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In silico Studies Combining QSAR Models, DFT-based Reactivity Descriptors and Docking Simulations of Phthalimide Congeners with Hypolipidemic Activity

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5. Supplementary material

5.1 Scores and loadings of the PCA.

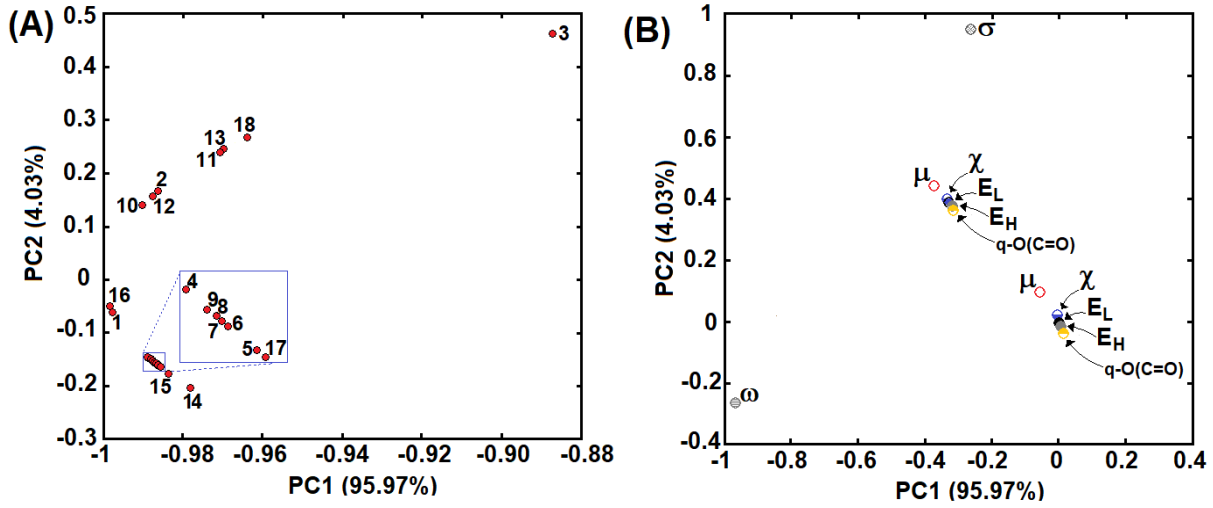

Figure SM-1. (**A**)**:** Isolated score graph; (**B**): Isolated loadings graph

5.2 Additional information of the chemometric procedure

According to a manual choice, see reference [84], some informations about the test set are placed bellow:

C_{16}: number of molecules for the test set = 3

molecules used as test set: **9**, **15** and **18**

T_{16}: number of molecules for the test set = 3

molecules used as test set: **3**, **10** and **14**

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5.3 Coordinates of the optimized geometries of the phthalimide congeners obtained through the B3LYP/6-311++G(d,p) calculations used in the QSAR studies.

