
32	8	0	-3.490021	3.692536	-0.371640
33	1	0	-3.007492	3.932310	0.428092
34	6	0	2.809019	0.856102	1.077027
35	6	0	2.277203	0.169813	2.365391
36	1	0	1.433536	-0.489294	2.163034
37	1	0	3.068880	-0.406056	2.853398
38	1	0	1.937554	0.939971	3.061317
39	6	0	3.889443	1.882378	1.461919
40	1	0	3.456068	2.638750	2.120403
41	1	0	4.715161	1.400006	1.988079
42	1	0	4.294689	2.380274	0.579792
43	8	0	4.555333	-0.060787	-0.308847
44	8	0	3.510996	-2.353907	-0.899380
45	1	0	4.322719	-1.853815	-1.085219
46	6	0	1.867614	-0.468813	-2.491679
47	1	0	2.264792	0.537229	-2.342417
48	1	0	2.638121	-1.078128	-2.966770
49	1	0	1.018686	-0.398217	-3.175165

Conformer f-1

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	1.211900	-2.171010	0.529607
2	6	0	2.407679	-2.534825	-0.002404

3	6	0	2.884026	-1.432918	-0.847476
4	6	0	1.897341	-0.251307	-0.716590
5	6	0	0.785118	-0.839766	0.129913
6	6	0	2.595449	0.917775	-0.004475
7	6	0	1.761385	2.158592	0.216025
8	6	0	0.421986	2.246345	0.201883
9	6	0	-0.599058	1.196960	-0.006079
10	6	0	-0.349888	-0.192920	0.471679
11	6	0	-1.742920	1.556878	-0.622323
12	6	0	-3.145641	-0.540147	-0.259634
13	6	0	-2.830657	-0.450208	1.225285
14	6	0	-1.334681	-0.809298	1.456623
15	6	0	3.152187	-3.818190	0.155495
16	8	0	3.860823	-1.409428	-1.576756
17	8	0	1.431462	0.112637	-2.014943
18	6	0	2.574352	3.412154	0.446281
19	8	0	3.454819	3.291729	1.572680
20	6	0	-2.868420	0.680921	-1.132722
21	6	0	-4.194615	1.494050	-1.107813
22	6	0	-2.560104	0.248712	-2.583530
23	8	0	-3.653217	-1.557546	-0.692220
24	8	0	-3.657680	-1.337965	1.955504
25	6	0	-0.949091	-0.447351	2.904291
26	1	0	0.633101	-2.809757	1.184974
27	1	0	3.472759	1.193679	-0.603986
28	1	0	3.000483	0.567833	0.952486
29	1	0	-0.000248	3.242903	0.312981
30	1	0	-1.835688	2.599862	-0.917384
31	1	0	-3.025232	0.563627	1.584102
32	1	0	-1.300526	-1.896467	1.350557
33	1	0	2.603844	-4.526786	0.777405
34	1	0	4.133251	-3.644226	0.608958
35	1	0	3.335707	-4.277979	-0.820536
36	1	0	2.216927	0.188421	-2.574406
37	1	0	3.234799	3.596107	-0.406779
38	1	0	1.913300	4.279023	0.557172
39	1	0	2.903541	3.152384	2.351326
40	1	0	-4.076625	2.390378	-1.721422
41	1	0	-4.460219	1.808708	-0.095718
42	1	0	-5.014857	0.900382	-1.515621
43	1	0	-2.454581	1.130650	-3.219385
44	1	0	-1.628761	-0.318480	-2.629087
45	1	0	-3.369955	-0.369956	-2.973647
46	1	0	-3.899881	-2.037498	1.328658

47	1	0	-0.935739	0.637265	3.043326
48	1	0	0.041627	-0.834721	3.150260
49	1	0	-1.674770	-0.877437	3.597431

Conformer f-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.098812	-2.319068	0.291802
2	6	0	2.321245	-2.628107	-0.213153
3	6	0	2.894712	-1.408606	-0.795257
4	6	0	1.933562	-0.231955	-0.515987
5	6	0	0.742141	-0.919475	0.122716
6	6	0	2.602407	0.754214	0.455078
7	6	0	1.789817	1.967751	0.836355
8	6	0	0.459679	2.117719	0.735939
9	6	0	-0.573299	1.162682	0.281449
10	6	0	-0.395787	-0.300807	0.505301
11	6	0	-1.661242	1.674848	-0.329423
12	6	0	-3.135992	-0.398200	-0.464431
13	6	0	-2.930642	-0.598568	1.029033
14	6	0	-1.465116	-1.049361	1.290493
15	6	0	3.013253	-3.949445	-0.250847
16	8	0	3.927925	-1.290311	-1.431652
17	8	0	1.584423	0.387432	-1.752900
18	6	0	2.621351	3.132264	1.327825
19	8	0	3.566790	3.588670	0.350279
20	6	0	-2.771541	0.955574	-1.066580
21	6	0	-2.378230	0.800227	-2.552551
22	6	0	-4.075926	1.797771	-0.965733
23	8	0	-3.629137	-1.298991	-1.116484
24	8	0	-3.830480	-1.575553	1.519881
25	6	0	-1.177834	-0.975164	2.803071
26	1	0	0.452919	-3.044159	0.770749
27	1	0	2.907893	0.214804	1.362011
28	1	0	3.530251	1.105579	-0.010078
29	1	0	0.061935	3.100960	0.978077
30	1	0	-1.704530	2.757284	-0.429439
31	1	0	-3.128580	0.336869	1.558607
32	1	0	-1.450532	-2.099217	0.987184
33	1	0	3.244330	-4.232111	-1.282635
34	1	0	3.968276	-3.902754	0.282086
35	1	0	2.404029	-4.735201	0.197521
36	1	0	2.414947	0.534971	-2.226361
37	1	0	3.229506	2.827654	2.185343
38	1	0	1.968034	3.950319	1.651214

39	1	0	3.063296	3.865860	-0.424039
40	1	0	-2.215027	1.784176	-2.997849
41	1	0	-3.173282	0.294153	-3.102624
42	1	0	-1.457196	0.223119	-2.651840
43	1	0	-3.893623	2.790852	-1.383627
44	1	0	-4.403028	1.920486	0.069500
45	1	0	-4.880520	1.325628	-1.532632
46	1	0	-4.035026	-2.142198	0.759648
47	1	0	-1.145128	0.063896	3.142336
48	1	0	-1.964281	-1.495856	3.353208
49	1	0	-0.219047	-1.440850	3.040049

Conformer g-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.240941	-2.194196	0.470726
2	1	0	-0.544175	-2.938949	0.830959
3	6	0	-2.424416	-2.507234	-0.115584
4	6	0	-3.062542	-1.262307	-0.559686
5	6	0	-2.207977	-0.081224	-0.038174
6	6	0	-0.932708	-0.768775	0.426673
7	6	0	-2.054484	1.081813	-1.009480
8	1	0	-1.408764	0.786327	-1.843719
9	1	0	-3.039419	1.302889	-1.433902
10	6	0	-1.491941	2.289911	-0.295895
11	6	0	-0.291932	2.282238	0.285971
12	1	0	0.067073	3.202327	0.737177
13	6	0	0.682440	1.155503	0.255530
14	6	0	0.294781	-0.226495	0.650920
15	6	0	1.920997	1.493722	-0.171706
16	1	0	2.071966	2.552191	-0.374589
17	6	0	2.781399	-0.803457	-0.719620
18	6	0	2.485788	-1.626028	0.534109
19	1	0	3.406206	-1.662550	1.131926
20	6	0	1.343277	-1.037676	1.413311
21	1	0	0.858040	-1.934921	1.790957
22	6	0	-3.034169	-3.852033	-0.332746
23	1	0	-3.231016	-4.021842	-1.395842
24	1	0	-3.998765	-3.926251	0.179996
25	1	0	-2.386222	-4.649586	0.033099
26	8	0	-4.118998	-1.129858	-1.152495
27	8	0	-2.896552	0.352892	1.161150
28	1	0	-3.813172	0.529379	0.909962
29	6	0	-2.390719	3.504070	-0.267103
30	1	0	-3.375545	3.197886	0.115334

31	1	0	-2.551643	3.858828	-1.291322
32	8	0	-1.886805	4.615033	0.459325
33	1	0	-1.862632	4.369586	1.391176
34	6	0	3.132258	0.678741	-0.604331
35	6	0	3.547867	1.200393	-1.999421
36	1	0	2.738260	1.087539	-2.721181
37	1	0	4.415342	0.650943	-2.370258
38	1	0	3.811100	2.258194	-1.931835
39	6	0	4.328394	0.882743	0.364403
40	1	0	4.572500	1.946314	0.412600
41	1	0	5.208856	0.349884	-0.004700
42	1	0	4.120125	0.541089	1.376450
43	8	0	2.722795	-1.368393	-1.795448
44	8	0	2.137664	-2.942492	0.145161
45	1	0	2.238365	-2.961029	-0.821728
46	6	0	1.822271	-0.283606	2.669448
47	1	0	2.299278	0.669668	2.446521
48	1	0	2.526765	-0.904093	3.229849
49	1	0	0.966788	-0.077900	3.317459

Conformer g-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.068276	2.282904	0.308112
2	1	0	0.316655	3.027810	0.532546
3	6	0	2.262318	2.579272	-0.264928
4	6	0	2.982659	1.322662	-0.508057
5	6	0	2.161531	0.176007	0.131254
6	6	0	0.833936	0.849635	0.445719
7	6	0	2.114676	-1.111910	-0.679199
8	1	0	1.496617	-0.962905	-1.571420
9	1	0	3.123204	-1.344968	-1.029713
10	6	0	1.578483	-2.245130	0.167320
11	6	0	0.347732	-2.225266	0.687178
12	1	0	0.008651	-3.088349	1.255270
13	6	0	-0.676420	-1.164181	0.472927
14	6	0	-0.373556	0.275673	0.696184
15	6	0	-1.875793	-1.620207	0.044350
16	1	0	-1.970558	-2.702573	-0.019451
17	6	0	-2.819848	0.545807	-0.825384
18	6	0	-2.626107	1.528706	0.329457
19	1	0	-3.571807	1.579763	0.885137
20	6	0	-1.491053	1.118659	1.312559
21	1	0	-1.064714	2.080205	1.590580
22	6	0	2.814486	3.914232	-0.639285

23	1	0	3.055967	3.949046	-1.706176
24	1	0	3.747328	4.111553	-0.100913
25	1	0	2.110190	4.716410	-0.415178
26	8	0	4.071682	1.172910	-1.033330
27	8	0	2.806236	-0.053714	1.409703
28	1	0	3.737444	-0.236773	1.225740
29	6	0	2.509459	-3.399418	0.431670
30	1	0	2.012754	-4.152397	1.054852
31	1	0	3.392876	-3.045118	0.971545
32	8	0	3.020858	-3.982258	-0.773883
33	1	0	2.265182	-4.303975	-1.278810
34	6	0	-3.097451	-0.930910	-0.546081
35	6	0	-3.406422	-1.640120	-1.885462
36	1	0	-2.566059	-1.565545	-2.576507
37	1	0	-4.281006	-1.192924	-2.361823
38	1	0	-3.614730	-2.696149	-1.701038
39	6	0	-4.335063	-1.084186	0.379163
40	1	0	-4.532882	-2.146157	0.540537
41	1	0	-5.216816	-0.644726	-0.094807
42	1	0	-4.199895	-0.617183	1.353024
43	8	0	-2.744539	0.981179	-1.958663
44	8	0	-2.337470	2.808446	-0.203710
45	1	0	-2.396240	2.705990	-1.168806
46	6	0	-1.986009	0.501359	2.635427
47	1	0	-2.416509	-0.491445	2.513869
48	1	0	-2.735904	1.153356	3.090990
49	1	0	-1.148890	0.413028	3.332070

Conformer h-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.335800	-2.258582	-0.415766
2	1	0	0.668274	-3.019320	-0.798823
3	6	0	2.523529	-2.554890	0.168118
4	6	0	3.147068	-1.297690	0.604297
5	6	0	2.288243	-0.133746	0.052662
6	6	0	1.006514	-0.835717	-0.375027
7	6	0	2.150817	1.066597	0.978713
8	1	0	1.514075	0.807931	1.831656
9	1	0	3.141324	1.301769	1.381901
10	6	0	1.582702	2.242302	0.217986
11	6	0	0.371808	2.209934	-0.339186
12	1	0	0.009196	3.105933	-0.833839
13	6	0	-0.609078	1.092235	-0.230509
14	6	0	-0.231733	-0.307011	-0.573678

