

Methylations with Methanol via Bioinspired Catalytic C–O Bond Cleavage

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1. Cartesian Coordinates of Optimized Structures

Int0

Zn	0.992925	1.197723	-0.017894
O	-0.832896	2.148555	-0.347673
S	-1.223838	3.289233	0.556727
O	-1.465375	2.855151	1.946866
O	-0.363746	4.474764	0.385286
C	-2.886345	3.756139	-0.127262
O	2.750721	0.088067	0.371772
S	3.148060	-1.108937	-0.436557
O	2.528876	-2.376943	0.028769
O	3.092263	-0.891626	-1.892849
C	4.945738	-1.293458	-0.005435
F	5.594559	-0.180918	-0.354428
F	5.074610	-1.490378	1.307747
F	5.454363	-2.332660	-0.665584
F	-2.757087	4.109736	-1.407898
F	-3.716044	2.714797	-0.036962
F	-3.380864	4.780127	0.569134
O	0.627930	1.111138	2.057909
H	-0.170304	1.650434	2.252900
C	0.571482	-0.133383	2.772811
H	-0.376421	-0.643698	2.589252
H	1.385889	-0.753019	2.402365
H	0.700807	0.052992	3.843307
O	1.374078	1.184078	-2.040727
O	1.991781	3.035323	0.235375
H	1.331121	3.760580	0.229662
H	1.992941	0.464731	-2.284203
C	0.462384	1.504688	-3.107294
H	-0.141784	0.634561	-3.371304
H	-0.185394	2.296743	-2.736162
H	1.029313	1.861677	-3.971609
C	2.904594	3.209520	1.331989
H	2.375891	3.192727	2.288948
H	3.603749	2.374912	1.290633
H	3.446789	4.151673	1.213586
S	-0.650684	-1.721112	-1.036049
O	0.372990	-2.893018	-1.289043
O	-1.154299	-1.235896	-2.306579
O	-0.043869	-0.763781	-0.091255
C	-2.004312	-2.511555	-0.174127
C	-1.841871	-3.240818	1.012540

C	-2.965364	-3.777520	1.641066
C	-4.235310	-3.586118	1.103403
C	-4.382032	-2.856594	-0.075789
C	-3.273601	-2.316771	-0.721888
H	-2.838491	-4.347238	2.554248
H	-3.378748	-1.751956	-1.639570
H	-5.105799	-4.002939	1.596342
Cl	-5.972777	-2.616047	-0.754032
Cl	-0.279540	-3.518023	1.731035
H	1.229858	-2.759222	-0.747565

TS1

Zn	0.373614	1.449692	0.977210
O	-0.718812	1.533299	-2.998666
H	-1.425346	2.001630	-2.501803
C	-0.992621	-0.429311	-2.557952
H	-1.993481	-0.342945	-2.949941
H	-0.175185	-0.637026	-3.229294
H	-0.807569	-0.247006	-1.510569
O	2.490507	1.977309	0.880062
S	2.538147	1.996265	-0.626541
O	3.172415	3.152428	-1.247075
O	1.094561	1.755464	-1.047705
C	3.481959	0.533160	-1.077402
C	3.480199	-0.017427	-2.363423
C	4.296488	-0.009828	-0.082840
C	4.283828	-1.122037	-2.644845
C	5.109531	-1.097300	-0.385785
H	4.274260	0.415205	0.911806
C	5.104206	-1.664181	-1.658908
H	4.270913	-1.548479	-3.641213
O	0.805645	-0.596549	0.523866
S	0.557924	-1.821161	1.350842
O	-0.330012	-1.578885	2.509141
O	0.240206	-3.010655	0.544511
C	2.225022	-2.202659	2.088303
O	-1.592677	1.036026	0.289016
S	-2.619444	2.108223	0.046242
O	-2.738709	3.062538	1.166831
O	-2.542895	2.701193	-1.300078
C	-4.209578	1.148759	0.050722
F	-4.204994	0.298399	-0.980819
F	-4.342452	0.468002	1.191612
F	-5.235770	1.990669	-0.079542