(1)				(2)				(3)			
O	-1.67292	-2.29955	0.00010	O	0.080420	2.295409	0.489045	O	1.59312	2.36397	0.00006
N	-2.01036	0.00000	0.00007	C	-0.334072	1.164153	-0.380117	C	1.19275	1.22244	-0.00011
C	2.55542	0.69939	0.00006	N	0.424273	0.000193	-0.574728	N	1.99865	0.07714	0.00000
C	2.55542	-0.69939	0.00006	O	0.080779	-2.295085	-0.489417	C	1.26662	-1.12143	-0.00003
C	1.35772	-1.42145	0.00000	C	-0.333892	-1.163912	-0.380304	C	-0.15463	-0.69527	-0.00003
C	0.17604	-0.69775	-0.00008	C	-1.709505	-0.696911	-0.030219	C	-0.20339	0.70018	-0.00004
C	0.17604	0.69775	-0.00009	C	-1.709613	0.696882	-0.030112	C	-1.40987	1.38576	0.00001
C	1.35772	1.42145	-0.00001	C	-2.854083	1.420976	0.260503	C	-2.58238	0.62786	0.00003
H	3.50038	1.23035	0.00011	C	-4.015553	0.698902	0.556617	C	-2.5346	-0.77168	0.00002
H	3.50038	-1.23035	0.00012	C	-4.015444	-0.699377	0.556511	C	-1.31618	-1.45451	-0.00001
H	1.34763	-2.50473	0.00001	C	-2.853862	-1.421225	0.260287	H	-1.43212	2.46894	0.00000
C	-1.24222	-1.17207	-0.00016	C	1.844138	0.000331	-0.916838	H	-3.54455	1.12704	0.00005
C	-1.24222	1.17207	-0.00020	C	2.755256	-0.000078	0.315892	H	-3.46161	-1.33378	0.00004
H	1.34763	2.50473	-0.00001	C	4.240848	0.000103	-0.060235	H	-1.26984	-2.53650	0.00000
O	-1.67292	2.29955	0.00009	C	5.163307	-0.000328	1.162365	H	3.00613	0.13603	0.00016
H	-3.02039	0.00000	0.00031	H	-2.844408	2.504326	0.257163	N	1.67479	-2.32568	0.00003
				H	-4.931239	1.230067	0.789925	H	2.69307	-2.39379	0.00007
				H	-4.931048	-1.230720	0.789738				
				H	-2.844021	-2.504573	0.256781				
				H	2.026119	-0.886558	-1.527391				
				H	2.026057	0.887667	-1.526755				
				H	2.528355	0.881013	0.925923				
				H	2.528415	-0.881610	0.925304				
				H	4.457933	-0.877064	-0.681526				
				H	4.457886	0.877742	-0.680877				
				H	6.215641	-0.000184	0.865998				
				H	4.992801	0.882851	1.785527				
				H	4.992854	-0.883987	1.784860				
E = -513.2374067 Hartree				E = -670.5356142 Hartree				E = -493.3446185 Hartree			
ZPE = 303.304 KJ.mol^{-1}				ZPE = 599.7928 KJ.mol^{-1}				ZPE = 335.2660 KJ.mol^{-1}			
Nº imaginary frequencies = 0				Nº imaginary frequencies = 0				Nº imaginary frequencies = 0			

