Supplemental Information

Tandem Mass Spectrometry of Heparan Sulfate Negative Ions: Sulfate Loss Patterns and Chemical Modification Methods for Improvement of Product Ion Profiles

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Table S1. Comparison of average charge state and FPI for oligosaccharides before and after chemical modification.

Composition (native)	**Average charge state**	**FPI of most abundant charge state**	**Composition (after modification)**	**Average charge state**	**Average charge State with sulfolane**	**FPI of most abundant charge state**
[1,2,3,1,3]	2.38	0.667	[1,2,3,3,1]-2d_3	1.94	1.96	0.333
[1,2,3,1,4]	2.54	0.833	[1,2,3,3,2]-2d_3	2.04	2.39	0.500
[1,2,3,1,5]	2.82	1.000	[1,2,3,3,3]-2d_3	2.24	2.92	0.500
[1,3,4,1,4]	2.89	0.750	[1,3,4,4,1]-3d_3	2.00	2.00	0.375
[1,3,4,1,5]	3.07	0.875	[1,3,4,4,2]-3d_3	2.19	2.64	0.375
[1,3,4,1,6]	3.14	0.625	[1,3,4,4,3]-3d_3	2.29	2.93	0.500
[1,3,4,1,7]	3.27	0.875	[1,3,4,4,4]-3d_3	2.56	3.57	0.500
[1,3,4,1,8]	3.28	1.000	[1,3,4,4,5]-3d_3	3.25	4.12	0.625
[1,3,4,2,3]	2.45	0.625	[1,3,4,4,1]-2d_3	2.00	2.00	0.375
[1,3,4,2,4]	2.61	0.625	[1,3,4,4,2]-2d_3	2.17	2.65	0.375
[1,3,4,2,5]	2.84	0.750	[1,3,4,4,3]-2d_3	2.29	2.86	0.500
[1,3,4,2,6]	3.14	0.875	[1,3,4,4,4]-2d_3	2.63	3.57	0.500
[1,3,4,2,7]	3.48	1.000	[1,3,4,4,5]-2d_3	3.00	4.19	0.625

Figure S1. CID behavior of singly, doubly, and sodium-adducted precursor ions of D2S0.

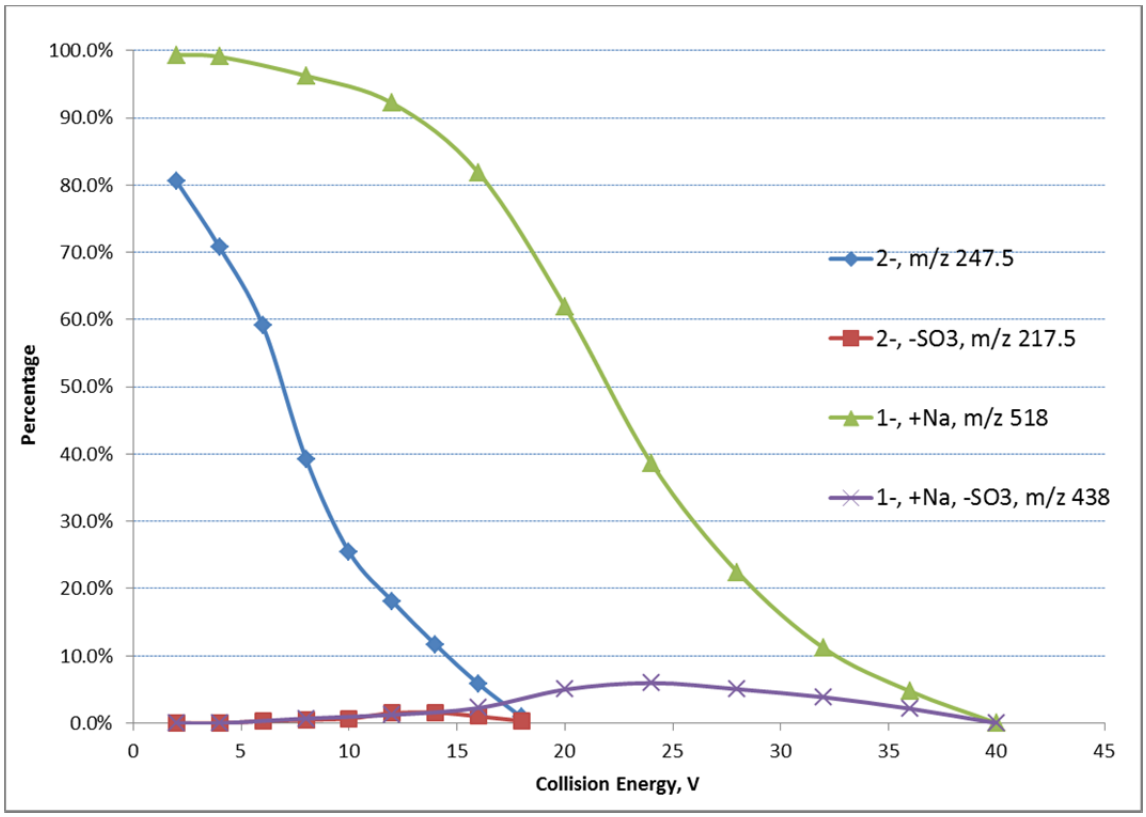


Figure S2. The energy of CH_3OSO_3H when the O-S bond is fixed at different lengths by ModRedundant calculation. The energy for the species that has the O-S bond length of 6 A and beyond was treated as the products are separated to infinite distance. The red curve is a fitting in Igor Pro.

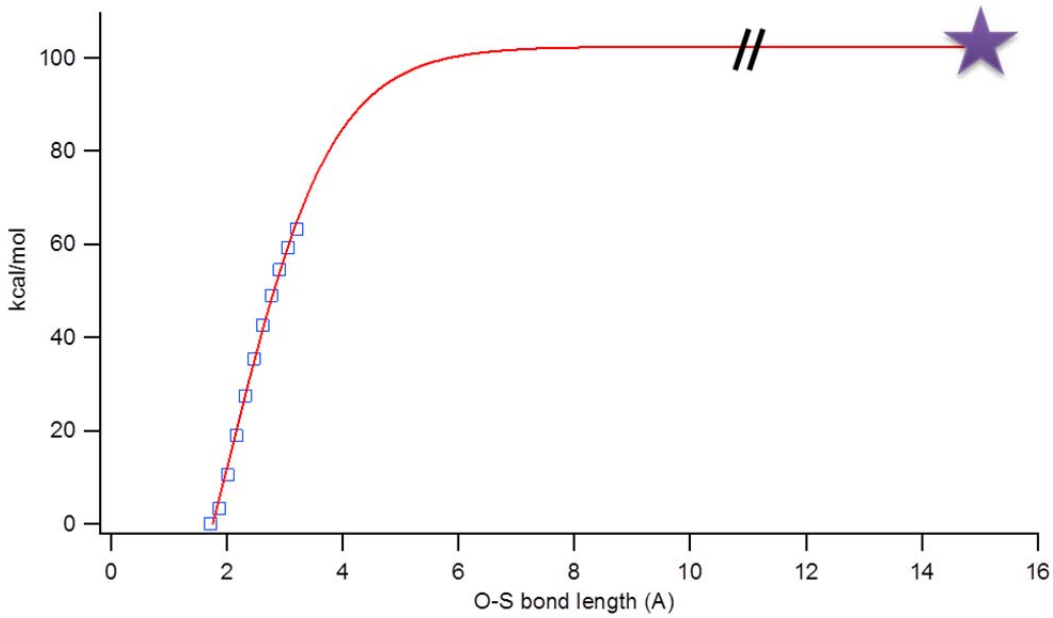


Figure S3. CID behaviors of singly charged precursor ions of D0S0 and D0A6.

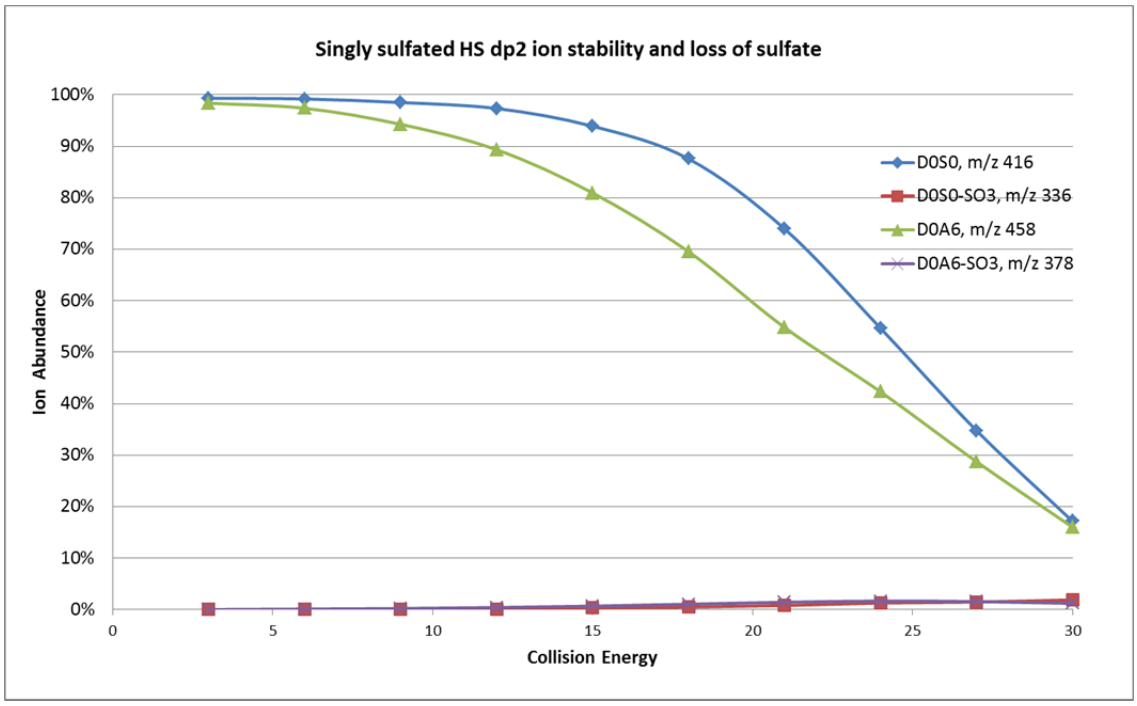
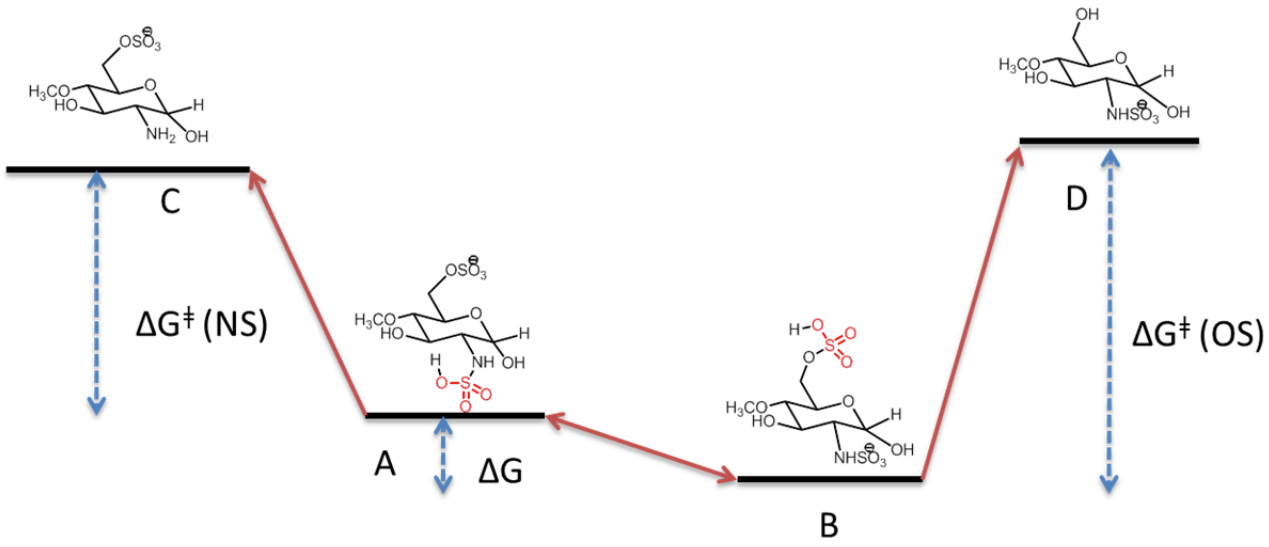
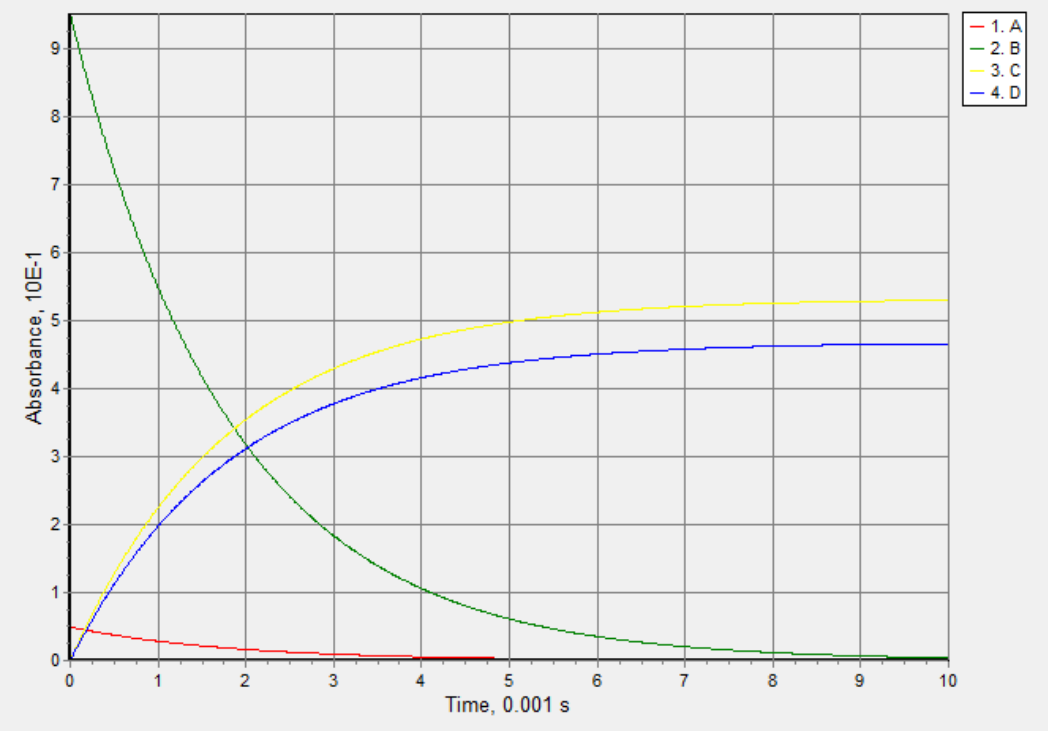


