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Supplementary Information for publication:

OH radical reactions with the hydrophilic component of sphingolipids

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Contents:

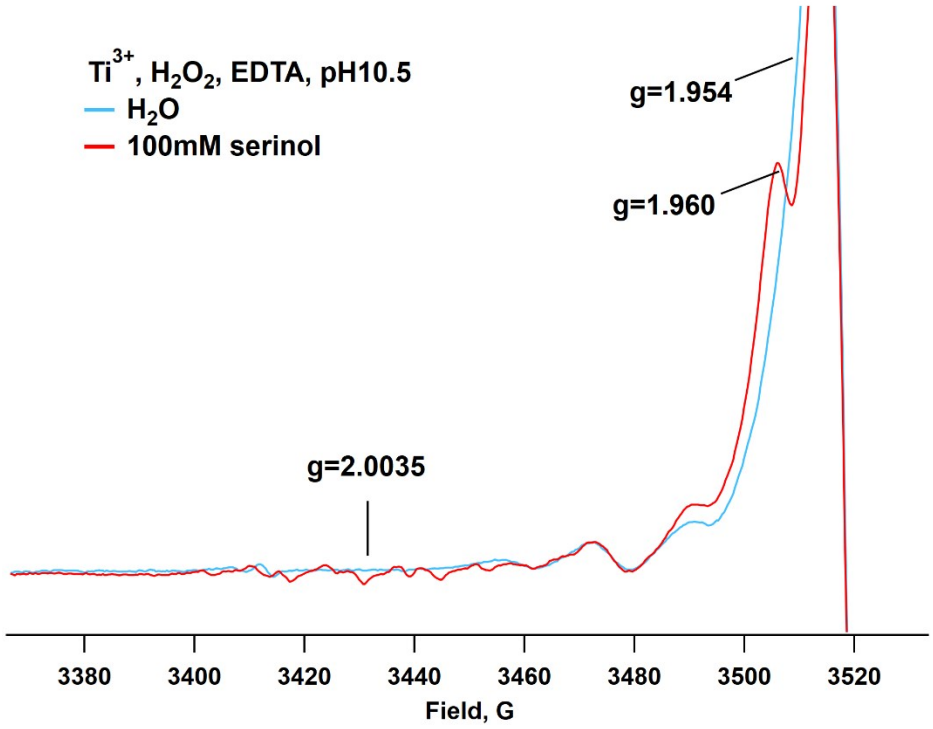

Figure S1. Comparison of EPR spectra of species formed in Ti^{3+}/EDTA/H_2O_2 –Fenton system at pH 10.5 (blue) - EDTA-Ti^{3+}complex (g = 1.954) and in the reaction of the Ti^{3+}/EDTA/H_2O_2 -Fenton with 100mM serinol at pH 10.5 (red) - EDTA-Ti^{3+}complex (g = 1.954) and serinol-EDTA-Ti^{3+}complex (g = 1.960). There is no signal from EDTA-based radicals formed during the attack of the OH radical at g = 2.0035 under these conditions.

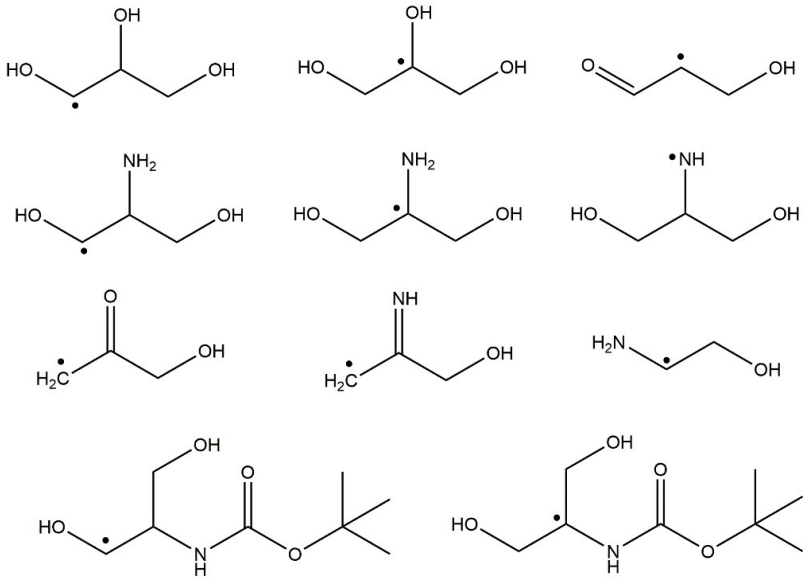

Figure S2. Structures of potential transients produced in the reaction of •OH radicals with glycerol, serinol and N-boc-serinol.

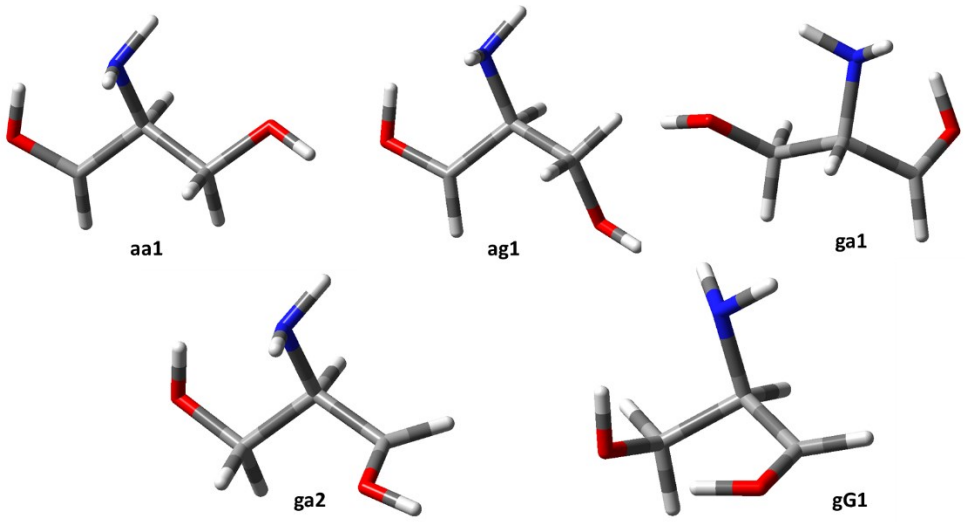

Figure S3. Optimized 3D structures of calculated C1 serinol radical conformers, labelled according to the values of the $\angle O_1CCC$ angle (first label) and the $\angle CCCO_2$ angle (second label) as G (+60°), g (−60°) and a (180°).