F	3.036255	-2.676451	1.140753
F	2.753537	-1.088562	2.609029
F	2.087814	-3.116075	3.049822
H	0.094458	1.725669	-2.481322
H	5.733971	-2.518258	-1.878459
S	-1.366043	-2.722748	-2.178194
H	-0.579164	-2.860147	-1.073574
C	-2.945373	-2.675322	-1.340359
C	-3.039173	-2.634244	0.055130
C	-4.099690	-2.653499	-2.126970
C	-4.295693	-2.559665	0.646833
H	-2.151751	-2.667784	0.673755
C	-5.348069	-2.568487	-1.512362
H	-4.028668	-2.702002	-3.209853
C	-5.467297	-2.510138	-0.119983
H	-4.361958	-2.522551	1.730399
H	-6.242389	-2.543193	-2.128368
C	-6.810286	-2.359567	0.547302
H	-7.630407	-2.512458	-0.158678
H	-6.930480	-3.071411	1.370155
H	-6.916322	-1.353999	0.971731
Cl	6.140370	-1.769333	0.856280
Cl	2.497644	0.637019	-3.652804
O	0.028619	1.006182	2.945517
H	-0.228762	0.053123	2.969388
C	-0.836289	1.787688	3.788686
H	-0.401904	2.784108	3.853836
H	-1.842930	1.855123	3.365835
H	-0.872023	1.336323	4.783467
O	-0.077567	3.482190	1.360853
H	-1.053545	3.567297	1.427724
C	0.434055	4.549332	0.535623
H	1.519784	4.484105	0.562427
H	0.085558	4.444638	-0.495363
H	0.111846	5.509536	0.946449

TS1b

Zn	1.405512	0.297049	0.562096
O	1.046416	0.654894	-1.622422
H	1.729148	1.306817	-1.939606
C	-0.851711	0.707343	-2.074067
H	-1.039381	1.449219	-1.316764
H	-0.714333	0.988401	-3.107510
H	-0.879889	-0.334838	-1.809926

O	1.617751	-1.694573	0.133239
S	1.435312	-2.580531	-1.075028
O	2.408971	-3.654647	-1.178475
O	1.282304	-1.731107	-2.308449
C	-0.202566	-3.286482	-0.812730
C	-0.521579	-4.027539	0.332049
C	-1.186944	-3.019502	-1.766472
C	-1.831941	-4.463437	0.529658
C	-2.487950	-3.459037	-1.549628
H	-0.918400	-2.482917	-2.667444
C	-2.823104	-4.174273	-0.403181
H	-2.073476	-5.017460	1.428866
O	-0.698593	0.402905	0.800751
S	-1.602089	-0.573320	1.500521
O	-2.768600	-0.943412	0.685696
O	-0.875417	-1.650102	2.188482
C	-2.291210	0.437855	2.906989
O	3.426070	0.631060	0.105255
S	3.866891	1.897687	-0.577256
O	3.255944	2.074786	-1.915229
O	3.809180	3.073493	0.312137
C	5.669535	1.572805	-0.890672
F	6.287070	1.351314	0.270642
F	5.800932	0.507264	-1.677818
F	6.208451	2.638457	-1.485331
F	-1.319962	0.701247	3.789099
F	-2.787988	1.604862	2.461845
F	-3.264158	-0.242139	3.514642
H	1.282563	-0.279370	-1.989170
H	-3.843754	-4.498242	-0.238548
S	-3.281465	0.509986	-2.303418
H	-3.295028	-0.217306	-1.159774
C	-3.711541	2.083120	-1.572408
C	-4.087749	2.182670	-0.231347
C	-3.639485	3.228699	-2.371459
C	-4.384975	3.434649	0.303576
H	-4.135766	1.297220	0.390219
C	-3.941629	4.470230	-1.818261
H	-3.346074	3.155451	-3.414809
C	-4.319762	4.596183	-0.474557
H	-4.666035	3.504787	1.350418
H	-3.879990	5.357530	-2.442072
C	-4.671157	5.942295	0.106755
H	-4.075172	6.740529	-0.344823