Figure S4. (A) Reaction schemes of E and F and equilibrium between them. (B) Simulated product distribution of N- and O-sulfate loss at 600 K. (C) Simulated product distribution of N- and O-sulfate loss at 1000 K.

(A)



(B)



(C)

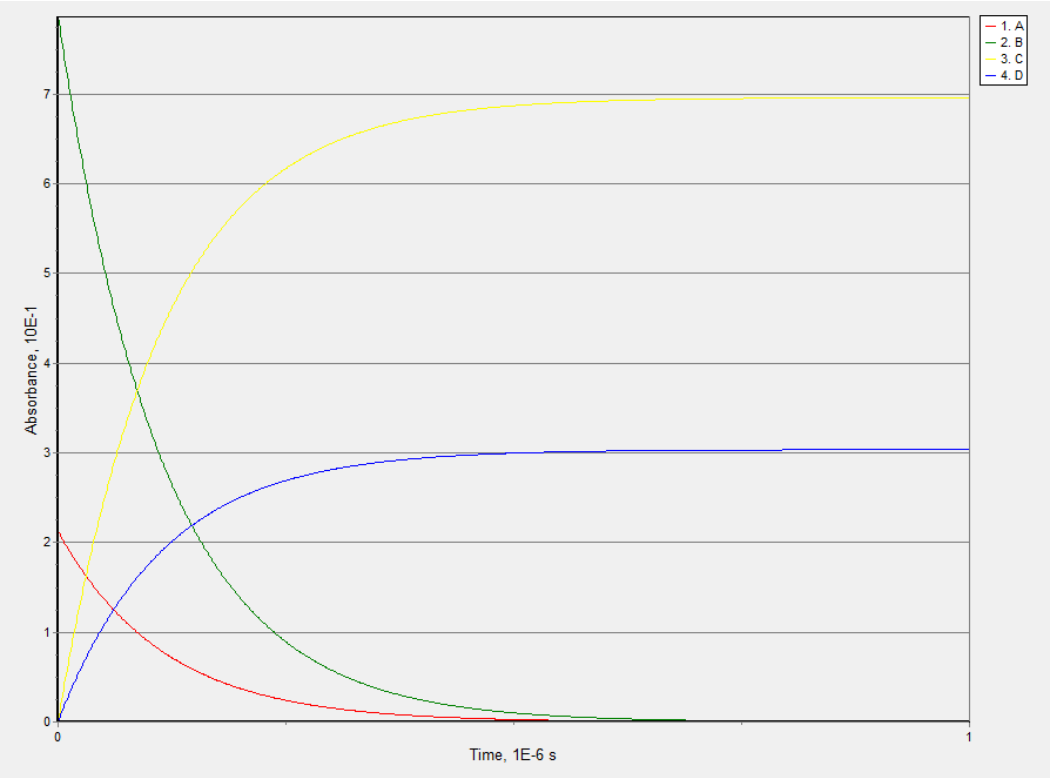
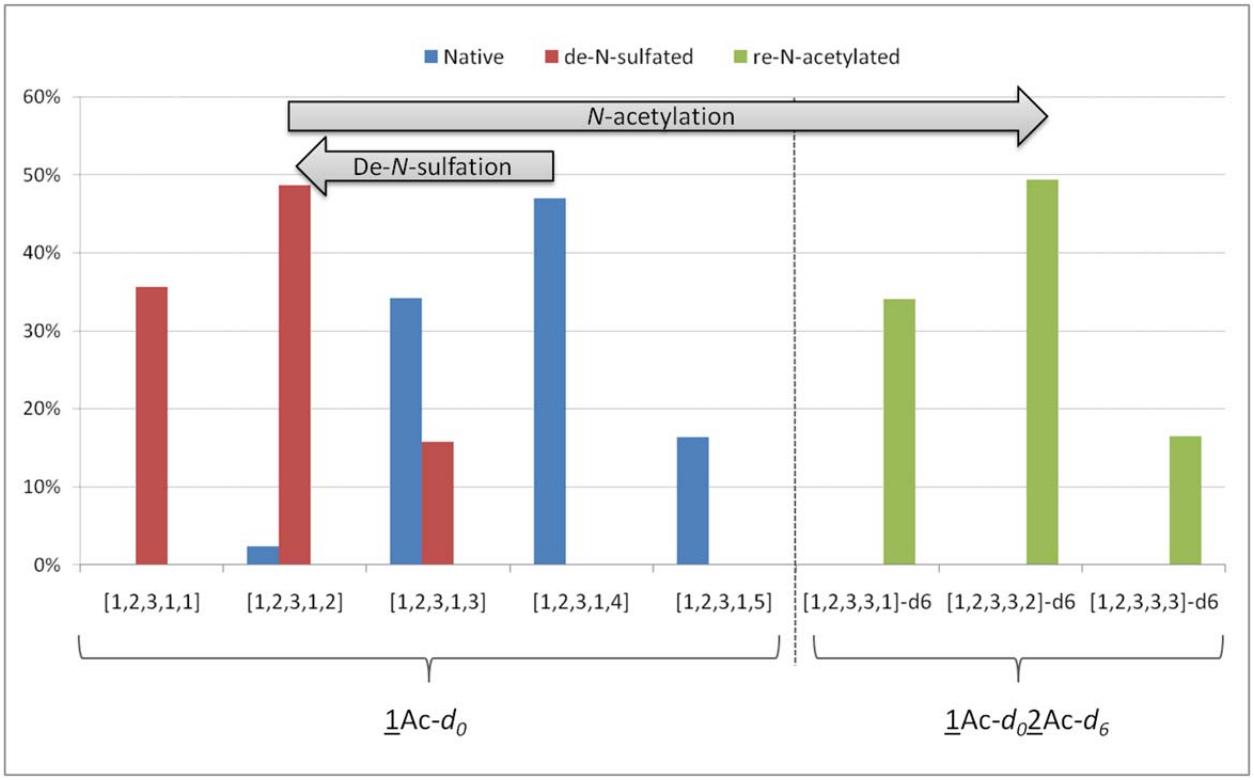


Figure S5. Product distribution of dp6 and dp8's before and after chemical modification.



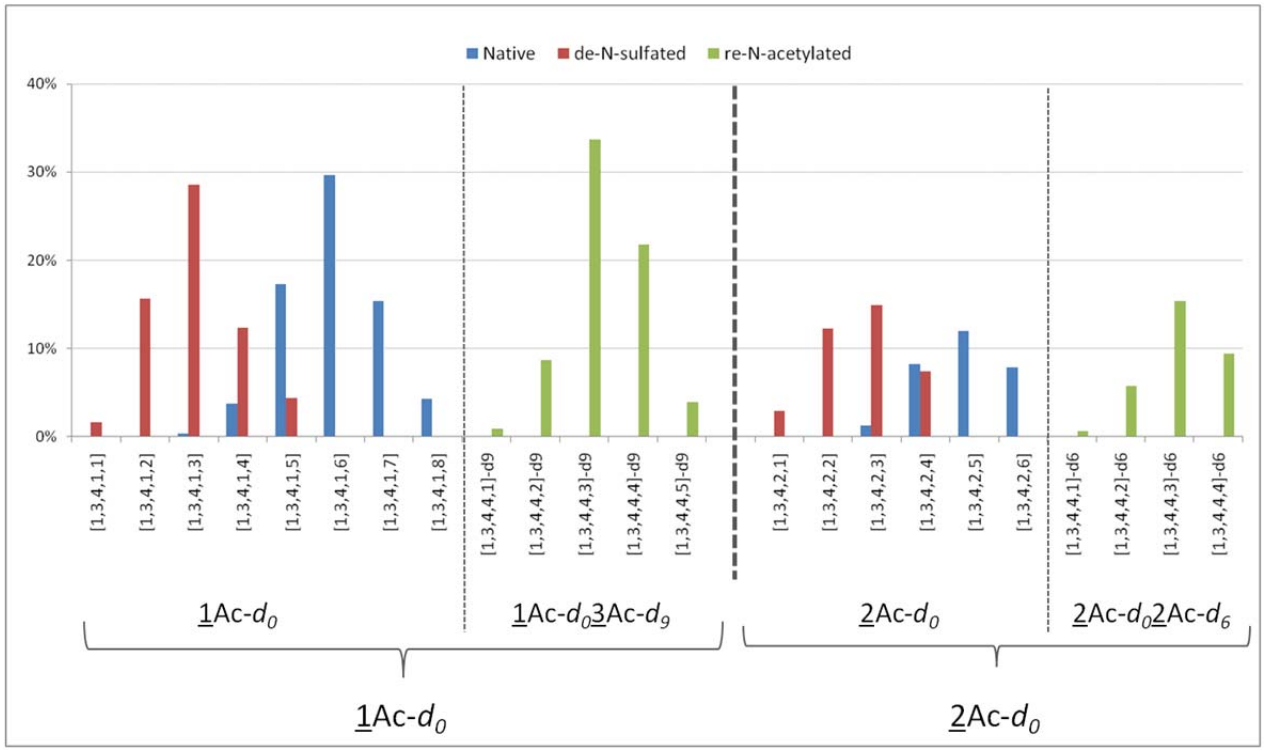


Figure S6(A). HILIC LC/MS profiles of species 2, 3 and 4 from the HS dp6 oligosaccharide, derivatization scheme shown in Figure 5.