(4)				(5)				(6)			
O	-0.043714	2.295155	-0.120498	O	-2.36219	-1.47321	-0.04763	O	-1.70156	1.92900	-0.02833
C	-0.380315	1.125173	-0.197110	C	-1.59805	-0.53135	0.02479	C	-1.10930	0.86384	-0.08213
C	5.243059	-0.512270	0.956643	N	-1.99580	0.81465	0.11920	N	-1.72319	-0.38525	-0.18907
C	4.273746	-0.046713	-0.133635	N	-0.89140	1.68977	-0.10208	N	-0.78906	-1.43876	0.01062
C	2.802434	-0.247416	0.244973	C	0.24690	0.86780	-0.03216	C	0.47457	-0.82490	-0.01137
C	1.844522	0.222486	-0.858165	C	-0.12686	-0.47628	0.01358	C	0.33095	0.56297	-0.02800
N	0.439640	0.064396	-0.524417	C	0.83079	-1.48999	0.02095	C	1.44421	1.40053	0.01820
C	-0.252282	-1.218939	-0.544589	C	2.17088	-1.12469	0.01301	C	2.70374	0.81428	0.05142
C	-1.665435	-0.842043	-0.173882	C	2.53832	0.23240	-0.00454	C	2.83932	-0.58471	0.04031
C	-1.729217	0.534253	0.029076	C	1.58932	1.24901	-0.02724	C	1.73250	-1.42726	0.00991
C	-2.915833	1.165967	0.383914	H	0.52258	-2.52868	0.04200	H	1.31531	2.47647	0.01910
C	-4.055780	0.378190	0.533878	H	2.94215	-1.88546	0.02242	H	3.59119	1.43501	0.08431
C	-3.995974	-1.005863	0.331601	H	3.59040	0.49486	-0.00836	H	3.83205	-1.02020	0.06388
C	-2.799004	-1.631807	-0.024236	H	1.88434	2.29153	-0.05667	H	1.84699	-2.50508	0.01779
H	6.282943	-0.354962	0.657840	H	-2.84218	1.07877	-0.36895	C	-3.10151	-0.62002	0.19088
H	5.079407	0.034549	1.890256	H	-0.89719	2.44232	0.58046	H	-3.62078	0.33286	0.09378
H	5.116657	-1.578282	1.170729					H	-3.56767	-1.35133	-0.47441
H	4.448206	1.014098	-0.348585					H	-0.91453	-2.16639	-0.68880
H	4.486643	-0.585795	-1.065127					H	-3.17120	-0.97360	1.22482
H	2.626106	-1.307821	0.463950								
H	2.575897	0.305694	1.163103								
H	2.049219	-0.318367	-1.790895								
H	1.994802	1.286809	-1.052550								
H	0.183989	-1.923336	0.174254								
H	-0.194382	-1.679938	-1.539568								
H	-2.938915	2.238789	0.535982								
H	-4.998448	0.837072	0.809542								
H	-4.893938	-1.601384	0.453297								
H	-2.765476	-2.705255	-0.178137								
E = -596.4785267 Hartree ZPE = 647.9724 KJ.mol^{-1} Nº imaginary frequencies = 0				E = -455.195397 Hartree ZPE = 322.0702 KJ.mol^{-1} Nº imaginary frequencies = 0				E = -494.5174687 Hartree ZPE = 394.2073 KJ.mol^{-1} Nº imaginary frequencies = 0			