H	-5.726387	6.182353	-0.071307
H	-4.508848	5.964474	1.187775
Cl	-3.726248	-3.080648	-2.734213
Cl	0.669353	-4.429113	1.536156
O	1.269826	2.368877	1.023198
H	2.154243	2.794085	0.989009
C	0.530379	2.854845	2.155888
H	-0.523498	2.673804	1.957688
H	0.826586	2.329102	3.067573
H	0.702072	3.928819	2.267184
O	1.595326	-0.375346	2.537377
H	0.855247	-1.017184	2.594289
C	2.833248	-1.052034	2.851307
H	3.635909	-0.338754	2.666401
H	2.829264	-1.344368	3.904910
H	2.962761	-1.922796	2.205580

TS1c

Zn	-0.835655	0.147186	-0.542322
O	-0.227213	-3.074569	2.867777
H	-0.910760	-3.508759	2.313122
C	-0.802450	-1.176348	2.630719
H	-1.763361	-1.527122	2.302822
H	-0.681404	-0.873638	3.660988
H	0.013390	-1.076372	1.943041
O	1.151003	-0.084129	0.244947
S	2.001600	-1.324921	0.053874
O	1.908609	-1.846819	-1.327668
O	1.796504	-2.324578	1.122488
C	3.686587	-0.729821	0.316952
C	4.365586	0.110446	-0.574200
C	4.306545	-1.121636	1.505635
C	5.654110	0.551536	-0.270697
C	5.590685	-0.671435	1.795890
H	3.777773	-1.778792	2.183327
C	6.272156	0.165988	0.915101
H	6.170789	1.197334	-0.971208
O	-0.552382	2.330736	-1.254524
S	-0.179663	3.622496	-0.661144
O	-0.645386	4.844601	-1.273117
O	-0.469776	3.639904	0.884062
C	1.687911	3.664031	-0.662500
O	-1.000792	-1.921415	-0.209210
S	-2.120782	-2.910418	-0.258819

O	-2.249203	-3.682513	0.989117
O	-3.374093	-2.339778	-0.796949
C	-1.522527	-4.114564	-1.541674
F	-1.335500	-3.471045	-2.698577
F	-0.371022	-4.655140	-1.143277
F	-2.431427	-5.076899	-1.714018
F	2.158196	2.672998	0.088346
F	2.103216	3.521338	-1.922343
F	2.101534	4.832650	-0.182208
H	0.556988	-3.019055	2.278235
H	7.272873	0.509179	1.149972
S	-1.390415	0.947023	1.677929
H	-0.718231	2.703079	1.249434
C	-3.159543	1.190211	1.759693
C	-3.668895	2.464350	2.034279
C	-4.046643	0.128421	1.547772
C	-5.047426	2.667773	2.084677
H	-2.993139	3.297762	2.197515
C	-5.420217	0.345121	1.608258
H	-3.681274	-0.862443	1.306811
C	-5.946339	1.615283	1.877819
H	-5.428316	3.664496	2.290463
H	-6.093033	-0.489828	1.432217
C	-7.435799	1.833432	1.967628
H	-7.701012	2.872750	1.754759
H	-7.975928	1.192278	1.264765
H	-7.807726	1.599118	2.972655
Cl	6.357920	-1.166222	3.288898
Cl	3.669941	0.639206	-2.084651
O	-0.049986	-0.380172	-2.421420
H	0.672607	-1.008002	-2.163287
C	0.443741	0.519890	-3.423134
H	-0.415263	1.014347	-3.876231
H	1.100710	1.275661	-2.990682
H	0.979752	-0.047255	-4.188800
O	-2.773409	0.245496	-1.346332
H	-3.163431	-0.647703	-1.202695
C	-3.030891	0.668866	-2.691118
H	-2.579447	-0.019415	-3.412012
H	-4.110216	0.729336	-2.857234
H	-2.593713	1.661371	-2.801236