15	6	0	-1.835999	1.472839	0.197005
16	1	0	-1.956628	2.545084	0.340925
17	6	0	-2.772558	-0.766351	0.908017
18	6	0	-2.362138	-1.692521	-0.255427
19	1	0	-1.916944	-2.546959	0.256906
20	6	0	-1.306379	-1.158271	-1.256286
21	1	0	-0.823675	-2.058989	-1.633133
22	6	0	3.153967	-3.889645	0.385034
23	1	0	3.358687	-4.052132	1.447729
24	1	0	4.116962	-3.950610	-0.132303
25	1	0	2.515918	-4.697941	0.025597
26	8	0	4.195458	-1.150164	1.205859
27	8	0	2.964242	0.249877	-1.171576
28	1	0	3.881889	0.444485	-0.938497
29	6	0	2.489131	3.445454	0.101142
30	1	0	3.466409	3.107934	-0.274089
31	1	0	2.666475	3.864332	1.098051
32	8	0	1.982541	4.510955	-0.688620
33	1	0	1.933253	4.201513	-1.600254
34	6	0	-3.066031	0.723840	0.686298
35	6	0	-3.464536	1.356134	2.039674
36	1	0	-2.661791	1.260712	2.772080
37	1	0	-4.352500	0.867105	2.443492
38	1	0	-3.685112	2.416761	1.899862
39	6	0	-4.261080	0.911545	-0.288780
40	1	0	-4.483585	1.977121	-0.382009
41	1	0	-5.152100	0.412983	0.100681
42	1	0	-4.061342	0.539103	-1.292424
43	8	0	-2.879030	-1.266963	2.008368
44	8	0	-3.532642	-2.228076	-0.878248
45	1	0	-3.953289	-1.545453	-1.411629
46	6	0	-1.840667	-0.461640	-2.524516
47	1	0	-2.293672	0.509907	-2.335693
48	1	0	-2.563771	-1.101253	-3.036060
49	1	0	-1.008895	-0.303940	-3.214999

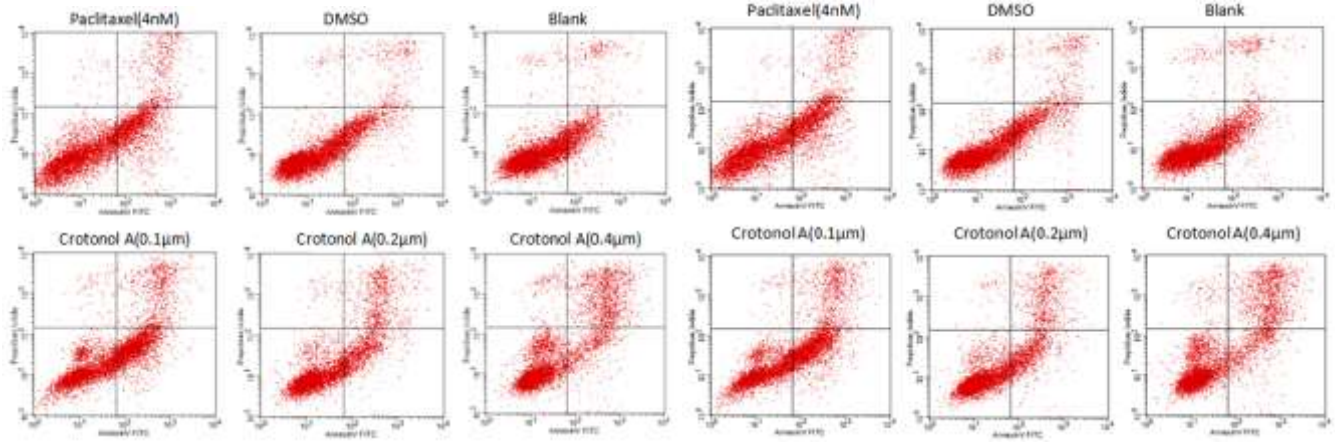
Conformer h-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.233997	2.245313	-0.345811
2	1	0	-0.566689	3.015663	-0.709480
3	6	0	-2.424388	2.521425	0.240423
4	6	0	-3.039379	1.251455	0.664133
5	6	0	-2.184133	0.105622	0.068949
6	6	0	-0.905391	0.820310	-0.344588

7	6	0	-2.036011	-1.126969	0.950691
8	1	0	-1.339625	-0.920264	1.769459
9	1	0	-3.011758	-1.353346	1.383433
10	6	0	-1.550549	-2.272067	0.089166
11	6	0	-0.361350	-2.222907	-0.518213
12	1	0	-0.054818	-3.054190	-1.148612
13	6	0	0.660240	-1.150297	-0.320698
14	6	0	0.321485	0.277622	-0.577927
15	6	0	1.870386	-1.596606	0.084957
16	1	0	1.960302	-2.679150	0.156462
17	6	0	2.865710	0.569809	0.932873
18	6	0	2.481942	1.578316	-0.171346
19	1	0	2.056518	2.409018	0.393823
20	6	0	1.417305	1.138751	-1.208846
21	1	0	0.960195	2.074770	-1.527433
22	6	0	-3.059918	3.847093	0.491534
23	1	0	-3.282543	3.971188	1.555665
24	1	0	-4.014573	3.923916	-0.039037
25	1	0	-2.417760	4.667876	0.169957
26	8	0	-4.050283	1.094908	1.317695
27	8	0	-2.951400	-0.245723	-1.126242
28	1	0	-2.320268	-0.414941	-1.836274
29	6	0	-2.511429	-3.412682	-0.136295
30	1	0	-2.614457	-4.004543	0.780878
31	1	0	-2.120978	-4.075041	-0.918657
32	8	0	-3.827967	-2.955180	-0.463713
33	1	0	-3.730873	-2.101900	-0.914825
34	6	0	3.117286	-0.913496	0.623726
35	6	0	3.490275	-1.636692	1.938502
36	1	0	2.687691	-1.561189	2.673423
37	1	0	4.390330	-1.198768	2.372777
38	1	0	3.680590	-2.693142	1.736327
39	6	0	4.311976	-1.077849	-0.356636
40	1	0	4.508371	-2.141986	-0.506984
41	1	0	5.212846	-0.624681	0.064255
42	1	0	4.128458	-0.646331	-1.339728
43	8	0	2.988901	1.000412	2.060388
44	8	0	3.667867	2.121082	-0.755937
45	1	0	4.076254	1.460005	-1.324753
46	6	0	1.941597	0.508873	-2.515248
47	1	0	2.365346	-0.485006	-2.384202
48	1	0	2.687847	1.158075	-2.978868
49	1	0	1.112698	0.419799	-3.221225

Results: The crotonol A induced K562 cells apoptosis

Figure S2. Trials for the crotonol A induced K562 cells apoptosis (n=3) A B



C

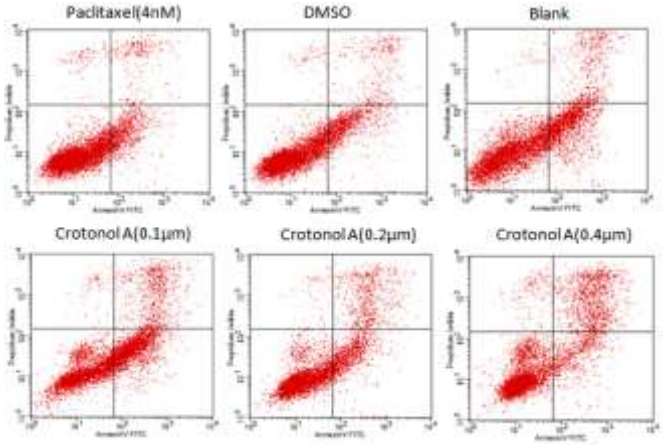


Table S4. Flow cytometry analyses of K562 cell apoptosis

Group	Upper left(UL)	Upper Right(UR)	Lower Left(LL)	Lower Right(LR)	Apoptosis rate （UR+LR）
Paclitaxel (4nM)	0.55	7.01	65.48	26.96	33.97
	0.58	6.78	65.95	26.69	33.47
	0.52	6.91	66.05	26.52	33.43
DMSO	0.74	4.08	77.27	17.91	21.99
	0.72	4.85	76.43	18.00	22.85
	0.83	4.32	77.92	16.93	21.25
Blank	1.21	3.20	82.74	12.85	16.05
	1.18	3.55	81.83	13.44	16.99
	1.06	3.01	82.81	13.12	16.13
Crotonol A(0.1μM)	1.07	10.34	53.06	35.53	45.87
	0.80	11.12	52.47	35.61	46.73
	0.90	10.82	52.72	35.56	46.38
Crotonol A(0.2μM)	0.77	9.80	73.73	15.70	25.50
	0.81	9.33	73.86	16.00	24.33
	0.82	8.87	74.91	15.40	24.27
Crotonol A(0.4μM)	1.59	16.43	72.49	9.49	25.92
	1.94	15.77	72.45	9.84	25.61
	1.89	16.04	72.95	9.12	25.16

Figure S3. Trials for Up-regulation levels of cleaved-PARP and bax as well as down-regulation level of bcl-2 in K562 cells treated with crotonol A.

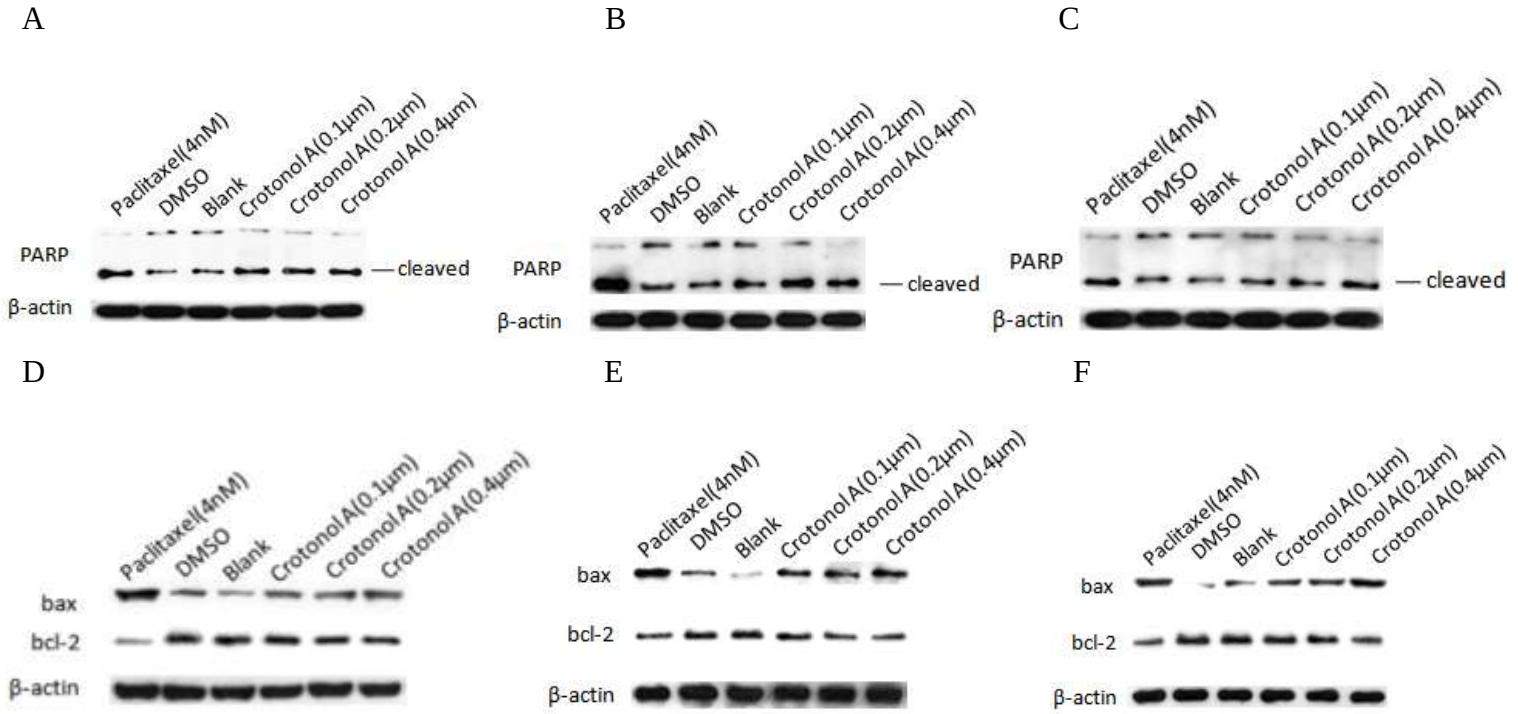


Table S5. The data of grey analyses using quantity one analysis software

Group	Paclitaxel (4nM)	DMSO	Blank	Crotonol A (0.1μM)	Crotonol A (0.2μM)	Crotonol A (0.4μM)
PARP	15.10	35.66	32.23	24.60	20.51	11.34
	10.49	28.53	29.06	20.20	15.18	11.22
	16.76	30.35	31.43	22.25	18.09	13.96
PARP -cleaved	71.72	42.92	39.36	50.79	58.65	53.02
	58.78	32.28	34.89	45.99	48.59	50.99
	50.16	33.83	31.94	37.84	41.56	47.47
β-actin	134.52	133.49	132.57	131.89	133.41	133.02
	139.70	136.87	137.43	139.56	136.74	137.51
	133.26	132.42	132.17	133.05	131.68	132.88
PARP/β-actin	0.11	0.27	0.24	0.19	0.15	0.09
	0.08	0.21	0.21	0.14	0.11	0.08
	0.13	0.23	0.24	0.17	0.14	0.11
PARP -cleaved /β-actin	0.53	0.32	0.30	0.39	0.44	0.40
	0.42	0.24	0.25	0.33	0.36	0.37
	0.38	0.26	0.24	0.28	0.32	0.36
bax	77.66	24.39	17.36	45.48	52.66	65.70
	71.57	13.46	27.27	42.57	53.69	72.29
	79.62	29.06	16.34	43.85	52.74	60.87
β-actin	133.66	134.01	132.23	134.48	132.83	130.24
	128.41	130.92	127.18	131.40	129.08	130.88
	132.48	134.34	129.44	129.00	131.17	128.43
bax/β-actin	0.58	0.18	0.13	0.34	0.40	0.50
	0.56	0.10	0.21	0.32	0.42	0.55

