Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Advances in predictive chemistry enable a multiscale rational design approach for biofuels with advantaged properties

SUPPORTING INFORMATION

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Potential Energy Surface Generation Details:

A) Additional Kinbot Settings and Capabilities

While KinBot does have the ability to automatically perform conformer searches to find the lowest energy configuration we did not use this feature because it substantially increased computational time. There are ways to limit the number of conformers searched including using keywords such as "random_conf" which sets the number of random conformers explored if an exhaustive conformer search is not selected. Additionally, the keyword "max_dihed", can be used to set the maximum number of dihedrals explored during an exhaustive conformer search. While these features may be useful in some settings, they were not utilized in our KinBot jobs, as we had other methods to identify the lowest energy conformer.

KinBot can also perform hindered rotor scans. The rotor scans are a combination of single point energy calculations thus making it somewhat difficult to view the potential because of the 36 separate jobs it creates (when scanning in 10-degree increments for 360 degrees). We also found for these larger chain molecules with multiple oxygens the rotors are not always straight forward resulting in large jumps or discontinuities in the KinBot rotor profiles. For these reasons we have chosen to set up the rotor scans in Gaussian manually resulting in a single job that allows us to view and diagnose issues in the rotor profiles more easily.

Another useful feature of KinBot is the automatic intrinsic reaction coordinate (IRC) calculations to confirm expected reactants and products of every transition states. These calculations help weed out unrealistic reactions or "bad" transition state structures identified by KinBot but scanning 3-5 steps in each direction of the transition state structure. While this provides a good first pass screening, we have seen times where unrealistic reactions are still reported by KinBot, thus the use of chemical intuition is still required at times to confirm the feasibility of reported reactions. Occasionally, additional IRC calculations performed at the M06-2x/cc-pVTZ level of theory confirmed expected

reactants and products for questionable transition states. Each scan used between 15-30 points in both directions of the TS structure.

Typically, the KinBot jobs for the ROO species completed with 24 hours, using 1 node and either 8 or 12 cores, at this level of theory. This combination of nodes and cores was found to work well for molecules of this size, with higher number of cores showing a decrease in job efficiency overall. Additional features in KinBot are available to further tailor the job to suit specific applications. (A full list of which can be found on their GitHub Wiki documentation):

https://github.com/zadorlab/KinBot/wiki/Input-and-Keywords##general-parameters

B) Comparison of calculated potential energy surfaces with previous literature data

To help further validate our method of calculating energetics, we compare the energies calculated in this work to previously published work for the ROO1 (O_2 addition to the carbon alpha to the OH group) and subsequent QOOH decompositions for both fuels via potential energy surfaces shown in Figure S1. Only pathways included in the rate constant calculations are shown. To our knowledge this is the only O_2 addition site that has been studied theoretically for both fuels. Energetics published by Welz et al.[1] calculated at the CBS-QB3 levels of for the n-butanol ROO1, and energetics published by Duan et al.[2] at the CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ level of theory for n-pentanol ROO1 are used for comparison. In most cases there was relatively good agreement between this work and the Welz et al.[1] and Duan et al.[2] studies which helps validates our chosen approach. The new energies calculated shown in Figure S1 differ from the Welz et al.[1] and Duan et al.[2] energies by a mean absolute error of 0.9 kcal/mol and 2.8 kcal/mol respectively. There was up 4.1 kcal/mol difference for transition states and up to 5.6 kcal/mol difference for stable products. Many of the starting structures were taken directly from Welz et al.[1] and Duan et al.[2] and confirmed to be the lowest energy conformer with hindered rotor scans, but in some cases lower energy conformers were identified. Thus, the difference in energy is assumed to come from the different level of theory used in this work and the lower energy conformers of select species. These comparisons further support the level of theory chosen for this work and our proposed methodology.

The other n-butanol pathways had similar energy differences as reported for the ROO1 when compared to the energies reported by Welz et al.[1]. In the case of n-pentanol, no other studies could be found to compare energetics for the ROO3 and ROO4. Full PESs for each ROO through QOOH decomposition pathways for which rate constants were calculated are presented in the next section.

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[1] O. Welz, J. Zádor, J. D. Savee, L. Sheps, D. L. Osborn, and C. A. Taatjes, "Low-Temperature Combustion Chemistry of n-Butanol: Principal Oxidation Pathways of Hydroxybutyl Radicals," *J. Phys. Chem. A*, vol. 117, no. 46, pp. 11983–12001, Nov. 2013, doi: 10.1021/jp403792t.

[2] Y. Duan *et al.*, "Oxidation kinetics of n-pentanol: A theoretical study of the reactivity of the 1-hydroxy-1-peroxypentyl radical," *Combust. Flame*, vol. 219, pp. 20–32, Sep. 2020, doi: 10.1016/j.combustflame.2020.05.014.

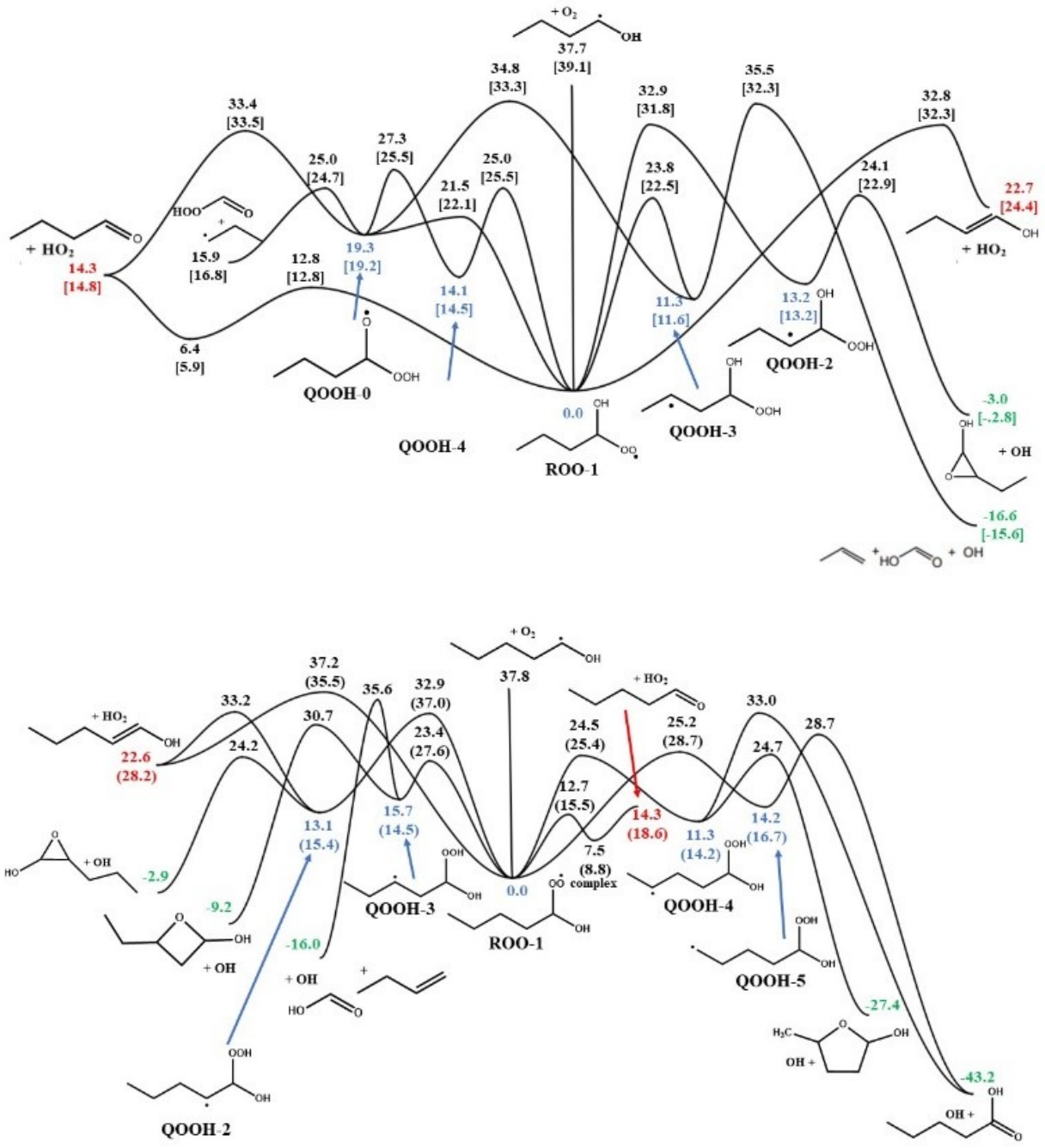


Figure S1. PESs calculated at the CCSD(T)/cc-pV∞Z//M06–2X/cc-pVTZ level of theory for the n-butanol ROO1 (top) and n-pentanol ROO1 (bottom) radicals compared to the corresponding energies from Welz et al.[1] (Top) and Duan et al.[2] (Bottom) in brackets. Energies are given in kcal/mol. Ignition suppression (red) and ignition promotion (green) product energies are highlighted. QOOH and ROO product energies are shown in blue. The pathways shown were turned into rate constants using MESS.

C) Detailed potential energy surfaces, energetics, geometries, and frequencies for species in the low temperature oxidation chemistry of n-butanol ROO and QOOH radicals originating from fuel radical + O_2.

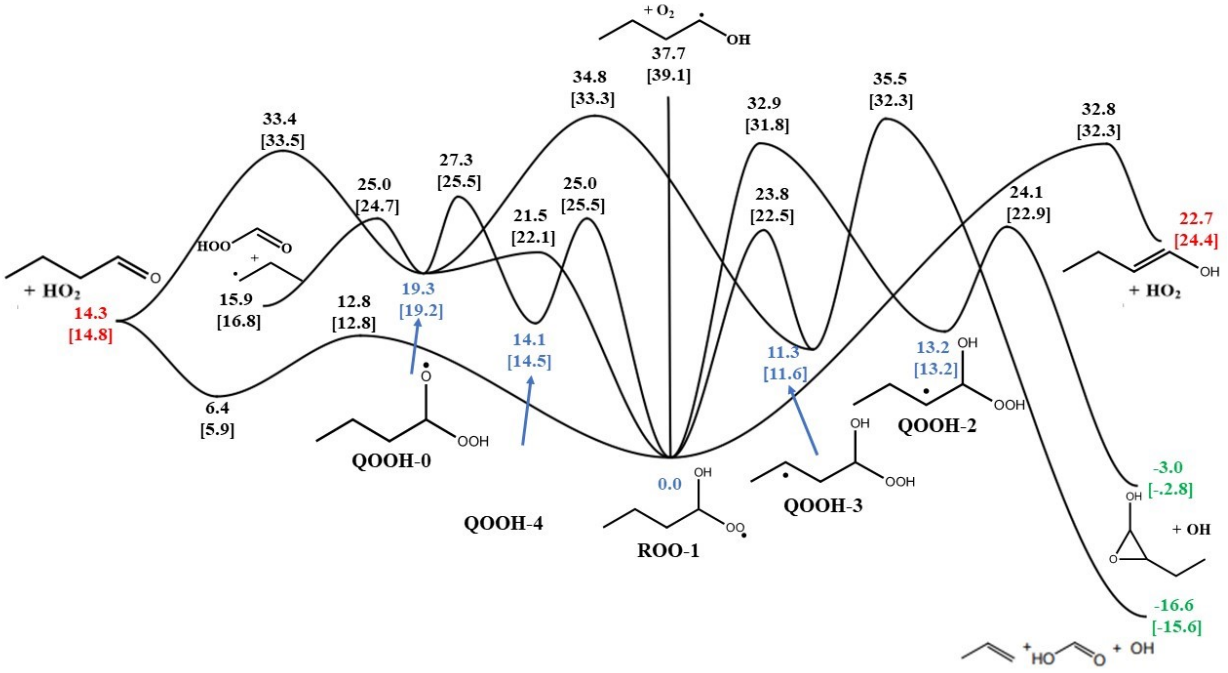


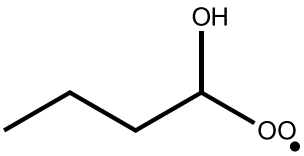
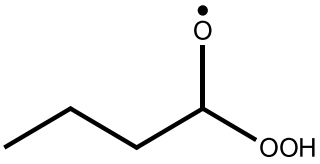
Figure S2. Potential energy surface for n-Butanol ROO1 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

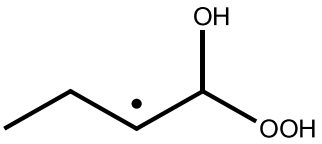
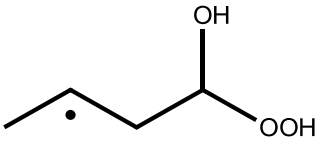
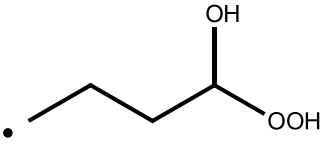
Table S1. Calculated relative energies for n-Butanol ROO1 PES for pathways included in the rate constant calculations

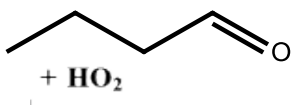
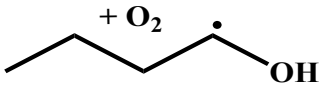
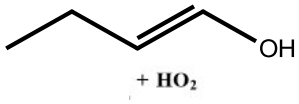
Species	Relative energy (kcal/mol)
N-Butanol ROO1	0.0
QOOH-0	19.3
QOOH-2	13.2
QOOH-3	11.3
QOOH-4	14.1
Butanal reaction complex	6.4
HO2 + Butanal	14.3
O2 + CH_3CH_2CHOH	37.7
HO2 + 1-Buten-1-ol	22.7
Propene + OH + Formic Acid	-16.6
3-ethyloxiran-2-ol + OH	-3.0
Performic acid + $CH_3CH_2CH_2$	15.9
Nbutanol-ROO1 = QOOH-0	21.5

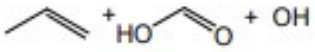
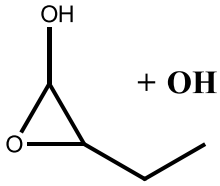
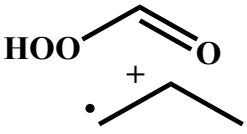
Nbutanol-ROO1 = QOOH-2	32.9
Nbutanol-ROO1 = QOOH-3	23.8
Nbutanol-ROO1 = QOOH-4	25.0
Nbutanol-ROO1 = HO2 butraldehyde complex	12.8
nbutanol-ROO1 = HO2 + 1buten1ol	32.8
QOOH-0 = QOOH-4	27.3
QOOH-0 = Performic acid + $CH_3CH_2CH_2$	25.0
QOOH-0 = QOOH-3	34.8
QOOH-0 = HO2 + Butraldehyde	33.4
QOOH-2 = OH + 3-ethyloxiran-2-ol	24.1
QOOH-3 = Propene + OH + Formic Acid	35.5

Table S2. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Butanol ROO1 PES

Species	Geometry				Frequencies (cm^{-1})
N-Butanol ROO1 	C	-0.0012355	0.00162506	0.00137161	155.68 328.89 338.14
	C	0.00186215	-0.0009091	1.52408339	400.53 545.95 644.98
	C	1.41788654	-0.0020271	2.08740614	754.05 879.03 905.01
	C	1.42363186	-0.0091047	3.59092188	950.11 1000.77 1072.58
	O	2.82341222	0.12477892	4.0042098	1116.27 1146.33 1207.45
	O	2.91514624	0.04672785	5.29447421	1245.26 1292.01 1305.72
	O	0.90989492	-1.1906936	4.06959732	1317.33 1340.29 1375.00
	H	0.51151693	0.88163362	-0.3891217	1407.67 1417.50 1478.20
	H	-1.0163285	0.00224155	-0.3927775	1493.30 1499.50 1505.12
	H	0.50925962	-0.8800235	-0.3877669	1514.19 3056.67 3057.97
	H	-0.5340104	0.87594211	1.89650903	3062.09 3072.41 3101.98
	H	-0.5290367	-0.8756366	1.90045703	3121.16 3134.75 3140.39
	H	1.9630224	-0.885928	1.74931238	3845.76 ! 78.93 87.21
	H	1.96662856	0.87783262	1.74585731	129.72 251.45 450.85
	H	0.92309107	0.86305039	4.02309004	!Torsions
	H	0.94690758	-1.1641646	5.03230196	
QOOH-0 	C	-0.0056103	-0.0135481	0.02118235	141.78 322.31 357.63
	C	-0.0020473	0.01229892	1.54421842	374.87 509.07 649.63
	H	1.00831273	-0.0156611	-0.3758086	748.91 859.44 917.29
	H	-0.5151599	-0.9021034	-0.353521	961.22 1018.81 1043.82
	H	-0.5213494	0.85941814	-0.3803917	1069.51 1088.08 1103.66
	C	-1.4157116	0.00697416	2.1060695	1164.63 1207.60 1266.44
	H	0.54197443	-0.8540994	1.92746594	1286.90 1324.71 1340.83
	H	0.52434946	0.89659781	1.90422072	1399.92 1417.95 1428.25
	C	-1.4379975	0.05944354	3.63830048	1487.64 1499.65 1505.02
	H	-1.9839512	0.86238146	1.7368336	1515.33 2940.14 3060.46
	H	-1.9529122	-0.8954122	1.81235685	3063.78 3080.34 3102.92
	H	-0.7921532	-0.7317138	4.06101387	3126.43 3137.24 3141.34
	O	-0.941113	1.22102374	4.09889991	3805.73 ! 70.14 86.13
	O	-2.7718837	-0.1734139	4.02940034	165.12 248.28 284.62
	O	-2.7960535	-0.2239881	5.44472678	!Torsions
	H	-2.8089651	0.71411406	5.67752487	
QOOH-2	C	-0.0036209	-0.0086895	-0.0024534	127.41 274.10 359.18
	C	-0.0001546	0.00310372	1.52121392	412.83 431.80 617.16

	C	1.37177871	0.00851441	2.09143197	639.91 770.40 914.26
	C	1.60709193	0.00099664	3.55930406	980.94 1040.26 1062.04
	O	2.91188367	0.37992608	3.90957672	1071.70 1110.32 1157.49
	H	0.50752274	0.87038812	-0.3952891	1163.92 1246.75 1271.22
	H	0.50791143	-0.8922706	-0.3853245	1310.84 1367.86 1411.04
	H	-0.5527461	0.86687714	1.90024623	1417.79 1439.84 1453.42
	H	-0.5487169	-0.8687183	1.90309042	1471.11 1503.94 1508.38
	H	2.21977724	-0.2599591	1.47454014	3000.24 3038.85 3063.72
	H	1.46276303	-0.9860723	4.01301969	3066.77 3131.66 3144.18
	H	3.14123097	1.15439041	3.38377416	3196.85 3788.49 3837.76 !
	H	-1.0193712	-0.0115943	-0.3938724	36.53 67.09 187.88
	O	0.6656101	0.88350203	4.12829432	241.36 324.28 466.27
	O	0.71432859	0.70838574	5.53326662	!Torsions
	H	1.58278532	1.07606071	5.75065216	
QOOH-3 	O	0.00783456	0.01028263	-0.0031942	234.64 289.37 380.37
	C	0.00274928	0.00438847	1.39524145	401.57 427.14 615.74
	C	1.40844996	0.00069203	1.9992394	705.74 838.16 887.70
	C	2.27412035	-1.104074	1.48912269	968.81 988.53 1011.14
	C	2.25074228	-2.4492443	2.12172708	1068.53 1123.14 1157.00
	H	0.68050291	-0.6195346	-0.2916531	1171.25 1243.67 1283.32
	O	-0.6410021	-1.1513506	1.87667924	1348.01 1371.94 1392.01
	O	-1.9968262	-1.083514	1.46786956	1418.97 1442.78 1449.88
	H	1.22738391	-2.7747673	2.31368367	1469.37 1482.40 1491.49
	H	2.76352122	-2.4330598	3.09242648	3003.09 3054.48 3090.96
	H	2.7492529	-3.1959935	1.50597893	3107.13 3119.84 3141.33
	H	-1.9181827	-1.1560954	0.50558872	3199.02 3783.37 3800.75 !
	H	3.06678313	-0.8630731	0.7948512	65.95 87.46 110.96
	H	1.29288625	-0.0674828	3.08474851	157.46 332.77 489.39
	H	1.84626806	0.97159433	1.76756465	!Torsions
	H	-0.5703688	0.88008902	1.70016268	
QOOH-4 	C	-0.0020762	0.00571731	0.00017475	210.16 331.91 407.58
	C	0.00202531	-0.0026237	2.50333111	439.95 463.42 563.59
	C	0.83977111	-0.0054702	3.76418032	639.10 746.71 892.29
	O	0.07745156	0.13480173	4.93343923	924.93 1032.60 1051.44
	H	-0.6839057	-0.4516337	4.86952136	1097.93 1109.64 1116.26
	H	-0.6310327	0.8851272	2.53177343	1149.93 1205.45 1263.83
	H	-0.6553567	-0.8779532	2.5255169	1317.82 1334.85 1383.78
	H	0.41607986	0.29872832	-0.9501347	1409.08 1440.98 1452.10
	H	-0.9820424	-0.4494413	0.00178614	1471.52 1474.70 1486.68
	H	1.56461613	0.8099579	3.78513092	3011.68 3046.08 3061.89
	O	1.52970382	-1.2301133	3.77937889	3099.39 3116.62 3168.80
	O	2.48287748	-1.1759618	4.82680806	3273.92 3788.11 3846.39 !
	H	1.91705655	-1.1705748	5.61204048	63.62 111.58 121.40
	C	0.83662635	-0.0168072	1.22540613	133.21 275.12 358.66
	H	1.47901359	-0.9062033	1.23940107	!Torsions
	H	1.52105587	0.83663903	1.2271309	
Butanal reaction complex	C	-0.0085244	-0.0009987	-0.00188	
	C	-0.0100987	-0.0009525	1.49250666	
	O	1.00115322	-0.0004474	2.15797469	
	O	-0.9060717	-0.0013469	4.51316228	
	O	0.37665648	-0.0007083	4.76915275	
	H	-0.5977748	0.86661093	-0.3210083	
	H	-0.5969461	-0.8691907	-0.3209535	
	H	-0.9887621	-0.0014057	1.99587556	
	H	0.79652379	-0.0005129	3.87318133	

	C	1.37397487	-0.0003586	-0.6311232	
	C	1.3040227	-0.0004411	-2.1521928	
	H	1.92607469	-0.8710574	-0.2756461	
	H	1.92524283	0.87088997	-0.2757023	
	H	2.29983167	2.023E-05	-2.5922618	
	H	0.77636359	-0.8814996	-2.5200825	
	H	0.77552229	0.88008914	-2.5201394	
HO_2 + Butanal 	O	0.5055325	2.59512924	1.6402416	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.5078306	
	H	-0.2367003	1.48037439	0.3500898	
	C	-0.00441	6.5214E-05	0.01515082	198.60 351.22 670.56
	C	-0.0010062	-0.0001334	1.53786123	702.76 793.34 871.50
	H	1.00927224	0.00029531	-0.3828154	954.96 971.92 1068.76
	H	-0.5164751	-0.8805809	-0.3756112	1144.92 1164.05 1257.19
	H	-0.5167844	0.88063386	-0.3753805	1314.53 1323.40 1404.53
	C	-1.4078027	-0.0004388	2.11022091	1418.67 1427.04 1455.41
	H	0.53550842	-0.8703149	1.91771071	1494.84 1506.11 1511.73
	H	0.53522414	0.87012322	1.91793976	1865.57 2942.87 3036.88
	H	-1.9800247	0.86885699	1.76638835	3057.95 3063.44 3081.03
	H	-1.9797315	-0.8698463	1.76618297	3107.91 3131.17 3137.91
	C	-1.4563209	-0.0006242	3.61189392	! 88.93 181.14 249.11
	O	-0.487602	-0.0005392	4.32036482	!Torsions
	H	-2.4711876	-0.0008527	4.05519724	
O_2 + $CH_3CH_2CH_2CHOH$ 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
					230.62 349.73 509.21
	C	-0.0039367	-0.0052607	0.01979238	620.02 747.83 869.06
	C	-0.0038201	0.00014303	1.54231085	890.43 997.97 1057.72
	H	1.00880764	-0.0059568	-0.3819927	1099.94 1104.61 1227.03
	H	-0.5173174	-0.88825	-0.3635314	1239.25 1290.48 1304.68
	H	-0.5195623	0.87282133	-0.3725567	1338.93 1371.20 1412.08
	C	-1.4278088	0.00559763	2.12005261	1455.26 1475.52 1497.40
	H	0.52059175	-0.8768464	1.92457696	1503.46 1511.29 3040.59
	H	0.53372927	0.8754132	1.91453435	3056.21 3062.40 3086.53
	C	-1.4693365	-0.0441979	3.6007418	3105.75 3127.87 3132.74
	H	-1.9552293	0.89929846	1.77948852	3153.23 3905.29 ! 97.06
	H	-1.9693541	-0.8584981	1.72216816	110.21 246.78 335.14
	H	-1.2919796	0.84711318	4.19314983	!Torsions
	O	-1.0300237	-1.2294756	4.1278098	
	H	-0.9957258	-1.1677106	5.0845094	
HO_2 + 1-Buten-1-ol 	O	0.5055325	2.59512924	1.6402416	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.5078306	
	H	-0.2367003	1.48037439	0.3500898	
	C	0.01129837	0.00358214	0.01477432	198.80 325.75 451.54
	C	-0.0023248	0.00030064	1.54312544	541.11 783.76 852.60
	C	1.37787198	-0.0043674	2.12660705	922.85 985.48 1034.78
	C	1.85338103	0.96644322	2.89334186	1097.01 1136.87 1162.38
	O	3.09505924	1.0376972	3.44299897	1252.01 1300.65 1339.99
	H	0.510588	0.89612038	-0.3616015	1353.79 1409.41 1411.50
	H	-0.999943	-0.0228673	-0.3905654	1487.78 1500.77 1509.73
	H	0.54933961	-0.864491	-0.3683461	1768.36 3051.37 3060.79
	H	-0.5441111	0.87381188	1.91078899	3091.05 3131.01 3138.61
					3143.67 3204.04 3864.71 !

	H	-0.5535529	-0.8764444	1.89279238	103.57 215.79 410.66
	H	2.01981761	-0.8478365	1.88197194	!Torsions
	H	1.25930771	1.83093605	3.16325846	
	H	3.59834683	0.25830996	3.18883928	
OH + Propene + Formic Acid 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
					183.19 300.73 449.63
	C	0.01585691	-0.0854882	0.00608506	534.72 617.79 774.75
	C	-0.0556418	0.08794094	1.3162727	841.90 870.41 966.21
	H	0.85520357	0.29776305	1.86853711	1040.69 1061.36 1101.47
	C	-1.3158007	0.01746241	2.11895409	1140.89 1185.22 1208.36
	H	0.95637244	-0.0231874	-0.5238575	1271.47 1293.58 1334.99
	H	-0.8698595	-0.2966194	-0.581535	1343.64 1412.14 1423.30
	H	-2.1742995	-0.1963687	1.48389568	1485.76 1504.24 1510.88
	H	-1.2484279	-0.7600202	2.88197701	1546.00 3063.21 3071.95
	H	-1.4981201	0.95851749	2.64087085	3121.21 3129.32 3141.70
					3144.81 3148.86 3870.71
					! 80.80 226.38 265.94
					!Torsions
	O	-0.0764726	0.175471670	0.09622945	
	C	0.0531058	0.034590623	1.42022032	645.59 1077.81 1164.30
	O	1.0902825	0.050749440	2.00881646	1323.84 1418.68 1881.20
	H	0.8111887	0.289072363	-0.27298859	3099.91 3799.57
	H	-0.9311085	-0.097335781	1.88192236	! Torsions 680.90 !
3-ethyloxiran-2-ol + OH 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.0048656182	0.0052648361	-0.0066756637	168.34 342.75 372.63
	C	0.002279904	0.0089069374	1.4542068967	500.79 584.58 770.58
	O	1.2174921893	0.0181235329	0.7573723213	850.82 929.21 968.18
	H	-0.1903033837	-0.9505528595	-0.4932385375	1030.65 1071.38 1125.08
	C	-0.2593001393	1.2262351708	-0.8407644511	1140.89 1158.60 1189.61
	C	0.6986887382	1.2959666262	-2.0253585486	1290.53 1300.74 1316.17
	H	-0.1401241053	2.1090528744	-0.2101407447	1349.14 1413.27 1420.67
	H	-1.2953249713	1.2091370732	-1.1852754197	1479.71 1503.13 1510.34
	H	0.5336526123	2.1961493629	-2.6150941313	1543.38 3064.26 3067.38
	H	1.7299090662	1.2997996172	-1.6738585087	3102.17 3120.26 3137.47
	H	0.5690261093	0.4345911019	-2.6817017176	3146.96 3180.00 3864.59
	O	-0.2726337925	-1.09454965	2.2246888182	! 92.07 213.70 246.40
	H	0.080091419	-1.8712621422	1.7788761453	!Torsions
	H	-0.2375900616	0.9137106846	2.0005081352	
Performic acid + $CH_3CH_2CH_2$ 	C	0.01538741	-2.696E-06	-0.0008042	365.53 458.65 872.98
	O	0.02467832	-1.014E-05	1.19505145	968.70 1035.30 1231.32
	O	1.11166835	1.635E-06	-0.7598789	1379.94 1516.73 1845.97
	O	2.28820566	-4.694E-06	0.02083889	3118.91 3630.83
	H	-0.8645358	1.6062E-06	-0.6498669	! 330.86 !Torsions
	H	1.93021958	-9.395E-06	0.9301233	
	C	0.00398392	-0.0002855	0.00920991	373.58 453.53 756.21
	C	-0.0088492	0.00032511	1.53512531	896.17 928.95 1053.02
	C	1.35655153	0.00925395	2.12046046	1101.17 1178.18 1271.23
	H	0.50409182	0.89025944	-0.3714512	1363.51 1410.57 1469.66

	H	-1.0058669	-0.0252347	-0.3981591	1474.78 1502.40 1508.75
	H	0.54159631	-0.870916	-0.3683077	2984.28 3059.08 3062.57
	H	-0.5754636	0.85926903	1.90453335	3130.39 3139.20 3166.94
	H	-0.5627097	-0.8813578	1.88703798	3270.35
	H	1.52056995	0.29075758	3.14940954	! 93.61 253.67 !Torsions
	H	2.18396319	-0.4237721	1.57666755	
Nbutanol-ROO1 = QOOH-0	C	0.00747065	-0.0439437	-0.0126139	1098.07i 88.28 200.68
	C	-0.0261458	-0.016094	1.51081071	331.31 362.44 525.63
	C	1.37462868	0.07839798	2.08962057	549.32 748.40 780.39
	C	1.32007162	0.06466735	3.65009247	827.57 881.61 895.11
	O	0.85755129	-1.0056744	4.18479723	920.82 966.41 1048.82
	O	2.689984	0.34982659	4.07454644	1067.80 1120.62 1167.87
	O	3.0758635	-0.6427866	4.91489909	1208.26 1248.29 1275.38
	H	0.57613684	-0.9019826	-0.3723315	1321.09 1348.94 1390.51
	H	1.98594992	-0.7761661	1.79810117	1415.24 1449.35 1481.31
	H	1.88016179	0.99286822	1.77838728	1497.99 1504.03 1512.94
	H	0.79131037	0.99676993	3.95931921	2742.74 2814.19 3061.15
	H	2.218672	-1.1904245	4.9250732	3064.37 3081.25 3110.02
	H	-0.6199505	0.83455143	1.85378181	3131.18 3140.53 3143.98
	H	-0.5073243	-0.9139054	1.89800799	! 76.88 128.70 250.66
	H	-0.9981364	-0.1117662	-0.4249484	!Torsions
	H	0.47458748	0.8570592	-0.4118992	
Nbutanol-ROO1 = QOOH-2	C	0.0080038	-0.009717	-0.0055653	2090.99i 134.44 177.61
	C	0.00227015	-0.0106888	1.52493428	218.56 370.23 456.61
	O	1.27561761	0.03629074	2.06724931	558.67 622.87 749.53
	O	-0.7682284	1.13774262	1.82804968	822.13 877.88 924.68
	O	-0.2056067	2.11480661	0.99426261	953.51 982.58 1032.55
	H	0.02615049	1.30950099	0.05229016	1070.05 1114.80 1123.71
	H	0.92440292	-0.3748644	-0.4634322	1164.07 1181.08 1255.83
	H	-0.5147904	-0.860282	1.97246764	1279.63 1318.74 1330.17
	H	1.67335986	0.87463157	1.80398	1400.33 1415.82 1434.75
	C	-1.2660435	-0.3991714	-0.6931981	1475.59 1504.49 1507.01
	C	-1.2711693	-0.0383514	-2.1739221	1745.36 3016.69 3065.17
	H	-2.1060621	0.07187733	-0.1788841	3090.36 3110.32 3134.03
	H	-1.3979394	-1.4820927	-0.5761087	3146.08 3147.30 3837.79
	H	-2.193794	-0.3608409	-2.6530191	! 73.33 254.60 349.46
	H	-1.1817953	1.04016537	-2.3044543	!Torsions
	H	-0.4372809	-0.5109585	-2.6937431	
Nbutanol-ROO1 = QOOH-3	C	0.00838912	0.02005395	0.01884293	1835.41i 62.71 152.66
	C	-0.0083423	7.3393E-05	1.52191768	306.32 359.23 422.57
	C	1.32340355	-0.0139021	2.22803325	468.10 487.72 548.88
	C	1.34886537	0.9704807	3.39670466	600.12 805.61 881.43
	O	2.64762227	1.10296939	3.8427768	932.59 971.64 1025.92
	H	2.65853618	1.70337554	4.59415038	1101.70 1107.89 1131.68
	H	-0.7536405	-0.6610368	1.96071592	1153.10 1193.29 1208.31
	H	1.56527253	-1.0060146	2.61677485	1237.09 1259.38 1317.11
	H	2.12419543	0.29393631	1.55427784	1374.21 1385.24 1410.81
	H	-0.9941838	0.11090404	-0.3949729	1451.48 1471.81 1488.74
	H	0.61269143	0.85034832	-0.3478695	1491.76 1590.08 3033.96
	H	0.44897415	-0.9028487	-0.3725932	3042.67 3060.23 3103.64
	H	0.64801964	0.68001341	4.18694946	3114.64 3127.62 3148.60
	O	0.92521298	2.23662407	2.90135051	3869.92
	O	-0.4364016	2.13734799	2.67359379	! 202.96 336.65 !Torsions
	H	-0.464266	1.18182095	1.94298723	
Nbutanol-ROO1 =	C	0.01906413	0.01044152	0.00941968	1899.51i 111.61 219.84

QOOH-4	C	0.00667583	0.01538379	1.51622653	246.43 329.59 371.31
	C	1.42496948	-0.0080907	2.10001868	453.07 462.45 548.56
	C	2.04661432	1.37670213	2.1526128	628.83 693.96 791.53
	O	1.70134217	2.18119583	1.0337892	872.18 920.39 962.40
	O	1.98561909	1.50978963	-0.1446932	1014.29 1047.32 1098.65
	H	1.02242799	0.84464557	-0.2890817	1110.41 1118.87 1162.25
	H	-0.5434991	-0.8609266	1.87092327	1178.47 1238.54 1258.05
	O	3.42029108	1.22915427	2.28893997	1300.70 1344.95 1375.87
	H	1.42661821	-0.4051203	3.11407845	1402.53 1454.27 1461.90
	H	2.07386299	-0.6459847	1.49891025	1480.45 1492.00 1492.22
	H	0.37912858	-0.9105027	-0.4435199	3041.10 3046.36 3087.01
	H	-0.8440812	0.4323375	-0.4957401	3100.36 3109.58 3137.65
	H	1.61709554	1.96691283	2.97039546	3198.16 3870.75
	H	3.82261629	2.10232999	2.31716014	! 339.12 !Torsions
	H	-0.5301336	0.89068643	1.88529892	
Nbutanol-ROO1 = HO_2 butraldehyde complex	O	0.00467053	0.00418071	-2.898E-05	666.65i 135.17 222.61
	C	0.00114948	0.00096984	1.26551269	281.31 347.96 577.37
	C	1.27935721	-0.0069829	2.05193898	660.56 722.75 742.93
	C	2.41458675	-0.7553949	1.36916843	801.25 854.87 879.79
	C	3.69657265	-0.7085305	2.1895961	982.85 1041.65 1060.01
	O	-0.5502711	-1.8138674	1.50814378	1071.50 1142.39 1191.69
	O	-0.6827677	-2.1789926	0.29612161	1263.34 1316.70 1334.13
	H	4.02426285	0.32093193	2.34138837	1385.25 1387.90 1411.30
	H	4.50324409	-1.2458839	1.69332117	1417.78 1462.74 1498.21
	H	3.54979803	-1.1583634	3.17246645	1505.11 1513.24 1675.46
	H	2.57871126	-0.3238466	0.38210236	1952.85 3036.73 3051.20
	H	2.11207726	-1.7924316	1.20942341	3059.26 3074.82 3089.33
	H	1.0739521	-0.4128653	3.04529139	3112.46 3133.61 3139.76
	H	1.55455522	1.04370379	2.19976223	!76.92 86.58 248.01
	H	-0.8742844	0.40569546	1.7869859	!Torsions
	H	-0.3845644	-1.1802757	-0.2060939	
nbutanol-ROO1 = HO_2 + 1-Buten-1-ol	C	0.01467613	0.03519313	0.02156411	1081.77i 103.68 144.57
	C	-0.0035916	-0.0308721	1.5458501	198.00 304.07 345.53
	C	1.38614925	-0.0419086	2.15329536	501.62 535.86 580.48
	C	2.04327527	1.16526004	2.3417863	688.66 780.34 906.70
	O	3.38112323	1.19652251	2.37551893	915.15 1019.33 1028.60
	O	1.69308687	1.33543993	4.44995578	1099.63 1131.49 1178.23
	O	1.20454828	0.19310566	4.6849473	1243.49 1284.80 1298.96
	H	0.56279135	-0.8110904	-0.3939178	1329.89 1363.01 1389.43
	H	1.20376964	-0.2193355	3.45715163	1398.80 1412.84 1492.44
	H	2.03542296	-0.8722734	1.88728978	1501.08 1509.18 1634.00
	H	1.52791903	2.11361163	2.24229916	1661.91 3057.75 3061.22
	H	3.68510753	2.02733371	2.75375722	3096.24 3130.44 3134.72
	H	-0.557304	0.82064514	1.94949413	3150.92 3184.71 3867.87
	H	-0.5450039	-0.9214473	1.867442	! 73.33 235.45 419.34
	H	-0.9941184	0.01934291	-0.3903706	!Torsions
	H	0.50807152	0.94644214	-0.3191627	
QOOH-0 = QOOH-4	C	0.0042460083	-0.0018600773	0.0061779677	1439.71i 97.86 204.60
	C	0.001924307	0.0110231285	1.5344424893	304.76 373.93 426.49
	C	1.4462872173	-0.0121316935	2.0398365522	471.54 597.66 624.23
	C	2.2250571547	1.1171548146	1.4150160047	717.76 856.74 876.27
	H	3.2853327232	0.9451055408	1.2550144832	903.03 963.22 987.37
	H	1.7089615332	1.1940393492	0.2813294398	1056.82 1071.41 1111.97
	H	1.4450966087	0.0805870461	3.1292017248	1140.84 1178.25 1213.01
	H	1.8992885654	-0.9695867448	1.7898409453	1249.10 1276.48 1300.65

	H	-0.5681710371	-0.840637328	1.9008434603	1342.12 1357.57 1371.98
	H	-0.4989202223	0.9264823004	1.8516250202	1442.09 1457.85 1477.66
	H	-1.0140962526	0.0900977571	-0.394846078	1491.07 1548.24 3013.36
	H	2.0219855866	2.1006306148	1.8331775934	3055.69 3088.69 3107.10
	O	0.7253799832	1.0313319319	-0.5374807566	3129.62 3147.47 3190.23
	O	0.5283974624	-1.258414381	-0.3700622598	3783.13
	O	0.4507364626	-1.3457775757	-1.7815761809	! 164.21 394.43 ! Torsions
	H	1.1012034305	-0.6834424575	-2.0559770482	
QOOH-0 = Performic acid + $CH_3CH_2CH_2$	C	0.00351519	0.04069615	0.02994893	440.26i 139.13 197.27
	C	0.00846726	-0.0184574	1.55378007	263.57 411.15 423.50
	C	1.37611531	-0.1154029	2.14021841	490.36 710.53 766.56
	C	2.41496583	1.45571162	1.56224275	833.68 902.53 933.76
	O	1.64296244	2.39176394	1.77330824	939.87 962.91 999.36
	O	3.55269112	1.28619261	2.32259537	1102.40 1128.51 1149.46
	O	3.37647257	1.89376147	3.58462164	1198.71 1285.32 1334.19
	H	0.43938622	0.9782587	-0.3150212	1375.26 1413.86 1462.14
	H	-1.011293	-0.0151431	-0.3594124	1473.41 1502.76 1508.61
	H	0.57334187	-0.786274	-0.3970951	1518.71 1595.83 3020.68
	H	-0.4981659	0.85337614	1.96607727	3044.57 3061.87 3111.89
	H	-0.5523325	-0.8999909	1.8886089	3120.29 3135.57 3146.24
	H	1.48497854	0.06219092	3.20435941	3215.56 3658.25
	H	2.02496564	-0.8967403	1.7551121	! 75.5532 95.7507
	H	2.62868328	1.05035795	0.56500106	280.7205 345.1318
	H	2.76751086	2.62474736	3.36889814	!Torsions
QOOH-0 = QOOH-3	O	0.51945611	0.37023462	0.18926944	1634.98i 100.88 152.33
	C	0.03761453	0.02380025	1.44665508	269.22 385.45 425.51
	O	1.0930949	-0.2191272	2.3518218	599.45 616.05 773.52
	O	1.82804164	-1.3210638	1.84876096	797.83 850.66 915.24
	C	-0.7076166	1.24431821	1.96922532	993.23 995.57 1035.97
	C	0.03287518	2.39876951	1.28671469	1074.10 1104.33 1141.78
	H	-0.6073406	3.11901652	0.78237381	1171.08 1214.26 1257.45
	C	1.16793198	3.02184486	2.05271176	1320.55 1330.76 1365.01
	H	0.49964858	1.69349501	0.3745359	1372.76 1410.25 1438.95
	H	-0.5487485	-0.8929725	1.33824818	1479.56 1488.22 1497.46
	H	2.25058568	-0.935358	1.06770386	1792.23 3042.13 3070.40
	H	-1.7438474	1.19846088	1.64135574	3096.45 3116.81 3128.04
	H	-0.6854078	1.29925581	3.05742617	3150.47 3158.07 3780.72
	H	0.76683359	3.58836601	2.89896519	! 178.85 223.88 363.23
	H	1.83375211	2.25753428	2.44991198	!Torsions
	H	1.74123913	3.71128734	1.43497497	
QOOH-0 = HO_2 + Butraldehyde	O	0.05888996	-9.565E-05	-0.01441	767.98i 52.68 247.36
	O	-0.0080097	-0.0090371	2.22939884	287.75 304.76 369.84
	O	1.32136373	0.01112815	2.49997722	415.74 494.37 591.03
	C	-0.3480131	0.87857224	0.80678085	780.61 867.75 914.45
	C	0.38762852	2.18792425	0.94511466	953.89 983.27 1075.29
	C	-0.025469	3.14718857	-0.1738863	1091.19 1158.52 1200.06
	C	0.41408457	2.68336646	-1.5572582	1238.98 1281.74 1349.82
	H	1.4974515	2.5644661	-1.59655	1362.16 1376.14 1422.27
	H	0.12414082	3.40459591	-2.3203845	1440.00 1473.93 1477.19
	H	-0.0285837	1.72054905	-1.8129608	1493.72 1502.76 1509.75
	H	0.40679131	4.12543013	0.04084628	2996.79 3056.13 3063.84
	H	-1.110265	3.28142853	-0.1524473	3078.09 3097.32 3133.38
	H	1.45747016	1.9858502	0.90157433	3139.20 3140.00 3785.83
	H	0.14687083	2.61259008	1.9206935	! 114.0272 130.6512
	H	-1.4303733	0.95237481	0.99367894	190.9324 !Torsions

	H	1.60962845	-0.8842058	2.27271847	
QOOH-2 = OH + 3-ethyloxiran-2-ol	O	-0.0276121	0.00176286	0.00960008	912.08i 148.59 217.63
	C	0.00739563	-0.0626291	1.39138799	243.49 293.96 350.85
	C	1.35504012	-0.0772199	1.98081549	426.13 428.74 569.47
	H	1.44812241	-0.4566903	2.9887123	667.92 723.09 792.20
	C	2.53343107	0.49762094	1.29750005	879.02 978.46 999.72
	C	3.27900504	1.51123775	2.16595791	1039.07 1065.30 1099.49
	O	-0.1163229	1.16381485	2.01107392	1167.54 1222.50 1262.87
	O	-1.6642465	1.71431072	1.51727814	1280.99 1311.88 1358.59
	H	-0.8259651	0.50671461	-0.1945617	1409.24 1430.75 1469.54
	H	-0.7017588	-0.7937072	1.78816977	1488.42 1502.09 1510.76
	H	3.2080535	-0.3304286	1.04673183	3021.64 3065.2124
	H	2.21564299	0.93942868	0.35527235	3067.5605 3128.7973
	H	3.60252295	1.05990895	3.10419794	3146.1021 3150.7622
	H	4.16056157	1.88738138	1.64939754	3217.1963 3809.5406
	H	2.62753839	2.35118693	2.4018222	3854.8755
	H	-1.400936	2.64115789	1.46517792	! 50.99 102.93 190.90
					!Torsions
QOOH-3 = Propene + OH + Formic Acid	O	-0.1007384	-0.1671138	0.07358496	1283.03i 57.30 76.50
	C	0.0010331	0.13445004	1.4010542	194.49 238.53 243.06
	O	1.13284525	-0.0877904	1.97592066	345.97 390.36 428.30
	O	1.25886227	-1.758209	2.19242289	503.85 612.37 692.86
	C	-0.079748	2.05181591	1.51442533	894.43 917.67 955.52
	C	-0.4253214	2.45415146	2.79765625	1017.01 1043.29 1049.70
	H	0.3616944	2.67069416	3.50907156	1103.34 1172.80 1200.96
	C	-1.8191667	2.39974487	3.31230047	1258.88 1304.05 1334.73
	H	0.79750018	-0.2710349	-0.2629328	1398.87 1426.13 1457.65
	H	-0.9188136	-0.133947	1.91692637	1475.63 1492.06 1546.66
	H	1.5713298	-1.6882267	3.10278648	3024.19 3085.96 3127.51
	H	0.91563023	2.28000539	1.15409886	3130.64 3132.93 3188.51
	H	-0.8514381	2.10038728	0.75240817	3221.75 3839.76 3854.11
	H	-2.0755165	3.30293339	3.86920253	! 111.96 128.97 139.42
	H	-2.5385194	2.27666781	2.50320998	!Torsions
	H	-1.9465325	1.56270288	4.00829681	

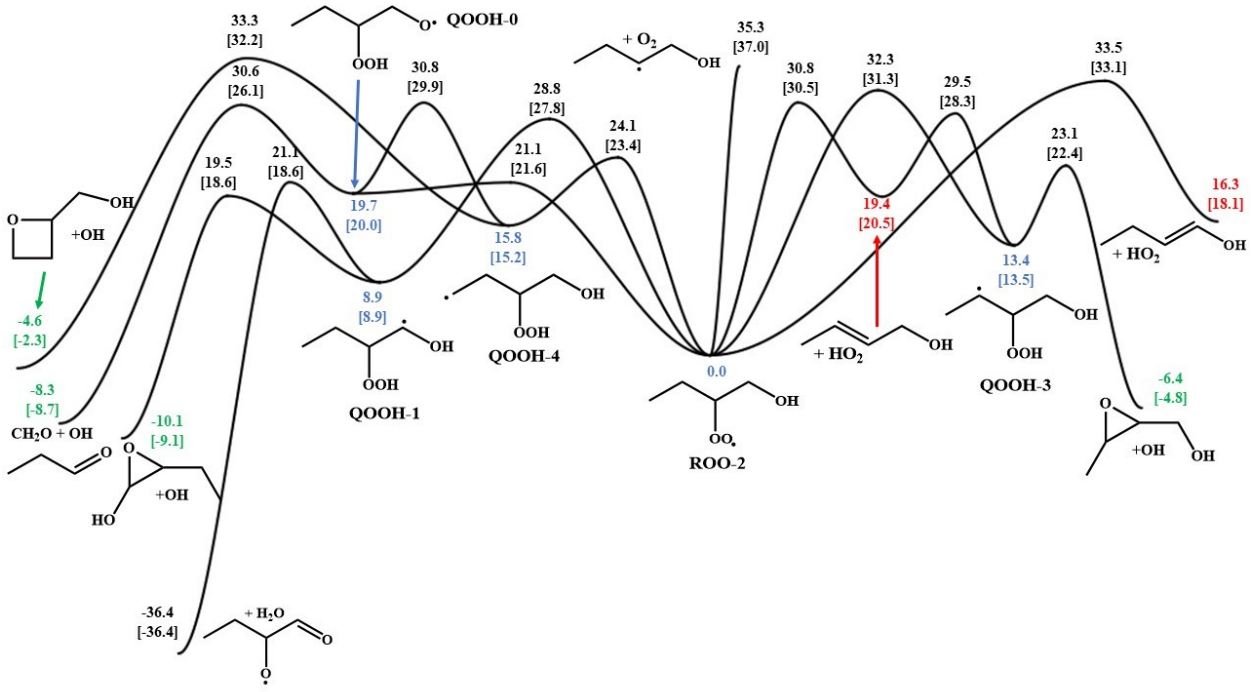


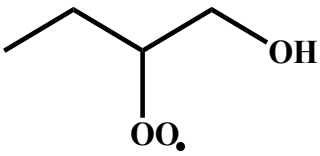
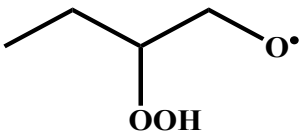
Figure S3. Potential energy surface for n-Butanol ROO2 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

