

# Supplementary Information for:

## Bioactivity of the Cannabigerol Cannabinoid and its Analogues – The role of Conformational Structure and Stability

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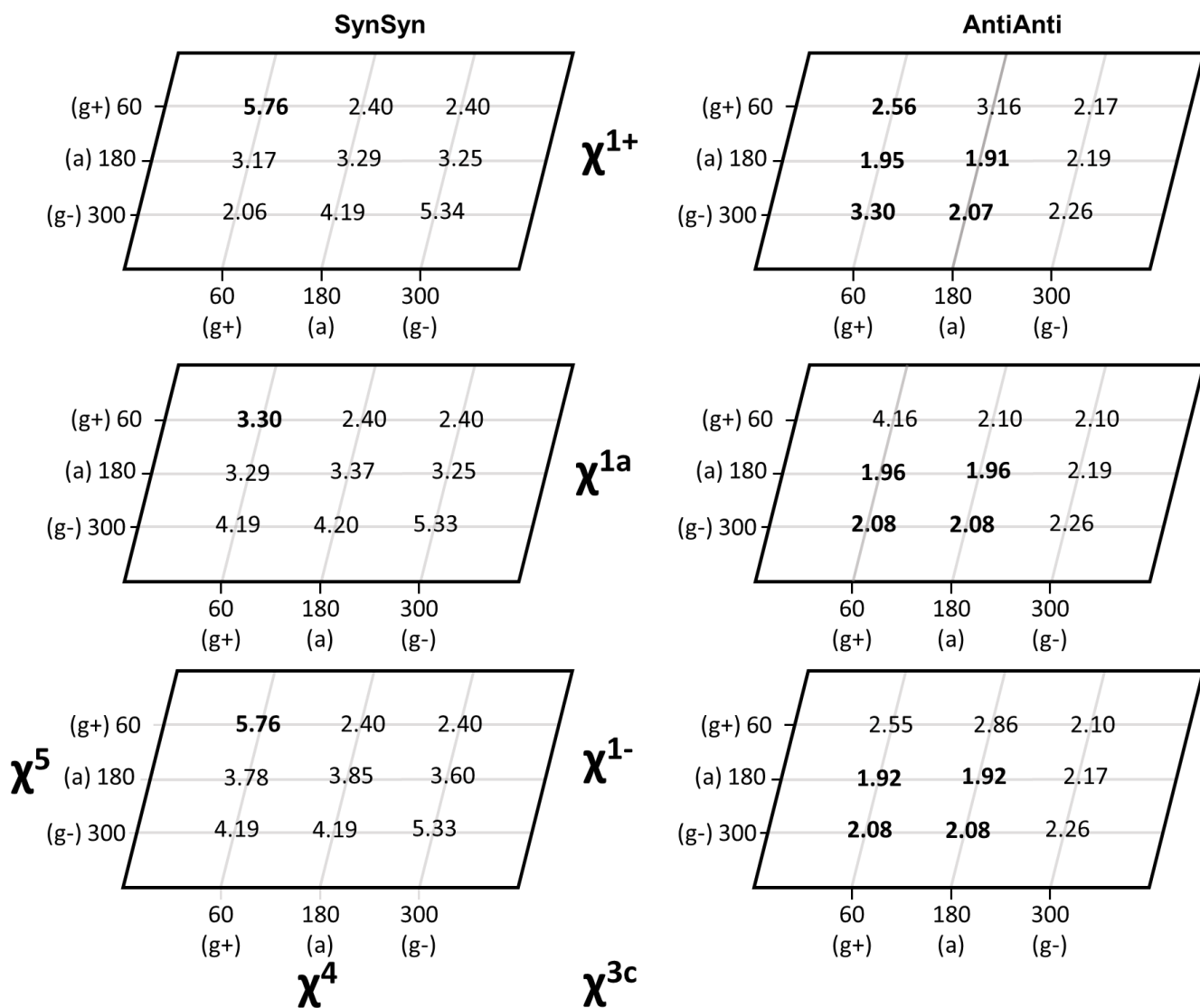
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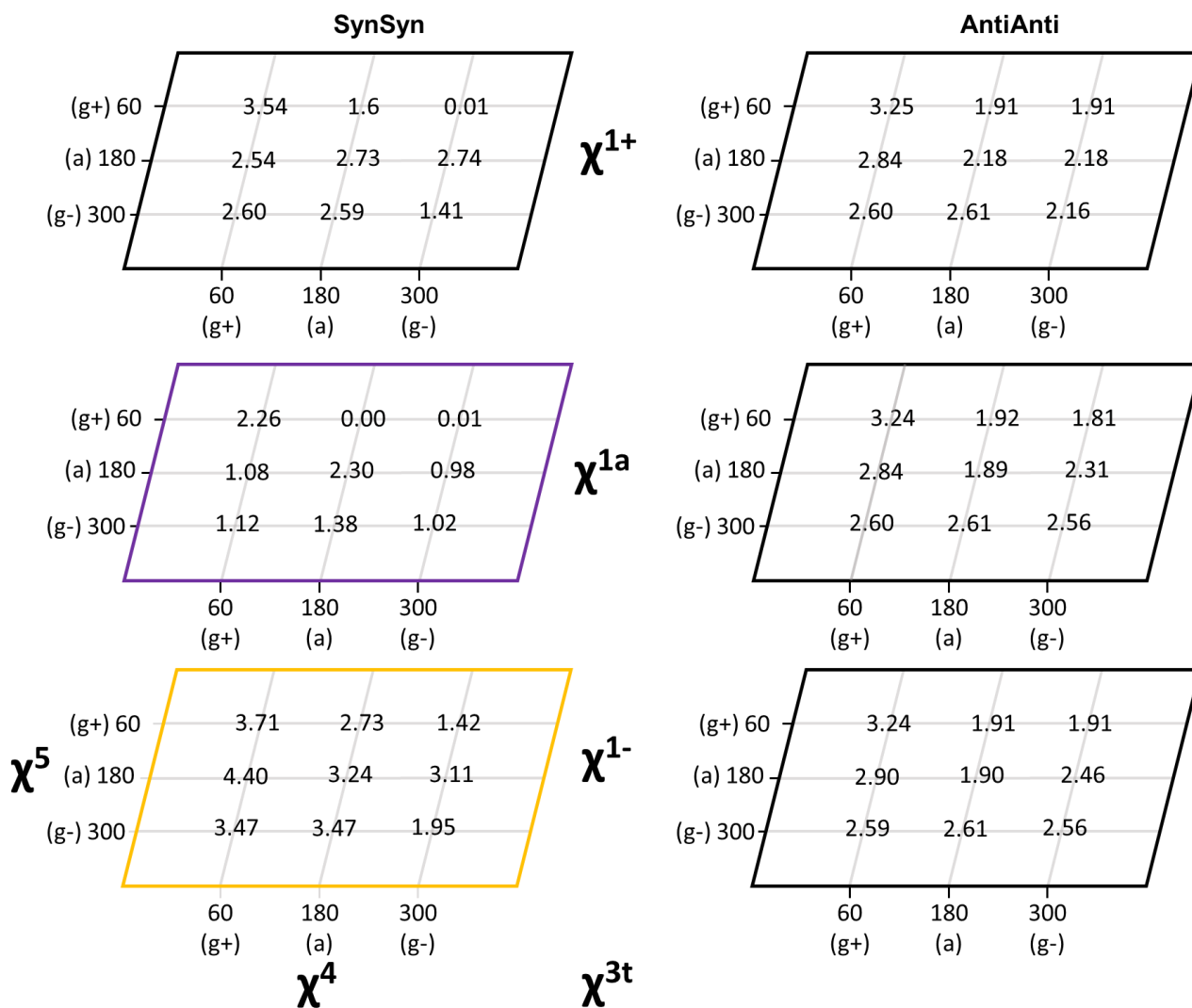
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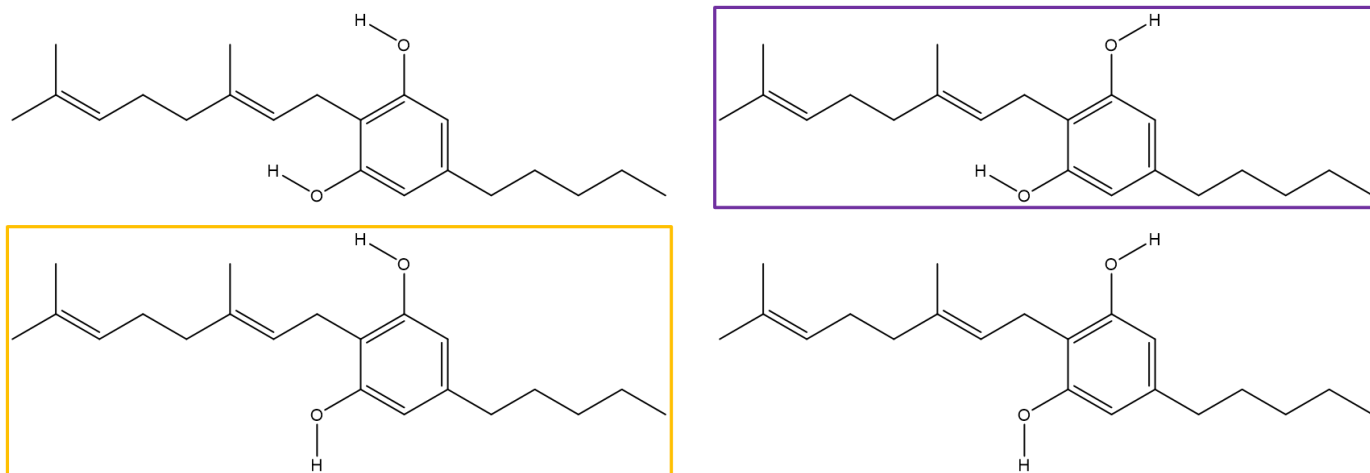
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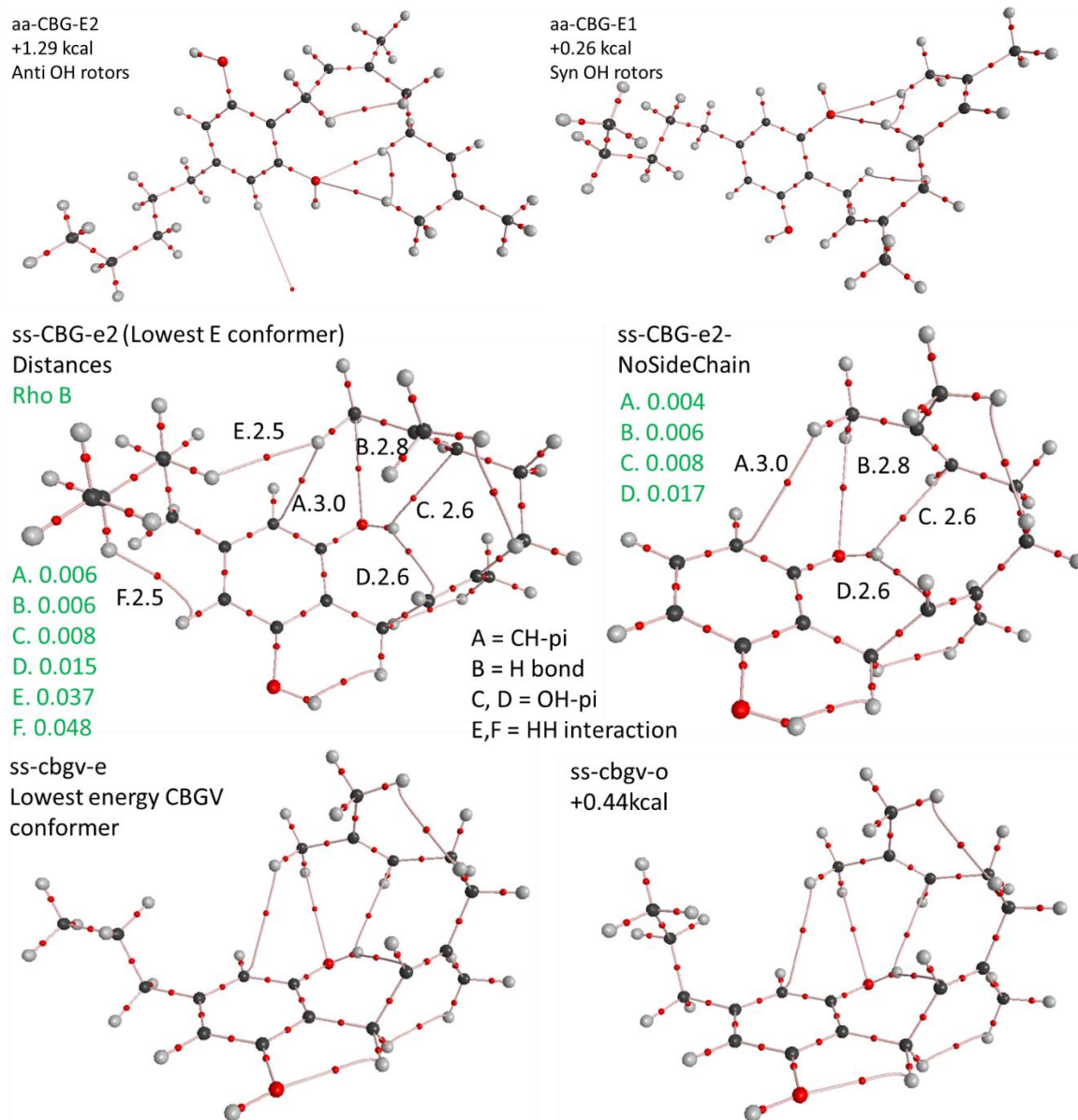
**Figure S1.** Ramachandran plots of the relative free-energies (kcal) for each of the differing geometries of the  $\chi^3$  *cis* isomers. The bold numbers highlight cases where alpha hydrogens bisected each other across opposite ends of the C=C double bond. Numbers that are adjacent and share the same value are indicative of degenerate cases or free-energy.



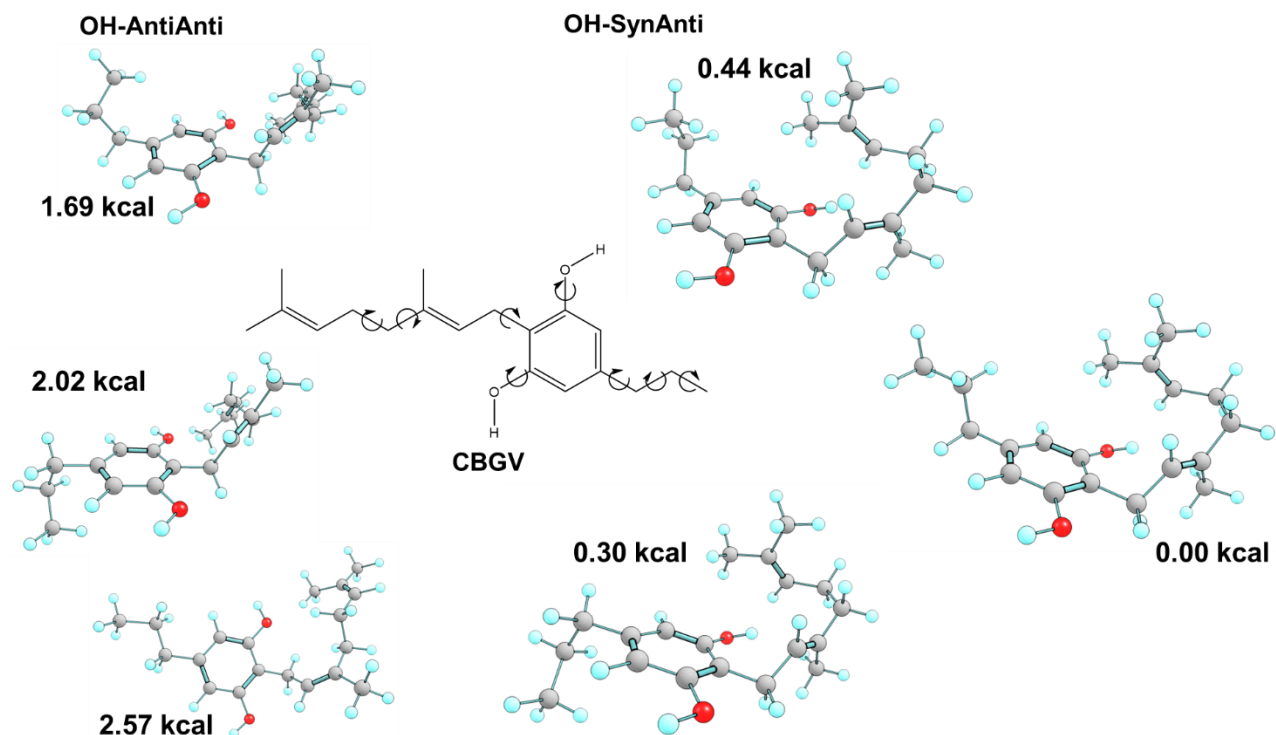
**Figure S2.** Ramachandran plots with the relative free energies (kcal) for each of the  $\chi^3$  *trans* conformers, with yellow and purple used to indicate differing structures resulting from differing orientations of the OH rotors (see **Figure S3**).



**Figure S3.** Schematic representation of the structural conformers generated by differing OH-rotor placements, defined relative to the geranyl chain. (*Top Left*) *syn-syn* conformer, (*Bottom Right*) *anti-anti*, (*Top Right* and *Bottom Left*) the mixed *anti-syn* and *syn-anti* cases, respectively.



**Figure S4** Molecular graphs plotted from the Atoms In Molecules (AIM) wavefunction analyses of the following CBG conformers: (*Top*) two *anti-anti* conformers, (*Middle Left*) the lowest free-energy conformer, (*Middle Right*) system conformer with H-atom as side-chain, (*Bottom*) two lowest free-energy conformers for CBGV; this conformer is devoid of the weakly-polar intra-molecular H-H interaction (between the geranyl and propyl side chains).

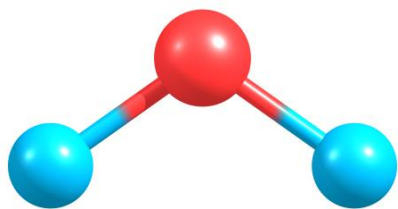


**Figure S5** CBGV Poses and relative energetics in kcal. Note the lowest energy conformer has the side chain extended outwards. CBGV's side chain is too short to successfully perform the H-H interaction stabilising the intramolecular 'staple'

## Exemplary Data Card of geometry optimised stationary points

**Example:** H<sub>2</sub>O molecule

### FILE NAME + Graphical Representation



### Cartesian Coordinates of all geometry optimised stationary points

Atom type	X	Y	Z
O	1.34146346	1.62020904	0.00000000
H	2.30146346	1.62020904	0.00000000
H	1.02100888	2.52514487	0.00000000

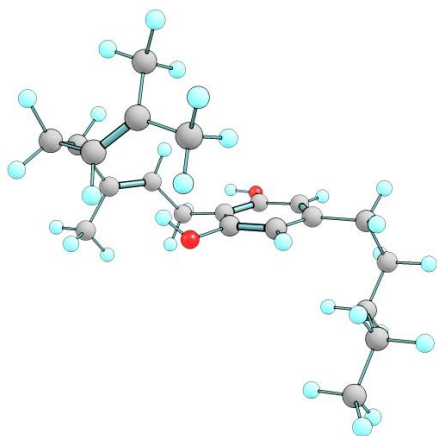
### Analytical frequencies of normal modes of vibration

Frequencies -- 1664.9645 3800.9563 3914.2425

### Thermodynamic properties reported

Zero-point correction= 0.021370 (Hartree/Particle)  
Thermal correction to Energy= 0.024205  
Thermal correction to Enthalpy= 0.025149  
Thermal correction to Gibbs Free Energy = 0.003713  
Sum of electronic and zero-point Energies = -76.398367  
Sum of electronic and thermal Energies = -76.395532  
Sum of electronic and thermal Enthalpies = -76.394588  
Sum of electronic and thermal Free Energies = -76.416024

**CBG**  
ss-CBG-U3



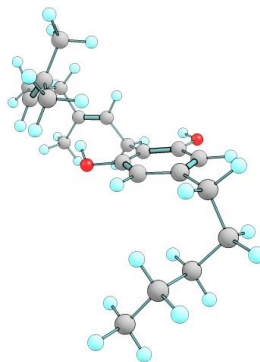
55 Atoms

C	-0.322421	-0.143469	-0.289287
C	-1.450953	0.447646	0.281379
C	-2.332993	-0.316874	1.05093
C	-2.051097	-1.670488	1.252639
C	-0.919986	-2.257916	0.677213
C	-0.039528	-1.513871	-0.130211
H	-1.617036	1.507798	0.122416
H	-2.702521	-2.291101	1.860273
O	0.489211	0.657166	-1.054745
H	1.416463	0.403651	-0.89927
O	-0.746939	-3.592908	0.934422
H	0.105454	-3.89054	0.590743
C	1.159422	-2.115537	-0.844509
C	2.466256	-1.560068	-0.325799
H	1.053398	-1.926012	-1.917019
H	1.165127	-3.209023	-0.745323
C	3.450163	-0.963015	-1.022002
H	2.579916	-1.629265	0.755786
C	4.639754	-0.382549	-0.289856
H	4.58724	-0.667968	0.765047
H	5.568945	-0.808969	-0.692303
C	4.733332	1.167592	-0.388787
C	3.432795	1.877758	-0.085794
H	5.061819	1.443997	-1.395999
H	5.529545	1.496144	0.290453
C	2.839326	1.993069	1.113154
H	2.910879	2.300898	-0.944124
C	1.499583	2.668805	1.269094
H	0.762155	1.971563	1.686827
H	1.566853	3.514325	1.96611
H	1.108076	3.027299	0.314642
C	3.452574	-0.771366	-2.519249
H	3.383173	0.292865	-2.77677
H	2.636797	-1.290138	-3.02483
H	4.39689	-1.132948	-2.943
C	3.424073	1.446094	2.391837
H	3.384778	2.199248	3.188281
H	4.46016	1.118205	2.285275
H	2.834261	0.589165	2.743352
C	-3.586449	0.294839	1.638483
H	-3.509734	1.386881	1.608421
H	-3.668444	0.017334	2.696461

Frequencies --	21.2300	24.9341	25.6674
Frequencies --	31.0639	39.7655	57.3746
Frequencies --	63.2080	84.6039	91.9227

Zero-point correction=	0.487662 (Hartree/Particle)
Thermal correction to Energy=	0.513948
Thermal correction to Enthalpy=	0.514893
Thermal correction to Gibbs Free Energy=	0.429460
Sum of electronic and zero-point Energies=	-969.567832
Sum of electronic and thermal Energies=	-969.541546
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Sum of electronic and thermal Free Energies=	-969.626034

**ss-CBG-u2**



55 Atoms

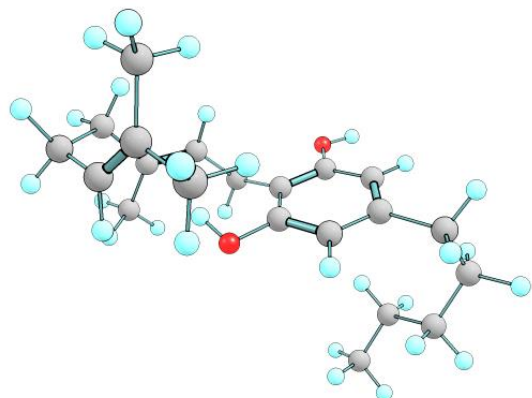
C	-0.331545	0.205912	0.294915
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C	-2.349532	0.490617	-1.014843
C	-2.034689	1.84407	-1.158449
C	-0.881624	2.375897	-0.571997
C	-0.013179	1.574248	0.191586
H	-1.670161	-1.392454	-0.177897
H	-2.676426	2.507437	-1.730259
O	0.464098	-0.647937	1.01833
H	1.396987	-0.412843	0.867343
O	-0.674922	3.715541	-0.774292
H	0.188823	3.974805	-0.427859
C	1.210844	2.111154	0.914697
C	2.493881	1.536079	0.358737
H	1.110983	1.882821	1.980238
H	1.249689	3.207039	0.858636
C	3.470606	0.890407	1.020826
H	2.593469	1.63557	-0.72188
C	4.63305	0.300921	0.252991
H	4.566325	0.610926	-0.794184
H	5.578758	0.698264	0.646768
C	4.694705	-1.252501	0.315034
C	3.373542	-1.926793	0.01942
H	5.035311	-1.559594	1.3093
H	5.471047	-1.58222	-0.386171
C	2.76317	-2.011569	-1.173593
H	2.852045	-2.348645	0.878677
C	1.406027	-2.65328	-1.322555
H	0.68075	-1.933181	-1.722406
H	1.445258	-3.490647	-2.031475
H	1.016915	-3.015099	-0.36844
C	3.490137	0.653864	2.511385
H	3.398333	-0.415596	2.737956
H	2.694779	1.176717	3.0445
H	4.449093	0.979861	2.931203
C	3.345235	-1.460721	-2.451847
C	3.282897	-2.203308	-3.256755
H	4.388542	-1.154147	-2.352712
H	2.768534	-0.58842	-2.786803
C	-3.627982	-0.058641	-1.609143
H	-3.544896	-1.144636	-1.722618
H	-3.767731	0.350286	-2.616933

Frequencies --	16.3917	24.7670	25.7267
Frequencies --	33.1665	43.8051	58.3892
Frequencies --	65.6944	89.3660	92.7062

Zero-point correction=	0.487790 (Hartree/Particle)
Thermal correction to Energy=	0.514001
Thermal correction to Enthalpy=	0.514946
Thermal correction to Gibbs Free Energy=	0.429672
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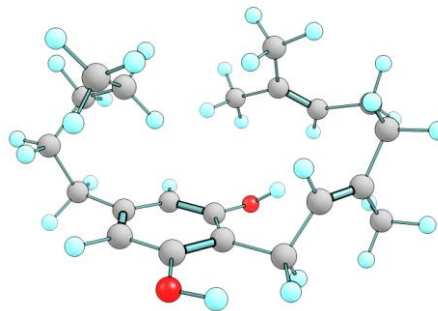
55 Atoms

C	-0.393797	0.00383	-0.188475
C	-1.41533	0.948817	-0.050992
C	-2.386358	0.795059	0.940311
C	-2.29838	-0.297249	1.810712
C	-1.274923	-1.238026	1.665037
C	-0.308611	-1.120931	0.650653
H	-1.439204	1.791476	-0.73388
H	-3.039533	-0.428588	2.596038
O	0.507314	0.197495	-1.203794
H	1.3821	-0.116805	-0.912158
O	-1.177993	-2.322644	2.498041
H	-1.910706	-2.304371	3.128722
C	0.775825	-2.164149	0.444199
C	2.159314	-1.583248	0.625437
H	0.664043	-2.600268	-0.554031
H	0.623434	-2.975015	1.162376
C	3.190877	-1.585601	-0.238325
H	2.302693	-1.07392	1.578545
C	4.476738	-0.875776	0.126192
H	4.41458	-0.530274	1.162651
H	5.317595	-1.581455	0.07222
C	4.802219	0.339251	-0.7885
C	3.636546	1.284801	-0.971975
H	5.123978	-0.024151	-1.770067
H	5.667866	0.857318	-0.358166
C	3.142344	2.137258	-0.060027
H	3.122564	1.224773	-1.931326
C	1.917976	2.972031	-0.342067
H	1.117202	2.732967	0.369568
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H	1.526598	2.798112	-1.346582
C	3.168686	-2.225551	-1.605517
H	3.252595	-1.465721	-2.39255
H	2.264629	-2.805127	-1.798008
H	4.030674	-2.892853	-1.724113
C	3.726424	2.317865	1.319405
H	3.855298	3.382856	1.548822
H	4.692028	1.824029	1.446279
H	3.041564	1.916322	2.078101
C	-3.551574	1.752822	1.040337
H	-3.30328	2.682568	0.515003
H	-3.720538	2.018248	2.09139

Frequencies --	19.1566	21.5965	25.9830
Frequencies --	36.9239	46.7935	54.4929
Frequencies --	66.4168	76.4720	90.3475

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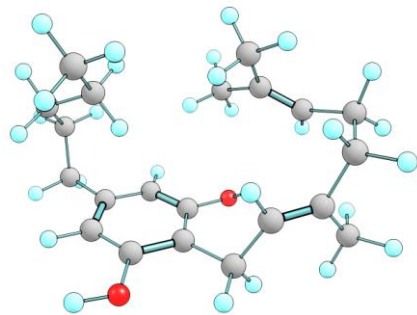
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C	-2.574478	-1.705654	0.056245
C	-1.354374	-2.244266	0.475356
C	-0.148063	-1.90811	-0.167105
H	-1.433636	0.261134	-2.472661
H	-3.473576	-1.982991	0.597427
O	0.911659	-0.602852	-1.90482
H	1.610937	-0.420252	-1.252356
O	-1.418371	-3.113352	1.532357
H	-0.52853	-3.372742	1.804644
C	1.206946	-2.461258	0.238459
C	2.068059	-1.378919	0.848833
H	1.686481	-2.895876	-0.643583
H	1.098652	-3.292141	0.948507
C	3.294051	-0.975968	0.472076
H	1.58377	-0.835286	1.659851
C	3.927221	0.217695	1.151312
H	3.28937	0.536463	1.981101
H	4.895849	-0.069099	1.583618
C	4.163081	1.425267	0.198589
C	2.983406	1.770093	-0.684382
H	5.026789	1.212681	-0.439556
H	4.450131	2.28373	0.818634
C	1.815811	2.311962	-0.301295
H	3.097184	1.52948	-1.741531
C	0.709003	2.582162	-1.290126
H	-0.207404	2.05661	-0.99925
H	0.464889	3.652501	-1.314264
C	0.972248	2.258928	-2.299811
C	4.108176	-1.605522	-0.63209
H	4.256036	-0.90133	-1.460191
H	3.658169	-2.511546	-1.040703
H	5.107518	-1.862953	-0.2613
C	1.491468	2.682524	1.124753
H	1.050709	3.685758	1.173452
H	2.362076	2.660906	1.78352
H	0.740567	1.993633	1.53312
C	-3.926065	-0.114865	-1.361436
H	-4.696708	-0.870634	-1.561239
H	-3.794669	0.452643	-2.290227
C	-4.45751	0.835841	-0.265096
H	-4.693306	0.25456	0.633838
H	-5.414689	1.237381	-0.620678
C	-3.539103	2.019935	0.099902
H	-3.157903	2.470109	-0.827349
H	-4.158299	2.791664	0.577615
C	-2.351006	1.728794	1.038508
H	-1.801013	2.668239	1.181278
H	-1.651113	1.036289	0.56333
C	-2.751092	1.172402	2.408683
H	-3.192902	0.17481	2.322425
H	-1.877615	1.085882	3.064086
H	-3.480771	1.822332	2.90664

Frequencies --	24.8953	33.7288	37.9852
Frequencies --	44.3797	59.3109	64.8072
Frequencies --	68.7141	75.8105	103.9804

Zero-point correction= 0.488213 (Hartree/Particle)  
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 Thermal correction to Enthalpy= 0.515088  
 Thermal correction to Gibbs Free Energy= 0.432242  
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 Sum of electronic and thermal Energies= -969.541956  
 Sum of electronic and thermal Enthalpies= -969.541012  
 Sum of electronic and thermal Free Energies= -969.623858

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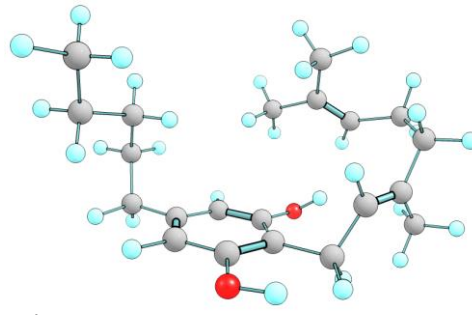
55 Atoms

C	0.236699	1.09175	-1.184398
C	1.46023	0.611551	-1.651801
C	2.642623	0.925825	-0.975568
C	2.581133	1.757084	0.146212
C	1.350682	2.247736	0.598837
C	0.151425	1.931384	-0.058164
H	1.466006	-0.050625	-2.51129
H	3.489052	2.002751	0.691566
O	-0.893588	0.733348	-1.878209
H	-1.599235	0.537349	-1.236453
O	1.267144	3.059316	1.70042
H	2.156034	3.215379	2.047793
C	-1.193741	2.44946	0.416977
C	-2.057786	1.31539	0.918148
H	-1.683831	2.984542	-0.402715
C	-1.030376	3.173314	1.220554
H	-3.276677	0.934535	0.496672
H	-1.58308	0.712875	1.692854
C	-3.915632	-0.304419	1.084218
H	-3.291832	-0.672238	1.904176
H	-4.893879	-0.050728	1.51603
C	-4.127779	-1.450368	0.053121
C	-2.928858	-1.733839	-0.825894
H	-4.979752	-1.200863	-0.587657
H	-4.423137	-2.347432	0.612013
C	-1.757466	-2.271101	-0.448802
H	-3.028292	-1.440884	-1.871113
C	-0.624745	-2.462848	-1.426091
H	0.267334	-1.920484	-1.092814
H	-0.34452	-3.522549	-1.492384
H	-0.878835	-2.103293	-2.425815
C	-4.079517	1.637235	-0.57146
H	-4.222458	0.987583	-1.443984
H	-3.620494	2.564517	-0.917697
H	-5.08139	1.875811	-0.194559
C	-1.449252	-2.701965	0.963864
H	-0.964438	-3.685673	0.973702
H	-2.334509	-2.752099	1.601449
H	-0.740842	-2.001136	1.424894
C	3.943048	0.269458	-1.377231
H	4.782662	0.81413	-0.929377
H	4.069171	0.329471	-2.465274
C	4.032839	-1.215811	-0.952576
H	5.006496	-1.593524	-1.28765
H	3.275683	-1.792732	-1.499484
C	3.873732	-1.466675	0.561505
H	4.474438	-2.340439	0.847024
H	4.296714	-0.6174	1.116701
C	2.42968	-1.708082	1.030096
H	2.039359	-2.6022	0.525526
H	1.789599	-0.877779	0.716889
C	2.325485	-1.886059	2.546941
H	2.661906	-0.982783	3.069424
H	1.294418	-2.085673	2.857942
H	2.946851	-2.719951	2.894411
H	-3.480771	1.822332	2.90664

Frequencies -- 23.1074 37.0585 40.8768  
 Frequencies -- 51.9819 61.6170 68.4963  
 Frequencies -- 74.4033 90.8889 96.6143

Zero-point correction= 0.488554 (Hartree/Particle)  
 Thermal correction to Energy= 0.514414  
 Thermal correction to Enthalpy= 0.515358  
 Thermal correction to Gibbs Free Energy= 0.432915  
 Sum of electronic and zero-point Energies= -969.570375  
 Sum of electronic and thermal Energies= -969.544515  
 Sum of electronic and thermal Enthalpies= -969.543571  
 Sum of electronic and thermal Free Energies= -969.626014

ss-cbg-e2.log



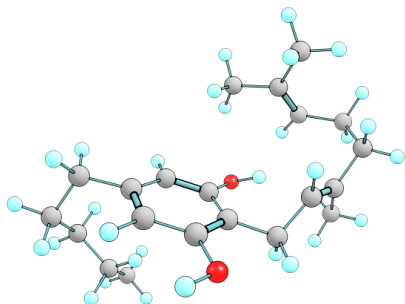
55 Atoms

C	0.08208	-1.116477	-1.159572
C	-1.15403	-0.743352	-1.680094
C	-2.334607	-1.114654	-1.025354
C	-2.245659	-1.868569	0.145093
C	-0.999435	-2.257354	0.653596
C	0.195067	-1.90633	0.003114
H	-1.175678	-0.13133	-2.575486
H	-3.137715	-2.161064	0.689662
O	1.206168	-0.710439	-1.839079
H	1.875769	-0.440121	-1.186807
O	-1.033813	-3.002023	1.80333
H	-0.13706	-3.149594	2.131154
C	1.573745	-2.32447	0.486014
C	2.357233	-1.137476	0.998096
C	2.098121	-2.817251	-0.338253
H	1.499125	-3.084362	1.275206
C	3.552483	-0.682285	0.582571
H	1.835592	-0.562362	1.762841
C	4.097343	0.608008	1.153907
H	3.475107	0.915808	1.999475
H	5.111357	0.44614	1.544299
C	4.154625	1.77222	0.121586
C	2.888443	1.943177	-0.68868
H	4.991531	1.603438	-0.563817
H	4.395657	2.689922	0.672306
C	1.703109	2.394608	-0.24832
H	2.946694	1.628458	-1.73061
C	0.496363	2.457338	-1.15121
H	-0.320841	1.847972	-0.745695
H	0.117222	3.484834	-1.227305
H	0.715256	2.086988	-2.155337
C	4.408159	-1.33915	-0.473418
H	4.524438	-0.683949	-1.34572
H	4.010899	-2.293215	-0.823348
H	5.41703	-1.516409	-0.082155
C	1.453365	2.848758	1.168334
H	0.926823	3.811011	1.179425
H	2.36864	2.955867	1.754112
H	0.803091	2.13183	1.687253
C	-3.67183	-0.624551	-1.537199
H	-4.477802	-1.110587	-0.977893
H	-3.797788	-0.921024	-2.58605
C	-3.820055	0.911886	-1.444553
H	-4.824264	1.186097	-1.793942
H	-3.112633	1.375998	-2.142866
C	-3.585025	1.496334	-0.044139
H	-2.561941	1.26025	0.277931
H	-3.641156	2.591536	-0.106588
C	-4.568695	1.008115	1.025839
H	-4.489093	-0.080503	1.130987
H	-5.596443	1.211035	0.694266
C	-4.32423	1.662	2.389121
H	-4.424453	2.751912	2.327811
H	-5.032627	1.302206	3.142664
H	-3.31237	1.443514	2.750082
H	-3.480771	1.822332	2.90664

Frequencies -- 17.1448 23.8720 29.4323  
 Frequencies -- 39.3377 44.0112 50.3915  
 Frequencies -- 62.4471 92.4218 97.6149

Zero-point correction= 0.487867 (Hartree/Particle)  
 Thermal correction to Energy= 0.514061  
 Thermal correction to Enthalpy= 0.515005  
 Thermal correction to Gibbs Free Energy= 0.430012  
 Sum of electronic and zero-point Energies= -969.568610  
 Sum of electronic and thermal Energies= -969.542416  
 Sum of electronic and thermal Enthalpies= -969.541472  
 Sum of electronic and thermal Free Energies= -969.626465

ss-cbg-e1.log

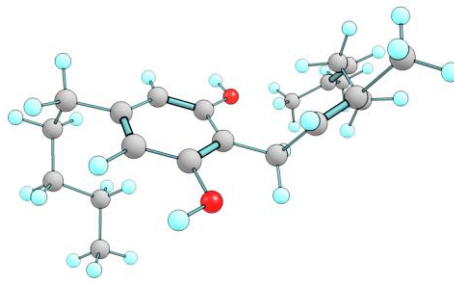


55 Atoms

C	0.393817	-0.003913	-0.188549
C	1.415213	-0.949052	-0.051109
C	2.386257	-0.795481	0.940259
C	2.298322	0.296714	1.810791
C	1.274973	1.23762	1.665165
C	0.308726	1.120777	0.650684
H	1.439025	-1.791615	-0.734121
H	3.039473	0.427922	2.596142
O	-0.507274	-0.197395	-1.203923
H	-1.382124	0.116572	-0.91214
O	1.178101	2.322143	2.4983
H	1.910806	2.303756	3.128987
C	-0.775519	2.164197	0.444232
C	-2.159087	1.583588	0.625763
H	-0.663781	2.600124	-0.554085
H	-0.622857	2.97513	1.162272
C	-3.190565	1.585515	-0.238091
H	-2.302551	1.074804	1.579149
C	-4.476463	0.875895	0.126629
H	-4.414205	0.530374	1.163072
H	-5.317235	1.581687	0.072765
C	-4.8022	-0.339078	-0.788059
C	-3.636549	-1.284593	-0.971933
H	-5.124202	0.024414	-1.769511
H	-5.667721	-0.857183	-0.357525
C	-3.141924	-2.136952	-0.06012
H	-3.122944	-1.224601	-1.931491
C	-1.917657	-2.971724	-0.342593
H	-1.116696	-2.732827	0.368886
H	-2.136546	-4.041253	-0.226207
H	-1.526512	-2.797639	-1.347167
C	-3.168109	2.224498	-1.605748
H	-3.249444	1.463853	-2.392284
H	-2.265034	2.805809	-1.797602
H	-4.031352	2.889874	-1.725928
C	-3.72544	-2.317508	1.319559
H	-3.85431	-3.382489	1.549029
H	-4.69094	-1.823584	1.446865
H	-3.040206	-1.916036	2.077954
C	3.55157	-1.753147	1.040006
H	3.303287	-2.682843	0.514585
H	3.720813	-2.018702	2.090985
C	4.870776	-1.19434	0.457388
H	5.641487	-1.961378	0.601105
H	5.188103	-0.326296	1.050268
C	4.802929	-0.802994	-1.032569
H	5.788192	-0.958945	-1.491981
H	4.116345	-1.484485	-1.554816
C	4.375721	0.648263	-1.300423
H	5.102853	1.322816	-0.827534
H	3.413366	0.848942	-0.819975
C	4.274697	0.9636	-2.795294
H	3.519297	0.331499	-3.276844
H	3.993548	2.007919	-2.967891
H	5.228525	0.785071	-3.305899
H	-3.480771	1.822332	2.90664

Frequencies -- 19.2087 21.6596 26.0368  
 Frequencies -- 37.0431 46.9182 55.2063  
 Frequencies -- 66.8094 76.6023 90.45017  
 Zero-point correction= 0.487884 (Hartree/Particle)  
 Thermal correction to Energy= 0.514112  
 Thermal correction to Enthalpy= 0.515057  
 Thermal correction to Gibbs Free Energy= 0.429825  
 Sum of electronic and zero-point Energies= -969.568165  
 Sum of electronic and thermal Energies= -969.541936  
 Sum of electronic and thermal Enthalpies= -969.540992  
 Sum of electronic and thermal Free Energies= -969.626224

aa-CBG-u.log



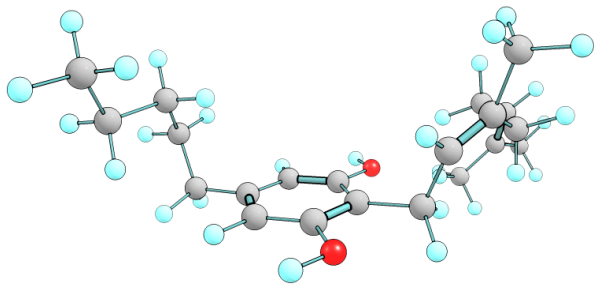
55 Atoms

C	0.5853	-0.21771	0.582761
C	1.710403	-0.546905	1.343666
C	2.870323	0.229589	1.25759
C	2.874409	1.3474	0.419832
C	1.739348	1.664325	-0.335498
C	0.574617	0.884089	-0.286781
H	1.685331	-1.420543	1.990827
H	3.764413	1.966488	0.339491
O	-0.563156	-0.964402	0.649388
H	-0.437378	-1.698691	1.265717
O	1.708585	2.756835	-1.162534
H	2.561796	3.210256	-1.122674
C	-0.649199	1.255426	-1.101754
C	-1.473476	2.320395	-0.412175
H	-1.241113	0.359012	-1.291376
H	-0.310357	1.636415	-2.073499
C	-2.78569	2.29318	-0.135271
H	-0.900876	3.197258	-0.109812
C	-3.706162	1.141608	-0.485223
H	-4.689111	1.5417	-0.768206
H	-3.340713	0.585971	-1.354093
C	-3.892915	0.140346	0.685342
C	-4.937939	-0.900882	0.379991
H	-4.194844	0.696961	1.582053
H	-2.92148	-0.308389	0.907113
C	-4.743313	-2.142452	-0.091854
H	-5.969183	-0.575432	0.52698
C	-5.906881	-3.063561	-0.371784
H	-5.921441	-3.368423	-1.426769
H	-5.823705	-3.988865	0.214157
H	-6.868715	-2.597977	-0.137917
C	-3.448441	3.440417	0.591335
H	-4.222806	3.904321	-0.033853
H	-2.731997	4.215057	0.879476
H	-3.954894	3.092326	1.500893
C	-3.389536	-2.740026	-0.390167
H	-3.217531	-3.633624	0.225237
H	-2.561846	-2.048723	-0.227426
C	-3.347773	-3.076791	-1.43448
H	4.118403	-0.182451	2.004455
H	3.859119	-0.433483	3.040501
C	4.811752	0.665707	2.049306
H	4.853668	-1.389717	1.378023
H	5.720958	-1.607537	2.013144
C	4.205649	-2.274488	1.431385
H	5.320865	-1.180631	-0.07639
H	6.233639	-1.766529	-0.248297
H	5.608414	-0.128819	-0.217293
C	4.294095	-1.573047	-1.149826
H	4.05853	-2.640484	-1.038563
H	3.356554	-1.033587	-0.98592
C	4.797839	-1.300764	-2.569821
H	5.732227	-1.838202	-2.771138
H	4.065319	-1.610125	-3.322853
H	4.994333	-0.231988	-2.715659
H	-3.480771	1.822332	2.90664

Frequencies -- 12.9313 22.1781 28.3680  
 Frequencies -- 31.3991 42.9823 44.3487  
 Frequencies -- 59.1177 74.7947 80.7858

Zero-point correction= 0.487959 (Hartree/Particle)  
 Thermal correction to Energy= 0.514343  
 Thermal correction to Enthalpy= 0.515287  
 Thermal correction to Gibbs Free Energy= 0.428735  
 Sum of electronic and zero-point Energies= -969.564628  
 Sum of electronic and thermal Energies= -969.538244  
 Sum of electronic and thermal Enthalpies= -969.537300  
 Sum of electronic and thermal Free Energies= -969.623852

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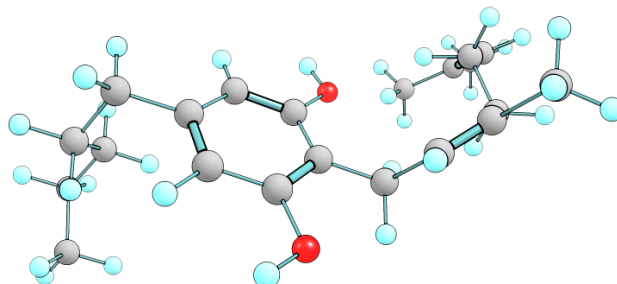
55 Atoms

C	0.269543	-0.989063	-0.553793
C	1.413162	-1.7499	-0.294285
C	2.671331	-1.292349	-0.700207
C	2.760454	-0.067782	-1.367256
C	1.606054	0.682821	-1.619038
C	0.333463	0.237807	-1.232179
H	1.321019	-2.69933	0.228302
H	3.727438	0.309439	-1.690327
O	-0.974266	-1.414615	-0.162616
H	-0.900144	-2.265942	0.289449
O	1.661717	1.894157	-2.258282
H	2.580809	2.094099	-2.483179
C	-0.902401	1.073629	-1.50258
C	-1.098468	2.132703	-0.440099
H	-1.772282	0.419011	-1.571193
H	-0.779696	1.560655	-2.478172
C	-2.203255	2.37687	0.280562
H	-0.215606	2.745081	-0.256064
C	-3.498115	1.602714	0.138741
H	-4.344022	2.291257	0.267989
H	-3.601929	1.176487	-0.863634
C	-3.630878	0.44993	1.168655
C	-4.983446	-0.21214	1.105869
H	-3.476338	0.854902	2.176886
H	-2.820045	-0.260698	0.988619
C	-5.327435	-1.300446	0.399046
H	-5.771463	0.290794	1.668798
C	-6.742621	-1.827214	0.413318
H	-7.167178	-1.838852	-0.599522
H	-6.770556	-2.865634	0.770028
H	-7.400033	-1.229916	1.05177
C	-2.219142	3.460755	1.333143
H	-2.962525	4.23169	1.09071
H	-1.244945	3.946662	1.439738
H	-2.504155	3.055981	2.312944
C	-4.376416	-2.090813	-0.466533
H	-4.325454	-3.135388	-0.130369
H	-3.363159	-1.687879	-0.483119
H	-4.744935	-2.121632	-1.500585
C	3.911982	-2.093184	-0.370412
H	4.738584	-1.773679	-1.013535
H	3.733188	-3.151273	-0.596343
C	4.326966	-1.97711	1.114293
H	3.51624	-2.3825	1.73254
H	5.199462	-2.622409	1.282319
C	4.64906	-0.551313	1.584908
H	4.822796	-0.571394	2.669243
H	3.772499	0.090824	1.426554
C	5.866955	0.083892	0.902749
H	6.738987	-0.570775	1.037759
H	5.698287	0.146803	-0.179271
C	6.180446	1.48252	1.442631
H	6.386138	1.452653	2.518914
H	7.053187	1.920451	0.946997
H	5.332788	2.160214	1.287743
H	-3.480771	1.822332	2.90664

Frequencies -- 11.4967 21.2697 27.3358  
 Frequencies -- 36.3500 38.0083 46.3954  
 Frequencies -- 58.8437 84.6576 91.1080

Zero-point correction= 0.488062 (Hartree/Particle)  
 Thermal correction to Energy= 0.514396  
 Thermal correction to Enthalpy= 0.515340  
 Thermal correction to Gibbs Free Energy= 0.428942  
 Sum of electronic and zero-point Energies= -969.566120  
 Sum of electronic and thermal Energies= -969.539787  
 Sum of electronic and thermal Enthalpies= -969.538842  
 Sum of electronic and thermal Free Energies= -969.625240

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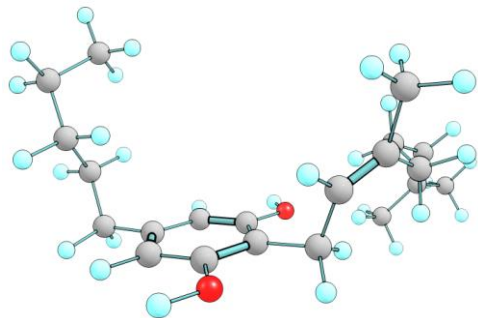
55 Atoms

C	-0.45987	-0.126175	-0.416231
C	-1.619281	-0.388973	-1.156015
C	-2.705491	0.486944	-1.097074
C	-2.611007	1.627018	-0.291245
C	-1.447739	1.874471	0.442447
C	-0.347653	1.001588	0.407691
H	-1.670688	-1.280979	-1.775336
H	-3.443061	2.324906	-0.235142
O	0.618879	-0.972194	-0.463198
H	0.427203	-1.709879	-1.058128
O	-1.316167	2.986821	1.2328
H	-2.132697	3.503683	1.194221
C	0.913005	1.304461	1.194184
C	1.789123	2.303916	0.471409
H	1.449782	0.374609	1.386333
H	0.618999	1.72161	2.165828
C	3.085459	2.179668	0.149821
H	1.271321	3.218256	0.18159
C	3.932697	0.966636	0.475895
H	4.950832	1.296692	0.722371
H	3.558752	0.441987	1.360325
C	4.008267	-0.05044	-0.69367
H	4.998319	-1.154248	-0.424823
C	4.306622	0.481392	-1.606327
H	3.002326	-0.439097	-0.872056
C	4.74894	-2.370488	0.08565
H	6.038602	-0.902928	-0.638329
C	5.861964	-3.364364	0.317849
H	5.916357	-3.652908	1.376095
H	5.683037	-4.290786	-0.244415
H	6.837986	-2.969376	0.021245
C	3.802785	3.27234	-0.60866
H	4.634692	3.677799	-0.017734
H	3.135404	4.098115	-0.871531
H	4.24419	2.885764	-1.536491
C	3.377738	-2.866331	0.475978
H	3.105658	-3.754394	-0.110774
H	2.59265	-2.119928	0.350131
H	3.376643	-3.183909	1.527096
C	-3.986401	0.195822	-1.849497
H	-3.794569	-0.550671	-2.629359
H	-4.322392	1.107021	-2.359191
C	-5.122574	-0.307226	-0.933362
H	-5.317887	0.454834	-0.169281
H	-6.041684	-0.394869	-1.528063
C	-4.819984	-1.655521	-0.269206
H	-3.908153	-1.566017	0.335734
H	-4.593492	-2.389982	-1.054464
C	-5.959575	-2.193529	0.609797
H	-6.874216	-2.277932	0.006696
H	-5.708084	-3.213797	0.926558
C	-6.242726	-1.341856	1.853108
H	-5.339034	-1.231415	2.464112
H	-6.587024	-0.337026	1.588354
H	-7.015752	-1.80007	2.478812
H	-3.480771	1.822332	2.90664

Frequencies -- 13.9572 19.7326 25.8665  
 Frequencies -- 32.1724 45.2049 46.5936  
 Frequencies -- 61.8014 67.3019 84.1439

Zero-point correction= 0.488187 (Hartree/Particle)  
 Thermal correction to Energy= 0.514483  
 Thermal correction to Enthalpy= 0.515427  
 Thermal correction to Gibbs Free Energy= 0.429090  
 Sum of electronic and zero-point Energies= -969.565310  
 Sum of electronic and thermal Energies= -969.539014  
 Sum of electronic and thermal Enthalpies= -969.538070  
 Sum of electronic and thermal Free Energies= -969.624407

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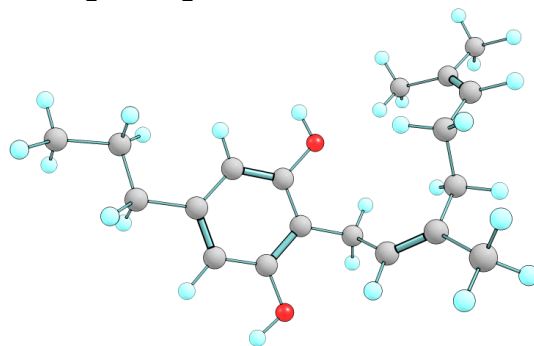


55 Atoms

C	0.406477	-0.366333	-1.136755
C	1.626957	-1.034009	-1.274516
C	2.810421	-0.31034	-1.4555
C	2.748026	1.084644	-1.499162
C	1.518534	1.738531	-1.358752
C	0.318622	1.033374	-1.184109
H	1.653649	-2.120468	-1.236362
H	3.65594	1.66741	-1.633646
O	-0.766537	-1.054596	-0.957778
H	-0.588591	-2.004922	-0.948997
O	1.424797	3.105938	-1.38267
H	2.30479	3.483505	-1.517843
C	-0.997527	1.766069	-1.009814
C	-1.181964	2.235172	0.417076
H	-1.816277	1.115923	-1.321044
H	-0.9971	2.636845	-1.677823
C	-2.232956	2.021317	1.222487
H	-0.337197	2.800812	0.81013
C	-3.471275	1.249031	0.81646
H	-4.351486	1.711374	1.283093
H	-3.637223	1.297999	-0.264019
C	-3.415682	-0.24558	1.229657
C	-4.718268	-0.95454	0.964216
H	-3.186329	-0.308521	2.301322
H	-2.580464	-0.713692	0.70242
C	-5.047246	-1.686775	-0.111703
H	-5.485825	-0.80891	1.726223
C	-6.415206	-2.31318	-0.242075
H	-6.929155	-1.948835	-1.141647
H	-6.33821	-3.403257	-0.352322
C	-7.050756	-2.102459	0.622989
C	-2.238122	2.535035	2.643416
H	-3.056454	3.250546	2.798761
H	-1.29804	3.028086	2.907218
H	-2.403839	1.718259	3.357905
C	-4.124767	-1.955508	-1.275954
H	-3.945821	-3.033793	-1.386219
H	-3.158811	-1.456228	-1.192097
H	-4.594575	-1.627562	-2.212701
C	4.135545	-1.035854	-1.550972
H	4.890746	-0.367204	-1.981006
H	4.035637	-1.884903	-2.237911
C	4.637354	-1.557374	-0.187448
H	3.885055	-2.241915	0.222546
H	5.545118	-2.153392	-0.351046
C	4.939865	-0.441671	0.819677
H	4.027213	0.1408	1.001535
H	5.65917	0.254208	0.365883
C	5.499626	-0.939178	2.161097
H	6.413976	-1.520916	1.979147
H	5.804711	-0.070821	2.758939
C	4.510664	-1.782029	2.975491
H	4.24475	-2.709296	2.457951
H	4.932169	-2.057146	3.947954
H	3.582688	-1.227068	3.157343
H	-3.480771	1.822332	2.90664