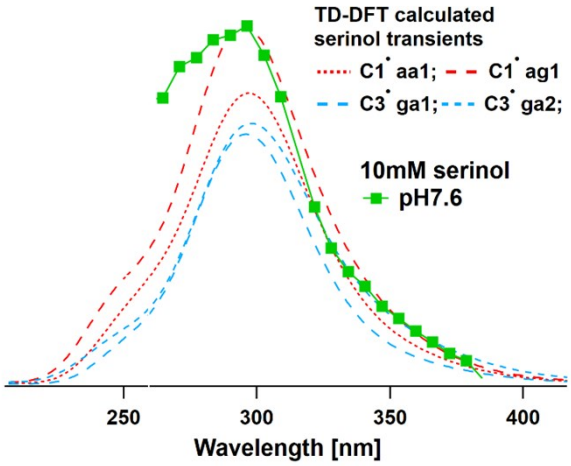

Figure S4. Experimental and TD-DFT calculated absorption spectra of serinol transients produced in reaction with •OH at pH 7.

Table S1. EPR parameters and excitation energies of the radicals formed in the reaction of serinol with OH radical

Radical	Conformer	Relative energies, kJ mol^{-1}	Significant Hyperfine coupling constant, Gauss	g value	Significant Excitation energies (oscillator strengths), nm
C1 serinol radical cation	aa1	0	17.5(βN), 23.5(αH)	2.0032	269(0.02), 323(0.01)
	ag1	6.43	18.5(βN), 25.6(αH)	2.0032	313(0.01), 321(0.014)
	ga1	6.68	17.6(βN), 21.5(αH)	2.0032	269(0.017), 320(0.01)
	ga2	-5.42	9.6(βN), 21.5(αH)	2.0033	341(0.01), 366(0.01)
	gG1	-5.16	15(βN), 19(αH)	2.0032	315(0.01), 339(0.018)
C3 serinol radical cation	aa1	-6.21	16.3(βN), 22.1(αH)	2.0032	367(0.02)
	ag1	-5.42	9.6(βN), 21.5(αH)	2.0033	341(0.01), 366(0.01)
	ga1	-3.17	18(βN), 26(αH)	2.0033	298(0.017), 325(0.007), 338(0.01)
	ga2	4.6	15(βN), 20(αH)	2.0032	315(0.01), 325(0.018)
	gG1	-2.54	17(βN), 32(αH)	2.0032	313(0.015), 354(0.012)
C2 serinol radical cation	aa1	25.59	11.4(αN), 25(3βH), 41.8(4βH)	2.0025	266(0.04), 284(0.008)
	ag1	29.61	20(3βH), 27(4βH)	2.0026	260(0.01), 295(0.006)
	ga1	29.45	31.6(3βH), 56 (4βH)	2.0026	269(0.008), 298(0.016)
	ga2	29.45	18(3βH), 21(4βH)	2.0026	283(0.01), 257(0.016)
	gG1	39.78	16.8(3βH), 9.6(4βH)	2.0025	233(0.07), 318(0.009)
C1 serinol radical	aa1	0.0	11(αH), 37.7(βH)	2.0033	263(0.008), 293(0.03)
	ag1	2.7	11.6(αH), 35.5(βH)	2.0032	261(0.007), 294(0.035)
	ga1	1.9	14(αH), 13.6(βH)	2.0033	307(0.018), 345(0.005)
	ga2	3.8	3(βN), 14.9(ɣH)	2.0032	264(0.02), 296(0.009), 350(0.009)
	gG1	2.1	11(αH), 37.8(βH)	2.0032	301(0.004), 347(0.014)
C3 serinol radical	aa1	2.1	13.5(αH), 6(βH), 4(βOH), 4(βN)	2.0031	261(0.03), 299(0.01), 343(0.009)
	ag1	6.1	11.4(αH), 33(βH)	2.0031	284(0.03), 311(0.005)
	ga1	8.7	14(αH), 34(βH)	2.0032	280(0.017), 297(0.015)
	ga2	1.6	11.5(αH), 38.5(βH), 4(βN)	2.0032	299(0.02), 352(0.006)
	gG1	14.5	10(βH), 13(βN), 13.4(ɣH), 6.7(ɣH)	2.0031	235(0.008), 283(0.007), 340(0.007)
C2 serinol radical	aa1	-18.9	29(βH), 26(βH), 2(αN)	2.0025	360(0.025), 384(0.08)
	ag1	-15.8	5.7(4βH), 6.5(αN), 3.7(βH)	2.0026	344(0.01), 368(0.07)
	ga1	-17.6	12.5(4βH), 4(αN), 4.5(2βH)	2.0027	304(0.02), 351(0.016), 405(0.02)
	ga2	-15.7	12.2(4βH), 4.2(αN), 5.3(βH)	2.0025	309(0.03), 368(0.018), 401(0.03)
	gG1	-21.7	29(βH), 26(βH), 2(αN)	2.0026	350(0.017), 352(0.018)
N-centered serinol radical	aa1	0	61(βH), 21(αH), 11(αN)	2.0045	224(0.015), 252(0.003), 316(0.002) 335(0.003), 534(0.002)
	ag1	7.29	66(βH), 21(αH), 11(αN)	2.0045	220 (0.015), 259 (0.002), 319(0.001), 346 (0.004), 540 (0.002)
	ga1	-1.45	53(βH), 21(αH), 11(αN)	2.0046	223(0.015), 251(0.006), 315 (0.002), 550(0.001)
	ga2	5.18	65(βH), 21(αH), 11(αN)	2.0046	217(0.003), 252(0.002), 302 (0.002), 355(0.003), 540(0.002)
	gG1	-4.58	52(βH), 21(αH), 11(αN)	2.0049	220(0.009), 245 (0.006), 325 (0.004), 330(0.001), 579 (0.001)