	0.60	0.22	0.13	0.34	0.40	0.47
bcl-2	36.37	52.25	57.94	47.33	37.81	35.48
	26.10	56.75	59.67	48.63	42.47	30.68
	20.77	52.35	51.67	48.30	40.80	37.43
β-actin	133.66	134.01	132.23	134.48	132.83	130.24
	128.41	130.92	127.18	131.40	129.08	130.88
	132.48	134.34	129.44	129.00	131.17	128.43
bcl-2/β-actin	0.27	0.38	0.44	0.35	0.28	0.27
	0.20	0.43	0.46	0.37	0.33	0.23
	0.16	0.39	0.40	0.37	0.31	0.29
bcl-2/bax	0.47	3.88	3.34	1.04	0.72	0.54
	0.36	1.95	2.16	1.14	0.79	0.42
	0.26	2.14	3.16	1.1o	0.77	0.61

Figure S4. The ^{1}H NMR spectrum of crotonol A (**1**) in CD_3OD

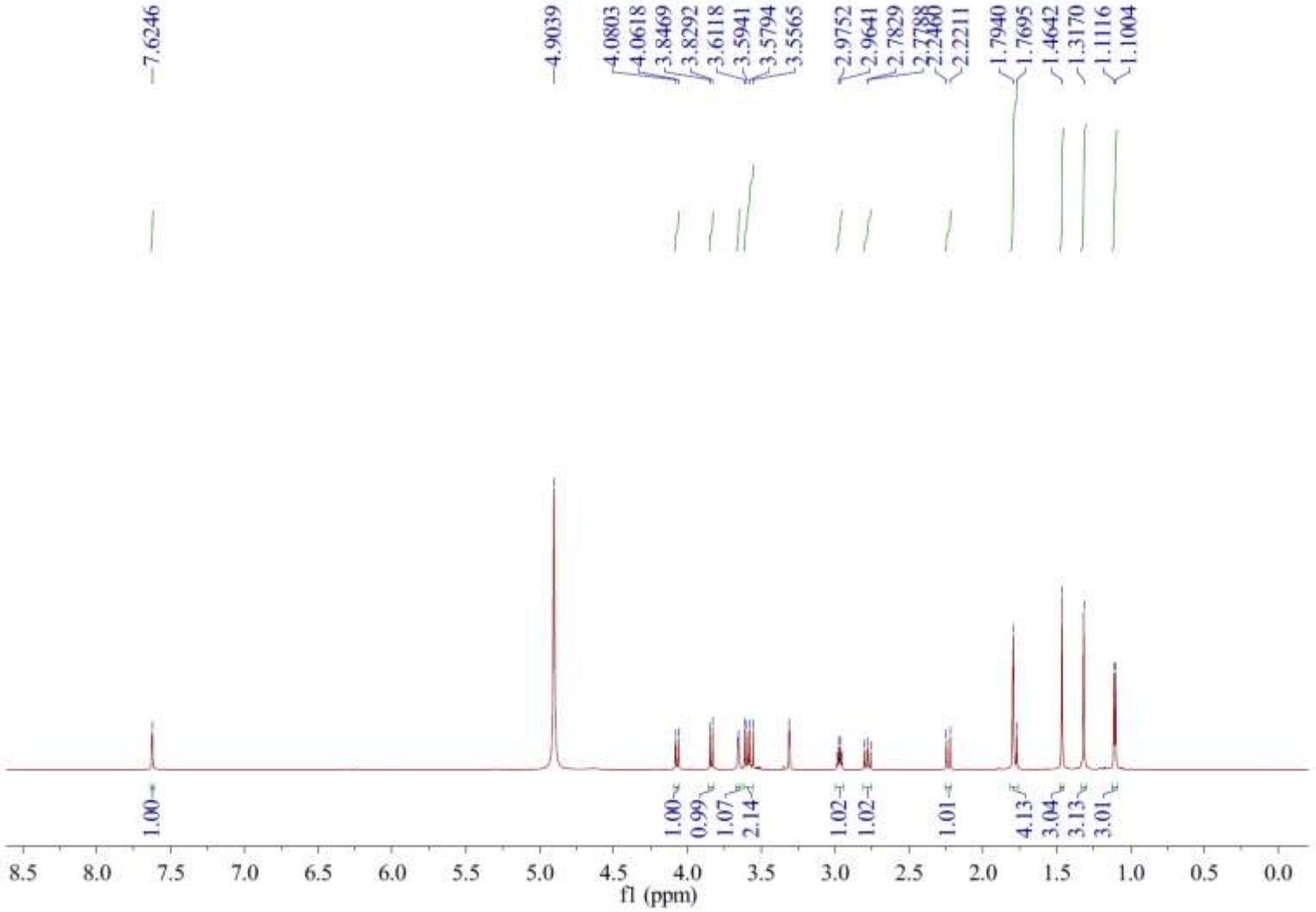


Figure S5. The ^{13}C NMR spectrum of crotonol A (**1**) in CD_3OD