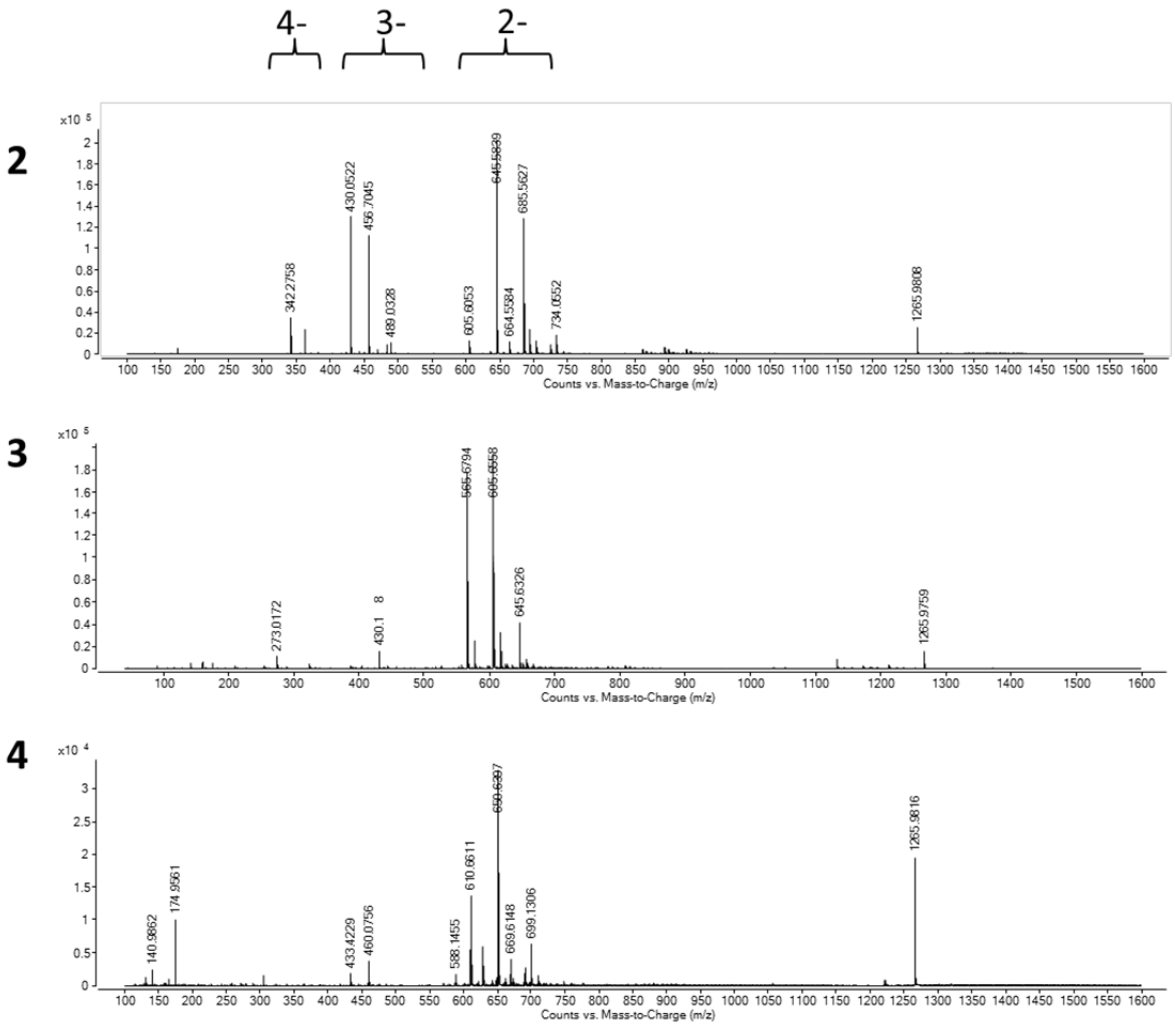


Figure S6(B). Extracted ion chromatograms (EIC)of products 2, 3, 4 of HS oligosaccharides. In 2, EICs are those of $[1,2,3,1,3]^{2-}$, $[1,2,3,1,4]^{2-}$, $[1,2,3,1,5]^{2-}$. In 3, EICs are those of $[1,2,3,1,1]^{2-}$, $[1,2,3,1,2]^{2-}$, $[1,2,3,1,3]^{2-}$. In 4, EICs are those of [1,2,3,3,1]-2d_3^{2-}, [1,2,3,1,2]-2d_3^{2-}, [1,2,3,1,3] -2d_3^{2-}. Please note there are multiple ionic species related to each molecular species including charge states and ammonium adducts. These EIC's are the most abundant ions and are representative.

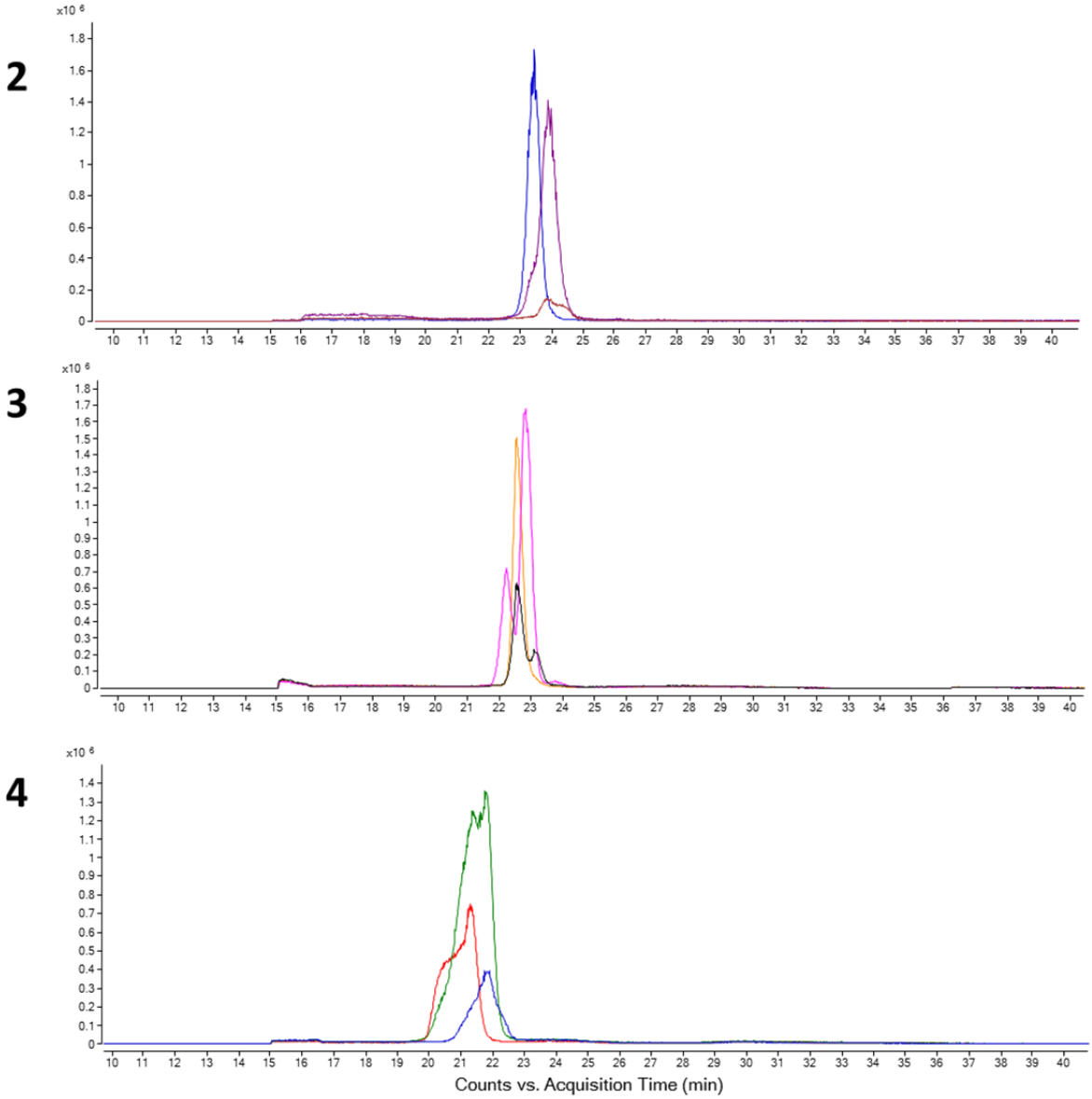


Figure S7. Charge state distribution of dp8's for chemical modification species 2, 3, 4 according to the scheme in Figure 5.

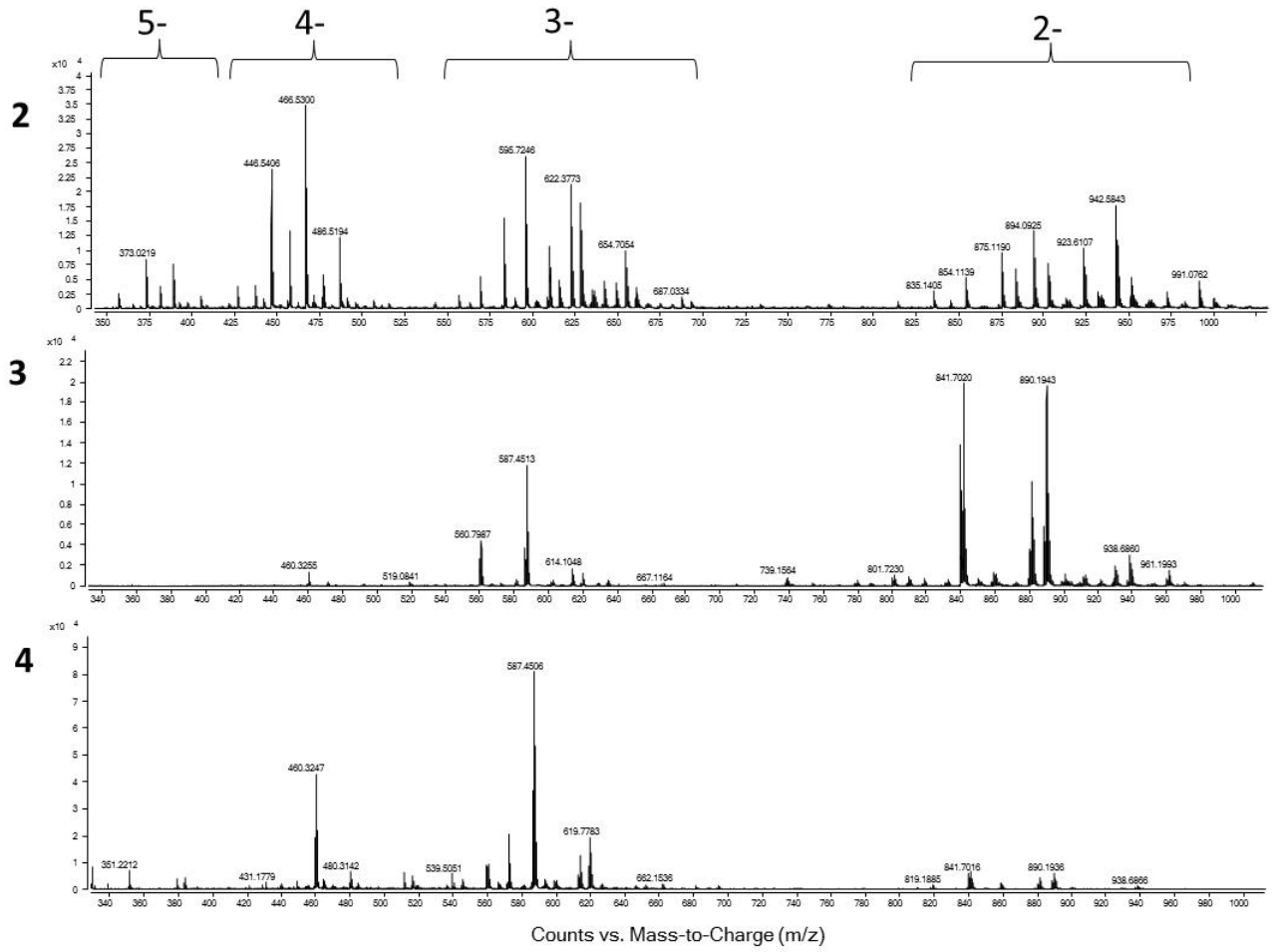
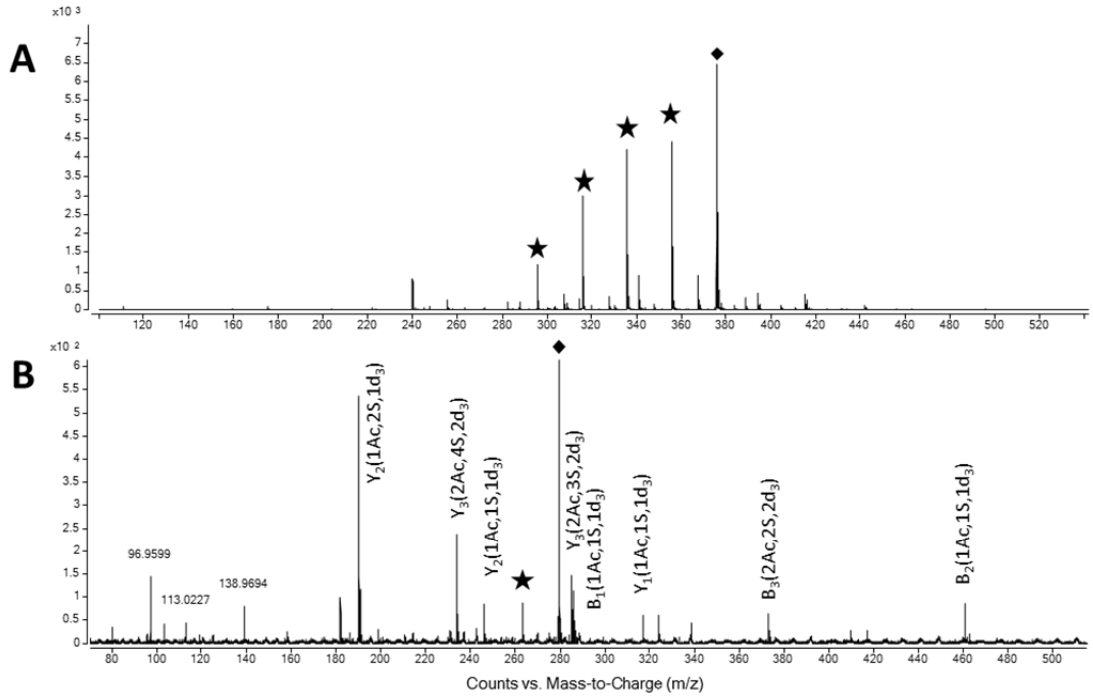