Frequencies --	7.2002	19.3532	23.4501
Frequencies --	28.2288	41.7405	43.3510
Frequencies --	54.7824	67.5545	78.5854
Zero-point correction=	0.487744 (Hartree/Particle)		
Thermal correction to Energy=	0.514211		
Thermal correction to Enthalpy=	0.515155		
Thermal correction to Gibbs Free Energy=	0.427437		
Sum of electronic and zero-point Energies=	-969.565741		
Sum of electronic and thermal Energies=	-969.539274		
Sum of electronic and thermal Enthalpies=	-969.538330		
Sum of electronic and thermal Free Energies=	-969.626048		

CBG-V  
aa-cbgv-e.log



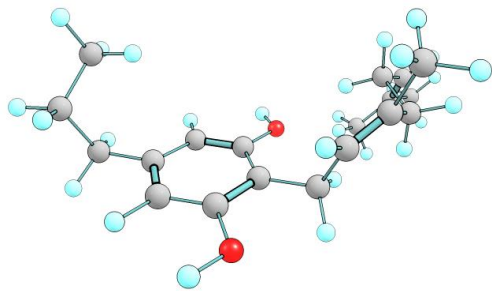
49 Atoms

C	1.036865	-0.336597	-0.33972
C	2.284899	-0.867975	0.0136
C	3.429451	-0.069487	-0.036154
C	3.298801	1.263379	-0.447631
C	2.048173	1.777673	-0.794403
C	0.885019	0.989985	-0.759106
H	2.342546	-1.905828	0.325656
H	4.175374	1.905907	-0.493945
O	-0.097853	-1.1071	-0.293084
H	0.125715	-1.998412	0.007195
O	1.88705	3.08098	-1.188506
H	2.746942	3.523499	-1.185896
C	-0.466811	1.578552	-1.114833
C	-1.050549	2.354249	0.045324
H	-1.136382	0.77868	-1.433894
H	-0.332966	2.255379	-1.968334
C	-2.250453	2.194331	0.623087
H	-0.384201	3.118634	0.445068
C	-3.278298	1.170075	0.187749
H	-4.281806	1.604318	0.291726
H	-3.165477	0.911374	-0.869464
C	-3.215359	-0.141344	1.014697
C	-4.363831	-1.065203	0.699533
H	-3.242244	0.11093	2.082378
H	-2.247725	-0.614929	0.828402
C	-4.385279	-2.065281	-0.195598
H	-5.289037	-0.852936	1.23779
C	-5.632207	-2.886563	-0.42154
H	-5.965185	-2.814866	-1.46567
H	-5.439806	-3.951332	-0.232927
H	-6.458151	-2.570267	0.222177
C	-2.657785	3.042147	1.806037
H	-3.546307	3.642828	1.570456
H	-1.859765	3.720877	2.120543
H	-2.928428	2.417025	2.666878
C	-3.209905	-2.465304	-1.053945
H	-2.927153	-3.509034	-0.860379
H	-2.329057	-1.839612	-0.9056
H	-3.484265	-2.416076	-2.116096
C	4.80489	-0.581795	0.354545
H	5.127993	-0.051709	1.262065
H	5.518968	-0.280614	-0.424017
C	4.937471	-2.089471	0.592259
H	4.276027	-2.394603	1.412757
H	4.597316	-2.632642	-0.298553
C	6.37631	-2.494445	0.925857
H	6.456139	-3.572063	1.100263
H	7.058505	-2.235438	0.108179
H	6.730461	-1.981691	1.827415

Frequencies --	10.9196	19.1188	32.5773
Frequencies --	39.1932	43.0707	58.5228
Frequencies --	76.7369	89.8641	103.6740

Zero-point correction=	0.430500 (Hartree/Particle)		
Thermal correction to Energy=	0.454440		
Thermal correction to Enthalpy=	0.455384		
Thermal correction to Gibbs Free Energy=	0.374446		
Sum of electronic and zero-point Energies=	-890.982838		
Sum of electronic and thermal Energies=	-890.958898		
Sum of electronic and thermal Enthalpies=	-890.957954		
Sum of electronic and thermal Free Energies=	-891.038892		

aa-cbgv-o.log



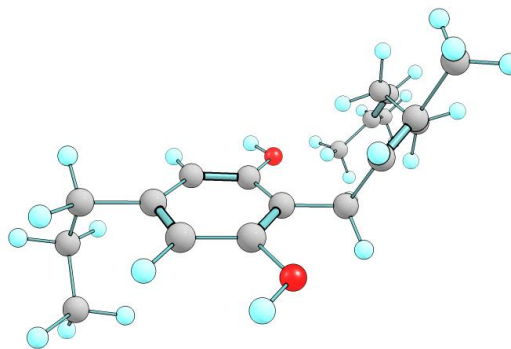
49 Atoms

C	1.011874	-0.714573	-0.531168
C	2.200741	-1.415986	-0.296608
C	3.435817	-0.791032	-0.4846
C	3.460993	0.541477	-0.910851
C	2.265626	1.228129	-1.140535
C	1.012694	0.616837	-0.967929
H	2.158891	-2.449144	0.03886
H	4.411781	1.047714	-1.060909
O	-0.211404	-1.307486	-0.348299
H	-0.090685	-2.219856	-0.052103
O	2.25205	2.536653	-1.548625
H	3.16178	2.850624	-1.64398
C	-0.270409	1.390076	-1.203723
C	-0.63059	2.239938	-0.004741
H	-1.072584	0.692198	-1.447309
H	-0.123995	2.040454	-2.075506
C	-1.799171	2.277267	0.652777
H	0.18105	2.876646	0.347453
C	-3.009438	1.444739	0.281441
H	-3.919649	2.029563	0.469822
H	-3.01727	1.203233	-0.785823
C	-3.097635	0.115306	1.07701
C	-4.380564	-0.625417	0.799585
H	-3.037021	0.33932	2.149714
H	-2.218019	-0.485656	0.832141
C	-4.58577	-1.588136	-0.113291
H	-5.240907	-0.296147	1.384528
C	-5.947645	-2.21408	-0.297781
H	-6.309914	-2.068663	-1.324356
H	-5.904877	-3.299892	-0.138045
H	-6.691015	-1.797806	0.388291
C	-1.980746	3.163138	1.863135
H	-2.76921	3.907439	1.6896
H	-1.061612	3.693893	2.127687
H	-2.296963	2.577976	2.736519
C	-3.51991	-2.13146	-1.033629
H	-3.392972	-3.212086	-0.882134
H	-2.548028	-1.653275	-0.906559
H	-3.825328	-2.004789	-2.080835
C	4.730603	-1.517292	-0.190357
H	5.450225	-1.31432	-0.992722
H	4.554139	-2.599666	-0.189222
C	5.362698	-1.109041	1.158016
H	6.342064	-1.595974	1.24389
H	5.551969	-0.028072	1.147829
C	4.499752	-1.470895	2.369673
H	4.985946	-1.174619	3.304733
H	3.524909	-0.975083	2.322878
H	4.318614	-2.551312	2.412399

Frequencies --	12.0208	23.7219	32.6120
Frequencies --	36.4882	46.6630	58.4835
Frequencies --	80.3583	85.7136	101.7585

Zero-point correction=	0.430698	(Hartree/Particle)
Thermal correction to Energy=	0.454473	
Thermal correction to Enthalpy=	0.455417	
Thermal correction to Gibbs Free Energy=	0.375223	
Sum of electronic and zero-point Energies=	-890.984804	
Sum of electronic and thermal Energies=	-890.961030	
Sum of electronic and thermal Enthalpies=	-890.960085	
Sum of electronic and thermal Free Energies=	-891.040279	

aa-cbgv-u.log



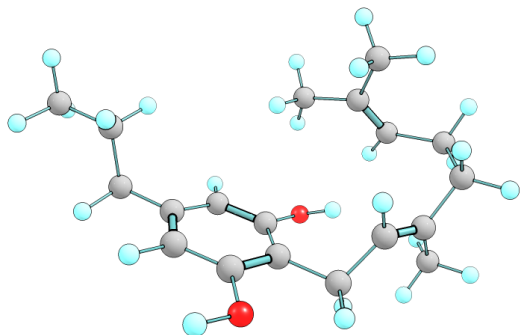
49 Atoms

C	-1.030721	-0.509032	-0.194768
C	-2.194835	-1.014473	-0.780856
C	-3.397532	-0.306033	-0.685795
C	-3.411194	0.909567	0.002896
C	-2.237354	1.401665	0.585574
C	-1.022807	0.704004	0.510579
H	-2.160931	-1.96043	-1.316304
H	-4.333287	1.479567	0.086502
O	0.161857	-1.181036	-0.282781
H	0.038462	-1.999031	-0.783188
O	-2.214447	2.596352	1.257337
H	-3.103039	2.977898	1.259397
C	0.242396	1.272018	1.123624
C	0.89215	2.28624	0.207622
H	0.927873	0.456235	1.357068
H	-0.023933	1.759569	2.070041
C	2.166056	2.316668	-0.211087
H	0.214709	3.064325	-0.144237
C	3.216373	1.30012	0.188089
H	4.18425	1.807927	0.295759
H	2.994538	0.856144	1.163263
C	3.368644	0.150583	-0.842604
C	4.522573	-0.758858	-0.507805
H	3.531737	0.585713	-1.836949
H	2.421199	-0.392363	-0.889583
C	4.481995	-1.911473	0.179178
H	5.501664	-0.399757	-0.829308
C	5.740137	-2.696714	0.463761
H	5.891974	-2.815573	1.544997
H	5.671022	-3.711742	0.049848
C	6.630082	-2.217957	0.044988
H	2.645723	3.390057	-1.160246
H	3.436192	3.996379	-0.698481
H	1.837574	4.059455	-1.469031
H	3.084708	2.949797	-2.065003
C	3.221728	-2.530462	0.733439
H	3.063523	-3.531068	0.308508
H	2.325842	-1.936204	0.549726
H	3.316732	-2.671904	1.81826
C	-4.662434	-0.877157	-1.289412
H	-4.443499	-1.259648	-2.293743
H	-5.406032	-0.080121	-1.409204
C	-5.276967	-2.016852	-0.448208
H	-6.120736	-2.443125	-1.004919
H	-4.535733	-2.819389	-0.343225
C	-5.748964	-1.56597	0.936526
H	-6.183995	-2.399443	1.497401
H	-4.919219	-1.159367	1.523374
H	-6.510767	-0.781802	0.854541

Frequencies --	19.3090	25.6588	30.9150
Frequencies --	37.6094	47.8754	59.3004
Frequencies --	74.9184	83.5266	103.6478

Zero-point correction=	0.430754	(Hartree/Particle)
Thermal correction to Energy=	0.454521	
Thermal correction to Enthalpy=	0.455465	
Thermal correction to Gibbs Free Energy=	0.375714	
Sum of electronic and zero-point Energies=	-890.984722	
Sum of electronic and thermal Energies=	-890.960956	
Sum of electronic and thermal Enthalpies=	-890.960012	
Sum of electronic and thermal Free Energies=	-891.039762	

ss-cbgv-e.log



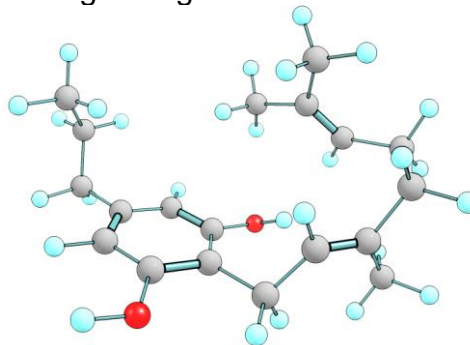
49 Atoms

C	0.55197	0.606766	-0.971544
C	1.801482	0.011051	-1.159729
C	2.919672	0.489916	-0.472523
C	2.763679	1.56692	0.406617
C	1.509547	2.161365	0.584005
C	0.37627	1.703357	-0.10823
H	1.879064	-0.834248	-1.835952
H	3.620653	1.947613	0.957926
O	-0.500587	0.102107	-1.692395
H	-1.305149	0.155101	-1.146172
O	1.337825	3.22589	1.431335
H	2.189879	3.459315	1.82437
C	-0.983956	2.362884	0.0407
C	-2.007126	1.408701	0.613398
H	-1.306654	2.742719	-0.934383
H	-0.882801	3.229393	0.700433
C	-3.19173	1.033486	0.097329
H	-1.703181	0.950379	1.554491
C	-4.023382	-0.008331	0.814541
H	-3.571977	-0.218009	1.789094
H	-5.031444	0.385851	1.004244
C	-4.162345	-1.345333	0.030991
C	-2.843755	-1.887707	-0.472326
H	-4.834994	-1.196646	-0.820197
H	-4.661507	-2.066603	0.689635
C	-1.865846	-2.437578	0.265096
H	-2.65685	-1.767347	-1.539348
C	-0.556331	-2.860517	-0.353209
H	0.278286	-2.306121	0.095139
H	-0.362574	-3.926037	-0.172715
H	-0.532891	-2.673109	-1.428727
C	-3.769629	1.54608	-1.199572
H	-3.869696	0.733488	-1.929855
H	-3.171424	2.334598	-1.658678
H	-4.779361	1.940242	-1.03309
C	-1.960813	-2.651985	1.755382
H	-1.648718	-3.669655	2.02035
H	-2.966426	-2.491685	2.149631
H	-1.280375	-1.970082	2.282439
C	4.258479	-0.198389	-0.612985
H	5.068698	0.525333	-0.459529
H	4.370625	-0.587007	-1.632775
C	4.428066	-1.360271	0.385349
H	3.613161	-2.079507	0.232905
H	4.308777	-0.971756	1.404716
C	5.780357	-2.063663	0.24757
H	5.87718	-2.886255	0.963578
H	6.606824	-1.365899	0.42473
H	5.907317	-2.478559	-0.758944

Frequencies --	17.6912	27.0209	31.3005
Frequencies --	43.3436	58.4183	68.5616
Frequencies --	84.5463	87.9587	110.1848

Zero-point correction=	0.430517 (Hartree/Particle)
Thermal correction to Energy=	0.454254
Thermal correction to Enthalpy=	0.455198
Thermal correction to Gibbs Free Energy=	0.376027
Sum of electronic and zero-point Energies=	-890.988489
Sum of electronic and thermal Energies=	-890.964753
Sum of electronic and thermal Enthalpies=	-890.963809
Sum of electronic and thermal Free Energies=	-891.042980

ss-cbgv-o.log



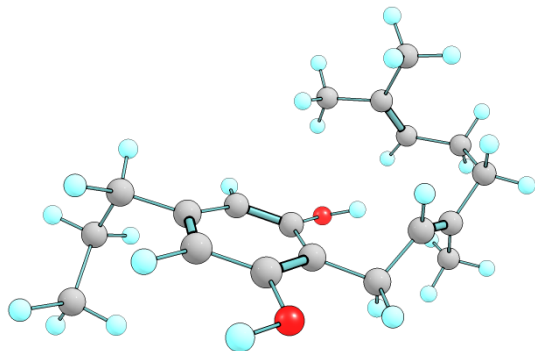
49 Atoms

C	-0.629572	-0.664682	-1.055328
C	-1.8442	-0.028739	-1.313787
C	-2.990094	-0.380446	-0.594111
C	-2.894644	-1.376887	0.381612
C	-1.673881	-2.018476	0.625391
C	-0.516335	-1.688293	-0.096136
H	-1.871401	0.755357	-2.063509
H	-3.771052	-1.655208	0.962127
O	0.457886	-0.274932	-1.797031
H	1.244721	-0.305075	-1.224783
O	-1.562083	-3.001984	1.574388
H	-2.425993	-3.148016	1.983448
C	0.809919	-2.393494	0.128732
C	1.850482	-1.444588	0.678361
H	1.143793	-2.836886	-0.815158
H	0.655845	-3.217761	0.831053
C	3.051717	-1.120252	0.166568
H	1.540724	-0.934931	1.590772
C	3.889426	-0.057737	0.845224
H	3.435703	0.193851	1.808592
H	4.894134	-0.45023	1.054622
C	4.039724	1.246454	0.009164
C	2.726958	1.775233	-0.523407
H	4.715998	1.059916	-0.831671
H	4.539366	1.990798	0.641344
C	1.742941	2.349214	0.186862
H	2.549126	1.62013	-1.587415
C	0.438019	2.749701	-0.45582
H	-0.401446	2.225198	0.018504
H	0.250806	3.824364	-0.331118
H	0.415301	2.506791	-1.520366
C	3.640823	-1.707279	-1.093354
H	3.768466	-0.93478	-1.862134
H	3.035212	-2.507243	-1.522069
H	4.640144	-2.110657	-0.890392
C	1.82537	2.614478	1.669641
H	1.50561	3.638755	1.897417
H	2.828876	2.473124	2.076363
H	1.144458	1.946863	2.214205
C	-4.287015	0.364727	-0.826128
H	-5.114764	-0.177376	-0.353212
H	-4.501646	0.396606	-1.901403
C	-4.253719	1.810036	-0.283914
H	-5.192724	2.30724	-0.557119
H	-3.450808	2.360696	-0.79025
C	-4.050442	1.885654	1.231648
H	-4.043909	2.923797	1.579003
H	-3.101963	1.424293	1.525088
H	-4.85186	1.357983	1.761922

Frequencies --	17.9757	30.3451	40.3201
Frequencies --	44.0039	57.2921	64.8426
Frequencies --	81.7078	107.1734	114.4724

Zero-point correction=	0.430862 (Hartree/Particle)
Thermal correction to Energy=	0.454396
Thermal correction to Enthalpy=	0.455340
Thermal correction to Gibbs Free Energy=	0.377137
Sum of electronic and zero-point Energies=	-890.988559
Sum of electronic and thermal Energies=	-890.965025
Sum of electronic and thermal Enthalpies=	-890.964081
Sum of electronic and thermal Free Energies=	-891.042284

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49 Atoms

C	-0.731498	-0.036221	-0.584836
C	-1.804163	0.850213	-0.468969
C	-2.8988	0.530446	0.340364
C	-2.890837	-0.681194	1.037795
C	-1.813051	-1.566242	0.912022
C	-0.715001	-1.272191	0.088657
H	-1.762572	1.790241	-1.009993
H	-3.727305	-0.944371	1.680762
O	0.299968	0.328489	-1.411978
H	1.135352	-0.002183	-1.035422
O	-1.793436	-2.763904	1.579478
H	-2.612145	-2.859027	2.08497
C	0.438865	-2.241987	-0.098447
C	1.749534	-1.656646	0.37544
H	0.497815	-2.524499	-1.154827
H	0.223175	-3.156272	0.462018
C	2.895347	-1.496233	-0.31133
H	1.725449	-1.296042	1.403857
C	4.075723	-0.815104	0.346032
H	3.844925	-0.634341	1.400455
H	4.950199	-1.480258	0.317578
C	4.469278	0.534544	-0.31938
C	3.296045	1.463947	-0.53494
H	4.948087	0.335436	-1.283839
H	5.236056	1.004621	0.308332
C	2.630566	2.1496	0.408263
H	2.930493	1.538243	-1.55912
C	1.419164	2.982893	0.071022
H	0.535132	2.610378	0.604532
H	1.561235	4.025989	0.382566
H	1.191105	2.960654	-0.996747
C	3.106291	-1.91832	-1.74543
H	3.262367	-1.043856	-2.389451
H	2.27202	-2.48897	-2.156059
H	4.010983	-2.532167	-1.82952
C	2.995337	2.128159	1.872078
H	3.034976	3.14702	2.276854
H	3.955355	1.646805	2.069707
H	2.22747	1.593984	2.447382
C	-4.08008	1.472657	0.427127
H	-3.715103	2.501682	0.530076
H	-4.664932	1.251931	1.328428
C	-5.006851	1.396493	-0.805497
H	-4.420416	1.628255	-1.70364
H	-5.766986	2.182776	-0.717927
C	-5.69019	0.036645	-0.971469
H	-6.34386	0.026285	-1.849627
H	-6.302005	-0.203561	-0.093957
H	-4.95321	-0.764185	-1.088417

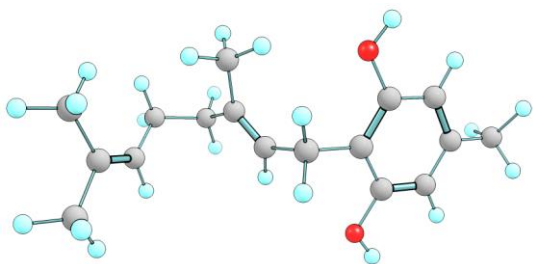
Frequencies --	21.3052	26.5084	29.9091
Frequencies --	44.1295	60.7222	61.8188
Frequencies --	76.1323	105.9411	106.5360

Zero-point correction=	0.430635 (Hartree/Particle)
Thermal correction to Energy=	0.454267
Thermal correction to Enthalpy=	0.455211
Thermal correction to Gibbs Free Energy=	0.376395
Sum of electronic and zero-point Energies=	-890.988265
Sum of electronic and thermal Energies=	-890.964633
Sum of electronic and thermal Enthalpies=	-890.963689
Sum of electronic and thermal Free Energies=	-891.042504



# Cannabigerocin-AA-1+3t

aa-1+4+5-.log



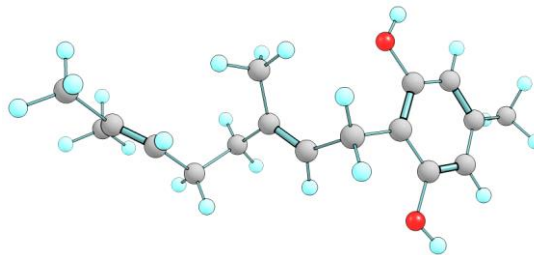
43 Atoms

C	2.589441	1.36346	-0.094305
C	3.942447	1.290958	0.254186
C	4.626304	0.074739	0.164662
C	3.937328	-1.056747	-0.282088
C	2.58359	-0.968497	-0.626159
C	1.880413	0.242891	-0.551998
H	4.458078	2.184142	0.59862
H	4.450705	-2.012106	-0.361308
O	1.88579	2.537316	-0.009491
H	2.473558	3.239852	0.300605
O	1.884557	-2.064049	-1.063784
H	2.470369	-2.83318	-1.077239
C	0.409154	0.334948	-0.908573
C	-0.475366	0.249813	0.315245
H	0.161197	-0.444922	-1.629739
H	0.231699	1.298376	-1.400819
C	-1.303447	-0.746493	0.661839
H	-0.397011	1.108907	0.981137
C	-2.136404	-0.650897	1.922571
H	-1.908774	-1.505242	2.576615
H	-1.869243	0.255348	2.47952
C	-3.664392	-0.644574	1.658526
C	-4.096421	0.547917	0.850524
H	-4.172103	-0.628066	2.633341
H	-3.956176	-1.583111	1.178576
C	-4.70278	0.576248	-0.346102
H	-3.84819	1.507869	1.307727
C	-5.033755	1.887493	-1.01905
H	-4.544351	1.957123	-1.999727
H	-6.112491	1.973219	-1.206427
H	-4.721663	2.748524	-0.421071
C	-1.501693	-2.005314	-0.152246
H	-1.615548	-2.872399	0.509729
H	-0.663991	-2.205049	-0.822119
H	-2.418126	-1.949561	-0.752907
C	-5.10922	-0.64222	-1.138817
H	-6.187186	-0.624668	-1.346018
H	-4.879688	-1.584169	-0.637752
H	-4.607365	-0.647738	-2.115246
C	6.07611	-0.023199	0.577184
H	6.601013	-0.799392	0.012574
H	6.164299	-0.277878	1.640517
H	6.600358	0.924826	0.425224

Frequencies --	16.5127	22.7803	34.4830
Frequencies --	36.9845	46.5963	49.9029
Frequencies --	79.4428	112.1908	132.6229

Zero-point correction= 0.372947 (Hartree/Particle)  
 Thermal correction to Energy= 0.394351  
 Thermal correction to Enthalpy= 0.395295  
 Thermal correction to Gibbs Free Energy= 0.320269  
 Sum of electronic and zero-point Energies= -812.401083  
 Sum of electronic and thermal Energies= -812.379679  
 Sum of electronic and thermal Enthalpies= -812.378734  
 Sum of electronic and thermal Free Energies= -812.453761

aa-1+4+5+.log



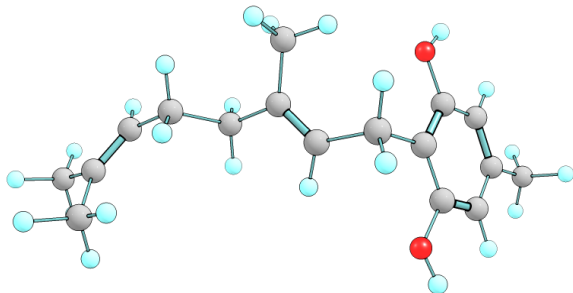
43 Atoms

C	-3.031451	-1.180002	-0.494099
C	-4.29923	-1.062732	0.086055
C	-4.765495	0.186376	0.507158
C	-3.948206	1.307212	0.332636
C	-2.681985	1.173978	-0.248784
C	-2.198061	-0.068109	-0.68555
H	-4.917662	-1.948293	0.212532
H	-4.292597	2.288318	0.651057
O	-2.537782	-2.390455	-0.908219
H	-3.197758	-3.077435	-0.742304
O	-1.858962	2.255384	-0.428264
H	-2.300048	3.050482	-0.099321
C	-0.816201	-0.216633	-1.293336
C	0.204336	-0.650996	-0.264955
H	-0.527226	0.723483	-1.765258
H	-0.864054	-0.975599	-2.082642
C	1.199168	0.071132	0.272464
H	0.075867	-1.677192	0.081556
C	2.1444	-0.575663	1.273065
H	2.562277	0.191418	1.936764
H	1.591136	-1.27953	1.906548
C	3.320629	-1.351243	0.617949
C	4.168329	-0.517777	-0.306059
H	2.891773	-2.185587	0.047612
H	3.924928	-1.796104	1.415574
C	5.368056	0.031279	-0.0576
H	3.723265	-0.326351	-1.282728
C	6.074401	0.86401	-1.100789
H	6.263607	1.879667	-0.728531
H	7.056438	0.437481	-1.345319
H	5.495998	0.942415	-2.02586
C	1.482993	1.518508	-0.046982
H	1.413401	2.119696	0.869195
H	0.787661	1.94429	-0.770851
C	2.507251	1.64085	-0.417743
H	6.122064	-0.105173	1.242486
H	7.112041	-0.547531	1.070521
H	5.602422	-0.71419	1.984514
H	6.299249	0.883804	1.684954
C	-6.115717	0.317817	1.171676
H	-6.561841	1.29814	0.98008
H	-6.029208	0.206293	2.259511

Frequencies --	12.6409	17.4362	23.5295
Frequencies --	36.7243	39.5012	50.7178
Frequencies --	92.3240	97.2866	109.8537

Zero-point correction= 0.372644 (Hartree/Particle)  
 Thermal correction to Energy= 0.394264  
 Thermal correction to Enthalpy= 0.395208  
 Thermal correction to Gibbs Free Energy= 0.318636  
 Sum of electronic and zero-point Energies= -812.398728  
 Sum of electronic and thermal Energies= -812.377108  
 Sum of electronic and thermal Enthalpies= -812.376164  
 Sum of electronic and thermal Free Energies= -812.452736

aa-1+4+5a.log



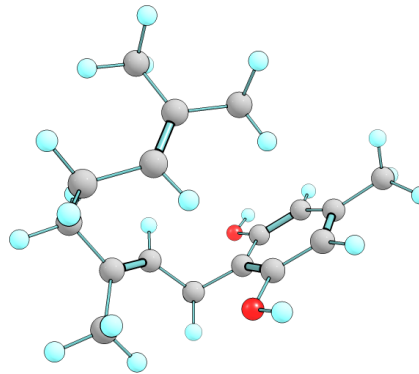
43 Atoms

C	-2.833649	-1.29422	-0.588621
C	-3.97141	-1.598784	0.166773
C	-4.659629	-0.584803	0.839705
C	-4.188041	0.728288	0.747795
C	-3.048597	1.017134	-0.011527
C	-2.351459	0.017558	-0.706214
H	-4.314198	-2.628663	0.231999
H	-4.703695	1.530841	1.269813
O	-2.126987	-2.265417	-1.24997
H	-2.556152	-3.121126	-1.113111
O	-2.561728	2.294781	-0.113976
H	-3.124337	2.893749	0.395544
C	-1.099807	0.328359	-1.504085
C	0.155913	0.083081	-0.69771
H	-1.145096	1.357811	-1.862148
H	-1.081305	-0.320847	-2.387372
C	1.037656	0.991084	-0.252506
H	0.3277	-0.964484	-0.450104
C	2.257551	0.552405	0.530166
H	2.285052	1.082885	1.493764
H	2.196674	-0.517365	0.760383
C	3.592876	0.819663	-0.209404
C	4.784719	0.422386	0.618218
H	3.661581	1.890464	-0.442744
H	3.571284	0.294865	-1.169589
C	5.62361	-0.60816	0.428656
H	4.950145	1.048261	1.497189
C	6.763108	-0.870418	1.384906
H	6.682203	-1.873206	1.825244
H	7.728544	-0.840762	0.86219
H	6.794465	-0.141532	2.199798
C	0.919621	2.479259	-0.495659
H	1.235613	3.03494	0.395585
H	-0.101142	2.782633	-0.732692
H	1.57433	2.805708	-1.313718
C	5.537224	-1.590591	-0.713883
H	6.462407	-1.57742	-1.304851
H	4.701833	-1.399241	-1.389578
H	5.431996	-2.61336	-0.329243
C	-5.909739	-0.896879	1.628015
H	-6.025477	-0.218887	2.478798
H	-5.898302	-1.923038	2.006632

Frequencies --	20.7712	21.8675	30.3120
Frequencies --	42.1729	50.7048	55.6290
Frequencies --	71.2281	88.4504	119.8437

Zero-point correction= 0.372624 (Hartree/Particle)  
 Thermal correction to Energy= 0.394277  
 Thermal correction to Enthalpy= 0.395221  
 Thermal correction to Gibbs Free Energy= 0.319427  
 Sum of electronic and zero-point Energies= -812.400190  
 Sum of electronic and thermal Energies= -812.378537  
 Sum of electronic and thermal Enthalpies= -812.377592  
 Sum of electronic and thermal Free Energies= -812.453387

aa-1+4-5+.log



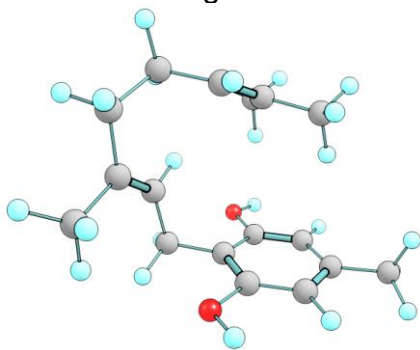
43 Atoms

C	-2.036059	-0.849104	1.192501
C	-3.009276	0.096709	0.847235
C	-3.112825	0.550705	-0.470026
C	-2.237752	0.037195	-1.432774
C	-1.267623	-0.903272	-1.071344
C	-1.152958	-1.382169	0.242589
H	-3.677169	0.484038	1.613051
H	-2.299864	0.376903	-2.463899
O	-1.896853	-1.294252	2.481672
H	-2.558563	-0.863087	3.039518
O	-0.375088	-1.399845	-1.984268
H	-0.538211	-0.990622	-2.844991
C	-0.049758	-2.350793	0.629977
C	1.208375	-1.566963	0.921557
H	0.104418	-3.068598	-0.178082
H	-0.36318	-2.910881	1.516673
C	2.32891	-1.491525	0.188636
H	1.120629	-0.902687	1.781742
C	3.372594	-0.445369	0.520194
H	3.212282	-0.069131	1.536835
H	4.38199	-0.878716	0.486816
C	3.320739	0.765891	-0.45719
C	1.935618	1.349755	-0.565913
H	3.650713	0.436092	-1.450582
H	4.050955	1.510291	-0.123823
C	1.442324	2.423719	0.06964
H	1.249151	0.775339	-1.186917
C	-0.002592	2.830481	-0.098518
H	-0.525613	2.813492	0.867289
H	-0.083223	3.859192	-0.47518
H	-0.54187	2.166447	-0.779065
C	2.607945	-2.310764	-1.046316
H	2.687047	-1.66701	-1.930585
H	1.833653	-3.049641	-1.253448
H	3.569011	-2.832349	-0.94959
C	2.23189	3.302216	1.009048
H	2.212541	4.347072	0.672115
H	3.275651	2.999087	1.1126
H	1.779481	3.293061	2.009506
C	-4.118761	1.614108	-0.840607
H	-4.468128	1.493825	-1.870377
H	-3.672094	2.613074	-0.762871

Frequencies --	24.6519	32.7819	37.2816
Frequencies --	51.6141	52.3952	72.8952
Frequencies --	86.0766	103.4222	111.4430

Zero-point correction= 0.373065 (Hartree/Particle)  
 Thermal correction to Energy= 0.394384  
 Thermal correction to Enthalpy= 0.395328  
 Thermal correction to Gibbs Free Energy= 0.321948  
 Sum of electronic and zero-point Energies= -812.403752  
 Sum of electronic and thermal Energies= -812.382433  
 Sum of electronic and thermal Enthalpies= -812.381489  
 Sum of electronic and thermal Free Energies= -812.454869

b-aa-1+4-5-.log



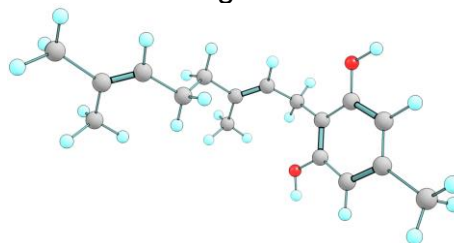
43 Atoms

C	1.580594	0.169445	1.387122
C	2.727028	-0.367026	0.790604
C	3.147536	0.091886	-0.461249
C	2.410481	1.097422	-1.094154
C	1.264566	1.621179	-0.485862
C	0.82739	1.178636	0.772198
H	3.283103	-1.149381	1.301385
H	2.719536	1.470484	-2.067719
O	1.127365	-0.283331	2.601647
H	1.736511	-0.954699	2.938541
O	0.512611	2.593694	-1.089545
H	0.902004	2.81093	-1.947497
C	-0.467332	1.688246	1.379014
C	-1.60612	0.813565	0.905091
H	-0.612874	2.73397	1.10399
H	-0.391644	1.64013	2.470491
C	-2.587951	1.119023	0.04537
H	-1.525461	-0.210229	1.257151
C	-3.587426	0.083687	-0.445654
H	-4.566776	0.283263	0.01485
H	-3.743169	0.254969	-1.521398
C	-3.227896	-1.403529	-0.244787
C	-1.974168	-1.793091	-0.986015
H	-4.075499	-1.994853	-0.620148
H	-3.15274	-1.630765	0.822702
C	-0.874123	-2.399062	-0.515129
H	-1.970552	-1.492995	-2.036024
C	0.332853	-2.619203	-1.39579
H	1.199814	-2.080783	-0.989848
H	0.611639	-3.680731	-1.434447
H	0.1656	-2.270764	-2.419247
C	-2.81186	2.492141	-0.540539
H	-2.668057	2.471338	-1.628419
H	-2.140306	3.249041	-0.134711
H	-3.84553	2.819995	-0.368146
C	-0.694661	-2.869743	0.907843
H	-0.350934	-3.911726	0.926349
H	-1.60961	-2.810353	1.500419
H	0.07179	-2.272513	1.41653
C	4.35087	-0.519914	-1.138299
H	4.857548	0.202573	-1.784799
H	4.052807	-1.367848	-1.767293

Frequencies --	21.7432	39.8787	43.9348
Frequencies --	48.7369	62.8473	71.2064
Frequencies --	100.0596	115.9059	120.6094

Zero-point correction= 0.373124 (Hartree/Particle)  
 Thermal correction to Energy= 0.394348  
 Thermal correction to Enthalpy= 0.395292  
 Thermal correction to Gibbs Free Energy= 0.322669  
 Sum of electronic and zero-point Energies= -812.404013  
 Sum of electronic and thermal Energies= -812.382789  
 Sum of electronic and thermal Enthalpies= -812.381845  
 Sum of electronic and thermal Free Energies= -812.454468

b-aa-1+4-5a.log



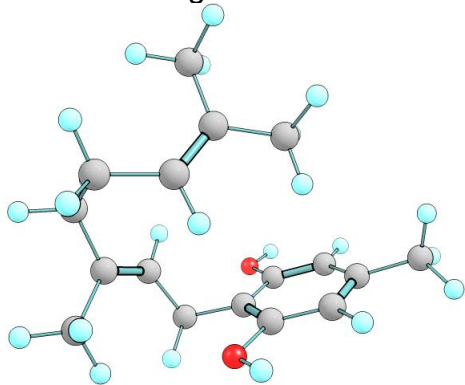
43 Atoms

C	2.986978	0.006968	1.237623
C	3.80813	-1.0882	0.949814
C	4.035774	-1.465242	-0.377499
C	3.426788	-0.73425	-1.401584
C	2.607663	0.359528	-1.097773
C	2.376118	0.762371	0.225429
H	4.264639	-1.6475	1.76307
H	3.584611	-1.014516	-2.440351
O	2.731212	0.397517	2.526834
H	3.208218	-0.182035	3.136505
O	1.995442	1.089579	-2.083757
C	2.231931	0.722807	-2.946554
H	1.460036	1.924738	0.558781
C	0.07182	1.450302	0.927655
H	1.431811	2.616602	-0.284022
H	1.884358	2.468042	1.410954
C	-1.055728	1.560433	0.209476
H	0.019366	0.934209	1.886519
C	-2.353643	0.976729	0.731486
H	-2.296197	0.834041	1.817188
H	-3.179015	1.678213	0.547971
C	-2.715158	-0.379507	0.072243
C	-4.001795	-0.946152	0.607601
H	-1.893478	-1.079663	0.274757
H	-2.755276	-0.259404	-1.014301
C	-5.188874	-1.040025	-0.012042
H	-3.948414	-1.287553	1.642974
C	-6.39236	-1.61934	0.693232
H	-7.212228	-0.889783	0.732858
H	-6.782132	-2.4912	0.151027
H	-6.161722	-1.929266	1.716554
C	-1.149546	2.228091	-1.142523
H	-1.723308	1.607321	-1.840912
H	-0.174702	2.412539	-1.594969
H	-1.688925	3.181587	-1.06451
C	-5.457925	-0.596506	-1.429552
H	-5.814707	-1.439065	-2.036285
H	-4.584891	-0.168659	-1.925547
H	-6.257063	0.15595	-1.447219
C	4.949521	-2.624333	-0.699159
H	4.679912	-3.094914	-1.649059
H	4.91634	-3.388119	0.083395

Frequencies --	13.5035	15.5923	26.2342
Frequencies --	35.8440	53.3222	60.9748
Frequencies --	66.0234	90.3536	105.8178

Zero-point correction= 0.372481 (Hartree/Particle)  
 Thermal correction to Energy= 0.394223  
 Thermal correction to Enthalpy= 0.395167  
 Thermal correction to Gibbs Free Energy= 0.318317  
 Sum of electronic and zero-point Energies= -812.400265  
 Sum of electronic and thermal Energies= -812.378523  
 Sum of electronic and thermal Enthalpies= -812.377579  
 Sum of electronic and thermal Free Energies= -812.454429

aa-1+4a5+.log

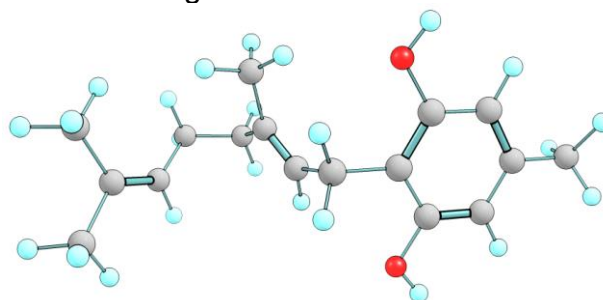


43 Atoms

C	-2.035963	-0.84889	1.192624
C	-3.009298	0.096741	0.847305
C	-3.113015	0.550531	-0.470043
C	-2.237939	0.037032	-1.432752
C	-1.267672	-0.903308	-1.07126
C	-1.152871	-1.382019	0.242697
H	-3.677179	0.484134	1.613099
H	-2.300117	0.376609	-2.463914
O	-1.896572	-1.293858	2.481838
H	-2.558678	-0.863169	3.039583
O	-0.375183	-1.399904	-1.984215
H	-0.538429	-0.990808	-2.844973
C	-0.04963	-2.350581	0.630152
C	1.208511	-1.566719	0.921632
H	0.104545	-3.068461	-0.17784
H	-0.36304	-2.910572	1.51691
C	2.329008	-1.491324	0.188649
H	1.120822	-0.902425	1.781807
C	3.372717	-0.445164	0.520121
H	3.212362	-0.068777	1.536699
H	4.382103	-0.878542	0.486843
C	3.320947	0.765973	-0.457429
C	1.935838	1.349828	-0.566323
H	3.650995	0.436047	-1.450752
H	4.051137	1.510405	-0.124078
C	1.442348	2.423557	0.069473
H	1.249535	0.77558	-1.187662
C	-0.002548	2.830324	-0.098886
H	-0.525725	2.81327	0.866833
H	-0.083109	3.859059	-0.475495
H	-0.541707	2.166337	-0.779571
C	2.607971	-2.310592	-1.046309
H	2.686414	-1.666925	-1.930696
H	1.833954	-3.049874	-1.253047
H	3.569306	-2.831722	-0.949859
C	2.231661	3.301708	1.009414
H	2.21199	4.34677	0.673148
H	3.275515	2.998818	1.112748
H	1.77928	3.291771	2.009878
C	-4.119251	1.613667	-0.840618
H	-4.468582	1.493284	-1.870382
H	-3.672936	2.612782	-0.762832
Frequencies --	24.6783	32.8113	37.2703
Frequencies --	51.3041	52.4024	72.8984
Frequencies --	86.0471	103.4322	111.4420

Zero-point correction= 0.373065 (Hartree/Particle)  
 Thermal correction to Energy= 0.394384  
 Thermal correction to Enthalpy= 0.395328  
 Thermal correction to Gibbs Free Energy= 0.321945  
 Sum of electronic and zero-point Energies= -812.403752  
 Sum of electronic and thermal Energies= -812.382433  
 Sum of electronic and thermal Enthalpies= -812.381489  
 Sum of electronic and thermal Free Energies= -812.454871

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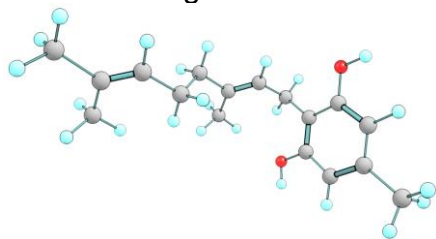


43 Atoms

C	2.588766	1.363379	-0.094416
C	3.941733	1.291156	0.254341
C	4.625871	0.075114	0.164852
C	3.937206	-1.056506	-0.282085
C	2.583528	-0.96854	-0.626399
C	1.880058	0.242693	-0.55228
H	4.45707	2.184428	0.598977
H	4.450815	-2.011747	-0.361254
O	1.884854	2.537086	-0.009664
H	2.472412	3.239722	0.300603
O	1.88484	-2.064226	-1.06426
C	2.470734	-2.833302	-1.077279
H	0.408814	0.334524	-0.909029
C	-0.47581	0.250186	0.314786
H	0.160894	-0.445791	-1.629716
H	0.231421	1.297649	-1.401886
C	-1.303255	-0.746305	0.662366
H	-0.398054	1.110018	0.979782
C	-2.136326	-0.64992	1.92296
H	-1.90856	-1.503733	2.577653
H	-1.869364	0.256786	2.479254
C	-3.664308	-0.644029	1.658869
C	-4.096553	0.548106	0.850456
H	-4.172032	-0.627239	2.633667
H	-3.955915	-1.582805	1.179273
C	-4.702258	0.575974	-0.346507
H	-3.849017	1.508246	1.307647
C	-5.03349	1.886958	-1.019831
H	-4.543715	1.956612	-2.000321
H	-6.112184	1.972205	-1.207666
H	-4.721996	2.748224	-0.42188
C	-1.500662	-2.006089	-0.150438
H	-1.613982	-2.872564	0.512422
H	-0.662802	-2.205964	-0.820071
H	-2.41711	-1.951566	-0.751189
C	-5.107654	-0.642824	-1.139243
H	-6.185448	-0.62566	-1.347367
H	-4.878255	-1.584557	-0.637714
H	-4.604968	-0.648462	-2.115244
C	6.075685	-0.022642	0.577407
H	6.601235	-0.797124	0.011036
H	6.163942	-0.279782	1.640133
Frequencies --	16.5772	22.7929	34.5234
Frequencies --	37.2963	46.5401	49.9144
Frequencies --	79.4872	112.1274	132.5322

Zero-point correction= 0.372946 (Hartree/Particle)  
 Thermal correction to Energy= 0.394350  
 Thermal correction to Enthalpy= 0.395295  
 Thermal correction to Gibbs Free Energy= 0.320278  
 Sum of electronic and zero-point Energies= -812.401083  
 Sum of electronic and thermal Energies= -812.379679  
 Sum of electronic and thermal Enthalpies= -812.378735  
 Sum of electronic and thermal Free Energies= -812.453751

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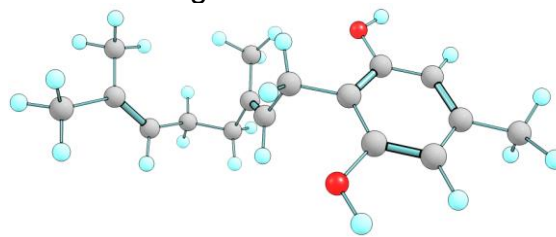
43 Atoms

C	2.986712	0.006116	1.237682
C	3.807834	-1.088912	0.949204
C	4.035674	-1.464992	-0.37834
C	3.426894	-0.733213	-1.401997
C	2.607813	0.360406	-1.097525
C	2.37606	0.762289	0.225948
H	4.264174	-1.648824	1.762141
H	3.584877	-1.012741	-2.440941
O	2.730747	0.395712	2.527143
H	3.207877	-0.184123	3.13645
O	1.995825	1.091227	-2.083086
H	2.232383	0.725022	-2.946107
C	1.459973	1.924445	0.560022
C	0.07174	1.449766	0.928558
H	1.431788	2.616868	-0.282325
H	1.88428	2.467161	1.412578
C	-1.055759	1.560211	0.210354
H	0.019234	0.933162	1.887147
C	-2.353676	0.976126	0.731931
H	-2.296352	0.832907	1.817572
H	-3.179102	1.677607	0.548648
C	-2.714942	-0.379833	0.071979
C	-4.001576	-0.946906	0.606909
H	-1.893197	-1.079981	0.274239
H	-2.754962	-0.259187	-1.014511
C	-5.188719	-1.040018	-0.012728
H	-3.948154	-1.289316	1.641948
C	-6.392225	-1.619861	0.692078
H	-7.212001	-0.890239	0.732439
H	-6.78213	-2.491166	0.149076
H	-6.161556	-1.930767	1.715099
C	-1.149538	2.228648	-1.141265
H	-1.723206	1.608236	-1.84005
H	-0.174683	2.413455	-1.593542
H	-1.689025	3.182042	-1.062715
C	-5.457845	-0.59501	-1.429757
H	-5.815253	-1.436795	-2.037196
H	-4.584684	-0.167188	-1.925558
H	-6.256558	0.157922	-1.446523
C	4.949402	-2.623912	-0.700673
H	4.680056	-3.093689	-1.651046
H	4.915903	-3.38833	0.081253
Frequencies --	13.5110	15.5528	26.1841
Frequencies --	35.8044	53.3847	61.1881
Frequencies --	66.0523	90.3954	105.8967

Zero-point correction= 0.372481 (Hartree/Particle)  
 Thermal correction to Energy= 0.394223  
 Thermal correction to Enthalpy= 0.395167  
 Thermal correction to Gibbs Free Energy= 0.318319  
 Sum of electronic and zero-point Energies= -812.400265  
 Sum of electronic and thermal Energies= -812.378523  
 Sum of electronic and thermal Enthalpies= -812.377579  
 Sum of electronic and thermal Free Energies= -812.454427

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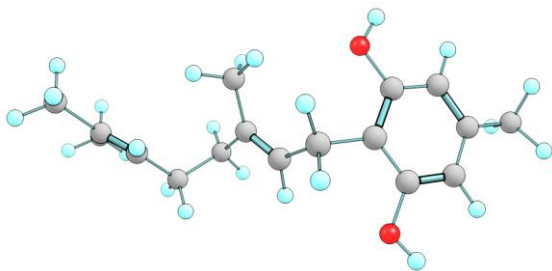
43 Atoms

C	2.589353	1.363426	-0.094395
C	3.942341	1.29092	0.254169
C	4.6262	0.074704	0.16468
C	3.937241	-1.056778	-0.282114
C	2.583522	-0.968526	-0.626252
C	1.88034	0.242856	-0.552112
H	4.457959	2.18411	0.598606
H	4.450626	-2.01213	-0.361344
O	1.885718	2.537295	-0.009671
H	2.473386	3.239762	0.300769
O	1.88452	-2.064072	-1.063952
H	2.470278	-2.833249	-1.077178
C	0.409083	0.334925	-0.908712
C	-0.475445	0.250136	0.315124
H	0.161066	-0.445094	-1.629693
H	0.231696	1.298243	-1.401194
C	-1.303335	-0.746199	0.662096
H	-0.397267	1.1095	0.980683
C	-2.136331	-0.650266	1.922775
H	-1.9086	-1.504357	2.577115
H	-1.869293	0.256202	2.479418
C	-3.664319	-0.644218	1.658713
C	-4.096508	0.548016	0.850425
H	-4.172031	-0.627525	2.633522
H	-3.955978	-1.582921	1.179008
C	-4.702751	0.575997	-0.346269
H	-3.848488	1.50811	1.307445
C	-5.033866	1.887048	-1.019521
H	-4.544427	1.956536	-2.000192
H	-6.112603	1.972587	-1.206973
H	-4.721922	2.748255	-0.421719
C	-1.501329	-2.005367	-0.151515
H	-1.615268	-2.872192	0.510784
H	-0.663462	-2.205315	-0.821118
H	-2.417637	-1.949935	-0.752398
C	-5.108888	-0.642704	-1.138772
H	-6.186812	-0.625329	-1.346202
H	-4.879349	-1.584501	-0.637426
H	-4.606837	-0.64841	-2.1151
C	6.075985	-0.023235	0.577267
H	6.600887	-0.799507	0.01277
H	6.164127	-0.277788	1.640634
H	6.600278	0.924754	0.425231

Frequencies -- 16.4983 22.7576 34.4854  
 Frequencies -- 36.8560 46.5817 49.8951  
 Frequencies -- 79.4422 112.1828 132.5979

Zero-point correction= 0.372946 (Hartree/Particle)  
 Thermal correction to Energy= 0.394351  
 Thermal correction to Enthalpy= 0.395295  
 Thermal correction to Gibbs Free Energy= 0.320262  
 Sum of electronic and zero-point Energies= -812.401083  
 Sum of electronic and thermal Energies= -812.379679  
 Sum of electronic and thermal Enthalpies= -812.378735  
 Sum of electronic and thermal Free Energies= -812.453767

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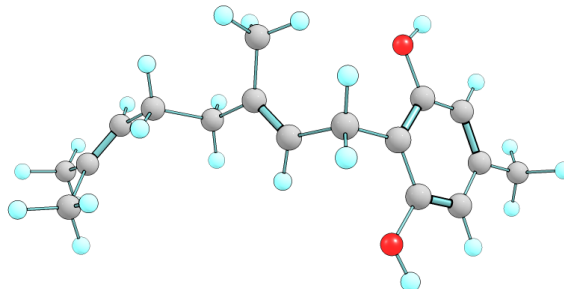
43 Atoms

C	-3.031624	-1.180042	-0.493986
C	-4.29936	-1.062637	0.086243
C	-4.7655	0.186529	0.507305
C	-3.948132	1.307294	0.332673
C	-2.681957	1.173923	-0.248807
C	-2.198162	-0.068228	-0.685552
H	-4.917854	-1.948143	0.212809
H	-4.292427	2.288444	0.651063
O	-2.53808	-2.390565	-0.90805
H	-3.198119	-3.077471	-0.742086
O	-1.858851	2.255242	-0.428408
H	-2.299853	3.050399	-0.099495
C	-0.816352	-0.216861	-1.293433
C	0.204254	-0.650972	-0.265012
H	-0.527446	0.723164	-1.765581
H	-0.864255	-0.976012	-2.082554
C	1.199227	0.071209	0.272069
H	0.075671	-1.677033	0.081865
C	2.144412	-0.575355	1.272864
H	2.562322	0.191902	1.936341
H	1.591075	-1.278982	1.906547
C	3.320603	-1.351209	0.618018
C	4.168521	-0.517993	-0.306032
H	2.891716	-2.18561	0.047796
H	3.924771	-1.795982	1.415793
C	5.368146	0.031192	-0.057371
H	3.723755	-0.326922	-1.282906
C	6.074794	0.863637	-1.100585
H	6.263809	1.879423	-0.728584
H	7.056935	0.43708	-1.344642
H	5.496702	0.941711	-2.025878
C	1.483232	1.518424	-0.047965
H	1.413655	2.120007	0.867952
H	0.787998	1.943966	-0.772071
H	2.50752	1.640505	-0.418728
C	6.12175	-0.104825	1.243
H	7.111871	-0.547018	1.071455
H	5.601988	-0.713788	1.984986
H	6.29858	0.884288	1.685307
C	-6.115675	0.318102	1.171899
H	-6.561703	1.298478	0.980348
H	-6.029118	0.206534	2.259725

Frequencies --	12.6379	17.4308	23.5160
Frequencies --	36.7219	39.4785	50.7282
Frequencies --	92.3026	97.2755	109.8182

