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Supplementary Information

Synthesis of 3-alkoxypropan-1,2-diols from glycidol: experimental and theoretical studies for the optimization of the synthesis of glycerol derived solvents

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Electronic Supplementary Material (ESI) for Green Chemistry.

1. Product characterization

Gas chromatography was carried out in a Hewlett Packard 7890 series II Gas Chromatograph using a column of phenyl silicone 5.5% (Zebron Inferno 30 m x 0.25 mm x 0.25 μm) and Helium as carrier gas.

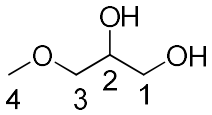
280 ºC injector temperature, 250 ºC detector temperature. Temperature program: initial T 80 º C for 3 min., Temperature gradient 5 ºC min^{-1} until 110 ºC, Temperature gradient 20 ºC min^{-1} until 230 ºC, 230 ºC isotherm for 5 min.

^{1}H- and ^{13}C-NMR spectra (DMSO, δ ppm, J Hz) were obtained using a Bruker AV-400 instrument with TMS as standard.

Mass spectroscopy was carried out in a Bruker MicroTof-Q, by electrospray ionization.

Boiling points were determined using differential scanning calorimetric (DSC) analysis in a TA Instruments DSC-Q20, calibrated with indium, using micropore aluminum pans, in a range of 298–673K, at atmospheric pressure. Boiling points were determined using onset temperature.

2. Products description



3-Methoxypropan-1,2-diol [1.0.0], CAS 623-39-2: Colorless liquid, b.p. = 222 ºC, **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 4.61 (d, 1H, *J* = 5.1 Hz, OH_2), 4.46 (t, 1H, *J* = 5.7 Hz, OH_1), 3.56 (sext, 1H, *J* = 5.1 Hz, H_2), 3.18-3.36 (m, 4H, H_1, H_{3a}, H_{3b}), 3.23 (s, 3H, H_4). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 74.2 (CH_2, C_3), 70.3 (CH, C_2), 62.9 (CH_2, C_1), 58.3 (CH_3, C_4). **HRMS** (ESI^+): *m/z* calc. = 129.0522, *m/z* found = 129.0527 ($M+Na^+$).

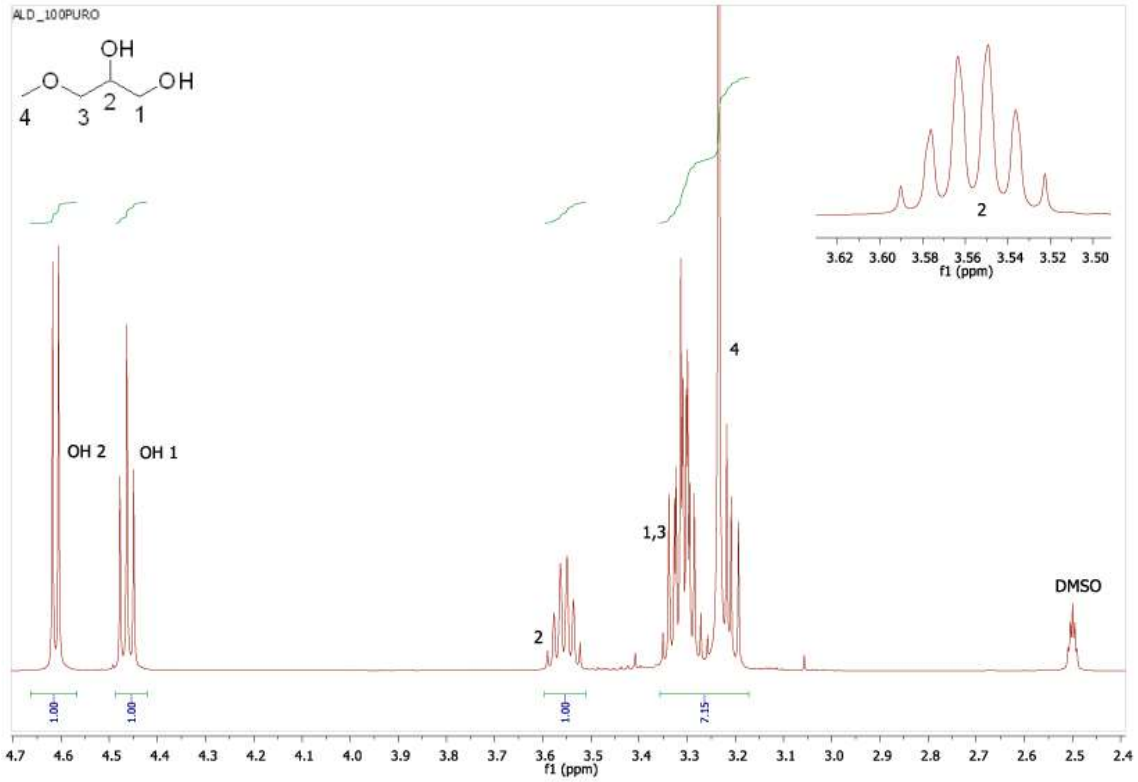


Figure S-1. [1]H-RMN of 3-methoxypropan-1,2-diol [1.0.0]

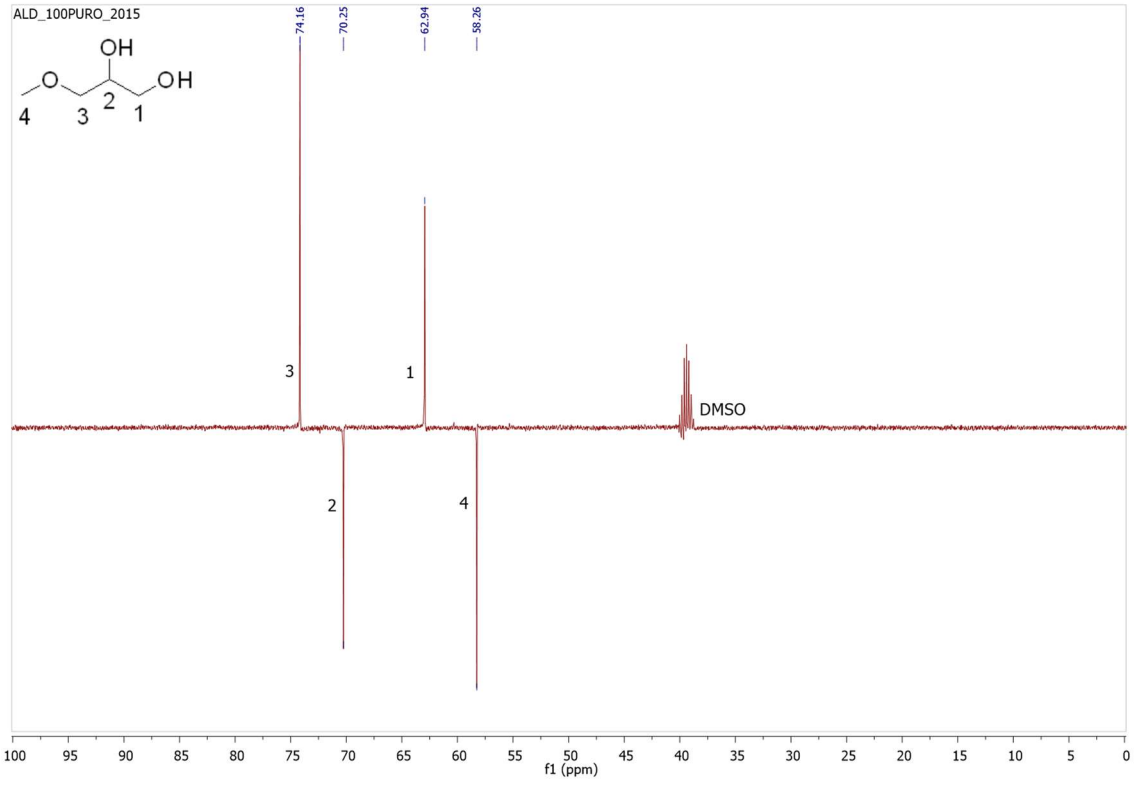


Figure S-2. [13]C-RMN (APT) of 3-methoxypropan-1,2-diol [1.0.0].

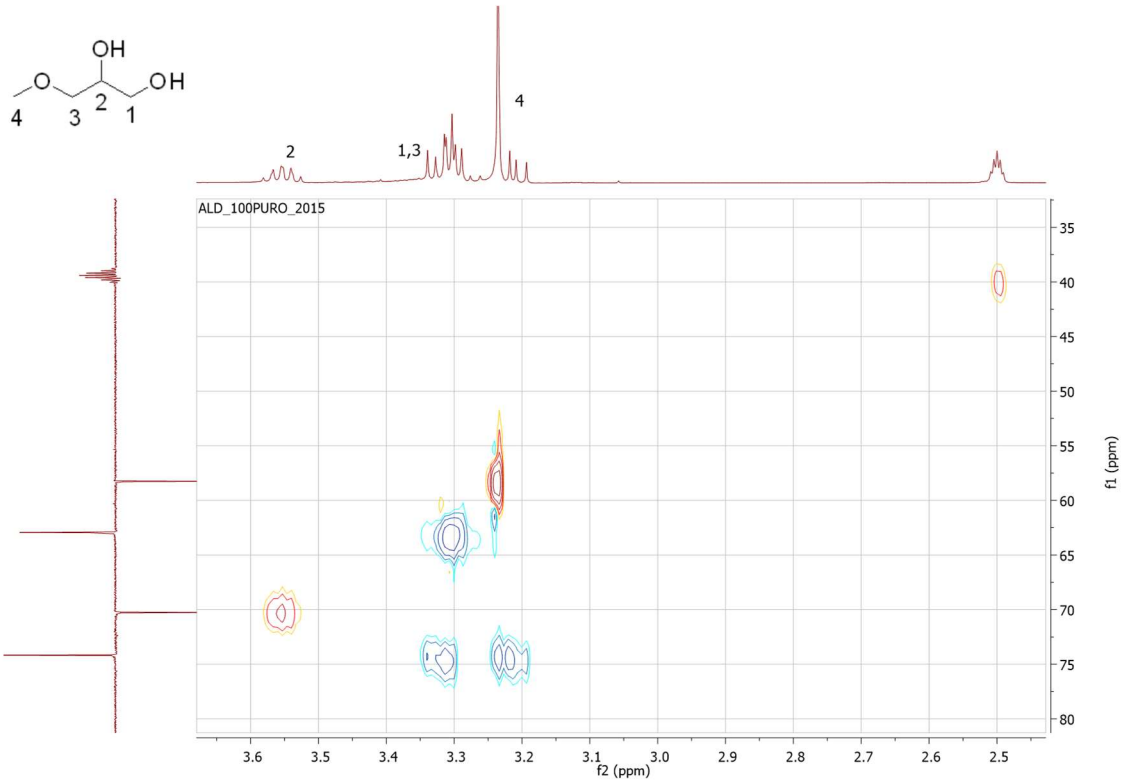
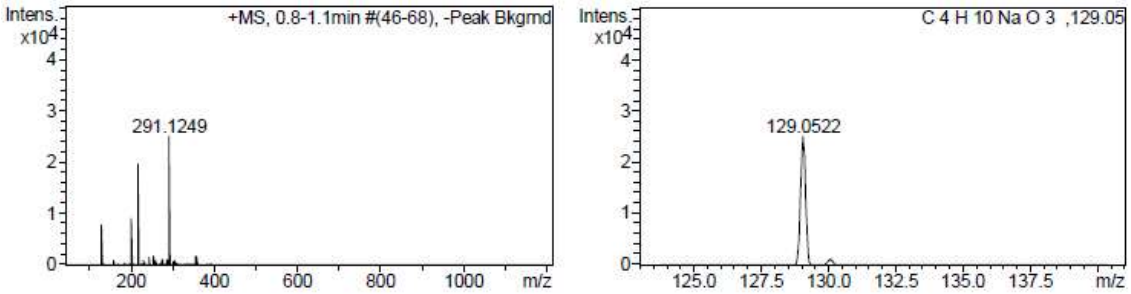


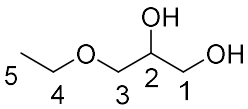
Figure S-3. HSQC of 3-methoxypropan-1,2-diol [1.0.0].



m/z	z	I	FWHM
129.0527		7855	0.0223
203.0909		9115	0.0297
217.1053		19677	0.0320

m/z	z	I	FWHM
129.0522		25044	0.2000
130.0556		1141	0.2000
131.0565		157	0.2000

Figure S4 . HRMS of 3-methoxypropan-1,2-diol [1.0.0].



3-ethoxypropan-1,2-diol [2.0.0], CAS 1874-62-0: Colorless liquid, b.p. = 221 ºC. **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 4.59 (d, 1H, *J* = 5.1 Hz, OH_2), 4.45 (t, 1H, *J* = 5.7 Hz, OH_1), 3.55 (sext, 1H, *J* = 5.3 Hz, H_2), 3.42 (q, 2H, *J* = 7.0 Hz, H_4), 3.21-3.37 (m, 4H, H_1, H_{3a}, H_{3b}), 1.10 (t, 3H, *J* = 7.0 Hz, H_5). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 72.3 (CH_2, C_3), 70.8 (CH, C_2), 66.0 (CH_2, C_4), 63.4 (CH_2, C_1), 15.4 (CH_3, C_5). **HRMS** (ESI^+): *m/z* calc. = 143.0679, *m/z* found = 143.0680 ($M+Na^+$).

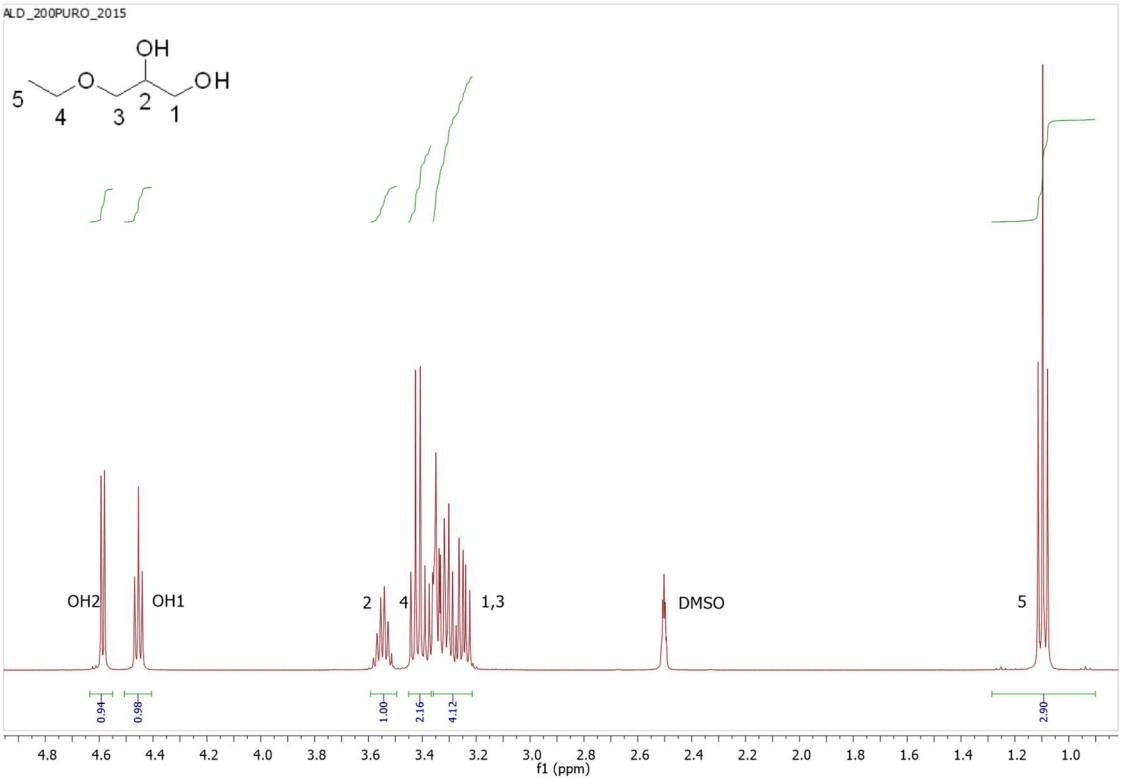


Figure S-5. ^{1}H-RMN of 3-ethoxypropan-1,2-diol [2.0.0]

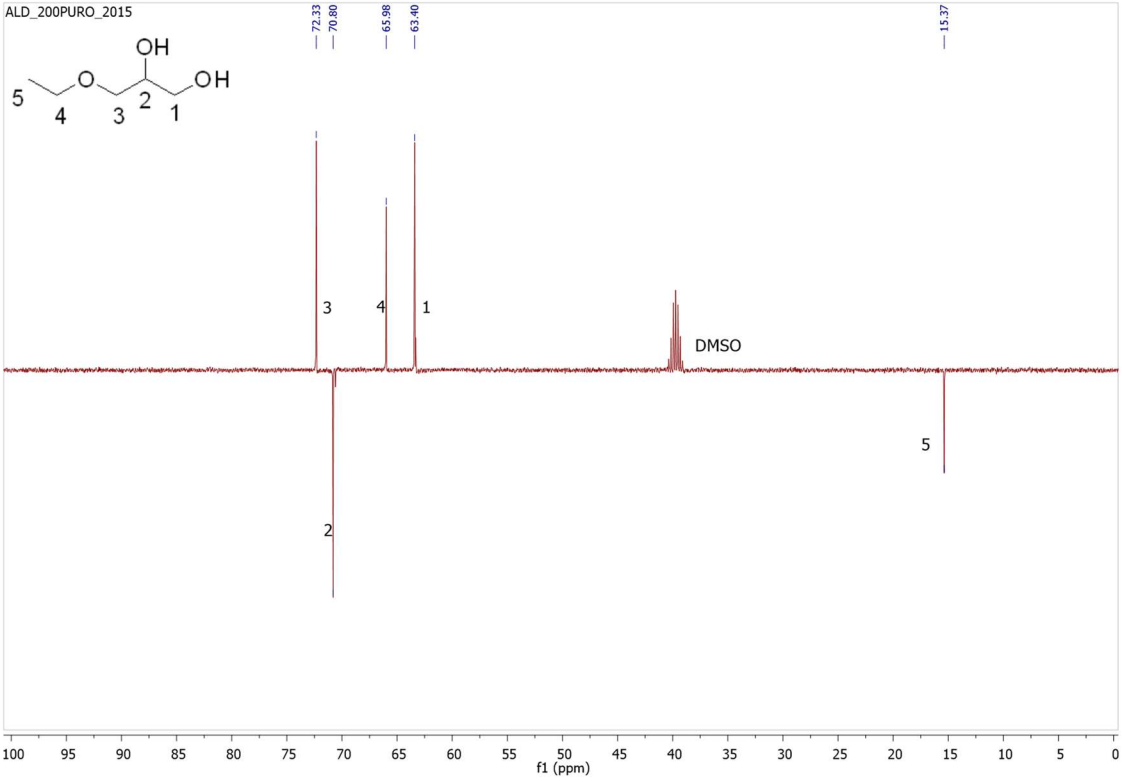


Figure S-6. ^{13}C-RMN (APT) of 3-ethoxypropan-1,2-diol [2.0.0].

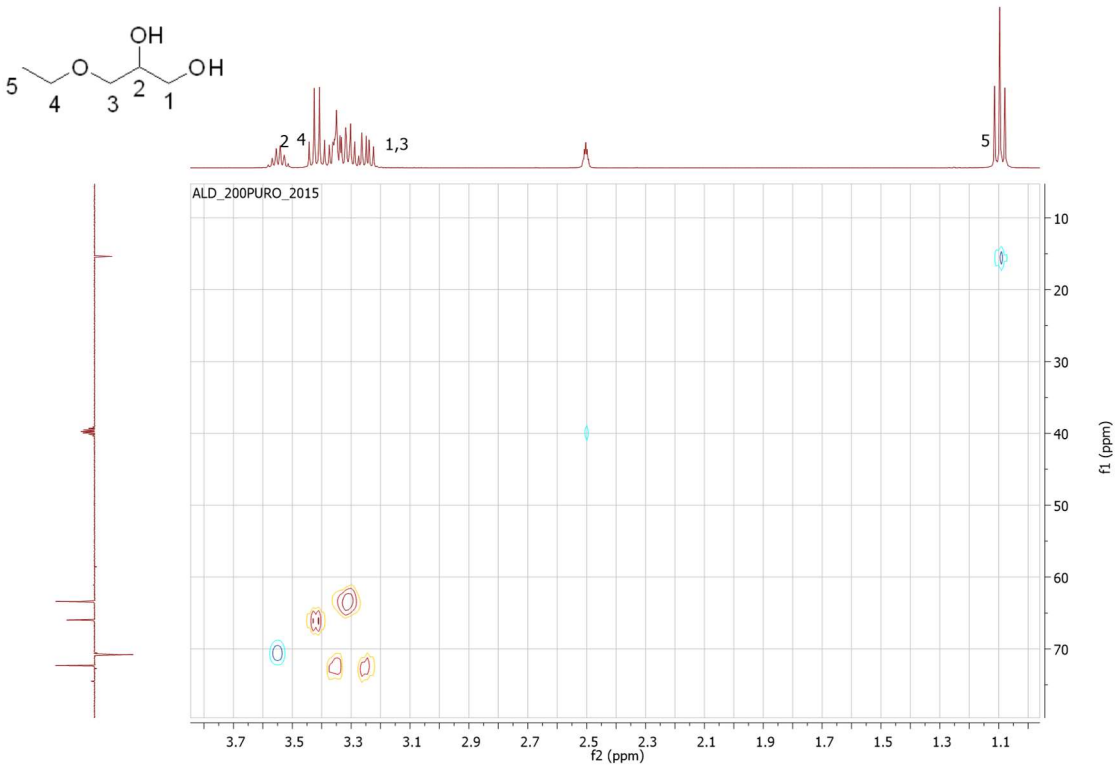
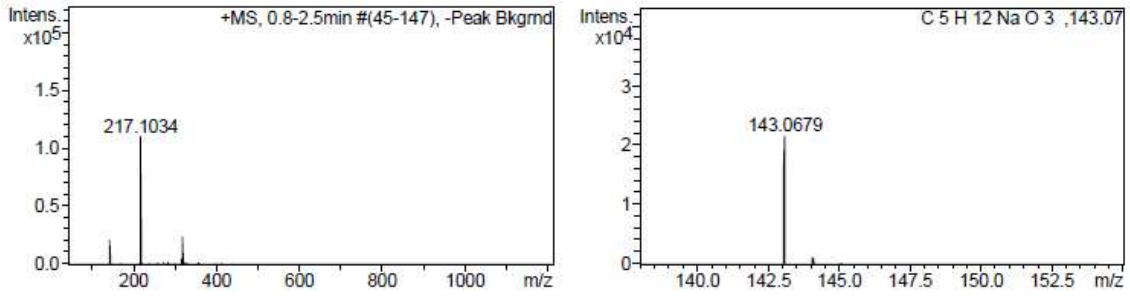


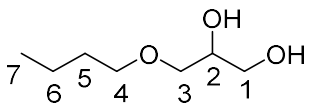
Figure S7. HSQC of 3-ethoxypropan-1,2-diol [2.0.0].



m/z	z	I	FWHM
143.0680		21514	0.0235
217.1034		110270	0.0341
218.1081		6986	0.0299

m/z	z	I	FWHM
143.0679		21514	0.0235
144.0712		1218	0.0235
145.0721		161	0.0235

Figure S-8 . HRMS of 3-ethoxypropan-1,2-diol [2.0.0].



3-Butoxypropan-1,2-diol [4.0.0], CAS 624-52-2: Colorless liquid, b.p. = 249 ºC: **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 4.54 (d, 1H, J = 5.1 Hz, OH_2), 4.41 (t, 1H, J = 5.7 Hz, OH_1), 3.49-3.57 (sext, 1H, J = 5.2 Hz, H_2), 3.34 (t, 2H, J = 6.7 Hz, H_4), 3.19-3.32 (m, 4H, H_1, H_{3a}, H_{3b}), 1.44 (quint, 2H, J = 7.6 Hz, H_5), 1.29 (sext, 2H, J = 7.3 Hz, H_6), 0.85 (t, 3H, J = 7.4 Hz, H_7). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 72.3 (CH_2, C_3), 70.6 (CH, C_2), 70.2 (CH_2, C_4), 63.2 (CH_2, C_1), 31.4 (CH_2, C_5), 18.9 (CH_2, C_6), 13.8 (CH_3, C_7). **HRMS** (ESI^+): *m/z* calc. = 171.0992, *m/z* found = 171.0996 ($M+Na^+$).

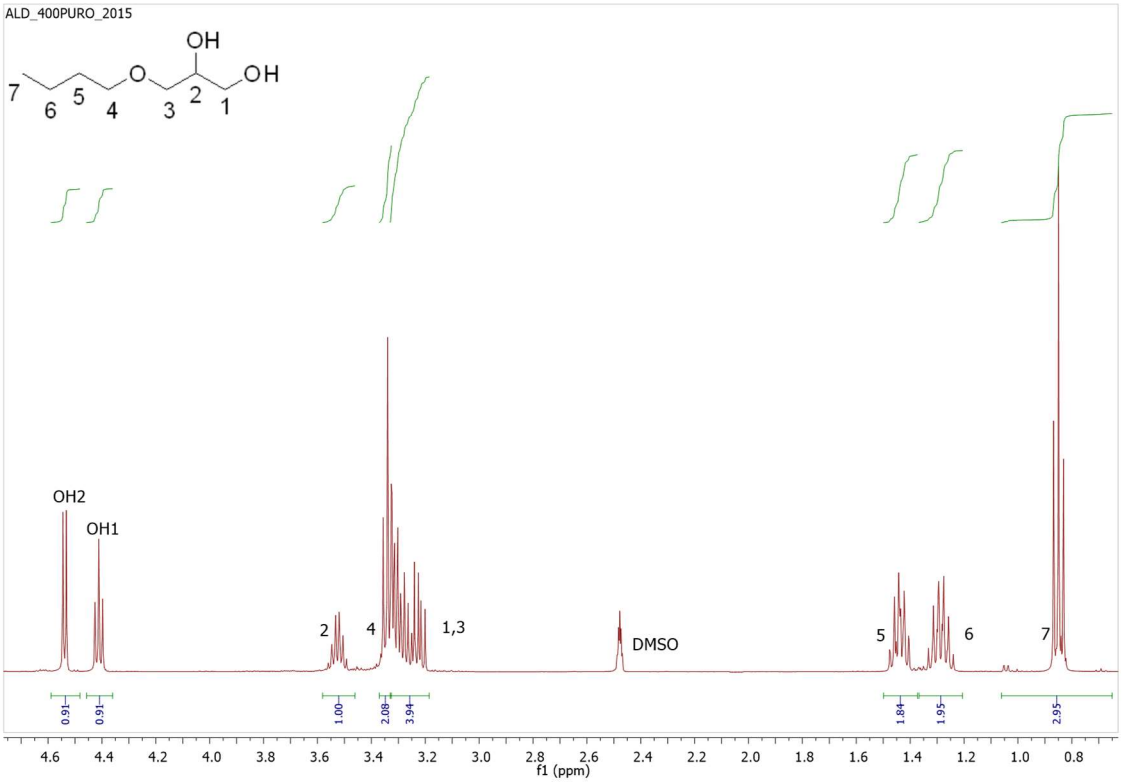


Figure S-9. ^{1}H-RMN of 3-butoxypropan-1,2-diol [4.0.0]

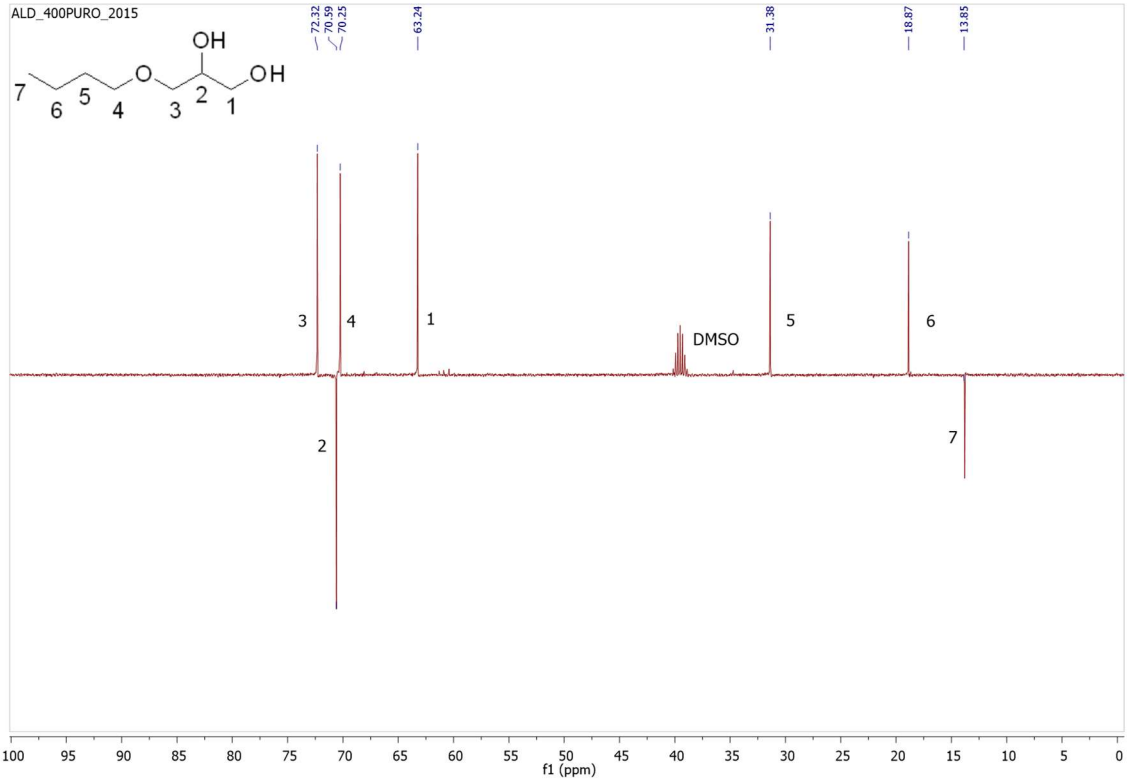


Figure S-10. ^{13}C-RMN (APT) of 3-butoxypropan-1,2-diol [4.0.0].

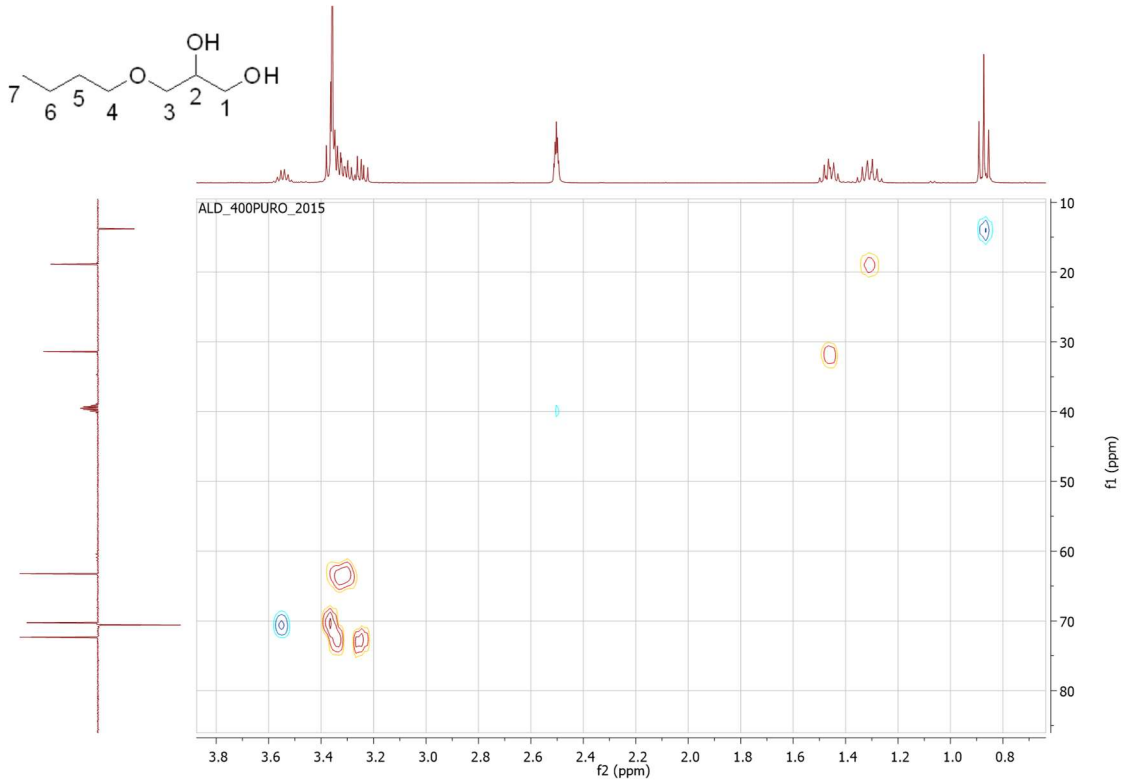
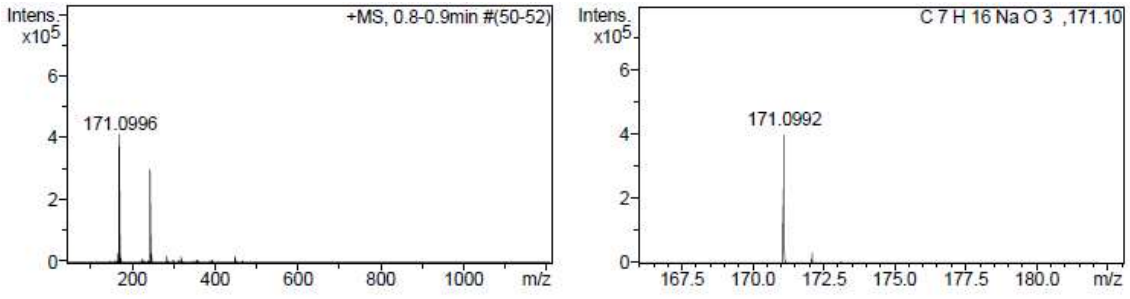


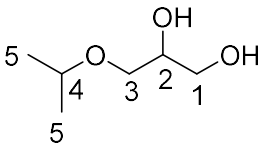
Figure S-11. HSQC of 3-butoxypropan-1,2-diol [4.0.0].



m/z	z	I	FWHM
168.0921		27789	0.0246
171.0996		413426	0.0267
172.1036		25679	0.0235

m/z	z	I	FWHM
171.0992		413426	0.0267
172.1025		32534	0.0267
173.1034		3659	0.0267

Figure S-12. HRMS of 3-butoxypropan-1,2-diol [4.0.0].