Table S2. EPR rarameters and excitation energies of the radicals formed in the reaction of serinol and N-boc-serinol with OH radical

Radical	Significant Hyperfine coupling constant, Gauss	g value	Significant Excitation energies (oscillator strengths), nm
Aminoethanol radical	15.5 (αH), 31.7(βH), 5(βH)	2.0027	x
Aminoethanol radical anion	4 (αH), 41(βH), 18(βH), 2(βN), 7(2βH)	2.0026	x
2-Iminopropanol radical	17.5(αH), 16.9(αH), 11.6(γH), 6(βN)	2.0034	x
C1 N-boc-serinol radical	14(αH), 38(βH)	2.0033	290(0.02), 306(0.004), 337(0.003)
C2 N-boc-serinol radical	18(4βH)	2.0027	284(0.06), 309(0.02), 343(0.02)
C1 N-boc-serinol radical cation	16.6(αH), 16.6 (βH), 11.8G(βN)	2.0033	235(0.009), 256(0.008), 326(0.05)
C2 N-boc-serinol radical cation	40(2βH), 8.4(2βH), 14.5(2βH), 3.6(αN)	2.0025	264 (0.01), 325(0.009)

*x - no calculations were made

Table S3. EPR parameters of the radicals formed in the reaction of glycerol with OH radical

Radical		g value	Significant Hyperfine coupling constant, Gauss
C1 glycerol radical	calculated	2.0031	16.4(αH), 4.3(βH), 1(OH)
	published	2.0029 [33]	17.3(αH), 10.6(βH), 1(OH) [33]
C2 glycerol radical	calculated	2.0029	10.0(4βH) (averaged)
	published	2.0028[33]	10.0(4βH) [33]
Hydroxypropanal radical (cis;trans)	calculated	2.0051	17.3(αH), 33 (2βH) (averaged)
	published	2.0045(cis);	17.1 (αH), 27.8(2βH), 1.2(CHO) (cis);
		2.0042 (trans)[33]	18.1(αH), 25.6(2βH), 1.5(CHO) (trans)[33]
Hydroxyacetone radical	calculated	2.0050	19 (αH), 18.9 (αH), 3.7(2γH) (C3) (averaged)
	published	2.0041[33]	19.6 (αH), 19.3(αH), 2.3(2γH) [33]

Table S4. Optimized Quantum Mechanical Geometries

C1 serinol radical_aa1				C1 serinol radical_ag1				C1 serinol radical_ga1			
0 2				0 2				0 2			
C	1.238642	-0.63352	0.302813	1.389659	0.413599	0.25506		-1.01539	-0.73445	-0.18637	
O	2.374997	0.03849	-0.24648	2.13207	-0.73065	-0.1753		-2.28499	-0.07635	-0.09499	
C	-0.0211	-0.00237	-0.2767	-0.02811	0.315083	-0.30435		0.019244	0.100843	0.574142	
N	-0.27185	1.389193	0.132864	-0.86121	1.489382	-0.00273		0.126218	1.424057	-0.06425	
C	-1.2388	-0.8063	0.070021	-0.75799	-0.89788	0.185797		1.375871	-0.53867	0.533623	
O	-2.43523	-0.16344	-0.05202	-2.11238	-0.89604	0.011669		2.134599	-0.28564	-0.57402	
H	3.168846	-0.30482	0.174938	3.021502	-0.67481	0.187605		-2.91139	-0.53031	-0.66757	
H	-2.20358	0.787922	-0.0414	-2.35104	0.046431	-0.08395		1.746574	0.525657	-0.95849	
H	-0.10473	1.506731	1.126886	-0.77007	1.761342	0.970389		-0.79367	1.751993	-0.33168	
H	0.344722	2.025229	-0.35471	-0.59814	2.283357	-0.57179		0.512815	2.102569	0.580953	
H	-1.28794	-1.87296	-0.09701	-0.3111	-1.88022	0.172368		1.580855	-1.48723	1.008535	
H	1.263801	-1.6983	0.049347	1.348983	0.458094	1.348518		-1.06625	-1.73102	0.258114	
H	1.226324	-0.54136	1.393278	1.853683	1.333452	-0.1125		-0.71146	-0.83071	-1.23265	
H	0.104928	0.025946	-1.37012	0.055739	0.275375	-1.40145		-0.31617	0.160236	1.616212	
C1 serinol radical_ga2				C1 serinol radical_gG1				C2 serinol radical_aa1			
0 2				0 2				0 2			
C	-1.41662	-0.13125	0.610323	-1.32367	0.287304	0.443474		1.27529	-0.62854	0.360327	
O	-1.99388	-0.51314	-0.57492	-1.67536	-0.77576	-0.34097		2.221852	-0.14903	-0.62454	
C	0.015124	0.263609	0.528959	0.099357	0.725601	0.52894		-0.01209	0.086901	0.19719	
N	0.291801	1.469965	-0.30029	0.537601	1.433773	-0.71018		0.02139	1.470403	0.282973	
C	0.914223	-0.86034	-0.00531	1.059077	-0.45665	0.712		-1.31915	-0.57984	0.413099	
O	2.265045	-0.41529	-0.10523	1.031989	-1.30516	-0.44848		-2.32897	-0.17213	-0.54274	
H	-2.94672	-0.60015	-0.4645	-0.85949	-1.26263	-0.56654		3.109141	-0.36181	-0.31577	
H	2.193454	0.509264	-0.3936	1.184668	-0.71051	-1.19905		-1.978	-0.34555	-1.42459	
H	-0.22132	1.414398	-1.17376	-0.18825	2.064523	-1.02799		-0.81777	1.944009	-0.01703	
H	-0.02842	2.305115	0.1748	1.354399	2.003798	-0.51396		0.855575	1.903053	-0.08546	
H	0.550274	-1.19227	-0.9835	0.763869	-1.07143	1.559709		-1.76192	-0.31268	1.379932	
H	0.893484	-1.71226	0.672991	2.075465	-0.09199	0.882863		-1.18876	-1.66392	0.392409	
H	-2.07439	0.278421	1.366185	-2.13849	0.971247	0.635129		1.116281	-1.70327	0.247125	
H	0.345327	0.50302	1.540781	0.183022	1.370462	1.410293		1.7084	-0.45448	1.357101	

