SUPPLEMENTARY MATERIAL

Figures captions

Figure S1. B3LYP and MPWB1K (distances given in parenthesis) optimized geometries of stationary points for the reaction of quercetin 3'OH site with methyl peroxide radical.

Figure S2. B3LYP and MPWB1K (distances given in parenthesis) optimized geometries of stationary points for the reaction of quercetin 3OH site with methyl peroxide radical.

Figure S3. B3LYP and MPWB1K (distances given in parenthesis) optimized geometries of stationary points for the reaction of quercetin 5OH site with methyl peroxide radical.

Figure S4. B3LYP and MPWB1K (distances given in parenthesis) optimized geometries of stationary points for the reaction of quercetin 7OH site with methyl peroxide radical.

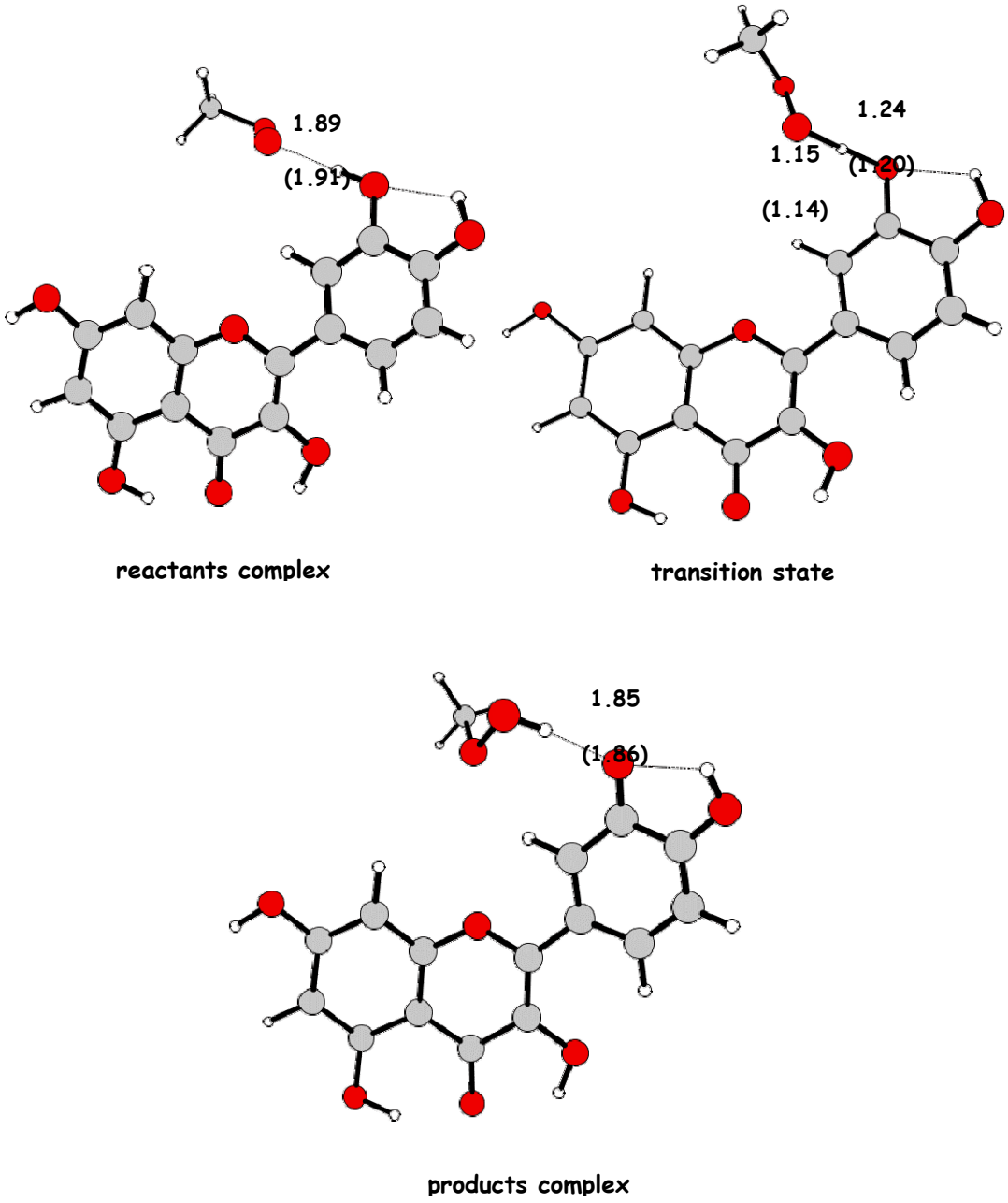

Figure S1

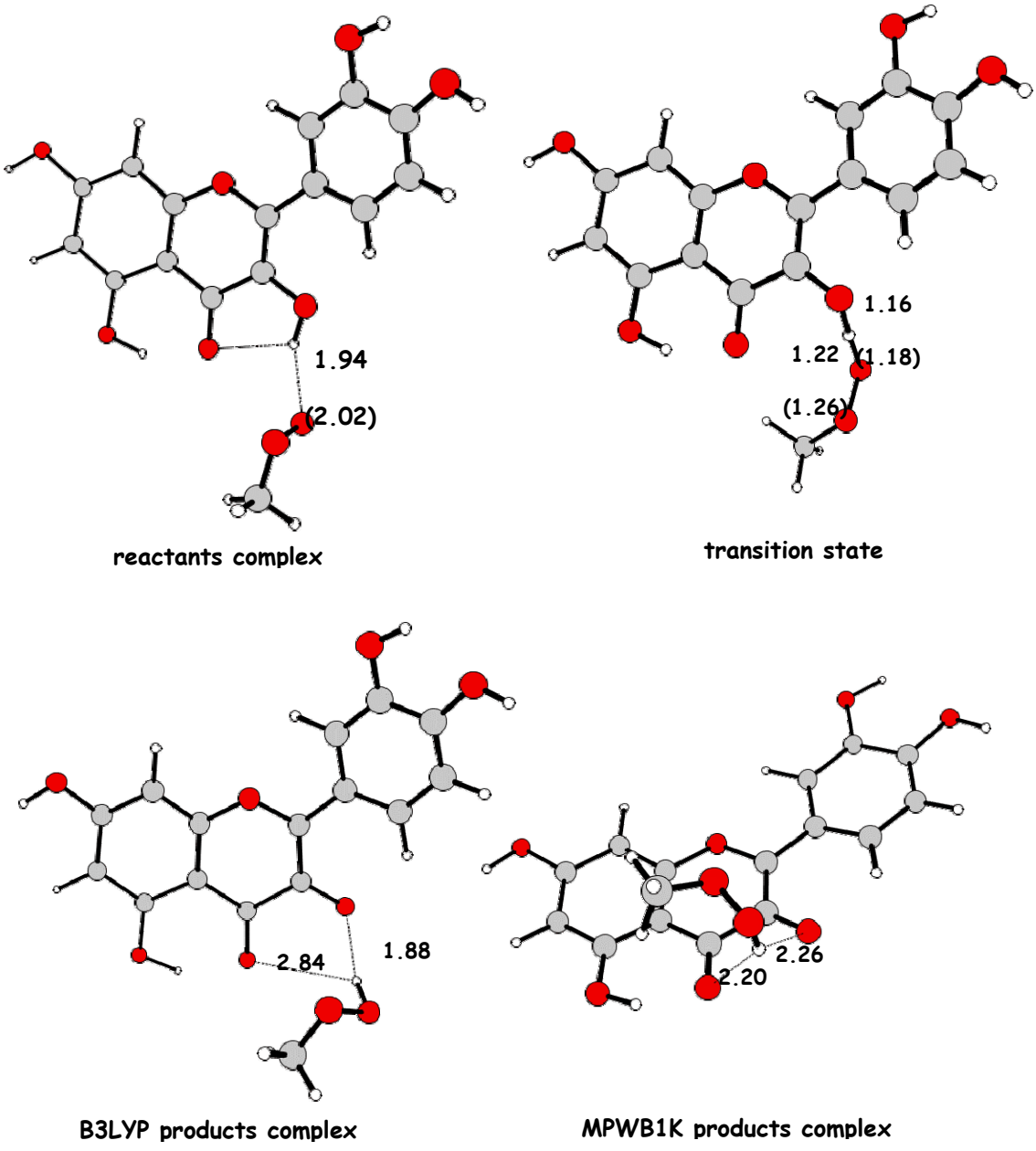

Figure S2

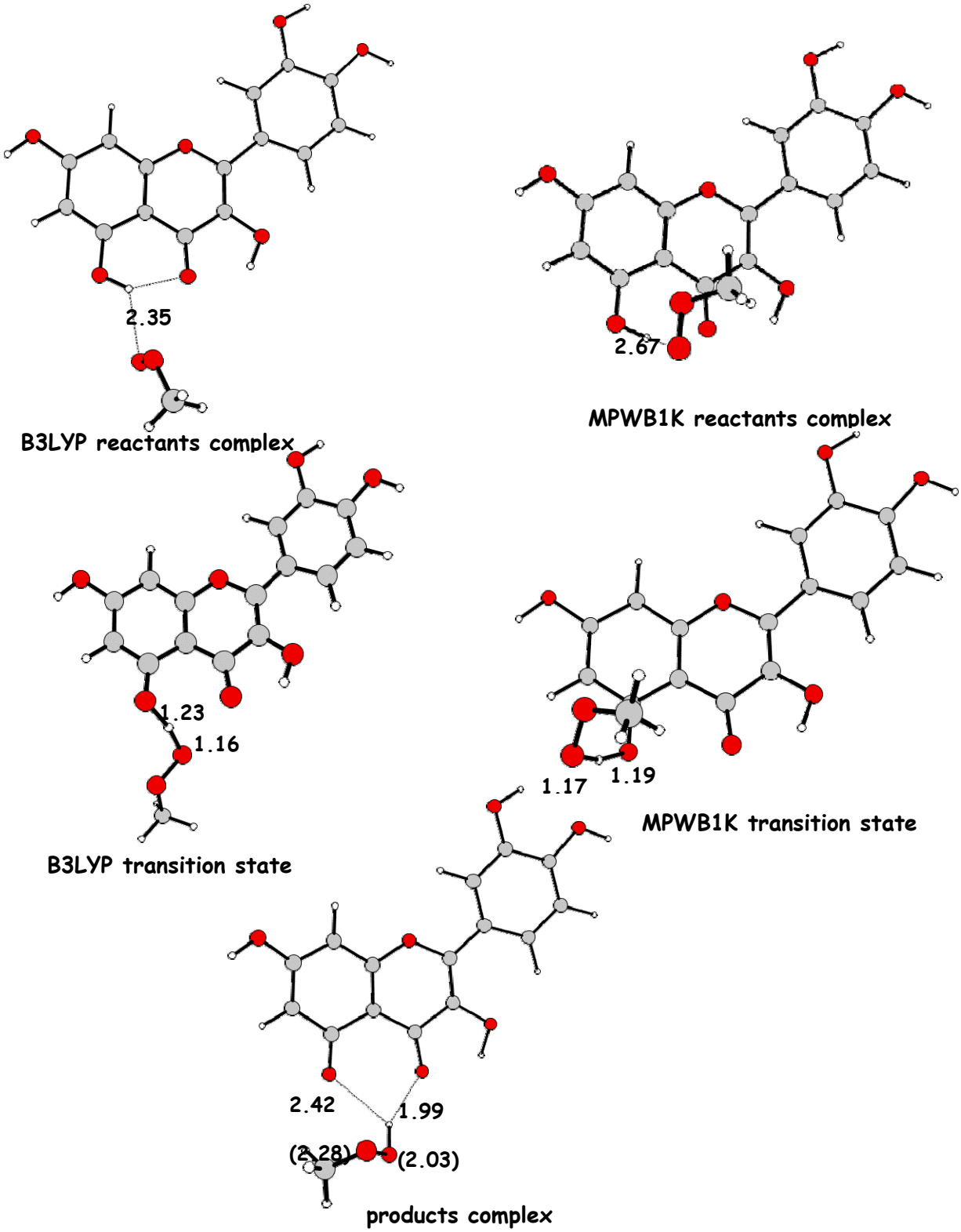

Figure S3

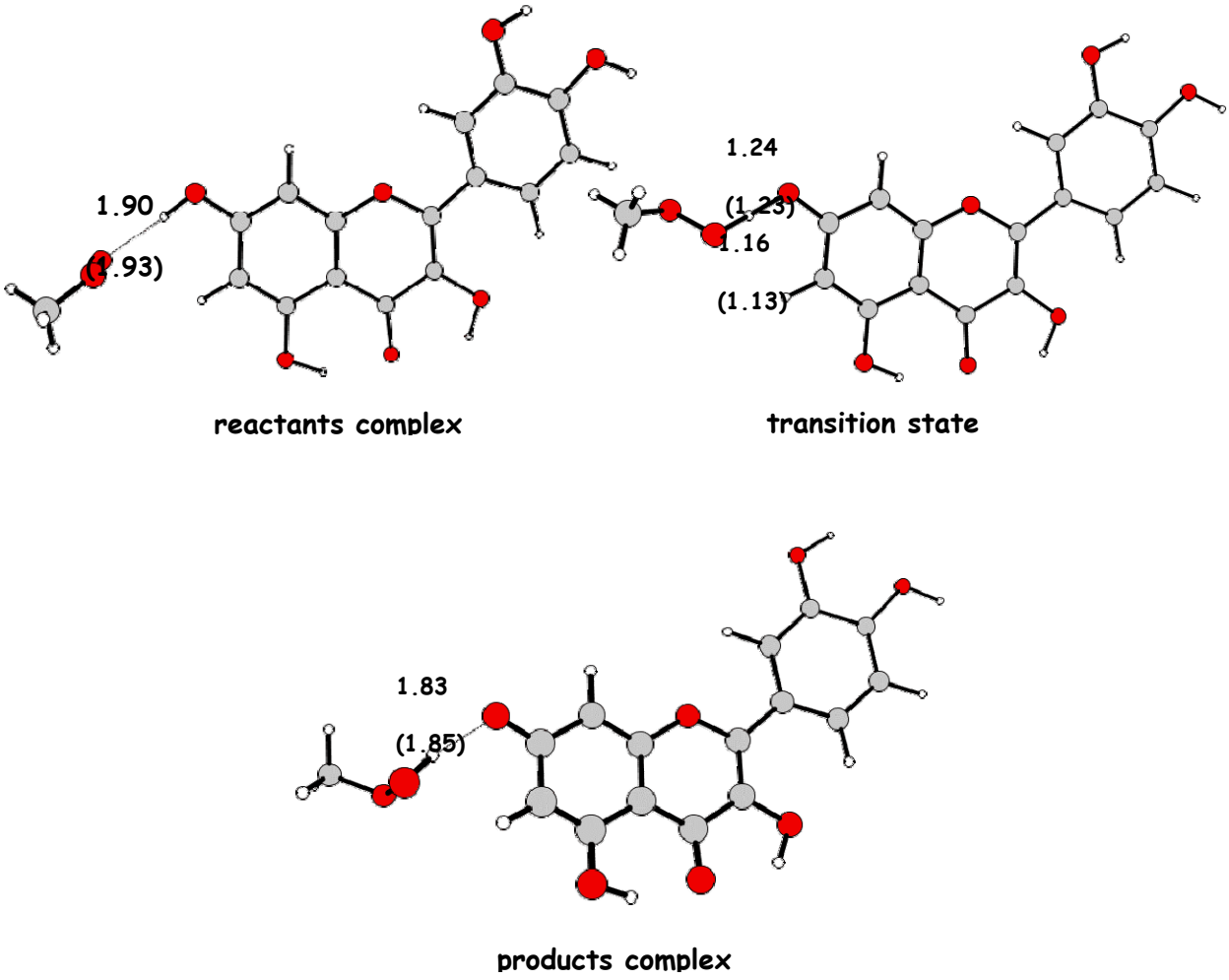

Figure S4

COORDINATES OF THE STATIONARY POINTS

B3LYP reactant complex (4'OH)

C	1.510210	1.442033	-0.166258
C	1.162053	0.075932	-0.199381