3-Isopropoxypropan-1,2-diol [3i.0.0], Colorless liquid, b.p. = 202 ºC,: **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 4.52 (d, 1H, J = 5.0 Hz, OH_2), 4.42 (t, 1H, J = 5.7 Hz, OH_1), 3.46-3.56 (m, 2H, H_2, H_4), 3.21-3.38 (m, 4H, H_1, H_{3a}, H_{3b}), 1.07 (d, 6H, J = 6.1 Hz, H_5). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 71.0 (CH, C_2 ó $_4$), 70.8 (CH, C_4 ó $_2$), 69.6 (CH_2, C_3), 63.3 (CH_2, C_1), 22.0 (CH_3, C_5). **HRMS** (ESI^+): *m/z* calc. = 157.0835, *m/z* found = 157.0839 ($M+Na^+$).

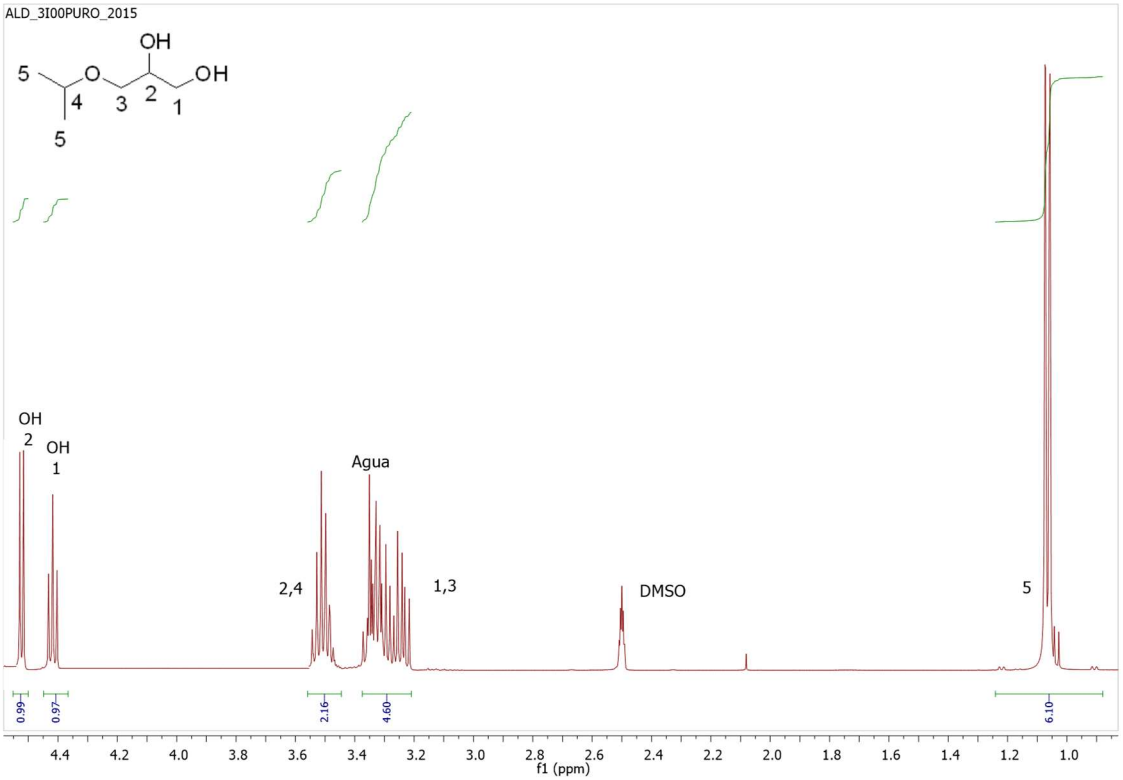


Figure S-13. [1]H-RMN of 3-isopropoxypropan-1,2-diol [3i.0.0]

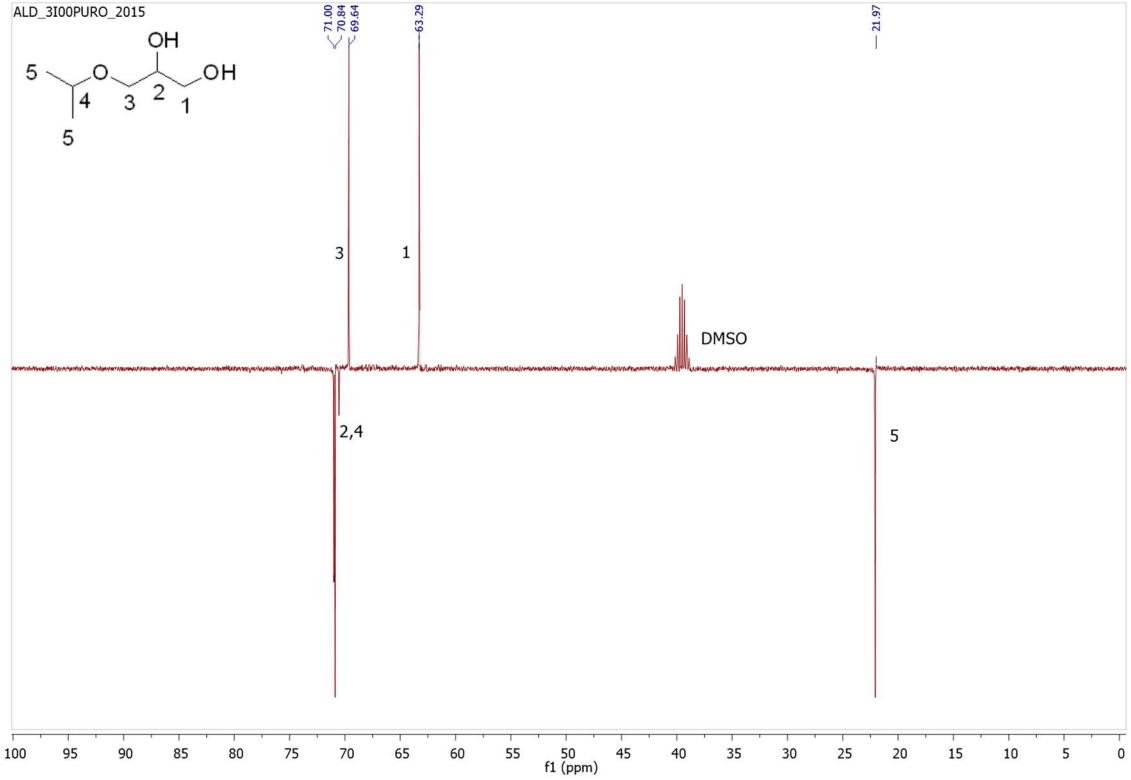


Figure S-14. [13]C-RMN (APT) of 3-isopropoxypropan-1,2-diol [3i.0.0].

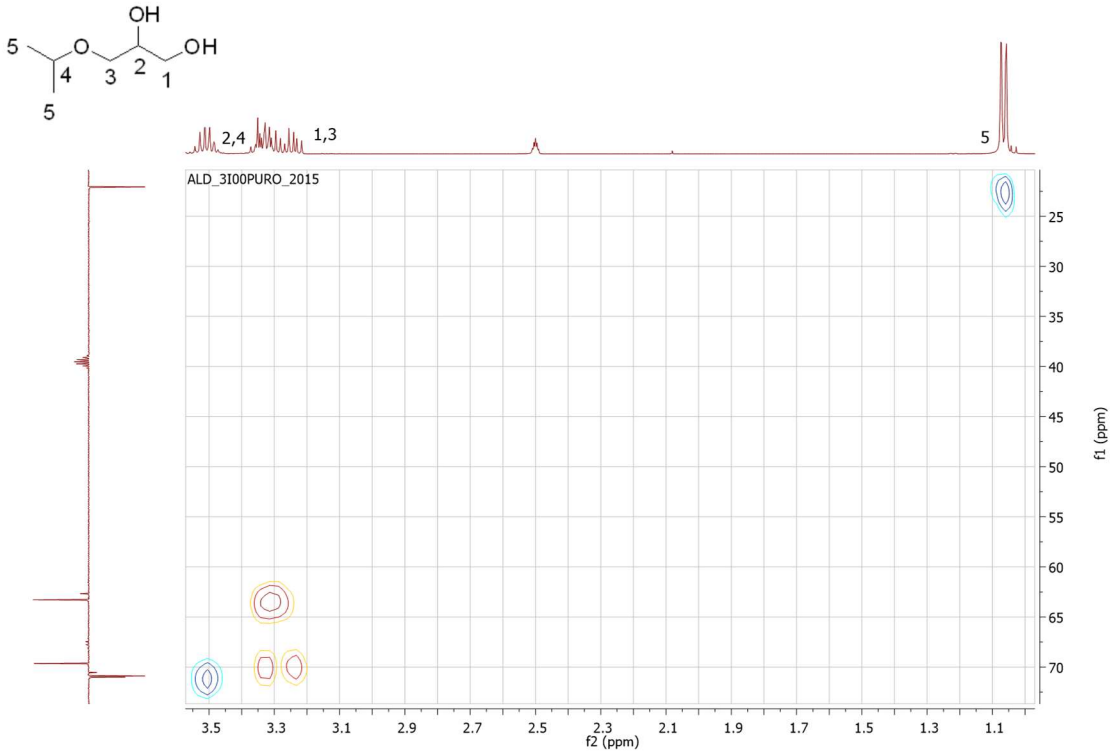
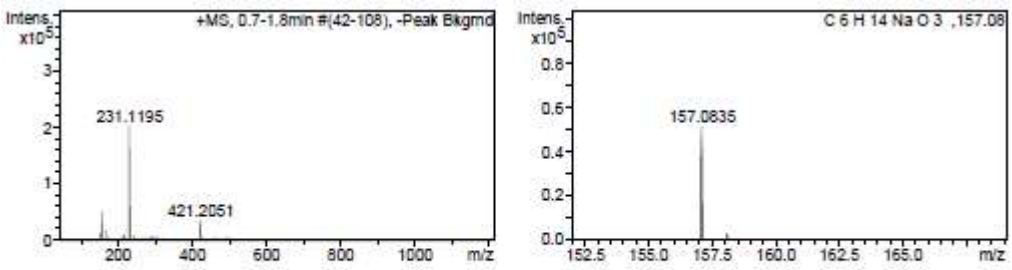


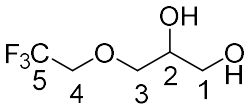
Figure S-15. HSQC of 3-isopropoxypropan-1,2-diol [3i.0.0].



m/z	z	I	FWHM
154.0747		13671	0.0214
157.0839		51624	0.0233
171.0624		18377	0.0241

m/z	z	I	FWHM
157.0835		51624	0.0233
158.0869		3492	0.0233
159.0878		418	0.0233

Figure S-16 . HRMS of 33-isopropoxypropan-1,2-diol [3i.0.0].



3-(2,2,2-Trifluoroethoxy)propan-1,2-diol [3F.0.0], Colorless liquid, b.p. = 213 ºC, **^{1}H NMR** (400 MHz, [D_6]DMSO, 25 ºC): δ 4.80 (d, 1H, *J* = 5.2 Hz, OH_2), 4.57 (t, 1H, *J* = 5.6 Hz, OH_1), 4.05 (q, 2H, *J* = 9.4 Hz, H_4), 3.57-3.64 (m, 2H, H_2, H_{3a}), 3.45-3.52 (m, 1H, H_{3b}), 3.32 (dd, 2H, *J* = 5.6 Hz, 5.7 Hz, H_1). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 124.6 (q, CF_3, *J* = 279.6 Hz, C_5), 73.9 (CH_2, C_3), 70.5 (CH, C_2), 67.7 (c, CH_2, *J* = 32.6 Hz, C_4), 62.7 (CH_2, C_1). **^{19}F NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ –73.0 (t, CF_3, *J* = 9.4 Hz, F_5). **HRMS** (ESI^+): *m/z* calc. = 197.0396, *m/z* found = 197.0400 ($M+Na^+$).

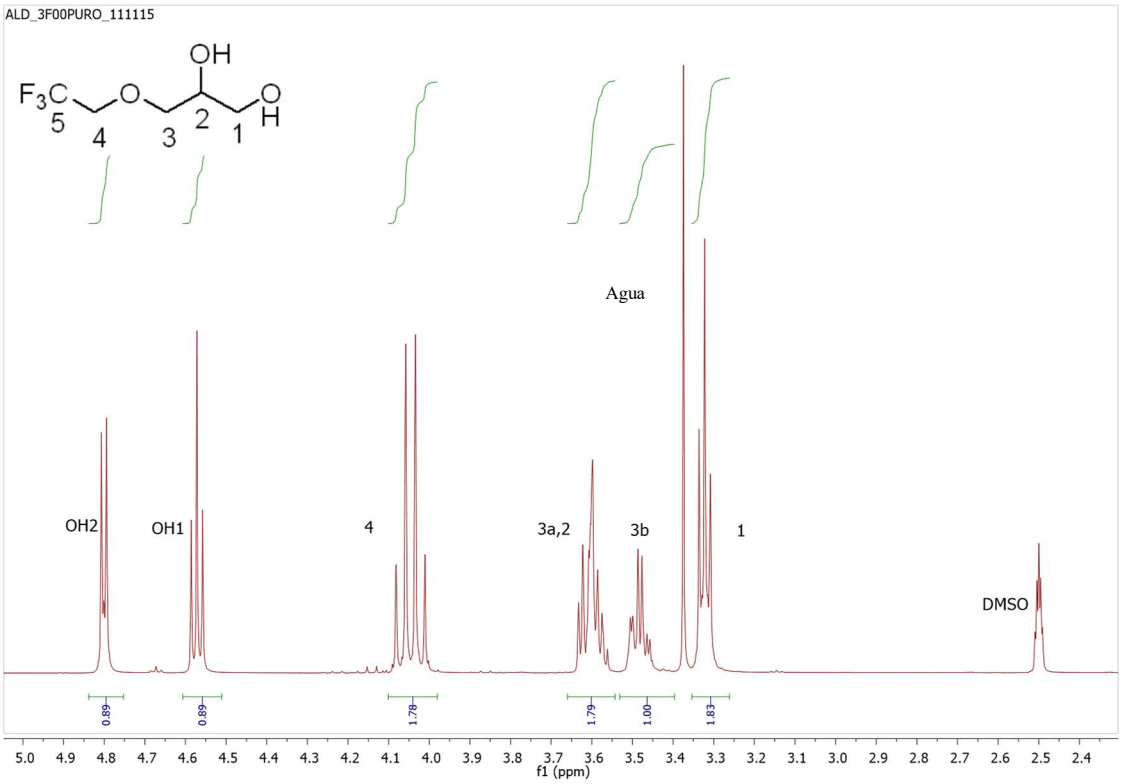


Figure S-17. [1]H-RMN of 3-(2,2,2-trifluoroethoxy)propan-1,2-diol [3F.0.0]

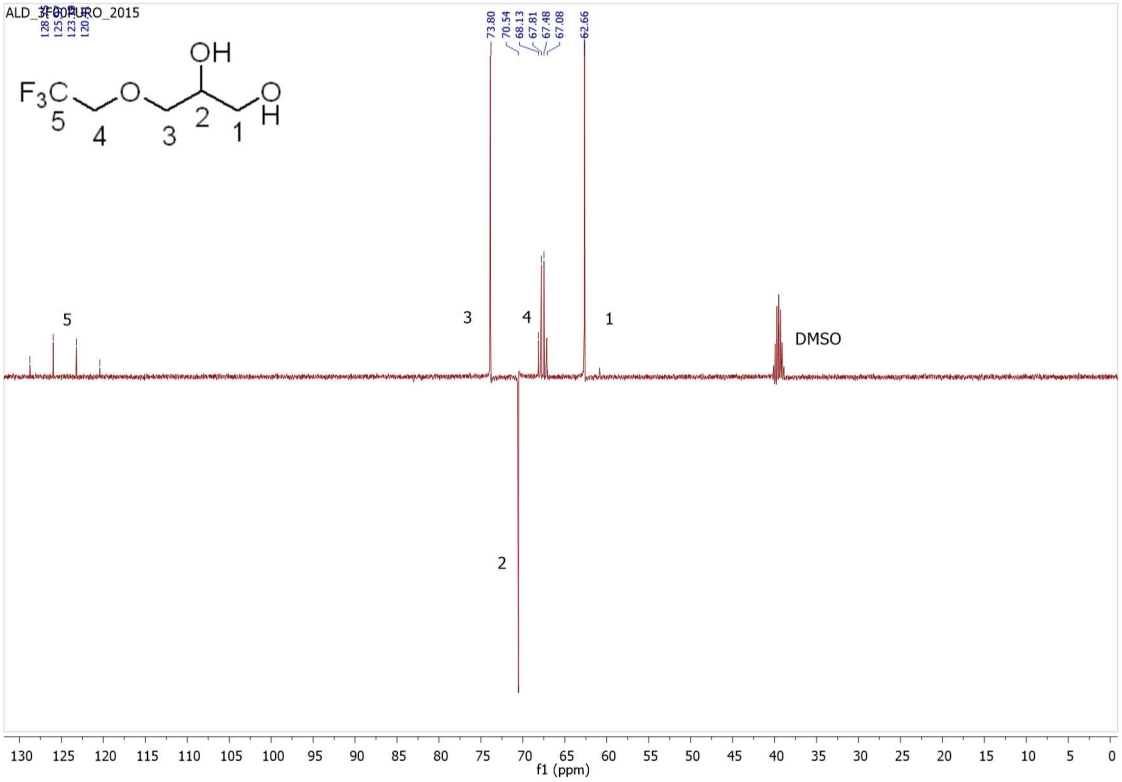


Figure S-18. [13]C-RMN (APT) of 3-(2,2,2-trifluoroethoxy)propan-1,2-diol [3F.0.0].

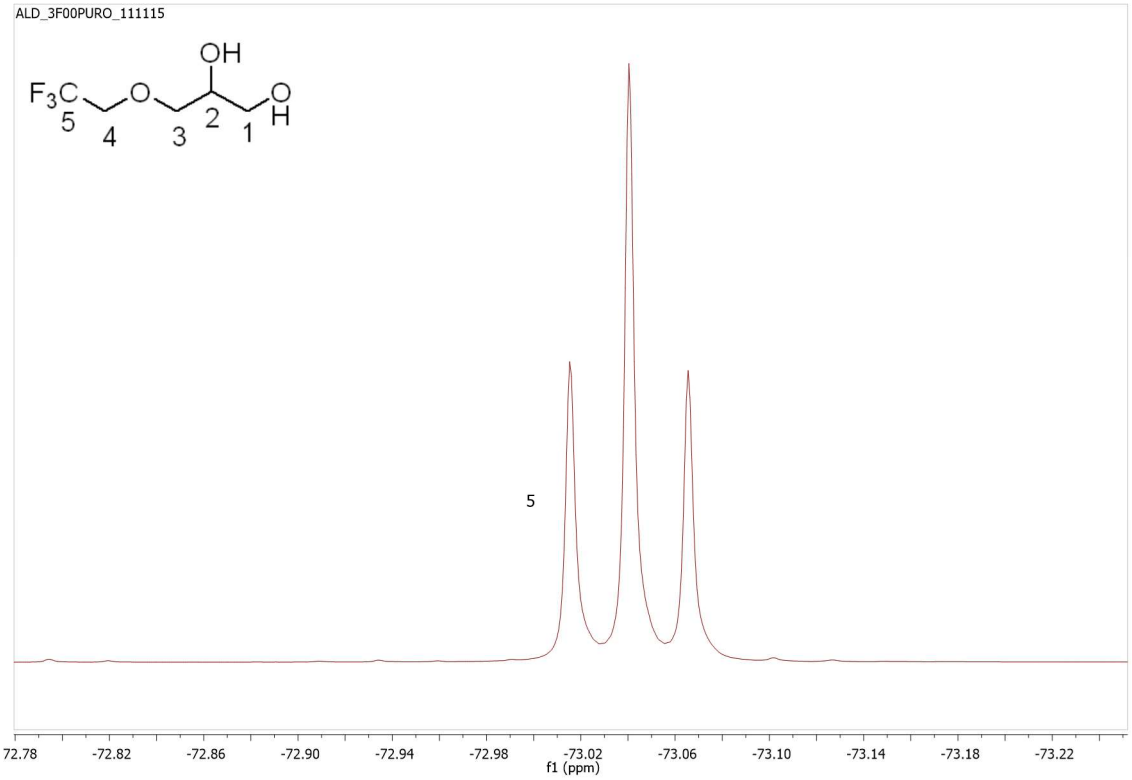


Figure S-19. ^{19}F-RMN of 3-(2,2,2-trifluoroethoxy)propan-1,2-diol [3F.0.0].

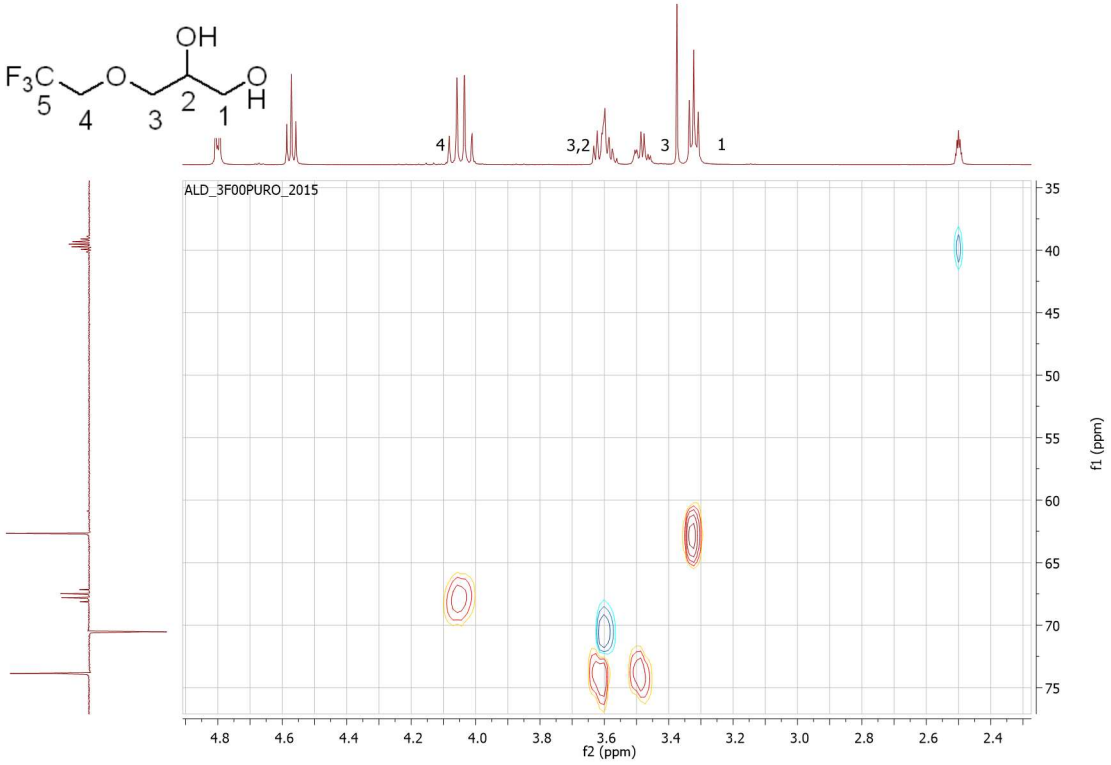


Figure S-20. HSQC of 3-(2,2,2-trifluoroethoxy)propan-1,2-diol [3F.0.0].

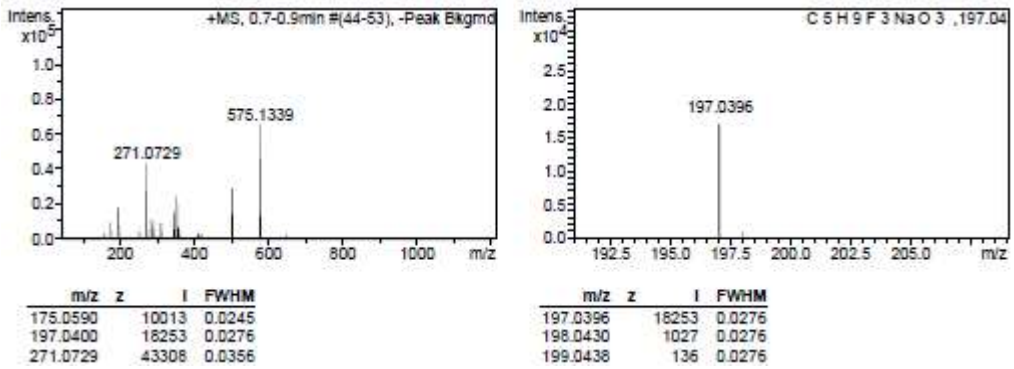
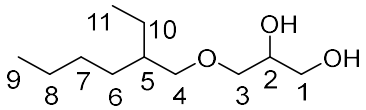


Figure S-21 . HRMS of 3-(2,2,2-trifluoroethoxy)propan-1,2-diol [3F.0.0].



3-(2-Ethylhexyloxy)propan-1,2-diol [6(2).0.0], CAS 70445-33-9: Colorless liquid, b.p. = 285 ºC, **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 4.57 (d, 1H, *J* = 5.0 Hz, OH_2), 4.45 (t, 1H, *J* = 5.7 Hz, OH_1), 3,55 (sext, 1H, *J* = 5.5 Hz, H_2), 3.20-3.38 (m, 6H, H_1, H_3, H_4), 1.43 (sept, 1H, *J* = 5.9 Hz, H_5), 1.15-1.37 (m, 8H, H_6, H_7, H_8, H_{10}), 0.86 (t, 3H, *J* = 6.6 Hz, H_9), 0.83 (t, 3H, *J* = 7.4 Hz, H_{11}). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 73.4 (CH_2, C_4), 72.6 (CH_2, C_3), 70.6 (CH, C_2), 63.3 (CH_2, C_1), 39.1 (CH, C_5), 30.0 (CH_2, C_6), 28.6 (CH_2, C_7), 23.4 (CH_2, C_{10}), 22.6 (CH_2, C_8), 14.0 (CH_3, C_9), 11.0 (CH_3, C_{11}). **HRMS** (ESI^+): *m/z* calc. = 227.1618, *m/z* found = 227.1607 (M+Na).

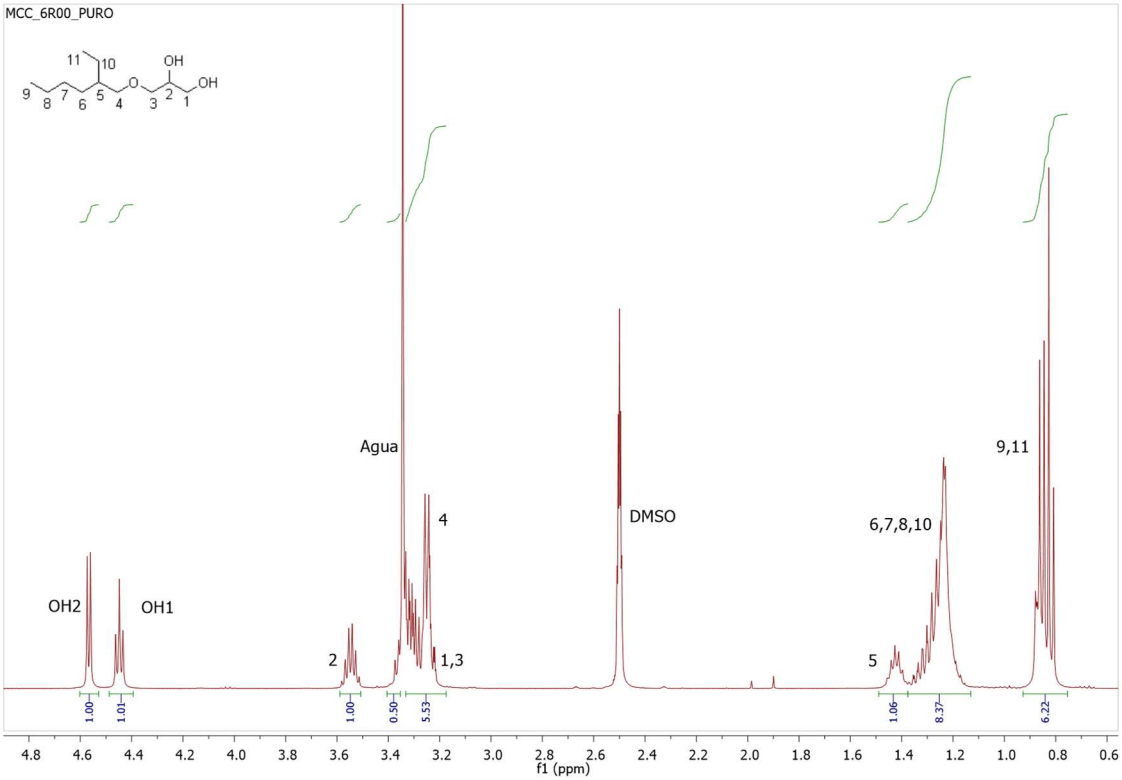


Figure S-22. ^{1}H-RMN of 3-(2-ethylhexyloxy)propan-1,2-diol [6(2).0.0].

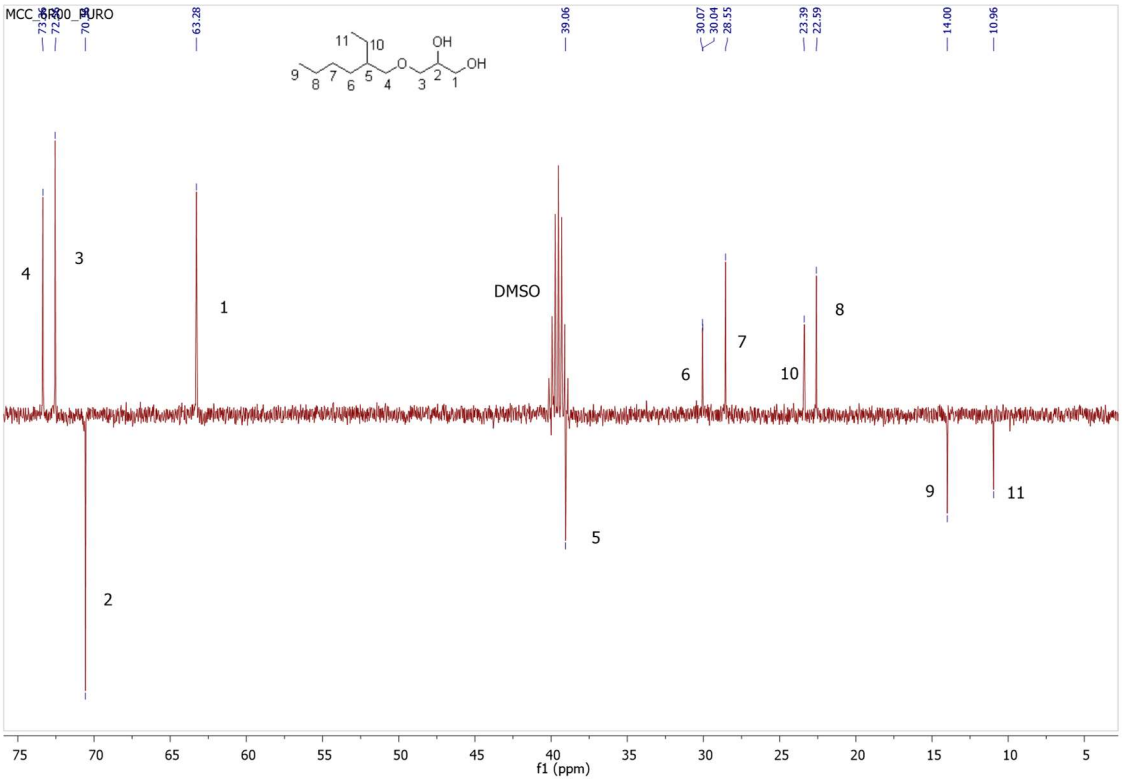


Figure S-23. ^{13}C-RMN (APT) of 3-(2-ethylhexyloxy)propan-1,2-diol [6(2).0.0].