Figure S8. Tandem mass spectra of Arixtra before chemical modification (A) and after chemical modification (B). C demonstrates major backbone cleavages observed in B, the notations in bold denote fragments with no secondary sulfate loss.



C

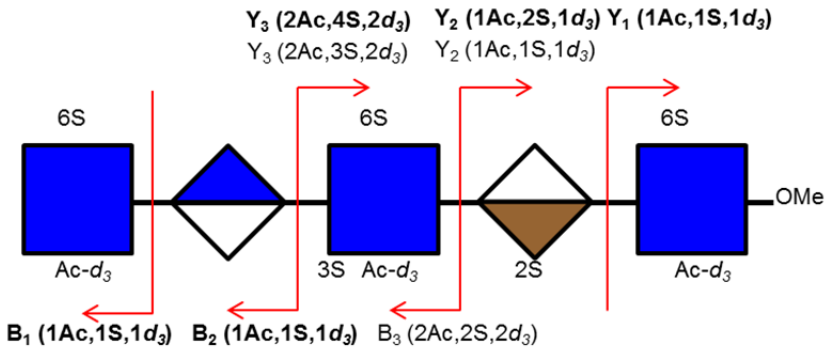
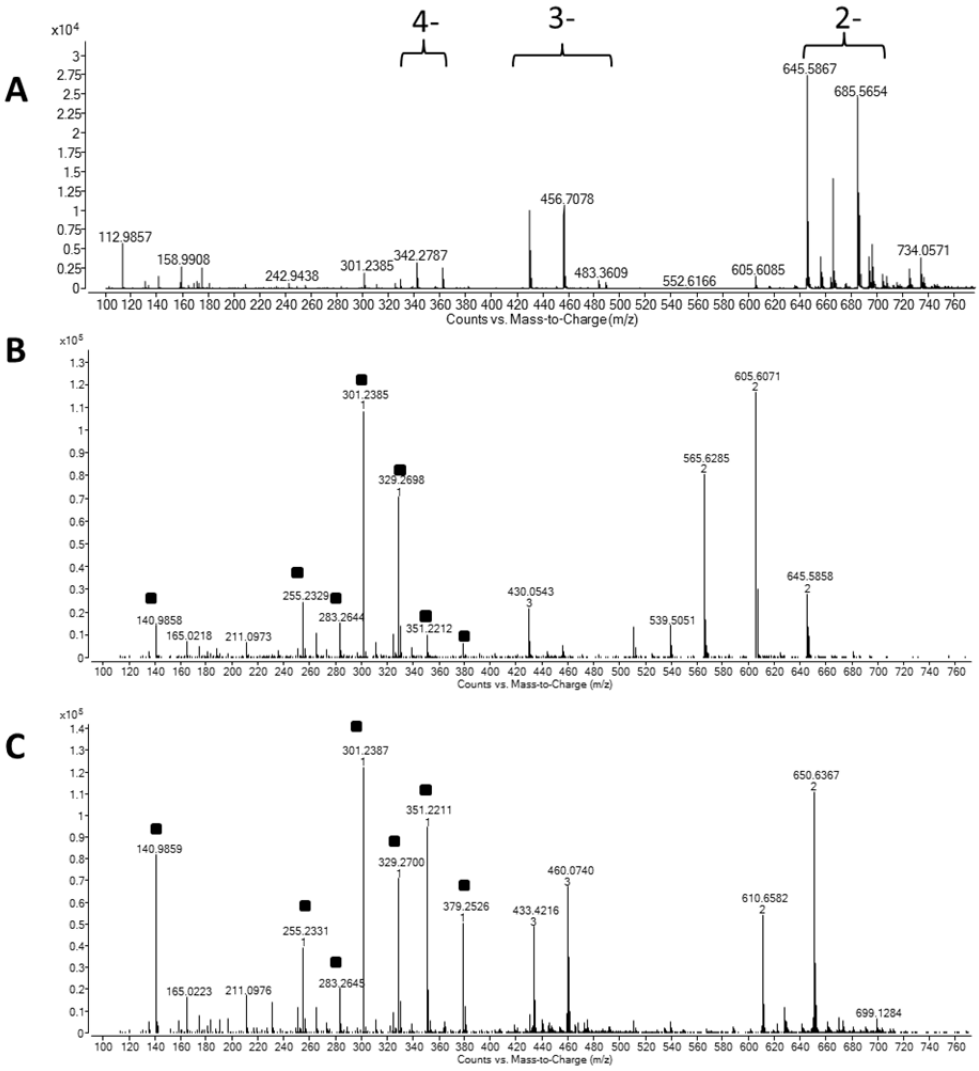
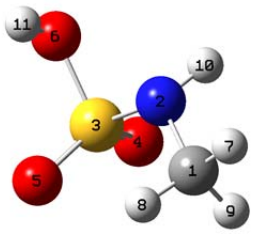


Figure S9. The charge distributions of (A) de-*N*-sulfated dp6 , (B) de-*N*-sulfated dp6 with sulfolane pulsing, and (C) de-*N*-sulfated and re-*N*-acetylated dp6 with sulfolane pulsing. The effect of charge state increase is more much pronounced in (C). Squares are background ions introduced by sulfolane pulsing.



Computational details, including coordinates, zero-point energies, thermal corrections, and frequencies.

CH3NHSO3H



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.244506	0.018826	-0.002428
2	7	0	0.981227	0.750213	-0.215312
3	16	0	-0.425127	-0.159869	-0.004199
4	8	0	-0.831399	-0.859639	-1.211477
5	8	0	-0.285688	-0.843675	1.273153
6	8	0	-1.491032	1.068409	0.131975
7	1	0	3.058706	0.742322	-0.091671
8	1	0	2.243654	-0.386561	1.009995
9	1	0	2.404153	-0.795714	-0.720270
10	1	0	0.936891	1.188758	-1.134974
11	1	0	-1.312051	1.523887	0.976661

SCF Done: E(RB+HF-LYP) = -719.783120040
Zero-point correction= 0.079732 (Hartree/Particle)
Thermal correction to Energy= 0.086674
Thermal correction to Enthalpy= 0.087618
Thermal correction to Gibbs Free Energy= 0.048693

Frequencies --	76.0841	167.3168	226.4834
Frequencies --	280.8891	358.3847	392.6806
Frequencies --	460.8321	494.3605	533.4588
Frequencies --	676.9081	804.0712	859.1654
Frequencies --	1060.2689	1147.2001	1159.7485
Frequencies --	1169.4230	1190.7027	1372.4449
Frequencies --	1454.2922	1476.1794	1522.5841
Frequencies --	1544.0390	3050.5391	3133.6128
Frequencies --	3181.5243	3508.3240	3696.9410

CH3NH2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705957	-0.000017	0.017641
2	7	0	0.752450	-0.000017	-0.126116
3	1	0	-1.115707	-0.880862	-0.488624
4	1	0	-1.085788	-0.001325	1.054627
5	1	0	-1.115331	0.882387	-0.486205
6	1	0	1.142662	0.812372	0.348575
7	1	0	1.142754	-0.812353	0.348590

SCF Done: E(RB+HF-LYP) = -95.8936373692

Zero-point correction= 0.064429 (Hartree/Particle)
 Thermal correction to Energy= 0.067811
 Thermal correction to Enthalpy= 0.068755
 Thermal correction to Gibbs Free Energy= 0.041535

Frequencies -- 332.0885 876.3208 987.7921
 Frequencies -- 1069.4850 1192.1576 1371.2456
 Frequencies -- 1484.8092 1528.1042 1546.8375
 Frequencies -- 1703.6716 2972.4273 3080.0606
 Frequencies -- 3119.8531 3466.4501 3549.9063

SO3

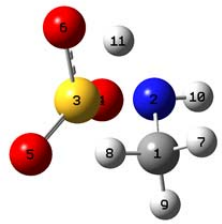
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000010	0.000000
2	8	0	-0.978321	-1.074830	0.000000
3	8	0	1.419962	-0.309904	0.000000
4	8	0	-0.441641	1.384714	0.000000

SCF Done: E(RB+HF-LYP) = -623.856339092

Zero-point correction= 0.011789 (Hartree/Particle)
 Thermal correction to Energy= 0.015384
 Thermal correction to Enthalpy= 0.016329
 Thermal correction to Gibbs Free Energy= -0.014686

Frequencies -- 455.0821 497.3102 498.2307
Frequencies -- 1022.3781 1350.6996 1350.9881

CH3NHSO3H loss of SO3 transition state



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.239807	0.215173	0.114914
2	7	0	1.064544	-0.646048	0.321743
3	16	0	-0.606664	0.107422	-0.008710
4	8	0	-1.432969	-0.092693	1.174292
5	8	0	-0.400683	1.444668	-0.547035
6	8	0	-0.702097	-1.023649	-1.073824
7	1	0	3.143177	-0.393576	0.210593
8	1	0	2.194073	0.638791	-0.888990
9	1	0	2.267358	1.030864	0.844214
10	1	0	1.051082	-1.076858	1.248602
11	1	0	0.446271	-1.313279	-0.644206