TS2

Zn	-0.411330	1.500358	-0.943748
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O	0.720384	1.520952	3.026420
H	1.423477	1.994908	2.529753
C	1.004603	-0.423209	2.549450
H	2.020936	-0.332308	2.898493
H	0.220097	-0.658378	3.250165
H	0.774043	-0.233821	1.512512
O	-2.529862	1.987958	-0.811532
S	-2.567771	1.960175	0.695605
O	-3.220535	3.084468	1.354106
O	-1.117084	1.734839	1.100066
C	-3.476469	0.464082	1.107440
C	-3.457936	-0.119787	2.378565
C	-4.276779	-0.074390	0.099029
C	-4.231147	-1.252709	2.631233
C	-5.059790	-1.191048	0.373705
H	-4.267003	0.377183	-0.884047
C	-5.037609	-1.790723	1.631599
H	-4.205731	-1.704659	3.616050
O	-0.804586	-0.567887	-0.555949
S	-0.517618	-1.758583	-1.418472
O	0.344830	-1.451445	-2.580780
O	-0.142120	-2.956423	-0.650250
C	-2.178805	-2.184017	-2.144368
O	1.555444	1.075470	-0.277376
S	2.594441	2.134049	-0.028312
O	2.682867	3.128564	-1.116579
O	2.562433	2.677392	1.340482
C	4.176642	1.165907	-0.122420
F	4.218737	0.299274	0.894315
F	4.242607	0.500948	-1.279100
F	5.213363	1.999016	-0.033745
F	-2.960364	-2.706562	-1.197372
F	-2.753414	-1.078682	-2.634072
F	-2.021951	-3.071237	-3.127304
H	-0.098571	1.713960	2.518062
H	-5.643918	-2.666913	1.828937
S	1.395317	-2.714275	2.120181
H	0.624752	-2.832598	1.003209
C	2.985029	-2.668578	1.304942
C	3.103612	-2.617717	-0.087132
C	4.131952	-2.665006	2.108888
C	4.367641	-2.562471	-0.666869
H	2.225933	-2.631158	-0.720703
C	5.391911	-2.598155	1.527377

H	4.042939	-2.716373	3.190207
C	5.513590	-2.541013	0.134204
H	4.455882	-2.519615	-1.749306
H	6.290031	-2.589441	2.134557
Cl	-6.074452	-1.857279	-0.884674
Cl	-2.491255	0.527259	3.683576
O	-0.084304	1.134099	-2.930673
H	0.193875	0.188343	-2.989550
C	0.748729	1.962941	-3.760446
H	0.294855	2.952585	-3.779435
H	1.762310	2.034174	-3.355012
H	0.772617	1.549866	-4.772123
O	0.019141	3.549069	-1.253109
H	0.993984	3.642607	-1.325899
C	-0.493729	4.581051	-0.385642
H	-1.579045	4.504769	-0.401731
H	-0.132118	4.445090	0.637195
H	-0.187111	5.558587	-0.766465
O	6.771341	-2.464687	-0.380430
H	6.721693	-2.433768	-1.344785

TS2b

Zn	0.601804	-1.156017	-1.038808
O	-0.795049	-2.087248	2.851671
H	-1.490235	-2.535535	2.328812
C	-1.222868	-0.061193	2.623712
H	-2.103671	-0.274449	3.205958
H	-0.295902	0.142222	3.135979
H	-1.218365	-0.229193	1.559497
O	2.482969	-1.669051	-0.486507
S	2.499290	-2.636803	0.685437
O	3.450807	-3.724269	0.534644
O	1.104898	-2.969578	1.067825
C	2.525067	2.470253	-0.291935
C	2.879097	3.812545	-0.491486
C	3.491068	1.464513	-0.355249
C	4.213176	4.138625	-0.734979
C	4.815862	1.812099	-0.607145
H	3.211637	0.429175	-0.217339
C	5.184953	3.143051	-0.793065
H	4.484761	5.177342	-0.882920
O	0.876481	0.488394	0.232177
S	0.825912	1.969677	-0.016347
O	0.065516	2.290108	-1.254646

