Electronic Supplementary Information

Ion-Molecule Reactions for the Differentiation of Primary, Secondary and Tertiary Hydroxyl Functionalities in Protonated Analytes in a Tandem Mass Spectrometer

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Table S1 Cartesian Coordinates of 1-Butanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.320697	0.477207	-0.000193
2	1	0	1.347103	1.132043	0.887373
3	1	0	1.345894	1.131641	-0.888129
4	6	0	0.034635	-0.338903	0.000722
5	1	0	0.040605	-0.996578	-0.878682
6	1	0	0.041084	-0.995110	0.881191
7	6	0	-2.520397	-0.296175	-0.000154
8	1	0	-2.577077	-0.941813	0.884617
9	1	0	-3.406850	0.348225	-0.000601
10	1	0	-2.576481	-0.942419	-0.884517
11	6	0	-1.229452	0.529227	-0.000101
12	1	0	-1.219884	1.190523	0.878195
13	1	0	-1.219319	1.190309	-0.878305
14	8	0	2.419507	-0.429640	-0.000896
15	1	0	3.235973	0.092167	0.004380

Total computed energy:

– 233.523344 Hartrees × 627.51 kcal/Hartrees = – 146538.2 kcal

Imaginary frequencies = 0

Table S2 Cartesian Coordinates of Protonated 1-Butanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.174078	0.564576	0.023448
2	1	0	-1.298732	1.202777	-0.851016
3	1	0	-1.302096	1.120105	0.954065
4	6	0	0.034327	-0.328799	-0.023201
5	1	0	0.033970	-1.015501	0.834565
6	1	0	0.022467	-0.924102	-0.943017
7	8	0	-2.453920	-0.347034	-0.084769
8	1	0	-3.303271	0.138854	-0.000234
9	1	0	-2.441501	-1.089141	0.558093
10	6	0	1.319582	0.535701	0.025021
11	1	0	1.316184	1.146863	0.936239
12	1	0	1.321052	1.228466	-0.825474
13	6	0	2.580682	-0.334709	-0.012121
14	1	0	3.473288	0.296381	0.020206
15	1	0	2.621173	-1.016325	0.844430
16	1	0	2.625748	-0.932721	-0.928589

Total computed energy:

– 233.825747 Hartrees × 627.51 kcal/Hartrees = – 146728.0 kcal

Imaginary frequencies = 0

Table S3. Cartesian Coordinates of 1-Pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.419870	-1.389721	0.000000
2	1	0	1.971277	-1.035795	0.887697
3	1	0	1.971277	-1.035795	-0.887697
4	6	0	0.013692	-0.804876	0.000000
5	1	0	-0.520347	-1.187509	-0.879910
6	1	0	-0.520347	-1.187509	0.879910
7	6	0	-1.414923	1.321485	0.000000
8	1	0	-1.962098	0.950069	0.877893
9	1	0	-1.962098	0.950069	-0.877893
10	6	0	0.000000	0.728219	0.000000
11	1	0	0.547132	1.101189	-0.878899
12	8	0	1.306830	-2.810071	0.000000
13	1	0	2.202705	-3.179279	0.000000
14	6	0	-1.426572	2.853302	0.000000
15	1	0	-2.449679	3.246223	0.000000
16	1	0	-0.915999	3.253632	0.884685
17	1	0	-0.915999	3.253632	-0.884685
18	1	0	0.547132	1.101189	0.878899

Total computed energy:

– 272.808558 Hartrees × 627.51 kcal/Hartrees = – 171190.1 kcal

Imaginary frequencies = 0

Table S4. Cartesian Coordinates of Protonated 1-Pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.769668	0.583960	0.020768
2	1	0	1.857653	1.152172	0.948317
3	1	0	1.855157	1.223274	-0.857493
4	6	0	0.625081	-0.388392	-0.024209
5	1	0	0.679804	-0.986849	-0.940324
6	1	0	0.667291	-1.068312	0.837856
7	6	0	-1.923977	-0.554917	-0.020975
8	1	0	-1.868767	-1.243795	0.832490
9	1	0	-1.871572	-1.173830	-0.926359
10	6	0	-0.713080	0.391444	0.014190
11	1	0	-0.755346	1.008025	0.921747
12	1	0	-0.759002	1.078094	-0.841161
13	8	0	3.112008	-0.239815	-0.077731
14	1	0	3.925384	0.303710	0.008693
15	6	0	-3.253915	0.203912	0.011684
16	1	0	-4.095898	-0.494388	-0.015120
17	1	0	-3.348975	0.805257	0.923039
18	1	0	-3.351603	0.876146	-0.848343
19	1	0	3.147142	-0.977025	0.569761

Total computed energy:

– 273.111806 Hartrees × 627.51 kcal/Hartrees = – 171380.4 kcal

Imaginary frequencies = 0

Table S5 Cartesian Coordinates of 2-Pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.472976	0.339227	0.312795
2	1	0	-1.334897	1.356075	-0.070996
3	1	0	-1.478544	0.420495	1.409546
4	6	0	-0.278710	-0.518966	-0.121992
5	1	0	-0.388407	-1.537487	0.276638
6	1	0	-0.265411	-0.607561	-1.217701
7	6	0	-2.815521	-0.223667	-0.163827
8	1	0	-3.650821	0.407137	0.161317
9	1	0	-2.852992	-0.285839	-1.258497
10	1	0	-2.988599	-1.233438	0.229687
11	6	0	1.075193	0.032473	0.326332
12	1	0	1.058175	0.148679	1.424721
13	6	0	2.237222	-0.887281	-0.054364
14	1	0	2.270942	-1.028151	-1.140526
15	1	0	3.197210	-0.458802	0.262355
16	1	0	2.140376	-1.869560	0.422814
17	8	0	1.220213	1.317757	-0.288492
18	1	0	2.060019	1.695674	0.014916

Total computed energy:

– 272.814995 Hartrees × 627.51 kcal/Hartrees = – 171194.1 kcal

Imaginary frequencies = 0

Table S6 Cartesian Coordinates of Protonated 2-Pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.489307	0.343201	0.276669
2	1	0	-1.396557	1.342560	-0.185447
3	1	0	-1.471415	0.493336	1.364474
4	6	0	-0.316006	-0.562016	-0.141060
5	1	0	-0.474574	-1.567102	0.274996
6	1	0	-0.275964	-0.684523	-1.230483
7	6	0	-2.844766	-0.237292	-0.143779
8	1	0	-3.658506	0.430087	0.152681
9	1	0	-2.899662	-0.375112	-1.228816
10	1	0	-3.016405	-1.208841	0.332029
11	6	0	1.043099	-0.143647	0.371694
12	1	0	1.041449	0.065915	1.444879
13	6	0	2.237225	-0.941604	-0.079024
14	1	0	2.262002	-1.050391	-1.166558
15	1	0	3.182667	-0.515358	0.273039
16	1	0	2.153134	-1.940593	0.364784
17	8	0	1.277995	1.323371	-0.259503
18	1	0	2.063947	1.781856	0.105977
19	1	0	0.484455	1.889339	-0.132532

Total computed energy:

– 273.125371 Hartrees × 627.51 kcal/Hartrees = – 171388.9 kcal

Imaginary frequencies = 0

Table S7 Cartesian Coordinates of 2-Methyl-2-butanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.658070	-0.858856	-0.341731
2	1	0	-1.581570	-1.841270	0.135815
3	1	0	-1.732936	-1.002496	-1.425204
4	6	0	-0.439925	-0.002347	0.014293
5	6	0	0.851945	-0.701893	-0.474089
6	1	0	0.831080	-1.732414	-0.097484
7	1	0	0.823176	-0.766532	-1.570409
8	6	0	2.165625	-0.043945	-0.036433
9	1	0	3.023391	-0.625692	-0.390995
10	1	0	2.276418	0.972449	-0.431578
11	1	0	2.241608	0.003811	1.056815
12	8	0	-0.452033	0.067954	1.451702
13	1	0	0.237954	0.694781	1.719505
14	6	0	-0.591034	1.410070	-0.572804
15	1	0	-0.624293	1.386629	-1.668329
16	1	0	-1.516318	1.867981	-0.208015
17	1	0	0.243184	2.060201	-0.280855
18	1	0	-2.576671	-0.379248	0.011703