Zero-point correction=	0.372644	(Hartree/Particle)
Thermal correction to Energy=	0.394264	
Thermal correction to Enthalpy=	0.395208	
Thermal correction to Gibbs Free Energy=	0.318633	
Sum of electronic and zero-point Energies=	-812.398728	
Sum of electronic and thermal Energies=	-812.377108	
Sum of electronic and thermal Enthalpies=	-812.376164	
Sum of electronic and thermal Free Energies=	-812.452738	

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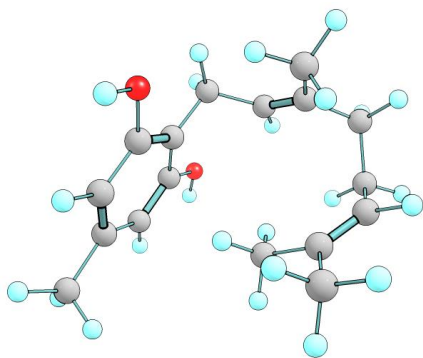
43 Atoms

C	-2.833383	-1.294326	-0.588332
C	-3.971278	-1.598915	0.166855
C	-4.659841	-0.584896	0.839376
C	-4.188429	0.728248	0.747318
C	-3.048826	1.017111	-0.011752
C	-2.35138	0.017497	-0.706085
H	-4.313948	-2.628825	0.23218
H	-4.704378	1.530838	1.268991
O	-2.126427	-2.265536	-1.249355
H	-2.555492	-3.121285	-1.112431
O	-2.562095	2.294802	-0.114313
H	-3.124944	2.893799	0.394913
C	-1.099662	0.328334	-1.503827
C	0.156017	0.083116	-0.697375
H	-1.144968	1.357781	-1.861899
H	-1.08105	-0.320866	-2.387121
C	1.037681	0.99117	-0.252128
H	0.327859	-0.964448	-0.449808
C	2.257635	0.552552	0.530479
H	2.285216	1.083064	1.494058
H	2.196797	-0.517212	0.760732
C	3.59289	0.819788	-0.20923
C	4.784806	0.422377	0.618227
H	3.661622	1.890595	-0.442526
H	3.571141	0.295045	-1.169443
H	5.623704	-0.608125	0.428425
C	4.950305	1.048114	1.497282
C	6.763274	-0.870518	1.384546
H	6.682425	-1.873381	1.824726
H	7.728671	-0.840759	0.861764
H	6.794679	-0.141769	2.199558
C	0.919486	2.479343	-0.495178
H	1.235351	3.034998	0.39613
H	-0.101295	2.782628	-0.732263
H	1.574209	2.805952	-1.313164
C	5.537231	-1.590394	-0.714249
H	6.462369	-1.577143	-1.305284
H	4.701797	-1.398942	-1.389859
H	5.432024	-2.613226	-0.329766
C	-5.910113	-0.896968	1.62744
H	-6.025833	-0.219189	2.478396
H	-5.898923	-1.923234	2.005763
H	-6.804337	-0.789028	1.001342

Frequencies --	20.7802	21.8944	30.3106
Frequencies --	42.1737	50.6913	55.6465
Frequencies --	71.2186	88.4438	119.8501

Zero-point correction=	0.372624	(Hartree/Particle)
Thermal correction to Energy=	0.394277	
Thermal correction to Enthalpy=	0.395221	
Thermal correction to Gibbs Free Energy=	0.319428	
Sum of electronic and zero-point Energies=	-812.400189	
Sum of electronic and thermal Energies=	-812.378536	
Sum of electronic and thermal Enthalpies=	-812.377592	
Sum of electronic and thermal Free Energies=	-812.453386	

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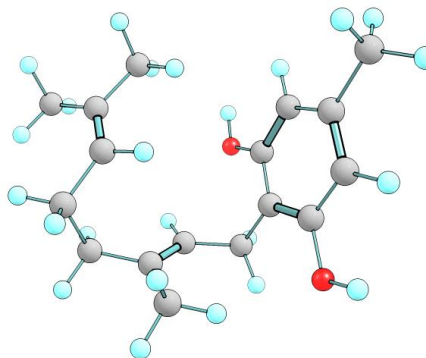
43 Atoms

C	1.737941	-1.036749	-1.061049
C	2.70539	-0.038717	-1.209473
C	3.127234	0.699926	-0.099874
C	2.578579	0.40786	1.151605
C	1.614846	-0.600386	1.284962
C	1.169543	-1.345382	0.183994
H	3.119302	0.167614	-2.193661
H	2.897516	0.96345	2.030224
O	1.28906	-1.767251	-2.130553
H	1.743182	-1.471833	-2.931571
O	1.075385	-0.905912	2.508776
H	1.437348	-0.30653	3.175513
C	0.088401	-2.405356	0.302569
C	-1.219464	-1.962984	-0.323309
H	-0.046682	-2.660742	1.354505
H	0.431087	-3.312955	-0.207949
C	-2.247166	-1.351819	0.283004
H	-1.282306	-2.117721	-1.399631
C	-3.444911	-0.897526	-0.536634
H	-3.710771	-1.66316	-1.275294
H	-4.317757	-0.773601	0.116944
C	-3.186667	0.431284	-1.296711
C	-2.87339	1.592183	-0.39235
H	-4.084013	0.665899	-1.886698
H	-2.376944	0.261158	-2.012364
C	-1.688593	2.195389	-0.204656
H	-3.719054	1.949541	0.198433
C	-1.543563	3.335931	0.774754
H	-0.811792	3.086134	1.554683
H	-1.165383	4.238315	0.275798
H	-2.490027	3.586735	1.262642
C	-2.296604	-1.007837	1.750333
H	-2.488792	0.065603	1.865733
H	-1.371814	-1.239197	2.280476
H	-3.128593	-1.529657	2.242364
C	-0.406776	1.818938	-0.904243
H	-0.017532	2.669539	-1.480269
H	-0.510149	0.965588	-1.57443
H	0.36559	1.559728	-0.17123
C	4.128163	1.81944	-0.259414
H	4.700109	1.980409	0.658957
H	3.621745	2.762524	-0.49918
H	4.832391	1.613294	-1.070837

Frequencies --	22.6180	39.3784	49.5636
Frequencies --	51.6668	72.2745	81.5849
Frequencies --	94.6132	110.4758	135.2503

Zero-point correction=	0.373414 (Hartree/Particle)
Thermal correction to Energy=	0.394476
Thermal correction to Enthalpy=	0.395420
Thermal correction to Gibbs Free Energy=	0.323536
Sum of electronic and zero-point Energies=	-812.403957
Sum of electronic and thermal Energies=	-812.382895
Sum of electronic and thermal Enthalpies=	-812.381951
Sum of electronic and thermal Free Energies=	-812.453835

aa-1a4-5+.log



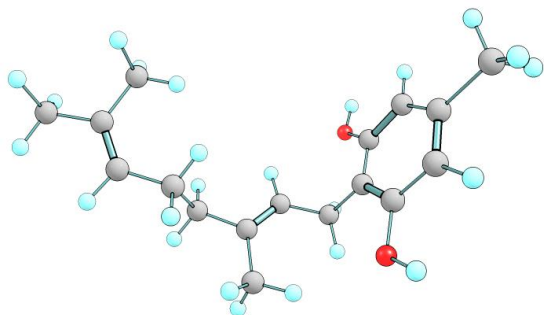
43 Atoms

C	-1.273981	0.668148	1.129891
C	-1.976191	1.675583	0.461645
C	-2.912913	1.344951	-0.523753
C	-3.141143	-0.002565	-0.80938
C	-2.433003	-1.00154	-0.128105
C	-1.474952	-0.693035	0.848009
H	-1.79359	2.716923	0.71512
O	-3.874136	-0.283917	-1.561786
H	-0.352041	0.958917	2.100788
H	-0.26885	1.918569	2.184084
O	-2.657745	-2.329998	-0.389015
H	-3.297782	-2.409368	-1.109297
C	-0.652454	-1.7611	1.549612
C	0.820477	-1.667484	1.195952
H	-1.057643	-2.742485	1.29524
H	-0.762449	-1.641242	2.633204
C	1.403429	-2.089481	0.064575
H	1.432528	-1.117366	1.906966
C	2.856826	-1.762877	-0.205638
H	3.338576	-1.429067	0.720319
C	3.393409	-2.658765	-0.548941
C	3.032906	-0.644035	-1.273209
C	2.228305	0.585839	-0.94366
H	2.716534	-1.029934	-2.250476
H	4.100209	-0.418167	-1.364484
C	2.64503	1.71044	-0.342568
H	1.164785	0.507566	-1.16713
C	1.674708	2.822626	-0.021997
H	1.659975	3.02414	1.058054
H	1.975136	3.762797	-0.503409
H	0.655954	2.583369	-0.339368
C	0.674357	-2.798275	-1.049716
H	0.645481	-2.170909	-1.950508
H	-0.357595	-3.045927	-0.798148
H	1.200538	-3.719269	-1.332334
C	4.066303	1.978851	0.086861
H	4.44411	2.900697	-0.374593
H	4.754251	1.168671	-0.162486
H	4.113015	2.136041	1.172531
C	-3.641671	2.42902	-1.281907
H	-4.599094	2.071399	-1.671361
H	-3.048126	2.774514	-2.13721

Frequencies --	15.1323	23.4531	29.5245
Frequencies --	40.8603	74.0035	75.7047
Frequencies --	91.3707	109.5558	123.5545

Zero-point correction=	0.372941 (Hartree/Particle)
Thermal correction to Energy=	0.394297
Thermal correction to Enthalpy=	0.395241
Thermal correction to Gibbs Free Energy=	0.321150
Sum of electronic and zero-point Energies=	-812.403232
Sum of electronic and thermal Energies=	-812.381875
Sum of electronic and thermal Enthalpies=	-812.380931
Sum of electronic and thermal Free Energies=	-812.455023

aa-1a4-5a.log



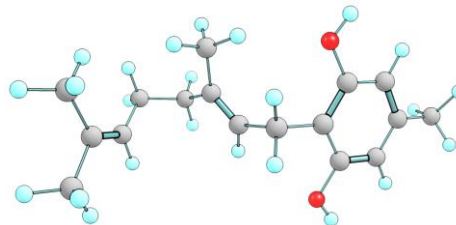
43 Atoms

C	2.51051	-0.594895	1.245417
C	3.256237	-1.621262	0.656994
C	3.732748	-1.481972	-0.650581
C	3.446777	-0.307417	-1.35191
C	2.698573	0.711225	-0.749362
C	2.219394	0.596403	0.563384
H	3.459131	-2.529766	1.219243
H	3.80209	-0.180703	-2.37191
O	2.019629	-0.700303	2.521367
H	2.285023	-1.551251	2.896242
O	2.403719	1.871228	-1.418774
H	2.790538	1.836386	-2.304155
C	1.376011	1.680818	1.207267
C	-0.097622	1.340248	1.166998
H	1.575917	2.633583	0.71544
H	1.683577	1.784691	2.254366
C	-1.047004	1.879934	0.387976
H	-0.386445	0.533718	1.840833
C	-2.471643	1.367274	0.460729
H	-2.639808	0.842582	1.408038
H	-3.173299	2.213285	0.439087
C	-2.825422	0.398838	-0.697332
C	-4.266636	-0.031297	-0.658258
H	-2.144278	-0.456342	-0.650714
H	-2.627455	0.898709	-1.654807
C	-4.765812	-1.223714	-0.296439
H	-4.979039	0.749715	-0.930147
C	-6.254684	-1.47711	-0.293045
H	-6.511811	-2.312331	-0.95819
H	-6.601185	-1.763548	0.708904
H	-6.823661	-0.59939	-0.612836
C	-0.808317	2.985538	-0.613325
H	-1.290238	2.750497	-1.569814
H	0.249775	3.156663	-0.81469
H	-1.258506	3.924848	-0.265154
C	-3.935422	-2.407994	0.13498
H	-4.229781	-2.732191	1.141614
H	-2.863158	-2.20486	0.149309
H	-4.110915	-3.265143	-0.528275
C	4.569173	-2.570367	-1.280964
H	4.49495	-2.551288	-2.372024
H	4.262343	-3.561548	-0.933811

Frequencies --	14.3904	17.5474	24.8631
Frequencies --	34.5154	57.2612	59.6850
Frequencies --	70.5197	93.9059	111.4176

Zero-point correction=	0.372544 (Hartree/Particle)
Thermal correction to Energy=	0.394256
Thermal correction to Enthalpy=	0.395201
Thermal correction to Gibbs Free Energy=	0.318632
Sum of electronic and zero-point Energies=	-812.400321
Sum of electronic and thermal Energies=	-812.378609
Sum of electronic and thermal Enthalpies=	-812.377665
Sum of electronic and thermal Free Energies=	-812.454234

aa-1a4a5-.log



43 Atoms

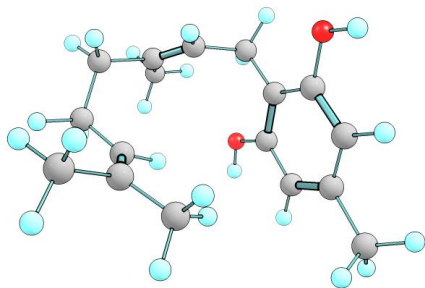
C	2.589014	1.363454	-0.094302
C	3.94199	1.29108	0.254353
C	4.625995	0.074947	0.164796
C	3.937202	-1.056574	-0.282139
C	2.583503	-0.968452	-0.626386
C	1.880166	0.242845	-0.552176
H	4.457466	2.184298	0.598929
H	4.450704	-2.011872	-0.361342
O	1.885216	2.537222	-0.009474
H	2.472901	3.239833	0.300614
O	1.884666	-2.064065	-1.064179
H	2.47059	-2.833111	-1.077669
C	0.408912	0.334789	-0.90882
C	-0.475643	0.249914	0.314997
H	0.160981	-0.445237	-1.629823
H	0.23145	1.29811	-1.401276
C	-1.303307	-0.746577	0.66207
H	-0.397655	1.109355	0.980482
C	-2.136328	-0.650683	1.922732
H	-1.908714	-1.504842	2.577025
H	-1.869234	0.25572	2.47946
C	-3.664314	-0.644454	1.658629
C	-4.096364	0.547963	0.850534
H	-4.172044	-0.627875	2.633431
H	-3.956059	-1.583045	1.178759
C	-4.702392	0.576208	-0.346262
H	-3.848431	1.507955	1.307819
C	-5.033425	1.887406	-1.019271
H	-4.543739	1.957157	-1.9998
H	-6.112121	1.972932	-1.206973
H	-4.721677	2.748481	-0.421174
C	-1.501005	-2.005896	-0.151372
H	-1.61418	-2.872726	0.511056
H	-0.663354	-2.20547	-0.821354
H	-2.417628	-1.950996	-0.751829
C	-5.108401	-0.64232	-1.1391
H	-6.18632	-0.624975	-1.34657
H	-4.87881	-1.584232	-0.637991
H	-4.6063	-0.647725	-2.115404
C	6.075798	-0.022892	0.57738
H	6.60115	-0.797945	0.011617
H	6.163967	-0.27921	1.640317
H	6.599596	0.925619	0.426938

Frequencies --	16.5841	22.8221	34.5217
Frequencies --	37.3261	46.5867	49.9251
Frequencies --	79.4833	112.1526	132.5897

Zero-point correction=	0.372947 (Hartree/Particle)
Thermal correction to Energy=	0.394350
Thermal correction to Enthalpy=	0.395295
Thermal correction to Gibbs Free Energy=	0.320284
Sum of electronic and zero-point Energies=	-812.401082
Sum of electronic and thermal Energies=	-812.379679
Sum of electronic and thermal Enthalpies=	-812.378735
Sum of electronic and thermal Free Energies=	-812.453746



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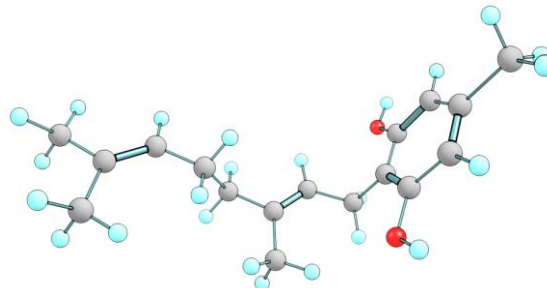
43 Atoms

C	-2.036289	-0.849391	1.192336
C	-3.009537	0.096495	0.847283
C	-3.113023	0.550874	-0.469843
C	-2.237788	0.037764	-1.432677
C	-1.267618	-0.90273	-1.071456
C	-1.153066	-1.382077	0.242339
H	-3.677507	0.483548	1.613174
H	-2.299846	0.377785	-2.463708
O	-1.897164	-1.294931	2.48138
H	-2.55918	-0.864246	3.039238
O	-0.374926	-1.398923	-1.984436
H	-0.537945	-0.989378	-2.845028
C	-0.049874	-2.350808	0.629463
C	1.208266	-1.567085	0.92126
H	0.104285	-3.06838	-0.178814
H	-0.363304	-2.911159	1.515994
C	2.328927	-1.491705	0.188524
H	1.12045	-0.902863	1.781487
C	3.37266	-0.445672	0.520338
H	3.212312	-0.06959	1.537032
H	4.38203	-0.87908	0.486948
C	3.320985	0.765772	-0.456851
C	1.935918	1.349717	-0.565676
H	3.651089	0.436117	-1.450253
H	4.051197	1.510069	-0.12324
C	1.442596	2.423666	0.06989
H	1.249492	0.775386	-1.18681
C	-0.002286	2.830487	-0.098415
H	-0.525459	2.813347	0.867308
H	-0.082839	3.859264	-0.47492
H	-0.541471	2.166581	-0.779166
C	2.608048	-2.310824	-1.046485
H	2.687067	-1.666969	-1.930693
H	1.833822	-3.049763	-1.253679
H	3.569164	-2.832319	-0.949812
C	2.232099	3.30207	1.009434
H	2.213013	4.346918	0.67245
H	3.275785	2.998759	1.113231
H	1.779458	3.293042	2.009791
C	-4.11912	1.614153	-0.840354
H	-4.470226	1.492408	-1.869375
H	-3.671934	2.613061	-0.764955

Frequencies -- 24.7289 32.8368 37.3697  
 Frequencies -- 52.0213 52.4122 72.8519  
 Frequencies -- 86.1130 103.4532 111.6132

Zero-point correction= 0.373067 (Hartree/Particle)  
 Thermal correction to Energy= 0.394383  
 Thermal correction to Enthalpy= 0.395327  
 Thermal correction to Gibbs Free Energy= 0.321964  
 Sum of electronic and zero-point Energies= -812.403750  
 Sum of electronic and thermal Energies= -812.382434  
 Sum of electronic and thermal Enthalpies= -812.381490  
 Sum of electronic and thermal Free Energies= -812.454853

aa-1a4a5a.log



43 Atoms

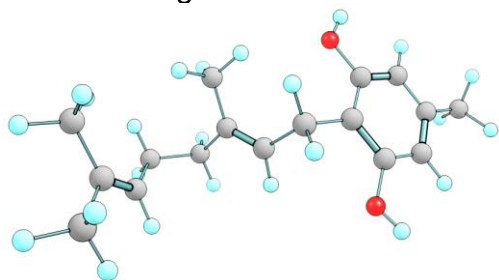
C	-2.97832	0.010011	1.240877
C	-3.805311	1.098654	0.943578
C	-4.042648	1.456834	-0.386937
C	-3.446301	0.707197	-1.40537
C	-2.621322	-0.379115	-1.092222
C	-2.375459	-0.759891	0.235234
H	-4.259331	1.666425	1.752299
H	-3.619615	0.967089	-2.447013
O	-2.715755	-0.364104	2.533592
H	-3.188958	0.223609	3.138405
O	-2.023383	-1.128507	-2.072546
H	-2.269249	-0.776322	-2.938784
C	-1.462022	-1.921513	0.578415
C	-0.071815	-1.447867	0.941166
H	-1.436882	-2.621403	-0.257799
H	-1.886483	-2.455558	1.43639
C	1.052683	-1.561025	0.218693
H	-0.014945	-0.929876	1.898707
C	2.35367	-0.978704	0.734546
H	2.301473	-0.835786	1.820482
H	3.177323	-1.681203	0.547278
C	2.71362	0.377013	0.07345
C	4.00342	0.942049	0.602829
H	1.893707	1.078114	0.279889
H	2.748394	0.256805	-1.013275
H	5.187026	1.037409	-0.023179
C	3.955898	1.280798	1.639367
C	6.394545	1.614557	0.676978
H	7.214479	0.884736	0.709854
H	6.781403	2.487914	0.135098
H	6.169732	1.92156	1.702475
C	1.139715	-2.230699	-1.132784
H	1.712751	-1.612363	-1.833942
H	0.162655	-2.412904	-1.58141
H	1.676708	-3.185622	-1.055653
C	5.448164	0.597804	-1.443388
H	5.801507	1.44209	-2.049735
H	4.572395	0.171313	-1.935722
H	6.247233	-0.154543	-1.46762
C	-4.900765	2.65467	-0.719426
H	-5.425714	2.518624	-1.669613
H	-4.289272	3.560598	-0.812341

Frequencies -- 9.1810 16.1652 27.2878  
 Frequencies -- 35.8744 48.3802 53.3949  
 Frequencies -- 66.5354 90.1495 106.8597

Zero-point correction= 0.372473 (Hartree/Particle)  
 Thermal correction to Energy= 0.394238  
 Thermal correction to Enthalpy= 0.395183  
 Thermal correction to Gibbs Free Energy= 0.317854  
 Sum of electronic and zero-point Energies= -812.400275  
 Sum of electronic and thermal Energies= -812.378510  
 Sum of electronic and thermal Enthalpies= -812.377565  
 Sum of electronic and thermal Free Energies= -812.454894

# Cannabigerocin-AA-1-3t

aa-1-4+5-.log



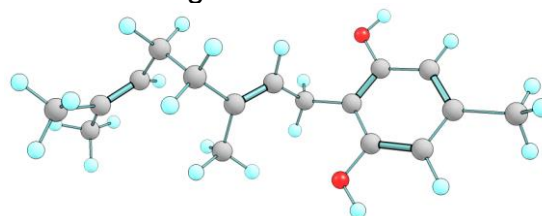
43 Atoms

C	2.583582	-0.968437	-0.62612
C	3.937341	-1.05669	-0.282106
C	4.626329	0.074785	0.164645
C	3.942462	1.290995	0.254261
C	2.589438	1.363498	-0.094155
C	1.880399	0.242938	-0.551876
H	4.450723	-2.012042	-0.361386
H	4.458102	2.184171	0.598711
O	1.884539	-2.063978	-1.06375
H	2.470391	-2.833078	-1.077392
O	1.885778	2.537339	-0.009225
H	2.473576	3.239879	0.300808
C	0.409126	0.334989	-0.908388
C	-0.475382	0.249502	0.315411
H	0.161194	-0.444716	-1.629747
H	0.231605	1.29853	-1.400391
C	-1.303489	-0.746896	0.661684
H	-0.397007	1.10838	0.981582
C	-2.136502	-0.651666	1.922395
H	-1.909036	-1.506279	2.576148
H	-1.869276	0.254338	2.47971
C	-3.664478	-0.645072	1.658242
C	-4.096348	0.547749	0.850646
H	-4.17225	-0.628871	2.63303
H	-3.956329	-1.583405	1.17793
C	-4.702707	0.576552	-0.345969
H	-3.847991	1.50752	1.308165
C	-5.033462	1.888064	-1.018509
H	-4.543842	1.958016	-1.999059
H	-6.112152	1.973926	-1.206088
H	-4.721442	2.748862	-0.420155
C	-1.501783	-2.005418	-0.152853
H	-1.616016	-2.872699	0.508796
H	-0.66394	-2.205106	-0.822567
H	-2.418036	-1.949257	-0.753761
C	-5.109352	-0.641596	-1.139071
H	-6.187383	-0.623979	-1.345938
H	-4.879652	-1.583752	-0.638466
H	-4.607791	-0.646702	-2.115655
C	6.076177	-0.023085	0.577048
H	6.600919	0.924313	0.422842
H	6.600502	-0.800815	0.014031

Frequencies --	16.5387	22.7584	34.4658
Frequencies --	36.4308	46.6298	49.9158
Frequencies --	79.4434	112.2214	132.6667

Zero-point correction=	0.372946 (Hartree/Particle)
Thermal correction to Energy=	0.394350
Thermal correction to Enthalpy=	0.395295
Thermal correction to Gibbs Free Energy=	0.320256
Sum of electronic and zero-point Energies=	-812.401084
Sum of electronic and thermal Energies=	-812.379679
Sum of electronic and thermal Enthalpies=	-812.378735
Sum of electronic and thermal Free Energies=	-812.453773

# aa-1-4+5+.log



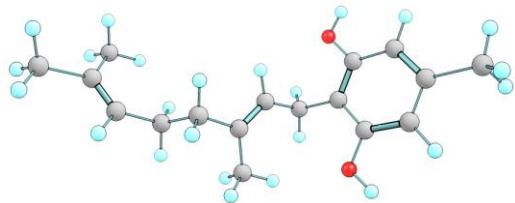
43 Atoms

C	-2.618654	1.129321	0.091645
C	-3.896725	1.20469	0.65371
C	-4.77715	0.122468	0.547049
C	-4.358472	-1.025385	-0.130469
C	-3.076933	-1.084228	-0.692354
C	-2.183565	-0.007569	-0.60806
H	-4.203021	2.107032	1.177745
H	-5.023982	-1.880698	-0.218974
O	-1.7303	2.169225	0.184022
H	-2.142916	2.901253	0.662358
O	-2.631564	-2.203981	-1.347018
H	-3.357658	-2.838133	-1.423252
C	-0.788498	-0.076227	-1.195639
C	0.218491	-0.599888	-0.197925
H	-0.501898	0.914398	-1.554217
H	-0.804969	-0.741979	-2.06637
C	1.317739	0.022567	0.255778
H	-0.006999	-1.595934	0.185932
C	2.254807	-0.702602	1.206367
H	2.720101	0.017956	1.889692
H	1.683967	-1.406304	1.824305
C	3.378857	-1.497202	0.485444
C	4.242644	-0.66108	-0.428573
H	2.898642	-2.288732	-0.101067
C	3.992991	-1.998069	1.244306
H	5.266848	0.093928	-0.06448
H	3.968586	-0.66786	-1.4828
C	6.03078	0.92095	-1.067774
H	5.90459	1.99258	-0.862519
H	7.108657	0.720112	-1.007368
H	5.704074	0.730555	-2.094301
C	1.714308	1.421202	-0.171787
H	2.332844	1.899393	0.594016
H	0.838684	2.052562	-0.342701
H	2.313875	1.408207	-1.089774
C	5.779307	0.17182	1.355215
H	6.620441	-0.519843	1.500105
H	5.01753	-0.073281	2.098858
H	6.157593	1.175595	1.578586
C	-6.143497	0.185609	1.188175
H	-6.823643	-0.554343	0.757421
H	-6.594364	1.175739	1.068196

Frequencies --	12.6454	17.4160	23.5254
Frequencies --	36.7194	39.4931	50.7008
Frequencies --	92.3118	97.2815	109.8432

Zero-point correction=	0.372644 (Hartree/Particle)
Thermal correction to Energy=	0.394264
Thermal correction to Enthalpy=	0.395208
Thermal correction to Gibbs Free Energy=	0.318634
Sum of electronic and zero-point Energies=	-812.398728
Sum of electronic and thermal Energies=	-812.377108
Sum of electronic and thermal Enthalpies=	-812.376164
Sum of electronic and thermal Free Energies=	-812.452738

aa-1-4+5a.log



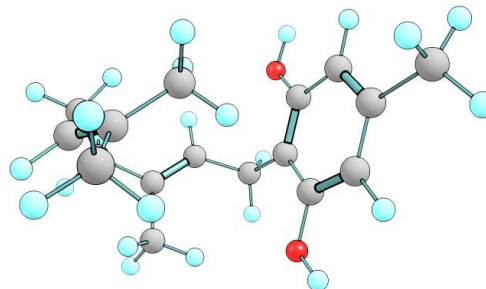
43 Atoms

C	3.072716	0.971143	-0.021362
C	4.209079	0.648779	-0.768927
C	4.663857	-0.673641	-0.826193
C	3.965302	-1.658976	-0.125021
C	2.82871	-1.320278	0.620296
C	2.362149	-0.001534	0.700249
H	4.737529	1.430499	-1.309675
H	4.297281	-2.69376	-0.158543
O	2.60162	2.256869	0.049074
H	3.168403	2.834942	-0.479629
O	2.113357	-2.265161	1.309909
H	2.532253	-3.129128	1.194906
C	1.115715	0.347452	1.490416
C	-0.143781	0.097253	0.691528
H	1.174927	1.385538	1.820406
H	1.089293	-0.277258	2.391025
C	-1.01593	1.004501	0.226131
H	-0.32778	-0.953914	0.469205
C	-2.242064	0.561575	-0.544207
H	-2.262437	1.065615	-1.522094
H	-2.196247	-0.514908	-0.744795
C	-3.573185	0.867912	0.187615
C	-4.771056	0.465795	-0.629579
H	-3.626187	1.94549	0.392173
H	-3.559061	0.368934	1.161422
C	-5.631135	-0.550231	-0.411718
H	-4.925439	1.069556	-1.525978
C	-6.773899	-0.820382	-1.362276
H	-6.708043	-1.835634	-1.775746
H	-7.739282	-0.762071	-0.841881
H	-6.793258	-0.112995	-2.19625
C	-0.879893	2.496629	0.433619
H	-1.19915	3.035137	-0.466913
H	0.146535	2.794074	0.653327
H	-1.52237	2.848891	1.250667
C	-5.563977	-1.50261	0.75779
H	-6.487838	-1.453413	1.348952
H	-4.723964	-1.31065	1.427283
H	-5.481119	-2.537643	0.401583
C	5.888789	-1.019062	-1.640089
H	6.133733	-2.081858	-1.567374
H	6.760601	-0.447146	-1.303292

Frequencies --	20.9632	22.1464	30.3184
Frequencies --	42.3922	50.3685	61.2337
Frequencies --	71.0713	88.6196	120.0543

Zero-point correction=	0.372643 (Hartree/Particle)
Thermal correction to Energy=	0.394286
Thermal correction to Enthalpy=	0.395230
Thermal correction to Gibbs Free Energy=	0.319538
Sum of electronic and zero-point Energies=	-812.400174
Sum of electronic and thermal Energies=	-812.378532
Sum of electronic and thermal Enthalpies=	-812.377587
Sum of electronic and thermal Free Energies=	-812.453279

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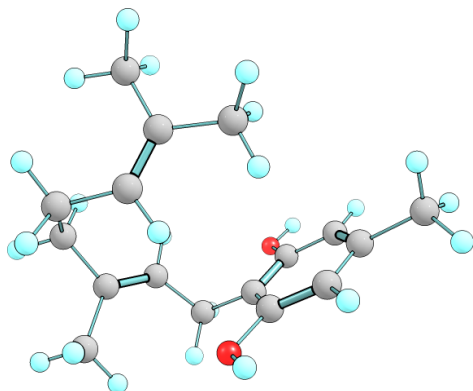
43 Atoms

C	1.614943	-0.600518	1.284883
C	2.578646	0.407739	1.151604
C	3.127259	0.699942	-0.099878
C	2.705379	-0.038566	-1.209524
C	1.737897	-1.036593	-1.061185
C	1.169553	-1.345356	0.183828
H	2.897649	0.963206	2.030278
H	3.119265	0.167858	-2.193697
O	1.075642	-0.906326	2.508699
H	1.437269	-0.306752	3.175447
O	1.288954	-1.766948	-2.130767
H	1.74295	-1.471381	-2.931805
C	0.088402	-2.405322	0.302343
C	-1.219477	-1.962824	-0.323401
H	-0.046605	-2.660865	1.354249
H	0.431033	-3.312859	-0.208325
C	-2.247191	-1.351795	0.283019
H	-1.282343	-2.117403	-1.399745
C	-3.444967	-0.89747	-0.536576
H	-3.710917	-1.663128	-1.275177
H	-4.317775	-0.77348	0.117038
C	-3.186674	0.431303	-1.296677
C	-2.873417	1.592137	-0.392245
H	-4.083985	0.665949	-1.886709
H	-2.376921	0.261166	-2.012294
C	-1.688667	2.195416	-0.204551
H	-3.71907	1.949368	0.198634
C	-1.54366	3.335842	0.77499
H	-0.811857	3.085958	1.554863
H	-1.165515	4.238309	0.27616
H	-2.490111	3.586549	1.262946
C	-2.296621	-1.00804	1.750392
H	-2.48882	0.065385	1.865936
H	-1.37181	-1.23945	2.280473
H	-3.128581	-1.529921	2.242403
C	-0.406858	1.819087	-0.904192
H	-0.017601	2.669768	-1.480087
H	-0.510228	0.965844	-1.574519
O	0.365494	1.559762	-0.171214
C	4.128284	1.819394	-0.259199
H	4.831546	1.614076	-1.071663
H	4.701326	1.979068	0.658725

Frequencies --	22.6065	39.3499	49.5556
Frequencies --	52.1015	72.2593	81.5780
Frequencies --	94.5701	110.4459	135.2450

Zero-point correction=	0.373415 (Hartree/Particle)
Thermal correction to Energy=	0.394477
Thermal correction to Enthalpy=	0.395421
Thermal correction to Gibbs Free Energy=	0.323542
Sum of electronic and zero-point Energies=	-812.403956
Sum of electronic and thermal Energies=	-812.382894
Sum of electronic and thermal Enthalpies=	-812.381950
Sum of electronic and thermal Free Energies=	-812.453829

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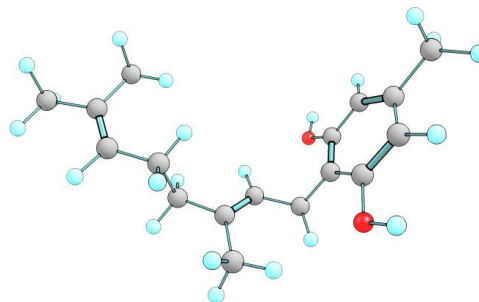
43 Atoms

C	-1.267648	-0.903314	-1.071355
C	-2.237863	0.037085	-1.432772
C	-3.112884	0.550601	-0.469986
C	-3.009208	0.096707	0.847305
C	-2.035947	-0.849066	1.192544
C	-1.152909	-1.382168	0.242581
H	-2.30008	0.376715	-2.463919
H	-3.677063	0.484067	1.613144
O	-0.37513	-1.399861	-1.984309
H	-0.538255	-0.990602	-2.845017
O	-1.896627	-1.294157	2.481723
H	-2.558282	-0.862957	3.03961
C	-0.0497	-2.350783	0.629952
C	1.20841	-1.566922	0.921535
H	0.10448	-3.06858	-0.178118
H	-0.363111	-2.910869	1.516654
C	2.328998	-1.49156	0.188689
H	1.120596	-0.902547	1.781643
C	3.372628	-0.445322	0.520163
H	3.212362	-0.069069	1.536808
H	4.382047	-0.878615	0.486733
C	3.320642	0.76594	-0.457229
C	1.935486	1.349744	-0.565804
H	3.650511	0.436144	-1.450662
H	4.050874	1.510359	-0.123941
C	1.442251	2.423847	0.069562
H	1.248933	0.775137	-1.186537
C	-0.002764	2.83038	-0.098337
H	-0.525577	2.813397	0.867583
H	-0.083627	3.859042	-0.475081
H	-0.542078	2.166199	-0.778722
C	2.608129	-2.310976	-1.046124
H	2.687215	-1.667357	-1.930493
H	1.833908	-3.049964	-1.25315
H	3.569233	-2.832473	-0.949276
C	2.231939	3.302663	1.008565
H	2.212351	4.347433	0.671377
H	3.275771	2.9997	1.111899
H	1.779798	3.29369	2.009149
C	-4.118938	1.613895	-0.840577
H	-4.989133	1.592156	-0.178264
H	-4.46807	1.493723	-1.870442
H	-3.672484	2.612935	-0.762565

Frequencies --	24.6343	32.7599	37.3012
Frequencies --	51.6847	52.4123	72.8591
Frequencies --	86.0679	103.4420	111.4358

Zero-point correction=	0.373065 (Hartree/Particle)
Thermal correction to Energy=	0.394383
Thermal correction to Enthalpy=	0.395327
Thermal correction to Gibbs Free Energy=	0.321949
Sum of electronic and zero-point Energies=	-812.403752
Sum of electronic and thermal Energies=	-812.382434
Sum of electronic and thermal Enthalpies=	-812.381490
Sum of electronic and thermal Free Energies=	-812.454868

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43 Atoms

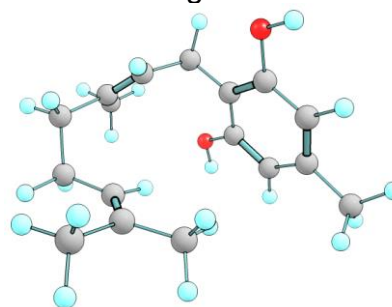
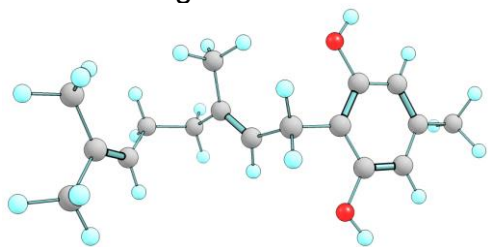
C	2.710405	0.713565	-0.742564
C	3.465869	-0.301557	-1.341038
C	3.743154	-1.480232	-0.642336
C	3.260019	-1.621751	0.66212
C	2.506785	-0.598216	1.246911
C	2.219444	0.594071	0.565819
H	3.834386	-0.169128	-2.355654
H	3.46391	-2.529183	1.225622
O	2.425872	1.878277	-1.40836
H	2.819143	1.845954	-2.290996
O	2.011761	-0.705259	2.521112
H	2.275879	-1.556703	2.895757
C	1.377078	1.679504	1.209329
C	-0.097184	1.341664	1.16669
H	1.579317	2.63235	0.718633
H	1.683066	1.781996	2.257047
C	-1.043231	1.880141	0.382795
H	-0.389571	0.538699	1.843217
C	-2.4694	1.371634	0.454431
H	-2.640998	0.851148	1.403441
H	-3.168665	2.219487	0.427955
C	-2.823536	0.399628	-0.700533
C	-4.265672	-0.027445	-0.661686
H	-2.144211	-0.456755	-0.649804
H	-2.623305	0.895512	-1.659602
C	-4.767687	-1.217286	-0.29536
H	-4.976157	0.753814	-0.937848
C	-6.257084	-1.467629	-0.29266
H	-6.51513	-2.30535	-0.954292
H	-6.605393	-1.748744	0.710171
H	-6.823861	-0.5902	-0.617134
C	-0.798915	2.980411	-0.623044
H	-1.27938	2.742363	-1.579521
H	0.260177	3.147393	-0.82277
H	-1.247048	3.922705	-0.280309
C	-3.940229	-2.401388	0.142138
H	-4.236462	-2.720672	1.149794
H	-2.867555	-2.20042	0.156909
H	-4.116691	-3.260996	-0.517671
C	4.522546	-2.595576	-1.298282
H	5.061224	-3.195711	-0.559238
H	5.248503	-2.206463	-2.018296
H	3.853594	-3.272475	-1.843823

Frequencies --	15.5131	18.2381	25.4708
Frequencies --	34.6357	57.6400	64.1595
Frequencies --	71.0902	93.9132	111.9739

Zero-point correction=	0.372582 (Hartree/Particle)
Thermal correction to Energy=	0.394268
Thermal correction to Enthalpy=	0.395213
Thermal correction to Gibbs Free Energy=	0.318889
Sum of electronic and zero-point Energies=	-812.400287
Sum of electronic and thermal Energies=	-812.378601
Sum of electronic and thermal Enthalpies=	-812.377656
Sum of electronic and thermal Free Energies=	-812.453980

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43 Atoms

C	2.589015	1.363437	-0.094465
C	3.941956	1.291029	0.254287
C	4.625925	0.074866	0.16482
C	3.937126	-1.056641	-0.28214
C	2.583432	-0.968495	-0.626437
C	1.880139	0.242823	-0.552312
H	4.457461	2.184243	0.598832
H	4.45061	-2.011941	-0.361398
O	1.885265	2.537244	-0.009783
H	2.472863	3.239792	0.300612
O	1.884608	-2.064102	-1.064279
H	2.470415	-2.833246	-1.07734
C	0.4089	0.334828	-0.909013
C	-0.475705	0.250364	0.314808
H	0.160906	-0.44536	-1.629814
H	0.23156	1.298031	-1.401738
C	-1.303185	-0.746139	0.662278
H	-0.397904	1.110105	0.979922
C	-2.136235	-0.649884	1.922898
H	-1.908382	-1.50372	2.577533
H	-1.869343	0.256812	2.479247
C	-3.664224	-0.644137	1.658821
C	-4.096608	0.548003	0.850488
H	-4.171938	-0.627467	2.63363
H	-3.95574	-1.582921	1.17918
C	-4.702499	0.575867	-0.346382
H	-3.849027	1.50815	1.307644
C	-5.033839	1.886856	-1.019647
H	-4.544106	1.956564	-2.000156
H	-6.112546	1.972048	-1.207436
H	-4.722365	2.748124	-0.421684
C	-1.50059	-2.005859	-0.150632
H	-1.613859	-2.87239	0.512169
H	-0.662745	-2.205669	-0.820308
H	-2.417062	-1.951327	-0.751348
C	-5.107992	-0.642924	-1.139077
H	-6.185847	-0.625846	-1.346904
H	-4.878366	-1.584669	-0.637669
H	-4.605573	-0.648448	-2.115215
C	6.075669	-0.023014	0.577558
H	6.600751	-0.799016	0.012847
H	6.163695	-0.277955	1.640841
H	6.599862	0.925095	0.425927

Frequencies --	16.5611	22.8098	34.5203
Frequencies --	37.1261	46.5845	49.9180
Frequencies --	79.4956	112.1552	132.5811

Zero-point correction=	0.372946 (Hartree/Particle)
Thermal correction to Energy=	0.394350
Thermal correction to Enthalpy=	0.395294
Thermal correction to Gibbs Free Energy=	0.320276
Sum of electronic and zero-point Energies=	-812.401083
Sum of electronic and thermal Energies=	-812.379679
Sum of electronic and thermal Enthalpies=	-812.378735
Sum of electronic and thermal Free Energies=	-812.453753

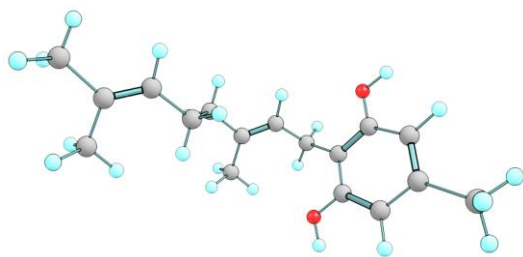
43 Atoms

C	-1.267588	-0.902771	-1.071496
C	-2.237736	0.037794	-1.432695
C	-3.11292	0.550899	-0.469854
C	-3.009443	0.096463	0.847283
C	-2.036263	-0.849462	1.19229
C	-1.153064	-1.382176	0.242246
H	-2.299701	0.377905	-2.463698
H	-3.677425	0.483521	1.613161
O	-0.37491	-1.398927	-1.984503
H	-0.537994	-0.989417	-2.845096
O	-1.897103	-1.295045	2.481315
H	-2.558929	-0.864174	3.039251
C	-0.049879	-2.350928	0.629358
C	1.208218	-1.567145	0.921248
H	0.10435	-3.06844	-0.17895
H	-0.363326	-2.911312	1.515855
C	2.328887	-1.49161	0.188543
H	1.120318	-0.902997	1.781522
C	3.372527	-0.445523	0.520483
H	3.211928	-0.069374	1.537114
H	4.381913	-0.87892	0.487358
C	3.321003	0.765842	-0.456776
C	1.93593	1.349765	-0.565787
H	3.651226	0.436159	-1.450125
H	4.051154	1.510175	-0.12311
C	1.442524	2.423622	0.069856
H	1.249611	0.775495	-1.187103
C	-0.002318	2.830553	-0.098625
H	-0.525593	2.813434	0.867042
H	-0.082742	3.859335	-0.475133
H	-0.541476	2.166682	-0.779426
C	2.608155	-2.310651	-1.046489
H	2.686883	-1.666784	-1.930713
H	1.834164	-3.049854	-1.2536
H	3.569457	-2.831822	-0.949893
C	2.231906	3.301887	1.009638
H	2.212807	4.346793	0.672841
H	3.275595	2.998599	1.113485
H	1.779163	3.292644	2.009944
C	-4.119095	1.614193	-0.840142
H	-4.989251	1.592165	-0.177781
H	-4.468316	1.494182	-1.869996
H	-3.672774	2.613266	-0.761936

Frequencies --	24.7528	32.8692	37.3346
Frequencies --	51.4509	52.4219	72.8688
Frequencies --	86.1161	103.4614	111.6021

Zero-point correction=	0.373066 (Hartree/Particle)
Thermal correction to Energy=	0.394384
Thermal correction to Enthalpy=	0.395328
Thermal correction to Gibbs Free Energy=	0.321955
Sum of electronic and zero-point Energies=	-812.403751
Sum of electronic and thermal Energies=	-812.382433
Sum of electronic and thermal Enthalpies=	-812.381489
Sum of electronic and thermal Free Energies=	-812.454862

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43 Atoms

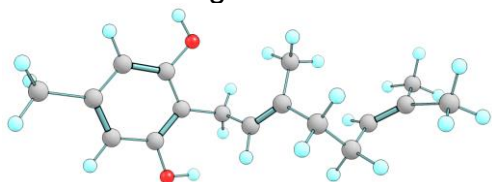
C	2.622056	0.380535	-1.091741
C	3.447176	-0.705414	-1.40583
C	4.042902	-1.456393	-0.388033
C	3.804838	-1.099901	0.942814
C	2.977734	-0.011614	1.241044
C	2.375442	0.759601	0.23605
H	3.621103	-0.963932	-2.447715
H	4.258424	-1.668698	1.751055
O	2.024766	1.131258	-2.07145
H	2.271064	0.780151	-2.937999
O	2.714507	0.360902	2.534082
H	3.187423	-0.227548	3.138403
C	1.461935	1.920875	0.580239
C	0.071693	1.446966	0.942525
H	1.436836	2.621519	-0.255346
H	1.886352	2.454151	1.438717
C	-1.052713	1.560684	0.219999
H	0.01471	0.928287	1.89968
C	-2.353807	0.978094	0.735282
H	-2.301719	0.834352	1.821111
H	-3.177372	1.68082	0.548469
C	-2.713815	-0.377112	0.073166
C	-4.003776	-0.942369	0.601929
H	-1.894022	-1.078457	0.279259
H	-2.748391	-0.256151	-1.013474
C	-5.187266	-1.037259	-0.024371
H	-3.956481	-1.281801	1.638254
C	-6.394954	-1.614781	0.675193
H	-7.214798	-0.884878	0.70851
H	-6.781848	-2.487686	0.132617
H	-6.17031	-1.922563	1.700493
C	-1.1395	2.23143	-1.130985
H	-1.713585	1.614319	-1.832353
H	-0.16238	2.41277	-1.579846
H	-1.675281	3.18696	-1.052945
C	-5.448094	-0.596842	-1.44439
H	-5.801112	-1.440828	-2.051345
H	-4.572269	-0.169897	-1.93623
H	-6.247292	0.15537	-1.468392
C	4.901068	-2.653898	-0.721587
H	5.644802	-2.843238	0.057852
H	5.427046	-2.516437	-1.671001
H	4.289392	-3.559485	-0.816671

Frequencies --	9.1659	16.1603	27.3019
Frequencies --	35.8391	49.2214	53.4601
Frequencies --	66.5738	90.2183	106.9393

Zero-point correction=	0.372475 (Hartree/Particle)
Thermal correction to Energy=	0.394239
Thermal correction to Enthalpy=	0.395183
Thermal correction to Gibbs Free Energy=	0.317869
Sum of electronic and zero-point Energies=	-812.400273
Sum of electronic and thermal Energies=	-812.378509
Sum of electronic and thermal Enthalpies=	-812.377565
Sum of electronic and thermal Free Energies=	-812.454879

# Cannabigerocin-ss-1-3t

b-ss-1-4+5+.log

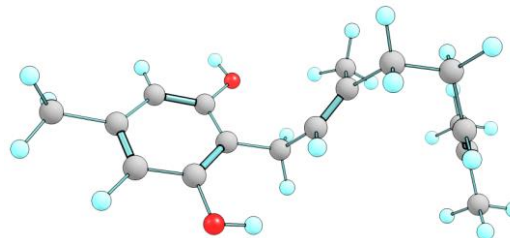


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.657843	1.149352	-0.275019
2	6	0	-3.909415	1.331877	0.317201
3	6	0	-4.755327	0.235950	0.530455
4	6	0	-4.326219	-1.033855	0.143904
5	6	0	-3.069263	-1.203760	-0.448750
6	6	0	-2.210246	-0.119465	-0.683571
7	1	0	-4.222010	2.329453	0.616744
8	1	0	-4.950518	-1.907925	0.299137
9	8	0	-1.803016	2.199108	-0.488107
10	1	0	-2.214077	3.015191	-0.171795
11	8	0	-2.726798	-2.490000	-0.777053
12	1	0	-1.868190	-2.501767	-1.220288
13	6	0	-0.825902	-0.297788	-1.281990
14	6	0	0.197640	-0.676613	-0.234198
15	1	0	-0.541615	0.618710	-1.799597
16	1	0	-0.853485	-1.074135	-2.062003
17	6	0	1.215857	0.062355	0.231486
18	1	0	0.052557	-1.666373	0.202637
19	6	0	2.151880	-0.521195	1.277830
20	1	0	2.575520	0.287626	1.885829
21	1	0	1.589508	-1.171962	1.958140
22	6	0	3.321916	-1.352644	0.683515
23	6	0	4.188422	-0.595571	-0.289423
24	1	0	2.888332	-2.220706	0.171028
25	1	0	3.916350	-1.746228	1.515296
26	6	0	5.347841	0.033114	-0.038727
27	1	0	3.796383	-0.536600	-1.304937
28	6	0	6.086121	0.773094	-1.128283
29	1	0	6.207169	1.833146	-0.868424
30	1	0	7.099268	0.370291	-1.259848
31	1	0	5.567797	0.715012	-2.089743
32	6	0	1.533321	1.468704	-0.213611
33	1	0	1.507196	2.143681	0.651627
34	1	0	0.832455	1.856908	-0.952919
35	1	0	2.550088	1.525840	-0.618665
36	6	0	6.018269	0.082079	1.312174
37	1	0	7.036955	-0.323019	1.254205
38	1	0	5.477008	-0.467176	2.084771
39	1	0	6.118495	1.122115	1.648950
40	6	0	-6.120744	0.437687	1.144166
41	1	0	-6.514037	-0.493587	1.560874
42	1	0	-6.838437	0.792979	0.394657
43	1	0	-6.092050	1.185735	-1.942661

Freq			
Frequencies --	10.2486	18.6965	25.7733
Frequencies --	31.7243	38.8923	45.0049
Frequencies --	90.9356	96.4803	111.8024

Zero-point correction=	0.372502 (Hartree/Particle)
Thermal correction to Energy=	0.394186
Thermal correction to Enthalpy=	0.395130
Thermal correction to Gibbs Free Energy=	0.318122
Sum of electronic and zero-point Energies=	-812.397619
Sum of electronic and thermal Energies=	-812.375934
Sum of electronic and thermal Enthalpies=	-812.374990
Sum of electronic and thermal Free Energies=	-812.451999

# b-ss-1-4+5-.log



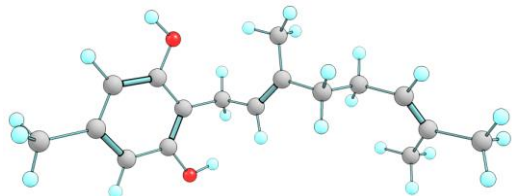
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.593317	-0.954867	-0.628003
2	6	0	3.943058	-1.049290	-0.281267
3	6	0	4.634771	0.080184	0.174176
4	6	0	3.956749	1.296030	0.266721
5	6	0	2.604430	1.377386	-0.084699
6	6	0	1.892528	0.261123	-0.549872
7	1	0	4.453515	-2.005962	-0.363395
8	1	0	4.459222	2.193338	0.613449
9	8	0	1.887730	-2.044120	-1.070138
10	1	0	2.468017	-2.817479	-1.085013
11	8	0	2.017369	2.608520	0.053609
12	1	0	1.106879	2.579138	-0.268752
13	6	0	0.417266	0.334729	-0.900905
14	6	0	-0.465960	0.230482	0.323078
15	1	0	0.181546	-0.446182	-1.624136
16	1	0	0.205022	1.281998	-1.420846
17	6	0	-1.306313	-0.764847	0.640631
18	1	0	-0.377842	1.064376	1.020530
19	6	0	-2.133371	-0.698067	1.906763
20	1	0	-1.906158	-1.570729	2.535920
21	1	0	-1.859867	0.191630	2.486605
22	6	0	-3.661801	-0.678668	1.647311
23	6	0	-4.089982	0.532100	0.864765
24	1	0	-4.165791	-0.679850	2.624043
25	1	0	-3.959520	-1.605686	1.149144
26	6	0	-4.704530	0.586495	-0.326811
27	1	0	-3.831885	1.481535	1.338099
28	6	0	-5.030639	1.912196	-0.973270
29	1	0	-4.548642	1.995825	-1.956526
30	1	0	-6.110116	2.009270	-1.150312
31	1	0	-4.707454	2.759956	-0.362385
32	6	0	-1.524403	-1.993239	-0.213172
33	1	0	-1.670307	-2.875913	0.420654
34	1	0	-0.682988	-2.195319	-0.877796
35	1	0	-2.430200	-1.893121	-0.823703
36	6	0	-5.127046	-0.614205	-1.138088
37	1	0	-6.206780	-0.584881	-1.334242
38	1	0	-4.899969	-1.567129	-0.657017
39	1	0	-4.634893	-0.605042	-2.119423
40	6	0	6.083705	-0.030006	0.586634
41	1	0	6.583200	0.942338	0.558442
42	1	0	6.632770	-0.716942	-0.064842
43	1	0	6.170767	-0.415599	1.609778

Frequencies --	16.9001	23.9657	33.3588
Frequencies --	46.4587	48.8619	51.3275
Frequencies --	77.8760	114.4658	136.3558