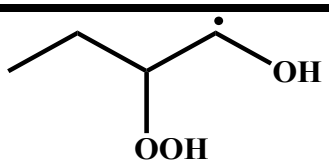
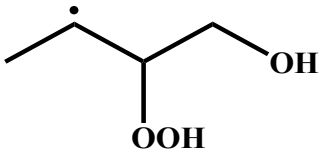
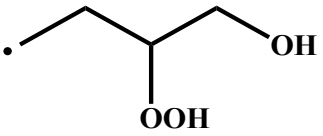
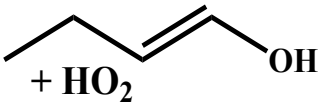
Table S3. Calculated relative energies for n-Butanol ROO2 PES

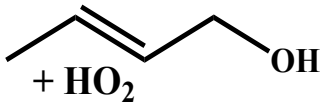
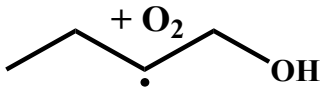
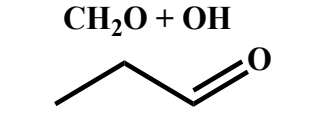
Species	Relative energy (kcal/mol)
n-Butanol ROO2	0.0
QOOH-0	19.7
QOOH-1	8.9
QOOH-3	13.4
QOOH-4	15.2
HO_2 + 1-Buten-1-ol	16.3
HO_2 + 2-Buten-1-ol	19.4
O2 + CH_3CH_2CHOH	35.3
CH_2O + OH + propanal	-8.3
OH + 3-ethyloxiran-2-ol	-10.1
OH + (3-methyloxiran-2-yl)methanol	-6.4
H_2O + C4H7O-2O	-36.4
OH + 2-Oxetanemethanol	-1.6
nbutanol-ROO2 = QOOH-0	21.1
nbutanol-ROO2 = QOOH-1	28.8
nbutanol-ROO2 = QOOH-3	32.3
nbutanol-ROO2 = QOOH-4	24.1

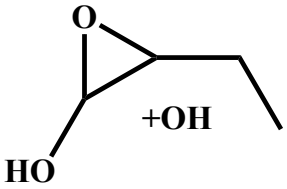
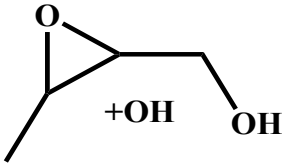
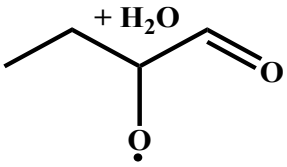
nbutanol-ROO2 = HO_2 + 1-Buten-1-ol	33.5
nbutanol-ROO2 = HO_2 + 2-Buten-1-ol	30.8
QOOH-0 = CH_2O + OH + propanal	30.6
QOOH-0 = QOOH4	30.8
QOOH-1 = OH + 3-ethyloxiran-2-ol	19.4
QOOH-1 = H_2O + C4H7O-2O	21.1
QOOH-3 = HO_2 + 2-Buten-1-ol	29.5
QOOH-3 = OH + (3-methyloxiran-2-yl)methanol	23.1
QOOH-4 = OH + 2-Oxetanemethanol	36.2

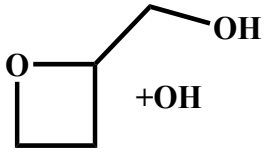
Table S4. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Butanol ROO2 PES

Species	Geometry				Frequencies (cm^{-1})
n-Butanol ROO2 	C	0.00414919	0.00039887	-0.0063532	203.81 276.18 389.42
	C	-0.0109508	0.00764199	1.51318833	442.79 462.16 568.03
	O	1.26887165	0.00992274	2.0899559	766.96 865.67 936.55
	H	1.78046719	0.70891454	1.66878779	987.76 1039.61 1106.81
	O	0.31252996	1.34129474	-0.4870088	1137.34 1144.57 1177.07
	O	1.50300129	1.73142785	-0.1515957	1241.43 1275.12 1305.12
	H	-0.5083835	-0.9017293	1.85191068	1309.36 1357.00 1395.95
	H	-0.6121841	0.86281382	1.84595797	1407.35 1420.94 1450.08
	H	0.80548265	-0.6473991	-0.3680143	1480.93 1503.96 1506.62
	C	-1.3339156	-0.3537085	-0.6216271	1512.17 3024.51 3066.06
	C	-1.3054069	-0.362323	-2.1450752	3072.01 3090.05 3106.23
	H	-2.0827033	0.35332231	-0.2567543	3116.72 3141.98 3154.96
	H	-1.6161182	-1.3375999	-0.2444141	3841.31
	H	-2.2772128	-0.6405759	-2.5487635	! 63.78 92.35 149.39
	H	-1.0440195	0.61913591	-2.5364848	223.85 418.89 !Torsions
	H	-0.5701531	-1.078781	-2.512897	
QOOH-0 	C	0.02515031	0.01467505	0.0233738	230.71 288.16 365.45
	C	0.00045171	-0.0272433	1.54600252	382.88 487.86 539.85
	C	1.40127358	-0.0174218	2.13294998	773.55 793.88 810.70
	O	1.95175722	1.2451521	1.8759065	943.83 984.36 1054.70
	O	3.3594867	1.16313329	1.98066816	1071.51 1098.18 1154.53
	C	1.33524642	-0.2584677	3.68839487	1189.34 1241.40 1281.50
	O	2.59704006	-0.1752249	4.165195	1293.38 1312.61 1371.96
	H	0.54924866	0.9021098	-0.325705	1391.71 1416.05 1459.07
	H	-0.9866688	0.03135768	-0.3783362	1481.84 1501.96 1511.51
	H	0.53402282	-0.8607874	-0.3805991	1523.99 2993.24 3054.94
	H	-0.5411864	0.83351355	1.94285122	3070.35 3073.46 3092.23
	H	-0.5136383	-0.9231203	1.89673088	3115.77 3141.59 3157.24
	H	2.03642635	-0.7838888	1.68946685	3704.39
	H	0.69099967	0.53914939	4.07844154	! 89.91 132.87 158.54
	H	0.88613193	-1.2474948	3.84002657	215.34 413.09 !Torsions
	H	3.48980385	1.16244545	2.94408323	
QOOH-1	O	-0.002582	-0.006918	0.00055695	278.87 290.74 314.20
	C	-6.882E-05	-0.0004697	1.35669363	441.61 492.35 570.58
	C	1.28068215	-0.0006635	2.09969217	744.47 814.85 864.50
	C	1.12002229	0.46673159	3.53714197	919.89 982.61 1047.91
	C	2.43165089	0.48727772	4.31126457	1052.49 1066.15 1144.40

	O	1.8604389	-1.3173887	2.19662692	1201.63 1234.52 1296.63
	O	2.05414783	-1.7953549	0.87054315	1335.55 1362.90 1388.97
	H	2.86121343	-0.5099067	4.37732624	1405.53 1412.01 1461.09
	H	2.27675413	0.86307535	5.32151077	1486.12 1500.19 1509.52
	H	3.15950537	1.13362709	3.81930942	3001.93 3059.54 3068.27
	H	0.39604313	-0.1877300	4.02743954	3108.77 3129.27 3157.83
	H	0.68166626	1.46529452	3.50720725	3205.03 3810.84 3875.46
	H	2.018706	0.6239563	1.57587519	!71.06 92.63 155.32 231.70
	H	1.35811015	-2.4616755	0.80723928	241.76 349.37 !Torsions
	H	0.85576866	-0.3310543	-0.2975655	
	H	-0.9343143	0.3073257	1.79874251	
QOOH-3	C	-0.0012412	-0.0007304	-0.0001854	211.07 284.09 327.94
	C	-0.0006018	0.00339384	1.48559919	388.96 423.03 573.45
	C	1.28593876	-0.000727	2.23048201	750.96 813.53 926.02
	O	2.06608824	1.17856759	1.94912333	965.28 985.18 1016.19
	O	1.38652275	2.31172299	2.47873745	1055.21 1118.33 1149.67
	C	1.12443433	-0.2243142	3.72800479	1169.68 1250.89 1274.93
	O	0.09955346	0.547305	4.31071664	1343.32 1385.33 1393.17
	H	0.85230782	0.5542085	-0.3945259	1409.52 1428.71 1446.21
	H	-0.9158943	0.42666027	-0.4094349	1484.97 1490.21 1498.78
	H	0.07661777	-1.0215377	-0.3957374	3006.38 3021.35 3044.74
	H	0.8247436	2.57941776	1.73960021	3082.41 3108.12 3132.58
	H	-0.9199387	-0.0998591	2.04193892	3227.24 3806.45 3863.48
	H	1.95998909	-0.7730101	1.83655623	! 75.77 96.89 118.96
	H	0.29616524	1.46777188	4.11062724	178.91 255.61 506.02
	H	0.85798607	-1.2688219	3.89521383	!Torsions
	H	2.09070081	-0.0370635	4.20692174	
QOOH-4	C	-0.0455713	0.08588109	0.02491216	234.35 286.96 347.56
	C	-0.0202544	-0.0012351	1.50727771	422.79 506.87 547.38
	H	0.86364244	0.27728827	-0.5242852	703.50 797.78 888.76
	H	-0.9187504	-0.2259744	-0.5290989	932.24 976.84 1002.49
	C	-1.4135157	-0.020828	2.12806889	1065.14 1106.02 1132.79
	H	0.49832953	-0.9107542	1.83943441	1175.97 1220.98 1253.42
	H	0.55366183	0.82272453	1.93633647	1293.67 1378.23 1380.70
	C	-1.3953021	0.16483606	3.63907218	1404.59 1414.13 1444.11
	H	-1.909573	-0.9695645	1.90326055	1467.43 1471.92 1503.41
	H	-2.4316956	0.22087915	3.98660613	3004.20 3042.00 3071.51
	H	-0.9318718	-0.7114171	4.09586201	3088.59 3103.00 3171.11
	O	-0.6490828	1.28205433	4.06580397	3275.30 3770.62 3859.27
	H	-0.976339	2.04831689	3.58372884	! 113.75 123.51 168.23
	O	-2.2947726	0.90891541	1.49668006	188.00 377.34 461.13
	O	-1.7370618	2.21415097	1.59559275	!Torsions
	H	-1.2437289	2.28126406	0.76500203	
HO_2 + 1-Buten-1-ol	O	0.5055325	2.59512924	1.6402416	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.5078306	
	H	-0.2367003	1.48037439	0.3500898	
	C	0.01129837	0.00358214	0.01477432	198.80 325.75 451.54 541.11 783.76 852.60 922.85 985.48 1034.78 1097.01 1136.87 1162.38 1252.01 1300.65 1339.99 1353.79 1409.41 1411.50 1487.78 1500.77 1509.73 1768.36 3051.37 3060.79
	C	-0.0023248	0.00030064	1.54312544	
	C	1.37787198	-0.0043674	2.12660705	
	C	1.85338103	0.96644322	2.89334186	
	O	3.09505924	1.0376972	3.44299897	
	H	0.510588	0.89612038	-0.3616015	
	H	-0.999943	-0.0228673	-0.3905654	

	H	0.54933961	-0.864491	-0.3683461	3091.05 3131.01 3138.61
	H	-0.5441111	0.87381188	1.91078899	3143.67 3204.04 3864.71 !
	H	-0.5535529	-0.8764444	1.89279238	103.57 215.79 410.66
	H	2.01981761	-0.8478365	1.88197194	!Torsions
	H	1.25930771	1.83093605	3.16325846	
	H	3.59834683	0.25830996	3.18883928	
HO_2 + 2-Buten-1-ol 	O	0.5055325	2.59512924	1.6402416	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.5078306	
	H	-0.2367003	1.48037439	0.3500898	
	C	0.00110526	0.00256459	-0.0011716	203.37 217.75 385.57
	C	0.00066903	0.01365029	1.49481965	664.25 761.91 886.05
	C	1.08837957	-0.0155826	2.25011467	992.44 1004.80 1024.36
	C	1.09180759	0.00119467	3.75055544	1079.05 1127.29 1159.84
	O	-0.1766844	0.20950003	4.32881862	1218.06 1309.76 1331.97
	H	-0.5095386	1.0554586	4.01701157	1381.01 1411.88 1423.68
	H	-0.495219	0.88895076	-0.4003137	1484.34 1497.31 1505.71
	H	-0.5430353	-0.8629292	-0.3832872	1773.11 3015.55 3055.25
	H	1.01553917	-0.0287349	-0.3963188	3082.49 3109.05 3137.25
	H	-0.9681528	0.02977415	1.98429173	3157.34 3172.01 3871.48
	H	2.06800524	-0.0534041	1.78101488	! 146.92 248.09 333.02
	H	1.81085974	0.75185766	4.10035097	!Torsions
	H	1.44131754	-0.9616869	4.1293429	
O_2 + $CH_3CH_2CHCH_2OH$ 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
	C	-0.0015825	0.01326112	0.01257112	219.96 338.55 423.36
	C	0.00034886	-0.0115301	1.53850701	571.99 776.65 854.61
	C	1.37035089	-0.0340186	2.11798744	961.22 1004.33 1044.34
	C	1.61174357	-0.5898045	3.47632502	1067.63 1131.85 1162.92
	O	1.13199109	-1.9235058	3.61561782	1213.38 1271.72 1312.65
	H	0.54397346	0.88098158	-0.3604318	1368.77 1410.95 1412.39
	H	0.48029449	-0.8788017	-0.3879407	1429.46 1478.28 1502.71
	H	-0.5384147	0.87167593	1.91113659	1505.02 1507.35 2983.10
	H	-0.5568254	-0.8747611	1.90833609	3022.07 3060.92 3061.61
	H	2.14707552	0.5534704	1.64448467	3083.67 3129.16 3138.57
	H	2.67346261	-0.529658	3.73168497	3186.48 3865.89
	H	1.06375403	-0.0196742	4.23517961	! 39.15 96.86 248.28
	H	1.52424115	-2.4474306	2.91160524	310.65 !Torsions
	H	-1.0156616	0.05855007	-0.3822163	
CH_2O + OH + propanal 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	1.75214387	-0.7145028	0.73740505	1218.60 1279.77 1546.46
	C	1.58204252	-0.4681554	-0.4198612	1877.08 2943.66 3014.59
	H	1.92664152	0.47856444	-0.870535	
	H	1.07176408	-1.1748522	-1.0968368	
	C	-0.0088334	0.00308834	0.00021537	266.82 673.44 677.86
	C	-0.0031765	0.0007975	1.48572907	873.63 908.86 1008.52
	C	1.4220078	-0.0026989	2.02869628	1121.87 1156.86 1283.93
	O	-1.2572665	-0.1552681	-0.5283629	1372.83 1414.21 1430.39
	O	-1.1755897	-0.1115346	-1.9431467	1457.55 1497.45 1504.73
	H	-0.5449389	0.8748294	1.86892114	1866.92 2945.02 3050.32
	H	-0.5497278	-0.8754972	1.84187402	3077.74 3081.28 3153.86

	H	1.42405644	0.00808997	3.117032	3156.87 ! 148.66 238.11
	H	1.96099697	-0.8880251	1.6929931	!Torsions
	H	1.96977516	0.87446604	1.6833002	
	H	-1.0570379	-1.0450961	-2.1614852	
	H	0.65665443	0.63494383	-0.5771534	
OH + 3-ethyloxiran-2-ol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.0048656182	0.0052648361	-0.0066756637	168.34 342.75 372.63
	C	0.002279904	0.0089069374	1.4542068967	500.79 584.58 770.58
	O	1.2174921893	0.0181235329	0.7573723213	850.82 929.21 968.18
	H	-0.1903033837	-0.9505528595	-0.4932385375	1030.65 1071.38 1125.08
	C	-0.2593001393	1.2262351708	-0.8407644511	1140.89 1158.60 1189.61
	C	0.6986887382	1.2959666262	-2.0253585486	1290.53 1300.74 1316.17
	H	-0.1401241053	2.1090528744	-0.2101407447	1349.14 1413.27 1420.67
	H	-1.2953249713	1.2091370732	-1.1852754197	1479.71 1503.13 1510.34
	H	0.5336526123	2.1961493629	-2.6150941313	1543.38 3064.26 3067.38
	H	1.7299090662	1.2997996172	-1.6738585087	3102.17 3120.26 3137.47
	H	0.5690261093	0.4345911019	-2.6817017176	3146.96 3180.00 3864.59
	O	-0.2726337925	-1.09454965	2.2246888182	! 92.07 213.70 246.40
	H	0.080091419	-1.8712621422	1.7788761453	!Torsions
	H	-0.2375900616	0.9137106846	2.0005081352	
OH + (3-methyloxiran-2-yl)methanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.0249967	-0.0096645	0.00557249	216.98 252.48 345.91
	C	0.02036494	-0.0109615	1.46669032	487.45 661.03 810.18
	O	1.2204231	-0.0527622	0.69066332	849.03 928.33 990.13
	H	-0.2921184	-0.9348947	-0.4976453	1043.17 1061.80 1120.59
	H	-0.1345916	0.94404806	1.95743573	1156.40 1178.21 1191.96
	C	-0.2506700	1.25480857	-0.7855856	1236.18 1295.03 1352.51
	H	-1.3181558	1.40124612	-0.9530579	1383.43 1416.82 1437.97
	H	0.23056504	1.14840617	-1.7646988	1481.56 1498.30 1513.48
	O	0.23144785	2.38691919	-0.1054971	1542.00 3025.36 3068.00
	H	1.12125414	2.17003775	0.19537663	3108.80 3138.49 3142.99
	C	-0.282753	-1.2391095	2.27009872	3144.84 3166.51 3836.21
	H	0.34283428	-1.2760561	3.16164578	! 139.24 195.56 432.82 !
	H	-1.3258835	-1.2390351	2.58640753	Torsions
	H	-0.0933594	-2.1339043	1.67888819	
H_2O + C4H7O-2O 	O	0.0000000	0.0000000	0.0000000	1627.56 3874.01 3976.38
	H	0.0000000	0.0000000	0.95889274	
	H	0.92689607	0.0000000	-0.2456399	
	C	0.01673954	0.00849452	0.00519858	195.17 301.77 424.03
	C	-0.0060448	0.01793886	1.52658674	452.05 624.65 776.61
	H	1.02296171	0.03766019	1.88485081	783.88 842.12 964.82
	C	0.91155131	1.09016937	-0.6215018	1009.56 1063.42 1108.40
	O	1.72905502	1.70338992	-0.0053043	1122.74 1188.85 1258.04
	H	0.72312133	1.25226796	-1.6979873	1306.11 1355.96 1387.11
	C	-0.7663696	-1.1765753	2.08247933	1417.19 1486.24 1503.61
	H	-0.8229522	-1.1332364	3.16859132	1512.04 1874.89 2874.99
	H	-1.7812291	-1.2014535	1.68803477	2975.91 3064.35 3081.31
	H	0.48426576	-0.9337066	-0.3571317	3120.59 3138.31 3150.94 !
	H	-0.2758252	-2.112597	1.81012312	78.62 125.20 234.48
	O	-1.1998539	0.03248776	-0.6015606	!Torsions

	H	-0.4667365	0.95360642	1.8480206	
OH + 2-Oxetanemethanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	0.01729099	0.09418816	0.03889921	73.95 235.30 391.41
	C	0.01294046	0.05392339	1.44599647	507.01 778.44 786.72
	C	1.42289723	-0.058538	1.97348474	891.81 920.57 984.23
	O	2.1944882	1.07727223	1.52470555	1022.86 1074.63 1098.29
	C	1.62799283	0.32220045	3.4451704	1133.85 1158.50 1185.74
	C	2.32085759	1.56696057	2.871867	1217.49 1235.81 1265.62
	H	3.36513036	1.70583709	3.14963112	1300.40 1343.39 1371.83
	H	1.78088468	2.50458691	3.01131355	1397.73 1444.51 1495.77
	H	0.6484262	0.77688137	-0.2141286	1505.15 1540.55 3009.12
	H	-0.4546666	0.95342704	1.86760298	3067.71 3085.35 3107.16
	H	-0.5770104	-0.8119478	1.75022915	3112.68 3116.91 3172.50
	H	1.88114855	-0.990674	1.63902836	3842.64
	H	0.71620687	0.49872574	4.01113018	! 135.48 442.69 !Torsions
	H	2.28238865	-0.3428488	3.9997329	
nbutanol-ROO2 = QOOH-0	C	0.00994688	0.00772352	0.01948832	1183.70i 150.47 195.06
	C	0.00278297	-0.0088118	1.54415913	306.09 369.34 456.40
	C	1.4008015	-0.001596	2.11599225	515.03 549.74 674.93
	O	1.97967107	1.23737352	1.90080381	747.20 777.11 897.39
	O	3.30825587	1.16814857	2.24973842	944.48 965.80 1006.79
	C	1.39325964	-0.1899622	3.72018332	1089.73 1103.13 1165.43
	O	2.62667843	0.03248468	4.19116809	1186.03 1229.20 1244.08
	H	0.51745655	0.89660626	-0.3513416	1269.35 1306.10 1314.03
	H	-1.006175	0.00504656	-0.3708355	1360.43 1409.01 1416.94
	H	0.52610682	-0.8668731	-0.3767032	1481.60 1502.77 1510.14
	H	-0.5323844	0.85803384	1.93487273	1515.76 1844.18 2979.86
	H	-0.5082568	-0.8984373	1.91543832	3046.56 3070.81 3076.06
	H	2.04598819	-0.7880051	1.71867877	3087.44 3117.07 3143.97
	H	0.63354934	0.5026477	4.10244845	3154.01
	H	1.07589268	-1.2353133	3.8391094	! 85.22 223.83 !Torsions
	H	3.22604303	0.73866895	3.25022422	
nbutanol-ROO2 = QOOH-1	H	0.01097354	-0.0104299	-0.0174892	2042.57i 140.94 183.46
	O	0.0380693	-0.0208266	1.27029283	278.70 304.57 474.12
	O	1.43061638	0.00303633	1.31607633	511.74 572.85 671.41
	C	1.82156182	-0.8026898	0.22354493	776.89 890.80 977.46
	H	1.52464785	-1.8457063	0.41103062	980.83 1020.29 1053.88
	C	0.94246899	-0.256955	-0.9057753	1095.39 1152.17 1170.68
	H	1.24721741	0.71238687	-1.2972592	1206.20 1244.62 1278.68
	O	0.61945354	-1.0954069	-1.929855	1299.91 1340.71 1364.99
	H	0.42543668	-1.972101	-1.5806121	1406.99 1415.19 1444.89
	C	3.31502186	-0.6880143	0.01425012	1481.12 1502.27 1510.00
	C	4.10984703	-1.2750282	1.1751433	1791.97 2988.23 3066.17
	H	3.55871748	0.36707617	-0.1233864	3069.76 3107.12 3134.01
	H	3.55907786	-1.2006622	-0.9187232	3139.60 3152.78 3843.35
	H	5.18049557	-1.1849815	0.99987439	! 89.33 210.83 409.97 !
	H	3.86904112	-0.7587827	2.10290036	Torsions
	H	3.87752626	-2.332238	1.30824888	
nbutanol-ROO2 = QOOH-3	C	-0.001553	0.00241565	0.0005299	2169.27i 134.78 225.32
	C	3.3694E-05	-0.0006967	1.49837104	252.67 323.08 373.15
	C	1.37274431	-0.0036366	2.17148711	595.35 621.27 769.77
	O	1.79530567	1.35673139	2.04450674	821.72 848.65 933.48
	O	0.65479777	2.08946266	2.39360384	973.51 1012.17 1029.44

	C	1.33077585	-0.4705436	3.61847046	1078.86 1105.09 1119.88
	O	0.25805062	0.06611223	4.35542317	1170.71 1194.47 1240.35
	H	0.70880661	0.73564777	-0.3819901	1276.31 1345.66 1375.66
	H	-0.989056	0.21994834	-0.4023109	1402.28 1413.20 1442.74
	H	0.29863984	-0.9814611	-0.3756775	1483.91 1490.95 1502.79
	H	-0.1475826	1.24162015	1.90911791	1739.10 3033.18 3038.68
	H	-0.7654569	-0.5974981	1.98505839	3073.56 3101.12 3108.03
	H	2.11689689	-0.5852721	1.6200449	3145.70 3165.96 3838.65
	H	0.28374246	1.02357196	4.25210588	! 119.41 213.67 474.26
	H	1.20895306	-1.5551002	3.63153197	!Torsions
	H	2.29501881	-0.2332749	4.07972522	
nbutanol-ROO2 = QOOH-4	C	0.01878856	-0.0058021	0.0150424	1819.70i 138.93 193.27
	C	0.00916222	-0.0078217	1.51716778	265.11 405.66 414.03
	C	1.44283581	0.00535571	2.07470711	473.45 500.91 551.93
	H	0.10994559	0.96492957	-0.4626804	659.87 828.35 866.08
	H	-0.5119767	0.8702543	1.90946558	931.09 1004.95 1054.18
	H	-0.491297	-0.8978941	1.89901086	1096.63 1116.01 1118.09
	H	1.95263999	0.93871235	1.82162961	1131.84 1150.20 1176.11
	O	2.14395064	-1.0692218	1.46931319	1226.55 1262.12 1286.43
	O	2.35770145	-0.7565159	0.13857351	1358.98 1371.34 1396.78
	H	1.25493711	-0.5219278	-0.208353	1442.33 1454.53 1479.35
	H	-0.6661267	-0.6791204	-0.4876924	1506.26 1586.80 3032.32
	C	1.51165355	-0.2484517	3.56490733	3049.91 3072.37 3114.37
	H	0.92272993	0.50678558	4.08469922	3123.37 3125.95 3215.00
	H	1.07005992	-1.2293722	3.77572357	3865.68 ! 112.16 374.61
	O	2.82812288	-0.1581741	4.05160261	!Torsions
	H	3.37293928	-0.7590015	3.53423236	
nbutanol-ROO2 = HO_2 + 1-Buten-1-ol	H	-0.0036614	0.0354777	0.03740466	1151.01i 121.64 161.80
	O	0.00498675	-0.0162248	0.99529826	196.63 309.77 320.47
	C	1.33023469	-0.0250713	1.44900867	517.78 546.15 568.69
	H	2.03336073	0.82293673	0.67906009	694.30 796.42 919.04
	C	1.6134402	0.72037259	2.58051205	953.98 1013.38 1020.00
	H	1.86413888	-0.9663362	1.31609134	1082.47 1145.23 1174.82
	H	0.82526364	1.34272595	2.98685604	1222.90 1267.65 1288.99
	O	2.57366647	1.9652575	0.46916787	1308.45 1346.20 1365.86
	O	2.47746422	2.38411732	1.65029142	1405.38 1411.02 1494.40
	C	2.77906698	0.40553886	3.45843009	1501.60 1513.22 1609.96
	C	2.36993411	-0.5519656	4.5807236	1661.65 3066.19 3070.82
	H	3.1755905	1.32814508	3.8814059	3105.41 3115.33 3141.37
	H	3.57293599	-0.0419753	2.85664614	3145.80 3199.50 3891.82 !
	H	3.21791549	-0.7643365	5.23010667	86.58 222.29 229.61
	H	1.57661453	-0.1195646	5.19042459	!Torsions
	H	2.00414518	-1.4941142	4.17392057	
nbutanol-ROO2 = HO_2 + 2-Buten-1-ol	C	0.00748144	-0.0032111	0.00522557	1061.14i 139.62 179.47
	C	-0.0169334	-0.000816	1.5210366	199.30 259.51 440.28
	C	1.15651263	0.08090975	2.25517124	449.24 524.65 533.45
	O	1.03137651	2.09743773	2.84098076	701.20 829.10 916.28
	O	-0.1060666	2.39306311	2.39323234	964.26 1050.87 1058.88
	C	1.27162232	-0.4324004	3.65518202	1092.43 1138.37 1157.04
	O	2.33413829	0.13949437	4.37438764	1223.74 1274.89 1287.12
	H	0.81203204	0.63344892	-0.3631571	1299.76 1383.61 1401.84
	H	-0.9279725	0.37102311	-0.4078601	1421.26 1428.28 1491.27
	H	0.16610857	-1.0071485	-0.3889948	1494.78 1508.19 1603.32
	H	-0.354236	1.23841274	1.85829041	1635.38 3026.94 3064.76
	H	-0.8308284	-0.5516629	1.98946087	3077.91 3121.71 3131.51

	H	2.09789567	0.2853099	1.75662342	3142.23 3183.26 3873.51
	H	0.31045588	-0.3055255	4.16716461	! 120.00 152.81 386.42
	H	1.47373301	-1.5060067	3.60970093	!Torsions
	H	2.18842313	1.08926975	4.41151457	
QOOH-0 = CH_2O + OH + propanal	O	-0.0537264	0.02999715	0.07688465	266.24i 113.48 162.58
	C	0.01083562	-0.006978	1.30069532	255.98 294.88 339.54
	C	2.13026194	-0.0174697	1.76946559	423.73 566.28 647.85
	C	2.73502899	0.83319693	0.70663192	768.14 875.09 924.14
	C	2.2402837	2.27708936	0.71486137	993.10 1066.66 1090.80
	O	2.23604764	0.52379943	3.00804276	1122.74 1143.26 1218.66
	O	1.78041926	-0.4369054	3.95214512	1252.92 1295.33 1370.60
	H	-0.0875416	0.91057349	1.90746257	1387.57 1416.67 1441.42
	H	-0.130083	-0.9478563	1.85629482	1462.39 1493.48 1504.16
	H	2.25891899	-1.0941776	1.74602371	1515.51 1664.42 2932.31
	H	3.82462097	0.80457528	0.81649354	3001.83 3034.93 3076.88
	H	2.48824897	0.36005428	-0.2437842	3116.49 3151.09 3155.36
	H	2.41347765	2.75071061	1.68001878	3166.49 3839.29
	H	2.76370896	2.85536492	-0.0440878	! 85.03 101.37 140.45
	H	1.1757174	2.30833625	0.4877695	211.20 ! Torsions
	H	1.26974898	0.12711229	4.54597338	
QOOH-0 = QOOH4	O	-0.0009855	0.00042169	-0.0050552	1640.39i 160.40 200.15
	C	-0.0088262	0.01476347	1.38391056	267.60 401.74 406.07
	C	1.42111414	0.00972573	1.93609069	458.98 481.82 546.63
	C	2.1423376	1.2565758	1.43830312	655.20 833.51 886.30
	C	2.08006623	1.29483598	-0.067393	968.67 1004.68 1024.51
	O	1.4405384	0.0687546	3.34620657	1098.37 1109.22 1121.23
	O	1.00005685	-1.1967772	3.83007479	1167.10 1174.90 1201.25
	H	-0.5399514	0.88337974	1.79651089	1245.31 1257.46 1310.81
	H	-0.5115413	-0.8991465	1.71729749	1325.05 1372.74 1390.12
	H	1.93533503	-0.895168	1.59955045	1407.24 1462.99 1487.13
	H	1.6542246	2.13019312	1.8732029	1502.33 1553.55 2996.64
	H	3.173475	1.23921549	1.79825021	3055.43 3062.53 3069.46
	H	0.96468512	0.75052569	-0.3115588	3110.58 3119.04 3199.04
	H	2.03959897	2.28099881	-0.518736	3840.24
	H	2.7835879	0.63623988	-0.5695926	! 106.42 170.03 !Torsions
	H	0.22362754	-0.9430074	4.34235484	
QOOH-1 = OH + 3-ethyloxiran-2-ol	H	0.06988136	-0.0442517	-0.013343	859.58i 115.92 153.66 231.08
	O	0.07675271	-0.031355	0.95100057	276.37 301.87 448.34
	O	1.80001686	0.01567789	1.06255721	501.86 530.65 723.96
	C	2.10461454	0.95125267	2.04363203	791.92 907.69 965.12
	H	1.70778534	0.66576573	3.02828674	982.43 1059.49 1111.44
	H	4.11896677	0.99203378	1.08357114	1148.13 1172.87 1245.66
	C	3.50429792	0.55859679	1.85706374	1253.05 1299.63 1331.00
	O	4.08301984	-0.4296349	2.52798962	1359.64 1412.85 1415.48
	H	3.46332019	-0.8008313	3.16742113	1496.53 1504.17 1511.41
	C	1.75564636	2.38368504	1.70228438	1538.98 3000.41 3059.46
	C	2.20830971	3.35352038	2.78509626	3071.31 3116.06 3138.98
	H	0.67665688	2.42274121	1.55919045	3143.65 3251.80 3834.90
	H	2.21641172	2.62592551	0.74176573	3859.27
	H	1.95142783	4.37915272	2.52654333	! 87.45 136.27 189.16
	H	1.73291692	3.12272547	3.73933994	403.42 !Torsions
	H	3.28897269	3.30680985	2.93124401	
QOOH-1 = H_2O + C4H7O-2O	C	-0.0034204	0.00716075	0.00069117	1685.87i 148.73 149.58
	C	-0.0184066	-0.0067565	1.5290771	266.46 295.45 333.81
	H	1.03143066	0.01781943	-0.3488384	391.88 420.31 505.07

	H	-0.4629412	0.94737003	-0.3069235	630.83 727.76 799.85
	C	0.92429461	0.97120184	2.12851732	838.33 897.38 952.33
	H	0.36032033	-0.984935	1.89198081	993.91 1033.65 1062.05
	H	1.98244794	0.92815757	1.90283895	1113.30 1150.38 1202.50
	O	0.58363576	1.7087304	3.14940714	1250.21 1269.10 1311.62
	H	-0.4077998	1.81266505	3.08682208	1362.85 1395.03 1413.15
	O	-1.2596307	0.01677719	2.08992751	1475.31 1499.74 1508.82
	O	-1.6829569	1.68453259	2.05177261	1551.21 2927.69 2960.76
	H	-2.5865775	1.51498049	2.33605789	3064.79 3067.77 3112.72
	C	-0.7615228	-1.1779608	-0.5774309	3136.78 3151.85 3214.37
	H	-1.7774646	-1.2001126	-0.1864536	3886.33
	H	-0.8124428	-1.1184881	-1.6633343	! 86.04 227.00
	H	-0.2781621	-2.1200807	-0.31356	!Torsions
QOOH-3 = HO_2 + 2-Buten-1-ol	C	0.01575077	0.01406454	0.00938249	594.58i 139.42 204.55
	C	-0.0002503	-0.0450457	1.37476775	228.78 285.02 349.19
	H	0.98095331	0.04096169	-0.4829141	394.37 679.06 767.30
	C	1.22959593	-0.3659149	2.18188152	878.97 937.62 964.61
	H	-0.9473167	-0.2269421	1.87226064	1000.29 1036.35 1085.25
	H	1.13655436	0.10851079	3.16251635	1130.35 1160.72 1230.51
	H	1.27823911	-1.4454733	2.33951102	1287.56 1300.89 1389.05
	O	2.42508718	0.00759066	1.53937472	1401.95 1414.36 1435.31
	H	2.42328645	0.97038785	1.50705666	1475.49 1485.61 1500.45
	O	-0.1948777	1.85676242	1.81112056	1595.34 3044.02 3051.47
	O	1.0003006	2.51542595	1.59420535	3092.28 3092.73 3141.44
	H	0.85570135	2.98008898	0.76059027	3169.42 3189.97 3802.24
	C	-1.2069568	0.15659492	-0.8251827	3842.49
	H	-1.206284	1.11175374	-1.3572267	! 68.49 124.35 155.45
	H	-1.2524071	-0.6228745	-1.5890269	439.10 527.51 ! Torsions
	H	-2.1107993	0.10709582	-0.2205602	
QOOH-3 = OH + (3-methyloxiran-2-yl)methanol	C	0.01942739	0.02006753	0.0128315	903.32i 90.03 173.92
	C	0.00984493	-0.0258782	1.48174581	222.97 272.95 353.00
	H	0.98408245	3.3403E-05	-0.4749996	401.84 472.90 538.62
	C	1.18223628	-0.6896175	2.16924929	709.54 881.51 920.48
	H	-0.9423748	-0.3222131	1.92946675	993.02 1011.31 1074.68
	H	1.16166509	-1.761376	1.96214707	1112.10 1143.21 1155.70
	H	2.10521613	-0.2755053	1.74240452	1202.28 1256.16 1263.36
	O	1.12715032	-0.5259392	3.56148621	1339.99 1389.00 1410.28
	H	0.94880286	0.41226094	3.71734766	1454.26 1470.36 1481.84
	O	0.1263543	1.36592555	1.36523941	1501.33 1505.08 3011.14
	O	0.20409846	2.03630644	2.92647772	3033.40 3074.23 3096.48
	H	0.80424057	2.74798226	2.67338475	3105.88 3154.27 3214.78
	C	-1.2133633	0.15960831	-0.7920251	3753.18 3857.53
	H	-1.0948274	0.89521201	-1.5871481	! 94.6938 148.94 213.04
	H	-1.4566754	-0.7952401	-1.2710047	633.04 !Torisons
	H	-2.0538673	0.44753758	-0.1637191	
QOOH-4 = OH + 2-Oxetanemethanol	O	-0.0003891	-0.0067862	0.0167562	1082.34i 72.58 187.36
	C	0.011674	0.01835499	1.41911223	197.80 266.58 305.17
	C	1.39753868	-0.005025	2.02959053	363.53 445.95 482.77
	O	2.01497231	1.30416568	2.13382616	581.67 621.10 809.88
	O	1.83131148	1.94331977	0.62017095	853.98 876.91 938.43
	C	1.42537804	-0.3178958	3.52097047	1061.82 1066.60 1095.66
	C	2.47032675	0.67955194	3.9186947	1113.42 1143.43 1155.28
	H	3.5131369	0.42052515	3.81301997	1232.46 1246.51 1277.97
	H	2.23935531	1.49345849	4.58702694	1341.74 1348.76 1415.01
	H	0.55314793	0.73122025	-0.2645626	1458.18 1473.20 1492.63

	H	-0.516817	0.89104867	1.82376289	1498.57	3017.99	3066.67
	H	-0.5147437	-0.8783302	1.75514673	3079.51	3088.27	3132.26
	H	2.04950573	-0.657259	1.44255527	3178.69	3284.65	3820.41
	H	2.76664672	2.10762496	0.45832806	3872.62		
	H	0.46405563	-0.0802816	3.97568305	! 153.22	557.03	!Torisons
	H	1.67882344	-1.353506	3.74541777			

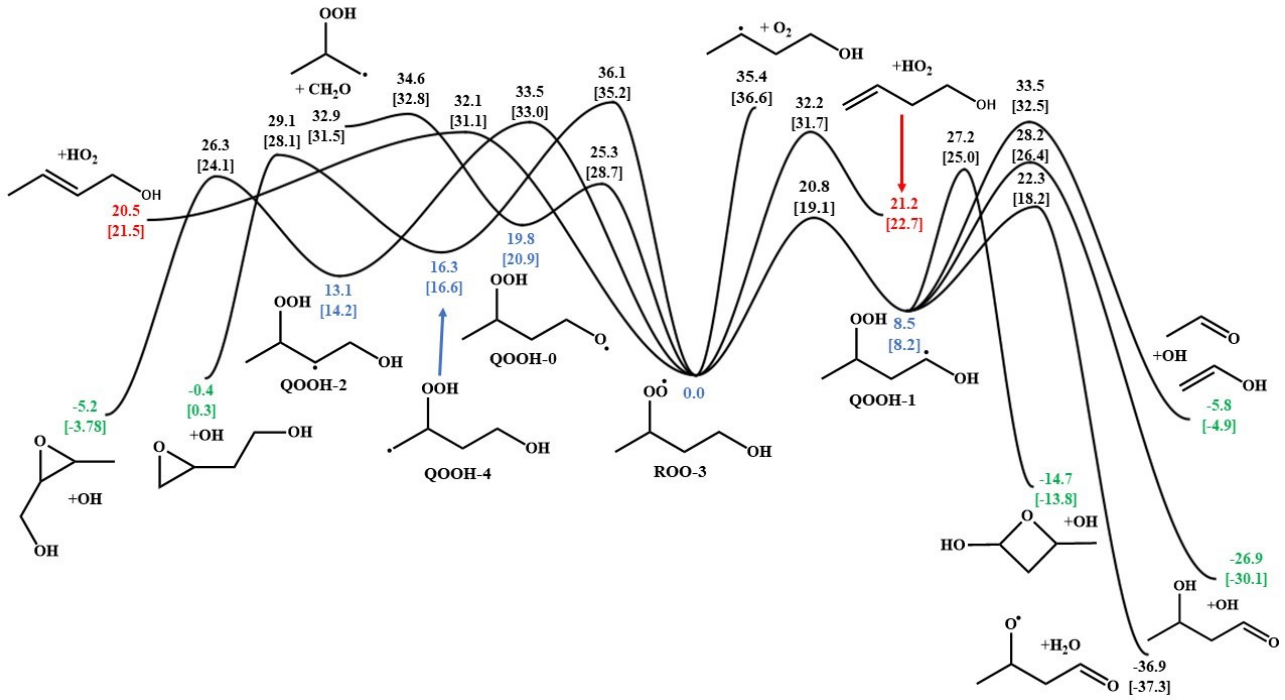


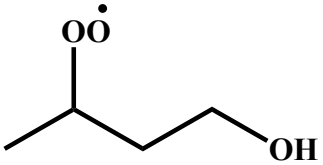
Figure S4. Potential energy surface for n-Butanol ROO3 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

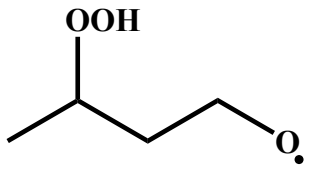
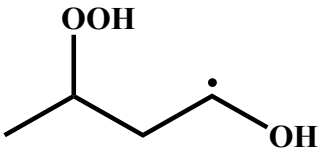
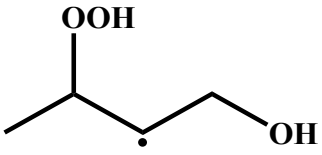
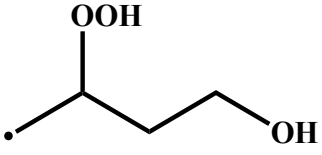
Table S5. Calculated relative energies for n-Butanol ROO3 PES

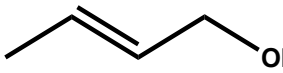
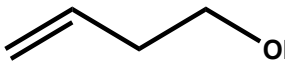
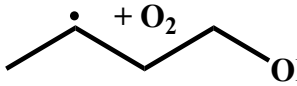
Species	Relative energy (kcal/mol)
n-Butanol-ROO3	0.0
QOOH-0	19.8
QOOH-1	8.5
QOOH-2	13.1
QOOH-4	16.3
HO_2 + 2-Buten-1-ol	20.5
HO_2 + 3-Buten-1-ol	21.2
O2 + $CH_3CHCH_2CH_2OH$	35.4
CH_2O + 1-methylethyl	32.9

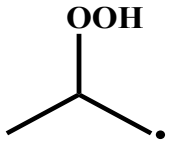
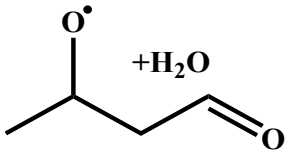
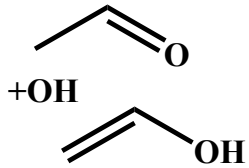
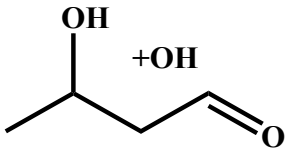
2-hydroperoxypropane	
H_2O + C4Y1-3OR	-36.9
acetaldehyde + vinyl alcohol + OH	-5.8
OH + 3-Hydroxybutanal	-26.9
OH + $C_4H_7OHCYO1$-3	-14.7
OH + (3-methyloxiran-2-yl)methanol	-5.2
OH + Oxiraneethanol	-0.4
nbutanol-ROO3 = QOOH-0	25.3
nbutanol-ROO3 = QOOH-1	20.8
nbutanol-ROO3 = QOOH-2	33.5
nbutanol-ROO3 = QOOH-4	36.1
nbutanol-ROO3 = HO_2 + 2-Buten-1-ol	32.1
nbutanol-ROO3 = HO_2 + 3-Buten-1-ol	32.2
QOOH-0 = CH_2O + 1-methylethyl 2-hydroperoxypropane	34.6
QOOH-1 = H_2O + C4Y1-3OR	22.3
QOOH-1 = acetaldehyde + vinyl + OH	33.5
QOOH-1 = OH + 3-Hydroxybutanal	28.2
QOOH-1 = OH + $C_4H_7OHCYO1$-3	27.2
QOOH-2 = OH + (3-methyloxiran-2-yl)methanol	26.3
QOOH-4 = OH + Oxiraneethanol	29.1

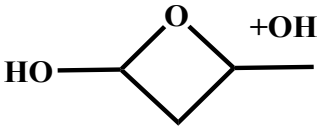
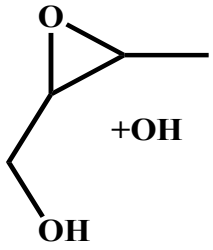
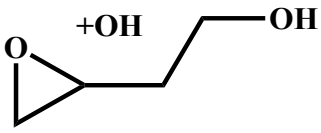
Table S6. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Butanol ROO3 PES

Species	Geometry				Frequencies (cm^{-1})
n-Butanol-ROO3 	C	-0.0027869	0.00175127	0.00131322	243.06 314.38 346.36
	C	0.00607111	0.00121713	1.51278024	426.48 520.15 588.71
	C	1.40425682	-0.0027727	2.10760087	791.65 870.10 887.54
	C	1.43052341	0.10851296	3.62835285	986.91 1001.51 1098.07
	O	0.628446	-0.873044	4.24973224	1119.66 1156.85 1170.54
	O	-0.6905465	1.21724529	1.91547463	1223.58 1273.69 1312.15
	O	-1.2327505	1.11290061	3.08872128	1336.31 1375.36 1400.24
	H	0.51519381	0.88159328	-0.3797204	1412.77 1419.61 1423.24
	H	-1.0209304	0.00021662	-0.3826888	1466.81 1490.98 1504.40
	H	0.51093683	-0.885517	-0.3652701	1519.83 3058.34 3060.21
	H	-0.5797459	-0.8228425	1.91827489	3075.09 3103.29 3114.66
	H	1.87043347	-0.9442397	1.80901277	3119.78 3153.06 3159.14
	H	1.98706437	0.81066795	1.66789442	3858.25 ! 108.03 150.10
	H	2.45087896	-0.0460864	3.97808279	177.16 215.94 495.47
	H	1.12763945	1.11244778	3.93689349	!Torsions
	H	-0.2798701	-0.5558906	4.21848952	
QOOH-0	C	0.02618606	0.0040594	0.01427711	259.47 293.35 356.73
	C	-0.0048392	0.00606076	1.53117297	443.14 523.35 575.76
	C	1.38395707	0.00196174	2.17440524	763.86 835.76 891.81
	C	2.10658736	1.33161065	2.01891322	932.70 974.17 1040.09
	O	1.56407941	2.36421183	2.74226294	1067.65 1082.95 1110.01
	O	-0.7274812	1.17836228	1.87486805	1183.20 1210.77 1244.61

	O	-0.9327153	1.18060141	3.27913033	1342.04 1370.04 1378.13
	H	0.54632601	0.88118285	-0.369283	1384.37 1402.60 1421.14
	H	-0.988512	0.01556666	-0.3782889	1454.49 1475.57 1489.02
	H	0.53229784	-0.8898445	-0.3474604	1508.87 2952.22 3019.27
	H	-0.5632476	-0.8614744	1.89329054	3056.05 3075.50 3080.55
	H	1.29221449	-0.2168052	3.23842077	3124.97 3149.87 3157.23
	H	1.97855041	-0.7964888	1.72623281	3739.39 ! 84.36 168.51
	H	3.13920679	1.2476154	2.40064686	199.33 212.69 513.16
	H	2.22224897	1.64196867	0.97210617	!Torsions
	H	-0.2051862	1.75555166	3.5647213	
QOOH-1 	C	0.00785346	-0.0081115	0.0220848	274.10 293.48 334.22
	C	0.01359971	-0.0045546	1.53649552	443.75 482.87 491.56
	H	1.02436871	0.01138624	-0.3669753	660.12 838.90 897.67
	H	-0.5013015	-0.8980758	-0.350258	918.65 1004.30 1057.12
	H	-0.5125576	0.87237831	-0.3534537	1098.54 1121.50 1148.29
	C	-1.3836945	-0.1252594	2.14113328	1225.48 1253.56 1314.46
	H	0.50852575	0.88849653	1.9253358	1372.81 1377.67 1392.52
	C	-1.4201165	0.02960668	3.62276517	1411.06 1416.19 1448.27
	H	-2.0108562	0.64417412	1.69040448	1470.90 1490.68 1506.25
	H	-1.794405	-1.0971499	1.82666255	2973.24 3065.79 3075.03
	H	-2.2943358	0.43893269	4.10700907	3116.12 3142.33 3150.94
	O	-0.7546063	-0.8590169	4.40568107	3216.87 3783.52 3834.30
	H	-0.0198547	-1.2249466	3.89539481	! 76.98 118.04 173.19
	O	0.7182908	-1.1445711	2.04702875	219.16 255.09 597.13
	O	2.10371041	-0.9671082	1.79128152	!Torsions
	H	2.26827683	-1.6503586	1.13050941	
QOOH-2 	C	-0.0151654	-0.0343884	-0.0004101	249.61 261.39 306.31
	C	0.00901618	0.0207445	1.52400098	333.08 508.50 574.55
	C	1.40550886	0.02165539	2.0594821	657.42 822.34 913.60
	C	2.13861588	1.29862332	2.26142557	981.68 1001.58 1018.62
	O	1.83127434	1.91522736	3.52911248	1057.17 1095.04 1105.47
	O	-0.6748136	1.21959616	1.85269078	1208.39 1213.47 1319.60
	O	-0.8941581	1.23781355	3.25537691	1353.16 1384.19 1385.76
	H	0.46574635	-0.9473105	-0.3474262	1402.03 1419.56 1485.47
	H	0.51950642	0.82069784	-0.4139506	1499.09 1503.53 1513.44
	H	-1.0434445	-0.0118348	-0.3573644	3054.23 3069.75 3070.82
	H	-0.5500848	-0.8242102	1.93588901	3125.70 3147.31 3156.38
	H	-0.0857963	1.68209758	3.56561869	3205.42 3675.78 3863.74
	H	1.88371759	-0.9221244	2.28325647	!77.69 152.93 217.45
	H	3.21700092	1.15116438	2.18348955	225.17 364.19 611.52
	H	1.83443415	2.0375253	1.52076281	!Torsions
	H	2.1380941	1.32646881	4.22513093	
QOOH-4 	C	-0.0037974	0.00167056	0.00620164	245.20 278.99 376.63
	C	-0.0010668	-0.0055718	1.48840117	417.40 447.22 550.62
	C	1.40560038	-0.0013005	2.07992852	657.05 808.53 907.40
	C	1.43175981	-0.1009935	3.59752774	918.34 959.63 1006.32
	O	0.9601115	-1.3544824	4.07907169	1064.20 1102.84 1131.76
	O	-0.7954949	-1.0834974	2.00353013	1149.22 1223.89 1265.10
	O	-0.1820585	-2.3114158	1.63576861	1310.07 1352.71 1398.48
	H	0.42528606	-2.4508396	2.38168776	1412.31 1421.84 1457.91
	H	-0.9161058	-0.2300575	-0.5203912	1471.64 1478.47 1513.15
	H	0.89108014	0.2259038	-0.5528241	2996.17 3041.00 3070.06
	H	-0.5553809	0.85855714	1.88243702	3114.03 3121.56 3180.20
	H	1.98093619	-0.8236169	1.65013071	3292.92 3706.94 3855.34
	H	1.89559853	0.92583395	1.77410595	! 103.06 103.44 174.38