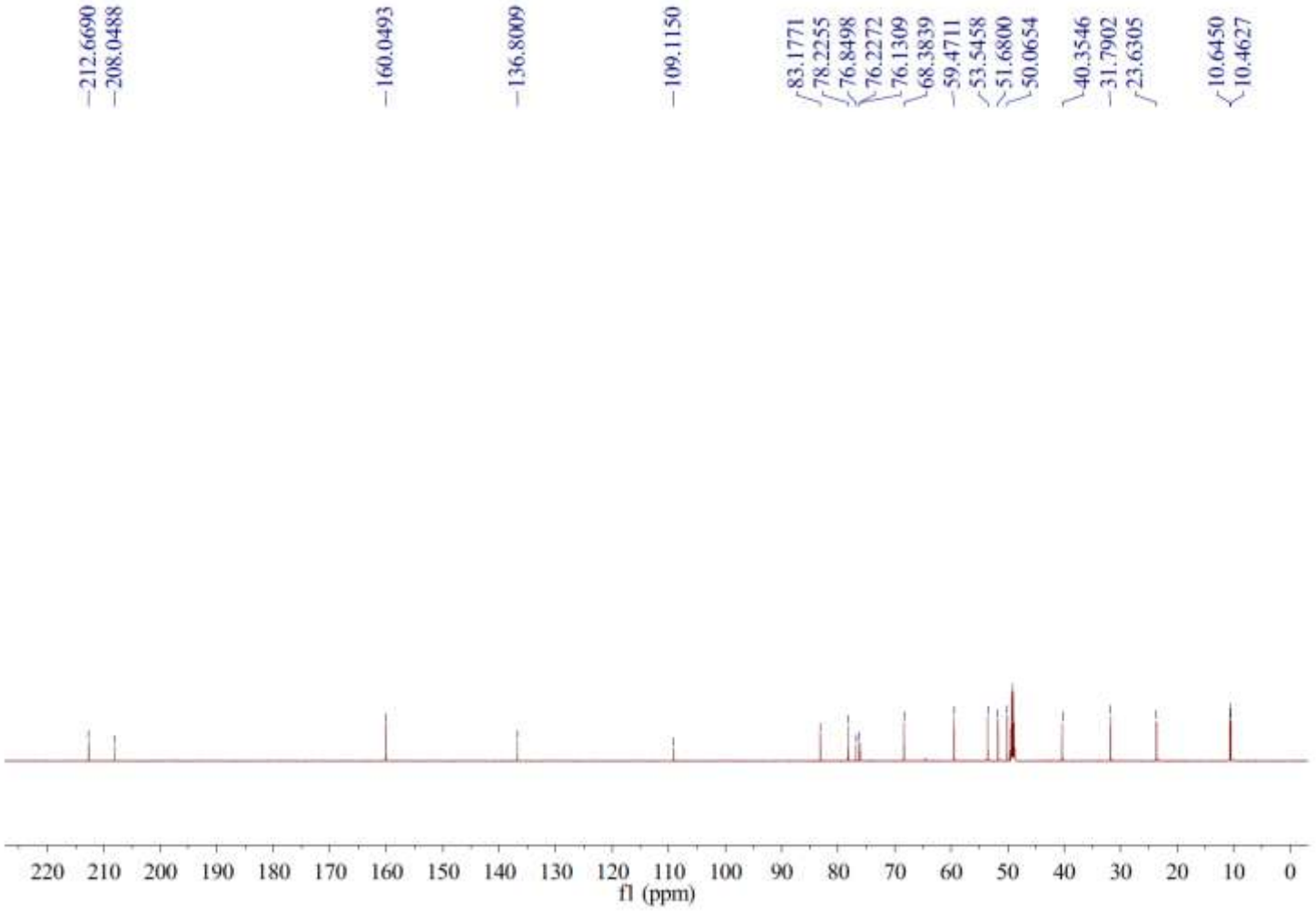


Figure S6. The HSQC spectrum of crotonol A (**1**) in CD_3OD

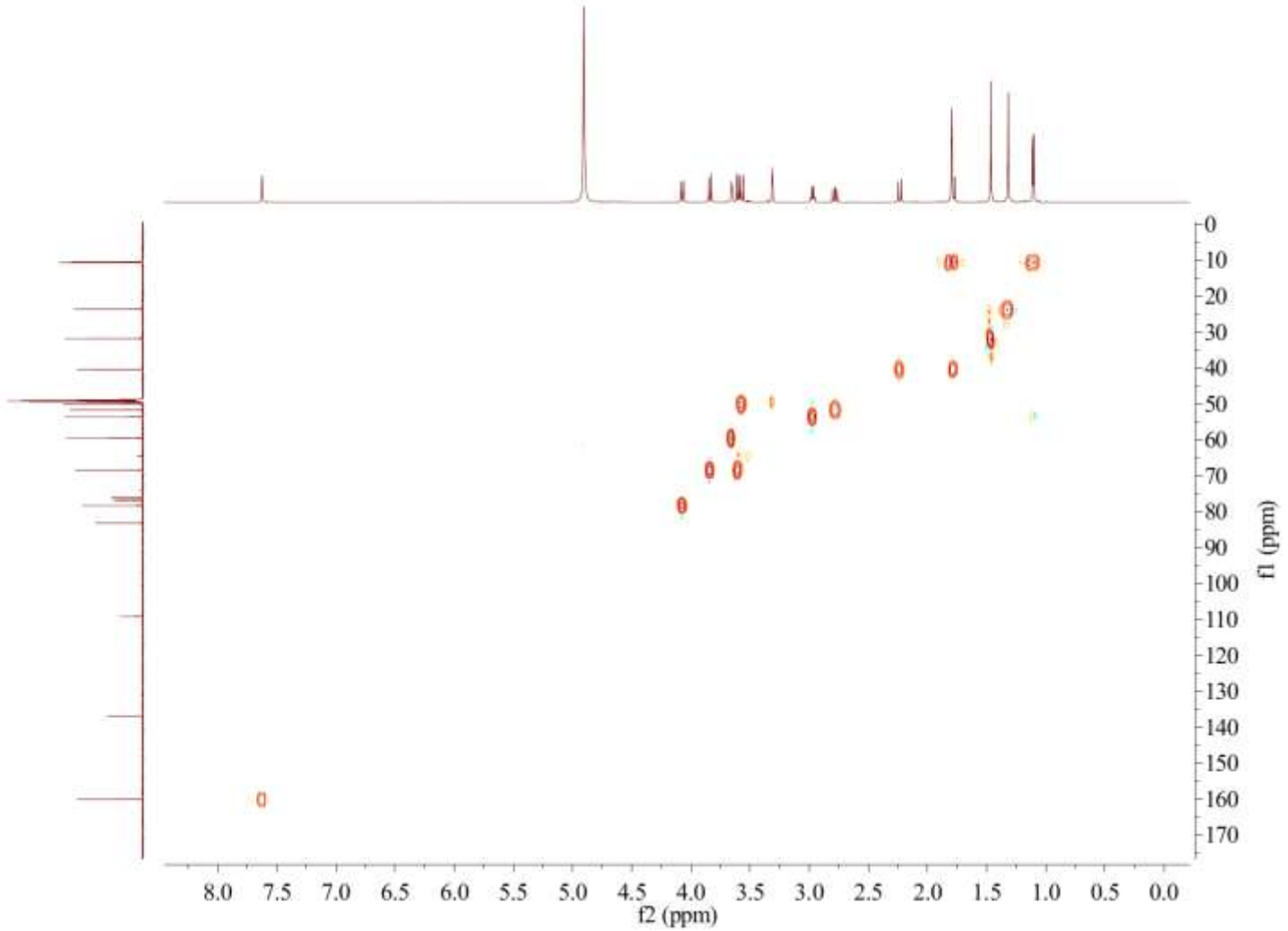


Figure S7. The ^{1}H-^{1}H COSY spectrum of crotonol A (**1**) in CD_3OD

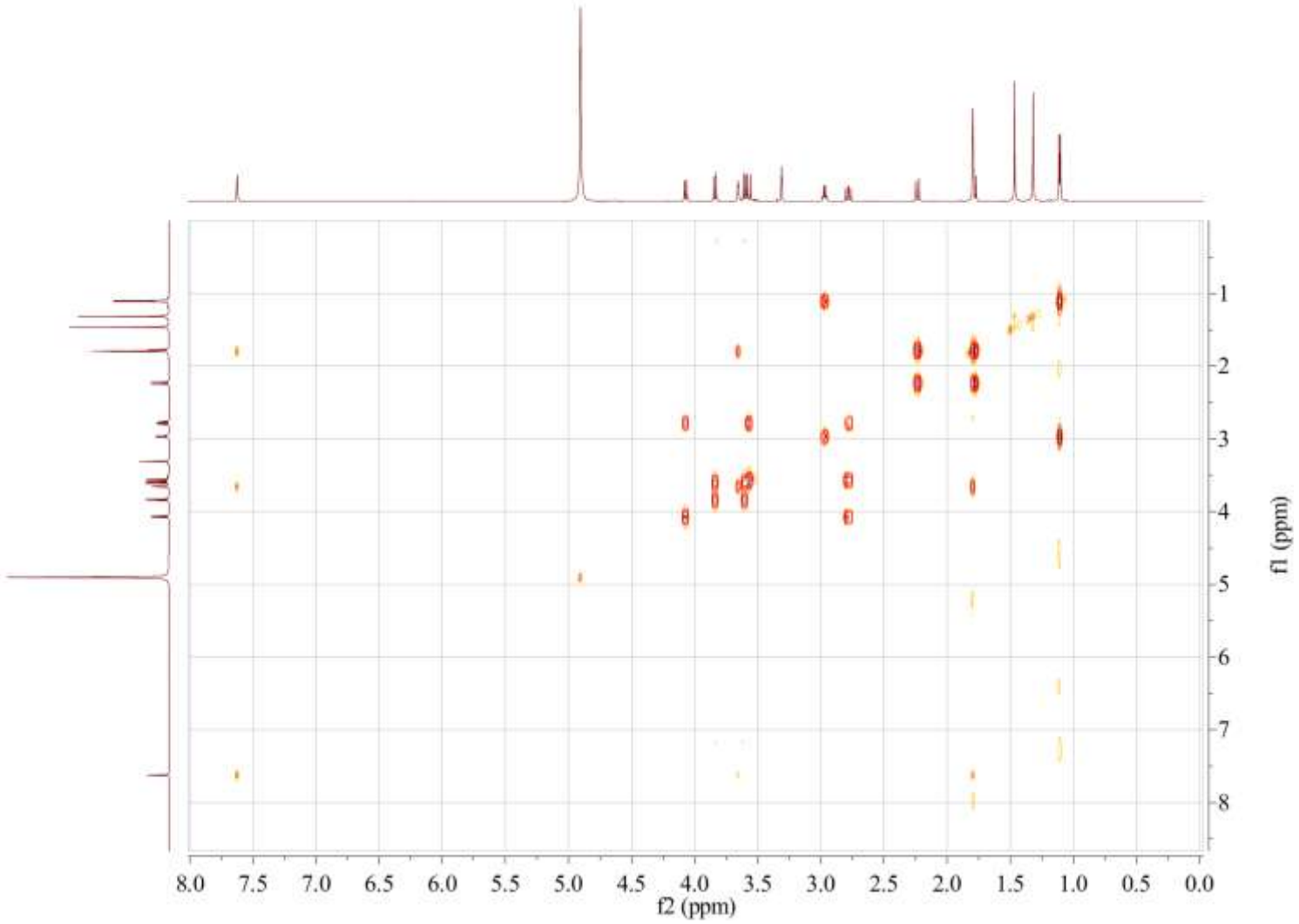


Figure S8. The HMBC spectrum of crotonol A (**1**) in CD_3OD

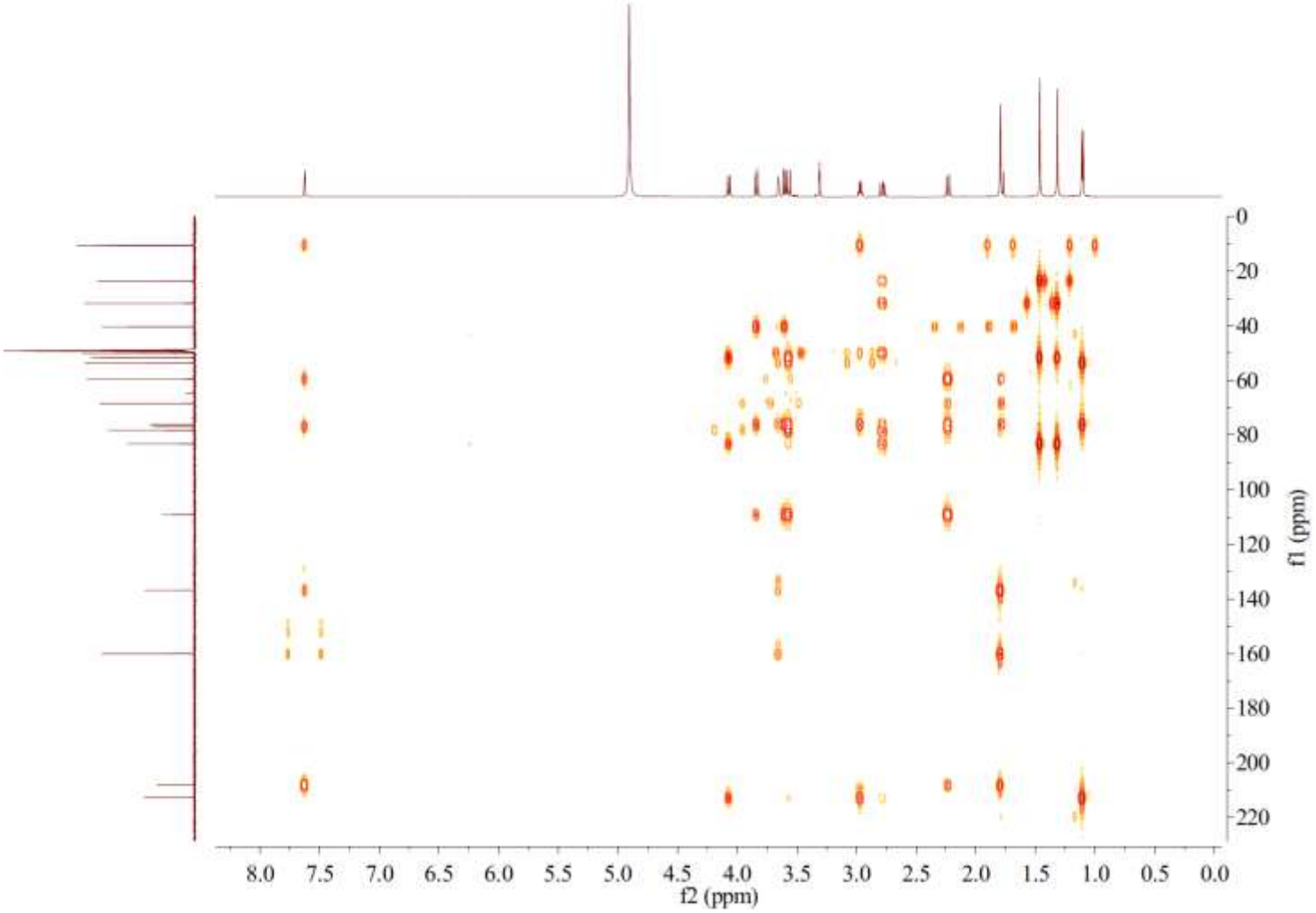


Figure S9. The enlarged HMBC spectrum of crotonol A (1) about correlation H-14/C-7 and H-5/C-4

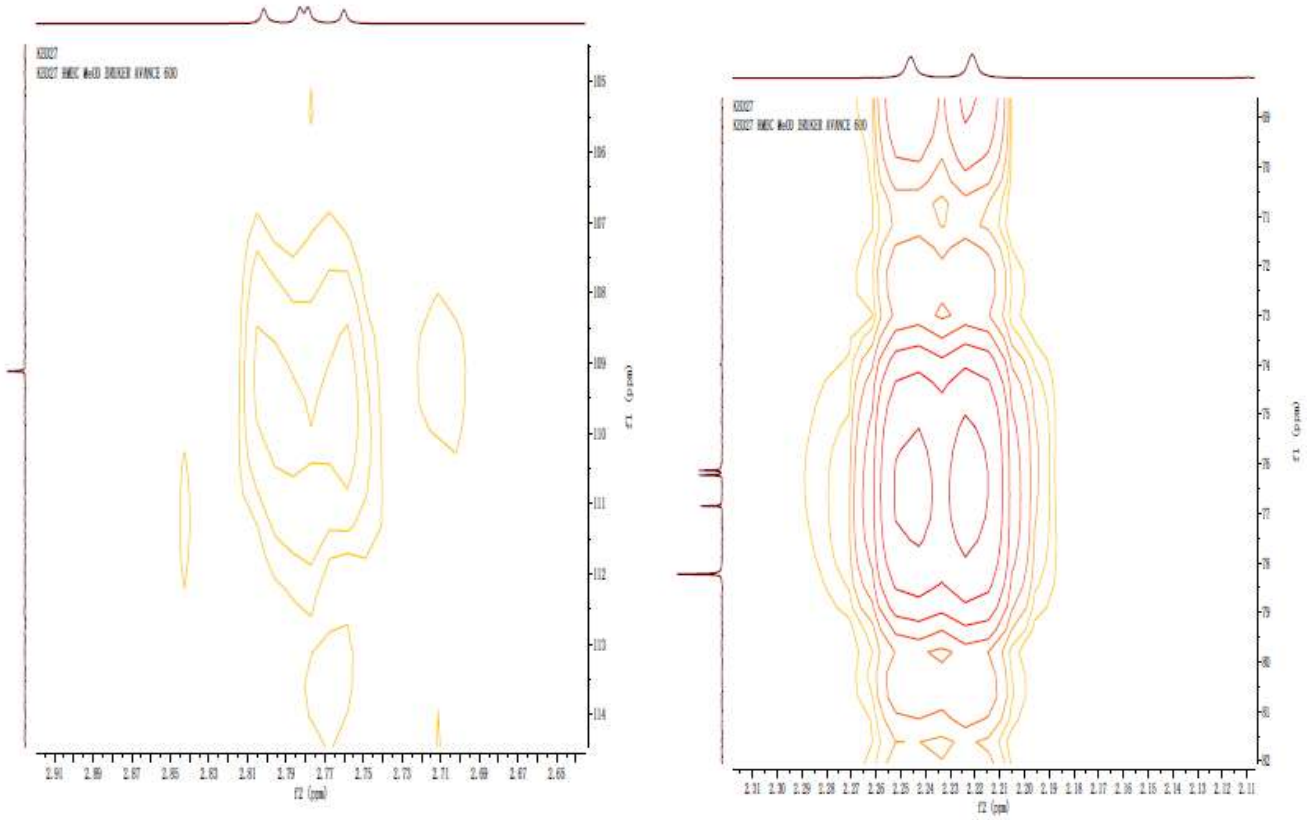


Figure S10. The enlarged HMBC spectrum of crotonol A (1) about the H-10/H-19b/H-8 signals and the C-13/C-4/C-9/C-6 signals