Continuation of the Table S4

C2 serinol radical_ag1				C2 serinol radical_ga1			C2 serinol radical_ga2		
0 2				0 2			0 2		
C	1.26617	-0.15287	0.621154	-1.00576	-0.75833	-0.21371	-1.34533	-0.15235	0.631336
O	1.761682	-0.8671	-0.55286	-2.32589	-0.30732	0.164649	-2.19698	-0.46387	-0.51789
C	-0.02021	0.51993	0.340168	-0.00164	0.243025	0.227623	0.006236	0.244093	0.192838
N	4.51E-05	1.648168	-0.46487	-0.18242	1.542599	-0.23079	0.211236	1.544318	-0.24324
C	-1.3319	-0.12131	0.59001	1.355268	-0.16625	0.649706	1.013063	-0.7625	-0.22666
O	-1.77974	-1.0417	-0.4535	2.231847	-0.58588	-0.44508	2.327469	-0.3285	0.193883
H	2.635635	-1.21375	-0.33767	-2.97073	-0.78153	-0.37068	-3.06011	-0.73195	-0.18058
H	-1.78591	-0.56023	-1.28793	2.307662	0.152281	-1.05965	2.982216	-0.79904	-0.33269
H	-0.81741	2.239951	-0.45098	-1.14486	1.824116	-0.3476	-0.36626	2.257203	0.176318
H	0.862523	2.169583	-0.50724	0.3715	2.256413	0.219342	1.177461	1.825475	-0.32197
H	-2.10676	0.639098	0.73479	1.30473	-1.03885	1.298525	1.0292	-0.88624	-1.31954
H	-1.28725	-0.73647	1.486734	1.847392	0.642594	1.198483	0.768686	-1.73121	0.215787
H	1.134853	-0.86078	1.442328	-0.7832	-1.72527	0.244332	-1.81531	0.654968	1.201651
H	2.024099	0.581324	0.916962	-0.9904	-0.89302	-1.30543	-1.28224	-1.03594	1.270647
C2 serinol radical_gG1				C3 serinol radical_aa1			C3 serinol radical_ag1		
0 2				0 2			0 2		
C	-1.27953	-0.11716	0.581398	1.295562	-0.53436	0.296945	1.433301	0.369314	0.171709
O	-1.55063	-1.09611	-0.46747	2.439959	-0.12522	-0.33779	2.168368	-0.74929	-0.1274
C	-0.03151	0.655837	0.364175	0.032318	0.038768	-0.23009	0.009918	0.339941	-0.27821
N	-0.06699	1.713491	-0.53564	-0.25645	1.439013	0.192633	-0.72978	1.565613	0.049265
C	1.272235	-0.0135	0.589179	-1.1731	-0.81664	0.172551	-0.76699	-0.84622	0.31193
O	1.541457	-1.09437	-0.36785	-2.38852	-0.20248	-0.2447	-2.1121	-0.84682	-0.15669
H	-0.71395	-1.55	-0.63404	3.213497	-0.42381	0.153028	3.096403	-0.59938	0.084142
H	1.678344	-0.69449	-1.23418	-2.22405	0.750238	-0.14787	-2.38024	0.0846	-0.14646
H	0.743016	2.314808	-0.56393	-0.07717	1.54868	1.185847	-0.54802	1.845786	1.007402
H	-0.93256	2.228044	-0.59825	0.356199	2.086131	-0.28821	-0.44748	2.333374	-0.54648
H	1.28096	-0.51333	1.556285	-1.17507	-0.96095	1.260384	-0.74073	-0.78273	1.4065
H	2.100058	0.699316	0.561109	-1.11469	-1.79703	-0.29782	-0.31404	-1.78956	0.013397
H	-2.15579	0.531732	0.59511	1.390282	-0.84449	1.331221	1.967776	1.308773	0.248435
H	-1.22496	-0.63774	1.541415	0.085985	0.06311	-1.32154	-0.03278	0.230474	-1.37162