Zero-point correction=	0.372845 (Hartree/Particle)
Thermal correction to Energy=	0.394239
Thermal correction to Enthalpy=	0.395183
Thermal correction to Gibbs Free Energy=	0.320459
Sum of electronic and zero-point Energies=	-812.399999
Sum of electronic and thermal Energies=	-812.378605
Sum of electronic and thermal Enthalpies=	-812.377661
Sum of electronic and thermal Free Energies=	-812.452385

b-ss-1-4+5a.log



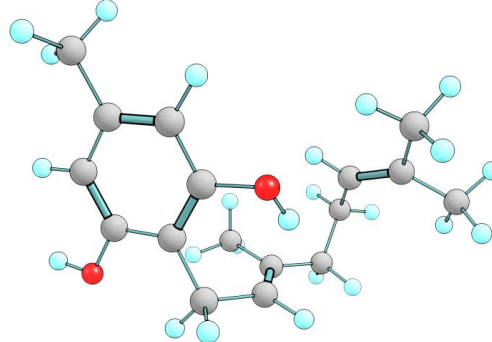
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.059518	1.009068	-0.015012
2	6	0	-4.196911	0.716797	0.739310
3	6	0	-4.663306	-0.601702	0.830468
4	6	0	-3.975376	-1.609439	0.155884
5	6	0	-2.835069	-1.302989	-0.597440
6	6	0	-2.356297	0.010016	-0.712130
7	1	0	-4.717977	1.517051	1.259593
8	1	0	-4.303964	-2.642539	0.204567
9	8	0	-2.573557	2.286988	-0.117867
10	1	0	-3.134849	2.885491	0.393761
11	8	0	-2.215089	-2.361158	-1.210043
12	1	0	-1.472133	-2.047594	-1.742517
13	6	0	-1.101116	0.345658	-1.497591
14	6	0	0.155895	0.089526	-0.695299
15	1	0	-1.153169	1.382908	-1.829077
16	1	0	-1.069738	-0.251463	-2.422339
17	6	0	1.036520	0.995054	-0.243641
18	1	0	0.332488	-0.958062	-0.448009
19	6	0	2.254837	0.551175	0.537831
20	1	0	2.278452	1.073812	1.505491
21	1	0	2.195573	-0.520519	0.758818
22	6	0	3.590489	0.827841	-0.197699
23	6	0	4.781137	0.421025	0.627103
24	1	0	3.658945	1.901202	-0.418625
25	1	0	3.570176	0.313823	-1.163719
26	6	0	5.617440	-0.609842	0.428256
27	1	0	4.947638	1.038816	1.511479
28	6	0	6.756289	-0.883575	1.381976
29	1	0	6.672968	-1.890281	1.812759
30	1	0	7.721697	-0.851304	0.859410
31	1	0	6.789508	-0.162567	2.203752
32	6	0	0.917738	2.484279	-0.477582
33	1	0	1.244413	3.033961	0.413126
34	1	0	-0.104769	2.791405	-0.702165
35	1	0	1.564382	2.812442	-1.301061
36	6	0	5.528545	-1.581723	-0.723037
37	1	0	6.453921	-1.565842	-1.313575
38	1	0	4.693905	-1.382015	-1.397223
39	1	0	5.420315	-2.607536	-0.347517
40	6	0	-5.890957	-0.913431	1.653574
41	1	0	-6.148758	-1.974440	1.604084
42	1	0	-6.755968	-0.337681	1.305862
43	1	0	-5.735942	-0.652143	2.706583

Frequencies -- -27.4587      20.3759      24.2156  
 Frequencies -- 29.1567      42.8860      50.0829  
 Frequencies -- 72.8049      88.3570      122.0995

Zero-point correction= 0.372401 (Hartree/Particle)  
 Thermal correction to Energy= 0.393230  
 Thermal correction to Enthalpy= 0.394174  
 Thermal correction to Gibbs Free Energy= 0.320628  
 Sum of electronic and zero-point Energies= -812.399122  
 Sum of electronic and thermal Energies= -812.378292  
 Sum of electronic and thermal Enthalpies= -812.377348  
 Sum of electronic and thermal Free Energies= -812.450895

b-ss-1-4-5+.log



Standard orientation:

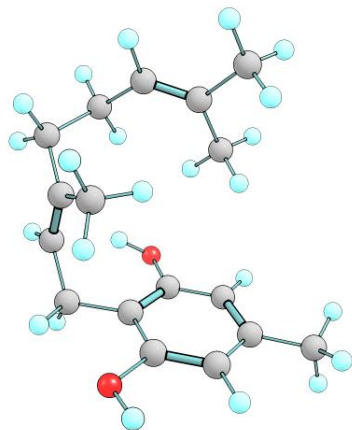
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			X	Y	Z
1	6	0	-2.856315	-0.815444	0.246853
2	6	0	-3.630519	0.162628	-0.384383
3	6	0	-3.171953	1.481739	-0.470802
4	6	0	-1.919248	1.793093	0.061781
5	6	0	-1.151890	0.805910	0.687772
6	6	0	-1.606728	-0.517645	0.815257
7	1	0	-4.593499	-0.109226	-0.810554
8	1	0	-1.513241	2.797242	-0.009008
9	8	0	-3.281766	-2.117981	0.328780
10	1	0	-4.133266	-2.203606	-0.121467
11	8	0	0.062697	1.195586	1.193880
12	1	0	0.689171	0.452799	1.125356
13	6	0	-0.790651	-1.569408	1.548318
14	6	0	0.646080	-1.716863	1.072769
15	1	0	-1.311202	-2.528773	1.476090
16	1	0	-0.770781	-1.314237	2.614918
17	6	0	1.043782	-1.935990	-0.192573
18	1	0	1.414551	-1.642056	1.842208
19	6	0	2.511661	-1.973709	-0.546457
20	1	0	3.117435	-1.942369	0.365846
21	1	0	2.743318	-2.915608	-1.063264
22	6	0	2.938003	-0.793600	-1.462515
23	6	0	2.622866	0.552006	-0.858413
24	1	0	2.422923	-0.886072	-2.426040
25	1	0	4.007138	-0.895769	-1.675427
26	6	0	3.415419	1.288492	-0.062746
27	1	0	1.623795	0.935025	-1.063488
28	6	0	2.952831	2.613037	0.494694
29	1	0	3.032114	2.623163	1.589642
30	1	0	3.587676	3.431803	0.130397
31	1	0	1.914441	2.825767	0.232561
32	6	0	0.080631	-2.098276	-1.345091
33	1	0	-0.055117	-1.149700	-1.879609
34	1	0	-0.906551	-2.432676	-1.020324
35	1	0	0.471116	-2.820584	-2.070605
36	6	0	4.810846	0.888126	0.348719
37	1	0	5.535388	1.661952	0.063600
38	1	0	5.135949	-0.059169	-0.085558
39	1	0	4.872167	0.795435	1.440765
40	6	0	-4.024003	2.547584	-1.118333
41	1	0	-3.412001	3.365988	-1.508087
42	1	0	-4.726940	2.979838	-0.395550
43	1	0	-4.616897	2.139917	-1.942764

Frequencies -- 23.0723      30.7035      37.4400  
 Frequencies -- 54.7526      75.6948      78.9959  
 Frequencies -- 99.5285      119.5327      123.6016

Zero-point correction= 0.373263 (Hartree/Particle)  
 Thermal correction to Energy= 0.394286  
 Thermal correction to Enthalpy= 0.395230  
 Thermal correction to Gibbs Free Energy= 0.322834  
 Sum of electronic and zero-point Energies= -812.405211  
 Sum of electronic and thermal Energies= -812.384188  
 Sum of electronic and thermal Enthalpies= -812.383243  
 Sum of electronic and thermal Free Energies= -812.455639



b-ss-1-4-5-.log



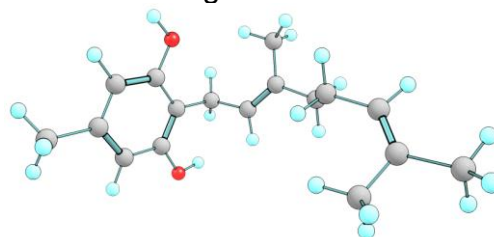
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.470133	-0.809661	0.747574
2	6	0	3.111393	0.430337	0.822009
3	6	0	2.864702	1.413314	-0.142744
4	6	0	1.951005	1.139811	-1.162477
5	6	0	1.310708	-0.101869	-1.222356
6	6	0	1.566031	-1.115498	-0.283020
7	1	0	3.803707	0.626791	1.637487
8	1	0	1.709212	1.884483	-1.913857
9	8	0	2.688137	-1.782111	1.691010
10	1	0	3.295566	-1.443068	2.362690
11	8	0	0.422919	-0.290905	-2.250610
12	1	0	-0.213755	-0.975720	-1.979261
13	6	0	0.899257	-2.478953	-0.381606
14	6	0	-0.613804	-2.441581	-0.536736
15	1	0	1.171448	-3.063830	0.501980
16	1	0	1.319240	-3.016408	-1.240817
17	6	0	-1.472456	-1.809400	0.284793
18	1	0	-1.024074	-2.987203	-1.387451
19	6	0	-2.948988	-1.768235	-0.046515
20	1	0	-3.186563	-2.570372	-0.754493
21	1	0	-3.541992	-1.953472	0.859047
22	6	0	-3.407671	-0.423117	-0.678224
23	6	0	-3.438207	0.736705	0.279290
24	1	0	-4.423177	-0.578720	-1.068266
25	1	0	-2.771953	-0.213807	-1.543816
26	6	0	-2.660642	1.830781	0.290977
27	1	0	-4.189472	0.646319	1.066045
28	6	0	-2.836243	2.894176	1.348855
29	1	0	-1.915142	3.014634	1.934695
30	1	0	-3.041861	3.871907	0.893323
31	1	0	-3.651830	2.660398	2.039141
32	6	0	-1.020725	-1.093893	1.536447
33	1	0	-0.899259	-0.021693	1.352681
34	1	0	-0.070463	-1.479777	1.913096
35	1	0	-1.774937	-1.192984	2.324081
36	6	0	-1.545025	2.109605	-0.685027
37	1	0	-1.713859	3.063207	-1.202474
38	1	0	-1.404911	1.331660	-1.436002
39	1	0	-0.591192	2.211745	-0.151669
40	6	0	3.584957	2.739737	-0.087640
41	1	0	4.543867	2.687248	-0.617888
42	1	0	3.800240	3.035844	0.943443
43	1	0	2.996174	3.533392	-0.556512

Frequencies --	31.3192	39.1079	44.8365
Frequencies --	55.8499	65.0189	72.3726
Frequencies --	83.2052	114.0158	136.9485

Zero-point correction= 0.373081 (Hartree/Particle)  
 Thermal correction to Energy= 0.394089  
 Thermal correction to Enthalpy= 0.395033  
 Thermal correction to Gibbs Free Energy= 0.323215  
 Sum of electronic and zero-point Energies= -812.404936  
 Sum of electronic and thermal Energies= -812.383927  
 Sum of electronic and thermal Enthalpies= -812.382983  
 Sum of electronic and thermal Free Energies= -812.454802

b-ss-1-4-5a.log



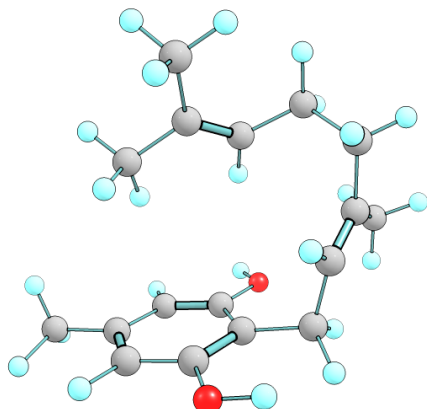
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.607332	0.630845	-0.837240
2	6	0	3.352422	-0.412318	-1.391481
3	6	0	3.732488	-1.504788	-0.601464
4	6	0	3.362393	-1.527266	0.743447
5	6	0	2.615291	-0.475697	1.286883
6	6	0	2.228786	0.631553	0.516634
7	1	0	3.632820	-0.373845	-2.441420
8	1	0	3.639711	-2.355425	1.387656
9	8	0	2.214741	1.710150	-1.585421
10	1	0	2.537298	1.606359	-2.491086
11	8	0	2.281747	-0.593237	2.611400
12	1	0	1.831870	0.207396	2.912199
13	6	0	1.380686	1.754592	1.087148
14	6	0	-0.088559	1.393736	1.094867
15	1	0	1.561286	2.665061	0.515570
16	1	0	1.706572	1.986086	2.112930
17	6	0	-1.066464	1.910179	0.335961
18	1	0	-0.354742	0.588171	1.780995
19	6	0	-2.477901	1.369344	0.448171
20	1	0	-2.614437	0.855140	1.406157
21	1	0	-3.196841	2.200364	0.429642
22	6	0	-2.834174	0.376801	-0.688604
23	6	0	-4.264325	-0.084241	-0.611417
24	1	0	-2.133267	-0.462372	-0.644674
25	1	0	-2.668167	0.867147	-1.656958
26	6	0	-4.727817	-1.281677	-0.220023
27	1	0	-4.999797	0.676035	-0.880373
28	6	0	-6.209937	-1.569154	-0.180630
29	1	0	-6.461507	-2.419712	-0.828197
30	1	0	-6.527788	-1.849064	0.832569
31	1	0	-6.806091	-0.709599	-0.500217
32	6	0	-0.876768	3.012828	-0.678028
33	1	0	-1.377665	2.759721	-1.619716
34	1	0	0.170882	3.208810	-0.908284
35	1	0	-1.339733	3.942853	-0.322696
36	6	0	-3.861018	-2.439325	0.211883
37	1	0	-4.128106	-2.755394	1.228595
38	1	0	-2.793898	-2.210527	0.202316
39	1	0	-4.028547	-3.310049	-0.435532
40	6	0	4.505800	-2.650774	-1.210005
41	1	0	5.017232	-3.240296	-0.444217
42	1	0	5.254262	-2.292382	-1.923739
43	1	0	3.837323	-3.327615	-1.755973

Frequencies --	14.5201	17.6006	29.2657
Frequencies --	34.2521	55.4171	62.1419
Frequencies --	66.5415	96.3657	108.7761

Zero-point correction= 0.372483 (Hartree/Particle)  
 Thermal correction to Energy= 0.394194  
 Thermal correction to Enthalpy= 0.395138  
 Thermal correction to Gibbs Free Energy= 0.318665  
 Sum of electronic and zero-point Energies= -812.399127  
 Sum of electronic and thermal Energies= -812.377416  
 Sum of electronic and thermal Enthalpies= -812.376472  
 Sum of electronic and thermal Free Energies= -812.452946

b-ss-1-4a5+.log



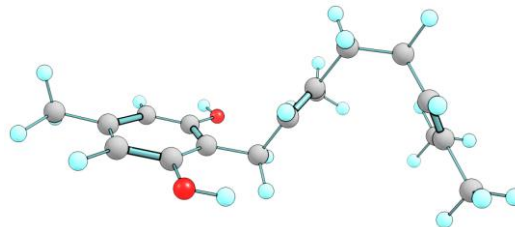
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.296504	-1.009591	-1.030252
2	6	0	-2.300461	-0.117750	-1.412891
3	6	0	-3.133140	0.461820	-0.447044
4	6	0	-2.949176	0.124154	0.893283
5	6	0	-1.942234	-0.776016	1.263358
6	6	0	-1.105791	-1.380079	0.312308
7	1	0	-2.423603	0.135040	-2.463321
8	1	0	-3.570168	0.557276	1.670852
9	8	0	-0.441803	-1.565406	-1.945528
10	1	0	-0.659846	-1.234436	-2.827534
11	8	0	-1.823193	-1.025675	2.605458
12	1	0	-1.103833	-1.651421	2.763083
13	6	0	0.034073	-2.307753	0.699533
14	6	0	1.277867	-1.488770	0.952321
15	1	0	0.187186	-3.038715	-0.095577
16	1	0	-0.234944	-2.892372	1.591881
17	6	0	2.382164	-1.407568	0.196283
18	1	0	1.191053	-0.799677	1.793127
19	6	0	3.403431	-0.326615	0.480425
20	1	0	3.248523	0.074671	1.488131
21	1	0	4.422730	-0.735043	0.443223
22	6	0	3.302371	0.854082	-0.530718
23	6	0	1.893445	1.374681	-0.655978
24	1	0	3.648003	0.512387	-1.514424
25	1	0	3.999426	1.637618	-0.216489
26	6	0	1.340513	2.417605	-0.018156
27	1	0	1.241701	0.773417	-1.288863
28	6	0	-0.120478	2.753821	-0.201012
29	1	0	-0.656746	2.688835	0.755164
30	1	0	-0.248156	3.784549	-0.558593
31	1	0	-0.615189	2.076898	-0.902094
32	6	0	2.657263	-2.252361	-1.021838
33	1	0	2.699252	-1.629502	-1.923404
34	1	0	1.900598	-3.018138	-1.193531
35	1	0	3.634723	-2.743231	-0.932459
36	6	0	2.075568	3.321167	0.941191
37	1	0	2.010217	4.368144	0.617082
38	1	0	3.131222	3.066213	1.054392
39	1	0	1.611886	3.277078	1.935525
40	6	0	-4.178294	1.473227	-0.852882
41	1	0	-4.972798	1.551579	-0.105627
42	1	0	-4.633976	1.214463	-1.813620
43	1	0	-3.730990	2.468700	-0.963945

Frequencies --	25.3496	34.1789	37.3625
Frequencies --	51.3321	60.0141	72.6522
Frequencies --	84.9353	105.9180	112.1561

Zero-point correction= 0.372994 (Hartree/Particle)  
 Thermal correction to Energy= 0.394315  
 Thermal correction to Enthalpy= 0.395260  
 Thermal correction to Gibbs Free Energy= 0.322040  
 Sum of electronic and zero-point Energies= -812.402603  
 Sum of electronic and thermal Energies= -812.381282  
 Sum of electronic and thermal Enthalpies= -812.380338  
 Sum of electronic and thermal Free Energies= -812.453558

b-ss-1-4a5-.log



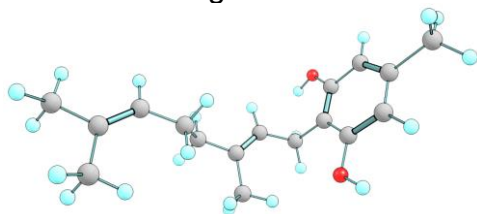
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.604381	1.377419	-0.084665
2	6	0	3.956705	1.296082	0.266739
3	6	0	4.634749	0.080252	0.174165
4	6	0	3.943058	-1.049225	-0.281300
5	6	0	2.593310	-0.954823	-0.628011
6	6	0	1.892499	0.261153	-0.549862
7	1	0	4.459162	2.193388	0.613493
8	1	0	4.453525	-2.005890	-0.363438
9	8	0	2.017290	2.608526	0.053728
10	1	0	1.106803	2.579147	-0.268642
11	8	0	1.887735	-2.044080	-1.070149
12	1	0	2.468048	-2.817418	-1.085086
13	6	0	0.417241	0.334729	-0.900921
14	6	0	-0.466017	0.230407	0.323030
15	1	0	0.181560	-0.446149	-1.624200
16	1	0	0.204975	1.282018	-1.420818
17	6	0	-1.306284	-0.764995	0.640575
18	1	0	-0.377972	1.064308	1.020482
19	6	0	-2.133374	-0.698284	1.906688
20	1	0	-1.906189	-1.570984	2.535800
21	1	0	-1.859895	0.191377	2.486597
22	6	0	-3.661799	-0.678866	1.647191
23	6	0	-4.089971	0.532013	0.864810
24	1	0	-4.165812	-0.680188	2.623911
25	1	0	-3.959491	-1.605818	1.148887
26	6	0	-4.704514	0.586584	-0.326759
27	1	0	-3.831884	1.481378	1.338288
28	6	0	-5.030618	1.912383	-0.973025
29	1	0	-4.548546	1.996187	-1.956229
30	1	0	-6.110084	2.009451	-1.150135
31	1	0	-4.707510	2.760050	-0.361974
32	6	0	-1.524235	-1.993424	-0.213204
33	1	0	-1.669909	-2.876121	0.420647
34	1	0	-0.682853	-2.195352	-0.877913
35	1	0	-2.430116	-1.893501	-0.823645
36	6	0	-5.127004	-0.613992	-1.138237
37	1	0	-6.206745	-0.584695	-1.334345
38	1	0	-4.899854	-1.566992	-0.657351
39	1	0	-4.634882	-0.604616	-2.119586
40	6	0	6.083674	-0.029938	0.586650
41	1	0	6.632720	-0.716994	-0.064717
42	1	0	6.170722	-0.415378	1.609853
43	1	0	6.583216	0.942378	0.558307

Frequencies --	16.9006	23.9491	33.3606
Frequencies --	46.4611	48.8792	51.3269
Frequencies --	77.8457	114.4549	136.3421

Zero-point correction= 0.372845 (Hartree/Particle)  
 Thermal correction to Energy= 0.394239  
 Thermal correction to Enthalpy= 0.395183  
 Thermal correction to Gibbs Free Energy= 0.320458  
 Sum of electronic and zero-point Energies= -812.399999  
 Sum of electronic and thermal Energies= -812.378605  
 Sum of electronic and thermal Enthalpies= -812.377661  
 Sum of electronic and thermal Free Energies= -812.452386

b-ss-1-4a5a.log



Standard orientation:

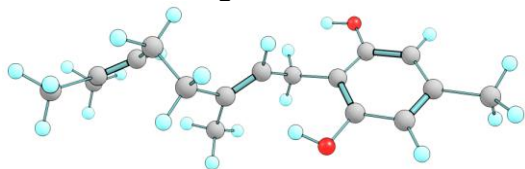
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-2.596899	-0.283982	-1.111366
2	6	0	-3.415794	0.819833	-1.359636
3	6	0	-4.044933	1.484343	-0.299292
4	6	0	-3.845863	1.020837	1.001410
5	6	0	-3.022677	-0.086422	1.237078
6	6	0	-2.387149	-0.771680	0.190341
7	1	0	-3.559406	1.162967	-2.381470
8	1	0	-4.317888	1.507865	1.848667
9	8	0	-1.963382	-0.950435	-2.128097
10	1	0	-2.181669	-0.529991	-2.971068
11	8	0	-2.872364	-0.458561	2.547951
12	1	0	-2.345880	-1.266878	2.605438
13	6	0	-1.460087	-1.947668	0.443271
14	6	0	-0.073287	-1.493860	0.844318
15	1	0	-1.427793	-2.576013	-0.446999
16	1	0	-1.877494	-2.588206	1.235413
17	6	0	1.055745	-1.569157	0.124334
18	1	0	-0.015175	-1.022318	1.826507
19	6	0	2.351470	-1.011632	0.678407
20	1	0	2.292700	-0.926848	1.769993
21	1	0	3.177279	-1.701528	0.458233
22	6	0	2.711236	0.378348	0.091909
23	6	0	3.995326	0.917580	0.660765
24	1	0	1.887684	1.065360	0.328505
25	1	0	2.755279	0.315410	-0.999288
26	6	0	5.185365	1.039213	0.051736
27	1	0	3.936665	1.209477	1.710798
28	6	0	6.385947	1.583178	0.789196
29	1	0	7.204234	0.850872	0.799346
30	1	0	6.780113	2.478292	0.289740
31	1	0	6.150465	1.846242	1.824454
32	6	0	1.153538	-2.168469	-1.258465
33	1	0	1.729405	-1.512389	-1.921587
34	1	0	0.181290	-2.330967	-1.724352
35	1	0	1.693867	-3.123737	-1.224664
36	6	0	5.460485	0.662600	-1.383785
37	1	0	5.819323	1.532770	-1.948886
38	1	0	4.589697	0.258108	-1.902766
39	1	0	6.260015	-0.087966	-1.433174
40	6	0	-4.900641	2.700368	-0.565033
41	1	0	-5.587179	2.895979	0.263211
42	1	0	-5.490855	2.580272	-1.478923
43	1	0	-4.279399	3.594605	-0.697088

Frequencies -- 16.7035            20.0514            27.6056  
 Frequencies -- 37.5058            49.4293            54.0728  
 Frequencies -- 65.3093            91.5509            106.7482

Zero-point correction=            0.372498 (Hartree/Particle)  
 Thermal correction to Energy=    0.394206  
 Thermal correction to Enthalpy=   0.395150  
 Thermal correction to Gibbs Free Energy= 0.318724  
 Sum of electronic and zero-point Energies= -812.399005  
 Sum of electronic and thermal Energies= -812.377297  
 Sum of electronic and thermal Enthalpies= -812.376353  
 Sum of electronic and thermal Free Energies= -812.452779

# Cannabigerocin-ss-1+3t

b-ss-1+4+5+.log



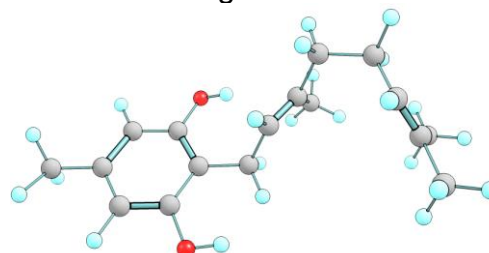
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.262357	1.369719	-0.084152
2	6	0	-4.573128	0.930430	-0.304718
3	6	0	-4.900096	-0.421008	-0.184396
4	6	0	-3.890986	-1.333134	0.140349
5	6	0	-2.584684	-0.890900	0.355014
6	6	0	-2.234311	0.472894	0.259177
7	1	0	-5.325842	1.667447	-0.566158
8	1	0	-4.098710	-2.395258	0.223652
9	8	0	-3.066795	2.719434	-0.214540
10	1	0	-2.138166	2.940488	-0.066712
11	8	0	-1.657907	-1.842717	0.688788
12	1	0	-0.769262	-1.512213	0.463339
13	6	0	-0.811327	0.910672	0.568409
14	6	0	0.224672	0.214934	-0.287803
15	1	0	-0.610605	0.748638	1.632667
16	1	0	-0.693845	1.992038	0.418848
17	6	0	1.329323	-0.441609	0.114174
18	1	0	0.026949	0.267970	-1.358804
19	6	0	2.269706	-1.032227	-0.923180
20	1	0	2.817769	-1.874287	-0.484873
21	1	0	1.691916	-1.426685	-1.766749
22	6	0	3.297107	-0.008647	-1.480428
23	6	0	4.159965	0.637480	-0.427400
24	1	0	2.737336	0.772499	-2.009885
25	1	0	3.907548	-0.519388	-2.232288
26	6	0	5.395618	0.276802	-0.045713
27	1	0	3.698044	1.475351	0.095174
28	6	0	6.122255	1.020605	1.048918
29	1	0	6.374714	0.346534	1.878055
30	1	0	7.073559	1.427776	0.681492
31	1	0	5.528619	1.847257	1.449513
32	6	0	1.751010	-0.628329	1.550961
33	1	0	1.776892	-1.697025	1.798165
34	1	0	1.099643	-0.128377	2.269657
35	1	0	2.770525	-0.253088	1.690672
36	6	0	6.170751	-0.874938	-0.636711
37	1	0	7.127457	-0.526935	-1.047436
38	1	0	5.632714	-1.401332	-1.427366
39	1	0	6.417901	-1.606077	0.143854
40	6	0	-6.322753	-0.889429	-0.380449
41	1	0	-6.356294	-1.891666	-0.818139
42	1	0	-6.882049	-0.211215	-1.031223
43	1	0	-6.853802	-0.936071	0.578247

Frequencies -- 12.0189      26.9582      31.1106  
 Frequencies -- 36.4686      45.8049      52.7694  
 Frequencies -- 86.2245      99.1428      121.9701

Zero-point correction= 0.372403 (Hartree/Particle)  
 Thermal correction to Energy= 0.393962  
 Thermal correction to Enthalpy= 0.394907  
 Thermal correction to Gibbs Free Energy= 0.319151  
 Sum of electronic and zero-point Energies= -812.399011  
 Sum of electronic and thermal Energies= -812.377452  
 Sum of electronic and thermal Enthalpies= -812.376508  
 Sum of electronic and thermal Free Energies= -812.452263

# b-ss-1+4+5-.log



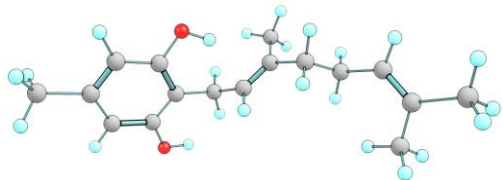
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.744322	1.461650	0.095971
2	6	0	-4.108737	1.300494	-0.173450
3	6	0	-4.677128	0.027107	-0.229548
4	6	0	-3.855821	-1.088339	-0.034673
5	6	0	-2.496043	-0.922171	0.230375
6	6	0	-1.904424	0.355899	0.318482
7	1	0	-4.710247	2.189402	-0.335114
8	1	0	-4.253637	-2.096539	-0.093465
9	8	0	-2.302913	2.757943	0.140675
10	1	0	-1.345909	2.782105	0.269952
11	8	0	-1.759378	-2.060416	0.430437
12	1	0	-0.827054	-1.874996	0.216473
13	6	0	-0.434671	0.477894	0.685438
14	6	0	0.480112	-0.239638	-0.282733
15	1	0	-0.288534	0.110420	1.706906
16	1	0	-0.124302	1.530362	0.721883
17	6	0	1.437388	-1.141745	0.002876
18	1	0	0.323718	0.026677	-1.327458
19	6	0	2.281779	-1.734899	-1.104247
20	1	0	2.186633	-2.829283	-1.085660
21	1	0	1.908593	-1.397208	-2.077832
22	6	0	3.785454	-1.376484	-0.985272
23	6	0	4.021352	0.107233	-1.054925
24	1	0	4.309557	-1.872102	-1.814067
25	1	0	4.192769	-1.806407	-0.066048
26	6	0	4.591179	0.908205	-0.141490
27	1	0	3.646587	0.575417	-1.967088
28	6	0	4.711246	2.394872	-0.380082
29	1	0	4.192823	2.958605	0.406978
30	1	0	5.761103	2.715037	-0.347888
31	1	0	4.292226	2.693241	-1.345266
32	6	0	1.786062	-1.598558	1.400154
33	1	0	2.043682	-2.663078	1.403879
34	1	0	0.976182	-1.444338	2.116131
35	1	0	2.662987	-1.056408	1.772314
36	6	0	5.157762	0.449421	1.180249
37	1	0	6.215634	0.730650	1.261929
38	1	0	5.086218	-0.628476	1.336203
39	1	0	4.641451	0.947122	2.011490
40	6	0	-6.156666	-0.145981	-0.480244
41	1	0	-6.359279	-1.048154	-1.065388
42	1	0	-6.575979	0.711347	-1.014411
43	1	0	-6.704029	-0.243375	0.465369

Frequencies -- 16.5607      25.0814      35.2200  
 Frequencies -- 44.6333      53.0606      54.8948  
 Frequencies -- 76.3896      105.2279      131.3438

Zero-point correction= 0.372558 (Hartree/Particle)  
 Thermal correction to Energy= 0.393977  
 Thermal correction to Enthalpy= 0.394921  
 Thermal correction to Gibbs Free Energy= 0.320122  
 Sum of electronic and zero-point Energies= -812.401334  
 Sum of electronic and thermal Energies= -812.379914  
 Sum of electronic and thermal Enthalpies= -812.378970  
 Sum of electronic and thermal Free Energies= -812.453769

b-ss-1+4+5a.log



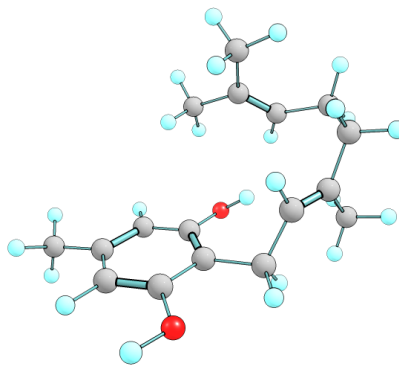
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.317335	-1.257889	0.538305
2	6	0	4.492062	-1.177390	-0.219131
3	6	0	4.757359	-0.054052	-1.003454
4	6	0	3.818997	0.982576	-1.037131
5	6	0	2.647546	0.895719	-0.283933
6	6	0	2.367674	-0.220222	0.533454
7	1	0	5.190018	-2.007548	-0.176225
8	1	0	3.976922	1.864092	-1.650457
9	8	0	3.175859	-2.400315	1.281158
10	1	0	2.335069	-2.391198	1.756577
11	8	0	1.788357	1.961094	-0.352250
12	1	0	0.890027	1.658736	-0.126621
13	6	0	1.112722	-0.230005	1.391290
14	6	0	-0.160763	-0.063970	0.591310
15	1	0	1.195801	0.545919	2.159928
16	1	0	1.028894	-1.170122	1.951880
17	6	0	-1.146169	0.832450	0.788939
18	1	0	-0.266506	-0.767117	-0.234330
19	6	0	-2.371790	0.822886	-0.098732
20	1	0	-2.507973	1.820259	-0.540288
21	1	0	-2.232466	0.122836	-0.929461
22	6	0	-3.668618	0.440823	0.659145
23	6	0	-4.872932	0.481605	-0.241607
24	1	0	-3.817497	1.146291	1.486999
25	1	0	-3.531769	-0.545800	1.112428
26	6	0	-5.603696	-0.546822	-0.699455
27	1	0	-5.151164	1.483328	-0.573727
28	6	0	-6.778588	-0.316262	-1.620170
29	1	0	-6.641155	-0.848628	-2.570718
30	1	0	-7.704730	-0.707940	-1.178859
31	1	0	-6.928325	0.744330	-1.841437
32	6	0	-1.147609	1.865965	1.892346
33	1	0	-1.579295	2.807083	1.534882
34	1	0	-0.149085	2.078591	2.279753
35	1	0	-1.764202	1.533601	2.735888
36	6	0	-5.355054	-1.997460	-0.366250
37	1	0	-6.235180	-2.436990	0.120941
38	1	0	-4.494529	-2.153487	0.286587
39	1	0	-5.190077	-2.575791	-1.284519
40	6	0	6.043439	0.051717	-1.788634
41	1	0	5.890823	0.580291	-2.734467
42	1	0	6.460670	-0.934793	-2.009621
43	1	0	6.800519	0.609805	-1.224142

Frequencies -- 12.9147 26.6004 30.9036  
 Frequencies -- 42.8494 46.4316 50.3958  
 Frequencies -- 76.7210 84.3304 111.1931

Zero-point correction= 0.372224 (Hartree/Particle)  
 Thermal correction to Energy= 0.393934  
 Thermal correction to Enthalpy= 0.394878  
 Thermal correction to Gibbs Free Energy= 0.318489  
 Sum of electronic and zero-point Energies= -812.400118  
 Sum of electronic and thermal Energies= -812.378408  
 Sum of electronic and thermal Enthalpies= -812.377464  
 Sum of electronic and thermal Free Energies= -812.453854

b-ss-1+4-5+.log



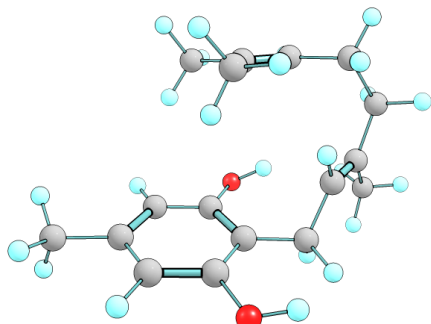
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.628005	-1.217069	-0.607177
2	6	0	3.626628	-0.238725	-0.552406
3	6	0	3.445655	0.918017	0.213486
4	6	0	2.243657	1.087103	0.905155
5	6	0	1.250679	0.105296	0.842484
6	6	0	1.422146	-1.076579	0.099719
7	1	0	4.548845	-0.383929	-1.110393
8	1	0	2.054011	1.979664	1.492440
9	8	0	2.790447	-2.360662	-1.346344
10	1	0	3.660294	-2.345133	-1.768409
11	8	0	0.106069	0.324240	1.565720
12	1	0	-0.650374	-0.045290	1.075579
13	6	0	0.350967	-2.153392	0.091591
14	6	0	-0.952013	-1.652731	-0.488351
15	1	0	0.206603	-2.519791	1.113354
16	1	0	0.711578	-3.000172	-0.499504
17	6	0	-2.173942	-1.644347	0.075069
18	1	0	-0.854725	-1.219172	-1.483756
19	6	0	-3.337858	-1.022544	-0.666188
20	1	0	-3.016763	-0.753077	-1.677099
21	1	0	-4.146674	-1.759111	-0.771704
22	6	0	-3.919421	0.241528	0.028936
23	6	0	-2.866689	1.251069	0.427527
24	1	0	-4.477122	-0.062046	0.921024
25	1	0	-4.655779	0.686193	-0.651686
26	6	0	-2.165584	2.048951	-0.393631
27	1	0	-2.627313	1.293504	1.489990
28	6	0	-1.082474	2.960848	0.127244
29	1	0	-0.112439	2.697464	-0.313642
30	1	0	-1.283239	4.004594	-0.147738
31	1	0	-0.977822	2.895116	1.212312
32	6	0	-2.493926	-2.186274	1.447103
33	1	0	-2.825884	-1.382535	2.115943
34	1	0	-1.649454	-2.687079	1.922782
35	1	0	-3.322229	-2.902460	1.386634
36	6	0	-2.360482	2.089740	-1.889046
37	1	0	-2.447877	3.125362	-2.240134
38	1	0	-3.244115	1.542207	-2.223374
39	1	0	-1.487085	1.660830	-2.398032
40	6	0	4.540089	1.955015	0.304553
41	1	0	4.131924	2.949227	0.507726
42	1	0	5.122841	2.005537	-0.620137
43	1	0	5.238047	1.716032	1.116392

Frequencies -- 21.6160 25.9006 42.3281  
 Frequencies -- 47.4208 58.9234 66.4962  
 Frequencies -- 98.5291 108.6373 113.4402

Zero-point correction= 0.372786 (Hartree/Particle)  
 Thermal correction to Energy= 0.394090  
 Thermal correction to Enthalpy= 0.395034  
 Thermal correction to Gibbs Free Energy= 0.321525  
 Sum of electronic and zero-point Energies= -812.406645  
 Sum of electronic and thermal Energies= -812.385341  
 Sum of electronic and thermal Enthalpies= -812.384397  
 Sum of electronic and thermal Free Energies= -812.457906

b-ss-1+4-5-.log



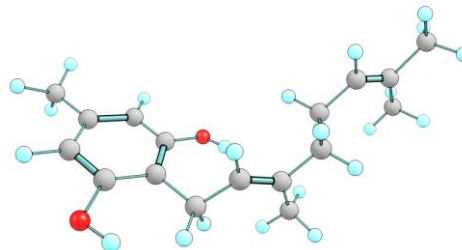
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.153421	-1.408748	0.738681
2	6	0	-3.291630	-0.603169	0.609392
3	6	0	-3.340171	0.412209	-0.346653
4	6	0	-2.217723	0.633988	-1.152418
5	6	0	-1.081282	-0.162111	-1.009655
6	6	0	-1.029297	-1.226592	-0.085393
7	1	0	-4.132706	-0.790951	1.269292
8	1	0	-2.204154	1.430543	-1.889393
9	8	0	-2.225832	-2.383268	1.699086
10	1	0	-1.368596	-2.817374	1.799117
11	8	0	-0.015451	0.114065	-1.827636
12	1	0	0.807039	-0.080830	-1.341846
13	6	0	0.202705	-2.115621	-0.037700
14	6	0	1.436419	-1.337857	0.362084
15	1	0	0.333536	-2.582926	-1.018807
16	1	0	0.057548	-2.951960	0.658979
17	6	0	2.624474	-1.285997	-0.264474
18	1	0	1.287601	-0.719588	1.241855
19	6	0	3.746313	-0.383636	0.222932
20	1	0	4.458828	-0.988829	0.801673
21	1	0	4.309108	-0.040518	-0.656136
22	6	0	3.332970	0.854147	1.047060
23	6	0	2.485334	1.807220	0.245306
24	1	0	4.257316	1.361814	1.355509
25	1	0	2.837125	0.547360	1.972281
26	6	0	1.251398	2.266553	0.505856
27	1	0	2.953133	2.135925	-0.685025
28	6	0	0.549948	3.195007	-0.456009
29	1	0	-0.396815	2.753033	-0.787145
30	1	0	0.302651	4.148664	0.028866
31	1	0	1.156242	3.406637	-1.341213
32	6	0	2.981400	-2.099132	-1.485097
33	1	0	3.162031	-1.441320	-2.344686
34	1	0	2.218512	-2.826851	-1.765685
35	1	0	3.916488	-2.645109	-1.309853
36	6	0	0.435300	1.920557	1.727545
37	1	0	0.099965	2.834841	2.233393
38	1	0	0.976794	1.316937	2.458440
39	1	0	-0.469391	1.372216	1.435730
40	6	0	-4.582777	1.253264	-0.517684
41	1	0	-4.331804	2.286927	-0.774572
42	1	0	-5.189232	1.262951	0.392330
43	1	0	-5.210705	0.861537	-1.327330

Frequencies -- 23.7312      35.1223      47.6543  
 Frequencies -- 56.5299      62.3031      89.8287  
 Frequencies -- 98.1389      109.2284      142.3774

Zero-point correction= 0.373001 (Hartree/Particle)  
 Thermal correction to Energy= 0.394153  
 Thermal correction to Enthalpy= 0.395097  
 Thermal correction to Gibbs Free Energy= 0.322844  
 Sum of electronic and zero-point Energies= -812.405506  
 Sum of electronic and thermal Energies= -812.384354  
 Sum of electronic and thermal Enthalpies= -812.383410  
 Sum of electronic and thermal Free Energies= -812.455663

b-ss-1+4-5a.log



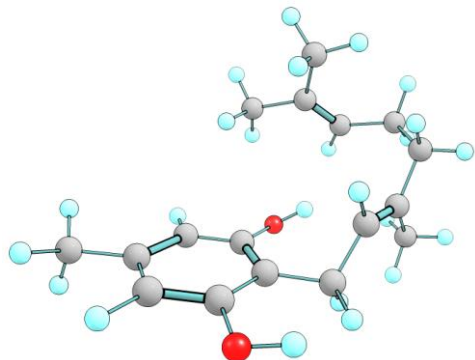
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.663588	0.753076	-0.598898
2	6	0	-4.570379	-0.313563	-0.602359
3	6	0	-4.257088	-1.515084	0.034359
4	6	0	-3.012841	-1.643032	0.660254
5	6	0	-2.111088	-0.578001	0.659155
6	6	0	-2.414826	0.654585	0.041168
7	1	0	-5.519878	-0.180221	-1.110952
8	1	0	-2.721616	-2.567883	1.148148
9	8	0	-4.086214	1.884419	-1.245700
10	1	0	-3.388776	2.552750	-1.243584
11	8	0	-0.922106	-0.778440	1.309365
12	1	0	-0.265353	-0.140368	0.977388
13	6	0	-1.421751	1.804046	0.116461
14	6	0	-0.066744	1.434541	-0.446465
15	1	0	-1.336722	2.139123	1.155842
16	1	0	-1.793109	2.679161	-0.432560
17	6	0	1.142145	1.583409	0.126692
18	1	0	-0.106687	0.968174	-1.430860
19	6	0	2.378121	1.058576	-0.574797
20	1	0	2.185352	0.947151	-1.647740
21	1	0	3.201511	1.776341	-0.469978
22	6	0	2.843567	-0.308537	-0.007763
23	6	0	4.035029	-0.849517	-0.750249
24	1	0	2.005180	-1.012933	-0.096840
25	1	0	3.051527	-2.098999	1.061597
26	6	0	5.309628	-0.912833	-0.334260
27	1	0	3.817696	-1.195790	-1.761916
28	6	0	6.393215	-1.467139	-1.228173
29	1	0	7.174410	-0.716446	-1.407106
30	1	0	6.891505	-2.323511	-0.754714
31	1	0	6.003511	-1.792039	-2.197041
32	6	0	1.388867	2.226312	1.469835
33	1	0	1.999250	1.578143	2.108395
34	1	0	0.474642	2.470820	2.013116
35	1	0	1.957301	3.154676	1.334048
36	6	0	5.796829	-0.456142	1.019031
37	1	0	6.261534	-1.289024	1.562584
38	1	0	5.008573	-0.039295	1.648579
39	1	0	6.574855	0.309587	0.904300
40	6	0	-5.248700	-2.654030	0.064228
41	1	0	-4.744840	-3.622840	-0.007202
42	1	0	-5.969425	-2.580436	-0.755023
43	1	0	-5.816260	-2.653087	1.002885

Frequencies -- 19.0394      28.7429      32.0003  
 Frequencies -- 39.2262      50.9480      51.9203  
 Frequencies -- 73.8577      95.4278      106.9868

Zero-point correction= 0.372490 (Hartree/Particle)  
 Thermal correction to Energy= 0.394085  
 Thermal correction to Enthalpy= 0.395030  
 Thermal correction to Gibbs Free Energy= 0.319471  
 Sum of electronic and zero-point Energies= -812.400518  
 Sum of electronic and thermal Energies= -812.378922  
 Sum of electronic and thermal Enthalpies= -812.377978  
 Sum of electronic and thermal Free Energies= -812.453537

b-ss-1+4a5+.log



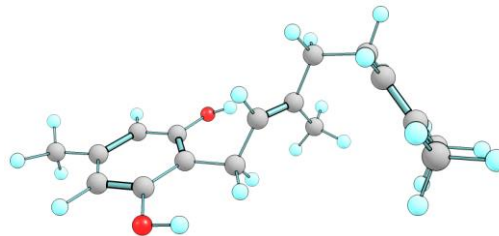
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.584021	-1.243287	0.626177
2	6	0	-3.594383	-0.274968	0.576599
3	6	0	-3.445276	0.871068	-0.205737
4	6	0	-2.255442	1.049301	-0.921447
5	6	0	-1.252746	0.081978	-0.867085
6	6	0	-1.398426	-1.101743	-0.115286
7	1	0	-4.492460	-0.437464	1.164284
8	1	0	-2.085692	1.939706	-1.518012
9	8	0	-2.842789	-2.330157	1.420179
10	1	0	-2.054477	-2.883881	1.493382
11	8	0	-0.120147	0.303659	-1.612130
12	1	0	0.654534	0.005207	-1.103194
13	6	0	-0.302815	-2.153740	-0.160814
14	6	0	0.979560	-1.659433	0.468741
15	1	0	-0.140098	-2.438621	-1.204672
16	1	0	-0.625226	-3.075743	0.340833
17	6	0	2.207992	-1.609228	-0.076478
18	1	0	0.854200	-1.259336	1.474652
19	6	0	3.343648	-0.971303	0.692986
20	1	0	2.999504	-0.723225	1.701579
21	1	0	4.169414	-1.688043	0.801390
22	6	0	3.902163	0.315509	0.020153
23	6	0	2.831652	1.296631	-0.402733
24	1	0	4.492289	0.034311	-0.858168
25	1	0	4.606123	0.778702	0.722238
26	6	0	2.078062	2.062266	0.402964
27	1	0	2.633713	1.351533	-1.473253
28	6	0	0.993400	2.956189	-0.145032
29	1	0	0.015587	2.672555	0.264633
30	1	0	1.166859	4.001458	0.142434
31	1	0	0.923589	2.896347	-1.233329
32	6	0	2.559745	-2.110847	-1.455989
33	1	0	2.849613	-1.280497	-2.111671
34	1	0	1.746288	-2.651232	-1.942223
35	1	0	3.425597	-2.781358	-1.402066
36	6	0	2.216526	2.085134	1.905053
37	1	0	2.255253	3.117323	2.274144
38	1	0	3.105848	1.562605	2.263457
39	1	0	1.340343	1.618562	2.374425
40	6	0	-4.549009	1.898715	-0.288697
41	1	0	-4.144261	2.912719	-0.362914
42	1	0	-5.206090	1.854271	0.584438
43	1	0	-5.170735	1.732642	-1.177028

Frequencies -- 24.2533 31.6299 45.6068  
 Frequencies -- 48.1223 59.3740 70.4912  
 Frequencies -- 104.9232 111.4927 113.4447

Zero-point correction= 0.372812 (Hartree/Particle)  
 Thermal correction to Energy= 0.394056  
 Thermal correction to Enthalpy= 0.395001  
 Thermal correction to Gibbs Free Energy= 0.322061  
 Sum of electronic and zero-point Energies= -812.404610  
 Sum of electronic and thermal Energies= -812.383366  
 Sum of electronic and thermal Enthalpies= -812.382422  
 Sum of electronic and thermal Free Energies= -812.455362

b-ss-1+4a5-.log



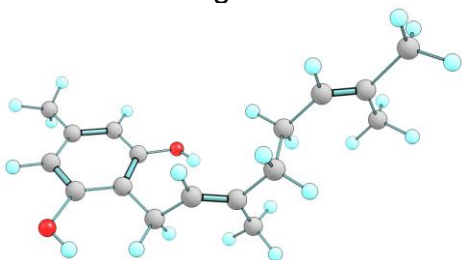
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.744170	1.461648	0.095951
2	6	0	-4.108583	1.300542	-0.173473
3	6	0	-4.677021	0.027166	-0.229600
4	6	0	-3.855768	-1.088314	-0.034760
5	6	0	-2.495977	-0.922191	0.230291
6	6	0	-1.904327	0.355837	0.318463
7	1	0	-4.710063	2.189455	-0.335209
8	1	0	-4.253591	-2.096502	-0.093683
9	8	0	-2.302701	2.757898	0.140681
10	1	0	-1.345682	2.782019	0.269845
11	8	0	-1.759333	-2.060466	0.430299
12	1	0	-0.827019	-1.875070	0.216279
13	6	0	-0.434578	0.477751	0.685456
14	6	0	0.480209	-0.239771	-0.282718
15	1	0	-0.288491	0.110222	1.706909
16	1	0	-0.124158	1.530204	0.721998
17	6	0	1.437436	-1.141935	0.002882
18	1	0	0.323878	0.026620	-1.327431
19	6	0	2.281884	-1.735020	-1.104229
20	1	0	2.186860	-2.829413	-1.085633
21	1	0	1.908675	-1.397370	-2.077818
22	6	0	3.785528	-1.376446	-0.985255
23	6	0	4.021268	0.107296	-1.054943
24	1	0	4.309676	-1.872037	-1.814035
25	1	0	4.192872	-1.806303	-0.066014
26	6	0	4.590886	0.908367	-0.141464
27	1	0	3.646551	0.575401	-1.967164
28	6	0	4.710799	2.395046	-0.380087
29	1	0	4.192254	2.958727	0.406928
30	1	0	5.760614	2.715333	-0.347830
31	1	0	4.291804	2.693341	-1.345302
32	6	0	1.786024	-1.598846	1.400157
33	1	0	2.043807	-2.663324	1.403801
34	1	0	0.976027	-1.444841	2.116047
35	1	0	2.662814	-1.056600	1.772493
36	6	0	5.157405	0.449698	1.180344
37	1	0	6.215208	0.731146	1.262141
38	1	0	5.086072	-0.628215	1.336281
39	1	0	4.640898	0.947282	2.011530
40	6	0	-6.156608	-0.145819	-0.480080
41	1	0	-6.359447	-1.048141	-1.064902
42	1	0	-6.575917	0.711424	-1.014373
43	1	0	-6.703794	-0.242879	0.465682

Frequencies -- 16.5349 25.0239 35.1866  
 Frequencies -- 44.6246 53.0935 54.8818  
 Frequencies -- 76.3677 105.1442 131.2652

Zero-point correction= 0.372556 (Hartree/Particle)  
 Thermal correction to Energy= 0.393977  
 Thermal correction to Enthalpy= 0.394921  
 Thermal correction to Gibbs Free Energy= 0.320115  
 Sum of electronic and zero-point Energies= -812.401335  
 Sum of electronic and thermal Energies= -812.379915  
 Sum of electronic and thermal Enthalpies= -812.378970  
 Sum of electronic and thermal Free Energies= -812.453777

b-ss-1+4a5a.log



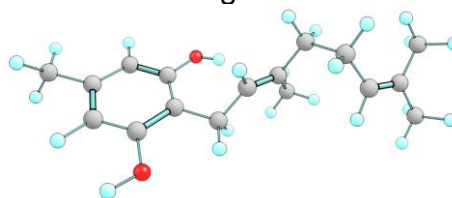
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.663590	0.752808	-0.599139
2	6	0	-4.570157	-0.314000	-0.602703
3	6	0	-4.256815	-1.515387	0.034275
4	6	0	-3.012748	-1.642992	0.660575
5	6	0	-2.111199	-0.577777	0.659578
6	6	0	-2.414973	0.654636	0.041301
7	1	0	-5.519568	-0.180914	-1.111528
8	1	0	-2.721493	-2.567691	1.148745
9	8	0	-4.086239	1.883993	-1.246206
10	1	0	-3.389001	2.552533	-1.243759
11	8	0	-0.922379	-0.777822	1.310240
12	1	0	-0.265491	-0.140109	0.977819
13	6	0	-1.422036	1.804214	0.116565
14	6	0	-0.066990	1.434787	-0.446316
15	1	0	-1.337066	2.139402	1.155913
16	1	0	-1.793430	2.679241	-0.432571
17	6	0	1.141872	1.583598	0.126919
18	1	0	-0.106873	0.968565	-1.430783
19	6	0	2.377922	1.059086	-0.574667
20	1	0	2.185080	0.947651	-1.647599
21	1	0	3.201107	1.777109	-0.469909
22	6	0	2.843829	-0.307891	-0.007749
23	6	0	4.035225	-0.848551	-0.750561
24	1	0	2.005588	-1.012500	-0.096643
25	1	0	3.052023	-0.209236	1.061560
26	6	0	5.309743	-0.912895	-0.334478
27	1	0	3.817883	-1.193712	-1.762613
28	6	0	6.393153	-1.466792	-1.228858
29	1	0	7.174708	-0.716277	-1.406975
30	1	0	6.891013	-2.323867	-0.756217
31	1	0	6.003383	-1.790544	-2.198086
32	6	0	1.388501	2.226409	1.470132
33	1	0	1.955636	3.155569	1.334320
34	1	0	2.000070	1.578848	2.108159
35	1	0	0.474257	2.469564	2.014001
36	6	0	5.797052	-0.457878	1.019338
37	1	0	6.261082	-1.291632	1.562133
38	1	0	5.009001	-0.041112	1.649195
39	1	0	6.575648	0.307408	0.905495
40	6	0	-5.248131	-2.654600	0.063798
41	1	0	-4.743943	-3.623273	-0.007250
42	1	0	-5.968414	-2.581337	-0.755875
43	1	0	-5.816210	-2.653711	1.002132

Frequencies -- 18.9418      28.7616      31.9083  
 Frequencies -- 39.1616      50.8807      51.9444  
 Frequencies -- 73.8714      95.4556      106.7223

Zero-point correction= 0.372487 (Hartree/Particle)  
 Thermal correction to Energy= 0.394084  
 Thermal correction to Enthalpy= 0.395028  
 Thermal correction to Gibbs Free Energy= 0.319456  
 Sum of electronic and zero-point Energies= -812.400521  
 Sum of electronic and thermal Energies= -812.378924  
 Sum of electronic and thermal Enthalpies= -812.377980  
 Sum of electronic and thermal Free Energies= -812.453551

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 b-ss-1a4+5+.log



Standard orientation:

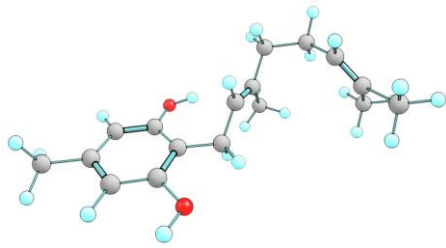
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-2.576769	-0.897565	0.343851
2	6	0	-3.893805	-1.337038	0.160256
3	6	0	-4.904678	-0.427078	-0.147729
4	6	0	-4.577528	0.928506	-0.279450
5	6	0	-3.261754	1.358561	-0.091525
6	6	0	-2.228400	0.460012	0.231205
7	1	0	-4.103692	-2.397348	0.258299
8	1	0	-5.349238	1.654524	-0.524992
9	8	0	-1.649240	-1.852833	0.660489
10	1	0	-0.760259	-1.507400	0.457449
11	8	0	-2.923197	2.683126	-0.200909
12	1	0	-3.712882	3.194881	-0.423479
13	6	0	-0.810336	0.938645	0.495575
14	6	0	0.231063	0.201954	-0.316736
15	1	0	-0.595467	0.855657	1.566871
16	1	0	-0.755399	2.004458	0.254595
17	6	0	1.330063	-0.442965	0.119095
18	1	0	0.047021	0.211643	-1.392022
19	6	0	2.280989	-1.070656	-0.887033
20	1	0	2.824503	-1.896954	-0.413991
21	1	0	1.711558	-1.494987	-1.721914
22	6	0	3.314238	-0.068249	-1.470770
23	6	0	4.164569	0.617077	-0.432945
24	1	0	2.759376	0.692716	-2.034027
25	1	0	3.933102	-0.604994	-2.197293
26	6	0	5.405535	0.288249	-0.039924
27	1	0	3.687236	1.460112	0.067011
28	6	0	6.116232	1.072337	1.036976
29	1	0	6.378397	0.424214	1.883673
30	1	0	7.061335	1.486564	0.661418
31	1	0	5.507580	1.898535	1.415484
32	6	0	1.735716	-0.581095	1.566303
33	1	0	1.753305	-1.640645	1.851473
34	1	0	1.077142	-0.054007	2.258632
35	1	0	2.755261	-0.205925	1.706369
36	6	0	6.203769	-0.863268	-0.599880
37	1	0	7.154373	-0.507458	-1.018099
38	1	0	5.677881	-1.420188	-1.377622
39	1	0	6.463670	-1.569135	0.199615
40	6	0	-6.330901	-0.883632	-0.346460
41	1	0	-6.691550	-0.627893	-1.349193
42	1	0	-7.003797	-0.396700	0.368501
43	1	0	-6.427975	-1.964781	-0.218257

Frequencies -- 15.7533      26.0754      27.8689  
 Frequencies -- 32.5737      37.6981      55.1217  
 Frequencies -- 87.6437      100.6302      127.5615

Zero-point correction= 0.372693 (Hartree/Particle)  
 Thermal correction to Energy= 0.394162  
 Thermal correction to Enthalpy= 0.395106  
 Thermal correction to Gibbs Free Energy= 0.319491  
 Sum of electronic and zero-point Energies= -812.401101  
 Sum of electronic and thermal Energies= -812.379632  
 Sum of electronic and thermal Enthalpies= -812.378687  
 Sum of electronic and thermal Free Energies= -812.454303



b-ss-1a4+5-.log



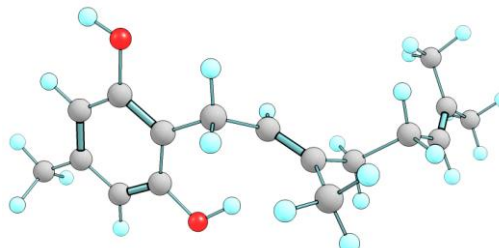
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.487728	-0.931832	0.203122
2	6	0	-3.853841	-1.098864	-0.047202
3	6	0	-4.681378	0.012913	-0.215279
4	6	0	-4.120047	1.292150	-0.134136
5	6	0	-2.753597	1.449755	0.118800
6	6	0	-1.904230	0.345156	0.301175
7	1	0	-4.249745	-2.107558	-0.111029
8	1	0	-4.746196	2.172125	-0.262147
9	8	0	-1.748548	-2.071089	0.376160
10	1	0	-0.809488	-1.864713	0.213625
11	8	0	-2.187401	2.694816	0.217733
12	1	0	-2.868301	3.365673	0.071807
13	6	0	-0.433710	0.515733	0.642549
14	6	0	0.485931	-0.249150	-0.282428
15	1	0	-0.265888	0.223796	1.685537
16	1	0	-0.184694	1.579490	0.582716
17	6	0	1.444181	-1.135597	0.047174
18	1	0	0.336500	-0.033755	-1.340383
19	6	0	2.296039	-1.776421	-1.027439
20	1	0	2.202482	-2.869243	-0.961207
21	1	0	1.927651	-1.483068	-2.017226
22	6	0	3.798915	-1.411815	-0.918223
23	6	0	4.035345	0.067068	-1.056188
24	1	0	4.327654	-1.945252	-1.720294
25	1	0	4.202162	-1.797725	0.022076
26	6	0	4.600601	0.909948	-0.178300
27	1	0	3.665617	0.492098	-1.991256
28	6	0	4.722971	2.383831	-0.485076
29	1	0	4.200132	2.983840	0.271654
30	1	0	5.772831	2.704816	-0.461643
31	1	0	4.309862	2.637282	-1.465539
32	6	0	1.785238	-1.529457	1.465604
33	1	0	2.037670	-2.594091	1.519705
34	1	0	0.972201	-1.338400	2.169038
35	1	0	2.663160	-0.975307	1.817576
36	6	0	5.158883	0.513175	1.166873
37	1	0	6.215932	0.799278	1.242717
38	1	0	5.087053	-0.556488	1.371485
39	1	0	4.636328	1.047778	1.970835
40	6	0	-6.150372	-0.159471	-0.522281
41	1	0	-6.743608	0.665196	-0.115952
42	1	0	-6.536948	-1.096174	-0.110553
43	1	0	-6.323976	-0.182155	-1.605161

Frequencies -- 15.4900 26.0603 31.3899  
 Frequencies -- 35.7135 45.3411 57.8837  
 Frequencies -- 73.7936 108.1444 127.5252

Zero-point correction= 0.372834 (Hartree/Particle)  
 Thermal correction to Energy= 0.394186  
 Thermal correction to Enthalpy= 0.395130  
 Thermal correction to Gibbs Free Energy= 0.320099  
 Sum of electronic and zero-point Energies= -812.403396  
 Sum of electronic and thermal Energies= -812.382045  
 Sum of electronic and thermal Enthalpies= -812.381101  
 Sum of electronic and thermal Free Energies= -812.456131

b-ss-1a4+5a.log



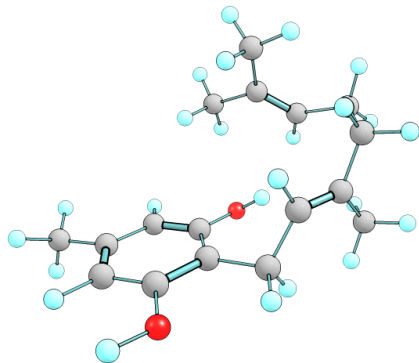
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.619682	0.885550	-0.347864
2	6	0	3.794776	0.944224	-1.101333
3	6	0	4.746526	-0.075043	-1.006035
4	6	0	4.497146	-1.154078	-0.153673
5	6	0	3.318016	-1.203302	0.599960
6	6	0	2.353828	-0.185731	0.527994
7	1	0	3.946218	1.792708	-1.761443
8	1	0	5.220840	-1.961221	-0.067615
9	8	0	1.747505	1.932396	-0.481344
10	1	0	0.863149	1.646075	-0.187552
11	8	0	3.064453	-2.246029	1.453782
12	1	0	3.797811	-2.874886	1.413948
13	6	0	1.104504	-0.209450	1.392263
14	6	0	-0.173610	-0.036430	0.602952
15	1	0	1.186590	0.556129	2.172321
16	1	0	1.064751	-1.169752	1.915249
17	6	0	-1.157177	0.862569	0.800310
18	1	0	-0.290476	-0.742639	-0.219362
19	6	0	-2.390337	0.845294	-0.077529
20	1	0	-2.547122	1.844875	-0.507089
21	1	0	-2.246649	0.156807	-0.917261
22	6	0	-3.675266	0.431407	0.684535
23	6	0	-4.886701	0.458293	-0.207419
24	1	0	-3.832121	1.124402	1.521213
25	1	0	-3.516215	-0.557419	1.125781
26	6	0	-5.579822	-0.581410	-0.697290
27	1	0	-5.204151	1.459157	-0.505082
28	6	0	-6.767291	-0.366008	-1.605422
29	1	0	-6.613231	-0.858961	-2.574527
30	1	0	-7.675009	-0.809630	-1.175116
31	1	0	-6.960202	0.694819	-1.788943
32	6	0	-1.150517	1.905317	1.894508
33	1	0	-1.541568	2.857318	1.518402
34	1	0	-0.155122	2.087203	2.304439
35	1	0	-1.798999	1.602957	2.725487
36	6	0	-5.272428	-2.031686	-0.415319
37	1	0	-6.134106	-2.524298	0.053721
38	1	0	-4.406505	-2.175383	0.233184
39	1	0	-5.082858	-2.569325	-1.353386
40	6	0	6.016380	-0.008862	-1.821903
41	1	0	6.658856	-0.874006	-1.638497
42	1	0	6.589756	0.894489	-1.585381
43	1	0	5.794448	0.025722	-2.894417

Frequencies -- 11.8044 24.6069 31.2892  
 Frequencies -- 38.0940 41.8618 52.4454  
 Frequencies -- 80.6151 85.9723 118.8669

Zero-point correction= 0.374550 (Hartree/Particle)  
 Thermal correction to Energy= 0.396022  
 Thermal correction to Enthalpy= 0.396966  
 Thermal correction to Gibbs Free Energy= 0.320804  
 Sum of electronic and zero-point Energies= -812.131713  
 Sum of electronic and thermal Energies= -812.110241  
 Sum of electronic and thermal Enthalpies= -812.109296  
 Sum of electronic and thermal Free Energies= -812.185458

b-ss-1a4-5+.log



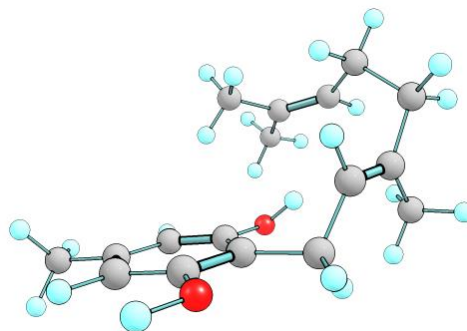
Standard orientation:

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			X	Y	Z
1	6	0	-1.250599	0.105135	-0.842560
2	6	0	-2.243499	1.087010	-0.905282
3	6	0	-3.445472	0.918093	-0.213522
4	6	0	-3.626481	-0.238545	0.552518
5	6	0	-2.627938	-1.216979	0.607320
6	6	0	-1.422126	-1.076673	-0.099699
7	1	0	-2.053799	1.979513	-1.492643
8	1	0	-4.548682	-0.383619	1.110567
9	8	0	-0.105986	0.323911	-1.565856
10	1	0	0.650434	-0.045416	-1.075533
11	8	0	-2.790496	-2.360544	1.346503
12	1	0	-3.659928	-2.344438	1.769403
13	6	0	-0.351023	-2.153576	-0.091476
14	6	0	0.951973	-1.652913	0.488423
15	1	0	-0.206676	-2.520102	-1.113193
16	1	0	-0.711698	-3.000251	0.499732
17	6	0	2.173857	-1.644326	-0.075090
18	1	0	0.854707	-1.219461	1.483880
19	6	0	3.337777	-1.022508	0.666153
20	1	0	3.016665	-0.753007	1.677053
21	1	0	4.146570	-1.759101	0.771702
22	6	0	3.919348	0.241539	-0.028971
23	6	0	2.866549	1.251042	-0.427516
24	1	0	4.477011	-0.062038	-0.921085
25	1	0	4.655722	0.686209	0.651627
26	6	0	2.165478	2.048935	0.393665
27	1	0	2.627056	1.293395	-1.489956
28	6	0	1.082198	2.960672	-0.127146
29	1	0	0.112234	2.697118	0.313797
30	1	0	1.282798	4.004457	0.147815
31	1	0	0.977487	2.894916	-1.212207
32	6	0	2.493788	-2.186047	-1.447220
33	1	0	2.824876	-1.382072	-2.116220
34	1	0	1.649540	-2.687537	-1.922577
35	1	0	3.322681	-2.901571	-1.387012
36	6	0	2.360602	2.089971	1.889042
37	1	0	2.448691	3.125643	2.239826
38	1	0	3.243945	1.541995	2.223405
39	1	0	1.487000	1.661762	2.398270
40	6	0	-4.539872	1.955105	-0.304781
41	1	0	-5.123915	2.004430	0.619147
42	1	0	-5.236660	1.717020	-1.117899
43	1	0	-4.131552	2.949606	-0.506231

Frequencies -- 21.6398 25.9208 42.3772  
 Frequencies -- 47.6654 59.0210 66.5515  
 Frequencies -- 98.6542 108.6444 113.4643

Zero-point correction= 0.372788 (Hartree/Particle)  
 Thermal correction to Energy= 0.394090  
 Thermal correction to Enthalpy= 0.395034  
 Thermal correction to Gibbs Free Energy= 0.321537  
 Sum of electronic and zero-point Energies= -812.406643  
 Sum of electronic and thermal Energies= -812.385341  
 Sum of electronic and thermal Enthalpies= -812.384397  
 Sum of electronic and thermal Free Energies= -812.457894

b-ss-1a4-5-.log



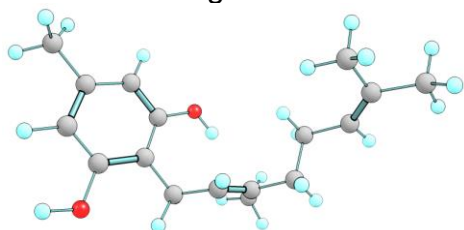
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.166608	0.268221	-0.754189
2	6	0	-2.126822	1.278735	-0.638334
3	6	0	-3.355820	1.015071	-0.031434
4	6	0	-3.600444	-0.271108	0.465353
5	6	0	-2.638032	-1.276210	0.336175
6	6	0	-1.403269	-1.036366	-0.293140
7	1	0	-1.888533	2.266594	-1.019305
8	1	0	-4.546373	-0.495137	0.953381
9	8	0	0.014148	0.596670	-1.375699
10	1	0	0.748250	0.140844	-0.928552
11	8	0	-2.862519	-2.544939	0.804404
12	1	0	-3.751982	-2.592149	1.180903
13	6	0	-0.380669	-2.136875	-0.512280
14	6	0	0.897221	-1.916610	0.264587
15	1	0	-0.172199	-2.215093	-1.584117
16	1	0	-0.823411	-3.089717	-0.208789
17	6	0	2.139161	-1.728375	-0.214078
18	1	0	0.765014	-1.897607	1.347180
19	6	0	3.296071	-1.488082	0.746976
20	1	0	3.306134	-2.259826	1.525485
21	1	0	4.243827	-1.580111	0.203617
22	6	0	3.241002	-0.099917	1.431841
23	6	0	3.177219	1.029013	0.440442
24	1	0	4.137545	0.004586	2.059944
25	1	0	2.383159	-0.076202	2.109342
26	6	0	2.260204	2.006947	0.353169
27	1	0	3.975356	1.022045	-0.304415
28	6	0	2.324785	3.035619	-0.749733
29	1	0	1.428747	2.959984	-1.377669
30	1	0	2.344986	4.054596	-0.341840
31	1	0	3.203914	2.902651	-1.386902
32	6	0	2.509100	-1.701527	-1.677548
33	1	0	3.024079	-0.762037	-1.914110
34	1	0	1.655324	-1.796928	-2.350624
35	1	0	3.214698	-2.509842	-1.905675
36	6	0	1.102457	2.196201	1.302375
37	1	0	1.006246	1.396581	2.038908
38	1	0	0.161097	2.255647	0.745827
39	1	0	1.211146	3.143997	1.845753
40	6	0	-4.405769	2.092311	0.105067
41	1	0	-4.677716	2.248500	1.154974
42	1	0	-5.324417	1.816611	-0.425265
43	1	0	-4.056632	3.045875	-0.299202

Frequencies -- 30.0617 38.1913 50.1589  
 Frequencies -- 57.0299 70.8461 84.0881  
 Frequencies -- 99.7699 116.4619 144.3144

Zero-point correction= 0.373308 (Hartree/Particle)  
 Thermal correction to Energy= 0.394305  
 Thermal correction to Enthalpy= 0.395250  
 Thermal correction to Gibbs Free Energy= 0.323713  
 Sum of electronic and zero-point Energies= -812.406695  
 Sum of electronic and thermal Energies= -812.385698  
 Sum of electronic and thermal Enthalpies= -812.384754  
 Sum of electronic and thermal Free Energies= -812.456290

b-ss-1a4-5a.log



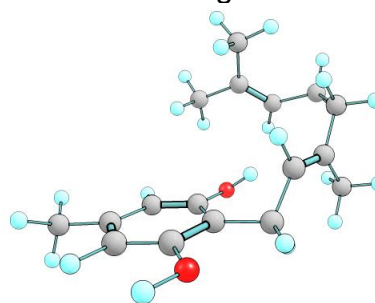
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.846530	0.382403	0.762511
2	6	0	2.649645	1.513968	0.943071
3	6	0	3.857702	1.641196	0.255957
4	6	0	4.249128	0.619883	-0.616751
5	6	0	3.441375	-0.508039	-0.790834
6	6	0	2.222817	-0.660147	-0.106211
7	1	0	2.309207	2.286047	1.625924
8	1	0	5.186925	0.696884	-1.162064
9	8	0	0.689809	0.333182	1.492394
10	1	0	0.103536	-0.346055	1.111397
11	8	0	3.814835	-1.526099	-1.630334
12	1	0	4.659501	-1.302239	-2.044272
13	6	0	1.376114	-1.913207	-0.268816
14	6	0	-0.073771	-1.601071	-0.562001
15	1	0	1.467351	-2.535535	0.628838
16	1	0	1.790419	-2.502956	-1.091880
17	6	0	-1.172697	-2.030179	0.087071
18	1	0	-0.219614	-0.914535	-1.396974
19	6	0	-2.536523	-1.504838	-0.313754
20	1	0	-2.519404	-1.147423	-1.348985
21	1	0	-3.278950	-2.312233	-0.265330
22	6	0	-2.999140	-0.338181	0.598170
23	6	0	-4.382456	0.139792	0.251750
24	1	0	-2.260266	0.466476	0.528027
25	1	0	-2.988104	-0.677312	1.642800
26	6	0	-4.736546	1.293340	-0.336082
27	1	0	-5.177510	-0.567976	0.492353
28	6	0	-6.184943	1.604250	-0.629826
29	1	0	-6.497153	2.528067	-0.124885
30	1	0	-6.338716	1.772993	-1.703926
31	1	0	-6.853165	0.799043	-0.311408
32	6	0	-1.168572	-2.990439	1.251321
33	1	0	-1.746664	-2.589480	2.091630
34	1	0	-0.168032	-3.230882	1.614460
35	1	0	-1.655082	-3.929130	0.958273
36	6	0	-3.773139	2.375902	-0.757091
37	1	0	-3.873668	2.577732	-1.831325
38	1	0	-2.728495	2.129910	-0.558864
39	1	0	-4.003813	3.318141	-0.243142
40	6	0	4.711005	2.876906	0.419112
41	1	0	5.774053	2.648128	0.297807
42	1	0	4.568210	3.333902	1.402564
43	1	0	4.453106	3.632528	-0.333090

Frequencies -- 17.2125 18.9064 30.0920  
 Frequencies -- 42.5926 46.5081 52.4544  
 Frequencies -- 77.8827 97.2340 120.6772

Zero-point correction= 0.372534 (Hartree/Particle)  
 Thermal correction to Energy= 0.394091  
 Thermal correction to Enthalpy= 0.395035  
 Thermal correction to Gibbs Free Energy= 0.319176  
 Sum of electronic and zero-point Energies= -812.402983  
 Sum of electronic and thermal Energies= -812.381426  
 Sum of electronic and thermal Enthalpies= -812.380482  
 Sum of electronic and thermal Free Energies= -812.456341

b-ss-1a4a5+.log



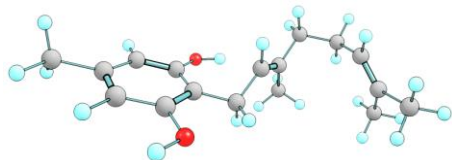
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-1.250646	0.105129	-0.842594
2	6	0	-2.243632	1.086940	-0.905321
3	6	0	-3.445564	0.917948	-0.213561
4	6	0	-3.626485	-0.238705	0.552504
5	6	0	-2.627879	-1.217035	0.607333
6	6	0	-1.422058	-1.076638	-0.099684
7	1	0	-2.053985	1.979435	-1.492704
8	1	0	-4.548669	-0.383815	1.110567
9	8	0	-0.106089	0.323991	-1.565956
10	1	0	0.650407	-0.045312	-1.075715
11	8	0	-2.790294	-2.360581	1.346574
12	1	0	-3.659896	-2.344771	1.769138
13	6	0	-0.350870	-2.153437	-0.091419
14	6	0	0.952121	-1.652642	0.488385
15	1	0	-0.206535	-2.520034	-1.113115
16	1	0	-0.711435	-3.000120	0.499844
17	6	0	2.174020	-1.644266	-0.075093
18	1	0	0.854864	-1.218968	1.483742
19	6	0	3.337945	-1.022375	0.666074
20	1	0	3.016907	-0.752978	1.677021
21	1	0	4.146818	-1.758894	0.771512
22	6	0	3.919341	0.241739	-0.029048
23	6	0	2.866483	1.251203	-0.427526
24	1	0	4.476989	-0.061761	-0.921200
25	1	0	4.655733	0.686446	0.651509
26	6	0	2.165356	2.048998	0.393695
27	1	0	2.627027	1.293644	-1.489969
28	6	0	1.082097	2.960770	-0.127093
29	1	0	0.112132	2.697253	0.313867
30	1	0	1.282743	4.004543	0.147869
31	1	0	0.977362	2.895018	-1.212151
32	6	0	2.493952	-2.186307	-1.447091
33	1	0	2.825987	-1.382635	-2.115976
34	1	0	1.649429	-2.687055	-1.922738
35	1	0	3.322188	-2.902567	-1.386592
36	6	0	2.360380	2.089865	1.889089
37	1	0	2.447938	3.125510	2.240072
38	1	0	3.243976	1.542263	2.223396
39	1	0	1.486971	1.661117	2.398191
40	6	0	-4.540069	1.954850	-0.304767
41	1	0	-5.237619	1.716001	-1.117003
42	1	0	-4.131966	2.949182	-0.507464
43	1	0	-5.123254	2.004998	0.619665

Frequencies -- 21.6104 25.8604 42.3220  
 Frequencies -- 47.4955 58.8958 66.4848  
 Frequencies -- 98.5054 108.6138 113.4293

Zero-point correction= 0.372786 (Hartree/Particle)  
 Thermal correction to Energy= 0.394090  
 Thermal correction to Enthalpy= 0.395034  
 Thermal correction to Gibbs Free Energy= 0.321523  
 Sum of electronic and zero-point Energies= -812.406645  
 Sum of electronic and thermal Energies= -812.385341  
 Sum of electronic and thermal Enthalpies= -812.384397  
 Sum of electronic and thermal Free Energies= -812.457908

b-ss-1a4a5-.log

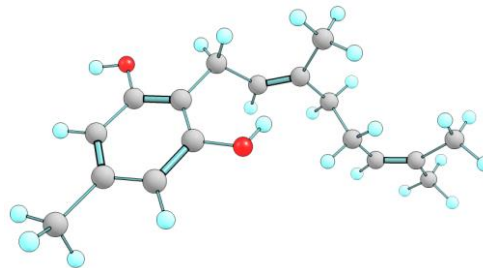


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.488619	-0.930995	0.197269
2	6	0	-3.852432	-1.095438	-0.057247
3	6	0	-4.679077	0.019341	-0.223690
4	6	0	-4.116047	1.295794	-0.141325
5	6	0	-2.748411	1.451351	0.116056
6	6	0	-1.902534	0.346385	0.299190
7	1	0	-4.249844	-2.103326	-0.126621
8	1	0	-4.739215	2.177216	-0.271951
9	8	0	-1.749677	-2.070648	0.368914
10	1	0	-0.810512	-1.864361	0.206962
11	8	0	-2.181957	2.696331	0.215010
12	1	0	-2.862450	3.367424	0.068459
13	6	0	-0.432082	0.513575	0.642109
14	6	0	0.487726	-0.251669	-0.282365
15	1	0	-0.265950	0.220383	1.685014
16	1	0	-0.181026	1.576950	0.583759
17	6	0	1.444495	-1.139477	0.047881
18	1	0	0.340399	-0.034890	-1.340316
19	6	0	2.298161	-1.779248	-1.025862
20	1	0	2.206358	-2.872209	-0.959776
21	1	0	1.930415	-1.486478	-2.016038
22	6	0	3.800399	-1.412318	-0.915030
23	6	0	4.035043	0.066630	-1.054614
24	1	0	4.331168	-1.946114	-1.715515
25	1	0	4.202779	-1.796440	0.026375
26	6	0	4.596829	0.911565	-0.176495
27	1	0	3.666912	0.489902	-1.991087
28	6	0	4.717690	2.385201	-0.484995
29	1	0	4.191819	2.985427	0.269459
30	1	0	5.766940	2.707982	-0.459120
31	1	0	4.306844	2.636669	-1.466901
32	6	0	1.782347	-1.535244	1.466518
33	1	0	2.034937	-2.599870	1.519710
34	1	0	0.967542	-1.345439	2.168228
35	1	0	2.659214	-0.981397	1.821594
36	6	0	5.152406	0.517473	1.170539
37	1	0	6.208733	0.805571	1.248804
38	1	0	5.081939	-0.552032	1.376418
39	1	0	4.626811	1.052201	1.972433
40	6	0	-6.153017	-0.161514	-0.501949
41	1	0	-6.672386	0.798244	-0.565994
42	1	0	-6.632506	-0.754520	0.284685
43	1	0	-6.313114	-0.694821	-1.445908

Frequencies -- 15.5967 26.3939 32.2372  
 Frequencies -- 45.1914 54.5629 57.7785  
 Frequencies -- 73.8930 108.5781 127.8166  
 Zero-point correction= 0.372860 (Hartree/Particle)  
 Thermal correction to Energy= 0.394169  
 Thermal correction to Enthalpy= 0.395113  
 Thermal correction to Gibbs Free Energy= 0.320527  
 Sum of electronic and zero-point Energies= -812.403379  
 Sum of electronic and thermal Energies= -812.382070  
 Sum of electronic and thermal Enthalpies= -812.381125  
 Sum of electronic and thermal Free Energies= -812.455712

b-ss-1a4a5a.log



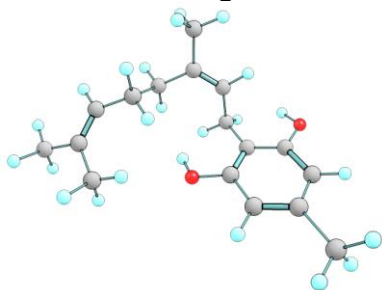
Standard orientation:

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1	6	0	-2.081007	-0.611551	0.604169
2	6	0	-2.992445	-1.670796	0.612115
3	6	0	-4.262567	-1.515326	0.050365
4	6	0	-4.600790	-0.286885	-0.523566
5	6	0	-3.682267	0.769668	-0.526643
6	6	0	-2.403676	0.638715	0.038152
7	1	0	-2.688710	-2.612660	1.058455
8	1	0	-5.581882	-0.143180	-0.969749
9	8	0	-0.866519	-0.843389	1.191577
10	1	0	-0.235805	-0.161325	0.896605
11	8	0	-4.002610	1.985146	-1.074961
12	1	0	-4.900333	1.944932	-1.432014
13	6	0	-1.424655	1.801740	0.063945
14	6	0	-0.064480	1.427699	-0.480144
15	1	0	-1.342931	2.189103	1.086005
16	1	0	-1.840474	2.615033	-0.538311
17	6	0	1.142316	1.587327	0.095121
18	1	0	-0.094825	0.947603	-1.458936
19	6	0	2.383614	1.058207	-0.594067
20	1	0	2.197147	0.934243	-1.666852
21	1	0	3.205344	1.778639	-0.493208
22	6	0	2.849004	-0.301558	-0.009303
23	6	0	4.049001	-0.846862	-0.734589
24	1	0	2.013539	-1.009555	-0.098000
25	1	0	3.047069	-0.191007	1.060823
26	6	0	5.320312	-0.898406	-0.306941
27	1	0	3.842144	-1.207207	-1.743562
28	6	0	6.414403	-1.459066	-1.183909
29	1	0	7.193502	-0.706947	-1.366069
30	1	0	6.912784	-2.306608	-0.694839
31	1	0	6.034766	-1.798754	-2.151719
32	6	0	1.381127	2.245463	1.432530
33	1	0	1.985154	1.603402	2.083537
34	1	0	0.462583	2.496713	1.965342
35	1	0	1.952458	3.171444	1.291710
36	6	0	5.793465	-0.420765	1.044127
37	1	0	6.258287	-1.243411	1.603002
38	1	0	4.997428	0.000092	1.661066
39	1	0	6.568001	0.347940	0.925571
40	6	0	-5.244673	-2.663261	0.060152
41	1	0	-6.189904	-2.389555	-0.415937
42	1	0	-5.462986	-2.986132	1.084264
43	1	0	-4.839412	-3.532915	-0.469203

Frequencies -- 19.4496 22.7228 33.2768  
 Frequencies -- 41.1988 46.0850 49.8778  
 Frequencies -- 75.5167 96.2284 110.5373

Zero-point correction= 0.372746 (Hartree/Particle)  
 Thermal correction to Energy= 0.394281  
 Thermal correction to Enthalpy= 0.395225  
 Thermal correction to Gibbs Free Energy= 0.319622  
 Sum of electronic and zero-point Energies= -812.402722  
 Sum of electronic and thermal Energies= -812.381187  
 Sum of electronic and thermal Enthalpies= -812.380243  
 Sum of electronic and thermal Free Energies= -812.455846

**Cannabigerocin-ss-1a3c**  
ss-1a3c4a5a.log



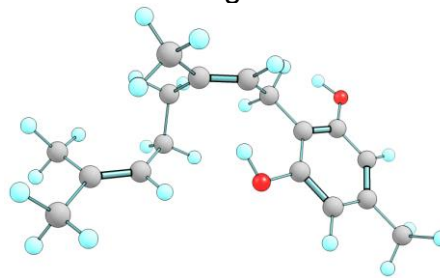
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.130942	0.614264	-0.479766
2	6	0	4.018793	-0.312078	0.068147
3	6	0	3.570397	-1.582676	0.444138
4	6	0	2.225611	-1.906154	0.257647
5	6	0	1.343656	-0.970609	-0.292268
6	6	0	1.771423	0.307588	-0.687296
7	1	0	5.056422	-0.021986	0.199961
8	1	0	1.838257	-2.880621	0.536669
9	8	0	3.657054	1.841069	-0.791978
10	1	0	2.994465	2.393314	-1.226816
11	8	0	0.041178	-1.383299	-0.417674
12	1	0	-0.486839	-0.710834	-0.866203
13	6	0	0.806193	1.351116	-1.226439
14	6	0	0.320311	2.275479	-0.132178
15	1	0	-0.027249	0.876455	-1.753541
16	1	0	1.299899	1.937183	-2.015931
17	6	0	-0.928805	2.438346	0.329359
18	1	0	1.116798	2.845424	0.346664
19	6	0	-2.142814	1.704074	-0.198340
20	1	0	-2.956501	2.426667	-0.349027
21	1	0	-1.953324	1.263966	-1.182790
22	6	0	-2.649168	0.589443	0.754526
23	6	0	-3.911929	-0.047115	0.241114
24	1	0	-2.846383	1.033014	1.739751
25	1	0	-1.850825	-0.143014	0.903136
26	6	0	-4.143315	-1.334976	-0.058003
27	1	0	-4.732082	0.657095	0.087861
28	6	0	-5.491076	-1.777524	-0.578004
29	1	0	-5.392619	-2.252320	-1.563276
30	1	0	-5.937693	-2.531545	0.083674
31	1	0	-6.193803	-0.944415	-0.669231
32	6	0	-1.203913	3.398712	1.463536
33	1	0	-1.927970	4.163906	1.155796
34	1	0	-0.294927	3.902944	1.802560
35	1	0	-1.644205	2.883978	2.326035
36	6	0	-3.142366	-2.454942	0.088129
37	1	0	-3.519896	-3.212405	0.787672
38	1	0	-2.161975	-2.130173	0.436912
39	1	0	-3.002470	-2.967990	-0.872495
40	6	0	4.535114	-2.581948	1.037785
41	1	0	4.035149	-3.518828	1.296502
42	1	0	5.003605	-2.185370	1.945391
43	1	0	5.343981	-2.812603	0.335426

Frequencies -- 18.5990 21.2656 23.8615  
 Frequencies -- 44.6567 51.4150 59.5102  
 Frequencies -- 92.4358 107.9664 125.3618

Zero-point correction= 0.372705 (Hartree/Particle)  
 Thermal correction to Energy= 0.394183  
 Thermal correction to Enthalpy= 0.395128  
 Thermal correction to Gibbs Free Energy= 0.320109  
 Sum of electronic and zero-point Energies= -812.399942  
 Sum of electronic and thermal Energies= -812.378463  
 Sum of electronic and thermal Enthalpies= -812.377519  
 Sum of electronic and thermal Free Energies= -812.452537

**ss-1a3c4+5+.log**



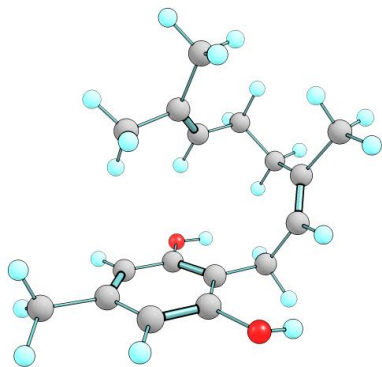
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.657274	0.701649	0.242260
2	6	0	-2.652211	1.682082	0.280513
3	6	0	-3.982795	1.356571	0.006810
4	6	0	-4.298283	0.034256	-0.310823
5	6	0	-3.299044	-0.942873	-0.351638
6	6	0	-1.952711	-0.644807	-0.061826
7	1	0	-2.362277	2.698823	0.526272
8	1	0	-5.316599	-0.259340	-0.545043
9	8	0	-0.381327	1.130234	0.495791
10	1	0	0.181250	0.358908	0.700962
11	8	0	-3.722305	-2.201393	-0.694520
12	1	0	-2.965674	-2.782771	-0.843195
13	6	0	-0.871981	-1.716429	-0.142756
14	6	0	0.181064	-1.639293	0.941027
15	1	0	-0.408017	-1.700417	-1.134991
16	1	0	-1.338593	-2.706849	-0.044069
17	6	0	1.515596	-1.594451	0.766705
18	1	0	-0.210323	-1.647480	1.958279
19	6	0	2.182897	-1.579060	-0.598422
20	1	0	3.215341	-1.927714	-0.488241
21	1	0	1.686047	-2.281856	-1.276284
22	6	0	2.210054	-0.179239	-1.272981
23	6	0	2.877118	0.892779	-0.443492
24	1	0	1.180319	0.130041	-1.480862
25	1	0	2.704663	-0.286878	-2.244839
26	6	0	4.193893	1.138865	-0.359301
27	1	0	2.208946	1.505355	0.160587
28	6	0	4.732282	2.231742	0.531159
29	1	0	5.426885	1.821849	1.276260
30	1	0	5.302747	2.966869	-0.051719
31	1	0	3.935231	2.759959	1.062068
32	6	0	2.450752	-1.532109	1.947942
33	1	0	3.101405	-2.415584	1.966038
34	1	0	1.915838	-1.477053	2.899987
35	1	0	3.109214	-0.660119	1.860161
36	6	0	5.246995	0.365672	-1.113877
37	1	0	5.878226	1.043886	-1.702196
38	1	0	4.830873	-0.384484	-1.789151
39	1	0	5.916427	-0.149359	-0.412579
40	6	0	-5.063076	2.409480	0.082369
41	1	0	-5.898306	2.174574	-0.583838
42	1	0	-4.676954	3.397469	-0.185310
43	1	0	-5.467279	2.482431	1.099514

Frequencies -- 19.5303 31.7631 39.7424  
 Frequencies -- 45.9296 49.6701 80.9073  
 Frequencies -- 94.7604 107.4599 136.0212

Zero-point correction= 0.373056 (Hartree/Particle)  
 Thermal correction to Energy= 0.394236  
 Thermal correction to Enthalpy= 0.395180  
 Thermal correction to Gibbs Free Energy= 0.321784  
 Sum of electronic and zero-point Energies= -812.401385  
 Sum of electronic and thermal Energies= -812.380205  
 Sum of electronic and thermal Enthalpies= -812.379261  
 Sum of electronic and thermal Free Energies= -812.452656

ss-1a3c4+5-.log



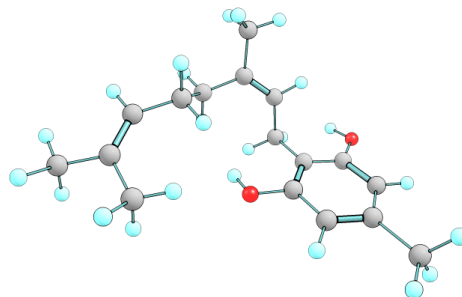
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.902458	-1.331203	-0.770285
2	6	0	2.932471	-0.419254	-1.004928
3	6	0	3.213495	0.581329	-0.070207
4	6	0	2.460422	0.634659	1.103753
5	6	0	1.423339	-0.276844	1.325029
6	6	0	1.102874	-1.274927	0.388043
7	1	0	3.509763	-0.512153	-1.919239
8	1	0	2.658842	1.384197	1.863171
9	8	0	1.703258	-2.278580	-1.743459
10	1	0	1.144046	-2.991303	-1.408623
11	8	0	0.747127	-0.117181	2.508335
12	1	0	0.059205	-0.788821	2.595578
13	6	0	-0.066100	-2.235713	0.565466
14	6	0	-1.195960	-1.985797	-0.414554
15	1	0	-0.438653	-2.214606	1.593376
16	1	0	0.289137	-3.270357	0.444622
17	6	0	-2.372920	-1.379691	-0.198858
18	1	0	-0.997669	-2.330981	-1.428413
19	6	0	-2.815598	-0.788312	1.120551
20	1	0	-3.771859	-1.241907	1.415288
21	1	0	-2.105853	-1.026180	1.918469
22	6	0	-3.003514	0.753771	1.072591
23	6	0	-1.728539	1.465417	0.711085
24	1	0	-3.336965	1.074319	2.069085
25	1	0	-3.816116	1.000592	0.384097
26	6	0	-1.465919	2.211981	-0.372687
27	1	0	-0.913180	1.297882	1.413484
28	6	0	-0.087669	2.787124	-0.599836
29	1	0	0.327417	2.429052	-1.551803
30	1	0	-0.121495	3.882643	-0.669431
31	1	0	0.611204	2.507100	0.192141
32	6	0	-3.362879	-1.230800	-1.331064
33	1	0	-4.349047	-1.615151	-1.040991
34	1	0	-3.037678	-1.763491	-2.228697
35	1	0	-3.503424	-0.178177	-1.600427
36	6	0	-2.460005	2.545186	-1.458233
37	1	0	-2.509839	3.630871	-1.611985
38	1	0	-3.471028	2.192123	-1.247053
39	1	0	-2.142873	2.111620	-2.415818
40	6	0	4.291915	1.603040	-0.339416
41	1	0	4.718083	1.990420	0.590449
42	1	0	3.885195	2.457566	-0.894137
43	1	0	5.102482	1.181041	-0.940842

Frequencies -- 22.7181 25.6540 39.9637  
 Frequencies -- 60.2922 68.2720 78.0593  
 Frequencies -- 106.7526 134.6666 140.0919

Zero-point correction= 0.373264 (Hartree/Particle)  
 Thermal correction to Energy= 0.394368  
 Thermal correction to Enthalpy= 0.395312  
 Thermal correction to Gibbs Free Energy= 0.322999  
 Sum of electronic and zero-point Energies= -812.400970  
 Sum of electronic and thermal Energies= -812.379866  
 Sum of electronic and thermal Enthalpies= -812.378922  
 Sum of electronic and thermal Free Energies= -812.451234

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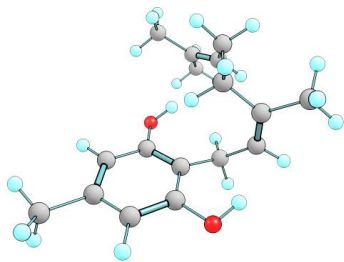
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.130627	0.614305	-0.479151
2	6	0	4.018363	-0.311964	0.069064
3	6	0	3.570032	-1.582772	0.444424
4	6	0	2.225421	-1.906479	0.257070
5	6	0	1.343572	-0.970985	-0.293109
6	6	0	1.771281	0.307423	-0.687498
7	1	0	5.055842	-0.021661	0.201578
8	1	0	1.838105	-2.881091	0.535639
9	8	0	3.656613	1.841350	-0.790674
10	1	0	2.994426	2.393213	-1.226611
11	8	0	0.041264	-1.383957	-0.419367
12	1	0	-0.486794	-0.711251	-0.867485
13	6	0	0.806213	1.351045	-1.226749
14	6	0	0.320529	2.275635	-0.132583
15	1	0	-0.027358	0.876497	-1.753732
16	1	0	1.299994	1.936910	-2.016349
17	6	0	-0.928540	2.438635	0.329019
18	1	0	1.117085	2.845626	0.346082
19	6	0	-2.142619	1.704261	-0.198398
20	1	0	-2.956538	2.426716	-0.348473
21	1	0	-1.953467	1.264506	-1.183071
22	6	0	-2.648273	0.589216	0.754357
23	6	0	-3.911461	-0.047093	0.241666
24	1	0	-2.844708	1.032357	1.739934
25	1	0	-1.849846	-0.143336	0.902046
26	6	0	-4.143227	-1.334878	-0.057480
27	1	0	-4.731629	0.657247	0.089083
28	6	0	-5.491391	-1.777171	-0.576645
29	1	0	-5.393668	-2.251790	-1.562075
30	1	0	-5.937635	-2.531266	0.085199
31	1	0	-6.194087	-0.943966	-0.667231
32	6	0	-1.203575	3.399323	1.462938
33	1	0	-1.927151	4.164815	1.154803
34	1	0	-0.294472	3.903177	1.802209
35	1	0	-1.644447	2.884936	2.325346
36	6	0	-3.142328	-2.454997	0.087832
37	1	0	-3.519404	-3.212414	0.787668
38	1	0	-2.161617	-2.130365	0.435839
39	1	0	-3.003272	-2.968052	-0.872911
40	6	0	4.534718	-2.582195	1.037870
41	1	0	4.033885	-3.517558	1.300377
42	1	0	5.006615	-2.184124	1.943031
43	1	0	5.341079	-2.816115	0.333685

Frequencies -- 17.2565 20.1733 23.7553  
 Frequencies -- 44.5896 51.2951 59.5143  
 Frequencies -- 92.3745 107.9936 125.3457

Zero-point correction= 0.372697 (Hartree/Particle)  
 Thermal correction to Energy= 0.394182  
 Thermal correction to Enthalpy= 0.395126  
 Thermal correction to Gibbs Free Energy= 0.319977  
 Sum of electronic and zero-point Energies= -812.399950  
 Sum of electronic and thermal Energies= -812.378465  
 Sum of electronic and thermal Enthalpies= -812.377521  
 Sum of electronic and thermal Free Energies= -812.452670

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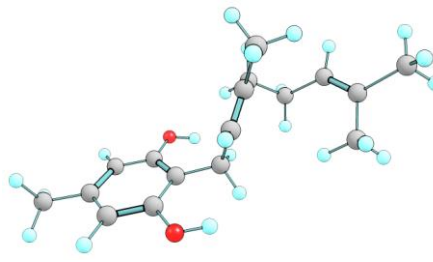
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.261796	0.959960	0.395631
2	6	0	-3.359950	0.332003	-0.194512
3	6	0	-3.344005	-1.047580	-0.425196
4	6	0	-2.196865	-1.772788	-0.091163
5	6	0	-1.099983	-1.136941	0.497609
6	6	0	-1.119420	0.237980	0.790651
7	1	0	-4.215395	0.938032	-0.476214
8	1	0	-2.127616	-2.836607	-0.295034
9	8	0	-2.350312	2.311932	0.604387
10	1	0	-1.449440	2.677288	0.650165
11	8	0	-0.014875	-1.926600	0.797310
12	1	0	0.806494	-1.422915	0.656120
13	6	0	-0.020838	0.927418	1.582422
14	6	0	0.626476	2.158577	0.962662
15	1	0	0.753099	0.201241	1.851209
16	1	0	-0.457633	1.240086	2.539360
17	6	0	1.110385	2.313631	-0.283792
18	1	0	0.746180	2.996794	1.649100
19	6	0	1.116147	1.228323	-1.340328
20	1	0	0.319947	0.503876	-1.160744
21	1	0	0.920758	1.682852	-2.319677
22	6	0	2.467740	0.466960	-1.425358
23	6	0	2.819146	-0.268589	-0.160184
24	1	0	3.267522	1.187122	-1.645080
25	1	0	2.421326	-0.211589	-2.281193
26	6	0	2.943120	-1.596794	0.025867
27	1	0	2.999050	0.376392	0.699862
28	6	0	3.320416	-2.158376	1.378256
29	1	0	2.546619	-2.845890	1.743181
30	1	0	4.247919	-2.740493	1.310162
31	1	0	3.461244	-1.372864	2.125813
32	6	0	1.751363	3.614402	-0.702812
33	1	0	2.778647	3.449444	-1.050346
34	1	0	1.780719	4.343400	0.111244
35	1	0	1.206873	4.058237	-1.545764
36	6	0	2.715360	-2.643612	-1.037481
37	1	0	3.601397	-3.281298	-1.142290
38	1	0	2.479174	-2.224575	-2.016760
39	1	0	1.885559	-3.296832	-0.741771
40	6	0	-4.544215	-1.738445	-1.028347
41	1	0	-4.254969	-2.643829	-1.569708
42	1	0	-5.078586	-1.080440	-1.720147
43	1	0	-5.255880	-2.036859	-0.248614

Frequencies -- 30.1611 49.7639 64.0313  
 Frequencies -- 68.5052 74.7182 82.1850  
 Frequencies -- 95.8108 121.3220 148.0192

Zero-point correction= 0.373684 (Hartree/Particle)  
 Thermal correction to Energy= 0.394448  
 Thermal correction to Enthalpy= 0.395392  
 Thermal correction to Gibbs Free Energy= 0.324741  
 Sum of electronic and zero-point Energies= -812.405137  
 Sum of electronic and thermal Energies= -812.384374  
 Sum of electronic and thermal Enthalpies= -812.383429  
 Sum of electronic and thermal Free Energies= -812.454080

ss-1a3c4-5-.log



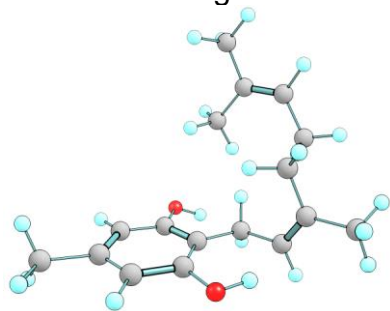
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.559299	1.336702	-0.217393
2	6	0	3.914008	1.228556	0.103719
3	6	0	4.529590	-0.025424	0.145523
4	6	0	3.772513	-1.159806	-0.158145
5	6	0	2.417901	-1.041749	-0.480202
6	6	0	1.774071	0.208075	-0.517741
7	1	0	4.470175	2.134606	0.322164
8	1	0	4.218607	-2.149115	-0.152659
9	8	0	2.034968	2.604071	-0.203805
10	1	0	1.136217	2.600254	-0.558024
11	8	0	1.760965	-2.218592	-0.743411
12	1	0	0.918050	-2.038805	-1.179228
13	6	0	0.280484	0.345177	-0.765823
14	6	0	-0.485626	0.523385	0.527461
15	1	0	-0.105027	-0.505553	-1.333995
16	1	0	0.086727	1.200184	-1.431240
17	6	0	-1.364823	-0.327899	1.074518
18	1	0	-0.251107	1.440381	1.067380
19	6	0	-1.765973	-1.645082	0.433143
20	1	0	-0.883504	-2.163489	0.041314
21	1	0	-2.182260	-2.306403	1.202082
22	6	0	-2.807855	-1.488272	-0.705766
23	6	0	-4.118953	-0.920876	-0.231251
24	1	0	-2.982259	-2.479982	-1.143895
25	1	0	-2.377584	-0.869699	-1.498516
26	6	0	-4.582693	0.328505	-0.392110
27	1	0	-4.735509	-1.616989	0.339619
28	6	0	-5.920271	0.740818	0.174632
29	1	0	-5.804694	1.573599	0.880913
30	1	0	-6.588920	1.100115	-0.618917
31	1	0	-6.419268	-0.081317	0.695587
32	6	0	-2.042613	-0.007337	2.383265
33	1	0	-3.131264	-0.006326	2.253380
34	1	0	-1.739479	0.966238	2.779400
35	1	0	-1.814930	-0.772200	3.137180
36	6	0	-3.851244	1.431085	-1.117835
37	1	0	-4.458981	1.818471	-1.945971
38	1	0	-2.883717	1.121675	-1.515137
39	1	0	-3.675713	2.275735	-0.439427
40	6	0	5.983491	-0.153292	0.534355
41	1	0	6.089585	-0.243419	1.622419
42	1	0	6.558877	0.723698	0.223563
43	1	0	6.440665	-1.040881	0.087641

Frequencies -- 17.5526 31.2567 37.4451  
 Frequencies -- 44.2492 54.6914 57.1697  
 Frequencies -- 83.5901 115.1336 134.1279

Zero-point correction= 0.372961 (Hartree/Particle)  
 Thermal correction to Energy= 0.394257  
 Thermal correction to Enthalpy= 0.395202  
 Thermal correction to Gibbs Free Energy= 0.321342  
 Sum of electronic and zero-point Energies= -812.397790  
 Sum of electronic and thermal Energies= -812.376494  
 Sum of electronic and thermal Enthalpies= -812.375550  
 Sum of electronic and thermal Free Energies= -812.449409

ss-1a3c4-5a.log



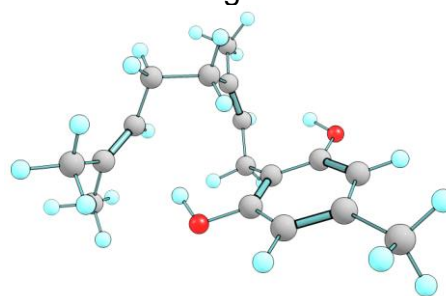
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.020197	1.116235	-0.379658
2	6	0	-3.135469	0.520469	-0.989568
3	6	0	-3.613791	-0.717739	-0.579038
4	6	0	-2.958955	-1.370246	0.466375
5	6	0	-1.851207	-0.773981	1.066045
6	6	0	-1.328432	0.470954	0.656632
7	1	0	-3.617610	1.068779	-1.792672
8	1	0	-3.304552	-2.327374	0.844157
9	8	0	-1.699865	2.347413	-0.869478
10	1	0	-0.855447	2.642851	-0.476531
11	8	0	-1.250085	-1.476117	2.085841
12	1	0	-0.747895	-0.861646	2.629292
13	6	0	-0.065859	0.931149	1.393699
14	6	0	0.594456	2.229580	0.969545
15	1	0	0.662666	0.119150	1.210991
16	1	0	-0.244236	0.952332	2.476946
17	6	0	1.559476	2.274142	0.030261
18	1	0	0.304574	3.145627	1.480305
19	6	0	2.008948	1.011159	-0.663826
20	1	0	1.202246	0.269475	-0.699134
21	1	0	2.282165	1.216241	-1.703693
22	6	0	3.238182	0.384627	0.058153
23	6	0	3.620969	-0.946563	-0.534008
24	1	0	2.999049	0.295226	1.123402
25	1	0	4.076216	1.086993	-0.010006
26	6	0	2.956890	-2.100945	-0.366956
27	1	0	4.471931	-0.940825	-1.214455
28	6	0	3.404482	-3.369104	-1.049393
29	1	0	3.664154	-4.144422	-0.314909
30	1	0	2.595582	-3.787108	-1.661946
31	1	0	4.272655	-3.207561	-1.694148
32	6	0	2.252279	3.548895	-0.353511
33	1	0	3.338765	3.446026	-0.235464
34	1	0	1.919756	4.397579	0.249949
35	1	0	2.073034	3.783051	-1.409838
36	6	0	1.723797	-2.255584	0.487514
37	1	0	0.814846	-2.317469	-0.123992
38	1	0	1.564041	-1.425070	1.179681
39	1	0	1.771666	-3.176457	1.081301
40	6	0	-4.783210	-1.373672	-1.267953
41	1	0	-5.597583	-1.564643	-0.562946
42	1	0	-4.494788	-2.350824	-1.683022
43	1	0	-5.165780	-0.766565	-2.090066

Frequencies -- 22.6446      28.1930      44.2415  
 Frequencies -- 47.8939      57.8674      80.2251  
 Frequencies -- 83.8436      105.4740      122.1346

Zero-point correction= 0.372801 (Hartree/Particle)  
 Thermal correction to Energy= 0.394079  
 Thermal correction to Enthalpy= 0.395023  
 Thermal correction to Gibbs Free Energy= 0.321682  
 Sum of electronic and zero-point Energies= -812.401052  
 Sum of electronic and thermal Energies= -812.379774  
 Sum of electronic and thermal Enthalpies= -812.378830  
 Sum of electronic and thermal Free Energies= -812.452171

ss-1a3c4a5+.log



Standard orientation:

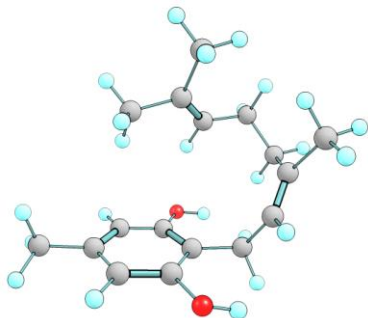
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.262304	0.959438	0.395876
2	6	0	-3.360451	0.331343	-0.194178
3	6	0	-3.344217	-1.048161	-0.425177
4	6	0	-2.196807	-1.773173	-0.091567
5	6	0	-1.099972	-1.137217	0.497135
6	6	0	-1.119714	0.237665	0.790525
7	1	0	-4.216044	0.937279	-0.475637
8	1	0	-2.127341	-2.836913	-0.295778
9	8	0	-2.351097	2.311357	0.604962
10	1	0	-1.450302	2.676901	0.650737
11	8	0	-0.014606	-1.926675	0.796376
12	1	0	0.806606	-1.422665	0.655469
13	6	0	-0.021149	0.927218	1.582236
14	6	0	0.625894	2.158509	0.962457
15	1	0	0.752906	0.201153	1.850952
16	1	0	-0.457910	1.239791	2.539212
17	6	0	1.109663	2.313672	-0.284029
18	1	0	0.745345	2.996790	1.648852
19	6	0	1.115772	1.228274	-1.340480
20	1	0	0.319785	0.503607	-1.160850
21	1	0	0.920276	1.682660	-2.319872
22	6	0	2.467592	0.467279	-1.425422
23	6	0	2.819258	-0.267856	-0.160070
24	1	0	3.267170	1.187597	-1.645378
25	1	0	2.421296	-0.211486	-2.281087
26	6	0	2.944295	-1.595925	0.026238
27	1	0	2.998267	0.377391	0.699960
28	6	0	3.321402	-2.156933	1.378910
29	1	0	2.548208	-2.845356	1.743383
30	1	0	4.249674	-2.737906	1.311488
31	1	0	3.460767	-1.371175	2.126483
32	6	0	1.750315	3.614585	-0.703113
33	1	0	2.777683	3.449853	-1.050514
34	1	0	1.779391	4.343685	0.110863
35	1	0	1.205808	4.058181	-1.546176
36	6	0	2.717940	-2.643143	-1.037025
37	1	0	3.604616	-3.280036	-1.141268
38	1	0	2.481882	-2.224515	-2.016506
39	1	0	1.888608	-3.297092	-0.741619
40	6	0	-4.544372	-1.739199	-1.028234
41	1	0	-4.255147	-2.644841	-1.569165
42	1	0	-5.078643	-1.081420	-1.720328
43	1	0	-5.256146	-2.037175	-0.248431