	H	2.45637643	-0.0060055	3.95372724	214.12 481.20 610.86
	H	0.85181363	0.71539751	4.03992566	!Torsion
	H	-0.0016683	-1.3234741	4.05967541	
HO_2 + 2-Buten-1-ol **+HO_2** 	O	0.5055325	2.59512924	1.6402416	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.5078306	
	H	-0.2367003	1.48037439	0.3500898	
	C	0.00110526	0.00256459	-0.0011716	203.37 217.75 385.57
	C	0.00066903	0.01365029	1.49481965	664.25 761.91 886.05
	C	1.08837957	-0.0155826	2.25011467	992.44 1004.80 1024.36
	C	1.09180759	0.00119467	3.75055544	1079.05 1127.29 1159.84
	O	-0.1766844	0.20950003	4.32881862	1218.06 1309.76 1331.97
	H	-0.5095386	1.0554586	4.01701157	1381.01 1411.88 1423.68
	H	-0.495219	0.88895076	-0.4003137	1484.34 1497.31 1505.71
	H	-0.5430353	-0.8629292	-0.3832872	1773.11 3015.55 3055.25
	H	1.01553917	-0.0287349	-0.3963188	3082.49 3109.05 3137.25
	H	-0.9681528	0.02977415	1.98429173	3157.34 3172.01 3871.48
	H	2.06800524	-0.0534041	1.78101488	! 146.92 248.09 333.02
	H	1.81085974	0.75185766	4.10035097	!Torsions
	H	1.44131754	-0.9616869	4.1293429	
HO_2 + 3-Buten-1-ol **+HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	-0.0057061	0.02884186	-0.0078678	286.62 434.83 450.48
	C	0.00263284	-0.0200608	1.31699621	680.08 858.08 895.61
	C	1.24134282	-0.0098615	2.15775766	978.94 993.88 1010.15
	C	1.54270448	-1.4143536	2.68326836	1052.50 1115.32 1168.54
	O	1.82739126	-2.3159744	1.63744258	1214.94 1259.79 1324.31
	H	-0.9263513	-0.0222759	-0.5732051	1350.40 1382.01 1429.52
	H	0.91543514	0.13962953	-0.5683053	1452.55 1484.24 1522.55
	H	-0.9386507	-0.1310315	1.84848231	1731.52 3018.97 3066.19
	H	2.09312042	0.33063104	1.5671235	3115.27 3119.65 3153.66
	H	1.12001114	0.66725427	3.00592175	3162.54 3246.55 3843.12
	H	1.12489172	-2.2402529	0.98347102	!90.62 169.52 387.54
	H	2.4263663	-1.3913679	3.31934447	!Torsions
	H	0.701864	-1.7694173	3.29102127	
O2 + $CH_3CHCH_2CH_2OH$ **+ O_2** 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
					257.30 380.64 479.05
					510.72 845.45 854.59
	C	0.00281341	-0.0019374	0.01484942	969.08 977.82 1028.25
	C	-0.001959	-0.0259303	1.50057013	1116.92 1137.02 1159.21
	C	1.2665421	-0.0032136	2.28178772	1213.96 1237.42 1322.01
	C	1.1149853	-0.6818202	3.63736618	1378.49 1403.96 1427.09
	O	0.82798446	-2.0594103	3.51015318	1431.43 1464.77 1481.25
	H	0.09050745	-2.1474037	2.89856753	1489.61 1523.41 2983.96
	H	-0.9137459	0.24347263	2.02209767	2998.46 3016.02 3075.03
	H	2.05967721	-0.5042282	1.72039471	3075.65 3118.68 3130.90
	H	1.60314877	1.03100269	2.44500852	3165.33 3849.70
	H	-0.976915	-0.2335666	-0.4004492	!60.37 123.22 184.04
	H	0.29228775	0.98431002	-0.3721617	354.16 ! Torsions
	H	0.72621429	-0.7151725	-0.3862884	
	H	2.04274727	-0.6143266	4.2035862	
	H	0.33362654	-0.1724965	4.21480034	

CH_2O + 1-methylethyl 2-hydroperoxypropane  + CH_2O					
H_2O + C4Y1-3OR 	O H H C C H H C O H C H H H H	0.0000000 0.0000000 0.9268960684 0.01197747 0.01065097 1.04155529 0.26396775 -0.7157058 -1.1788435 -0.7938646 -1.3446658 -1.6156672 -2.1090029 -0.4259251 -1.2957672	0.0000000 0.0000000 0.0000000 0.00182073 -0.0048425 -0.0229089 -1.0324709 -1.1646563 -2.072412 -1.1583638 0.35402668 1.37118222 -0.3321692 0.92659534 0.29857716	0.00000000 0.95889274 -0.24563991 0.01066192 1.53918978 -0.3584002 1.8637255 -0.595048 0.04035131 -1.6980611 2.14060679 1.85609164 1.78028195 -0.377324 3.22568146	1627.56 3874.01 3976.38 192.69 342.28 367.58 446.62 687.52 709.00 846.04 929.95 945.73 977.70 1029.13 1121.58 1164.04 1189.65 1230.85 1268.18 1355.47 1392.79 1421.74 1445.32 1494.89 1497.83 1855.08 2921.83 2958.94 3055.85 3071.02 3093.21 3148.44 3166.59 ! 85.79 159.78 228.12 !Torsions
OH + acetaldehyde + vinyl alcohol 	O H C C O H H H C C H H H O H	0.00000000 0.00000000 -0.0018794 -0.0031285 0.98635722 1.01686213 -0.5402751 -0.5402500 -1.0033142 0.00108637 -0.00237744 0.922217046 -0.931617023 -0.916296910 1.082393644 1.881163785	0.00000000 0.00000000 -1.897E-06 -1.48E-06 1.3699E-05 1.266E-05 0.87702138 -0.8770407 -1.645E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000	-0.00571069 0.96571069 -0.0001381 1.49919735 2.17677025 -0.3774697 -0.3636967 -0.3636964 1.97459753 0.00545105 1.329579641 -0.563562232 -0.535007759 1.908645540 2.142130840 1.605445553	3776.00 513.29 776.08 900.41 1138.06 1146.18 1379.68 1433.59 1464.85 1474.90 1874.28 2942.79 3063.52 3127.31 3180.67 ! 157.82 !Torsions 498.84 728.26 861.80 972.01 1017.42 1140.88 1334.37 1359.87 1452.26 1739.13 3176.70 3216.02 3281.22 3861.17 ! 449.99 !Torsions
OH + 3-Hydroxybutanal 	O H C C C H H H O	0.00000000 0.00000000 0.00700152 0.01103546 1.53420836 -0.463008 -0.3789321 -0.2531019 -0.7067605	0.00000000 0.00000000 0.01152681 0.00010228 0.00354836 -0.8283539 0.94940125 -0.9553511 0.95840844	-0.00571069 0.96571069 -5.053E-05 1.53388032 0.14270351 -0.5025336 -0.3991921 1.98926856 2.21959151	3776.00 213.21 338.50 409.14 464.65 676.87 772.36 855.07 940.04 980.30 988.62 1082.15 1143.22 1191.40 1247.18 1302.59 1333.80 1399.46 1405.54 1420.14 1439.87 1454.22

	H	-0.4160401	1.82359764	1.91293559	1487.25 1504.84 1849.49
	O	1.42199051	0.2254861	1.56571319	2964.86 3025.08 3045.73
	C	2.33365908	1.07954854	-0.544105	3067.42 3084.91 3140.69
	H	3.35718482	1.08934345	-0.1706696	3154.55 3848.24
	H	2.35852185	0.90607726	-1.620527	! 109.96 173.47 236.01
	H	1.88832736	2.05696839	-0.3564474	529.40 !Torsions
	H	1.9687381	-0.9810236	-0.0462515	
OH + $C_4H_7OHCYO1-3$ 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.0070015235	0.0115268149	-0.000050534	72.14 332.67 423.56
	C	0.0110354569	0.0001022818	1.5338803225	454.62 524.24 676.53
	C	1.5342083582	0.003548358	0.1427035088	840.88 917.8424 931.87
	H	-0.4630079731	-0.828353897	-0.5025336453	953.69 1029.17 1080.46
	H	-0.3789321417	0.9494012497	-0.3991921367	1112.78 1133.61 1200.05
	H	-0.2531018529	-0.9553511458	1.9892685632	1204.59 1249.96 1288.24
	O	-0.7067605096	0.9584084366	2.2195915148	1330.43 1358.75 1392.10
	H	-0.4160400513	1.8235976392	1.9129355901	1416.72 1459.27 1483.67
	O	1.4219905058	0.2254860992	1.5657131945	1496.22 1498.83 3059.44
	C	2.3336590804	1.0795485354	-0.544104959	3061.31 3093.34 3097.13
	H	3.3571848241	1.0893434452	-0.1706696453	3137.26 3142.30 3170.74
	H	2.358521847	0.9060772597	-1.6205269725	3852.65
	H	1.8883273633	2.0569683862	-0.3564473748	! 223.93 309.76 !Torsions
	H	1.9687380988	-0.9810236182	-0.0462515032	
OH + (3-methyloxiran-2-yl)methanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.0249967	-0.0096645	0.00557249	216.98 252.48 345.91
	C	0.02036494	-0.0109615	1.46669032	487.45 661.03 810.18
	O	1.2204231	-0.0527622	0.69066332	849.03 928.33 990.13
	H	-0.2921184	-0.9348947	-0.4976453	1043.17 1061.80 1120.59
	H	-0.1345916	0.94404806	1.95743573	1156.40 1178.21 1191.96
	C	-0.2506700	1.25480857	-0.7855856	1236.18 1295.03 1352.51
	H	-1.3181558	1.40124612	-0.9530579	1383.43 1416.82 1437.97
	H	0.23056504	1.14840617	-1.7646988	1481.56 1498.30 1513.48
	O	0.23144785	2.38691919	-0.1054971	1542.00 3025.36 3068.00
	H	1.12125414	2.17003775	0.19537663	3108.80 3138.49 3142.99
	C	-0.282753	-1.2391095	2.27009872	3144.84 3166.51 3836.21
	H	0.34283428	-1.2760561	3.16164578	! 139.24 195.56 432.82 !
	H	-1.3258835	-1.2390351	2.58640753	Torsions
	H	-0.0933594	-2.1339043	1.67888819	
OH + Oxiraneethanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	-0.0161659	0.05500447	0.02027366	243.59 372.40 402.01
	C	0.01372416	0.00237712	1.43843015	533.05 794.14 873.02
	C	1.2566078	0.01099717	0.66567049	906.01 956.93 980.27
	C	2.10946765	1.23984057	0.51650521	1031.81 1109.26 1130.62
	C	2.50749579	1.46341828	-0.9385673	1161.74 1166.98 1183.99
	O	1.41550286	1.87510826	-1.7297556	1241.43 1259.51 1309.05
	H	0.65618725	1.32816116	-1.5025392	1352.46 1386.32 1448.12
	H	1.76716602	-0.9374901	0.52532892	1454.23 1476.40 1525.93
	H	1.56209406	2.11687007	0.86711725	1544.54 3007.76 3067.44
	H	3.00247223	1.1268698	1.13479366	3108.70 3114.89 3131.63
	H	-0.350445	-0.9235414	1.86556452	3143.47 3225.64 3846.96

	H	-0.2958442	0.91297212	1.9377506	! 78.08 173.72 445.42 !
	H	3.25475097	2.25378374	-1.003621	Torsions
	H	2.96151369	0.547849	-1.339243	
nbutanol-ROO3 = QOOH-0	C	0.02837215	0.00766156	0.02122633	1811.93i 106.63 233.95
	C	-0.0025126	-0.0200743	1.55979562	248.04 343.44 372.21
	C	1.39709421	0.00120872	2.17169536	413.86 482.96 530.88
	O	2.33938915	-0.6348994	1.29173946	619.63 792.18 879.61
	O	1.89866551	-1.9153466	1.01754956	900.15 962.87 998.82
	H	1.27042307	-1.7778534	0.14956522	1013.85 1037.76 1063.26
	H	-0.9721039	0.27802825	-0.3387796	1146.52 1179.32 1192.13
	H	-0.5534222	0.84702198	1.92378204	1221.06 1263.77 1323.37
	H	-0.5432937	-0.9160101	1.86575761	1366.90 1379.14 1391.48
	H	1.7729604	1.02637961	2.18316818	1412.15 1474.62 1476.52
	H	0.74449784	0.75248794	-0.340154	1487.44 1504.16 1643.98
	C	1.45007081	-0.6029266	3.55768575	3005.14 3061.25 3070.17
	H	2.45007257	-0.5130885	3.97810499	3083.11 3086.30 3135.41
	H	0.7447733	-0.0944919	4.21566426	3145.10 3156.94
	H	1.18109312	-1.6572329	3.5081386	! 231.03 !Torisons
	O	0.28349822	-1.2517366	-0.5009957	
nbutanol-ROO3 = QOOH-1	C	-0.0019545	-0.0111867	0.0178515	1934.17i 109.56 166.75
	C	-0.0050799	-0.0195949	1.51690615	264.42 319.91 391.77
	C	1.43413368	0.00679581	2.0604952	477.17 525.01 533.52
	H	-0.5504508	0.85186339	1.88819602	676.88 835.61 888.88
	H	-0.4895257	-0.9233846	1.88694474	908.83 984.71 1020.15
	H	1.93860809	0.91039458	1.70900418	1073.90 1097.17 1139.36
	O	2.10454303	-1.120275	1.51743083	1170.90 1195.46 1226.35
	O	2.28317061	-0.9120486	0.16185905	1241.83 1282.14 1319.52
	H	1.12956666	-0.6517777	-0.1830846	1367.98 1379.48 1415.36
	H	-0.7849898	-0.5888028	-0.4755646	1419.16 1458.70 1487.59
	O	0.15201438	1.27460822	-0.4690927	1503.95 1602.74 3061.32
	H	0.18813209	1.25969673	-1.4287089	3071.14 3074.83 3087.69
	C	1.49895066	-0.1246912	3.56432622	3127.65 3148.94 3158.78
	H	2.53278857	-0.1181842	3.90339758	3889.21
	H	0.9698457	0.70327871	4.03396043	! 205.34 328.32 !Torsions
	H	1.03414276	-1.0587721	3.87996013	
nbutanol-ROO3 = QOOH-2	C	0.04257816	0.01464322	0.02091842	2167.29i 179.80 208.95
	C	0.00377908	0.00993475	1.53171742	261.87 338.20 431.94
	C	1.36161629	0.00397873	2.24527703	535.27 623.90 716.05
	C	2.46707336	0.85162416	1.69273848	804.04 854.97 898.92
	O	2.07247322	2.14220797	1.28992576	972.35 1026.72 1035.80
	O	-0.5837283	1.23624457	1.9726572	1052.68 1102.17 1162.73
	O	-0.3090095	1.26320944	3.34233719	1175.50 1190.63 1253.99
	H	0.62676145	0.85914523	-0.3396463	1305.05 1355.29 1381.04
	H	-0.968365	0.08214999	-0.3779647	1386.05 1417.15 1440.65
	H	0.4903096	-0.9119201	-0.3377109	1486.18 1499.07 1510.25
	H	-0.5932531	-0.8210606	1.91588356	1743.89 3007.45 3039.36
	H	0.77887611	0.65956187	3.24005874	3064.86 3074.57 3147.49
	H	1.69902541	-0.9586535	2.61995454	3155.68 3165.04 3850.69
	H	3.27783672	0.90722567	2.42759416	! 125.90 129.43 233.19 !
	H	2.88363201	0.35280603	0.80740176	Torsions
	H	1.28147127	2.40284715	1.77308943	
nbutanol-ROO3 = QOOH-4	H	0.0132293	-0.0064427	-0.0293898	2253.95i 183.78 241.08
	O	0.02427883	-0.0303989	1.20445396	335.83 408.08 423.20
	O	1.41539903	-0.0144147	1.30263488	478.29 496.39 598.35
	C	1.83292057	-0.7864595	0.17288498	677.31 842.41 889.12

	H	1.56796585	-1.8339395	0.34980521	925.05 990.30 1009.08
	C	0.96379773	-0.2256395	-0.9415369	1031.25 1066.65 1124.81
	H	1.24287472	0.76475378	-1.2924803	1134.00 1155.77 1163.08
	C	3.32912053	-0.6306096	-0.0015121	1233.79 1264.44 1337.72
	H	3.61877526	-1.1899179	-0.8941788	1357.96 1394.49 1410.69
	H	3.56795798	0.42137233	-0.1696171	1440.11 1458.24 1463.42
	H	0.61541662	-0.899855	-1.7151653	1519.27 1753.59 3012.50
	C	4.12035513	-1.141316	1.19943882	3049.69 3066.90 3115.38
	H	5.17629062	-1.1999952	0.93868938	3117.83 3120.91 3221.31
	H	3.78658432	-2.1560977	1.45063511	3853.00
	O	4.04111142	-0.2865024	2.31562407	! 64.03 155.77 423.20
	H	3.11382866	-0.1420083	2.52971335	!Torsions
nbutanol-ROO3 = HO_2 + 2-Buten-1-ol	C	0.01072864	0.00320116	0.00049234	1065.07i 129.95 144.32
	C	-0.0088239	-0.0029563	1.38638316	242.49 254.71 371.25
	O	2.10354408	-0.0153769	-0.265801	463.78 529.36 644.34
	O	2.48870731	-0.1240274	0.92946977	686.00 854.25 888.26
	H	1.32424504	-0.1557602	1.45353854	974.67 1015.94 1033.14
	H	-0.0178758	0.96172606	-0.5029914	1093.21 1124.65 1162.31
	H	-0.3538591	-0.9103295	1.87624555	1202.78 1279.48 1291.27
	C	-0.2601245	-1.2072835	-0.8254219	1308.57 1385.22 1390.86
	H	0.30640864	-1.1880593	-1.7544336	1411.79 1423.50 1476.73
	H	-0.0170468	-2.1179736	-0.2794124	1492.99 1531.57 1604.89
	H	-1.3223266	-1.2380152	-1.0811524	1649.55 3041.04 3056.39
	C	-0.2221951	1.29593409	2.15027853	3101.67 3122.81 3145.25
	H	0.12731278	1.18045855	3.18060928	3152.11 3200.80 3860.51
	H	-1.2817491	1.54924967	2.19468096	! 83.90 196.17 349.64 !
	O	0.40625888	2.39245823	1.51858984	Torsions
	H	1.35445545	2.23233525	1.49118181	
nbutanol-ROO3 = HO_2 + 3-Buten-1-ol	C	0.05269011	0.00087746	0.0104665	1064.03i 126.22 213.99
	C	-0.0286668	0.02354654	1.39393965	304.51 383.95 469.72
	O	2.16031404	-0.0549500	-0.1424562	489.03 551.93 619.49
	O	2.48466384	-0.110566	1.07298547	688.10 814.37 909.58
	H	1.30354465	-0.0699214	1.55100815	972.22 1008.28 1019.21
	H	0.07801056	0.94089962	-0.5294789	1068.68 1122.30 1165.68
	H	-0.4001453	-0.8626732	1.8965529	1233.74 1254.31 1287.25
	C	-0.2776839	-1.2040886	-0.8094636	1313.07 1341.96 1401.11
	H	-0.1369528	-2.1144766	-0.2238199	1408.07 1436.96 1442.32
	H	-1.3511200	-1.1265243	-1.0201251	1461.12 1512.72 1584.88
	H	-0.2315419	0.96600135	1.8877827	1639.39 3022.36 3032.91
	C	0.46615997	-1.3456697	-2.1387424	3103.46 3116.20 3139.99
	H	-0.1447906	-1.9281648	-2.8267291	3179.48 3227.94 3858.21
	H	0.61055079	-0.3554702	-2.5874409	! 62.46 156.36 452.64
	O	1.68338715	-2.0434949	-2.0287721	!Torsions
	H	2.29549969	-1.5125243	-1.5108527	
QOOH-0 = CH_2O + 1-methylethyl 2-hydroperoxypropane	O	0.02979523	0.00584293	0.02918248	388.01i 183.09 209.83
	C	0.04956406	0.04312022	1.26156121	278.92 342.56 376.52
	C	2.1323739	-0.015354	1.71408852	464.94 553.18 606.72
	C	2.59724857	1.41009453	1.68397651	650.39 846.82 898.07
	C	4.1157114	1.47561204	1.5539977	935.72 959.58 1005.14
	O	1.96014692	2.17566629	0.67210774	1105.91 1130.36 1162.08
	O	2.21938127	1.57098782	-0.5864587	1192.96 1252.75 1336.27
	H	-0.0356346	0.99905908	1.79682142	1384.01 1396.42 1461.28
	H	-0.1631165	-0.8644803	1.84462586	1475.90 1484.55 1487.86
	H	2.11275351	-0.5078584	2.6785269	1502.41 1628.81 2970.72
	H	2.40601219	-0.6410487	0.87513639	3051.13 3071.61 3083.01

	H	2.28021893	1.92198543	2.59526418	3147.70 3149.79 3162.86
	H	4.41990686	1.03398811	0.60716816	3251.33 3643.94 ! 102.67
	H	4.4354821	2.51625448	1.57773787	160.02 227.97 629.99
	H	4.59846547	0.93718229	2.36920739	!Torsions
	H	1.37624569	1.10274193	-0.7273716	
QOOH-1 = H_2O + C4Y1-3OR	C	0.00684864	-0.0014551	0.02135046	2453.88i 123.16 157.80
	C	0.019483	0.00599331	1.54026536	255.75 272.24 288.55
	H	1.0265929	0.02276984	-0.3592989	373.51 410.00 455.18
	H	-0.4729832	-0.914551	-0.329004	534.38 552.36 652.10
	H	-0.5363642	0.85771873	-0.3734844	778.56 890.21 918.74
	C	-1.4706716	0.11716868	2.10912873	995.04 1004.91 1016.03
	H	0.54209002	0.88256505	1.93341918	1082.03 1103.00 1124.84
	C	-1.5706177	-0.1406051	3.534448	1208.61 1248.75 1280.30
	H	-1.8642893	1.09995542	1.86203615	1296.90 1345.21 1398.08
	H	-2.0112748	-0.6434345	1.54027206	1432.40 1464.37 1486.50
	H	-1.8058115	0.62979903	4.25589548	1501.56 1579.83 2682.36
	O	-1.3281409	-1.3179688	4.05327386	3051.50 3067.27 3068.54
	H	-0.993164	-1.9268564	3.33156805	3143.11 3152.71 3155.64
	O	0.6689598	-1.0677438	2.07869303	3219.14 3882.22
	O	-0.3966111	-2.3990109	1.90713138	! 221.99 !Torsions
	H	0.32896908	-3.0313457	1.9032993	
QOOH-1 = acetaldehyde + vinyl + OH	C	-0.0120445	0.0296084	0.02046295	1017.50i 60.73 78.29
	C	0.01780292	0.00348952	1.52952604	140.72 194.22 281.63
	H	1.02150687	0.02944579	-0.3237746	313.95 363.54 432.58
	H	-0.5061246	-0.8619507	-0.3669405	491.92 502.29 534.23
	H	-0.5153115	0.91934701	-0.3578456	766.92 877.56 897.03
	C	-1.6679734	-0.1653827	2.15296106	918.56 1001.49 1026.68
	H	0.27849684	0.97810149	1.96817471	1089.43 1120.57 1159.45
	C	-2.4039865	0.91289897	1.64276661	1194.54 1287.42 1335.06
	H	-1.968572	-1.1379569	1.78485762	1365.36 1388.66 1440.11
	H	-1.4735416	-0.1538669	3.22131091	1458.69 1476.02 1501.14
	H	-2.9158384	0.88359343	0.69224073	1555.35 2981.25 3062.97
	O	-2.3048136	2.15740289	2.12746848	3128.07 3141.31 3150.29
	H	-1.8347402	2.15062721	2.96948284	3218.10 3236.99 3834.86
	O	0.58051524	-1.0243817	2.08911093	3848.92
	O	2.34303488	-0.8857776	1.74182874	! 150.76 229.22 !Torsions
	H	2.41182637	-1.8370625	1.5921557	
QOOH-1 = OH + 3-Hydroxybutanal	C	-0.0008636	-0.0161437	0.03651247	1956.68i 88.10 109.26
	C	0.0242361	0.01786314	1.5521211	158.72 194.72 245.01
	H	1.02453835	0.03077935	-0.32333307	308.64 335.26 435.85
	H	-0.45338599	-0.94630430	-0.308065	495.91 570.27 641.37
	H	-0.56148083	0.82666302	-0.3668178	759.39 883.31 901.69
	C	-1.51464161	-0.0797284	2.09328545	938.77 969.18 997.79
	H	0.42866867	0.96914732	1.91462564	1057.66 1123.52 1133.89
	C	-1.50191370	-0.0612784	3.53630941	1219.85 1254.00 1297.22
	H	-2.08815622	0.74112538	1.6704430	1301.26 1327.95 1391.18
	H	-1.86246901	-1.02760412	1.67912763	1411.37 1474.86 1487.74
	H	-1.93311109	0.72544510	4.1414815	1504.14 1566.23 2616.29
	O	-0.78218893	-0.94883087	4.16898422	3034.36 3066.93 3069.71
	H	-0.0841746	-1.27042726	3.50629707	3144.16 3158.13 3164.88
	O	0.6620020	-1.04332094	2.11161189	3209.63 3851.90
	O	2.3478571	-0.90392102	1.66076907	! 228.22 !Torsions
	H	2.40864571	-1.82793579	1.38881437	
QOOH-1 = OH + C_4H_7OHCYO1-3	C	0.01835109	-0.0632498	0.03350746	977.68i 75.45 124.32
	C	0.00689553	0.00859215	1.52778557	198.40 269.30 327.40

	H	0.94629892	-0.0588759	-0.5179687	393.19 436.08 464.74
	C	0.26730159	-1.4638362	1.83153037	475.96 628.55 764.30
	H	0.74610383	0.69302452	1.9506436	856.57 916.58 952.93
	H	-0.9827274	0.31199545	1.87240847	978.54 1060.37 1100.26
	O	-0.2102031	-2.0054786	0.58902837	1114.46 1155.83 1209.40
	O	-0.4375951	-3.5854798	1.03623899	1247.32 1287.21 1323.25
	H	-0.2959905	-3.9538791	0.15752182	1370.70 1381.70 1411.74
	H	-0.3477613	-1.856669	2.64112517	1463.44 1482.65 1496.08
	C	1.72440934	-1.8037081	2.056907	1504.97 3053.84 3060.80
	H	2.06989284	-1.3956934	3.00763209	3091.01 3112.37 3130.91
	H	1.84522945	-2.8844677	2.06927483	3162.17 3230.40 3850.93
	H	2.34140307	-1.3898731	1.25726934	3873.09 ! 110.16 242.50
	O	-1.0137116	0.36428932	-0.7096955	!Torsions
	H	-1.8291915	0.28723839	-0.2031573	
QOOH-2 = OH + (3-methyloxiran-2-yl)methanol	O	0.01706775	0.06405506	0.00849643	995.66i 114.20 146.99
	C	0.00618249	-0.0035700	1.41935226	233.34 234.26 267.54
	C	1.38189735	0.01064954	1.97962154	370.08 423.36 480.16
	H	2.1048509	-0.6954651	1.59388884	515.69 740.18 874.74
	C	1.85847836	1.08786432	2.86416377	908.23 961.52 1008.46
	C	3.11698205	0.8574901	3.65869828	1077.85 1107.55 1123.97
	O	2.05390427	1.73928192	1.63927445	1152.01 1202.48 1228.14
	O	2.60278575	3.31772898	1.95112733	1268.71 1332.93 1388.68
	H	0.51335934	0.85540155	-0.2260538	1404.58 1423.38 1469.37
	H	-0.5749249	0.81410592	1.85583751	1495.08 1497.35 1504.74
	H	-0.4894811	-0.9437992	1.67486339	3042.65 3070.16 3075.26
	H	1.06968546	1.56604179	3.44913827	3084.41 3146.59 3160.71
	H	3.86391274	0.35877462	3.04098838	3212.35 3846.07 3849.53
	H	3.5141402	1.81610891	3.98608252	! 62.43 215.17 459.43
	H	2.90969362	0.24154176	4.53327617	!Torsions
	H	3.41098119	3.23016136	1.43029688	
QOOH-4 = OH + Oxiraneethanol	O	0.15091019	-0.1138643	-0.0191668	976.47i 202.06 234.14
	C	0.02868792	0.01853398	1.37408865	242.13 274.06 359.57
	C	1.37743459	0.01884924	2.09178014	403.73 443.21 538.77
	C	2.1195153	1.3360852	2.04680336	555.84 787.18 798.35
	C	3.56393238	1.30265652	2.32457116	912.68 949.02 971.89
	H	4.13001503	0.41171432	2.10257112	1037.88 1055.82 1130.64
	H	4.07836222	2.19170582	2.64881771	1155.66 1195.28 1247.81
	O	2.571705	1.76125712	0.78917292	1267.65 1302.99 1354.00
	O	1.26195637	2.41003075	-0.0581483	1413.66 1434.42 1456.67
	H	0.53867848	0.70792872	-0.35062	1471.82 1482.70 1512.49
	H	-0.5333167	0.9219793	1.64184039	3018.77 3054.05 3077.04
	H	-0.5498509	-0.8392904	1.71671273	3105.51 3108.88 3191.13
	H	1.22976746	-0.2267494	3.14729307	3312.99 3744.82 3859.04 !
	H	2.00010499	-0.7613367	1.64830567	65.12 139.07 611.21
	H	1.58373000	2.13965734	2.55682525	!Torsions
	H	1.8015484	2.92235564	-0.6724881	

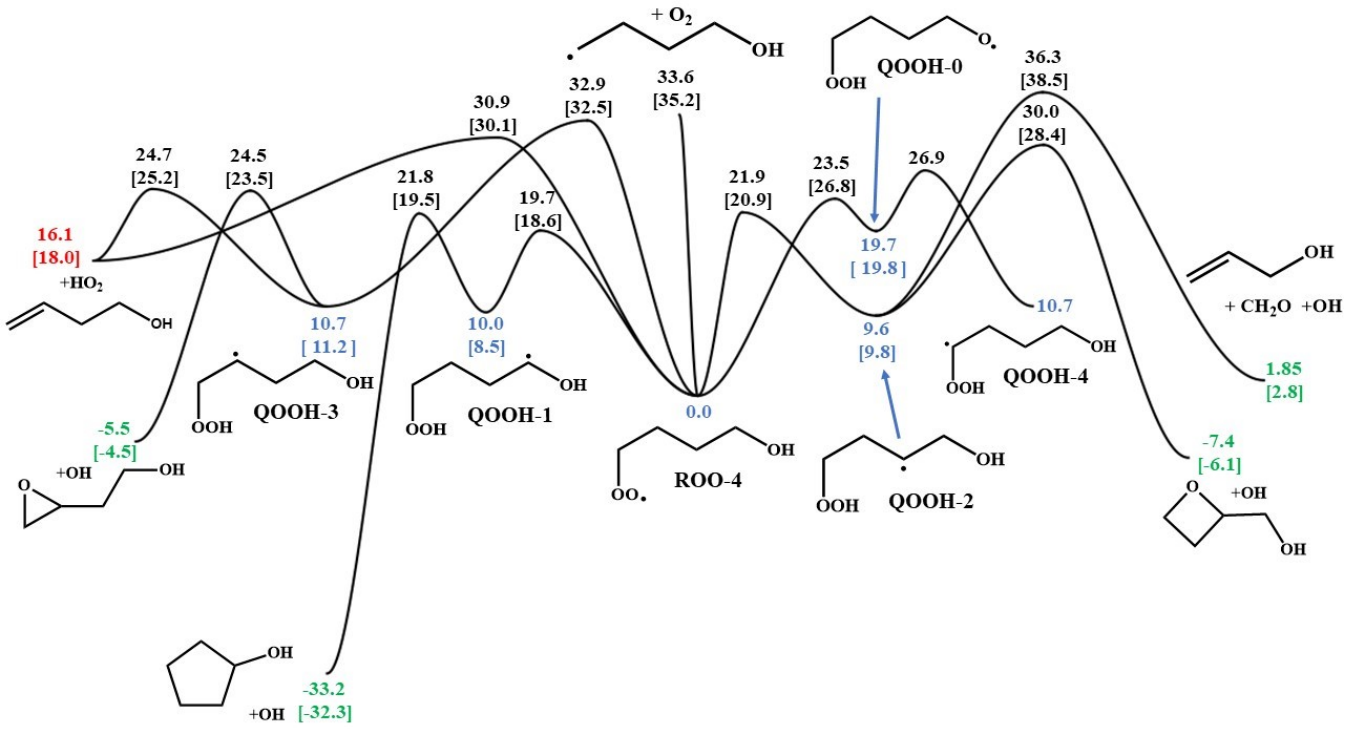


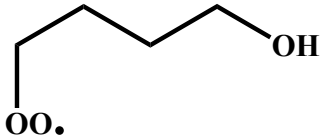
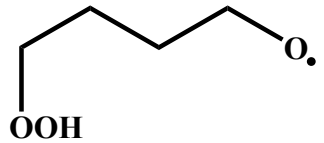
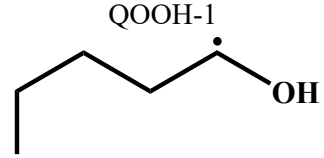
Figure S5. Potential energy surface for n-Butanol ROO4 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

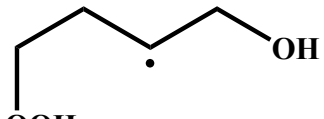
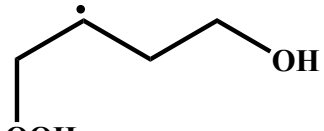
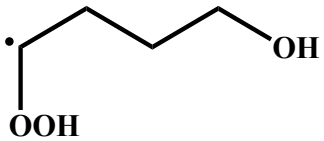
Table S7. Calculated relative energies for n-Butanol ROO4 PES

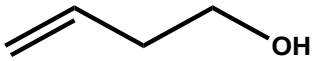
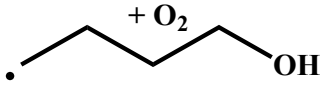
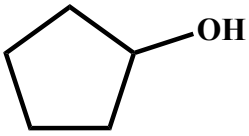
Species	Relative energy (kcal/mol)
n-Butanol ROO4	0.0
QOOH-0	19.7
QOOH-1	10.0
QOOH-2	9.6
QOOH-3	10.7
QOOH-4	10.7
HO_2 + 3-Buten-1-ol	16.1
O_2 + $CH_2CH_2CH_2CH_2OH$	33.6
OH + THF-2-ol	-33.2
OH + 2-Oxetanemethanol	-7.4
CH_2O + OH + 2-Propen-1-ol	1.85
OH + Oxiraneethanol	-5.5
n-Butanol ROO4 = QOOH-0	23.5
n-Butanol ROO4 = QOOH-1	19.7
n-Butanol ROO4 = QOOH-2	21.9
n-Butanol ROO4 = QOOH-3	32.9

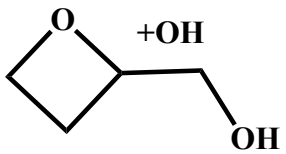
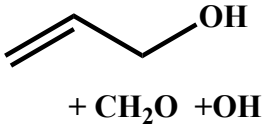
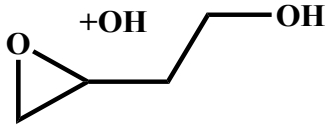
n-Butanol ROO4 = HO_2 + 3-Buten-1-ol	30.9
QOOH-0 = QOOH-4	26.9
QOOH-1 = OH + THF-2ol	21.8
QOOH-2 = OH + 2-Oxetanemethanol	30.0
QOOH-2 = CH_2O + OH + 2-Propen-1-ol	36.3
QOOH-3 = HO_2 + 3-Buten-1-ol	24.7
QOOH-3 = OH + Oxiraneethanol	24.5

Table S8. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Butanol ROO4 PES

Species	Geometry				Frequencies (cm^{-1})
n-Butanol ROO4 	O	-0.0130851	0.00629347	0.05977797	259.90 284.87 375.39
	O	0.0023087	0.01475211	1.35613569	481.09 589.77 751.65
	C	1.3528848	0.0037788	1.87355977	849.03 896.72 969.27
	C	1.26874927	0.09887914	3.37712934	991.21 1063.31 1101.03
	C	0.6697028	1.41722808	3.8539023	1136.14 1149.87 1200.80
	C	0.63736811	1.51201332	5.36451086	1236.75 1280.13 1292.80
	O	1.97477144	1.43921778	5.83126884	1301.32 1338.53 1343.99
	H	1.97721894	1.47217723	6.78950011	1401.76 1422.09 1458.64
	H	0.67700808	-0.7389712	3.75469322	1478.12 1491.69 1504.92
	H	2.27364492	-0.0104187	3.78529941	1532.76 3020.46 3054.47
	H	1.26227209	2.24960079	3.46599572	3064.56 3073.87 3082.92
	H	-0.344427	1.53069509	3.46783679	3108.56 3128.89 3139.65
	H	1.87294437	0.85377788	1.43112666	3905.22
	H	1.8176574	-0.9212493	1.53509979	! 46.95 69.55 118.32
	H	0.17082286	2.4536398	5.66832618	158.19 226.14 ! Torsions
	H	0.03928357	0.68940853	5.77326874	
QOOH-0 	O	0.02464409	-0.0268757	0.00409709	250.88 272.06 357.05
	C	0.01465634	-0.0028538	1.4212582	480.82 570.59 648.01
	C	1.46154597	0.0014534	1.86721264	768.23 884.61 916.86
	C	2.21169375	-1.2607669	1.46192344	982.29 1041.52 1051.15
	C	3.627158	-1.2774647	2.01825619	1090.29 1117.99 1128.20
	O	3.70515265	-1.2122584	3.38352606	1196.24 1238.60 1263.15
	H	1.95997545	0.88117858	1.45135892	1325.67 1331.15 1370.77
	H	1.4858798	0.10187306	2.95349702	1383.12 1403.12 1410.75
	H	1.6797052	-2.1398467	1.83407053	1420.18 1480.31 1494.57
	H	2.2490366	-1.3469369	0.37522351	1530.83 2936.33 2999.93
	H	-0.5095336	-0.8880252	1.79071313	3041.16 3056.02 3068.29
	H	-0.5130997	0.88926415	1.77021959	3088.96 3104.89 3123.82
	H	4.20763759	-2.1399519	1.66102403	3831.70
	H	4.19336709	-0.3970266	1.66185334	! 47.38 91.91 119.95
	O	-1.3228200	-0.1515247	-0.4258104	157.42 212.30 !Torsions
	H	-1.499442	0.73167175	-0.7708975	
QOOH-1 	O	-0.0398211	0.09814278	0.11582629	213.43 286.01 359.90
	C	-0.0067455	-0.0365094	1.52588128	455.24 557.46 600.13
	C	1.45032801	0.02069187	1.93545128	766.98 905.80 938.52
	C	2.27240649	-1.1307811	1.36439255	1035.66 1061.53 1089.37
	C	3.68283805	-1.0859019	1.83092704	1108.94 1125.07 1203.77
	O	4.59667722	-1.9278614	1.2664951	1229.19 1239.72 1282.00
	H	4.31383102	-2.1505307	0.37483814	1315.33 1346.59 1400.64
	H	1.88046989	0.97223503	1.61812759	1404.23 1414.86 1454.32
	H	1.49325402	-0.0015193	3.02661061	1478.44 1490.98 1530.32

	H	1.79626345	-2.0841225	1.64119609	2966.97 3040.80 3050.86
	H	2.24256058	-1.085438	0.270869	3067.13 3086.33 3113.12
	H	-0.4599554	-0.9914156	1.80472375	3199.19 3830.70 3869.06
	H	-0.5805373	0.7726055	1.98649359	! 73.14 80.24 94.43
	H	3.91481081	-0.8709467	2.86548799	133.19 239.58 348.51
	O	-1.3900528	-0.0672799	-0.291365	!Torsions
	H	-1.6284625	0.8329373	-0.5425581	
QOOH-2 	O	0.02104178	-0.024847	3.048E-05	249.19 300.18 378.92
	C	0.01434769	-0.0154919	1.41305806	435.39 567.46 579.85
	C	1.42010271	0.01052827	2.02267447	838.86 856.94 943.34
	C	2.27288848	-1.1279928	1.58612474	972.68 997.06 1023.33
	C	3.30095691	-0.9499383	0.52811635	1116.15 1128.49 1160.66
	O	2.74603918	-0.4568918	-0.7000024	1212.54 1250.65 1281.87
	H	1.97763139	-1.0025206	-0.9066919	1339.52 1367.23 1392.67
	H	1.89161707	0.95864004	1.75664866	1415.28 1425.67 1476.43
	H	1.29673134	0.00477898	3.10949824	1486.68 1489.59 1510.21
	H	2.08779398	-2.114084	1.99014901	3048.46 3049.54 3063.93
	H	-0.5032827	-0.9391245	1.67804521	3092.52 3100.48 3120.66
	H	-0.5685969	0.83792347	1.76602937	3200.51 3661.14 3824.51
	H	4.03369527	-0.1933228	0.82168744	! 92.69 120.08 190.23
	H	3.83853084	-1.8819385	0.34418645	223.58 469.90 633.69 !
	O	0.52852126	1.22956233	-0.4352162	Torsions
	H	1.45403165	0.99325796	-0.6252546	
QOOH-3 	O	-0.0383301	0.03668115	0.00898374	281.89 288.95 383.14
	C	0.00033851	0.0038947	1.44240615	441.06 535.35 595.66
	C	1.38164164	-0.0076368	1.99382155	834.42 855.87 918.51
	C	2.32622369	1.13002858	1.81227615	967.37 994.63 1060.69
	C	3.36088233	0.84719157	0.71518234	1092.11 1130.17 1156.86
	O	2.76011783	0.60215535	-0.5473278	1206.79 1238.87 1306.53
	H	2.24267866	-0.2104996	-0.4859949	1334.63 1369.87 1393.58
	H	1.75798382	-0.9207482	2.4376077	1415.44 1422.38 1473.63
	H	1.77797991	2.03892728	1.55994528	1479.73 1502.13 1518.44
	H	2.87791504	1.32008411	2.73830597	3041.34 3047.54 3055.93
	H	-0.5306685	-0.9114069	1.70169734	3106.84 3126.48 3127.55
	H	-0.5755893	0.86100322	1.80136561	3186.34 3660.80 3814.06
	H	4.00937023	1.71101428	0.57949182	!113.41 124.07 181.46
	H	3.98479347	-0.0028298	1.00621103	205.52 507.51 624.45
	O	0.09018081	1.39104137	-0.4059516	!Torsions
	H	1.02850182	1.42238974	-0.6636588	
QOOH-4 	O	-0.1064605	-0.1275668	0.07671376	278.19 292.88 365.81
	C	-0.0273185	-0.0585422	1.43602176	507.81 535.75 728.52
	C	1.2754078	-0.0058849	2.16080863	790.28 872.31 916.50
	C	2.10596218	-1.3019313	2.19762379	933.89 994.10 1066.37
	C	1.28290972	-2.5647585	2.39233381	1086.34 1124.61 1179.62
	O	0.50315326	-2.8940879	1.23945538	1235.59 1257.32 1299.09
	H	1.89868565	0.79727233	1.74990024	1366.61 1374.78 1394.14
	H	1.02948514	0.27849742	3.18558897	1417.36 1428.30 1460.43
	H	2.68516274	-1.4024515	1.28069161	1497.33 1507.56 1524.53
	H	2.82325684	-1.2312519	3.01804534	3016.41 3052.52 3074.35
	H	-0.3590268	-2.4781077	1.33940393	3090.90 3118.21 3129.73
	H	-0.8833635	0.49534232	1.79779339	3204.04 3603.84 3848.41
	H	1.94259158	-3.414112	2.56485158	! 100.27 147.62 173.56
	H	0.62997868	-2.4665957	3.26415025	235.95 441.29 613.89 !
	O	1.04193304	-0.7389758	-0.4850704	Torsions
	H	0.94328428	-1.6634539	-0.1842166	

HO_2 + 3-Buten-1-ol **+HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	-0.0057061	0.02884186	-0.0078678	286.62 434.83 450.48
	C	0.00263284	-0.0200608	1.31699621	680.08 858.08 895.61
	C	1.24134282	-0.0098615	2.15775766	978.94 993.88 1010.15
	C	1.54270448	-1.4143536	2.68326836	1052.50 1115.32 1168.54
	O	1.82739126	-2.3159744	1.63744258	1214.94 1259.79 1324.31
	H	-0.9263513	-0.0222759	-0.5732051	1350.40 1382.01 1429.52
	H	0.91543514	0.13962953	-0.5683053	1452.55 1484.24 1522.55
	H	-0.9386507	-0.1310315	1.84848231	1731.52 3018.97 3066.19
	H	2.09312042	0.33063104	1.5671235	3115.27 3119.65 3153.66
	H	1.12001114	0.66725427	3.00592175	3162.54 3246.55 3843.12
	H	1.12489172	-2.2402529	0.98347102	!90.62 169.52 387.54
	H	2.4263663	-1.3913679	3.31934447	!Torsions
	H	0.701864	-1.7694173	3.29102127	
O_2 + $CH_2CH_2CH_2CH_2OH$ **+ O_2** 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
	O	-0.0157085	-0.0454836	0.01723871	261.97 405.05 470.79
	C	0.00380591	-0.0054972	1.4339125	519.18 775.43 853.07
	C	1.417527	0.01273545	1.99448638	880.61 971.15 1011.87
	C	2.21820165	-1.2307331	1.59863213	1080.35 1114.44 1134.62
	C	1.69281399	-2.4717552	2.225826	1182.15 1226.16 1302.87
	H	2.2099766	-1.328096	0.51224026	1363.08 1374.81 1396.07
	H	3.26658164	-1.0772014	1.88696161	1424.74 1465.60 1475.09
	H	1.36486258	0.08687766	3.08423476	1488.37 1515.93 2995.15
	H	1.93030363	0.91295801	1.64256562	3034.36 3046.64 3080.19
	H	-0.5125723	-0.9092115	1.76006916	3101.46 3109.42 3163.47
	H	-0.561635	0.85493299	1.80527013	3270.19 3878.78
	H	0.39671117	0.75584465	-0.3145096	! 81.02 138.29 201.55
	H	1.41773886	-2.4735255	3.27157604	305.73 !Torsions
	H	1.71268876	-3.4183773	1.70937533	
OH + THF-2-ol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.00816229	-0.0011848	0.01204743	77.98 198.57 419.52
	O	0.01021311	-0.0193392	1.44441117	512.71 634.03 787.46
	C	1.33072775	-0.004553	1.91752801	870.86 878.78 943.02
	C	2.16458116	-0.6230945	0.81175024	956.44 963.06 1015.23
	C	1.47545795	-0.0438799	-0.4252665	1054.12 1128.18 1160.55
	H	-0.5446259	-0.8776807	-0.3298246	1201.49 1214.01 1255.99
	H	-0.5072726	0.8924968	-0.3380839	1266.18 1327.82 1348.71
	H	1.33702987	-0.5572262	2.85874334	1372.04 1409.74 1445.13
	H	3.21416216	-0.3563014	0.89777679	1484.50 1501.45 1539.18
	H	2.06158428	-1.7075157	0.8473418	3068.66 3081.11 3098.38
	H	1.8469762	0.961033	-0.6139868	3104.36 3114.84 3155.35
	H	1.62204483	-0.6441213	-1.3198357	3166.38 3875.36
	O	1.79068146	1.31102552	2.11348575	! 314.06 ! Torsions
	H	1.15055035	1.76358306	2.67000414	
OH + 2-Oxetanemethanol	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	

	O	0.01729099	0.09418816	0.03889921	73.95 235.30 391.41
	C	0.01294046	0.05392339	1.44599647	507.01 778.44 786.72
	C	1.42289723	-0.058538	1.97348474	891.81 920.57 984.23
	O	2.1944882	1.07727223	1.52470555	1022.86 1074.63 1098.29
	C	1.62799283	0.32220045	3.4451704	1133.85 1158.50 1185.74
	C	2.32085759	1.56696057	2.871867	1217.49 1235.81 1265.62
	H	3.36513036	1.70583709	3.14963112	1300.40 1343.39 1371.83
	H	1.78088468	2.50458691	3.01131355	1397.73 1444.51 1495.77
	H	0.6484262	0.77688137	-0.2141286	1505.15 1540.55 3009.12
	H	-0.4546666	0.95342704	1.86760298	3067.71 3085.35 3107.16
	H	-0.5770104	-0.8119478	1.75022915	3112.68 3116.91 3172.50
	H	1.88114855	-0.990674	1.63902836	3842.64
	H	0.71620687	0.49872574	4.01113018	! 135.48 442.69 !Torsions
	H	2.28238865	-0.3428488	3.9997329	
CH_2O + OH + 2-Propen-1-ol  **+ CH_2O +OH**	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	1.75214387	-0.7145028	0.73740505	1218.60 1279.77 1546.46
	C	1.58204252	-0.4681554	-0.4198612	1877.08 2943.66 3014.59
	H	1.92664152	0.47856444	-0.870535	
	H	1.07176408	-1.1748522	-1.0968368	
	C	-0.0004217	-0.0002202	-0.0004019	298.67 346.97 583.42
	C	-5.909E-05	0.00030874	1.49945498	621.43 904.96 971.41
	C	1.09008346	0.00027396	2.24896454	1003.02 1030.14 1052.03
	O	1.27818412	0.1238833	-0.5764257	1162.15 1224.07 1320.44
	H	-0.4086313	-0.9456428	-0.3640804	1382.30 1421.27 1449.20
	H	-0.674537	0.78741572	-0.3584569	1503.79 1739.63 3019.80
	H	-0.9807471	0.00565347	1.96449649	3086.64 3167.25 3179.27
	H	1.03126243	0.00823147	3.32808457	3260.43 3869.53
	H	2.07549285	-0.0272614	1.80209603	! 199.8541 346.9718 !Torsions
	H	1.66177723	0.95253574	-0.2765586	
OH + Oxiraneethanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	-0.0161659	0.05500447	0.02027366	243.59 372.40 402.01
	C	0.01372416	0.00237712	1.43843015	533.05 794.14 873.02
	C	1.2566078	0.01099717	0.66567049	906.01 956.93 980.27
	C	2.10946765	1.23984057	0.51650521	1031.81 1109.26 1130.62
	C	2.50749579	1.46341828	-0.9385673	1161.74 1166.98 1183.99
	O	1.41550286	1.87510826	-1.7297556	1241.43 1259.51 1309.05
	H	0.65618725	1.32816116	-1.5025392	1352.46 1386.32 1448.12
	H	1.76716602	-0.9374901	0.52532892	1454.23 1476.40 1525.93
	H	1.56209406	2.11687007	0.86711725	1544.54 3007.76 3067.44
	H	3.00247223	1.1268698	1.13479366	3108.70 3114.89 3131.63
	H	-0.350445	-0.9235414	1.86556452	3143.47 3225.64 3846.96
	H	-0.2958442	0.91297212	1.9377506	! 78.08 173.72 445.42 !
	H	3.25475097	2.25378374	-1.003621	Torsions
	H	2.96151369	0.547849	-1.339243	
n-Butanol ROO4 = QOOH-0	C	-0.0162700	-0.0028148	-0.0158818	1231.96i 67.35 204.36
	C	0.01732763	0.05530325	1.51123333	260.43 287.14 297.68
	H	1.01887131	-0.0186419	-0.3632714	462.88 476.24 510.24
	H	0.04955386	-0.9508995	1.95633965	610.98 738.81 818.21
	H	-0.4698611	-0.9468507	-0.3234873	846.62 900.71 930.77