Continuation of the Table S4

C3 serinol radical_ga1 0 2				C3 serinol radical_ga2 0 2			C3 serinol radical_gG1 0 2		
C	-1.01473	-0.7174	-0.04801	-1.40489	-0.25067	0.574702	-1.1175	-0.41801	0.670133
O	-2.27968	-0.20096	-0.17078	-1.84085	-0.38063	-0.78148	-1.18896	-1.29211	-0.45847
C	-0.01972	0.203702	0.564271	0.052533	0.204244	0.588709	-0.12376	0.743329	0.487889
N	0.050074	1.471448	-0.19479	0.317418	1.448311	-0.15399	-0.40419	1.58331	-0.701
C	1.381996	-0.41643	0.574445	0.985015	-0.84667	0.063199	1.296827	0.28603	0.494213
O	1.926143	-0.48397	-0.73997	2.228352	-0.41735	-0.30227	1.582901	-0.77845	-0.33228
H	-2.88451	-0.88102	-0.48666	-2.79732	-0.48251	-0.78798	-0.29724	-1.62271	-0.62425
H	1.603731	0.320693	-1.17731	2.115557	0.54377	-0.45135	2.530423	-0.95233	-0.3409
H	-0.87397	1.745074	-0.50452	-0.21646	1.454543	-1.01619	-0.45412	0.992142	-1.52386
H	0.394043	2.217915	0.398473	0.041337	2.259152	0.384395	-1.31861	2.013771	-0.6052
H	1.351508	-1.42924	0.976577	0.951866	-1.86764	0.417165	2.104852	0.982384	0.680655
H	2.029738	0.184723	1.221734	-2.01606	0.487756	1.099762	-2.12151	-0.01307	0.797315
H	-0.92563	-1.79018	0.062445	-1.49332	-1.20684	1.101241	-0.86025	-0.97821	1.575189
H	-0.30244	0.39212	1.614509	0.296507	0.416072	1.641257	-0.23917	1.391233	1.360686
C1 serinol radical cation_aa1 .+1 2				C1 serinol radical cation_ag1 +1 2			C1 serinol radical cation_ga1 +1 2		
C	1.111883	-0.85276	0.185357	1.435885	0.245797	0.250933	-0.83494	-0.89307	0.00737
O	2.277026	-0.20495	-0.31831	2.009163	-0.94248	-0.27112	-2.17597	-0.41573	0.01823
C	-0.08488	0.001259	-0.22009	-0.00571	0.287088	-0.24604	0.037996	0.249259	0.516354
N	0.261741	1.465197	0.189641	-0.55428	1.724407	-0.00898	-0.33603	1.49967	-0.33721
C	-1.34544	-0.47398	0.364469	-0.87431	-0.70968	0.386324	1.487602	-0.00532	0.560028
O	-2.54951	-0.24344	-0.20974	-2.05822	-0.93647	-0.23376	2.183277	-0.57606	-0.45395
H	3.058841	-0.57131	0.107286	2.902856	-1.03248	0.076141	-2.74076	-1.02852	-0.46391
H	-2.4613	0.05461	-1.12447	-2.59711	-1.55417	0.275077	1.620233	-1.0574	-1.07291
H	0.157164	1.604457	1.194435	-0.52423	1.978061	0.979024	-1.35633	1.536602	-0.41817
H	1.240229	1.638949	-0.06078	-0.02992	2.424611	-0.53584	-0.00258	2.355209	0.103091
H	-1.4096	-0.83869	1.377551	-0.68883	-1.13319	1.361066	2.117136	0.489595	1.281131
H	0.984782	-1.8431	-0.25349	1.455651	0.250548	1.344677	-0.70439	-1.74354	0.678023
H	1.158355	-0.95528	1.27183	1.97324	1.128931	-0.10486	-0.54935	-1.19893	-1.00321
H	-0.13916	0.051332	-1.30799	-0.02683	0.186084	-1.33157	-0.29042	0.522768	1.516628
H	-0.331	2.142631	-0.28596	-1.52761	1.773071	-0.30904	0.056316	1.455643	-1.27699

Continuation of the Table S4

C1 serinol radical cation_ga2 +1 2				C1 serinol radical cation_gG1 +1 2				C2 serinol radical cation_aa1 +1 2			
C	-1.46006	-0.12194	0.58924	1.304998	-0.43295	0.405025		1.297803	-0.78918	0.202148	
O	-1.99254	-0.5338	-0.58922	1.79387	0.570712	-0.35864		2.237983	0.010251	-0.51896	
C	-0.02913	0.210367	0.563821	-0.14157	-0.64853	0.588641		-0.01239	-0.09731	0.16596	
N	0.252076	1.482587	-0.2783	-0.76168	-1.45403	-0.6064		0.04722	1.361642	0.259848	
C	0.872444	-0.88285	-0.00521	-0.96968	0.62325	0.718842		-1.36094	-0.69577	0.326194	
O	2.194821	-0.34979	-0.04004	-0.79148	1.352194	-0.50271		-2.33298	0.017329	-0.44535	
H	-2.94754	-0.64476	-0.50982	1.06186	1.160429	-0.62316		3.115481	-0.11407	-0.14333	
H	2.754014	-0.91324	-0.58442	-1.30438	2.167384	-0.48084		-2.22955	-0.2212	-1.37431	
H	-0.2128	1.431624	-1.18458	-0.17649	-2.25439	-0.84125		-0.7703	1.77223	-0.20009	
H	-0.07255	2.322827	0.19678	-1.69562	-1.79951	-0.38169		0.90424	1.687908	-0.19932	
H	0.540684	-1.17593	-1.00264	-0.60521	1.189898	1.576009		-1.7036	-0.62534	1.363669	
H	0.807584	-1.74946	0.654286	-2.02355	0.388891	0.876169		-1.32198	-1.75366	0.063278	
H	-2.11564	0.167282	1.394894	2.033448	-1.16515	0.713179		1.189425	-1.78074	-0.24442	
H	0.301975	0.469472	1.565969	-0.30308	-1.2871	1.452885		1.637194	-0.93047	1.237364	
H	1.262011	1.549345	-0.43547	-0.83683	-0.85609	-1.43076		0.061674	1.70671	1.226844	
C2 serinol radical cation_ag1 +1 2				C2 serinol radical cation_ga1 +1 2				C2 serinol radical cation_ga2 +1 2			
C	1.187504	-0.82852	-0.19154	-1.18006	-0.83809	-0.14322		-1.36957	-0.59826	0.480868	
O	2.37015	-0.03808	-0.1668	-2.33235	-0.01104	-0.02		-2.19062	-0.07691	-0.57635	
C	0.002953	-0.06331	0.297606	0.00274	-0.05717	0.301578		-0.00277	-0.05743	0.301251	
N	0.070112	1.383513	0.080816	-0.08291	1.387643	0.08204		0.082846	1.387449	0.082271	
C	-1.36127	-0.61294	0.483533	1.369698	-0.59753	0.481522		1.180339	-0.83801	-0.1434	
O	-2.20022	-0.06603	-0.54642	2.19015	-0.07778	-0.57693		2.33245	-0.0108	-0.01973	
H	2.759123	-0.07091	0.714733	-3.01295	-0.31799	-0.62746		-3.10815	-0.06691	-0.28366	
H	-3.11172	-0.05501	-0.23548	3.107793	-0.06711	-0.28464		3.012892	-0.31682	-0.62787	
H	-0.60223	1.676778	-0.63703	-1.04753	1.621115	-0.1804		-0.15567	1.922081	0.921707	
H	-0.14606	1.914885	0.928464	0.154869	1.922507	0.921528		1.047725	1.620963	-0.17926	
H	-1.7537	-0.3423	1.469242	1.332692	-1.68822	0.455661		1.04815	-1.16333	-1.18579	
H	-1.32269	-1.7024	0.425086	1.777575	-0.2971	1.45229		1.263951	-1.74203	0.46784	
H	1.036844	-1.12395	-1.2376	-1.26364	-1.74204	0.468143		-1.77713	-0.29965	1.452343	
H	1.292173	-1.7494	0.386145	-1.04756	-1.16354	-1.18553		-1.33239	-1.6889	0.45307	
H	1.022946	1.629318	-0.21108	0.56248	1.686186	-0.65772		-0.56185	1.68635	-0.65794	