Frequencies -- 30.1800      49.7598      64.0544  
 Frequencies -- 68.5236      74.6874      82.1251  
 Frequencies -- 95.7216      121.2861      147.9515

Zero-point correction= 0.373683 (Hartree/Particle)  
 Thermal correction to Energy= 0.394447  
 Thermal correction to Enthalpy= 0.395392  
 Thermal correction to Gibbs Free Energy= 0.324738  
 Sum of electronic and zero-point Energies= -812.405139  
 Sum of electronic and thermal Energies= -812.384374  
 Sum of electronic and thermal Enthalpies= -812.383430  
 Sum of electronic and thermal Free Energies= -812.454083



ss-1a3c4a5-.log



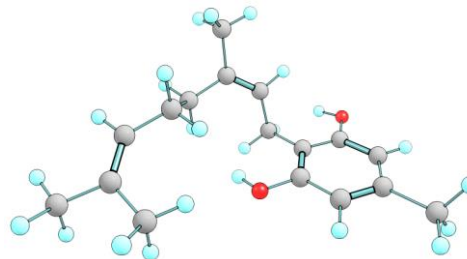
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.902549	-1.331354	-0.770020
2	6	0	2.932663	-0.419584	-1.004841
3	6	0	3.213767	0.581206	-0.070342
4	6	0	2.460640	0.634920	1.103546
5	6	0	1.423441	-0.276424	1.325006
6	6	0	1.102918	-1.274707	0.388276
7	1	0	3.510012	-0.512803	-1.919083
8	1	0	2.659090	1.384621	1.862797
9	8	0	1.703270	-2.278961	-1.742959
10	1	0	1.144220	-2.991683	-1.407850
11	8	0	0.747242	-0.116422	2.508269
12	1	0	0.058692	-0.787452	2.595261
13	6	0	-0.066150	-2.235322	0.565943
14	6	0	-1.195894	-1.985677	-0.414258
15	1	0	-0.438767	-2.213803	1.593826
16	1	0	0.289011	-3.270049	0.445538
17	6	0	-2.373008	-1.379790	-0.198794
18	1	0	-0.997369	-2.330898	-1.428057
19	6	0	-2.815993	-0.788322	1.120466
20	1	0	-3.772333	-1.241857	1.415027
21	1	0	-2.106457	-1.026153	1.918589
22	6	0	-3.003894	0.753777	1.072302
23	6	0	-1.728876	1.465415	0.710971
24	1	0	-3.337551	1.074423	2.068695
25	1	0	-3.816366	1.000505	0.383623
26	6	0	-1.466066	2.211888	-0.372821
27	1	0	-0.913634	1.298004	1.413541
28	6	0	-0.087788	2.787034	-0.599775
29	1	0	0.327441	2.428969	-1.551681
30	1	0	-0.121600	3.882556	-0.669383
31	1	0	0.610977	2.507022	0.192301
32	6	0	-3.362817	-1.231196	-1.331174
33	1	0	-4.349005	-1.615548	-1.041175
34	1	0	-3.037448	-1.764047	-2.228651
35	1	0	-3.503382	-0.178636	-1.600775
36	6	0	-2.459971	2.545030	-1.458551
37	1	0	-2.509994	3.630730	-1.612155
38	1	0	-3.470970	2.191732	-1.247654
39	1	0	-2.142525	2.111675	-2.416125
40	6	0	4.292295	1.602734	-0.339797
41	1	0	4.718381	1.990447	0.589966
42	1	0	3.885685	2.457071	-0.894892
43	1	0	5.102905	1.180461	-0.940970

Frequencies -- 22.8604      25.6389      39.9721  
 Frequencies -- 60.3651      68.3171      78.0619  
 Frequencies -- 106.7666      134.7087      140.1025

Zero-point correction= 0.373269 (Hartree/Particle)  
 Thermal correction to Energy= 0.394370  
 Thermal correction to Enthalpy= 0.395314  
 Thermal correction to Gibbs Free Energy= 0.323014  
 Sum of electronic and zero-point Energies= -812.400965  
 Sum of electronic and thermal Energies= -812.379864  
 Sum of electronic and thermal Enthalpies= -812.378920  
 Sum of electronic and thermal Free Energies= -812.451220

ss-1a3c4a5a.log



Standard orientation:

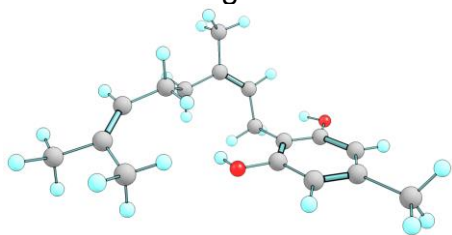
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	3.130942	0.614264	-0.479766
2	6	0	4.018793	-0.312078	0.068147
3	6	0	3.570397	-1.582676	0.444138
4	6	0	2.225611	-1.906154	0.257647
5	6	0	1.343656	-0.970609	-0.292268
6	6	0	1.771423	0.307588	-0.687296
7	1	0	5.056422	-0.021986	0.199961
8	1	0	1.838257	-2.880621	0.536669
9	8	0	3.657054	1.841069	-0.791978
10	1	0	2.994465	2.393314	-1.226816
11	8	0	0.041178	-1.383299	-0.417674
12	1	0	-0.486839	-0.710834	-0.866203
13	6	0	0.806193	1.351116	-1.226439
14	6	0	0.320311	2.275479	-0.132178
15	1	0	-0.027249	0.876455	-1.753541
16	1	0	1.299899	1.937183	-2.015931
17	6	0	-0.928805	2.438346	0.329359
18	1	0	1.116798	2.845424	0.346664
19	6	0	-2.142814	1.704074	-0.198340
20	1	0	-2.956501	2.426667	-0.349027
21	1	0	-1.953324	1.263966	-1.182790
22	6	0	-2.649168	0.589443	0.754526
23	6	0	-3.911929	-0.047115	0.241114
24	1	0	-2.846383	1.033014	1.739751
25	1	0	-1.850825	-0.143014	0.903136
26	6	0	-4.143315	-1.334976	-0.058003
27	1	0	-4.732082	0.657095	0.087861
28	6	0	-5.491076	-1.777524	-0.578004
29	1	0	-5.392619	-2.252320	-1.563276
30	1	0	-5.937693	-2.531545	0.083674
31	1	0	-6.193803	-0.944415	-0.669231
32	6	0	-1.203913	3.398712	1.463536
33	1	0	-1.927970	4.163906	1.155796
34	1	0	-0.294927	3.902944	1.802560
35	1	0	-1.644205	2.883978	2.326035
36	6	0	-3.142366	-2.454942	0.088129
37	1	0	-3.519896	-3.212405	0.787672
38	1	0	-2.161975	-2.130173	0.436912
39	1	0	-3.002470	-2.967990	-0.872495
40	6	0	4.535114	-2.581948	1.037785
41	1	0	4.035149	-3.518828	1.296502
42	1	0	5.003605	-2.185370	1.945391
43	1	0	5.343981	-2.812603	0.335426

Frequencies -- 18.5990      21.2656      23.8615  
 Frequencies -- 44.6567      51.4150      59.5102  
 Frequencies -- 92.4358      107.9664      125.3618

Zero-point correction= 0.372705 (Hartree/Particle)  
 Thermal correction to Energy= 0.394183  
 Thermal correction to Enthalpy= 0.395128  
 Thermal correction to Gibbs Free Energy= 0.320109  
 Sum of electronic and zero-point Energies= -812.399942  
 Sum of electronic and thermal Energies= -812.378463  
 Sum of electronic and thermal Enthalpies= -812.377519  
 Sum of electronic and thermal Free Energies= -812.452537

# Cannabigerocin-ss-1+3c

## ss-1+3c4a5a.log



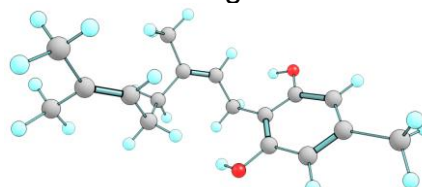
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.131273	0.613963	-0.481037
2	6	0	4.019379	-0.312517	0.066239
3	6	0	3.570910	-1.582788	0.443246
4	6	0	2.225917	-1.906020	0.257862
5	6	0	1.343743	-0.970391	-0.291561
6	6	0	1.771502	0.307580	-0.687296
7	1	0	5.057277	-0.022800	0.196735
8	1	0	1.838591	-2.880381	0.537279
9	8	0	3.657494	1.840441	-0.794307
10	1	0	2.994507	2.392910	-1.228257
11	8	0	0.041115	-1.382855	-0.416135
12	1	0	-0.486993	-0.710378	-0.864542
13	6	0	0.806057	1.351037	-1.226166
14	6	0	0.320293	2.275144	-0.131637
15	1	0	-0.027433	0.876301	-1.753133
16	1	0	1.299489	1.937245	-2.015720
17	6	0	-0.928776	2.437900	0.330084
18	1	0	1.116849	2.844925	0.347286
19	6	0	-2.142884	1.703940	-0.197833
20	1	0	-2.956303	2.426780	-0.348796
21	1	0	-1.953302	1.263701	-1.182202
22	6	0	-2.649901	0.589550	0.754968
23	6	0	-3.912455	-0.046938	0.240965
24	1	0	-2.847606	1.033323	1.739997
25	1	0	-1.851740	-0.142987	0.904180
26	6	0	-4.143645	-1.334722	-0.058638
27	1	0	-4.732574	0.657275	0.087551
28	6	0	-5.491153	-1.777183	-0.579356
29	1	0	-5.392247	-2.251687	-1.564723
30	1	0	-5.938017	-2.531423	0.081907
31	1	0	-6.193883	-0.944084	-0.670639
32	6	0	-1.203683	3.397788	1.464715
33	1	0	-1.928472	4.162601	1.157773
34	1	0	-0.294764	3.902488	1.803221
35	1	0	-1.642966	2.882498	2.327404
36	6	0	-3.142688	-2.454675	0.087547
37	1	0	-3.520488	-3.212435	0.786620
38	1	0	-2.162491	-2.129986	0.436943
39	1	0	-3.002290	-2.967342	-0.873206
40	6	0	4.535124	-2.580890	1.039664
41	1	0	4.041216	-3.527875	1.271869
42	1	0	4.979007	-2.194729	1.964120
43	1	0	5.361684	-2.789301	0.351263

Frequencies -- 16.8366 20.3320 23.8338  
 Frequencies -- 44.7285 51.4985 59.5221  
 Frequencies -- 92.4804 107.9473 125.3849

Zero-point correction= 0.372703 (Hartree/Particle)  
 Thermal correction to Energy= 0.394185  
 Thermal correction to Enthalpy= 0.395129  
 Thermal correction to Gibbs Free Energy= 0.319981  
 Sum of electronic and zero-point Energies= -812.399944  
 Sum of electronic and thermal Energies= -812.378462  
 Sum of electronic and thermal Enthalpies= -812.377518  
 Sum of electronic and thermal Free Energies= -812.452666

# ss-1+3c4+5+.log



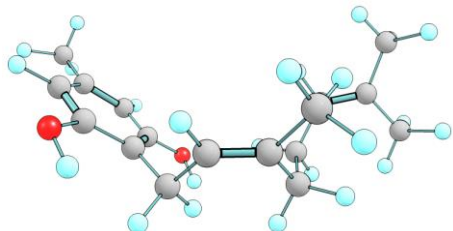
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.012988	0.941869	0.296384
2	6	0	3.934546	0.023823	0.803267
3	6	0	3.859137	-1.323363	0.439447
4	6	0	2.864349	-1.724112	-0.455531
5	6	0	1.947853	-0.797235	-0.959261
6	6	0	1.985343	0.558314	-0.586368
7	1	0	4.704988	0.380853	1.479173
8	1	0	2.787371	-2.756198	-0.782241
9	8	0	3.153920	2.237355	0.727232
10	1	0	2.606559	2.830735	0.196450
11	8	0	1.009448	-1.302202	-1.826311
12	1	0	0.565786	-0.582865	-2.293748
13	6	0	0.938983	1.569362	-1.030919
14	6	0	-0.017709	1.920058	0.089720
15	1	0	0.390893	1.213456	-1.906892
16	1	0	1.439003	2.483259	-1.389808
17	6	0	-1.352941	1.795000	0.102718
18	1	0	0.465603	2.310177	0.984844
19	6	0	-2.166343	1.234143	-1.049056
20	1	0	-3.167070	1.681789	-1.029352
21	1	0	-1.722915	1.512442	-2.011649
22	6	0	-2.326597	-0.312264	-1.018267
23	6	0	-2.955216	-0.846032	0.243018
24	1	0	-1.335452	-0.765522	-1.129138
25	1	0	-2.905211	-0.606945	-1.900260
26	6	0	-4.247831	-1.141674	0.452718
27	1	0	-2.268589	-0.975842	1.079646
28	6	0	-4.724262	-1.650949	1.791824
29	1	0	-5.481426	-0.979539	2.218120
30	1	0	-5.204842	-2.633089	1.690345
31	1	0	-3.906227	-1.743258	2.511921
32	6	0	-2.149838	2.217675	1.314611
33	1	0	-2.832173	3.038146	1.056168
34	1	0	-1.508101	2.552113	2.134850
35	1	0	-2.778038	1.395538	1.674870
36	6	0	-5.336548	-0.994419	-0.581624
37	1	0	-5.849561	-1.951516	-0.742409
38	1	0	-4.972668	-0.637469	-1.546961
39	1	0	-6.101316	-0.289631	-0.230248
40	6	0	4.825152	-2.331175	1.015607
41	1	0	5.004773	-3.155709	0.319567
42	1	0	4.428401	-2.766206	1.941130
43	1	0	5.786852	-1.870053	1.258517

Frequencies -- 12.6349 28.9805 43.4014  
 Frequencies -- 48.5557 54.3655 79.3490  
 Frequencies -- 82.1730 100.5374 134.3855

Zero-point correction= 0.373083 (Hartree/Particle)  
 Thermal correction to Energy= 0.394352  
 Thermal correction to Enthalpy= 0.395297  
 Thermal correction to Gibbs Free Energy= 0.321294  
 Sum of electronic and zero-point Energies= -812.396937  
 Sum of electronic and thermal Energies= -812.375668  
 Sum of electronic and thermal Enthalpies= -812.374724  
 Sum of electronic and thermal Free Energies= -812.448726

ss-1+3c4+5-.log



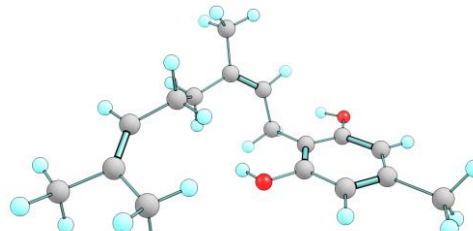
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-2.867588	1.165697	0.406652
2	6	0	-3.954447	0.346865	0.080816
3	6	0	-3.753313	-0.980919	-0.301691
4	6	0	-2.445756	-1.471894	-0.376294
5	6	0	-1.367094	-0.648019	-0.052001
6	6	0	-1.548085	0.681326	0.374418
7	1	0	-4.952586	0.770637	0.128063
8	1	0	-2.244494	-2.489741	-0.695090
9	8	0	-3.178487	2.449077	0.773994
10	1	0	-2.372524	2.974740	0.860141
11	8	0	-0.120775	-1.211260	-0.129427
12	1	0	0.569342	-0.538900	-0.253417
13	6	0	-0.344435	1.509931	0.779172
14	6	0	0.521728	1.898720	-0.401069
15	1	0	0.231910	0.949791	1.523229
16	1	0	-0.664300	2.417916	1.309192
17	6	0	1.863586	1.883222	-0.486078
18	1	0	-0.040822	2.244464	-1.268164
19	6	0	2.780941	1.481877	0.649273
20	1	0	3.256458	2.391900	1.043657
21	1	0	2.208652	1.053898	1.476309
22	6	0	3.901411	0.485111	0.257801
23	6	0	3.404174	-0.771209	-0.420012
24	1	0	4.457722	0.239084	1.169568
25	1	0	4.614850	0.986506	-0.404692
26	6	0	2.877588	-1.854359	0.174598
27	1	0	3.479895	-0.785134	-1.507095
28	6	0	2.427620	-3.050655	-0.627768
29	1	0	2.963316	-3.954711	-0.309940
30	1	0	1.359578	-3.235084	-0.469265
31	1	0	2.595816	-2.912002	-1.699758
32	6	0	2.549554	2.343666	-1.750899
33	1	0	3.282937	3.129301	-1.529326
34	1	0	1.835760	2.735425	-2.480106
35	1	0	3.102731	1.525683	-2.226588
36	6	0	2.658806	-1.974940	1.662130
37	1	0	1.581666	-1.984916	1.870199
38	1	0	3.104433	-1.156418	2.231390
39	1	0	3.066222	-2.919688	2.042393
40	6	0	-4.927465	-1.877276	-0.617263
41	1	0	-4.673195	-2.611627	-1.387378
42	1	0	-5.790152	-1.300852	-0.963428
43	1	0	-5.242462	-2.435653	0.272866

Frequencies -- 17.6737 37.5135 50.2638  
 Frequencies -- 60.9814 62.6204 81.3158  
 Frequencies -- 97.5376 127.1548 138.7150

Zero-point correction= 0.372999 (Hartree/Particle)  
 Thermal correction to Energy= 0.394131  
 Thermal correction to Enthalpy= 0.395076  
 Thermal correction to Gibbs Free Energy= 0.322614  
 Sum of electronic and zero-point Energies= -812.404245  
 Sum of electronic and thermal Energies= -812.383113  
 Sum of electronic and thermal Enthalpies= -812.382169  
 Sum of electronic and thermal Free Energies= -812.454630

ss-1+3c4+5a.log



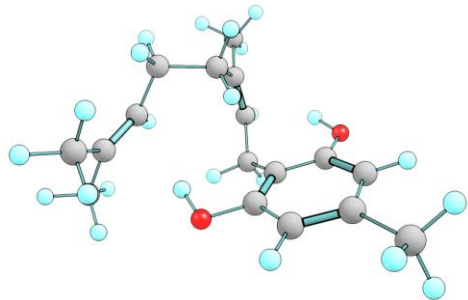
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.131056	0.614163	-0.480011
2	6	0	4.018807	-0.312209	0.068058
3	6	0	3.570259	-1.582669	0.444290
4	6	0	2.225357	-1.905898	0.258144
5	6	0	1.343491	-0.970306	-0.291835
6	6	0	1.771468	0.307694	-0.687273
7	1	0	5.056474	-0.022212	0.199783
8	1	0	1.837826	-2.880191	0.537537
9	8	0	3.657449	1.840728	-0.792670
10	1	0	2.994491	2.393672	-1.226050
11	8	0	0.040909	-1.382710	-0.416980
12	1	0	-0.487271	-0.709774	-0.864611
13	6	0	0.806285	1.351269	-1.226458
14	6	0	0.320393	2.275523	-0.132068
15	1	0	-0.027149	0.876615	-1.753559
16	1	0	1.300053	1.937307	-2.015898
17	6	0	-0.928685	2.438174	0.329646
18	1	0	1.116861	2.845474	0.346812
19	6	0	-2.142727	1.704121	-0.198304
20	1	0	-2.956158	2.426929	-0.349404
21	1	0	-1.953043	1.263852	-1.182643
22	6	0	-2.649812	0.589807	0.754522
23	6	0	-3.912147	-0.046978	0.240313
24	1	0	-2.847879	1.033722	1.739411
25	1	0	-1.851598	-0.142604	0.904077
26	6	0	-4.143255	-1.334987	-0.058361
27	1	0	-4.732191	0.657151	0.086112
28	6	0	-5.490620	-1.777860	-0.579099
29	1	0	-5.391440	-2.253204	-1.564031
30	1	0	-5.937679	-2.531519	0.082695
31	1	0	-6.193305	-0.944818	-0.671271
32	6	0	-1.203734	3.398188	1.464139
33	1	0	-1.928438	4.163002	1.156997
34	1	0	-0.294844	3.902874	1.802739
35	1	0	-1.643179	2.882969	2.326782
36	6	0	-3.142346	-2.454826	0.089101
37	1	0	-3.520132	-3.211761	0.789067
38	1	0	-2.162107	-2.129713	0.437995
39	1	0	-3.002005	-2.968575	-0.871080
40	6	0	4.535061	-2.582338	1.037132
41	1	0	4.033329	-3.516008	1.303917
42	1	0	5.010968	-2.182716	1.939488
43	1	0	5.338440	-2.819816	0.330710

Frequencies -- 13.9228 20.0389 23.9412  
 Frequencies -- 44.5551 51.5876 59.5345  
 Frequencies -- 92.5058 107.9481 125.3441

Zero-point correction= 0.372695 (Hartree/Particle)  
 Thermal correction to Energy= 0.394185  
 Thermal correction to Enthalpy= 0.395129  
 Thermal correction to Gibbs Free Energy= 0.319789  
 Sum of electronic and zero-point Energies= -812.399952  
 Sum of electronic and thermal Energies= -812.378462  
 Sum of electronic and thermal Enthalpies= -812.377518  
 Sum of electronic and thermal Free Energies= -812.452858

ss-1+3c4-5+.log



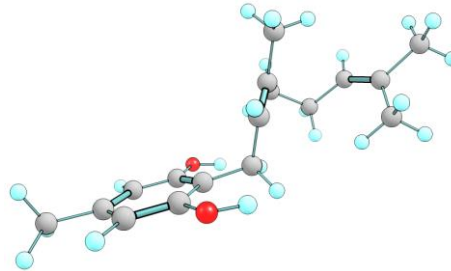
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.262329	0.959420	0.395980
2	6	0	-3.360592	0.331518	-0.193991
3	6	0	-3.344509	-1.048001	-0.425117
4	6	0	-2.197117	-1.773116	-0.091770
5	6	0	-1.100101	-1.137288	0.496828
6	6	0	-1.119689	0.237507	0.790370
7	1	0	-4.216223	0.937512	-0.475206
8	1	0	-2.127735	-2.836846	-0.296068
9	8	0	-2.351009	2.311307	0.605394
10	1	0	-1.450194	2.676856	0.650731
11	8	0	-0.014768	-1.926922	0.795641
12	1	0	0.806470	-1.422747	0.655554
13	6	0	-0.021099	0.926956	1.582092
14	6	0	0.625973	2.158287	0.962401
15	1	0	0.752971	0.200879	1.850811
16	1	0	-0.457853	1.239466	2.539099
17	6	0	1.109719	2.313539	-0.284086
18	1	0	0.745476	2.996500	1.648882
19	6	0	1.115856	1.228142	-1.340523
20	1	0	0.319925	0.503415	-1.160836
21	1	0	0.920284	1.682455	-2.319930
22	6	0	2.467742	0.467255	-1.425489
23	6	0	2.819524	-0.267714	-0.160085
24	1	0	3.267250	1.187625	-1.645570
25	1	0	2.421436	-0.211594	-2.281087
26	6	0	2.944550	-1.595765	0.026374
27	1	0	2.998641	0.377630	0.699851
28	6	0	3.321689	-2.156625	1.379102
29	1	0	2.548319	-2.844739	1.743807
30	1	0	4.249765	-2.737917	1.311693
31	1	0	3.461388	-1.370772	2.126512
32	6	0	1.750296	3.614492	-0.703132
33	1	0	2.777699	3.449855	-1.050482
34	1	0	1.779266	4.343580	0.110860
35	1	0	1.205795	4.058057	-1.546218
36	6	0	2.718134	-2.643109	-1.036739
37	1	0	3.604659	-3.280260	-1.140715
38	1	0	2.482352	-2.224598	-2.016343
39	1	0	1.888569	-3.296775	-0.741352
40	6	0	-4.544823	-1.738877	-1.028039
41	1	0	-4.255697	-2.644333	-1.569350
42	1	0	-5.079279	-1.080909	-1.719811
43	1	0	-5.256393	-2.037141	-0.248163

Frequencies -- 30.1792 49.7760 64.0647  
 Frequencies -- 68.5757 74.6983 82.1474  
 Frequencies -- 95.6772 121.2873 148.0086

Zero-point correction= 0.373683 (Hartree/Particle)  
 Thermal correction to Energy= 0.394447  
 Thermal correction to Enthalpy= 0.395391  
 Thermal correction to Gibbs Free Energy= 0.324740  
 Sum of electronic and zero-point Energies= -812.405139  
 Sum of electronic and thermal Energies= -812.384375  
 Sum of electronic and thermal Enthalpies= -812.383431  
 Sum of electronic and thermal Free Energies= -812.454082

ss-1+3c4-5-.log



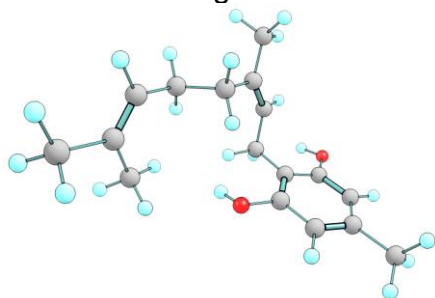
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.559261	1.336712	-0.217274
2	6	0	3.913987	1.228563	0.103770
3	6	0	4.529589	-0.025414	0.145457
4	6	0	3.772512	-1.159785	-0.158262
5	6	0	2.417873	-1.041719	-0.480233
6	6	0	1.774025	0.208093	-0.517644
7	1	0	4.470153	2.134609	0.322254
8	1	0	4.218611	-2.149093	-0.152859
9	8	0	2.034928	2.604079	-0.203557
10	1	0	1.136133	2.600280	-0.557667
11	8	0	1.760935	-2.218566	-0.743444
12	1	0	0.918020	-2.038778	-1.179264
13	6	0	0.280423	0.345174	-0.765657
14	6	0	-0.485681	0.523287	0.527645
15	1	0	-0.105057	-0.505537	-1.333882
16	1	0	0.086626	1.200219	-1.431014
17	6	0	-1.364898	-0.328010	1.074651
18	1	0	-0.251139	1.440245	1.067631
19	6	0	-1.766022	-1.645170	0.433206
20	1	0	-0.883529	-2.163558	0.041397
21	1	0	-2.182332	-2.306525	1.202106
22	6	0	-2.807854	-1.488308	-0.705734
23	6	0	-4.118916	-0.920804	-0.231253
24	1	0	-2.982321	-2.480005	-1.143875
25	1	0	-2.377516	-0.869763	-1.498471
26	6	0	-4.582595	0.328584	-0.392236
27	1	0	-4.735489	-1.616833	0.339708
28	6	0	-5.920155	0.741027	0.174457
29	1	0	-5.804523	1.573830	0.880705
30	1	0	-6.588758	1.100346	-0.619123
31	1	0	-6.419232	-0.081047	0.695434
32	6	0	-2.042678	-0.007513	2.383420
33	1	0	-3.131327	-0.006427	2.253511
34	1	0	-1.739496	0.966021	2.779626
35	1	0	-1.815058	-0.772442	3.137289
36	6	0	-3.851108	1.431037	-1.118118
37	1	0	-4.458724	1.818144	-1.946476
38	1	0	-2.883476	1.121610	-1.515157
39	1	0	-3.675789	2.275890	-0.439904
40	6	0	5.983559	-0.153237	0.534058
41	1	0	6.089812	-0.243609	1.622084
42	1	0	6.558815	0.723885	0.223385
43	1	0	6.440755	-1.040665	0.087040

Frequencies -- 17.5417 31.2681 37.4484  
 Frequencies -- 44.2523 54.7741 57.1804  
 Frequencies -- 83.5981 115.1438 134.1323

Zero-point correction= 0.372962 (Hartree/Particle)  
 Thermal correction to Energy= 0.394257  
 Thermal correction to Enthalpy= 0.395201  
 Thermal correction to Gibbs Free Energy= 0.321345  
 Sum of electronic and zero-point Energies= -812.397790  
 Sum of electronic and thermal Energies= -812.376494  
 Sum of electronic and thermal Enthalpies= -812.375550  
 Sum of electronic and thermal Free Energies= -812.449406

ss-1+3c4-5a.log



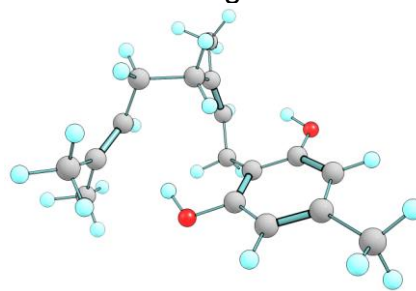
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.874066	0.605252	0.581812
2	6	0	-3.870223	-0.153784	-0.033881
3	6	0	-3.573644	-1.417255	-0.553226
4	6	0	-2.274431	-1.911133	-0.419212
5	6	0	-1.284178	-1.145338	0.202898
6	6	0	-1.548640	0.143699	0.699517
7	1	0	-4.872904	0.257227	-0.094699
8	1	0	-2.009685	-2.898156	-0.784491
9	8	0	-3.257803	1.836242	1.049584
10	1	0	-2.571199	2.212134	1.615013
11	8	0	-0.041088	-1.729910	0.272386
12	1	0	0.512700	-1.262013	0.909865
13	6	0	-0.473381	1.042689	1.295554
14	6	0	-0.144597	2.254575	0.437370
15	1	0	0.441230	0.474270	1.487036
16	1	0	-0.783615	1.382876	2.293336
17	6	0	0.779444	2.308893	-0.532632
18	1	0	-0.731155	3.150836	0.633288
19	6	0	1.660298	1.133615	-0.901693
20	1	0	1.137468	0.184935	-0.757035
21	1	0	1.907426	1.183889	-1.969319
22	6	0	2.981851	1.098512	-0.088514
23	6	0	3.850830	-0.063835	-0.488054
24	1	0	2.737768	1.071049	0.978399
25	1	0	3.523715	2.038420	-0.252269
26	6	0	3.956301	-1.253932	0.123414
27	1	0	4.409051	0.077316	-1.414362
28	6	0	4.831079	-2.348503	-0.438376
29	1	0	5.602556	-2.644395	0.284760
30	1	0	4.241046	-3.250756	-0.647104
31	1	0	5.328020	-2.044266	-1.363805
32	6	0	1.031184	3.578604	-1.306830
33	1	0	2.085896	3.874597	-1.238123
34	1	0	0.419958	4.411605	-0.948443
35	1	0	0.820542	3.430340	-2.373776
36	6	0	3.225257	-1.635238	1.388167
37	1	0	2.509010	-2.442660	1.185148
38	1	0	2.688063	-0.801921	1.848641
39	1	0	3.922470	-2.027577	2.138668
40	6	0	-4.636809	-2.225245	-1.258676
41	1	0	-4.421127	-3.296527	-1.214243
42	1	0	-4.699125	-1.946764	-2.317802
43	1	0	-5.624629	-2.054566	-0.820276

Frequencies -- 11.8227 25.8758 41.2874  
 Frequencies -- 57.2180 68.7852 77.6582  
 Frequencies -- 83.4283 100.4432 135.3828

Zero-point correction= 0.373101 (Hartree/Particle)  
 Thermal correction to Energy= 0.394372  
 Thermal correction to Enthalpy= 0.395317  
 Thermal correction to Gibbs Free Energy= 0.321545  
 Sum of electronic and zero-point Energies= -812.397736  
 Sum of electronic and thermal Energies= -812.376465  
 Sum of electronic and thermal Enthalpies= -812.375521  
 Sum of electronic and thermal Free Energies= -812.449292

ss-1+3c4a5+.log



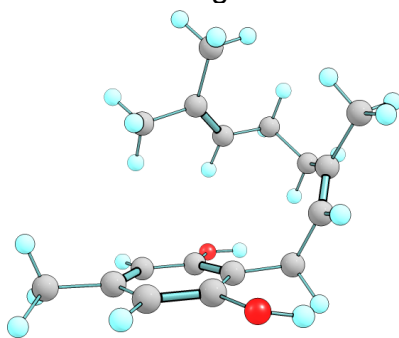
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.262587	0.959203	0.395991
2	6	0	-3.360658	0.331041	-0.194048
3	6	0	-3.344247	-1.048471	-0.425163
4	6	0	-2.196715	-1.773329	-0.091767
5	6	0	-1.099873	-1.137261	0.496888
6	6	0	-1.119832	0.237537	0.790478
7	1	0	-4.216393	0.936833	-0.475382
8	1	0	-2.127056	-2.837031	-0.296107
9	8	0	-2.351482	2.311080	0.605327
10	1	0	-1.450702	2.676744	0.650556
11	8	0	-0.014336	-1.926608	0.795756
12	1	0	0.806788	-1.422321	0.655363
13	6	0	-0.021366	0.927254	1.582178
14	6	0	0.625597	2.158540	0.962322
15	1	0	0.752740	0.201285	1.851015
16	1	0	-0.458223	1.239886	2.539089
17	6	0	1.109352	2.313675	-0.284174
18	1	0	0.744960	2.996876	1.648665
19	6	0	1.115675	1.228188	-1.340526
20	1	0	0.319792	0.503411	-1.160870
21	1	0	0.920164	1.682448	-2.319972
22	6	0	2.467641	0.467412	-1.425360
23	6	0	2.819384	-0.267552	-0.159944
24	1	0	3.267087	1.187857	-1.645375
25	1	0	2.421444	-0.211442	-2.280960
26	6	0	2.944798	-1.595572	0.026442
27	1	0	2.998155	0.377790	0.700064
28	6	0	3.321823	-2.156396	1.379209
29	1	0	2.548784	-2.845090	1.743508
30	1	0	4.250317	-2.737041	1.312035
31	1	0	3.460707	-1.370572	2.126800
32	6	0	1.749776	3.614665	-0.703365
33	1	0	2.777124	3.450082	-1.050895
34	1	0	1.778838	4.343798	0.110582
35	1	0	1.205094	4.058152	-1.546374
36	6	0	2.718803	-2.642921	-1.036770
37	1	0	3.605043	-3.280609	-1.139768
38	1	0	2.484257	-2.224393	-2.016659
39	1	0	1.888549	-3.296044	-0.742114
40	6	0	-4.544395	-1.739610	-1.028117
41	1	0	-4.255032	-2.644812	-1.569722
42	1	0	-5.079228	-1.081636	-1.719588
43	1	0	-5.255705	-2.038367	-0.248190

Frequencies -- 30.1931 49.7708 64.0701  
 Frequencies -- 68.6043 74.6984 82.1510  
 Frequencies -- 95.7058 121.3381 148.0860

Zero-point correction= 0.373684 (Hartree/Particle)  
 Thermal correction to Energy= 0.394448  
 Thermal correction to Enthalpy= 0.395392  
 Thermal correction to Gibbs Free Energy= 0.324743  
 Sum of electronic and zero-point Energies= -812.405138  
 Sum of electronic and thermal Energies= -812.384374  
 Sum of electronic and thermal Enthalpies= -812.383430  
 Sum of electronic and thermal Free Energies= -812.454079

ss-1+3c4a5-.log



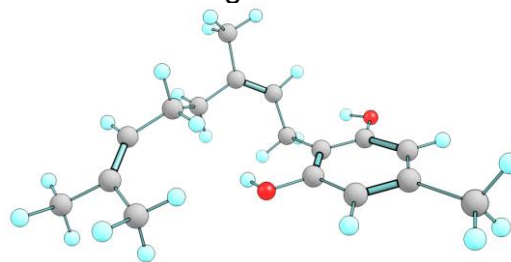
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.902776	-1.330915	-0.770480
2	6	0	2.932552	-0.418666	-1.004985
3	6	0	3.213309	0.581858	-0.070119
4	6	0	2.460209	0.634836	1.103833
5	6	0	1.423375	-0.276987	1.324978
6	6	0	1.103178	-1.275020	0.387860
7	1	0	3.509866	-0.511276	-1.919308
8	1	0	2.658421	1.384309	1.863368
9	8	0	1.703844	-2.278230	-1.743768
10	1	0	1.144602	-2.991021	-1.409129
11	8	0	0.747148	-0.117699	2.508329
12	1	0	0.059493	-0.789615	2.595547
13	6	0	-0.065612	-2.236064	0.565068
14	6	0	-1.195546	-1.986102	-0.414859
15	1	0	-0.438149	-2.215284	1.592989
16	1	0	0.289801	-3.270617	0.443959
17	6	0	-2.372540	-1.380115	-0.199001
18	1	0	-0.997276	-2.331068	-1.428794
19	6	0	-2.815208	-0.789004	1.120523
20	1	0	-3.771383	-1.242768	1.415273
21	1	0	-2.105372	-1.026869	1.918358
22	6	0	-3.003354	0.753059	1.072780
23	6	0	-1.728579	1.464922	0.711033
24	1	0	-3.336609	1.073441	2.069393
25	1	0	-3.816167	0.999839	0.384519
26	6	0	-1.466493	2.212063	-0.372470
27	1	0	-0.912914	1.297135	1.413015
28	6	0	-0.088416	2.787520	-0.599875
29	1	0	0.326203	2.430307	-1.552363
30	1	0	-0.122389	3.883097	-0.668536
31	1	0	0.610890	2.506918	0.191516
32	6	0	-3.362519	-1.231005	-1.331157
33	1	0	-4.348683	-1.615413	-1.041147
34	1	0	-3.037333	-1.763514	-2.228902
35	1	0	-3.503061	-0.178324	-1.600301
36	6	0	-2.461091	2.545727	-1.457401
37	1	0	-2.511314	3.631505	-1.610386
38	1	0	-3.471927	2.192215	-1.246080
39	1	0	-2.144197	2.112928	-2.415411
40	6	0	4.291499	1.603858	-0.339145
41	1	0	4.717550	1.991202	0.590789
42	1	0	3.884595	2.458378	-0.893740
43	1	0	5.102179	1.182133	-0.940607

Frequencies --	22.6951	25.8359	39.9484
Frequencies --	60.1927	68.2675	78.0250
Frequencies --	106.7216	134.6628	140.1756

Zero-point correction= 0.373264 (Hartree/Particle)  
 Thermal correction to Energy= 0.394368  
 Thermal correction to Enthalpy= 0.395312  
 Thermal correction to Gibbs Free Energy= 0.323003  
 Sum of electronic and zero-point Energies= -812.400970  
 Sum of electronic and thermal Energies= -812.379866  
 Sum of electronic and thermal Enthalpies= -812.378922  
 Sum of electronic and thermal Free Energies= -812.451230

ss-1+3c4a5a.log



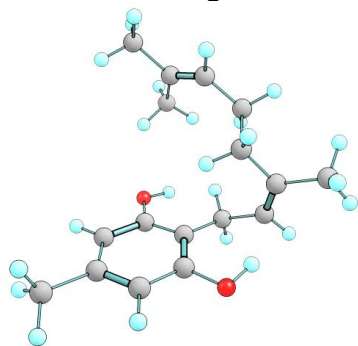
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.131273	0.613963	-0.481037
2	6	0	4.019379	-0.312517	0.066239
3	6	0	3.570910	-1.582788	0.443246
4	6	0	2.225917	-1.906020	0.257862
5	6	0	1.343743	-0.970391	-0.291561
6	6	0	1.771502	0.307580	-0.687296
7	1	0	5.057277	-0.022800	0.196735
8	1	0	1.838591	-2.880381	0.537279
9	8	0	3.657494	1.840441	-0.794307
10	1	0	2.994507	2.392910	-1.228257
11	8	0	0.041115	-1.382855	-0.416135
12	1	0	-0.486993	-0.710378	-0.864542
13	6	0	0.806057	1.351037	-1.226166
14	6	0	0.320293	2.275144	-0.131637
15	1	0	-0.027433	0.876301	-1.753133
16	1	0	1.299489	1.937245	-2.015720
17	6	0	-0.928776	2.437900	0.330084
18	1	0	1.116849	2.844925	0.347286
19	6	0	-2.142884	1.703940	-0.197833
20	1	0	-2.956303	2.426780	-0.348796
21	1	0	-1.953302	1.263701	-1.182202
22	6	0	-2.649901	0.589550	0.754968
23	6	0	-3.912455	-0.046938	0.240965
24	1	0	-2.847606	1.033323	1.739997
25	1	0	-1.851740	-0.142987	0.904180
26	6	0	-4.143645	-1.334722	-0.058638
27	1	0	-4.732574	0.657275	0.087551
28	6	0	-5.491153	-1.777183	-0.579356
29	1	0	-5.392247	-2.251687	-1.564723
30	1	0	-5.938017	-2.531423	0.081907
31	1	0	-6.193883	-0.944084	-0.670639
32	6	0	-1.203683	3.397788	1.464715
33	1	0	-1.928472	4.162601	1.157773
34	1	0	-0.294764	3.902488	1.803221
35	1	0	-1.642966	2.882498	2.327404
36	6	0	-3.142688	-2.454675	0.087547
37	1	0	-3.520488	-3.212435	0.786620
38	1	0	-2.162491	-2.129986	0.436943
39	1	0	-3.002290	-2.967342	-0.873206
40	6	0	4.535124	-2.580890	1.039664
41	1	0	4.041216	-3.527875	1.271869
42	1	0	4.979007	-2.194729	1.964120
43	1	0	5.361684	-2.789301	0.351263

Frequencies --	16.8366	20.3320	23.8338
Frequencies --	44.7285	51.4985	59.5221
Frequencies --	92.4804	107.9473	125.3849

Zero-point correction= 0.372703 (Hartree/Particle)  
 Thermal correction to Energy= 0.394185  
 Thermal correction to Enthalpy= 0.395129  
 Thermal correction to Gibbs Free Energy= 0.319981  
 Sum of electronic and zero-point Energies= -812.399944  
 Sum of electronic and thermal Energies= -812.378462  
 Sum of electronic and thermal Enthalpies= -812.377518  
 Sum of electronic and thermal Free Energies= -812.452666

**Cannabigerocin-ss-1-3c**  
ss-1-3c4-5a.log



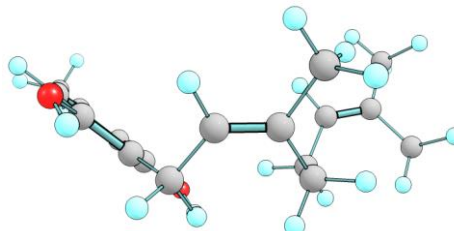
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.444251	-0.972674	1.038167
2	6	0	-2.370888	-1.761533	0.352713
3	6	0	-3.218218	-1.188592	-0.597894
4	6	0	-3.115750	0.180946	-0.847850
5	6	0	-2.183188	0.967438	-0.162907
6	6	0	-1.314002	0.410951	0.800207
7	1	0	-2.420690	-2.820720	0.584425
8	1	0	-3.753546	0.666437	-1.579960
9	8	0	-0.678321	-1.636722	1.963873
10	1	0	-0.099138	-1.019186	2.428377
11	8	0	-2.183402	2.298421	-0.473525
12	1	0	-1.340952	2.689252	-0.175232
13	6	0	-0.312680	1.233940	1.608922
14	6	0	0.283008	2.474702	0.959091
15	1	0	0.531586	0.586447	1.884515
16	1	0	-0.776362	1.532159	2.557106
17	6	0	1.086116	2.484697	-0.122114
18	1	0	0.077862	3.419788	1.460075
19	6	0	1.498978	1.213363	-0.829119
20	1	0	0.743868	0.434536	-0.696433
21	1	0	1.582605	1.393653	-1.907836
22	6	0	2.856095	0.670885	-0.300802
23	6	0	3.180242	-0.667769	-0.905546
24	1	0	2.807091	0.613818	0.790887
25	1	0	3.647222	1.393100	-0.539223
26	6	0	3.055751	-1.872961	-0.327268
27	1	0	3.490109	-0.636784	-1.951055
28	6	0	3.343390	-3.140033	-1.095975
29	1	0	4.144531	-3.717703	-0.616291
30	1	0	2.460395	-3.792900	-1.112795
31	1	0	3.637690	-2.938599	-2.129935
32	6	0	1.673081	3.764674	-0.656934
33	1	0	2.768690	3.709574	-0.672498
34	1	0	1.382467	4.634715	-0.062081
35	1	0	1.355514	3.930089	-1.693828
36	6	0	2.604545	-2.098162	1.095979
37	1	0	1.588676	-2.511723	1.121549
38	1	0	2.601054	-1.185597	1.696000
39	1	0	3.256388	-2.824844	1.596201
40	6	0	-4.196789	-2.041381	-1.369997
41	1	0	-5.081826	-1.468936	-1.662928
42	1	0	-4.523581	-2.905439	-0.784113
43	1	0	-3.738508	-2.425671	-2.289741

Frequencies --	22.6446	28.1930	44.2415
Frequencies --	47.8939	57.8674	80.2251
Frequencies --	83.8436	105.4740	122.1346

Zero-point correction= 0.372801 (Hartree/Particle)  
 Thermal correction to Energy= 0.394079  
 Thermal correction to Enthalpy= 0.395023  
 Thermal correction to Gibbs Free Energy= 0.321682  
 Sum of electronic and zero-point Energies= -812.401052  
 Sum of electronic and thermal Energies= -812.379774  
 Sum of electronic and thermal Enthalpies= -812.378830  
 Sum of electronic and thermal Free Energies= -812.452171

ss-1-3c4+5+.log



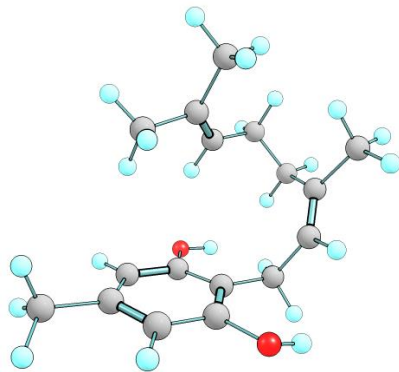
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.947762	-0.797103	-0.959340
2	6	0	2.864208	-1.724082	-0.455676
3	6	0	3.858963	-1.323489	0.439383
4	6	0	3.934413	0.023670	0.803361
5	6	0	3.012921	0.941800	0.296549
6	6	0	1.985290	0.558392	-0.586305
7	1	0	2.787167	-2.756134	-0.782488
8	1	0	4.704836	0.380566	1.479360
9	8	0	1.009378	-1.301960	-1.826476
10	1	0	0.565734	-0.582566	-2.293844
11	8	0	3.153838	2.237229	0.727599
12	1	0	2.606811	2.830734	0.196606
13	6	0	0.939045	1.569558	-1.030832
14	6	0	-0.017740	1.920218	0.089741
15	1	0	0.391023	1.213817	-1.906920
16	1	0	1.439174	2.483464	-1.389545
17	6	0	-1.352963	1.795097	0.102672
18	1	0	0.465526	2.310333	0.984896
19	6	0	-2.166297	1.234237	-1.049148
20	1	0	-3.167013	1.681919	-1.029500
21	1	0	-1.722809	1.512514	-2.011719
22	6	0	-2.326567	-0.312160	-1.018348
23	6	0	-2.955051	-0.845964	0.242989
24	1	0	-1.335423	-0.765415	-1.129317
25	1	0	-2.905251	-0.606846	-1.900290
26	6	0	-4.247617	-1.141761	0.452778
27	1	0	-2.268352	-0.975690	1.079572
28	6	0	-4.723892	-1.651115	1.791910
29	1	0	-5.480855	-0.979615	2.218423
30	1	0	-5.204670	-2.633156	1.690405
31	1	0	-3.905740	-1.743661	2.511845
32	6	0	-2.149965	2.217763	1.314502
33	1	0	-2.831872	3.038611	1.056102
34	1	0	-1.508279	2.551718	2.134979
35	1	0	-2.778596	1.395795	1.674375
36	6	0	-5.336411	-0.994726	-0.581519
37	1	0	-5.848510	-1.952191	-0.743070
38	1	0	-4.972808	-0.636701	-1.546561
39	1	0	-6.101869	-0.290943	-0.229641
40	6	0	4.824987	-2.331362	1.015413
41	1	0	5.786881	-1.870375	1.257820
42	1	0	5.004127	-3.156114	0.319514
43	1	0	4.428530	-2.766051	1.941226

Frequencies --	12.6102	28.9964	43.4104
Frequencies --	48.5593	54.3118	79.3660
Frequencies --	82.1694	100.5467	134.3844

Zero-point correction= 0.373083 (Hartree/Particle)  
 Thermal correction to Energy= 0.394352  
 Thermal correction to Enthalpy= 0.395297  
 Thermal correction to Gibbs Free Energy= 0.321293  
 Sum of electronic and zero-point Energies= -812.396937  
 Sum of electronic and thermal Energies= -812.375668  
 Sum of electronic and thermal Enthalpies= -812.374723  
 Sum of electronic and thermal Free Energies= -812.448727

ss-1-3c4+5-.log



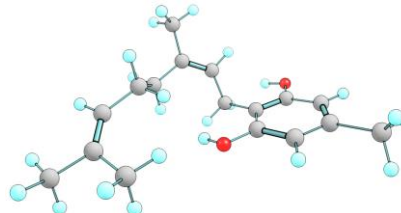
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423293	-0.277218	1.325084
2	6	0	2.460104	0.634630	1.103806
3	6	0	3.213056	0.581683	-0.070216
4	6	0	2.932235	-0.418894	-1.005043
5	6	0	1.902491	-1.331111	-0.770428
6	6	0	1.102993	-1.275218	0.387995
7	1	0	2.658357	1.384120	1.863314
8	1	0	3.509509	-0.511546	-1.919388
9	8	0	0.747211	-0.117926	2.508511
10	1	0	0.059276	-0.789573	2.595605
11	8	0	1.703269	-2.278382	-1.743730
12	1	0	1.145179	-2.991803	-1.408487
13	6	0	-0.065859	-2.236175	0.565223
14	6	0	-1.195663	-1.986165	-0.414836
15	1	0	-0.438481	-2.215250	1.593112
16	1	0	0.289457	-3.270779	0.444255
17	6	0	-2.372556	-1.379929	-0.199128
18	1	0	-0.997306	-2.331268	-1.428698
19	6	0	-2.815290	-0.788713	1.120342
20	1	0	-3.771538	-1.242389	1.414995
21	1	0	-2.105564	-1.026653	1.918255
22	6	0	-3.003252	0.753342	1.072559
23	6	0	-1.728334	1.465110	0.711109
24	1	0	-3.336712	1.073802	2.069084
25	1	0	-3.815868	1.000222	0.384102
26	6	0	-1.465993	2.212315	-0.372288
27	1	0	-0.912827	1.297269	1.413258
28	6	0	-0.087841	2.787720	-0.599368
29	1	0	0.327209	2.430068	-1.551508
30	1	0	-0.121839	3.883258	-0.668549
31	1	0	0.611150	2.507507	0.192439
32	6	0	-3.362427	-1.230776	-1.331375
33	1	0	-4.348678	-1.615011	-1.041427
34	1	0	-3.037239	-1.763399	-2.229052
35	1	0	-3.502788	-0.178095	-1.600618
36	6	0	-2.460285	2.545883	-1.457528
37	1	0	-2.510207	3.631612	-1.610912
38	1	0	-3.471251	2.192678	-1.246305
39	1	0	-2.143288	2.112653	-2.415314
40	6	0	4.291101	1.603767	-0.339495
41	1	0	5.101972	1.181940	-0.940627
42	1	0	4.716896	1.991653	0.590326
43	1	0	3.884102	2.457928	-0.894585

Frequencies --	22.7060	25.7392	39.9542
Frequencies --	60.4068	68.2914	78.0421
Frequencies --	106.7354	134.6668	140.1435

Zero-point correction= 0.373266 (Hartree/Particle)  
 Thermal correction to Energy= 0.394369  
 Thermal correction to Enthalpy= 0.395313  
 Thermal correction to Gibbs Free Energy= 0.323006  
 Sum of electronic and zero-point Energies= -812.400968  
 Sum of electronic and thermal Energies= -812.379865  
 Sum of electronic and thermal Enthalpies= -812.378921  
 Sum of electronic and thermal Free Energies= -812.451227

ss-1-3c4+5a.log



Standard orientation:

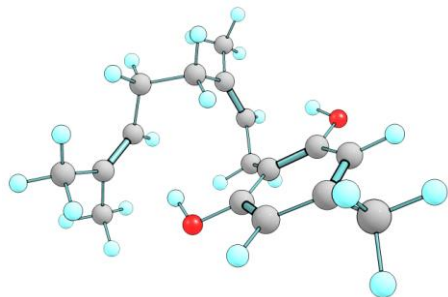
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.345569	-0.966260	-0.284799
2	6	0	2.225192	-1.901482	0.260876
3	6	0	3.574842	-1.580538	0.440430
4	6	0	4.023709	-0.314774	0.060599
5	6	0	3.133884	0.615827	-0.485469
6	6	0	1.775732	0.312981	-0.685379
7	1	0	1.837780	-2.875156	0.543729
8	1	0	5.062283	-0.026313	0.185756
9	8	0	0.040258	-1.371672	-0.405220
10	1	0	-0.484781	-0.697992	-0.855284
11	8	0	3.665979	1.838824	-0.801598
12	1	0	3.002229	2.397641	-1.226285
13	6	0	0.809071	1.356277	-1.222436
14	6	0	0.319946	2.276223	-0.125915
15	1	0	-0.022488	0.881668	-1.752721
16	1	0	1.302965	1.945955	-2.009021
17	6	0	-0.929974	2.436728	0.334365
18	1	0	1.115211	2.845427	0.355880
19	6	0	-2.142862	1.703609	-0.197470
20	1	0	-2.954744	2.427314	-0.352661
21	1	0	-1.949943	1.262106	-1.180639
22	6	0	-2.655285	0.591065	0.754623
23	6	0	-3.914183	-0.047394	0.234186
24	1	0	-2.859587	1.036989	1.737307
25	1	0	-1.857642	-0.140617	0.910573
26	6	0	-4.142346	-1.335964	-0.064362
27	1	0	-4.734081	0.655745	0.074794
28	6	0	-5.486507	-1.780832	-0.591657
29	1	0	-5.381694	-2.256944	-1.575638
30	1	0	-5.936103	-2.534431	0.068490
31	1	0	-6.189662	-0.948681	-0.688155
32	6	0	-1.207072	3.393412	1.471204
33	1	0	-1.933958	4.156991	1.166160
34	1	0	-0.299337	3.899746	1.810431
35	1	0	-1.644602	2.875168	2.332999
36	6	0	-3.141017	-2.454560	0.089511
37	1	0	-3.520804	-3.210234	0.789779
38	1	0	-2.162366	-2.127739	0.441238
39	1	0	-2.996633	-2.970372	-0.868949
40	6	0	4.522039	-2.594086	1.038063
41	1	0	5.543895	-2.209298	1.087193
42	1	0	4.535076	-3.517076	0.447843
43	1	0	4.214654	-2.868496	2.053519