	H	-0.9226945	0.49223703	1.90195261	967.62 1004.49 1080.94
	C	-0.3519293	2.53060366	-0.232523	1121.63 1134.92 1197.09
	H	0.7283697	2.66501444	-0.2753598	1224.98 1271.40 1291.05
	H	-0.8282996	3.29503439	-0.8489085	1303.91 1373.07 1375.25
	C	-0.7805958	1.14189472	-0.6790014	1389.71 1398.13 1403.00
	H	-1.8488982	1.04277584	-0.4729195	1475.12 1483.45 1497.62
	H	-0.6640762	1.08194129	-1.7627933	1660.82 2906.79 2977.61
	O	-0.7795534	2.75439075	1.11508593	3062.25 3065.61 3070.63
	O	0.29751401	3.00893674	1.93862719	3102.37 3112.87 3132.61
	H	0.78374697	2.07369055	2.02346751	
	O	1.06730258	0.76002457	2.0375091	
n-Butanol ROO4 = QOOH-1	C	0.00916285	-0.0040599	0.0146658	1895.07i 86.08 159.95
	C	0.00890337	-0.0009137	1.52907232	263.34 315.66 356.42
	C	1.43916137	-0.0034619	2.07554152	410.54 459.38 568.73
	C	2.02350205	1.40812304	2.13036711	618.42 793.94 871.51
	O	1.5562046	2.2247296	1.06615171	916.91 948.65 1009.47
	O	1.89973437	1.63018444	-0.1334719	1057.28 1097.56 1111.11
	H	0.96640605	0.81928554	-0.275953	1128.47 1185.63 1220.76
	H	-0.5502505	-0.8702638	1.8835903	1251.17 1267.98 1301.94
	H	1.47011257	-0.4281057	3.07856783	1312.97 1356.48 1393.37
	H	2.06294364	-0.6381503	1.44436201	1402.96 1430.66 1478.20
	H	0.35702004	-0.9375156	-0.4274314	1491.88 1502.76 1522.64
	H	1.67940969	1.93437776	3.02194696	3046.67 3067.06 3076.84
	H	-0.5208300	0.88786495	1.88448409	3088.68 3113.29 3115.98
	O	-1.1608733	0.37247109	-0.6008337	3129.48 3857.39
	H	-1.5059603	1.15902324	-0.1663564	! 396.69 ! Torsions
	H	3.11480742	1.38771585	2.12560654	
n-Butanol ROO4 = QOOH-2	C	0.02115178	-0.0148928	-0.0017448	1826.48i 104.66 182.65
	C	0.0124551	0.02503675	1.50571697	277.85 380.06 475.38
	C	1.43579848	-0.0195427	2.09384408	512.22 550.67 685.50
	H	-0.4587673	0.94839917	1.85699795	812.61 850.27 874.89
	H	-0.5474767	-0.820794	1.90037925	952.01 975.70 1028.65
	H	1.95651152	0.92251368	1.92537597	1062.05 1111.92 1117.88
	O	2.14928085	-1.0799093	1.49112321	1147.03 1195.64 1232.21
	O	2.35487329	-0.7472467	0.16230871	1253.08 1280.77 1340.95
	H	1.22436903	-0.5877314	-0.1909243	1354.65 1380.26 1403.00
	H	-0.6777932	-0.7111893	-0.4583958	1423.87 1466.23 1499.70
	H	1.41611771	-0.2515893	3.15728177	1507.22 1568.97 3030.98
	C	0.1481352	1.2968647	-0.7313902	3047.59 3064.74 3092.26
	H	-0.7581007	1.89170575	-0.5792816	3124.24 3146.46 3155.27
	H	0.24217559	1.12166269	-1.8078373	3836.91
	O	1.21472032	2.08647137	-0.2453551	! 164.39 434.33 !Torsions
	H	2.02251214	1.56571207	-0.3139752	
n-Butanol ROO4 = QOOH-3	H	-0.0023204	0.03255345	-0.0053347	2173.87i 125.76 261.67
	O	-0.0082942	0.05234675	1.24906028	315.58 390.61 532.34
	O	1.38262626	0.02014996	1.35077217	560.25 674.93 765.79
	C	1.75641466	-0.8459716	0.29119252	871.77 899.74 957.26
	H	1.53232844	-1.882481	0.55466154	978.44 1024.66 1055.50
	C	0.8983419	-0.3854763	-0.8844799	1083.37 1130.26 1147.94
	H	1.24187331	0.53980703	-1.3423364	1218.00 1227.05 1244.89
	H	2.82917551	-0.7252902	0.14292914	1266.36 1321.12 1379.18
	C	0.29804717	-1.3843522	-1.829278	1395.95 1409.97 1428.56
	C	-0.4777093	-2.5091583	-1.1427125	1455.62 1504.06 1527.59
	H	1.08992867	-1.8302797	-2.4456168	1735.20 3014.31 3040.32
	H	-0.3708043	-0.8624053	-2.515311	3067.28 3098.21 3119.01

	H	-0.9420301	-3.1313162	-1.9066881	3125.25 3139.55 3823.03
	H	0.19880803	-3.1557706	-0.5752309	! 63.52 206.62 490.84
	O	-1.5226049	-2.0266409	-0.3300617	!Torsions
	H	-1.1529308	-1.6405729	0.47208236	
n-Butanol ROO4 = HO_2 + 3-Buten-1-ol	C	-0.0131762	0.00593394	-0.0162	1083.85i 122.82 203.69
	C	0.05155562	-0.0148193	1.37151615	320.09 398.53 477.17
	O	2.06114037	-0.0290737	1.6429523	485.54 584.60 701.94
	O	2.47237664	0.03590718	0.46056298	821.57 848.27 879.20
	H	1.32964956	0.0677524	-0.1023721	960.89 1011.18 1016.25
	H	-0.2870913	0.95145342	-0.4790631	1093.63 1109.51 1156.66
	H	-0.0635567	-0.9434443	1.91553593	1213.42 1263.04 1266.23
	C	-0.3889083	-1.2436637	-0.7886382	1291.81 1366.77 1389.15
	H	0.05936789	-1.2294409	-1.7840569	1416.35 1419.90 1439.48
	H	0.00297881	-2.1203218	-0.2679899	1479.30 1515.87 1580.02
	H	-0.0592376	0.88834965	1.95538753	1658.31 3023.76 3062.93
	C	-1.8992626	-1.3957648	-0.9367117	3106.54 3117.68 3136.51
	H	-2.3002447	-0.5574341	-1.5179685	3168.16 3255.77 3871.26
	H	-2.1277412	-2.3130263	-1.4780383	! 65.22 134.00 262.80
	O	-2.5560537	-1.5031942	0.30897885	!Torsions
	H	-2.4291345	-0.6787665	0.78619386	
QOOH-0 = QOOH-4	O	0.01977475	-0.0079464	0.01009262	1163.85i 118.52 180.76
	C	-0.0104246	-0.0279879	1.39380167	305.32 342.65 481.38
	C	1.31140155	-0.0141601	2.13959793	523.74 532.58 751.02
	C	1.91108261	-1.4102218	2.33115744	807.04 876.24 901.15
	C	0.81842641	-2.3905859	2.76589	945.59 985.85 1051.98
	O	-0.2390943	-2.4332775	1.85520144	1069.27 1104.62 1131.46
	H	2.0074595	0.63547025	1.6050363	1176.43 1210.19 1237.64
	H	1.12367006	0.43133749	3.11835884	1279.59 1339.29 1359.24
	H	2.35934092	-1.7543134	1.40139545	1364.19 1386.72 1419.96
	H	2.69129274	-1.385654	3.09267222	1462.27 1484.22 1495.75
	H	-0.4947391	-1.0993495	1.7060766	1503.69 1617.34 3002.08
	H	-0.7078232	0.75919352	1.67621948	3044.18 3063.24 3089.97
	H	1.23757828	-3.4029582	2.80110772	3109.35 3131.60 3146.49
	H	0.46135944	-2.1400956	3.77276518	3679.76
	O	0.87688535	-1.0368471	-0.4575483	! 202.49 420.37 ! Torsions
	H	0.43603949	-1.8367398	-0.1185141	
QOOH-1 = OH + THF-2ol	C	0.07971896	-0.0234601	0.01587591	941.05i 76.01 116.92
	C	0.0088284	-0.0233529	1.49491269	224.44 278.54 297.49
	C	1.44647441	0.01578411	2.00165377	361.63 433.58 464.04
	C	2.1982644	-1.1271746	1.3379374	552.66 741.75 863.01
	H	-0.5755922	0.81750696	1.88212629	903.37 935.91 961.13
	H	-0.4845469	-0.9446876	1.81053965	1042.42 1087.75 1110.77
	H	1.90840914	0.96408182	1.71956361	1123.52 1195.79 1229.50
	H	1.50149436	-0.0709448	3.0872309	1249.56 1277.73 1305.89
	H	0.47900572	0.83412378	-0.5109601	1334.50 1371.96 1393.50
	H	3.2731772	-1.0234039	1.47851387	1469.00 1486.57 1514.51
	H	1.88476643	-2.0900601	1.75397224	1526.83 3034.60 3038.29
	O	-0.8364247	-0.7745037	-0.6311407	3068.80 3100.74 3115.07
	H	-0.7066406	-0.7017717	-1.5803821	3123.19 3182.80 3860.99
	O	1.91342465	-1.097337	-0.055751	3884.25
	O	3.09490907	-2.084277	-0.6248571	! 171.52 394.10 ! Torsions
	H	2.50671411	-2.7042522	-1.0702372	
QOOH-2 = OH + 2-Oxetanemethanol	C	0.0330003	-0.0156664	-0.015213	1077.93i 72.35 95.25
	C	0.09883016	0.02618678	1.48627568	252.68 261.56 306.55

	H	0.94278836	0.08055206	-0.5914036	419.37 572.13 634.67
	C	-0.1222686	-1.4612158	1.75083465	743.23 834.27 902.63
	H	1.06401497	0.37601305	1.84373347	952.51 1002.78 1034.38
	H	-0.6922256	0.64531828	1.9072578	1049.77 1126.62 1131.67
	H	0.68391382	-1.958489	2.28738802	1157.77 1208.07 1220.71
	O	-0.1571127	-1.9278317	0.38840553	1248.37 1291.64 1354.28
	O	-0.6018933	-3.5052862	0.6396386	1377.51 1405.14 1423.47
	H	-0.0760901	-3.8756675	-0.0784929	1486.42 1488.66 1531.37
	H	-1.0734024	-1.6867499	2.23231977	3018.65 3049.87 3081.29
	C	-1.2543912	0.25666177	-0.7129983	3093.37 3130.65 3154.45
	H	-1.4266603	1.33816632	-0.7651552	3208.52 3816.10 3862.29
	H	-1.196612	-0.1114791	-1.7431181	! 150.64 204.00 514.54
	O	-2.3602845	-0.2866593	-0.0298608	!Torsions
	H	-2.1946328	-1.2343139	0.04811537	
QOOH-2 = CH_2O + OH + 2-Propen-1-ol	O	-0.0263675	-0.0565191	-0.0105816	470.47i 73.77 143.63
	C	0.01465276	0.06823669	1.42190459	191.58 284.80 382.68
	C	1.43427777	0.02099158	1.86219966	465.06 480.73 572.73
	H	1.98816016	-0.8749144	1.60854773	727.96 867.79 911.84
	C	2.05122304	1.06479337	2.45967516	963.90 967.13 979.78
	C	2.84627114	2.46404387	0.87018827	1004.91 1054.56 1156.49
	O	1.87933448	2.52175404	-0.0761162	1212.70 1234.49 1241.72
	O	2.05544885	1.44074911	-0.9757914	1278.69 1291.87 1408.70
	H	-0.9376756	-0.0178581	-0.3113092	1451.27 1460.86 1515.46
	H	-0.4399427	1.01299476	1.73015452	1530.87 1608.20 3030.94
	H	-0.5579622	-0.7566309	1.85753752	3080.26 3123.77 3153.49
	H	1.4639414	1.89756786	2.8269319	3189.09 3241.92 3255.12
	H	3.03955384	0.95188767	2.88433386	3508.75 3883.09
	H	2.90455955	3.40108252	1.41108871	! 93.52 246.54 298.22
	H	3.75941647	1.96697156	0.57060209	689.62 !Torsions
	H	1.30166092	0.86660033	-0.7235423	
QOOH-3 = HO_2 + 3-Buten-1-ol	O	-0.0304979	0.0582797	0.00595778	702.17i 203.21 275.08
	C	0.00635944	-0.021568	1.91149104	324.87 353.53 432.33
	C	1.3484798	-0.0026922	2.1849056	506.22 733.88 859.45
	C	2.18338481	1.23123875	2.1143104	887.54 945.19 987.39
	C	3.22684799	1.12500338	0.9984461	1010.08 1033.35 1093.44
	O	2.64124923	0.93808968	-0.2786025	1106.37 1165.47 1220.48
	H	2.11245861	0.12831811	-0.2559268	1251.65 1283.59 1341.02
	H	1.87436303	-0.9454755	2.30149142	1396.92 1423.51 1445.36
	H	1.5482189	2.10203326	1.9421066	1475.94 1512.66 1522.52
	H	2.71819407	1.39049666	3.05620402	1569.11 3038.29 3043.43
	H	-0.5482694	-0.9439077	2.01100805	3103.04 3127.83 3158.32
	H	-0.5711978	0.89016419	1.97830547	3170.14 3259.43 3634.88
	H	3.80581837	2.04474471	0.93842945	3776.23
	H	3.91902687	0.30602813	1.21906167	! 97.97 170.61 179.55
	O	-0.1049556	1.38517425	-0.3318465	573.60 659.85 ! Torsions
	H	0.82188345	1.61272506	-0.5296646	
QOOH-3 = OH + Oxiraneethanol	O	0.24522865	-0.2904877	0.07490023	955.78i 83.25 260.94
	C	0.03462535	0.0787164	1.40595562	278.28 315.69 364.04
	C	1.49512185	-0.0516918	1.50706602	427.34 533.37 697.21
	C	2.38450874	1.10828436	1.24417947	830.78 872.75 951.41
	C	2.21164635	1.75093142	-0.1491776	987.75 1022.01 1079.53
	O	0.96889382	2.3796171	-0.3214347	1100.44 1143.29 1195.22
	H	0.32330149	1.72907569	-0.6301766	1202.25 1212.46 1285.24
	H	1.90711771	-1.0308482	1.69888422	1319.36 1333.48 1404.26
	H	2.17491867	1.89230438	1.9796051	1415.03 1437.34 1477.66

	H	3.42735206	0.81209467	1.35828319	1507.85 1530.90 3038.37
	H	-0.574849	-0.6333287	1.96007312	3059.97 3078.59 3110.76
	H	-0.3299534	1.10163298	1.50108496	3115.41 3143.52 3230.43
	H	2.97696491	2.52131388	-0.2500444	3771.86 3849.70
	H	2.38725792	0.99226007	-0.9149287	! 119.83 209.55 236.54
	O	-1.1220467	0.21068205	-0.8080901	660.12 ! Torsions
	H	-1.0025588	-0.4229549	-1.5266772	

D) Detailed potential energy surfaces, energetics, geometries, and frequencies for species in the low temperature oxidation chemistry of n-pentanol ROO and QOOH radicals originating from fuel radical + O_2

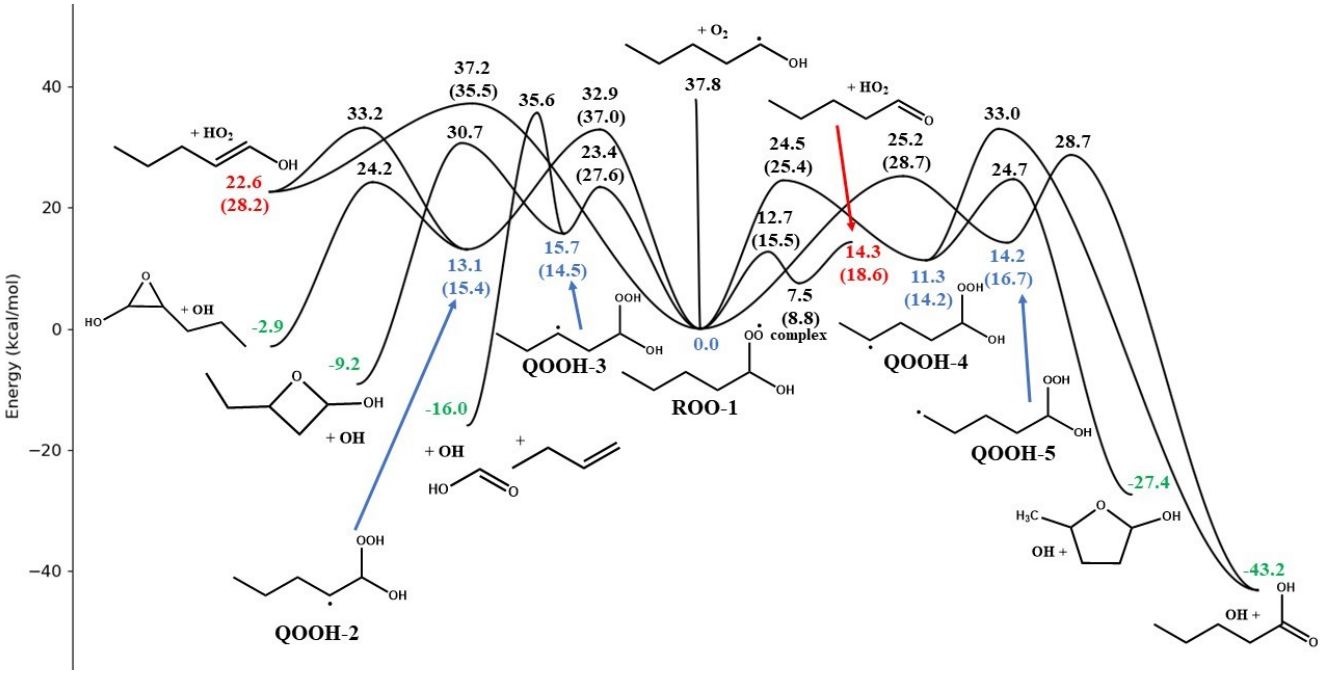


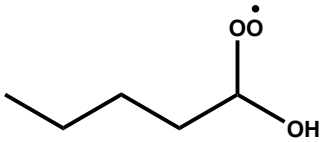
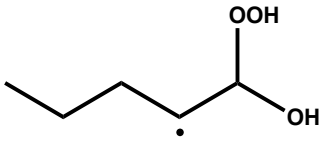
Figure S6. Potential energy surface for n-Pentanol ROO1 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

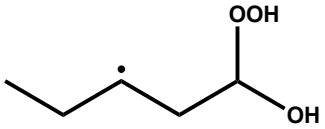
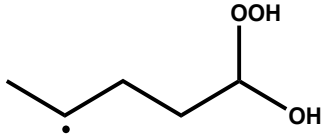
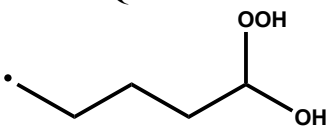
Table S9. Calculated relative energies for n-Pentanol ROO1 PES

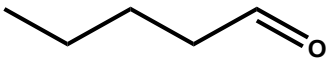
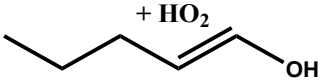
Species	Relative energy (kcal/mol)
n-Pentanol ROO1	0.0
QOOH-2	13.1
QOOH-3	15.7
QOOH-4	11.3
QOOH-5	14.2
HO_2_Pentanal complex	7.5
HO_2 + Pentanal	14.3
HO_2 + 1-Penten-1-ol	22.6
O_2 + $CH_3CH_2CH_2CH_2CHOH$	37.8
OH + 3-propyloxiran-2-ol	-2.9
OH + 4-ethyloxetan-2-ol	-9.2
OH + Formic acid +1-Butene	-16.0
OH+ 5-methylTHF-2ol	-27.4
OH + Pentanoic Acid	-43.2

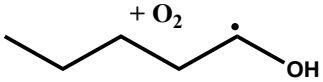
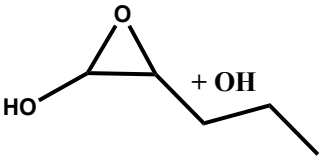
n-Pentanol ROO1= QOOH-2	32.9
n-Pentanol ROO1= QOOH-3	23.4
n-Pentanol ROO1= QOOH-4	24.5
n-Pentanol ROO1= QOOH-5	25.2
n-Pentanol ROO1= HO_2 Pentanal complex	12.7
n-Pentanol ROO1= HO_2 + 1-Penten-1-ol	37.2
QOOH-2 = OH + 3-propyloxiran-2-ol	24.2
QOOH-2 = HO_2 + 1-Penten-1-ol	33.2
QOOH-3 = OH + 4-ethyloxetan-2-ol	30.7
QOOH-3 = OH + Formic acid +1-Butene	35.6
QOOH-4 = OH+ 5-methylTHF-2ol	24.7
QOOH-4 = OH + Pentanoic Acid	33.0
QOOH-5 = OH + Pentanoic Acid	28.7

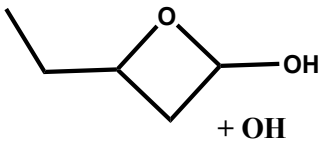
Table S10. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Pentanol ROO1 PES

Species	Geometry				Frequencies (cm^{-1})
n-Pentanol ROO1 	C	3.2004E-06	-9.365E-05	-1.547E-05	102.34 266.08 305.34
	C	6.88907E-05	0.00020074	1.52347904	363.14 454.06 551.82
	C	1.408302143	2.5291E-05	2.10426175	644.07 741.10 804.85
	C	1.394814927	-0.0029003	3.60777463	898.70 929.54 949.72
	O	0.874620953	-1.1827784	4.08358881	1011.93 1050.85 1091.22
	O	2.789634907	0.13134737	4.03804421	1120.42 1149.65 1205.69
	O	2.865998907	0.05541531	5.32940258	1233.57 1275.29 1296.73
	H	0.546736497	-0.8763037	-0.3570209	1301.11 1334.74 1338.88
	H	1.957673143	-0.8849839	1.77632044	1352.94 1387.09 1415.89
	H	1.962010835	0.8788074	1.76818049	1417.04 1478.57 1492.06
	H	0.88956778	0.87084003	4.03113256	1493.67 1503.29 1504.55
	H	0.901490944	-1.1540221	5.04657176	1516.01 3042.87 3053.17
	H	-0.544264075	0.87842914	1.88464374	3057.04 3060.19 3071.11
	H	-0.539497313	-0.8743362	1.89215327	3079.91 3099.72 3122.85
	H	0.54851258	0.87351324	-0.3614037	3128.64 3137.06 3847.63
	C	-1.408846712	-0.0005034	-0.5780732	! 59.84 78.40 124.99
	H	-1.395119046	-0.0039136	-1.6671791	154.68 247.48 444.57
	H	-1.962877819	-0.8795634	-0.2463766	!Torsions
	H	-1.962128871	0.88153449	-0.2525545	
QOOH-2 	C	-0.1466462	-0.0783408	0.03937137	152.95 310.39 319.39
	C	0.0814575	0.04211347	1.50211574	380.01 413.93 507.05
	O	1.41782367	0.36222199	1.82416926	600.53 638.96 741.90
	O	-0.7876764	1.04561333	1.9620233	865.07 907.52 985.95
	O	-0.7262371	1.04613809	3.37680985	1021.31 1052.05 1072.43
	H	0.17259551	1.36697371	3.53829727	1100.22 1118.11 1155.00
	H	-0.9962303	0.44231808	-0.3815346	1174.80 1240.86 1251.97
	H	-0.1209423	-0.8832567	2.05111658	1275.35 1322.77 1341.70
	H	1.70520649	1.04878189	1.21100077	1389.22 1416.39 1428.54
	C	0.56743122	-1.115118	-0.7479975	1442.09 1456.96 1475.30
	C	0.75105062	-0.7364085	-2.2169228	1496.32 1503.71 1511.84
	H	0.01280239	-2.0642379	-0.6995761	2978.46 3053.99 3055.68
	H	1.53994113	-1.3176166	-0.2902457	3060.15 3066.69 3093.15

	H	-0.2269094	-0.5219126	-2.6540172	3127.95 3138.04 3205.35
	H	1.32522473	0.19077518	-2.275929	3786.13 3828.93
	C	1.44660082	-1.833144	-3.0111547	! 32.75 49.93 91.26
	H	0.8682373	-2.7576773	-2.9846378	162.89 243.15 259.23
	H	1.57713751	-1.5491317	-4.0544122	449.05 !Torsions
	H	2.43218205	-2.0474913	-2.595734	
QOOH-3 	O	-0.0053923	0.04695772	0.01323672	93.44 263.90 308.99
	C	-0.0033418	-0.0003343	1.40666042	351.97 447.28 477.34
	C	1.42705269	0.00170959	1.90050675	556.67 635.51 769.75
	C	2.13861576	1.26129789	1.55680917	872.48 927.17 1004.08
	C	3.38866164	1.64407867	2.26519703	1021.44 1056.33 1069.84
	C	3.84901385	3.0595739	1.93479134	1090.00 1118.30 1153.03
	H	-0.8936309	0.26923664	-0.2773892	1181.79 1194.88 1263.55
	H	-1.9372342	-1.8852509	0.81390645	1275.18 1307.29 1347.48
	H	1.91970029	-0.8725883	1.45193141	1391.30 1411.65 1413.97
	H	1.42221506	-0.1601439	2.98066199	1440.33 1463.10 1472.44
	H	3.24189773	1.53887243	3.3453848	1478.43 1502.23 1509.00
	H	4.19185232	0.93507456	2.01584525	2978.29 2996.60 3040.67
	H	-0.5773993	0.83542103	1.81894076	3056.11 3063.59 3090.34
	O	-0.5711211	-1.2015721	1.88432768	3131.29 3140.55 3190.82
	O	-1.9365768	-1.1938421	1.48651649	3833.25 3887.36
	H	1.91046597	1.72698387	0.60646346	! 44.35 54.30 133.73
	H	3.08580098	3.78618979	2.21361076	163.94 201.09 246.09
	H	4.76880401	3.31248572	2.4601948	435.28 ! Torsions
	H	4.03238523	3.16306581	0.86488791	
QOOH-4 	O	-0.0388879	-0.0153509	0.02282351	262.34 313.45 370.81
	C	-0.0041691	0.01043814	1.43387517	437.35 441.38 515.83
	C	1.46071892	-0.0218438	1.80745212	532.53 627.26 810.16
	C	1.65683328	-0.0929635	3.31972911	863.63 941.64 986.98
	C	1.13626595	-1.3494926	3.92550891	999.89 1029.40 1064.01
	C	0.87957971	-1.4348451	5.38675257	1096.22 1109.78 1141.05
	O	-1.4106498	-0.0551495	-0.3527207	1173.56 1219.25 1230.83
	H	-1.5269864	0.82885078	-0.7205793	1308.57 1333.02 1344.40
	H	2.72975577	0.01322529	3.5335596	1398.05 1404.99 1416.21
	O	-0.578292	1.17884374	1.93691439	1429.66 1468.81 1476.14
	H	1.92334151	0.87832525	1.40115974	1479.80 1487.46 1490.17
	H	1.91878841	-0.884237	1.32124044	2985.33 2995.06 3056.05
	H	1.24023857	-2.2672269	3.35898079	3071.59 3072.59 3083.50
	H	-0.5424911	-0.8677084	1.80408146	3130.00 3132.00 3174.46
	H	-1.5331991	1.08146631	1.90305525	3835.70 3889.75
	H	1.17314356	0.76937763	3.78562287	! 38.70 50.88 89.59
	H	0.33037932	-2.3368519	5.65242588	127.18 167.33 200.41
	H	1.8145019	-1.4435279	5.96340178	213.38 ! Torsions
	H	0.3107636	-0.5696866	5.73560144	
QOOH-5 	O	0.0031939	0.0315515	-0.004783	120.62 276.49 324.96
	C	0.00205268	-0.0006595	1.40710808	397.69 422.70 484.62
	C	1.45315602	0.02493378	1.82320204	564.97 638.06 775.08
	C	1.61849965	-0.1310312	3.32961623	837.46 900.83 937.01
	C	3.08746384	-0.0927615	3.75512622	1003.39 1009.27 1067.65
	C	3.87799837	-1.2336433	3.22310952	1089.65 1114.27 1123.72
	O	-1.3568674	-0.0572496	-0.4152029	1165.23 1206.49 1226.51
	H	1.064303	0.66047497	3.83377416	1293.00 1309.30 1331.03
	O	-0.6509029	1.11002103	1.94199054	1369.42 1382.49 1405.17
	H	1.87539143	0.97732962	1.49421685	1417.30 1467.16 1471.96
	H	1.97942041	-0.7709306	1.29445437	1477.04 1485.45 1505.43

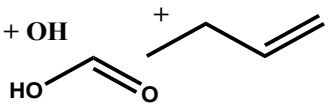
	H	3.53429267	0.85283981	3.43760105	2990.79 3039.27 3047.04
	H	3.1295029	-0.087106	4.85283403	3071.32 3075.71 3109.97
	H	-0.4982691	-0.9236403	1.72095701	3129.74 3164.09 3269.88
	H	-1.5965016	0.98228552	1.829447	3836.63 3884.21
	H	1.17958907	-1.0814474	3.64862704	! 50.31 78.07 129.25
	H	-1.4947023	0.82192142	-0.7869496	163.93 180.79 210.14
	H	4.93318369	-1.1420757	3.01796375	451.75 !Torsions
	H	3.44558764	-2.2245096	3.20312953	
HO_2_Pentanal complex	C	-0.0004214	-0.0039481	-6.246E-05	35.54 77.14 99.39 139.71
	C	-0.0015487	0.00322176	1.52352085	229.45 293.06 304.79
	C	1.40168828	0.00246401	2.10249048	401.34 521.44 665.13
	C	1.4552599	0.05253883	3.59548226	700.43 750.75 864.36
	O	0.49014245	0.18305465	4.31342461	912.76 934.66 989.17
	O	0.65998746	-2.618094	3.60192447	1057.22 1091.57 1148.15
	O	-0.4405133	-2.3253929	4.23437595	1167.59 1244.55 1286.09
	H	0.54932807	-0.8791088	-0.355564	1294.49 1315.16 1335.87
	H	1.96475342	-0.8838446	1.79404005	1376.60 1414.84 1417.58
	H	1.98418862	0.85847072	1.73966242	1424.27 1447.79 1490.89
	H	2.46182654	-0.0084293	4.04387593	1499.32 1503.88 1513.74
	H	-0.3821498	-1.354651	4.40779828	1535.02 1820.35 2985.40
	H	-0.5451105	0.8758727	1.89196689	3035.01 3047.68 3061.05
	H	-0.5403423	-0.8727956	1.89190122	3067.75 3075.27 3079.85
	H	0.54336676	0.87124896	-0.3654591	3111.02 3129.79 3138.40
	C	-1.4096574	-0.0122433	-0.5771198	3430.61
	H	-1.9665926	0.86744743	-0.2518966	! 69.10 121.82 172.95
	H	-1.3964235	-0.0174101	-1.6662015	247.04 !Torsions
	H	-1.958586	-0.893619	-0.2434553	
HO_2 + Pentanal + **HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	6.0184E-05	0.00124921	-4.284E-05	140.56 299.20 400.66
	C	2.7293E-05	-0.0012722	1.52329305	670.32 697.98 745.75
	C	1.40164882	0.00011679	2.10655102	859.48 908.45 931.11
	C	1.43853024	-0.0022977	3.60855584	981.37 1054.92 1090.15
	O	0.46478417	-0.0050813	4.31006192	1146.97 1167.55 1240.50
	H	0.54839838	-0.872008	-0.3634906	1281.45 1312.22 1329.48
	H	1.97825565	-0.867757	1.76669019	1372.14 1412.36 1416.18
	H	1.97533776	0.8710381	1.76955942	1425.60 1454.31 1489.45
	H	2.45008232	-0.0013491	4.05939334	1499.00 1504.76 1513.63
	H	-0.5445329	0.86808521	1.89787802	1865.27 2940.81 3036.12
	H	-0.5416076	-0.873689	1.89499537	3044.41 3060.11 3062.26
	H	0.54545994	0.87754198	-0.3605941	3067.79 3073.87 3108.09
	C	-1.4091651	-0.0001614	-0.5776584	3128.31 3136.97
	H	-1.963843	0.87854282	-0.2461224	! 76.72 113.55 186.14
	H	-1.3968797	0.00166412	-1.6668882	252.13 !Torsions
	H	-1.9608856	-0.8818184	-0.2490396	
HO_2 + 1-Penten-1-ol + **HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	0.00025799	-0.0001046	0.00078112	201.42 287.30 415.29 563.33 664.50 753.58 768.18 881.43 902.93 983.92 989.49 1063.95
	H	-0.000575	-0.0001886	1.0917344	
	H	1.03698763	0.00013268	-0.3334129	

	H	-0.4574812	-0.9343578	-0.3287795	1089.11 1120.74 1146.50
	C	-0.7634959	1.20066828	-0.5404506	1232.78 1269.62 1299.59
	H	-0.2847981	2.12752309	-0.2183988	1326.13 1350.50 1381.26
	H	-0.732841	1.20829388	-1.6328675	1413.82 1436.05 1493.71
	C	-2.2262138	1.21582364	-0.0836282	1503.09 1504.42 1518.38
	H	-2.2568877	1.19808253	1.00767246	1757.41 3021.52 3055.19
	H	-2.7066605	0.28176563	-0.3985029	3058.58 3079.19 3096.84
	C	-2.9905041	2.4055515	-0.5884645	3125.29 3136.16 3208.54
	H	-2.9948155	3.30749023	0.00745224	3232.69 3867.09
	C	-3.6345672	2.44593275	-1.7482587	! 37.26 97.92 241.49
	H	-4.1630401	3.32468709	-2.090451	350.56 !Torsions
	O	-3.7333116	1.43447291	-2.6516855	
	H	-3.250494	0.66788088	-2.328376	
O_2 + $CH_3CH_2CH_2CH_2CHOH$ + O_2 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
	O	0.00501895	-0.0357187	-0.0005619	177.95 298.67 405.41
	C	0.00247524	0.00803873	1.36835868	500.38 617.97 736.16
	C	1.3569991	0.00295021	1.97057654	794.88 914.26 923.54
	C	2.1143249	-1.3183802	1.7710259	988.31 1028.24 1078.41
	C	3.5239174	-1.2815165	2.34648108	1105.39 1125.99 1225.83
	C	4.26984305	-2.5947686	2.14790562	1230.81 1267.16 1286.59
	H	3.74256301	-3.4172317	2.63350177	1329.01 1335.09 1351.08
	H	4.35160422	-2.8360038	1.08716929	1393.80 1413.66 1455.71
	H	4.08022075	-0.4660752	1.87709176	1475.74 1491.41 1501.13
	H	1.54906578	-2.1309505	2.23706212	1503.40 1513.91 3039.08
	H	1.94342361	0.81321505	1.52606132	3044.50 3052.74 3057.79
	H	-0.8306124	-0.4740845	1.86880677	3072.57 3087.17 3105.86
	H	-0.8935249	-0.1216736	-0.3253481	3125.72 3131.95 3154.14
	H	5.27724443	-2.5526049	2.56096741	3904.33
	H	3.47185428	-1.0435823	3.41240669	!79.63 91.70 134.41
	H	2.15602323	-1.5396235	0.70197478	247.90 354.46 !Torsions
	H	1.27133629	0.21688699	3.03806022	
OH + 3-propyloxiran-2-ol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	0.00858541	0.00788023	-0.0033215	138.26 279.43 331.25
	C	0.00080935	-0.0060384	1.37336832	461.79 545.72 611.66
	C	1.28041175	-0.0048183	2.07309725	747.53 837.86 866.75
	C	2.59229054	-0.0788749	1.34906652	908.98 918.13 1035.04
	C	3.57826926	-0.9969758	2.06557279	1066.15 1089.50 1103.82
	C	4.9121342	-1.0856464	1.33659938	1150.02 1182.93 1207.71
	H	1.31229708	0.44116013	3.0637562	1265.99 1272.53 1302.29
	O	0.45084506	-1.1742052	2.00883774	1329.73 1334.60 1386.71
	H	4.77378697	-1.466265	0.32379592	1415.06 1425.11 1481.83
	H	5.60681993	-1.7479306	1.85173792	1498.58 1504.30 1513.37
	H	5.37993578	-0.1029602	1.2592956	1544.51 3052.65 3057.93
	H	3.13021948	-1.9885882	2.15161947	3060.33 3092.74 3119.51
	H	3.73616948	-0.6359088	3.08518372	3127.35 3134.40 3135.90
	H	3.00814019	0.93017088	1.27696458	3144.23 3871.14
	H	2.41779992	-0.432493	0.3330755	! 73.55 94.77 247.47
	H	-0.8810854	0.43763417	1.82633978	259.38 !Torsions
	H	-0.749394	-0.4888337	-0.3241442	
OH + 4-ethyloxetan-2-ol	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	



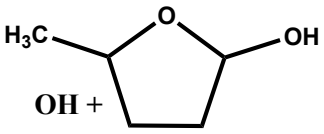
C	0.01920659	0.03079032	0.03037982	66.42 192.09 353.77
C	0.00840188	0.01182081	1.55268745	425.53 480.75 558.56
C	1.40908004	-0.041704	2.12042403	736.08 794.61 823.57
H	1.92872353	-0.9342214	1.76326786	934.75 972.91 978.59
C	1.54913121	0.25705172	3.61783354	1007.65 1030.66 1079.43
C	2.1727325	1.58036322	3.15162295	1110.19 1117.41 1196.56
O	3.43074937	1.92176132	3.60644288	1208.93 1252.80 1278.38
O	2.16891186	1.14483516	1.79023049	1299.66 1319.50 1339.72
H	0.60322644	0.87740349	-0.3285103	1365.62 1412.67 1417.69
H	-0.9884317	0.1110834	-0.3744358	1458.12 1479.63 493.99
H	0.46941738	-0.8809127	-0.3650476	1502.45 1512.18 3049.38
H	-0.4878003	0.9063537	1.9388332	3059.51 3065.33 3092.16
H	-0.5491728	-0.8513297	1.92566819	3097.41 3105.15 3134.55
H	0.624911	0.32444392	4.18638022	3147.81 3164.65 3851.28
H	2.26351364	-0.3730825	4.14336717	! 118.43 237.81 314.50
H	1.55476492	2.46771152	3.2930619	!Torsions
H	4.0302396	1.1978027	3.39739093	

OH + Formic acid +1-Butene

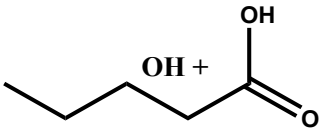


O	0.00000000	0.00000000	-0.00571069	3776.00
H	0.00000000	0.00000000	0.96571069	
O	-0.0764726	0.175471670	0.09622945	645.59 1077.81 1164.30
C	0.0531058	0.034590623	1.42022032	1323.84 1418.68 1881.20
O	1.0902825	0.050749440	2.00881646	3099.91 3799.57
H	0.8111887	0.289072363	-0.27298859	! Torsions 680.90 !
H	-0.9311085	-0.097335781	1.88192236	
C	-0.0001742	-8.287E-05	-5.112E-05	299.14 546.33 569.16 805.15
C	-1.753E-05	-0.0003164	1.52049125	857.37 966.78 1008.83
C	1.3601832	0.00014863	2.15352469	1034.78 1047.28 1111.79
C	2.51874127	0.00073991	1.51187936	1150.60 1292.45 1333.69
H	-1.0183445	-0.0004479	-0.3858087	1379.83 1411.66 1455.24
H	0.50907585	-0.8810468	-0.3915306	1479.40 1502.34 1514.07
H	0.5083415	0.88142428	-0.3912617	1736.20 3045.26 3065.53
H	-0.5517142	0.86826892	1.8918808	3068.56 3133.54 3141.30
H	-0.5509953	-0.8694723	1.89161272	3158.65 3175.71 3254.10
H	1.36738514	-2.699E-05	3.23933663	!174.80 281.55 !Torsions
H	3.45592633	0.00104351	2.0512206	
H	2.57642953	0.00094226	0.43106708	

OH+ 5-methylTHF-2ol



O	0.00000000	0.00000000	-0.00571069	3776.00
H	0.00000000	0.00000000	0.96571069	
C	0.00028358	-0.001144	-0.0001249	54.27 187.04 339.41
C	-0.0032182	-0.0007748	1.51360539	417.03 458.27 516.60
H	1.02407629	-0.0013279	1.88712538	615.00 785.05 829.06
C	-0.7974287	1.15357383	2.13818207	876.81 919.85 926.47
C	-1.4798701	0.48981129	3.33384933	976.14 1011.56 1033.32
C	-1.7430339	-0.8953466	2.77402096	1057.29 1141.55 1147.09
O	-2.9021967	-0.8189038	1.97650438	1163.60 1208.63 1235.80
O	-0.6144895	-1.2076519	2.00475315	1257.52 1314.95 1345.70
H	0.53533923	-0.8685227	-0.3838225	1366.88 1391.19 1399.58
H	0.48266026	0.90063253	-0.3795674	1414.97 1444.00 1482.11
H	-1.0260335	-0.0307837	-0.3671379	1488.82 1499.57 1505.50

	H	-0.1566794	1.98773494	2.4146197	3052.74 3061.56 3081.22
	H	-1.5487815	1.51119904	1.43451457	3093.09 3098.50 3136.50
	H	-0.7995758	0.41132959	4.18164594	3144.50 3148.80 3163.01
	H	-2.3958333	0.98122292	3.65018686	3873.78
	H	-1.8470984	-1.6807751	3.52483674	! 253.91 311.31 !Torsions
	H	-2.9669824	-1.6392377	1.47919626	
	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
OH + Pentanoic Acid 	O	0.02014808	0.2180686	0.01052076	253.78 280.32 354.70
	C	0.01382496	0.03673468	1.19650654	537.29 631.61 662.26
	C	1.21984147	0.01800089	2.09735199	745.91 829.53 854.70
	C	2.53221328	0.01034601	1.32938042	915.33 956.40 1041.65
	C	2.80354534	-1.3147695	0.62577134	1081.65 1130.34 1130.60
	C	4.11601917	-1.2945265	-0.1462067	1195.93 1241.89 1277.61
	H	1.97899527	-1.532213	-0.0550909	1318.51 1331.60 1338.98
	O	-1.1272159	-0.1548257	1.88744595	1408.59 1414.89 1433.29
	H	4.30576562	-2.2475127	-0.6384612	1463.22 1484.87 1497.60
	H	4.95634995	-1.0867968	0.51820866	1504.79 1511.48 1871.61
	H	4.09919428	-0.5189778	-0.9128656	3050.08 3058.08 3064.51
	H	3.3484219	0.22570063	2.02221554	3072.27 3092.86 3106.64
	H	2.51656091	0.81442672	0.5912845	3114.98 3129.00 3135.52
	H	1.1319498	-0.8468128	2.75807537	3816.27
	H	1.13359719	0.89712251	2.74037013	! 50.34 81.29 117.85
	H	2.82380059	-2.1167193	1.36896301	243.91 522.79! Torsions
	H	-1.8534149	-0.1049200	1.2512832	
n-Pentanol ROO1= QOOH-2	C	8.8485E-05	0.00012417	-4.416E-05	2089.05i 123.64 180.62
	C	6.0188E-05	-9.89E-05	1.53057582	220.11 318.37 336.19
	O	1.27642122	0.000171	2.06800445	496.79 566.42 624.17
	O	-0.7262066	1.17616577	1.83616576	735.48 801.75 828.72
	O	-0.1310915	2.13158639	0.999846	910.04 922.31 949.47
	H	0.06859892	1.31699712	0.0575313	990.24 1030.98 1061.22
	H	0.90053782	-0.3995113	-0.4605117	1083.68 1117.41 1133.80
	H	-0.5462871	-0.8298068	1.98054492	1165.82 1181.43 1243.93
	H	1.70364411	0.82321109	1.80266165	1260.66 1301.78 1323.61
	C	-1.2896888	-0.3393215	-0.6832248	1331.52 1367.91 1408.25
	C	-1.3070559	0.03527961	-2.1618682	1417.53 1437.53 1471.46
	H	-2.1143508	0.15221944	-0.1604269	1495.52 1504.90 1510.93
	H	-1.4597372	-1.4200354	-0.5830179	1745.19 3003.27 3054.97
	H	-1.1514065	1.11252534	-2.2532931	3061.65 3076.14 3095.42
	H	-0.465117	-0.4455968	-2.6656663	3113.71 3129.78 3139.79
	C	-2.6121246	-0.3593492	-2.8394234	3146.25 3835.93
	H	-2.7711199	-1.4368586	-2.7795563	! 63.52 77.06 247.99
	H	-3.4606302	0.12887788	-2.3587993	376.47 ! Torsions
	H	-2.6152042	-0.0780794	-3.8914231	
n-Pentanol ROO1= QOOH-3	C	2.5421E-05	0.00012482	2.155E-05	1833.19i 100.55 128.59
	C	2.5934E-05	0.00010875	1.50599253	280.16 302.64 353.27
	C	1.33575855	2.1092E-05	2.20001529	418.18 487.97 536.12
	C	1.87050911	-1.4250411	2.36143567	567.78 652.47 751.55
	O	2.97964642	-1.3963491	3.18132211	843.39 855.98 912.17
	H	3.33066489	-2.2882614	3.26165548	984.77 1034.87 1052.51
	H	-0.404394	-1.2346438	1.82380774	1090.82 1106.50 1131.78
	H	2.07703379	0.57048297	1.63245342	1150.27 1200.17 1214.96
	H	1.27371636	0.41759138	3.20370972	1236.92 1263.84 1290.52
	H	0.36690614	0.97176605	-0.351255	1314.83 1333.75 1379.70

	H	0.71678317	-0.7426769	-0.3603363	1403.98 1416.79 1450.82
	H	2.06490038	-1.8960581	1.39138876	1470.68 1478.20 1504.11
	O	0.86805173	-2.1968287	3.01258184	1507.41 1581.68 3022.54
	O	-0.1533574	-2.3799666	2.0969362	3041.98 3053.34 3062.30
	H	-0.7592453	0.63697214	1.95531764	3071.72 3125.96 3130.86
	C	-1.3774249	-0.2779947	-0.5880746	3139.15 3142.55 3868.38
	H	-2.102284	0.45839206	-0.2390207	! 69.55 249.47 334.14
	H	-1.3594353	-0.243726	-1.6761788	!Torsions
	H	-1.7304996	-1.2644728	-0.2858555	
n-Pentanol ROO1= QOOH-4	C	4.2261E-05	-1.905E-05	-4.127E-05	1862.03i 66.17 118.86
	C	8.7379E-06	-9.098E-06	1.51211111	234.54 262.67 321.86
	C	1.41853513	-5.728E-05	2.09173692	374.90 395.52 491.46
	C	2.03305211	1.39825635	2.13311163	567.61 571.73 682.54
	O	1.62267213	2.18042757	1.01802004	790.05 838.97 885.57
	O	1.97409776	1.50681635	-0.1400836	898.21 980.60 1021.69
	H	1.0325814	0.76229656	-0.281174	1054.02 1077.16 1105.82
	H	-0.5438988	-0.8809314	1.86582538	1129.11 1145.72 1161.49
	O	3.41399804	1.36943648	2.25858411	1177.95 1221.19 1252.33
	H	1.43225987	-0.3896466	3.10868801	1315.23 1329.39 1366.45
	H	2.06033949	-0.6517457	1.49440974	1391.90 1399.58 1409.92
	H	0.33090093	-0.9475672	-0.4268865	1432.07 1477.00 1482.78
	H	1.64796344	1.9698976	2.97798704	1489.41 1489.79 1503.20
	H	3.76662198	0.95605926	1.46244929	3031.12 3044.07 3070.04
	H	-0.5465025	0.87244436	1.87773876	3087.05 3099.22 3107.89
	C	-1.1816447	0.62448246	-0.684413	3109.65 3131.18 3146.87
	H	-1.0861228	0.59801629	-1.7681928	3844.27
	H	-2.102408	0.09591324	-0.4149424	! 197.63 342.75 !Torsions
n-Pentanol ROO1= QOOH-5	C	-0.0004533	-0.0002369	0.00019493	1901.04i 97.40 160.45
	C	0.00040915	0.00013177	1.53217177	183.80 220.10 319.46
	C	1.40694508	0.00035332	2.14666068	353.49 411.93 479.09
	C	1.86380919	1.33839917	2.71329078	521.93 572.67 637.91
	O	1.69367557	2.40971517	1.79651363	671.03 780.54 793.45
	O	2.41480436	2.12711196	0.64746146	878.10 915.81 970.47
	H	-0.5379879	-0.8849129	1.86984973	995.63 1044.86 1059.93
	O	3.17070369	1.27866998	3.18069779	1098.32 1114.30 1137.29
	H	1.46826254	-0.7062671	2.97356522	1157.93 1186.80 1226.05
	H	2.14311617	-0.3246328	1.40741093	1262.48 1273.85 1325.61
	H	0.62151891	-0.8235698	-0.3580492	1359.57 1379.11 1389.45
	H	-1.0174701	-0.2147781	-0.3503834	1405.87 1431.50 1454.40
	H	1.23829396	1.64382019	3.55292847	1468.57 1478.45 1488.74
	H	3.73945718	1.09193313	2.42561523	1495.51 3016.31 3058.76
	H	-0.5642946	0.86388465	1.8931926	3069.56 3082.32 3101.12
	C	0.43770792	1.29083292	-0.6285737	3106.16 3112.87 3127.32
	H	1.58369268	1.68077868	-0.066018	3187.96 3847.28
	H	0.67370726	1.25379833	-1.6883883	! 311.49 !Torisons
	H	-0.1523223	2.16240843	-0.3509003	
n-Pentanol ROO1= HO_2 Pentanal complex	C	0	0	0	668.84i 104.81 171.76
	C	0	0	1.52350303	275.70 312.95 403.38
	C	1.40625508	0	2.10270102	574.52 657.60 720.85
	C	1.44270643	0.03528892	3.60269179	734.99 783.20 804.18
	O	0.55503711	0.6413259	4.27082707	903.09 927.01 941.93
	O	0.87348572	-1.747869	3.99197183	1053.06 1057.48 1062.27
	O	-0.1167296	-1.5125966	4.75615309	1091.39 1146.01 1191.17
	H	0.54819615	-0.8734043	-0.3625439	1246.30 1285.74 1317.08