C	2.186859	-0.878192	-0.316250
C	3.516402	-0.475904	-0.395913
C	3.850752	0.873240	-0.360160
C	2.832232	1.837795	-0.244840
C	-0.245782	-0.310647	-0.111933
C	-0.785846	-1.568423	-0.085203
C	-2.215825	-1.776951	0.010996
C	-3.038521	-0.605555	0.077409
C	-2.433980	0.661994	0.045911
O	-1.084703	0.776571	-0.046312
C	-4.454576	-0.687346	0.175044
C	-5.205764	0.477890	0.236084
C	-4.561337	1.723321	0.201065
C	-3.174790	1.834727	0.106026
O	-5.064558	-1.879119	0.208147
O	-5.263911	2.884632	0.258421
O	-2.654733	-2.954876	0.032922
O	-0.053124	-2.708943	-0.142531
O	5.115581	1.372694	-0.430644
O	3.153658	3.160795	-0.210180
H	1.947787	-1.928932	-0.345814
H	0.752062	2.206461	-0.078143
H	4.302397	-1.217075	-0.489100
H	-0.724006	-3.417843	-0.101128
H	-2.696715	2.803427	0.080163
H	-6.284985	0.404238	0.309813
H	5.775602	0.659311	-0.494848
H	4.115657	3.222271	-0.279850
H	-4.360022	-2.568950	0.154173
H	-6.204367	2.686848	0.320942
O	7.047476	-0.715402	-0.618528
O	7.527888	-0.907005	0.590423
C	8.516098	-1.972412	0.603178
H	8.843252	-2.040735	1.638790
H	9.336453	-1.695404	-0.058184
H	8.040016	-2.895163	0.272905