Frequencies --	20.8170	23.8482	38.0217
Frequencies --	44.2363	52.6989	59.4846
Frequencies --	93.2658	107.7240	124.2487

Zero-point correction= 0.372773 (Hartree/Particle)  
 Thermal correction to Energy= 0.394205  
 Thermal correction to Enthalpy= 0.395149  
 Thermal correction to Gibbs Free Energy= 0.320802  
 Sum of electronic and zero-point Energies= -812.399914  
 Sum of electronic and thermal Energies= -812.378482  
 Sum of electronic and thermal Enthalpies= -812.377537  
 Sum of electronic and thermal Free Energies= -812.451885



ss-1-3c4-5+.log



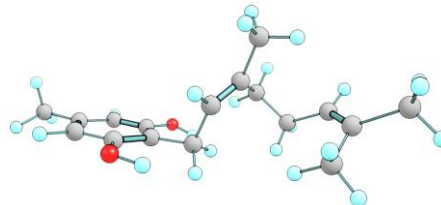
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.102052	-1.136036	0.503917
2	6	0	-2.200436	-1.772656	-0.076551
3	6	0	-3.348307	-1.046074	-0.412471
4	6	0	-3.362709	0.332341	-0.185794
5	6	0	-2.260215	0.962748	0.397806
6	6	0	-1.118844	0.241912	0.791465
7	1	0	-2.135139	-2.838327	-0.273060
8	1	0	-4.219910	0.937768	-0.462923
9	8	0	-0.017033	-1.924456	0.807844
10	1	0	0.804231	-1.422301	0.660786
11	8	0	-2.350041	2.314989	0.603917
12	1	0	-1.449467	2.680907	0.650695
13	6	0	-0.019389	0.931254	1.582271
14	6	0	0.628958	2.160915	0.960705
15	1	0	0.753942	0.204751	1.851841
16	1	0	-0.455549	1.245566	2.538973
17	6	0	1.111678	2.314153	-0.286410
18	1	0	0.750535	2.999565	1.646281
19	6	0	1.114721	1.227790	-1.341884
20	1	0	0.317617	0.504748	-1.160662
21	1	0	0.918996	1.681630	-2.321486
22	6	0	2.465024	0.464282	-1.427631
23	6	0	2.816737	-0.270843	-0.162283
24	1	0	3.265739	1.183010	-1.648707
25	1	0	2.416748	-0.214838	-2.282914
26	6	0	2.939238	-1.599081	0.024554
27	1	0	2.998498	0.374513	0.697095
28	6	0	3.317974	-2.160225	1.376729
29	1	0	2.543814	-2.846332	1.743506
30	1	0	4.244510	-2.743751	1.307463
31	1	0	3.461258	-1.374369	2.123452
32	6	0	1.754155	3.613592	-0.707260
33	1	0	2.780907	3.446815	-1.055507
34	1	0	1.785268	4.343311	0.106085
35	1	0	1.209609	4.057437	-1.550169
36	6	0	2.708609	-2.646363	-1.037721
37	1	0	3.594208	-3.284354	-1.144407
38	1	0	2.470103	-2.227750	-2.016619
39	1	0	1.879391	-3.299254	-0.739634
40	6	0	-4.528090	-1.741444	-1.050390
41	1	0	-5.372246	-1.059903	-1.184009
42	1	0	-4.866051	-2.585974	-0.439940
43	1	0	-4.262729	-2.144716	-2.034537

Frequencies -- 30.1841 49.7727 64.0632  
 Frequencies -- 68.4741 74.6998 82.1699  
 Frequencies -- 95.6864 121.3005 148.0483

Zero-point correction= 0.373683 (Hartree/Particle)  
 Thermal correction to Energy= 0.394447  
 Thermal correction to Enthalpy= 0.395392  
 Thermal correction to Gibbs Free Energy= 0.324740  
 Sum of electronic and zero-point Energies= -812.405139  
 Sum of electronic and thermal Energies= -812.384374  
 Sum of electronic and thermal Enthalpies= -812.383430  
 Sum of electronic and thermal Free Energies= -812.454082

ss-1-3c4-5-.log



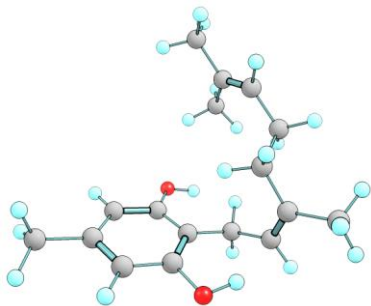
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.417715	-1.041656	-0.480253
2	6	0	3.772306	-1.159922	-0.158243
3	6	0	4.529541	-0.025659	0.145488
4	6	0	3.914139	1.228398	0.103746
5	6	0	2.559429	1.336752	-0.217306
6	6	0	1.774039	0.208255	-0.517681
7	1	0	4.218280	-2.149282	-0.152848
8	1	0	4.470423	2.134379	0.322174
9	8	0	1.760541	-2.218387	-0.743484
10	1	0	0.918080	-2.038447	-1.180116
11	8	0	2.035309	2.604210	-0.203678
12	1	0	1.136372	2.600483	-0.557421
13	6	0	0.280469	0.345522	-0.765758
14	6	0	-0.485669	0.523502	0.527536
15	1	0	-0.105074	-0.505037	-1.334164
16	1	0	0.086811	1.200725	-1.430952
17	6	0	-1.364795	-0.327902	1.074517
18	1	0	-0.251244	1.440461	1.067558
19	6	0	-1.765830	-1.645062	0.433035
20	1	0	-0.883327	-2.163327	0.041116
21	1	0	-2.182016	-2.306505	1.201925
22	6	0	-2.807767	-1.488218	-0.705811
23	6	0	-4.118849	-0.920876	-0.231216
24	1	0	-2.982155	-2.479906	-1.143999
25	1	0	-2.377542	-0.869579	-1.498532
26	6	0	-4.582679	0.328463	-0.392126
27	1	0	-4.735313	-1.616982	0.339757
28	6	0	-5.920227	0.740739	0.174726
29	1	0	-5.804629	1.573627	0.880875
30	1	0	-6.589014	1.099867	-0.618779
31	1	0	-6.419080	-0.081362	0.695866
32	6	0	-2.042576	-0.007522	2.383315
33	1	0	-3.131229	-0.006596	2.253471
34	1	0	-1.739515	0.966042	2.779528
35	1	0	-1.814801	-0.772430	3.137153
36	6	0	-3.851338	1.431044	-1.117942
37	1	0	-4.459299	1.818625	-1.945817
38	1	0	-2.883994	1.121559	-1.515633
39	1	0	-3.675465	2.275575	-0.439475
40	6	0	5.983429	-0.153660	0.534313
41	1	0	6.559070	0.722848	0.222627
42	1	0	6.440292	-1.041838	0.088469
43	1	0	6.089544	-0.242677	1.622464

Frequencies -- 17.5667 31.2623 37.4448  
 Frequencies -- 44.2690 54.3989 57.1635  
 Frequencies -- 83.5784 115.1340 134.1171

Zero-point correction= 0.372960 (Hartree/Particle)  
 Thermal correction to Energy= 0.394258  
 Thermal correction to Enthalpy= 0.395202  
 Thermal correction to Gibbs Free Energy= 0.321337  
 Sum of electronic and zero-point Energies= -812.397791  
 Sum of electronic and thermal Energies= -812.376493  
 Sum of electronic and thermal Enthalpies= -812.375549  
 Sum of electronic and thermal Free Energies= -812.449414

ss-1-3c4-5a.log



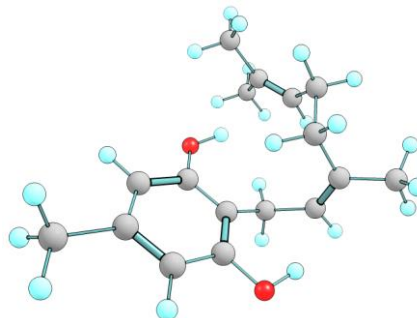
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.444251	-0.972674	1.038167
2	6	0	-2.370888	-1.761533	0.352713
3	6	0	-3.218218	-1.188592	-0.597894
4	6	0	-3.115750	0.180946	-0.847850
5	6	0	-2.183188	0.967438	-0.162907
6	6	0	-1.314002	0.410951	0.800207
7	1	0	-2.420690	-2.820720	0.584425
8	1	0	-3.753546	0.666437	-1.579960
9	8	0	-0.678321	-1.636722	1.963873
10	1	0	-0.099138	-1.019186	2.428377
11	8	0	-2.183402	2.298421	-0.473525
12	1	0	-1.340952	2.689252	-0.175232
13	6	0	-0.312680	1.233940	1.608922
14	6	0	0.283008	2.474702	0.959091
15	1	0	0.531586	0.586447	1.884515
16	1	0	-0.776362	1.532159	2.557106
17	6	0	1.086116	2.484697	-0.122114
18	1	0	0.077862	3.419788	1.460075
19	6	0	1.498978	1.213363	-0.829119
20	1	0	0.743868	0.434536	-0.696433
21	1	0	1.582605	1.393653	-1.907836
22	6	0	2.856095	0.670885	-0.300802
23	6	0	3.180242	-0.667769	-0.905546
24	1	0	2.807091	0.613818	0.790887
25	1	0	3.647222	1.393100	-0.539223
26	6	0	3.055751	-1.872961	-0.327268
27	1	0	3.490109	-0.636784	-1.951055
28	6	0	3.343390	-3.140033	-1.095975
29	1	0	4.144531	-3.717703	-0.616291
30	1	0	2.460395	-3.792900	-1.112795
31	1	0	3.637690	-2.938599	-2.129935
32	6	0	1.673081	3.764674	-0.656934
33	1	0	2.768690	3.709574	-0.672498
34	1	0	1.382467	4.634715	-0.062081
35	1	0	1.355514	3.930089	-1.693828
36	6	0	2.604545	-2.098162	1.095979
37	1	0	1.588676	-2.511723	1.121549
38	1	0	2.601054	-1.185597	1.696000
39	1	0	3.256388	-2.824844	1.596201
40	6	0	-4.196789	-2.041381	-1.369997
41	1	0	-5.081826	-1.468936	-1.662928
42	1	0	-4.523581	-2.905439	-0.784113
43	1	0	-3.738508	-2.425671	-2.289741

Frequencies -- 22.6446 28.1930 44.2415  
 Frequencies -- 47.8939 57.8674 80.2251  
 Frequencies -- 83.8436 105.4740 122.1346

Zero-point correction= 0.372801 (Hartree/Particle)  
 Thermal correction to Energy= 0.394079  
 Thermal correction to Enthalpy= 0.395023  
 Thermal correction to Gibbs Free Energy= 0.321682  
 Sum of electronic and zero-point Energies= -812.401052  
 Sum of electronic and thermal Energies= -812.379774  
 Sum of electronic and thermal Enthalpies= -812.378830  
 Sum of electronic and thermal Free Energies= -812.452171

ss-1-3c4a5+.log



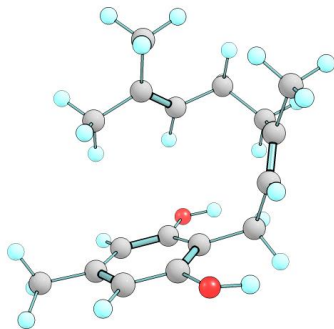
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.102078	-1.136236	0.503764
2	6	0	-2.200723	-1.772761	-0.076438
3	6	0	-3.348540	-1.046121	-0.412152
4	6	0	-3.362850	0.332340	-0.185430
5	6	0	-2.260221	0.962604	0.397936
6	6	0	-1.118759	0.241688	0.791338
7	1	0	-2.135606	-2.838472	-0.272816
8	1	0	-4.220126	0.937771	-0.462303
9	8	0	-0.017172	-1.924799	0.807441
10	1	0	0.804124	-1.422476	0.661187
11	8	0	-2.349854	2.314843	0.604297
12	1	0	-1.449204	2.680617	0.650734
13	6	0	-0.019301	0.930959	1.582213
14	6	0	0.628951	2.160703	0.960726
15	1	0	0.754015	0.204452	1.851792
16	1	0	-0.455508	1.245270	2.538898
17	6	0	1.111578	2.314167	-0.286391
18	1	0	0.750408	2.999331	1.646346
19	6	0	1.114925	1.227909	-1.341982
20	1	0	0.317792	0.504825	-1.161020
21	1	0	0.919454	1.681844	-2.321586
22	6	0	2.465310	0.464466	-1.427509
23	6	0	2.816903	-0.270698	-0.162175
24	1	0	3.265984	1.183261	-1.648493
25	1	0	2.417138	-0.214613	-2.282836
26	6	0	2.939407	-1.598945	0.024574
27	1	0	2.998534	0.374600	0.697265
28	6	0	3.318029	-2.160183	1.376746
29	1	0	2.544164	-2.846826	1.743133
30	1	0	4.244930	-2.743146	1.307610
31	1	0	3.460656	-1.374423	2.123695
32	6	0	1.753657	3.613814	-0.707246
33	1	0	2.780143	3.447191	-1.056335
34	1	0	1.785306	4.343286	0.106299
35	1	0	1.208424	4.057874	-1.549597
36	6	0	2.708866	-2.646136	-1.037783
37	1	0	3.594274	-3.284464	-1.144111
38	1	0	2.470948	-2.227462	-2.016794
39	1	0	1.879312	-3.298758	-0.740034
40	6	0	-4.528159	-1.741094	-1.050834
41	1	0	-5.375807	-1.062058	-1.174780
42	1	0	-4.859645	-2.592503	-0.446496
43	1	0	-4.265477	-2.134320	-2.039791

Frequencies -- 30.1923 49.7701 64.0624  
 Frequencies -- 68.4666 74.6905 82.1404  
 Frequencies -- 95.6779 121.2921 148.0207

Zero-point correction= 0.373683 (Hartree/Particle)  
 Thermal correction to Energy= 0.394447  
 Thermal correction to Enthalpy= 0.395391  
 Thermal correction to Gibbs Free Energy= 0.324739  
 Sum of electronic and zero-point Energies= -812.405139  
 Sum of electronic and thermal Energies= -812.384374  
 Sum of electronic and thermal Enthalpies= -812.383430  
 Sum of electronic and thermal Free Energies= -812.454083

ss-1-3c4a5-.log



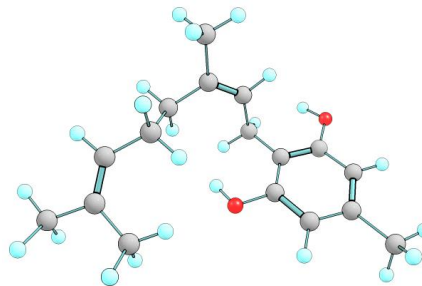
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423324	-0.277080	1.324986
2	6	0	2.460146	0.634744	1.103867
3	6	0	3.213248	0.581808	-0.070100
4	6	0	2.932499	-0.418681	-1.004987
5	6	0	1.902714	-1.330946	-0.770511
6	6	0	1.103127	-1.275094	0.387826
7	1	0	2.658345	1.384227	1.863397
8	1	0	3.509790	-0.511252	-1.919331
9	8	0	0.747113	-0.117868	2.508351
10	1	0	0.059171	-0.789518	2.595326
11	8	0	1.703817	-2.278222	-1.743833
12	1	0	1.144494	-2.990979	-1.409263
13	6	0	-0.065659	-2.236150	0.565035
14	6	0	-1.195619	-1.986167	-0.414862
15	1	0	-0.438180	-2.215393	1.592964
16	1	0	0.289765	-3.270694	0.443897
17	6	0	-2.372559	-1.380078	-0.198992
18	1	0	-0.997444	-2.331199	-1.428794
19	6	0	-2.815187	-0.788916	1.120530
20	1	0	-3.771375	-1.242648	1.415283
21	1	0	-2.105365	-1.026817	1.918367
22	6	0	-3.003280	0.753144	1.072757
23	6	0	-1.728481	1.464999	0.711056
24	1	0	-3.336574	1.073570	2.069345
25	1	0	-3.816052	0.999926	0.384452
26	6	0	-1.466357	2.212116	-0.372453
27	1	0	-0.912862	1.297252	1.413098
28	6	0	-0.088285	2.787617	-0.599794
29	1	0	0.326385	2.430428	-1.552269
30	1	0	-0.122295	3.883193	-0.668441
31	1	0	0.611001	2.507028	0.191621
32	6	0	-3.362540	-1.230901	-1.331145
33	1	0	-4.348835	-1.614876	-1.041016
34	1	0	-3.037572	-1.763736	-2.228775
35	1	0	-3.502695	-0.178230	-1.600538
36	6	0	-2.460888	2.545729	-1.457464
37	1	0	-2.511146	3.631504	-1.610453
38	1	0	-3.471729	2.192171	-1.246232
39	1	0	-2.143886	2.112939	-2.415441
40	6	0	4.291400	1.603865	-0.339087
41	1	0	5.101853	1.182346	-0.941001
42	1	0	4.717801	1.990785	0.590863
43	1	0	3.884350	2.458636	-0.893182

Frequencies --	22.6947	25.8353	39.9485
Frequencies --	59.9999	68.2866	78.0273
Frequencies --	106.7296	134.6768	140.1766

Zero-point correction=	0.373264 (Hartree/Particle)
Thermal correction to Energy=	0.394368
Thermal correction to Enthalpy=	0.395313
Thermal correction to Gibbs Free Energy=	0.323002
Sum of electronic and zero-point Energies=	-812.400969
Sum of electronic and thermal Energies=	-812.379865
Sum of electronic and thermal Enthalpies=	-812.378921
Sum of electronic and thermal Free Energies=	-812.451232

ss-1-3c4a5a.log



Standard orientation:

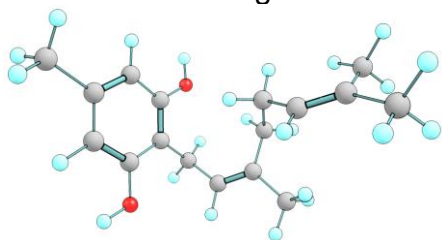
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.345529	-0.966656	-0.285604
2	6	0	2.225132	-1.901885	0.260111
3	6	0	3.574632	-1.580728	0.440365
4	6	0	4.023420	-0.314768	0.061078
5	6	0	3.133631	0.615815	-0.485054
6	6	0	1.775603	0.312797	-0.685564
7	1	0	1.837804	-2.875748	0.542432
8	1	0	5.061902	-0.026163	0.186667
9	8	0	0.040381	-1.372362	-0.406803
10	1	0	-0.484784	-0.698323	-0.856184
11	8	0	3.665592	1.839019	-0.800641
12	1	0	3.002171	2.397453	-1.226343
13	6	0	0.809067	1.356176	-1.222686
14	6	0	0.320166	2.276323	-0.126229
15	1	0	-0.022629	0.881675	-1.752837
16	1	0	1.302993	1.945672	-2.009393
17	6	0	-0.929696	2.436942	0.334154
18	1	0	1.115509	2.845566	0.355381
19	6	0	-2.142667	1.703760	-0.197426
20	1	0	-2.954748	2.427356	-0.352059
21	1	0	-1.950066	1.262577	-1.180801
22	6	0	-2.654481	0.590837	0.754551
23	6	0	-3.913807	-0.047320	0.234766
24	1	0	-2.858037	1.036349	1.737579
25	1	0	-1.856787	-0.140974	0.909633
26	6	0	-4.142371	-1.335790	-0.063907
27	1	0	-4.733693	0.655983	0.076042
28	6	0	-5.486926	-1.780322	-0.590471
29	1	0	-5.382813	-2.256202	-1.574637
30	1	0	-5.936214	-2.534019	0.069774
31	1	0	-6.190021	-0.948044	-0.686313
32	6	0	-1.206683	3.393883	1.470800
33	1	0	-1.933223	4.157686	1.165488
34	1	0	-0.298842	3.899937	1.810161
35	1	0	-1.644607	2.875915	2.332559
36	6	0	-3.141133	-2.454583	0.089114
37	1	0	-3.520505	-3.210228	0.789638
38	1	0	-2.162150	-2.127963	0.440106
39	1	0	-2.997593	-2.970367	-0.869487
40	6	0	4.521640	-2.594009	1.038750
41	1	0	5.544593	-2.211480	1.082392
42	1	0	4.530130	-3.519632	0.452633
43	1	0	4.217495	-2.863119	2.056622

Frequencies --	20.9647	23.9840	41.8089
Frequencies --	44.6317	53.0046	59.5329
Frequencies --	93.2743	107.7085	124.2463

Zero-point correction=	0.372784 (Hartree/Particle)
Thermal correction to Energy=	0.394206
Thermal correction to Enthalpy=	0.395150
Thermal correction to Gibbs Free Energy=	0.320919
Sum of electronic and zero-point Energies=	-812.399902
Sum of electronic and thermal Energies=	-812.378480
Sum of electronic and thermal Enthalpies=	-812.377536
Sum of electronic and thermal Free Energies=	-812.451767

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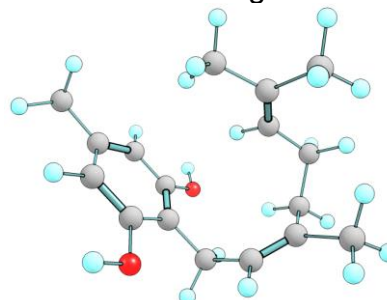
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.651588	-0.750480	0.728953
2	6	0	-3.306873	0.405057	1.165034
3	6	0	-3.240636	1.578427	0.406674
4	6	0	-2.516088	1.568673	-0.787891
5	6	0	-1.869864	0.401698	-1.214853
6	6	0	-1.911622	-0.781412	-0.463175
7	1	0	-3.864698	0.387557	2.098372
8	1	0	-2.452773	2.468512	-1.395351
9	8	0	-2.692906	-1.917203	1.446505
10	1	0	-3.231432	-1.785409	2.238853
11	8	0	-1.160686	0.372739	-2.388830
12	1	0	-1.157866	1.256616	-2.780375
13	6	0	-1.177529	-2.040294	-0.887893
14	6	0	-0.007408	-2.398352	0.009978
15	1	0	-0.846804	-1.918484	-1.921417
16	1	0	-1.886379	-2.876156	-0.874869
17	6	0	1.252757	-1.944397	-0.084853
18	1	0	-0.243811	-3.084729	0.820902
19	6	0	1.699520	-0.933475	-1.120930
20	1	0	2.729006	-1.156565	-1.429430
21	1	0	1.069850	-0.996438	-2.013106
22	6	0	1.648112	0.544370	-0.634950
23	6	0	2.558158	0.869526	0.523424
24	1	0	0.616260	0.771722	-0.353162
25	1	0	1.879736	1.181083	-1.496706
26	6	0	3.847001	1.240431	0.461712
27	1	0	2.113464	0.766095	1.513398
28	6	0	4.645437	1.518217	1.712105
29	1	0	5.517106	0.853189	1.776213
30	1	0	5.039718	2.543282	1.707890
31	1	0	4.048910	1.385498	2.619322
32	6	0	2.320307	-2.429829	0.868095
33	1	0	3.121496	-2.941832	0.318041
34	1	0	1.920972	-3.124266	1.613445
35	1	0	2.796481	-1.593069	1.390821
36	6	0	4.619330	1.401563	-0.824463
37	1	0	5.043524	2.411438	-0.899329
38	1	0	4.015597	1.218197	-1.715413
39	1	0	5.469644	0.707397	-0.848328
40	6	0	-3.969961	2.823266	0.853811
41	1	0	-3.477633	3.728588	0.487052
42	1	0	-4.027526	2.882441	1.944684
43	1	0	-4.998428	2.833114	0.472433

Frequencies -- 17.5299 33.5680 36.8641  
 Frequencies -- 45.4124 56.3702 73.2879  
 Frequencies -- 78.5951 106.2842 130.0438

Zero-point correction= 0.373159 (Hartree/Particle)  
 Thermal correction to Energy= 0.394484  
 Thermal correction to Enthalpy= 0.395428  
 Thermal correction to Gibbs Free Energy= 0.321630  
 Sum of electronic and zero-point Energies= -812.399753  
 Sum of electronic and thermal Energies= -812.378429  
 Sum of electronic and thermal Enthalpies= -812.377484  
 Sum of electronic and thermal Free Energies= -812.451283

# b-aa-1a3c4+5-.log



Standard orientation:

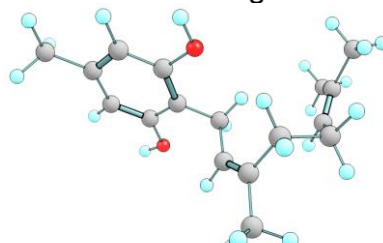
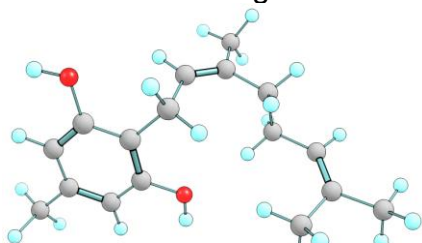
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	1.732740	-1.222821	-0.969021
2	6	0	2.774568	-0.295899	-1.074185
3	6	0	3.118738	0.500150	0.022588
4	6	0	2.414337	0.340190	1.218609
5	6	0	1.371003	-0.589535	1.306032
6	6	0	0.999585	-1.388401	0.216392
7	1	0	3.313532	-0.195938	-2.013345
8	1	0	2.670293	0.942258	2.087181
9	8	0	1.373311	-2.024642	-2.020429
10	1	0	1.939167	-1.828777	-2.779735
11	8	0	0.660827	-0.748147	2.470300
12	1	0	0.988689	-0.123526	3.131493
13	6	0	-0.147773	-2.380193	0.290288
14	6	0	-1.338848	-1.990024	-0.564596
15	1	0	-0.439056	-2.504790	1.334029
16	1	0	0.215106	-3.354701	-0.058111
17	6	0	-2.418566	-1.283374	-0.196654
18	1	0	-1.273379	-2.314638	-1.601442
19	6	0	-2.638554	-0.719963	1.190749
20	1	0	-3.575198	-1.128023	1.598305
21	1	0	-1.832958	-1.021784	1.864542
22	6	0	-2.739142	0.830236	1.226236
23	6	0	-1.465757	1.487352	0.770645
24	1	0	-2.947164	1.120538	2.265777
25	1	0	-3.600436	1.161952	0.639535
26	6	0	-1.263204	2.288117	-0.286611
27	1	0	-0.597551	1.224071	1.372299
28	6	0	0.120844	2.797664	-0.614267
29	1	0	0.422481	2.479626	-1.621535
30	1	0	0.149628	3.895710	-0.615133
31	1	0	0.870465	2.427846	0.089938
32	6	0	-3.516075	-0.995244	-1.195477
33	1	0	-4.495066	-1.298189	-0.801191
34	1	0	-3.351875	-1.518500	-2.141689
35	1	0	-3.587689	0.076224	-1.415669
36	6	0	-2.334967	2.748009	-1.244320
37	1	0	-2.336418	3.843091	-1.322165
38	1	0	-3.339792	2.432911	-0.957125
39	1	0	-2.136810	2.367144	-2.255003
40	6	0	4.202504	1.544613	-0.097213
41	1	0	4.687856	1.731470	0.865097
42	1	0	3.784488	2.498046	-0.443328
43	1	0	4.969990	1.245026	-0.816856

Frequencies -- 28.7095 36.4418 42.6487  
 Frequencies -- 67.3777 70.8291 79.3333  
 Frequencies -- 96.9463 126.5120 141.1476

Zero-point correction= 0.373542 (Hartree/Particle)  
 Thermal correction to Energy= 0.394571  
 Thermal correction to Enthalpy= 0.395516  
 Thermal correction to Gibbs Free Energy= 0.323959  
 Sum of electronic and zero-point Energies= -812.405014  
 Sum of electronic and thermal Energies= -812.383985  
 Sum of electronic and thermal Enthalpies= -812.383041  
 Sum of electronic and thermal Free Energies= -812.454598

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Standard orientation:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.030749	0.661927	-0.652861
2	6	0	4.094442	-0.080037	-0.129304
3	6	0	3.856569	-1.318022	0.475873
4	6	0	2.543633	-1.791009	0.550967
5	6	0	1.490280	-1.036005	0.022816
6	6	0	1.705741	0.201108	-0.600623
7	1	0	5.106636	0.312425	-0.191850
8	1	0	2.333787	-2.747378	1.023831
9	8	0	3.226320	1.884603	-1.241166
10	1	0	4.169829	2.096492	-1.231880
11	8	0	0.193906	-1.479317	0.092169
12	1	0	0.166175	-2.335644	0.540203
13	6	0	0.567410	1.038920	-1.150729
14	6	0	0.146583	2.111824	-0.170540
15	1	0	-0.269215	0.387651	-1.407344
16	1	0	0.909854	1.514348	-2.078846
17	6	0	-1.086743	2.364218	0.292289
18	1	0	0.969187	2.728444	0.191420
19	6	0	-2.322985	1.586249	-0.109786
20	1	0	-3.180143	2.271598	-0.151524
21	1	0	-2.221651	1.161804	-1.113402
22	6	0	-2.654870	0.431672	0.872655
23	6	0	-3.981044	-0.211901	0.562851
24	1	0	-2.683247	0.834336	1.893635
25	1	0	-1.832728	-0.287814	0.841862
26	6	0	-4.204841	-1.331932	-0.142387
27	1	0	-4.852769	0.333330	0.928836
28	6	0	-5.608177	-1.833873	-0.386162
29	1	0	-5.820957	-1.897692	-1.461684
30	1	0	-5.736211	-2.849184	0.012924
31	1	0	-6.363562	-1.189833	0.073458
32	6	0	-1.325591	3.462675	1.302064
33	1	0	-1.996434	4.230511	0.894374
34	1	0	-0.395626	3.949397	1.609865
35	1	0	-1.816872	3.071799	2.202664
36	6	0	-3.121727	-2.187307	-0.753590
37	1	0	-3.147247	-3.202003	-0.333282
38	1	0	-2.117735	-1.784971	-0.614113
39	1	0	-3.293573	-2.300078	-1.832197
40	6	0	5.002901	-2.143489	1.010398
41	1	0	4.678869	-2.799666	1.823339
42	1	0	5.812263	-1.509218	1.383878
43	1	0	5.425577	-2.781054	0.224220

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.488327	0.294945	1.195546
2	6	0	-3.817103	0.056131	0.835526
3	6	0	-4.112727	-0.599893	-0.365254
4	6	0	-3.060689	-1.006546	-1.188481
5	6	0	-1.733095	-0.759605	-0.813364
6	6	0	-1.414272	-0.111977	0.387248
7	1	0	-4.620691	0.385117	1.490304
8	1	0	-3.266844	-1.515823	-2.126857
9	8	0	-2.160870	0.940943	2.359987
10	1	0	-2.970438	1.161165	2.840978
11	8	0	-0.684795	-1.149839	-1.607324
12	1	0	-1.028252	-1.589857	-2.396704
13	6	0	0.020704	0.175923	0.783560
14	6	0	0.419042	1.603556	0.479805
15	1	0	0.688763	-0.529789	0.290511
16	1	0	0.123865	0.010423	1.862804
17	6	0	1.285932	2.029647	-0.451297
18	1	0	-0.085310	2.348677	1.094818
19	6	0	2.041222	1.113223	-1.394717
20	1	0	1.481216	0.190767	-1.569975
21	1	0	2.134809	1.615117	-2.367234
22	6	0	3.468988	0.748350	-0.902505
23	6	0	3.453337	-0.052457	0.371137
24	1	0	4.035785	1.675450	-0.740119
25	1	0	3.983485	0.211280	-1.705287
26	6	0	3.693911	-1.363442	0.529778
27	1	0	3.156702	0.512189	1.254667
28	6	0	3.576676	-2.014611	1.887421
29	1	0	2.821525	-2.811893	1.872845
30	1	0	4.522123	-2.489969	2.181075
31	1	0	3.298302	-1.297675	2.665159
32	6	0	1.588837	3.501071	-0.612566
33	1	0	2.664643	3.695894	-0.512729
34	1	0	1.065428	4.114200	0.126794
35	1	0	1.304580	3.852582	-1.613435
36	6	0	4.078179	-2.311174	-0.579848
37	1	0	5.039198	-2.794600	-0.360417
38	1	0	4.157450	-1.828767	-1.555664
39	1	0	3.339032	-3.118690	-0.663539
40	6	0	-5.549322	-0.860597	-0.752891
41	1	0	-5.621167	-1.343717	-1.730802
42	1	0	-6.122854	0.072092	-0.793153
43	1	0	-6.043779	-1.508255	-0.019930

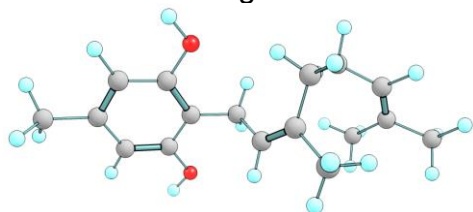
Frequencies -- 17.0119      27.6452      44.6116  
 Frequencies -- 47.5104      58.5809      60.8764  
 Frequencies -- 75.3379      103.4950      127.1853

Frequencies -- 16.0108      21.9752      32.5897  
 Frequencies -- 39.3313      51.9472      55.8540  
 Frequencies -- 66.4534      106.8026      125.6573

Zero-point correction= 0.373059 (Hartree/Particle)  
 Thermal correction to Energy= 0.394438  
 Thermal correction to Enthalpy= 0.395382  
 Thermal correction to Gibbs Free Energy= 0.321238  
 Sum of electronic and zero-point Energies= -812.402964  
 Sum of electronic and thermal Energies= -812.381585  
 Sum of electronic and thermal Enthalpies= -812.380641  
 Sum of electronic and thermal Free Energies= -812.454786

Zero-point correction= 0.372878 (Hartree/Particle)  
 Thermal correction to Energy= 0.394358  
 Thermal correction to Enthalpy= 0.395302  
 Thermal correction to Gibbs Free Energy= 0.320112  
 Sum of electronic and zero-point Energies= -812.401802  
 Sum of electronic and thermal Energies= -812.380322  
 Sum of electronic and thermal Enthalpies= -812.379378  
 Sum of electronic and thermal Free Energies= -812.454568

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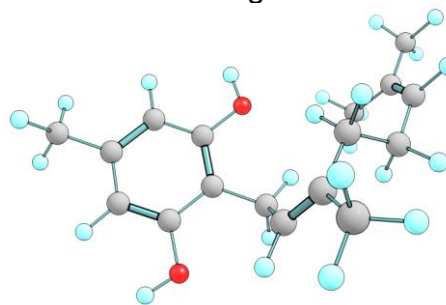
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.589555	1.343012	-0.185934
2	6	0	3.956027	1.216050	0.085665
3	6	0	4.552901	-0.048319	0.107691
4	6	0	3.763796	-1.172899	-0.151195
5	6	0	2.398025	-1.029492	-0.421526
6	6	0	1.780389	0.229203	-0.455487
7	1	0	4.550572	2.104955	0.282721
8	1	0	4.207885	-2.165492	-0.141810
9	8	0	1.968886	2.565418	-0.205830
10	1	0	2.618833	3.256529	-0.018341
11	8	0	1.602865	-2.117286	-0.677372
12	1	0	2.138044	-2.921454	-0.635806
13	6	0	0.296133	0.382950	-0.726121
14	6	0	-0.495403	0.511549	0.556409
15	1	0	-0.049509	-0.463580	-1.320624
16	1	0	0.142799	1.286441	-1.328381
17	6	0	-1.391260	-0.358223	1.045945
18	1	0	-0.274343	1.410670	1.131189
19	6	0	-1.777183	-1.643021	0.333271
20	1	0	-0.887304	-2.119047	-0.091533
21	1	0	-2.193881	-2.349277	1.062411
22	6	0	-2.815234	-1.430103	-0.800969
23	6	0	-4.140811	-0.909116	-0.313263
24	1	0	-2.974127	-2.395452	-1.300775
25	1	0	-2.382503	-0.760963	-1.550293
26	6	0	-4.614907	0.344105	-0.394657
27	1	0	-4.761915	-1.648951	0.194819
28	6	0	-5.968226	0.703575	0.170859
29	1	0	-5.875285	1.477730	0.944221
30	1	0	-6.621088	1.121807	-0.606957
31	1	0	-6.473723	-0.160040	0.612579
32	6	0	-2.100858	-0.091892	2.351069
33	1	0	-3.186765	-0.081825	2.199264
34	1	0	-1.804433	0.863554	2.794566
35	1	0	-1.892688	-0.887436	3.079248
36	6	0	-3.878973	1.501139	-1.025092
37	1	0	-4.458910	1.923160	-1.856575
38	1	0	-2.887459	1.233930	-1.392671
39	1	0	-3.751818	2.309806	-0.293908
40	6	0	6.018766	-0.199023	0.439801
41	1	0	6.165926	-0.309675	1.521166
42	1	0	6.592694	0.676196	0.121500
43	1	0	6.448575	-1.083604	-0.039194

Frequencies -- 15.1760 19.1004 34.6814  
 Frequencies -- 41.8599 50.3521 60.3542  
 Frequencies -- 80.6909 112.2697 128.4631

Zero-point correction= 0.372990 (Hartree/Particle)  
 Thermal correction to Energy= 0.394355  
 Thermal correction to Enthalpy= 0.395299  
 Thermal correction to Gibbs Free Energy= 0.320566  
 Sum of electronic and zero-point Energies= -812.401883  
 Sum of electronic and thermal Energies= -812.380518  
 Sum of electronic and thermal Enthalpies= -812.379574  
 Sum of electronic and thermal Free Energies= -812.454307

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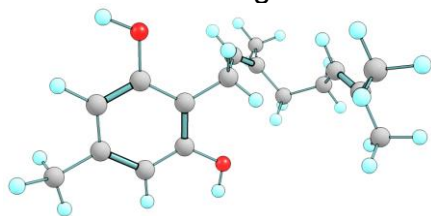
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.860517	0.644763	0.754037
2	6	0	-3.998603	0.001121	0.258569
3	6	0	-3.873170	-1.191844	-0.460634
4	6	0	-2.598064	-1.726622	-0.662985
5	6	0	-1.467954	-1.070926	-0.159501
6	6	0	-1.569976	0.128215	0.560065
7	1	0	-4.980859	0.433418	0.433770
8	1	0	-2.477576	-2.656079	-1.214424
9	8	0	-2.944754	1.815872	1.461803
10	1	0	-3.873204	2.074142	1.542600
11	8	0	-0.208404	-1.584322	-0.344475
12	1	0	-0.266446	-2.402827	-0.855556
13	6	0	-0.350876	0.859624	1.091212
14	6	0	-0.000370	2.085838	0.272914
15	1	0	0.489327	0.166497	1.135578
16	1	0	-0.560296	1.179250	2.119182
17	6	0	1.010131	2.201020	-0.601932
18	1	0	-0.664044	2.936434	0.421685
19	6	0	1.977973	1.072875	-0.897598
20	1	0	1.477387	0.104746	-0.819477
21	1	0	2.334054	1.158353	-1.932518
22	6	0	3.208183	1.063788	0.048485
23	6	0	4.121432	-0.100536	-0.237481
24	1	0	2.845232	1.038041	1.081621
25	1	0	3.756957	2.007150	-0.062261
26	6	0	4.034249	-1.331536	0.291540
27	1	0	4.878717	0.070371	-1.003508
28	6	0	4.959165	-2.441732	-0.144644
29	1	0	5.538510	-2.828479	0.704321
30	1	0	4.387722	-3.292448	-0.539858
31	1	0	5.661102	-2.115470	-0.917644
32	6	0	1.271546	3.494434	-1.334879
33	1	0	2.295488	3.846847	-1.152652
34	1	0	0.581489	4.288203	-1.034010
35	1	0	1.182886	3.355063	-2.420506
36	6	0	3.007016	-1.735735	1.322698
37	1	0	2.205182	-2.324677	0.859351
38	1	0	2.535328	-0.881492	1.812759
39	1	0	3.460072	-2.364721	2.098501
40	6	0	-5.093358	-1.871238	-1.035974
41	1	0	-4.929352	-2.944442	-1.168492
42	1	0	-5.346090	-1.454556	-2.018669
43	1	0	-5.967163	-1.734777	-0.391767

Frequencies -- 14.9499 21.5263 41.3450  
 Frequencies -- 49.3413 55.4876 57.7551  
 Frequencies -- 70.4805 98.0272 121.8467

Zero-point correction= 0.372798 (Hartree/Particle)  
 Thermal correction to Energy= 0.394338  
 Thermal correction to Enthalpy= 0.395282  
 Thermal correction to Gibbs Free Energy= 0.320221  
 Sum of electronic and zero-point Energies= -812.401835  
 Sum of electronic and thermal Energies= -812.380295  
 Sum of electronic and thermal Enthalpies= -812.379351  
 Sum of electronic and thermal Free Energies= -812.454412

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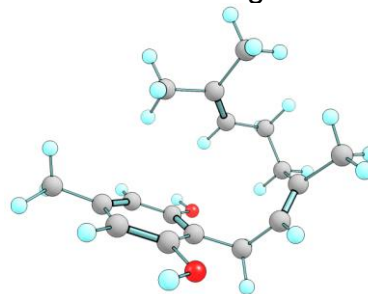
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.488285	0.294877	1.195597
2	6	0	-3.817070	0.056140	0.835576
3	6	0	-4.112731	-0.599786	-0.365255
4	6	0	-3.060720	-1.006421	-1.188518
5	6	0	-1.733110	-0.759555	-0.813396
6	6	0	-1.414247	-0.112035	0.387262
7	1	0	-4.620644	0.385111	1.490378
8	1	0	-3.266903	-1.515607	-2.126936
9	8	0	-2.160781	0.940793	2.360068
10	1	0	-2.970331	1.160877	2.841151
11	8	0	-0.684839	-1.149766	-1.607407
12	1	0	-1.028335	-1.589533	-2.396910
13	6	0	0.020743	0.175809	0.783588
14	6	0	0.419098	1.603448	0.479872
15	1	0	0.688782	-0.529893	0.290501
16	1	0	0.123896	0.010273	1.862825
17	6	0	1.285965	2.029568	-0.451236
18	1	0	-0.085256	2.348551	1.094907
19	6	0	2.041274	1.113187	-1.394681
20	1	0	1.481317	0.190700	-1.569912
21	1	0	2.134831	1.615089	-2.367196
22	6	0	3.469074	0.748406	-0.902487
23	6	0	3.453507	-0.052393	0.371158
24	1	0	4.035798	1.675549	-0.740118
25	1	0	3.983572	0.211358	-1.705283
26	6	0	3.693923	-1.363414	0.529738
27	1	0	3.157076	0.512280	1.254739
28	6	0	3.576772	-2.014612	1.887381
29	1	0	2.821595	-2.811871	1.872856
30	1	0	4.522234	-2.489995	2.180937
31	1	0	3.298484	-1.297677	2.665150
32	6	0	1.588785	3.501012	-0.612551
33	1	0	2.664607	3.695875	-0.513011
34	1	0	1.065547	4.114112	0.126954
35	1	0	1.304226	3.852515	-1.613339
36	6	0	4.077759	-2.311198	-0.579996
37	1	0	5.038341	-2.795415	-0.360420
38	1	0	4.157647	-1.828629	-1.555684
39	1	0	3.337991	-3.118110	-0.664055
40	6	0	-5.549344	-0.860435	-0.752880
41	1	0	-5.621227	-1.343246	-1.730941
42	1	0	-6.122922	0.072239	-0.792800
43	1	0	-6.043715	-1.508359	-0.020096

Frequencies -- 16.0252            21.9780            32.5826  
 Frequencies -- 39.6579            51.9569            55.8859  
 Frequencies -- 66.4497            106.8036            125.6576

Zero-point correction=            0.372879 (Hartree/Particle)  
 Thermal correction to Energy=    0.394358  
 Thermal correction to Enthalpy= 0.395302  
 Thermal correction to Gibbs Free Energy= 0.320121  
 Sum of electronic and zero-point Energies= -812.401801  
 Sum of electronic and thermal Energies= -812.380322  
 Sum of electronic and thermal Enthalpies= -812.379378  
 Sum of electronic and thermal Free Energies= -812.454559

b-aa-1a3c4a5-.log



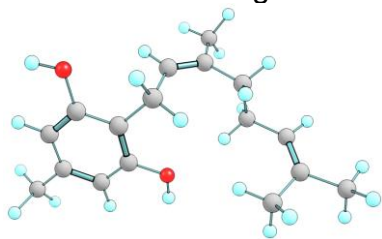
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	1.732670	-1.222740	-0.969125
2	6	0	2.774523	-0.295822	-1.074203
3	6	0	3.118712	0.500096	0.022644
4	6	0	2.414311	0.340033	1.218668
5	6	0	1.370966	-0.589677	1.306002
6	6	0	0.999548	-1.388451	0.216281
7	1	0	3.313455	-0.195749	-2.013371
8	1	0	2.670313	0.942005	2.087291
9	8	0	1.373192	-2.024415	-2.020620
10	1	0	1.939011	-1.828457	-2.779924
11	8	0	0.660733	-0.748373	2.470225
12	1	0	0.988518	-0.123759	3.131460
13	6	0	-0.147786	-2.380279	0.290112
14	6	0	-1.338922	-1.990062	-0.564677
15	1	0	-0.439019	-2.505019	1.333849
16	1	0	0.215120	-3.354720	-0.058437
17	6	0	-2.418583	-1.283378	-0.196637
18	1	0	-1.273549	-2.314660	-1.601537
19	6	0	-2.638443	-0.719967	1.190793
20	1	0	-3.575058	-1.128012	1.598433
21	1	0	-1.832781	-1.021768	1.864507
22	6	0	-2.739018	0.830226	1.226264
23	6	0	-1.465635	1.487306	0.770623
24	1	0	-2.947020	1.120561	2.265800
25	1	0	-3.600313	1.161940	0.639560
26	6	0	-1.263115	2.288162	-0.286570
27	1	0	-0.597406	1.223955	1.372214
28	6	0	0.120936	2.797727	-0.614215
29	1	0	0.422508	2.479851	-1.621555
30	1	0	0.149743	3.895773	-0.614903
31	1	0	0.870577	2.427785	0.089909
32	6	0	-3.516131	-0.995105	-1.195379
33	1	0	-4.495146	-1.297818	-0.800982
34	1	0	-3.352126	-1.518455	-2.141574
35	1	0	-3.587535	0.076365	-1.415627
36	6	0	-2.334920	2.748160	-1.244169
37	1	0	-2.336396	3.843255	-1.321858
38	1	0	-3.339725	2.433003	-0.956961
39	1	0	-2.136802	2.367445	-2.254916
40	6	0	4.202523	1.544525	-0.097029
41	1	0	4.686909	1.732287	0.865586
42	1	0	3.784762	2.497601	-0.444432
43	1	0	4.970741	1.244366	-0.815662

Frequencies -- 28.7025            36.4567            42.6549  
 Frequencies -- 67.4411            70.8945            79.3509  
 Frequencies -- 96.9457            126.5157            141.1566

Zero-point correction=            0.373543 (Hartree/Particle)  
 Thermal correction to Energy=    0.394572  
 Thermal correction to Enthalpy= 0.395516  
 Thermal correction to Gibbs Free Energy= 0.323962  
 Sum of electronic and zero-point Energies= -812.405014  
 Sum of electronic and thermal Energies= -812.383985  
 Sum of electronic and thermal Enthalpies= -812.383041  
 Sum of electronic and thermal Free Energies= -812.454595

b-aa-1a3c4a5a.log



Standard orientation:

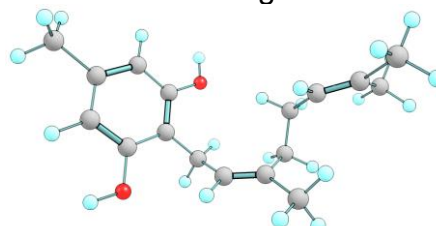
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	3.030844	0.661881	-0.652898
2	6	0	4.094401	-0.080165	-0.129182
3	6	0	3.856356	-1.318168	0.475917
4	6	0	2.543389	-1.791108	0.550745
5	6	0	1.490160	-1.036001	0.022471
6	6	0	1.705790	0.201137	-0.600875
7	1	0	5.106636	0.312221	-0.191620
8	1	0	2.333403	-2.747515	1.023475
9	8	0	3.226590	1.884550	-1.241151
10	1	0	4.170091	2.096457	-1.231559
11	8	0	0.193746	-1.479250	0.091663
12	1	0	0.165913	-2.335562	0.539715
13	6	0	0.567559	1.039097	-1.150979
14	6	0	0.146700	2.111827	-0.170590
15	1	0	-0.269078	0.387934	-1.407824
16	1	0	0.910128	1.514746	-2.078926
17	6	0	-1.086618	2.364113	0.292317
18	1	0	0.969296	2.728402	0.191475
19	6	0	-2.322860	1.586151	-0.109764
20	1	0	-3.179958	2.271557	-0.151755
21	1	0	-2.221399	1.161450	-1.113255
22	6	0	-2.654958	0.431793	0.872887
23	6	0	-3.981125	-0.211776	0.562986
24	1	0	-2.683485	0.834640	1.893783
25	1	0	-1.832856	-0.287745	0.842316
26	6	0	-4.204807	-1.331793	-0.142300
27	1	0	-4.852880	0.333439	0.928915
28	6	0	-5.608114	-1.833761	-0.386330
29	1	0	-5.820830	-1.897133	-1.461892
30	1	0	-5.736070	-2.849240	0.012336
31	1	0	-6.363563	-1.189959	0.073519
32	6	0	-1.325445	3.462431	1.302285
33	1	0	-1.996429	4.230224	0.894759
34	1	0	-0.395480	3.949221	1.609983
35	1	0	-1.816527	3.071396	2.202918
36	6	0	-3.121610	-2.187132	-0.753428
37	1	0	-3.146957	-3.201729	-0.332878
38	1	0	-2.117667	-1.784604	-0.614124
39	1	0	-3.293545	-2.300146	-1.831992
40	6	0	5.002532	-2.143586	1.010911
41	1	0	4.678286	-2.799265	1.824173
42	1	0	5.811895	-1.509213	1.384208
43	1	0	5.425211	-2.781606	0.225123

Frequencies -- 17.0596 27.6230 44.6080  
 Frequencies -- 47.5187 58.4138 60.8439  
 Frequencies -- 75.3415 103.5018 127.1725

Zero-point correction= 0.373058 (Hartree/Particle)  
 Thermal correction to Energy= 0.394437  
 Thermal correction to Enthalpy= 0.395381  
 Thermal correction to Gibbs Free Energy= 0.321235  
 Sum of electronic and zero-point Energies= -812.402966  
 Sum of electronic and thermal Energies= -812.381586  
 Sum of electronic and thermal Enthalpies= -812.380642  
 Sum of electronic and thermal Free Energies= -812.454789

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Standard orientation:

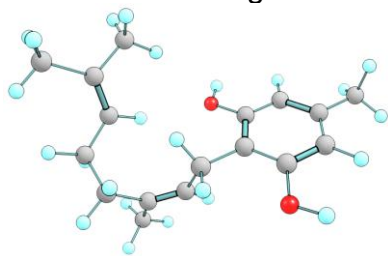
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2	6	0	4.007470	0.078729	0.707934
3	6	0	3.935383	-1.284754	0.406295
4	6	0	2.877874	-1.745267	-0.382443
5	6	0	1.905488	-0.854517	-0.852810
6	6	0	1.953402	0.515686	-0.557947
7	1	0	4.824905	0.462656	1.313796
8	1	0	2.806522	-2.799918	-0.637513
9	8	0	3.068110	2.297640	0.509071
10	1	0	3.845580	2.487813	1.051733
11	8	0	0.869477	-1.287492	-1.640338
12	1	0	0.929349	-2.245978	-1.752580
13	6	0	0.894283	1.490964	-1.038135
14	6	0	-0.044754	1.898049	0.076779
15	1	0	0.351288	1.051597	-1.875354
16	1	0	1.402932	2.389256	-1.413635
17	6	0	-1.384433	1.831922	0.088316
18	1	0	0.459928	2.293150	0.957583
19	6	0	-2.217274	1.298379	-1.064220
20	1	0	-3.211289	1.761032	-1.028998
21	1	0	-1.774496	1.584750	-2.024775
22	6	0	-2.395500	-0.245471	-1.058689
23	6	0	-2.981106	-0.789953	0.217628
24	1	0	-1.410482	-0.697695	-1.215594
25	1	0	-3.011849	-0.518094	-1.922396
26	6	0	-4.252132	-1.149597	0.457933
27	1	0	-2.273799	-0.872846	1.043506
28	6	0	-4.674430	-1.666718	1.812446
29	1	0	-5.457899	-1.031798	2.247313
30	1	0	-5.103747	-2.674474	1.732703
31	1	0	-3.838579	-1.706855	2.516899
32	6	0	-2.169764	2.299005	1.292052
33	1	0	-2.821574	3.142279	1.026629
34	1	0	-1.518340	2.616401	2.111870
35	1	0	-2.829186	1.503995	1.659809
36	6	0	-5.369080	-1.075530	-0.554304
37	1	0	-5.822978	-2.064053	-0.704107
38	1	0	-5.048178	-0.698355	-1.527059
39	1	0	-6.170982	-0.420894	-0.188659
40	6	0	4.965945	-2.246792	0.948420
41	1	0	5.089781	-3.112297	0.291095
42	1	0	4.668117	-2.625030	1.934051
43	1	0	5.940375	-1.763753	1.066598

Frequencies -- 7.9814 20.1348 35.6910  
 Frequencies -- 40.5196 45.5850 71.7371  
 Frequencies -- 82.3710 98.1719 132.5435

Zero-point correction= 0.372822 (Hartree/Particle)  
 Thermal correction to Energy= 0.394299  
 Thermal correction to Enthalpy= 0.395243  
 Thermal correction to Gibbs Free Energy= 0.319640  
 Sum of electronic and zero-point Energies= -812.400653  
 Sum of electronic and thermal Energies= -812.379176  
 Sum of electronic and thermal Enthalpies= -812.378232  
 Sum of electronic and thermal Free Energies= -812.453835



b-aa-1+3c4+5-.log



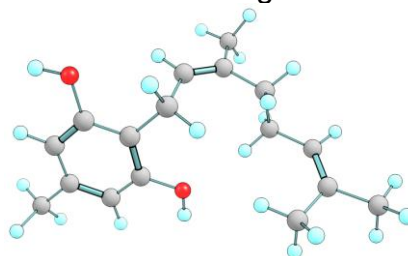
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-2.671801	0.802118	0.975262
2	6	0	-3.922318	0.269944	0.636758
3	6	0	-4.021170	-0.759210	-0.302844
4	6	0	-2.852565	-1.240431	-0.901716
5	6	0	-1.611568	-0.699225	-0.553230
6	6	0	-1.485090	0.325675	0.397717
7	1	0	-4.818675	0.666060	1.107972
8	1	0	-2.904451	-2.034221	-1.643085
9	8	0	-2.555824	1.818917	1.887339
10	1	0	-3.432797	2.038357	2.230483
11	8	0	-0.449737	-1.143429	-1.130997
12	1	0	-0.652217	-1.848948	-1.760483
13	6	0	-0.131164	0.902590	0.745987
14	6	0	0.415642	1.814901	-0.338772
15	1	0	0.570542	0.081361	0.921529
16	1	0	-0.216280	1.452691	1.689692
17	6	0	1.694487	2.184415	-0.499505
18	1	0	-0.324293	2.196245	-1.042292
19	6	0	2.816756	1.741329	0.418428
20	1	0	3.470829	2.602893	0.609206
21	1	0	2.425743	1.424820	1.390599
22	6	0	3.688217	0.593441	-0.161161
23	6	0	2.925161	-0.697818	-0.279217
24	1	0	4.575372	0.479617	0.468680
25	1	0	4.053236	0.898959	-1.152465
26	6	0	3.216517	-1.888104	0.270768
27	1	0	2.006935	-0.625478	-0.860161
28	6	0	2.299008	-3.073737	0.077517
29	1	0	2.804801	-3.880280	-0.470839
30	1	0	2.005387	-3.499247	1.046703
31	1	0	1.388615	-2.800423	-0.461299
32	6	0	2.109101	3.089081	-1.635907
33	1	0	2.548114	4.021347	-1.256474
34	1	0	1.265948	3.347244	-2.283106
35	1	0	2.879507	2.617350	-2.259444
36	6	0	4.438054	-2.184039	1.106639
37	1	0	4.145171	-2.534675	2.105075
38	1	0	5.100175	-1.325403	1.231769
39	1	0	5.022926	-2.996364	0.655144
40	6	0	-5.362303	-1.364051	-0.644779
41	1	0	-5.397387	-1.694229	-1.687277
42	1	0	-6.176130	-0.651377	-0.483379
43	1	0	-5.566359	-2.241482	-0.018956