	H	1.97925371	-0.8654456	1.76188058	1334.36 1374.88 1387.69
	H	1.95520958	0.88597888	1.76338975	1388.53 1415.47 1418.75
	H	2.43000651	-0.1105875	4.05662885	1463.17 1492.19 1501.43
	H	-0.0597594	-0.3570995	4.74177686	1504.61 1514.79 1675.88
	H	-0.5401999	0.87205121	1.89552337	1950.83 3036.37 3046.59
	H	-0.5400432	-0.8782498	1.88772655	3050.20 3059.94 3063.13
	H	0.54510051	0.87673139	-0.3596369	3077.04 3090.41 3113.45
	C	-1.4095452	-0.0015874	-0.5766425	3128.63 3137.64
	H	-1.9640099	0.87737126	-0.2453524	! 63.20 69.04 145.78
	H	-1.3972966	-0.000182	-1.6658233	246.81 !Torsions
	H	-1.9609971	-0.8835436	-0.2481134	
n-Pentanol ROO1= HO_2 + 1-Penten-1-ol	C	0	0	0	1087.80i 88.62 143.20
	H	0	0	1.08942524	235.59 254.75 277.95
	H	1.03795626	0	-0.3356393	359.83 473.58 601.55
	H	-0.4558752	-0.9329245	-0.3351361	656.69 719.16 756.53
	C	-0.748102	1.20160852	-0.5612819	858.89 879.84 924.52
	H	-1.7794232	1.20062512	-0.1995349	984.26 1018.10 1067.55
	H	-0.2915225	2.12702709	-0.2041818	1086.48 1129.53 1157.27
	C	-0.7546363	1.21457387	-2.0888944	1245.32 1288.90 1294.97
	H	-1.1932368	0.28449737	-2.4564085	1297.89 1322.57 1336.18
	H	0.27434004	1.23838222	-2.4533841	1389.59 1397.73 1413.25
	C	-1.5178899	2.38855297	-2.6704342	1435.71 1487.81 1497.15
	H	-1.4274414	2.2704569	-3.990239	1503.26 1511.66 1626.55
	H	-2.593107	2.39434125	-2.518242	1653.58 3053.21 3058.63
	C	-0.9390347	3.65261946	-2.6756706	3066.57 3086.08 3108.22
	H	-1.5356103	4.55234871	-2.7484571	3128.10 3135.20 3157.63
	O	0.33765227	3.79880741	-2.2950497	3204.50 3869.92
	H	0.66971916	4.66034992	-2.5652512	! 66.75 97.96 239.16
	O	-0.610808	3.80412871	-4.7793246	420.41 !Torsions
	O	-1.0396935	2.67687513	-5.1589191	
QOOH-2 = OH + 3-propyloxiran-2-ol	C	0.11379485	0.07602079	-0.0063842	906.29i 135.24 146.16
	C	0.04608932	-0.0185864	1.51273894	175.72 216.96 296.09
	C	1.43053841	-0.0030253	2.16358438	306.73 395.08 441.11
	C	2.15762549	1.27081981	1.97878144	575.12 669.32 710.27
	H	1.62240642	2.20994906	2.00722747	780.97 851.06 901.06
	C	3.59945885	1.32892165	1.69717482	934.20 1040.09 1072.26
	O	4.31589792	0.21274789	2.0927225	1088.17 1105.80 1165.94
	O	3.21756369	1.30753267	0.37203768	1213.62 1244.20 1267.46
	O	4.71093013	1.27401642	-0.4785249	1281.89 1328.82 1361.83
	H	0.5880503	1.00498913	-0.3220752	1376.50 1419.76 1432.69
	H	-0.8811469	0.03036522	-0.4472502	1455.02 1486.60 1498.05
	H	0.70503425	-0.7448062	-0.4148193	1502.05 1509.87 3009.60
	H	-0.5479003	0.80764749	1.9116057	3056.93 3063.72 3067.59
	H	-0.4647618	-0.9367541	1.80549319	3096.77 3116.65 3132.80
	H	1.32776012	-0.1642116	3.24515601	3142.33 3214.76 3808.23
	H	2.05106168	-0.8199274	1.79429139	3856.03
	H	4.10787558	2.26023933	1.96009686	! 49.12 74.11 243.76
	H	5.02685518	0.1315159	1.44313177	426.14 974.80 !Torsions
	H	4.37781473	0.71212644	-1.1888082	
QOOH-2 = HO_2 + 1-Penten-1-ol	O	-0.0267702	-0.0078786	0.01390689	654.52i 72.13 193.57
	C	-0.0089391	-0.0136927	1.36556389	254.90 308.96 350.25
	C	1.14544198	0.01903844	2.10641832	417.87 456.46 573.43
	C	1.15390982	0.13974823	3.59238924	743.69 773.88 877.11
	C	1.24050035	-1.2128538	4.32325106	880.40 955.97 1001.26
	C	2.39539893	-2.0775911	3.83705537	1064.93 1070.35 1107.65

	H	2.07788216	-0.2114935	1.60078604	1142.05 1163.33 1234.77
	O	-0.4132305	-1.8992246	1.72209613	1271.70 1286.03 1328.53
	O	0.15537475	-2.5834106	0.67515829	1349.59 1371.83 1410.02
	H	2.22549997	-2.3990405	2.80913347	1419.76 1427.61 1485.81
	H	2.49900465	-2.9715138	4.45058561	1491.63 1502.32 1513.98
	H	3.34177907	-1.5332053	3.87668468	1577.76 3046.57 3052.38
	H	0.30513824	-1.7510307	4.17492083	3069.57 3094.77 3113.82
	H	1.34184474	-1.0135798	5.39175499	3132.37 3138.63 3166.22
	H	0.25894789	0.67026268	3.9229441	3225.10 3781.09 3849.34
	H	2.01338301	0.74866806	3.88668055	! 43.49 117.99 156.44
	H	-0.9502777	0.3140611	1.7831418	272.45 302.95 535.17 !
	H	0.83693475	-0.2864984	-0.3095862	Torsions
	H	-0.4526998	-2.4117612	-0.0568071	
QOOH-3 = OH + 4-ethyloxetan-2-ol	C	0.05049378	0.08798737	0.03836736	1118.54i 58.94 118.64
	C	0.01662771	-0.0127245	1.55984329	248.79 274.55 316.72
	C	1.37910342	0.005878	2.14931381	337.20 344.21 459.95
	H	2.1185855	-0.6348762	1.68271629	485.26 576.49 669.87
	C	1.65214562	0.50323719	3.5408879	740.40 804.90 869.61
	C	2.42475393	1.76320951	3.15852555	908.82 982.81 1028.54
	O	3.80769195	1.67283602	3.3050148	1030.77 1082.93 1084.68
	O	2.04577051	1.80386773	1.78289778	1096.87 1141.70 1158.5527
	O	2.50675491	3.33234592	1.33008003	1217.81 1267.94 1284.19
	H	0.53894943	1.01477142	-0.2592905	1302.89 1323.07 1337.59
	H	-0.9552436	0.07347268	-0.378304	1413.61 1433.34 1450.22
	H	0.60600142	-0.7457063	-0.3930131	1468.89 1487.61 1503.11
	H	-0.558082	0.81528359	1.97967665	1511.87 3004.95 3065.48
	H	-0.496377	-0.9352377	1.86300559	3082.36 3086.93 3135.94
	H	0.72712505	0.7478279	4.06047905	3136.48 3150.31 3153.14
	H	2.24250662	-0.1681915	4.16416318	3172.88 3837.52 3846.85
	H	2.12957507	2.68578865	3.64987585	! 76.39 170.30 246.32
	H	4.10432311	0.84588413	2.91053466	!Torsions
	H	3.44581249	3.13953195	1.21114359	
QOOH-3 = OH + Formic acid +1-Butene	C	0.05786964	0.08723536	0.04047765	1071.94i 61.53 65.91
	C	0.03165049	0.03330042	1.56335532	169.96 183.75 278.92
	C	1.36229795	-0.0376459	2.22237173	324.54 334.15 456.52
	H	1.37061207	-0.2620981	3.28074571	534.89 543.98 638.78
	C	2.5443102	0.48081311	1.65014307	678.45 796.38 856.58
	C	2.40090077	2.21535203	1.93797468	916.79 952.38 1000.64
	O	2.18740799	2.36338257	3.29838625	1031.28 1071.90 1107.75
	O	3.52897148	2.66393203	1.50019693	1146.53 1175.97 1202.71
	O	3.47372398	4.401536	1.90369135	1250.96 1272.82 1325.85
	H	0.55773111	0.98568171	-0.3209921	1352.15 1376.84 1403.07
	H	-0.9548975	0.09122181	-0.35801	1413.53 1439.41 1460.95
	H	0.58113586	-0.7763508	-0.3707797	1504.06 1511.96 1527.36
	H	-0.4812881	0.924416	1.95588148	2984.65 3015.66 3068.28
	H	-0.5734244	-0.8098298	1.904975	3073.59 3135.96 3144.13
	H	3.46588169	0.24791064	2.16878465	3147.63 3200.18 3226.73
	H	2.63152321	0.43682983	0.57060285	3777.71 3852.77
	H	1.51226535	2.49073676	1.35598512	! 95.43 132.55 237.32
	H	2.63438052	3.19561482	3.5123699	407.78 ! Torsions
	H	4.43101118	4.48623757	1.81305774	
QOOH-4 = OH+ 5-methylTHF-2ol	C	-0.0006046	-0.0015207	0.00074015	965.05i 56.02 113.73
	C	0.00128907	0.00125208	1.48724403	213.52 239.86 278.66
	H	0.9667455	0.00586158	1.97226609	327.40 379.01 497.43
	C	-1.1665107	0.52587738	2.25235678	520.93 560.58 626.89

	C	-2.3115598	-0.4680175	2.0930555	744.41 832.74 868.16
	C	-1.8088081	-1.8596345	2.43334162	902.16 982.67 996.09
	O	-2.6366518	-2.7817201	1.80869163	1020.53 1057.08 1110.73
	O	-0.4587196	-1.9803715	1.97631656	1132.21 1156.09 1171.08
	O	-0.1784095	-3.5274207	2.44183494	1218.53 1237.62 1303.82
	H	0.70387139	-0.7358814	-0.388153	1344.09 1365.14 1391.39
	H	0.3007383	0.97851019	-0.3884613	1393.37 1421.11 1468.23
	H	-0.986371	-0.2279133	-0.4037338	1475.68 1482.19 1492.99
	H	-0.9055269	0.63325592	3.30530737	1502.70 3019.13 3033.48
	H	-1.4734091	1.51186476	1.88698527	3037.60 3090.55 3103.83
	H	-3.1681617	-0.2255489	2.7208872	3106.88 3138.61 3145.19
	H	-2.6583406	-0.4968636	1.06019894	3208.26 3829.35 3870.46
	H	-1.780899	-2.0302052	3.5152007	! 135.56 187.44 443.60
	H	-2.2404423	-3.643596	1.98329788	!Torisons
	H	0.3617114	-3.7618784	1.67905044	
QOOH-4 = OH + Pentanoic Acid	C	0.00208335	-0.0001258	-0.0001084	1851.87i 55.87 135.77
	C	0.00045862	0.00016927	1.50027435	189.93 292.53 374.81
	H	0.98635538	0.00184249	1.96233964	415.03 438.41 519.91
	C	-1.0238219	-0.8472651	2.22929335	549.42 750.32 774.92
	C	-1.4770029	-0.0127388	3.4406249	829.81 843.71 882.83
	C	-1.541089	1.39242983	2.8988228	941.22 985.32 994.86
	O	-2.7318058	1.60724963	2.21831581	1048.30 1085.29 1123.85
	O	-1.1884078	2.43251549	3.71413759	1141.90 1186.12 1227.68
	O	-2.0367258	2.40215905	4.89803091	1253.62 1297.08 1318.80
	H	0.70125527	0.73067382	-0.4050895	1364.79 1371.40 1388.13
	H	-0.9941824	0.22375852	-0.3860726	1404.84 1419.77 1478.34
	H	0.28698764	-0.9811221	-0.3960314	1488.59 1492.25 1496.05
	H	-1.8784700	-1.0246199	1.57391405	1656.28 3024.91 3069.67
	H	-0.6312215	-1.818849	2.53163228	3088.44 3091.70 3107.69
	H	-2.4276368	-0.335852	3.86157957	3120.98 3135.40 3146.88
	H	-0.7223595	-0.0278753	4.22692674	3816.64 3854.03
	H	-0.5391725	1.19001648	2.01099195	! 127.30 164.55 235.22
	H	-2.6560647	2.43116493	1.72600456	357.50 !Torsions
	H	-2.8556776	2.78257755	4.55411529	
QOOH-5 = OH + Pentanoic Acid	C	0.00179151	-0.0134966	-0.0045788	1798.67i 87.19 115.11
	H	0.00229687	-0.0151468	1.0845067	262.27 283.63 324.00
	H	1.00097335	-0.0168818	-0.4272928	381.69 423.30 506.76
	C	-1.0130856	-0.9394692	-0.6311794	558.41 570.54 662.83
	C	-2.4434201	-0.4325314	-0.4087368	817.57 832.81 855.62
	C	-2.6550464	0.93752188	-1.0533968	921.61 969.89 996.88
	C	-1.6726709	1.94519795	-0.5224291	1010.75 1039.01 1095.19
	O	-1.4992491	3.02005224	-1.3590414	1095.84 1145.77 1205.90
	O	-2.0655684	2.31082105	0.7703029	1217.35 1265.63 1292.79
	O	-1.0197148	3.10950208	1.31587218	1335.92 1363.84 1377.92
	H	-0.8270323	-1.0130576	-1.7055447	1387.39 1392.36 1448.05
	H	-0.9210599	-1.9526499	-0.2290326	1458.97 1474.69 1488.64
	H	-3.159999	-1.1420809	-0.8217997	1498.46 1561.05 3038.64
	H	-2.6428754	-0.362908	0.66329921	3059.39 3063.42 3081.44
	H	-2.4951139	0.87899394	-2.1310671	3097.49 3111.15 3121.35
	H	-3.6711522	1.30532672	-0.8892121	3190.67 3808.91 3843.47
	H	-0.5904777	1.22286451	-0.3364421	! 142.20 268.59 446.18
	H	-0.9464475	3.66058381	-0.8967061	!Torsions
	H	-0.4839108	2.44743117	1.77251772	

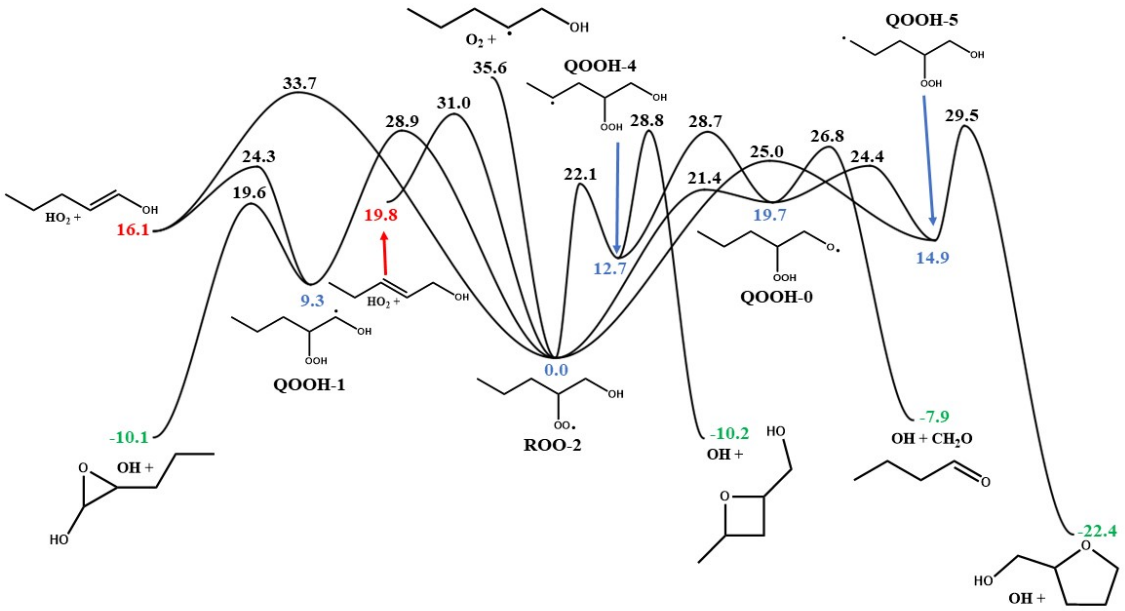


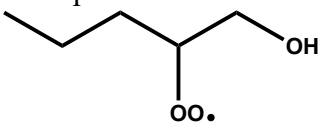
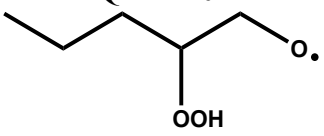
Figure S7. Potential energy surface for n-Pentanol ROO2 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

Table S11. Calculated relative energies for n-Pentanol ROO2 PES

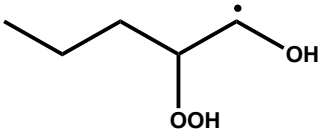
Species	Relative energy (kcal/mol)
N-pentanol ROO2	0.0
QOOH-0	19.7
QOOH-1	9.3
QOOH-4	12.7
QOOH-5	14.9
HO_2 + 1-Penten-1-ol	16.1
HO_2 + 2-Penten-1-ol	19.8
O_2 + $CH_3CH_2CH_2CHCH_2OH$	35.6
OH + CH_2O + butanal	-7.9
OH + 3-propyloxiran-2-ol	-10.1
OH + (4-methyl-2-oxetanyl)methanol	-10.2
OH + Tetrahydrofurfuryl alcohol	-22.4
N-pentanol ROO2 = QOOH-0	21.4
N-pentanol ROO2 = QOOH-1	28.9
N-pentanol ROO2 = QOOH-4	22.1
N-pentanol ROO2 = QOOH-5	25.0

N-pentanol ROO2 = HO_2 + 1-Penten-1-ol	33.7
N-pentanol ROO3 = HO_2 + 2-Penten-1-ol	31.0
QOOH-0 = OH + CH_2O + butanal	26.8
QOOH-0 = QOOH-4	28.7
QOOH-1 = OH + 3-propyloxiran-2-ol	19.6
QOOH-1 = HO_2 + 1-Penten-1-ol	24.3
QOOH-4 = OH + (4-methyl-2-oxetanyl)methanol	28.8
QOOH-5 = QOOH-0	24.4
QOOH-5 = OH + Tetrahydrofurfuryl alcohol	29.5

Table S12. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Pentanol ROO2 PES

Species	Geometry				Frequencies (cm^{-1})		
N-pentanol ROO2 	O	-0.0137725585	0.0351188265	-0.0017996434	133.52	265.55	319.59
	C	0.0089685856	-0.0004797956	1.4013799905	367.38	423.65	461.92
	O	2.7420061517	-0.0366680441	0.6565751435	615.61	739.88	829.87
	O	2.381677761	0.1306136745	1.891028599	886.14	918.21	999.27
	C	1.1149780663	0.8415367247	2.0160082765	1039.84	1076.04	1105.12
	C	0.932854332	1.0878337691	3.4986630891	1136.35	1152.55	1179.21
	C	2.0286731862	1.9510156159	4.1145537474	1239.82	1255.49	1280.7
	C	1.7947533654	2.1899868081	5.6001599505	1308.44	1333.59	1337.76
	H	0.8403882607	2.6906073973	5.7696614127	1373.0	1397.8	1417.98
	H	2.5793891	2.8098963387	6.031107338	1418.43	1449.04	1477.29
	H	1.7760796818	1.2461269085	6.146488758	1498.51	1505.59	1505.76
	H	2.0678675744	2.9065597041	3.5858477367	1513.78	3024.13	3051.19
	H	2.9958813752	1.470759379	3.9625242383	3059.68	3064.89	3086.9
	H	0.8827175834	0.123259302	4.0123603444	3095.05	3108.11	3115.14
	H	-0.0369949322	1.5706122876	3.6383342813	3131.7	3140.81	3843.49
	H	1.2285694706	1.7721085073	1.4559869283	! 55.35	76.44 91.11	180.59
	H	0.1046953865	-1.0241663679	1.784028979	250.58	436.72	! Torsions
	H	-0.9480796231	0.3951129139	1.7427311165			
	H	0.8785022437	-0.1473229366	-0.3151303291			
QOOH-0 	O	-0.0114362634	0.0144662915	0.0055735152	113.44	275.5	317.48
	C	0.0005462864	-0.0090862534	1.3562267161	361.2	377.57	483.35
	O	2.6586367505	0.0394888668	-0.0432641139	588.39	743.27	793.46
	O	2.4138821232	-0.3290115141	1.2996567402	820.75	853.17	915.79
	C	1.4160540919	0.5023169529	1.8256030459	988.67	1060.11	1069.79
	C	1.5179783832	0.4287849059	3.3382659699	1074.72	1116.44	1155.67
	C	2.7814319272	1.0967610179	3.8697195992	1189.53	1235.1	1269.07
	C	2.8849174525	0.9848931206	5.3850672337	1282.89	1292.79	1334.34
	H	2.0285223296	1.4538212718	5.8719519241	1343.32	1381.19	1406.16
	H	3.7872272861	1.4680625357	5.7568601482	1416.11	1459.68	1478.05
	H	2.9126547817	-0.0601991446	5.6959158582	1498.99	1504.4	1513.8
	H	2.781893151	2.1484089181	3.5740064657	1524.27	2992.84	3053.95
	H	3.6499546723	0.6374978025	3.3974047022	3056.67	3059.3	3067.42
	H	1.499112876	-0.6232515446	3.6344209068	3090.02	3100.88	3114.14
	H	0.6341648011	0.9015692792	3.7723123523	3132.82	3139.63	3703.6
	H	1.5574839307	1.5183496566	1.4529298587	! 73.56	91.19 155.41	
	H	-0.0863589872	-1.0273503472	1.7549397337	202.91	246.48 405.13 !	
	H	-0.7441997869	0.6616137328	1.8016703307	Torsions		
	H	1.9017011888	-0.3615655883	-0.5031840149			

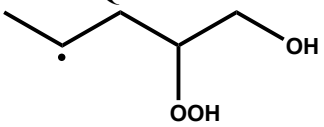
QOOH-1



C	-0.0006741622	0.0051559382	-0.0039797398
C	-0.0019374669	-0.010233894	1.5203225107
C	1.3966656133	-0.0146330658	2.1304618713
C	2.2458936845	1.1680192806	1.6952120962
O	1.5424045945	2.4213732435	1.7367573737
O	1.0158573082	2.6133404642	3.0416501684
C	3.5052102263	1.3010329697	2.4730073805
O	4.3097122608	2.3567580832	2.190394273
H	0.3895176051	0.9476667412	-0.3879343412
H	-1.0099415223	-0.1141137831	-0.3958406505
H	0.611142916	-0.8052784798	-0.4058709437
H	-0.5450800141	0.8573307576	1.896204915
H	-0.5321415848	-0.8942191478	1.8778241312
H	1.3264479549	-0.0167267268	3.2185120988
H	1.9315046169	-0.9227112902	1.8381620475
H	2.4665363417	1.1026421955	0.6201518107
H	1.8040864736	2.8219373076	3.5640349521
H	4.0172946152	0.4551714206	2.9047496086
H	3.7789575823	3.0234570056	1.73541942

192.8	282.31	323.67
368.8	437.83	455.81
604.54	691.14	768.05
851.93	896.91	921.63
1003.73	1042.97	1049.0
1094.13	1151.21	1163.43
1198.35	1238.55	1273.06
1314.65	1345.55	1362.23
1383.71	1398.07	1417.25
1425.43	1466.41	1481.95
1496.34	1504.74	1515.94
3001.4	3056.34	3058.96
3074.61	3107.94	3114.6
3130.32	3138.01	3239.27
3770.83	3808.96	
! 71.1	91.85	120.6
166.06	246.14	262.89
556.08!Torsions		

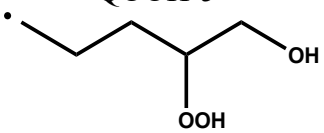
QOOH-4



C	-0.0031563251	0.0261434753	0.0163391195
C	0.0051924389	0.0234881087	1.5041583883
C	1.2932094869	0.0217879875	2.2560362621
C	2.2959691568	1.0610918754	1.7585405006
O	1.6862006905	2.3224569899	1.4799570469
O	1.0040472341	2.7658224204	2.6454899863
C	3.4555751917	1.254304707	2.7176048685
O	4.3945460635	2.1707216015	2.2088132967
H	0.5168145852	0.9006398147	-0.3819815366
H	-1.0158368504	0.0226028906	-0.3809970813
H	0.5126391608	-0.8560836522	-0.3852874216
H	0.1081513496	2.4424858327	2.4726333835
H	-0.8876228393	-0.2815828648	2.032262258
H	1.1101758779	0.1774035325	3.320278347
H	1.7859620696	-0.957495677	2.1694693457
H	2.6898318669	0.7854812018	0.7769193682
H	3.0623461133	1.5796268829	3.6864431589
H	3.9721104808	0.30457683	2.8604039423
H	3.9094492778	2.96736204	1.9706237813

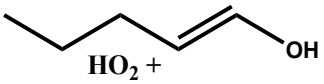
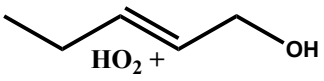
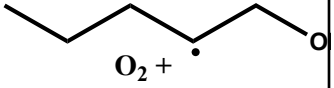
204.55	265.13	305.84
342.87	423.55	474.06
578.45	643.31	846.18
877.05	907.33	974.3
999.67	1017.41	1083.88
1098.84	1126.68	1159.41
1173.69	1222.63	1257.85
1273.35	1370.52	1377.84
1390.61	1403.37	1414.8
1421.76	1439.23	1467.58
1479.94	1495.48	1508.93
2990.07	3002.97	3044.18
3078.03	3082.29	3098.95
3114.78	3144.47	3199.08
3775.64	3854.16	
! 75.16	113.51	172.46 100.96
147.3	386.11	400.42
!Torsions		

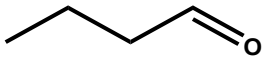
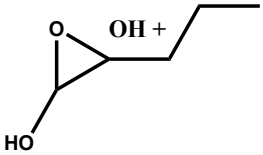
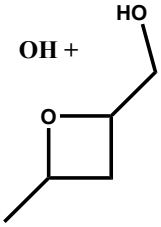
QOOH-5

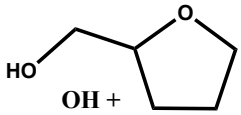


C	-0.0166249891	0.088259702	0.0246507428
C	0.0079394488	-0.0269897986	1.5063690839
C	1.4246018052	-0.0244058393	2.0845983071
C	2.1960872591	1.2495903324	1.7818639741
C	3.593873891	1.2551514553	2.3813073039
O	3.5543574948	1.1364909216	3.786153703
O	1.4257721011	2.3035447691	2.3627315133
O	1.9904608592	3.5430141346	1.954155226
H	1.3443413618	3.8403402591	1.3024427268
H	-0.8580450391	0.5272722088	-0.4888886069
H	0.7064072685	-0.4519538591	-0.5713152957
H	-0.5714230285	0.7804506942	1.9552583811
H	-0.4831930269	-0.9586204286	1.8181267816
H	1.3986246137	-0.1676029168	3.1647273527
H	1.9957910119	-0.8566540075	1.6656442918
H	2.2525598997	1.4150354962	0.7005994159
H	4.1536713667	0.4000522281	2.0013543876
H	4.1125040176	2.1678156181	2.0773942226

218.61	260.6	306.55
347.52	453.61	508.31
526.87	686.75	785.01
865.76	892.79	921.9
963.53	1008.35	1053.12
1092.77	1116.21	1135.12
1177.28	1211.8	1237.83
1272.48	1320.4	1366.37
1377.61	1384.76	1407.23
1423.95	1427.81	1465.7
1474.95	1489.12	1511.9
2994.4	3046.33	3063.66
3067.63	3100.04	3116.41
3125.87	3162.86	3267.16
3828.09	3853.47	
!40.48	81.33	121.96
151.83	171.78	241.76 405.8
!Torsions		

	H 2.9845397019 1.8405050378 4.1124985004	
HO_2 + 1-Penten-1-ol 	O 0.50553254 2.59512924 1.64024162 O -0.1679742 2.44348437 0.50783059 H -0.2367003 1.48037439 0.35008979 C 0.0002579884 -0.0001046157 0.0007811153 H -0.0005750367 -0.0001885655 1.0917343967 H 1.036987631 0.0001326844 -0.3334129125 H -0.457481237 -0.9343578466 -0.3287794854 C -0.7634959325 1.200668278 -0.5404506435 H -0.2847980538 2.127523091 -0.2183987848 H -0.7328410033 1.2082938787 -1.6328674925 C -2.2262137848 1.2158236436 -0.0836282254 H -2.2568877069 1.19808253 1.0076724603 H -2.7066604701 0.2817656292 -0.3985029262 C -2.9905040891 2.4055515018 -0.5884645294 H -2.9948154737 3.3074902263 0.007452236 C -3.6345671979 2.4459327453 -1.7482586839 H -4.1630400515 3.3246870882 -2.0904510077 O -3.7333116157 1.4344729089 -2.6516855017 H -3.2504940332 0.6678808764 -2.3283760216	1161.48 1475.38 3553.10 201.42 287.30 415.29 563.33 664.50 753.58 768.18 881.43 902.93 983.92 989.49 1063.95 1089.11 1120.74 1146.50 1232.78 1269.62 1299.59 1326.13 1350.50 1381.26 1413.82 1436.05 1493.71 1503.09 1504.42 1518.38 1757.41 3021.52 3055.19 3058.58 3079.19 3096.84 3125.29 3136.16 3208.54 3232.69 3867.09 ! 37.26 97.92 241.49 350.56 !Torsions
HO_2 + 2-Penten-1-ol 	O 0.50553254 2.59512924 1.64024162 O -0.1679742 2.44348437 0.50783059 H -0.2367003 1.48037439 0.35008979 O -0.000519 -0.0065331 0.00055603 C -0.000325 0.0021708 1.41000729 C 1.36752406 0.0054969 2.02862908 C 2.49830442 -0.1306882 1.35124778 C 3.88213291 -0.1264388 1.93148228 C 3.95085596 0.05489942 3.43977648 H 3.50308669 1.00214471 3.74206539 H 4.98437523 0.04757593 3.78232763 H 3.42017156 -0.7459438 3.95551955 H 4.46145392 0.66011685 1.43908344 H 4.37403529 -1.0620802 1.65020816 H 2.43683489 -0.2763714 0.27700455 H 1.38431859 0.13218972 3.10648502 H -0.540868 -0.895914 1.71667489 H -0.5712518 0.8550729 1.79663322 H 0.46723818 0.77699436 -0.3009978	1161.48 1475.38 3553.10 186.84 211.96 263.32 511.73 666.54 717.51 834.34 897.61 952.18 1009.01 1028.98 1050.91 1112.86 1117.79 1158.51 1218.88 1294.18 1299.47 1339.65 1379.45 1383.16 1416.67 1422.59 1481.87 1503.34 1506.78 1512.30 1767.83 3015.22 3044.94 3063.49 3067.58 3083.51 3130.49 3140.36 3166.05 3174.59 3869.89 ! 82.75 231.01 301.73 359.59 !Torsions
O_2 + $CH_3CH_2CH_2CHCH_2OH$ 	O 0.00000000 0.000000000 0.0079491871 O 0.00000000 0.000000000 1.1978125329 O 0.4169203025 0.2520378597 -0.0441896204 C 0.1115273511 0.0514116198 1.3320800493 C 1.3261393348 -0.1628669692 2.1630193742 C 2.375267668 -1.139978931 1.7605796537 C 3.7734955206 -0.5156371674 1.6415628588 C 3.8425059103 0.5626231706 0.567216665 H 2.1012880769 -1.5823810758 0.8002616877 H 2.4223778676 -1.9559777492 2.4909054459 H -0.5322072421 -0.8355165242 1.3428464339 H -0.4803616786 0.8826933349 1.7260680624 H 1.0601347958 0.9641254273 -0.1012516677 H 4.0613861415 -0.0929446286 2.6070992342	1758.25 233.86 318.73 373.01 482.42 566.71 777.81 833.4 884.27 918.51 976.17 1028.97 1065.37 1084.49 1135.69 1164.75 1208.3 1244.88 1282.08 1338.98 1363.35 1375.08 1404.64 1413.92 1426.9 1476.88 1494.28 1501.64 1502.53 1513.52 3018.03 3021.05 3051.18 3057.32 3058.0 3086.04 3097.29

	H 4.4934750885 -1.3045231978 1.4173519748 H 4.8575879855 0.9372720622 0.4411711695 H 3.2080181561 1.4118463651 0.8290556603 H 3.5036498481 0.1708663143 -0.3937586388 H 1.39405882 0.3118660948 3.133530662	3119.86 3134.03 3188.11 3867.8 !60.58 87.63 149.04 270.77 329.41! !Torsions
OH + CH_2O + butanal **OH + CH_2O** 	O 0.0000 0.0000 -0.0057106914 H 0.0000 0.0000 0.9657106914 O 1.7521438715 -0.7145028218 0.7374050535 C 1.5820425223 -0.4681554342 -0.4198612336 H 1.9266415225 0.4785644408 -0.8705350011 H 1.0717640837 -1.1748521847 -1.0968368189 C -0.00441 6.5214E-05 0.01515082 C -0.0010062 -0.0001334 1.53786123 H 1.00927224 0.00029531 -0.3828154 H -0.5164751 -0.8805809 -0.3756112 H -0.5167844 0.88063386 -0.3753805 C -1.4078027 -0.0004388 2.11022091 H 0.53550842 -0.8703149 1.91771071 H 0.53522414 0.87012322 1.91793976 H -1.9800247 0.86885699 1.76638835 H -1.9797315 -0.8698463 1.76618297 C -1.4563209 -0.0006242 3.61189392 O -0.487602 -0.0005392 4.32036482 H -2.4711876 -0.0008527 4.05519724	3776.00 1218.60 1279.77 1546.46 1877.08 2943.66 3014.59 198.60 351.22 670.56 702.76 793.34 871.50 954.96 971.92 1068.76 1144.92 1164.05 1257.19 1314.53 1323.40 1404.53 1418.67 1427.04 1455.41 1494.84 1506.11 1511.73 1865.57 2942.87 3036.88 3057.95 3063.44 3081.03 3107.91 3131.17 3137.91 ! 88.93 181.14 249.11 !Torsions
OH + 3-propyloxiran-2-ol 	O 0.0000 0.0000 -0.0057106914 H 0.0000 0.0000 0.9657106914 C -0.0015425449 0.0425658773 -0.0068077915 C -0.0024275245 -0.0277787832 1.5141137344 C 1.4095505263 -0.0528049347 2.0920743573 C 1.3995437881 -0.082587317 3.5913421869 C 2.3055280743 0.705725944 4.4235498173 H 3.0751666634 1.3173013291 3.9671799678 O 2.6766408932 0.3534867992 5.6984173772 O 0.9870977841 1.1394811938 4.2360600239 H 0.5101336965 0.9419227254 -0.3521202489 H -1.0145502579 0.0600571194 -0.4065023965 H 0.5139503148 -0.8175237247 -0.436850982 H -0.5327523943 0.8304212575 1.9307354686 H -0.5414425083 -0.9193128839 1.8444679658 H 1.9514096126 -0.9266121567 1.7200710439 H 1.9568051437 0.8334372143 1.7610281308 H 0.9643738645 -0.9697590678 4.0475005686 H 1.924113323 -0.0650954912 6.1284381045	3776.00 124.0 319.13 334.82 349.58 538.27 590.39 745.17 819.41 894.6 909.85 970.22 1022.84 1070.28 1086.61 1131.47 1147.87 1155.82 1189.98 1265.45 1296.49 1302.48 1317.52 1333.01 1388.15 1415.88 1423.61 1474.51 1497.37 1504.76 1511.79 1542.57 3049.26 3057.08 3060.71 3085.29 3103.05 3120.02 3128.14 3137.31 3177.42 3863.49 ! Torsions 74.88 97.38 234.01 248.25!
OH + (4-methyl-2-oxetanyl)methanol 	O 0.0000 0.0000 -0.0057106914 H 0.0000 0.0000 0.9657106914 C 0.0628472265 -0.0652191921 0.0107090042 C -0.0068669249 -0.0034407848 1.514175257 H 0.9957505578 0.0335840719 1.9474178052 C -0.9776649968 1.0012231204 2.1517029988 C -1.5795241984 -0.2306612892 2.8398818927 C -3.0354680207 -0.5422470306 2.5780635062 O -3.3101910399 -0.5742580069 1.1959802291	3776.00 71.12 255.91 333.95 351.22 450.13 635.4 686.38 827.2 887.46 924.11 932.08 945.72 1014.96 1065.41 1118.18 1129.08 1148.46 1162.35 1211.34 1221.92 1257.13 1296.16 1343.98 1364.53

	O -0.7360838036 -1.1182937036 2.0777873244 H -0.9416972371 -0.0550503705 -0.4139208566 H 0.573809418 -0.973008901 -0.3097333864 H 0.6103412429 0.7947360282 -0.3769290029 H -0.5442740466 1.7550597509 2.8015104081 H -1.6542174872 1.4580935106 1.4322629294 H -1.3610615397 -0.3006993013 3.9087609385 H -3.2876988806 -1.4985317363 3.0494685603 H -3.663947984 0.23224619713 .0197114653 H -2.6760713034 -1.1903373206 0.8126779326	1389.38 1405.42 1423.32 1432.14 1487.96 1493.25 1501.88 1503.58 3031.33 3057.94 3059.59 3063.71 3109.12 3109.99 3135.51 3140.17 3174.63 3839.48 ! Torsions 149.51 237.64 463.45 !
OH + Tetrahydrofurfuryl alcohol 	O 0.0000 0.0000 -0.0057106914 H 0.0000 0.0000 0.9657106914 C -0.0564289428 0.0272043052 0.0252307586 H -0.192675142 0.0649189491 1.1107763046 H 1.0109997989 0.0036635767 -0.1903642779 C -0.8259303424 -1.1433282038 -0.5737195824 C -2.2081345103 -0.5233847959 -0.7608395769 C -1.8633943207 0.8987153906 -1.1915680994 C -2.8625407584 1.9549526268 -0.7538146093 O -2.9519373538 2.0176595743 0.6516450064 O -0.6133780559 1.2009300009 -0.5621582771 H -0.3996870358 -1.4207747323 -1.5386158554 H -0.8228400675 -2.0199768011 0.0703441174 H -2.8223816779 -1.0380703766 -1.496535529 H -2.745538138 -0.4908919395 0.1879961633 H -1.731501943 0.9529695445 -2.2778426197 H -2.5692133962 2.9237312792 -1.1702595823 H -3.8544665165 1.7067927215 -1.133130579 H -2.0525147347 2.1517731618 0.9689553957	3776.00 58.66 222.25 286.83 322.3 567.07 650.0 676.6 845.49 881.67 901.7 925.51 951.41 1005.39 1009.95 1060.53 1111.57 1159.29 1160.29 1209.27 1213.89 1243.72 1274.48 1309.75 1339.76 1359.59 1369.64 1400.97 1416.98 1431.87 1490.16 1503.46 1511.31 1539.65 3028.33 3035.5 3045.39 3080.02 3086.42 3111.76 3114.48 3141.46 3149.0 3848.78 ! Torsions 144.94 448.18 !
N-pentanol ROO2 = QOOH-0	O -0.0300528101 0.0179732736 0.0196678131 O -0.0080238851 0.0120186465 1.3948522282 C 1.3105872798 -0.0010822117 1.8161339122 C 1.3592659703 -0.21891761 3.3089866684 C 0.968877213 -1.6395796858 3.7073103684 C 1.0200001518 -1.8374863836 5.2161561577 C 1.8990007186 1.446798684 1.4027798995 O 1.639856837 1.6694308078 0.1086264874 H 2.0230802479 -1.6485431191 5.6011405136 H 0.7414257035 -2.853450852 5.4914479098 H 0.3359610501 -1.154038132 5.720503938 H 1.6400305964 -2.3476349288 3.2159477843 H -0.0344864522 -1.8486952499 3.3339883485 H 0.6922857311 0.501900695 3.7876197458 H 2.3720957187 0.0014128931 3.6543077055 H 1.8779020534 -0.7357231884 1.2409804653 H 1.4336845996 2.1675557456 2.0861163552 H 2.9729179724 1.3377204285 1.6085715919 H 0.6457263452 0.8516511955 -0.1831678824	1186.70*i* 118.38 188.92 295.2 313.89 348.6 466.71 513.1 588.52 685.15 739.08 751.46 858.21 898.12 918.72 971.8 1006.91 1068.34 1100.9 1121.07 1165.66 1185.16 1226.15 1243.39 1253.94 1289.19 1306.51 1329.26 1337.16 1386.1 1414.7 1417.73 1478.11 1498.23 1504.46 1513.0 1516.04 1844.49 2979.09 3046.13 3057.92 3060.77 3068.12 3086.63 3096.93 3114.24 3132.11 3141.48 !78.52 85.92 246.48 !Torsions
N-pentanol ROO2 = QOOH-1	O 0.0097096129 -0.0102553878 -0.0038213484 C -0.0007070226 0.0007679089 1.4204965433 C 1.3833501906 0.0071814328 2.0410717112 C 2.2291002313 1.1806976214 1.5635951761 C 3.6093630442 1.1884158521 2.2066318384	2056.98*i* 126.95 170.15 266.84 311.48 354.09 377.25 593.57 647.11 735.19 780.35 878.81 908.55 933.69 952.85

	O	0.4631965622	-1.292492079	-0.3192005205	1005.33	1030.98	1071.18
	C	-0.7646300983	-1.2947414749	1.720292136	1105.56	1131.03	1165.21
	O	-2.1063822278	-1.2555174546	1.4817017457	1184.14	1228.92	1243.01
	H	3.5353404983	1.2624047107	3.2926489146	1273.34	1323.22	1332.91
	H	4.2077131806	2.0272606147	1.8538845312	1343.97	1383.97	1413.81
	H	4.1495393761	0.270180202	1.9726835417	1416.54	1445.73	1478.7
	H	1.7089013287	2.1158655777	1.7871662058	1498.1	1505.18	1513.07
	H	2.3195319873	1.1264638161	0.4780976359	1761.28	3053.04	3058.14
	H	1.8856941567	-0.9324107036	1.8014941068	3061.23	3074.0	3097.25
	H	1.268028888	0.0447851625	3.1280051429	3111.56	3130.73	3138.12
	H	-0.5704491729	0.8904428828	1.702832153	3166.46	3803.61	
	H	-0.1454065011	-1.8313045032	0.702234314	! 63.45	82.12	241.64
	H	-0.5573760335	-1.8103719642	2.6531232772	523.53	!Torsions	
	H	-2.2533649448	-0.7529521974	0.6694129022			
N-pentanol ROO2 = QOOH-4	C	0.0022110592	-0.0028992745	0.0016432789	1821.49*i*	96.83	154.29
	C	-0.0025362459	0.0029780678	1.5065240836	203.91	311.59	393.04
	C	1.3394977424	0.00312671	2.1907096722	398.33	488.97	494.52
	C	1.9032385083	1.4287655358	2.3303569211	626.08	678.1	789.82
	O	0.9136498094	2.2316976279	2.952838763	870.23	891.53	929.82
	O	-0.1475907237	2.3860640952	2.0797120288	932.94	1013.63	1052.48
	C	3.1184340779	1.5052528271	3.2371213726	1098.68	1118.68	1134.04
	O	2.8512636541	1.0172726612	4.5324837828	1142.31	1153.78	1206.45
	H	0.6507133088	0.7831749888	-0.3884275497	1251.17	1253.39	1290.18
	H	-0.9955532161	0.1481125437	-0.4069472567	1352.74	1368.18	1368.99
	H	0.3775312634	-0.9584373847	-0.3772076637	1402.48	1412.61	1431.21
	H	-0.3935958091	1.2329044893	1.8260619244	1473.51	1490.02	1494.61
	H	-0.7537129263	-0.6348842271	1.9649527535	1505.06	1574.28	3036.3
	H	1.2777534526	-0.4212847664	3.1908665865	3040.57	3048.67	3063.15
	H	2.0629139314	-0.5850193264	1.6153236835	3104.44	3121.77	3130.65
	H	2.1353097354	1.8544348994	1.3495247508	3139.25	3149.02	3863.74
	H	3.9140816144	0.8871468865	2.8218817743	! 108.86	194.79	304.53 !
	H	3.4690467481	2.5409020143	3.268846955			
	H	2.1228459686	1.5307716043	4.8949471171			
N-pentanol ROO2 = QOOH-5	C	0.0005194676	-0.0140854838	-0.001284831	1900.84*i*	70.74	188.02
	C	0.0013888028	-0.0166519051	1.504237436	262.22	289.01	298.07
	C	1.4275278925	0.0016265151	2.0739240855	375.05	452.67	475.51
	C	2.0453831301	1.4050946894	2.0943997798	529.03	605.6	634.5
	O	1.4693605264	2.2484306038	1.0937510486	836.24	838.01	876.91
	O	1.7518321747	1.7393374517	-0.1597159688	892.52	996.46	1033.68
	C	1.760790443	2.144067407	3.3893515245	1055.44	1086.41	1119.6
	O	2.3164178269	3.4359095808	3.397308783	1124.26	1130.31	1150.29
	H	0.9003154023	0.9396474943	-0.2978377896	1170.81	1246.27	1250.57
	H	-0.9085828105	0.3142780682	-0.495434338	1271.05	1336.23	1352.03
	H	0.4561629815	-0.8860780573	-0.4651394361	1378.96	1388.09	1399.95
	H	-0.5646149816	0.8356041544	1.8812570679	1447.71	1456.71	1479.41
	H	-0.5148464415	-0.9147937813	1.8575449431	1494.99	1501.54	1507.41
	H	1.4295956173	-0.3847504056	3.0947312092	3019.35	3039.93	3070.93
	H	2.0514607489	-0.6697600676	1.4829764272	3080.92	3101.77	3108.67
	H	3.1235707653	1.3691468594	1.9246995135	3116.4	3120.81	3197.52
	H	0.6762978223	2.1716807193	3.5552526196	3864.7		
	H	2.2133828012	1.5941552361	4.2139184184	!141.25	393.95	! Torsions
	H	2.0421828511	3.8758609478	2.5868675086			
N-pentanol ROO2 = HO_2 + 1-Penten-1-ol	O	0.0471378659	0.0108086336	-0.008837734	1155.31*i*	92.12	160.14
	C	0.0343129125	0.0210812779	1.39238747	258.11	274.05	323.96
	C	1.2636934305	-0.0268638273	2.0282056557	396.93	521.36	542.84
	C	1.4713253167	0.5055199582	3.4062470457	573.32	696.36	783.94