B3LYP transition state (4'OH)

C	1.520890	1.247603	0.060271
C	1.100146	-0.095802	0.147554
C	2.079051	-1.117331	0.270023
C	3.422341	-0.808962	0.308330
C	3.852474	0.530432	0.214126
C	2.864430	1.558551	0.087801
C	-0.320210	-0.401116	0.117113
C	-0.935506	-1.628029	0.187138
C	-2.383676	-1.755208	0.141185
C	-3.136046	-0.545174	0.020970
C	-2.457060	0.684556	-0.045929
O	-1.100171	0.724953	0.002234
C	-4.558096	-0.546908	-0.031758
C	-5.240943	0.655231	-0.147226
C	-4.523548	1.858568	-0.210543
C	-3.128738	1.891553	-0.161336

O	-5.239105	-1.697051	0.029663
O	-5.153975	3.053494	-0.322814
O	-2.881734	-2.905019	0.209805
O	-0.278114	-2.799782	0.301937
O	5.101474	0.927629	0.242375
O	3.286892	2.835204	-0.005363
H	1.768569	-2.146999	0.345313
H	0.803832	2.049183	-0.037060
H	4.169367	-1.586158	0.411285
H	-0.990708	-3.470083	0.326303
H	-2.595479	2.829972	-0.211619
H	-6.324241	0.642505	-0.186065
H	5.828123	0.110749	-0.051651
H	4.257447	2.801357	0.025738
H	-4.582474	-2.427838	0.110047
H	-6.107131	2.915774	-0.345501
O	6.618674	-0.771145	-0.502127
O	7.647243	-0.774034	0.418223
C	8.824457	-1.267075	-0.216765
H	9.591958	-1.267891	0.557796
H	9.107930	-0.608356	-1.041725
H	8.651321	-2.279903	-0.589534

B3LYP product complex (4'OH)

C	1.537713	1.318163	-0.296806
C	1.145443	-0.037054	-0.266382
C	2.146468	-1.065115	-0.361852
C	3.471165	-0.762304	-0.479059
C	3.907811	0.607801	-0.510925
C	2.870745	1.640027	-0.413695
C	-0.256924	-0.364077	-0.137660
C	-0.847854	-1.607150	-0.065814
C	-2.293486	-1.755370	0.073992
C	-3.064386	-0.555145	0.129028
C	-2.410851	0.689132	0.048461
O	-1.059528	0.752018	-0.078956
C	-4.481841	-0.578328	0.263609
C	-5.185091	0.616228	0.310368
C	-4.493397	1.833113	0.225473
C	-3.103439	1.887321	0.094136
O	-5.139098	-1.740091	0.344715
O	-5.141822	3.020734	0.266675
O	-2.760251	-2.916516	0.136585
O	-0.178540	-2.770196	-0.111926
O	5.096315	0.996030	-0.617008
O	3.300289	2.902578	-0.445843
H	1.838136	-2.098187	-0.339480
H	0.806456	2.109623	-0.227344
H	4.230253	-1.531887	-0.550415
H	-0.876717	-3.453377	-0.034798
H	-2.591540	2.836747	0.030593
H	-6.263860	0.587097	0.412124
H	6.324950	-0.369007	-0.669466
H	4.272613	2.836590	-0.532057
H	-4.476162	-2.466115	0.294249
H	-6.089552	2.872155	0.356513
O	6.786308	-1.232992	-0.714450
O	7.155246	-1.417576	0.678496
C	8.568075	-1.365950	0.733887
H	8.813902	-1.557246	1.781880
H	8.948780	-0.381432	0.437838

H	9.018807	-2.139274	0.103024

B3LYP reactant complex (3'OH)

C	1.576272	1.515251	0.093990
C	1.200115	0.174791	-0.141205
C	2.209479	-0.773452	-0.381410
C	3.547231	-0.394643	-0.386507
C	3.909847	0.926660	-0.157507
C	2.907810	1.886006	0.083224
C	-0.215290	-0.185288	-0.125616
C	-0.794983	-1.392135	-0.414337
C	-2.229934	-1.575382	-0.360478
C	-3.016467	-0.434371	0.009686
C	-2.373170	0.779061	0.298966
O	-1.021716	0.874560	0.224398
C	-4.433962	-0.496756	0.097382
C	-5.149278	0.635528	0.463842
C	-4.466706	1.826924	0.746665
C	-3.077712	1.917531	0.669463
O	-5.080822	-1.637163	-0.171466
O	-5.132558	2.955533	1.110312
O	-2.708564	-2.703553	-0.638826
O	-0.095279	-2.496728	-0.772691
O	5.213750	1.298313	-0.164921
O	3.369640	3.154524	0.297358
H	1.949487	-1.803997	-0.562928
H	0.820533	2.264386	0.285521
H	4.329410	-1.121286	-0.569377
H	-0.782661	-3.175747	-0.913611
H	-2.568800	2.841907	0.902084
H	-6.230117	0.576792	0.526310
H	5.240189	2.249338	0.011083
H	2.632504	3.781066	0.406315
H	-4.398632	-2.311734	-0.407418
H	-6.077268	2.771191	1.143695
O	1.214799	5.007533	0.605319
O	1.072306	5.621403	-0.548938
C	-0.042992	6.551899	-0.518644
H	0.131885	7.281993	0.271099
H	-0.961176	5.992698	-0.340022
H	-0.046945	7.018807	-1.501739

B3LYP transition state (3'OH)

C	1.288562	1.612248	-0.381414
C	1.028908	0.241763	-0.271101
C	2.117507	-0.671006	-0.311099
C	3.421741	-0.225015	-0.449149
C	3.680071	1.138511	-0.543781
C	2.601515	2.080309	-0.515447
C	-0.347950	-0.223173	-0.128292
C	-0.810482	-1.507505	-0.010491
C	-2.229781	-1.791772	0.128346
C	-3.116494	-0.669171	0.137003
C	-2.587556	0.627708	0.012803
O	-1.248411	0.813921	-0.115455
C	-4.524405	-0.825052	0.269934
C	-5.340380	0.296937	0.273997
C	-4.770066	1.572047	0.147613
C	-3.393088	1.756367	0.015408
O	-5.065124	-2.043327	0.390806

O	-5.535086	2.692120	0.148179
O	-2.590547	-2.989178	0.232249
O	-0.019428	-2.603413	-0.010258
O	4.926907	1.611706	-0.664271
O	2.947280	3.344567	-0.633583
H	1.926499	-1.729705	-0.236433
H	0.485354	2.334144	-0.362717
H	4.250303	-0.921594	-0.475622
H	-0.646304	-3.347464	0.089018
H	-2.973047	2.747344	-0.079957
H	-6.411875	0.166839	0.375494
H	4.840221	2.581331	-0.703340
H	2.193054	4.057955	-0.146290
H	-4.328935	-2.698603	0.366027
H	-6.462248	2.449418	0.244799
O	1.446517	4.814315	0.500063
O	1.274710	5.889892	-0.350352
C	1.054834	7.058824	0.435043
H	1.928199	7.259042	1.061260
H	0.168334	6.928024	1.061024
H	0.902493	7.864876	-0.283439

B3LYP product complex (3'OH)

C	1.511733	1.694757	0.073898
C	1.187839	0.374555	-0.181399
C	2.233562	-0.572390	-0.448527
C	3.566487	-0.201338	-0.460725
C	3.905578	1.123057	-0.204193
C	2.873873	2.121989	0.075860
C	-0.217996	-0.035014	-0.168285
C	-0.758552	-1.260542	-0.441463
C	-2.199904	-1.480623	-0.378155
C	-3.009013	-0.358418	-0.020597
C	-2.394102	0.878618	0.249443
O	-1.045121	1.004349	0.167972
C	-4.426093	-0.451287	0.075339
C	-5.161959	0.669474	0.428792
C	-4.505021	1.882147	0.690341
C	-3.117145	2.005801	0.605111
O	-5.051110	-1.608713	-0.173070
O	-5.193219	2.995649	1.039013
O	-2.633670	-2.626946	-0.639903
O	-0.043143	-2.352413	-0.786719
O	5.160035	1.553889	-0.194123
O	3.269646	3.299363	0.301946
H	1.970723	-1.600413	-0.645326
H	0.755131	2.442945	0.266701
H	4.346438	-0.924602	-0.663033
H	-0.718475	-3.049498	-0.910938
H	-2.621826	2.943841	0.814625
H	-6.240800	0.588435	0.498352
H	5.095709	2.509734	0.015561
H	2.041103	4.528733	0.935203
H	-4.364904	-2.275894	-0.403619
H	-6.135123	2.796826	1.075384
O	1.326367	5.105648	1.280319
O	0.218466	4.706879	0.435109
C	0.080252	5.701084	-0.566737
H	0.963061	5.742012	-1.214669
H	-0.094145	6.683708	-0.118557

