Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information to:
Proposed Mechanisms for the Formation of an α-O-4 Coniferyl Alcohol Linkage in Lignin: A Density Functional Theory Study

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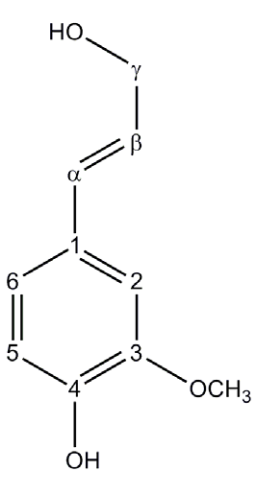
Contents

Structure Notes

1. Compound information for structure **3** is not included in this Supporting Information, because **3** was used in the manuscript as a structural reference point only. No thermodynamic or Fukui function calculations for **3** were performed for this work.
2. For compounds that have chiral C_α, C_β, or both:
    a. (R,R) or (S,S), (R,S) or (S,R) notation is used to specify the stereochemistry of C_α and C_β, respectively. For example, compound information is provided for the four stereoisomers of **5** are given in the following manner: **(R,R)-5**, **(S,S)-5**, **(R,S)-5**, and **(S,R)-5**.
    b. The quinone methide, **4**, has a chiral C_β, but not a chiral C_α; therefore, **(R)-4** and **(S)-4** designate the stereochemistry of C_β for **4**.
    c. When structures have a radical electron centered at C_α or C_β, coupled with a chiral center at C_β or C_α, respectively, only the stereochemistry of the chiral carbon is represented in the structure name. For instance, **9** has a chiral C_α and a radical electron at C_β; therefore, the name given for this structure is either **(R)-9** or **(S)-9**, because **9** has only one chiral carbon.
3. For each compound (pages 7-31), the following results are given.
    a. Total electronic energy in atomic units (au)
    b. Zero-point correction (au)
    c. Sum of electronic and thermal Free Energies (au)
    d. Number of imaginary frequencies: (**0 for all cases**)
    e. Cartesian coordinates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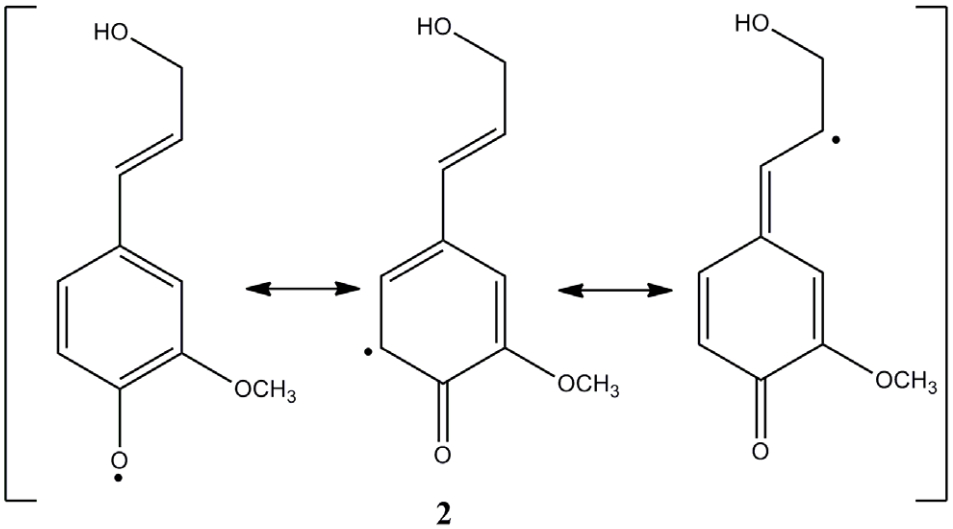
γ
β
α
1
2
3
4
5
6
OCH3
OH

1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O

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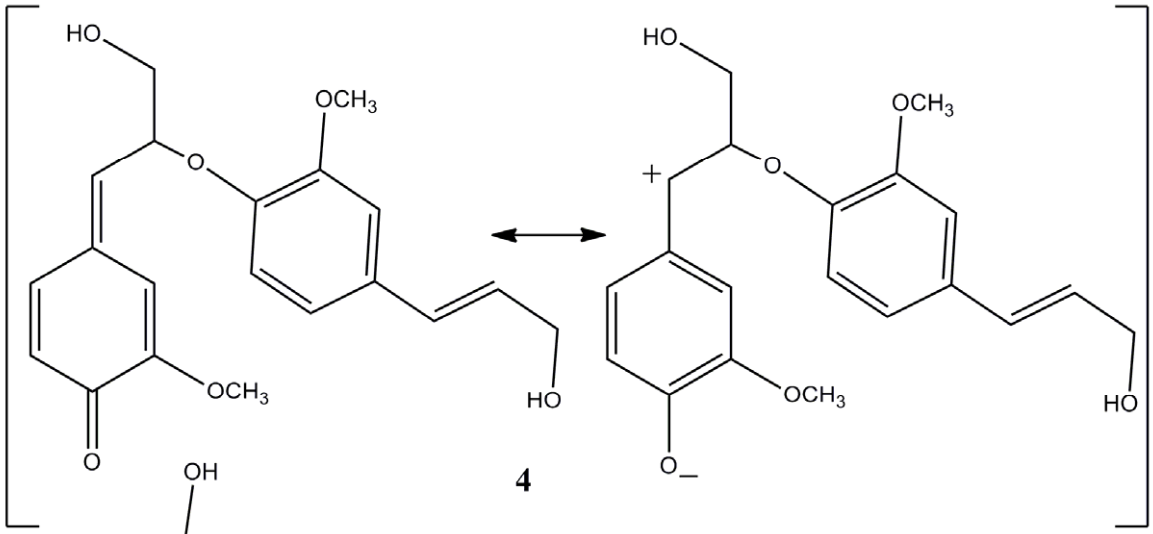
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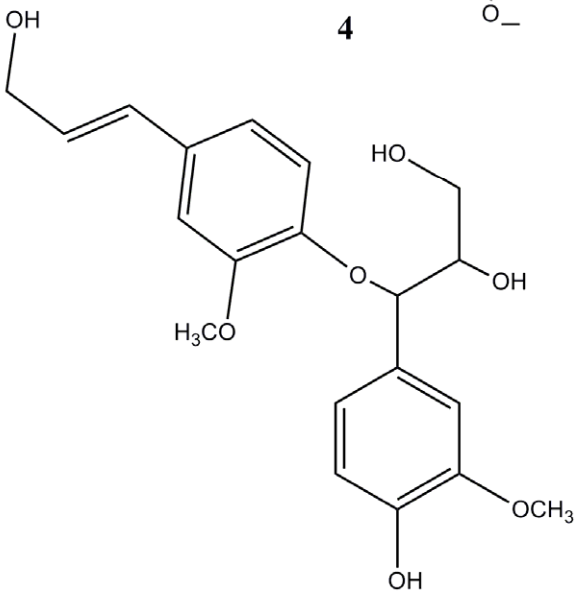
OCH3
O

4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OH
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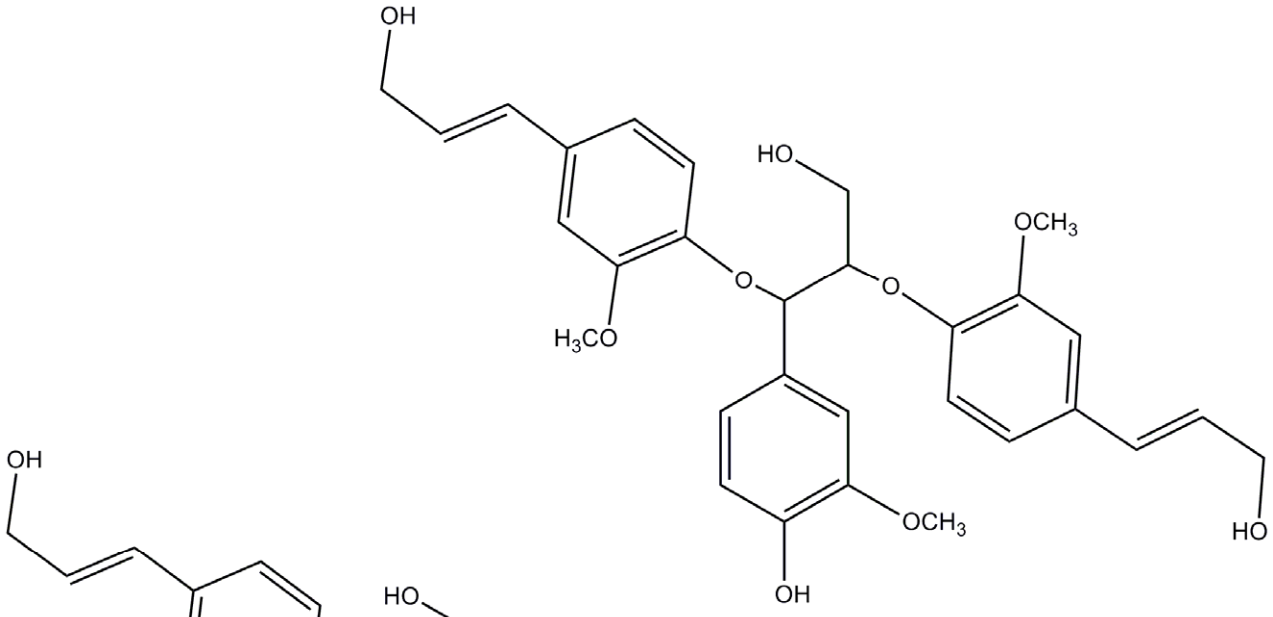
OH