SCF Done: E(RB+HF-LYP) = -719.741805740

Zero-point correction= 0.075907 (Hartree/Particle)
 Thermal correction to Energy= 0.082332
 Thermal correction to Enthalpy= 0.083277
 Thermal correction to Gibbs Free Energy= 0.045311

Frequencies -- -1653.6221 106.6640 172.0125
 Frequencies -- 202.3221 289.5682 406.4738
 Frequencies -- 469.5911 509.2549 638.4670
 Frequencies -- 649.9993 880.8321 956.8046
 Frequencies -- 1061.1579 1104.0877 1163.4860
 Frequencies -- 1207.8001 1313.1552 1347.5647
 Frequencies -- 1425.8110 1477.2258 1518.9438
 Frequencies -- 1528.9354 1993.4130 3073.5462
 Frequencies -- 3146.0020 3182.3104 3493.8062

CH3NHSO3 anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.015904	0.688208	-0.000222
2	16	0	0.537781	-0.046694	0.000036
3	8	0	1.402994	1.160718	-0.000472
4	8	0	0.591470	-0.866894	1.238383
5	8	0	0.591287	-0.867869	-1.237671
6	6	0	-2.241375	-0.053885	-0.000094
7	1	0	-1.005765	1.695456	-0.000075
8	1	0	-1.989873	-1.118834	-0.000579
9	1	0	-2.867412	0.134025	0.892130
10	1	0	-2.867882	0.134677	-0.891844

SCF Done: E(RB+HF-LYP) = -719.268824222

Zero-point correction= 0.067895 (Hartree/Particle)
 Thermal correction to Energy= 0.074154
 Thermal correction to Enthalpy= 0.075098
 Thermal correction to Gibbs Free Energy= 0.037549

Frequencies -- 89.9617 216.7902 230.9182
 Frequencies -- 359.0570 391.7007 503.4149
 Frequencies -- 522.8191 564.6501 672.8558
 Frequencies -- 854.6617 999.2294 1067.6908
 Frequencies -- 1144.4050 1158.2249 1217.1329
 Frequencies -- 1247.0990 1417.4183 1455.7955
 Frequencies -- 1513.8924 1548.1013 2989.4563
 Frequencies -- 3043.2923 3121.9600 3471.9615

CH_3NH^- anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.856226	0.749327	-0.000459
2	6	0	-6.810792	-0.289495	0.000015
3	1	0	-6.416719	1.625176	0.000089
4	1	0	-6.294194	-1.279938	-0.000108
5	1	0	-7.549044	-0.402494	0.886171
6	1	0	-7.549425	-0.402476	-0.885807

SCF Done: E(RB+HF-LYP) = -95.2362797958

Zero-point correction= 0.046112 (Hartree/Particle)
Thermal correction to Energy= 0.049305
Thermal correction to Enthalpy= 0.050250
Thermal correction to Gibbs Free Energy= 0.023570

Frequencies -- 456.5459 1042.9312 1082.9411
Frequencies -- 1138.5268 1382.8227 1444.7973
Frequencies -- 1501.6566 1547.5048 2233.5357
Frequencies -- 2426.8364 2822.7789 3159.8992

$CH_3NHSO_3^-Na^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.162337	0.039820	-0.001410
2	7	0	0.991839	-0.742733	-0.391302
3	16	0	-0.526639	0.054399	0.011471
4	8	0	-0.423943	0.416120	1.454002
5	8	0	-0.552795	1.221499	-0.902531
6	8	0	-1.507237	-1.019706	-0.276929
7	1	0	3.076083	-0.493299	-0.301387
8	1	0	2.125460	0.989541	-0.543752
9	1	0	2.214791	0.266034	1.076158
10	1	0	0.964794	-1.615751	0.136690

SCF Done: E(RB+HF-LYP) = -719.268824222
Zero-point correction= 0.067895 (Hartree/Particle)
Thermal correction to Energy= 0.074154
Thermal correction to Enthalpy= 0.075098
Thermal correction to Gibbs Free Energy= 0.037549

Frequencies -- 456.5459 1042.9312 1082.9411
Frequencies -- 1138.5268 1382.8227 1444.7973
Frequencies -- 1501.6566 1547.5048 2233.5357
Frequencies -- 2426.8364 2822.7789 3159.8992

CH3NHNa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.570800	-0.274150	0.020592
2	7	0	0.349097	0.502481	-0.103624
3	1	0	2.425307	0.161788	-0.538143
4	1	0	1.944220	-0.433164	1.054679
5	1	0	1.422139	-1.279627	-0.403929
6	1	0	0.530320	1.416618	0.319244
7	11	0	-1.653678	-0.158008	0.015452

SCF Done: E(RB+HF-LYP) = -257.569681316

Zero-point correction= 0.051287 (Hartree/Particle)
 Thermal correction to Energy= 0.056091
 Thermal correction to Enthalpy= 0.057035
 Thermal correction to Gibbs Free Energy= 0.024408

Frequencies -- 126.5566 153.5348 410.7465
 Frequencies -- 469.9118 1053.5354 1077.7392
 Frequencies -- 1120.8450 1378.0848 1479.8795
 Frequencies -- 1507.5488 1544.1630 2875.5705
 Frequencies -- 2894.2727 3010.9615 3409.1083

CH3NHSO3Li

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.926475	-0.159709	0.000063
2	7	0	-0.449148	0.308094	-0.000304
3	1	0	1.513793	0.157256	-0.884152
4	1	0	1.513299	0.157425	0.884477
5	1	0	0.948068	-1.260481	0.000114
6	1	0	-0.427952	1.329489	0.000727
7	3	0	-1.987340	-0.527363	0.000194

SCF Done: E(RB+HF-LYP) = -102.814442491

Zero-point correction= 0.052803 (Hartree/Particle)
 Thermal correction to Energy= 0.057232
 Thermal correction to Enthalpy= 0.058176
 Thermal correction to Gibbs Free Energy= 0.027761

Frequencies -- 75.9665 142.9554 198.1931
 Frequencies -- 220.7764 375.9115 379.7170
 Frequencies -- 407.8821 516.4443 547.6077
 Frequencies -- 594.6857 634.4476 690.8219
 Frequencies -- 832.7698 982.3886 1056.7644
 Frequencies -- 1077.7671 1161.4481 1171.5984
 Frequencies -- 1280.1539 1431.4758 1471.2563
 Frequencies -- 1518.6620 1543.8594 3048.2748
 Frequencies -- 3125.7542 3158.5750 3494.3673

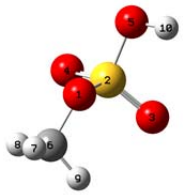
CH3NHLi

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.926475	-0.159709	0.000063
2	7	0	-0.449148	0.308094	-0.000304
3	1	0	1.513793	0.157256	-0.884152
4	1	0	1.513299	0.157425	0.884477
5	1	0	0.948068	-1.260481	0.000114
6	1	0	-0.427952	1.329489	0.000727
7	3	0	-1.987340	-0.527363	0.000194

SCF Done: E(RB+HF-LYP) = -102.814442491
Zero-point correction= 0.052803 (Hartree/Particle)
Thermal correction to Energy= 0.057232
Thermal correction to Enthalpy= 0.058176
Thermal correction to Gibbs Free Energy= 0.027761

Frequencies -- 182.8471 184.1900 478.9401
Frequencies -- 773.0027 1058.1169 1117.7051
Frequencies -- 1139.6853 1394.4074 1485.3242
Frequencies -- 1509.3910 1547.6084 2919.1961
Frequencies -- 2926.9959 3021.3152 3439.0377

CH3OSO3H



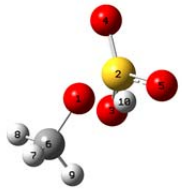
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.919551	-0.663540	-0.436476
2	16	0	-0.400654	0.140935	0.070868
3	8	0	-0.518901	-0.006038	1.514226
4	8	0	-0.466608	1.434282	-0.574107
5	8	0	-1.489075	-0.811460	-0.652577
6	6	0	2.177469	-0.076667	-0.016942
7	1	0	2.942787	-0.728561	-0.437568
8	1	0	2.274821	0.933773	-0.422414
9	1	0	2.244828	-0.065730	1.074323
10	1	0	-1.676537	-1.560399	-0.055095

SCF Done: E(RB+HF-LYP) = -739.649374080

Zero-point correction= 0.066874 (Hartree/Particle)
Thermal correction to Energy= 0.073805
Thermal correction to Enthalpy= 0.074749
Thermal correction to Gibbs Free Energy= 0.035477

Frequencies --	98.8836	163.2628	178.8839
Frequencies --	245.6891	361.3020	402.6203
Frequencies --	464.3004	508.1796	556.5350
Frequencies --	740.2636	809.0907	1031.8512
Frequencies --	1142.4569	1182.9868	1199.6958
Frequencies --	1205.9312	1399.8774	1485.1605
Frequencies --	1515.1616	1529.7647	3081.5867
Frequencies --	3169.0466	3193.9389	3706.2772

CH3OSO3H TS to lose SO3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.056464	-0.582282	0.452127
2	16	0	0.628376	0.096091	-0.031934
3	8	0	0.376791	1.348359	-0.724267
4	8	0	1.470771	0.050094	1.145176
5	8	0	0.615264	-1.174664	-0.905398
6	6	0	-2.210123	0.229575	0.150164
7	1	0	-3.085486	-0.386143	0.367118
8	1	0	-2.197200	1.101647	0.807091
9	1	0	-2.209207	0.547414	-0.895667
10	1	0	-0.552283	-1.309879	-0.409690

SCF Done: E(RB+HF-LYP) = -739.599141032

Zero-point correction= 0.062586 (Hartree/Particle)
 Thermal correction to Energy= 0.069045
 Thermal correction to Enthalpy= 0.069989
 Thermal correction to Gibbs Free Energy= 0.031814

Frequencies -- -1603.3488 98.5581 143.0414
 Frequencies -- 202.5839 278.2833 395.3636
 Frequencies -- 476.3110 502.4168 622.7171
 Frequencies -- 651.1720 962.0941 1039.5226
 Frequencies -- 1107.9760 1186.1849 1218.0329
 Frequencies -- 1254.0150 1379.2096 1487.0541
 Frequencies -- 1513.8603 1522.3002 2011.4837
 Frequencies -- 3077.4449 3167.2125 3175.4495

CH3OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.662031	-0.019516	0.000078
2	8	0	-0.748930	0.122482	-0.000099
3	1	0	1.079457	0.991134	-0.000112
4	1	0	1.036787	-0.543538	0.893374
5	1	0	1.036970	-0.543952	-0.892896
6	1	0	-1.133966	-0.766402	-0.000047

SCF Done: E(RB+HF-LYP) = -115.764786860

Zero-point correction= 0.051476 (Hartree/Particle)
 Thermal correction to Energy= 0.054767
 Thermal correction to Enthalpy= 0.055711
 Thermal correction to Gibbs Free Energy= 0.028756

Frequencies -- 346.1513 1067.9019 1097.5621
 Frequencies -- 1183.6041 1399.9051 1511.4787
 Frequencies -- 1524.9230 1541.8263 2996.3354
 Frequencies -- 3038.4909 3131.7942 3755.5354

CH3OSO3 anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.947434	0.834987	-0.000135
2	16	0	0.516533	-0.055029	0.000042
3	8	0	1.497113	1.044890	-0.000034
4	8	0	0.448974	-0.855917	1.245585
5	8	0	0.449097	-0.856200	-1.245327
6	6	0	-2.100167	0.016368	-0.000152
7	1	0	-2.969309	0.687302	-0.000200
8	1	0	-2.138081	-0.623586	-0.893039
9	1	0	-2.138142	-0.623532	0.892771

SCF Done: E(RB+HF-LYP) = -739.145860683

Zero-point correction= 0.055194 (Hartree/Particle)
 Thermal correction to Energy= 0.061391
 Thermal correction to Enthalpy= 0.062336
 Thermal correction to Gibbs Free Energy= 0.024786