O	0.349836	2.690966	1.190462
C	3.132442	-1.592188	2.099885
O	-1.333017	-1.244736	-0.347107
S	-2.337598	-2.374268	-0.407304
O	-2.168046	-3.223389	-1.601578
O	-2.527837	-3.054283	0.877292
C	-3.926760	-1.442822	-0.695157
F	-4.259970	-0.792641	0.420922
F	-3.772830	-0.561346	-1.692239
F	-4.892413	-2.301771	-1.013953
F	3.402044	-2.384929	3.137064
F	4.237879	-0.940901	1.735006
F	2.201406	-0.698428	2.469848
H	0.015720	-2.299836	2.345467
H	6.220344	3.399340	-0.985067
O	-1.685999	1.758236	2.458218
H	-0.911796	2.171724	1.955908
C	-2.883627	1.926478	1.761335
C	-2.899527	2.240229	0.403729
C	-4.067428	1.726326	2.466845
C	-4.123512	2.334029	-0.254297
H	-1.981037	2.401778	-0.147122
C	-5.286374	1.823707	1.802549
H	-4.029294	1.507615	3.528741
C	-5.322109	2.114647	0.432705
H	-4.131942	2.557916	-1.316116
H	-6.210031	1.669546	2.351145
Cl	6.028247	0.557007	-0.693979
Cl	1.707074	5.100987	-0.457010
O	0.334938	0.065711	-2.658275
H	0.182918	0.975471	-2.293620
C	-0.687710	-0.249105	-3.622271
H	-0.474478	-1.248208	-3.998519
H	-1.677736	-0.233829	-3.157802
H	-0.645269	0.472142	-4.442501
O	0.380072	-2.854648	-2.239561
H	-0.558078	-3.143677	-2.145772
C	1.242257	-4.009842	-2.186578
H	2.268968	-3.651995	-2.230802
H	1.089260	-4.563743	-1.257054
H	1.035103	-4.651856	-3.046787
S	-6.908853	2.114886	-0.381096
H	-6.509126	2.729161	-1.508446

TS3

Zn	0.448304	-1.161733	-1.042429
O	-1.117362	-2.012912	2.807313
H	-1.819919	-2.420171	2.260915
C	-1.415844	0.021808	2.578140
H	-2.336899	-0.136130	3.113826
H	-0.506023	0.175421	3.136078
H	-1.370782	-0.129717	1.512673
O	2.269836	-1.772170	-0.417132
S	2.225887	-2.721992	0.768712
O	3.148799	-3.838408	0.654651
O	0.815969	-3.010242	1.126094
C	2.498134	2.379438	-0.311785
C	2.913452	3.699691	-0.537430
C	3.421827	1.332867	-0.328670
C	4.264655	3.962935	-0.761999
C	4.764970	1.617544	-0.561350
H	3.096066	0.314534	-0.167887
C	5.194162	2.926194	-0.774360
H	4.583078	4.985072	-0.930637
O	0.761298	0.479745	0.217600
S	0.773892	1.958526	-0.054053
O	0.046730	2.288792	-1.309147
O	0.313953	2.717679	1.134047
C	2.858415	-1.673332	2.180253
O	-1.492960	-1.156398	-0.376784
S	-2.573959	-2.207454	-0.481971
O	-2.427572	-3.057754	-1.678549
O	-2.854841	-2.881793	0.789265
C	-4.075112	-1.156922	-0.812412
F	-4.401270	-0.492673	0.296468
F	-3.819358	-0.282767	-1.794094
F	-5.091448	-1.939126	-1.175866
F	3.084186	-2.456456	3.235259
F	3.989248	-1.058573	1.829588
F	1.945198	-0.748401	2.516617
H	-0.301500	-2.271685	2.330642
H	6.243139	3.133432	-0.951231
O	-1.769022	1.876812	2.411186
H	-0.978440	2.247298	1.906745
C	-2.960717	2.124805	1.725594
C	-2.969326	2.451367	0.370942
C	-4.146463	2.001627	2.444652
C	-4.196216	2.655994	-0.258998

H	-2.046255	2.551601	-0.187271
C	-5.360567	2.200274	1.791238
H	-4.109431	1.767835	3.503625
C	-5.407598	2.524305	0.429437
H	-4.206016	2.914120	-1.314179
H	-6.286592	2.104517	2.351064
C	-6.726520	2.689499	-0.283324
H	-7.506392	3.048143	0.394415
H	-6.646393	3.395949	-1.114360
H	-7.069174	1.733576	-0.698564
Cl	5.924417	0.310389	-0.588239
Cl	1.796821	5.036861	-0.556766
O	0.279489	0.046243	-2.682886
H	0.143094	0.964141	-2.330469
C	-0.711367	-0.244012	-3.686752
H	-0.512132	-1.250727	-4.050162
H	-1.718776	-0.197173	-3.263747
H	-0.614534	0.471809	-4.507090
O	0.166289	-2.868871	-2.223103
H	-0.792609	-3.090675	-2.166673
C	0.941125	-4.079449	-2.100167
H	1.991629	-3.795542	-2.108220
H	0.709338	-4.592636	-1.163601
H	0.726285	-4.731139	-2.951184