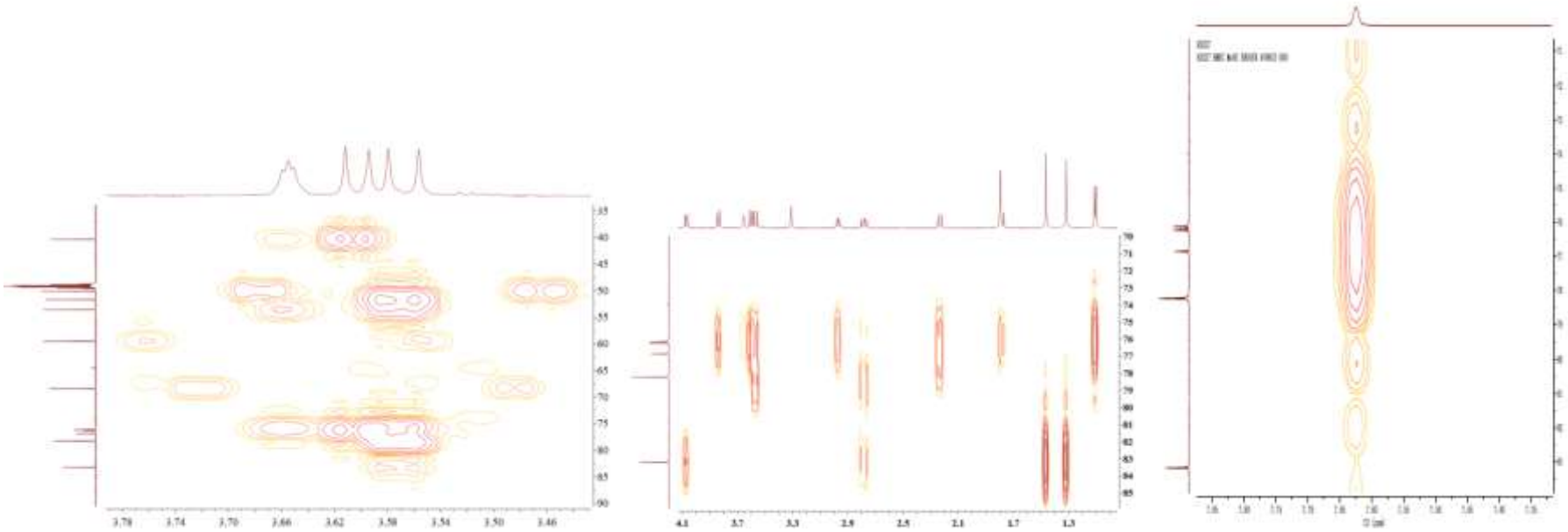


Figure S11. The NOESY spectrum of crotonol A (**1**) in CD_3OD

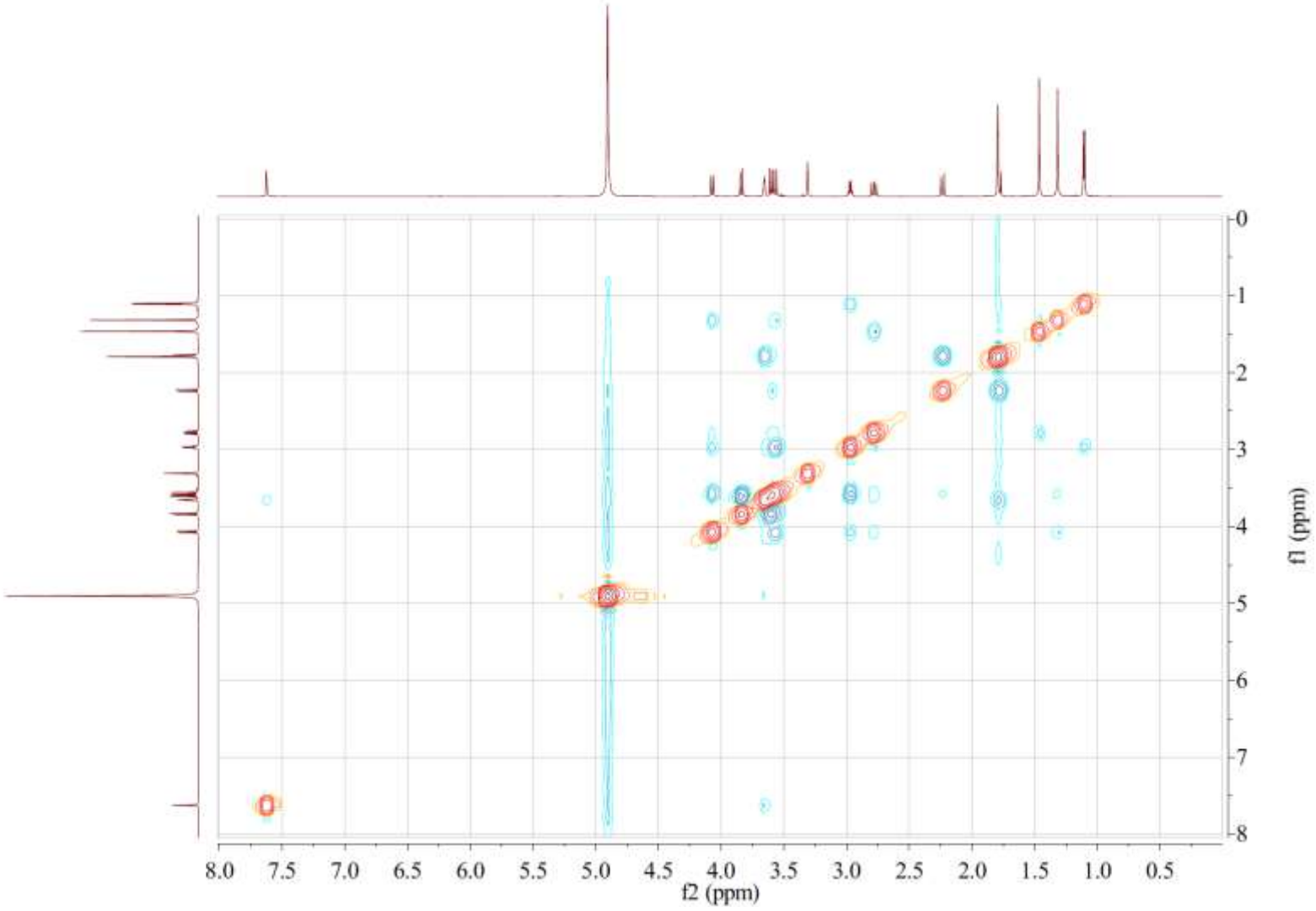


Figure S12. The enlarged NOESY spectrum of crotonol A (1) about H-10/H-19b/H-8 signals

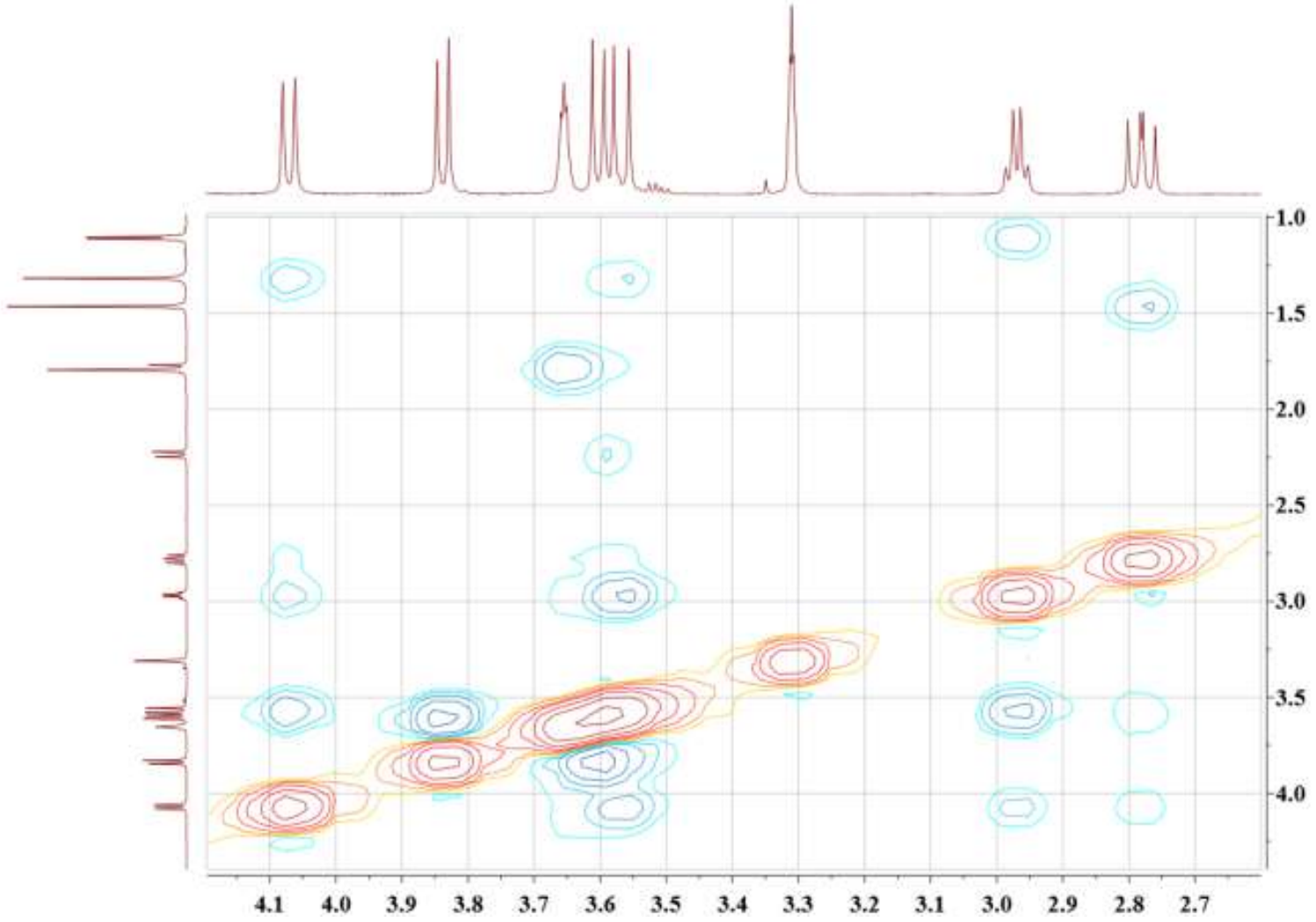


Figure S13. The HRESIMS spectrum of crotonol A (**1**)

Qualitative Analysis Report

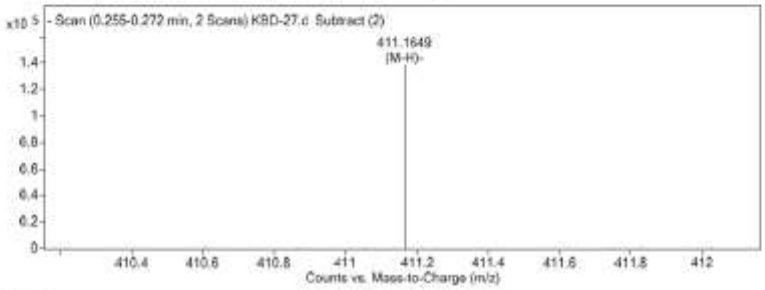
Data Filename	KBD-27.d	**Sample Name**	KBD-27
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	12/25/2015 4:12:24 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group **Info.**

Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
411.1649	1	138945.25	C20 H28 O9	(M-H)-
412.1685	1	35033.69	C20 H28 O9	(M-H)-
447.1412	1	15735.56		
474.1602	1	48911.79		
509.1412	1	12887.99		
525.1574	1	184300.78		
526.161	1	48794.4		
823.3359	1	17181.43		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H28 O9	412.1733	411.1661	411.1649	1.1	2.5	7.0000