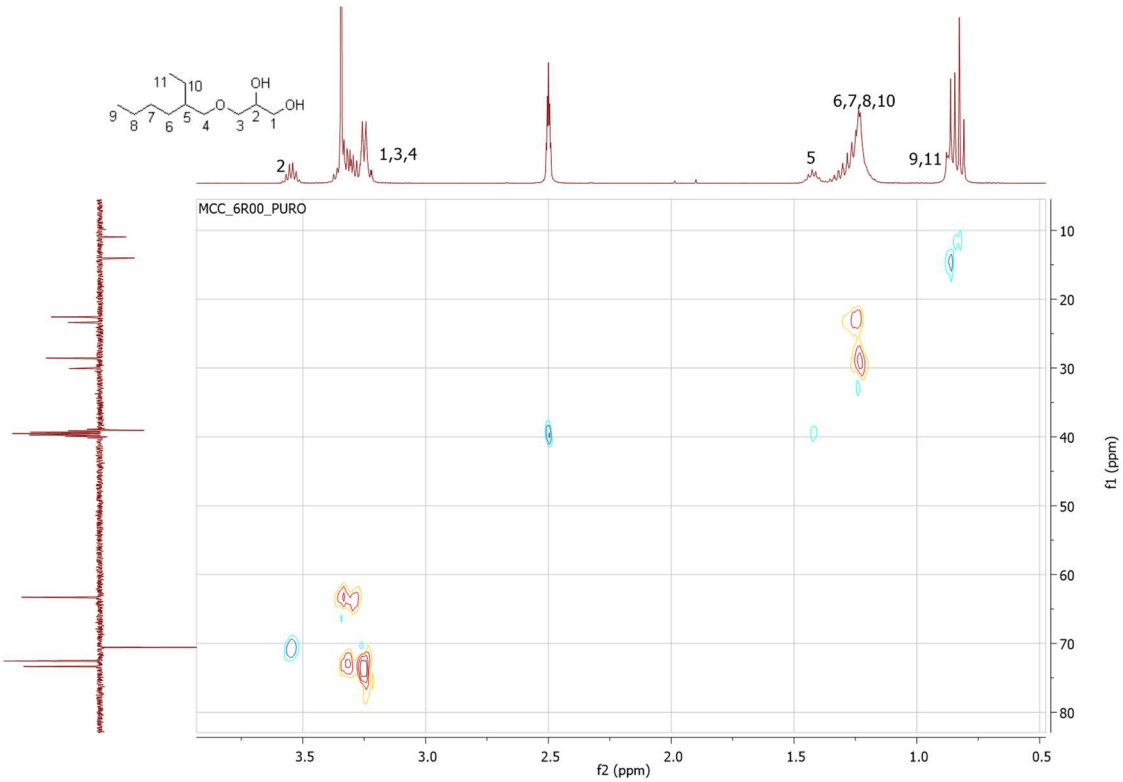
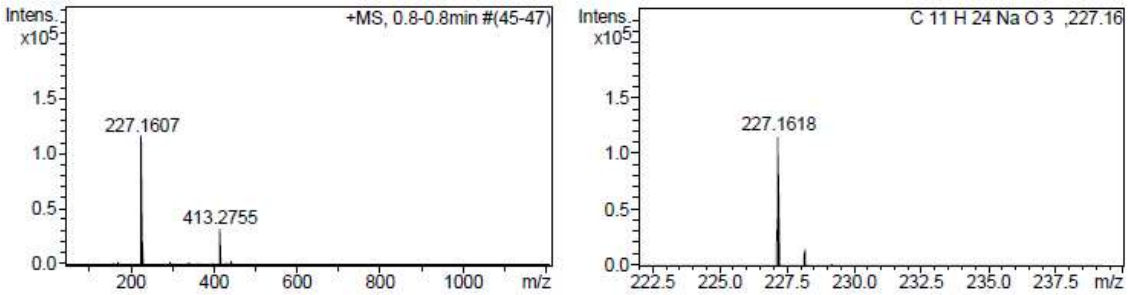


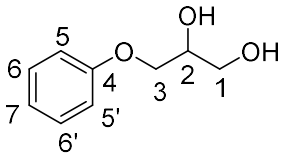
Figure S-24. HSQC of 3-(2-ethylhexyloxy)propan-1,2-diol [6(2).0.0].



m/z	z	I	FWHM
171.0997		1589	0.0260
226.9523		3414	0.0322
227.1607		116094	0.0363

m/z	z	I	FWHM
227.1618		116094	0.0363
228.1651		14265	0.0363
229.1685		1517	0.0363

Figure S-25 . HRMS of 3-(2-ethylhexyloxy)propan-1,2-diol [6(2).0.0].



3-Phenoxypropan-1,2-diol, [Ph.0.0], White solid CAS 538-43-2: **^{1}H NMR** (400 MHz, [d_6]DMSO, 25 ºC): δ 7.24-7.30 (m, 2H, $H_{6,6'}$), 6.89-6.94 (m, 3H, $H_{5,5'}$, H_7), 4.95 (d, 1H, J = 5.1 Hz, OH_2), 4.67 (t, 1H, J = 5.7 Hz, OH_1), 3.98 (dd, 1H, J_{gem} = 9.7 Hz, J = 5.1 Hz, H_{3a}), 3.84 (dd, 1H, J_{gem} = 9.7 Hz, J = 5.1 Hz, H_{3b}), 3.79 (sext, 1H, J = 5.1 Hz, H_2), 3.44 (t, 2H, J = 5.5 Hz, H_1). **^{13}C NMR** (100 MHz, [d_6]DMSO, 25 ºC): δ 158.7 (C, C_4), 129.5 (CH, $C_{6,6'}$), 120.4 (CH, C_7), 114.5 (CH, $C_{5,5'}$), 70.0 (CH, C_2), 69.4 (CH_2, C_3), 62.7 (CH_2, C_1). **HRMS** (ESI^+): *m/z* calc. = 191.0679, *m/z* found = 191.0674 ($M+Na^+$).

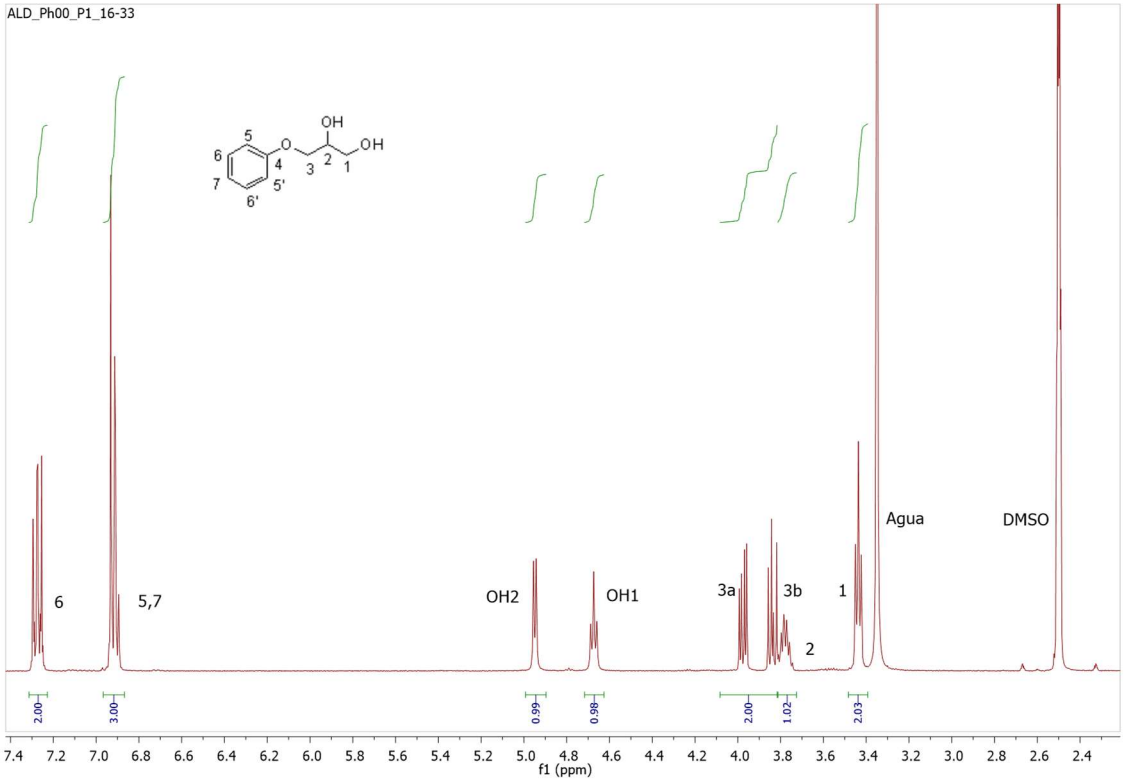


Figure S-26. ^{1}H-RMN of 3-phenoxypropan-1,2-diol, [Ph.0.0.]

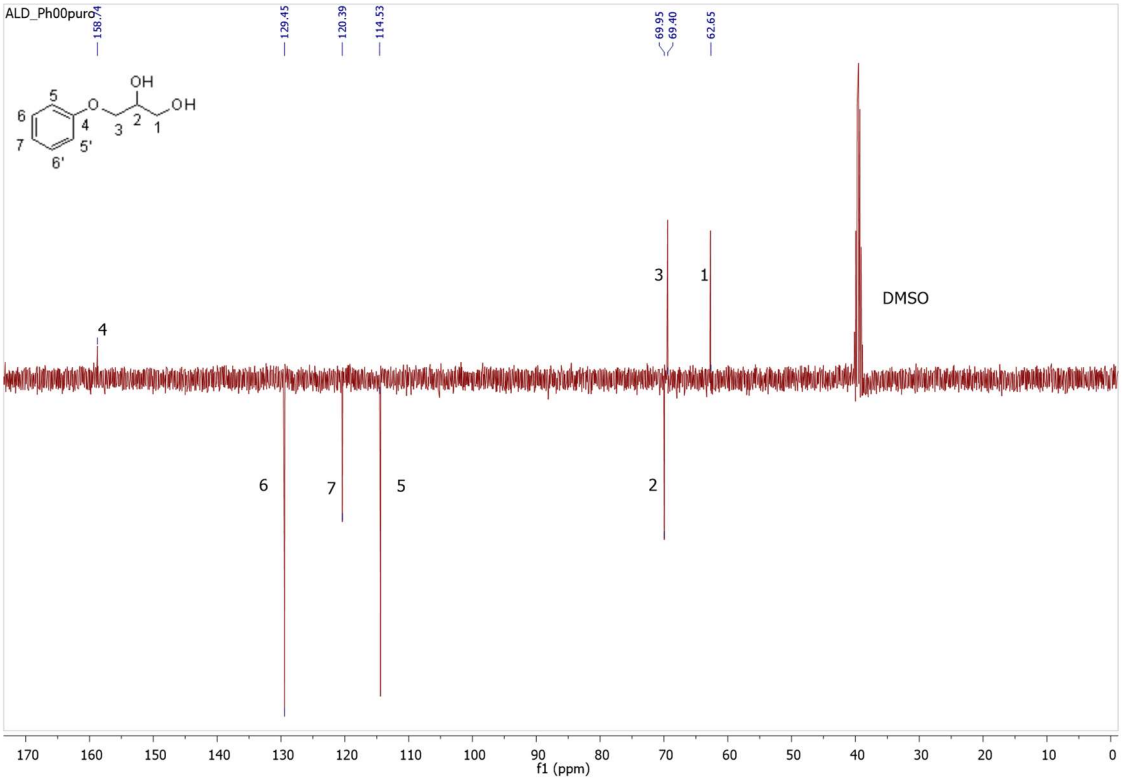


Figure S-27. ^{13}C-RMN (APT) 3-phenoxypropan-1,2-diol, [Ph.0.0.]

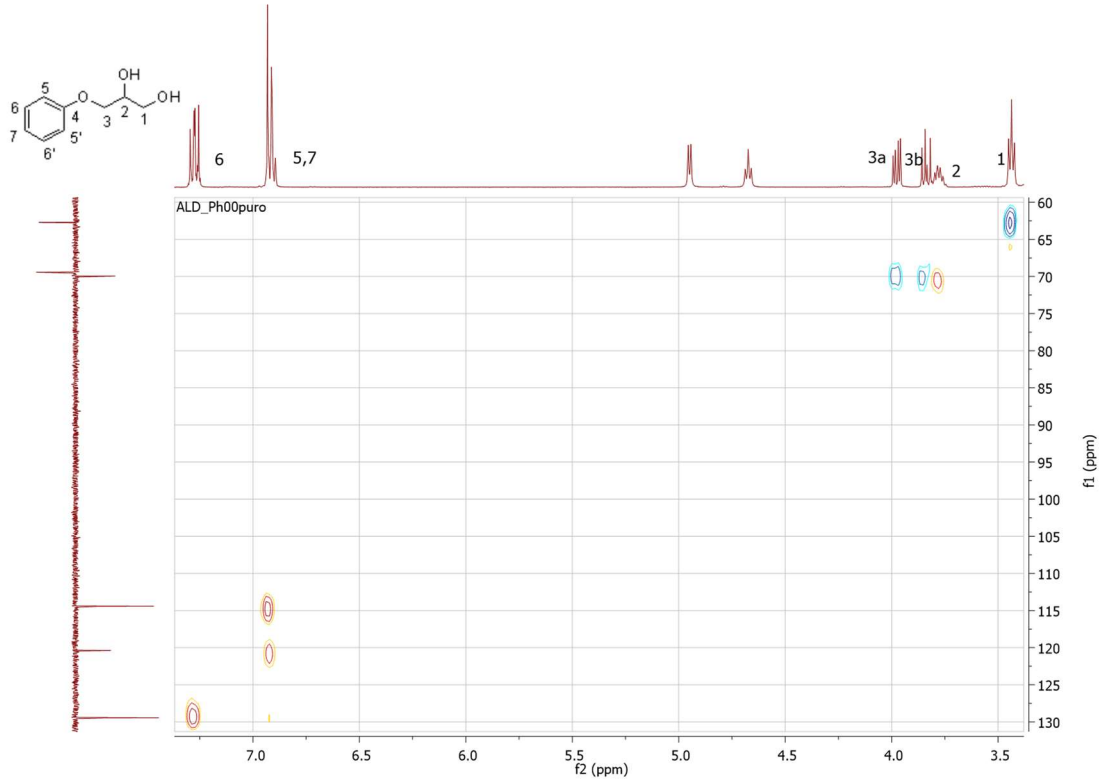
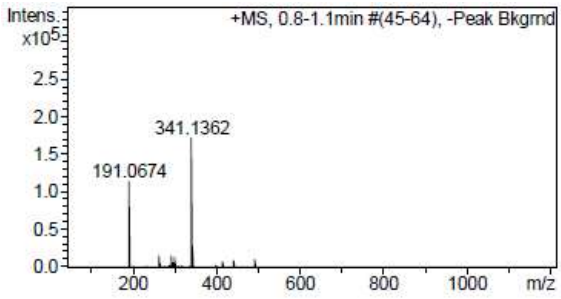
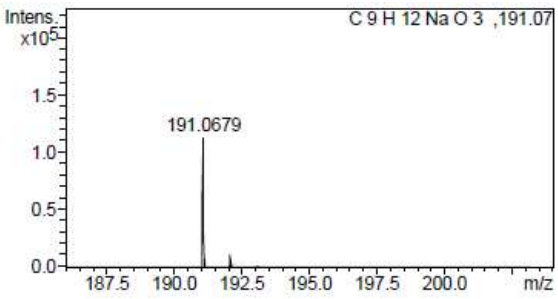


Figure S-28. HSQC of 3-phenoxypropan-1,2-diol, [Ph.0.0.].



m/z	z	I	FWHM
191.0674		114151	0.0307
192.0710		8612	0.0260
263.0882		15625	0.0354



m/z	z	I	FWHM
191.0679		114151	0.0307
192.0712		11400	0.0307
193.0721		1213	0.0307

Figure S-29 . HRMS 3-phenoxypropan-1,2-diol, [Ph.0.0.].

3. Comparison of at once and dropwise addition of glycidol in its reactions with methanol and butanol.

Table S1. Time evolution of the conversion of glycidol and yield of [1.0.0] in the reaction of glycidol with methanol, catalyzed by KOH (20% mol) at 65 ºC, when glycidol is added either at once or dropwise during the first 15 min. of reaction.

	Dropwise addition		At once addition	
Time (min)	**Conversion (%)**	**Yield (Select.) (%)**	**Conversion (%)**	**Yield (Select.) (%)**
0	0	0(0)	0	0(0)
5	-	-	58	29(50)
15	52	34(65)	71	42(59)
30	70	58(83)	82	56(68)
45	82	73(89)	89	62(70)
60	90	84(93)	93	67(72)
90	97	91(93)	97	69(71)
120	100	93(93)	100	70(70)

Table S2. Time evolution of the conversion of glycidol and yield of [4.0.0] in the reaction of glycidol with butanol, catalyzed by KOH (20% mol) at 65 ºC, when glycidol is added either at once or dropwise during the first 15 min. of reaction.

	Dropwise addition		At once addition	
Time (min)	**Conversion (%)**	**Yield (Select.) (%)**	**Conversion (%)**	**Yield (Select.) (%)**
0	0	0(0)	0	0(0)
5	-	-	68	17(25)
15	82	46(56)	80	30(38)
30	95	51(54)	91	38(42)
45	99	52(53)	95	39(41)
60	99	52(53)	96	40(42)
90	100	57(57)	98	42(43)
120	100	60(60)	98	42(43)

4. Scheme of the catalytic cycles involved in the reactions of glycidol.

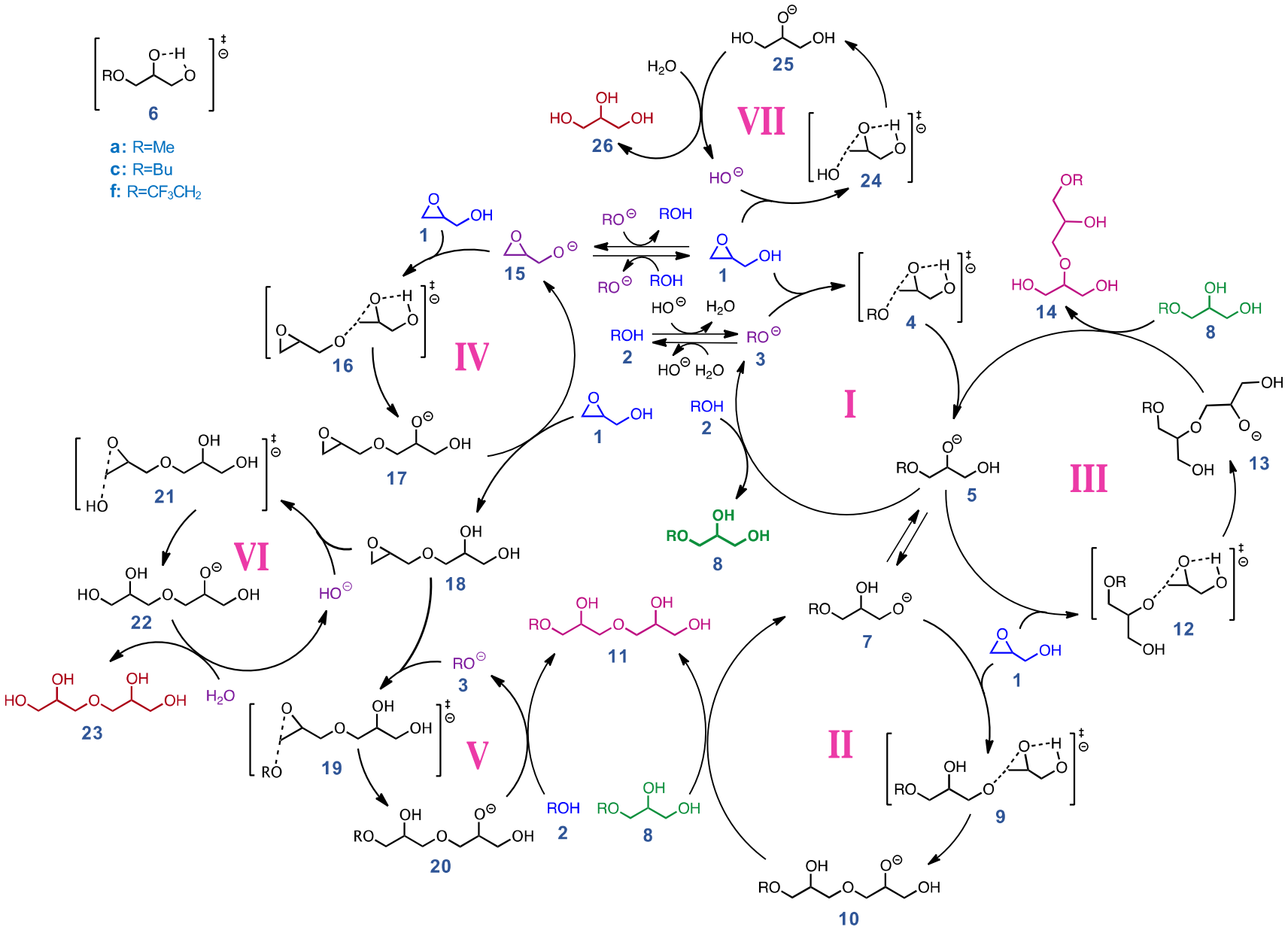


Figure S-30. Possible catalytic cycles involved in the reaction of glycidol **1** and alcohols **2** catalyzed by bases, considered in this work.

5. Table of the calculated energies of all structures described.

Table S3. Electronic and Gibbs Free Energies (at 298.15 K) of the reactants. transition structures. intermediates and products described in this work. calculated at the PCM(solvent)/B3LYP/6-311++G(d.p) theoretical level.

		Methanol		Butanol		2.2.2-Trifluoroethanol	
Cycle	**Structure**	**E_0 (a.u.)**	**G (a.u.)**	**E_0 (a.u.)**	**G (a.u.)**	**E_0 (a.u.)**	**G (a.u.)**
	HO^-	-75.961466	-75.969015	-75.957551	-75.965101	-75.542275	-75.549077
	H_2O	-76.467344	-76.464447	-76.466959	-76.464066	-76.062468	-76.057166
	1	-268.416454	-268.354654	-268.416025	-268.354195	-268.416345	-268.354537
	2	-115.771691	-115.743490	-233.749720	-233.643889	-452.925555	-452.899813
	3	-115.262408	-115.248195	-233.236762	-233.144552	-452.435097	-452.421582
I	**4**	-383.661927	-383.569770	-501.636463	-501.464818	-720.831154	-720.738752
	5	-383.728778	-383.629825	-501.703386	-501.526297	-720.882975	-720.785868
	6	-383.724367	-383.629083	-501.698695	-501.525801	-720.878212	-720.784413
	7	-383.728346	-383.629513	-501.702728	-501.525869	-720.881939	-720.783911
	8	-384.227265	-384.115416	-502.204884	-502.015358	-721.380085	-721.269738
	9-rr	-652.124598	-651.946996	-770.099471	-769.842757		
	10-rr	-652.180243	-651.997048	-770.154293	-769.892859		
II	**11-rr**	-652.680414	-652.484366	-770.657697	-770.383556		
	9-sr	-652.118289	-651.940278	-770.092888	-769.836843		
	10-sr	-652.180021	-651.996892	-770.154426	-769.893830		
	11-sr	-652.679994	-652.483719	-770.657359	-770.383671		
	12-rr	-652.117186	-651.939490	-770.094902	-769.837116		
	13-rr	-652.189940	-652.004575	-770.164653	-769.900935		
III	**14-rr**	-652.677764	-652.479165	-770.649351	-770.374105		
	12-sr	-652.123804	-651.946161	-770.089570	-769.834197		
	13-sr	-652.188344	-652.002379	-770.163000	-769.899174		
	14-sr	-652.677266	-652.480318	-770.654618	-770.381124		
	15	-267.912127	-267.864115	-267.908402	-267.860454	-267.911190	-267.863196
	16-rr	-536.310232	-536.183879	-536.307334	-536.181318	-536.309503	-536.183200
IV	**17-rr**	-536.371308	-536.238681	-536.368007	-536.235466	-536.370478	-536.237870
	18-rr	-536.869097	-536.723705	-536.868434	-536.722976	-536.868929	-536.723511
	16-sr	-536.310060	-536.182816	-536.307173	-536.179913	-536.309334	-536.182051
	17-sr	-536.367762	-536.235910	-536.364484	-536.232556	-536.371685	-536.239162
	18-sr	-536.869073	-536.723526	-536.868451	-536.722801	-536.870432	-536.724802
	19-rr	-652.110970	-651.935237	-770.087520	-769.831350		
	20-rr	-652.176297	-651.991528	-770.149451	-769.887552		
V	**11-rr**	-652.680414	-652.484366	-770.657697	-770.383556		
	19-sr	-652.113780	-651.937353	-770.087761	-769.831853		
	20-sr	-652.173010	-651.991523	-770.147014	-769.887042		
	11-sr	-652.679994	-652.483719	-770.657359	-770.383671		
	21-rr	-612.807670	-612.655278	-612.803374	-612.651426		
	22-rr	-612.875129	-612.717588	-612.869815	-612.712407		
	23-rr	-613.372760	-613.202503	-613.371947	-613.201577		
VI	**21-sr**	-612.809649	-612.656823	-612.806025	-612.653281		
	22-sr	-612.873495	-612.716475	-612.870001	-612.712867		
	23-sr	-613.372543	-613.202143	-613.371672	-613.201044		
	24	-344.357955	-344.290107	-344.354769	-344.286865		
VII	**25**	-344.419338	-344.346050	-344.416018	-344.342698		
	26	-344.917849	-344.831784	-344.917275	-344.831157		

6. Reaction coordinates calculated for the reactions of glycidol with methanol, butanol and trifluoroethanol.

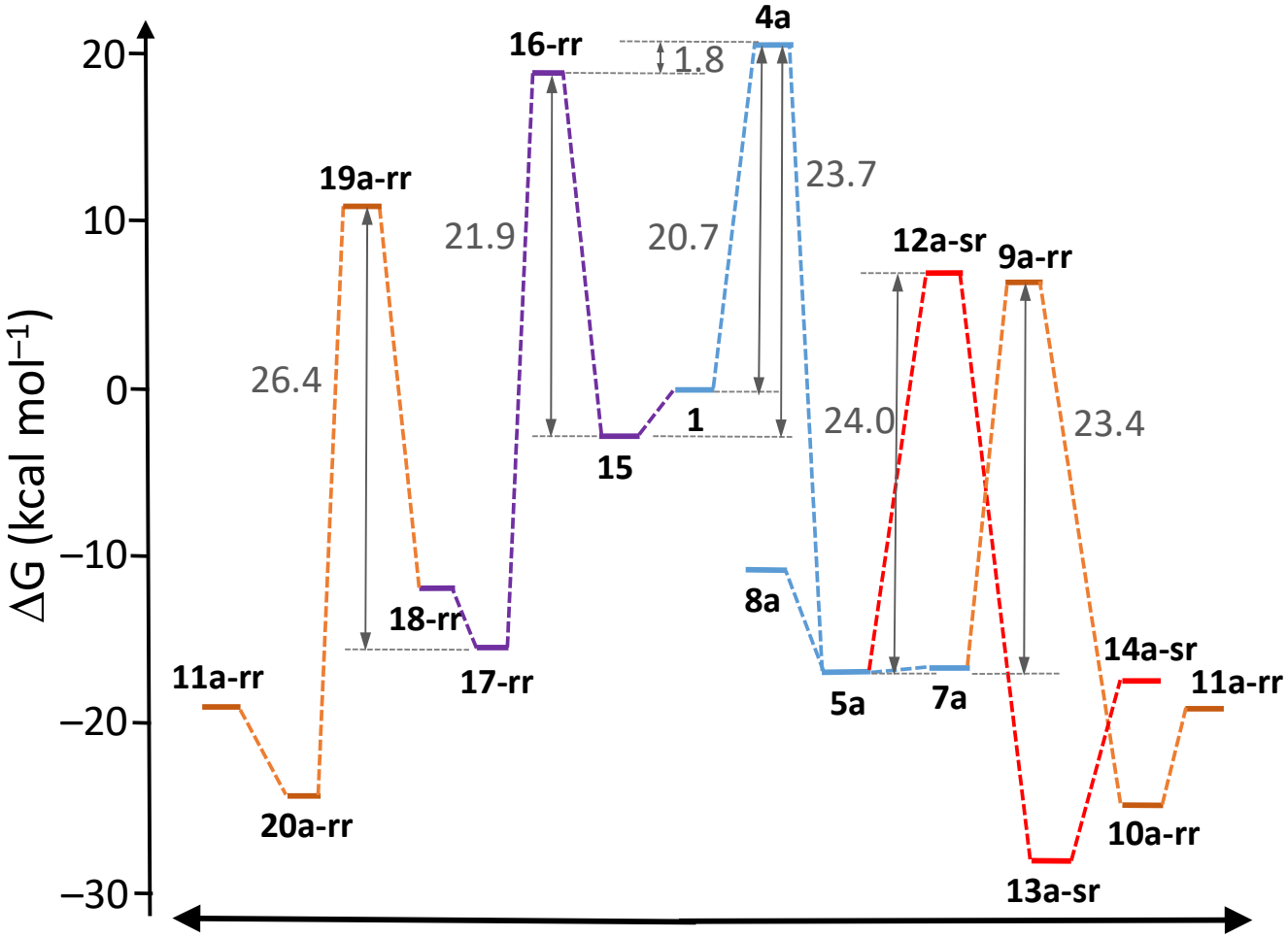


Figure S-31. Calculated (at the PCM(solvent)/B3LYP/6-311++G(d,p) theoretical level) reaction profiles for the reaction of glycidol (**1**) with methanol (**2a**), catalyzed by bases. Only cycles **I**, **II**, **III** and **IV** are shown.

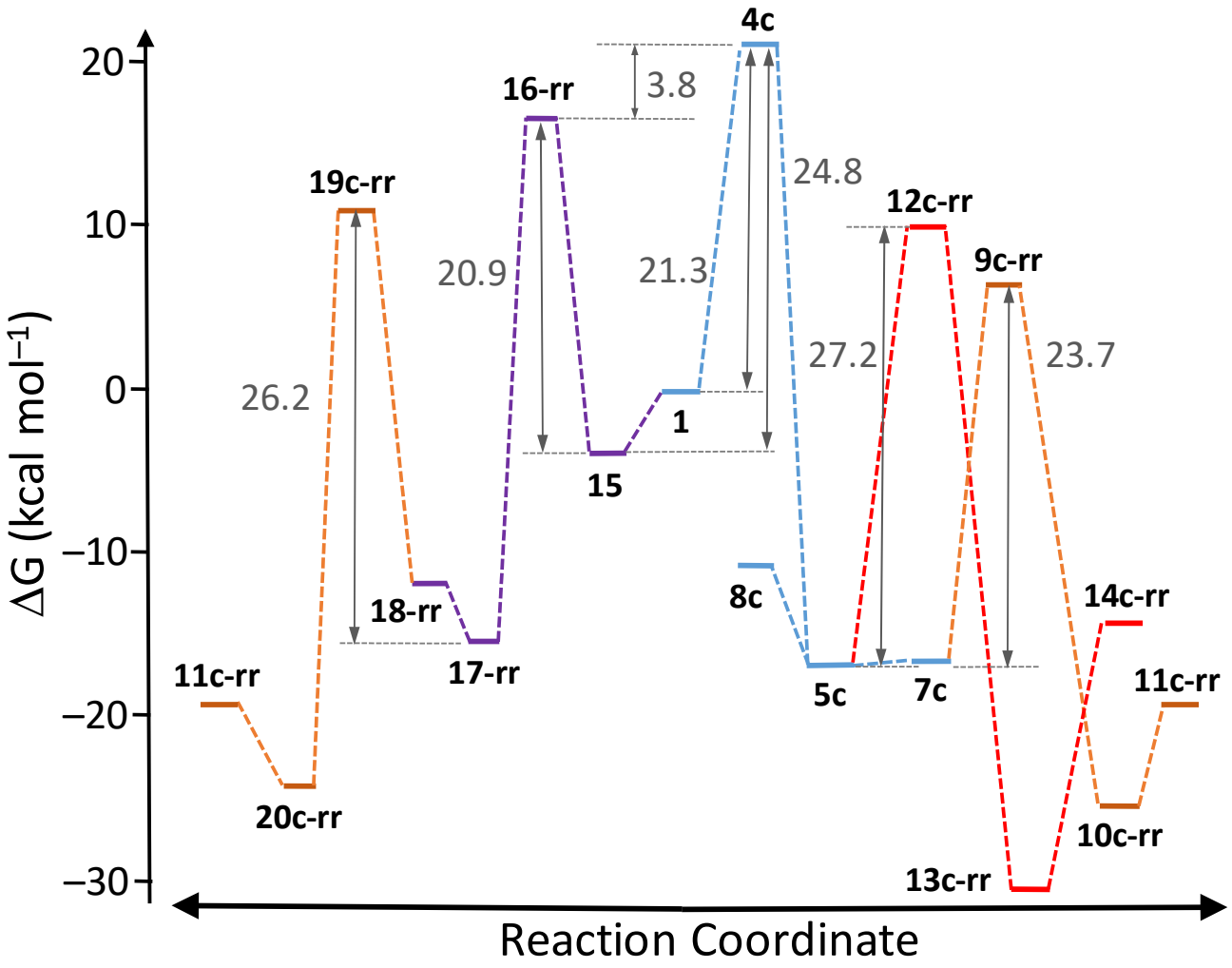


Figure S-32. Calculated (at the PCM(solvent)/B3LYP/6-311++G(d,p) theoretical level) reaction profiles for the reaction of glycidol (**1**) with butanol (**2c**), catalyzed by bases. Only cycles **I**, **II**, **III** and **IV** are shown.

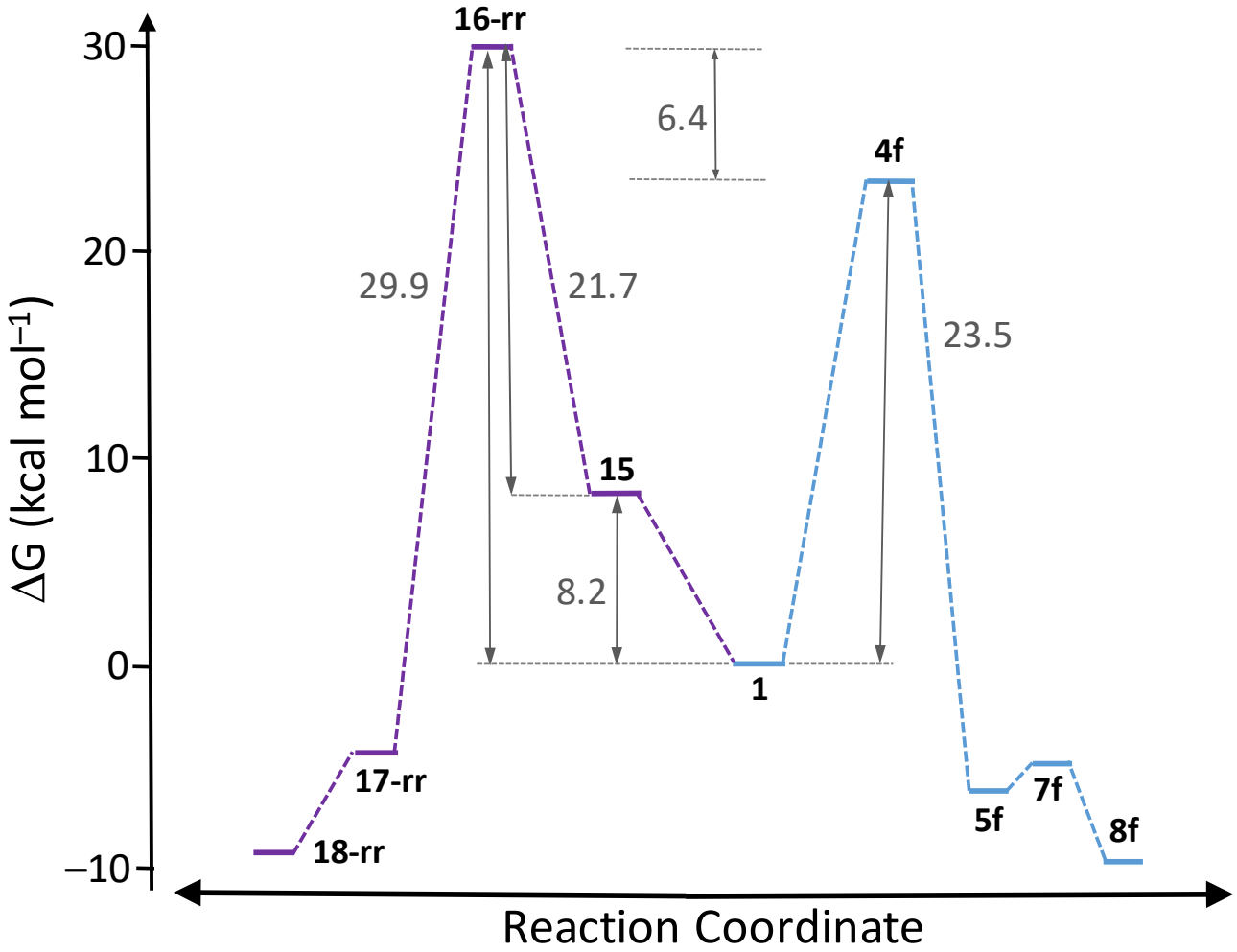


Figure S-33. Calculated (at the PCM(solvent)/B3LYP/6-311++G(d,p) theoretical level) reaction profiles for the reaction of glycidol (**1**) with 2,2,2-trifluoroethanol (**2f**), catalyzed by bases. Only cycles **I** and **IV** are shown.