MeOH

C	-0.099263	0.547205	0.012089
H	0.273505	-0.480351	0.027582
H	0.257614	1.022179	-0.914643
H	-1.198801	0.507279	-0.022778
O	0.391584	1.181917	1.180080
H	0.069754	2.091425	1.179615

H₂O

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	0.760060
H	0.000000	0.000000	-0.760060

1o

C	-0.548877	-0.741244	-0.006671
C	0.842759	-0.750608	-0.016072
C	1.552901	0.456413	0.000073
C	0.846300	1.662640	0.026146
C	-0.547767	1.654611	0.032549

C	-1.271920	0.458288	0.014374
H	-1.083956	-1.687312	-0.015997
H	1.377079	-1.696038	-0.033065
H	1.377626	2.609755	0.046172
H	-1.080426	2.601766	0.054709
S	3.338284	0.377542	-0.000572
H	3.555612	1.703714	-0.043987
C	-2.780391	0.456446	-0.008275
H	-3.186457	1.391239	0.388573
H	-3.162368	0.340800	-1.030224
H	-3.187820	-0.368360	0.584565

2o

C	-0.544395	-0.730012	-0.065702
C	0.844232	-0.729216	-0.079090
C	1.554858	0.481579	-0.028928
C	0.839454	1.680489	0.034462
C	-0.557574	1.661781	0.047096
C	-1.275663	0.466015	-0.002278
H	-1.073641	-1.678905	-0.105299
H	1.385320	-1.670173	-0.128661
H	1.352206	2.634071	0.074402
H	-1.095221	2.605269	0.096724
S	3.332427	0.368365	-0.051476
C	-2.784020	0.449196	0.011637
H	-3.192689	1.462010	0.062328
H	-3.186769	-0.028884	-0.888711
H	-3.169612	-0.110038	0.871863
C	3.854794	2.106908	0.025461
H	3.517960	2.584760	0.948382
H	4.946375	2.088787	0.014133
H	3.500788	2.669148	-0.841804

1y

C	2.114196	0.980700	0.363453
C	0.867461	1.576271	0.214706
C	-0.228328	0.835044	-0.249024
C	-0.050341	-0.515055	-0.560600
C	1.199840	-1.115566	-0.411993
C	2.287502	-0.371463	0.050183
H	2.965234	1.549486	0.721707
H	0.746582	2.626859	0.461710
H	-0.883217	-1.111094	-0.921582
H	1.323053	-2.167784	-0.658337

O	3.535412	-0.903106	0.216630
H	3.517996	-1.834911	-0.036180
S	-1.800032	1.674404	-0.414002
H	-2.498986	0.615236	-0.857553

2y

C	1.682413	1.175248	0.000680
C	0.307472	1.363684	0.000471
C	-0.573145	0.268648	-0.000455
C	-0.037192	-1.021637	-0.001071
C	1.346630	-1.214444	-0.000700
C	2.211811	-0.120706	0.000129
H	2.362505	2.020162	0.001369
H	-0.091509	2.373923	0.001074
H	-0.681197	-1.892672	-0.001856
H	1.746995	-2.226026	-0.001094
O	3.573777	-0.246476	0.000557
H	3.802290	-1.184681	-0.000834
S	-2.317805	0.639452	-0.001062
C	-3.081383	-1.010601	0.001959
H	-2.813412	-1.576866	-0.893277
H	-2.811043	-1.574480	0.897988
H	-4.159603	-0.839929	0.003103

2y'

C	-0.547511	1.406345	-0.000156
C	0.831788	1.259587	-0.000217
C	1.412452	-0.018063	-0.000108
C	0.579573	-1.136978	-0.000050
C	-0.810965	-0.995804	-0.000289
C	-1.381777	0.279792	-0.000252
H	-1.005033	2.389787	-0.000220
H	1.462985	2.143094	-0.000431
H	1.004827	-2.136170	0.000206
H	-1.428100	-1.885764	-0.000426
O	-2.723417	0.532474	-0.000439
S	3.197201	-0.127454	0.000649
H	3.273393	-1.471338	-0.006350
C	-3.604233	-0.577388	0.000657
H	-3.468579	-1.200404	0.894425
H	-4.613484	-0.163487	0.001180
H	-3.469865	-1.201184	-0.892770