5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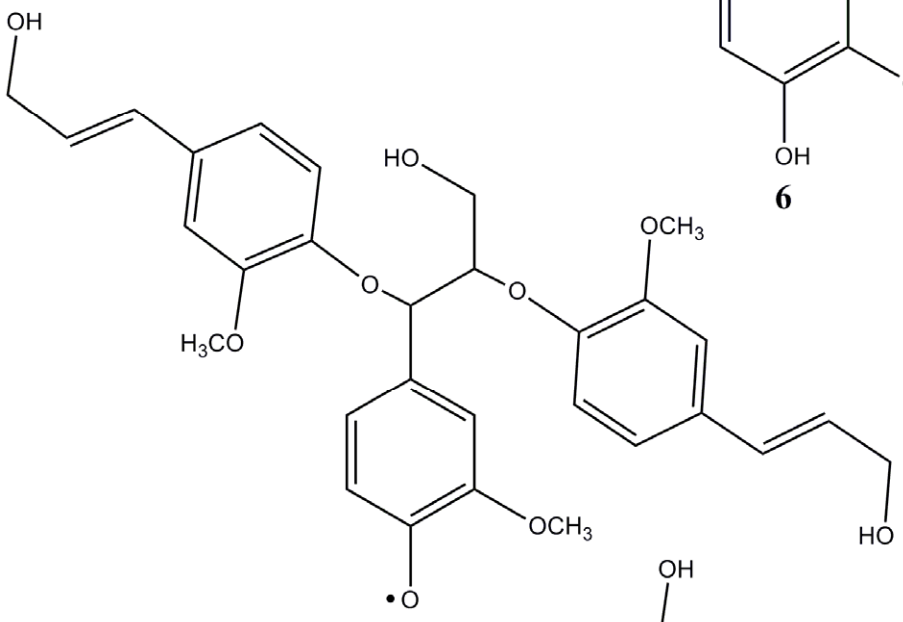
OH

6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O
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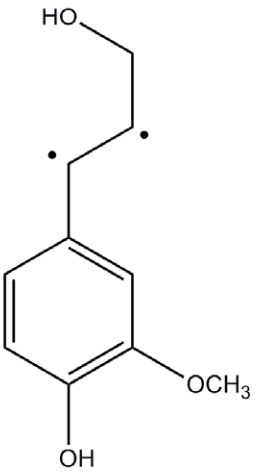
HO
•O

7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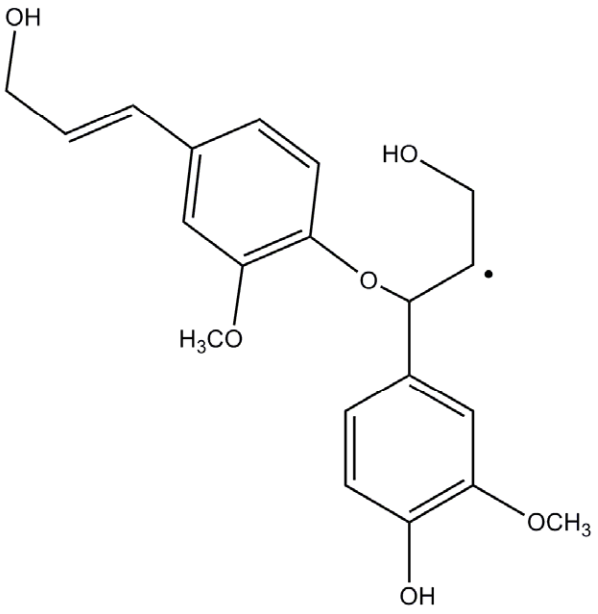
OCH3
OH

8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O
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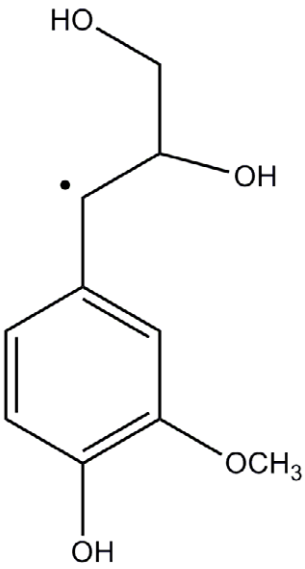
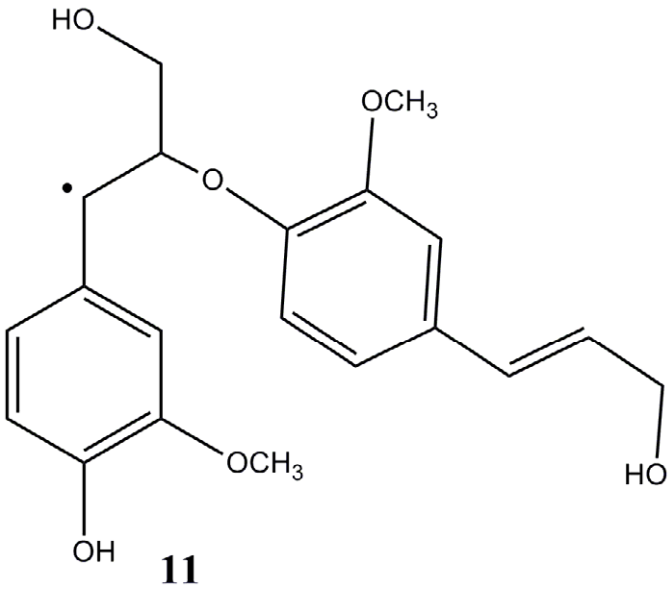
OCH3
OH

9



10



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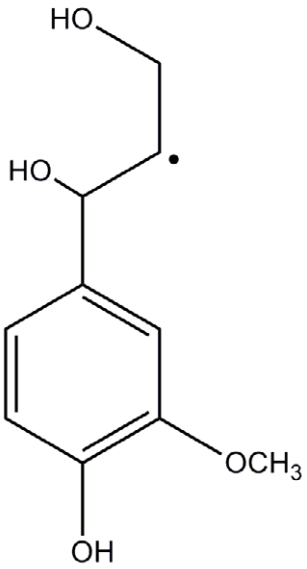

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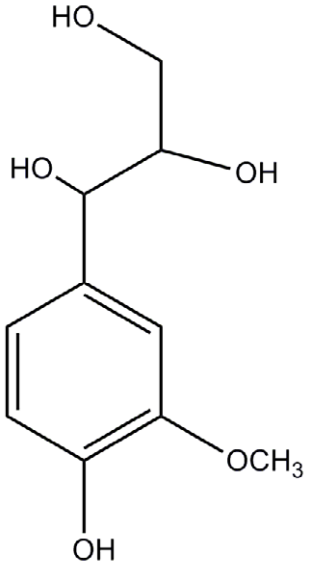

13

Compound Information for **1**
Total electronic energy (au): -614.094943
Zero-point correction (au): 0.202048
Sum of electronic and thermal Free Energies (au): -613.933690
Number of imaginary frequencies: 0

C	-1.467071	0.704401	0.170911
C	-0.338384	0.123421	0.240832
C	0.926584	-1.252502	0.192931
C	1.094111	-2.095434	0.068135
C	0.213819	-1.530283	-0.001433
C	-0.702855	-0.146069	0.049750
C	-0.370154	2.154355	0.224780
C	-0.921359	3.125237	0.319728
C	-2.154481	4.581335	0.335882
O	-2.667943	5.166612	1.526170
H	-0.564511	0.763727	0.337984
O	1.792868	-1.888024	0.257457
O	2.093284	-3.440344	0.023542
H	1.260514	-2.178971	-0.095513
H	-1.763101	0.271377	-0.004431
H	0.717819	2.451202	0.177967
H	-0.804327	2.896704	0.386657
H	-0.893273	4.722150	0.299949
H	0.277714	5.070979	-0.548430
H	-3.842540	6.124433	1.437162
H	-4.668753	-3.900117	-0.057561
C	-3.825422	-1.101357	0.394242
H	-3.977481	-1.809326	0.431370
H	-1.467071	-0.513783	1.318706
H	-0.338384	-0.430787	-0.461704

Compound Information for **2**
Total electronic energy (au): -613.462851
Zero-point correction (au): 0.189489
Sum of electronic and thermal Free Energies (au): -613.314317
Number of imaginary frequencies: 0

C	-0.361064	-0.796165	0.080069
C	0.332633	0.439650	0.079902
C	1.708032	0.484569	0.009287
C	2.512534	-0.759169	-0.063900
C	1.753298	-1.996703	-0.061722
C	0.389965	-2.005663	0.005874
C	-1.805295	-0.888518	0.148433
C	-2.690459	0.124376	0.236892
C	-4.167238	-0.069245	0.345848
O	-4.804191	0.750316	-0.640690
H	-0.234154	1.358939	0.132601
O	2.446112	1.602659	-0.000964
O	3.748083	-0.733407	-0.122997
H	2.330072	-2.912364	-0.117404
H	-0.148157	-2.948020	0.004183
H	-2.200255	-1.902345	0.126042
H	-2.364972	1.160503	0.244563
H	-4.425889	-1.126852	0.208478
H	-4.498658	0.231287	1.351556
H	-5.745546	0.793532	-0.445729
C	1.791729	2.866502	0.058462
H	2.586007	3.609509	0.032075
H	1.128073	3.007029	-0.800610
H	1.221531	2.971442	0.987083