Continuation of the Table S4

C2 serinol radical cation_gG1 +1 2				C3 serinol radical cation_aa1 +1 2			C3 serinol radical cation_ag1 +1 2		
C	-1.02918	-0.56415	0.736144	1.334919	-0.51819	0.31773	1.460064	-0.12194	-0.58924
O	-1.40289	-1.20948	-0.49384	2.458482	-0.14715	-0.34256	1.992538	-0.5338	0.589218
C	-0.07429	0.539059	0.447209	0.071205	-0.01609	-0.22798	0.029135	0.210367	-0.56382
N	-0.63592	1.605715	-0.40126	-0.22024	1.452145	0.200455	-0.25208	1.482587	0.2783
C	1.394211	0.324876	0.416985	-1.13702	-0.84345	0.187561	-0.87244	-0.88285	0.005205
O	1.662457	-0.74836	-0.50523	-2.29189	-0.16934	-0.30546	-2.19482	-0.34979	0.040037
H	-0.60785	-1.62441	-0.85486	3.242821	-0.46499	0.120929	2.947542	-0.64476	0.509821
H	2.478872	-1.1869	-0.24081	-3.07877	-0.5303	0.115192	-2.75401	-0.91324	0.584417
H	0.08328	2.230107	-0.76881	-0.12555	1.572735	1.208649	0.212801	1.431624	1.184577
H	-1.30743	2.182652	0.113232	0.41454	2.104108	-0.25649	0.072549	2.322827	-0.19678
H	1.724842	0.048093	1.420636	-1.1783	-0.94675	1.274535	-0.54068	-1.17593	1.00264
H	1.927543	1.231306	0.12207	-1.0363	-1.83648	-0.25278	-0.80758	-1.74946	-0.65429
H	-1.95534	-0.19347	1.174505	1.419094	-0.991	1.284529	2.115641	0.167282	-1.39489
H	-0.57284	-1.26607	1.433773	0.120649	0.047972	-1.31484	-0.30197	0.469472	-1.56597
H	-1.14066	1.202614	-1.20042	-1.18383	1.678016	-0.0626	-1.26201	1.549345	0.435467
C3 serinol radical cation_ga1 +1 2				C3 serinol radical cation_ga2 +1 2			C3 serinol radical cation_gG1 +1 2		
C	-1.02646	-0.7295	-0.08106	-1.28515	-0.43871	0.679374	-0.95758	-0.63677	0.736239
O	-2.31518	-0.30321	-0.04655	-1.82731	-0.58016	-0.63085	-1.0811	-1.32782	-0.50093
C	-0.06257	0.177072	0.561941	0.090722	0.196856	0.522598	-0.1217	0.644492	0.592491
N	0.029578	1.509382	-0.22962	-0.14169	1.541265	-0.23235	-0.75082	1.421421	-0.6
C	1.344849	-0.38994	0.649927	1.048639	-0.66248	-0.19568	1.318944	0.423626	0.396698
O	1.825785	-0.52654	-0.68476	2.385112	-0.43614	-0.1443	1.677344	-0.63187	-0.38112
H	-2.87964	-0.88174	-0.57314	-2.75711	-0.82137	-0.56845	-0.22313	-1.71105	-0.7227
H	2.769071	-0.71737	-0.66651	2.637037	0.069195	0.640039	2.637249	-0.69568	-0.45128
H	-0.89962	1.826637	-0.50383	-0.74799	1.355774	-1.03471	-0.90154	0.767251	-1.37207
H	0.468055	2.251476	0.316937	-0.59698	2.236206	0.361021	-1.65322	1.82722	-0.35044
H	1.298817	-1.35217	1.163111	0.747735	-1.29726	-1.01294	2.07213	1.132462	0.702297
H	1.982828	0.280252	1.228997	-1.9217	0.195526	1.299513	-1.96894	-0.38421	1.049761
H	-0.74203	-1.50697	-0.77232	-1.16727	-1.40327	1.175158	-0.50666	-1.26023	1.50858
H	-0.41366	0.473355	1.55045	0.47744	0.491207	1.497707	-0.26725	1.290024	1.454956
H	0.58939	1.353023	-1.07073	0.732954	1.941573	-0.56752	-0.14092	2.173733	-0.91529