Frequencies -- 21.5606      38.8250      42.8070  
 Frequencies -- 45.6046      49.9985      69.3290  
 Frequencies -- 91.2376      119.3700      145.2982

Zero-point correction= 0.372781 (Hartree/Particle)  
 Thermal correction to Energy= 0.394159  
 Thermal correction to Enthalpy= 0.395103  
 Thermal correction to Gibbs Free Energy= 0.321580  
 Sum of electronic and zero-point Energies= -812.401455  
 Sum of electronic and thermal Energies= -812.380077  
 Sum of electronic and thermal Enthalpies= -812.379132  
 Sum of electronic and thermal Free Energies= -812.452655

b-aa-1+3c4+5a.log



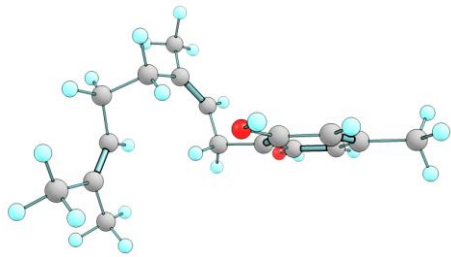
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.030758	0.661739	-0.653820
2	6	0	4.094655	-0.080055	-0.130401
3	6	0	3.856944	-1.317544	0.475849
4	6	0	2.543955	-1.790201	0.552209
5	6	0	1.490409	-1.035379	0.024186
6	6	0	1.705699	0.201208	-0.600380
7	1	0	5.106885	0.312179	-0.193905
8	1	0	2.334238	-2.746165	1.025955
9	8	0	3.226201	1.883994	-1.243034
10	1	0	4.169766	2.095671	-1.234504
11	8	0	0.193975	-1.478316	0.094787
12	1	0	0.166419	-2.334521	0.543068
13	6	0	0.567092	1.038724	-1.150362
14	6	0	0.146112	2.111592	-0.170182
15	1	0	-0.269419	0.387229	-1.406793
16	1	0	0.909271	1.514181	-2.078554
17	6	0	-1.087261	2.363847	0.292618
18	1	0	0.968623	2.728309	0.191846
19	6	0	-2.323415	1.585768	-0.109502
20	1	0	-3.180522	2.271150	-0.151829
21	1	0	-2.221769	1.160864	-1.112889
22	6	0	-2.655731	0.431607	0.873300
23	6	0	-3.981544	-0.212437	0.562829
24	1	0	-2.684918	0.834732	1.894065
25	1	0	-1.833404	-0.287702	0.843392
26	6	0	-4.204535	-1.332214	-0.143065
27	1	0	-4.853657	0.332227	0.928732
28	6	0	-5.607545	-1.834646	-0.387759
29	1	0	-5.819723	-1.898200	-1.463418
30	1	0	-5.735365	-2.850135	0.010939
31	1	0	-6.363432	-1.191055	0.071670
32	6	0	-1.326223	3.462215	1.302479
33	1	0	-1.997321	4.229898	0.894925
34	1	0	-0.396322	3.949150	1.610146
35	1	0	-1.817247	3.071182	2.203153
36	6	0	-3.120784	-2.186709	-0.754387
37	1	0	-3.146413	-3.201849	-0.335167
38	1	0	-2.116961	-1.784325	-0.613771
39	1	0	-3.291830	-2.298367	-1.833242
40	6	0	5.003550	-2.142853	1.010063
41	1	0	4.679936	-2.798766	1.823374
42	1	0	5.813108	-1.508446	1.382891
43	1	0	5.425842	-2.780647	0.223855

Frequencies -- 16.7987      27.6087      44.5120  
 Frequencies -- 47.4371      58.6351      60.8994  
 Frequencies -- 75.2694      103.4805      127.0931

Zero-point correction= 0.373056 (Hartree/Particle)  
 Thermal correction to Energy= 0.394435  
 Thermal correction to Enthalpy= 0.395380  
 Thermal correction to Gibbs Free Energy= 0.321219  
 Sum of electronic and zero-point Energies= -812.402968  
 Sum of electronic and thermal Energies= -812.381588  
 Sum of electronic and thermal Enthalpies= -812.380644  
 Sum of electronic and thermal Free Energies= -812.454804

b-aa-1+3c4-5+.log



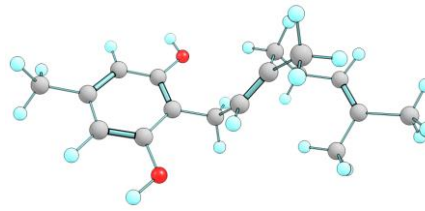
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.488052	0.293760	1.196067
2	6	0	-3.816944	0.055108	0.836348
3	6	0	-4.112938	-0.599884	-0.364908
4	6	0	-3.061166	-1.005993	-1.188742
5	6	0	-1.733453	-0.759234	-0.813917
6	6	0	-1.414258	-0.112484	0.387080
7	1	0	-4.620322	0.383412	1.491731
8	1	0	-3.267648	-1.514697	-2.127361
9	8	0	-2.160209	0.938758	2.360954
10	1	0	-2.969619	1.158424	2.842470
11	8	0	-0.685399	-1.149011	-1.608430
12	1	0	-1.029128	-1.588097	-2.398216
13	6	0	0.020845	0.175054	0.783215
14	6	0	0.419080	1.602889	0.480260
15	1	0	0.688729	-0.530355	0.289496
16	1	0	0.124290	0.008855	1.862324
17	6	0	1.285919	2.029592	-0.450606
18	1	0	-0.085378	2.347600	1.095696
19	6	0	2.041368	1.113754	-1.394459
20	1	0	1.481514	0.191281	-1.570147
21	1	0	2.134878	1.616121	-2.366742
22	6	0	3.469197	0.748895	-0.902406
23	6	0	3.453685	-0.052253	0.371026
24	1	0	4.035896	1.676016	-0.739792
25	1	0	3.983698	0.212079	-1.705359
26	6	0	3.694168	-1.363307	0.529246
27	1	0	3.157242	0.512169	1.254766
28	6	0	3.577075	-2.014855	1.886729
29	1	0	2.822027	-2.812231	1.871980
30	1	0	4.522613	-2.490148	2.180197
31	1	0	3.298640	-1.298139	2.664653
32	6	0	1.588580	3.501152	-0.611155
33	1	0	2.664377	3.696075	-0.511451
34	1	0	1.065228	4.113807	0.128644
35	1	0	1.304026	3.853124	-1.611781
36	6	0	4.077987	-2.310787	-0.580757
37	1	0	5.038368	-2.795379	-0.361145
38	1	0	4.158236	-1.827864	-1.556244
39	1	0	3.337975	-3.117432	-0.665283
40	6	0	-5.549706	-0.858426	-0.753364
41	1	0	-5.620975	-1.357603	-1.723229
42	1	0	-6.117065	0.077140	-0.812102
43	1	0	-6.051064	-1.490012	-0.011228

Frequencies -- 16.1350 21.9760 32.6515  
 Frequencies -- 43.9855 52.0195 55.9109  
 Frequencies -- 66.4558 106.8094 125.6878

Zero-point correction= 0.372890 (Hartree/Particle)  
 Thermal correction to Energy= 0.394359  
 Thermal correction to Enthalpy= 0.395303  
 Thermal correction to Gibbs Free Energy= 0.320230  
 Sum of electronic and zero-point Energies= -812.401790  
 Sum of electronic and thermal Energies= -812.380321  
 Sum of electronic and thermal Enthalpies= -812.379377  
 Sum of electronic and thermal Free Energies= -812.454450

b-aa-1+3c4-5-.log



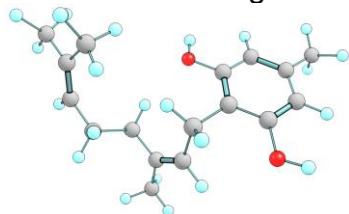
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.589508	1.343018	-0.185895
2	6	0	3.955991	1.216088	0.085676
3	6	0	4.552900	-0.048263	0.107668
4	6	0	3.763821	-1.172861	-0.151233
5	6	0	2.398042	-1.029489	-0.421536
6	6	0	1.780370	0.229192	-0.455460
7	1	0	4.550513	2.105008	0.282744
8	1	0	4.207941	-2.165442	-0.141882
9	8	0	1.968805	2.565409	-0.205740
10	1	0	2.618744	3.256535	-0.018275
11	8	0	1.602905	-2.117298	-0.677394
12	1	0	2.138113	-2.921451	-0.635886
13	6	0	0.296110	0.382904	-0.726082
14	6	0	-0.495415	0.511459	0.556462
15	1	0	-0.049513	-0.463630	-1.320592
16	1	0	0.142749	1.286397	-1.328332
17	6	0	-1.391269	-0.358330	1.045973
18	1	0	-0.274347	1.410562	1.131269
19	6	0	-1.777206	-1.643089	0.333238
20	1	0	-0.887331	-2.119113	-0.091584
21	1	0	-2.193918	-2.349374	1.062342
22	6	0	-2.815250	-1.430106	-0.800996
23	6	0	-4.140797	-0.909066	-0.313268
24	1	0	-2.974187	-2.395441	-1.300818
25	1	0	-2.382491	-0.760973	-1.550311
26	6	0	-4.614857	0.344168	-0.394676
27	1	0	-4.761915	-1.648870	0.194843
28	6	0	-5.968155	0.703688	0.170863
29	1	0	-5.875175	1.477877	0.944186
30	1	0	-6.621034	1.121896	-0.606953
31	1	0	-6.473656	-0.159898	0.612639
32	6	0	-2.100880	-0.092032	2.351097
33	1	0	-3.186785	-0.081906	2.199265
34	1	0	-1.804419	0.863377	2.794650
35	1	0	-1.892769	-0.887625	3.079238
36	6	0	-3.878916	1.501171	-1.025159
37	1	0	-4.458863	1.923171	-1.856646
38	1	0	-2.887412	1.233937	-1.392754
39	1	0	-3.751740	2.309858	-0.294002
40	6	0	6.018770	-0.198944	0.439759
41	1	0	6.165970	-0.309285	1.521152
42	1	0	6.592732	0.676155	0.121184
43	1	0	6.448511	-1.083688	-0.038995

Frequencies -- 15.1888 19.0996 34.6721  
 Frequencies -- 41.8553 50.3490 60.3794  
 Frequencies -- 80.6952 112.2715 128.4619

Zero-point correction= 0.372990 (Hartree/Particle)  
 Thermal correction to Energy= 0.394355  
 Thermal correction to Enthalpy= 0.395299  
 Thermal correction to Gibbs Free Energy= 0.320567  
 Sum of electronic and zero-point Energies= -812.401883  
 Sum of electronic and thermal Energies= -812.380518  
 Sum of electronic and thermal Enthalpies= -812.379574  
 Sum of electronic and thermal Free Energies= -812.454306

b-aa-1+3c4-5a.log



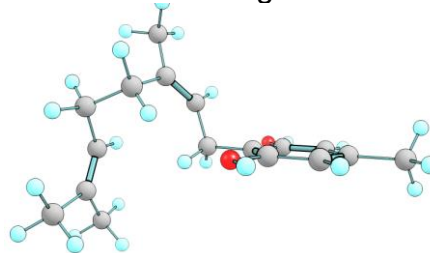
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.860373	0.644822	0.754101
2	6	0	-3.998479	0.001214	0.258669
3	6	0	-3.873076	-1.191717	-0.460630
4	6	0	-2.597994	-1.726454	-0.663112
5	6	0	-1.467841	-1.070786	-0.159646
6	6	0	-1.569828	0.128290	0.560010
7	1	0	-4.980734	0.433470	0.433972
8	1	0	-2.477518	-2.655871	-1.214626
9	8	0	-2.944547	1.815912	1.461904
10	1	0	-3.873024	2.073939	1.543189
11	8	0	-0.208310	-1.584179	-0.344774
12	1	0	-0.266422	-2.402746	-0.855749
13	6	0	-0.350704	0.859670	1.091133
14	6	0	-0.000167	2.085861	0.272815
15	1	0	0.489474	0.166517	1.135494
16	1	0	-0.560095	1.179332	2.119097
17	6	0	1.010402	2.201053	-0.601951
18	1	0	-0.663890	2.936435	0.421516
19	6	0	1.978217	1.072884	-0.897591
20	1	0	1.477597	0.104776	-0.819404
21	1	0	2.334223	1.158290	-1.932546
22	6	0	3.208501	1.063762	0.048393
23	6	0	4.121433	-0.100861	-0.237386
24	1	0	2.845623	1.038340	1.081569
25	1	0	3.757480	2.006970	-0.062618
26	6	0	4.033727	-1.331803	0.291689
27	1	0	4.878842	0.069723	-1.003362
28	6	0	4.958191	-2.442400	-0.144422
29	1	0	5.537374	-2.829341	0.704564
30	1	0	4.386394	-3.292902	-0.539589
31	1	0	5.660262	-2.116477	-0.917446
32	6	0	1.271855	3.494465	-1.334892
33	1	0	2.295775	3.846892	-1.152573
34	1	0	0.581759	4.288223	-1.034082
35	1	0	1.183293	3.355089	-2.420527
36	6	0	3.006242	-1.735524	1.322794
37	1	0	2.203870	-2.323646	0.859338
38	1	0	2.535316	-0.881045	1.813186
39	1	0	3.458855	-2.365122	2.098358
40	6	0	-5.093300	-1.871061	-1.035955
41	1	0	-4.929407	-2.944304	-1.168308
42	1	0	-5.345874	-1.454502	-2.018746
43	1	0	-5.967146	-1.734392	-0.391853

Frequencies -- 14.8548 21.4924 41.3708  
 Frequencies -- 49.3186 55.5067 57.7812  
 Frequencies -- 70.4585 98.0526 121.7778

Zero-point correction= 0.372797 (Hartree/Particle)  
 Thermal correction to Energy= 0.394337  
 Thermal correction to Enthalpy= 0.395281  
 Thermal correction to Gibbs Free Energy= 0.320213  
 Sum of electronic and zero-point Energies= -812.401836  
 Sum of electronic and thermal Energies= -812.380296  
 Sum of electronic and thermal Enthalpies= -812.379352  
 Sum of electronic and thermal Free Energies= -812.454420

b-aa-1+3c4a5+.log



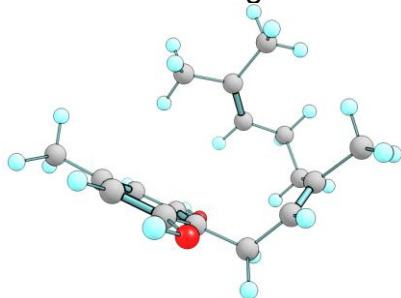
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.488296	0.294807	1.195636
2	6	0	-3.817052	0.055881	0.835664
3	6	0	-4.112662	-0.600126	-0.365145
4	6	0	-3.060619	-1.006809	-1.188329
5	6	0	-1.733023	-0.759756	-0.813250
6	6	0	-1.414217	-0.112076	0.387327
7	1	0	-4.620647	0.384732	1.490501
8	1	0	-3.266760	-1.516160	-2.126666
9	8	0	-2.160830	0.940782	2.360086
10	1	0	-2.970399	1.160809	2.841172
11	8	0	-0.684720	-1.150040	-1.607185
12	1	0	-1.028183	-1.589879	-2.396661
13	6	0	0.020747	0.175846	0.783688
14	6	0	0.419050	1.603485	0.479905
15	1	0	0.688839	-0.529848	0.290661
16	1	0	0.123870	0.010370	1.862937
17	6	0	1.285851	2.029590	-0.451272
18	1	0	-0.085289	2.348604	1.094931
19	6	0	2.041141	1.113192	-1.394718
20	1	0	1.481210	0.190677	-1.569881
21	1	0	2.134641	1.615056	-2.367256
22	6	0	3.468978	0.748487	-0.902570
23	6	0	3.453505	-0.052276	0.371097
24	1	0	4.035663	1.675663	-0.740255
25	1	0	3.983465	0.211442	-1.705375
26	6	0	3.693974	-1.363285	0.529701
27	1	0	3.157101	0.512409	1.254679
28	6	0	3.576916	-2.014451	1.887365
29	1	0	2.821784	-2.811754	1.872894
30	1	0	4.522414	-2.489775	2.180897
31	1	0	3.298617	-1.297513	2.665127
32	6	0	1.588601	3.501037	-0.612685
33	1	0	2.664428	3.695948	-0.513284
34	1	0	1.065427	4.114153	0.126852
35	1	0	1.303910	3.852484	-1.613455
36	6	0	4.077765	-2.311089	-0.580032
37	1	0	5.038292	-2.795399	-0.360428
38	1	0	4.157734	-1.828514	-1.555710
39	1	0	3.337925	-3.117931	-0.664131
40	6	0	-5.549293	-0.859940	-0.753244
41	1	0	-5.620723	-1.351621	-1.726911
42	1	0	-6.119755	0.074197	-0.803301
43	1	0	-6.047315	-1.499181	-0.015376

Frequencies -- 16.0266 21.9868 32.6031  
 Frequencies -- 39.3866 51.9586 55.8862  
 Frequencies -- 66.4548 106.8037 125.6575

Zero-point correction= 0.372879 (Hartree/Particle)  
 Thermal correction to Energy= 0.394358  
 Thermal correction to Enthalpy= 0.395302  
 Thermal correction to Gibbs Free Energy= 0.320116  
 Sum of electronic and zero-point Energies= -812.401802  
 Sum of electronic and thermal Energies= -812.380322  
 Sum of electronic and thermal Enthalpies= -812.379378  
 Sum of electronic and thermal Free Energies= -812.454564

b-aa-1+3c4a5-.log



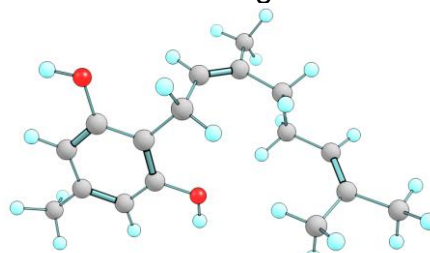
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.732683	-1.222717	-0.969159
2	6	0	2.774409	-0.295683	-1.074284
3	6	0	3.118585	0.500261	0.022562
4	6	0	2.414242	0.340109	1.218587
5	6	0	1.371015	-0.589737	1.305976
6	6	0	0.999613	-1.388513	0.216277
7	1	0	3.313307	-0.195563	-2.013467
8	1	0	2.670236	0.942031	2.087245
9	8	0	1.373233	-2.024449	-2.020622
10	1	0	1.938905	-1.828337	-2.780001
11	8	0	0.660922	-0.748539	2.470275
12	1	0	0.988966	-0.124162	3.131609
13	6	0	-0.147712	-2.380349	0.290128
14	6	0	-1.338804	-1.990091	-0.564678
15	1	0	-0.438949	-2.505079	1.333864
16	1	0	0.215175	-3.354818	-0.058376
17	6	0	-2.418471	-1.283402	-0.196665
18	1	0	-1.273413	-2.314634	-1.601546
19	6	0	-2.638427	-0.720042	1.190762
20	1	0	-3.575036	-1.128147	1.598365
21	1	0	-1.832777	-1.021837	1.864494
22	6	0	-2.739045	0.830145	1.226284
23	6	0	-1.465695	1.487301	0.770667
24	1	0	-2.947000	1.120405	2.265852
25	1	0	-3.600385	1.161915	0.639671
26	6	0	-1.263207	2.288154	-0.286517
27	1	0	-0.597479	1.224078	1.372332
28	6	0	0.120789	2.797910	-0.614072
29	1	0	0.422523	2.479989	-1.621351
30	1	0	0.149441	3.895964	-0.614874
31	1	0	0.870427	2.428158	0.090151
32	6	0	-3.515964	-0.995157	-1.195469
33	1	0	-4.495010	-1.297765	-0.801065
34	1	0	-3.351985	-1.518610	-2.141610
35	1	0	-3.587313	0.076295	-1.415835
36	6	0	-2.335046	2.748098	-1.244093
37	1	0	-2.336922	3.843221	-1.321378
38	1	0	-3.339781	2.432459	-0.957165
39	1	0	-2.136618	2.367832	-2.254949
40	6	0	4.202413	1.544683	-0.097085
41	1	0	4.688193	1.730875	0.865136
42	1	0	3.784411	2.498388	-0.442443
43	1	0	4.969579	1.245433	-0.817214

Frequencies -- 28.6869 36.4086 42.6332  
 Frequencies -- 67.2573 70.6266 79.3396  
 Frequencies -- 96.9453 126.4998 141.1410

Zero-point correction= 0.373541 (Hartree/Particle)  
 Thermal correction to Energy= 0.394571  
 Thermal correction to Enthalpy= 0.395516  
 Thermal correction to Gibbs Free Energy= 0.323953  
 Sum of electronic and zero-point Energies= -812.405016  
 Sum of electronic and thermal Energies= -812.383986  
 Sum of electronic and thermal Enthalpies= -812.383041  
 Sum of electronic and thermal Free Energies= -812.454604

b-aa-1+3c4a5a.log



Standard orientation:

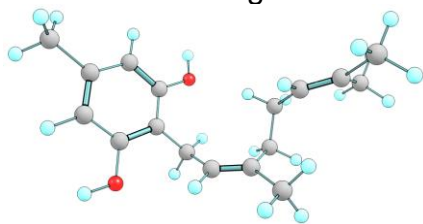
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	3.031412	0.657852	-0.656979
2	6	0	4.094706	-0.090775	-0.141813
3	6	0	3.854828	-1.330246	0.459096
4	6	0	2.541558	-1.803571	0.528411
5	6	0	1.488722	-1.041780	0.009352
6	6	0	1.705559	0.199879	-0.604783
7	1	0	5.108264	0.297469	-0.208103
8	1	0	2.331251	-2.765731	0.989279
9	8	0	3.229530	1.881089	-1.243238
10	1	0	4.173672	2.090218	-1.235167
11	8	0	0.192278	-1.485991	0.071654
12	1	0	0.163279	-2.344543	0.515327
13	6	0	0.568903	1.040779	-1.153689
14	6	0	0.150568	2.112258	-0.170865
15	1	0	-0.269054	0.391834	-1.411798
16	1	0	0.912373	1.517776	-2.080631
17	6	0	-1.081515	2.364308	0.295422
18	1	0	0.974288	2.727858	0.190304
19	6	0	-2.319201	1.587651	-0.104741
20	1	0	-3.176264	2.273374	-0.141821
21	1	0	-2.221315	1.165823	-1.109805
22	6	0	-2.648284	0.430600	0.875741
23	6	0	-3.977378	-0.209346	0.570819
24	1	0	-2.670576	0.830031	1.898129
25	1	0	-1.827797	-0.290501	0.838391
26	6	0	-4.207183	-1.325564	-0.138494
27	1	0	-4.845996	0.335541	0.944618
28	6	0	-5.612734	-1.824139	-0.376364
29	1	0	-5.831895	-1.882647	-1.450906
30	1	0	-5.740060	-2.841072	0.018794
31	1	0	-6.364365	-1.181024	0.090649
32	6	0	-1.317378	3.461110	1.307725
33	1	0	-1.988704	4.230053	0.902938
34	1	0	-0.386424	3.946732	1.614272
35	1	0	-1.806838	3.068872	2.208729
36	6	0	-3.129011	-2.179483	-0.760362
37	1	0	-3.153499	-3.196225	-0.344977
38	1	0	-2.123658	-1.779213	-0.624811
39	1	0	-3.307410	-2.286585	-1.838478
40	6	0	4.991269	-2.127627	1.054187
41	1	0	4.783216	-3.201213	1.028438
42	1	0	5.155196	-1.851916	2.103145
43	1	0	5.928805	-1.947131	0.520181

Frequencies -- 16.9348 27.4577 44.9187  
 Frequencies -- 47.6582 54.4543 60.4548  
 Frequencies -- 75.9054 103.7095 127.1874

Zero-point correction= 0.373049 (Hartree/Particle)  
 Thermal correction to Energy= 0.394438  
 Thermal correction to Enthalpy= 0.395382  
 Thermal correction to Gibbs Free Energy= 0.321166  
 Sum of electronic and zero-point Energies= -812.402973  
 Sum of electronic and thermal Energies= -812.381585  
 Sum of electronic and thermal Enthalpies= -812.380641  
 Sum of electronic and thermal Free Energies= -812.454857

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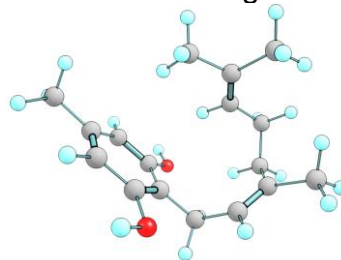
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.905392	-0.854597	-0.852666
2	6	0	2.877824	-1.745331	-0.382386
3	6	0	3.935443	-1.284789	0.406202
4	6	0	4.007580	0.078697	0.707773
5	6	0	3.027681	0.955487	0.231845
6	6	0	1.953378	0.515631	-0.557899
7	1	0	2.806413	-2.800001	-0.637359
8	1	0	4.825064	0.462644	1.313554
9	8	0	0.869256	-1.287598	-1.640009
10	1	0	0.929168	-2.246074	-1.752303
11	8	0	3.068235	2.297618	0.508910
12	1	0	3.845994	2.487855	1.051135
13	6	0	0.894260	1.490912	-1.038075
14	6	0	-0.044725	1.898062	0.076860
15	1	0	0.351203	1.051526	-1.875245
16	1	0	1.402915	2.389179	-1.413630
17	6	0	-1.384411	1.832038	0.088403
18	1	0	0.459998	2.293092	0.957669
19	6	0	-2.217321	1.298643	-1.064148
20	1	0	-3.211304	1.761360	-1.028831
21	1	0	-1.774560	1.585051	-2.024701
22	6	0	-2.395654	-0.245187	-1.058726
23	6	0	-2.981174	-0.789730	0.217594
24	1	0	-1.410679	-0.697466	-1.215747
25	1	0	-3.012088	-0.517701	-1.922407
26	6	0	-4.252131	-1.149628	0.457882
27	1	0	-2.273852	-0.872475	1.043473
28	6	0	-4.674354	-1.666823	1.812393
29	1	0	-5.457884	-1.031999	2.247290
30	1	0	-5.103560	-2.674625	1.732630
31	1	0	-3.838488	-1.706889	2.516830
32	6	0	-2.169706	2.299132	1.292160
33	1	0	-2.821385	3.142528	1.026798
34	1	0	-1.518258	2.616365	2.112021
35	1	0	-2.829247	1.504179	1.659827
36	6	0	-5.369067	-1.075836	-0.554384
37	1	0	-5.822487	-2.064539	-0.704450
38	1	0	-5.048291	-0.698277	-1.527029
39	1	0	-6.171293	-0.421667	-0.188618
40	6	0	4.966019	-2.246842	0.948277
41	1	0	5.940400	-1.763753	1.066633
42	1	0	5.089976	-3.112226	0.290816
43	1	0	4.668117	-2.625280	1.933809

Frequencies -- 7.9315 20.1070 35.6779  
 Frequencies -- 40.4453 45.5817 71.7259  
 Frequencies -- 82.3716 98.1725 132.5488

Zero-point correction= 0.372821 (Hartree/Particle)  
 Thermal correction to Energy= 0.394299  
 Thermal correction to Enthalpy= 0.395243  
 Thermal correction to Gibbs Free Energy= 0.319630  
 Sum of electronic and zero-point Energies= -812.400653  
 Sum of electronic and thermal Energies= -812.379176  
 Sum of electronic and thermal Enthalpies= -812.378231  
 Sum of electronic and thermal Free Energies= -812.453844

# b-aa-1-3c4+5-.log



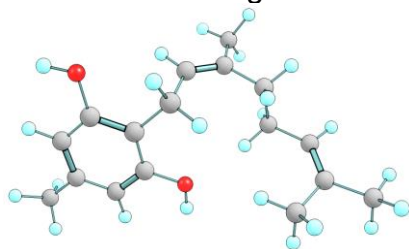
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.371001	-0.589694	1.306007
2	6	0	2.414382	0.339969	1.218687
3	6	0	3.118779	0.500040	0.022667
4	6	0	2.774553	-0.295847	-1.074194
5	6	0	1.732637	-1.222699	-0.969142
6	6	0	0.999512	-1.388403	0.216259
7	1	0	2.670401	0.941916	2.087327
8	1	0	3.313528	-0.195848	-2.013344
9	8	0	0.660794	-0.748390	2.470245
10	1	0	0.988806	-0.124001	3.131584
11	8	0	1.373141	-2.024352	-2.020657
12	1	0	1.938925	-1.828346	-2.779980
13	6	0	-0.147868	-2.380175	0.290069
14	6	0	-1.338981	-1.989909	-0.564715
15	1	0	-0.439113	-2.504903	1.333805
16	1	0	0.214993	-3.354635	-0.058485
17	6	0	-2.418643	-1.283238	-0.196655
18	1	0	-1.273610	-2.314478	-1.601582
19	6	0	-2.638511	-0.719899	1.190795
20	1	0	-3.575155	-1.127931	1.598383
21	1	0	-1.832880	-1.021796	1.864511
22	6	0	-2.738999	0.830303	1.226416
23	6	0	-1.465610	1.487344	0.770715
24	1	0	-2.946879	1.120510	2.266011
25	1	0	-3.600335	1.162140	0.639843
26	6	0	-1.263075	2.288052	-0.286587
27	1	0	-0.597385	1.224016	1.372321
28	6	0	0.120997	2.797457	-0.614370
29	1	0	0.422561	2.479200	-1.621590
30	1	0	0.149867	3.895501	-0.615448
31	1	0	0.870610	2.427718	0.089883
32	6	0	-3.516240	-0.995041	-1.195362
33	1	0	-4.495183	-1.298094	-0.801034
34	1	0	-3.352084	-1.518156	-2.141657
35	1	0	-3.587943	0.076454	-1.415394
36	6	0	-2.334886	2.748081	-1.244173
37	1	0	-2.336449	3.843189	-1.321701
38	1	0	-3.339679	2.432814	-0.957055
39	1	0	-2.136692	2.367533	-2.254964
40	6	0	4.202572	1.544485	-0.097024
41	1	0	4.970106	1.244932	-0.816633
42	1	0	4.687847	1.731344	0.865321
43	1	0	3.784549	2.497905	-0.443167

Frequencies -- 28.7108 36.4203 42.6597  
 Frequencies -- 67.4012 70.8620 79.3392  
 Frequencies -- 96.9506 126.5106 141.1451

Zero-point correction= 0.373542 (Hartree/Particle)  
 Thermal correction to Energy= 0.394571  
 Thermal correction to Enthalpy= 0.395516  
 Thermal correction to Gibbs Free Energy= 0.323960  
 Sum of electronic and zero-point Energies= -812.405014  
 Sum of electronic and thermal Energies= -812.383985  
 Sum of electronic and thermal Enthalpies= -812.383041  
 Sum of electronic and thermal Free Energies= -812.454597

b-aa-1-3c4+5a.log



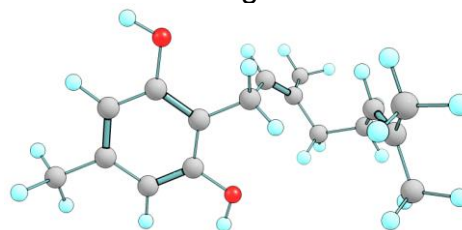
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.488761	-1.041916	0.009242
2	6	0	2.541622	-1.803649	0.528289
3	6	0	3.854872	-1.330221	0.459064
4	6	0	4.094670	-0.090696	-0.141726
5	6	0	3.031330	0.657890	-0.656890
6	6	0	1.705522	0.199827	-0.604777
7	1	0	2.331384	-2.765870	0.989057
8	1	0	5.108193	0.297647	-0.207966
9	8	0	0.192347	-1.486231	0.071426
10	1	0	0.163402	-2.344896	0.514887
11	8	0	3.229390	1.881198	-1.243018
12	1	0	4.173542	2.090291	-1.235093
13	6	0	0.568837	1.040692	-1.153665
14	6	0	0.150551	2.112249	-0.170916
15	1	0	-0.269142	0.391743	-1.411689
16	1	0	0.912252	1.517616	-2.080670
17	6	0	-1.081529	2.364375	0.295341
18	1	0	0.974283	2.727845	0.190223
19	6	0	-2.319232	1.587710	-0.104749
20	1	0	-3.176327	2.273401	-0.141673
21	1	0	-2.221464	1.165977	-1.109866
22	6	0	-2.648153	0.430577	0.875686
23	6	0	-3.977272	-0.209372	0.570908
24	1	0	-2.670303	0.829947	1.898103
25	1	0	-1.827657	-0.290506	0.838190
26	6	0	-4.207176	-1.325579	-0.138396
27	1	0	-4.845847	0.335516	0.944801
28	6	0	-5.612759	-1.824103	-0.376120
29	1	0	-5.832036	-1.882625	-1.450639
30	1	0	-5.740096	-2.841028	0.019059
31	1	0	-6.364323	-1.180957	0.090955
32	6	0	-1.317367	3.461241	1.307568
33	1	0	-1.988532	4.230266	0.902666
34	1	0	-0.386394	3.946751	1.614230
35	1	0	-1.807017	3.069110	2.208519
36	6	0	-3.129085	-2.179506	-0.760379
37	1	0	-3.153553	-3.196258	-0.345012
38	1	0	-2.123711	-1.779268	-0.624907
39	1	0	-3.307574	-2.286600	-1.838481
40	6	0	4.991333	-2.127518	1.054207
41	1	0	5.928835	-1.947160	0.520091
42	1	0	4.783257	-3.201102	1.028739
43	1	0	5.155380	-1.851562	2.103087

Frequencies -- 16.9374 27.4513 44.9426  
 Frequencies -- 47.6658 54.4350 60.4486  
 Frequencies -- 75.9154 103.7063 127.2088

Zero-point correction= 0.373050 (Hartree/Particle)  
 Thermal correction to Energy= 0.394439  
 Thermal correction to Enthalpy= 0.395383  
 Thermal correction to Gibbs Free Energy= 0.321166  
 Sum of electronic and zero-point Energies= -812.402973  
 Sum of electronic and thermal Energies= -812.381584  
 Sum of electronic and thermal Enthalpies= -812.380640  
 Sum of electronic and thermal Free Energies= -812.454856

b-aa-1-3c4-5+.log



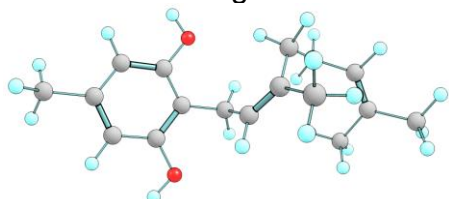
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.733750	-0.760565	-0.810299
2	6	0	-3.060009	-1.004308	-1.187285
3	6	0	-4.113341	-0.592475	-0.366074
4	6	0	-3.818334	0.068587	0.830601
5	6	0	-2.488335	0.304202	1.193408
6	6	0	-1.414929	-0.108899	0.389621
7	1	0	-3.266361	-1.514772	-2.125142
8	1	0	-4.621758	0.405477	1.481340
9	8	0	-0.684101	-1.153974	-1.600811
10	1	0	-1.026345	-1.594723	-2.390319
11	8	0	-2.162952	0.956418	2.354963
12	1	0	-2.973360	1.179788	2.833064
13	6	0	0.020160	0.179726	0.785191
14	6	0	0.419509	1.605967	0.476153
15	1	0	0.688005	-0.528335	0.295249
16	1	0	0.122696	0.018431	1.865139
17	6	0	1.286440	2.028192	-0.456662
18	1	0	-0.084190	2.353601	1.088644
19	6	0	2.404826	1.108057	-1.397191
20	1	0	1.480128	0.185412	-1.569168
21	1	0	2.134445	1.606643	-2.371407
22	6	0	3.468505	0.743887	-0.904237
23	6	0	3.452646	-0.053623	0.371458
24	1	0	4.035716	1.671172	-0.744335
25	1	0	3.982650	0.204497	-1.705688
26	6	0	3.693269	-1.364184	0.533508
27	1	0	3.155827	0.513297	1.253470
28	6	0	3.575766	-2.011941	1.892773
29	1	0	2.820932	-2.809555	1.879934
30	1	0	4.521297	-2.486184	2.187954
31	1	0	3.296838	-1.293151	2.668598
32	6	0	1.590242	3.498866	-0.623130
33	1	0	2.666261	3.693250	-0.524783
34	1	0	1.067824	4.114846	0.114562
35	1	0	1.305449	3.847200	-1.624960
36	6	0	4.077754	-2.314786	-0.573601
37	1	0	5.038039	-2.798686	-0.352053
38	1	0	4.158569	-1.834664	-1.550419
39	1	0	3.337856	-3.121728	-0.656262
40	6	0	-5.545835	-0.882792	-0.747342
41	1	0	-6.219302	-0.094026	-0.398818
42	1	0	-5.887393	-1.823472	-0.298247
43	1	0	-5.660894	-0.977328	-1.830925

Frequencies -- 16.0367 21.9851 32.6107  
 Frequencies -- 39.5734 51.9644 55.8889  
 Frequencies -- 66.4636 106.8059 125.6609

Zero-point correction= 0.372879 (Hartree/Particle)  
 Thermal correction to Energy= 0.394358  
 Thermal correction to Enthalpy= 0.395302  
 Thermal correction to Gibbs Free Energy= 0.320121  
 Sum of electronic and zero-point Energies= -812.401801  
 Sum of electronic and thermal Energies= -812.380322  
 Sum of electronic and thermal Enthalpies= -812.379378  
 Sum of electronic and thermal Free Energies= -812.454559

b-aa-1-3c4-5-.log



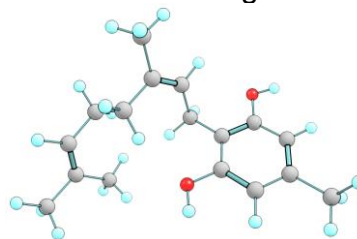
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.398059	-1.029526	-0.421454
2	6	0	3.763815	-1.172954	-0.151079
3	6	0	4.552953	-0.048377	0.107752
4	6	0	3.956120	1.216004	0.085610
5	6	0	2.589654	1.342987	-0.186034
6	6	0	1.780462	0.229187	-0.455520
7	1	0	4.207877	-2.165558	-0.141621
8	1	0	4.550685	2.104912	0.282599
9	8	0	1.602863	-2.117310	-0.677233
10	1	0	2.138010	-2.921495	-0.635576
11	8	0	1.969029	2.565413	-0.206039
12	1	0	2.618986	3.256506	-0.018513
13	6	0	0.296223	0.382975	-0.726230
14	6	0	-0.495363	0.511701	0.556258
15	1	0	-0.049435	-0.463580	-1.320686
16	1	0	0.142957	1.286437	-1.328550
17	6	0	-1.391240	-0.358021	1.045849
18	1	0	-0.274319	1.410879	1.130953
19	6	0	-1.777145	-1.642882	0.333284
20	1	0	-0.887269	-2.118910	-0.091522
21	1	0	-2.193790	-2.349099	1.062494
22	6	0	-2.815241	-1.430075	-0.800934
23	6	0	-4.140878	-0.909209	-0.313240
24	1	0	-2.974062	-2.395449	-1.300712
25	1	0	-2.382580	-0.760914	-1.550282
26	6	0	-4.615061	0.343983	-0.394573
27	1	0	-4.761960	-1.649134	0.194739
28	6	0	-5.968450	0.703316	0.170865
29	1	0	-5.875606	1.477337	0.944373
30	1	0	-6.621236	1.121667	-0.606950
31	1	0	-6.473968	-0.160393	0.612375
32	6	0	-2.100883	-0.091565	2.350924
33	1	0	-3.186786	-0.081600	2.199096
34	1	0	-1.804528	0.863957	2.794302
35	1	0	-1.892668	-0.887002	3.079209
36	6	0	-3.879156	1.501107	-1.024879
37	1	0	-4.458938	1.922991	-1.856540
38	1	0	-2.887495	1.234034	-1.392154
39	1	0	-3.752335	2.309830	-0.293699
40	6	0	6.018803	-0.199120	0.439906
41	1	0	6.592714	0.676233	0.121943
42	1	0	6.448676	-1.083518	-0.039373
43	1	0	6.165908	-0.310141	1.521241

Frequencies -- 15.1587 19.1261 34.7484  
 Frequencies -- 41.9246 50.3578 60.4508  
 Frequencies -- 80.6977 112.2778 128.4730

Zero-point correction= 0.372991 (Hartree/Particle)  
 Thermal correction to Energy= 0.394355  
 Thermal correction to Enthalpy= 0.395300  
 Thermal correction to Gibbs Free Energy= 0.320572  
 Sum of electronic and zero-point Energies= -812.401882  
 Sum of electronic and thermal Energies= -812.380518  
 Sum of electronic and thermal Enthalpies= -812.379573  
 Sum of electronic and thermal Free Energies= -812.454301

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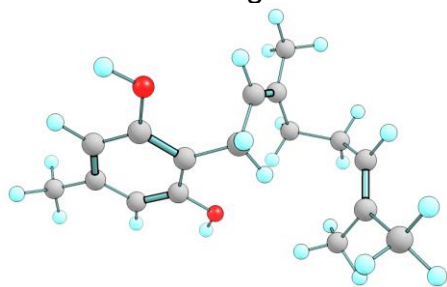
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.466343	-1.069184	-0.160657
2	6	0	-2.597813	-1.722463	-0.667812
3	6	0	-3.871271	-1.186391	-0.467028
4	6	0	-3.995834	0.008940	0.250841
5	6	0	-2.858460	0.648761	0.749283
6	6	0	-1.567526	0.128617	0.558261
7	1	0	-2.477276	-2.650859	-1.220848
8	1	0	-4.977764	0.444108	0.421216
9	8	0	-0.207732	-1.584662	-0.345486
10	1	0	-0.267050	-2.402283	-0.857733
11	8	0	-2.939856	1.821371	1.454967
12	1	0	-3.867638	2.082563	1.534307
13	6	0	-0.347514	0.858598	1.088856
14	6	0	0.004714	2.083452	0.270041
15	1	0	0.491906	0.163970	1.133286
16	1	0	-0.556070	1.179009	2.116732
17	6	0	1.012628	2.194205	-0.602176
18	1	0	-0.656848	2.935775	0.417788
19	6	0	1.975736	1.061711	-0.894976
20	1	0	1.471168	0.095524	-0.815580
21	1	0	2.332917	1.144028	-1.929742
22	6	0	3.204970	1.049640	0.052259
23	6	0	4.117223	-0.113471	-0.234344
24	1	0	2.841132	1.022735	1.085406
25	1	0	3.754985	1.992443	-0.056621
26	6	0	4.030162	-1.323990	0.290233
27	1	0	4.873892	0.054212	-1.001236
28	6	0	4.953846	-2.435335	-0.142729
29	1	0	5.531433	-2.821247	0.707819
30	1	0	4.381731	-3.285887	-0.537325
31	1	0	5.657446	-2.111281	-0.915182
32	6	0	1.278346	3.485598	-1.336992
33	1	0	2.303603	3.834624	-1.155578
34	1	0	0.591233	4.282262	-1.037039
35	1	0	1.188833	3.344983	-2.422394
36	6	0	3.002765	-1.718828	1.322551
37	1	0	2.212865	-2.329658	0.866771
38	1	0	2.515914	-0.860325	1.790862
39	1	0	3.459436	-2.325048	2.114285
40	6	0	-5.099718	-1.873219	-1.015694
41	1	0	-5.822782	-2.084412	-0.220092
42	1	0	-4.848414	-2.818612	-1.503466
43	1	0	-5.609415	-1.240134	-1.750994

Frequencies -- 14.9499 21.5263 41.3450  
 Frequencies -- 49.3413 55.4876 57.7551  
 Frequencies -- 70.4805 98.0272 121.8467

Zero-point correction= 0.372798 (Hartree/Particle)  
 Thermal correction to Energy= 0.394338  
 Thermal correction to Enthalpy= 0.395282  
 Thermal correction to Gibbs Free Energy= 0.320221  
 Sum of electronic and zero-point Energies= -812.401835  
 Sum of electronic and thermal Energies= -812.380295  
 Sum of electronic and thermal Enthalpies= -812.379351  
 Sum of electronic and thermal Free Energies= -812.454412

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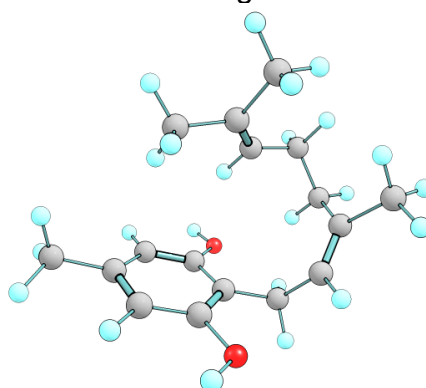
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.556806	-1.008248	-0.427946
2	6	0	-2.850876	-1.324386	-0.860761
3	6	0	-3.952249	-0.630118	-0.356448
4	6	0	-3.740715	0.375796	0.592836
5	6	0	-2.443534	0.678895	1.014455
6	6	0	-1.319810	0.001136	0.514904
7	1	0	-2.993299	-2.114336	-1.593484
8	1	0	-4.584545	0.924978	1.003715
9	8	0	-0.463742	-1.684101	-0.911466
10	1	0	-0.747198	-2.322658	-1.579479
11	8	0	-2.194794	1.659007	1.940809
12	1	0	-3.032048	2.045909	2.230763
13	6	0	0.080405	0.371552	0.970392
14	6	0	0.535909	1.714535	0.436128
15	1	0	0.779209	-0.413526	0.686932
16	1	0	0.085043	0.422302	2.065858
17	6	0	1.342365	1.941685	-0.611938
18	1	0	0.122404	2.571988	0.965077
19	6	0	1.935204	0.849906	-1.479649
20	1	0	1.349610	-0.068024	-1.399690
21	1	0	1.878525	1.169633	-2.529342
22	6	0	3.418137	0.525513	-1.158046
23	6	0	3.609488	-0.053771	0.223040
24	1	0	4.020007	1.436575	-1.257876
25	1	0	3.785416	-0.167543	-1.925387
26	6	0	3.445197	-1.338335	0.574247
27	1	0	3.858705	0.659155	1.008022
28	6	0	3.585697	-1.785911	2.009566
29	1	0	2.647944	-2.230482	2.369061
30	1	0	4.354013	-2.563746	2.108705
31	1	0	3.845378	-0.958371	2.675427
32	6	0	1.704865	3.351943	-1.018166
33	1	0	2.793318	3.491189	-1.041050
34	1	0	1.285083	4.098019	-0.337665
35	1	0	1.345673	3.571382	-2.032183
36	6	0	3.036255	-2.427576	-0.389146
37	1	0	3.593373	-3.351229	-0.193845
38	1	0	3.189923	-2.151242	-1.434808
39	1	0	1.969275	-2.655563	-0.270057
40	6	0	-5.349887	-0.936783	-0.841268
41	1	0	-6.055475	-0.999410	-0.006179
42	1	0	-5.386696	-1.881268	-1.390370
43	1	0	-5.713224	-0.147961	-1.510096

Frequencies -- 16.0266            21.9868            32.6031  
 Frequencies -- 39.3866            51.9586            55.8862  
 Frequencies -- 66.4548            106.8037            125.6575

Zero-point correction=            0.372879 (Hartree/Particle)  
 Thermal correction to Energy=    0.394358  
 Thermal correction to Enthalpy= 0.395302  
 Thermal correction to Gibbs Free Energy= 0.320116  
 Sum of electronic and zero-point Energies= -812.401802  
 Sum of electronic and thermal Energies= -812.380322  
 Sum of electronic and thermal Enthalpies= -812.379378  
 Sum of electronic and thermal Free Energies= -812.454564

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Standard orientation:

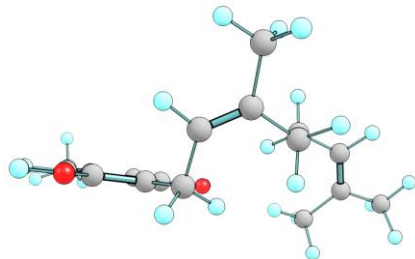
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.370904	-0.589025	1.306060
2	6	0	2.414029	0.340936	1.218550
3	6	0	3.118681	0.500632	0.022644
4	6	0	2.774925	-0.295857	-1.073955
5	6	0	1.733248	-1.222935	-0.968734
6	6	0	0.999912	-1.388321	0.216597
7	1	0	2.669609	0.943399	2.086962
8	1	0	3.314094	-0.196095	-2.013019
9	8	0	0.660505	-0.747421	2.470217
10	1	0	0.988594	-0.123019	3.131504
11	8	0	1.374058	-2.025057	-2.019990
12	1	0	1.940206	-1.829546	-2.779166
13	6	0	-0.147317	-2.380241	0.290553
14	6	0	-1.338358	-1.990168	-0.564412
15	1	0	-0.438609	-2.504803	1.334298
16	1	0	0.215640	-3.354718	-0.057832
17	6	0	-2.418195	-1.283620	-0.196647
18	1	0	-1.272701	-2.314743	-1.601267
19	6	0	-2.638471	-0.720235	1.190735
20	1	0	-3.575099	-1.128467	1.598168
21	1	0	-1.832910	-1.021952	1.864612
22	6	0	-2.739297	0.829928	1.226261
23	6	0	-1.466099	1.487296	0.770505
24	1	0	-2.947217	1.120169	2.265842
25	1	0	-3.600714	1.161543	0.639685
26	6	0	-1.263822	2.287905	-0.286923
27	1	0	-0.597800	1.224425	1.372209
28	6	0	0.120058	2.797849	-0.614683
29	1	0	0.421701	2.479963	-1.622000
30	1	0	0.148545	3.895906	-0.615497
31	1	0	0.869839	2.428211	0.089450
32	6	0	-3.515641	-0.995707	-1.195595
33	1	0	-4.494537	-1.299350	-0.801594
34	1	0	-3.350985	-1.518535	-2.141966
35	1	0	-3.587827	0.075796	-1.415405
36	6	0	-2.335749	2.747254	-1.244713
37	1	0	-2.337132	3.842284	-1.323265
38	1	0	-3.340544	2.432418	-0.957107
39	1	0	-2.137844	2.365722	-2.255196
40	6	0	4.202389	1.545151	-0.097239
41	1	0	4.970433	1.245062	-0.816083
42	1	0	4.687047	1.732845	0.865256
43	1	0	3.784534	2.498251	-0.444443

Frequencies -- 28.7458            36.4724            42.6788  
 Frequencies -- 67.3636            70.7438            79.3538  
 Frequencies -- 96.9920            126.5334            141.1504

Zero-point correction=            0.373543 (Hartree/Particle)  
 Thermal correction to Energy=    0.394571  
 Thermal correction to Enthalpy= 0.395516  
 Thermal correction to Gibbs Free Energy= 0.323961  
 Sum of electronic and zero-point Energies= -812.405014  
 Sum of electronic and thermal Energies= -812.383985  
 Sum of electronic and thermal Enthalpies= -812.383041  
 Sum of electronic and thermal Free Energies= -812.454595



b-aa-1-3c4a5a.log



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.488663	-1.042031	0.008760
2	6	0	2.541386	-1.803889	0.527907
3	6	0	3.854662	-1.330460	0.459112
4	6	0	4.094635	-0.090825	-0.141390
5	6	0	3.031429	0.657881	-0.656666
6	6	0	1.705595	0.199838	-0.604949
7	1	0	2.331019	-2.766202	0.988430
8	1	0	5.108181	0.297514	-0.207304
9	8	0	0.192232	-1.486363	0.070497
10	1	0	0.163126	-2.344924	0.514150
11	8	0	3.229653	1.881296	-1.242522
12	1	0	4.173805	2.090371	-1.234310
13	6	0	0.569063	1.040878	-1.153920
14	6	0	0.150822	2.112365	-0.171060
15	1	0	-0.268956	0.392049	-1.412104
16	1	0	0.912656	1.517859	-2.080824
17	6	0	-1.081226	2.364433	0.295306
18	1	0	0.974595	2.727898	0.190092
19	6	0	-2.318970	1.587858	-0.104825
20	1	0	-3.176022	2.273607	-0.141674
21	1	0	-2.221233	1.166198	-1.109975
22	6	0	-2.647969	0.430658	0.875511
23	6	0	-3.977219	-0.209038	0.570771
24	1	0	-2.669994	0.829914	1.897976
25	1	0	-1.827582	-0.290542	0.837868
26	6	0	-4.207378	-1.325403	-0.138200
27	1	0	-4.845670	0.336218	0.944427
28	6	0	-5.613079	-1.823639	-0.375847
29	1	0	-5.832312	-1.882472	-1.450355
30	1	0	-5.740688	-2.840396	0.019680
31	1	0	-6.364499	-1.180143	0.090980
32	6	0	-1.316987	3.461159	1.307714
33	1	0	-1.988228	4.230214	0.902998
34	1	0	-0.385989	3.946652	1.614328
35	1	0	-1.806508	3.068875	2.208667
36	6	0	-3.129473	-2.179819	-0.759851
37	1	0	-3.154000	-3.196330	-0.343901
38	1	0	-2.124040	-1.779608	-0.624746
39	1	0	-3.308130	-2.287493	-1.837866
40	6	0	4.990936	-2.127895	1.054438
41	1	0	5.928883	-1.946406	0.521496
42	1	0	4.783420	-3.201554	1.027444
43	1	0	5.153750	-1.853171	2.103834

Frequencies -- 17.0411      27.5302      44.9705  
 Frequencies -- 47.7020      54.7163      60.4578  
 Frequencies -- 75.9226      103.7202      127.2206

Zero-point correction= 0.373051 (Hartree/Particle)  
 Thermal correction to Energy= 0.394439  
 Thermal correction to Enthalpy= 0.395383  
 Thermal correction to Gibbs Free Energy= 0.321181  
 Sum of electronic and zero-point Energies= -812.402972  
 Sum of electronic and thermal Energies= -812.381584  
 Sum of electronic and thermal Enthalpies= -812.380640  
 Sum of electronic and thermal Free Energies= -812.454841