Compound Information for **(R)-4**
Total electronic energy (au): -1226.949685
Zero-point correction (au): 0.385618
Sum of electronic and thermal Free Energies (au): -1226.623875
Number of imaginary frequencies: 0

C	-2.758298	0.225752	-0.690359	C	-4.864477	-3.591923	-4.165584
C	-2.718979	1.668407	-0.866617	C	-4.788616	-2.203518	-4.378752
C	-3.481478	2.498694	-0.110366	C	-3.607867	-1.500679	-4.162480
C	-4.411307	1.974745	0.940367	C	-2.462697	-2.187576	-3.701197
C	-4.426231	0.515674	1.097061	C	-2.530994	-3.560156	-3.506348
C	-3.658269	-0.289352	0.341391	C	-3.712843	-4.260218	-3.738366
C	-2.040463	-0.696658	-1.386556	C	-6.097284	-4.360827	-4.385603
C	-0.999177	-0.597275	-2.461163	C	-7.315982	-3.888021	-4.670286
C	-0.671777	0.739952	-3.127180	C	-8.523696	-4.750233	-4.846729
O	0.347299	0.566205	-4.098741	O	-9.105832	-4.462192	-6.126003
H	-2.067893	2.081737	-1.618500	H	-5.661614	-1.676624	-4.737021
O	-3.507660	3.840120	-0.197664	O	-3.460192	-0.163345	-4.379891
O	-5.107753	2.717156	1.614445	O	-1.245242	-1.562727	-3.544330
H	-5.094339	0.127100	1.856770	H	-1.633916	-4.073110	-3.179533
H	-3.692329	-1.365175	0.479610	H	-3.740492	-5.332658	-3.581285
H	-2.210182	-1.729988	-1.095950	H	-5.979494	-5.438886	-4.290251
H	-0.060389	-0.964302	-2.023998	H	-7.496219	-2.822117	-4.781128
H	-1.570552	1.170338	-3.576632	H	-8.248719	-5.809911	-4.770927
H	-0.263194	1.428259	-2.384274	H	-9.251441	-4.530743	-4.051594
H	0.058089	-0.147472	-4.681136	H	-9.984388	-4.853507	-6.158706
C	-2.653340	4.478007	-1.139328	C	-4.574297	0.573557	-4.873778
H	-2.833056	5.545187	-1.026583	H	-4.224803	1.598375	-4.987403
H	-1.601200	4.258193	-0.929040	H	-4.902106	0.193495	-5.846520
H	-2.893554	4.171721	-2.163106	H	-5.410505	0.551234	-4.167880

Compound Information for **(S)-4**

Total electronic energy (au): -1226.958254
Zero-point correction (au): 0.384964
Sum of electronic and thermal Free Energies (au): -1226.633844
Number of imaginary frequencies: 0

C	-2.310428	0.118914	-0.173169	C	-5.097096	-3.484931	-4.060555
C	-2.710475	1.451418	-0.591567	C	-4.710179	-2.244578	-4.601060
C	-3.359561	2.291633	0.251934	C	-3.482155	-1.672725	-4.290155
C	-3.704728	1.883546	1.649940	C	-2.609869	-2.333173	-3.394380
C	-3.274069	0.534731	2.042940	C	-2.984384	-3.561354	-2.870197
C	-2.622608	-0.281126	1.194349	C	-4.209852	-4.137008	-3.199388
C	-1.666439	-0.765769	-0.976997	C	-6.383827	-4.120382	-4.375024
C	-1.264461	-0.582385	-2.409272	C	-7.381730	-3.628670	-5.118386
C	0.199895	-0.158871	-2.574537	C	-8.671890	-4.343803	-5.356640
O	0.299222	1.199135	-2.154596	O	-8.877993	-4.453226	-6.772846
H	-2.440846	1.773328	-1.586647	H	-5.373495	-1.737992	-5.287693
O	-3.756532	3.546403	-0.033714	O	-3.029102	-0.492996	-4.808711
O	-4.303767	2.627420	2.411874	O	-1.355525	-1.842780	-3.112522
H	-3.516276	0.239118	3.057154	H	-2.291918	-4.066503	-2.207448
H	-2.317634	-1.274543	1.508104	H	-4.479952	-5.098840	-2.778089
H	-1.390105	-1.730114	-0.557226	H	-6.518239	-5.106409	-3.933660
H	-1.883740	0.159533	-2.914188	H	-7.305459	-2.654234	-5.593369
H	0.847454	-0.813393	-1.979210	H	-8.649268	-5.335142	-4.886408
H	0.461394	-0.270919	-3.632621	H	-9.498065	-3.773751	-4.906605
H	1.226799	1.430682	-2.056422	H	-9.786557	-4.728766	-6.929981
C	-3.472299	4.064197	-1.327041	C	-3.825031	0.175439	-5.780974
H	-3.863054	5.079970	-1.331957	H	-3.256839	1.057493	-6.071685
H	-2.394064	4.081958	-1.517600	H	-3.990803	-0.456361	-6.659429
H	-3.970087	3.475655	-2.105716	H	-4.789419	0.485225	-5.364822

Compound Information for **(R,R)-5**
Total electronic energy (au): -1303.451529
Zero-point correction (au): 0.413640
Sum of electronic and thermal Free Energies (au): -1303.099835
Number of imaginary frequencies: 0

C	2.225249	-0.092099	0.104608	C	-2.047703	1.121138	0.521484
C	3.070667	-0.903872	-0.668284	C	-0.855461	0.603912	-0.049360
C	3.823206	-1.904070	-0.065921	C	-0.902761	-0.607405	-0.726818
C	3.741487	-2.110973	1.324618	C	-2.108960	-1.301231	-0.855982
C	2.904380	-1.310114	2.086107	C	-4.532363	-1.572460	-0.470585
C	2.151186	-0.301800	1.480145	C	-5.747871	-1.284964	0.010967
C	1.462418	1.040341	-0.564186	C	-6.946657	-2.152851	-0.191305
C	2.314906	2.325786	-0.647853	O	-7.979650	-1.374110	-0.815761
C	1.565019	3.504315	-1.259457	H	-4.140496	0.824751	0.817932
O	2.432895	4.612439	-1.467308	O	-1.917014	2.310857	1.168741
H	3.127378	-0.751139	-1.739666	O	0.257257	1.373298	0.123432
O	4.677255	-2.765486	-0.706227	H	-0.000603	-1.033675	-1.142872
O	4.472472	-3.094916	1.916194	H	-2.119528	-2.245186	-1.389746
H	2.846470	-1.487172	3.153373	H	-4.424213	-2.482650	-1.058600
H	1.488997	0.311495	2.078490	H	-5.926103	-0.384875	0.593116
H	1.222005	0.756717	-1.597815	H	-6.685736	-3.021584	-0.809369
H	3.172203	2.090474	-1.295224	H	-7.304218	-2.523920	0.780625
H	1.173501	3.229053	-2.241622	H	-8.807169	-1.862050	-0.758322
H	0.725838	3.771338	-0.609885	C	-3.072150	2.890947	1.758108
H	2.829544	4.820731	-0.613353	H	-2.735985	3.822683	2.209956
C	4.840295	-2.646983	-2.115510	H	-3.839301	3.107420	1.006636
H	5.552552	-3.418858	-2.400997	H	-3.494001	2.242766	2.534190
H	3.892390	-2.814979	-2.636580	O	2.780539	2.778738	0.619940
H	5.240341	-1.664119	-2.384135	H	4.983374	-3.541978	1.227873
C	-3.290963	-0.807449	-0.305886	H	3.283186	2.074123	1.044902
C	-3.235666	0.418843	0.388276				

Compound Information for **(S,S)-5**
Total electronic energy (au): -1303.449717
Zero-point correction (au): 0.413308
Sum of electronic and thermal Free Energies (au): -1303.098654
Number of imaginary frequencies: 0

C	2.167544	0.195150	-0.691893	C	-1.841636	-1.202054	0.602177
C	2.367213	0.755686	0.578761	C	-0.790895	-0.854581	-0.285366
C	2.964321	2.001664	0.702355	C	-1.066393	-0.029686	-1.367116
C	3.377009	2.712694	-0.441191	C	-2.364081	0.439934	-1.585506
C	3.178124	2.160820	-1.697056	C	-4.758251	0.616767	-1.005919
C	2.572019	0.908780	-1.818385	C	-5.889019	0.368568	-0.333598
C	1.564414	-1.186304	-0.839366	C	-7.221591	0.924052	-0.717075
C	2.496631	-2.360994	-0.446814	O	-7.766371	1.631771	0.407868
C	3.851866	-2.286656	-1.127388	H	-3.919524	-1.004621	1.049477
O	4.436068	-3.588088	-1.105358	O	-1.483747	-2.002803	1.647253
H	2.055002	0.202764	1.452494	O	0.424661	-1.389753	0.016978
O	3.215893	2.657218	1.881241	H	-0.273591	0.271160	-2.037031
O	3.961251	3.935892	-0.314060	H	-2.553196	1.086247	-2.435496
H	3.491343	2.721859	-2.569249	H	-4.817921	1.277895	-1.869135
H	2.414313	0.493929	-2.808819	H	-5.895118	-0.272445	0.543943
H	1.265228	-1.340226	-1.882614	H	-7.119767	1.588889	-1.584355
H	2.002451	-3.283319	-0.780634	H	-7.899000	0.103623	-0.997082
H	3.726240	-1.944421	-2.163369	H	-8.694462	1.816350	0.232501
H	4.473578	-1.558228	-0.597047	C	-2.492348	-2.401246	2.565787
H	5.388567	-3.502866	-1.198227	H	-1.990951	-3.024784	3.304321
C	2.845412	2.025928	3.103859	H	-2.942780	-1.536892	3.065658
H	3.142557	2.711054	3.895842	H	-3.275766	-2.985220	2.070586
H	1.764419	1.861537	3.148418	O	2.701324	-2.407619	0.957943
H	3.368300	1.072704	3.227272	H	4.005193	4.144732	0.629129
C	-3.412830	0.098859	-0.732205	H	1.833547	-2.524737	1.363523
C	-3.124393	-0.732037	0.370101				