7. Tables of specific calculations carried out to test temperature and theoretical level dependencies.

Table S4. Calculated (PCM(solvent)/B3LYP/6-311++G(d.p)) Gibbs Free Energies (at 298.15 K and 338.15 K).

Structure	G_{298} (a.u.)	$\Delta G^{\ddagger}_{298}$ (kcal mol^{-1})	G_{338} (a.u.)	$\Delta G^{\ddagger}_{338}$ (kcal mol^{-1})	$\Delta\Delta G^{\ddagger}$ (kcal mol^{-1})[a]
1	-268.354654		-268.359423		
2a	-115.743490		-115.747170		
3a	-115.248195		-115.251739		
4a	-383.569770	20.76	-383.576015	22.05	1.30
7a	-383.629513		-383.635266		
9a-rr	-651.946996	23.32	-651.955367	24.67	1.35
9a-sr	-651.940278	27.54	-651.948597	28.92	1.38
15	-267.864115		-267.868754		
16-rr	-536.183879	21.89	-536.191171	23.22	1.33
16-sr	-536.182816	22.56	-536.190000	23.96	1.40

[a] Note that the selectivities, defined by the difference between activation energies of two different reaction pathways, do no change with the temperature. For instance, the selectivity of cycle **I** against cycle **II** is 2.56 kcal mol^{-1} at 298.15 K and 2.62 kcal mol^{-1} at 338.15 K.

Table S5. Calculated (PCM(solvent)/Functional/6-311++G(d.p)) Gibbs Free Energies (at 298.15 K) and activation barriers for the aperture of glycidol with methoxide, using eight different pure, hybrid and double hybrid density functionals.

	G_{298} (a.u.)			$\Delta G^{\ddagger}$ (kcal mol^{-1})
Functional	**1**	**3a**	**4**	
B3LYP	-268.354654	-115.248195	-383.569770	20.76
PBEPBE	-268.041330	-115.107505	-383.121947	16.87
τHCTH	-268.286566	-115.222475	-383.477446	19.83
PBE1PBE	-268.048350	-115.106302	-383.119674	21.95
MPW1PW91	-268.282688	-115.208462	-383.455369	22.45
HSEH1PBE	-268.071039	-115.116821	-383.153822	21.36
M06	-268.188207	-115.172393	-383.327432	20.81
M06-2X	-268.238596	-115.184419	-383.386132	23.14
B2PLYP-D3	-267.825726	-115.007432	-382.793180	25.09

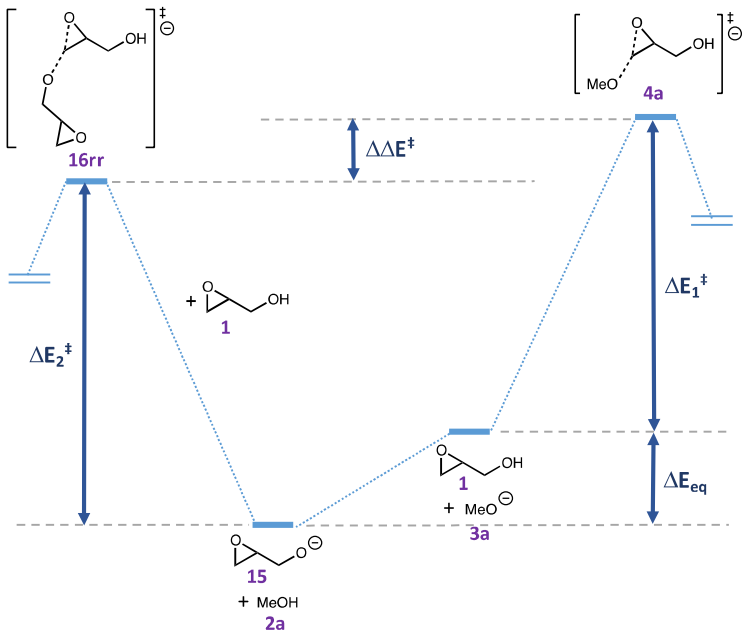


Figure S-34. Reaction profiles for the reactions of glycidol (**1**) with methanol (**2a**) and glycidol dimerization (**1** + **15**) used for the comparison of theoretical levels in Table S6.

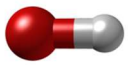
Table S6. Calculated energy differences and activation barriers for the aperture of glycidol with methoxide and glycidol dimerization, using different theoretical methods. See Figure S-31.[a]

Method	Basis set	$\Delta E_1^{\ddagger}$ [a]	ΔE_{eq}	$\Delta E_2^{\ddagger}$	$\Delta\Delta E^{\ddagger}$
PCM(methanol)/B3LYP	6-311++G(d,p)	10.6	3.1	11.5	2.2
PCM(methanol)/B2PLYP-D3	6-311++G(d,p)	14.3	2.9	14.8	2.4
SMD(methanol)/DLPNO-CCSD(T)[b]	aug-cc-pTZ + aug-cc-pVTZ/C	12.6	2.9	13.9	1.6
SMD(methanol)/DLPNO-CCSD(T)[c]	aug-cc-pTZ + aug-cc-pVTZ/C	12.7	3.2	13.4	2.5

[a] All energy values in kcal mol^{-1}. [b] Single point energies using B3LYP geometries. [c] Single point energies using B2PLYP-D3 geometries.

8. Calculated (PCM(solvent)/B3LYP/6-311++G(d.p)) energies and optimized geometries of all the structures discussed in the paper.

HO^-



```
Solvent = Methanol

E0 =   -75.961466 Hartree
 H =   -75.949461 Hartree
 G =   -75.969015 Hartree
 S =    41.156000 Cal/mol K

O         0.812443     -0.000018      0.000004
H        -0.151127      0.000043     -0.000001

Solvent = Butanol

E0 =   -75.957551 Hartree
 H =   -75.945546 Hartree
 G =   -75.965101 Hartree
 S =    41.156000 Cal/mol K

O         0.812443     -0.000018      0.000004
H        -0.151127      0.000043     -0.000001

Solvent = 2.2.2-Trifluoroethanol

E0 =   -75.542275 Hartree
 H =   -75.529563 Hartree
 G =   -75.549077 Hartree
 S =    41.070000 Cal/mol K

O        -0.110770     -0.126827      0.000000
H        -0.425512      0.761979      0.000000

=====================================================================
```

H_2O

```
Solvent = Methanol

E0 =   -76.467344 Hartree
 H =   -76.442363 Hartree
 G =   -76.464447 Hartree
 S =    46.480000 Cal/mol K

O        -0.763200      0.138187     -0.000008
H        -1.126342     -0.754667     -0.000005
H         0.192248      0.010728      0.000002

Solvent = Butanol

E0 =   -76.466959 Hartree
 H =   -76.441982 Hartree
 G =   -76.464066 Hartree
 S =    46.480000 Cal/mol K
```

```
O       -0.763200      0.138187     -0.000008
H       -1.126342     -0.754667     -0.000005
H        0.192248      0.010728      0.000002

Solvent = 2.2.2-Trifluoroethanol

E0 =   -76.062468 Hartree
 H =   -76.035802 Hartree
 G =   -76.057166 Hartree
 S =    44.965000 Cal/mol K

O       -0.114389     -0.144055      0.000000
H        0.828659     -0.111466      0.000000
H       -0.398466      0.755780      0.000000
```

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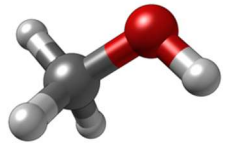
CH_3OH (**2a**)



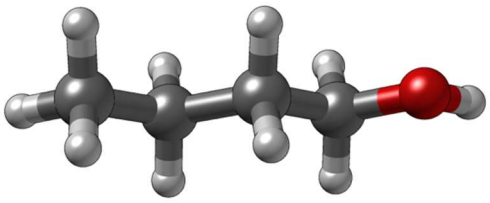
```
Solvent = Methanol

E0 =  -115.771691 Hartree
 H =  -115.716400 Hartree
 G =  -115.743490 Hartree
 S =    57.017000 Cal/mol K

C       -1.329282      0.490490     -0.000002
H       -1.334206      1.124876     -0.892125
H       -1.334201      1.124899      0.892105
O       -2.430404     -0.425934      0.000013
H       -3.248263      0.082620      0.000009
H       -0.418575     -0.108781      0.000003
```

==========

C_4H_9OH (**2c**)



```
Solvent = Butanol

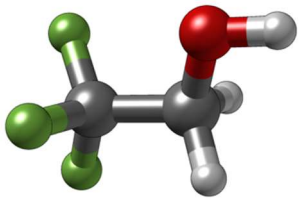
E0 =  -233.749719 Hartree
 H =  -233.605681 Hartree
 G =  -233.643889 Hartree
 S =    80.415000 Cal/mol K

C        2.522271     -0.294673     -0.000001
H        2.579589     -0.938001     -0.883619
H        2.579595     -0.937969      0.883640
H        3.404486      0.351394     -0.000016
C        1.230777      0.528703     -0.000011
H        1.218742      1.186337      0.877200
```

H	1.218737	1.186307	-0.877244
C	-0.031425	-0.341898	0.000007
H	-0.029937	-0.994896	0.880609
H	-0.029945	-0.994922	-0.880575
C	-1.311113	0.478723	0.000000
H	-1.347741	1.122915	-0.887374
H	-1.347736	1.122938	0.887359
O	-2.433431	-0.420155	0.000016
H	-3.242429	0.102485	0.000012

==========

CF_3CH_2OH (**2f**)



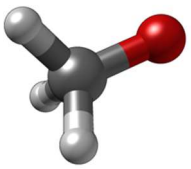
Solvent = 2.2.2-Trifluoroethanol

E0 = -452.925555 Hartree
H = -452.862166 Hartree
G = -452.899813 Hartree
S = 79.236000 Cal/mol K

C	0.653438	-0.021720	0.000006
H	1.026319	-0.534450	0.891859
H	1.026335	-0.534464	-0.891831
O	-0.756090	0.104118	-0.000007
H	-1.140373	-0.779538	-0.000003
C	1.241911	1.374093	0.000000
F	0.875278	2.092555	1.085330
F	0.875298	2.092537	-1.085349
F	2.593609	1.311337	0.000013

==========

CH_3O^- (**3a**)



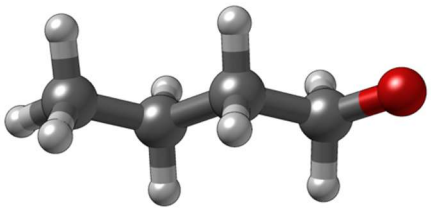
Solvent = Methanol

E0 = -115.262408 Hartree
H = -115.222059 Hartree
G = -115.248195 Hartree
S = 55.008000 Cal/mol K

C	1.447787	0.431876	0.000001
H	1.372410	1.112267	0.882598
H	1.372414	1.112260	-0.882602
O	2.569126	-0.370490	0.000007
H	0.482710	-0.131190	0.000001

==========

$C_4H_9O^-$ (**3c**)



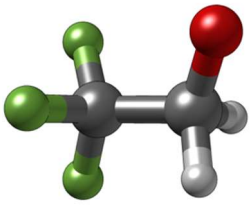
```
Solvent = Butanol

E0 =  -233.129166 Hartree
 H =  -232.999581 Hartree
 G =  -233.036527 Hartree
 S =    77.759000 Cal/mol K

C        -4.935795      0.195749     -0.002581
H        -4.607514     -0.850780     -0.045082
H        -4.604697      0.680119     -0.930245
H        -6.033479      0.199146     -0.000199
C        -4.360190      0.906384      1.228298
H        -4.741203      1.938567      1.259384
H        -4.743969      0.419401      2.137748
C        -2.829447      0.934264      1.281341
H        -2.433033      1.428307      0.378835
H        -2.435803     -0.095455      1.259845
C        -2.219037      1.653278      2.526843
H        -2.733400      1.146649      3.416578
H        -2.730632      2.678522      2.530887
O        -0.883446      1.676477      2.571137
```

==========

$CF_3CH_2O^-$ (**3f**)



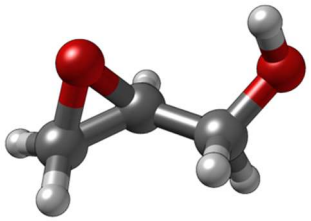
```
Solvent = 2.2.2-Trifluoroethanol

E0 =  -452.435097 Hartree
 H =  -452.385925 Hartree
 G =  -452.421582 Hartree
 S =    75.047000 Cal/mol K

C         0.581777     -0.020858      0.000006
H         1.047343     -0.517460      0.884748
H         1.047356     -0.517473     -0.884721
O        -0.771131      0.012632     -0.000004
C         1.233687      1.366246      0.000000
F         0.900121      2.118369      1.085861
F         0.900142      2.118349     -1.085881
F         2.602569      1.300845      0.000014
```

==========

Glycidol (**1**)



Solvent = Methanol

E0 = -268.416454 Hartree
H = -268.319754 Hartree
G = -268.354654 Hartree
S = 73.454000 Cal/mol K

C	0.350982	-0.138608	0.493767
C	1.670916	-0.400651	-0.086982
O	1.075723	0.908902	-0.192671
H	0.282389	0.017330	1.568166
H	1.745859	-0.943497	-1.024798
H	2.537097	-0.460062	0.564580
C	-0.910870	-0.611586	-0.173994
H	-1.208358	-1.572018	0.252916
H	-0.735795	-0.748164	-1.246853
O	-2.009345	0.278454	0.052303
H	-1.809772	1.118689	-0.377151

Solvent = Butanol

E0 = -268.416025 Hartree
H = -268.319314 Hartree
G = -268.354195 Hartree
S = 73.413000 Cal/mol K

C	0.358515	-0.142925	0.494101
C	1.676610	-0.404850	-0.091210
O	1.083046	0.905498	-0.190360
H	0.292864	0.009240	1.569267
H	1.748247	-0.944535	-1.031192
H	2.544493	-0.468085	0.557809
C	-0.906194	-0.610574	-0.172108
H	-1.205367	-1.571980	0.251546
H	-0.733645	-0.743458	-1.245967
O	-2.001457	0.281230	0.060241
H	-1.799096	1.123634	-0.363578

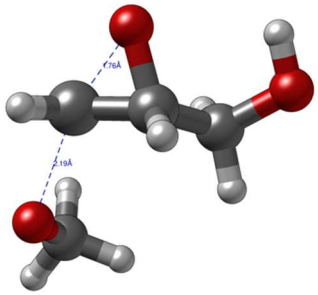
Solvent = 2.2.2-Trifluoroethanol

E0 = -268.416345 Hartree
H = -268.319643 Hartree
G = -268.354537 Hartree
S = 73.441000 Cal/mol K

C	0.350776	-0.138734	0.493500
C	1.670729	-0.400683	-0.087249
O	1.075443	0.908827	-0.192937
H	0.282173	0.017198	1.567899
H	1.745711	-0.943524	-1.025065
H	2.536914	-0.460032	0.564313
C	-0.911041	-0.611802	-0.174260
H	-1.208461	-1.572256	0.252650
H	-0.735957	-0.748368	-1.247120
O	-2.009580	0.278159	0.052036
H	-1.810067	1.118408	-0.377418

==========

TS **4a**



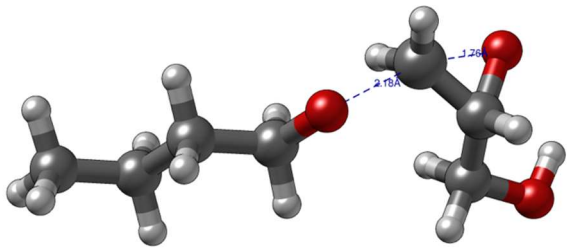
Solvent = Methanol

E0 = -383.661927 Hartree
H = -383.524221 Hartree
G = -383.569772 Hartree
S = 95.871000 Cal/mol K

O	-0.475970	1.909602	0.003697
C	-0.233019	0.588699	-0.445971
H	-0.598422	0.385696	-1.459306
C	-0.666017	-0.483459	0.531811
H	-0.160427	-0.334950	1.493668
H	-0.422192	-1.479616	0.156818
C	1.085921	1.183302	-0.334782
H	1.471318	1.767189	-1.151218
H	1.579946	1.204354	0.622093
O	2.682447	-0.201868	-0.898647
C	2.979525	-1.046904	0.155470
H	2.282557	-1.908672	0.254632
H	2.958718	-0.539479	1.148003
H	3.992974	-1.493466	0.080285
O	-2.089628	-0.451321	0.711603
H	-2.316120	0.462322	0.929959

==========

TS **4c**



Solvent = Butanol

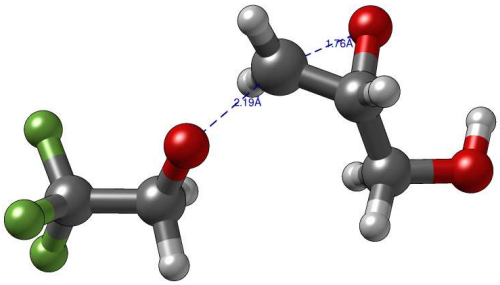
E0 = -501.636462 Hartree
H = -501.409817 Hartree
G = -501.464818 Hartree
S = 115.761000 Cal/mol K

O	3.193813	-1.051754	0.802286
C	2.549808	-0.429339	-0.295089
H	2.917888	-0.755823	-1.274600

C	2.488560	1.080639	-0.193711
H	1.969422	1.369803	0.728319
H	1.958926	1.512359	-1.045689
C	1.515016	-1.239085	0.318555
H	1.434524	-2.278944	0.057722
H	0.972870	-0.853451	1.165597
O	-0.393899	-1.074403	-0.727843
C	-1.185593	-0.074634	-0.197016
H	-1.020546	0.911202	-0.692331
H	-0.955335	0.112944	0.880274
O	3.811993	1.635728	-0.209604
H	4.314399	1.154783	0.461446
C	-2.697094	-0.368295	-0.277451
H	-2.966554	-0.522071	-1.331158
H	-2.891463	-1.319681	0.235763
C	-3.584332	0.728457	0.322432
H	-3.380658	1.679106	-0.186483
H	-3.309547	0.881664	1.373786
C	-5.082765	0.419133	0.232878
H	-5.686696	1.218903	0.672740
H	-5.398685	0.298343	-0.808577
H	-5.325369	-0.509255	0.760439

==========

TS **4f**



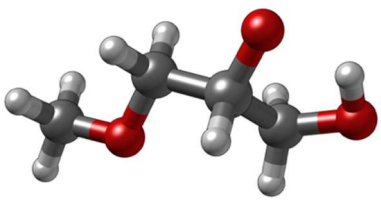
Solvent = 2.2.2-Trifluoroethanol

E0 = -452.925555 Hartree
H = -452.862166 Hartree
G = -452.899813 Hartree
S = 79.236000 Cal/mol K

C	0.653438	-0.021720	0.000006
H	1.026319	-0.534450	0.891859
H	1.026335	-0.534464	-0.891831
O	-0.756090	0.104118	-0.000007
H	-1.140373	-0.779538	-0.000003
C	1.241911	1.374093	0.000000
F	0.875278	2.092555	1.085330
F	0.875298	2.092537	-1.085349
F	2.593609	1.311337	0.000013

==========

INT **5a**



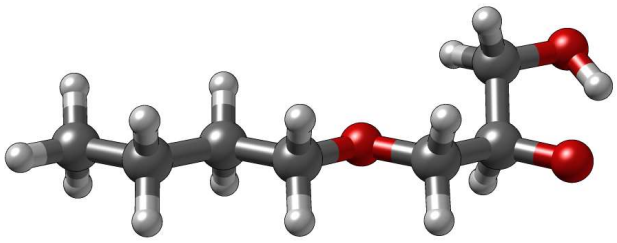
Solvent = Methanol

E0 = -383.728778 Hartree
 H = -383.587711 Hartree
 G = -383.629825 Hartree
 S =   88.637000 Cal/mol K

H	1.100002	-1.076947	1.228016
C	1.032504	-0.952456	0.135873
H	0.885148	-1.946857	-0.309750
C	2.339135	-0.348569	-0.387763
H	2.205455	-0.204121	-1.485177
C	2.586738	1.060095	0.223734
H	2.314610	1.052831	1.291500
H	2.016286	1.848065	-0.275539
O	-0.081291	-0.113123	-0.186352
O	3.427135	-1.151408	-0.101672
O	3.984767	1.330909	0.082371
H	4.315416	0.394645	0.040519
C	-1.316862	-0.645149	0.262608
H	-1.516056	-1.625725	-0.190568
H	-1.329867	-0.756729	1.355239
H	-2.103393	0.050455	-0.033512

==========

INT **5c**



Solvent = Butanol

E0 = -501.703386 Hartree
 H = -501.473459 Hartree
 G = -501.526297 Hartree
 S =   111.205000 Cal/mol K

H	1.097691	-1.020323	1.250112
C	1.023007	-0.933071	0.154879
H	0.876667	-1.942289	-0.255054
C	2.328184	-0.350670	-0.396089
H	2.182689	-0.226049	-1.494773
C	2.597855	1.067081	0.185506
H	2.330245	1.085539	1.254517
H	2.035422	1.852302	-0.327523
O	-0.095043	-0.108498	-0.190944
O	3.409893	-1.159842	-0.107839
O	3.998300	1.315680	0.032601
H	4.314214	0.373112	0.001443
C	-1.335573	-0.635924	0.265335
H	-1.474735	-1.651215	-0.136625
H	-1.322381	-0.717568	1.363051
C	-2.472824	0.269427	-0.184701
H	-2.302515	1.277607	0.210549
H	-2.451335	0.348633	-1.277877

```
C        -3.846680      -0.238319       0.268889
H        -4.004202      -1.252513      -0.117159
H        -3.860790      -0.320546       1.362208
C        -4.997612       0.662915      -0.188057
H        -5.963193       0.275398       0.148888
H        -4.887258       1.676423       0.210332
H        -5.030486       0.737069      -1.279654
```

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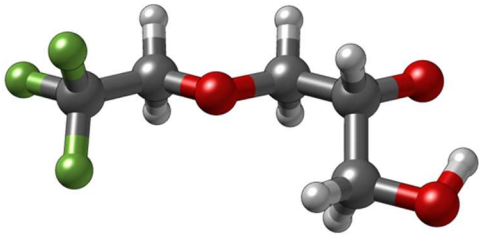
INT **5f**



```
Solvent = 2.2.2-Trifluoroethanol

E0 =  -720.882975 Hartree
 H =  -720.733534 Hartree
 G =  -720.785868 Hartree
 S =   110.147000 Cal/mol K

H         0.812836       0.639663       1.264939
C         0.807540       0.641600       0.165930
H         1.191353       1.608911      -0.182349
C        -0.622934       0.440571      -0.341030
H        -0.565379       0.401014      -1.453440
C        -1.193539      -0.927561       0.130106
H        -0.894128      -1.114284       1.174025
H        -0.853316      -1.765062      -0.484880
O         1.664895      -0.412414      -0.317469
O        -1.456110       1.447910       0.099981
O        -2.617957      -0.832579       0.044341
H        -2.712901       0.151380       0.128750
C         2.994849      -0.264478       0.101555
H         3.444846       0.666131      -0.267717
H         3.091265      -0.290093       1.194642
C         3.805230      -1.417744      -0.453966
F         3.362999      -2.620517      -0.020974
F         3.793476      -1.462407      -1.805580
F         5.100667      -1.310349      -0.071334
```

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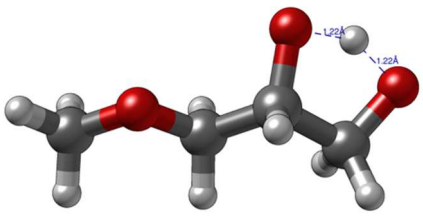
TS **6a**




```
Solvent = Methanol
```

```
E0 =  -383.724367 Hartree
 H =  -383.587766 Hartree
 G =  -383.629083 Hartree
 S =    86.959000 Cal/mol K

C       -1.356726     -0.557068     -0.244665
O       -0.191521      0.102792      0.224921
C        1.008182     -0.598067     -0.105528
H        1.083305     -0.711689     -1.197654
H        0.972513     -1.606423      0.339577
C        2.226624      0.144220      0.411086
H        2.070140      0.328034      1.489816
C        3.536845     -0.735133      0.218535
H        3.343765     -1.538301     -0.516717
H        3.814734     -1.221984      1.164759
O        2.503287      1.339334     -0.265595
O        4.513301      0.161644     -0.237870
H       -1.448681     -1.561433      0.190429
H       -1.349060     -0.649141     -1.338799
H        3.675740      1.030769     -0.399929
H       -2.217071      0.042142      0.056797
```

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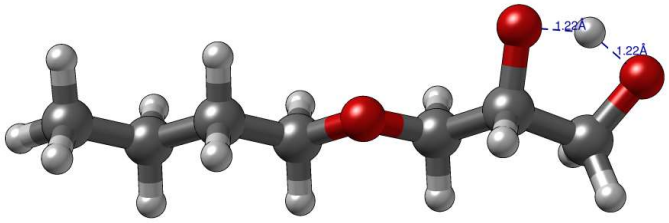
TS **6c**




```
Solvent = Butanol

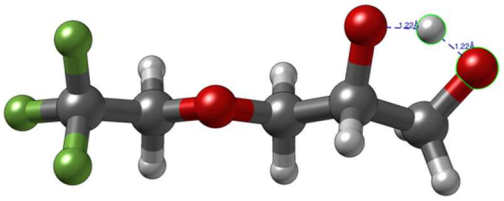
E0 =  -501.698695 Hartree
 H =  -501.473342 Hartree
 G =  -501.525801 Hartree
 S =   110.408000 Cal/mol K

C       -1.368183     -0.554566     -0.222549
O       -0.191855      0.105388      0.232083
C        1.006696     -0.597012     -0.098319
H        1.075917     -0.723262     -1.189411
H        0.976418     -1.600403      0.358929
C        2.228554      0.152665      0.401540
H        2.070172      0.363574      1.475203
C        3.535158     -0.737241      0.234513
H        3.340550     -1.557905     -0.481502
H        3.807179     -1.202382      1.193670
O        2.513078      1.328663     -0.303107
O        4.517379      0.142426     -0.240207
H       -1.420292     -1.563530      0.215366
H       -1.327820     -0.673547     -1.315946
H        3.683913      1.010250     -0.428259
C       -2.590035      0.259959      0.176635
H       -2.504321      1.262602     -0.258084
H       -2.591501      0.385406      1.265648
C       -3.906535     -0.386267     -0.270039
H       -3.894795     -0.520905     -1.358177
```

```
H        -3.983817      -1.390751       0.162952
C        -5.137488       0.434143       0.127078
H        -6.061141      -0.050233      -0.201976
H        -5.194440       0.558651       1.213113
H        -5.106356       1.432702      -0.320174
```

==========

TS **6f**



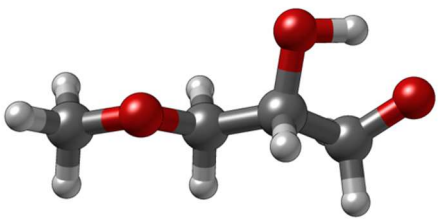
```
Solvent = 2.2.2-Trifluoroethanol

E0 =  -720.878212 Hartree
 H =  -720.733305 Hartree
 G =  -720.784413 Hartree
 S =   107.566000 Cal/mol K

C        -3.074347      -0.104048      -0.225224
O        -1.854036       0.337938       0.307697
C        -0.739248      -0.462505      -0.124236
H        -0.705585      -0.480032      -1.221849
H        -0.881793      -1.491743       0.238511
C         0.556533       0.108912       0.416410
H         0.437562       0.228171       1.508207
C         1.761144      -0.889955       0.128019
H         1.464371      -1.622776      -0.645336
H         2.009351      -1.459727       1.035388
O         0.944155       1.311684      -0.184224
O         2.812740      -0.072923      -0.306538
H        -3.287026      -1.149276       0.034234
H        -3.112568       0.000295      -1.317065
H         2.067667       0.890438      -0.383192
C        -4.187021       0.744228       0.356004
F        -4.046264       2.058430       0.072127
F        -4.270335       0.642811       1.702055
F        -5.384365       0.355425      -0.145924
```

==========

INT **7a**



```
Solvent = Methanol

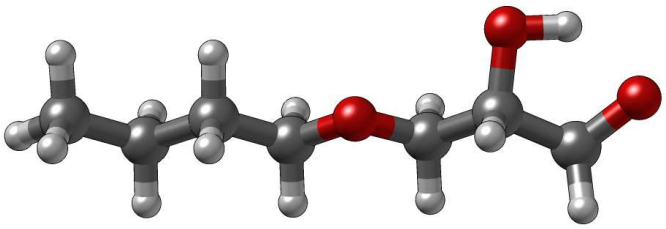
E0 =  -383.728346 Hartree
 H =  -383.587567 Hartree
 G =  -383.629513 Hartree
```

```
 S =    88.281000 Cal/mol K

C       -1.363462      -0.552199      -0.263947
O       -0.188415       0.089795       0.207912
C        1.003666      -0.599122      -0.172971
H        1.048495      -0.686957      -1.267879
H        0.987919      -1.616278       0.250116
C        2.228404       0.128577       0.328811
H        2.083454       0.365891       1.394595
C        3.534393      -0.719433       0.162917
H        3.401112      -1.364842      -0.736706
H        3.591736      -1.414857       1.024782
O        2.455644       1.341000      -0.391443
O        4.619611       0.125916       0.048181
H       -1.444668      -1.574006       0.130423
H       -1.379553      -0.597779      -1.360857
H        3.456737       1.310910      -0.410846
H       -2.216738       0.032503       0.081394
```

==========

INT **7c**



```
Solvent = Butanol

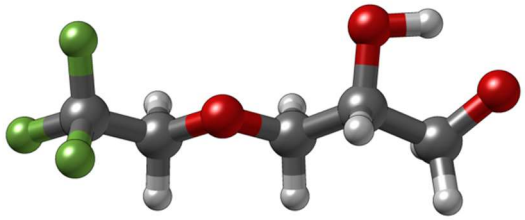
E0 =  -501.702727 Hartree
 H =  -501.473152 Hartree
 G =  -501.525869 Hartree
 S =   110.952000 Cal/mol K

C        1.371812      -0.550954       0.243481
O        0.187410       0.098362      -0.209380
C       -1.003762      -0.596255       0.162058
H       -1.056711      -0.685823       1.256416
H       -0.981424      -1.613179      -0.261912
C       -2.230674       0.122925      -0.348193
H       -2.080438       0.360620      -1.413234
C       -3.531226      -0.735479      -0.190454
H       -3.399485      -1.375806       0.713545
H       -3.572808      -1.436244      -1.049711
O       -2.472748       1.333896       0.368497
O       -4.625070       0.098836      -0.090278
H        1.418113      -1.568216      -0.174824
H        1.345618      -0.647153       1.339304
C        2.586786       0.256443      -0.188677
H        2.510097       1.265194       0.233325
H        2.569621       0.366130      -1.279176
C        3.909512      -0.386479       0.244671
H        3.913733      -0.511158       1.334037
H        3.979570      -1.394871      -0.180234
C        5.135022       0.429243      -0.177941
H        6.062951      -0.054007       0.140494
H        5.175303       0.545261      -1.265630
```

```
H         5.112192      1.431182      0.262138
H        -3.473356      1.297927      0.377704
```

==========

INT **7f**



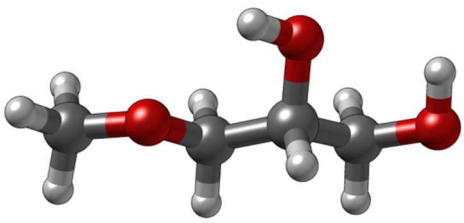
```
Solvent = 2.2.2-Trifluoroethanol

E0 =  -720.881939 Hartree
 H =  -720.732848 Hartree
 G =  -720.783911 Hartree
 S =   107.470000 Cal/mol K

C         3.087465     -0.130636      0.143828
O         1.847380      0.297546     -0.355835
C         0.745496     -0.458436      0.177655
H         0.760340     -0.401290      1.273324
H         0.856596     -1.511008     -0.120473
C        -0.560913      0.083129     -0.347645
H        -0.484839      0.187603     -1.441070
C        -1.770231     -0.853268     -0.000658
H        -1.532342     -1.363635      0.961804
H        -1.800763     -1.654566     -0.766365
O        -0.870744      1.351861      0.224886
O        -2.921606     -0.097781      0.072822
H         3.282760     -1.187171     -0.080737
H         3.172219      0.019037      1.227600
H        -1.862461      1.231546      0.310974
C         4.177949      0.686175     -0.519254
F         4.055258      2.011276     -0.283241
F         4.202375      0.529248     -1.862042
F         5.393442      0.310024     -0.053378
```

==========

3-Methoxypropane-1.2-diol. **[1.0.0]** (**8a**)