	C 2.0500358125 1.9284588956 3.3809055944 C 1.1309911723 2.9494840471 2.7217365412 O 1.2552403627 -2.0571270422 2.5521545345 O 0.0760900121 -2.3709204981 2.2530873492 H 0.9804078468 2.7293099635 1.6650214446 H 1.545691252 3.9535989552 2.7991277496 H 0.1507732127 2.9544242126 3.2024339927 H 3.0134806326 1.9107985762 2.8665603124 H 2.25390145 2.226625678 4.4103003941 H 2.1507030185 -0.1515428692 3.9494265274 H 0.5186384764 0.5071579786 3.942797345 H 2.1417724999 -0.1840059079 1.4125117367 H -0.2692507123 -1.2171665819 1.8075094902 H -0.747214914 0.6291318727 1.8476782313 H -0.6803976402 -0.5252123448 -0.3309306495	863.65 896.92 958.39 993.42 1018.3 1065.57 1098.89 1143.07 1172.82 1217.69 1245.64 1279.57 1291.57 1314.14 1340.38 1370.59 1378.26 1406.15 1421.21 1491.1 1496.26 1506.1 1510.12 1609.64 1658.94 3057.16 3059.15 3064.16 3099.85 3110.88 3113.93 3129.31 3140.99 3193.43 3890.91 ! 58.65 123.16 206.96 242.37 !Torsions
N-pentanol ROO3 = HO_2 + 2-Penten-1-ol	C 0.0033335461 -0.0065120178 0.0027735939 C 0.0007687337 -0.0005236896 1.5289815609 C 1.4045464121 0.0026241782 2.1054848143 C 2.1038943983 1.1913356013 2.2417845759 O 1.3292973124 0.3465529574 4.6267815428 O 1.9285204369 1.4131649622 4.3308672814 C 3.5992249222 1.2696733597 2.2852627991 O 4.1956991796 0.1030656124 2.7989167684 H 0.4989888227 0.8849589104 -0.3839031259 H -1.0097559411 -0.0342347064 -0.3976557916 H 0.541471054 -0.8753511654 -0.3778037385 H -0.5362983908 0.8770388388 1.8965306189 H -0.5456398981 -0.8710189159 1.8950528119 H 1.2338683482 -0.109543793 3.4174999232 H 2.0130051279 -0.8785581607 1.9133205222 H 1.5910727442 2.1333897149 2.0730554073 H 3.9695791808 1.3840759641 1.262687988 H 3.9041067309 2.158147244 2.8451862651 H 3.9561213362 0.0337501259 3.7282912241	1074.87*i* 113.79 140.23 197.16 250.68 310.91 397.24 460.41 558.2 673.02 706.33 782.09 871.18 902.4 946.74 976.46 1043.05 1056.19 1101.83 1129.49 1163.59 1208.46 1253.1 1278.59 1292.84 1334.32 1370.0 1393.16 1397.2 1411.33 1422.78 1491.78 1496.59 1501.68 1508.64 1597.49 1632.67 3045.27 3056.91 3061.4 3083.1 3094.53 3129.57 3134.55 3140.26 3169.33 3861.26 !69.44 89.11 263.54 365.85 !Torsions
QOOH-0 = OH + CH_2O + butanal	O -0.0443797021 -0.3926062991 -0.1142452292 C -0.2469597048 -0.1983767976 1.074026377 O 2.6559666625 0.0482556937 -0.172224231 O 2.5626495329 -0.2246943962 1.2128091259 C 1.768738449 0.6882618443 1.8121665973 C 1.7844174903 0.5918270572 3.2950395372 C 3.0652136209 1.1634803726 3.9206659842 C 3.0549780321 1.038311601 5.4379010434 H 2.2076892416 1.5743784948 5.8678550596 H 3.9656231349 1.4456588568 5.8745993752 H 2.9760047171 -0.0065464981 5.7405496217 H 3.16708973 2.2109858275 3.6304695116 H 3.9226433337 0.6356755061 3.5015106219 H 1.6803479792 -0.4572212588 3.5848888031 H 0.9152271781 1.125422949 3.6875472063 H 1.6983569363 1.639866669 1.2973937701 H -0.0692336521 -0.9846885469 1.823199785 H -0.808520522 0.682226695 1.4233875653 H 1.801361895 -0.3056213973 -0.4876939253	103.62*i* 97.76 200.19 297.05 316.49 330.17 395.45 561.31 585.75 743.98 808.94 858.66 907.24 998.44 1054.76 1069.1 1109.41 1125.65 1168.35 1237.24 1254.94 1274.43 1304.31 1332.95 1376.07 1412.35 1416.04 1472.65 1495.47 1497.5 1504.33 1509.45 1511.49 1706.66 2959.02 3033.69 3050.87 3059.42 3070.6 3090.97 3110.78 3132.43 3139.16 3177.41 3622.98 ! Torsions 63.88 68.92 82.55 227.0 245.28 533.27!
QOOH-0 = QOOH-4	C -0.0020345799 -0.000506947 0.0002193437 C -0.0002254167 -0.0008535282 1.5100886662	1484.46*i* 88.89 127.94 182.82 266.32 348.92

	C 1.3615869993 0.0004476247 2.1727195989 C 1.9122246021 1.4223945812 2.2251108915 C 0.8848743855 2.3256844925 2.9115420494 O -0.3018258768 2.3444442048 2.188493212 O 3.1189280661 1.3545071706 2.9577881314 O 3.7212771448 2.6430952759 2.9161803643 H 0.6158158603 0.8064191736 -0.3935399528 H -1.0084303104 0.1237822553 -0.3958821374 H 0.3955279335 -0.9446631421 -0.3819549382 H -0.4531704475 1.1074950541 1.848494137 H -0.6931642205 -0.7202998674 1.9415176115 H 1.3004170103 -0.3700050044 3.1969949236 H 2.0614906869 -0.6391500535 1.6277895594 H 2.1120631883 1.8045927054 1.219199555 H 0.750498711 1.9844234936 3.9461520695 H 1.276037767 3.3480253274 2.9308126206 H 4.499917514 2.4699782245 2.3742022889	411.93 471.83 488.14 544.3 656.52 839.33 871.01 900.12 926.85 1008.06 1025.2 1051.65 1105.19 1114.18 1138.15 1163.48 1177.73 1194.9 1229.66 1279.85 1305.38 1324.63 1357.83 1378.51 1390.59 1412.27 1413.42 1480.87 1489.39 1496.44 1498.03 1562.59 3006.71 3047.71 3052.31 3054.25 3069.94 3109.31 3115.45 3126.92 3147.88 3837.09 ! Torsions 151.44 193.9 208.6 !
QOOH-1 = OH + 3-propyloxiran-2-ol	C 0.0001567803 0.0073470956 -0.0005065549 C 0.0001725882 -0.0106348476 1.5225878171 C 1.4106964654 -0.0050276438 2.0970137448 C 1.4243301045 -0.021373086 3.6095777247 C 1.149598752 -1.3099517728 4.2512436027 H 1.433467402 -2.2453497569 3.7947930025 O 0.6507186016 -1.4262424035 5.4757236225 O 2.6848910236 -0.098364501 4.1909943879 O 3.4850562718 1.3876789591 3.8236324853 H 0.5111204561 0.8947964672 -0.3753982186 H -1.0126023353 0.0072857781 -0.4012683944 H 0.5190690167 -0.865766362 -0.3980803533 H -0.5463139808 0.8575574887 1.8997521757 H -0.5375856348 -0.893212053 1.8806853859 H 1.9740440746 -0.8715010769 1.73827258 H 1.9566895248 0.8841648634 1.7798157808 H 0.8250248985 0.8004842849 4.0260644805 H 0.465172604 -0.5524525546 5.8400809311 H 4.3182023967 0.9621550676 3.5891307995	859.66*i* 111.24 120.04 205.36 250.53 278.48 350.6 404.48 512.54 549.68 724.4 750.87 865.31 922.72 967.42 985.52 1043.68 1084.61 1124.88 1150.57 1172.91 1237.86 1251.28 1281.12 1301.06 1326.94 1352.84 1387.62 1415.56 1415.74 1492.3 1499.85 1504.25 1513.82 1538.68 3000.82 3044.53 3057.49 3061.75 3078.36 3119.8 3130.4 3138.01 3250.98 3834.59 3858.45 ! Torsions 74.17 81.28 163.17 249.63 442.07!
QOOH-1 = HO_2 + 1-Penten-1-ol	C -0.0122406607 -0.0133914825 0.0042082766 C 0.0003956143 0.0043585191 1.5274505416 C 1.4132068428 0.0097453805 2.1179724401 C 2.181807216 -1.2367387549 1.8093449092 C 3.1710065666 -1.2575422589 0.8703251019 H 3.5605267391 -0.3602494623 0.4087250731 O 3.8532627362 -2.3638459577 0.5283341702 O 3.2456405495 -1.3978465328 3.4590639292 O 3.9511287182 -2.5828620587 3.344827416 H 0.5386825515 0.8400726467 -0.3957109945 H -1.0290899172 0.0327118489 -0.3836892114 H 0.4552940873 -0.9180533185 -0.3851477873 H -0.5283289714 0.8878498487 1.888433637 H -0.5440042171 -0.8608786303 1.9134281583 H 1.9651954396 0.8767318346 1.7463951444 H 1.3563536544 0.1076274249 3.2036264924 H 1.7076334369 -2.1794764527 2.0629224037 H 3.6062977895 -3.0750393561 1.1346505786 H 4.8469187846 -2.2891822423 3.1352026978	481.93*i* 165.73 253.02 261.58 318.9 358.39 456.0 544.6 580.86 783.53 832.64 866.62 901.81 968.07 1004.02 1032.56 1077.6 1100.62 1158.07 1178.76 1237.43 1288.51 1299.53 1323.03 1362.59 1377.03 1395.88 1414.29 1423.21 1486.32 1493.8 1503.09 1508.91 1626.83 3055.9 3057.64 3060.96 3095.86 3104.08 3126.36 3137.8 3163.54 3218.65 3799.2 3801.48 ! Torsions 39.43 89.83 111.42 170.25 279.57 422.65!

QOOH-4 = OH + (4-methyl-2-oxetanyl)methanol	C 0.0070084561 -0.0005111943 0.0010446917 C -0.0001476523 0.0011600122 1.4829083891 H 0.9490547731 0.0019168864 2.0002837288 C -1.2242928975 0.4188711671 2.2445549557 C -1.6979670507 -0.9513426241 2.7313624067 C -3.1206688128 -1.3015474324 2.3221341075 O -3.2206235898 -1.4127840178 0.9210127202 O -0.7414272817 -1.7621662287 2.0137086641 O -1.3347585763 -3.2815523834 2.2830366733 H 0.7591032343 -0.6838367532 -0.3921363233 H 0.2329253683 0.999018423 -0.3890027763 H -0.9737649988 -0.2914474293 -0.3761109583 H -1.0124600128 1.1066639002 3.0615231248 H -1.961335987 0.8667490504 1.5774830058 H -1.5638317928 -1.1022827148 3.8044652395 H -3.4395090007 -2.2211146404 2.8138715597 H -3.7822472883 -0.4918979464 2.6357904355 H -2.6457187893 -2.1493635323 0.6809706775 H -0.4909191045 -3.7319695337 2.1697576929	1025.53*i* 50.36 133.27 220.92 298.27 306.02 362.44 399.2 434.57 581.73 673.12 736.75 837.73 913.0 919.03 951.76 1005.24 1040.66 1059.6 1109.35 1148.65 1157.5 1165.52 1222.23 1242.49 1287.39 1327.82 1375.18 1386.23 1405.15 1422.76 1429.59 1480.73 1485.53 1493.69 1509.74 3021.16 3067.32 3077.4 3081.52 3098.03 3116.02 3134.66 3140.84 3201.98 3830.28 3874.37 ! Torsions 103.03 175.37 232.79 489.0!
QOOH-5 = QOOH-0	C -0.0250682387 -0.0124211015 -0.0000273162 H -0.0409016835 -0.0054985072 1.085497627 H 0.977412806 0.0265168594 -0.4205436561 C -1.0489811918 0.831937371 -0.7121652156 C -1.295817943 0.3369798433 -2.1437092094 C -2.2916562573 -0.8215234623 -2.2040584656 C -2.1676954503 -1.6632907717 -3.4657381562 O -0.8581715047 -2.11715957 -3.7199586289 O -2.2329297547 -1.6400484445 -1.0271495181 O -0.9524995778 -2.1476802871 -0.8685478999 H -1.9851083399 0.8398118517 -0.1523795862 H -0.6915784156 1.8659768039 -0.7422394705 H -1.6914551005 1.1416511085 -2.7640113642 H -0.3518951258 0.0256846623 -2.5928257165 H -3.3130458351 -0.4366067187 -2.1451631509 H -2.870919669 -2.4989005131 -3.3882481582 H -2.4599389917 -1.0540211941 -4.323159953 H -0.538042099 -2.5348890403 -2.913200093 H -0.3920876071 -1.2583333538 -0.3240738401	1906.39*i* 79.69 227.26 233.44 292.93 327.01 391.88 401.77 471.41 565.66 619.02 717.02 771.03 850.0 890.36 933.7 966.0 999.01 1041.38 1054.64 1098.74 1122.31 1145.29 1167.81 1176.48 1245.98 1256.47 1266.05 1318.95 1356.45 1379.82 1389.15 1411.12 1443.67 1456.26 1478.71 1489.9 1500.07 1503.4 3038.59 3040.36 3076.82 3080.4 3098.73 3101.24 3109.29 3125.2 3197.7 3840.55 ! 145.46 458.79 Torsions !
QOOH-5 = OH + Tetrahydrofurfuryl alcohol	C -0.0538662377 0.115948198 0.0297842229 H -0.0999017012 0.0994042181 1.1089262602 H 0.9293033347 0.0734119897 -0.412191341 C -1.2545766281 -0.3029433459 -0.7357691443 C -2.3383530549 0.728858961 -0.4413449669 C -1.7773793365 2.114477367 -0.7314525958 C -2.6411652629 3.1985097468 -0.0850204552 O -2.4834776418 3.2065119936 1.3125308266 O -0.4492083849 2.1391513868 -0.1893301452 O -0.0799537377 3.7428419432 -0.246575029 H -1.0363942608 -0.3278675957 -1.8041389697 H -1.5904063282 -1.3030284693 -0.4440974927 H -3.2391163534 0.5656036937 -1.0346757133 H -2.6128300198 0.6904020155 0.614940729 H -1.7147252736 2.2888650017 -1.8108600802 H -2.4024141617 4.170363066 -0.5164963229 H -3.6889848859 2.9761500143 -0.2936490028	988.09*i* 57.07 153.36 252.73 276.59 311.59 348.84 406.67 489.78 525.07 564.92 694.77 798.3 823.8 887.95 896.69 936.26 979.44 1012.87 1064.81 1090.71 1121.02 1145.37 1171.05 1212.16 1239.76 1268.47 1324.76 1354.51 1358.96 1386.66 1414.55 1433.66 1473.93 1483.75 1500.69 1519.27 3038.75 3040.11 3068.77 3077.57 3099.69 3119.54 3122.75 3173.65 3276.32 3839.36 3871.06 ! Torsions 137.76 238.79

	H -1.5581899477 3.428641911 1.4677958838 H 0.8744332442 3.610826148 -0.2514234184	473.17!

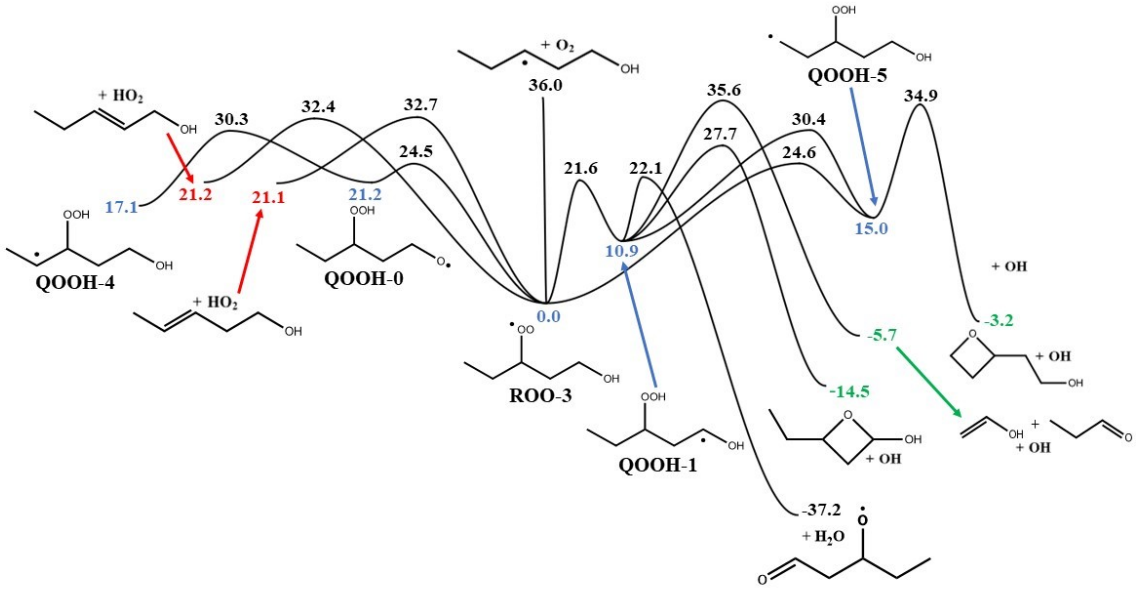


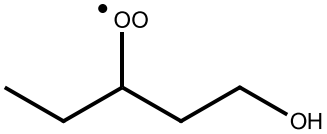
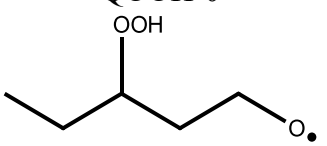
Figure S8. Potential energy surface for n-Pentanol ROO3 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

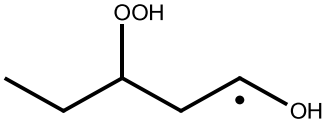
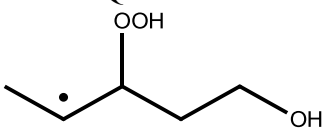
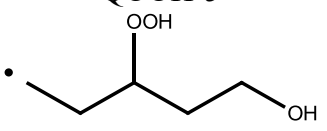
Table S13. Calculated relative energies for n-Pentanol ROO3 PES

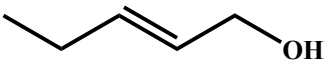
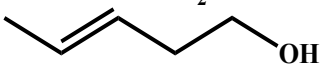
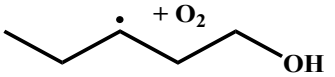
Species	Relative energy (kcal/mol)
N-pentanol ROO3	0.0
QOOH-0	21.2
QOOH-1	10.9
QOOH-4	17.1
QOOH-5	15.0
HO_2 + 2-Penten-1-ol	21.2
HO_2 + 3-Penten-1-ol	21.1
O_2 + $CH_3CH_2CHCH_2CH_2OH$	36.0
OH + 4-ethyloxetan-2-ol	-14.5
OH + Vinyl Alcohol + Propanal	-5.7
H_2O + 3-hydroxy-pentanal radical	-37.2
OH + 2-Oxetaneethanol	-3.2
N-pentanol ROO3 = QOOH-0	24.5

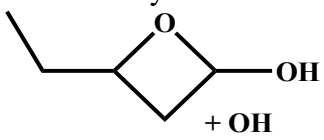
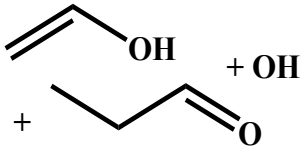
N-pentanol ROO3 = QOOH-1	21.6
N-pentanol ROO3 = QOOH-5	24.6
N-pentanol ROO3 = HO_2 + 2-Penten-1-ol	32.4
N-pentanol ROO3 = HO_2 + 3-Penten-1-ol	32.7
QOOH-0 = QOOH-4	30.3
QOOH-1 = OH + 4-ethyloxetan-2-ol	27.7
QOOH-1 = OH + Vinyl Alcohol + Propanal	35.6
QOOH-1 = QOOH-5	30.4
QOOH-1 = H_2O + 3-hydroxy-pentanal radical	22.1
QOOH-5 = OH + 2-Oxetaneethanol	34.9

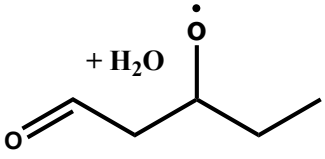
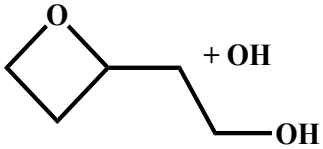
Table S14. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Pentanol ROO3 PES

Species	Geometry				Frequencies (cm^{-1})		
N-pentanol ROO3 	C	-0.0008115	-0.0006878	0.00179856	266.98	324.17	383.59
	C	0.00080367	0.00361901	1.51723721	456.44	501.04	519.59
	C	1.39167295	0.02245808	2.12776093	585.86	765.21	798.53
	C	1.39483503	0.15182536	3.64745537	913.44	927.25	952.90
	O	0.59923357	-0.8352066	4.26882821	1030.95	1061.13	1105.77
	H	0.64355172	-0.8185407	-0.3248117	1122.37	1144.09	1172.52
	H	1.87250198	-0.9171501	1.84767801	1221.46	1253.51	1303.40
	H	1.97121312	0.83754444	1.68680353	1313.81	1321.95	1372.55
	H	2.41214659	0.01740666	4.01384168	1387.48	1412.20	1413.09
	H	-0.3144394	-0.5364937	4.21569285	1420.41	1425.62	1466.04
	H	-0.5804286	-0.8290469	1.91533509	1482.91	1505.13	1511.52
	H	0.46570699	0.92476714	-0.3436748	1524.46	3058.72	3060.82
	C	-1.3960835	-0.1509304	-0.5896113	3066.03	3069.79	3097.93
	H	-1.3625609	-0.1414646	-1.6776289	3104.51	3113.44	3120.19
	H	-1.8503952	-1.0911091	-0.275097	3140.08	3149.10	3853.21
	H	-2.0447397	0.66131638	-0.2643588	! 83.98	114.22	122.11
	O	-0.7150142	1.21068974	1.91478696	168.07	211.76	238.69
	O	-1.2949757	1.09200825	3.06838012	!Torsions		
	H	1.07166004	1.15432898	3.93985891			
QOOH-0 	O	-0.0140267	0.0272476	-0.0120434	248.01	259.48	314.98
	C	-0.0062348	-0.0009675	1.35365691	367.74	490.78	523.82
	C	1.38849443	-0.0141578	1.96812687	601.40	679.45	786.74
	C	2.14586513	1.26734955	1.66460033	849.92	895.07	945.62
	C	3.63613011	1.19985733	1.96782445	992.35	1021.68	1055.69
	C	3.95067258	0.80665054	3.40661622	1089.18	1098.55	1109.03
	H	3.42433758	1.45352254	4.1094881	1158.86	1195.09	1253.86
	H	5.01780853	0.88616669	3.60776397	1292.34	1322.50	1358.77
	H	3.65149019	-0.2206431	3.61471378	1374.94	1383.64	1397.04
	H	4.07061975	2.17396919	1.73783822	1398.38	1418.81	1430.01
	H	4.0891354	0.49069198	1.27195545	1469.21	1493.42	1504.58
	H	1.99417329	1.53256136	0.61497168	1514.29	2945.49	3007.89
	H	1.94825214	-0.8630983	1.57159625	3064.00	3067.18	3073.28
	H	1.3098582	-0.1455889	3.04933296	3077.97	3104.05	3119.82
	H	-0.6326743	-0.8266728	1.71752726	3135.25	3140.52	3834.45

	H	-0.534372	0.92007043	1.65988511	!66.28 78.97 114.64
	O	1.48889627	2.25213753	2.46459451	152.29 213.44 220.79
	O	1.88876567	3.53415922	2.00181977	!Torsions
	H	2.43645463	3.84470943	2.73239753	
QOOH-1 	O	0.4797866	0.56887088	-0.0921436	250.24 291.28 350.32
	C	0.10152967	0.02837029	1.1091012	395.10 435.41 515.40
	C	1.19674953	-0.1377885	2.09190607	540.97 700.91 764.42
	C	2.03636471	-1.4111172	1.91051054	839.76 898.04 952.26
	C	2.66092891	-1.549782	0.53226159	988.65 1044.66 1060.24
	C	3.64099927	-2.7124161	0.44200994	1088.81 1111.04 1189.32
	H	4.45724202	-2.589319	1.1557182	1212.46 1224.94 1279.96
	H	4.07696408	-2.7807005	-0.5537667	1309.08 1313.19 1350.99
	H	3.14314754	-3.6561814	0.65899446	1375.05 1404.76 1413.20
	H	3.1574609	-0.6070947	0.29654004	1415.62 1455.16 1474.35
	H	1.85909771	-1.6646393	-0.1985618	1483.81 1503.49 1512.80
	H	2.81984886	-1.4319987	2.67793844	3020.07 3063.21 3067.30
	H	0.77712719	-0.1616211	3.09789138	3077.95 3113.84 3122.56
	H	1.86580643	0.72423552	2.0298553	3134.05 3147.09 3184.68
	H	-0.2683817	0.57285845	-0.6932314	3834.47 3898.52
	H	-0.7475638	-0.6432935	1.10450696	! 50.64 98.2584 113.6531
	O	1.22998404	-2.5755052	2.06903841	132.9152 189.3343
	O	0.76508123	-2.6149421	3.4121852	212.3903 232.5440 !Torsions
	H	1.2931449	-3.3361367	3.77396182	
QOOH-4 	C	-0.0039635	0.00461944	-0.0027947	95.37 150.85 253.65
	C	0.0102238	0.00254397	1.48043157	334.27 386.29 488.27
	C	1.13856753	-0.0179562	-2.2418599	545.40 599.29 658.07
	C	2.48245385	-0.0666749	-2.9567762	799.53 906.31 943.00
	O	3.23011158	1.14056719	-2.7969077	975.93 995.61 1015.68
	H	2.34386641	-0.270485	-4.0203846	1051.92 1075.50 1114.19
	H	3.10615222	-0.8574931	-2.5415688	1135.22 1161.15 1205.59
	H	0.69976326	0.9739516	-2.3760224	1264.90 1289.25 1352.51
	H	0.44931778	-0.7334157	-2.6950687	1371.19 1391.27 1402.14
	H	1.45929677	-1.4113848	-0.6372335	1420.21 1428.83 1474.12
	C	1.23268444	-0.3409975	-0.7505806	1474.67 1484.40 1489.86
	O	2.39563823	0.22523966	-0.143944	1509.55 2992.18 3023.87
	O	2.29399157	1.64191539	-0.210753	3060.01 3066.94 3078.80
	H	2.79924815	1.80303491	-1.0254763	3107.74 3126.01 3137.73
	H	2.89308183	1.78869578	-3.4199789	3206.85 3696.30 3887.21
	H	0.53314382	0.88653379	1.86265144	! 50.86 129.09 194.07 212.59
	H	-0.8531943	0.3981206	-0.5432567	277.13 321.00 !Torsions
	H	-0.9958883	-0.0006997	1.89592252	
	H	0.55388089	-0.8630476	1.86674643	
QOOH-5 	O	0.00359539	-0.0169837	-0.0044402	320.75 340.94 362.33
	C	0.00751494	0.00223526	1.40500645	465.85 482.65 498.84
	C	1.41115326	-0.0030191	1.99928379	532.69 596.07 805.39
	C	2.07819503	-1.3677983	1.95060032	853.85 926.88 938.37
	C	3.48319907	-1.364002	2.54448713	965.50 1013.29 1070.22
	C	4.22853411	-2.6229153	2.28740856	1074.14 1114.38 1136.60
	O	2.07125122	-1.9160869	0.62837706	1163.97 1204.17 1241.89
	O	2.95391913	-1.1506631	-0.1837103	1269.21 1303.95 1369.19
	H	3.7466101	-1.7055444	-0.1732688	1394.81 1396.82 1407.16
	H	5.28907262	-2.6790292	2.47896357	1411.34 1440.61 1461.20
	H	3.69754453	-3.5416344	2.08626873	1467.59 1472.08 1519.68
	H	3.38303349	-1.1801407	3.62255669	3003.61 3006.16 3056.11
	H	4.03735433	-0.5060100	2.15447793	3063.83 3073.75 3109.07

	H	1.4591668	-2.0988185	2.48103212	3114.90 3172.56 3277.33
	H	1.36873748	0.31105734	3.04537694	3782.03 3861.85
	H	2.0248874	0.72142127	1.46022784	! 50.2920 115.3722
	H	-0.5673068	-0.8399642	1.81296411	133.6292 171.4489
	H	-0.5091441	0.91658415	1.69488106	179.1650 211.1462
	H	0.52817396	-0.7710673	-0.290611	287.2927 !Torsions
HO_2 + 2-Penten-1-ol + **HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	O	-0.000519	-0.0065331	0.00055603	186.84 211.96 263.32
	C	-0.000325	0.0021708	1.41000729	511.73 666.54 717.51
	C	1.36752406	0.0054969	2.02862908	834.34 897.61 952.18
	C	2.49830442	-0.1306882	1.35124778	1009.01 1028.98 1050.91
	C	3.88213291	-0.1264388	1.93148228	1112.86 1117.79 1158.51
	C	3.95085596	0.05489942	3.43977648	1218.88 1294.18 1299.47
	H	3.50308669	1.00214471	3.74206539	1339.65 1379.45 1383.16
	H	4.98437523	0.04757593	3.78232763	1416.67 1422.59 1481.87
	H	3.42017156	-0.7459438	3.95551955	1503.34 1506.78 1512.30
	H	4.46145392	0.66011685	1.43908344	1767.83 3015.22 3044.94
	H	4.37403529	-1.0620802	1.65020816	3063.49 3067.58 3083.51
	H	2.43683489	-0.2763714	0.27700455	3130.49 3140.36 3166.05
	H	1.38431859	0.13218972	3.10648502	3174.59 3869.89
	H	-0.540868	-0.895914	1.71667489	! 82.75 231.01 301.73
	H	-0.5712518	0.8550729	1.79663322	359.59 !Torsions
	H	0.46723818	0.77699436	-0.3009978	
HO_2 + 3-Penten-1-ol + **HO_2** 	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	0.30741342	0.53663611	0.31779885	212.22 305.22 404.48
	C	0.11748188	-0.2747225	1.56168933	487.97 585.71 736.62
	C	1.06960779	-0.8340096	2.29993048	813.19 914.17 1006.86
	C	2.54829385	-0.7549825	2.05604885	1025.31 1038.79 1052.87
	C	3.17925167	0.36835798	2.86244458	1072.29 1112.21 1160.14
	O	4.57819267	0.32537583	2.64856422	1233.77 1238.47 1291.00
	H	-0.1404099	1.52489465	0.43670741	1319.37 1325.18 1402.26
	H	-0.1914926	0.06548623	-0.5312159	1441.33 1454.06 1487.48
	H	1.35635719	0.67217956	0.06445755	1490.90 1512.54 1534.21
	H	-0.9115007	-0.4093642	1.87881797	1759.41 3015.82 3049.79
	H	0.76532983	-1.3789717	3.18759787	3059.11 3080.81 3108.21
	H	3.02779919	-1.690201	2.34904747	3126.12 3151.02 3160.00
	H	2.77763966	-0.5958202	1.00303124	3180.40 3900.10
	H	2.75657684	1.32554537	2.5376014	! 28.3354 111.1528
	H	2.9376226	0.24020201	3.92346677	137.1140 268.8076 !Torsions
	H	4.99400023	1.02664967	3.15358488	
O_2 + $CH_3CH_2CHCH_2CH_2OH$ + **O_2** 	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
	C	0.0105688	0.00707752	-0.0032427	238.12 303.93 407.60
	C	0.01645146	-0.0160225	1.48786038	432.01 539.75 772.27
	H	1.03661934	-0.0577798	1.87005522	821.14 880.02 928.67
	H	-0.4500800	0.89547021	1.88158779	1024.13 1040.12 1063.37
	C	-0.7522976	-1.2174856	2.04745852	1104.68 1127.69 1172.27
	H	-0.7453851	-1.1917241	3.13637166	1195.38 1243.50 1272.95

	H	-1.7971446	-1.1725427	1.71874708	1320.92 1346.91 1380.95
	O	-0.1609198	-2.4442397	1.67538546	1413.04 1416.06 1434.40
	H	-0.0679867	-2.4425472	0.71768904	1470.99 1477.28 1501.93
	C	-1.1802979	0.48461104	-0.7581735	1507.42 1521.75 2982.64
	H	-2.0917918	0.21802457	-0.2144502	3016.46 3024.76 3054.25
	H	-1.1757695	1.58375251	-0.7908957	3061.23 3107.50 3119.48
	C	-1.2437534	-0.057132	-2.1828845	3128.21 3139.76 3189.45
	H	-2.1070157	0.33281431	-2.7203273	3848.64
	H	-1.3086446	-1.145612	-2.1782739	! 40.21 65.77 153.14
	H	-0.3473115	0.21990777	-2.7387395	242.56 357.57 ! Torsions
	H	0.93310565	-0.1446784	-0.5484748	
OH + 4-ethyloxetan-2-ol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	O	0.34346164	-0.2561859	0.34660115	58.32 184.39 353.97
	C	-0.0790514	0.01090735	1.64663722	414.38 471.37 567.93
	H	0.77500421	0.12743212	2.31805924	751.62 798.63 846.59
	C	-1.1612041	1.08515517	1.65024272	931.74 960.66 992.52
	C	-2.1056542	-0.0755866	1.99844696	1004.91 1042.82 1059.41
	O	-0.9778608	-0.9713651	2.15142669	1117.93 1147.44 1172.91
	C	-2.9226474	0.02105638	3.26232865	1207.41 1242.39 1262.68
	C	-3.5594424	-1.3147545	3.62334215	1284.44 1314.89 1336.08
	H	0.87916496	-1.0547976	0.35768183	1382.31 1412.82 1418.43
	H	-1.0624719	1.81887219	2.44660243	1449.47 1478.28 1491.82
	H	-1.3036969	1.57181538	0.69078423	1502.57 1511.82 3051.64
	H	-2.7289109	-0.3997974	1.16052208	3057.02 3064.83 3066.73
	H	-2.268393	0.3587361	4.06971465	3095.10 3117.16 3134.36
	H	-3.687823	0.78890837	3.12070759	3145.84 3184.47 3868.84
	H	-2.7901735	-2.0780768	3.73462733	! 116.7807 237.2156
	H	-4.1169919	-1.2505213	4.55650614	291.4149 !Torsions
	H	-4.2466826	-1.640844	2.8415018	
OH + Vinyl Alcohol + Propanal 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.00108637	0.00000000	0.00545105	498.84 728.26 861.80
	C	-0.00237744	0.00000000	1.329579641	972.01 1017.42 1140.88
	H	0.922217046	0.00000000	-0.563562232	1334.37 1359.87 1452.26
	H	-0.931617023	0.00000000	-0.535007759	1739.13 3176.70 3216.02
	H	-0.916296910	0.00000000	1.908645540	3281.22 3861.17 ! 449.99
	O	1.082393644	0.00000000	2.142130840	!Torsions
	H	1.881163785	0.00000000	1.605445553	
	C	-0.0088334	0.00308834	0.00021537	266.82 673.44 677.86
	C	-0.0031765	0.0007975	1.48572907	873.63 908.86 1008.52
	C	1.4220078	-0.0026989	2.02869628	1121.87 1156.86 1283.93
	O	-1.2572665	-0.1552681	-0.5283629	1372.83 1414.21 1430.39
	O	-1.1755897	-0.1115346	-1.9431467	1457.55 1497.45 1504.73
	H	-0.5449389	0.8748294	1.86892114	1866.92 2945.02 3050.32
	H	-0.5497278	-0.8754972	1.84187402	3077.74 3081.28 3153.86
	H	1.42405644	0.00808997	3.117032	3156.87 ! 148.66 238.11
	H	1.96099697	-0.8880251	1.6929931	!Torsions
	H	1.96977516	0.87446604	1.6833002	
	H	-1.0570379	-1.0450961	-2.1614852	
	H	0.65665443	0.63494383	-0.5771534	

H_2O + 3-hydroxy-pentanal radical 	O	0.00000000	0.00000000	0.00000000	1627.56 3874.01 3976.38
	H	0.00000000	0.00000000	0.95889274	
	H	0.9268960684	0.00000000	-0.2456399095	
	C	-0.0070795451	-0.0058596137	0.0018583396	234.1 252.17 344.87
	C	0.004421028	0.0038721129	1.5330767205	427.58 459.61 690.96
	H	1.0317303898	-0.0161474754	-0.337816993	716.39 777.48 866.18
	H	-0.4687883252	-0.9379835638	-0.3265022671	911.91 978.78 1007.21
	C	0.5558053965	-1.2851413647	2.1411282838	1045.62 1066.41 1103.2
	H	-1.0463285361	0.1066076096	1.8708704255	1155.65 1194.38 1223.59
	C	-0.4013562567	-2.44050143	2.0586164848	1253.01 1307.89 1350.73
	H	1.4951955209	-1.5756605354	1.6606483305	1357.34 1413.72 1423.55
	H	0.7932358778	-1.1259100079	3.1970271152	1445.27 1484.05 1500.97
	H	-0.0155032507	-3.4080525301	2.4296815842	1510.34 1854.81 2910.47
	O	-1.5240278967	-2.3557629196	1.6407887908	2961.0 3056.14 3060.85
	O	0.6145304852	1.1145294398	2.0464595789	3067.78 3093.5 3111.98
	C	-0.7454084911	1.1912909571	-0.5748102452	3137.6 3150.15
	H	-0.319774325	2.1195951269	-0.1970529326	! 79.39 89.83 153.9 187.2 !
	H	-0.6864169098	1.2037482596	-1.6619074721	Torsions
	H	-1.7995951717	1.1629489196	-0.2961397423	
OH + 2-Oxetaneethanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.0536885	0.03510669	0.03780999	31.31 233.15 410.15
	C	-0.0498954	-0.0279208	1.57330041	501.00 522.11 760.07
	C	1.29694893	-0.0250411	2.26191506	789.47 861.35 889.91
	C	1.21221735	-0.5355606	3.69589186	941.96 982.37 997.06
	O	0.99919762	-1.9280406	3.75850064	1025.21 1076.70 1119.80
	C	-0.6109167	-1.3929804	0.11727113	1133.41 1162.52 1186.09
	H	0.05744707	-2.1770422	-0.2396784	1221.16 1232.15 1257.47
	H	-1.6045266	-1.5426175	-0.3039401	1265.38 1305.02 1343.51
	O	-0.6513672	-1.3473654	1.55421569	1375.48 1396.73 1416.65
	H	0.2911173	-2.1400398	3.13912561	1457.59 1469.97 1496.44
	H	0.4224639	0.00913643	4.2304461	1525.08 1541.20 3002.53
	H	2.14953223	-0.3407717	4.21655223	3051.20 3060.81 3073.20
	H	1.68485772	0.9971578	2.25047504	3102.58 3106.07 3114.95
	H	1.99549461	-0.6565004	1.70625687	3119.86 3172.96 3816.76
	H	-0.7261897	0.67645752	2.06413726	! 79.5697 187.8029 349.9802
	H	-0.7322995	0.76622328	-0.3908789	!Torsions
	H	0.92901393	0.13379559	-0.4162295	
N-pentanol ROO3 = QOOH-0	C	-0.0116315	-0.0489422	0.03655817	1846.94i 71.39 190.21
	C	0.01765543	-0.013301	1.55924282	266.03 296.37 318.57
	C	1.42609122	0.00911691	2.12798354	385.92 438.48 482.88
	C	1.45577047	0.00819477	3.66061089	514.38 619.86 768.01
	C	1.52292571	-1.4152297	4.24208774	835.76 861.44 908.54
	O	2.81486168	-1.9180732	4.203102	969.64 977.54 1013.40
	O	2.04895339	-1.1812752	1.62371829	1057.63 1070.59 1087.74
	O	3.35598846	-1.2180259	2.06408002	1134.57 1181.27 1189.24
	H	0.52267232	0.80687953	-0.378104	1205.08 1249.66 1306.36
	H	-1.0356095	-0.0170112	-0.3323258	1335.26 1343.87 1375.22
	H	0.46098386	-0.9529281	-0.3413992	1379.75 1412.56 1417.28
	H	-0.4948423	0.87803239	1.92544366	1469.12 1476.01 1482.81
	H	-0.5116661	-0.8763484	1.97190124	1501.57 1511.84 1644.72

	H	1.97860385	0.86510347	1.73129744	3003.04 3053.35 3060.63
	H	2.31840226	0.55352776	4.039483	3063.54 3069.63 3089.56
	H	0.55587241	0.5003723	4.0301266	3103.31 3137.19 3140.65
	H	1.26362052	-1.3640316	5.3073131	3156.88
	H	0.81073088	-2.0814293	3.74533951	! 110.4340 216.6845 !Torsions
	H	3.2855579	-1.7283796	3.01433195	
N-pentanol ROO3 = QOOH-1	C	0.00193634	0.03372559	0.03445692	1914.25i 71.00 144.02
	C	0.01093883	-0.0395859	1.55569123	246.19 303.69 336.42
	C	1.41326164	-0.0313322	2.1316962	431.97 448.52 486.44
	C	1.43062946	-0.0246296	3.66368213	525.43 605.98 770.90
	C	2.81946433	-0.2273600	4.20391228	828.32 925.91 962.80
	O	2.81333616	-0.9399588	5.38574808	1009.73 1023.34 1061.69
	O	2.04749423	-1.2289558	1.70571	1099.91 1120.69 1137.49
	O	3.39821646	-1.1245169	1.98729967	1173.87 1195.33 1224.24
	H	0.47455099	0.95372326	-0.3116867	1258.84 1294.77 1311.26
	H	-1.0157404	0.01259685	-0.3522175	1315.66 1346.75 1379.01
	H	0.54859622	-0.8052984	-0.39201	1411.09 1416.70 1431.21
	H	-0.5342447	0.80415932	1.98302955	1468.69 1482.67 1502.04
	H	-0.4900754	-0.9481538	1.89726873	1511.98 1599.78 3040.60
	H	1.98957781	0.81363984	1.73902132	3052.99 3064.59 3065.82
	H	1.00140258	0.91339367	4.0260701	3069.37 3104.00 3115.65
	H	0.80736165	-0.845719	4.02238637	3137.37 3153.97 3886.80
	H	3.35219788	-0.8774255	3.20070688	!106.9532 208.5363
	H	3.44532139	0.66877775	4.2283576	381.6076 !Torsions
	H	3.7024731	-0.9775666	5.74699592	
N-pentanol ROO3 = QOOH-5	C	-0.0007219	-0.0019987	-0.0004187	1808.74i 132.18 149.31
	C	-0.002922	-0.0075344	1.50032772	267.00 327.72 409.65
	C	1.43173857	0.01209121	2.06288855	473.59 475.23 498.87
	C	1.49205446	-0.1928886	3.56378609	540.90 652.87 826.87
	C	2.91426885	-0.219923	4.11346179	837.33 890.90 931.84
	O	3.57996782	-1.4355403	3.86030193	997.06 1018.59 1066.50
	O	2.13271632	-1.0634942	1.44908677	1087.11 1108.57 1128.88
	O	2.33620771	-0.7507042	0.116092	1132.13 1154.16 1174.89
	H	1.22718995	-0.5195761	-0.2271999	1226.71 1236.60 1272.33
	H	0.09055526	0.96865388	-0.4785344	1307.50 1351.52 1375.90
	H	-0.6882762	-0.6740651	-0.5013686	1396.02 1406.77 1442.59
	H	-0.5268338	0.86600406	1.8992283	1453.52 1465.05 1481.00
	H	-0.4949514	-0.9008408	1.88453708	1520.02 1578.12 3011.73
	H	1.93351778	0.94198646	1.77674803	3049.67 3051.88 3066.34
	H	0.93267903	0.6220487	4.02840615	3111.59 3112.72 3119.97
	H	0.99372428	-1.1287601	3.82631758	3126.11 3215.23 3853.26
	H	3.47798585	0.63217654	3.71272383	! 57.1545 196.1244 445.4986
	H	2.88677191	-0.1112662	5.19706794	!Torsions
	H	3.54717048	-1.6018671	2.91295985	
N-pentanol ROO3 = HO_2 + 2-Penten-1-ol	C	0.00434483	0.00452462	-0.0018131	1069.47i 138.96 236.77
	C	-0.0043862	-0.0115109	1.38514414	262.36 288.93 352.73
	C	1.21446775	-0.0092679	2.25094392	444.19 469.50 566.06
	C	2.46235295	-0.5953533	1.60484828	653.23 688.86 768.34
	O	-0.4314368	-2.0669232	1.64366236	857.91 907.21 958.68
	O	-0.4220622	-2.4619624	0.44599512	1015.06 1024.84 1069.80
	H	2.27407269	-1.6121905	1.25918531	1106.37 1122.33 1144.9256
	H	3.28133263	-0.6279886	2.32103328	1201.18 1269.52 1275.72
	H	2.79358369	-0.0019288	0.75342896	1306.96 1307.85 1378.55
	H	0.98169862	-0.545037	3.17221516	1386.45 1396.67 1420.53

	H	1.39698654	1.03030962	2.54527798	1421.07 1470.29 1505.00
	H	-0.9401928	0.22205717	1.87912661	1511.19 1530.08 1599.30
	H	-0.1380454	-1.3241608	-0.075326	1643.49 3039.79 3041.62
	C	-1.2240691	0.49732001	-0.7552246	3071.12 3094.95 3101.14
	O	-2.4275025	0.11841712	-0.1196277	3140.64 3147.50 3163.43
	H	0.95604175	0.14416829	-0.5058232	3192.75 3860.24
	H	-2.4759658	-0.8421056	-0.0958168	! 78.6100 88.0240
	H	-1.2422915	1.58675144	-0.7946387	128.5818 217.3702 !Torsions
	H	-1.1925053	0.13553673	-1.7873001	
N-pentanol ROO3 = HO_2 + 3-Penten-1-ol	C	0.01127585	-0.0260352	0.03150441	1071.03i 159.08 171.58
	C	-0.0235847	-0.0016891	1.54826717	238.24 258.71 282.30
	C	1.1334812	0.10584054	2.31376319	384.89 437.67 495.78
	C	2.51855781	0.21819177	1.76996752	566.30 588.45 701.92
	C	3.45374607	1.10852877	2.59286158	790.40 857.64 917.06
	O	3.33135454	0.88373403	3.98147202	964.17 1004.17 1043.23
	O	0.8841267	2.11611629	2.9481286	1070.05 1086.56 1117.69
	O	-0.2385099	2.37848285	2.44328441	1152.68 1201.61 1250.86
	H	0.57359641	0.81628686	-0.3706846	1283.67 1290.18 1333.16
	H	-0.9977079	0.03739747	-0.3714854	1397.20 1403.63 1405.26
	H	0.4646222	-0.9428044	-0.3487019	1423.16 1436.91 1463.86
	H	-0.4145767	1.21918199	1.87910464	1500.34 1505.54 1522.60
	H	-0.8302664	-0.5666045	2.00695437	1585.76 1625.22 3031.40
	H	1.08338864	-0.1932758	3.35315	3062.98 3074.91 3117.09
	H	2.91553379	-0.8040345	1.76884802	3123.58 3126.69 3139.79
	H	2.51279239	0.55616686	0.73377207	3152.03 3199.41 3876.32
	H	4.48630062	0.88621155	2.32591979	! 76.4005 124.0313
	H	3.26522336	2.15575238	2.3526202	132.9519 384.8940 !Torsions
	H	2.59569104	1.41303626	4.30173614	
QOOH-0 = QOOH-4	O	0.01144233	0.02382876	-0.0190251	1462.55i 74.44 211.34
	C	-0.0059826	0.01428251	1.37418066	230.04 263.39 341.10
	C	1.41000817	0.00229721	1.95369961	422.01 451.40 535.65
	C	2.15553333	-1.2173812	1.42164628	583.14 656.71 792.08
	O	1.52922606	-2.4321223	1.81301468	843.03 895.36 925.44
	O	1.66598157	-2.5500721	3.22287724	970.49 1014.36 1063.12
	C	2.14562673	-1.2037928	-0.0897315	1069.78 1093.95 1103.49
	C	2.31299146	-2.5188727	-0.8093802	1168.89 1176.23 1202.34
	H	-0.5111746	0.93289391	1.693089	1241.42 1296.04 1307.98
	H	-0.5727538	-0.840589	1.76238905	1350.12 1360.34 1372.69
	H	1.94160038	0.90086059	1.63557009	1387.27 1407.75 1412.28
	H	1.38393125	-0.009751	3.04265073	1476.46 1487.77 1495.25
	H	3.18438962	-1.2282009	1.80104936	1499.10 1577.18 3008.05
	H	0.74576626	-2.511284	3.50912077	3024.30 3047.25 3051.10
	H	1.02631759	-0.717244	-0.3227852	3085.42 3116.68 3127.59
	H	2.80607052	-0.4187425	-0.4561324	3136.36 3164.72 3834.44
	H	1.52566112	-3.2196705	-0.5427792	! 123.0578 170.5756
	H	2.30425991	-2.3708856	-1.8873278	204.5424 !Torsions
	H	3.26685781	-2.9790954	-0.5366431	
QOOH-1 = OH + 4-ethyloxetan-2-ol	O	0.02120162	-0.0080163	0.01383048	985.06i 64.05 101.26
	C	0.00808888	-0.0157496	1.36063209	158.39 205.92 268.11
	H	0.96388859	-0.0259089	1.86721341	368.17 398.65 430.60
	C	-1.2168887	0.52485033	2.01466021	462.50 534.72 673.21
	C	-1.6207255	-0.6939093	2.84621232	754.49 790.34 821.07
	O	-0.8038731	-1.6747299	2.18029237	944.79 974.60 998.48
	O	-1.3787143	-3.0621116	2.88253559	1007.84 1083.94 1098.11
	C	-1.2995499	-0.6022271	4.32916327	1139.40 1148.55 1182.74