Compound Information for **(R,S)-5**
Total electronic energy (au): -1303.452052
Zero-point correction (au): 0.413540
Sum of electronic and thermal Free Energies (au): -1303.100610
Number of imaginary frequencies: 0

C	2.204627	-0.093187	0.220741	C	-2.076574	1.097394	0.612675
C	3.097478	-0.829751	-0.569707	C	-0.872057	0.620679	0.034223
C	3.812169	-1.883227	-0.015772	C	-0.902707	-0.538184	-0.730037
C	3.638299	-2.224422	1.337562	C	-2.104964	-1.220143	-0.933109
C	2.752479	-1.495880	2.116948	C	-4.535010	-1.521792	-0.612146
C	2.041642	-0.430950	1.561725	C	-5.756598	-1.279528	-0.120917
C	1.466425	1.086618	-0.387418	C	-6.948937	-2.133368	-0.404480
C	2.276922	2.394340	-0.315220	O	-7.983561	-1.309240	-0.965346
C	1.477725	3.602972	-0.793431	H	-4.175169	0.780038	0.844956
O	2.409979	4.695454	-0.828267	O	-1.962731	2.242110	1.344567
H	3.242205	-0.551869	-1.605286	O	0.236839	1.371274	0.289911
O	4.720222	-2.674771	-0.677813	H	0.010641	-0.932868	-1.152697
O	4.333797	-3.264636	1.878723	H	-2.102508	-2.124299	-1.531835
H	2.627413	-1.771699	3.157205	H	-4.416340	-2.382017	-1.269285
H	1.348121	0.129394	2.176315	H	-5.944534	-0.431202	0.531765
H	1.262459	0.892370	-1.447628	H	-6.679268	-2.943585	-1.093929
H	2.584197	2.566293	0.724932	H	-7.309716	-2.589300	0.529427
H	1.078217	3.409374	-1.797388	H	-8.807527	-1.806450	-0.958088
H	0.654311	3.806408	-0.105822	C	-3.129228	2.762909	1.965919
H	1.984239	5.465139	-1.215469	H	-2.807206	3.657452	2.496756
C	5.022020	-2.372439	-2.035314	H	-3.890826	3.033681	1.226329
H	5.779321	-3.092033	-2.341907	H	-3.553782	2.050159	2.681366
H	4.136923	-2.483416	-2.670240	O	3.422589	2.208016	-1.139570
H	5.418521	-1.357135	-2.133000	H	4.898038	-3.633172	1.185652
C	-3.298988	-0.768060	-0.372387	H	3.819900	3.081114	-1.250819
C	-3.260507	0.406349	0.406985				

Compound Information for **(S,R)-5**
Total electronic energy (au): -1303.437049
Zero-point correction (au): 0.413429
Sum of electronic and thermal Free Energies (au): -1303.085526
Number of imaginary frequencies: 0

C	-2.610206	0.546819	-0.489081	C	1.972081	1.199369	-0.974352
C	-2.733827	-0.624147	0.278925	C	0.696199	0.586578	-0.881626
C	-3.757151	-1.528235	0.024473	C	0.622949	-0.768561	-0.585443
C	-4.680558	-1.285962	-1.009440	C	1.776175	-1.509971	-0.324481
C	-4.564030	-0.132107	-1.768969	C	4.224875	-1.731732	-0.095912
C	-3.538001	0.775121	-1.504904	C	5.508612	-1.352106	-0.104441
C	-1.499223	1.565721	-0.282662	C	6.648429	-2.278931	0.165297
C	-1.047663	1.751766	1.170854	O	7.423919	-1.754573	1.255259
C	-2.206077	2.169506	2.077912	H	4.084135	0.923798	-0.781350
O	-1.630030	2.384037	3.375157	O	1.977933	2.506876	-1.331840
H	-2.032941	-0.828933	1.076709	O	-0.389182	1.357044	-1.197426
O	-3.985745	-2.698437	0.706602	H	-0.344486	-1.251291	-0.580709
O	-5.682693	-2.172764	-1.257416	H	1.691051	-2.565718	-0.090039
H	-5.282168	0.045753	-2.560351	H	4.007613	-2.771018	0.146623
H	-3.456127	1.672125	-2.108537	H	5.791784	-0.325778	-0.321601
H	-1.872341	2.535491	-0.620541	H	6.272822	-3.282677	0.402307
H	-0.622364	0.816656	1.561208	H	7.282055	-2.357330	-0.730562
H	-2.646138	3.097944	1.694532	H	8.263442	-2.223963	1.286095
H	-2.977499	1.396493	2.122198	C	3.215013	3.200451	-1.350417
H	-2.256000	2.862357	3.925901	H	2.972675	4.228205	-1.616274
C	-3.114140	-3.051492	1.775002	H	3.696890	3.184150	-0.366562
H	-3.479647	-4.002415	2.158443	H	3.900233	2.786029	-2.099002
H	-2.085301	-3.172517	1.421650	O	-0.050122	2.762586	1.186613
H	-3.143347	-2.301791	2.572172	H	-5.592168	-2.905198	-0.632739
C	3.038455	-0.915056	-0.380138	H	0.113496	2.963814	2.116645
C	3.115036	0.449244	-0.719230				

Compound Information for **(R,S)-6**
Total electronic energy (au): -1841.081891
Zero-point correction (au): 0.591465
Sum of electronic and thermal Free Energies (au): -1840.570371
Number of imaginary frequencies: 0

C	-0.349770	0.845226	-0.605459	H	-2.562956	1.201824	0.950272
C	0.343973	1.839899	0.096894	H	-4.861998	1.872367	1.487324
C	0.728767	3.007601	-0.549564	H	-7.183026	1.560927	1.426952
C	0.421576	3.201447	-1.908018	H	-8.340334	-0.747236	-0.221865
C	-0.265623	2.215699	-2.600377	H	-9.520918	1.566898	1.435511
C	-0.647599	1.040822	-1.952349	H	-10.177857	1.022309	-0.123513
C	-0.733704	-0.445116	0.098239	H	-11.317650	-0.045986	1.499817
C	0.373938	-1.523689	-0.008328	C	-4.964883	-3.245950	-1.824522
C	-0.076249	-2.880063	0.519122	H	-4.480932	-4.060948	-2.360434
O	0.959011	-3.824430	0.237335	H	-5.578998	-3.656792	-1.015706
H	0.600595	1.676636	1.135312	H	-5.602008	-2.684773	-2.516786
O	1.413934	4.052770	0.020927	C	5.501825	-1.042100	-0.276555
O	0.793930	4.350355	-2.539465	C	5.012352	-0.313427	0.825388
H	-0.497989	2.380411	-3.645698	C	3.666258	-0.323251	1.156530
H	-1.191977	0.280589	-2.498889	C	2.749381	-1.073238	0.376774
H	-0.897294	-0.255140	1.165537	C	3.230010	-1.809454	-0.698009
H	0.674041	-1.617045	-1.054504	C	4.586990	-1.786336	-1.022023
H	-0.248649	-2.798306	1.600120	C	6.918979	-1.058299	-0.654694
H	-1.009372	-3.160747	0.025030	C	7.932073	-0.387666	-0.091829
H	0.733450	-4.663683	0.648305	C	9.342354	-0.453869	-0.578947
C	1.780975	3.952238	1.392743	O	10.187065	-0.869015	0.507163
H	2.339384	4.858668	1.620913	H	5.701820	0.262859	1.426273
H	0.893673	3.899394	2.032474	O	3.130010	0.357875	2.216173
H	2.409133	3.074156	1.566873	O	1.450738	-1.017858	0.789290
C	-5.788032	0.230954	0.456229	H	2.560326	-2.442149	-1.261819
C	-5.532174	-0.927984	-0.304856	H	4.935655	-2.374478	-1.863950
C	-4.237563	-1.326339	-0.599711	H	7.148909	-1.699957	-1.504046
C	-3.140025	-0.558359	-0.133206	H	7.772883	0.260052	0.766141
C	-3.385440	0.587532	0.611260	H	9.419401	-1.152921	-1.421536
C	-4.695930	0.972431	0.905476	H	9.661672	0.538137	-0.931633
C	-7.145138	0.678284	0.790291	H	11.103987	-0.725922	0.252197
C	-8.308717	0.140028	0.404872	C	4.023014	0.929641	3.161420
C	-9.643761	0.694736	0.780689	H	3.397602	1.323824	3.961669
O	10.401443	-0.333963	1.437779	H	4.609176	1.747297	2.725918
H	-6.362753	-1.523007	-0.657299	H	1.265539	4.898862	-1.898136
O	-3.911481	-2.437975	-1.318297	H	4.704911	0.176851	3.570831
O	-1.907338	-1.037926	-0.466723				