--- End Of Report ---

Figure S14. The UV spectrum of crotonol A (**1**) in MeOH

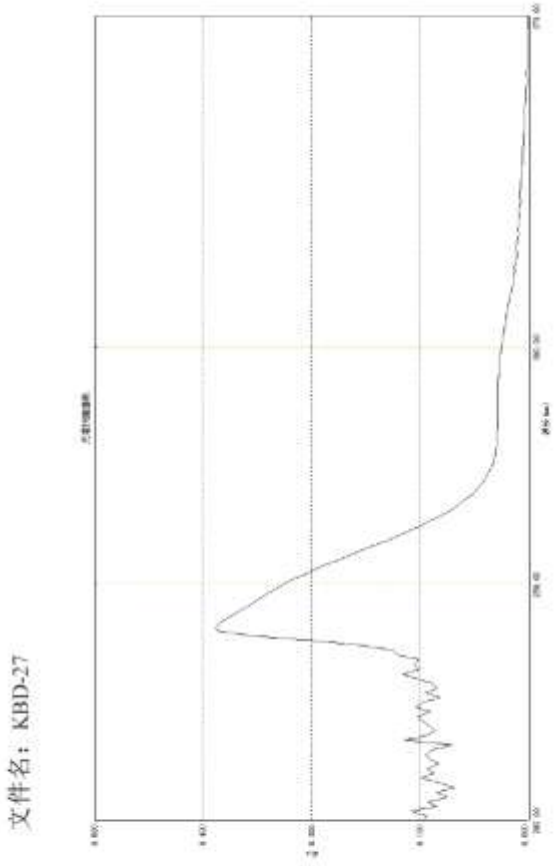


Figure S15. The ^{1}H NMR spectrum of crotonol B (**2**) in CD_3OD

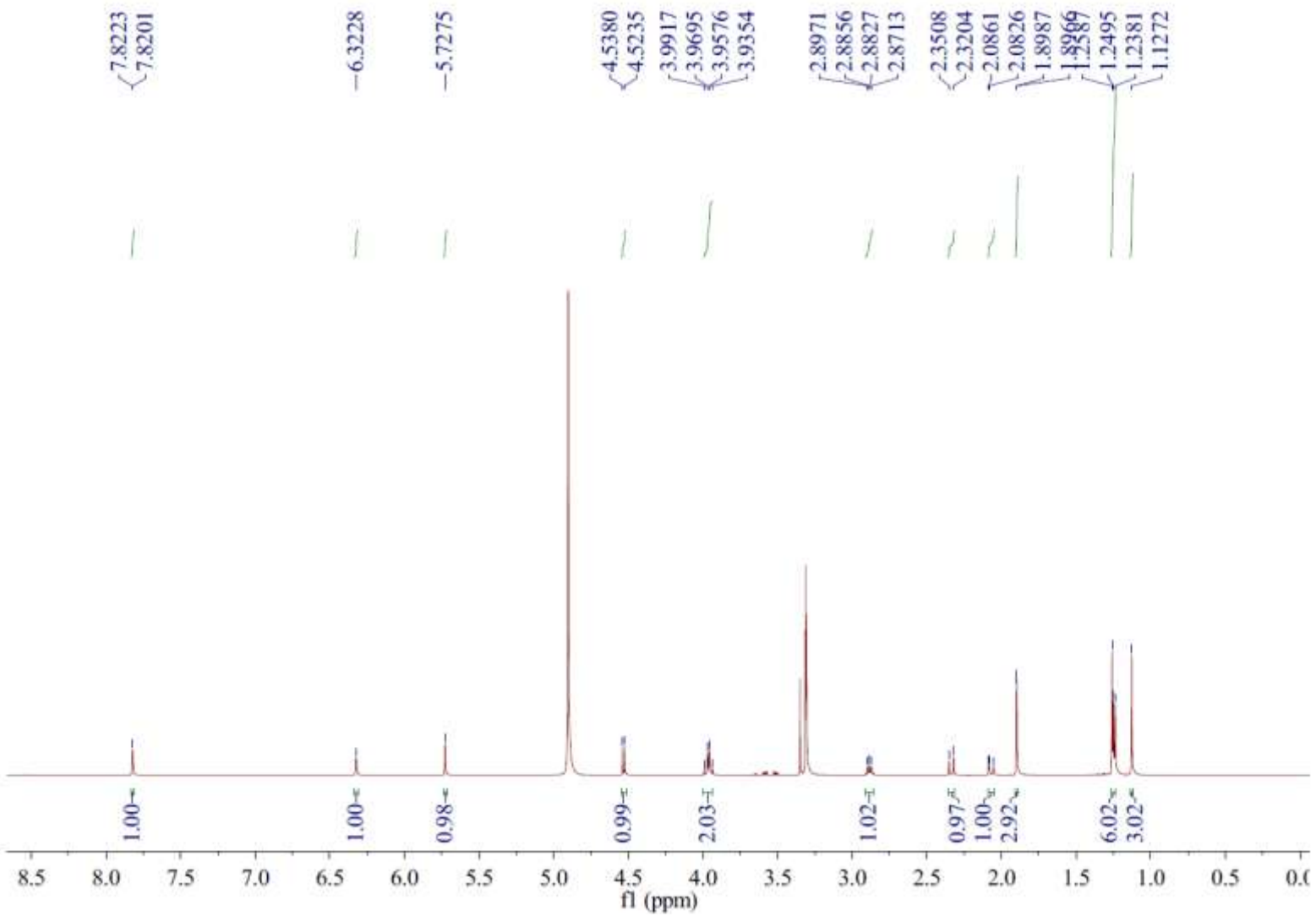


Figure S16. The ^{13}C NMR spectrum of crotonol B (**2**) in CD_3OD

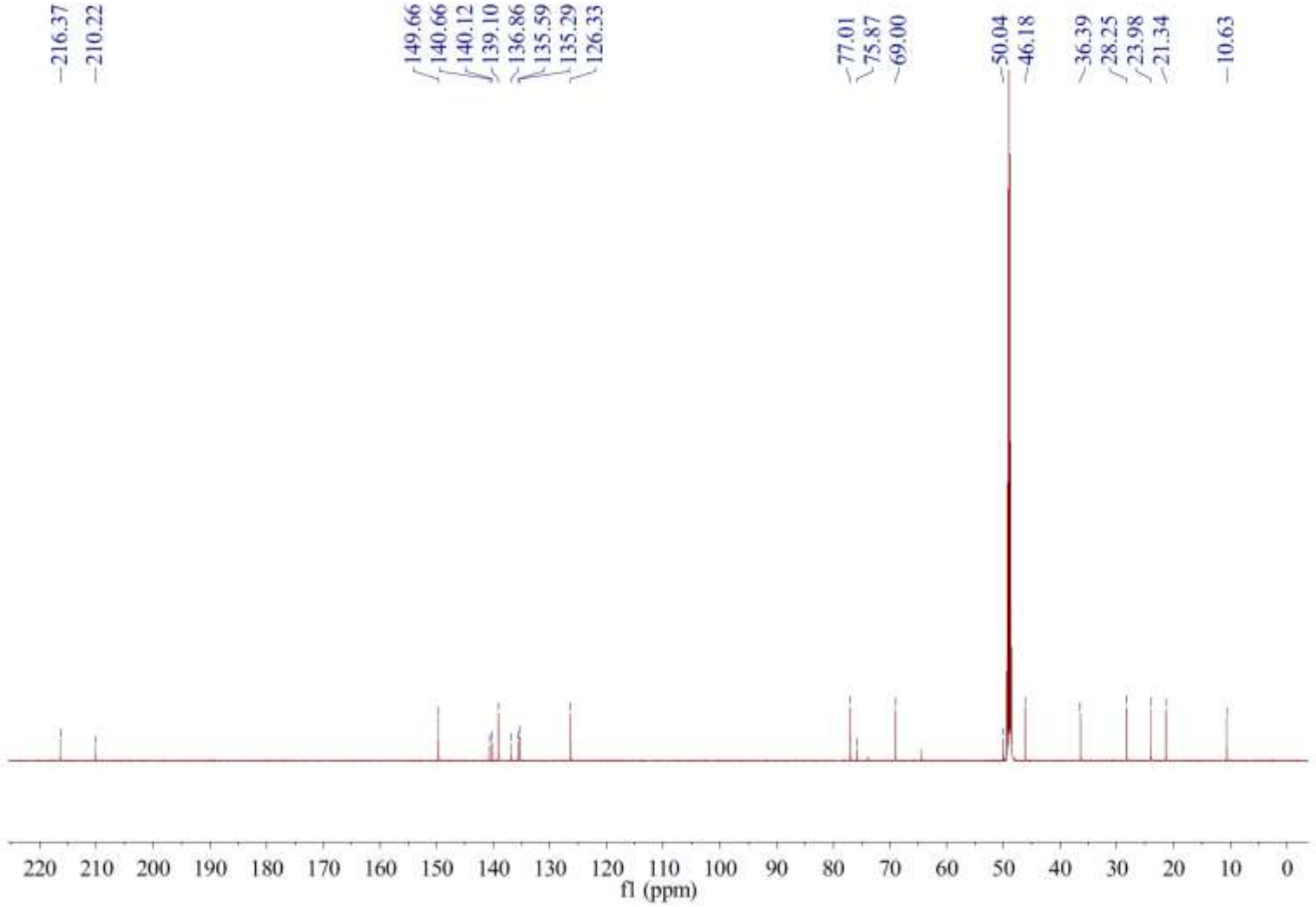


Figure S17. The HSQC spectrum of crotonol B (**2**) in CD_3OD