(7)				(8)				(9)			
O	-1.19409	2.13226	-0.17743	C	1.18174	0.59346	-0.04579	O	-0.498601	2.387304	0.041793
C	-0.68404	1.02641	-0.26050	C	2.36018	1.23779	0.32785	C	-0.879566	1.252369	0.282063
N	-1.37589	-0.14962	-0.55238	C	3.50032	0.46445	0.50949	N	-0.153697	0.305019	1.003103
N	-0.55603	-1.29494	-0.34605	C	3.45502	-0.92787	0.32044	N	-0.753833	-0.982624	0.915145
C	0.74336	-0.79475	-0.16128	C	2.27932	-1.58004	-0.03725	C	-2.117341	0.554821	-0.104606
C	0.71092	0.59713	-0.06545	C	1.13980	-0.79258	-0.20416	C	-3.250946	0.999311	-0.783403
C	1.87156	1.32647	0.18851	N	-0.16848	-1.20283	-0.50889	C	-4.286169	0.096028	-0.991598
C	3.06798	0.63093	0.31375	N	-0.90035	-0.00065	-0.72100	C	-4.182013	-1.226789	-0.527361
C	3.09520	-0.76895	0.18775	C	-0.16585	1.11676	-0.32617	C	-3.047695	-1.682119	0.137103
C	1.93895	-1.50513	-0.05008	O	-0.61450	2.24859	-0.23351	H	-3.312004	2.025845	-1.125247
H	1.82740	2.40583	0.27434	C	-2.35409	-0.05581	-0.66299	H	-5.183332	0.408442	-1.512644
H	3.98995	1.16605	0.50764	C	-2.91585	-0.38207	0.72610	H	-5.003602	-1.913558	-0.697930
H	4.04062	-1.29071	0.28636	C	-4.44526	-0.44672	0.72180	H	-2.970636	-2.708434	0.477282
H	1.96784	-2.58579	-0.12934	H	2.37294	2.31324	0.46067	C	1.289480	0.384732	1.184616
C	-2.81415	-0.28793	-0.35732	H	4.43442	0.93257	0.79647	C	2.100621	-0.127435	-0.011676
H	-3.17937	-1.05887	-1.04332	H	4.35783	-1.51099	0.46437	H	1.497734	1.441105	1.365165
C	-3.21601	-0.60241	1.08493	H	2.25072	-2.65605	-0.16519	C	3.610960	-0.032577	0.227966
H	-0.64793	-1.94268	-1.12487	H	-2.70145	-0.78668	-1.40192	H	1.818755	-1.165037	-0.219386
H	-3.23689	0.66510	-0.67862	H	-2.69244	0.92898	-0.99186	H	1.827403	0.461064	-0.893928
H	-4.30174	-0.71219	1.15338	H	-2.57528	0.38562	1.42759	C	4.445185	-0.524121	-0.960818
H	-2.75374	-1.53030	1.42800	H	-2.49819	-1.33459	1.06618	H	3.880357	1.007832	0.450713
H	-2.91264	0.20669	1.75283	H	-4.81141	-1.22084	0.03953	H	3.878820	-0.614724	1.119939
				H	-4.88324	0.50635	0.40985	H	1.552648	-0.163133	2.096143
				H	-4.83013	-0.67691	1.71829	C	-2.011241	-0.767824	0.327820
				H	-0.23799	-1.80939	-1.32256	H	4.175998	-1.563503	-1.184427
								H	4.178217	0.057489	-1.851058
								H	-0.789267	-1.421576	1.832021
								C	5.954435	-0.426995	-0.721033
								H	6.258186	-1.026020	0.143447
								H	6.519101	-0.784221	-1.586575
								H	6.258886	0.606826	-0.530028
E = -533.844269 Hartree				E = -573.1687359 Hartree				E = -651.8174347 Hartree			
ZPE = 468.5724 KJ.mol^{-1}				ZPE = 543.0304 KJ.mol^{-1}				ZPE = 691.5988 KJ.mol^{-1}			
Nº imaginary frequencies = 0				Nº imaginary frequencies = 0				Nº imaginary frequencies = 0			