Compound Information for **(S,R)-6**
Total electronic energy (au): -1841.090244
Zero-point correction (au): 0.592616
Sum of electronic and thermal Free Energies (au): -1840.576155
Number of imaginary frequencies: 0

C	0.413728	1.270258	-0.663687	H	2.699739	1.409262	0.834360
C	-0.322079	2.215318	0.065918	H	5.023040	1.700460	1.600536
C	-0.620610	3.448733	-0.497704	H	7.251336	1.006302	1.777274
C	-0.179352	3.762163	-1.796194	H	8.154000	-1.511211	0.282633
C	0.550887	2.826795	-2.513778	H	9.542582	0.607465	2.036884
C	0.842609	1.583339	-1.951323	H	9.886424	-1.133746	2.125902
C	0.682240	-0.091943	-0.052929	H	11.383414	-0.221535	0.709128
C	-0.469382	-1.098431	-0.279094	C	4.532394	-3.527403	-1.523929
C	-0.100627	-2.542240	0.114951	H	3.953698	-4.271818	-2.067593
O	0.572738	-3.245357	-0.912579	H	5.334909	-3.148055	-2.164435
H	-0.677094	1.962425	1.056163	H	4.961234	-3.983289	-0.625663
O	-1.338050	4.453426	0.104258	C	-5.578703	-1.415092	-0.163998
O	-0.465060	4.976326	-2.344467	C	-5.142554	-0.630801	0.923390
H	0.885735	3.082916	-3.511777	C	-3.796982	-0.377761	1.137667
H	1.416538	0.860305	-2.517441	C	-2.826511	-0.916981	0.254294
H	0.820926	0.000027	1.030891	C	-3.250681	-1.694746	-0.816199
H	-0.755931	-1.074175	-1.334406	C	-4.611163	-1.934417	-1.023050
H	0.480269	-2.528996	1.047356	C	-6.995104	-1.699392	-0.421244
H	-1.022951	-3.091158	0.313130	C	-8.053980	-1.346048	0.317700
H	1.435041	-2.825903	-1.048327	C	-9.461740	-1.714637	-0.019585
C	-1.863044	4.224608	1.407678	O	-10.245921	-0.513485	-0.093926
H	-2.421530	5.122391	1.667382	H	-5.875098	-0.212218	1.598829
H	-2.530368	3.357643	1.416286	O	-3.305807	0.378916	2.163706
H	-1.057477	4.073241	2.133789	O	-1.530821	-0.612940	0.549728
C	5.748049	-0.113342	0.706429	H	-2.531097	-2.131478	-1.495189
C	5.375356	-1.244208	-0.049295	H	-4.914468	-2.544162	-1.866880
C	4.067941	-1.422020	-0.470495	H	-7.180221	-2.273673	-1.327669
C	3.083634	-0.457961	-0.145361	H	-7.938850	-0.763037	1.227596
C	3.439775	0.656040	0.599769	H	-9.492975	-2.260944	-0.970973
C	4.760830	0.820582	1.023607	H	-9.871046	-2.371838	0.762066
C	7.123981	0.116275	1.163180	H	-11.176530	-0.757333	-0.120589
C	8.208807	-0.626152	0.910883	C	-4.218842	0.844413	3.147732
C	9.566713	-0.322724	1.454771	H	-3.616105	1.369140	3.887764
O	10.487307	-0.216537	0.358288	H	-4.742132	0.012547	3.631396
H	6.119845	-1.988177	-0.295257	H	-0.986069	5.475527	-1.701046
O	3.612634	-2.493295	-1.187216	H	-4.954209	1.536130	2.721610
O	1.833216	-0.731604	-0.619586				

Compound Information for **(R,S)-7**
Total electronic energy (au): -1840.43906222
Zero-point correction (au): 0.578210
Sum of electronic and thermal Free Energies (au): -1839.942015
Number of imaginary frequencies: 0

C	0.160603	0.869798	-0.189466	O	1.733003	-0.882029	0.468985
C	0.438075	1.567307	0.993136	H	2.428294	0.654882	-1.682125
C	0.046025	2.891113	1.139814	H	4.738524	1.135038	-2.347612
C	-0.669952	3.592221	0.055478	H	7.058268	0.945513	-2.081585
C	-0.929113	2.809769	-1.136004	H	8.168830	-0.567367	0.340271
C	-0.530300	1.504908	-1.249907	H	9.398752	0.984415	-2.020297
C	0.582711	-0.582245	-0.323269	H	9.989401	1.090513	-0.347555
C	-0.526359	-1.558007	0.153385	H	11.208360	-0.488609	-1.401479
C	-0.060060	-3.008902	0.133328	C	4.754754	-2.334826	2.668532
O	-1.059588	-3.796801	0.781949	H	4.255922	-2.894791	3.457847
H	0.977200	1.057479	1.780113	H	5.394625	-3.011086	2.091526
O	0.269148	3.640019	2.225698	H	5.368461	-1.545421	3.115965
O	-1.022610	4.779234	0.165872	C	-5.601083	-0.780703	0.350990
H	-1.459087	3.316222	-1.934172	C	-5.102765	-0.386390	-0.906251
H	-0.762377	0.936500	-2.142447	C	-3.776027	-0.593155	-1.254628
H	0.785753	-0.809883	-1.376162	C	-2.894220	-1.206295	-0.330206
H	-0.825657	-1.284566	1.168530	C	-3.383806	-1.619390	0.900771
H	0.069248	-3.319447	-0.911188	C	-4.720436	-1.400541	1.238312
H	0.896748	-3.084801	0.655662	C	-6.998012	-0.577171	0.751943
H	-0.856313	-4.727536	0.653278	C	-7.979445	0.007485	0.054060
C	0.955013	3.067139	3.337380	C	-9.367221	0.196204	0.573141
H	1.013205	3.857326	4.082896	O	-10.290126	-0.413176	-0.344063
H	0.400271	2.216404	3.744588	H	-5.768102	0.089081	-1.612714
H	1.963660	2.750356	3.055720	O	-3.229462	-0.245182	-2.455941
C	5.637628	0.039752	-0.732373	O	-1.606438	-1.371979	-0.763365
C	5.362256	-0.745803	0.405515	H	-2.737642	-2.152616	1.583569
C	4.060584	-1.036027	0.784624	H	-5.080699	-1.733944	2.205363
C	2.977332	-0.535868	0.018756	H	-7.239249	-0.953098	1.745081
C	3.240708	0.243570	-1.098920	H	-7.808773	0.390629	-0.948437
C	4.558163	0.523277	-1.470828	H	-9.461469	-0.247017	1.572800
C	7.003198	0.360851	-1.164773	H	-9.589076	1.270419	0.656547
C	8.154491	0.026252	-0.569914	H	-11.178774	-0.115065	-0.126039
C	9.499989	0.430006	-1.078606	C	-4.078220	0.334923	-3.437120
O	10.293172	-0.752394	-1.263578	H	-3.448989	0.507116	-4.309201
H	6.183313	-1.137173	0.989203	H	-4.493124	1.289455	-3.095231
O	3.715289	-1.791808	1.865038	H	-4.895665	-0.341493	-3.708854

Compound Information for **(S,R)-7**
Total electronic energy (au): -1840.42948274
Zero-point correction (au): 0.578384
Sum of electronic and thermal Free Energies (au): -1839.932654
Number of imaginary frequencies: 0

C	-0.419142	1.652491	0.362468	O	-1.851668	-0.088879	1.318039
C	0.429126	1.992346	-0.698195	H	-2.084234	0.392916	-1.360573
C	0.632244	3.321565	-1.044698	H	-4.094530	-0.088471	-2.682991
C	-0.061992	4.403320	-0.318170	H	-6.312750	-0.808748	-2.899467
C	-0.930296	3.980926	0.762429	H	-7.781696	-1.895638	-0.440133
C	-1.096357	2.661645	1.088554	H	-8.492344	-1.495942	-3.411252
C	-0.565937	0.197206	0.764186	H	-8.941633	-2.934556	-2.469209
C	0.428076	-0.185523	1.901595	H	-10.673049	-1.490890	-2.375359
C	0.332513	-1.650316	2.322191	C	-5.101397	-1.554013	3.152569
O	1.129808	-1.806968	3.493349	H	-4.795458	-1.633907	4.194329
H	0.945601	1.204076	-1.231387	H	-5.949149	-0.865168	3.074498
O	1.438844	3.743626	-2.024099	H	-5.398157	-2.542206	2.784318
O	0.094799	5.598237	-0.622198	C	4.711279	-1.480977	-0.773659
H	-1.442099	4.770157	1.300542	C	5.005151	-0.563169	0.255196
H	-1.754544	2.372916	1.899313	C	4.006214	-0.011945	1.044500
H	-0.404179	-0.439271	-0.111569	C	2.647176	-0.368748	0.822109
H	0.146516	0.411049	2.772448	C	2.356869	-1.264451	-0.201072
H	-0.721752	-1.858553	2.526627	C	3.375030	-1.818111	-0.983188
H	0.676008	-2.321637	1.528517	C	5.745455	-2.089250	-1.618785
H	1.091241	-2.726994	3.770344	C	7.066153	-1.872907	-1.588372
C	2.185569	2.785391	-2.773114	C	8.036001	-2.527893	-2.517059
H	2.780975	3.364516	-3.475686	O	9.028247	-3.211877	-1.736655
H	2.843369	2.203015	-2.121744	H	6.034162	-0.289792	0.440795
H	1.519898	2.113147	-3.323498	O	4.218557	0.876648	2.047476
C	-5.240675	-0.835141	-1.025955	O	1.755400	0.268762	1.627737
C	-5.208325	-1.092321	0.359891	H	1.334912	-1.548449	-0.406352
C	-4.074904	-0.835646	1.116093	H	3.114560	-2.520798	-1.767224
C	-2.918478	-0.305529	0.489880	H	5.366185	-2.798654	-2.352805
C	-2.945067	-0.043440	-0.872705	H	7.510260	-1.190140	-0.869017
C	-4.094991	-0.308464	-1.621269	H	7.511983	-3.226944	-3.181539
C	-6.426566	-1.088368	-1.853373	H	8.522351	-1.765227	-3.143185
C	-7.598518	-1.610767	-1.472729	H	9.760422	-3.451130	-2.313571
C	-8.740886	-1.854781	-2.404276	C	5.553972	1.256527	2.348907
O	-9.900410	-1.180952	-1.892542	H	5.479664	1.955282	3.180241
H	-6.086270	-1.496405	0.843564	H	6.030884	1.755247	1.497813
O	-3.965737	-1.059095	2.454845	H	6.156351	0.393255	2.651892