Total computed energy:

– 272.817816 Hartrees × 627.51 kcal/Hartrees = – 171195.9 kcal

Imaginary frequencies = 0

Table S8 Cartesian Coordinates of Protonated 2-Methyl-2-butanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.665509	0.956565	-0.077498
2	1	0	-1.595813	1.547363	-0.994059
3	1	0	-1.747603	1.649572	0.767899
4	6	0	-0.431900	0.110272	0.139434
5	6	0	0.879950	0.868660	-0.006341
6	1	0	0.828981	1.478934	-0.914673
7	1	0	0.883891	1.577707	0.832877
8	6	0	2.178557	0.050465	0.020611
9	1	0	3.030551	0.729418	-0.071076
10	1	0	2.306961	-0.509937	0.950808
11	1	0	2.265542	-0.650480	-0.822160
12	8	0	-0.436615	-0.836903	-1.251225
13	1	0	0.379011	-1.377950	-1.307752
14	6	0	-0.528345	-0.876989	1.281548
15	1	0	-0.490833	-0.307908	2.218350
16	1	0	-1.477946	-1.421614	1.274339
17	1	0	0.301564	-1.588187	1.301714
18	1	0	-2.582410	0.358036	-0.091246
19	1	0	-1.205494	-1.443575	-1.281735

Total computed energy:

– 273.133804 Hartrees × 627.51 kcal/Hartrees = 171394.2 kcal

Imaginary frequencies = 0

Table S9 Cartesian Coordinates of 3-Heptanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.371373	-0.718714	-0.186121
2	1	0	2.381997	-0.803051	-1.281210
3	1	0	2.259857	-1.737247	0.209063
4	6	0	1.136668	0.091152	0.213630
5	6	0	3.687937	-0.107190	0.301250
6	1	0	3.716423	-0.050619	1.396853
7	1	0	3.810238	0.906474	-0.090689
8	6	0	-0.171931	-0.601782	-0.195045
9	1	0	-0.152619	-0.768614	-1.281023
10	1	0	-0.202959	-1.593223	0.279411
11	6	0	-1.439199	0.176893	0.181139
12	1	0	-1.433352	0.389966	1.261644
13	1	0	-1.435654	1.151235	-0.329496
14	1	0	4.545063	-0.708102	-0.023051
15	8	0	1.269472	1.374069	-0.410335
16	1	0	0.593151	1.957799	-0.035992
17	1	0	1.139768	0.215234	1.312098
18	6	0	-2.736865	-0.559239	-0.177643
19	1	0	-2.751391	-1.532693	0.332434
20	1	0	-2.739483	-0.779956	-1.254238
21	6	0	-3.999371	0.228431	0.186492
22	1	0	-4.906769	-0.324020	-0.082653
23	1	0	-4.042167	0.434370	1.263228
24	1	0	-4.029553	1.192589	-0.335917

Total computed energy:

– 351.385017 Hartrees × 627.51 kcal/Hartrees = – 220497.6 kcal

Imaginary frequencies = 0

Table S10 Cartesian Coordinates of Protonated 3-Heptanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.377909	-0.775262	-0.182134
2	1	0	2.359038	-0.902433	-1.270429
3	1	0	2.319228	-1.784104	0.248944
4	6	0	1.106903	-0.091515	0.266407
5	6	0	3.677323	-0.099676	0.278411
6	1	0	3.695761	0.055264	1.363262
7	1	0	3.854515	0.863047	-0.220655
8	6	0	-0.210943	-0.647605	-0.221909
9	1	0	-0.170354	-0.789393	-1.308700
10	1	0	-0.273677	-1.652872	0.218354
11	6	0	-1.458025	0.156912	0.187792
12	1	0	-1.442022	0.343726	1.270971
13	1	0	-1.467794	1.145242	-0.307632
14	1	0	4.533973	-0.728978	0.023624
15	8	0	1.184131	1.384375	-0.378009
16	1	0	0.356178	1.883821	-0.204322
17	1	0	1.100150	0.129443	1.338309
18	6	0	-2.767248	-0.556929	-0.187166
19	1	0	-2.787960	-1.533756	0.313777
20	1	0	-2.769208	-0.760762	-1.265904
21	6	0	-4.012809	0.248061	0.192516
22	1	0	-4.921683	-0.295181	-0.082495
23	1	0	-4.053170	0.438379	1.271228
24	1	0	-4.037174	1.215516	-0.322871
25	1	0	1.952495	1.894120	-0.044890

Total computed energy:

– 351.698615 Hartrees × 627.51 kcal/Hartrees = – 220694.4 kcal

Imaginary frequencies = 0

Table S11 Cartesian Coordinates of 3-Hexanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.753595	-0.757808	-0.239507
2	1	0	1.719620	-0.805622	-1.336334
3	1	0	1.605772	-1.782343	0.127116
4	6	0	0.576723	0.097708	0.232820
5	6	0	3.116154	-0.227646	0.215813
6	1	0	3.188889	-0.211234	1.310714
7	1	0	3.272727	0.792224	-0.146633
8	6	0	-0.779260	-0.513044	-0.151423
9	1	0	-0.807267	-0.639701	-1.242742
10	1	0	-0.846510	-1.518840	0.288080
11	6	0	-1.990720	0.314024	0.298354
12	1	0	-1.940211	0.475408	1.385610
13	1	0	-1.946342	1.308243	-0.168334
14	1	0	3.929815	-0.856989	-0.162095
15	8	0	0.752928	1.394147	-0.351655
16	1	0	0.124808	1.998599	0.070657
17	1	0	0.624618	0.182049	1.334047
18	6	0	-3.330170	-0.340067	-0.056050
19	1	0	-3.428348	-1.323149	0.420339
20	1	0	-3.423447	-0.486502	-1.138906
21	1	0	-4.175475	0.275686	0.271681

Total computed energy:

– 312.099898 Hartrees × 627.51 kcal/Hartrees = – 195845.8 kcal

Imaginary frequencies = 0

Table S12 Cartesian Coordinates of Protonated 3-Hexanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.759738	-0.820560	-0.237379
2	1	0	1.696411	-0.911189	-1.327681
3	1	0	1.657822	-1.837824	0.164858
4	6	0	0.546139	-0.081317	0.277515
5	6	0	3.111059	-0.235068	0.196850
6	1	0	3.174702	-0.114767	1.284375
7	1	0	3.328585	0.730493	-0.280587
8	6	0	-0.816514	-0.545267	-0.183812
9	1	0	-0.823487	-0.636708	-1.276767
10	1	0	-0.916094	-1.565977	0.211826
11	6	0	-2.004415	0.300456	0.311473
12	1	0	-1.941523	0.422131	1.401300
13	1	0	-1.970925	1.313563	-0.126884
14	1	0	3.920343	-0.904528	-0.105858
15	8	0	0.689203	1.409602	-0.319961
16	1	0	-0.089549	1.959532	-0.084885
17	1	0	0.587636	0.101841	1.355728
18	6	0	-3.354057	-0.324358	-0.061386
19	1	0	-3.463921	-1.314510	0.393883
20	1	0	-3.455180	-0.435438	-1.146197
21	1	0	-4.179043	0.300539	0.291462
22	1	0	1.508896	1.852704	-0.014446

Total computed energy:

– 312.412507 Hartrees × 627.51 kcal/Hartrees = – 196042.0 kcal

Imaginary frequencies = 0

Table S13 Cartesian Coordinates of 3-Methyl-3-pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.256752	-0.761666	-0.405575
2	1	0	-1.156398	-1.755141	0.050051
3	1	0	-1.239970	-0.912682	-1.493293
4	6	0	-0.004128	0.045848	-0.008426
5	6	0	-2.597626	-0.154609	0.020163
6	1	0	-2.817986	0.778092	-0.511204
7	1	0	-2.599896	0.056138	1.093571
8	6	0	1.255648	-0.726383	-0.474663
9	1	0	1.159085	-1.759645	-0.117790
10	1	0	1.255155	-0.771708	-1.572362
11	6	0	2.596633	-0.164759	0.012174
12	1	0	3.422210	-0.804319	-0.318455
13	1	0	2.793795	0.843171	-0.370610
14	1	0	2.636793	-0.129468	1.107583
15	1	0	-3.416010	-0.851565	-0.193262
16	8	0	-0.036313	0.102443	1.429993
17	1	0	0.650512	0.724667	1.714874
18	6	0	-0.037897	1.470457	-0.584039
19	1	0	-0.077660	1.456497	-1.679588
20	1	0	-0.909939	2.016164	-0.213164
21	1	0	0.855549	2.036922	-0.294104

Total computed energy:

– 312.101023 Hartrees × 627.51 kcal/Hartrees = – 195846.5 kcal

Imaginary frequencies = 0

Table S14 Cartesian Coordinates of Protonated 3-Methyl-3-pentanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.974556	-0.446384	0.841869
2	1	0	0.412437	-0.892486	1.674818
3	6	0	-0.034974	0.436632	0.128376
4	8	0	0.963001	1.230551	-1.017139
5	1	0	0.435656	1.770784	-1.641214
6	6	0	-0.588271	1.565582	0.968685
7	1	0	-1.246935	1.130187	1.728922
8	1	0	0.196680	2.109544	1.504211
9	1	0	-1.191371	2.265785	0.381971
10	1	0	1.613720	1.822988	-0.586741
11	1	0	1.723890	0.195264	1.324987
12	6	0	1.651630	-1.549692	0.021087
13	1	0	2.372269	-2.076926	0.652017
14	1	0	0.933816	-2.290239	-0.343099
15	1	0	2.195173	-1.145911	-0.838446
16	6	0	-1.026022	-0.242204	-0.799921
17	1	0	-1.594700	0.522457	-1.345792
18	1	0	-0.480784	-0.842865	-1.534007
19	6	0	-2.017767	-1.144022	-0.036645
20	1	0	-2.705486	-1.596580	-0.755707
21	1	0	-1.506249	-1.954969	0.489750
22	1	0	-2.617028	-0.580913	0.684739

Total computed energy:

– 312.418738 Hartrees × 627.51 kcal/Hartrees = – 196045.9 kcal

Imaginary frequencies = 0

Table S15 Cartesian Coordinates of 1-Heptanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.520016	-2.867613	0.000000
2	1	0	-0.992541	-3.256191	0.887738
3	1	0	-0.992541	-3.256191	-0.887738
4	6	0	-1.475477	-1.345429	0.000000
5	1	0	-2.023640	-0.983231	-0.879847
6	1	0	-2.023640	-0.983231	0.879847
7	6	0	0.000000	0.747893	0.000000
8	1	0	-0.543104	1.126841	0.878323
9	1	0	-0.543104	1.126841	-0.878323
10	6	0	-0.047814	-0.785408	0.000000
11	1	0	0.495477	-1.163639	-0.878850
12	8	0	-2.887275	-3.268619	0.000000
13	1	0	-2.912580	-4.237258	0.000000
14	6	0	1.424698	1.316448	0.000000
15	1	0	1.968234	0.937270	0.878482
16	1	0	1.968234	0.937270	-0.878482
17	6	0	1.473411	2.849583	0.000000
18	1	0	0.931015	3.228574	0.877931
19	1	0	0.931015	3.228574	-0.877931
20	6	0	2.899619	3.409401	0.000000
21	1	0	3.456503	3.076131	-0.884581
22	1	0	2.900369	4.505448	0.000000
23	1	0	3.456503	3.076131	0.884581
24	1	0	0.495477	-1.163639	0.878850

Total computed energy:

– 351.378720 Hartrees × 627.51 kcal/Hartrees = – 220493.7 kcal

Imaginary frequencies = 0

Table S16 Cartesian Coordinates of Protonated 1-Heptanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.056143	0.577123	0.014250
2	1	0	-3.162938	1.203259	-0.871108
3	1	0	-3.162243	1.152266	0.935570
4	6	0	-1.881739	-0.358856	-0.020290
5	1	0	-1.902712	-1.030436	0.849021
6	1	0	-1.916510	-0.968375	-0.930032
7	6	0	0.671186	-0.443343	-0.014505
8	1	0	0.640128	-1.074070	-0.913721
9	1	0	0.638446	-1.125724	0.846381
10	6	0	-0.568887	0.464133	0.010347
11	1	0	-0.545671	1.142745	-0.852122
12	8	0	-4.373151	-0.290652	-0.073739
13	1	0	-5.203257	0.226653	0.014108
14	6	0	1.983648	0.351413	0.010494
15	1	0	2.011266	1.036435	-0.849105
16	1	0	2.009687	0.984353	0.909293
17	6	0	3.228454	-0.546482	-0.015199
18	1	0	3.199918	-1.178234	-0.913853
19	1	0	3.197453	-1.232371	0.842797
20	6	0	4.537160	0.249080	0.011287
21	1	0	4.611322	0.862998	0.916772
22	1	0	5.404274	-0.418991	-0.009305
23	1	0	4.612776	0.919387	-0.853128
24	1	0	-4.380603	-1.024245	0.578654
25	1	0	-0.548194	1.091157	0.911388

Total computed energy:

– 351.682674 Hartrees × 627.51 kcal/Hartrees = – 220684.4 kcal

Imaginary frequencies = 0

Table S17 Cartesian Coordinates of 1-Hexanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.544605	0.649099	0.000000
2	1	0	2.515489	1.303631	0.887740
3	1	0	2.515489	1.303631	-0.887740
4	6	0	1.332626	-0.273033	0.000000
5	1	0	1.395235	-0.927037	-0.879866
6	1	0	1.395235	-0.927037	0.879866
7	6	0	-1.223346	-0.439981	0.000000
8	1	0	-1.178600	-1.100883	0.878332
9	1	0	-1.178600	-1.100883	-0.878332
10	6	0	0.000000	0.485556	0.000000
11	1	0	-0.046632	1.145959	-0.878854
12	8	0	3.716034	-0.162057	0.000000
13	1	0	4.485120	0.427369	0.000000
14	6	0	-2.560657	0.311378	0.000000
15	1	0	-2.604884	0.971604	0.878036
16	1	0	-2.604884	0.971604	-0.878036
17	6	0	-3.776793	-0.620380	0.000000
18	1	0	-3.778809	-1.269273	0.884548
19	1	0	-4.715601	-0.054758	0.000000
20	1	0	-3.778809	-1.269273	-0.884548
21	1	0	-0.046632	1.145959	0.878854

Total computed energy:

– 312.093564 Hartrees × 627.51 kcal/Hartrees = – 195841.8 kcal

Imaginary frequencies = 0

Table S18 Cartesian Coordinates of Protonated 1-Hexanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.439483	0.535888	0.015432
2	1	0	-2.567836	1.161975	-0.867112
3	1	0	-2.568302	1.102263	0.939285
4	6	0	-1.230910	-0.355794	-0.021327
5	1	0	-1.228466	-1.031243	0.845214
6	1	0	-1.242221	-0.962480	-0.933565
7	6	0	1.323194	-0.346646	-0.011934
8	1	0	1.317500	-0.974851	-0.913489
9	1	0	1.315287	-1.032887	0.846518
10	6	0	0.050660	0.514582	0.014365
11	1	0	0.047342	1.138604	0.917742
12	8	0	-3.722424	-0.379836	-0.079230
13	1	0	-4.571540	0.105554	0.009228
14	6	0	2.606001	0.495743	0.017999
15	1	0	2.607770	1.183293	-0.838818
16	1	0	2.605212	1.124985	0.918637
17	6	0	3.875026	-0.362129	-0.008892
18	1	0	3.921872	-0.975346	-0.916376
19	1	0	4.771231	0.265674	0.014894
20	1	0	3.917976	-1.036884	0.854067
21	1	0	-3.703696	-1.116611	0.569365
22	1	0	0.050332	1.196778	-0.845603