	C	0.17869229	-0.3711751	4.61622528	1251.25 1275.28 1291.77
	H	0.84193315	-0.3872273	-0.3124234	1316.78 1345.73 1372.41
	H	-1.0467476	1.42840808	2.60433678	1386.32 1417.37 1463.49
	H	-1.951961	0.74080732	1.24204777	1484.19 1502.81 1511.56
	H	-2.6675561	-0.9673936	2.7144416	1513.91 3057.35 3060.06
	H	-1.3048334	-3.6002249	2.08724473	3063.78 3091.56 3116.27
	H	-1.9044395	0.20495554	4.75134452	3133.84 3141.27 3145.34
	H	-1.6226479	-1.530349	4.79876669	3196.30 3871.12 3881.53
	H	0.53315748	0.57257118	4.19579687	! 188.6313 248.6320
	H	0.36517349	-0.3386853	5.6885079	293.4371 !Torsions
	H	0.77069851	-1.1819085	4.19284954	
QOOH-1 = OH + Vinyl Alcohol + Propanal	O	0.00302825	-0.0075957	-0.0211216	1084.91i 45.61 67.28
	C	0.00591269	0.00487667	1.32598863	87.86 139.68 193.20
	H	0.96711319	0.00859062	1.82191775	263.67 299.94 349.21
	C	-1.1922961	-0.223498	1.99785648	411.38 462.91 473.71
	C	-1.579235	-2.0287116	1.9805789	622.70 717.11 789.81
	O	-0.9303456	-2.4601521	3.01772987	878.31 890.85 924.72
	O	-1.1699696	-4.2314155	3.02487746	984.63 1032.39 1046.73
	C	-3.090764	-2.1487403	2.03187754	1073.22 1114.13 1137.66
	C	-3.6854863	-1.6681824	3.34606239	1184.06 1284.18 1292.01
	H	0.89962127	0.02506929	-0.3634704	1304.94 1338.33 1358.42
	H	-1.1900881	0.01142658	3.05285048	1399.07 1445.51 1448.61
	H	-2.0811935	0.10560057	1.46819103	1478.15 1502.11 1508.84
	H	-1.1669503	-2.301381	1.00154295	1579.78 3018.37 3060.01
	H	-0.283696	-4.3711724	3.37942167	3065.93 3099.63 3132.14
	H	-3.5317131	-1.6375667	1.1739359	3140.19 3154.28 3203.91
	H	-3.2879156	-3.2171865	1.90923425	3241.78 3857.01 3896.37
	H	-3.5490622	-0.5936298	3.47961319	! 115.5927 205.7723
	H	-4.753942	-1.8735025	3.38788198	245.8156 !Torsions
	H	-3.201429	-2.1800894	4.17578049	
QOOH-1 = QOOH-5	O	0.0241252	0.00033466	0.00541997	1713.12i 126.69 160.58
	C	0.00795953	-0.0138374	1.40708372	243.65 297.06 341.98
	H	1.0278129	-0.0209325	1.7809061	395.94 514.99 551.48
	C	-0.9076879	1.00663369	2.03863485	570.10 602.06 713.03
	C	-2.3743865	0.63030251	1.82042485	811.81 851.97 874.45
	O	-2.6628119	0.4451395	0.43400619	943.34 967.17 1005.11
	O	-2.4014525	1.65820199	-0.2534973	1030.27 1050.32 1064.66
	C	-2.7070571	-0.7155005	2.46773518	1098.28 1141.60 1172.88
	C	-1.790072	-1.823297	2.00038587	1204.07 1256.89 1285.81
	H	-0.7911371	-0.4191417	-0.2958864	1340.73 1355.83 1371.38
	H	-0.7220307	1.04506301	3.11389839	1389.72 1413.52 1445.30
	H	-0.7108946	2.00546713	1.64123739	1455.83 1463.02 1471.13
	H	-3.0307711	1.41337641	2.20594937	1482.88 1524.73 3052.01
	H	-1.4653999	1.55519116	-0.4902599	3059.23 3080.06 3104.77
	H	-2.6255687	-0.5832221	3.54733803	3109.34 3122.51 3147.02
	H	-3.7533245	-0.9462835	2.25019164	3204.95 3725.12 3806.33 !
	H	-0.6041437	-1.1234125	1.77484697	133.1663 437.4065 456.7591
	H	-1.5556727	-2.5927801	2.72748244	!Torsions
	H	-2.0192936	-2.2304406	1.01964261	
QOOH-1 = H_2O + 3-hydroxy-pentanal radical	C	0.0115820101	0.0283450476	0.000903117	2528.23i 116.18 147.26
	C	0.0073767955	0.0052944358	1.5234152431	220.51 262.42 283.49
	H	1.0537098559	0.0243679851	-0.3239475479	318.09 369.91 403.94
	H	-0.4497170872	-0.8896281083	-0.3715573388	474.09 532.53 545.61
	C	0.6007815541	-1.3736388827	2.0660108157	681.7 790.25 816.08
	H	-1.0148764869	0.0582735368	1.9137020169	907.54 927.13 992.78

	C	0.8778187669	-1.36981484	3.4918537172	993.96 1025.32 1043.11
	H	-0.0876605635	-2.1738967892	1.8063485138	1086.82 1113.17 1139.08
	H	1.5245212953	-1.4916039555	1.4937101562	1202.26 1245.09 1271.13
	H	0.3070155358	-1.9512891404	4.2026616398	1283.54 1302.1 1340.24
	O	1.8070786959	-0.6165175164	4.0246580635	1380.37 1410.71 1434.24
	H	2.1891638785	-0.0230870379	3.3141228865	1464.14 1483.36 1502.72
	O	0.6543779034	1.0715271353	2.0822913618	1510.16 1579.56 2686.9
	O	2.3277919748	0.7551237208	1.9041164852	3036.4 3061.27 3062.82
	H	2.5503790477	1.6913154538	1.9255887856	3065.95 3105.3 3131.78
	C	-0.7102491513	1.2502909415	-0.5499516241	3146.28 3154.99 3221.19
	H	-0.2545226401	2.1619066241	-0.1660548446	3883.99
	H	-0.6696890666	1.2782760374	-1.6380318294	! 79.18 232.19 ! Torsions
	H	-1.7604687513	1.2503026823	-0.2534645648	
QOOH-5 = OH + 2-Oxetaneethanol	O	0.20463065	-0.0810622	-0.0323656	1053.36i 66.05 130.72
	C	0.06192631	0.00512799	1.36413216	187.93 230.65 245.23
	C	1.39839297	0.01916686	2.10059362	262.93 285.78 338.45
	C	2.16046931	1.33232647	2.08891902	407.22 438.64 505.10
	C	3.58587173	1.18812324	2.62105134	576.92 657.08 782.08
	C	4.2609934	1.01315019	1.29423663	826.29 863.73 920.46
	H	4.24432574	0.04696203	0.81297991	961.99 1000.58 1041.71
	H	5.00575387	1.71267954	0.95012023	1058.71 1067.56 1117.36
	O	2.53621799	1.77292493	0.75790914	1142.60 1158.94 1226.81
	O	1.14500409	2.49021308	0.21459996	1248.06 1262.52 1299.48
	H	0.53655754	0.77761914	-0.3258395	1317.02 1357.25 1414.21
	H	-0.5266844	0.88491972	1.6496052	1417.18 1451.99 1468.90
	H	-0.4971639	-0.8786716	1.6729631	1475.80 1498.90 1509.81
	H	1.22735604	-0.2275935	3.15334984	3025.86 3043.11 3077.23
	H	2.02663199	-0.7703677	1.67853241	3084.98 3099.73 3104.58
	H	1.57660481	2.12687971	2.55378914	3146.99 3180.51 3285.46
	H	3.9223203	2.09660172	3.1141128	3774.96 3867.36
	H	3.70869747	0.34182215	3.29834437	! 605.8016 !Torsions
	H	1.58111434	3.11544815	-0.3751096	

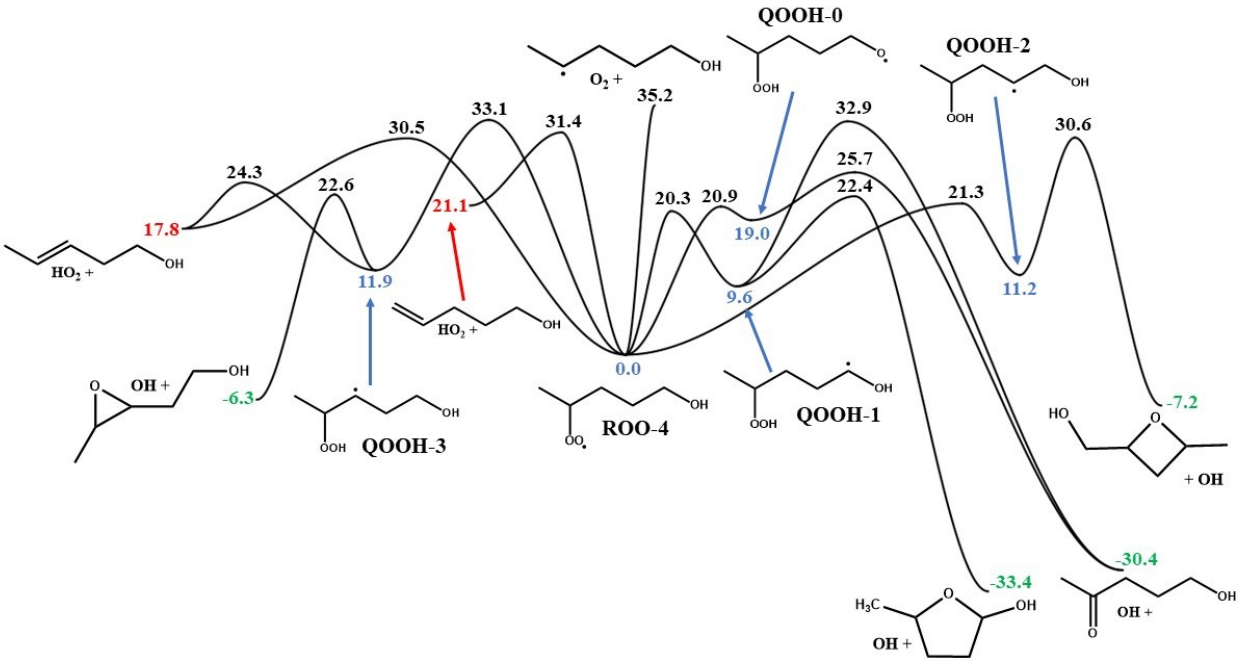


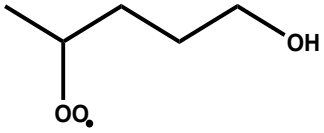
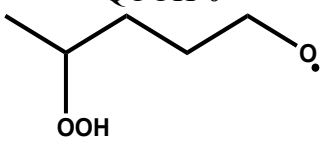
Figure S9. Potential energy surface for n-Pentanol ROO4 calculated at CCSD(T)/cc-pV∞Z//M06-2X/cc-pVTZ level of theory. Energies are given in kcal/mol. QOOH energies are given in blue, HO_2 producing routes in red, OH producing rates in green.

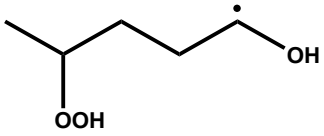
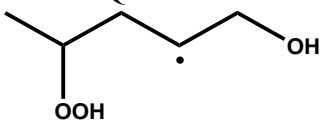
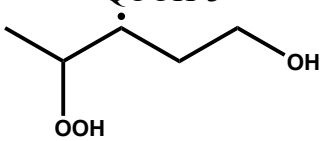
Table S15. Calculated relative energies for n-Pentanol ROO4 PES

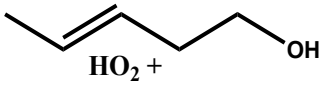
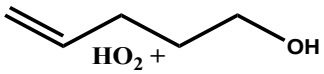
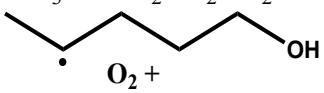
Species	Relative energy (kcal/mol)
N-pentanol ROO-4	0.0
QOOH-0	19.0
QOOH-1	9.6
QOOH-2	21.3
QOOH-3	33.1
HO_2 + 3-Penten-1-ol	17.8
HO_2 + 4-Penten-1-ol	21.1
O_2 + $CH_3CHCH_2CH_2CH_2OH$	35.2
OH + 5-Hydroxy-2-pentanone	-30.4
OH + 5-methylTHF-2ol	-33.4
OH + (4-methyloxetan-2-yl)methanol	-7.2
OH + 2-(3-methyloxiran-2-yl)ethanol	-6.3
N-pentanol ROO-4 = QOOH-0	20.9
N-pentanol ROO-4 = QOOH-1	20.3
N-pentanol ROO-4 = QOOH-2	21.3
N-pentanol ROO-4 = QOOH-3	33.1
N-pentanol ROO-4 = HO_2 + 3-Penten-1-ol	30.5
N-pentanol ROO-4 = HO_2 + 4-Penten-1-ol	31.4

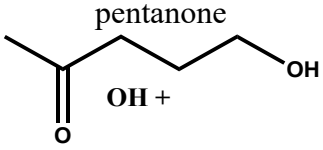
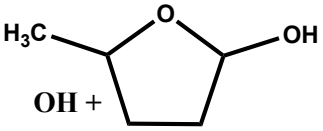
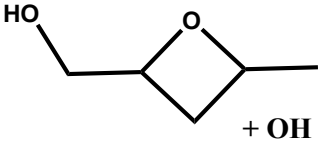
QOOH-0 = OH + 5-Hydroxy-2-pentanone	25.7
QOOH-1 = OH + 5-Hydroxy-2-pentanone	32.9
QOOH-1 = OH + 5-methyl-THF-2ol	22.4
QOOH-2 = OH + (4-methyloxetan-2-yl)methanol	30.6
QOOH-3 = HO_2 + 3-Penten-1-ol	24.3
QOOH-3 = OH + 2-(3-methyloxiran-2-yl)ethanol	22.6

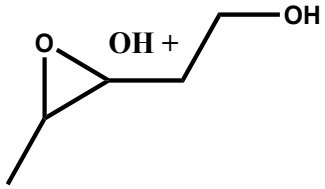
Table S16. Optimized geometries and frequencies (m062x/cc-pVTZ) of relevant stationary points on the calculated n-Pentanol ROO4 PES

Species	Geometry				Frequencies (cm^{-1})
N-pentanol ROO-4 	C	0.00049362	-0.026066	0.00457709	163.27 234.54 343.00
	C	0.00445625	0.01110842	1.51648964	378.37 430.86 515.70
	C	1.41360792	0.03227082	2.09758397	568.62 803.20 833.10
	C	1.52348936	0.20342873	3.61174046	886.78 915.85 930.28
	C	1.07554782	-0.9995585	4.42970393	1018.88 1047.12 1109.13
	O	-0.2755494	-1.3624142	4.22363831	1139.76 1164.02 1166.44
	H	2.56949613	0.39770952	3.85877068	1196.45 1276.38 1301.30
	H	0.9682776	1.08952029	3.92886912	1314.53 1338.84 1383.64
	H	1.26126581	-0.7983675	5.49011495	1387.06 1401.23 1407.08
	H	-0.8058625	-0.5579782	4.19069711	1418.97 1445.18 1472.34
	H	-1.0169741	-0.0266949	-0.3811419	1490.31 1491.87 1502.70
	H	1.89181861	-0.9055932	1.80095851	1526.18 3029.04 3050.65
	H	1.96158661	0.83714081	1.60129368	3061.66 3072.86 3082.06
	H	-0.5864131	-0.7935624	1.94531206	3092.69 3104.75 3140.40
	H	0.50401588	-0.9287659	-0.3381572	3157.31 3160.37 3825.52
	H	1.66931277	-1.8742818	4.15594567	! 97.92 120.44 137.59
	O	-0.6734535	1.25267427	1.87683433	212.18 484.62 308.56
	H	0.52891537	0.83783828	-0.398703	!Torsions
	O	-1.2914273	1.18531145	3.01431852	
QOOH-0 	C	0.06221615	0.08532497	0.03924041	164.3 204.93 330.4 375.23
	C	0.00704607	0.00400062	1.55277974	466.83 514.21 620.1 749.77
	O	1.37256442	-0.0343389	1.95858031	798.97 868.23 923.61 932.19
	O	1.42528193	-0.3156086	3.34698949	963.94 1024.43 1050.97
	C	-0.7642516	1.14813057	2.20616256	1056.89 1080.24 1141.54
	C	-0.3253828	2.56065409	1.82839067	1178.57 1201.82 1225.92
	C	1.12450213	2.90401345	2.18670797	1249.94 1304.19 1370.13
	O	1.49969278	2.54768253	3.45024705	1381.0 1386.96 1400.7 1409.64
	H	0.62381569	0.96230235	-0.2837073	1427.81 1462.95 1484.48
	H	-0.9458035	0.15212616	-0.3689483	1485.86 1495.41 1513.45
	H	0.55032349	-0.7973737	-0.3682488	2911.77 3027.72 3056.43
	H	-0.455513	-0.9384871	1.85860643	3068.07 3072.76 3079.9
	H	-1.8158791	1.02786892	1.93764398	3104.52 3123.6 3143.05
	H	-0.7106681	1.02496714	3.28777837	3158.23 3708.87
	H	-0.4537103	2.73888127	0.75883208	! 76.45 162.29 225.88 265.64
	H	-0.9739719	3.27501842	2.33825302	296.3 544.24 !Torsions
	H	1.80566923	2.29917938	1.55703634	
	H	1.35342722	3.95666504	1.98240548	
	H	1.48639998	0.57874246	3.72163779	

QOOH-1 	C	0.00210814	-0.0215518	0.0070221	189.54 293.03 304.81
	C	-0.0036911	0.00349908	1.52213092	401.16 474.54 489.06
	C	1.39529058	0.03189375	2.11542921	545.52 669.15 789.69
	C	1.41252988	0.04841853	3.64667451	867.79 907.40 948.69
	C	0.64400944	-1.0606545	4.26489732	975.75 1040.35 1063.91
	O	0.99509488	-2.3062239	3.81565471	1111.15 1129.62 1161.83
	H	2.45894549	0.01757401	3.97922573	1207.55 1216.46 1272.97
	H	0.99494534	0.99248186	3.99454342	1294.20 1336.69 1372.13
	H	1.89904825	-0.899751	1.76863679	1382.76 1402.82 1404.61
	H	1.94673749	0.85795094	1.71883736	1419.82 1453.64 1468.49
	H	-1.0134686	0.04599254	-0.3770138	1481.29 1489.00 1506.95
	H	0.57863755	0.82034217	-0.3777256	2993.67 3045.42 3066.79
	H	0.45118549	-0.9473372	-0.3528131	3075.25 3112.26 3126.87
	H	-0.5653442	-0.8500874	1.91542293	3140.13 3157.88 3170.45
	H	0.28967149	-0.9922745	5.2864948	3825.52 3903.26
	O	-0.6149694	1.19597742	2.01157799	! 36.81 74.74 118.53
	O	-1.9947029	1.15451662	1.67864894	187.70 225.19 240.96
	H	-2.3846174	0.89111069	2.52082406	349.87 !Torsions
	H	0.51451249	-2.9773909	4.30457482	
QOOH-2 	C	0.03138482	0.09627912	0.01277276	186.07 233.12 302.27
	C	-0.0061633	-0.0390503	1.52244477	339.97 363.99 497.16
	C	1.41373962	-0.1056085	2.11453295	544.74 590.00 838.39
	C	1.47861376	-0.0925931	3.59961437	886.57 899.00 939.79
	C	1.83480569	1.1540712	4.32814696	1000.24 1017.30 1055.76
	O	0.83432842	2.18177314	4.20553261	1102.02 1128.97 1158.02
	H	1.10181056	-0.9440285	4.14899426	1170.33 1214.45 1271.60
	H	2.78906132	1.54923443	3.96187469	1292.63 1355.07 1365.07
	H	1.87821529	-1.016201	1.72169888	1381.87 1403.55 1410.29
	H	1.9807604	0.74028958	1.70988485	1426.80 1474.82 1488.86
	H	-0.9773152	0.0942289	-0.3940473	1502.63 1505.89 1514.03
	H	0.51624422	1.03206955	-0.2676226	3023.13 3026.71 3064.33
	H	0.59433153	-0.7267727	-0.4256827	3070.88 3090.16 3141.25
	H	1.93274545	0.97386357	5.39573858	3143.71 3161.24 3205.11
	O	-0.7173629	1.09990904	1.99493596	3637.97 3823.38
	H	-0.5723487	-0.9235899	1.81870884	! 86.41 102.53 143.47
	O	-1.3460008	0.7664622	3.22571599	221.78 403.37 462.68
	H	-0.7798351	1.24177141	3.86085197	632.97 !Torsions
	H	0.77082697	2.43046986	3.27548817	
QOOH-3 	C	-0.0723748	-0.1066942	0.06365031	279.61 308.50 358.68
	C	0.0397236	0.08963324	1.56225359	424.27 501.51 525.15
	C	1.43991401	0.04660772	2.06124504	554.32 594.06 830.21
	C	1.78992249	-0.4600822	3.41481538	876.64 902.91 929.21
	C	1.62397318	0.60403829	4.51401697	1014.37 1015.89 1078.24
	O	0.28813314	1.03063354	4.64670247	1098.74 1117.87 1149.19
	H	1.14574929	-1.3033438	3.67700965	1189.13 1214.92 1253.57
	H	2.825026	-0.8081415	3.43178422	1315.51 1342.41 1355.53
	H	2.28995801	1.44842572	4.3063242	1399.75 1405.74 1410.87
	H	2.19300845	0.54879658	1.46673812	1444.18 1451.89 1478.01
	H	-1.1040198	0.02181378	-0.2568428	1489.14 1500.89 1517.01
	H	0.55111874	0.62473796	-0.4504875	3030.97 3046.95 3052.18
	H	-0.5666336	-0.6462306	2.10001796	3070.99 3102.27 3113.48
	H	1.91382709	0.17630063	5.47347359	3145.33 3161.16 3186.10
	O	-0.4683664	1.3979965	1.9242821	3782.09 3801.00
	H	0.26182482	-1.1070204	-0.2098496	! 44.07 72.85 111.82
	O	-1.8745411	1.40743708	1.7097246	206.05 229.11 248.33

	H	-2.2129364	1.2125776	2.59375214	290.68 !Torsions
	H	0.03689112	1.46982719	3.82439152	
HO_2 + 3-Penten-1-ol  **HO_2 +**	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	0.30741342	0.53663611	0.31779885	212.22 305.22 404.48
	C	0.11748188	-0.2747225	1.56168933	487.97 585.71 736.62
	C	1.06960779	-0.8340096	2.29993048	813.19 914.17 1006.86
	C	2.54829385	-0.7549825	2.05604885	1025.31 1038.79 1052.87
	C	3.17925167	0.36835798	2.86244458	1072.29 1112.21 1160.14
	O	4.57819267	0.32537583	2.64856422	1233.77 1238.47 1291.00
	H	-0.1404099	1.52489465	0.43670741	1319.37 1325.18 1402.26
	H	-0.1914926	0.06548623	-0.5312159	1441.33 1454.06 1487.48
	H	1.35635719	0.67217956	0.06445755	1490.90 1512.54 1534.21
	H	-0.9115007	-0.4093642	1.87881797	1759.41 3015.82 3049.79
	H	0.76532983	-1.3789717	3.18759787	3059.11 3080.81 3108.21
	H	3.02779919	-1.690201	2.34904747	3126.12 3151.02 3160.00
	H	2.77763966	-0.5958202	1.00303124	3180.40 3900.10
	H	2.75657684	1.32554537	2.5376014	! 28.3354 111.1528
	H	2.9376226	0.24020201	3.92346677	137.1140 268.8076 !Torsions
	H	4.99400023	1.02664967	3.15358488	
HO_2 + 4-Penten-1-ol  **HO_2 +**	O	0.50553254	2.59512924	1.64024162	1161.48 1475.38 3553.10
	O	-0.1679742	2.44348437	0.50783059	
	H	-0.2367003	1.48037439	0.35008979	
	C	-0.0272666	0.01693358	0.00420408	170.18 293.55 422.78
	C	-0.0057323	0.00997062	1.33040751	489.29 654.55 811.08
	H	0.89122364	0.00506179	-0.5711245	877.73 918.93 955.32
	H	-0.9563146	0.04644576	-0.5488319	975.65 1015.47 1048.14
	C	1.23635754	-0.0225536	2.16850263	1067.96 1128.09 1156.01
	C	1.32734663	-1.2423691	3.09262829	1213.17 1247.29 1285.07
	C	1.39779665	-2.5695416	2.34866035	1325.90 1360.53 1382.68
	O	0.15964152	-2.9645816	1.79168399	1399.38 1433.00 1455.56
	H	-0.9465082	0.01964466	1.87470355	1475.09 1487.08 1515.31
	H	2.11257198	0.00673123	1.51592775	1729.36 3012.47 3048.02
	H	1.26459168	0.88177872	2.78220093	3059.31 3089.01 3106.74
	H	2.21852562	-1.1406455	3.71569009	3110.17 3152.13 3161.30
	H	0.46515928	-1.2708675	3.76303536	3246.67 3863.45
	H	2.1756791	-2.5181256	1.57619265	! 78.69 114.61 335.54
	H	1.67919752	-3.3636631	3.03965912	432.24 !Torsions
	H	-0.0787164	-2.3321037	1.10820512	
O_2 + $CH_3CHCH_2CH_2CH_2OH$  **O_2 +**	O	0.0000000	0.0000000	0.00794919	1758.25
	O	0.0000000	0.0000000	1.19781253	
	O	0.00438981	0.0433413	-0.0062954	145.40 316.58 366.63
	C	0.0004821	-0.0074812	1.41018085	408.92 519.09 754.61
	C	1.39985003	-0.0034647	2.00182314	877.67 915.74 945.66
	C	2.23783258	-1.1953123	1.55263137	984.93 1038.53 1079.86
	C	3.63009569	-1.1712338	2.07375895	1115.18 1128.32 1147.60
	C	4.51111614	-2.3585353	1.92362181	1181.01 1244.79 1289.25
	H	1.74478895	-2.1241901	1.86521948	1314.33 1372.87 1386.65
	H	2.23592022	-1.2299798	0.45398613	1409.92 1423.78 1432.48
	H	1.3259407	0.00709056	3.09218877	1474.13 1478.81 1489.24
	H	1.90639242	0.92542063	1.71698058	1492.23 1518.69 2990.54

	H	-0.5101887	-0.9364771	1.66777244	2996.13 3022.99 3031.73
	H	-0.5877283	0.81739825	1.82464317	3039.49 3065.26 3085.36
	H	0.42441303	0.8629837	-0.2785423	3104.10 3132.49 3183.01
	H	5.43139152	-2.2605105	2.49715389	3878.75
	H	4.79572612	-2.5225477	0.87554931	! 48.39 79.93 121.34
	H	4.00136138	-3.2698933	2.24759197	185.59 280.74 ! Torsions
	H	4.07178636	-0.2140255	2.31995981	
OH + 5-Hydroxy-2-pentanone 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	-0.00090238	-0.03722963	-0.01381492	265.28 310.42 374.60
	C	-0.00393088	0.02417681	1.48996651	485.29 535.70 599.45
	C	1.356399012	0.02769792	2.16088620	760.52 834.90 884.82
	C	1.328577951	0.56601908	3.58353934	912.75 977.18 1029.06
	C	1.272512439	2.08814268	3.60467380	1037.48 1110.12 1140.94
	O	0.276355238	2.61189646	2.748053951	1180.32 1205.72 1241.19
	O	-1.032469402	0.05785116	2.122496665	1296.78 1363.92 1384.46
	H	0.7309707731	-0.760026	-0.37477947	1390.76 1408.83 1436.17
	H	0.2998361598	0.94486196	-0.38549287	1452.61 1467.68 1480.27
	H	-0.99348451	-0.275492201	-0.38397966	1484.61 1525.86 1837.73
	H	-0.548667946	2.146827108	2.92234571	3037.18 3051.21 3065.07
	H	1.698296767	-1.012194277	2.14045054	3074.40 3090.18 3092.96
	H	2.054398212	0.590013033	1.535343514	3121.70 3131.65 3182.10
	H	0.458525844	0.153509337	4.097146228	3848.01 ! 31.47 127.75
	H	2.214107828	0.241386953	4.131481995	148.55 159.41 464.24
	H	1.133943487	2.441568892	4.631238671	!Torsions
	H	2.216709420	2.497574561	3.24076278	
OH + 5-methylTHF-2ol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.00028358	-0.001144	-0.0001249	54.27 187.04 339.41
	C	-0.0032182	-0.0007748	1.51360539	417.03 458.27 516.60
	H	1.02407629	-0.0013279	1.88712538	615.00 785.05 829.06
	C	-0.7974287	1.15357383	2.13818207	876.81 919.85 926.47
	C	-1.4798701	0.48981129	3.33384933	976.14 1011.56 1033.32
	C	-1.7430339	-0.8953466	2.77402096	1057.29 1141.55 1147.09
	O	-2.9021967	-0.8189038	1.97650438	1163.60 1208.63 1235.80
	O	-0.6144895	-1.2076519	2.00475315	1257.52 1314.95 1345.70
	H	0.53533923	-0.8685227	-0.3838225	1366.88 1391.19 1399.58
	H	0.48266026	0.90063253	-0.3795674	1414.97 1444.00 1482.11
	H	-1.0260335	-0.0307837	-0.3671379	1488.82 1499.57 1505.50
	H	-0.1566794	1.98773494	2.4146197	3052.74 3061.56 3081.22
	H	-1.5487815	1.51119904	1.43451457	3093.09 3098.50 3136.50
	H	-0.7995758	0.41132959	4.18164594	3144.50 3148.80 3163.01
	H	-2.3958333	0.98122292	3.65018686	3873.78
	H	-1.8470984	-1.6807751	3.52483674	! 253.91 311.31 !Torsions
	H	-2.9669824	-1.6392377	1.47919626	
OH + (4-methyloxetan-2-yl)methanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.00299798	0.01159375	-0.0120154	74.82 246.13 272.2 404.68
	H	0.0342442	0.02840066	1.07776395	443.52 596.35 746.6 816.24
	H	1.02623614	0.01386001	-0.3872219	901.0 911.4 941.15 957.84
	H	-0.4827179	-0.9096893	-0.3367822	1023.96 1073.88 1095.89

	C	-0.7487566	1.21004624	-0.5296356	1115.32 1151.22 1172.15
	H	-0.793433	1.21032601	-1.6206069	1203.07 1233.97 1262.36
	C	-2.1001722	1.54794635	0.11795922	1279.22 1304.92 1360.04
	H	-2.3127749	0.96184758	1.00915906	1378.55 1400.93 1419.55
	H	-2.9594286	1.56649504	-0.5448162	1452.01 1484.3 1492.5 1499.85
	C	-1.4514541	2.91050069	0.40638995	1507.09 3018.7 3058.21
	O	-0.1766464	2.45240752	-0.0651885	3066.46 3071.7 3072.78
	C	-1.9656052	4.07250457	-0.4075171	3110.18 3134.3 3139.21 3177.0
	H	-1.2098627	4.86301098	-0.3843273	3919.15
	H	-2.8851877	4.45347686	0.05246626	! 129.21 155.4 233.68
	O	-2.2067507	3.63366609	-1.7314856	!Torsions
	H	-2.1995262	4.38820339	-2.321457	
	H	-1.4031861	3.20615449	1.45732439	
OH + 2-(3-methyloxiran-2-yl)ethanol 	O	0.00000000	0.00000000	-0.00571069	3776.00
	H	0.00000000	0.00000000	0.96571069	
	C	0.01710404	0.00788610	0.01580231	252.47 359.52 428.56
	C	-0.01102377	-0.02190248	1.51376145	440.67 451.56 543.16
					796.70 854.80 896.61
	C	1.20911727	0.01417474	2.32303375	952.82 960.30 1021.38
	H	2.15330109	0.09126179	1.78915540	1060.60 1098.24 1132.38
					1147.02 1179.66 1183.50
	C	1.29324860	-0.54390900	3.71648982	1240.69 1257.42 1293.86
					1343.89 1385.66 1391.63
	C	1.93995626	0.45161926	4.67422545	1418.66 1449.87 1466.16
	O	1.09792639	1.54923240	4.94624002	1482.52 1496.81 1524.34
					1540.69 3007.73 3066.04
	O	0.39059840	1.17804169	2.16646753	3068.73 3107.51 3112.36
					3132.13 3137.87 3139.74
	H	0.93009267	0.48778620	-0.33328506	3156.87 3843.87
					! 64.15 149.60 179.40
	H	-0.83525879	0.56621964	-0.37048527	206.54 !Torsions
	H	-0.02694916	-1.00412422	-0.38660753	
	H	-0.88132759	-0.48628238	1.96844145	
	H	0.29310323	-0.78069116	4.08429001	
	H	1.8741710	-1.4683148	3.69213285	
	H	2.14409858	-0.02927151	5.63056296	
	H	2.90125406	0.78493515	4.26211731	
	H	0.71234012	1.84337954	4.1140472	
N-pentanol ROO-4 = QOOH-0	C	0.01684972	0.04755285	0.02341064	1431.21i 90.46 231.41
	C	0.0113658	0.0044988	1.53777266	267.89 285.03 328.81
	O	1.4016177	0.01239899	1.89827827	341.82 381.68 494.14
	O	1.54988812	-0.0618106	3.26232317	536.38 629.56 641.77
	C	-0.7668723	1.143496	2.19515405	741.30 799.25 839.33
	C	-0.2294468	2.54815734	1.92490162	887.75 913.99 939.37
	C	1.20107514	2.72147954	2.42636564	981.53 1020.92 1054.04
	O	1.41330022	2.27484662	3.69995595	1126.76 1135.68 1181.26
	H	0.4892662	0.96052133	-0.3379009	1201.27 1227.30 1251.99
	H	-1.0055304	0.01427541	-0.3502811	1283.08 1357.15 1361.49

	H	0.56452316	-0.8023887	-0.3787604	1372.09 1381.87 1387.48
	H	-0.4036674	-0.9438909	1.88870676	1408.63 1424.33 1481.64
	H	-1.7985223	1.06712581	1.84766581	1486.62 1496.23 1511.14
	H	-0.7883387	0.97498259	3.27142085	1626.80 2870.56 2987.17
	H	-0.2664579	2.78989892	0.86080378	3063.19 3069.63 3076.32
	H	-0.8732331	3.26632844	2.43534074	3086.43 3108.05 3128.91
	H	1.89871758	2.17786591	1.7559168	3150.30 3157.71
	H	1.54079289	3.76648385	2.3676235	! 188.94 !Torsions
	H	1.47324421	0.95379359	3.60964188	
N-pentanol ROO-4 = QOOH-1	C	0.00088503	0.00186379	-0.001276	1968.46i 86.10 166.42
	C	-0.0005538	-0.0012238	1.51453124	179.98 284.57 310.28
	O	1.38418026	-0.0027648	1.8726542	333.14 385.12 483.81
	O	1.50638783	0.00056748	3.24687009	526.40 619.18 635.42
	C	-0.7289791	1.20911195	2.11342017	797.26 875.83 888.58
	C	0.16301111	2.45470293	2.19949621	916.46 960.39 1018.64
	C	1.00126958	2.43787651	3.45315059	1032.28 1084.74 1107.45
	O	0.21788423	2.69259879	4.56436794	1116.58 1170.66 1195.30
	H	0.39327633	0.94456193	-0.3841269	1213.55 1236.16 1268.20
	H	-1.0142724	-0.1278296	-0.373011	1306.73 1345.38 1373.12
	H	0.6201349	-0.8082766	-0.3822573	1377.73 1396.40 1411.60
	H	-0.4465034	-0.9249409	1.89149917	1418.37 1471.07 1487.56
	H	-1.6066626	1.41184246	1.4990287	1499.04 1504.94 1542.79
	H	-1.0878989	0.9743856	3.11500226	3060.20 3063.05 3070.96
	H	0.81875968	2.5212303	1.33168211	3074.12 3087.50 3121.60
	H	-0.4512466	3.35804081	2.21972872	3130.77 3144.35 3155.75
	H	1.40383647	1.20395502	3.5012246	3888.27
	H	1.92185052	3.02495865	3.41850706	! 223.59 361.82 !Torsions
	H	0.76702077	2.72049041	5.35175016	
N-pentanol ROO-4 = QOOH-2	C	-0.0118187	-0.0091735	0.03665625	1814.78i 102.41 121.30
	C	-0.0193682	-0.005286	1.54792281	259.22 281.36 338.66
	O	1.34010656	-0.0119519	1.95998056	467.94 480.46 509.01
	O	1.38147693	-0.2102012	3.32869871	550.23 686.14 794.00
	C	-0.689516	1.25623285	2.13620023	857.29 901.60 910.98
	C	-0.4031624	1.44441386	3.6033338	930.54 1010.45 1050.78
	C	-1.3241281	0.76751000	4.58458107	1097.26 1111.27 1134.71
	O	-1.5210998	-0.6003246	4.28840726	1144.40 1174.15 1218.49
	H	0.54449229	0.84982097	-0.3380321	1232.36 1255.69 1301.66
	H	-1.032937	0.04693831	-0.3378743	1351.74 1372.96 1381.66
	H	0.45090578	-0.9183168	-0.3417664	1395.83 1417.32 1424.86
	H	-0.5078607	-0.8958577	1.94552673	1463.75 1488.16 1503.77
	H	-0.3336271	2.11541514	1.56746955	1506.87 1568.37 3029.55
	H	-1.7673371	1.15469365	1.972617	3043.15 3063.34 3073.56
	H	0.72520972	0.71889051	3.69255427	3094.36 3116.53 3146.19
	H	-0.0975493	2.44474701	3.89974151	3150.45 3158.71 3836.32
	H	-0.9518523	0.90274431	5.60511561	! 168.65 210.94 414.24
	H	-2.3155045	1.2294013	4.5388717	!Torsions
	H	-0.6553962	-1.0221321	4.25449542	
N-pentanol ROO-4 = QOOH-3	C	0.0771364	0.03746421	0.03875113	2195.11i 92.01 170.45
	C	-0.0273143	0.01288019	1.54956355	241.49 311.71 366.81
	O	1.25151534	0.08753601	2.18699457	497.30 512.71 615.11
	O	1.60658393	1.4335538	2.04952588	749.22 785.74 865.24
	C	-0.7355251	1.24042138	2.12077949	905.36 917.73 958.38
	C	-1.1322049	1.17811331	3.56677066	990.03 1026.34 1074.53
	C	-1.3021513	2.55811586	4.1906764	1089.83 1118.23 1136.46
	O	-0.1513756	3.36271575	4.03895473	1144.85 1173.11 1227.11

	H	0.54617209	0.9639728	-0.2887711	1256.91 1289.73 1327.17
	H	-0.9147259	-0.0313949	-0.4080869	1371.90 1378.30 1408.64
	H	0.67613169	-0.8014823	-0.3102292	1418.45 1430.62 1470.86
	H	-0.4629722	-0.9260994	1.90159295	1487.97 1502.20 1524.79
	H	0.42260265	1.86056675	2.10536747	1744.50 3026.00 3043.43
	H	-1.424455	1.76499069	1.46233521	3069.13 3072.11 3073.41
	H	-2.0707611	0.62170323	3.67410903	3104.97 3140.75 3148.40
	H	-0.3691737	0.61770916	4.11560709	3159.49 3855.15
	H	-2.1096276	3.09813046	3.69427671	! 60.10 199.70 220.30
	H	-1.5729754	2.4522545	5.24552651	304.39 !Torsions
	H	0.62522016	2.85717964	4.29871527	
N-pentanol ROO-4 = HO_2 + 3-Penten-1-ol	C	0.0121498	-0.0133698	-0.0007314	1073.04i 98.17 148.46
	C	0.01533442	-0.011382	1.4923931	241.53 266.45 303.08
	O	2.06950056	0.03545925	1.68469244	437.07 486.68 523.57
	O	2.23471941	1.10150401	2.32983413	588.18 698.82 838.71
	C	-0.2976025	1.11090596	2.25476558	878.35 921.51 939.63
	C	-0.8489103	0.96153657	3.65933722	998.67 1025.55 1082.08
	C	-2.3643907	0.79264546	3.67017743	1094.17 1121.37 1158.01
	O	-2.7851714	-0.3528052	2.9569887	1207.58 1246.20 1270.64
	H	0.22593717	0.98141991	-0.390111	1296.89 1331.65 1378.62
	H	-0.9715278	-0.3166038	-0.369168	1388.52 1401.42 1418.12
	H	0.74503025	-0.7136117	-0.3969053	1423.10 1477.01 1479.87
	H	-0.0118463	-0.9819622	1.97523218	1492.13 1514.30 1597.05
	H	0.99933981	1.40355115	2.43656756	1656.76 3024.30 3053.26
	H	-0.6324786	1.98764369	1.70117249	3062.31 3103.73 3117.19
	H	-0.3938823	0.0886349	4.13278163	3119.84 3120.61 3151.52
	H	-0.591169	1.83057146	4.26811735	3182.60 3873.00 ! 61.10
	H	-2.7167553	0.65742378	4.69201272	128.49 202.78 331.57
	H	-2.8404769	1.6955271	3.27094094	!Torsions
	H	-2.5587583	-0.2273975	2.03179611	
N-pentanol ROO-4 = HO_2 + 4-Penten-1-ol	C	-0.0060239	-0.0150327	0.00804138	1076.69i 169.09 238.64
	C	0.09289433	-4.374E-06	1.3904838	261.15 354.17 424.97
	O	2.51684058	0.0227121	0.27943958	443.98 510.75 553.34
	O	2.21806869	-0.0395674	1.50086711	624.01 690.76 773.00
	C	-0.096538	1.24419659	2.20627437	845.78 915.14 955.73
	C	-0.017434	1.0409011	3.71623009	1014.24 1018.86 1041.10
	C	1.3492898	0.59339003	4.21880318	1099.44 1123.60 1157.54
	O	2.36050577	1.52597827	3.89551348	1207.85 1225.60 1287.91
	H	1.3202772	0.01146495	-0.174229	1310.89 1316.14 1346.77
	H	-0.3318472	0.89270032	-0.4887602	1390.92 1406.95 1410.56
	H	-0.2754543	-0.9420279	-0.4829333	1422.27 1452.81 1469.00
	H	0.06278261	-0.9424777	1.9264836	1479.92 1522.55 1582.05
	H	0.6328079	1.99466516	1.89100508	1632.61 3049.31 3053.36
	H	-1.0769752	1.65450882	1.94934291	3057.36 3088.57 3098.02
	H	-0.2680792	1.98275536	4.20631509	3110.92 3137.46 3176.73
	H	-0.7664322	0.30689713	4.02746947	3226.21 3873.79
	H	1.31947861	0.51442232	5.3062703	! 72.88 121.86 164.40
	H	1.59906015	-0.3981816	3.82981306	396.67 ! Torsions
	H	2.75363326	1.25773304	3.06040976	
QOOH-0 = OH + 5-Hydroxy-2-pentanone	C	0.01695065	-0.0242648	0.03187801	1035.61i 122.30 127.64
	C	-0.0141507	0.00761998	1.54087475	273.00 305.16 358.30
	C	1.33550527	0.00552315	2.23069579	387.31 480.81 491.35
	C	1.85454428	-1.4249334	2.36845105	537.21 640.20 822.84
	C	0.80281976	-2.2739956	3.08423788	867.29 909.97 937.04
	O	-0.3889024	-2.3179689	2.36748254	950.28 1018.59 1031.92

	O	-0.7532197	1.06696813	2.08265333	1043.20 1100.82 1144.68
	O	-2.0543487	1.06996801	1.51808583	1182.91 1196.64 1225.24
	H	0.62753745	-0.862079	-0.3009305	1240.83 1266.43 1329.96
	H	0.45166227	0.90536253	-0.3417503	1355.29 1365.83 1384.82
	H	-0.9820911	-0.1347286	-0.3795738	1401.90 1416.42 1472.18
	H	-0.4997967	-1.0367103	1.89892952	1478.92 1484.39 1494.86
	H	2.04075759	0.62590192	1.67281226	1501.46 1642.35 2994.43
	H	1.21573426	0.44715662	3.22195807	3035.81 3059.32 3063.49
	H	2.0474299	-1.8579629	1.38523177	3075.94 3107.63 3125.72
	H	2.78983971	-1.4389566	2.92818178	3142.74 3175.67 3813.66 !
	H	1.16160244	-3.307988	3.15844909	69.73 195.59 248.82
	H	0.65215514	-1.8949263	4.10398667	!Torsions
	H	-2.5612329	0.6147707	2.20283306	
QOOH-1 = OH + 5-Hydroxy-2-pentanone	C	-0.0295187	0.06691702	0.0807124	1798.30i 144.46 181.85
	C	0.05071393	0.04555399	1.58179911	198.82 268.01 356.40
	C	1.43659969	0.03222528	2.1955439	365.28 415.88 463.67
	C	1.88776867	-1.4375333	2.13721213	548.70 658.17 764.66
	C	0.65160702	-2.2404043	2.45678002	808.23 860.39 886.09
	H	0.39273929	-2.2969222	3.51653115	964.25 986.04 1018.11
	O	0.59782728	-3.4511849	1.79235925	1056.83 1086.06 1124.52
	O	-0.8857455	0.82735329	2.22506111	1189.03 1227.59 1231.61
	O	-0.5201203	2.23072901	2.02055987	1247.95 1278.27 1321.98
	H	0.55301585	-0.7501851	-0.3460019	1330.94 1336.79 1395.62
	H	0.37019125	1.00595388	-0.3128461	1414.16 1451.82 1480.39
	H	-1.0626855	-0.0399104	-0.2487214	1481.76 1498.44 1501.91
	H	-0.1915607	-1.2635922	1.98297618	1655.01 3042.60 3072.01
	H	2.13316656	0.70169484	1.68920222	3074.36 3077.54 3112.27
	H	1.34650976	0.36168926	3.23154834	3116.21 3128.55 3140.21
	H	2.20297012	-1.7035271	1.12668956	3840.18 3893.57
	H	2.72127871	-1.6477725	2.8072383	! 230.39 330.36 52.79
	H	-0.1402709	-3.9681818	2.12315608	95.11 !Torsions
	H	-1.2305439	2.51243609	1.43234487	
QOOH-1 = OH + 5-methyl-THF-2ol	C	-0.0612467	0.31024799	0.19047991	962.1i 67.53 97.36 182.72
	C	-0.0044726	-0.1844537	1.62162638	256.54 277.25 317.92 411.72
	C	1.4007998	-0.0646468	2.21393548	439.52 462.16 498.49 566.39
	C	1.28389837	-0.0523928	3.73108954	708.9 824.97 882.99 914.78
	C	0.4017245	1.0940543	4.07298867	953.82 993.24 1040.6 1078.77
	O	-0.4780585	1.04223808	5.08848517	1116.37 1135.45 1157.66
	H	0.82332761	-0.9794094	4.08376407	1210.19 1239.26 1251.01
	H	2.26631288	0.02834277	4.20750187	1318.51 1332.32 1372.58
	H	2.02973531	-0.877714	1.8496617	1374.73 1393.56 1409.48
	H	1.85342103	0.87320778	1.88097142	1461.75 1481.54 1486.03
	H	-1.0563561	0.16882538	-0.2212935	1500.22 1509.7 3032.3 3039.56
	H	0.18896186	1.37179369	0.16034987	3058.01 3063.59 3082.72
	H	0.6592435	-0.2323633	-0.4235919	3112.63 3130.14 3172.18
	H	-0.3238084	-1.2304005	1.66951761	3207.87 3824.79 3867.38
	H	0.7313538	2.1025842	3.86348427	! 139.06 223.65 379.51 !
	O	-0.8796839	0.55703018	2.47508586	Torsions
	O	-2.3422701	0.08075699	1.9092393	
	H	-2.7657256	0.94156239	2.00107021	
	H	-0.9217868	0.18598469	5.07120594	
QOOH-2 = OH + (4-methyloxetan-2-yl)methanol	C	0.15803556	0.70338753	0.55795944	1097.26i 60.21 98.05 188.38
	C	0.00265683	-0.149192	1.79496188	232.72 319.2 349.55 421.71
	C	1.31693601	-0.5311123	2.48889245	442.99 513.89 636.34 758.75
	C	1.15035101	0.28478101	3.73813062	842.81 885.5 929.85 953.14

	C	1.67025275	1.67692356	3.84325139	1004.7 1075.87 1102.15
	O	0.76968062	2.51283829	4.53242233	1119.96 1125.68 1137.56
	H	0.88055533	-0.2006519	4.66554713	1160.85 1212.06 1236.93
	H	1.89055257	2.06413936	2.84177726	1285.2 1315.31 1346.94
	H	1.38054792	-1.5959756	2.69834645	1383.21 1403.12 1415.13
	H	2.19141658	-0.2339529	1.90737565	1443.6 1480.09 1493.31
	H	-0.8129163	1.03968708	0.20354945	1499.48 1506.35 3023.71
	H	0.77597801	1.57568073	0.77445822	3058.33 3064.94 3073.72
	H	0.64315607	0.1226899	-0.2279866	3088.92 3134.39 3143.42
	H	2.60557973	1.69389688	4.41223201	3168.1 3209.53 3831.34
	O	-0.5835727	0.59665869	2.89286592	3859.46
	H	-0.6392416	-1.0065151	1.59144078	! 137.27 259.73 283.77
	O	-2.0791035	0.97891889	2.30063556	497.29 !Torisons
	H	-2.5741878	0.59817636	3.03532151	
	H	-0.0795766	2.41677344	4.08558916	
QOOH-3 = HO_2 + 3-Penten-1-ol	C	0.00239958	0.00125709	-0.00274575	670.57i 154.71 178.28
	C	0.00165012	-0.00526931	1.49396613	271.72 311.07 344.23
	C	1.16862193	-0.00259766	2.21948275	363.80 479.86 511.53
	H	2.09669035	0.228625945	1.70212909	758.24 869.08 898.29
	C	1.22561387	-0.08923378	3.70700160	929.49 989.88 1019.64
	C	1.84942999	1.171435233	4.31150279	1030.95 1094.21 1102.01
	O	1.11918943	2.345180629	3.99891359	1118.18 1163.28 1219.08
	O	-0.60419505	1.783934343	1.83624039	1228.18 1290.88 1311.54
	O	-1.38828606	1.742478565	2.96287261	1371.46 1395.69 1410.43
	H	0.89163377	0.496940519	-0.39032505	1425.44 1469.99 1482.02
	H	-0.87860622	0.517297191	-0.37801952	1494.75 1511.24 1522.21
	H	-0.01208929	-1.02102395	-0.38364818	1579.36 3035.30 3040.44
	H	-0.887658876	-0.39738200	1.9733908228	3067.47 3103.33 3126.41
	H	0.222283489	-0.23480742	4.1110951176	3132.83 3143.00 3156.41
	H	1.834790539	-0.94363431	4.0204403009	3183.15 3637.84 3771.88
	H	1.863473670	1.09951000	5.3976224862	! 95.84 136.89 185.97
	H	2.884586279	1.26911289	3.9681703254	237.04 585.09 661.51 !
	H	1.059525007	2.41807051	3.0358515192	Torsions
	H	-0.787842508	2.06747453	3.6580280623	
QOOH-3 = OH + 2-(3-methyloxiran-2-yl)ethanol	C	-0.0949763	-0.0795021	0.05922951	943.82i 101.03 200.08
	C	0.0809583	0.03467175	1.55043724	238.75 282.62 304.07
	C	1.4360673	-0.0239198	2.12594839	379.73 439.89 497.65
	H	2.25524164	0.31444683	1.5068125	532.58 642.06 708.84
	C	1.66399509	-0.433219	3.53503272	815.62 897.67 907.81
	C	0.94557028	0.44289688	4.58426657	923.25 1006.74 1033.27
	O	-0.4520400	0.32096256	4.54789774	1076.56 1117.02 1123.07
	O	0.11129039	1.3556302	2.0186762	1148.82 1200.87 1216.26
	O	-1.4998325	1.89429733	2.09440496	1270.25 1301.89 1328.95
	H	0.67647049	0.49317985	-0.4554211	1365.18 1404.19 1412.50
	H	-1.0700318	0.31972557	-0.215247	1419.15 1465.81 1477.24
	H	-0.0382722	-1.1206175	-0.2573968	1494.78 1501.20 1510.20
	H	-0.6389405	-0.5619308	2.1152962	3038.42 3059.49 3068.10
	H	1.29642851	-1.4552166	3.67525114	3083.02 3110.54 3114.30
	H	2.7313925	-0.4272712	3.75659733	3145.77 3154.39 3210.86
	H	1.26945317	0.10557254	5.56941753	3784.35 3849.88
	H	1.26108398	1.48090507	4.45733478	! 76.48 179.45 216.04
	H	-0.8034056	0.92741385	3.8821339	253.59 !Torsions
	H	-1.2897793	2.82739792	1.96391122	

Rate Constant Calculation and Modeling Details:

A) Updated Rate Constants in Chemkin-PLOG Format:

Table S17. Reaction rate constants and updated thermo calculated in this work for the n-butanol ROO and QOOH decompositions. A species glossary is given in the supplemental material as an excel document.