Compound Information for **8**
Total electronic energy (au): -614.009935
Zero-point correction (au): 0.197469
Sum of electronic and thermal Free Energies (au): -613.854670
Number of imaginary frequencies: 0

C	0.281412	0.693921	0.505684
C	-1.079896	0.267804	0.442999
C	-1.420642	-1.027815	0.101519
C	-0.398356	-1.964841	-0.196942
C	0.936837	-1.564343	-0.139249
C	1.281628	-0.267253	0.203168
C	0.631137	2.016955	0.857343
C	-0.319293	3.076504	1.186799
C	-0.756088	4.083458	0.178461
O	-1.927302	4.749338	0.658270
H	-1.849552	0.990254	0.678966
O	-2.690150	-1.508280	0.022599
O	-0.783958	-3.229915	-0.529343
H	1.713212	-2.289613	-0.367825
H	2.325817	0.021151	0.242673
H	1.696968	2.249076	0.897648
H	-0.596082	3.281063	2.219959
H	0.052492	4.818111	0.002478
H	-0.946995	3.590540	-0.786929
H	-2.106744	5.504882	0.090767
H	-0.001720	-3.763614	-0.704837
C	-3.763606	-0.622917	0.312365
H	-4.671508	-1.211276	0.190794
H	-3.706392	-0.248084	1.339874
H	-3.781844	0.223831	-0.382157

Compound Information for **(R)-9**
Total electronic energy (au): -1227.532909
Zero-point correction (au): 0.393718
Sum of electronic and thermal Free Energies (au): -1227.201765
Number of imaginary frequencies: 0

C	2.630824	0.709213	-0.355970	C	-2.218448	-0.549701	0.917697
C	2.941936	-0.595286	-0.761327	C	-0.943663	-0.282449	0.430082
C	4.103984	-1.206397	-0.311370	C	-0.783043	0.198084	-0.891456
C	4.985414	-0.523421	0.545393	C	-1.912540	0.363125	-1.683932
C	4.683504	0.770972	0.937167	C	-3.185714	0.077967	-1.194680
C	3.511908	1.384249	0.486350	C	-4.722454	-0.637382	0.604150
C	1.398821	1.411242	-0.908406	C	-5.096744	-1.018502	1.831372
C	0.769658	2.384692	0.018561	C	-6.512003	-1.299093	2.218407
C	-0.050289	3.520750	-0.470279	O	-6.850959	-0.478829	3.346874
O	-0.084591	4.533839	0.538704	H	-2.331887	-0.915039	1.928727
H	2.253189	-1.117833	-1.409197	O	0.204190	-0.460249	1.139083
O	4.511749	-2.482336	-0.624936	O	0.442879	0.411707	-1.464215
O	6.125175	-1.130295	0.987847	H	-1.771140	0.713158	-2.699941
H	5.369701	1.290406	1.595419	H	-4.049470	0.215308	-1.835901
H	3.294408	2.398632	0.800210	H	-5.502475	-0.497222	-0.142461
H	1.693408	1.941904	-1.822604	H	-4.368985	-1.149746	2.627695
H	0.805859	2.214876	1.087469	H	-7.183306	-1.098422	1.373578
H	0.367201	3.915202	-1.410245	H	-6.617536	-2.359961	2.489859
H	-1.075542	3.178181	-0.697084	H	-7.673808	-0.803692	3.725638
H	-0.791787	5.151700	0.330905	C	0.121006	-0.918850	2.482335
C	3.706136	-3.254340	-1.507838	H	1.148147	-0.969660	2.839144
H	4.215664	-4.209898	-1.621129	H	-0.448506	-0.222637	3.107334
H	2.708220	-3.418916	-1.089380	H	-0.333532	-1.913955	2.536226
H	3.616388	-2.769142	-2.484977	H	6.153717	-2.015538	0.600653
C	-3.362359	-0.371676	0.117562				

Compound Information for **(S)-9**
Total electronic energy (au): -1227.538469
Zero-point correction (au): 0.393792
Sum of electronic and thermal Free Energies (au): -1227.207444
Number of imaginary frequencies: 0

C	-2.973964	0.283710	-0.148442	C	2.681904	-0.506148	-0.605468
C	-3.628614	-0.389471	0.894053	C	1.292424	-0.475273	-0.637001
C	-4.959551	-0.755647	0.755820	C	0.561851	-0.390749	0.574029
C	-5.665072	-0.447980	-0.423155	C	1.260266	-0.364910	1.774907
C	-5.017458	0.217104	-1.452366	C	2.652946	-0.406825	1.799996
C	-3.675456	0.576276	-1.315109	C	4.854583	-0.482444	0.679021
C	-1.538266	0.725549	0.008236	C	5.723889	-0.452655	-0.338297
C	-1.402743	1.925462	0.875307	C	7.206796	-0.504081	-0.164891
C	-0.379404	2.973287	0.635012	O	7.783961	0.638187	-0.815628
O	-0.742812	4.156060	1.350923	H	3.232917	-0.577811	-1.532634
H	-3.075545	-0.640669	1.788558	O	0.548702	-0.534251	-1.779920
O	-5.708893	-1.428944	1.690397	O	-0.804860	-0.429477	0.592647
O	-6.972530	-0.810518	-0.555031	H	0.687802	-0.317556	2.693723
H	-5.569853	0.440071	-2.357241	H	3.172736	-0.384334	2.751510
H	-3.176972	1.089456	-2.130044	H	5.258671	-0.516688	1.689493
H	-1.113343	0.912650	-0.979546	H	5.384905	-0.388989	-1.368912
H	-1.976495	1.983507	1.793723	H	7.463730	-0.517658	0.902038
H	0.613269	2.619068	0.967947	H	7.600836	-1.424943	-0.619809
H	-0.291280	3.178577	-0.444075	H	8.734810	0.505288	-0.881728
H	0.007855	4.757428	1.350889	C	1.218016	-0.715126	-3.021648
C	-5.090584	-1.797678	2.917928	H	0.433889	-0.772375	-3.774761
H	-5.854395	-2.316132	3.495035	H	1.879071	0.128448	-3.248104
H	-4.243106	-2.468434	2.745463	H	1.796228	-1.644960	-3.028287
H	-4.753152	-0.913977	3.468897	H	-7.234117	-1.266458	0.256326
C	3.387668	-0.466355	0.611893				

Compound Information for **(R)-10**
Total electronic energy (au): -689.914272
Zero-point correction (au): 0.216535
Sum of electronic and thermal Free Energies (au): -689.740631
Number of imaginary frequencies: 0

C	0.190646	-0.164308	-0.227134
C	-1.034637	-0.878120	-0.033710
C	-2.253538	-0.235748	0.062596
C	-2.303598	1.178141	-0.036023
C	-1.121903	1.890652	-0.233032
C	0.104200	1.251153	-0.331432
C	1.400145	-0.889798	-0.301318
C	2.796580	-0.340661	-0.424663
C	3.328586	0.201185	0.902880
O	4.745273	0.331936	0.808415
H	-0.987139	-1.956327	0.044417
O	-3.453572	-0.848911	0.251019
O	-3.526358	1.771132	0.063610
H	-1.171027	2.973197	-0.316409
H	0.999826	1.828010	-0.511674
H	1.334507	-1.967833	-0.184799
H	3.464201	-1.166266	-0.707012
H	2.849872	1.165528	1.108054
H	3.058205	-0.499708	1.702552
H	5.054369	0.901004	1.518558
H	-3.424160	2.724879	-0.024317
C	-3.478260	-2.265166	0.350859
H	-4.523907	-2.532887	0.493015
H	-3.103151	-2.737433	-0.563884
H	-2.893396	-2.616566	1.208164
O	2.922588	0.717906	-1.386868
H	2.639333	0.378044	-2.242098