H	-0.793697	5.399068	-1.150132

B3LYP reactant complex (3OH)

C	1.520985	1.563528	-0.309869
C	1.230936	0.188383	-0.203892
C	2.295879	-0.728116	-0.242992
C	3.604171	-0.275343	-0.383448
C	3.875219	1.081626	-0.486174
C	2.823252	2.010074	-0.448965
C	-0.163853	-0.239727	-0.056773
C	-0.655673	-1.513792	0.070416
C	-2.083586	-1.752520	0.210705
C	-2.933923	-0.593353	0.207964
C	-2.370617	0.685010	0.075108
O	-1.028836	0.828747	-0.051980
C	-4.346383	-0.704337	0.339599
C	-5.129753	0.441386	0.333682
C	-4.523056	1.698509	0.198244
C	-3.142852	1.839623	0.067369
O	-4.921654	-1.906607	0.468791
O	-5.258190	2.841513	0.188401
O	-2.513791	-2.924278	0.326326
O	0.148702	-2.596642	0.072114
O	5.129920	1.622396	-0.627029
O	3.076448	3.345144	-0.548861
H	2.103109	-1.785103	-0.164104
H	0.731947	2.300562	-0.284671
H	4.421043	-0.990517	-0.413102
H	-0.396140	-3.404560	0.174485
H	-2.692095	2.816209	-0.036353
H	-6.204888	0.342724	0.433824
H	5.790338	0.922919	-0.642637
H	4.030931	3.458374	-0.640363
H	-4.190553	-2.574035	0.445865
H	-6.190918	2.621848	0.284040
O	-0.729521	-5.307879	0.321518
O	-1.014057	-5.525996	1.587350
C	-1.820655	-6.719790	1.741748
H	-1.949673	-6.841007	2.816073
H	-1.289739	-7.566253	1.306154
H	-2.777171	-6.559950	1.244600

B3LYP Transition state (3OH)

C	1.447002	1.291296	-0.610044
C	1.208234	0.069969	0.058197
C	2.312761	-0.714439	0.445104
C	3.604477	-0.291203	0.159332
C	3.823237	0.908178	-0.506506
C	2.733033	1.708645	-0.893602
C	-0.167951	-0.335546	0.320977
C	-0.618559	-1.574422	0.789093
C	-2.066115	-1.803930	0.952494
C	-2.936058	-0.697214	0.638873
C	-2.399830	0.524366	0.207520
O	-1.053194	0.671051	0.070824
C	-4.349855	-0.800737	0.771400
C	-5.155198	0.291903	0.469825
C	-4.571107	1.488779	0.040055
C	-3.187408	1.623288	-0.096490

O	-4.909709	-1.940645	1.185601
O	-5.320080	2.578301	-0.265172
O	-2.497537	-2.911577	1.331167
O	0.209798	-2.527165	1.113548
O	5.055367	1.407213	-0.830554
O	2.938283	2.885176	-1.544950
H	2.151843	-1.642183	0.968643
H	0.627839	1.922723	-0.921259
H	4.450673	-0.899444	0.464161
H	0.037933	-3.586666	0.671529
H	-2.750879	2.554886	-0.426884
H	-6.229858	0.194192	0.574758
H	5.746878	0.800750	-0.546449
H	3.890156	3.004306	-1.655302
H	-4.166736	-2.575743	1.351480
H	-6.252636	2.373634	-0.137463
O	-0.103361	-4.642522	0.082020
O	-0.594712	-5.516719	1.015877
C	-1.883232	-5.976998	0.602109
H	-2.182338	-6.705451	1.356590
H	-1.809186	-6.445394	-0.382383
H	-2.571253	-5.129900	0.579534

B3LYP product complex (3OH)

C	1.481641	1.396641	-0.230723
C	1.169436	0.017960	-0.323692
C	2.228362	-0.912094	-0.438075
C	3.541975	-0.470336	-0.462402
C	3.831703	0.887376	-0.377350
C	2.789907	1.830856	-0.260988
C	-0.210121	-0.401361	-0.274349
C	-0.708174	-1.740655	-0.482380
C	-2.192220	-1.972414	-0.316684
C	-3.002302	-0.818389	-0.026387
C	-2.418982	0.451272	0.113608
O	-1.067206	0.616373	-0.006240
C	-4.415390	-0.927269	0.120637
C	-5.175680	0.206815	0.393663
C	-4.545882	1.446562	0.522819
C	-3.158220	1.586355	0.384827
O	-5.019439	-2.108106	-0.003675
O	-5.239446	2.578656	0.788426
O	-2.656692	-3.111318	-0.449045
O	0.024010	-2.693486	-0.792763
O	5.089575	1.415165	-0.395464
O	3.070529	3.157718	-0.179004
H	2.007607	-1.965113	-0.501592
H	0.699942	2.136472	-0.139405
H	4.351273	-1.189267	-0.543541
H	-0.160866	-4.417800	-0.070733
H	-2.687932	2.553211	0.492290
H	-6.249397	0.103269	0.500597
H	5.747802	0.716266	-0.471622
H	4.029375	3.266903	-0.214475
H	-4.313324	-2.775765	-0.198834
H	-6.177788	2.373892	0.866390
O	0.025089	-5.174160	0.518621
O	-0.545807	-4.685327	1.758948
C	-1.735728	-5.422520	1.976471
H	-2.115425	-5.065629	2.938434

H	-1.528765	-6.496160	2.039390
H	-2.471568	-5.228878	1.189545

B3LYP reactant complex (5OH)

C	1.619853	1.576976	-0.254143
C	1.221772	0.226259	-0.260299
C	2.205371	-0.767537	-0.396426
C	3.545125	-0.412731	-0.520216
C	3.924926	0.922122	-0.510788
C	2.953375	1.926523	-0.377076
C	-0.198535	-0.106017	-0.123814
C	-0.782746	-1.338631	-0.069937
C	-2.221905	-1.496974	0.078733
C	-2.998529	-0.294064	0.162018
C	-2.342360	0.949206	0.097846
O	-0.992125	1.013138	-0.038923
C	-4.414302	-0.309512	0.307441
C	-5.106423	0.893635	0.377945
C	-4.412126	2.107887	0.308434
C	-3.025945	2.154698	0.168410
O	-5.104243	-1.451007	0.377166
O	-5.060250	3.300213	0.374522
O	-2.687717	-2.657101	0.124691
O	-0.101816	-2.508126	-0.143912
O	5.218035	1.370221	-0.625540
O	3.314579	3.239650	-0.367471
H	1.927290	-1.809068	-0.405689
H	0.892448	2.368965	-0.152285
H	4.300427	-1.186038	-0.625147
H	-0.806208	-3.184014	-0.075772
H	-2.504153	3.099438	0.116151
H	-6.184867	0.867138	0.487399
H	5.819627	0.624574	-0.713778
H	4.274225	3.283052	-0.465174
H	-4.497637	-2.222024	0.322421
H	-6.006207	3.144300	0.466221
O	-5.200058	-4.451027	0.604757
O	-4.835688	-4.714135	1.842345
C	-4.854038	-6.139279	2.100835
H	-4.556384	-6.248524	3.142850
H	-4.143552	-6.628983	1.434598
H	-5.863163	-6.517832	1.936486

B3LYP transition state (5OH)

C	1.553127	1.611548	-0.685399
C	1.369896	0.311580	-0.175023
C	2.486881	-0.533843	-0.059652
C	3.745428	-0.085022	-0.446074
C	3.913006	1.198331	-0.948132
C	2.806426	2.055015	-1.069073
C	0.030662	-0.125335	0.218189
C	-0.365832	-1.337411	0.708086
C	-1.765748	-1.637575	1.040442
C	-2.713488	-0.573005	0.821316
C	-2.231015	0.656817	0.340569
O	-0.918212	0.848763	0.048342
C	-4.128347	-0.682549	1.105178
C	-4.940776	0.458603	0.888644
C	-4.408859	1.652988	0.421655
C	-3.046297	1.767209	0.133037
O	-4.692279	-1.742354	1.570023