(10)				(11)				(12)			
C	2.48160	-0.75684	0.20791	O	-0.95697	2.31859	0.32638	C	2.191032	0.695224	-0.004327
C	3.56203	-1.60893	0.37259	C	-1.31617	1.17764	0.16828	C	3.333472	1.407552	0.321675
C	4.82413	-1.12358	0.01543	N	-0.46812	0.04920	0.05236	C	4.480322	0.673525	0.643425
C	4.98358	0.17205	-0.48743	C	-1.21281	-1.14259	-0.12309	C	4.468478	-0.724788	0.633120
C	3.88599	1.02382	-0.64800	C	-2.70650	0.65126	0.05460	C	3.309524	-1.434983	0.300861
C	2.64060	0.53283	-0.28972	C	-3.91769	1.32307	0.10186	C	2.179694	-0.698679	-0.015271
C	1.30250	1.18815	-0.34590	C	-5.08205	0.56003	-0.03322	N	0.067147	0.019754	-0.610526
N	0.38317	0.22535	0.13783	C	-5.02028	-0.82640	-0.20918	C	0.829315	1.176237	-0.386392
C	1.03535	-0.98052	0.49324	C	-3.79208	-1.49403	-0.25381	O	0.428321	2.311986	-0.502595
O	0.50322	-1.96935	0.93487	H	-3.95436	2.39722	0.23769	C	-1.340364	0.032508	-0.999610
O	1.02859	2.30175	-0.72062	H	-3.73281	-2.56731	-0.38860	C	-2.293846	-0.001886	0.200441
C	-1.02465	0.44520	0.25710	C	0.95842	0.10545	0.10990	C	-3.763905	0.013070	-0.230122
C	-1.49664	1.59878	0.88604	O	-0.75330	-2.25119	-0.24845	H	3.332660	2.490968	0.326662
C	-2.86836	1.79446	0.98461	C	1.65312	1.03183	-0.66744	H	5.393650	1.195329	0.905044
C	-3.76177	0.84967	0.47840	C	1.65843	-0.76164	0.94871	H	5.373057	-1.265872	0.886173
C	-3.29746	-0.31100	-0.14531	C	-2.64515	-0.72824	-0.11731	H	3.291742	-2.518075	0.288438
C	-1.91436	-0.49388	-0.25735	H	-5.94031	-1.39029	-0.31176	H	-1.502625	-0.835352	-1.642265
C	-4.22266	-1.38593	-0.68979	C	3.04739	-0.70183	0.99784	H	-1.499578	0.938044	-1.588576
C	-5.69758	-1.00497	-0.83451	C	3.76462	0.22086	0.22900	H	-2.086717	0.860466	0.843406
H	3.42736	-2.61086	0.76191	C	3.04153	1.08692	-0.59773	H	-2.089315	-0.901364	0.790938
H	5.69412	-1.76016	0.12869	H	-6.04901	1.04889	-0.00198	C	-4.740436	-0.027376	0.951374
H	5.97465	0.51944	-0.75579	H	1.11126	1.71425	-1.30895	C	-6.209306	-0.011796	0.519158
H	3.99815	2.02919	-1.03559	H	3.57037	1.81956	-1.19893	H	-3.960007	-0.843026	-0.888550
H	-0.80204	2.33106	1.27475	C	5.27631	0.25477	0.26139	H	-3.959938	0.911822	-0.828937
H	-3.24699	2.69061	1.46297	H	1.12127	-1.48103	1.55240	H	-4.543425	0.826874	1.610013
H	-4.82572	1.02839	0.57241	C	5.91971	-0.68080	-0.77751	H	-4.543876	-0.925405	1.548994
H	-1.52801	-1.38302	-0.74088	H	3.58083	-1.38179	1.65444	H	-6.444166	-0.872576	-0.114911
H	-4.14280	-2.26653	-0.04027	H	5.61971	1.27929	0.08639	H	-6.444537	0.892505	-0.050930
H	-3.83772	-1.70627	-1.66416	H	5.62399	-0.02332	1.26143	H	-6.879480	-0.043193	1.382571
H	-5.82548	-0.13153	-1.48018	H	7.01094	-0.62964	-0.72426	C	0.811679	-1.151239	-411006
H	-6.15841	-0.78079	0.13118	H	5.61994	-1.71873	-0.60964	O	0.391500	-2.278690	-0.539198
H	-6.25766	-1.83209	-1.27773	H	5.61643	-0.40832	-1.79199				
E = -822.9879058 Hartree				E = -822.9895286 Hartree				E = -709.8600116 Hartree			
ZPE = 660.4537 KJ.mol^{-1}				ZPE = 660.2783 KJ.mol^{-1}				ZPE = 673.8681 KJ.mol^{-1}			
Nº imaginary frequencies = 0				Nº imaginary frequencies = 0				Nº imaginary frequencies = 0			