Compound Information for **(S)-10**
Total electronic energy (au): -689.920667
Zero-point correction (au): 0.216913
Sum of electronic and thermal Free Energies (au): -689.746313
Number of imaginary frequencies: 0

C	-0.125491	0.615207	0.242086
C	-1.252722	-0.223632	-0.027636
C	-1.122914	-1.579996	-0.252364
C	0.166548	-2.171129	-0.219667
C	1.277144	-1.371873	0.043137
C	1.150482	-0.009395	0.270198
C	-0.323671	1.991095	0.465231
C	0.741943	3.003034	0.729615
C	1.292598	3.605458	-0.567959
O	2.256644	4.597557	-0.186384
H	-2.231976	0.235808	-0.047570
O	-2.148399	-2.435380	-0.510371
O	0.247782	-3.512498	-0.449009
H	2.260602	-1.833474	0.070566
H	2.039594	0.572104	0.477208
H	-1.332937	2.388458	0.433922
H	1.588385	2.549385	1.265535
H	1.757926	2.821733	-1.176270
H	0.469190	4.059867	-1.131144
H	2.464575	5.150317	-0.944925
H	1.168416	-3.789243	-0.390240
C	-3.468707	-1.912471	-0.544613
H	-4.116736	-2.761273	-0.756196
H	-3.748904	-1.471447	0.418220
H	-3.581262	-1.162664	-1.335473
O	0.175602	4.038423	1.535011
H	0.815286	4.762028	1.539090

Compound Information for **(R)-11**
Total electronic energy (au): -1227.558437
Zero-point correction (au): 0.394920
Sum of electronic and thermal Free Energies (au): -1227.225796
Number of imaginary frequencies: 0

C	2.679305	0.358306	-0.478962	C	-2.611160	-0.035679	1.585563
C	3.985533	-0.035141	-0.048428	C	-1.425101	0.687497	1.576485
C	4.432618	-1.326255	-0.223328	C	-1.097014	1.483508	0.450175
C	3.602845	-2.296459	-0.832230	C	-1.981447	1.537944	-0.621212
C	2.324795	-1.937274	-1.251731	C	-3.165118	0.800025	-0.602221
C	1.866202	-0.641165	-1.082252	C	-4.759088	-0.753057	0.468442
C	2.266168	1.692812	-0.290157	C	-5.236461	-1.596596	1.392301
C	0.935174	2.255977	-0.661380	C	-6.520975	-2.344492	1.244597
C	1.046136	3.708268	-1.103863	O	-7.362967	-2.046591	2.370390
O	-0.196472	4.114130	-1.675575	H	-2.856461	-0.644285	2.444584
H	4.619095	0.707777	0.418801	O	-0.518877	0.697345	2.592434
O	5.661297	-1.814398	0.147198	O	0.062414	2.199222	0.510684
O	4.046861	-3.569625	-1.002323	H	-1.752676	2.191126	-1.453721
H	1.699175	-2.695484	-1.707524	H	-3.841691	0.860865	-1.447839
H	0.862006	-0.398794	-1.404440	H	-5.359122	-0.594323	-0.426505
H	2.940063	2.358606	0.242257	H	-4.694906	-1.790257	2.314494
H	0.472275	1.684897	-1.468697	H	-7.014493	-2.066208	0.304572
H	1.302149	4.321162	-0.231522	H	-6.320019	-3.425773	1.214444
H	1.853357	3.791312	-1.843065	H	-8.091617	-2.675160	2.380904
H	-0.264028	5.072056	-1.644057	C	-0.787449	-0.087182	3.743947
C	6.580565	-0.931807	0.780790	H	0.058221	0.069509	4.411984
H	7.470642	-1.523175	0.988106	H	-1.708151	0.233974	4.243764
H	6.841110	-0.097168	0.122202	H	-0.860310	-1.152239	3.496315
H	6.170522	-0.545771	1.719340	H	4.945283	-3.619865	-0.647396
C	-3.500824	0.001582	0.493936				

Compound Information for **(S)-11**
Total electronic energy (au): -1227.546123
Zero-point correction (au): 0.395290
Sum of electronic and thermal Free Energies (au): -1227.212069
Number of imaginary frequencies: 0

C	2.057035	0.506058	-0.236316	C	-2.248329	0.001295	0.690224
C	3.003436	-0.405543	0.333339	C	-1.307747	0.984916	0.979826
C	3.188677	-1.667567	-0.186893	C	-1.091842	2.039000	0.059901
C	2.434272	-2.100688	-1.300398	C	-1.863953	2.091803	-1.094332
C	1.496773	-1.240205	-1.862086	C	-2.807703	1.105291	-1.375865
C	1.306908	0.033527	-1.348094	C	-3.996408	-0.992905	-0.833157
C	1.942582	1.784792	0.357746	C	-4.222912	-2.149898	-0.200147
C	1.181372	3.002668	-0.066505	C	-5.236530	-3.154864	-0.640921
C	1.273738	3.402549	-1.545054	O	-6.126232	-3.420192	0.454633
O	2.641197	3.726085	-1.800472	H	-2.414007	-0.801092	1.395137
H	3.587667	-0.073101	1.181675	O	-0.565746	1.024622	2.117783
O	4.073570	-2.612231	0.274831	O	-0.224573	3.052963	0.370879
O	2.616635	-3.347899	-1.811798	H	-1.727481	2.930410	-1.767244
H	0.911924	-1.592240	-2.703631	H	-3.396793	1.168651	-2.284209
H	0.539271	0.652553	-1.787701	H	-4.596835	-0.769986	-1.713846
H	2.518977	1.926141	1.265762	H	-3.656025	-2.428423	0.684043
H	1.601156	3.842520	0.489289	H	-5.789980	-2.779511	-1.511095
H	0.932844	2.604977	-2.209533	H	-4.729786	-4.085444	-0.936500
H	0.631146	4.278945	-1.692867	H	-6.644072	-4.203730	0.244961
H	2.765887	3.823353	-2.748578	C	-0.730160	-0.015514	3.070914
C	4.914766	-2.277296	1.372397	H	-0.041678	0.216088	3.882155
H	5.532823	-3.154442	1.556128	H	-1.752928	-0.043167	3.462397
H	5.554346	-1.422534	1.130546	H	-0.475004	-0.991705	2.644555
H	4.324729	-2.052639	2.266761	H	3.306288	-3.782178	-1.290922
C	-3.004363	0.037032	-0.495542				

Compound Information for **(R)-12**
Total electronic energy (au): -689.894634
Zero-point correction (au): 0.214928
Sum of electronic and thermal Free Energies (au): -689.725134
Number of imaginary frequencies: 0

C	0.064182	0.520881	0.746112
C	-1.039642	-0.094135	0.139984
C	-0.959613	-1.390437	-0.369377
C	0.257050	-2.092771	-0.262627
C	1.350268	-1.481350	0.342752
C	1.263265	-0.182818	0.840236
C	-0.056827	1.941586	1.295474
C	0.911438	2.889208	0.671700
C	0.688400	3.457441	-0.678801
O	1.954895	3.723020	-1.290556
H	-1.971639	0.453255	0.071033
O	-1.980554	-2.058071	-0.973043
O	0.296418	-3.359895	-0.769884
H	2.285606	-2.029182	0.417783
H	2.129016	0.279538	1.298530
H	-1.085578	2.280798	1.082005
H	1.788838	3.187255	1.232327
H	0.096182	2.762765	-1.294512
H	0.106095	4.395594	-0.608077
H	1.809208	4.258389	-2.076648
H	1.179264	-3.723302	-0.644506
C	-3.229540	-1.398394	-1.115711
H	-3.882520	-2.108534	-1.620246
H	-3.660248	-1.138966	-0.142103
H	-3.137719	-0.493304	-1.726579
O	0.167045	1.983435	2.712962
H	-0.279290	1.225996	3.106773

Compound Information for **(S)-12**
Total electronic energy (au): -689.894783
Zero-point correction (au): 0.215284
Sum of electronic and thermal Free Energies (au): -689.725066
Number of imaginary frequencies: 0

C	0.456582	-0.283930	0.686354
C	-0.545129	0.658890	0.428011
C	-1.778153	0.271500	-0.094227
C	-2.016317	-1.089643	-0.370824
C	-1.019292	-2.021623	-0.110756
C	0.210699	-1.626724	0.415972
C	1.818549	0.135544	1.225889
C	2.893145	0.084758	0.184139
C	2.848146	0.898439	-1.058539
O	3.584001	0.210355	-2.077249
H	-0.350320	1.694566	0.663999
O	-2.808212	1.120131	-0.363115
O	-3.239436	-1.424698	-0.882112
H	-1.208069	-3.071107	-0.318700
H	0.972963	-2.373673	0.608550
H	2.086823	-0.554603	2.034818
H	3.742333	-0.577712	0.311883
H	1.806768	1.065800	-1.366047
H	3.294401	1.893521	-0.885852
H	3.662037	0.788830	-2.842052
H	-3.271066	-2.376446	-1.023768
C	-2.634011	2.501374	-0.081692
H	-3.571893	2.979120	-0.360465
H	-2.440055	2.672541	0.982644
H	-1.817632	2.931490	-0.672482
O	1.683114	1.468919	1.777258
H	2.556976	1.752033	2.066662

Compound Information for **(R,R)-13**
Total electronic energy (au): -765.805939
Zero-point correction (au): 0.234784
Sum of electronic and thermal Free Energies (au): -765.614722
Number of imaginary frequencies: 0