Continuation of the Table S4

N-centered serinol radical_aa1				N-centered serinol radical_ag1				N-centered serinol radical_ga1			
0 2				0 2				0 2			
C	1.263642	-0.64901	0.236993	1.4323	0.383827	0.234923		-0.98442	-0.72833	-0.11467	
O	2.377566	0.066588	-0.2965	2.062338	-0.80494	-0.24383		-2.29821	-0.17346	-0.04472	
C	-0.01488	0.060286	-0.21679	-0.021	0.385826	-0.24983		-0.00721	0.284651	0.503895	
N	-0.13137	1.404154	0.278655	-0.71472	1.609832	0.043053		0.014135	1.528157	-0.21912	
C	-1.27513	-0.7281	0.150755	-0.83631	-0.78978	0.297518		1.412991	-0.26668	0.622782	
O	-2.45101	-0.0171	-0.22088	-2.18641	-0.73597	-0.15308		2.02562	-0.45725	-0.65271	
H	3.178923	-0.22941	0.146195	2.937854	-0.86855	0.150882		-2.8743	-0.65842	-0.64343	
H	-2.32383	0.893632	0.077685	-2.49097	0.16836	-0.00046		1.985175	0.388771	-1.11557	
H	0.792338	1.838536	0.205479	-0.08778	2.396714	-0.14474		-0.96047	1.803012	-0.36828	
H	-1.29714	-1.68012	-0.3772	-0.79569	-0.77359	1.392702		1.408071	-1.23935	1.113021	
H	1.252774	-1.67964	-0.12891	-0.42138	-1.73365	-0.04664		2.008234	0.41945	1.231891	
H	1.307214	-0.67067	1.329023	1.939701	1.272993	-0.15117		-0.9274	-1.66132	0.452696	
H	0.032374	0.136266	-1.31673	0.005969	0.296654	-1.35025		-0.70491	-0.93207	-1.14976	
H	-1.27739	-0.93262	1.227163	1.45796	0.420285	1.327887		-0.38082	0.490726	1.520722	
N-centered serinol radical_ga2				N-centered serinol radical_gG1				2-iminopropanol radical			
0 2				0 2				0 2			
C	-1.41228	-0.1343	0.610299	-1.29787	-0.07658	0.558956		C	-0.71384	-1.34988	0.070368
O	-1.92045	-0.44231	-0.69033	-1.39555	-1.10305	-0.42427		C	-0.59633	0.048206	0.023406
C	0.042985	0.314001	0.481425	-0.03942	0.806618	0.407658		H	-1.68748	-1.81702	-0.02627
N	0.238406	1.488856	-0.32753	0.020254	1.491152	-0.85796		H	0.156887	-1.97944	0.199392
C	0.979555	-0.79288	-0.01668	1.255955	0.025371	0.631427		C	0.770946	0.69959	0.174369
O	2.322613	-0.32457	-0.10704	1.446618	-0.99113	-0.36573		H	0.805099	1.582646	-0.47148
H	-2.83233	-0.73648	-0.60051	-0.51041	-1.48205	-0.53034		H	0.874044	1.042252	1.206937
H	2.284782	0.522316	-0.57134	1.580375	-0.54616	-1.2114		N	-1.60669	0.87207	-0.1166
H	-0.52115	2.147188	-0.13635	-0.86105	1.997163	-0.98222		H	-2.47971	0.345705	-0.16927
H	0.634191	-1.15584	-0.98805	1.227068	-0.4916	1.589235		O	1.86262	-0.16478	-0.0657
H	0.979831	-1.6276	0.68285	2.105565	0.711296	0.63492		H	1.912374	-0.34795	-1.00636
H	-1.99602	0.668633	1.070096	-2.19154	0.53988	0.461234					
H	0.366736	0.584491	1.501591	-1.29082	-0.50486	1.567054					
H	-1.46376	-1.01067	1.263098	-0.12149	1.559289	1.209002					

Continuation of the Table S4

Aminoethanol radical 0 2				Aminoethanol radical anion -1 2			
C	0.714471	0.596562	0.217301	C	0.646375	0.670639	-0.18636
C	-0.70029	0.58403	-0.25988	C	-0.83771	0.52012	0.092181
H	1.219815	1.492078	-0.16516	H	1.139704	1.632865	-0.06161
H	0.758629	0.622965	1.321134	H	-1.34282	1.306938	-0.52854
H	-1.19723	1.528029	-0.4607	H	-1.00119	0.905873	1.145908
O	1.382774	-0.60628	-0.23642	N	1.387613	-0.46691	0.153347
H	2.179696	-0.70943	0.298196	H	0.75942	-1.25834	0.025584
N	-1.5209	-0.46754	0.182556	H	2.256117	-0.58499	-0.34575
H	-1.05038	-1.36574	0.171072	O	-1.29707	-0.73482	-0.09299
H	-2.41151	-0.52844	-0.29557				
C1 glycerol radical 0 2				C2 glycerol radical 0 2			
C	0.969351	-0.59019	0.626035		-1.36771	0.52498	0.391914
C	0.068005	0.568121	0.443674		-0.02548	0.03277	0.115276
H	1.589278	-0.70448	1.504308		-1.32562	-1.61191	0.367155
C	-1.15808	0.28086	-0.42352		-1.7149	-0.22175	1.389187
H	-0.2654	0.89425	1.428429		1.234056	-0.7491	0.206297
H	-0.84048	-0.06118	-1.41275		1.563005	-0.8611	1.250973
H	-1.71724	1.211512	-0.54199		1.085333	-1.74957	-0.20642
O	0.756023	1.725168	-0.11593		2.248558	-0.03028	-0.51959
H	1.228704	1.436252	-0.90513		3.108145	-0.24252	-0.14208
O	1.375422	-1.21334	-0.52264		-2.36682	-0.14541	-0.5804
H	2.064014	-1.85757	-0.32561		-2.44568	0.814621	-0.56517
O	-1.95587	-0.71197	0.22449		0.080093	1.386057	0.294096
H	-2.73907	-0.87046	-0.31179		0.98984	1.637164	0.072577
Hydroxypropanal radical 0 2				Hydroxyacetone radical 0 2			
C	-1.16514	0.472255	0.164344	C	-0.75712	0.710602	-0.00061
C	0.120594	-0.27454	0.167466	C	0.627263	0.072737	-0.00021
H	-1.34069	0.870783	1.181715	H	-0.81829	1.363284	0.883522
H	-1.09964	1.347563	-0.50223	H	-0.81895	1.360516	-0.88672
C	1.381487	0.331447	-0.10486	C	0.758996	-1.35067	-0.00038
H	0.102532	-1.32887	0.434187	H	1.75563	-1.77917	0.00004
H	1.365557	1.400233	-0.39266	H	-0.10514	-2.00275	-0.00087
O	-2.21237	-0.41041	-0.22003	O	-1.76869	-0.2844	0.001275
H	-3.0518	0.048177	-0.05812	H	-2.62628	0.167997	-0.00301
O	2.462671	-0.27869	-0.03304	O	1.623461	0.821165	0.000502