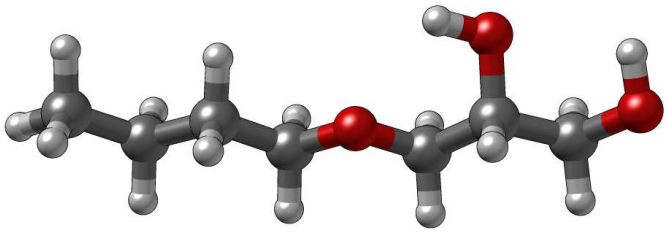
```
Solvent = Methanol

E0 =  -384.227265 Hartree
 H =  -384.071671 Hartree
 G =  -384.115416 Hartree
 S =    92.068000 Cal/mol K
```

```
C         1.387194      -0.665072       0.191471
O         0.180363      -0.025481      -0.209814
C        -0.984413      -0.779824       0.105908
H        -0.995726      -1.022178       1.177624
H        -1.001374      -1.717353      -0.466325
C        -2.187832       0.078422      -0.252600
H        -2.155375       0.303741      -1.326665
C        -3.507943      -0.605850       0.068589
H        -3.555200      -0.828411       1.141815
H        -3.587749      -1.542899      -0.484577
O        -2.175263       1.308312       0.487128
O        -4.625284       0.194452      -0.321889
H        -1.318033       1.726835       0.339174
H         1.507680      -1.630503      -0.314483
H         1.405332      -0.825538       1.276186
H        -4.518375       1.057909       0.096164
H         2.208951      -0.006595      -0.089818
```

==========

3-Butoxypropane-1.2-diol. **[4.0.0]** (**8c**)



```
Solvent = Butanol

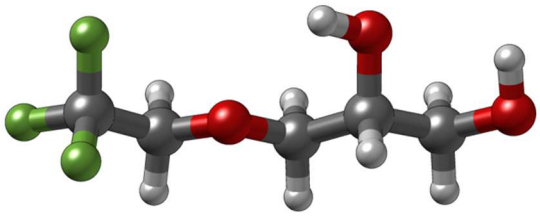
E0 =  -502.204884 Hartree
 H =  -501.960494 Hartree
 G =  -502.015358 Hartree
 S =   115.472000 Cal/mol K

C         1.397618      -0.655968       0.183686
O         0.180710      -0.018581      -0.211699
C        -0.982432      -0.778265       0.094811
H        -0.994922      -1.032303       1.163826
H        -0.998122      -1.709959      -0.487108
C        -2.188774       0.080358      -0.254641
H        -2.157185       0.317933      -1.326026
C        -3.507013      -0.611326       0.059202
H        -3.550556      -0.850734       1.129053
H        -3.586316      -1.539807      -0.508197
O        -2.180136       1.301802       0.498772
O        -4.627134       0.191983      -0.315500
H        -1.324661       1.724957       0.354075
H         1.480540      -1.628956      -0.321009
H         1.376186      -0.842236       1.266784
H        -4.519852       1.049460       0.114552
C         2.570772       0.238594      -0.183861
H         2.443924       1.209473       0.308862
H         2.551106       0.423887      -1.263858
C         3.921609      -0.369617       0.211737
H         3.932011      -0.560960       1.291209
H         4.037272      -1.345362      -0.274766
C         5.107562       0.526167      -0.157582
H         6.056340       0.067405       0.133988
```

```
H         5.142708       0.709047      -1.236133
H         5.038926       1.497512       0.342215

=====================================================================
```

3-(2.2.2-trifluoroethoxy)propane-1.2-diol. **[3F.0.0]** (**8f**)



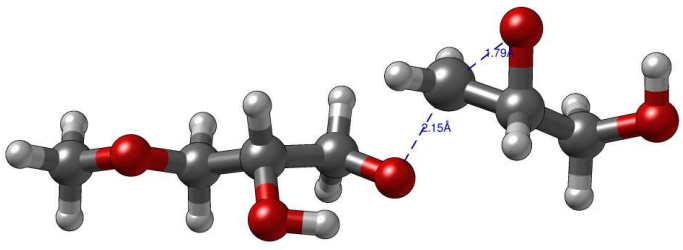
```
Solvent = 2.2.2-Trifluoroethanol

E0 =  -721.380085 Hartree
 H =  -721.216176 Hartree
 G =  -721.269738 Hartree
 S =   112.731000 Cal/mol K

C         3.097899      -0.169705       0.049565
O         1.814976       0.244330      -0.354372
C         0.766867      -0.591836       0.147000
H         0.841790      -0.665061       1.238878
H         0.846828      -1.596196      -0.286436
C        -0.549048       0.056006      -0.252454
H        -0.581937       0.148106      -1.345343
C        -1.751849      -0.753802       0.211930
H        -1.733049      -0.844995       1.305091
H        -1.719530      -1.754508      -0.221069
O        -0.685490       1.355229       0.338652
O        -2.977858      -0.161647      -0.216626
H         0.040203       1.907034       0.023296
H         3.348565      -1.165785      -0.333821
H         3.204149      -0.170859       1.140658
H        -2.972154       0.755481       0.084953
C         4.107952       0.810343      -0.512671
F         3.914481       2.069852      -0.061839
F         4.079815       0.869424      -1.862465
F         5.360199       0.444596      -0.153528

=====================================================================
```

TS **9a-rr**



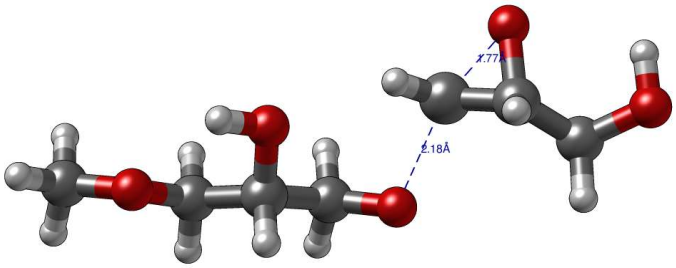

```
Solvent = Methanol

E0 =  -652.124598 Hartree
 H =  -651.886266 Hartree
 G =  -651.946996 Hartree
 S =   127.817000 Cal/mol K
```

O	4.675877	1.780727	-0.563221
C	4.521970	0.674978	0.306356
H	4.453836	0.946343	1.366834
C	5.539700	-0.424450	0.076147
H	5.453131	-0.801141	-0.950847
H	5.390595	-1.254979	0.769177
C	3.279821	0.666447	-0.442070
H	2.479119	1.316330	-0.136127
H	3.256907	0.219182	-1.421349
O	2.092888	-1.009704	0.191425
C	0.964943	-1.141529	-0.604338
H	0.656473	-2.203318	-0.690966
H	1.116306	-0.780277	-1.640479
O	6.865026	0.073521	0.309098
H	6.934996	0.893519	-0.198309
C	-0.221516	-0.340971	0.015292
H	-0.159325	0.709653	-0.305793
C	-1.563028	-0.892733	-0.408142
H	-1.575426	-1.015466	-1.502617
H	-1.716196	-1.881681	0.047025
O	-0.062283	-0.401229	1.435266
H	0.907110	-0.593350	1.490230
O	-2.613562	-0.010643	-0.016087
C	-3.897966	-0.495691	-0.379573
H	-3.981480	-0.623813	-1.466980
H	-4.112305	-1.457237	0.104857
H	-4.630327	0.241684	-0.049524

==========

TS **9a-sr**



Solvent = Methanol

E0 = -652.123804 Hartree
H = -651.885229 Hartree
G = -651.946161 Hartree
S = 128.243000 Cal/mol K

O	4.478890	-0.705719	0.646303
C	3.110304	-1.051109	0.706778
H	2.799050	-1.484730	1.665225
C	2.641255	-1.895960	-0.461044
H	2.820210	-1.360241	-1.401558
H	1.576133	-2.123377	-0.382356
C	3.058956	0.395886	0.607215
H	3.191757	0.986442	1.496035
H	3.162947	0.858040	-0.360420
O	1.026405	1.057643	0.638561
C	0.561557	1.510979	-0.590555
O	3.330975	-3.154055	-0.470954
H	4.272006	-2.945180	-0.399042
C	-0.904083	1.092725	-0.779072
H	-0.986513	0.008428	-0.622165

H	-1.537241	1.593865	-0.032155
O	-1.353773	1.426930	-2.094258
C	-2.711857	1.081258	-2.315506
H	-2.964750	1.376361	-3.334876
H	-3.375161	1.605745	-1.614880
C	0.732731	3.053537	-0.652650
H	1.761481	3.295960	-0.953911
H	0.045414	3.518634	-1.364151
O	0.476528	3.579879	0.654077
H	0.703760	2.794275	1.204349
H	1.125666	1.082366	-1.442644
H	-2.871348	0.000193	-2.205443

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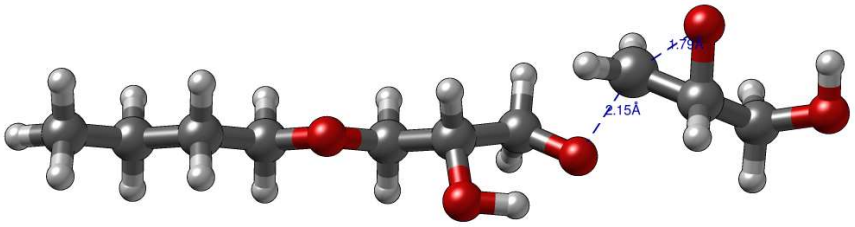
TS **9c-rr**



Solvent = Butanol

E0 = -770.099471 Hartree
H = -769.772359 Hartree
G = -769.842757 Hartree
S = 148.165000 Cal/mol K

O	4.688965	1.718435	-0.706554
C	4.514115	0.689178	0.248579
H	4.420037	1.048276	1.280644
C	5.536778	-0.423631	0.136800
H	5.475152	-0.885276	-0.856853
H	5.369634	-1.193557	0.892854
C	3.291413	0.614066	-0.526321
H	2.481819	1.283559	-0.294848
H	3.292519	0.085900	-1.464579
O	2.102405	-1.014723	0.217260
C	0.967575	-1.185217	-0.560332
H	0.656669	-2.249606	-0.589830
H	1.110024	-0.878256	-1.615479
O	6.856017	0.094869	0.359341
H	6.933377	0.875524	-0.205771
C	-0.213363	-0.352270	0.027069
H	-0.153681	0.680599	-0.347721
C	-1.558997	-0.923258	-0.357810
H	-1.577321	-1.102599	-1.444568
H	-1.707761	-1.887789	0.148250
O	-0.042672	-0.340400	1.446210
H	0.927103	-0.529179	1.502903
O	-2.606969	-0.022726	-0.004673
C	-3.901148	-0.523190	-0.330600
H	-3.959079	-0.720344	-1.411947
H	-4.069150	-1.478898	0.187947
C	-4.952980	0.495478	0.081430
H	-4.752800	1.441317	-0.435032
H	-4.853158	0.691932	1.155115
C	-6.380664	0.029798	-0.227884

```
H        -6.472517      -0.173018      -1.301556
H        -6.570510      -0.922104       0.282081
C        -7.443385       1.050764       0.189222
H        -7.299949       2.003586      -0.330081
H        -8.450430       0.692838      -0.042520
H        -7.398801       1.248929       1.264805
```

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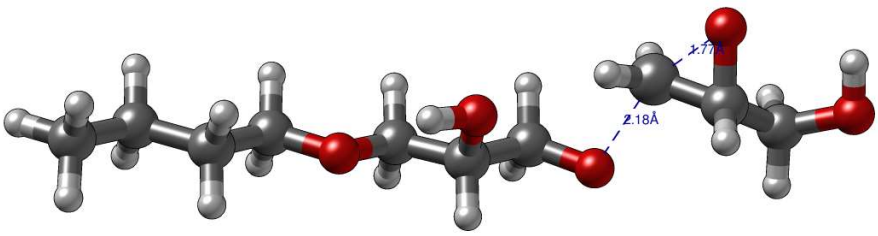
TS **9c-sr**




```
Solvent = Butanol

E0 =  -770.092888 Hartree
 H =  -769.765873 Hartree
 G =  -769.836843 Hartree
 S =   149.369000 Cal/mol K

O        -4.556649       1.651932       0.683173
C        -4.478453       0.655398      -0.322124
H        -4.346644       1.052399      -1.335564
C        -5.598385      -0.361762      -0.258090
H        -5.586182      -0.864929       0.716973
H        -5.496470      -1.114220      -1.043016
C        -3.277892       0.452828       0.462376
H        -2.396731       1.033150       0.254987
H        -3.332035      -0.131690       1.364940
O        -2.161139      -1.240784      -0.337136
C        -0.985469      -1.369037       0.366572
H        -0.695301      -2.433789       0.508458
H        -1.057053      -0.949520       1.397859
O        -6.865360       0.280511      -0.465309
H        -6.879344       1.040102       0.132399
C         0.235533      -0.689906      -0.279516
H         0.296767      -1.015262      -1.328221
C         1.538849      -1.049923       0.419436
H         1.484723      -0.783692       1.485001
H         1.728827      -2.128478       0.338497
O         0.050924       0.738751      -0.248765
H         0.892480       1.128631      -0.518477
O         2.594999      -0.317829      -0.203419
C         3.856176      -0.471864       0.446663
H         3.769706      -0.149168       1.494344
H         4.139888      -1.534341       0.448692
C         4.901749       0.357194      -0.283290
H         4.582614       1.405815      -0.288785
H         4.945953       0.031895      -1.329022
C         6.292737       0.244276       0.352210
H         6.239320       0.557827       1.401453
H         6.603991      -0.806996       0.360657
C         7.348740       1.081515      -0.375478
H         7.082256       2.143122      -0.370409
H         8.329443       0.981628       0.097912
H         7.448729       0.769137      -1.419743
```

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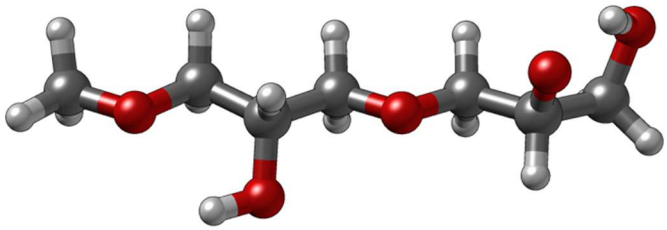
INT **10a-rr**



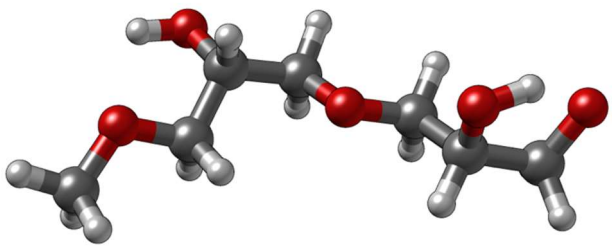
Solvent = Methanol

E0 = -652.180243 Hartree
H = -651.939073 Hartree
G = -651.997048 Hartree
S = 122.018000 Cal/mol K

C	-0.235330	-0.187400	-0.054190
H	-0.154113	-0.508935	0.992574
C	-1.432682	0.746745	-0.184757
H	-1.507169	1.129702	-1.212376
H	-1.331670	1.597551	0.501475
C	1.054052	0.507657	-0.450781
H	1.103889	1.488822	0.043528
H	1.059665	0.675181	-1.537832
O	2.162206	-0.287717	-0.066646
C	3.414124	0.291452	-0.442118
H	3.501159	1.295677	0.001322
H	3.443780	0.394533	-1.538454
C	4.575821	-0.591616	0.040438
H	4.429586	-1.579027	-0.445744
C	5.925537	-0.000907	-0.511104
H	5.790098	0.600664	-1.416777
H	6.617718	-0.821638	-0.746562
O	-2.594097	-0.012797	0.133307
O	-0.414089	-1.337814	-0.890511
H	-1.309846	-1.660632	-0.725750
O	4.672501	-0.680946	1.413740
O	6.472925	0.815680	0.523764
H	5.956801	0.430253	1.293221
C	-3.807643	0.696373	-0.089602
H	-3.860734	1.593675	0.538730
H	-3.903275	0.991609	-1.141566
H	-4.625337	0.025282	0.172548

==========

INT **10a-sr**



Solvent = Methanol

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E0 =  -652.180021 Hartree
 H =  -651.938920 Hartree
 G =  -651.996892 Hartree
 S =   122.012000 Cal/mol K

C       -0.208264      1.394037      0.310791
H       -0.137555      1.160856      1.381144
C       -1.043435      0.319872     -0.368329
H       -0.585020     -0.665457     -0.224389
H       -1.112919      0.524749     -1.446339
C        1.199201      1.498409     -0.263967
H        1.701181      2.365902      0.185494
H        1.149939      1.662728     -1.350508
O        1.903534      0.303846      0.030248
C        3.241021      0.306761     -0.474794
H        3.792794      1.162184     -0.058717
H        3.214809      0.414698     -1.569213
C        3.946226     -0.990784     -0.114407
H        3.349262     -1.826136     -0.499969
C        5.413524     -1.027351     -0.697231
H        5.439901     -0.389302     -1.603815
H        5.597788     -2.063298     -1.054592
O       -2.341342      0.361637      0.218610
O       -0.814346      2.681375      0.139205
H       -1.754708      2.573047      0.331715
O        4.090355     -1.137479      1.296355
H        5.073676     -0.926188      1.362599
O        6.307247     -0.634454      0.280758
C       -3.264602     -0.528179     -0.397884
H       -3.398733     -0.284316     -1.458959
H       -2.926523     -1.568003     -0.311949
H       -4.216557     -0.415740      0.120810
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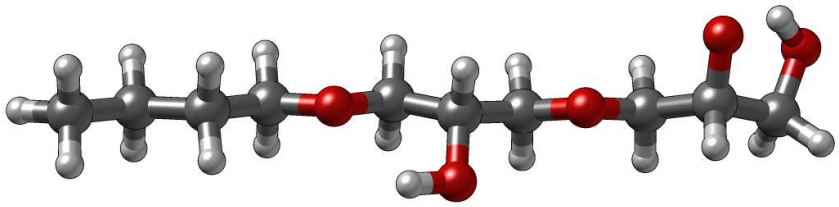
INT **10c-rr**



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Solvent = Butanol

E0 =  -770.154293 Hartree
 H =  -769.824368 Hartree
 G =  -769.892859 Hartree
 S =   144.150000 Cal/mol K

C       -0.236792     -0.167868     -0.125802
H       -0.154226     -0.769390      0.788973
C       -1.439080      0.759905      0.008754
H       -1.511312      1.419237     -0.867995
H       -1.341920      1.381248      0.908554
C        1.050259      0.615621     -0.307971
H        1.084175      1.435079      0.425192
H        1.066496      1.060480     -1.313889
O        2.161125     -0.244387     -0.128145
```

```
C         3.410905      0.410109     -0.360352
H         3.493756      1.290790      0.295608
H         3.441326      0.754131     -1.406699
C         4.576495     -0.550917     -0.079685
H         4.421711     -1.419565     -0.753728
C         5.924502      0.139847     -0.517573
H         5.773823      0.939161     -1.252361
H         6.595648     -0.608597     -0.962313
O        -2.597609     -0.062347      0.094284
O        -0.410069     -1.038323     -1.251479
H        -1.304375     -1.397678     -1.183219
O         4.687744     -0.915355      1.245308
O         6.512688      0.682478      0.662573
H         5.990396      0.146140      1.334695
C        -3.822655      0.673538      0.077298
H        -3.831643      1.385874      0.914403
H        -3.886707      1.252779     -0.854785
C        -4.988607     -0.295918      0.189087
H        -4.882438     -0.872633      1.114936
H        -4.937094     -1.011025     -0.639982
C        -6.347462      0.414601      0.175444
H        -6.385788      1.140443      0.996275
H        -6.446314      0.992291     -0.751111
C        -7.526264     -0.555174      0.299011
H        -7.472917     -1.123212      1.233062
H        -8.480938     -0.022066      0.286789
H        -7.534478     -1.273652     -0.526692
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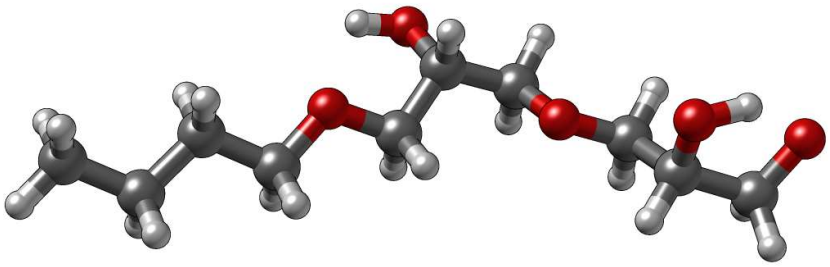
INT **10c-sr**



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Solvent = Butanol

E0 =  -770.154426 Hartree
 H =  -769.824587 Hartree
 G =  -769.893830 Hartree
 S =   145.734000 Cal/mol K

C        -0.198693      1.366628      0.322996
H        -0.114023      1.122180      1.389841
C        -1.051907      0.306122     -0.357351
H        -0.613246     -0.687675     -0.209349
H        -1.110618      0.510435     -1.436217
C         1.200623      1.469426     -0.271293
H         1.710639      2.334067      0.174879
H         1.135000      1.639793     -1.356269
O         1.907368      0.273469      0.007180
C         3.242165      0.284193     -0.505717
H         3.781559      1.158003     -0.113469
H         3.208035      0.365582     -1.602378
C         3.972038     -0.992143     -0.117915
H         3.392335     -1.847689     -0.485117
C         5.439078     -1.012093     -0.697856
```

```
H         5.445120      -0.429107      -1.641966
H         5.656631      -2.061731      -0.993780
O        -2.352153       0.375613       0.221212
O        -0.800469       2.658735       0.173120
H        -1.741247       2.546198       0.361996
O         4.118399      -1.105391       1.295724
H         5.089428      -0.850035       1.361083
O         6.317196      -0.534237       0.254165
C        -3.305406      -0.479864      -0.412294
H        -3.371232      -0.224716      -1.479581
H        -2.965856      -1.522624      -0.338665
C        -4.656689      -0.307436       0.263426
H        -4.947266       0.748069       0.208918
H        -4.557020      -0.556597       1.325991
C        -5.748516      -1.176704      -0.371834
H        -5.446977      -2.229816      -0.327393
H        -5.838502      -0.926844      -1.435554
C        -7.111121      -1.008785       0.306985
H        -7.454378       0.029041       0.250677
H        -7.870170      -1.637359      -0.166811
H        -7.061266      -1.285436       1.364763
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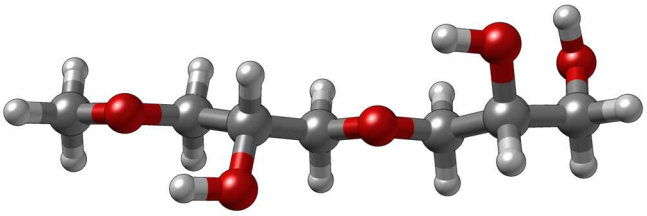
(*R*)-3-((*R*)-2-hydroxy-3-methoxypropoxy)propane-1.2-diol (**11a-rr**)



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Solvent = Methanol

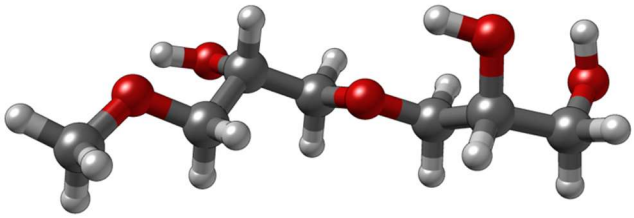
E0 =  -652.680414 Hartree
 H =  -652.424532 Hartree
 G =  -652.484366 Hartree
 S =   125.932000 Cal/mol K

 C      1.77914400    0.23854300    0.08036600
 H      1.60260100    0.44264100    1.14488300
 C      3.00361300   -0.66118200   -0.04504800
 H      3.17414300   -0.92867400   -1.09722600
 H      2.86304200   -1.58249900    0.53492200
 C      0.54505200   -0.42722200   -0.49713300
 H      0.46000500   -1.44893800   -0.10374000
 H      0.63007600   -0.48231200   -1.59032200
 O     -0.60685800    0.32709500   -0.13541200
 C     -1.82438800   -0.22728100   -0.62953600
 H     -1.91234100   -1.27494700   -0.31712500
 H     -1.85242500   -0.18052200   -1.72581400
 C     -2.96017500    0.60080700   -0.04432800
 H     -2.88513800    1.62515900   -0.43335800
 C     -4.34143700    0.06176200   -0.39569400
 H     -4.45422500    0.00110500   -1.47959500
 H     -5.09671100    0.75685200   -0.01111900
 O      4.11359200    0.07681300    0.45301300
 O      1.99827000    1.47372900   -0.60985600
 H      2.87302700    1.78606000   -0.34300300
 O     -2.87622800    0.62423900    1.38816900
 H     -1.94353800    0.73585700    1.61495800
 O     -4.56766000   -1.25239400    0.11760300
 H     -4.38774800   -1.22074900    1.06573600
```

```
 C      5.36009900   -0.58376400    0.26138800
 H      5.38269800   -1.54300900    0.79220200
 H      5.55170000   -0.76048600   -0.80382600
 H      6.13445100    0.06863400    0.66420100
```

==========

(*S*)-3-((*R*)-2-hydroxy-3-methoxypropoxy)propane-1.2-diol (**11a-sr**)



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Solvent = Methanol

E0 =  -652.679994 Hartree
 H =  -652.423983 Hartree
 G =  -652.483719 Hartree
 S =   125.723000 Cal/mol K

 C      1.77914400    0.23854300    0.08036600
 H      1.60260100    0.44264100    1.14488300
 C      3.00361300   -0.66118200   -0.04504800
 H      3.17414300   -0.92867400   -1.09722600
 H      2.86304200   -1.58249900    0.53492200
 C      0.54505200   -0.42722200   -0.49713300
 H      0.46000500   -1.44893800   -0.10374000
 H      0.63007600   -0.48231200   -1.59032200
 O     -0.60685800    0.32709500   -0.13541200
 C     -1.82438800   -0.22728100   -0.62953600
 H     -1.91234100   -1.27494700   -0.31712500
 H     -1.85242500   -0.18052200   -1.72581400
 C     -2.96017500    0.60080700   -0.04432800
 H     -2.88513800    1.62515900   -0.43335800
 C     -4.34143700    0.06176200   -0.39569400
 H     -4.45422500    0.00110500   -1.47959500
 H     -5.09671100    0.75685200   -0.01111900
 O      4.11359200    0.07681300    0.45301300
 O      1.99827000    1.47372900   -0.60985600
 H      2.87302700    1.78606000   -0.34300300
 O     -2.87622800    0.62423900    1.38816900
 H     -1.94353800    0.73585700    1.61495800
 O     -4.56766000   -1.25239400    0.11760300
 H     -4.38774800   -1.22074900    1.06573600
 C      5.36009900   -0.58376400    0.26138800
 H      5.38269800   -1.54300900    0.79220200
 H      5.55170000   -0.76048600   -0.80382600
 H      6.13445100    0.06863400    0.66420100
```

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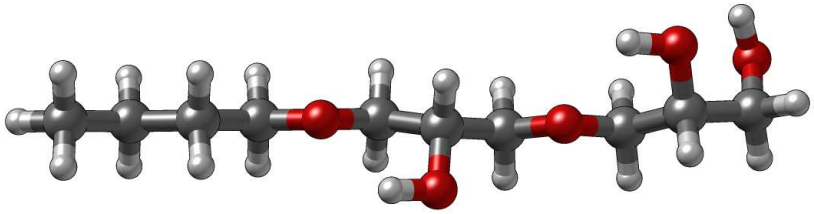
(*R*)-3-((*R*)-2-hydroxy-3-butoxypropoxy)propane-1.2-diol (**11c-rr**)



Solvent = Butanol

E0 = -770.657697 Hartree
 H = -770.312969 Hartree
 G = -770.383556 Hartree
 S =   148.562000 Cal/mol K

C	-0.21692900	-0.17494900	-0.16518400
H	-0.11893000	-0.62627500	0.83120900
C	-1.41551000	0.76783800	-0.15527600
H	-1.50761800	1.27598900	-1.12552300
H	-1.29798500	1.52674300	0.62929500
C	1.06498200	0.56758700	-0.48962300
H	1.13140300	1.47492100	0.12559600
H	1.06299000	0.86444500	-1.54658200
O	2.17820200	-0.27859200	-0.22259700
C	3.43326900	0.32521800	-0.52776600
H	3.51861900	1.29153000	-0.01594000
H	3.52967900	0.48764200	-1.60917000
C	4.51613100	-0.63055100	-0.04635200
H	4.44307900	-1.56277100	-0.62233200
C	5.92623600	-0.07914300	-0.21698100
H	6.10362100	0.17539300	-1.26345900
H	6.64305100	-0.85614900	0.07272600
O	-2.56878200	-0.02775500	0.08849900
O	-0.40663900	-1.20815300	-1.13785000
H	-1.30322200	-1.54469700	-1.00810900
O	4.34818000	-0.91491200	1.35008600
H	3.40301700	-1.04855400	1.49975700
O	6.14884100	1.11085300	0.54152000
H	5.91105400	0.91196400	1.45594700
C	-3.79671900	0.69611500	-0.02672500
H	-3.79112800	1.53719200	0.68077300
H	-3.87957900	1.11232400	-1.04053700
C	-4.95719200	-0.24117900	0.26658300
H	-4.83460200	-0.65283000	1.27484000
H	-4.91610200	-1.08610100	-0.43042100
C	-6.31825900	0.45614000	0.15456300
H	-6.34577600	1.31137400	0.84012600
H	-6.43392100	0.86736900	-0.85510700
C	-7.49181100	-0.47862900	0.46131700
H	-7.42056900	-0.88019000	1.47699800
H	-8.44793800	0.04499100	0.37588900
H	-7.51274100	-1.32651900	-0.23057800

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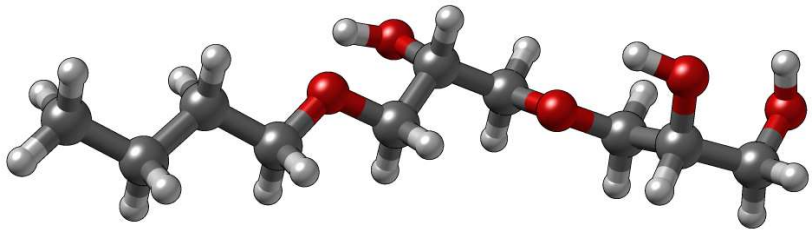
(*S*)-3-((*R*)-2-hydroxy-3-butoxypropoxy)propane-1.2-diol (**11c-sr**)



Solvent = Butanol

E0 = -770.657359 Hartree
H = -770.312567 Hartree
G = -770.383671 Hartree
S = 149.651000 Cal/mol K

C	-0.18073900	1.33157100	0.33208200
H	-0.08657700	1.02227800	1.38130800
C	-1.05957200	0.32631500	-0.39807300
H	-0.63050800	-0.68001300	-0.32296100
H	-1.13584700	0.59984700	-1.46026400
C	1.21206300	1.44961500	-0.27354700
H	1.74583300	2.27274200	0.21777800
H	1.14021300	1.67919100	-1.34532700
O	1.90267500	0.22226500	-0.07526200
C	3.24198900	0.23948200	-0.56634800
H	3.78488300	1.09070800	-0.13864600
H	3.24876700	0.32819500	-1.66037800
C	3.88981000	-1.07249200	-0.14645500
H	3.36366300	-1.89938400	-0.64239400
C	5.36467800	-1.15942900	-0.51964400
H	5.48625100	-1.01849700	-1.59510200
H	5.73278700	-2.15900900	-0.26122800
O	-2.34546600	0.37443800	0.21111300
O	-0.75860000	2.63966800	0.26653300
H	-1.69975600	2.53463800	0.45831900
O	3.81105600	-1.23809800	1.27645400
H	2.92742000	-0.95633100	1.54722700
O	6.15533400	-0.15666400	0.12029100
H	5.98958100	-0.22734600	1.06886300
C	-3.32177800	-0.43417300	-0.44971900
H	-3.40585500	-0.11857100	-1.49924300
H	-2.99246600	-1.48278000	-0.44139700
C	-4.65661300	-0.28592500	0.26304700
H	-4.93982200	0.77291600	0.26743100
H	-4.53610500	-0.58846500	1.30949000
C	-5.76875100	-1.11505100	-0.39041700
H	-5.87738200	-0.81461800	-1.43918200
H	-5.47605500	-2.17154400	-0.40155000
C	-7.11607100	-0.96804700	0.32272400
H	-7.45171700	0.07375700	0.32064800
H	-7.88949200	-1.56858800	-0.16392100
H	-7.04790700	-1.29319000	1.36559900

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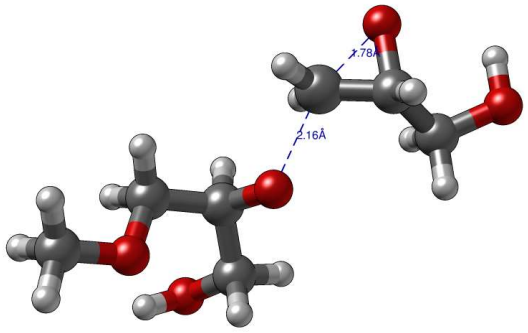
TS **12a-rr**

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Solvent = Methanol

E0 =  -652.117186 Hartree
 H =  -651.878637 Hartree
 G =  -651.939490 Hartree
 S =   128.076000 Cal/mol K

O         3.877686     -1.968283      1.010329
C         3.551696     -1.328862     -0.210357
H         3.387755     -2.018747     -1.046659
C         4.504658     -0.211718     -0.584410
H         4.505916      0.553478      0.201926
H         4.217361      0.255345     -1.528563
C         2.408079     -1.042337      0.633582
H         1.624575     -1.773134      0.722157
H         2.460725     -0.227336      1.336411
O         0.997286      0.182831     -0.450552
C         0.369965      1.101157      0.364310
H         0.869891      1.185645      1.359457
O         5.829179     -0.732182     -0.768880
H         6.018079     -1.266714      0.014107
C         0.451368      2.502962     -0.279893
H         1.499869      2.803117     -0.332978
H         0.060977      2.444446     -1.301200
C        -1.083158      0.735803      0.721022
H        -1.112750     -0.319487      1.026235
H        -1.444378      1.340665      1.567908
O        -1.947677      0.941325     -0.398829
O        -0.222972      3.550954      0.447431
H        -1.170782      3.409609      0.344322
C        -3.286559      0.554206     -0.136115
H        -3.869776      0.754147     -1.036147
H        -3.710531      1.126021      0.700622
H        -3.351678     -0.515456      0.103718
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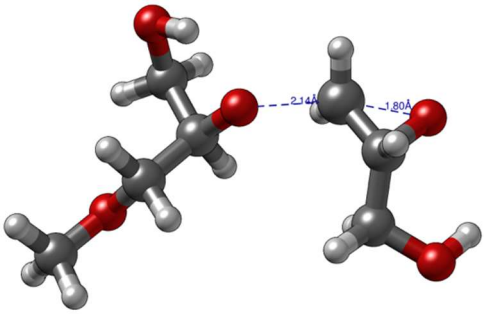
TS **12a-sr**