O	-5.169527	2.759886	0.212395
O	-1.994782	-2.774056	1.478647
O	0.464437	-2.372042	0.932416
O	5.110827	1.730393	-1.354438
O	2.959800	3.315184	-1.560397
H	2.373325	-1.533565	0.327796
H	0.718612	2.289694	-0.789000
H	4.604415	-0.743083	-0.354381
H	-0.147511	-3.065690	1.271730
H	-2.631830	2.694585	-0.236150
H	-5.997632	0.357211	1.109304
H	5.816101	1.086145	-1.238473
H	3.894132	3.440286	-1.769674
H	-4.381898	-2.914851	1.358954
H	-6.082891	2.566810	0.449879
O	-4.393578	-4.014881	0.997963
O	-5.561898	-4.535922	1.501399
C	-5.916963	-5.677674	0.722835
H	-6.827214	-6.063431	1.181719
H	-5.117917	-6.421551	0.765367
H	-6.100291	-5.379970	-0.312624

B3LYP product complex (5OH)

C	1.526475	1.691780	-0.296207
C	1.334221	0.296160	-0.262006
C	2.458731	-0.545170	-0.327406
C	3.733708	0.000938	-0.424882
C	3.910533	1.377599	-0.459347
C	2.795845	2.231966	-0.394302
C	-0.019662	-0.240461	-0.157976
C	-0.430637	-1.549015	-0.154074
C	-1.842618	-1.940467	-0.043507
C	-2.782326	-0.852534	0.067366
C	-2.294075	0.450162	0.053424
O	-0.976258	0.735269	-0.056180
C	-4.238636	-1.049763	0.191431
C	-5.062940	0.142310	0.292808
C	-4.516650	1.407936	0.273786
C	-3.125290	1.579163	0.153366
O	-4.756194	-2.173858	0.208740
O	-5.245910	2.548766	0.365667
O	-2.073746	-3.157189	-0.058493
O	0.402997	-2.592490	-0.249010
O	5.121764	2.009087	-0.555032
O	2.957534	3.581500	-0.427379
H	2.339804	-1.616303	-0.301417
H	0.688032	2.371292	-0.247782
H	4.598151	-0.654096	-0.474074
H	-0.205753	-3.367112	-0.209973
H	-2.695693	2.571665	0.138969
H	-6.131086	-0.021148	0.383898
H	5.834294	1.363140	-0.593617
H	3.902549	3.768241	-0.496928
H	-3.594399	-4.253817	0.615475
H	-6.180851	2.330009	0.447683
O	-3.925732	-5.085984	1.001085
O	-4.487661	-4.610667	2.249299
C	-5.895184	-4.672505	2.111268
H	-6.286765	-4.360956	3.084510
H	-6.226557	-5.694374	1.895008

H	-6.248618	-3.991258	1.331144

B3LYP reactant complex (7OH)

C	1.768413	1.512553	-0.382485
C	1.310591	0.191782	-0.210654
C	2.254976	-0.845110	-0.126590
C	3.614400	-0.561079	-0.212366
C	4.052821	0.744843	-0.381258
C	3.121337	1.791625	-0.467064
C	-0.129190	-0.065069	-0.123135
C	-0.769739	-1.259146	0.054813
C	-2.218085	-1.338942	0.125444
C	-2.940042	-0.111305	-0.000633
C	-2.231909	1.090270	-0.183744
O	-0.873238	1.083796	-0.239869
C	-4.361186	-0.062520	0.054615
C	-5.013635	1.153061	-0.072062
C	-4.269604	2.333009	-0.252965
C	-2.872752	2.312292	-0.311209
O	-5.070526	-1.187872	0.229227
O	-4.867500	3.533568	-0.378269
O	-2.747033	-2.466990	0.292938
O	-0.135788	-2.451014	0.182234
O	5.369436	1.123750	-0.476324
O	3.540695	3.076804	-0.632604
H	1.931582	-1.864973	0.005209
H	1.072477	2.335827	-0.451505
H	4.338923	-1.367465	-0.146592
H	-0.867087	-3.089867	0.295281
H	-2.314678	3.227161	-0.450615
H	-6.095121	1.179239	-0.032817
H	5.940730	0.352363	-0.410659
H	4.505494	3.070176	-0.670030
H	-4.427314	-1.932081	0.295866
H	-5.834913	3.444594	-0.309844
O	-7.721726	3.368591	-0.119813
O	-7.972562	3.598798	1.150569
C	-9.397073	3.536803	1.426863
H	-9.756501	2.535519	1.190800
H	-9.903735	4.288264	0.821931
H	-9.487803	3.752047	2.489836

B3LYP transition state (7OH)

C	1.594482	1.583974	-0.250514
C	1.233547	0.221341	-0.240291
C	2.249862	-0.750356	-0.285733
C	3.583688	-0.363080	-0.338525
C	3.926631	0.982726	-0.346693
C	2.922329	1.966310	-0.302591
C	-0.179110	-0.142924	-0.180382
C	-0.734396	-1.399608	-0.140265
C	-2.171338	-1.599677	-0.069940
C	-2.982193	-0.425058	-0.039506
C	-2.363802	0.839652	-0.091448
O	-1.005574	0.945251	-0.160941
C	-4.416105	-0.491631	0.034417
C	-5.160770	0.665394	0.045521
C	-4.519368	1.938030	0.000678
C	-3.092212	2.009913	-0.063824
O	-5.019379	-1.687241	0.077940

O	-5.181933	3.045176	-0.000123
O	-2.601580	-2.779935	-0.034257
O	-0.017185	-2.540992	-0.156550
O	5.207915	1.462276	-0.395850
O	3.248567	3.285803	-0.310710
H	2.000870	-1.799078	-0.279586
H	0.841496	2.357828	-0.217112
H	4.363936	-1.117284	-0.373366
H	-0.699605	-3.243382	-0.115701
H	-2.611090	2.977636	-0.091431
H	-6.240718	0.610197	0.082104
H	5.837410	0.734658	-0.423461
H	4.210845	3.356848	-0.350405
H	-4.320927	-2.380590	0.050796
H	-6.343311	2.965236	0.412909
O	-7.373556	2.918727	0.937145
O	-8.136455	3.822201	0.212415
C	-9.193553	4.281573	1.048056
H	-8.784877	4.800849	1.918706
H	-9.811106	3.439099	1.370128
H	-9.771538	4.966108	0.426979

B3LYP product complex (7OH)

C	1.642925	1.579303	-0.139711
C	1.235752	0.237925	-0.295962
C	2.207045	-0.738092	-0.587252
C	3.542003	-0.375532	-0.716940
C	3.930501	0.949050	-0.561341
C	2.971434	1.937084	-0.269404
C	-0.175451	-0.098215	-0.151665
C	-0.778448	-1.332231	-0.275378
C	-2.205594	-1.510661	-0.103996
C	-2.970755	-0.337601	0.202638
C	-2.302280	0.897528	0.316829
O	-0.951780	0.982890	0.140803
C	-4.403963	-0.392258	0.395427
C	-5.101089	0.750416	0.686108
C	-4.420697	2.016748	0.804757
C	-2.977981	2.060311	0.609456
O	-5.034381	-1.568677	0.285999
O	-5.021256	3.085384	1.071568
O	-2.676284	-2.666543	-0.233977
O	-0.109997	-2.463478	-0.562447
O	5.214387	1.403448	-0.669717
O	3.342151	3.233918	-0.115192
H	1.923329	-1.770476	-0.710849
H	0.926191	2.355672	0.084102
H	4.287532	-1.131929	-0.941412
H	-0.807802	-3.151902	-0.581622
H	-2.469532	3.010501	0.698571
H	-6.173857	0.724519	0.828349
H	5.814606	0.677823	-0.869954
H	4.298145	3.292874	-0.239516
H	-4.368876	-2.259991	0.073289
H	-6.840719	2.960633	1.239197
O	-7.783321	2.701544	1.320326
O	-8.272791	3.037833	-0.004694
C	-9.161868	4.126447	0.155069
H	-8.646529	5.017950	0.531611
H	-9.988374	3.869132	0.825954

H	-9.550192	4.320779	-0.848400

MPWB1K reactant complex (4'OH)