(3a + MeOH)₂

C	-1.317726	-2.288024	-0.924029
C	0.072924	-2.375023	-0.909980
C	0.798605	-1.828538	0.150170
C	0.125606	-1.245559	1.226149
C	-1.263576	-1.164114	1.211383
C	-1.986963	-1.651063	0.122327
H	-1.891564	-2.676865	-1.758549
H	0.606447	-2.840353	-1.732397
H	0.689558	-0.820241	2.048946
H	-1.780062	-0.666539	2.027370
O	-3.349986	-1.485362	0.016260
O	2.177094	-1.853167	0.085135
H	2.539078	-1.284010	0.814174
O	3.014413	0.040444	1.766130
H	2.706705	0.803405	1.223362
C	4.382673	0.239994	2.098408
H	4.515761	1.133338	2.720869
H	4.716741	-0.631585	2.666090
H	5.015869	0.338842	1.205752
C	-1.318489	2.287571	0.924310
C	0.072136	2.374958	0.910167
C	0.797899	1.828696	-0.150043
C	0.124988	1.245564	-1.225995
C	-1.264173	1.163769	-1.211151
C	-1.987622	1.650479	-0.122031
H	-1.892379	2.676233	1.758879
H	0.605586	2.840416	1.732559
H	0.689003	0.820409	-2.048830
H	-1.780580	0.666094	-2.027128
O	-3.350600	1.484425	-0.015895
O	2.176390	1.853716	-0.085081
H	2.538545	1.284731	-0.814162
O	3.014128	-0.039606	-1.766228
H	2.707001	-0.802719	-1.223342
C	4.382096	-0.238840	-2.099867
H	4.514763	-1.132121	-2.722511
H	4.715411	0.632840	-2.667835
H	5.016209	-0.337594	-1.207851
H	-3.632985	0.887024	-0.722460
H	-3.632468	-0.887918	0.722749

(4a + H₂O)₂

C	-1.261888	-2.363556	-0.919747
C	0.127944	-2.361492	-0.915301

C	0.822200	-1.797409	0.158545
C	0.116476	-1.252212	1.229678
C	-1.278924	-1.251576	1.224505
C	-1.974624	-1.801548	0.146014
H	-1.816826	-2.790616	-1.748442
H	0.685557	-2.784591	-1.744626
H	0.655129	-0.797998	2.053889
H	-1.803520	-0.791646	2.051729
O	-3.342623	-1.821069	0.033651
O	2.201885	-1.781727	0.107963
H	2.544218	-1.220174	0.851585
O	2.971903	0.082105	1.856012
H	2.729715	0.828045	1.255719
C	-4.092868	-1.316068	1.129045
H	-3.872397	-1.868188	2.051721
H	-3.903079	-0.248017	1.286778
H	-5.142261	-1.461879	0.867097
C	-1.262438	2.363388	0.919815
C	0.127392	2.361665	0.915387
C	0.821800	1.797683	-0.158416
C	0.116227	1.252236	-1.229519
C	-1.279173	1.251223	-1.224346
C	-1.975020	1.801101	-0.145904
H	-1.817494	2.790363	1.748475
H	0.684892	2.784961	1.744687
H	0.655001	0.798093	-2.053689
H	-1.803643	0.791082	-2.051532
O	-3.343023	1.820236	-0.033534
O	2.201486	1.782332	-0.107811
H	2.543955	1.220864	-0.851433
O	2.971922	-0.081289	-1.855886
H	2.729939	-0.827285	-1.255588
C	-4.093115	1.314828	-1.128844
H	-3.872789	1.866846	-2.051616
H	-3.903016	0.246802	-1.286382
H	-5.142552	1.460382	-0.866932
H	3.899336	0.211190	2.086229
H	3.899378	-0.210151	-2.086137

(4a + MeOH)₂

C	-13.473013	7.872430	-9.417071
C	-14.149846	7.019119	-8.553881
C	-14.915206	7.545375	-7.509578
C	-15.008846	8.926513	-7.347080