Frequencies -- 86.0850 167.0440 250.7604
 Frequencies -- 372.5162 394.3641 503.4220
 Frequencies -- 543.4119 574.1570 676.6090
 Frequencies -- 1001.3284 1089.1989 1188.0329
 Frequencies -- 1201.4697 1233.8833 1265.8303
 Frequencies -- 1475.1882 1506.0856 1548.0606
 Frequencies -- 3006.6437 3066.1697 3077.2014

CH3O anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.788560	-0.000001	-0.000002
2	6	0	-0.520653	0.000003	-0.000003
3	1	0	-1.061524	1.028302	-0.054433
4	1	0	-1.061541	-0.561309	-0.863290
5	1	0	-1.061501	-0.467008	0.917757

SCF Done: E(RB+HF-LYP) = -115.144818297

Zero-point correction= 0.034705 (Hartree/Particle)
 Thermal correction to Energy= 0.037595
 Thermal correction to Enthalpy= 0.038539
 Thermal correction to Gibbs Free Energy= 0.012476

Frequencies -- 1232.3686 1232.4336 1270.3482
 Frequencies -- 1459.5982 1459.6732 1608.4680
 Frequencies -- 2251.2081 2251.4078 2468.2249

CH3OSO3Na

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.172087	-0.589424	0.728570
2	16	0	-0.071733	0.381735	-0.023733
3	8	0	0.534882	-0.468742	-1.114116
4	8	0	-0.768935	1.579276	-0.486655
5	8	0	0.948377	0.564272	1.060346
6	6	0	-2.365133	-0.853052	-0.029925
7	1	0	-2.989553	-1.470730	0.618278
8	1	0	-2.879961	0.080959	-0.271767
9	1	0	-2.126240	-1.399259	-0.948824
10	11	0	2.454216	-0.625771	-0.031234

SCF Done: E(RB+HF-LYP) = -901.436209959

Zero-point correction= 0.057054 (Hartree/Particle)
 Thermal correction to Energy= 0.064912
 Thermal correction to Enthalpy= 0.065856
 Thermal correction to Gibbs Free Energy= 0.023841

Frequencies -- 64.1708 84.9692 154.3309
 Frequencies -- 225.6321 266.4206 300.4160
 Frequencies -- 374.5533 443.7489 511.5138
 Frequencies -- 556.4783 604.3504 735.5879
 Frequencies -- 985.2514 1047.2707 1122.0645
 Frequencies -- 1184.1829 1202.7352 1285.1987
 Frequencies -- 1482.6409 1512.5309 1536.7339
 Frequencies -- 3059.4911 3138.2390 3165.3277

CH3ONa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.640293	-0.000392	0.000000
2	1	0	2.086125	1.020494	-0.000062
3	1	0	2.084527	-0.511612	-0.884469
4	1	0	2.084527	-0.511503	0.884531
5	8	0	0.270839	0.001033	0.000000
6	11	0	-1.660332	-0.000299	0.000000

SCF Done: E(RB+HF-LYP) = -277.474542374
Zero-point correction= 0.039626 (Hartree/Particle)
Thermal correction to Energy= 0.044316
Thermal correction to Enthalpy= 0.045260
Thermal correction to Gibbs Free Energy= 0.012596

Frequencies -- 77.0103 77.1287 485.1653
Frequencies -- 1197.7772 1197.9077 1217.3592
Frequencies -- 1521.3845 1521.5628 1536.2413
Frequencies -- 2853.7424 2853.7558 2854.8811

CH3OSO3Li

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.973026	-0.506739	-0.670882
2	16	0	-0.328499	0.215501	0.010024
3	8	0	-0.731433	-0.666612	1.177737
4	8	0	0.020233	1.589114	0.342076
5	8	0	-1.387121	-0.009646	-1.038632
6	6	0	2.214023	-0.348836	0.048260
7	1	0	2.964580	-0.842566	-0.570466
8	1	0	2.455058	0.710752	0.164911
9	1	0	2.154978	-0.835815	1.026821
10	3	0	-2.200134	-1.212104	0.148797

SCF Done: E(RB+HF-LYP) = -746.671457071

Zero-point correction= 0.058324 (Hartree/Particle)
 Thermal correction to Energy= 0.065618
 Thermal correction to Enthalpy= 0.066562
 Thermal correction to Gibbs Free Energy= 0.026609

Frequencies -- 73.9131 141.6825 157.6270
 Frequencies -- 245.8788 363.3850 395.1718
 Frequencies -- 417.9579 514.6190 566.4536
 Frequencies -- 601.6380 639.2273 749.3009
 Frequencies -- 981.9994 1038.0094 1098.1187
 Frequencies -- 1183.5443 1202.7292 1304.3204
 Frequencies -- 1484.7880 1513.7357 1533.4923
 Frequencies -- 3067.2611 3149.4305 3177.0109

CH3OLi

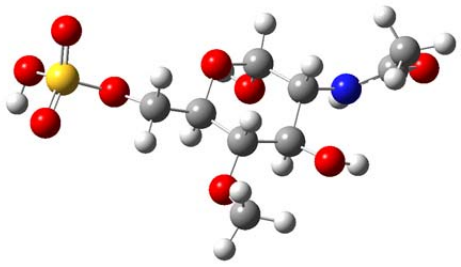
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.931525	0.000000	-0.000207
2	1	0	-1.358864	-0.000126	1.022761
3	1	0	-1.358281	-0.885732	-0.511399
4	1	0	-1.358281	0.885858	-0.511181
5	8	0	0.443495	0.000000	0.000194
6	3	0	2.038872	0.000000	-0.000164

SCF Done: E(RB+HF-LYP) = -122.723975661

Zero-point correction= 0.041536 (Hartree/Particle)
Thermal correction to Energy= 0.045722
Thermal correction to Enthalpy= 0.046666
Thermal correction to Gibbs Free Energy= 0.016942

Frequencies -- 167.0821 167.2318 841.0863
Frequencies -- 1205.4147 1205.4395 1281.5453
Frequencies -- 1526.0103 1526.4572 1529.5306
Frequencies -- 2912.8665 2933.1752 2936.4660

GlcNAc, 6-sulfate, 4-OCH3, alpha anomer



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.482344	1.342599	0.024441
2	6	0	-1.887215	0.952667	-0.450978
3	6	0	-2.300182	-0.426164	0.108607
4	6	0	-1.224188	-1.478753	-0.189719
5	8	0	0.033412	-1.046093	0.280527
6	6	0	0.495009	0.187387	-0.279843
7	6	0	1.865531	0.455856	0.306915
8	8	0	-1.240774	-1.708631	-1.582285
9	1	0	-1.422466	-2.403673	0.364844
10	8	0	-2.809325	1.946214	-0.016561
11	8	0	2.783956	-0.504112	-0.294668
12	16	0	4.296988	-0.456433	0.296747
13	8	0	4.938285	-1.520256	-0.741584
14	8	0	4.859373	0.862353	0.043834
15	8	0	4.339386	-1.067520	1.606902
16	7	0	-3.599222	-0.833203	-0.400467
17	8	0	-5.760641	-1.481813	-0.263771
18	6	0	-4.788785	-0.985029	0.285714
19	6	0	-4.830948	-0.487343	1.723464
20	8	0	0.024320	2.476387	-0.655484
21	6	0	-0.330194	3.740250	-0.101556
22	1	0	-0.514524	1.523222	1.112111
23	1	0	-1.863006	0.905162	-1.548981
24	1	0	-2.361802	-0.335390	1.195509
25	1	0	0.586225	0.096679	-1.369427
26	1	0	2.189612	1.467628	0.056857
27	1	0	1.852554	0.306623	1.391101
28	1	0	-0.624278	-2.434373	-1.772361
29	1	0	-3.663376	1.726218	-0.424422
30	1	0	-3.604239	-1.246654	-1.327326
31	1	0	-4.436476	0.529653	1.816873
32	1	0	-5.870127	-0.512943	2.053146
33	1	0	-4.240723	-1.136784	2.381650
34	1	0	0.219159	4.489026	-0.677744
35	1	0	-1.405341	3.926536	-0.175479

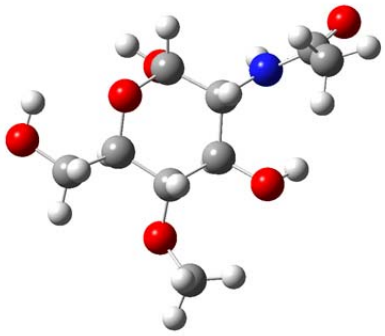
```
   36          1             0       -0.026073    3.808535    0.953897
   37          1             0        5.183577   -1.035147   -1.552468
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1483.42011519

Zero-point correction=                           0.291319 (Hartree/Particle)
 Thermal correction to Energy=                    0.313056
 Thermal correction to Enthalpy=                  0.314000
 Thermal correction to Gibbs Free Energy=         0.237910

Frequencies --    17.0689               23.8120               34.6244
 Frequencies --    43.3543               57.4580               71.2950
 Frequencies --    81.3786               89.7646              104.4703
 Frequencies --   141.5219              163.2568              171.0559
 Frequencies --   180.2990              193.0926              225.0328
 Frequencies --   243.4909              252.9742              257.1889
 Frequencies --   271.1744              307.0954              344.8071
 Frequencies --   355.6847              370.3085              384.6023
 Frequencies --   392.8330              405.8325              440.0502
 Frequencies --   443.3066              474.9553              485.5781
 Frequencies --   490.9858              511.8729              539.2524
 Frequencies --   557.8660              561.7360              612.8912
 Frequencies --   617.2624              634.6480              682.0869
 Frequencies --   782.2623              801.7805              841.6327
 Frequencies --   848.1382              873.4663              935.5026
 Frequencies --   981.8188              992.2323             1030.1476
 Frequencies --  1042.3232             1061.8496             1068.2519
 Frequencies --  1085.9191             1088.3974             1110.1610
 Frequencies --  1133.5476             1152.7079             1155.1250
 Frequencies --  1159.9014             1173.2561             1177.0383
 Frequencies --  1182.5608             1189.5506             1220.3980
 Frequencies --  1229.1545             1241.8386             1285.2538
 Frequencies --  1302.3709             1317.1500             1343.5971
 Frequencies --  1351.6361             1366.6447             1378.8677
 Frequencies --  1388.1765             1398.9963             1407.4955
 Frequencies --  1414.2486             1423.0648             1445.5796
 Frequencies --  1451.6422             1458.9918             1500.4351
 Frequencies --  1503.8512             1511.0639             1513.0075
 Frequencies --  1517.9533             1526.7791             1546.1283
 Frequencies --  1798.0504             2992.8416             3018.3424
 Frequencies --  3037.8436             3058.4099             3066.2336
 Frequencies --  3070.8701             3088.3182             3111.6748
 Frequencies --  3121.7965             3124.6501             3153.4545
 Frequencies --  3164.3614             3179.0799             3575.3650
 Frequencies --  3698.4334             3725.7230             3740.8910
```