C	1.503335	1.447890	-0.135252
C	1.170392	0.094116	-0.198563
C	2.183876	-0.843085	-0.353685
C	3.498768	-0.434187	-0.440494
C	3.820246	0.902389	-0.372942
C	2.810266	1.849718	-0.220048
C	-0.225320	-0.297563	-0.103107
C	-0.739720	-1.546496	-0.048295
C	-2.156245	-1.762789	0.049432
C	-2.978523	-0.604437	0.090140
C	-2.385765	0.652454	0.034563
O	-1.056880	0.769387	-0.058774
C	-4.379077	-0.696759	0.187131
C	-5.132346	0.452033	0.224303
C	-4.501827	1.689627	0.166325
C	-3.129130	1.810483	0.071193
O	-4.971160	-1.876567	0.242194
O	-5.207152	2.827165	0.200393
O	-2.575580	-2.926977	0.097716
O	-0.010172	-2.669315	-0.076842
O	5.065239	1.405993	-0.445693
O	3.129232	3.153126	-0.155234
H	1.951623	-1.888113	-0.409798
H	0.743198	2.198345	-0.017282
H	4.285243	-1.161322	-0.564134
H	-0.666104	-3.375123	-0.017890
H	-2.661850	2.776616	0.026612
H	-6.204617	0.372923	0.298370
H	5.720320	0.706696	-0.516109
H	4.079991	3.217800	-0.231090
H	-4.276917	-2.558435	0.204161
H	-6.135802	2.626989	0.265141
O	7.008118	-0.687910	-0.622391
O	7.359528	-0.982849	0.575445
C	8.350244	-2.008128	0.589600
H	8.564899	-2.187215	1.633908
H	9.228145	-1.653850	0.063819
H	7.946419	-2.893329	0.114390

MPWB1K transition state (4'OH)

C	1.539372	1.172888	0.183036
C	1.117540	-0.149244	0.323531
C	2.065310	-1.159399	0.554902
C	3.394200	-0.853399	0.651237
C	3.829322	0.467129	0.506316
C	2.870555	1.479686	0.261111
C	-0.296386	-0.437381	0.229996
C	-0.915934	-1.640397	0.304245
C	-2.350700	-1.747917	0.181631
C	-3.067445	-0.539001	-0.016114
C	-2.368292	0.662669	-0.081066
O	-1.036751	0.679767	0.039664
C	-4.470102	-0.518787	-0.145919
C	-5.115836	0.679432	-0.332349
C	-4.379004	1.856909	-0.390983
C	-3.002522	1.867647	-0.267499

O	-5.166219	-1.639345	-0.089269
O	-4.976040	3.039045	-0.570607
O	-2.859530	-2.871541	0.255168
O	-0.294165	-2.803716	0.487780
O	5.066019	0.846467	0.584206
O	3.306526	2.726743	0.115586
H	1.744157	-2.176208	0.666710
H	0.833876	1.961469	-0.000081
H	4.129535	-1.617953	0.835549
H	-1.005838	-3.457637	0.490623
H	-2.451702	2.788569	-0.315015
H	-6.189057	0.685386	-0.430071
H	5.742818	0.047476	0.143902
H	4.263082	2.688406	0.198893
H	-4.544901	-2.373966	0.046621
H	-5.918250	2.918883	-0.641099
O	6.380998	-0.774528	-0.486015
O	7.489299	-0.984472	0.240707
C	8.589688	-1.081695	-0.624457
H	9.445603	-1.280213	0.008705
H	8.722045	-0.148296	-1.164350
H	8.438395	-1.896026	-1.327008

MPWB1K product complex (4'OH)

C	1.615603	1.337380	-0.380399
C	1.256774	-0.011066	-0.348053
C	2.256256	-1.015759	-0.484625
C	3.558925	-0.694903	-0.648254
C	3.964017	0.672341	-0.682123
C	2.928183	1.678141	-0.541311
C	-0.127611	-0.355047	-0.172969
C	-0.681608	-1.594190	-0.088585
C	-2.106820	-1.762422	0.098454
C	-2.883604	-0.580624	0.183232
C	-2.253483	0.658178	0.086065
O	-0.928041	0.735300	-0.082823
C	-4.280836	-0.624817	0.361711
C	-4.991470	0.548479	0.434433
C	-4.324434	1.763299	0.331936
C	-2.953818	1.837344	0.157778
O	-4.910635	-1.780278	0.459016
O	-4.982374	2.922972	0.397587
O	-2.545551	-2.913956	0.170565
O	-0.008367	-2.734991	-0.161079
O	5.126145	1.078458	-0.826609
O	3.336632	2.928933	-0.580495
H	1.965012	-2.047537	-0.457281
H	0.876029	2.109477	-0.280175
H	4.320802	-1.449407	-0.742556
H	-0.683401	-3.421577	-0.064147
H	-2.459753	2.788002	0.080960
H	-6.059564	0.505624	0.570351
H	6.389796	-0.241226	-1.044280
H	4.294110	2.879826	-0.703282
H	-4.254693	-2.492590	0.386037
H	-5.914039	2.763459	0.516074
O	6.865649	-1.083182	-1.056530
O	6.558544	-1.591019	0.218974
C	7.681906	-1.397141	1.023101
H	7.435620	-1.846615	1.979881
H	7.892737	-0.337558	1.159423

H	8.552498	-1.890341	0.597706

MPWB1K reactant complex (3'OH)

C	1.587176	1.533475	0.157016
C	1.210092	0.216732	-0.115935
C	2.199364	-0.726567	-0.365235
C	3.529627	-0.362275	-0.345317
C	3.896186	0.937804	-0.082456
C	2.909263	1.889067	0.169205
C	-0.201101	-0.120184	-0.124715
C	-0.783043	-1.281551	-0.499987
C	-2.209234	-1.444774	-0.459792
C	-2.969056	-0.327927	-0.011728
C	-2.308815	0.836624	0.360373
O	-0.976006	0.909613	0.293716
C	-4.373094	-0.372515	0.070370
C	-5.061993	0.731913	0.513720
C	-4.363955	1.876589	0.878517
C	-2.986672	1.948535	0.808359
O	-5.030862	-1.463697	-0.276015
O	-5.004658	2.968968	1.316366
O	-2.694889	-2.525535	-0.817037
O	-0.110974	-2.353677	-0.935980
O	5.183418	1.301870	-0.065189
O	3.373152	3.131823	0.417634
H	1.933073	-1.744692	-0.572227
H	0.838604	2.278653	0.360495
H	4.304058	-1.085802	-0.535264
H	-0.798455	-3.002682	-1.128550
H	-2.464484	2.837682	1.109607
H	-6.137295	0.688789	0.572842
H	5.212041	2.238119	0.130695
H	2.648026	3.753777	0.518670
H	-4.376757	-2.127347	-0.559293
H	-5.941924	2.801992	1.340073
O	1.114138	4.891782	0.572443
O	0.969416	5.378285	-0.605376
C	-0.218918	6.159981	-0.704681
H	-0.185033	6.945211	0.040008
H	-1.076499	5.516628	-0.549942
H	-0.213689	6.566778	-1.706319

MPWB1K transition state (3'OH)

C	1.185466	1.628408	-0.535277
C	0.978341	0.284553	-0.288182
C	2.088758	-0.571739	-0.200716
C	3.370300	-0.095072	-0.345388
C	3.579236	1.248295	-0.573791
C	2.475064	2.126420	-0.683932
C	-0.381166	-0.201248	-0.127125
C	-0.805626	-1.472204	0.042698
C	-2.209265	-1.773297	0.186407
C	-3.106398	-0.672703	0.140436
C	-2.598630	0.610421	-0.038426
O	-1.282243	0.805524	-0.167965
C	-4.497786	-0.841381	0.274504
C	-5.320945	0.257943	0.227063
C	-4.771841	1.522599	0.047176

C	-3.411015	1.718388	-0.088337
O	-5.015162	-2.044585	0.445301
O	-5.545706	2.612046	-0.002481
O	-2.543201	-2.953486	0.338025
O	-0.003659	-2.539621	0.091818
O	4.793276	1.755627	-0.703337
O	2.754981	3.373531	-0.928197
H	1.936029	-1.617727	-0.016416
H	0.362670	2.315509	-0.610324
H	4.219033	-0.752507	-0.269373
H	-0.605749	-3.284484	0.215923
H	-3.005222	2.703564	-0.224947
H	-6.384649	0.119305	0.330976
H	4.673933	2.699766	-0.847746
H	2.069806	4.049950	-0.309608
H	-4.285653	-2.686994	0.452484
H	-6.459410	2.363807	0.100372
O	1.438432	4.689629	0.488016
O	1.037806	5.783000	-0.179421
C	1.294732	6.917565	0.605940
H	2.362936	7.018606	0.776724
H	0.774923	6.837146	1.556013
H	0.919407	7.759678	0.037689

MPWB1K product complex (3'OH)