Continuation of the Table S4

C1 N-boc-serinol radical 0 2				C2 N-boc-serinol radical 0 2		
C	-2.59384	1.265044	-0.45931	3.281072	1.095019	0.226467
O	-2.29694	2.396687	0.337141	2.853057	2.261623	-0.46059
C	-2.33896	0.022157	0.380628	2.240126	0.035082	0.098589
N	-0.95357	-0.12076	0.822506	0.938698	0.515834	0.129973
C	-2.80758	-1.21408	-0.31691	2.570542	-1.38177	0.418934
O	-2.43992	-2.41482	0.200567	2.192552	-2.31735	-0.58137
H	-2.31362	3.172443	-0.22356	3.293911	3.019749	-0.07671
H	-1.64049	-2.27372	0.722015	1.226122	-2.28315	-0.58656
H	-0.74671	0.180151	1.758391	0.855173	1.517695	0.037076
H	-3.76883	-1.23059	-0.81066	2.127118	-1.66688	1.382069
H	-3.64527	1.261752	-0.76439	3.652255	-1.45726	0.526108
H	-1.97352	1.236889	-1.35631	4.223361	0.717215	-0.1814
H	-2.90295	0.149973	1.314331	3.458162	1.335574	1.285598
C	0.110258	-0.12075	-0.03349	-0.22473	-0.1862	0.073466
O	0.028918	-0.27499	-1.2335	-0.3072	-1.40377	0.041614
O	1.238376	0.045471	0.664408	-1.25088	0.663767	0.059526
C	2.553918	0.018956	0.028365	-2.641	0.208671	-0.00343
C	2.802247	-1.34125	-0.6097	-2.88674	-0.55362	-1.29829
C	2.67969	1.16017	-0.97232	-2.97947	-0.61581	1.230939
C	3.497614	0.236096	1.202282	-3.41853	1.516461	-0.00021
H	2.650849	-2.1347	0.122463	-2.57025	0.043522	-2.15359
H	2.142338	-1.50803	-1.45659	-2.35616	-1.5015	-1.30981
H	3.834511	-1.38935	-0.95623	-3.95419	-0.7503	-1.39628
H	2.425203	2.107707	-0.49695	-2.73358	-0.05937	2.135474
H	3.711724	1.218325	-1.31798	-4.0497	-0.82139	1.237506
H	2.031872	1.008074	-1.83097	-2.44363	-1.56085	1.237399
H	4.528482	0.233397	0.850521	-4.48649	1.30727	-0.04398
H	3.297404	1.193543	1.68244	-3.21247	2.082565	0.907607
H	3.380357	-0.55733	1.939843	-3.14835	2.125018	-0.8626

Continuation of the Table S4

C1 N-boc-serinol radical cation +1 2				C2 N-boc-serinol radical cation +1 2			
C	2.238961	1.10241	0.983184	C	3.206607	1.042776	-0.10851
C	1.827657	-0.26196	0.46595	O	2.475957	2.184218	-0.55191
H	1.359721	1.666761	1.298828	C	2.246066	0.054001	0.462605
H	2.883306	0.955911	1.852057	N	0.922757	0.587138	0.746866
C	2.960948	-1.13983	0.154996	C	2.559889	-1.37735	0.704782
H	1.125603	-0.7503	1.141103	O	2.611533	-2.13757	-0.51049
H	3.945206	-0.76143	-0.07681	H	2.99458	2.98154	-0.40636
O	2.608612	-2.38086	-0.23604	H	1.752214	-2.04785	-0.94313
H	3.372791	-2.86378	-0.55964	H	0.960185	1.581358	0.453801
O	2.912913	1.747963	-0.07696	H	1.850281	-1.81519	1.411158
H	2.99827	2.681248	0.121364	H	3.555048	-1.45977	1.142164
N	1.006283	-0.01742	-0.84158	H	3.75217	0.58183	-0.93795
H	0.944659	-0.90406	-1.34219	H	3.946341	1.324578	0.650551
C	-0.35399	0.534949	-0.60474	C	-0.26361	-0.07048	-0.00139
O	-1.11382	-0.44195	-0.23496	O	-0.04532	-0.87334	-0.85414
O	-0.54762	1.701395	-0.74161	O	-1.33478	0.437245	0.495399
C	-2.54307	-0.22887	0.166916	C	-2.74253	0.051194	-0.0047
C	-2.57416	0.695049	1.370522	C	-2.84381	0.458004	-1.464
C	-3.30947	0.31274	-1.02562	C	-2.93409	-1.43635	0.232881
C	-2.9863	-1.63348	0.527253	C	-3.62533	0.897001	0.894224
H	-1.93908	0.30814	2.166585	H	-2.61322	1.515066	-1.58919
H	-2.25915	1.70349	1.114523	H	-2.1867	-0.13275	-2.0974
H	-3.59707	0.740322	1.741735	H	-3.86933	0.29354	-1.79367
H	-3.18603	-0.33991	-1.88881	H	-2.7554	-1.68865	1.277215
H	-4.36734	0.341585	-0.76808	H	-3.96759	-1.68822	-0.00377
H	-2.99345	1.319712	-1.28572	H	-2.28641	-2.03731	-0.4003
H	-4.02831	-1.60668	0.841402	H	-4.66756	0.716591	0.634344
H	-2.89971	-2.29754	-0.33128	H	-3.4811	0.633969	1.940871
H	-2.38704	-2.02918	1.345763	H	-3.41552	1.95698	0.760844
H	1.539455	0.659209	-1.39397	H	0.694436	0.577144	1.746555