Total computed energy:

– 312.397289 Hartrees × 627.51 kcal/Hartrees = – 186032.4 kcal

Imaginary frequencies = 0

Table S19 Cartesian Coordinates of 1-Octanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.881811	-0.190043	0.000000
2	1	0	-3.942823	-0.842322	0.887779
3	1	0	-3.942823	-0.842322	-0.887779
4	6	0	-2.554616	0.556818	0.000000
5	1	0	-2.526925	1.213218	-0.879888
6	1	0	-2.526925	1.213218	0.879888
7	6	0	0.000000	0.371472	0.000000
8	1	0	0.045081	1.032177	0.878303
9	1	0	0.045081	1.032177	-0.878303
10	8	0	-4.930668	0.774418	0.000000
11	1	0	-5.773464	0.296282	0.000000
12	6	0	1.220997	-0.556998	0.000000
13	1	0	1.174776	-1.217988	0.878472
14	1	0	1.174776	-1.217988	-0.878472
15	6	0	2.560283	0.190994	0.000000
16	1	0	2.607602	0.852072	0.878386
17	1	0	2.607602	0.852072	-0.878386
18	6	0	3.781952	-0.736757	0.000000
19	1	0	3.735064	-1.396862	-0.877979
20	1	0	3.735064	-1.396862	0.877979
21	6	0	5.115193	0.018113	0.000000
22	1	0	5.207124	0.660429	0.884620
23	1	0	5.966791	-0.671962	0.000000
24	1	0	5.207124	0.660429	-0.884620
25	6	0	-1.338916	-0.377699	0.000000
26	1	0	-1.383135	-1.038258	0.878839
27	1	0	-1.383135	-1.038258	-0.878839

Total computed energy:

– 390.663760 Hartrees × 627.51 kcal/Hartrees = – 245145.4 kcal

Imaginary frequencies = 0

Table S20 Cartesian Coordinates of Protonated 1-Octanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.712875	0.517910	0.011518
2	1	0	3.842363	1.090771	0.931256
3	1	0	3.842893	1.137105	-0.875620
4	6	0	2.503311	-0.372140	-0.019138
5	1	0	2.513650	-0.985449	-0.926928
6	1	0	2.499177	-1.041130	0.852384
7	6	0	-0.050937	-0.358271	-0.010514
8	1	0	-0.043622	-1.037632	0.853299
9	1	0	-0.044610	-0.993591	-0.906966
10	6	0	1.223186	0.501052	0.009755
11	1	0	1.225095	1.176819	-0.855243
12	8	0	4.995549	-0.400525	-0.075694
13	1	0	5.845156	0.084475	0.009921
14	6	0	-1.331924	0.486559	0.011775
15	1	0	-1.331976	1.123884	0.907758
16	1	0	-1.332919	1.168269	-0.850795
17	6	0	-2.609924	-0.363061	-0.009149
18	1	0	-2.606351	-1.046957	0.852200
19	1	0	-2.608357	-1.000421	-0.905436
20	6	0	-3.894889	0.475496	0.014751
21	1	0	-3.896231	1.159681	-0.845301
22	1	0	-3.894791	1.111606	0.911017
23	6	0	-5.166570	-0.378197	-0.007734
24	1	0	-5.210100	-1.049185	0.858578
25	1	0	-6.064362	0.248503	0.011726
26	1	0	-5.212944	-0.998252	-0.911045
27	1	0	4.975268	-1.132093	0.578679
28	1	0	1.227498	1.131709	0.908475

Total computed energy:

– 390.967886 Hartrees × 627.51 kcal/Hartrees = – 245336.3 kcal

Imaginary frequencies = 0