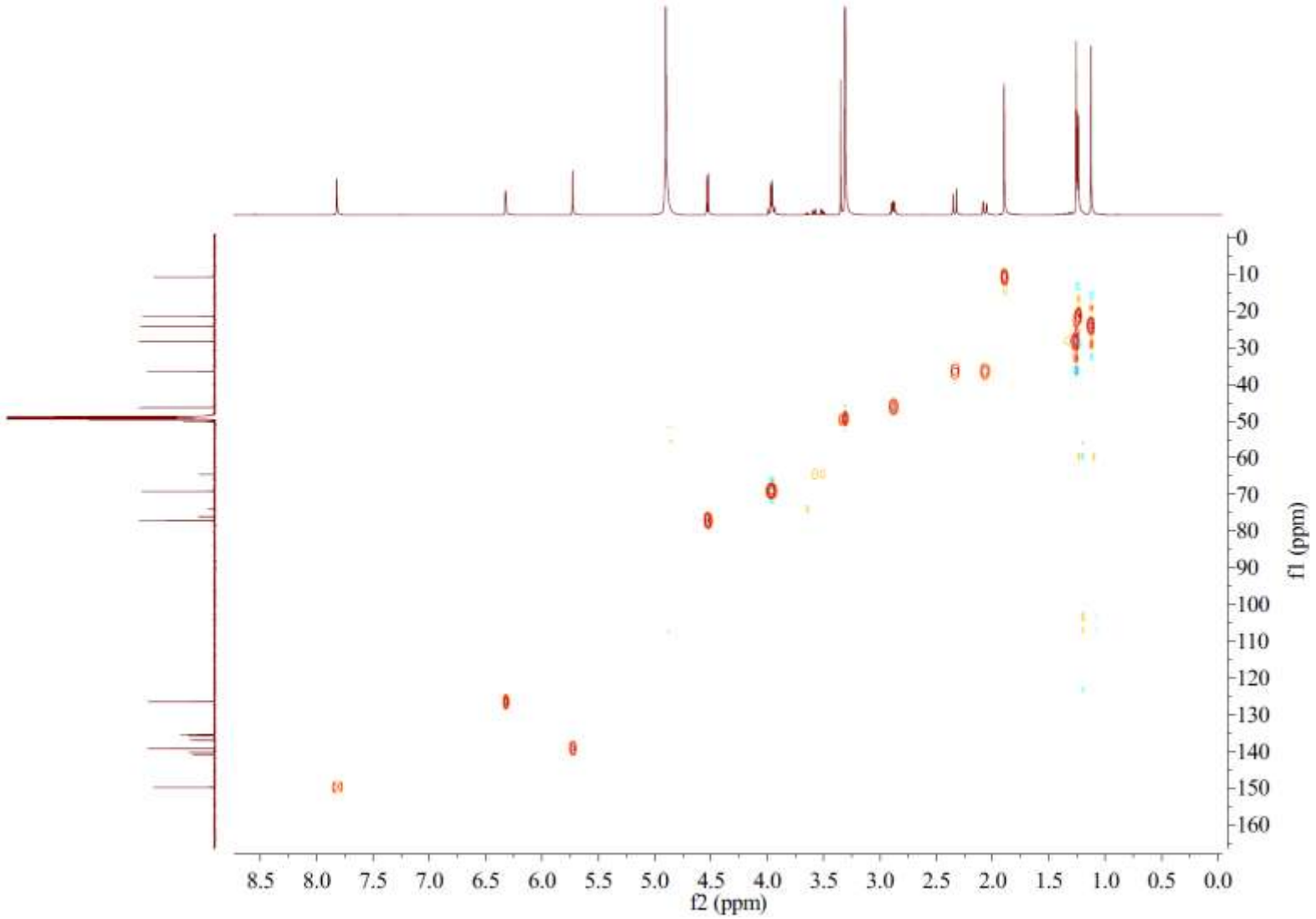


Figure S18. The ^{1}H-^{1}H COSY spectrum of crotonol B (**2**) in CD_3OD

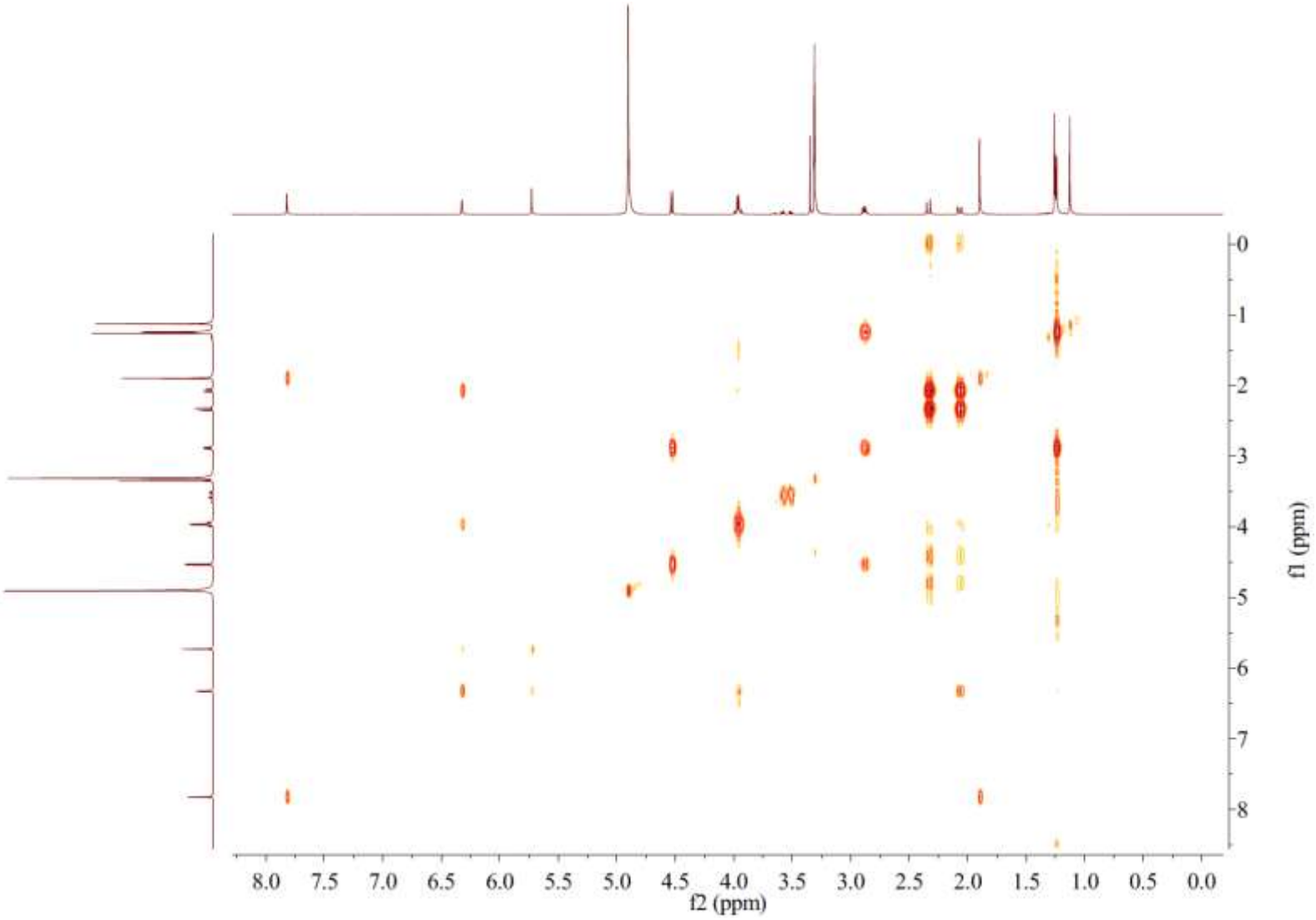


Figure S19. The HMBC spectrum of crotonol B (**2**) in CD_3OD

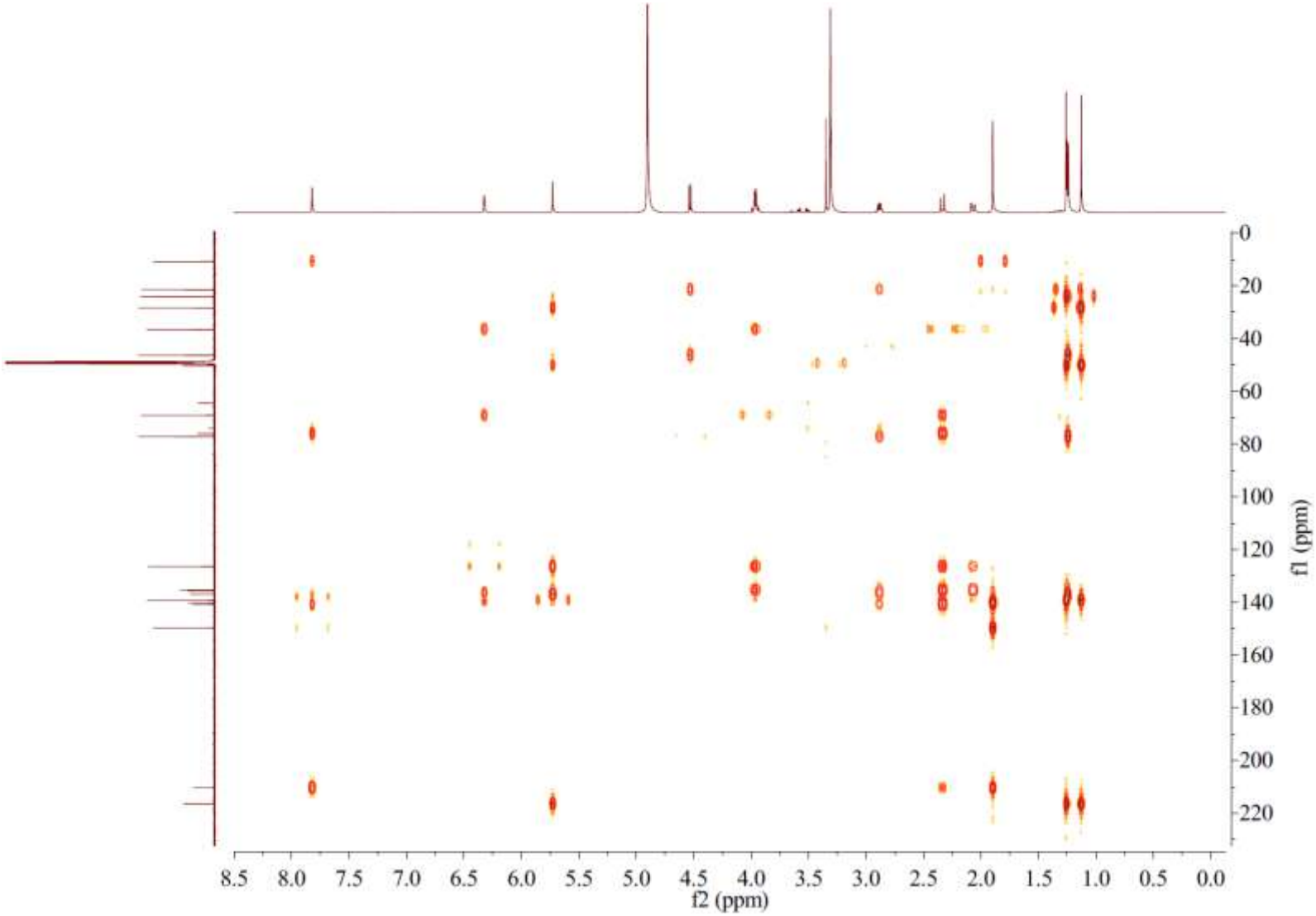


Figure S20. The enlarged HMBC spectrum of crotonol B (**2**) about correlation H12/C13