C	1.488625	1.678462	0.059058
C	1.175358	0.371651	-0.189981
C	2.211370	-0.562992	-0.457003
C	3.532417	-0.191252	-0.477443
C	3.864852	1.123926	-0.229182
C	2.840813	2.105281	0.050258
C	-0.222894	-0.032543	-0.170655
C	-0.749296	-1.250172	-0.413396
C	-2.178054	-1.464877	-0.344145
C	-2.976011	-0.339941	-0.013264
C	-2.361029	0.888050	0.221538
O	-1.031822	1.003051	0.135495
C	-4.377793	-0.428692	0.089715
C	-5.103039	0.690769	0.416264
C	-4.447760	1.897288	0.641308
C	-3.073531	2.016639	0.547709
O	-4.997391	-1.575451	-0.124733
O	-5.127823	3.002006	0.960195
O	-2.604877	-2.600448	-0.574738
O	-0.044970	-2.339098	-0.728208
O	5.100906	1.558326	-0.227217
O	3.222335	3.271575	0.268156
H	1.952214	-1.587109	-0.648281
H	0.732844	2.419073	0.253696
H	4.309350	-0.907541	-0.680877
H	-0.711010	-3.031418	-0.834770
H	-2.577026	2.952554	0.730455
H	-6.175274	0.614446	0.493502
H	5.039192	2.502508	-0.023383
H	1.947568	4.451767	0.940597
H	-4.328125	-2.245126	-0.340586
H	-6.059140	2.807683	1.005580
O	1.195330	4.946696	1.294473
O	0.178300	4.626755	0.379724
C	0.067603	5.697201	-0.510597
H	0.977097	5.817945	-1.096568

H	-0.147933	6.619220	0.022828
H	-0.760388	5.448258	-1.166724

MPWB1K reactant complex (3OH)

C	1.487888	1.531171	-0.394120
C	1.237278	0.174256	-0.191133
C	2.310307	-0.705881	-0.129292
C	3.599276	-0.232867	-0.269879
C	3.834109	1.105884	-0.473213
C	2.769564	1.997097	-0.535579
C	-0.142417	-0.268244	-0.047423
C	-0.609730	-1.535596	0.024232
C	-2.022858	-1.792290	0.153257
C	-2.874590	-0.650075	0.199721
C	-2.321506	0.622660	0.123641
O	-1.000801	0.776426	0.003685
C	-4.270845	-0.776347	0.325053
C	-5.054290	0.352136	0.370413
C	-4.459793	1.606483	0.292298
C	-3.093907	1.761667	0.167959
O	-4.830512	-1.971379	0.398624
O	-5.195164	2.724875	0.334374
O	-2.426659	-2.958444	0.211213
O	0.184510	-2.604505	-0.027338
O	5.059041	1.663698	-0.624463
O	2.998045	3.306322	-0.733886
H	2.144831	-1.752556	0.029127
H	0.682928	2.240819	-0.445584
H	4.431079	-0.919182	-0.219553
H	-0.366424	-3.395852	0.037166
H	-2.651734	2.738865	0.109387
H	-6.122393	0.243733	0.465807
H	5.736062	0.997094	-0.574657
H	3.942056	3.431281	-0.809613
H	-4.113128	-2.629742	0.344974
H	-6.116350	2.499348	0.419356
O	-0.679080	-5.376092	0.277764
O	-1.081086	-5.404393	1.496616
C	-1.973958	-6.488213	1.719190
H	-2.197185	-6.471483	2.777441
H	-1.487413	-7.413765	1.435729
H	-2.869846	-6.328139	1.131871

MPWB1K transition state (3OH)

C	1.411695	1.236521	-0.637523
C	1.189314	0.054313	0.073992
C	2.283679	-0.692654	0.502057
C	3.562175	-0.267831	0.212744
C	3.767757	0.891587	-0.498207
C	2.682963	1.653225	-0.926808
C	-0.176580	-0.345304	0.335262
C	-0.613390	-1.569276	0.806915
C	-2.046641	-1.807690	0.952359
C	-2.909473	-0.706251	0.651176
C	-2.374350	0.504164	0.231686
O	-1.046635	0.642983	0.084231
C	-4.306712	-0.807925	0.788923
C	-5.102858	0.279969	0.506910
C	-4.521913	1.468804	0.090964
C	-3.152045	1.599314	-0.054082

O	-4.860120	-1.936526	1.188654
O	-5.262405	2.546687	-0.190273
O	-2.460519	-2.912222	1.296540
O	0.198830	-2.513569	1.123564
O	4.978080	1.388060	-0.830858
O	2.887596	2.783967	-1.619945
H	2.131949	-1.591384	1.065163
H	0.588703	1.836509	-0.980178
H	4.409415	-0.844198	0.551624
H	0.038784	-3.567083	0.612003
H	-2.716393	2.526835	-0.376269
H	-6.170867	0.186279	0.617350
H	5.673174	0.817428	-0.518828
H	3.829917	2.903529	-1.722130
H	-4.136403	-2.574564	1.337753
H	-6.184352	2.347642	-0.058049
O	-0.149467	-4.554184	0.026393
O	-0.611697	-5.420218	0.933392
C	-1.865320	-5.900468	0.522204
H	-2.191041	-6.571184	1.307744
H	-1.762983	-6.435747	-0.417801
H	-2.551145	-5.068780	0.415005

MPWB1K product complex (3OH)

C	1.530297	1.168554	0.015262
C	1.284939	-0.144068	-0.411154
C	2.359509	-0.930778	-0.833181
C	3.633768	-0.411077	-0.828312
C	3.859577	0.880620	-0.408659
C	2.797780	1.679151	0.017670
C	-0.060564	-0.634559	-0.395772
C	-0.503355	-1.920883	-0.822930
C	-1.968210	-2.212226	-0.736505
C	-2.805907	-1.187527	-0.205740
C	-2.257612	0.026407	0.194267
O	-0.936996	0.259989	0.078069
C	-4.194409	-1.373877	-0.065116
C	-4.973451	-0.366763	0.463031
C	-4.380897	0.824430	0.848197
C	-3.015897	1.037889	0.720491
O	-4.759620	-2.507177	-0.430099
O	-5.095185	1.828373	1.362506
O	-2.383362	-3.300263	-1.107017
O	0.237063	-2.798496	-1.247443
O	5.068257	1.475376	-0.368461
O	3.025530	2.936694	0.424991
H	2.187346	-1.938210	-1.155468
H	0.727533	1.799998	0.347875
H	4.463757	-1.019982	-1.152359
H	-0.799657	-4.438819	-0.085129
H	-2.574509	1.968739	1.024828
H	-6.034468	-0.525960	0.563453
H	5.748954	0.877685	-0.661691
H	3.963139	3.107468	0.359143
H	-4.059192	-3.083039	-0.790283
H	-6.015123	1.584541	1.405386
O	-0.677596	-4.702192	0.833792
O	-1.042130	-3.532419	1.520452
C	-2.278977	-3.781217	2.120783
H	-2.510814	-2.886786	2.690889
H	-2.217296	-4.637357	2.787104

H	-3.050352	-3.956524	1.372372

MPWB1K reactant complex (5OH)

C	1.493110	1.664728	-0.365161
C	1.339029	0.283193	-0.261528
C	2.466532	-0.528115	-0.285848
C	3.718250	0.039214	-0.411638
C	3.859613	1.402732	-0.515025
C	2.737607	2.224653	-0.491833
C	0.001598	-0.265085	-0.126337
C	-0.384957	-1.561134	-0.112240
C	-1.776251	-1.956818	0.024952
C	-2.711666	-0.876467	0.142939
C	-2.234747	0.409366	0.116711
O	-0.944081	0.696097	-0.011953
C	-4.145697	-1.077842	0.279560
C	-4.974116	0.092383	0.389754
C	-4.442821	1.354466	0.364947
C	-3.069882	1.528470	0.226304
O	-4.648897	-2.194358	0.297760
O	-5.173729	2.470762	0.466285
O	-2.014803	-3.153364	0.023229
O	0.449563	-2.586821	-0.220423
O	5.038823	2.051660	-0.642831
O	2.873872	3.555764	-0.593102
H	2.371383	-1.593353	-0.205510
H	0.642414	2.320756	-0.349442
H	4.594153	-0.591184	-0.428423
H	-0.131979	-3.362160	-0.169832
H	-2.645144	2.516453	0.204512
H	-6.033132	-0.081003	0.494207
H	5.763001	1.434290	-0.651938
H	3.805140	3.753932	-0.672290
H	-3.600030	-4.160290	0.790560
H	-6.095520	2.250181	0.563153
O	-3.903998	-4.958722	1.235492
O	-4.702403	-4.444217	2.269284
C	-6.029379	-4.627366	1.883512
H	-6.626823	-4.278080	2.720973
H	-6.238458	-5.679793	1.701610
H	-6.264178	-4.045115	0.994942

MPWB1K transition state (5OH)