(13)				(14)				(15)			
O	0.45053	-2.30394	-0.92579	O	0.04395	2.34665	-0.68102	O	0.04966	2.35947	-0.63925
C	0.03085	-1.20784	-0.62976	C	-0.41138	1.24115	-0.47605	C	-0.40287	1.25130	-0.44551
C	-1.35605	-0.87027	-0.19808	C	-1.82243	0.91989	-0.10807	C	-1.81721	0.91853	-0.10285
C	-2.41275	-1.76296	-0.06118	C	-2.86562	1.82917	0.02322	C	-2.86609	1.82168	0.02548
C	-3.64658	-1.27105	0.36411	C	-4.12549	1.34715	0.37815	C	-4.12874	1.32981	0.35602
C	-3.82115	0.08737	0.64323	C	-4.33739	-0.01752	0.59664	C	-4.33774	-0.03845	0.55371
C	-2.76514	0.99056	0.50412	C	-3.29367	-0.93650	0.46643	C	-3.28839	-0.95137	0.42641
C	-1.54899	0.47605	0.08690	C	-2.05277	-0.43194	0.11531	C	-2.04483	-0.43721	0.09949
S	-0.03888	1.39403	-0.19391	S	-0.54090	-1.36024	-0.12005	S	-0.52703	-1.35796	-0.12654
O	0.54669	1.92230	1.03058	O	-0.62481	-2.25551	-1.26537	O	-0.58575	-2.22669	-1.29371
O	-0.16134	2.28001	-1.34533	O	-0.01433	-1.87894	1.13878	O	-0.02164	-1.90199	1.12947
N	0.79171	-0.04352	-0.67122	N	0.32212	0.06756	-0.55123	N	0.33987	0.08201	-0.51157
C	2.23361	-0.06296	-0.79145	C	1.76633	0.02646	-0.80904	C	1.78238	0.05050	-0.76611
C	2.94449	-0.49241	0.50665	C	2.58683	0.32550	0.44708	C	2.59283	0.32638	0.50343
C	4.45059	-0.36542	0.48488	C	4.08575	0.25130	0.19628	C	4.07743	0.26286	0.24272
H	-2.26079	-2.81251	-0.28130	H	-2.68544	2.88285	-0.15153	H	-2.68789	2.87839	-0.13211
H	-4.48276	-1.95073	0.48081	H	-4.95315	2.03828	0.48544	H	-4.96068	2.01609	0.46097
H	-4.78830	0.44785	0.97326	H	-5.32458	-0.37045	0.87071	H	-5.32708	-0.39902	0.80942
H	-2.89326	2.04442	0.71708	H	-3.45059	-1.99490	0.63270	H	-3.44311	-2.01241	0.57715
H	2.58725	0.92042	-1.11301	H	1.97261	0.75680	-1.59132	H	1.98948	0.80053	-1.52962
H	2.49965	-0.77386	-1.58000	H	2.00997	-0.95633	-1.21441	H	2.03168	-0.92284	-1.19083
H	4.87706	-0.88811	1.33966	C	4.98180	0.56230	1.37679	O	4.78927	0.55228	1.35699
H	4.72291	0.69416	0.54097	O	4.53265	-0.04256	-0.89183	O	4.59603	-0.01034	-0.81112
O	2.32599	-0.90393	1.45454	H	4.80515	1.58510	1.72450	H	2.34761	-0.39767	1.28590
H	4.87012	-0.76075	-0.44478	H	4.75372	-0.10436	2.21419	H	2.35413	1.31519	0.90458
				H	6.02621	0.44917	1.08940	H	5.72822	0.48900	1.12443
				H	2.32989	-0.37802	1.24685				
				H	2.34431	1.32380	0.82782				
E = -1140.4913995 Hartree				E = -1179.8211546 Hartree				E= -1215.766435 Hartree			
ZPE = 472.8416 KJ.mol^{-1}				ZPE = 547.4428 KJ.mol^{-1}				ZPE = 490.3942 KJ.mol^{-1}			
Nº imaginary frequencies = 0				Nº imaginary frequencies = 0				Nº imaginary frequencies = 0			