Solvent = Methanol

E0 = -652.121767 Hartree
 H = -651.883022 Hartree
 G = -651.943004 Hartree
 S =   126.243000 Cal/mol K

O	4.414775	-0.804788	0.679800
C	3.028031	-1.076608	0.712534
H	2.680557	-1.524167	1.651779
C	2.525404	-1.851539	-0.488502
H	2.763486	-1.304834	-1.409160
H	1.444896	-2.001346	-0.436929
C	3.074228	0.373559	0.665842
H	3.224488	0.921151	1.578908
H	3.211419	0.865482	-0.282599
O	1.096732	1.215711	0.696776
C	0.630250	1.579002	-0.551776
O	3.118265	-3.158012	-0.522936
H	4.072225	-3.025689	-0.443700
C	-0.784529	1.007786	-0.754331
H	-0.753371	-0.085411	-0.658298
H	-1.447673	1.403675	0.028630
O	-1.310123	1.361570	-2.045836
C	-2.647679	0.923546	-2.247317
H	-2.949627	1.239224	-3.246441
H	-3.324411	1.367995	-1.506883
C	0.639665	3.113085	-0.721984
H	-0.068417	3.556254	-0.005725
H	1.638369	3.483929	-0.478909
O	0.344631	3.567137	-2.057001
H	-0.402393	3.026384	-2.359431
H	1.259931	1.172867	-1.375242
H	-2.715192	-0.169207	-2.178250

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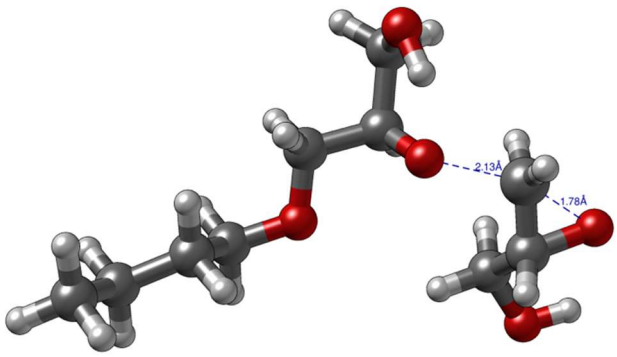
TS **12c-rr**



Solvent = Butanol

E0 = -770.094902 Hartree
 H = -769.767364 Hartree
 G = -769.837116 Hartree
 S =   146.805000 Cal/mol K

O	-4.384414	0.554780	1.005221
C	-3.034049	0.959355	0.902642
H	-2.636829	1.433406	1.808329
C	-2.742698	1.788746	-0.331926
H	-2.997284	1.215969	-1.232262

H	-1.690326	2.074413	-0.381810
C	-2.947524	-0.487431	0.839765
H	-2.958866	-1.053187	1.753999
H	-3.138439	-0.984409	-0.096300
O	-0.919768	-1.108409	0.698344
C	-0.489249	-1.347367	-0.598629
O	-3.500421	3.007275	-0.293776
H	-4.410253	2.748467	-0.094028
C	0.991085	-1.001426	-0.807868
H	1.600720	-1.562677	-0.087206
H	1.301454	-1.294734	-1.823321
O	1.194472	0.403347	-0.652188
C	2.521248	0.842857	-0.939374
H	2.445480	1.925019	-1.082302
H	2.856783	0.404655	-1.891385
C	3.535380	0.542354	0.165919
H	3.623971	-0.539836	0.309817
H	3.160402	0.958615	1.108259
C	4.920049	1.124876	-0.142647
H	4.833598	2.209002	-0.284419
H	5.280920	0.719281	-1.095664
C	5.949998	0.836056	0.953638
H	6.925164	1.265016	0.705988
H	5.633529	1.258084	1.912663
H	6.085221	-0.241071	1.093727
C	-0.723058	-2.859067	-0.929335
H	-1.739213	-2.996145	-1.324156
H	-0.016428	-3.243583	-1.672137
O	-0.571401	-3.600598	0.282586
H	-0.742647	-2.880003	0.940209
H	-1.057570	-0.753843	-1.341482

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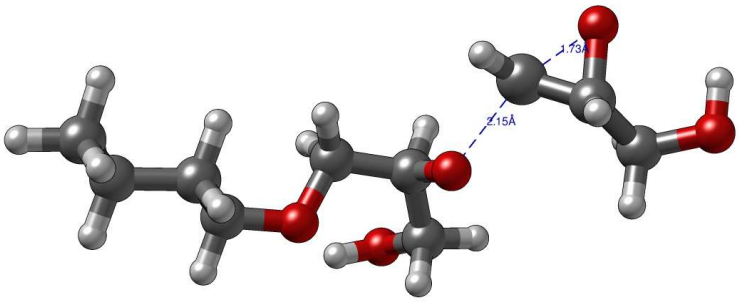
TS **12c-sr**



Solvent = Butanol

E0 = -770.089528 Hartree
H = -769.762013 Hartree
G = -769.834197 Hartree
S = 151.923000 Cal/mol K

O	3.905273	-2.068563	0.869211
C	3.550825	-1.384104	-0.323214
H	3.383566	-2.041825	-1.183343
C	4.467446	-0.228773	-0.661964
H	4.478659	0.490943	0.165753
H	4.137166	0.283002	-1.568064
C	2.440030	-1.188610	0.585613
H	1.670224	-1.935756	0.646307
H	2.479986	-0.397633	1.315850

```
O         0.941478      0.031586     -0.365978
C         0.358215      0.930883      0.496496
H         0.845181      0.914730      1.503736
O         5.796813     -0.704253     -0.921500
H         6.035676     -1.264053     -0.170930
C         0.532775      2.367365     -0.048624
H         1.590640      2.635709     -0.009343
H         0.216900      2.379398     -1.096722
C        -1.122336      0.637336      0.815595
H        -1.220112     -0.439634      0.995043
H        -1.438405      1.165583      1.728828
O        -1.964451      1.054378     -0.266511
O        -0.165679      3.393195      0.687917
H        -1.106137      3.255230      0.524017
C        -3.359528      0.840959     -0.050530
H        -3.870890      1.496577     -0.762038
H        -3.630592      1.173689      0.962532
C        -3.808552     -0.603869     -0.270697
H        -3.299150     -1.266041      0.437723
H        -3.501329     -0.916731     -1.275430
C        -5.325733     -0.769820     -0.117574
H        -5.836039     -0.104137     -0.824274
H        -5.627962     -0.442184      0.884460
C        -5.797032     -2.209300     -0.344736
H        -6.881718     -2.294870     -0.233360
H        -5.535993     -2.554572     -1.350028
H        -5.332732     -2.893790      0.372192
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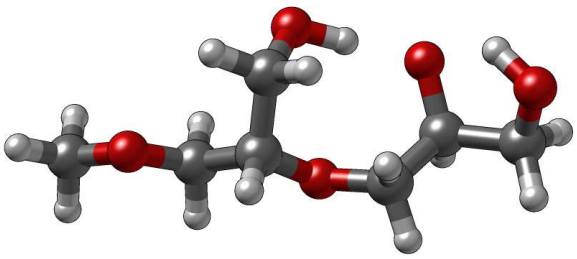
INT **13a-rr**



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Solvent = Methanol

E0 =  -652.189940 Hartree
 H =  -651.948916 Hartree
 G =  -652.004575 Hartree
 S =   117.144000 Cal/mol K

H        -0.947566     -1.778196     -0.589221
C        -0.885370     -0.694190     -0.426051
H        -0.806372     -0.201602     -1.403953
C         0.350062     -0.382531      0.414232
H         0.189219     -0.784806      1.426913
C         0.623292      1.127170      0.537791
H         1.354254      1.294255      1.341066
H        -0.308282      1.611818      0.846734
O        -2.041103     -0.234303      0.264882
C        -3.238070     -0.451438     -0.468741
H        -3.216612      0.079815     -1.428850
H        -3.397555     -1.520353     -0.660958
O         1.411495     -1.087469     -0.230082
O         1.071365      1.709765     -0.668277
H         2.030231      1.372594     -0.797710
```

```
C         2.702300      -1.065183       0.398230
H         2.662737      -0.508785       1.340092
H         2.973413      -2.104267       0.626209
C         3.753040      -0.442085      -0.538622
H         3.775546      -1.079647      -1.444579
C         5.161128      -0.527155       0.120294
H         5.929458      -0.574943      -0.663606
H         5.274109      -1.406499       0.762815
O         3.494088       0.889881      -0.839876
H         4.729545       1.263519       0.444479
O         5.348542       0.649748       0.910723
H        -4.062334      -0.069406       0.134024
```

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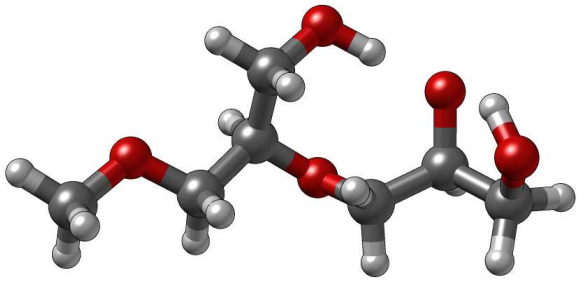
INT **13a-sr**



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Solvent = Methanol

E0 =  -652.188344 Hartree
 H =  -651.947147 Hartree
 G =  -652.002379 Hartree
 S =   116.247000 Cal/mol K

C         0.343150       0.634596      -0.814159
C         0.624159       1.392363       0.491564
H         0.830426       0.676366       1.301547
H        -0.288300       1.928253       0.767430
O         1.512840       0.051163      -1.400010
O         1.678764       2.323202       0.363840
C         2.321572      -0.837854      -0.608524
H         1.889750      -0.985711       0.385510
H         2.337694      -1.808356      -1.120056
C         3.752277      -0.287006      -0.475311
H         4.143827      -0.188773      -1.507112
C         4.649572      -1.322584       0.262893
H         5.693045      -1.194729      -0.056444
H         4.354950      -2.357443       0.060712
O         3.808507       0.912541       0.225747
H         4.289170      -0.121688       1.650718
O         4.539866      -1.077459       1.667773
C        -0.760364      -0.417883      -0.665249
H        -0.506440      -1.144774       0.119993
H        -0.861812      -0.964346      -1.612893
O        -1.983243       0.234428      -0.341273
C        -3.068495      -0.673325      -0.204113
H        -2.884819      -1.391073       0.605531
H        -3.240538      -1.227810      -1.135558
H         0.016954       1.363375      -1.563033
H         2.542304       1.776474       0.268632
H        -3.955505      -0.085257       0.032296
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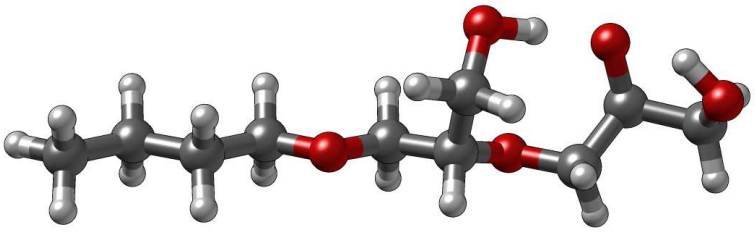
INT **13c-rr**



Solvent = Butanol

E0 = -770.164653 Hartree
 H = -769.834786 Hartree
 G = -769.900935 Hartree
 S =   139.223000 Cal/mol K

H	-0.941905	-1.783573	-0.587512
C	-0.883617	-0.701085	-0.412833
H	-0.808869	-0.198612	-1.385823
C	0.355691	-0.393281	0.424193
H	0.199205	-0.798899	1.436441
C	0.628854	1.116255	0.551449
H	1.365528	1.280957	1.350180
H	-0.301417	1.597382	0.870031
O	-2.038421	-0.252817	0.286756
C	-3.241126	-0.429006	-0.459505
H	-3.173256	0.132204	-1.402932
H	-3.363984	-1.491956	-0.715183
O	1.414363	-1.096432	-0.226948
O	1.065370	1.705315	-0.655157
H	2.021624	1.366528	-0.798943
C	2.710343	-1.068110	0.389380
H	2.678998	-0.508908	1.330249
H	2.986917	-2.105901	0.617960
C	3.751695	-0.443922	-0.558150
H	3.771318	-1.086774	-1.460700
C	5.163781	-0.518561	0.092905
H	5.927922	-0.557259	-0.695649
H	5.288725	-1.398511	0.732606
O	3.485317	0.884510	-0.863087
H	4.719180	1.267574	0.421097
O	5.344237	0.657825	0.885275
C	-4.420756	0.058425	0.367679
H	-4.258272	1.109887	0.630824
H	-4.450904	-0.504332	1.307811
C	-5.758717	-0.089637	-0.366335
H	-5.721487	0.472579	-1.306847
H	-5.907974	-1.140322	-0.642002
C	-6.950687	0.391368	0.466528
H	-7.889726	0.278184	-0.082371
H	-7.036915	-0.178594	1.396980
H	-6.844793	1.447787	0.732624

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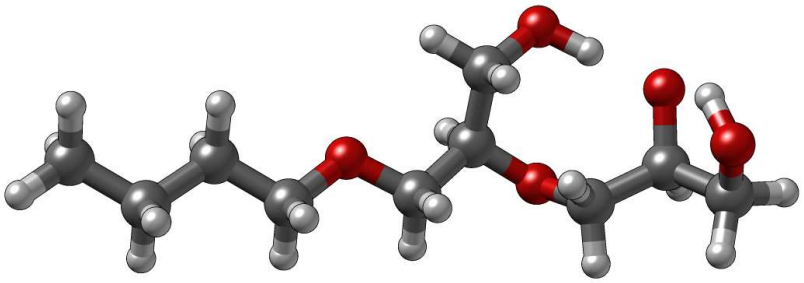
INT **13c-sr**



Solvent = Butanol

E0 = -770.163000 Hartree
 H = -769.833038 Hartree
 G = -769.899174 Hartree
 S =   139.196000 Cal/mol K

C	-0.350777	0.657555	0.803389
C	-0.635308	1.396104	-0.513082
H	-0.840458	0.666807	-1.311514
H	0.275622	1.929984	-0.798251
O	-1.519198	0.083605	1.401576
O	-1.691494	2.325508	-0.397760
C	-2.326844	-0.823342	0.629311
H	-1.889440	-1.000887	-0.357456
H	-2.349673	-1.778798	1.168747
C	-3.755655	-0.273142	0.470376
H	-4.148383	-0.132398	1.497111
C	-4.655382	-1.334648	-0.227409
H	-5.699206	-1.188206	0.082851
H	-4.366653	-2.361787	0.018998
O	-3.806353	0.895981	-0.278868
H	-4.282662	-0.194275	-1.661234
O	-4.539318	-1.148744	-1.640406
C	0.751946	-0.397878	0.667771
H	0.490540	-1.140588	-0.099954
H	0.857450	-0.925016	1.625912
O	1.973523	0.245100	0.322199
C	3.070028	-0.662308	0.217558
H	2.847702	-1.421675	-0.546339
H	3.205008	-1.185552	1.175664
C	4.327380	0.110639	-0.149524
H	4.158518	0.632192	-1.098565
H	4.504045	0.880753	0.610140
C	5.561122	-0.792043	-0.267544
H	5.373772	-1.567876	-1.019354
H	5.719671	-1.316308	0.682285
C	6.830079	-0.019375	-0.639621
H	7.692798	-0.686920	-0.716713
H	6.714017	0.488847	-1.602040
H	7.062524	0.741508	0.112036
H	-0.023099	1.397401	1.540661
H	-2.554393	1.775477	-0.310703

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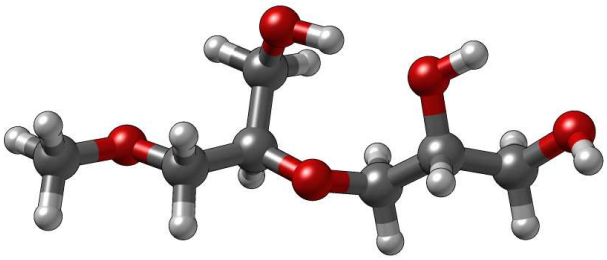
(*R*)-3-(((*R*)-1-hydroxy-3-methoxypropan-2-yl)oxy)propane-1.2-diol (**14a-rr**)



Solvent = Methanol

E0 = -652.189940 Hartree
H = -651.948916 Hartree
G = -652.004575 Hartree
S = 117.144000 Cal/mol K

H	-0.947566	-1.778196	-0.589221
C	-0.885370	-0.694190	-0.426051
H	-0.806372	-0.201602	-1.403953
C	0.350062	-0.382531	0.414232
H	0.189219	-0.784806	1.426913
C	0.623292	1.127170	0.537791
H	1.354254	1.294255	1.341066
H	-0.308282	1.611818	0.846734
O	-2.041103	-0.234303	0.264882
C	-3.238070	-0.451438	-0.468741
H	-3.216612	0.079815	-1.428850
H	-3.397555	-1.520353	-0.660958
O	1.411495	-1.087469	-0.230082
O	1.071365	1.709765	-0.668277
H	2.030231	1.372594	-0.797710
C	2.702300	-1.065183	0.398230
H	2.662737	-0.508785	1.340092
H	2.973413	-2.104267	0.626209
C	3.753040	-0.442085	-0.538622
H	3.775546	-1.079647	-1.444579
C	5.161128	-0.527155	0.120294
H	5.929458	-0.574943	-0.663606
H	5.274109	-1.406499	0.762815
O	3.494088	0.889881	-0.839876
H	4.729545	1.263519	0.444479
O	5.348542	0.649748	0.910723
H	-4.062334	-0.069406	0.134024

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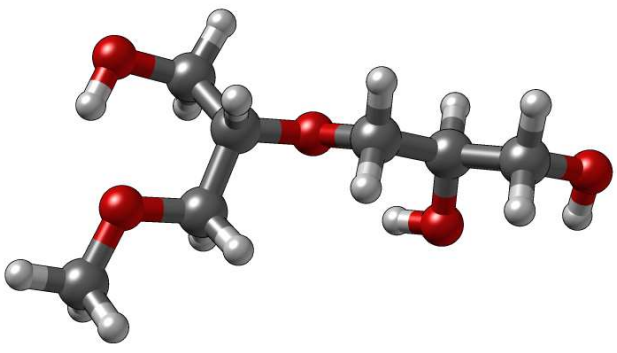
(*R*)-3-(((*S*)-1-hydroxy-3-methoxypropan-2-yl)oxy)propane-1.2-diol (**14a-sr**)



Solvent = Methanol

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E0 =  -652.188344 Hartree
 H =  -651.947147 Hartree
 G =  -652.002379 Hartree
 S =   116.247000 Cal/mol K

C         0.343150      0.634596     -0.814159
C         0.624159      1.392363      0.491564
H         0.830426      0.676366      1.301547
H        -0.288300      1.928253      0.767430
O         1.512840      0.051163     -1.400010
O         1.678764      2.323202      0.363840
C         2.321572     -0.837854     -0.608524
H         1.889750     -0.985711      0.385510
H         2.337694     -1.808356     -1.120056
C         3.752277     -0.287006     -0.475311
H         4.143827     -0.188773     -1.507112
C         4.649572     -1.322584      0.262893
H         5.693045     -1.194729     -0.056444
H         4.354950     -2.357443      0.060712
O         3.808507      0.912541      0.225747
H         4.289170     -0.121688      1.650718
O         4.539866     -1.077459      1.667773
C        -0.760364     -0.417883     -0.665249
H        -0.506440     -1.144774      0.119993
H        -0.861812     -0.964346     -1.612893
O        -1.983243      0.234428     -0.341273
C        -3.068495     -0.673325     -0.204113
H        -2.884819     -1.391073      0.605531
H        -3.240538     -1.227810     -1.135558
H         0.016954      1.363375     -1.563033
H         2.542304      1.776474      0.268632
H        -3.955505     -0.085257      0.032296

=====================================================================
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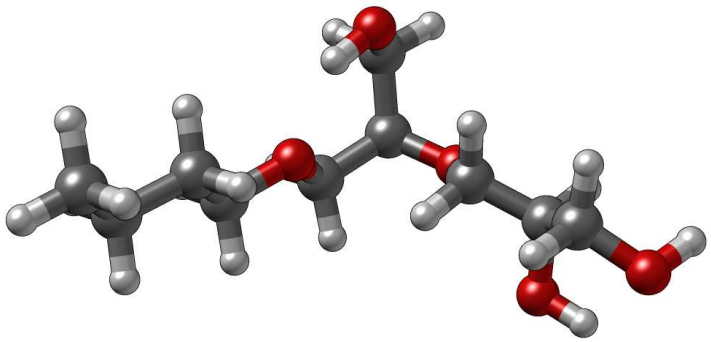
(*R*)-3-(((*R*)-1-hydroxy-3-butoxypropan-2-yl)oxy)propane-1.2-diol (**14c-rr**)



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Solvent = Butanol

E0 =  -770.649351 Hartree
 H =  -770.304224 Hartree
 G =  -770.374105 Hartree
 S =   147.077000 Cal/mol K

H        -0.272106      1.016965     -2.006632
C        -0.615265      1.577406     -1.127695
H        -1.271230      2.385958     -1.476900
C         0.587179      2.206149     -0.418453
H         0.880669      3.054576     -1.046156
C         0.252033      2.809688      0.951972
H        -0.499828      3.596550      0.797443
```

```
H         1.150124      3.281586      1.355334
O        -1.352006      0.719034     -0.252931
C        -2.523603      0.163952     -0.860276
H        -3.172680      0.980508     -1.206098
H        -2.228404     -0.425485     -1.739048
O         1.766815      1.391912     -0.415598
O        -0.195316      1.876611      1.938058
H        -0.876064      1.334692      1.509020
C         1.698031      0.079558      0.149518
H         1.492584      0.135702      1.222860
H         0.905187     -0.506506     -0.326224
C         3.034878     -0.599803     -0.079475
H         3.833255      0.089356      0.231542
C         3.155752     -1.889397      0.733948
H         2.338095     -2.569462      0.484929
H         3.119286     -1.670016      1.805383
O         3.178381     -0.888213     -1.475046
H         3.924469     -1.498002     -1.554150
O         4.360696     -2.590427      0.396058
H         5.106707     -2.138867      0.808380
C        -3.247014     -0.706592      0.154698
H        -2.566995     -1.495339      0.495910
H        -3.495562     -0.097239      1.031312
C        -4.524057     -1.335861     -0.415107
H        -5.195033     -0.542503     -0.764854
H        -4.271146     -1.936440     -1.296724
C        -5.258930     -2.211801      0.603674
H        -6.163906     -2.647404      0.171386
H        -4.623926     -3.034383      0.947327
H        -5.555165     -1.630832      1.482693
```

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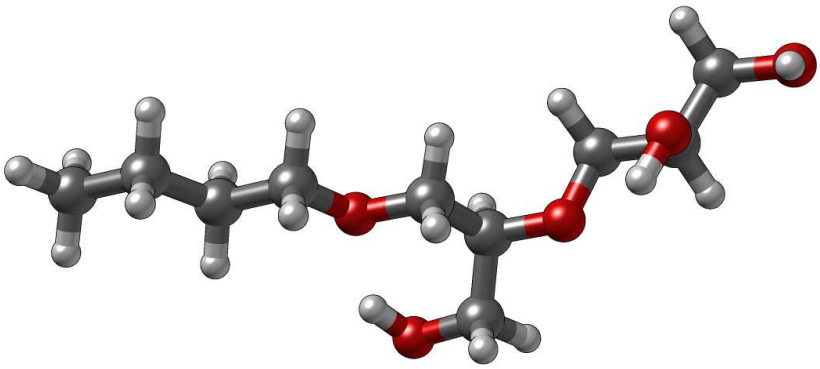
(*R*)-3-(((*R*)-1-hydroxy-3-butoxypropan-2-yl)oxy)propane-1.2-diol (**14c-sr**)



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Solvent = Butanol

E0 =  -770.654618 Hartree
 H =  -770.309713 Hartree
 G =  -770.381124 Hartree
 S =   150.298000 Cal/mol K

H         0.175148     -1.028734     -0.076709
C         0.522453     -0.061847      0.308478
H         0.486351     -0.095885      1.406051
C        -0.385312      1.066937     -0.190333
H        -0.353295      1.107728     -1.285840
C         0.015575      2.440017      0.359232
H         0.049698      2.396682      1.456279
H        -0.742618      3.170460      0.071760
O         1.854456      0.192400     -0.133551
```

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C         2.803528      -0.782593       0.315728
H         2.813121      -0.799928       1.414055
H         2.488890      -1.775019      -0.034291
O        -1.721142       0.811980       0.253205
O         1.260168       2.896450      -0.171328
H         1.874826       2.146788      -0.125530
C        -2.536610       0.084953      -0.668321
H        -2.709098       0.683485      -1.571513
H        -2.052223      -0.856708      -0.953624
C        -3.855291      -0.200360       0.032870
H        -4.311277       0.752617       0.330426
C        -4.831054      -0.960033      -0.854063
H        -4.385827      -1.916854      -1.154215
H        -5.049390      -0.381200      -1.752725
O        -3.653117      -1.012311       1.198571
H        -3.043868      -0.543658       1.781747
O        -6.078910      -1.177505      -0.194953
H        -5.884177      -1.602001       0.649979
C         4.176236      -0.428052      -0.232145
H         4.123714      -0.396095      -1.326250
H         4.443522       0.580209       0.104699
C         5.258236      -1.422646       0.205544
H         5.304512      -1.450941       1.300467
H         4.975949      -2.431728      -0.117062
C         6.641452      -1.078241      -0.354177
H         7.392586      -1.802032      -0.026321
H         6.634468      -1.076747      -1.448648
H         6.965845      -0.086883      -0.022567
```

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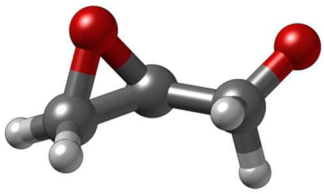
oxiran-2-ylmethanolate (**15**)



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Solvent = Methanol

E0 =  -267.912127 Hartree
 H =  -267.830129 Hartree
 G =  -267.864115 Hartree
 S =    71.530000 Cal/mol K

C         0.336745      -0.115877       0.479802
C         1.659743      -0.418782      -0.075801
O         1.107345       0.907566      -0.214159
H         0.274436       0.073134       1.551984
H         1.730659      -0.979451      -1.004921
H         2.525518      -0.490487       0.577664
C        -0.963762      -0.573995      -0.162509
H        -1.103079      -1.622275       0.208603
H        -0.734219      -0.691976      -1.249391
O        -2.036679       0.240928       0.092496

Solvent = Butanol

E0 =  -267.908402 Hartree
 H =  -267.826471 Hartree
 G =  -267.860454 Hartree
 S =    71.522000 Cal/mol K
```

```
C         0.336207      -0.112215       0.478151
C         1.659561      -0.420603      -0.074490
O         1.111233       0.906140      -0.217888
H         0.272697       0.080768       1.549512
H         1.730260      -0.985069      -1.001504
H         2.524442      -0.492950       0.580412
C        -0.964982      -0.572502      -0.162607
H        -1.095534      -1.625137       0.202220
H        -0.736681      -0.682717      -1.251192
O        -2.040497       0.233070       0.101152

Solvent = 2.2.2-Trifluoroethanol

E0 =  -267.911190 Hartree
 H =  -267.829209 Hartree
 G =  -267.863196 Hartree
 S =    71.533000 Cal/mol K

C         0.336621      -0.114913       0.479425
C         1.659643      -0.419244      -0.075459
O         1.108366       0.907269      -0.215069
H         0.274035       0.075063       1.551414
H         1.730432      -0.980847      -1.004066
H         2.525231      -0.491192       0.578303
C        -0.964056      -0.573569      -0.162541
H        -1.101085      -1.622957       0.207035
H        -0.734763      -0.689697      -1.249856
O        -2.037719       0.238873       0.094580
```

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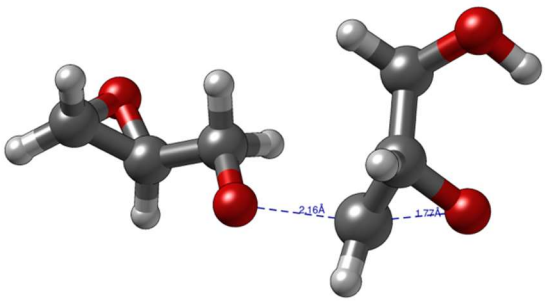
TS **16-rr**

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Solvent = Methanol

E0 =  -536.310232 Hartree
 H =  -536.130837 Hartree
 G =  -536.183879 Hartree
 S =   111.638000 Cal/mol K

 O      3.04850100   -1.15761800   -0.36603900
 C      2.20063700   -0.35208400    0.42994400
 H      2.38653700   -0.43382500    1.50753700
 C      2.13647700    1.09444300   -0.01716300
 H      1.78768000    1.14737600   -1.05575900
 H      1.45759000    1.67376900    0.61210400
 C      1.29740500   -1.33037300   -0.14825300
 H      1.19957000   -2.29396000    0.31889400
 H      0.92026600   -1.17694100   -1.14566200
 O     -0.74108500   -1.05077800    0.50612400
 C     -1.37397700   -0.05495200   -0.20926700
 H     -1.21537200    0.96526900    0.20434400
 H     -1.02493400    0.00036300   -1.26662000
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```
 O      3.42869100    1.70699000    0.10110000
 H      4.04869100    1.11729000   -0.34846400
 C     -2.87659700   -0.27935600   -0.25729400
 C     -3.79090100    0.36109400    0.69075300
 O     -3.71288600    0.83470300   -0.67319200
 H     -3.18602400   -1.23097600   -0.68829800
 H     -4.73259000   -0.11328200    0.95388300
 H     -3.38544200    1.04591500    1.43177400

Solvent = Butanol

E0 =  -536.307334 Hartree
 H =  -536.127967 Hartree
 G =  -536.181318 Hartree
 S =   112.287000 Cal/mol K

 O      3.04944800   -1.15277100   -0.36247100
 C      2.19815300   -0.35011900    0.43295400
 H      2.38175600   -0.43270200    1.51084800
 C      2.13375200    1.09647900   -0.01407100
 H      1.77921700    1.14959100   -1.05079400
 H      1.45997000    1.67796900    0.61866200
 C      1.30022400   -1.33041500   -0.14915300
 H      1.20184300   -2.29428500    0.31734100
 H      0.92402800   -1.17652200   -1.14684500
 O     -0.74182300   -1.05425000    0.50148100
 C     -1.37397400   -0.05916700   -0.21352300
 H     -1.21244800    0.96214400    0.19718400
 H     -1.02869000   -0.00595400   -1.27271000
 O      3.42873500    1.70466700    0.09591000
 H      4.04436700    1.10419100   -0.34560800
 C     -2.87743000   -0.27999900   -0.25662100
 C     -3.78691400    0.36419000    0.69324700
 O     -3.71352700    0.83491300   -0.67164400
 H     -3.19028200   -1.23202000   -0.68425100
 H     -4.72843900   -0.10794100    0.96139000
 H     -3.37685000    1.04925000    1.43157300

Solvent = 2.2.2-Trifluoroethanol

E0 =  -536.309503 Hartree
 H =  -536.130115 Hartree
 G =  -536.183200 Hartree
 S =   111.727000 Cal/mol K

 O      3.04893900   -1.15619000   -0.36466200
 C      2.19993400   -0.35135800    0.43086600
 H      2.38511400   -0.43301600    1.50858100
 C      2.13550000    1.09506100   -0.01659500
 H      1.78530900    1.14770600   -1.05476000
 H      1.45777100    1.67499100    0.61335800
 C      1.29832400   -1.33046900   -0.14822800
 H      1.20043800   -2.29403300    0.31896800
 H      0.92155300   -1.17722800   -1.14580600
 O     -0.74124200   -1.05190600    0.50488000
 C     -1.37412600   -0.05706100   -0.21135300
 H     -1.21394000    0.96399100    0.19983100
 H     -1.02697500   -0.00404000   -1.26957500
 O      3.42831900    1.70673700    0.09948200
 H      4.04735000    1.11418300   -0.34773300
 C     -2.87710400   -0.27993600   -0.25640500
 C     -3.78901600    0.36347100    0.69187300
 O     -3.71319700    0.83404400   -0.67316900
 H     -3.18823300   -1.23222900   -0.68468700
 H     -4.73064900   -0.10944300    0.95792500
 H     -3.38136800    1.04938400    1.43069500
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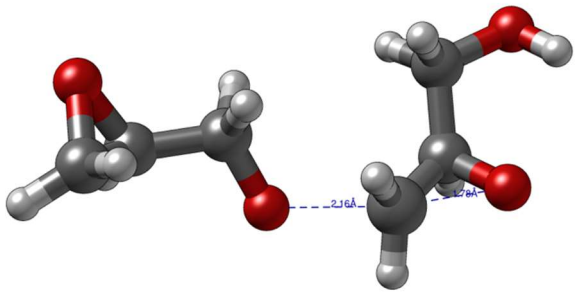
TS **16-sr**



Solvent = Methanol

E0 = -536.310060 Hartree
 H = -536.130574 Hartree
 G = -536.182816 Hartree
 S =   109.952000 Cal/mol K

O	2.891247	-1.377544	-0.056589
C	2.221907	-0.243139	-0.571673
H	2.510068	0.020816	-1.596298
C	2.265645	0.961247	0.346815
H	1.823339	0.704801	1.317276
H	1.716558	1.803731	-0.078705
C	1.161766	-1.225329	-0.429341
H	1.012893	-1.951783	-1.208049
H	0.700183	-1.368884	0.533304
O	-0.756340	-0.482734	-1.077510
C	-1.337077	0.337320	-0.131033
H	-0.993432	1.394252	-0.197153
H	-1.118933	0.023254	0.914619
O	3.619873	1.401874	0.523145
H	4.127975	0.619599	0.776045
C	-2.850307	0.356897	-0.271372
C	-3.721389	-0.503397	0.532263
O	-3.622920	0.908281	0.830019
H	-3.217516	0.669602	-1.248271
H	-3.273923	-1.155684	1.278471
H	-4.687977	-0.820118	0.149526

Solvent = Butanol

E0 = -536.307173 Hartree
 H = -536.127681 Hartree
 G = -536.179913 Hartree
 S =   109.932000 Cal/mol K