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!! Final N-butanol Lockwood Rates 11-18-21!
!
! ROO1 Decomposition Rates
!
PC4H8OH-1O2=NC3H7CHO+HO2 1.0 0.0 0.0 !well skipping over the complex so no HP rates
   PLOG/ 0.100 2.019E+43 -10.604 18999.5/
   PLOG/ 1.000 5.585E+36 -8.150 18370.3/
   PLOG/ 10.000 6.713E+28 -5.363 17157.6/
   PLOG/ 100.000 2.504E+24 -3.795 16768.0/
PC4H8OH-1O2=>O2+PC4H8OH-1  7.914E+23 -2.477 39847.7
   PLOG/ 0.100 1.688E+129 -41.274 61279.9/
   PLOG/ 1.000 8.667E+49 -12.577 43656.0/
   PLOG/ 10.000 1.391E+46 -10.228 44399.5/
   PLOG/ 100.000 1.087E+35 -6.166 42695.9/
O2+PC4H8OH-1=>PC4H8OH-1O2   1.274E+12 0.283 116.9
   PLOG/ 0.100 3.799E-30 11.222 -10994.2/
   PLOG/ 1.000 1.935E+40 -10.522 4475.3/
   PLOG/ 10.000 6.660E+35 -7.947 5068.5/
   PLOG/ 100.000 2.140E+24 -3.753 3291.8/
O2+PC4H8OH-1=NC3H7CHO+HO2 1.0 0.0 0.0  !well skipping over the complex so no HP rates
   PLOG/ 0.100 3.169E+20 -2.543 2046.3/
   PLOG/ 0.100 4.836E+32 -5.872 11186.3/
   PLOG/ 1.000 3.787E+20 -2.563 2093.3/
   PLOG/ 1.000 6.490E+32 -5.909 11285.0/
   PLOG/ 10.00 1.766E+22 -3.087 3083.2/
   PLOG/ 10.00 2.706E+31 -5.502 10263.1/
   PLOG/ 100.0 1.023E+18 -1.829 2729.4/
   PLOG/ 100.0 3.951E+31 -5.435 12245.1/
!
!
!ROO2 & Subsequent QOOH Decomp:
!
!
PC4H8OH-2O2=SQC4H7OHP-4  8.656E-02 3.648 17799.4
   PLOG/ 0.100 1.215E-04 4.207 15799.0/
   PLOG/ 1.000 2.214E-06 4.988 15978.9/
   PLOG/ 10.000 4.242E-06 4.988 16367.3/
```

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   PLOG/ 100.000 3.578E+06 1.211 20063.4/
PC4H8OH-2O2=C4H7OH-2OOH-1   1.319E-09 6.153 16809.1
   PLOG/ 0.100 5.878E+08 -1.267 15607.8/
   PLOG/ 1.000 3.215E-06 3.963 13709.0/
   PLOG/ 10.000 1.228E-16 7.864 12660.0/
   PLOG/ 100.000 1.270E-18 8.817 13243.8/
PC4H8OH-2O2=>PC4H8OH-2+O2 3.240E+24 -2.557 37791.4
   PLOG/ 0.100 8.185E+64 -15.954 47842.2/
   PLOG/ 1.000 8.358E+53 -12.205 45511.1/
   PLOG/ 10.000 9.788E+43 -8.880 43183.0/
   PLOG/ 100.000 5.771E+37 -6.804 41695.6/
PC4H8OH-2+O2=>PC4H8OH-2O2  1.0 0.0 0.0
   PLOG/ 0.100 5.047E+54 -14.275 8833.4/
   PLOG/ 0.100 5.782E+79 -21.458 21226.6/
   PLOG/ 1.000 1.601E+45 -10.943 7117.5/
   PLOG/ 1.000 3.593E+75 -19.733 22179.3/
   PLOG/ 10.000 3.658E+36 -7.952 5430.0/
   PLOG/ 10.000 5.525E+68 -17.249 22297.5/
   PLOG/ 100.000 7.284E+29 -5.651 4066.9/
   PLOG/ 100.000 3.333E+60 -14.411 21770.4/
PC4H8OH-2O2=OH+CH2O+C2H5CHO  1.0 0.0 0.0 !well skipping
   PLOG/ 0.100 5.972E+51 -12.692 41483.3/
   PLOG/ 1.000 8.617E+40 -9.063 38932.9/
   PLOG/ 10.000 1.125E+33 -6.438 37033.0/
   PLOG/ 100.000 8.999E+29 -5.385 36388.9/
PC4H8OH-2O2=C4H7OHCYO1-2+OH   1.0 0.0 0.0 !well skipping
   PLOG/ 0.100 2.291E+23 -4.249 26500.4/
   PLOG/ 1.000 4.390E+20 -3.166 27038.3/
   PLOG/ 10.000 4.272E+21 -3.237 29214.1/
   PLOG/ 100.000 8.524E+18 -2.188 30516.1/
SQC4H7OHP-4=>PC4H8OH-2+O2 1.0 0.0 0.0  !well skipping
   PLOG/ 0.100 4.887E-75 29.791 2191.5/
   PLOG/ 1.000 5.943E+03 3.314 18694.6/
   PLOG/ 10.000 2.692E+10 1.254 21607.4/
   PLOG/ 100.000 5.112E+22 -2.763 26355.6/
PC4H8OH-2+O2=>SQC4H7OHP-4 1.0 0.0 0.0 ! well skipping
   PLOG/ 10.000 1.140E+00 3.270 153.9/
   PLOG/ 10.000 1.143E+16 -1.401 8387.4/
   PLOG/ 100.000 9.120E+06 0.878 2812.2/
   PLOG/ 100.000 2.591E+45 -10.151 23978.4/
SQC4H7OHP-4=CH2O+OH+C2H5CHO   1.0 0.0 0.0  !well skipping
   PLOG/ 0.100 2.265E-83 31.221 -3844.0/
   PLOG/ 1.000 1.484E+07 1.018 15359.9/
   PLOG/ 10.000 5.654E+11 -0.095 17498.3/
   PLOG/ 100.000 1.720E+18 -2.034 19979.8/
SQC4H7OHP-4=CY(CCCO)COH+OH  3.223E+13 -0.461 16084.2
   PLOG/ 0.100 1.543E-04 3.892 9039.1/
   PLOG/ 1.000 3.372E+18 -2.642 15912.3/
   PLOG/ 10.000 3.555E+16 -1.576 16498.5/
   PLOG/ 100.000 6.446E+15 -1.218 16690.8/
C4H7OH-2OOH-1=C4H7OHCYO1-2+OH 4.193E+12 0.125 10258.6
   PLOG/ 0.100 2.944E+36 -8.698 13319.7/
   PLOG/ 1.000 4.610E+34 -7.680 14036.8/
   PLOG/ 10.000 1.509E+27 -4.892 13172.1/
   PLOG/ 100.000 2.897E+19 -2.188 11777.4/
C4H7OH-2OOH-1=C4H7O-2O+H2O 8.842E+05 1.596 7226.3
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    PLOG/ 0.100 5.122E+17 -3.134 7253.2/
    PLOG/ 1.000 1.683E+13 -1.316 7205.8/
    PLOG/ 10.000 3.636E+08 0.477 6893.0/
    PLOG/ 100.000 3.130E+05 1.630 6636.7/
!
!
!ROO3 & Subsequent QOOH Decomp:
!
!
PC4H8OH-3O2=C4H7OH-3OOH-1   1.585E+06 1.646 14594.2
    PLOG/ 0.100 1.341E+10 0.027 14435.2/
    PLOG/ 1.000 7.695E+06 1.286 14284.4/
    PLOG/ 10.000 1.788E+11 -0.021 15920.9/
    PLOG/ 100.000 3.187E+10 0.269 15914.9/
PC4H8OH-3O2=>PC4H8OH-3+O2  5.917E+29 -4.038 39548.8
    PLOG/ 0.100 4.668E+69 -17.461 48834.9/
    PLOG/ 1.000 8.279E+61 -14.662 47702.3/
    PLOG/ 10.000 2.484E+53 -11.742 45940.7/
    PLOG/ 100.000 7.335E+43 -8.583 43580.5/
PC4H8OH-3+O2=>PC4H8OH-3O2  5.326E+13 -0.219 357.6
    PLOG/ 0.100 1.041E+56 -14.765 9059.8/
    PLOG/ 0.100 7.780E+79 -21.732 20274.2/
    PLOG/ 1.000 4.174E+51 -13.099 8623.5/
    PLOG/ 1.000 8.764E+75 -19.997 21412.6/
    PLOG/ 10.000 1.490E+35 -7.456 5212.7/
    PLOG/ 10.000 1.441E+76 -19.713 23978.0/
    PLOG/ 100.000 4.935E+32 -6.570 4828.0/
    PLOG/ 100.000 3.417E+62 -15.137 21450.8/
PC4H8OH-3O2=H2O+C4Y1-3OR    1.0 0.0 0.0   !well skipping no HP rates
    PLOG/ 0.100 3.387E+33 -7.100 25595.7/
    PLOG/ 1.000 3.140E+22 -3.421 24275.3/
    PLOG/ 10.000 2.115E+16 -1.596 23361.2/
    PLOG/ 100.000 1.147E+19 -2.665 25004.7/
C4H7OH-3OOH-1=>PC4H8OH-3+O2   1.0 0.0 0.0   !well skipping
    PLOG/ 0.100 6.612E+11 0.915 26372.2/
    PLOG/ 1.000 7.872E+30 -5.108 32136.7/
    PLOG/ 10.000 3.735E+39 -7.753 36288.7/
    PLOG/ 100.000 3.652E+33 -5.868 35928.0/
PC4H8OH-3+O2=>C4H7OH-3OOH-1   1.0 0.0 0.0   !well skipping
    PLOG/ 1.000 1.271E+26 -4.782 3967.4/
    PLOG/ 1.000 7.347E+35 -7.556 9650.3/
    PLOG/ 10.000 1.296E+30 -6.061 6171.3/
    PLOG/ 10.000 3.107E+63 -15.762 22804.1/
    PLOG/ 100.000 2.841E+13 -0.672 2969.5/
    PLOG/ 100.000 6.994E+59 -14.382 25697.5/
C4H7OH-3OOH-1=H2O+C4Y1-3OR   3.844E-03 3.754 2892.4
    PLOG/ 0.100 2.823E+04 1.209 3672.4/
    PLOG/ 1.000 8.674E-05 4.169 2056.3/
    PLOG/ 10.000 1.412E-03 3.868 2755.0/
    PLOG/ 100.000 6.886E+00 2.744 4099.3/
C4H7OH-3OOH-1=OH+CH3CHO+C2H3OH  1.279E+12 0.209 24453.8
    PLOG/ 0.100 8.709E-22 10.287 14400.0/
    PLOG/ 1.000 2.732E+20 -3.005 25113.7/
    PLOG/ 10.000 7.810E+20 -2.765 26428.8/
    PLOG/ 100.000 1.113E+17 -1.387 25864.1/
C4H7OH-3OOH-1=OH+C4H7OHCYO1-3   5.042E+13 -0.535 18181.4
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    PLOG/ 0.100 1.816E+07 0.875 14543.7/
    PLOG/ 1.000 1.017E+22 -3.534 19409.8/
    PLOG/ 10.000 2.381E+19 -2.443 19495.2/
    PLOG/ 100.000 6.405E+16 -1.535 19079.2/
C4H7OH-3OOH-1=CC(O)CCO+OH  1.281E-03 4.252 9750.7
    PLOG/ 0.100 9.548E-25 10.360 1196.5/
    PLOG/ 1.000 7.159E-17 8.192 4665.9/
    PLOG/ 10.000 1.443E-06 5.077 8383.8/
    PLOG/ 100.000 3.788E+00 3.139 10788.8/
!
!
! ROO4 & Subsequent QOOH Decomposition
!
!
PC4H8OH-4O2=C4H7OH-4OOH-1 7.353E-04 3.780 11442.9
    PLOG/ 0.100 2.137E-05 4.206 10733.4/
    PLOG/ 1.000 3.451E-05 4.177 10938.6/
    PLOG/ 10.000 1.215E+03 1.794 13314.3/
    PLOG/ 100.000 6.427E+01 2.219 13015.6/
PC4H8OH-4O2=C4H7OH-4OOH-2  7.843E-09 5.418 12350.7
    PLOG/ 0.100 6.263E+14 -2.842 15714.2/
    PLOG/ 1.000 6.711E+04 0.792 14330.6/
    PLOG/ 10.000 8.720E-05 3.928 12802.5/
    PLOG/ 100.000 4.486E-11 6.084 11509.1/
PC4H8OH-4O2=>O2+PC4H8OH-4  1.151E+19 -1.247 34587.8
    PLOG/ 0.100 1.660E+50 -11.484 42702.3/
    PLOG/ 1.000 1.809E+40 -8.136 40417.8/
    PLOG/ 10.000 7.348E+33 -5.998 38927.3/
    PLOG/ 100.000 7.907E+27 -4.053 37315.4/
O2+PC4H8OH-4=>PC4H8OH-4O2   1.507E+12 0.169 -3.1
    PLOG/ 0.100 1.229E+48 -12.003 7922.5/
    PLOG/ 0.100 1.930E+78 -20.705 23095.9/
    PLOG/ 1.000 1.059E+38 -8.536 5899.7/
    PLOG/ 1.000 2.261E+70 -17.871 22740.6/
    PLOG/ 10.000 2.013E+31 -6.220 4560.2/
    PLOG/ 10.000 5.915E+62 -15.207 22559.8/
    PLOG/ 100.000 8.294E+24 -4.060 3143.2/
    PLOG/ 100.000 1.246E+51 -11.427 20046.7/
C4H7OH-4OOH-1=>O2+PC4H8OH-4  1.0 0.0 0.0   !well skipping
    PLOG/ 0.100 2.221E+24 -3.770 27638.7/
    PLOG/ 1.000 1.271E+17 -1.378 27114.0/
    PLOG/ 10.000 1.394E+22 -3.087 29822.6/
    PLOG/ 100.000 1.444E+11 0.184 27195.7/
O2+PC4H8OH-4=>C4H7OH-4OOH-1  1.0 0.0 0.0   !well skipping
    PLOG/ 1.000 1.060E+17 -2.216 3514.4/
    PLOG/ 1.000 3.752E+52 -12.764 19864.8/
    PLOG/ 10.000 3.578E+08 0.459 2364.2/
    PLOG/ 10.000 4.684E+62 -15.508 29307.4/
    PLOG/ 100.000 2.638E+04 1.534 1730.2/
    PLOG/ 100.000 1.506E+39 -8.311 22710.2/
C4H7OH-4OOH-1=C4H7OHCYO1-4+OH  4.423E+05 1.373 8801.5
    PLOG/ 0.100 2.483E+14 -1.577 10804.0/
    PLOG/ 1.000 1.817E+09 0.181 9727.4/
    PLOG/ 10.000 4.035E+07 0.745 9381.5/
    PLOG/ 100.000 1.439E+06 1.210 8958.9/
C4H7OH-4OOH-2=CY(CCCO)COH+OH  2.888E+12 0.437 19917.7
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    PLOG/ 0.100 4.989E+14 -2.465 15064.5/
    PLOG/ 1.000 3.082E+33 -7.639 21800.4/
    PLOG/ 10.000 6.253E+29 -5.714 22799.8/
    PLOG/ 100.000 1.651E+17 -1.263 20607.2/
C4H7OH-4OOH-2=OH+CH2O+C3H5OH  2.854E+16 -0.511 28873.6
    PLOG/ 0.100 6.346E-54 20.834 13293.3/
    PLOG/ 1.000 3.757E+35 -8.687 29884.0/
    PLOG/ 10.000 5.351E+40 -9.292 32749.3/
    PLOG/ 100.000 2.417E+27 -4.313 30957.8/
!
!
!
! Updated thermo for new species not previously in mechanism. Estimated using  RMG (Reaction Mechanism Generator)
!
!
C4H7O-2O              C   4H   7O   2     G   100.000  5000.000 1058.65      1
 1.06252120E+01 2.37944840E-02-9.55578605E-06 1.77797221E-09-1.24965013E-13    2
-2.11411408E+04-2.23361290E+01 1.78185997E+00 4.07274573E-02-1.01967347E-05    3
-1.25234239E-08 6.72487245E-12-1.83452017E+04 2.51937987E+01                   4
 C4Y1-3OR             C   4H   7O   2     G   100.000  5000.000 1260.66      1
 7.62973590E+00 3.05137232E-02-1.35884872E-05 2.57256707E-09-1.79175557E-13    2
-2.17218129E+04-7.62305377E+00 1.90572393E+00 4.86758726E-02-3.51990075E-05    3
 1.40008421E-08-2.44552781E-12-2.02786220E+04 2.13178171E+01                   4
CC(O)CCO              C   4H   8O   2     G   100.000  5000.000 1126.09      1
 7.24007111E+00 3.30850383E-02-1.46258211E-05 2.76720370E-09-1.93081454E-13    2
-4.92173629E+04-5.07633596E+00 1.74065590E+00 5.26193902E-02-4.06461494E-05    3
 1.81715764E-08-3.61292730E-12-4.79787831E+04 2.21082827E+01                   4
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Table S18. Reaction rate constants calculated in this work for the n-pentanol ROO and QOOH decompositions. A species glossary is given in the supplemental material as an excel document.

```
! Lockwood Updated N-pentanol ROO & QOOH Rates 11-17-2021
!
! ROO1 Rates
!
C5H10OH-1O2=HO2+PC4H9CHO 1.0 0 0 ! Well skipping, no HP rates.
    PLOG/ 0.100 4.912E+35 -8.137 17182.6/
    PLOG/ 1.000 2.245E+23 -3.892 14662.1/
    PLOG/ 10.000 5.528E+18 -2.311 13718.2/
    PLOG/ 100.000 3.124E+17 -1.826 13864.5/
C5H10OH-1O2=>C5H10OH11+O2 2.449E+25 -3.034 39734.5
    PLOG/ 0.100 1.159E+49 -12.896 42374.7/
    PLOG/ 1.000 2.893E+55 -13.689 45428.6/
    PLOG/ 10.000 7.194E+41 -8.576 43598.9/
    PLOG/ 100.000 8.444E+33 -5.801 42120.7/
C5H10OH11+O2=>C5H10OH-1O2  3.089E+12 0.162 5.2
    PLOG/ 0.100 7.319E+39 -10.944 3485.6/
    PLOG/ 1.000 4.995E+44 -11.197 6236.6/
    PLOG/ 10.000 1.160E+32 -6.367 4845.2/
    PLOG/ 100.000 1.381E+21 -2.622 2584.2/
C5H10OH11+O2=HO2+PC4H9CHO     1.0 0.0 0.0 ! Well skipping, no HP rates.
    PLOG/ 0.100 8.528E+22 -3.329 2480.5/
    PLOG/ 0.100 6.721E+36 -7.129 12732.7/
    PLOG/ 1.000 2.284E+24 -3.736 3306.7/
```

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    PLOG/ 1.000 6.711E+36 -7.128 12792.3/
    PLOG/ 10.00 2.878E+24 -3.853 4090.4/
    PLOG/ 10.00 1.231E+37 -7.151 13226.9/
    PLOG/ 100.0 6.673E+09 0.842 1298.7/
    PLOG/ 100.0 1.924E+44 -9.284 19708.5/
!
!
! ROO2 Rates
!
C5H10OH-2O2=>O2+C5H10OH12 2.743E+22 -2.097 38053.0
    PLOG/ 0.100 6.010E+54 -12.718 46427.8/
    PLOG/ 1.000 1.641E+45 -9.502 44251.8/
    PLOG/ 10.000 2.494E+36 -6.596 42014.9/
    PLOG/ 100.000 1.501E+31 -4.886 40655.4/
O2+C5H10OH12=>C5H10OH-2O2 1.0 0.0 0.0
    PLOG/ 0.10 1.302E+23 -4.125 -0.3/
    PLOG/ 0.10 1.568E+71 -18.525 19110.2/
    PLOG/ 1.000 5.084E+40 -9.251 6752.3/
    PLOG/ 1.000 7.795E+83 -21.864 28807.9/
    PLOG/ 10.000 3.467E+31 -6.164 4669.2/
    PLOG/ 10.000 3.557E+70 -17.456 26224.7/
    PLOG/ 100.000 6.129E+25 -4.244 3301.7/
    PLOG/ 100.000 4.674E+51 -11.540 20008.9/
C5H10OH-2O2=C5H9OH-2OOH-1 8.287E-12 6.616 16058.0
    PLOG/ 0.100 5.163E-25 10.477 10850.6/
    PLOG/ 1.000 3.250E-21 9.469 12684.1/
    PLOG/ 10.000 9.940E-06 4.614 17605.2/
    PLOG/ 100.000 2.163E-05 4.568 17971.8/
C5H10OH-2O2=C5H9OH-2OOH-4 2.307E-01 3.330 15359.3
    PLOG/ 1.000 3.987E-05 4.363 13661.8/
    PLOG/ 10.000 5.299E-06 4.768 13828.0/
    PLOG/ 100.000 9.595E+03 1.856 16739.0/
C5H10OH-2O2=C5H9OH-2OOH-5  5.603E-04 3.910 16993.7
    PLOG/ 0.100 6.984E+00 2.697 18093.5/
    PLOG/ 1.000 1.145E+04 1.730 19215.1/
    PLOG/ 10.000 6.941E+11 -0.733 21594.4/
    PLOG/ 100.000 7.853E+09 -0.087 21123.2/
C5H10OH-2O2=CH2O+OH+NC3H7CHO 1.0 0.0 0.0 ! well skipping over QOOH-0 well
    PLOG/ 0.100 2.665E+38 -8.523 32832.2/
    PLOG/ 1.000 2.227E+33 -6.848 31554.6/
    PLOG/ 10.000 1.729E+29 -5.510 30449.0/
    PLOG/ 100.000 9.042E+26 -4.768 29820.3/
C5H9OH-2OOH-1=C5H9O1-2OH-1+OH 9.473E+12 -0.797 9651.1
    PLOG/ 0.100 1.028E+25 -4.921 12160.2/
    PLOG/ 1.000 3.034E+17 -2.311 10691.1/
    PLOG/ 10.000 2.603E+14 -1.269 10029.1/
    PLOG/ 100.000 1.873E+14 -1.210 10043.1/
C5H9OH-2OOH-1=HO2+C5H9OH1-1 1.012E+10 -0.171 13784.2
    PLOG/ 0.100 1.233E+32 -7.726 18481.2/
    PLOG/ 1.000 4.001E+19 -3.374 16094.7/
    PLOG/ 10.000 7.558E+12 -1.110 14551.5/
    PLOG/ 100.000 1.192E+12 -0.832 14400.8/
C5H9OH-2OOH-4=>O2+C5H10OH12 1.0 0.0 0.0 ! well skipping
    PLOG/ 1.000 4.560E-14 8.956 18613.8/
    PLOG/ 10.000 7.052E-02 5.075 22762.2/
    PLOG/ 100.000 1.101E+17 -0.884 28939.0/
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O2+C5H10OH12=>C5H9OH-2OOH-4 1.0 0.0 0.0 ! well skipping
   PLOG/ 10.000 2.984E-07 5.509 -1050.8/
   PLOG/ 10.000 3.944E-27 12.522 -0.9/
   PLOG/ 100.000 3.742E-02 3.639 881.8/
   PLOG/ 100.000 4.722E+29 -5.243 19230.8/
C5H9OH-2OOH-4=CH2O+OH+NC3H7CHO 1.0 0.0 0.0 ! well skipping
   PLOG/ 1.000 1.356E+25 -4.730 18053.6/
   PLOG/ 10.000 1.247E+23 -3.636 18704.0/
   PLOG/ 100.000 2.030E+24 -3.878 19687.3/
C5H9OH-2OOH-4=OH+C5H9O2-4OH-1  3.412E+13 -0.668 14951.8
   PLOG/ 1.000 5.588E+23 -4.514 16130.1/
   PLOG/ 10.000 1.758E+18 -2.321 15825.2/
   PLOG/ 100.000 2.448E+16 -1.601 15718.2/
C5H9OH-2OOH-5=CH2O+OH+NC3H7CHO 1.0 0.0 0.0  ! well skipping
   PLOG/ 0.100 2.901E+26 -5.352 14115.3/
   PLOG/ 1.000 2.641E+21 -3.451 13556.0/
   PLOG/ 10.000 9.962E+16 -1.942 12605.6/
   PLOG/ 100.000 6.489E+14 -1.218 12110.0/
C5H9OH-2OOH-5=>O2+C5H10OH12 1.0 0 0 ! well skipping
   PLOG/ 0.100 1.580E-01 4.485 19000.8/
   PLOG/ 1.000 8.897E+06 2.054 22221.9/
   PLOG/ 10.000 2.564E+19 -2.051 26832.0/
   PLOG/ 100.000 8.089E+11 0.122 25320.1/
O2+C5H10OH12=>C5H9OH-2OOH-5 1.0 0 0 ! well skipping
   PLOG/ 1.000 3.735E-01 3.418 240.7/
   PLOG/ 1.000 1.168E+07 1.349 5079.6/
   PLOG/ 10.000 6.686E+05 1.239 2709.1/
   PLOG/ 10.000 2.854E+47 -10.887 24293.9/
   PLOG/ 100.000 2.502E-02 3.420 1315.7/
   PLOG/ 100.000 3.386E+28 -5.177 18844.4/
C5H9OH-2OOH-5=OH+C5H9O2-5OH-1 1.346E+07 0.870 11174.9
   PLOG/ 0.100 5.487E+22 -4.606 14143.8/
   PLOG/ 1.000 2.257E+16 -2.220 13370.0/
   PLOG/ 10.000 1.019E+12 -0.715 12517.9/
   PLOG/ 100.000 1.618E+10 -0.114 12086.8/
!
!
! ROO3 Rates
!
C5H10OH-3O2=C5H9OH-3OOH-1   2.856E+04 2.219 15174.2
   PLOG/ 0.100 3.353E+01 2.978 13700.9/
   PLOG/ 1.000 5.608E+00 3.343 13870.4/
   PLOG/ 10.000 1.877E+12 -0.341 17228.6/
   PLOG/ 100.000 6.809E+10 0.157 16960.9/
C5H10OH-3O2=C5H9OH-3OOH-5   3.016E+02 2.772 18660.3
   PLOG/ 1.000 1.021E+04 2.022 18172.2/
   PLOG/ 10.000 1.144E-05 5.114 16387.1/
   PLOG/ 100.000 6.273E+11 -0.256 21195.2/
C5H10OH-3O2=>C5H10OH13+O2   1.665E+28 -3.431 39175.6
   PLOG/ 0.100 4.397E+69 -17.315 48899.7/
   PLOG/ 1.000 6.876E+60 -14.233 47283.1/
   PLOG/ 10.000 7.041E+58 -13.407 47434.8/
   PLOG/ 100.000 1.145E+44 -8.563 43556.3/
C5H10OH-3O2=H2O+NC5KET13O 1.0 0.0 0.0 ! well skipping, no HP rates
   PLOG/ 0.010 8.661E+33 -7.472 24614.9/
   PLOG/ 0.100 4.639E+15 -1.373 21364.6/
```

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   PLOG/ 1.000 9.344E-02 3.983 17966.2/
   PLOG/ 10.000 3.004E+40 -9.750 29772.1/
   PLOG/ 100.000 4.871E+09 -0.055 21745.8/
C5H10OH13+O2=>C5H10OH-3O2 3.003E+12 0.166 0.6
   PLOG/ 1.000 2.081E+43 -10.632 5393.9/
   PLOG/ 1.000 4.441E+73 -19.388 19731.9/
   PLOG/ 10.000 3.031E+21 -3.485 -11.1/
   PLOG/ 10.000 3.726E+56 -13.859 14341.3/
   PLOG/ 100.000 4.902E+32 -6.635 4627.4/
   PLOG/ 100.000 3.955E+65 -16.153 22066.2/
C5H9OH-3OOH-1=>C5H10OH13+O2    1.0 0.0 0.0   ! Well skipping, no HP rates
   PLOG/ 0.100 4.578E+21 -2.306 26972.3/
   PLOG/ 1.000 1.682E+36 -6.885 32095.9/
   PLOG/ 10.000 2.417E+42 -8.851 35271.3/
   PLOG/ 100.000 1.060E+37 -7.211 34993.3/
C5H10OH13+O2=>C5H9OH-3OOH-1 1.0 0.0 0.0 ! well skipping, no HP rates
   PLOG/ 1.000 1.560E+09 0.657 0.9/
   PLOG/ 1.000 6.938E+45 -10.645 12930.5/
   PLOG/ 10.000 3.195E+26 -4.943 5931.7/
   PLOG/ 10.000 7.297E+67 -17.067 25562.2/
   PLOG/ 100.000 2.548E-06 4.726 -4086.1/
   PLOG/ 100.000 1.671E+39 -8.294 15632.4/
C5H9OH-3OOH-1=H2O+NC5KET13O 1.393E-03 3.588 614.1
   PLOG/ 0.100 1.791E-04 3.740 -97.3/
   PLOG/ 1.000 5.814E-07 4.635 -470.7/
   PLOG/ 10.000 6.534E-03 3.366 821.5/
   PLOG/ 100.000 1.663E-01 2.938 1327.0/
C5H9OH-3OOH-1=C5H9O1-3OH-1+OH   7.315E+09 0.355 14740.9
   PLOG/ 0.100 3.034E+18 -2.881 15778.4/
   PLOG/ 1.000 1.270E+16 -1.782 16066.0/
   PLOG/ 10.000 1.039E+14 -0.998 15866.4/
   PLOG/ 100.000 3.981E+12 -0.518 15556.5/
C5H9OH-3OOH-1=OH+C2H5CHO+C2H3OH 7.074E+08 1.126 22608.3
   PLOG/ 0.100 1.725E+04 1.948 19694.6/
   PLOG/ 1.000 1.053E+17 -1.765 24065.1/
   PLOG/ 10.000 2.413E+15 -1.024 24301.4/
   PLOG/ 100.000 2.834E+13 -0.357 23923.2/
C5H9OH-3OOH-5=C5H9OH-3OOH-1  2.513E+04 2.077 9217.4
   PLOG/ 1.000 7.814E-13 7.263 4041.6/
   PLOG/ 10.000 2.767E-10 6.525 5065.8/
   PLOG/ 100.000 1.099E+04 2.158 8965.9/
C5H9OH-3OOH-5=>C5H10OH13+O2   1.0 0.0 0.0  ! Well skipping, no HP rates
   PLOG/ 1.000 5.113E+08 1.907 21503.0/
   PLOG/ 10.000 5.335E+13 0.515 24388.5/
   PLOG/ 100.000 1.927E+24 -2.904 28678.5/
C5H10OH13+O2=>C5H9OH-3OOH-5 1.0 0.0 0.0  ! Well skipping, no HP rates
      PLOG/ 1.000 1.040E+09 0.180 941.3/
   PLOG/ 1.000 4.524E-68 25.830 -13979.4/
   PLOG/ 10.000 3.677E+02 2.452 601.4/
   PLOG/ 10.000 2.540E+15 -1.322 6629.4/
   PLOG/ 100.000 1.761E+10 -0.084 3761.1/
   PLOG/ 100.000 5.775E+54 -13.071 26273.2/
C5H9OH-3OOH-5=C5H9O3-5OH-1+OH    2.038E+11 -0.119 18286.1
   PLOG/ 1.000 2.132E+28 -6.460 20456.4/
   PLOG/ 10.000 7.774E+19 -3.135 19843.5/
   PLOG/ 100.000 3.925E+15 -1.550 19314.5/
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NC5KET13O=C2H5CHO+CH2CHO  7.769E+11 0.408 11384.3
   PLOG/ 1.000 2.639E+38 -8.786 16598.2/
   PLOG/ 10.000 4.434E+29 -5.613 15292.2/
   PLOG/ 100.000 6.320E+20 -2.564 13512.6/
!
! ROO4 Rates
!
C5H10OH-4O2=>O2+C5H10OH14  2.958E+34 -5.116 39813.8
   PLOG/ 0.100 9.490E+83 -21.957 50595.9/
   PLOG/ 1.000 2.072E+76 -19.138 49619.4/
   PLOG/ 10.000 2.967E+67 -16.033 48056.9/
   PLOG/ 100.000 3.819E+57 -12.680 45901.2/
O2+C5H10OH14=>C5H10OH-4O2 3.003E+12 0.166 0.6
   PLOG/ 0.100 6.107E+73 -20.669 13533.7/
   PLOG/ 0.100 2.455E+101 -28.891 26378.5/
   PLOG/ 1.000 2.420E+59 -15.686 10609.1/
   PLOG/ 1.000 6.234E+102 -28.918 28426.3/
   PLOG/ 10.000 3.527E+57 -14.962 10578.0/
   PLOG/ 10.000 1.825E+89 -24.166 26283.8/
   PLOG/ 100.000 6.181E+46 -11.264 8399.4/
   PLOG/ 100.000 1.389E+81 -21.200 26269.0/
C5H10OH-4O2=C5H9O1-4OH-1+OH  1.0 0.0 0.0   ! well skipping, no HP rates
   PLOG/ 0.100 2.106E+37 -8.005 29669.3/
   PLOG/ 1.000 6.867E+63 -16.768 37707.1/
   PLOG/ 10.000 2.803E+65 -17.495 38862.4/
   PLOG/ 100.000 1.396E+24 -4.289 28331.1/
C5H10OH-4O2=C5H9OH-4OOH-1     3.662E+07 1.052 14523.6
   PLOG/ 0.100 1.479E+06 1.343 13549.7/
   PLOG/ 1.000 1.568E+13 -0.875 15688.3/
   PLOG/ 10.000 1.254E+13 -0.798 15837.7/
   PLOG/ 100.000 2.191E+12 -0.522 15752.3/
C5H10OH-4O2=C5H9OH-4OOH-2   3.131E+05 1.876 15964.5
   PLOG/ 1.000 6.972E+06 1.055 14976.2/
   PLOG/ 10.000 2.467E+02 2.723 14516.9/
   PLOG/ 100.000 8.198E+08 0.695 16618.9/
C5H9OH-4OOH-1=>O2+C5H10OH14 1.0 0.0 0.0  ! well skipping, no HP rates
   PLOG/ 0.100 3.622E+54 -13.138 34098.9/
   PLOG/ 1.000 3.001E+64 -16.146 38452.4/
   PLOG/ 10.000 1.170E+58 -13.968 38453.5/
   PLOG/ 100.000 6.401E+49 -11.341 37505.2/
O2+C5H10OH14=>C5H9OH-4OOH-1 1.0 0.0 0.0  ! well skipping, no HP rates
   PLOG/ 1.000 2.965E+51 -13.524 9840.1/
   PLOG/ 1.000 6.245E+76 -20.838 21768.8/
   PLOG/ 10.000 5.600E+186 -59.319 41632.0/
   PLOG/ 10.000 8.123E+52 -13.152 15595.4/
   PLOG/ 100.000 5.214E+20 -3.488 4410.8/
   PLOG/ 100.000 1.394E+59 -14.825 22087.6/
C5H9OH-4OOH-1=C5H9O1-4OH-1+OH  1.720E+10 0.183 10706.9
   PLOG/ 0.100 3.446E+22 -4.042 13276.6/
   PLOG/ 1.000 2.573E+17 -2.203 12466.1/
   PLOG/ 10.000 5.641E+13 -0.956 11685.5/
   PLOG/ 100.000 1.267E+12 -0.412 11267.5/
C5H9OH-4OOH-1=OH+C3H6OHCOCH3      2.896E-05 4.553 12534.7! new species in mechanism
!(5_hydroxy_2_pentanone, SMILES=CC(=O)CCCO )
   PLOG/ 0.100 4.629E+00 2.763 13184.7/
   PLOG/ 1.000 9.409E-03 3.568 12450.4/
```

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   PLOG/ 10.000 2.006E-01 3.272 13430.2/
   PLOG/ 100.000 8.907E-02 3.434 13548.9/
C5H9OH-4OOH-2=>O2+C5H10OH14   1.0 0.0 0.0   ! well skipping, no HP rates
   PLOG/ 1.000 5.519E-16 10.387 17735.2/
   PLOG/ 10.000 1.879E+23 -2.248 27690.1/
   PLOG/ 100.000 9.667E+34 -5.931 32396.6/
O2+C5H10OH14=>C5H9OH-4OOH-2  1.0 0.0 0.0   ! well skipping, no HP rates
   PLOG/ 100.000 1.903E+21 -3.680 4905.7/
   PLOG/ 100.000 1.576E+58 -14.538 22360.9/
C5H9OH-4OOH-2=OH+C5H9O2-4OH-1  1.186E+14 -0.172 19194.2
   PLOG/ 1.000 5.732E+21 -3.968 17536.3/
   PLOG/ 10.000 6.375E+23 -3.859 20047.1/
   PLOG/ 100.000 3.618E+16 -1.128 19304.9/
!
```

B) Predicted modeling data:

Table S19. Predicted IDT values for n-butanol.

P = 15 bar, Phi = 1						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Weber[3])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Saggese et al.[4])**	**Predicted IDT (current work)**
725	1.38	66.76	725	1.38	36.4	80.0
737	1.36	49.8	737	1.36	33.3	73.0
758	1.32	36.16	758	1.32	28.1	66.0
784	1.27	28.64	784	1.27	21.8	46.7
787	1.27	23.24	787	1.27	21.0	46.3
816	1.23	20.64	816	1.23	14.7	32.5
826	1.21	17.6	826	1.21	12.9	28.6
839	1.19	15.32	839	1.19	10.7	24.8
P = 20 bar, Phi = 1						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Agbro[5])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Saggese et al.[4])**	**Predicted IDT (current work)**
848	1.18	5.8	854	1.17	6.6	12.3
828	1.21	6.5	830	1.20	7.9	14.5
805	1.24	8.5	810	1.23	8.5	19.8
775	1.29	13.0	781	1.28	14.9	29.8
756	1.32	14.5	763	1.31	17.7	33.1
737	1.36	19.7	744	1.34	24.3	53.4
722	1.38	29.5	726	1.38	28.2	51.8
696	1.44	37.9	700	1.43	50	80.3

[3] B. W. Weber, K. Kumar, Y. Zhang, and C.-J. Sung, Autoignition of n-butanol at elevated pressure and low-to-intermediate temperature, *Combust. Flame* 158 (5) (2001) 809–819.

[4] C. Saggese *et al.*, An improved detailed chemical kinetic model for C3-C4 linear and iso-alcohols and their blends with gasoline at engine-relevant conditions, *Proc. Combust. Inst.* 38 (2020) 415-423.

[5] E. Agbro, A. S. Tomlin, M. Lawes, S. Park, and S. M. Sarathy, "The influence of n-butanol blending on the ignition delay times of gasoline and its surrogate at high pressures," *Fuel* 187 (2017) 211–219.

671	1.49	59.2	678	1.47	111.5	179
P = 30 bar, Phi = 1						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Weber[3])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Saggese et al.[4])**	**Predicted IDT (current work)**
678	1.474	72.32	678	1.474	60.9	95.4
680	1.470	67.8	680	1.471	51.9	80.4
695	1.44	42.24	695	1.44	29.0	43.9
708	1.41	23.24	708	1.41	18.9	29.9
725	1.38	13.32	725	1.38	14.3	24.3
739	1.35	12.24	739	1.35	10.6	19.3
750	1.33	9.96	750	1.33	8.3	15.8
761	1.31	7.72	761	1.31	7.1	14.0

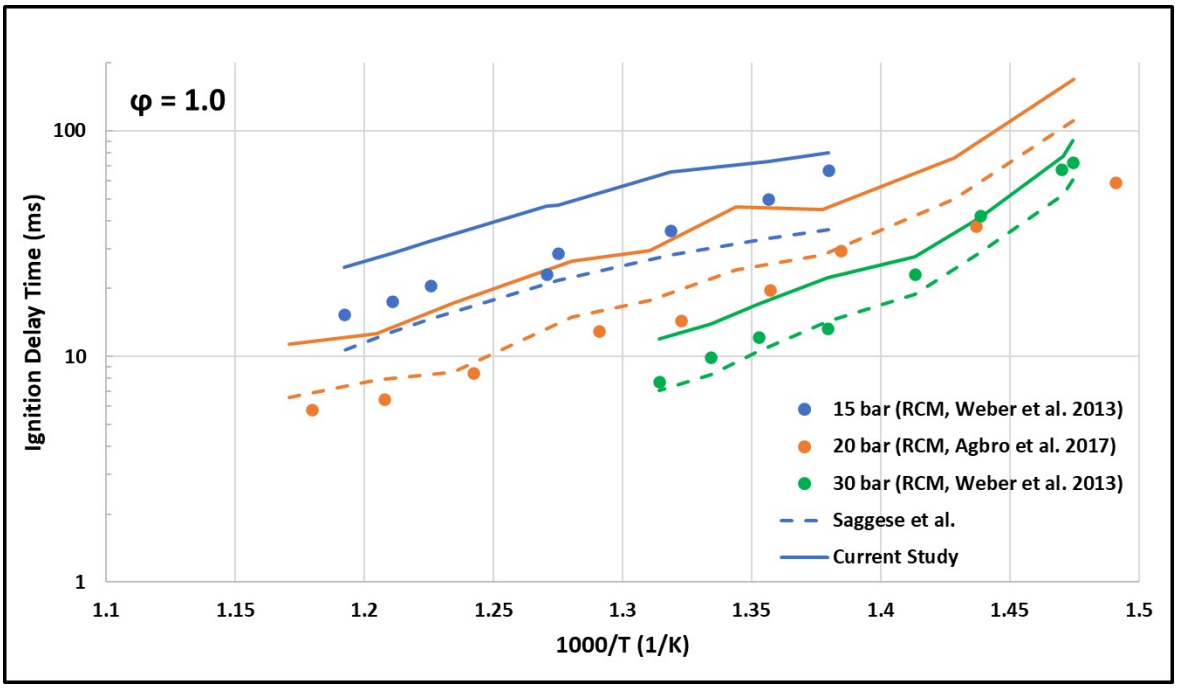

Figure S10. Comparison of predicted n-butanol IDTs between the Saggese et al.[4] and updated mechanisms.

Table S20. Predicted IDT values for n-pentanol.

P = 9 bar, Phi = 1 (Shock Tube)						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Heufer et al.[6])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Sarathy et al.[7])**	**Predicted IDT (current work)**
1209	0.83	0.10	880	1.14	18.38	21.90
1149	0.87	0.19	900	1.11	15.41	17.80
1086	0.92	0.45	920	1.09	12.27	13.70
1069	0.94	0.65	940	1.06	9.39	10.20

[6] K. A. Heufer, J. Bugler, and H. J. Curran, A comparison of longer alkane and alcohol ignition including new experimental results for n-pentanol and n-hexanol, *Proc. Combust. Inst.* 34 (2013) 511-518.
[7] S. M. Sarathy, P. Oßwald, N. Hansen, and K. Kohse-Höinghaus, Alcohol combustion chemistry, *Prog. Energy Combust. Sci.* 44 (2014) 40–102.

1012	0.99	0.98	960	1.04	6.98	7.40
950	1.05	1.94	980	1.02	5.10	5.34
963	1.04	2.08	1000	1.00	3.70	3.83
920	1.09	3.15	1020	0.98	2.68	2.75
882	1.13	5.13	1040	0.96	1.95	2.00
			1060	0.94	1.43	1.47
			1080	0.93	1.06	1.09
			1100	0.91	0.80	0.83
			1120	0.89	0.61	0.63
			1140	0.88	0.47	0.48
			1160	0.86	0.36	0.38
			1180	0.85	0.29	0.30
			1200	0.83	0.22	0.23
			1220	0.82	0.18	0.19
P = 30 bar, Phi = 1 (Shock Tube)						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Heufer et al.[6])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Sarathy et al.[8])**	**Predicted IDT (current work)**
1124	0.89	0.09	720	1.39	15.70	14.5
1090	0.92	0.19	740	1.35	8.89	8.1
1091	0.92	0.22	760	1.32	5.52	5.0
1038	0.96	0.33	780	1.28	3.79	3.4
980	1.02	0.81	800	1.25	2.92	2.6
925	1.08	1.01	820	1.22	2.51	2.3
914	1.09	1.20	840	1.19	2.37	2.3
885	1.13	1.35	860	1.16	2.40	2.5
834	1.20	1.77	880	1.14	2.45	2.8
819	1.22	1.65	900	1.11	2.40	2.9
752	1.33	2.33	920	1.09	2.22	2.7
736	1.36	3.79	940	1.06	1.94	2.30
			960	1.04	1.61	1.90
			980	1.02	1.29	1.50
			1000	1.00	1.01	1.10
			1020	0.98	0.77	0.83
			1040	0.96	0.59	0.62
			1060	0.94	0.44	0.46
			1080	0.93	0.34	0.34
			1100	0.91	0.26	0.26
			1120	0.89	0.20	0.2
			1140	0.88	0.15	0.15
P = 10 bar, Phi = 1 (RCM)						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Pelucchi et al.[8])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Sarathy et al.[8])**	**Predicted IDT (current work)**
711	1.406	85.0	710	1.4075	837.20	684.00

[8] M. Pelucchi *et al.*, Combustion of n-C3–C6 Linear Alcohols: An Experimental and Kinetic Modeling Study. Part II: Speciation Measurements in a Jet-Stirred Reactor, Ignition Delay Time Measurements in a Rapid Compression Machine, Model Validation, and Kinetic Analysis, *Energy Fuels*, 34 (11) (2020) 14708–14725.

710	1.408	77.7	725	1.3793	157.20	133.20
711	1.406	76.3	743	1.3459	56.90	51.20
710	1.408	77.2	762	1.3123	25.90	24.20
725	1.379	45.4	780	1.2821	19.00	20.20
725	1.379	47.5	797	1.2547	17.91	19.60
725	1.379	44.1	817	1.224	19.00	22.00
743	1.346	26.9	837	1.1947	21.95	27.00
744	1.344	30.3				
742	1.348	28.9				
743	1.346	27.1				
761	1.314	25.9				
762	1.312	24.1				
762	1.312	23.1				
779	1.284	26.2				
781	1.280	24.5				
780	1.282	23.9				
797	1.255	27.6				
796	1.256	26.6				
797	1.255	27.0				
817	1.224	30.5				
816	1.225	31.3				
818	1.222	31.1				
837	1.195	32.0				
836	1.196	31.6				
838	1.193	33.3				
P = 19 bar, Phi = 1 (RCM)						
Temp (K)	**1000/T (1/K)**	**Experimental IDT (Heufer et al.[6])**	**Temp (K)**	**1000/T (1/K)**	**Predicted IDT (Sarathy et al.[8])**	**Predicted IDT (current work)**
675	1.481	78.0	357	1.48	1252	1112
675	1.481	84.0	364	1.45	420	344
691	1.447	43.0	382	1.42	59	51
688	1.453	34.8				
704	1.420	20.8				
705	1.418	16.3				

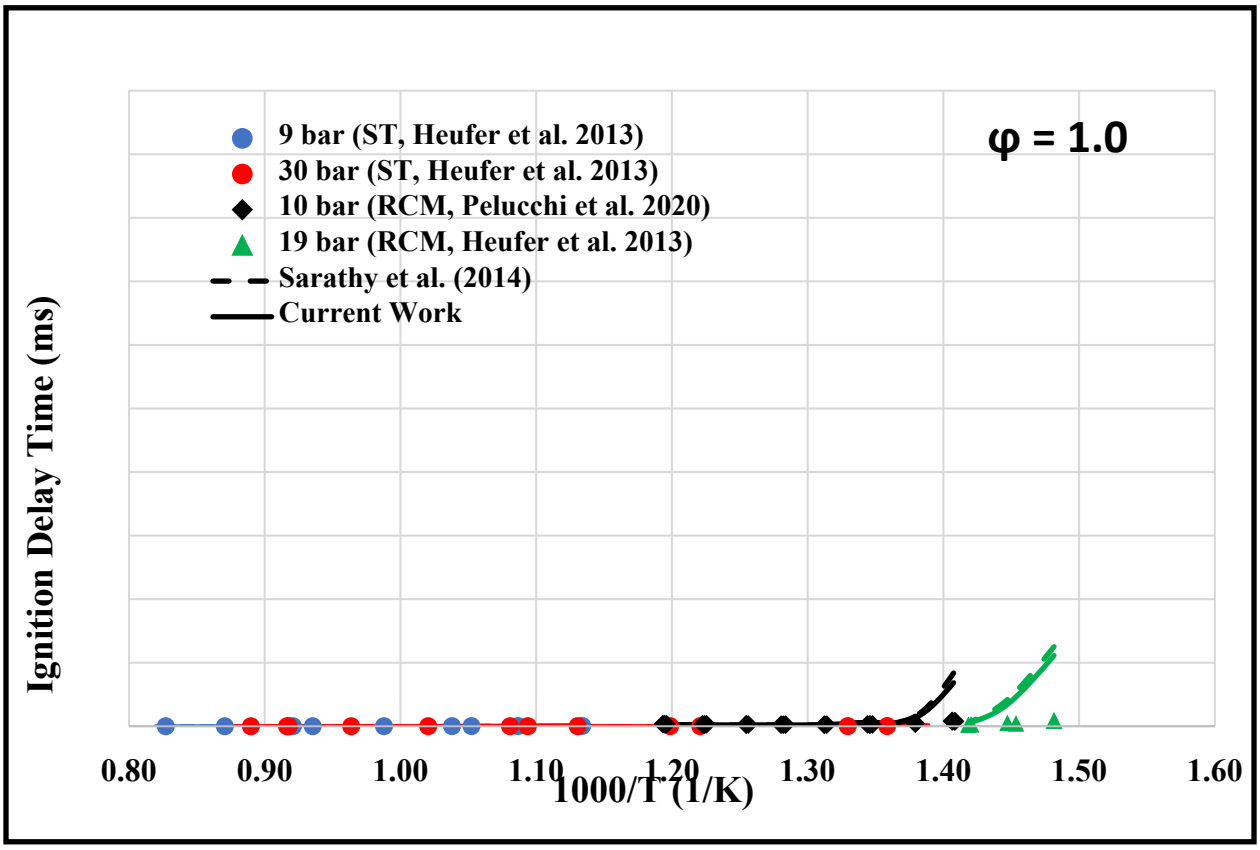

Figure S11. Comparison of predicted n-pentanol IDTs between the base and updated mechanisms.