(16)				(17)				(18)			
O	-0.362798	2.268461	-0.950710	O	0.859093	2.345897	0.778757	O	0.399186	2.293855	-0.524026
C	-0.815540	1.196599	-0.609492	C	1.300759	1.249680	0.507367	C	-0.027447	1.167071	-0.429221
C	-2.198132	0.938267	-0.108372	C	2.694735	0.941384	0.069713	C	-1.407919	0.697276	-0.112367
C	-3.197873	1.887364	0.069910	C	3.721636	1.860787	-0.110245	C	-2.558519	1.421148	0.153475
C	-4.437681	1.463485	0.548112	C	4.968338	1.390930	-0.523173	C	-3.725484	0.699091	0.425453
C	-4.672120	0.116863	0.842286	C	5.183040	0.028310	-0.751553	C	-3.725443	-0.699234	0.425414
C	-3.671895	-0.841850	0.665788	C	4.155475	-0.900677	-0.573169	C	-2.558437	-1.421207	0.153387
C	-2.450883	-0.395127	0.189073	C	2.928125	-0.408415	-0.161972	C	-1.407885	-0.697251	-0.112436
S	-0.995553	-1.385112	-0.134334	S	1.438414	-1.351797	0.142914	C	-0.027435	-1.166946	-0.429535
O	-1.181733	-2.278357	-1.271528	O	1.561894	-2.212330	1.312936	N	0.727998	0.000093	-0.629517
O	-0.417970	-1.923642	1.090793	O	0.892864	-1.915746	-1.086269	C	2.154220	0.000129	-0.826828
N	-0.109204	0.003885	-0.638980	N	0.569031	0.073525	0.568938	C	2.939179	-0.000085	0.496054
C	1.276909	-0.108284	-1.102935	C	-0.834994	0.009853	0.989735	C	4.444404	0.000070	0.354963
C	2.297944	0.141550	0.011622	C	-1.818587	0.185367	-0.171972	H	-2.548354	2.504405	0.152519
H	-2.999873	2.926517	-0.162806	H	3.538997	2.912839	0.071560	H	-4.645375	1.230274	0.641309
H	-5.231455	2.186446	0.694517	H	5.783191	2.090105	-0.669273	H	-4.645306	-1.230484	0.641223
H	-5.642807	-0.190473	1.213173	H	6.159739	-0.315051	-1.071571	H	-2.548221	-2.504463	0.152310
H	-3.846027	-1.886323	0.892080	H	4.314399	-1.957400	-0.748000	H	2.430675	0.885913	-1.405114
H	1.390881	0.621896	-1.907894	H	-0.965983	0.800194	1.732395	H	2.430683	-0.885459	-1.405411
H	1.396360	-1.103449	-1.540901	H	-0.984343	-0.948171	1.495508	H	4.772495	-0.880933	-0.205773
H	2.134982	-0.568897	0.825107	H	-1.635784	-0.593965	-0.918081	H	4.907517	-0.000054	1.340423
H	2.143317	1.140209	0.425503	H	-1.623309	1.147944	-0.655112	O	0.399314	-2.293698	-0.524207
C	4.775090	0.302926	0.531392	C	-3.272168	0.125205	0.307268	O	2.374268	-0.000349	1.562039
C	3.725662	0.015789	-0.517420	H	-3.464485	-0.833417	0.798764	H	4.772349	0.881309	-0.205486
H	3.921600	-0.984669	-0.918373	H	-3.446765	0.907359	1.055005				
H	3.904841	0.707845	-1.348949	C	-4.267401	0.305868	-0.854146				
O	4.573393	0.678403	1.657659	H	-4.120390	-0.493108	-1.587954				
O	6.024656	0.090342	0.045451	H	-4.109548	1.263846	-1.351321				
H	6.648188	0.298346	0.757664	C	-5.705866	0.271612	-0.397773				
				O	-6.477740	1.197384	-0.416475				
				O	-6.058475	-0.956126	0.066948				
				H	-6.983184	-0.899136	0.351246				
E= -1255.0913657 Hartree				E= -1294.4156352 Hartree				E= -705.2452768 Hartree			
ZPE = 564.9612 KJ.mol^{-1}				ZPE = 640.2767 KJ.mol^{-1}				ZPE = 473312.7 KJ.mol^{-1}			
Nº imaginary frequencies = 0				Nº imaginary frequencies = 0				Nº imaginary frequencies = 1			