O	2.890942	-1.375221	-0.057284
C	2.221702	-0.240588	-0.572112
H	2.508846	0.023118	-1.597039
C	2.268435	0.963343	0.346919
H	1.822294	0.708630	1.316158
H	1.724894	1.808986	-0.079436
C	1.162654	-1.223347	-0.427932
H	1.011897	-1.949220	-1.206760
H	0.701355	-1.366209	0.534919
O	-0.757283	-0.482374	-1.074834
C	-1.338510	0.337770	-0.130254
H	-0.996206	1.395466	-0.196997
H	-1.121418	0.025620	0.916655
O	3.624743	1.395917	0.527244

```
H         4.128116      0.607440      0.770495
C        -2.851702      0.355622     -0.271789
C        -3.722175     -0.504833      0.531974
O        -3.627567      0.907301      0.827500
H        -3.217821      0.665568     -1.249945
H        -3.274091     -1.155117      1.279636
H        -4.687464     -0.824815      0.148369

Solvent = 2.2.2-Trifluoroethanol

E0 =  -536.309334 Hartree
 H =  -536.129845 Hartree
 G =  -536.182051 Hartree
 S =   109.878000 Cal/mol K

O         2.874625      1.246965     -0.586562
C         2.213713      0.422624      0.353592
H         2.532097      0.580858      1.390960
C         2.220107     -1.047692     -0.012809
H         1.748233     -1.188497     -0.992983
H         1.679897     -1.642443      0.726638
C         1.157082      1.288257     -0.139251
H         1.037896      2.266438      0.291119
H         0.666257      1.047310     -1.067351
O        -0.745318      0.900832      0.800008
C        -1.361438     -0.216248      0.273360
H        -1.023677     -1.166470      0.745342
H        -1.174381     -0.347941     -0.816377
O         3.565247     -1.546891     -0.036959
H         4.069813     -0.936519     -0.591014
C        -2.869579     -0.149257      0.449445
C        -3.759298      0.337538     -0.606966
O        -3.681142     -1.077757     -0.320917
H        -3.207755     -0.040526      1.479376
H        -3.330821      0.630634     -1.562509
H        -4.710769      0.799309     -0.356725
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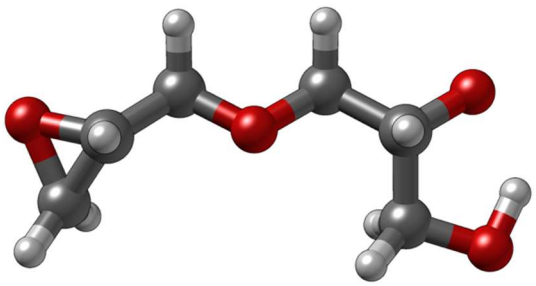
INT **17-rr**



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Solvent = Methanol

E0 =  -536.371308 Hartree
 H =  -536.188796 Hartree
 G =  -536.238681 Hartree
 S =   104.992000 Cal/mol K

O        -2.680332     -2.715933      0.084580
C        -1.588899     -2.138110      0.703391
H        -0.913367     -2.901291      1.155218
C        -2.093482     -1.238648      1.867667
H        -2.400551     -0.257346      1.471371
H        -1.337648     -1.080660      2.641760
```

```
C       -0.738888     -1.332279     -0.283755
H       -0.400132     -1.988439     -1.097470
H       -1.349758     -0.529195     -0.722956
O        0.400369     -0.763610      0.378263
C        1.246953     -0.036753     -0.496588
H        0.721770      0.827293     -0.927191
H        1.579942     -0.678970     -1.325275
O       -3.222239     -1.902786      2.443550
H       -3.502034     -2.437638      1.654798
C        2.442623      0.434146      0.291967
C        2.500886      1.775885      0.878404
O        3.227371      1.467350     -0.332528
H        3.035111     -0.353377      0.752342
H        3.123691      1.956288      1.749105
H        1.661243      2.451682      0.743683

Solvent = Butanol

E0 =  -536.368007 Hartree
 H =  -536.185517 Hartree
 G =  -536.235466 Hartree
 S =   105.126000 Cal/mol K

O       -2.681600     -2.712994      0.084671
C       -1.589446     -2.138817      0.702936
H       -0.913676     -2.903555      1.152568
C       -2.091154     -1.240552      1.869985
H       -2.393223     -0.256506      1.476251
H       -1.334784     -1.088384      2.644911
C       -0.739737     -1.332069     -0.283977
H       -0.400269     -1.987858     -1.097845
H       -1.351885     -0.529863     -0.723134
O        0.399281     -0.761580      0.378007
C        1.246917     -0.037257     -0.496628
H        0.723357      0.826534     -0.930101
H        1.581234     -0.680906     -1.323920
O       -3.223096     -1.901308      2.442235
H       -3.502674     -2.433958      1.651235
C        2.441619      0.434412      0.293029
C        2.499752      1.777212      0.876846
O        3.228989      1.465806     -0.331374
H        3.031815     -0.352872      0.756763
H        3.120432      1.958859      1.748901
H        1.660780      2.453263      0.738979

Solvent = 2.2.2-Trifluoroethanol

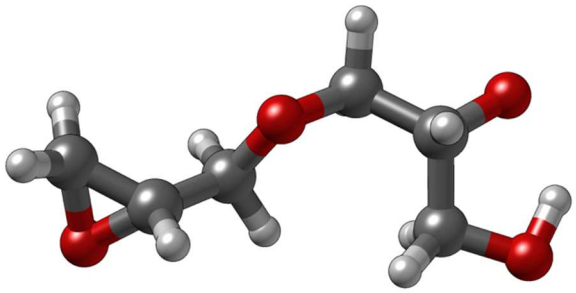
E0 =  -536.371308 Hartree
 H =  -536.188796 Hartree
 G =  -536.238681 Hartree
 S =   104.992000 Cal/mol K

O       -2.680332     -2.715933      0.084580
C       -1.588899     -2.138110      0.703391
H       -0.913367     -2.901291      1.155218
C       -2.093482     -1.238648      1.867667
H       -2.400551     -0.257346      1.471371
H       -1.337648     -1.080660      2.641760
C       -0.738888     -1.332279     -0.283755
H       -0.400132     -1.988439     -1.097470
H       -1.349758     -0.529195     -0.722956
O        0.400369     -0.763610      0.378263
C        1.246953     -0.036753     -0.496588
H        0.721770      0.827293     -0.927191
H        1.579942     -0.678970     -1.325275
O       -3.222239     -1.902786      2.443550
```

```
H        -3.502034      -2.437638       1.654798
C         2.442623       0.434146       0.291967
C         2.500886       1.775885       0.878404
O         3.227371       1.467350      -0.332528
H         3.035111      -0.353377       0.752342
H         3.123691       1.956288       1.749105
H         1.661243       2.451682       0.743683
```

==========

INT **17-sr**



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Solvent = Methanol

E0 =  -536.367762 Hartree
 H =  -536.185164 Hartree
 G =  -536.235910 Hartree
 S =   106.804000 Cal/mol K

O         3.551041       0.904280      -0.146437
C         2.306182       0.499437       0.292256
H         2.121336       0.789244       1.353713
C         2.247967      -1.050882       0.242531
H         2.071335      -1.382913      -0.792987
H         1.469723      -1.473881       0.885313
C         1.179161       1.152006      -0.526474
H         1.330390       2.235366      -0.510299
H         1.230183       0.818647      -1.571017
O        -0.142650       0.916028       0.004322
C        -0.916387      -0.044018      -0.700916
H        -0.391449      -1.005805      -0.764369
H        -1.128731       0.295934      -1.723684
O         3.522582      -1.527626       0.686582
H         4.077870      -0.749410       0.427530
C        -2.210180      -0.230265       0.050940
C        -3.417951       0.524938      -0.292481
O        -3.273750      -0.857127      -0.690764
H        -2.107347      -0.596632       1.069925
H        -3.384123       1.238749      -1.110453
H        -4.174881       0.703154       0.465089

Solvent = Butanol

E0 =  -536.364484 Hartree
 H =  -536.181909 Hartree
 G =  -536.232556 Hartree
 S =   106.596000 Cal/mol K

O         3.551451       0.898434      -0.147625
C         2.306260       0.500043       0.292442
H         2.122010       0.793288       1.353410
C         2.242177      -1.050893       0.247100
H         2.060718      -1.384960      -0.787127
H         1.464481      -1.469454       0.893801
```

```
C         1.181574      1.154467     -0.528205
H         1.334205      2.237556     -0.511811
H         1.234657      0.820771     -1.572619
O        -0.142677      0.920914     -0.000568
C        -0.914402     -0.039925     -0.705522
H        -0.386926     -1.000171     -0.772070
H        -1.130356      0.300613     -1.727544
O         3.516397     -1.530154      0.687509
H         4.071806     -0.751821      0.426433
C        -2.205976     -0.232120      0.048704
C        -3.416734      0.520673     -0.289118
O        -3.270192     -0.859540     -0.691624
H        -2.099209     -0.600793      1.066481
H        -3.387006      1.237247     -1.104904
H        -4.171936      0.695050      0.471178

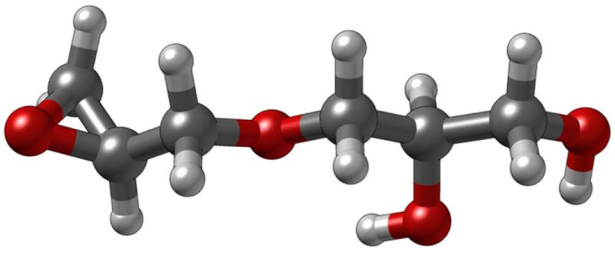
Solvent = 2.2.2-Trifluoroethanol

E0 =  -536.371685 Hartree
 H =  -536.189299 Hartree
 G =  -536.239162 Hartree
 S =   104.945000 Cal/mol K

O         1.098354     -4.317594      4.244505
C         1.610071     -3.859825      3.045987
H         0.998983     -4.196393      2.176247
C         3.033731     -4.454327      2.851116
H         3.767229     -3.850467      3.409247
H         3.339210     -4.491381      1.801997
C         1.641579     -2.329083      2.990369
H         0.625265     -1.936908      3.136736
H         2.276247     -1.945889      3.803825
O         2.151323     -1.878690      1.727473
C         2.149629     -0.465432      1.600609
H         2.783695     -0.004871      2.370975
H         1.127720     -0.074444      1.722286
O         3.001428     -5.784501      3.377269
H         2.252492     -5.675051      4.020156
C         2.653628     -0.096387      0.236333
C         3.328552      1.181075     -0.008762
O         4.086102     -0.043914      0.057506
H         2.131819     -0.567960     -0.593370
H         3.496538      1.865439      0.817985
H         3.271263      1.634574     -0.993497

=====================================================================
```

(*R*)-3-(((*R*)-oxiran-2-yl)methoxy)propane-1.2-diol (**18-rr**)



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Solvent = Methanol

E0 =  -536.869097 Hartree
 H =  -536.672063 Hartree
 G =  -536.723705 Hartree
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```
 S =   108.690000 Cal/mol K

O        1.923859      1.349598     -0.356933
C        1.839192      0.047076      0.239273
H        1.731318      0.153846      1.326362
C        3.158666     -0.649038     -0.061022
H        3.278267     -0.756492     -1.146264
H        3.169661     -1.642349      0.389861
C        0.642852     -0.720918     -0.300917
H        0.721414     -0.831472     -1.390563
H        0.594572     -1.719319      0.153086
O       -0.524091      0.030025      0.027371
C       -1.720081     -0.511574     -0.522844
H       -1.927494     -1.503923     -0.102144
H       -1.621845     -0.612105     -1.612280
O        4.266411      0.062575      0.492769
H        4.213234      0.970326      0.168589
C       -2.848193      0.432536     -0.194457
C       -3.698457      0.234847      0.982723
O       -4.169021     -0.118728     -0.337185
H       -2.741969      1.439870     -0.590431
H       -4.199875      1.086644      1.431300
H       -3.510466     -0.609804      1.639051
H        1.088401      1.803210     -0.191198

Solvent = Butanol

E0 =  -536.868434 Hartree
 H =  -536.671380 Hartree
 G =  -536.722976 Hartree
 S =   108.594000 Cal/mol K

O        1.958802      1.251699     -0.582770
C        1.877381      0.072599      0.230562
H        1.772948      0.366077      1.283084
C        3.196918     -0.664000      0.051290
H        3.313214     -0.957397     -0.999516
H        3.210551     -1.564502      0.667055
C        0.680030     -0.777993     -0.164215
H        0.755785     -1.076786     -1.218168
H        0.633659     -1.682058      0.457125
O       -0.486407      0.018314      0.031381
C       -1.683587     -0.611369     -0.411781
H       -1.889018     -1.515003      0.176546
H       -1.588663     -0.901019     -1.467168
O        4.304936      0.133339      0.470181
H        4.247950      0.972241     -0.004034
C       -2.811818      0.374926     -0.250255
C       -3.658762      0.385675      0.945746
O       -4.132122     -0.193501     -0.290341
H       -2.707579      1.297575     -0.816593
H       -4.159870      1.302548      1.239901
H       -3.467942     -0.330814      1.739388
H        1.123202      1.726425     -0.495987

Solvent = 2.2.2-Trifluoroethanol

E0 =  -536.868929 Hartree
 H =  -536.671892 Hartree
 G =  -536.723511 Hartree
 S =   108.641000 Cal/mol K

O        1.958920      1.251912     -0.583523
C        1.877136      0.073044      0.230587
H        1.772196      0.367397      1.282796
C        3.196416     -0.664147      0.052229
```

```
H         3.313087      -0.958848      -0.998076
H         3.209598      -1.563785       0.669125
C         0.680010      -0.777788      -0.164162
H         0.755633      -1.076326      -1.218145
H         0.633931      -1.681921       0.456865
O        -0.486713       0.018335       0.031772
C        -1.683727      -0.611304      -0.412265
H        -1.889038      -1.515346       0.175377
H        -1.588440      -0.899928      -1.467843
O         4.305037       0.133494       0.470445
H         4.250106       0.970920      -0.006664
C        -2.811800       0.375068      -0.249976
C        -3.658590       0.384975       0.946114
O        -4.132506      -0.193200      -0.290705
H        -2.707625       1.298126      -0.815585
H        -4.159549       1.301642       1.241004
H        -3.467978      -0.332429       1.738920
H         1.123505       1.727088      -0.496859
```

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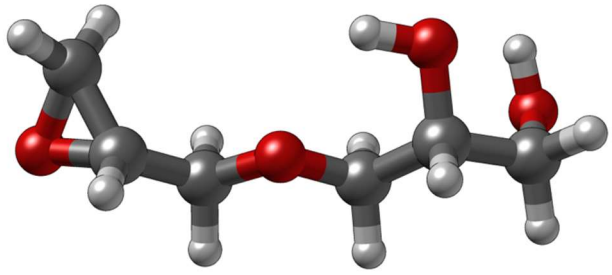
(*R*)-3-(((*S*)-oxiran-2-yl)methoxy)propane-1.2-diol (**18-sr**)



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Solvent = Methanol

E0 =  -536.869073 Hartree
 H =  -536.672025 Hartree
 G =  -536.723526 Hartree
 S =   108.394000 Cal/mol K

O         2.950674      -1.344575      -0.367903
C         1.901303      -0.365953      -0.376990
H         1.710502      -0.041227      -1.408685
C         2.411355       0.835430       0.409303
H         1.641238       1.607578       0.451929
H         3.283114       1.249359      -0.110358
C         0.619197      -0.955571       0.193117
H         0.758337      -1.234606       1.244125
H        -0.195310      -0.223426       0.124116
O         0.313145      -2.115419      -0.581288
C        -0.798222      -2.852507      -0.082491
H        -1.687031      -2.208464      -0.038449
H        -0.593134      -3.227137       0.928502
O         2.745271       0.509650       1.759825
H         3.369598      -0.226247       1.728094
C        -1.047620      -4.005385      -1.020824
C        -0.492821      -5.338194      -0.767312
O        -1.883016      -5.051738      -0.495540
H        -1.275488      -3.728814      -2.047642
H         0.117782      -5.501622       0.115882
H        -0.322077      -6.015079      -1.598521
H         2.562110      -2.180596      -0.657232

Solvent = Butanol
```

```
E0 =  -536.868451 Hartree
 H =  -536.671374 Hartree
 G =  -536.722801 Hartree
 S =   108.238000 Cal/mol K

O        2.950006     -1.343834     -0.369298
C        1.901012     -0.365219     -0.377239
H        1.709986     -0.039346     -1.408617
C        2.411381      0.834926      0.410827
H        1.640991      1.606770      0.455768
H        3.282417      1.250176     -0.109067
C        0.618889     -0.955190      0.192644
H        0.757933     -1.233346      1.243906
H       -0.195966     -0.223325      0.123127
O        0.313433     -2.115326     -0.581378
C       -0.798352     -2.852151     -0.083392
H       -1.687326     -2.208171     -0.040685
H       -0.594661     -3.226132      0.928158
O        2.746486      0.506586      1.760051
H        3.371499     -0.228588      1.725989
C       -1.046904     -4.005801     -1.021028
C       -0.492915     -5.338615     -0.765375
O       -1.882947     -5.051270     -0.495915
H       -1.273067     -3.729989     -2.048450
H        0.116623     -5.501403      0.118734
H       -0.321162     -6.016418     -1.595692
H        2.561552     -2.178877     -0.661411

Solvent = 2.2.2-Trifluoroethanol

E0 =  -536.870432 Hartree
 H =  -536.673456 Hartree
 G =  -536.724802 Hartree
 S =   108.066000 Cal/mol K

O       -0.170568     -0.845890     -4.250889
C       -0.946931      0.314998     -4.581125
H       -1.920987     -0.002249     -4.975224
C       -0.183326      1.044078     -5.676905
H        0.794524      1.361610     -5.293849
H       -0.736353      1.929342     -5.994084
C       -1.172525      1.184711     -3.353996
H       -0.210346      1.509451     -2.935569
H       -1.759462      2.073549     -3.620543
O       -1.875284      0.393407     -2.399368
C       -2.056809      1.046835     -1.146111
H       -2.649143      1.961732     -1.274390
H       -1.081366      1.321586     -0.720357
O       -0.020719      0.227023     -6.837113
H        0.382959     -0.600943     -6.548216
C       -2.756982      0.105610     -0.211930
C       -3.622370      0.604423      0.860566
O       -4.192895      0.019404     -0.327166
H       -2.273246     -0.858878     -0.075839
H       -3.785068      1.673320      0.964834
H       -3.739710      0.017040      1.765807
H       -0.631222     -1.315156     -3.544577

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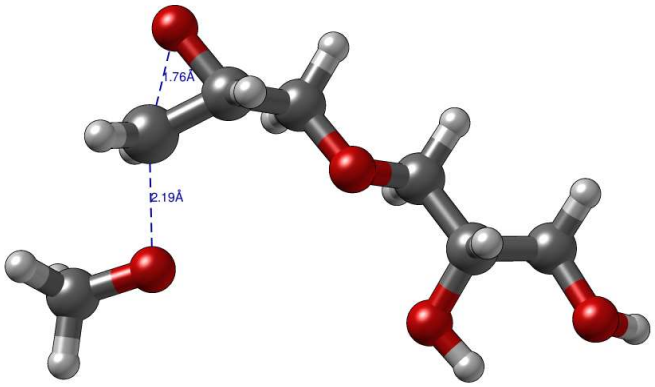
TS **19a-rr**

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Solvent = Methanol

E0 =  -652.110970 Hartree
 H =  -651.873315 Hartree
 G =  -651.935237 Hartree
 S =   130.326000 Cal/mol K

O         3.100278      -2.096260      -0.152057
C         2.059990      -1.269121       0.324003
H         1.821418      -1.392954       1.386845
C         0.804628      -1.326598      -0.525872
H         0.465146      -2.372707      -0.568717
H         1.025317      -0.999489      -1.551209
C         3.137765      -0.346030       0.004468
H         3.922081      -0.178810       0.721580
H         3.260260      -0.011056      -1.011508
O         2.635918       1.740765       0.433011
C         3.768785       2.445641       0.073997
H         4.022223       2.365222      -1.008554
H         4.688936       2.118734       0.612634
O        -0.212573      -0.511338       0.048881
H         3.683935       3.533045       0.275211
C        -1.435016      -0.575517      -0.671901
H        -1.810512      -1.608636      -0.680091
H        -1.279960      -0.258520      -1.712481
C        -2.459642       0.328300      -0.013740
H        -2.465378       0.125290       1.065953
O        -2.082344       1.690787      -0.237956
H        -2.832855       2.232056       0.041122
C        -3.859001       0.071257      -0.561625
H        -3.869976       0.213921      -1.647696
H        -4.169860      -0.953382      -0.331459
O        -4.731129       1.017775       0.072788
H        -5.548041       1.078343      -0.433301

=====================================================================
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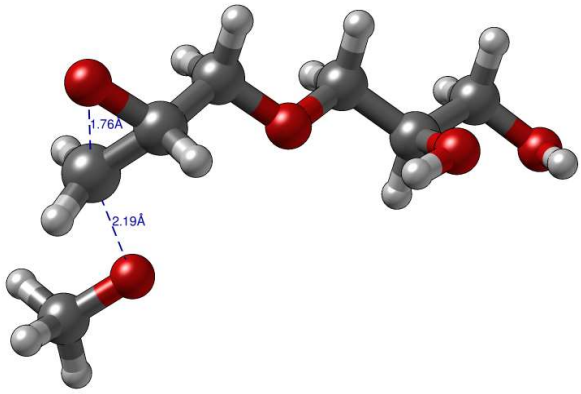
TS **19a-sr**

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Solvent = Methanol

E0 =  -652.113780 Hartree
 H =  -651.876020 Hartree
 G =  -651.937353 Hartree
 S =   129.086000 Cal/mol K

O       -1.210279      1.516463      0.062519
C       -0.594099      0.378863     -0.500691
H       -0.622324      0.333757     -1.595797
C       -1.054948     -0.933090      0.106164
H       -2.148828     -0.998367      0.011719
H       -0.801046     -0.969743      1.173859
C        0.501972      1.130349      0.089261
H        0.949926      1.937261     -0.464647
H        0.712554      1.018937      1.138804
O        2.432668      0.144207     -0.202944
C        3.382560      1.074397      0.173906
H        3.338906      1.349438      1.253103
H        3.303079      2.041615     -0.375618
O       -0.445256     -2.020909     -0.586708
H        4.421698      0.726644      0.001565
C       -0.820479     -3.296123     -0.079354
H       -1.915625     -3.379357     -0.044273
H       -0.424659     -3.438089      0.935261
C       -0.245281     -4.342274     -1.021866
H        0.847249     -4.238135     -1.044341
O       -0.762151     -4.168442     -2.349944
H       -0.591741     -3.253938     -2.608202
C       -0.598827     -5.761578     -0.604170
H       -0.201759     -5.969190      0.390549
H       -1.689676     -5.876126     -0.575965
O       -0.021782     -6.728675     -1.484058
H       -0.285877     -6.489929     -2.381426

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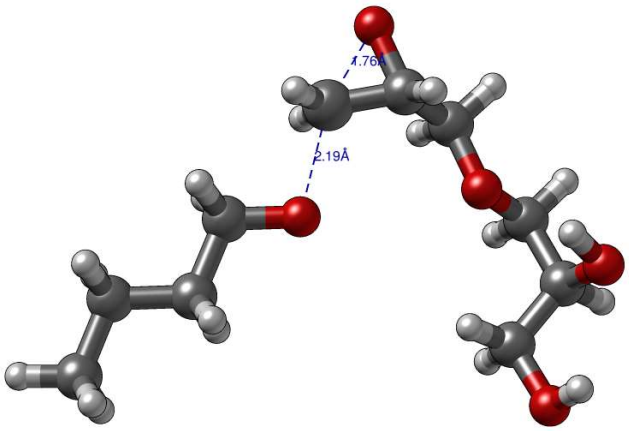
TS **19c-rr**

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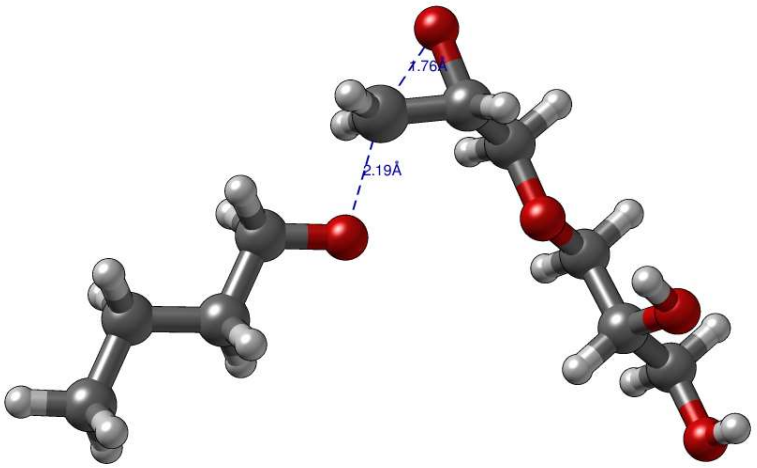
Solvent = Butanol

E0 =  -770.087520 Hartree
 H =  -769.760491 Hartree
 G =  -769.831350 Hartree
 S =   149.137000 Cal/mol K

O       -0.302271      3.794126      0.060079
C        0.186032      2.517714      0.410789
H        0.485969      2.408469      1.459669
C        1.269403      2.008815     -0.521024
H        2.100045      2.730041     -0.518174
H        0.883527      1.936131     -1.546436
C       -1.219358      2.296588      0.109976
H       -1.958240      2.483864      0.868901
H       -1.524334      2.157423     -0.913112
O       -1.821123      0.203142      0.355455
C       -3.175843      0.185568      0.093902
H       -3.421129      0.650418     -0.892569
H       -3.759798      0.784068      0.835247
O        1.735453      0.736505     -0.076663
C        2.787245      0.211359     -0.877497
H        3.600371      0.945342     -0.955864
H        2.429612     -0.016629     -1.890723
C        3.305722     -1.052178     -0.203727
H        4.205314     -1.383709     -0.729562
O        3.724230     -0.773852      1.143066
H        3.036488     -0.220222      1.538900
C        2.289979     -2.194137     -0.200438
H        1.364468     -1.871565      0.289298
H        2.054240     -2.488683     -1.225217
O        2.822669     -3.352512      0.447649
H        3.160700     -3.058478      1.303610
C       -3.791089     -1.227379      0.080835
H       -3.266317     -1.828050     -0.674331
H       -3.590589     -1.702898      1.050329
C       -5.297984     -1.251373     -0.200330
H       -5.816621     -0.645691      0.553578
H       -5.494294     -0.768087     -1.165778
C       -5.895959     -2.662373     -0.212041
H       -6.971243     -2.642650     -0.415170
H       -5.423894     -3.284230     -0.979812
H       -5.748749     -3.160676      0.751847

=====================================================================
```

TS **19c-sr**

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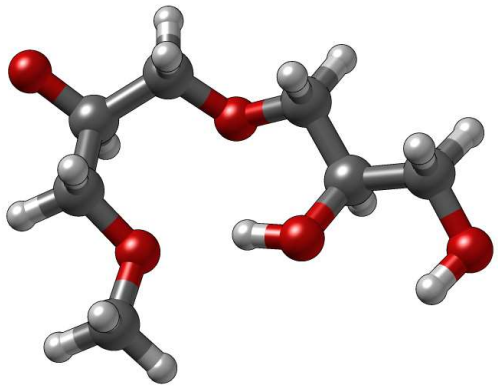
Solvent = Butanol

E0 =  -770.087761 Hartree
 H =  -769.760950 Hartree
 G =  -769.831853 Hartree
 S =   149.227000 Cal/mol K

O         3.071435      -2.151080       0.000865
C         2.041868      -1.266121       0.385264
H         1.773257      -1.302856       1.447605
C         0.806362      -1.358599      -0.489938
H         0.447770      -2.398423      -0.474173
H         1.053898      -1.098679      -1.527801
C         3.148874      -0.395344       0.025445
H         3.917637      -0.189340       0.749566
H         3.305312      -0.141115      -1.008801
O         2.647010       1.720439       0.274059
C         3.809123       2.415051       0.006710
H         4.202482       2.204734      -1.017832
H         4.644001       2.123166       0.689953
O        -0.209898      -0.491610       0.009209
C        -1.423634      -0.567499      -0.727277
H        -1.769482      -1.609923      -0.773268
H        -1.276491      -0.201560      -1.752492
C        -2.448903       0.294192      -0.005275
H        -2.094524       1.332750       0.009973
O        -2.635888      -0.159329       1.343714
H        -1.765977      -0.185329       1.761756
C        -3.816514       0.246106      -0.669080
H        -3.746953       0.605405      -1.696965
H        -4.180333      -0.789000      -0.684317
O        -4.756539       1.091929      -0.003643
H        -4.742422       0.851742       0.931251
C         3.658213       3.944857       0.119248
H         2.866131       4.267517      -0.569915
H         3.306306       4.185331       1.131530
C         4.944043       4.725595      -0.176133
H         5.735026       4.393189       0.507976
H         5.293199       4.479596      -1.186955
C         4.778185       6.244461      -0.055503
H         5.712586       6.770440      -0.274857
H         4.017370       6.614325      -0.750780
H         4.466552       6.527970       0.955187

=====================================================================
```

INT **20a-rr**



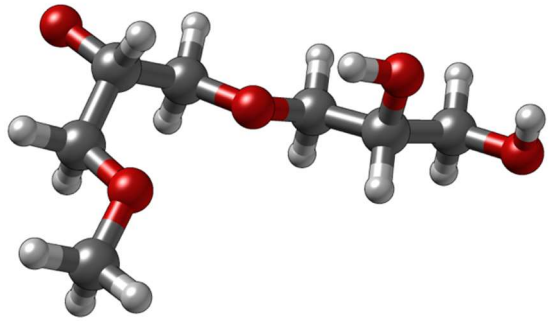
Solvent = Methanol

E0 = -652.176297 Hartree
 H = -651.934674 Hartree
 G = -651.991528 Hartree
 S =   119.659000 Cal/mol K

O	2.356622	-1.035097	1.589956
C	2.355268	-1.088949	0.215001
H	3.059181	-1.849099	-0.199347
C	0.955912	-1.477615	-0.302430
H	0.257800	-0.649003	-0.118389
H	0.605229	-2.350488	0.264338
C	2.821586	0.276208	-0.339172
H	2.088377	1.049681	-0.064172
H	3.770649	0.518951	0.155262
O	3.032791	0.311214	-1.765506
C	3.689352	1.503929	-2.180571
H	4.674543	1.592639	-1.706321
H	3.095931	2.392551	-1.929625
O	0.985563	-1.785192	-1.702175
H	3.815840	1.451971	-3.262763
C	-0.214352	-1.582375	-2.433836
H	-0.823539	-0.802873	-1.958888
H	-0.808123	-2.505333	-2.485387
C	0.201684	-1.127836	-3.827694
H	0.802965	-1.922533	-4.292262
O	0.980597	0.068417	-3.744700
H	1.635734	-0.032899	-3.023825
C	-0.986355	-0.823770	-4.726947
H	-1.589322	-1.721325	-4.875106
H	-1.613534	-0.053775	-4.259734
O	-0.566090	-0.394360	-6.025783
H	0.070070	0.319374	-5.890201

==========

INT **20a-sr**



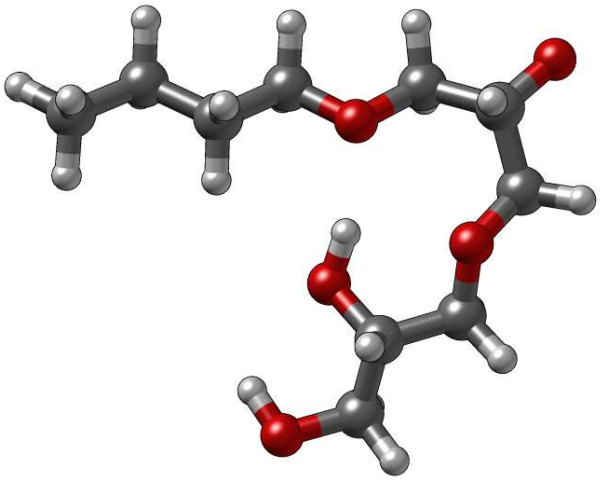
Solvent = Methanol

E0 = -652.173010 Hartree
 H = -651.931655 Hartree
 G = -651.991523 Hartree
 S =   126.003000 Cal/mol K

O	2.721586	-2.426605	0.167374
C	2.052585	-1.239405	0.373453
H	1.755504	-1.077246	1.436953
C	0.740361	-1.250428	-0.438379
H	0.261706	-2.224286	-0.272149
H	0.967779	-1.162290	-1.511891
C	2.979882	-0.064723	-0.000705
H	3.946266	-0.240019	0.492685
H	3.152531	-0.073351	-1.089038
O	2.479046	1.216444	0.396162
C	3.373822	2.267982	0.077450
H	3.542449	2.335854	-1.006272
H	4.345723	2.129926	0.571626
O	-0.175632	-0.212434	-0.057065
H	2.927121	3.200717	0.425963
C	-1.429369	-0.296805	-0.716334
H	-1.858949	-1.300773	-0.584319
H	-1.320384	-0.104655	-1.792992
C	-2.337324	0.750166	-0.085989
H	-1.915762	1.746463	-0.275458
O	-2.430447	0.543519	1.331755
H	-1.527956	0.417146	1.653627
C	-3.755727	0.701688	-0.630437
H	-3.749350	0.877108	-1.707413
H	-4.188824	-0.288130	-0.439834
O	-4.579084	1.720986	-0.057542
H	-4.528971	1.623310	0.901370

==========

INT **20c-rr**



Solvent = Butanol

E0 = -770.149451 Hartree
H = -769.819119 Hartree
G = -769.887552 Hartree
S = 144.029000 Cal/mol K