GlcNAc, 4-OMe, alpha anomer



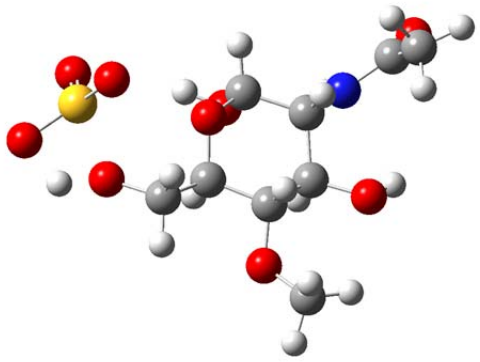
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.268076	0.876337	0.093294
2	6	0	-0.158448	0.852177	-0.468992
3	6	0	-0.968421	-0.316648	0.135616
4	6	0	-0.212701	-1.644172	-0.014223
5	8	0	1.085454	-1.534697	0.525517
6	6	0	1.912465	-0.509541	-0.066443
7	6	0	3.264487	-0.635692	0.628089
8	8	0	-0.215776	-1.968401	-1.388009
9	1	0	-0.696005	-2.432567	0.576429
10	8	0	-0.798314	2.087877	-0.163208
11	8	0	3.812732	-1.930641	0.457066
12	7	0	-2.297307	-0.399300	-0.448255
13	8	0	-4.558264	-0.406944	-0.449974
14	6	0	-3.520029	-0.155292	0.144224
15	6	0	-3.507090	0.452957	1.539497
16	8	0	2.110414	1.779082	-0.602093
17	6	0	2.087361	3.124734	-0.141045
18	1	0	1.220422	1.138513	1.163812
19	1	0	-0.085151	0.718526	-1.557466
20	1	0	-1.067088	-0.127273	1.207036
21	1	0	2.038172	-0.721112	-1.135037
22	1	0	3.963860	0.075722	0.184550
23	1	0	3.146027	-0.386263	1.696067
24	1	0	0.193592	-2.842279	-1.493569
25	1	0	-1.645983	2.085353	-0.637825
26	1	0	-2.359930	-0.866421	-1.346955
27	1	0	-2.840466	1.318989	1.602392
28	1	0	-4.527726	0.751813	1.780924
29	1	0	-3.173922	-0.280653	2.284014
30	1	0	2.856338	3.654834	-0.709244
31	1	0	1.112914	3.594363	-0.305816
32	1	0	2.334146	3.181325	0.930293
33	1	0	3.127780	-2.547145	0.763685

SCF Done: E(RB+HF-LYP) = -859.539234254
Zero-point correction= 0.277041 (Hartree/Particle)
Thermal correction to Energy= 0.294372

```
 Thermal correction to Enthalpy=                 0.295316
 Thermal correction to Gibbs Free Energy=        0.231890

Frequencies --    41.0633               52.9714               59.3583
 Frequencies --    79.1262               82.0837              113.6815
 Frequencies --   140.3248              160.5573              169.5519
 Frequencies --   191.0000              200.0307              228.7141
 Frequencies --   256.0545              269.5251              297.0480
 Frequencies --   315.7573              346.0031              357.2933
 Frequencies --   377.2972              391.3506              425.0599
 Frequencies --   438.9359              458.0425              486.3035
 Frequencies --   495.0328              551.9786              560.8148
 Frequencies --   613.3770              620.5478              632.5776
 Frequencies --   679.3592              786.3197              845.4937
 Frequencies --   854.4850              933.9142              984.1258
 Frequencies --  1011.8236             1034.7863             1052.6937
 Frequencies --  1067.2072             1069.9698             1087.8989
 Frequencies --  1089.9715             1109.7501             1133.0878
 Frequencies --  1138.7291             1149.2035             1157.9211
 Frequencies --  1172.4298             1189.1426             1215.7016
 Frequencies --  1228.1724             1234.5110             1254.2472
 Frequencies --  1299.6222             1315.6094             1342.2669
 Frequencies --  1353.4079             1359.4959             1382.2989
 Frequencies --  1388.0486             1405.8000             1411.3769
 Frequencies --  1414.7015             1425.5139             1448.1358
 Frequencies --  1455.3273             1457.8860             1500.3407
 Frequencies --  1503.3795             1511.0156             1512.8341
 Frequencies --  1520.1251             1533.4030             1546.3044
 Frequencies --  1796.7507             2987.8835             2994.5259
 Frequencies --  3014.5407             3039.8529             3058.4843
 Frequencies --  3059.9367             3073.9005             3105.5366
 Frequencies --  3122.8514             3125.8051             3145.4610
 Frequencies --  3147.4079             3178.8916             3576.9442
 Frequencies --  3726.9531             3729.9299             3741.8265
```

GlcNAc with 6-sulfate, 4-OCH3, alpha anomer, TS to lose 6-sulfate



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.531058	1.729177	0.104269
2	6	0	-1.812705	1.043600	-0.390834
3	6	0	-1.867109	-0.434918	0.064110
4	6	0	-0.573213	-1.182275	-0.290201
5	8	0	0.543357	-0.463412	0.196211
6	6	0	0.666727	0.863717	-0.321101
7	6	0	2.001549	1.382168	0.179795
8	8	0	-0.540667	-1.352638	-1.686720
9	1	0	-0.526376	-2.145994	0.229205
10	8	0	-2.940489	1.743839	0.121633
11	8	0	3.041431	0.606056	-0.458897
12	16	0	3.647205	-1.008618	0.284227
13	8	0	4.999464	-0.318217	0.023530
14	8	0	3.217150	-1.031892	1.670273
15	8	0	3.288425	-2.075509	-0.631383
16	7	0	-3.035328	-1.105431	-0.481857
17	8	0	-4.964060	-2.282677	-0.401279
18	6	0	-4.140491	-1.598280	0.186776
19	6	0	-4.287685	-1.227439	1.655501
20	8	0	-0.321572	3.003470	-0.477199
21	6	0	-0.987936	4.090777	0.158620
22	1	0	-0.566649	1.805229	1.203916
23	1	0	-1.804088	1.083997	-1.489730
24	1	0	-1.939392	-0.435296	1.154156
25	1	0	0.700791	0.836125	-1.417272
26	1	0	2.147507	2.417965	-0.130805
27	1	0	2.088737	1.290359	1.267347
28	1	0	0.241113	-1.889573	-1.900477
29	1	0	-3.723372	1.346226	-0.294805
30	1	0	-2.944757	-1.450408	-1.432203
31	1	0	-4.142808	-0.155686	1.824785
32	1	0	-5.288797	-1.520736	1.973371

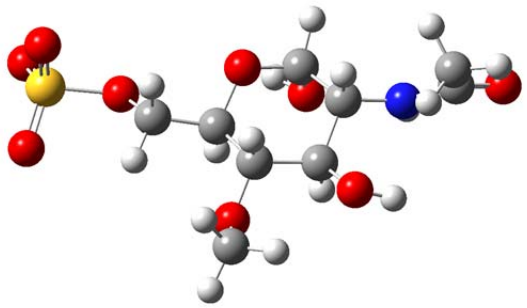
```
   33          1             0       -3.555905   -1.765501    2.270614
   34          1             0       -0.634228    4.997246   -0.339241
   35          1             0       -2.074276    4.011445    0.062421
   36          1             0       -0.726972    4.143581    1.226524
   37          1             0        4.248701    0.675615   -0.313404
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1483.37241243

Zero-point correction=                           0.287189 (Hartree/Particle)
 Thermal correction to Energy=                    0.308264
 Thermal correction to Enthalpy=                  0.309208
 Thermal correction to Gibbs Free Energy=         0.235063

Frequencies -- -1596.8083               18.8413               30.2712
 Frequencies --    40.1202               49.9244               59.5444
 Frequencies --    71.6955               81.7192               88.3797
 Frequencies --   131.5244              148.8304              159.2519
 Frequencies --   173.4294              193.9325              204.6141
 Frequencies --   229.2782              252.1729              269.0468
 Frequencies --   275.7552              297.3087              314.1237
 Frequencies --   348.0394              373.7659              393.2327
 Frequencies --   403.7125              416.0200              437.8040
 Frequencies --   455.1010              477.4166              482.9947
 Frequencies --   490.9937              501.8749              547.9494
 Frequencies --   560.5164              587.3956              610.9055
 Frequencies --   620.1247              631.2615              681.8274
 Frequencies --   714.2511              788.9504              847.0079
 Frequencies --   870.8114              933.2107              956.6078
 Frequencies --   984.6358             1012.1304             1035.8171
 Frequencies --  1048.2261             1058.3487             1068.7477
 Frequencies --  1069.4771             1088.6024             1107.8668
 Frequencies --  1113.2148             1136.2064             1153.8621
 Frequencies --  1156.7074             1162.1029             1174.8102
 Frequencies --  1189.9504             1221.7170             1224.3685
 Frequencies --  1229.8646             1245.6105             1286.7599
 Frequencies --  1300.9293             1318.1854             1342.5940
 Frequencies --  1349.9480             1361.1369             1373.1379
 Frequencies --  1379.7806             1387.8378             1406.7463
 Frequencies --  1412.4238             1425.3142             1444.2003
 Frequencies --  1454.0128             1460.5468             1499.8786
 Frequencies --  1502.3581             1508.7637             1511.3180
 Frequencies --  1512.3546             1519.7689             1545.8134
 Frequencies --  1798.8934             2022.3095             2996.6962
 Frequencies --  3017.9611             3033.1852             3059.3193
 Frequencies --  3067.1002             3080.8729             3090.9045
 Frequencies --  3112.5225             3123.0019             3126.1106
 Frequencies --  3153.5083             3168.1732             3179.4741
 Frequencies --  3573.3497             3723.8245             3726.7486
```

GlcNAc, 6-sulfate anion, 4-OMe, anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.433827	1.271470	-0.009759
2	6	0	-1.851186	0.895563	-0.454901
3	6	0	-2.298057	-0.447339	0.154166
4	6	0	-1.231663	-1.527264	-0.082436
5	8	0	0.018269	-1.097899	0.357506
6	6	0	0.530700	0.099075	-0.272478
7	6	0	1.929218	0.329376	0.274428
8	8	0	-1.262460	-1.844350	-1.466598
9	1	0	-1.455718	-2.420031	0.517876
10	8	0	-2.753527	1.936390	-0.065292
11	8	0	2.763880	-0.689790	-0.232530
12	16	0	4.423467	-0.488345	0.191840
13	8	0	5.004431	-1.666055	-0.472970
14	8	0	4.774543	0.825125	-0.394263
15	8	0	4.411278	-0.517755	1.671513
16	7	0	-3.596571	-0.867624	-0.359630
17	8	0	-5.812471	-1.325201	-0.284533
18	6	0	-4.818857	-0.859519	0.263928
19	6	0	-4.882624	-0.238234	1.653770
20	8	0	0.028357	2.391092	-0.751675
21	6	0	-0.099157	3.641203	-0.098320
22	1	0	-0.442250	1.497038	1.068364
23	1	0	-1.834511	0.805506	-1.549528
24	1	0	-2.374250	-0.314329	1.235892
25	1	0	0.601749	-0.059665	-1.354974
26	1	0	2.277942	1.317809	-0.051317
27	1	0	1.904119	0.307740	1.374217
28	1	0	-0.489507	-2.409287	-1.635903