C	1.492345	1.146442	0.297174
C	1.183853	-0.069907	-0.308870
C	2.208892	-0.833952	-0.850520
C	3.512570	-0.386188	-0.781755
C	3.806716	0.814818	-0.181353
C	2.788334	1.589008	0.363701
C	-0.203565	-0.498902	-0.363420
C	-0.701445	-1.683428	-0.770822
C	-2.127279	-1.971883	-0.766061
C	-2.972117	-0.897726	-0.318124
C	-2.375358	0.272025	0.121009
O	-1.056353	0.452305	0.085192
C	-4.396506	-0.956627	-0.313887
C	-5.119114	0.105892	0.244568
C	-4.474394	1.231399	0.723346
C	-3.102243	1.334100	0.644569
O	-5.013679	-1.961036	-0.817289

O	-5.136094	2.260051	1.265847
O	-2.468104	-3.092507	-1.106563
O	0.040752	-2.703470	-1.197296
O	5.050029	1.336120	-0.059630
O	3.074739	2.760682	0.952749
H	1.994930	-1.771279	-1.324597
H	0.722328	1.763038	0.722230
H	4.308439	-0.982054	-1.202197
H	-0.617154	-3.390342	-1.387500
H	-2.595693	2.216723	0.990056
H	-6.192321	0.009278	0.289390
H	5.682873	0.804853	-0.531480
H	4.017103	2.900530	0.884195
H	-5.756843	-2.422935	-0.016777
H	-6.072068	2.084096	1.256591
O	-6.282880	-2.718879	0.981918
O	-5.431250	-2.274670	1.920725
C	-4.390867	-3.217048	2.075636
H	-3.703765	-2.787519	2.793982
H	-3.905688	-3.384098	1.115984
H	-4.804766	-4.150158	2.445679

MPWB1K product complex (5OH)

C	1.493110	1.664728	-0.365161
C	1.339029	0.283193	-0.261528
C	2.466532	-0.528115	-0.285848
C	3.718250	0.039214	-0.411638
C	3.859613	1.402732	-0.515025
C	2.737607	2.224653	-0.491833
C	0.001598	-0.265085	-0.126337
C	-0.384957	-1.561134	-0.112240
C	-1.776251	-1.956818	0.024952
C	-2.711666	-0.876467	0.142939
C	-2.234747	0.409366	0.116711
O	-0.944081	0.696097	-0.011953
C	-4.145697	-1.077842	0.279560
C	-4.974116	0.092383	0.389754
C	-4.442821	1.354466	0.364947
C	-3.069882	1.528470	0.226304
O	-4.648897	-2.194358	0.297760
O	-5.173729	2.470762	0.466285
O	-2.014803	-3.153364	0.023229
O	0.449563	-2.586821	-0.220423
O	5.038823	2.051660	-0.642831
O	2.873872	3.555764	-0.593102
H	2.371383	-1.593353	-0.205510
H	0.642414	2.320756	-0.349442
H	4.594153	-0.591184	-0.428423
H	-0.131979	-3.362160	-0.169832
H	-2.645144	2.516453	0.204512
H	-6.033132	-0.081003	0.494207
H	5.763001	1.434290	-0.651938
H	3.805140	3.753932	-0.672290
H	-3.600030	-4.160290	0.790560
H	-6.095520	2.250181	0.563153
O	-3.903998	-4.958722	1.235492
O	-4.702403	-4.444217	2.269284
C	-6.029379	-4.627366	1.883512
H	-6.626823	-4.278080	2.720973
H	-6.238458	-5.679793	1.701610

H	-6.264178	-4.045115	0.994942

MPWB1K reactant complex (7OH)

C	1.493110	1.664728	-0.365161
C	1.339029	0.283193	-0.261528
C	2.466532	-0.528115	-0.285848
C	3.718250	0.039214	-0.411638
C	3.859613	1.402732	-0.515025
C	2.737607	2.224653	-0.491833
C	0.001598	-0.265085	-0.126337
C	-0.384957	-1.561134	-0.112240
C	-1.776251	-1.956818	0.024952
C	-2.711666	-0.876467	0.142939
C	-2.234747	0.409366	0.116711
O	-0.944081	0.696097	-0.011953
C	-4.145697	-1.077842	0.279560
C	-4.974116	0.092383	0.389754
C	-4.442821	1.354466	0.364947
C	-3.069882	1.528470	0.226304
O	-4.648897	-2.194358	0.297760
O	-5.173729	2.470762	0.466285
O	-2.014803	-3.153364	0.023229
O	0.449563	-2.586821	-0.220423
O	5.038823	2.051660	-0.642831
O	2.873872	3.555764	-0.593102
H	2.371383	-1.593353	-0.205510
H	0.642414	2.320756	-0.349442
H	4.594153	-0.591184	-0.428423
H	-0.131979	-3.362160	-0.169832
H	-2.645144	2.516453	0.204512
H	-6.033132	-0.081003	0.494207
H	5.763001	1.434290	-0.651938
H	3.805140	3.753932	-0.672290
H	-3.600030	-4.160290	0.790560
H	-6.095520	2.250181	0.563153
O	-3.903998	-4.958722	1.235492
O	-4.702403	-4.444217	2.269284
C	-6.029379	-4.627366	1.883512
H	-6.626823	-4.278080	2.720973
H	-6.238458	-5.679793	1.701610
H	-6.264178	-4.045115	0.994942

MPWB1K transition state (7OH)

C	1.455575	1.614337	-0.241280
C	1.136075	0.257496	-0.181722
C	2.162512	-0.678729	-0.137008
C	3.476502	-0.261425	-0.152084
C	3.781281	1.077925	-0.210809
C	2.762982	2.025592	-0.255935
C	-0.260358	-0.138989	-0.169888
C	-0.769332	-1.394051	-0.115368
C	-2.186800	-1.626790	-0.112658
C	-3.023211	-0.477459	-0.166117
C	-2.432787	0.784518	-0.223517
O	-1.097974	0.915314	-0.223702
C	-4.437046	-0.588706	-0.171861
C	-5.202500	0.538896	-0.248540
C	-4.589816	1.809981	-0.295660

C	-3.185543	1.928356	-0.264221
O	-5.006724	-1.780722	-0.120420
O	-5.290000	2.879121	-0.390357
O	-2.587865	-2.795784	-0.061755
O	-0.031898	-2.504807	-0.060280
O	5.033294	1.586471	-0.230322
O	3.061919	3.332257	-0.313814
H	1.942029	-1.726587	-0.091185
H	0.684624	2.362137	-0.277542
H	4.272606	-0.989364	-0.117862
H	-0.683028	-3.218717	-0.031681
H	-2.731989	2.902147	-0.291529
H	-6.275205	0.461149	-0.274872
H	5.680135	0.889090	-0.200075
H	4.013300	3.419568	-0.317429
H	-4.306545	-2.453039	-0.084564
H	-6.370109	2.769356	0.177638
O	-7.252247	2.735639	0.875176
O	-8.145208	3.576627	0.320372
C	-8.672834	4.399729	1.326260
H	-7.885769	5.012809	1.756555
H	-9.134457	3.793071	2.099822
H	-9.413693	5.019551	0.836821

MPWB1K product complex (7OH)

C	1.560679	1.585172	-0.185338
C	1.179020	0.248108	-0.301899
C	2.149375	-0.717146	-0.546948
C	3.471216	-0.344864	-0.671135
C	3.837242	0.975787	-0.556143
C	2.874351	1.951705	-0.311636
C	-0.222655	-0.090454	-0.155352
C	-0.811562	-1.306377	-0.310272
C	-2.222114	-1.486299	-0.134059
C	-2.978467	-0.324721	0.212286
C	-2.307010	0.887127	0.352541
O	-0.981032	0.970871	0.167738
C	-4.394418	-0.387519	0.415749
C	-5.079234	0.736404	0.747510
C	-4.394842	1.982242	0.895934
C	-2.973352	2.034615	0.687226
O	-5.020688	-1.543339	0.278367
O	-4.984914	3.030430	1.203850
O	-2.694066	-2.616807	-0.291805
O	-0.151367	-2.416138	-0.634218
O	5.099945	1.438977	-0.662992
O	3.232038	3.238527	-0.200831
H	1.879678	-1.750755	-0.638182
H	0.833891	2.353387	0.004485
H	4.225292	-1.093499	-0.859312
H	-0.834068	-3.099423	-0.673954
H	-2.464528	2.975043	0.800230
H	-6.144939	0.710332	0.898186
H	5.709272	0.727048	-0.830279
H	4.178413	3.298292	-0.317993
H	-4.373371	-2.224945	0.040192
H	-6.824124	2.908736	1.354543
O	-7.755502	2.650849	1.351040
O	-8.127434	2.939347	0.025790
C	-8.929284	4.079160	0.067858

H	-8.372861	4.944510	0.425574
H	-9.799716	3.920304	0.700296
H	-9.246681	4.247440	-0.956423