O	-0.394407	4.333388	-0.030353
C	-0.194067	3.017694	0.317543
H	-0.341459	2.818879	1.406018
C	1.255698	2.606791	-0.003756
H	1.933421	3.360844	0.417862
H	1.392091	2.597248	-1.094117
C	-1.228089	2.134665	-0.420514
H	-2.208114	2.602458	-0.266322
H	-1.014355	2.146598	-1.500354
O	-1.303238	0.768150	0.037595
C	-2.461833	0.095904	-0.462810
H	-2.381969	-0.014648	-1.554749
H	-3.349574	0.711386	-0.259582
O	1.567827	1.316051	0.535647
C	2.571739	0.564662	-0.128109
H	3.559864	0.737609	0.320721
H	2.617479	0.841868	-1.189127
C	2.164450	-0.897743	0.002103
H	2.133380	-1.160131	1.069269
O	0.871303	-1.099836	-0.573276
H	0.271601	-0.399343	-0.246508
C	3.118239	-1.846170	-0.706484
H	3.176291	-1.583102	-1.770512
H	4.117869	-1.771466	-0.274649
O	2.709244	-3.209453	-0.558153
H	1.777141	-3.247957	-0.807518
C	-2.606550	-1.265518	0.202566
H	-1.704564	-1.857751	0.015724
H	-2.675842	-1.123128	1.287332
C	-3.837659	-2.031179	-0.297771
H	-4.737152	-1.429366	-0.121323
H	-3.765547	-2.164275	-1.383793
C	-4.001927	-3.398868	0.371677
H	-4.884526	-3.922526	-0.006332
H	-3.131057	-4.035537	0.186433
H	-4.113461	-3.296227	1.455724

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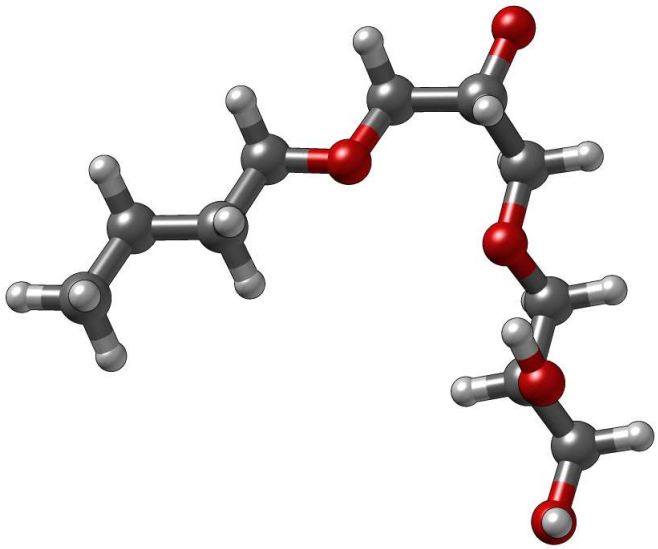
INT **20c-sr**



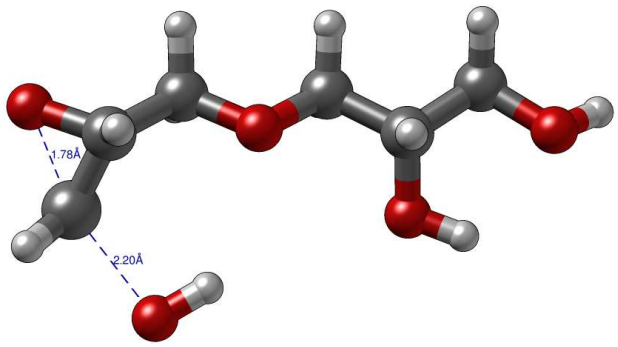
Solvent = Butanol

E0 = -770.147014 Hartree
 H = -769.816883 Hartree
 G = -769.887042 Hartree
 S =   147.661000 Cal/mol K

O	0.262553	4.068649	0.414372
C	0.111105	2.702297	0.492128
H	0.131866	2.311640	1.537724
C	1.289214	2.029487	-0.242182
H	2.216061	2.476234	0.141053
H	1.222687	2.255662	-1.317447
C	-1.263049	2.297242	-0.083592
H	-1.999450	3.011413	0.309949
H	-1.250112	2.399615	-1.180899
O	-1.660740	0.969320	0.273311
C	-2.951642	0.627707	-0.212887
H	-2.963263	0.681863	-1.312859
H	-3.693063	1.353674	0.156616
O	1.347735	0.606026	-0.057480
C	2.495131	0.009537	-0.639712
H	3.406860	0.498959	-0.266188
H	2.474077	0.104234	-1.734715
C	2.485684	-1.460188	-0.241530
H	1.600349	-1.941167	-0.678604
O	2.431692	-1.591166	1.186879
H	1.737583	-0.992436	1.493474
C	3.729575	-2.203093	-0.701942
H	3.811851	-2.158868	-1.789239
H	4.619933	-1.734370	-0.264501
O	3.678166	-3.588906	-0.353723
H	3.515255	-3.637666	0.596415
C	-3.311861	-0.776664	0.251002
H	-2.549308	-1.476211	-0.110979
H	-3.275393	-0.807081	1.346329
C	-4.695814	-1.227402	-0.230799
H	-5.453217	-0.518609	0.124839
H	-4.729701	-1.188767	-1.326172
C	-5.060149	-2.638674	0.239661
H	-6.050007	-2.934550	-0.119198
H	-4.338086	-3.374989	-0.127310
H	-5.069598	-2.699558	1.332580

==========

TS **21-rr**



Solvent = Methanol

E0 = -612.807670 Hartree
 H = -612.598757 Hartree
 G = -612.655278 Hartree
 S =   118.959000 Cal/mol K

O	-3.294913	-2.037871	0.085316
C	-2.218974	-1.274542	-0.411303
H	-2.085028	-1.315583	-1.498717
C	-0.906318	-1.511984	0.310418
H	-0.608833	-2.561941	0.168503
H	-1.033327	-1.337198	1.387686
C	-3.157389	-0.284478	0.086957
H	-3.972616	0.034984	-0.536049
H	-3.156883	-0.041753	1.134460
O	-2.412164	1.748894	-0.222937
O	0.094073	-0.646281	-0.219902
C	1.368729	-0.851495	0.373313
H	1.709525	-1.878963	0.182453
H	1.309740	-0.705726	1.460700
C	2.363487	0.128606	-0.218306
H	2.277476	0.098136	-1.313150
O	2.043663	1.444804	0.245843
H	2.784140	2.011833	-0.007621
C	3.794694	-0.231881	0.163260
H	3.899359	-0.254182	1.253469
H	4.055469	-1.215112	-0.242627
O	4.638022	0.785110	-0.396720
H	5.496099	0.754983	0.038919
H	-1.468668	1.551371	-0.203279

Solvent = Butanol

E0 = -612.803374 Hartree
 H = -612.594528 Hartree
 G = -612.651426 Hartree
 S =   119.753000 Cal/mol K

O	3.775820	-1.262003	-0.156459
C	2.600349	-0.669343	0.342144
H	2.415688	-0.833549	1.410812
C	1.359532	-0.976186	-0.475435
H	1.184796	-2.062733	-0.457311
H	1.514707	-0.674152	-1.520421
C	3.428722	0.475517	0.003314
H	4.171988	0.815397	0.701392
H	3.456933	0.817520	-1.015945

```
O         2.419705      2.371282      0.462951
O         0.238189     -0.292948      0.078710
C        -0.971094     -0.572840     -0.610754
H        -1.201029     -1.645954     -0.543631
H        -0.873642     -0.308710     -1.672872
C        -2.101863      0.226065      0.008968
H        -2.063660      0.099882      1.099673
O        -1.919065      1.607877     -0.316060
H        -2.726134      2.063316     -0.042363
C        -3.460739     -0.257309     -0.484882
H        -3.511805     -0.183802     -1.576782
H        -3.619621     -1.299428     -0.187276
O        -4.445379      0.594775      0.117838
H        -5.272796      0.508620     -0.366653
H         1.512609      2.058332      0.368164
```

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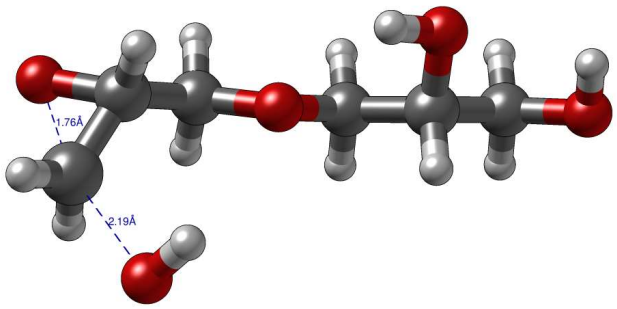
TS **21-sr**




```
Solvent = Methanol
E0 =  -612.809649 Hartree
 H =  -612.600661 Hartree
 G =  -612.656823 Hartree
 S =   118.201000 Cal/mol K

O         3.132553     -2.102689      0.014931
C         2.109301     -1.196221      0.355444
H         1.881044     -1.135811      1.426568
C         0.842246     -1.375327     -0.459643
H         0.492537     -2.410562     -0.335703
H         1.048937     -1.209746     -1.525254
C         3.192646     -0.351761     -0.125960
H         3.985521     -0.076751      0.544094
H         3.303784     -0.192205     -1.183510
O         2.727563      1.786867     -0.112494
O        -0.160929     -0.469954     -0.002629
C        -1.393894     -0.597149     -0.701282
H        -1.737586     -1.640430     -0.668932
H        -1.273274     -0.299582     -1.751491
C        -2.400689      0.309207     -0.009938
H        -2.037534      1.343965     -0.056538
O        -2.567396     -0.069789      1.364661
H        -1.690535     -0.085195      1.768255
C        -3.779935      0.239373     -0.647562
H        -3.724389      0.543910     -1.693751
H        -4.153637     -0.791215     -0.603059
O        -4.700648      1.128585     -0.012083
H        -4.684421      0.928585      0.932139
H         2.156578      1.879675      0.658767

Solvent = Butanol
```

```
E0 =  -612.806025 Hartree
 H =  -612.597087 Hartree
 G =  -612.653281 Hartree
 S =   118.268000 Cal/mol K

O         3.119804      -2.122215       0.030047
C         2.110925      -1.198515       0.358278
H         1.877419      -1.126916       1.428208
C         0.843028      -1.370490      -0.458217
H         0.491457      -2.405458      -0.337322
H         1.051137      -1.202242      -1.523137
C         3.193221      -0.351336      -0.123515
H         3.989743      -0.083637       0.545388
H         3.311632      -0.206216      -1.182513
O         2.729305       1.795304      -0.118943
O        -0.159866      -0.464856      -0.000510
C        -1.390015      -0.588566      -0.703309
H        -1.732756      -1.632591      -0.678935
H        -1.267047      -0.283862      -1.751323
C        -2.400569       0.311409      -0.009128
H        -2.041863       1.347741      -0.052194
O        -2.565498      -0.073142       1.364075
H        -1.687646      -0.090307       1.765532
C        -3.779712       0.237428      -0.646359
H        -3.726476       0.546725      -1.691344
H        -4.147840      -0.795493      -0.605991
O        -4.704591       1.118678      -0.006386
H        -4.679204       0.920340       0.937991
H         2.133255       1.873998       0.634637
```

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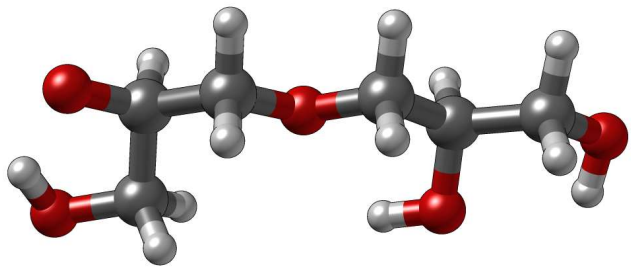
INT **22-rr**



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Solvent = Methanol

E0 =  -612.875129 Hartree
 H =  -612.662937 Hartree
 G =  -612.717588 Hartree
 S =   115.024000 Cal/mol K

O         3.739197      -1.291359       0.037566
C         2.590430      -0.644709      -0.374481
H         2.466312      -0.679960      -1.481837
C         1.334859      -1.284137       0.226669
H         1.382271      -1.226276       1.324437
H         1.291966      -2.344069      -0.058692
C         2.693947       0.856363       0.018731
H         2.061267       1.502636      -0.595958
H         2.405048       0.983600       1.074439
O         4.062108       1.236038      -0.157512
O         0.153781      -0.616206      -0.240438
C        -1.051639      -1.186169       0.249333
```

```
H        -1.039486      -1.210776       1.348286
H        -1.171353      -2.213859      -0.120896
C        -2.198039      -0.315607      -0.243036
H        -2.198323      -0.317053      -1.341099
O        -2.048110       1.033610       0.224604
H        -1.152947       1.316460      -0.001476
C        -3.552378      -0.798260       0.252245
H        -3.737093      -1.815140      -0.097258
H        -3.564073      -0.797892       1.349251
O        -4.618925       0.007203      -0.254984
H        -4.418562       0.923169      -0.025571
H         4.482716       0.342868      -0.051922

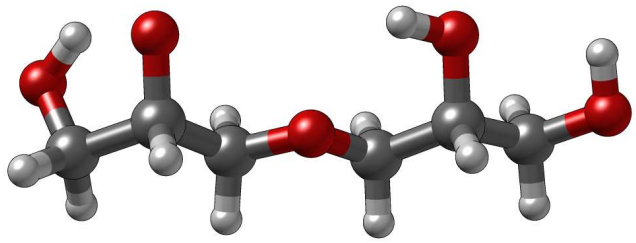
Solvent = Butanol

E0 =  -612.869815 Hartree
 H =  -612.657800 Hartree
 G =  -612.712407 Hartree
 S =   114.932000 Cal/mol K

O        -2.619728       1.408469      -0.095373
C        -2.432964       0.194745       0.529172
H        -2.218869       0.295927       1.614451
C        -1.272946      -0.628978      -0.051798
H        -1.415956      -0.759878      -1.134822
H        -1.236581      -1.624418       0.417853
C        -3.762108      -0.640102       0.395833
H        -3.582812      -1.718870       0.324326
H        -4.400634      -0.457767       1.271874
O        -4.416867      -0.187475      -0.787447
O        -0.025941       0.033575       0.185492
C         1.093986      -0.670020      -0.328260
H         1.066488      -0.696840      -1.426662
H         1.095668      -1.704811       0.044806
C         2.341880       0.058897       0.149652
H         2.341575       1.075567      -0.264959
O         2.359650       0.137378       1.583178
H         1.495632       0.472287       1.856403
C         3.625103      -0.644721      -0.262759
H         3.633819      -1.662087       0.148105
H         3.685119      -0.708463      -1.350488
O         4.784373       0.072486       0.167287
H         4.692130       0.219338       1.116857
H        -3.935975       0.688951      -0.885178

=====================================================================
```

INT **22-sr**



```
Solvent = Methanol

E0 =  -612.873495 Hartree
 H =  -612.661496 Hartree
```

```
 G =  -612.716475 Hartree
 S =   115.715000 Cal/mol K

O        2.267193     -1.333766      1.476713
C        2.333057     -0.864872      0.180991
H        2.515328      0.228946      0.127639
C        1.054280     -1.118642     -0.632227
H        0.812241     -2.191873     -0.622270
H        1.196383     -0.803549     -1.677562
C        3.542068     -1.570416     -0.539329
H        3.367359     -1.729420     -1.609283
H        4.446300     -0.955202     -0.429494
O        3.728540     -2.829865      0.104490
O       -0.038595     -0.380418     -0.074881
C       -1.270989     -0.600191     -0.744411
H       -1.493216     -1.676132     -0.782770
H       -1.231097     -0.216234     -1.773545
C       -2.346938      0.129621      0.046395
H       -2.124184      1.205045      0.040895
O       -2.375979     -0.336330      1.403777
H       -1.462421     -0.340723      1.719008
C       -3.739736     -0.088873     -0.522857
H       -3.783384      0.271093     -1.552068
H       -3.975086     -1.160355     -0.516690
O       -4.730942      0.640312      0.205236
H       -4.649914      0.385162      1.132536
H        3.232225     -2.626746      0.953155

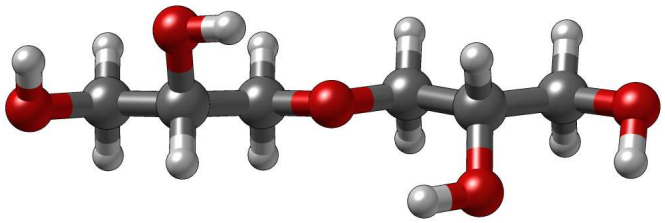
Solvent = Butanol

E0 =  -612.870001 Hartree
 H =  -612.658002 Hartree
 G =  -612.712867 Hartree
 S =   115.473000 Cal/mol K

O        2.258716     -1.336200      1.476092
C        2.330986     -0.864637      0.183326
H        2.516096      0.229233      0.131969
C        1.054747     -1.114027     -0.635725
H        0.809620     -2.186459     -0.625319
H        1.201927     -0.799912     -1.680934
C        3.540838     -1.572497     -0.534511
H        3.370323     -1.727743     -1.605951
H        4.446688     -0.960444     -0.418918
O        3.719599     -2.833747      0.106466
O       -0.038134     -0.371962     -0.083671
C       -1.270462     -0.596205     -0.749832
H       -1.490453     -1.672825     -0.785576
H       -1.234741     -0.214193     -1.780132
C       -2.346169      0.132134      0.042938
H       -2.127605      1.208488      0.032675
O       -2.367108     -0.329319      1.401497
H       -1.450655     -0.339561      1.708860
C       -3.740599     -0.093956     -0.519270
H       -3.791750      0.265358     -1.548471
H       -3.969876     -1.166858     -0.511443
O       -4.731832      0.629792      0.213799
H       -4.637645      0.381681      1.141793
H        3.219978     -2.629572      0.953789

=====================================================================
```

(2*R*.2'*R*)-3.3'-oxybis(propane-1.2-diol) **23-rr**



Solvent = Methanol

E0 = -613.372760 Hartree
H = -613.146018 Hartree
G = -613.202503 Hartree
S = 118.883000 Cal/mol K

O	2.358590	1.259297	0.511194
C	2.371907	0.028581	-0.226365
H	2.302150	0.249742	-1.299352
C	1.199159	-0.854433	0.171108
H	1.234586	-1.070350	1.246986
H	1.228597	-1.802571	-0.381112
C	3.714719	-0.629445	0.055712
H	3.798197	-0.850977	1.126940
H	3.796367	-1.564773	-0.499926
O	4.803412	0.192543	-0.367741
O	0.006631	-0.137736	-0.141367
C	-1.184918	-0.779705	0.307437
H	-1.212986	-0.805193	1.404406
H	-1.220234	-1.809590	-0.071397
C	-2.358813	0.020309	-0.235627
H	-2.289688	1.050301	0.137754
O	-2.346643	0.036521	-1.670396
H	-1.491713	0.384165	-1.952443
C	-3.700757	-0.565770	0.178418
H	-3.783776	-1.594344	-0.194009
H	-3.781252	-0.582562	1.266297
O	-4.790595	0.224658	-0.298720
H	-4.683215	0.313356	-1.253915
H	1.503754	1.681500	0.361893
H	4.694360	1.052764	0.056457

Solvent = Butanol

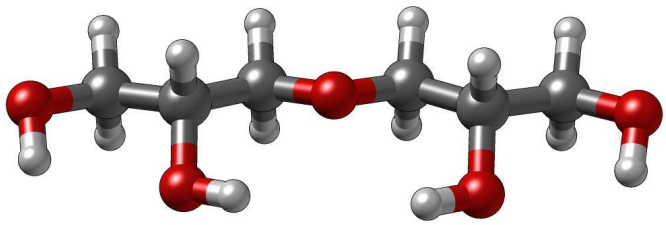
E0 = -613.371947 Hartree
H = -613.145170 Hartree
G = -613.201577 Hartree
S = 118.720000 Cal/mol K

O	2.366442	1.258123	0.549127
C	2.375772	0.044112	-0.215170
H	2.305743	0.288654	-1.283087
C	1.201211	-0.844422	0.164176
H	1.237553	-1.083937	1.235061
H	1.227521	-1.780335	-0.408839
C	3.717345	-0.623049	0.051296
H	3.800834	-0.867894	1.117531
H	3.796388	-1.546458	-0.524418
O	4.807165	0.205132	-0.355221
O	0.010053	-0.118289	-0.130825
C	-1.182378	-0.766741	0.305963
H	-1.208910	-0.815183	1.402278
H	-1.220603	-1.788340	-0.094501

```
C        -2.355333       0.046881      -0.218608
H        -2.283658       1.068697       0.176233
O        -2.345376       0.092682      -1.652464
H        -1.490355       0.444353      -1.928961
C        -3.698082      -0.544925       0.184770
H        -3.783278      -1.565383      -0.209154
H        -3.777470      -0.584547       1.272198
O        -4.786362       0.257454      -0.274238
H        -4.677913       0.368612      -1.226951
H         1.512345       1.685441       0.410944
H         4.698579       1.057273       0.085070
```

==========

(2*s*.2'*r*)-3.3'-oxybis(propane-1.2-diol) **23-sr**



```
Solvent = Methanol

E0 =  -613.372543 Hartree
 H =  -613.145832 Hartree
 G =  -613.202143 Hartree
 S =   118.517000 Cal/mol K

O         2.344652       1.281156       0.335359
C         2.377147      -0.004475      -0.301872
H         2.324355       0.129761      -1.389913
C         1.206739      -0.865917       0.145400
H         1.218546      -0.985167       1.236723
H         1.267367      -1.859023      -0.318745
C         3.720953      -0.623649       0.055022
H         3.785660      -0.760679       1.141627
H         3.823621      -1.598062      -0.424653
O         4.808186       0.177497      -0.409760
O         0.009078      -0.205899      -0.258477
C        -1.177428      -0.837272       0.216630
H        -1.154123      -0.899008       1.312624
H        -1.256486      -1.853151      -0.192359
C        -2.360953       0.001085      -0.240854
H        -2.349910       0.063689      -1.336436
O        -2.303699       1.325639       0.309111
H        -1.490430       1.742414       0.000965
C        -3.691470      -0.587574       0.207149
H        -3.812830      -1.592800      -0.198825
H        -3.715969      -0.648224       1.302343
O        -4.794232       0.183002      -0.272236
H        -4.642829       1.096379       0.001508
H         1.503028       1.699173       0.117922
H         4.672151       1.069149      -0.065519

Solvent = Butanol

E0 =  -613.371672 Hartree
 H =  -613.144911 Hartree
 G =  -613.201044 Hartree
 S =   118.142000 Cal/mol K
```

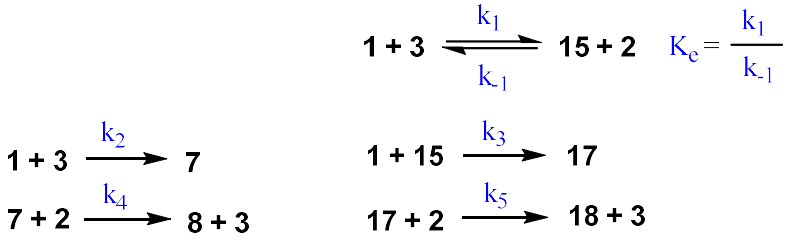
O	2.345074	1.279950	0.338414
C	2.377279	-0.004065	-0.301562
H	2.324477	0.132177	-1.389373
C	1.206721	-0.866019	0.144231
H	1.218828	-0.987111	1.235380
H	1.266937	-1.858387	-0.321834
C	3.721204	-0.623895	0.054111
H	3.785525	-0.762921	1.140565
H	3.824118	-1.597497	-0.427320
O	4.808053	0.177918	-0.409086
O	0.009106	-0.205204	-0.258184
C	-1.177243	-0.836337	0.217340
H	-1.154193	-0.896649	1.313457
H	-1.255673	-1.852821	-0.190548
C	-2.361225	0.000691	-0.241392
H	-2.350769	0.060916	-1.337126
O	-2.304174	1.326102	0.305901
H	-1.491291	1.742563	-0.003392
C	-3.691493	-0.587262	0.208495
H	-3.813008	-1.593449	-0.195264
H	-3.715019	-0.645612	1.303915
O	-4.794267	0.181828	-0.271819
H	-4.641948	1.096012	-0.001396
H	1.502951	1.697983	0.123347
H	4.671155	1.069134	-0.064128

==========

9. Simulations of the reaction kinetics.

Simplified reaction kinetics scheme used in the simulations:

Main reaction leading to [1.0.0] **Reactions leading to byproducts**



Equations used to calculate equilibrium and kinetic constants:

Eq. 1: $k_c = \frac{k_B \cdot T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}}$ Eq. 2: $K_e = e^{\frac{-\Delta G^0}{RT}}$

Values of the equilibrium and kinetic constants used in the simulations:

Table S7. Kinetic and equilibrium constants used in the simulations.

	Alcohol		
	Methanol	**Butanol**	**TFE**
K_e[a]	84.88	185.98	0.01[b]
k_1[c]	2300.25	2269.0	5
k_{-1}[c]	27.1	12.2	500
k_2[d]	0.27082680	0.12245300	0.0049395
k_3[d]	0.06841425	0.27167443	0.0934904
k_4[e]	30	30	30
k_5[e]	30	30	30

[a] Calculated using the Gibbs free energies of **1**, **2**, **3** and **15**, except in the case of **2f** (Table S1), using eq. 2.
[b] The actual value is *ca.* $5 \cdot 10^{-6}$, but it led to problems with the numerical integration of the kinetic equations, so an arbitrary value of 0.01 was used instead.
[c] The forward and reverse kinetic constants were given arbitrarily high values (much higher than those of the reaction constants) to simulate rapid pre-equilibrium. The quotient k_1/k_{-1} matches with the value of K_e.
[d] Calculated using eq. 1 from the activation barrier of the corresponding reactions (Table S1). In the case of k_3, the final value is the sum of the kinetic constants leading to the *RR* and *SR* diastereomers.
[c] The constants for the protonation process leading to the final products were given arbitrarily high values to speed-up the simulations.

Formulae used for the numerical integration of the kinetic equations:

$$[\mathbf{2}]_n = [\mathbf{2}]_{n-1} + (k_1 \cdot [\mathbf{1}]_{n-1} \cdot [\mathbf{3}]_{n-1} - k_1 \cdot [\mathbf{2}]_{n-1} \cdot [\mathbf{15}]_{n-1} - k_4 \cdot [\mathbf{2}]_{n-1} \cdot [\mathbf{7}]_{n-1} - k_5 \cdot [\mathbf{2}]_{n-1} \cdot [\mathbf{17}]_{n-1}) \cdot \delta t$$

$$[\mathbf{3}]_n = [\mathbf{3}]_{n-1} + (k_{-1} \cdot [\mathbf{15}]_{n-1} \cdot [\mathbf{2}]_{n-1} + k_4 \cdot [\mathbf{2}]_{n-1} \cdot [\mathbf{7}]_{n-1} + k_5 \cdot [\mathbf{2}]_{n-1} \cdot [\mathbf{17}]_{n-1} - (k_1 + k_2) \cdot [\mathbf{1}]_{n-1} \cdot [\mathbf{3}]_{n-1}) \cdot \delta t$$

$$[\mathbf{1}]_n = [\mathbf{1}]_{n-1} + (k_{-1} \cdot [\mathbf{15}]_{n-1} \cdot [\mathbf{2}]_{n-1} - ((k_1 + k_2) \cdot [\mathbf{3}]_{n-1} + k_3 \cdot [\mathbf{15}]_{n-1}) \cdot [\mathbf{1}]_{n-1}) \cdot \delta t$$

$$[\mathbf{15}]_n = [\mathbf{15}]_{n-1} + (k_1 \cdot [\mathbf{1}]_{n-1} \cdot [\mathbf{3}]_{n-1} - (k_{-1} \cdot [\mathbf{2}]_{n-1} + k_3 \cdot [\mathbf{1}]_{n-1}) \cdot [\mathbf{15}]_{n-1}) \cdot \delta t$$

$$[\mathbf{7}]_n = [\mathbf{7}]_{n-1} + (k_2 \cdot [\mathbf{1}]_{n-1} \cdot [\mathbf{3}]_{n-1} - k_4 \cdot [\mathbf{7}]_{n-1} \cdot [\mathbf{2}]_{n-1}) \cdot \delta t$$

$$[\mathbf{17}]_n = [\mathbf{17}]_{n-1} + (k_3 \cdot [\mathbf{1}]_{n-1} \cdot [\mathbf{15}]_{n-1} - k_5 \cdot [\mathbf{17}]_{n-1} \cdot [\mathbf{2}]_{n-1}) \cdot \delta t$$

$$[\mathbf{8}]_n = [\mathbf{8}]_{n-1} + (k_4 \cdot [\mathbf{7}]_{n-1} \cdot [\mathbf{2}]_{n-1}) \cdot \delta t$$

$$[\mathbf{18}]_n = [\mathbf{18}]_{n-1} + (k_5 \cdot [\mathbf{17}]_{n-1} \cdot [\mathbf{2}]_{n-1}) \cdot \delta t$$

Figures of the kinetic simulations:

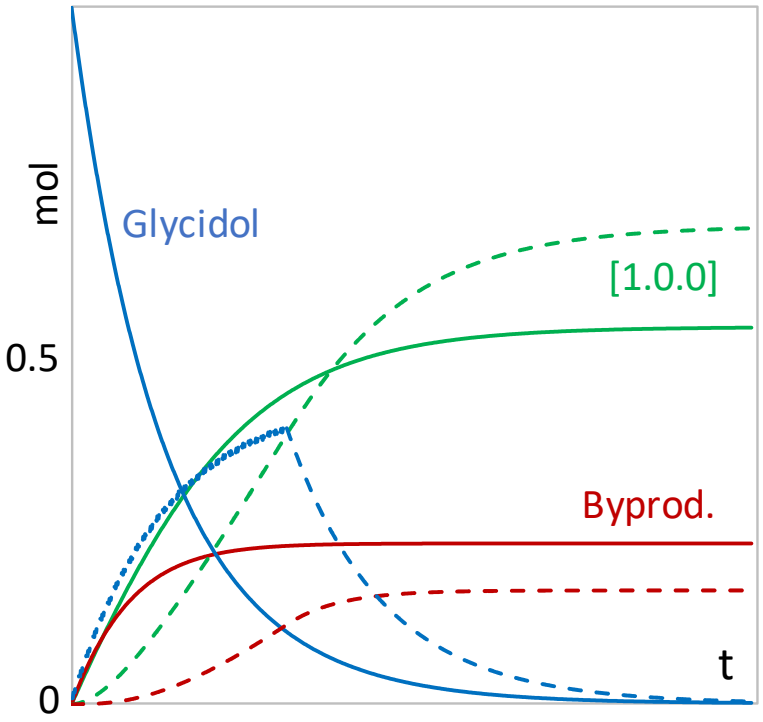


Figure S-35. Simulations of the kinetics of the reaction of glycidol (**1**) with methanol (**2a**), catalyzed by bases. Continuous line: At once glycidol addition; Dashed line: Dropwise glycidol addition.

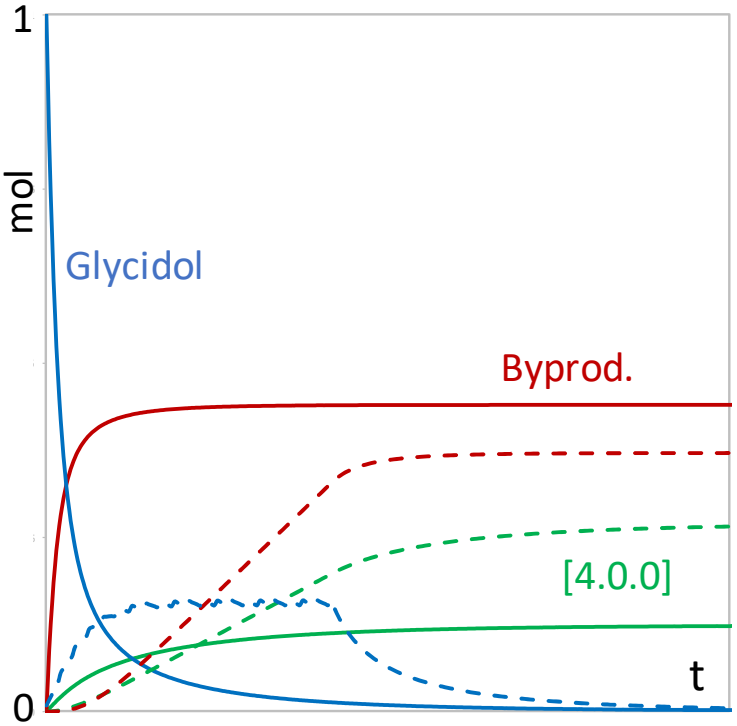


Figure S-36. Simulations of the kinetics of the reaction of glycidol (**1**) with butanol (**2c**), catalyzed by bases. Continuous line: At once glycidol addition; Dashed line: Dropwise glycidol addition.

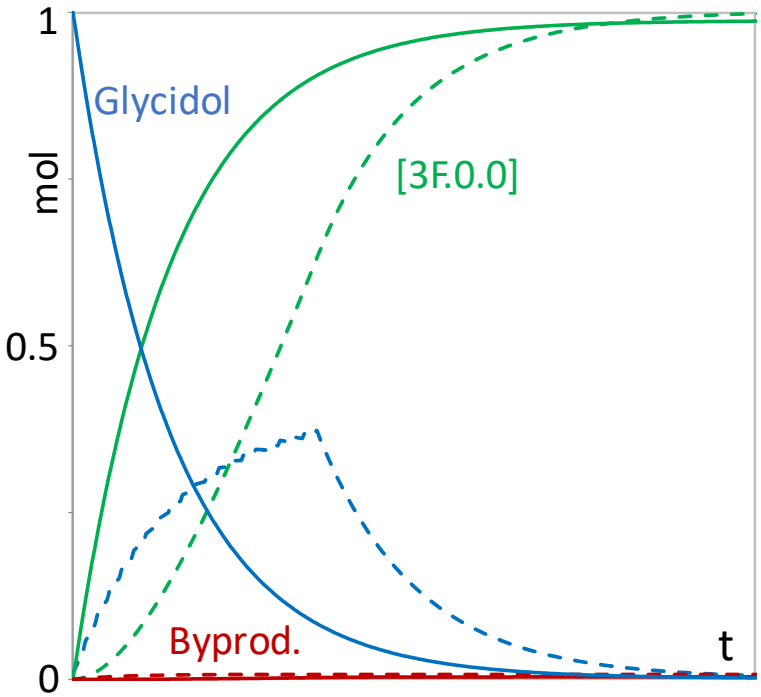


Figure S-35. Simulations of the kinetics of the reaction of glycidol (**1**) with 2,2,2-trifluoroethanol (**2f**), catalyzed by bases. Continuous line: At once glycidol addition; Dashed line: Dropwise glycidol addition.