C	0.046785	0.532124	0.887830
C	-1.003479	-0.041919	0.156831
C	-0.888455	-1.311769	-0.407269
C	0.310692	-2.032441	-0.232482
C	1.346607	-1.467056	0.501761
C	1.221881	-0.195029	1.061424
C	-0.102042	1.928528	1.466684
C	0.716289	2.993567	0.725194
C	0.571984	2.920270	-0.793336
O	1.304972	4.039712	-1.311165
H	-1.923528	0.516355	0.036593
O	-1.859663	-1.939746	-1.123896
O	0.383618	-3.273983	-0.796506
H	2.264091	-2.032442	0.640488
H	2.035107	0.221441	1.643098
H	-1.154596	2.235655	1.398949
H	1.775348	2.843928	0.980369
H	0.979094	1.980280	-1.176417
H	-0.487325	2.996156	-1.070334
H	1.109880	4.142810	-2.246469
H	1.240141	-3.664081	-0.592990
C	-3.093151	-1.266110	-1.327368
H	-3.707239	-1.946291	-1.915064
H	-3.595518	-1.053034	-0.377329
H	-2.953240	-0.332179	-1.883176
O	0.332775	1.982659	2.828265
H	-0.192247	1.354121	3.334621
O	0.278608	4.264652	1.187517
H	0.699610	4.921821	0.619176

Compound Information for **(S,S)-13**
Total electronic energy (au): -765.807142
Zero-point correction (au): 0.235223
Sum of electronic and thermal Free Energies (au): -765.615101
Number of imaginary frequencies: 0

C	-0.123698	-0.550975	-0.543956
C	0.843465	0.454032	-0.677030
C	2.113964	0.308929	-0.123176
C	2.428557	-0.867088	0.585318
C	1.467865	-1.862620	0.711053
C	0.198674	-1.714383	0.149634
C	-1.510327	-0.376905	-1.136666
C	-2.633819	-0.157241	-0.095626
C	-2.326676	0.920174	0.933038
O	-3.488028	1.005703	1.774994
H	0.591010	1.341964	-1.237326
O	3.112019	1.232197	-0.214999
O	3.686980	-0.969814	1.111899
H	1.716881	-2.772288	1.250765
H	-0.537659	-2.498994	0.266742
H	-1.774649	-1.296818	-1.672723
H	-3.531145	0.158919	-0.652401
H	-1.447634	0.632904	1.517721
H	-2.134096	1.873577	0.429890
H	-3.276406	1.528811	2.553149
H	3.777073	-1.825594	1.543644
C	2.863213	2.422435	-0.948082
H	3.787878	2.995697	-0.902059
H	2.620458	2.206318	-1.994200
H	2.051195	3.007413	-0.501754
O	-1.483053	0.727982	-2.046371
H	-2.315738	0.747172	-2.528007
O	-2.895241	-1.403202	0.539511
H	-3.476006	-1.216017	1.287688

Compound Information for **(R,S)-13**
Total electronic energy (au): -765.811314
Zero-point correction (au): 0.235654
Sum of electronic and thermal Free Energies (au): -765.618880
Number of imaginary frequencies: 0

C	-0.140627	-0.449333	-0.440938
C	0.878730	0.488030	-0.671961
C	2.169726	0.298247	-0.182851
C	2.456566	-0.869256	0.553436
C	1.449852	-1.801571	0.774622
C	0.158576	-1.599864	0.287003
C	-1.525730	-0.181202	-0.993146
C	-2.645641	0.052247	0.040922
C	-2.313184	1.097573	1.094898
O	-3.433804	1.366703	1.926790
H	0.650669	1.377999	-1.245085
O	3.208676	1.156885	-0.363478
O	3.732907	-1.023039	1.010629
H	1.678284	-2.698727	1.343292
H	-0.611645	-2.331567	0.488652
H	-1.476195	0.724458	-1.612871
H	-3.528611	0.390866	-0.518488
H	-1.457340	0.755681	1.689204
H	-2.045786	2.043262	0.617360
H	-3.743311	0.517215	2.262940
H	3.797297	-1.849807	1.500143
C	2.977398	2.357334	-1.086715
H	3.930399	2.883336	-1.097521
H	2.665810	2.151180	-2.116778
H	2.223782	2.982379	-0.595096
O	-2.015059	-1.273003	-1.796064
H	-1.283651	-1.621879	-2.316210
O	-2.972095	-1.144607	0.747639
H	-3.192232	-1.811518	0.086119

Compound Information for **(S,R)-13**
Total electronic energy (au): -765.812986
Zero-point correction (au): 0.235778
Sum of electronic and thermal Free Energies (au): -765.620094
Number of imaginary frequencies: 0

C	-0.125032	-0.574989	-0.460895
C	0.831949	0.433430	-0.627890
C	2.123601	0.290244	-0.124701
C	2.468997	-0.886244	0.570720
C	1.519208	-1.887509	0.727651
C	0.230384	-1.740610	0.211615
C	-1.535838	-0.399985	-0.986273
C	-2.572051	-0.172336	0.133020
C	-2.274332	1.029122	1.022579
O	-3.431736	1.196598	1.857924
H	0.550566	1.320880	-1.175457
O	3.114366	1.214129	-0.255095
O	3.745877	-0.983028	1.049996
H	1.792868	-2.799604	1.250648
H	-0.485082	-2.546742	0.333150
H	-1.838379	-1.324961	-1.496421
H	-2.616000	-1.071500	0.761383
H	-1.382526	0.836508	1.625967
H	-2.111417	1.919296	0.406409
H	-3.367280	2.032595	2.327828
H	3.856949	-1.836809	1.480814
C	2.838389	2.398993	-0.989194
H	3.765113	2.970486	-0.984932
H	2.553418	2.172116	-2.021990
H	2.045696	2.989018	-0.515964
O	-1.577846	0.680301	-1.912218
H	-2.513017	0.830688	-2.103078
O	-3.824388	0.007613	-0.533465
H	-4.432651	0.389147	0.113042

Table S1: Spin-contamination for the free radical models used for this work, resulting from the unrestricted B3LYP calculations. $<S^2>$ is the eigenfunction of the total spin.

Structure	$<S^2>$ Pre-annihilation	$<S^2>$ Post-annihilation	s(s+1), where s=1/2(# unpaired electrons)	% difference from pre-annihilation	% difference from post-annihilation
2	0.7855	0.7508	0.75	-4.7	-0.1
SR-7	0.7765	0.7505	0.75	-3.5	-0.1
RS-7	0.7763	0.7505	0.75	-3.5	-0.1
8	2.0133	2.0001	2.00	-0.7	0.0
R-9	0.7542	0.7500	0.75	-0.6	0.0
S-9	0.7546	0.7500	0.75	-0.6	0.0
R-10	0.7774	0.7505	0.75	-3.7	-0.1
S-10	0.7785	0.7505	0.75	-3.8	-0.1
R-11	0.7778	0.7505	0.75	-3.7	-0.1
S-11	0.7773	0.7505	0.75	-3.6	-0.1
R-12	0.7547	0.7500	0.75	-0.6	0.0
S-12	0.7543	0.7500	0.75	-0.6	0.0
$OH^{\cdot}$	0.7519	0.7500	0.75	-0.3	0.0

Table S2: NMR chemical shifts for the erythro stereoisomers of **6**. The rings are labeled in the included structure for **6**, shown in Figure S1. MUE, RMSE, and ME are the mean unsigned, root mean-squared, and maximum errors in ppm. Experimental chemical shifts are from reference 71 and the mPW1PW91/6-31G(d)//B3LYP/6-311++G(d,p) calculated NMR shifts were obtained as in reference 66. The experimental data was collected in acetone and the NMR calculated shifts were performed using the permittivity of acetone within a polarized continuum, as in references 71 and 66, respectively.

Ring	Carbon	δ_{exp}	$\delta_{erythro,\ weighted}$
A	1	130.39	130.5
	2	112.11	112.0
	3	148.1	144.9
	4	147.18	144.9
	5	115.23	114.6
	6	121.49	118.3
	α	81.15	89.1
	β	85.31	85.7
	γ	61.75	61.7
	OMe	56.18	53.9
B	1	132.74	128.7
	2	110.93	108.1
	3	151.71	148.4
	4	148.61	146.1
	5	119.04	112.4
	6	120.15	124.0
	α	129.85	133.3
	β	129.45	125.9
	γ	63.25	65.5
	OMe	56.2	53.8
C	1	132.05	129.6
	2	110.74	107.6
	3	151.17	148.0
	4	147.77	146.8
	5	117.02	114.6
	6	119.9	124.2
	α	129.85	133.2
	β	129.22	126.8
	γ	63.25	65.5
	OMe	56.32	53.9
	MUE (ppm)		112.6
	RMSE (ppm)		116.9
	ME (ppm)		151.7
	slope		0.97
	y-intercept (ppm)		2.10
	r^2		0.9905

Ring	Hydrogen	δ_{exp}	$\delta_{erythro,\ weighted}$
A	α	5.46	5.1
	β	4.56	4.4
	γ1	3.81	3.9
	γ2	3.93	3.7
	MUE (ppm)		4.3
	RMSE (ppm)		4.3
	ME (ppm)		5.1
	slope		0.81
	y-intercept (ppm)		0.68
	r^2		0.9821

Figure 1S: Labeling scheme used for NMR chemical shift results in Table 2S for **6**.