C	-14.327121	9.783860	-8.211724
C	-13.550452	9.259896	-9.247147
H	-12.869180	7.481336	-10.229175
H	-14.085326	5.942493	-8.674184
H	-15.589587	9.333554	-6.526501
H	-14.388290	10.851194	-8.044210
O	-12.820401	10.016157	-10.129647
O	-15.540309	6.664384	-6.650564
H	-15.920835	7.174316	-5.887042
O	-16.128471	8.040277	-4.450973
H	-15.189279	8.085891	-4.151817
C	-12.920862	11.428526	-10.016281
H	-13.957896	11.766039	-10.140400
H	-12.532202	11.781895	-9.054197
H	-12.312437	11.838600	-10.824196
C	-16.917101	7.498856	-3.399102
H	-16.908802	8.151793	-2.517623
H	-17.944584	7.418279	-3.761619
H	-16.575052	6.499343	-3.095838
C	-12.135987	10.818040	-5.513160
C	-12.824377	9.986400	-4.638012
C	-12.756508	8.599216	-4.794027
C	-11.985278	8.054256	-5.819195
C	-11.296088	8.888835	-6.700037
C	-11.373849	10.275451	-6.554623
H	-12.182436	11.897145	-5.410903
H	-13.425138	10.401321	-3.835087
H	-11.946676	6.978258	-5.949648
H	-10.731672	8.442618	-7.508331
O	-10.758859	11.179099	-7.384627
O	-13.485586	7.808871	-3.928710
H	-13.453896	6.868154	-4.247602
O	-13.713345	5.426151	-5.089278
H	-14.356551	5.745897	-5.765790
C	-9.935343	10.659121	-8.418630
H	-9.121456	10.046194	-8.010379
H	-10.517131	10.067377	-9.134796
H	-9.509477	11.525531	-8.927591
C	-14.271771	4.300984	-4.423220
H	-14.423785	3.463007	-5.114685
H	-13.566354	3.988859	-3.649524
H	-15.232585	4.536594	-3.944367

(4a' + H₂O)₂

C	-0.888211	0.610512	1.512312
C	-1.098605	-0.734648	1.266771
C	-1.944056	-1.128331	0.220354
C	-2.575343	-0.170136	-0.564318
C	-2.356307	1.192006	-0.314845
C	-1.510810	1.586459	0.720866
H	-0.221970	0.932162	2.304313
H	-0.599136	-1.498084	1.852910
H	-3.228279	-0.453191	-1.380610
H	-2.846905	1.922441	-0.945635
O	-1.222021	2.885626	1.039995
O	-2.075879	-2.496040	0.028694
H	-0.788391	-3.645067	1.311393
O	0.119061	-3.710314	1.639480
H	0.637270	-3.297133	0.932603
C	-1.726885	3.893591	0.179918
H	-1.348284	3.762806	-0.840497
H	-2.824385	3.904449	0.169691
H	-1.366998	4.842046	0.581723
C	0.877849	0.659929	-1.543364
C	1.100242	-0.689718	-1.335920
C	1.948979	-1.105361	-0.300716
C	2.571553	-0.164109	0.510991
C	2.340422	1.202529	0.300082
C	1.491595	1.618607	-0.724395
H	0.208885	0.997889	-2.326227
H	0.607684	-1.440571	-1.943745
H	3.226879	-0.464271	1.319212
H	2.824367	1.919158	0.951512
O	1.191295	2.923643	-1.006740
O	2.093227	-2.476722	-0.147861
H	0.814601	-3.600199	-1.463115
O	-0.093117	-3.663233	-1.790932
H	-0.612488	-3.271495	-1.072753
C	1.687618	3.911374	-0.118659
H	1.310197	3.748840	0.897616
H	2.784985	3.931274	-0.107966
H	1.319624	4.867610	-0.493790
C	3.108952	-2.938511	0.741170
H	4.085797	-2.529583	0.460484
H	2.877138	-2.671676	1.778192
H	3.117897	-4.024628	0.648500
C	-3.087254	-2.941847	-0.873381
H	-4.067837	-2.550073	-0.581500

H	-2.857834	-2.643598	-1.902339
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