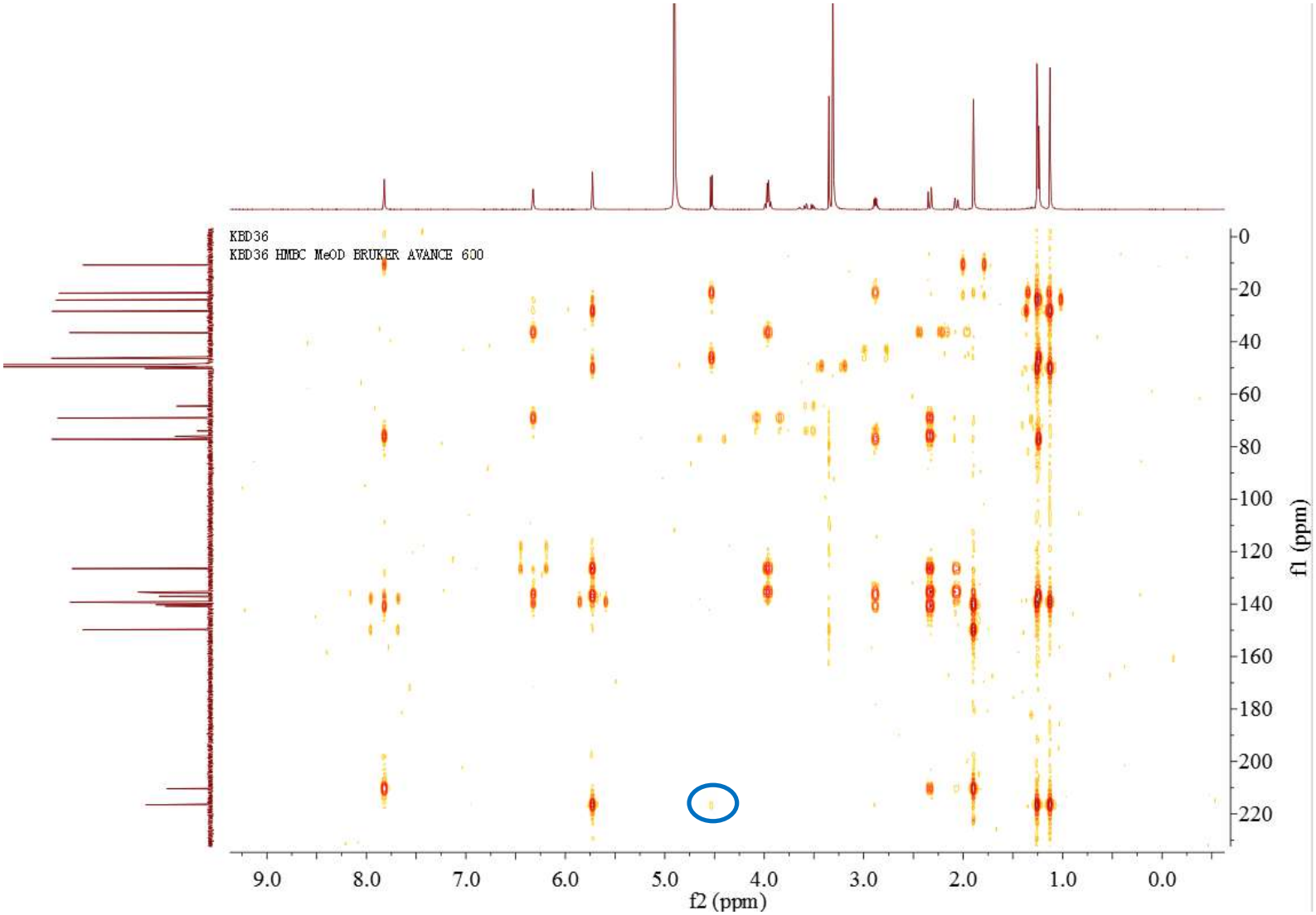


Figure S21. The enlarged HMBC spectrum of 2 between 135 and 141 ppm

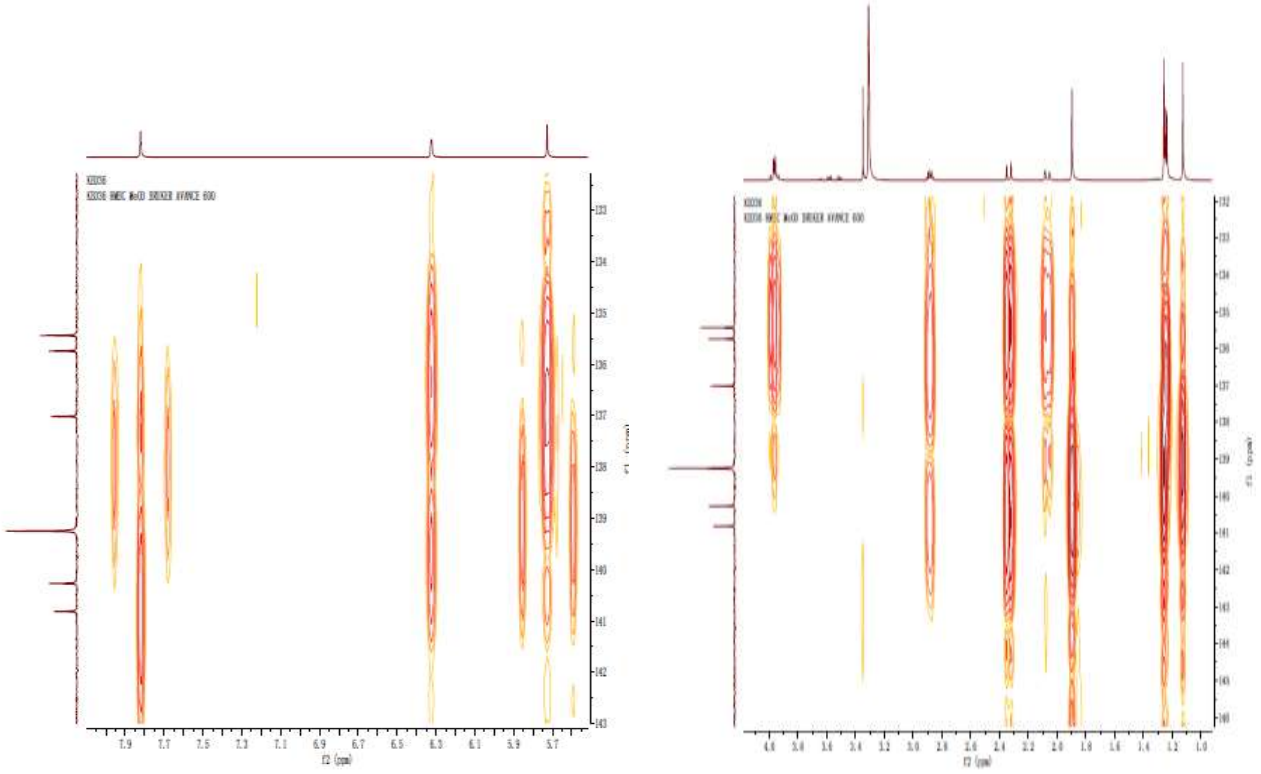
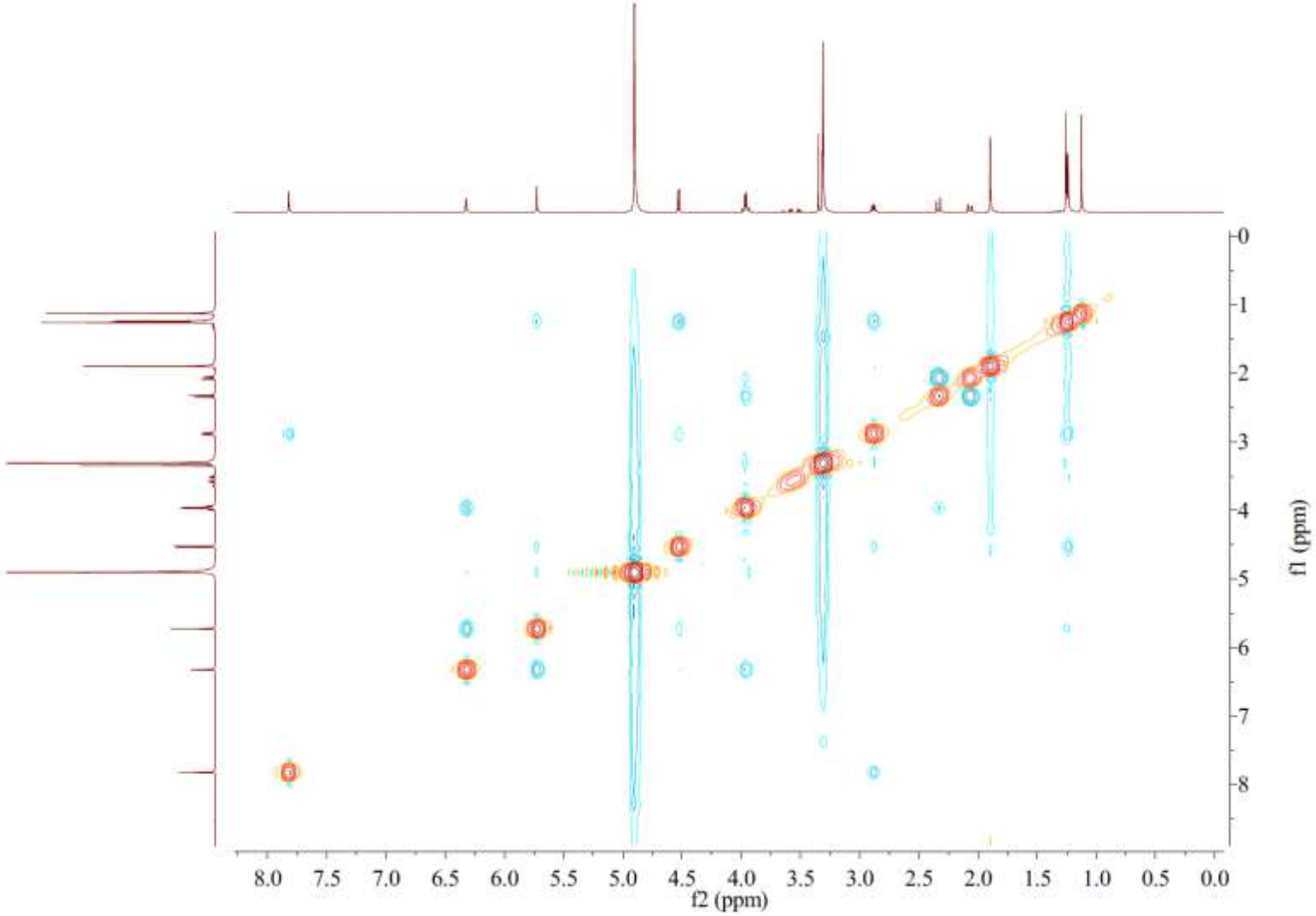


Figure S22. The NOESY spectrum of crotonol B (**2**) in CD_3OD



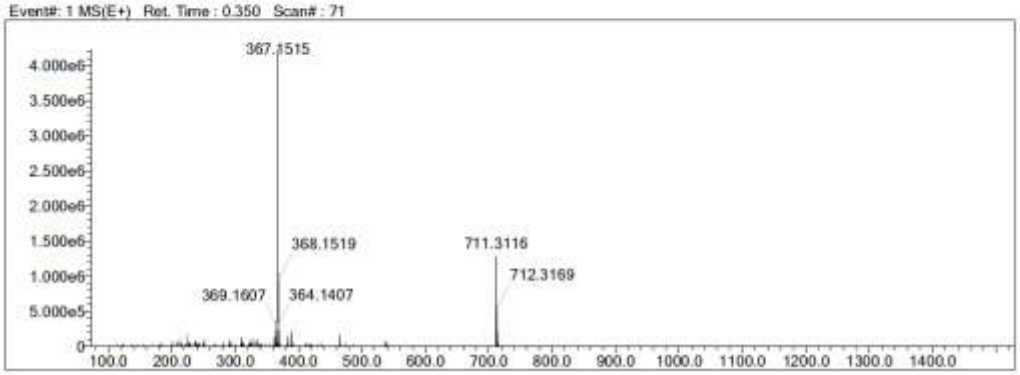
Formula Predictor Report - KBD36.lcd

Data File: E:\DATA\2016\0418\KBD36.lcd

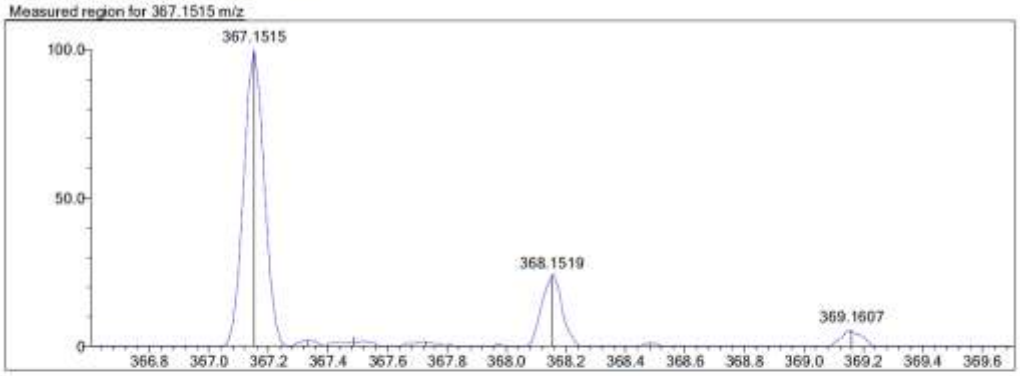
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	N	3	0	20	Si	4	0	0	Pt	2	0	0	Na
B	3	0	0	O	2	0	40	S	2	0	0					
C	4	0	80	F	1	0	0	Br	1	0	0					

Error Margin (ppm):	10	DBE Range:	-2.0 - 100.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	10

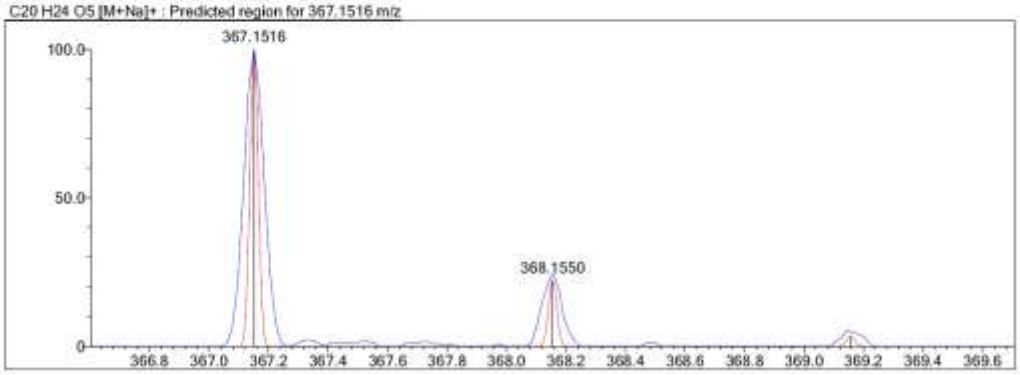
Event#: 1 MS(E+) Ret. Time : 0.350 Scan# : 71



Measured region for 367.1515 m/z



C20 H24 O5 [M+Na]+ : Predicted region for 367.1516 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	84.47	C20 H24 O5	[M+Na]+	367.1515	367.1516	-0.1	-0.27	84.47	9.0

Figure S23. The HRESIMS spectrum of crotonol B (**2**)

Figure S24. The UV spectrum of crotonol B (**2**) in MeOH

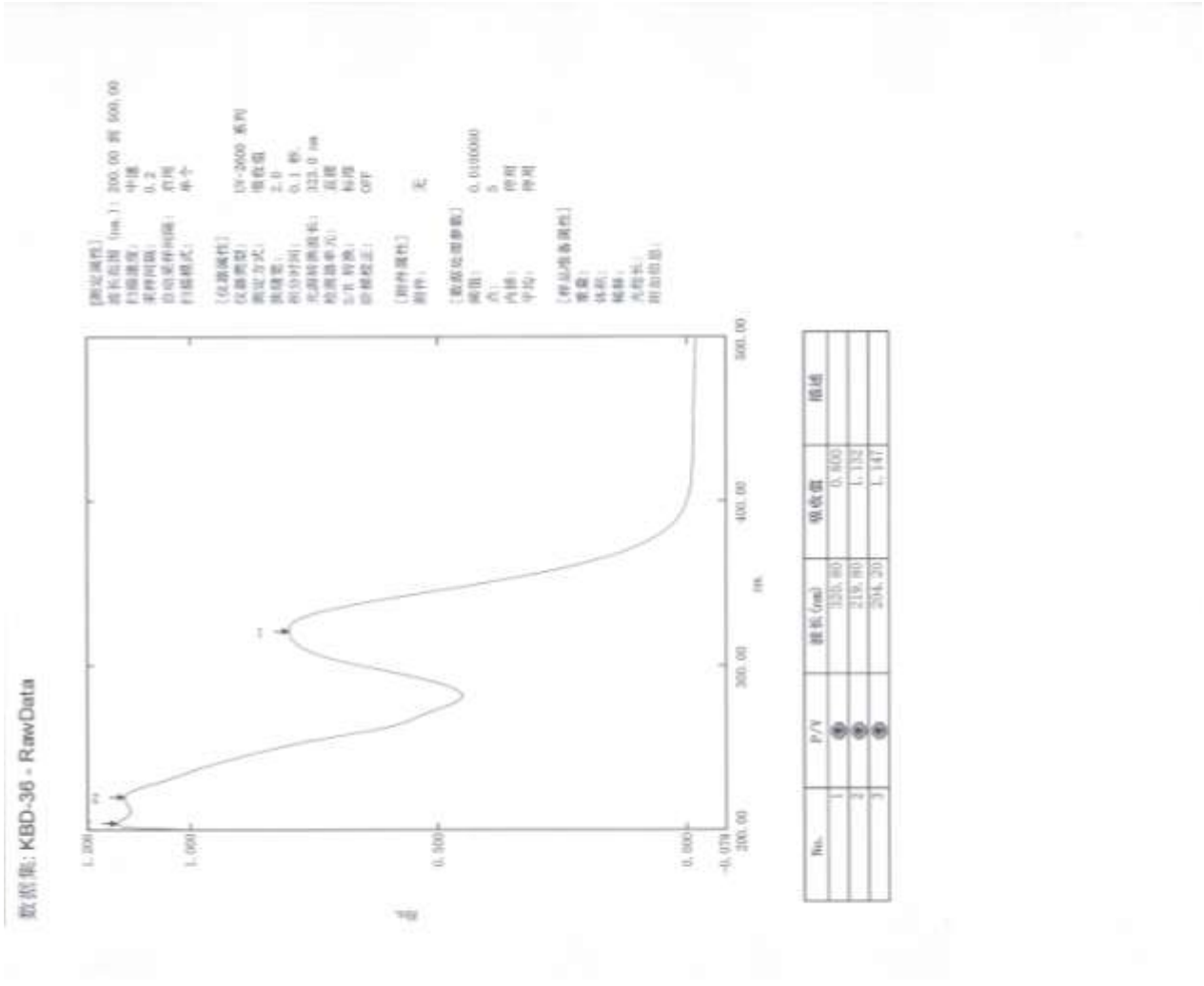


Figure S25. The MMFF calculations picture between H-11 and H-12