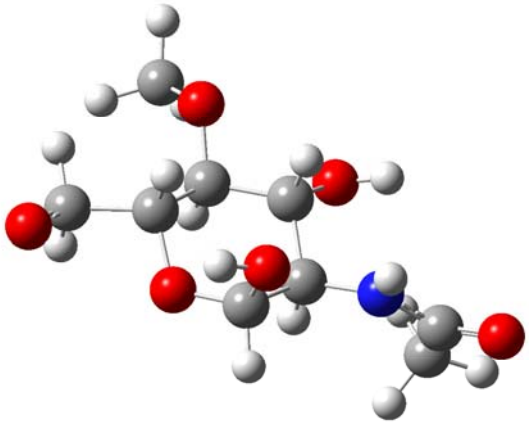
```
   29          1             0       -3.583219    1.770580   -0.540679
   30          1             0       -3.583860   -1.342779   -1.256025
   31          1             0       -4.408929    0.747896    1.679411
   32          1             0       -5.933704   -0.157793    1.934604
   33          1             0       -4.370303   -0.871928    2.388127
   34          1             0        0.340905    4.386184   -0.767894
   35          1             0       -1.148902    3.895882    0.093538
   36          1             0        0.455296    3.655620    0.852593
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1482.92278557

Zero-point correction=                           0.279417 (Hartree/Particle)
 Thermal correction to Energy=                    0.300583
 Thermal correction to Enthalpy=                  0.301527
 Thermal correction to Gibbs Free Energy=         0.226334

Frequencies --    12.9048               27.5629               30.9360
 Frequencies --    48.4859               61.5572               63.3271
 Frequencies --    82.6754               91.6780              119.9457
 Frequencies --   140.6752              167.9784              170.8444
 Frequencies --   179.1982              184.6291              233.1546
 Frequencies --   247.8710              254.6043              274.0891
 Frequencies --   300.2459              338.9990              356.9560
 Frequencies --   366.6289              369.1609              373.1666
 Frequencies --   410.7421              439.4714              452.2599
 Frequencies --   474.9811              497.7671              518.8385
 Frequencies --   540.7286              549.8142              561.8827
 Frequencies --   567.7935              610.2711              619.9325
 Frequencies --   634.6177              681.1170              718.5391
 Frequencies --   791.3697              849.1754              861.2939
 Frequencies --   931.1132              991.8020              999.5098
 Frequencies --  1019.5342             1036.3190             1061.5227
 Frequencies --  1069.0597             1073.2570             1093.0412
 Frequencies --  1105.9615             1116.0187             1132.0460
 Frequencies --  1154.1691             1155.4040             1160.6864
 Frequencies --  1170.4241             1189.5777             1220.1173
 Frequencies --  1230.2022             1235.7823             1241.5936
 Frequencies --  1272.2619             1276.1947             1296.5376
 Frequencies --  1315.6914             1338.8131             1362.1895
 Frequencies --  1364.0499             1374.7911             1389.2029
 Frequencies --  1405.9222             1412.3613             1426.3535
 Frequencies --  1432.7590             1450.1333             1456.6392
 Frequencies --  1498.8485             1501.7856             1511.2949
 Frequencies --  1515.5206             1520.5726             1538.8746
 Frequencies --  1544.1306             1782.5996             3004.6327
 Frequencies --  3012.7752             3019.4266             3037.5443
 Frequencies --  3045.3175             3058.6594             3069.0204
 Frequencies --  3078.7218             3079.5634             3120.3580
 Frequencies --  3126.3356             3129.1636             3173.8755
 Frequencies --  3578.7387             3726.9817             3736.3359
```

GlcNAc, 6-O anion, 4-OMe, anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.251977	0.843321	0.049860
2	6	0	-0.195529	0.816828	-0.444532
3	6	0	-1.004007	-0.316482	0.209919
4	6	0	-0.235219	-1.646221	0.152160
5	8	0	1.048501	-1.509086	0.639189
6	6	0	1.907342	-0.545875	-0.047864
7	6	0	3.340120	-0.737067	0.582701
8	8	0	-0.279965	-2.106523	-1.201767
9	1	0	-0.728153	-2.385358	0.803640
10	8	0	-0.818266	2.082267	-0.167046
11	8	0	3.848655	-1.918941	0.358582
12	7	0	-2.329826	-0.456682	-0.390887
13	8	0	-4.586859	-0.306793	-0.523888
14	6	0	-3.547643	-0.060973	0.086216
15	6	0	-3.557021	0.703151	1.405703
16	8	0	1.935451	1.790479	-0.776662
17	6	0	2.732001	2.718904	-0.076695
18	1	0	1.263149	1.175334	1.100599
19	1	0	-0.163619	0.651618	-1.530229
20	1	0	-1.122667	-0.072294	1.268574
21	1	0	1.983828	-0.830149	-1.105385
22	1	0	3.919056	0.167785	0.169357
23	1	0	3.165828	-0.426749	1.679017
24	1	0	0.492263	-2.692257	-1.286937
25	1	0	-1.611653	2.121241	-0.723981
26	1	0	-2.365893	-1.004883	-1.243850
27	1	0	-2.831909	1.522450	1.402082
28	1	0	-4.565812	1.089611	1.560318

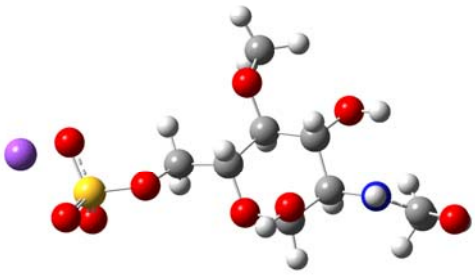
```
   29          1             0       -3.302118    0.039234    2.241014
   30          1             0        3.150619    3.402022   -0.825137
   31          1             0        2.135141    3.307948    0.639431
   32          1             0        3.558462    2.226482    0.455632
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -858.939391630

Range of M.O.s used for correlation:     1   272
 Zero-point correction=                           0.260343 (Hartree/Particle)
 Thermal correction to Energy=                    0.277552
 Thermal correction to Enthalpy=                  0.278496
 Thermal correction to Gibbs Free Energy=         0.214509

Frequencies --    18.6918               46.0088               58.7609
 Frequencies --    73.5167               86.9702              123.1714
 Frequencies --   138.8258              165.1238              176.2066
 Frequencies --   193.9091              199.2094              243.5954
 Frequencies --   250.8068              272.4267              286.4951
 Frequencies --   305.7264              324.9234              350.8221
 Frequencies --   364.9541              374.0327              412.4809
 Frequencies --   442.0259              483.6258              498.8757
 Frequencies --   555.0685              563.9219              583.9908
 Frequencies --   613.7282              628.5500              688.3853
 Frequencies --   777.8905              813.6888              849.1107
 Frequencies --   912.0686              944.7128              989.3174
 Frequencies --  1030.5675             1042.1424             1062.4779
 Frequencies --  1070.3536             1079.7042             1097.6026
 Frequencies --  1114.0013             1121.6957             1148.6038
 Frequencies --  1157.4715             1169.9414             1187.6934
 Frequencies --  1207.2518             1231.6963             1248.2461
 Frequencies --  1279.6013             1293.6321             1302.4346
 Frequencies --  1309.1550             1325.2391             1338.3963
 Frequencies --  1366.7744             1371.0718             1383.6972
 Frequencies --  1397.0117             1406.3034             1418.3458
 Frequencies --  1426.9328             1444.2976             1456.8242
 Frequencies --  1495.9713             1498.1663             1512.1805
 Frequencies --  1512.5975             1523.3222             1535.9087
 Frequencies --  1540.0230             1773.2194             2385.0429
 Frequencies --  2497.0913             2981.0585             2997.1787
 Frequencies --  3002.3645             3039.1483             3045.7425
 Frequencies --  3047.9473             3057.4264             3095.5315
 Frequencies --  3115.1595             3125.8399             3169.8735
 Frequencies --  3579.4942             3713.4479             3732.9568
```

GlcNAc 6-OSO3Na, 4-OMe, alpha aomer



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843824	1.330536	0.052248
2	6	0	-2.227129	0.933408	-0.476722
3	6	0	-2.669928	-0.432493	0.088628
4	6	0	-1.580744	-1.490502	-0.133238
5	8	0	-0.349590	-1.049281	0.382303
6	6	0	0.147315	0.172197	-0.183346
7	6	0	1.496468	0.440014	0.455733
8	8	0	-1.535809	-1.756704	-1.521299
9	1	0	-1.808460	-2.402744	0.431982
10	8	0	-3.167449	1.938617	-0.107331
11	8	0	2.425225	-0.524015	-0.082126
12	16	0	3.942940	-0.469624	0.561192
13	8	0	4.605661	-1.604807	-0.160913
14	8	0	4.538918	0.826762	0.068051
15	8	0	3.823656	-0.586198	2.012073
16	7	0	-3.942484	-0.851018	-0.478171
17	8	0	-6.115012	-1.477456	-0.445735
18	6	0	-5.168408	-0.974628	0.142939
19	6	0	-5.284551	-0.441149	1.563836
20	8	0	-0.319274	2.456084	-0.631756
21	6	0	-0.665224	3.722799	-0.084133
22	1	0	-0.920911	1.534764	1.132978
23	1	0	-2.153294	0.864225	-1.571322
24	1	0	-2.785818	-0.320620	1.169128
25	1	0	0.283479	0.053902	-1.265495
26	1	0	1.827158	1.451522	0.204534
27	1	0	1.434753	0.320863	1.542209
28	1	0	-0.873110	-2.452315	-1.663608
29	1	0	-3.998871	1.715331	-0.557593
30	1	0	-3.898305	-1.288057	-1.393011
31	1	0	-4.880366	0.572022	1.655625
32	1	0	-6.340894	-0.445330	1.834937
33	1	0	-4.741161	-1.082489	2.268615

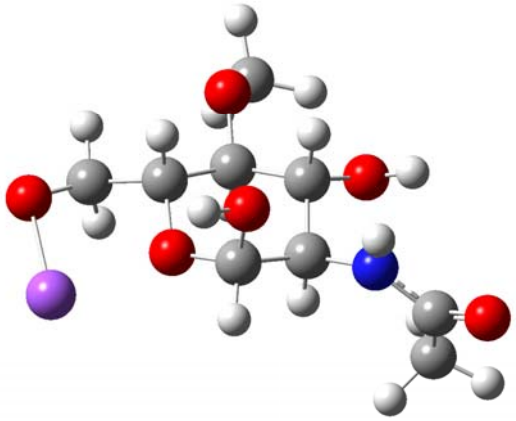
```
   34          1             0       -0.115830    4.467521   -0.666317
   35          1             0       -1.740175    3.914950   -0.154567
   36          1             0       -0.355691    3.797354    0.969543
   37         11             0        5.918492   -0.234083   -1.293756
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1645.20717800

Zero-point correction=                           0.281408 (Hartree/Particle)
 Thermal correction to Energy=                    0.304177
 Thermal correction to Enthalpy=                  0.305121
 Thermal correction to Gibbs Free Energy=         0.225732

Frequencies --    11.2634               19.4428               32.4956
 Frequencies --    40.5554               56.8681               57.9204
 Frequencies --    78.3103               80.7449              101.8027
 Frequencies --   107.1123              141.5196              165.6270
 Frequencies --   171.0354              179.2747              186.2668
 Frequencies --   232.3785              246.8415              254.5806
 Frequencies --   258.1180              270.6815              303.4572
 Frequencies --   308.2312              345.0377              356.6353
 Frequencies --   367.5867              392.8520              401.5216
 Frequencies --   423.7741              441.7077              458.9301
 Frequencies --   476.5044              496.3242              523.4181
 Frequencies --   549.4585              558.5334              563.0874
 Frequencies --   587.4666              615.6793              625.6638
 Frequencies --   643.1358              680.4598              778.1393
 Frequencies --   798.1809              848.3582              870.5638
 Frequencies --   933.8753              978.7478              987.0033
 Frequencies --  1013.0926             1034.3461             1053.9135
 Frequencies --  1062.7404             1068.2372             1085.9231
 Frequencies --  1092.0554             1111.2932             1123.3652
 Frequencies --  1134.7563             1153.9975             1156.0336
 Frequencies --  1159.6237             1173.1743             1189.2443
 Frequencies --  1220.4911             1229.3177             1242.1036
 Frequencies --  1275.9392             1293.9470             1302.3795
 Frequencies --  1317.3947             1341.5326             1354.4147
 Frequencies --  1368.2206             1377.5529             1388.5100
 Frequencies --  1407.9197             1413.6409             1423.1713
 Frequencies --  1443.5611             1451.6976             1459.3706
 Frequencies --  1499.6183             1502.1183             1510.0499
 Frequencies --  1513.0138             1518.0780             1532.2874
 Frequencies --  1546.6640             1795.0975             2997.7511
 Frequencies --  3015.6588             3037.7527             3058.6070
 Frequencies --  3063.4243             3065.2042             3080.5157
 Frequencies --  3105.2389             3121.9465             3125.2030
 Frequencies --  3140.8070             3146.3712             3178.2013
 Frequencies --  3576.0218             3726.6019             3737.4869
```

GlcNAc, 6-ONa, 4-OMe, alpha anomer



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.854174	1.258396	0.052499
2	6	0	-0.584863	1.032656	-0.423767
3	6	0	-1.122227	-0.331177	0.054101
4	6	0	-0.152454	-1.448689	-0.341232
5	8	0	1.140004	-1.194525	0.171504
6	6	0	1.773118	0.066067	-0.266465
7	6	0	3.158010	0.151313	0.433660
8	8	0	-0.184318	-1.538382	-1.747915
9	1	0	-0.458006	-2.401192	0.117727
10	8	0	-1.403252	2.082910	0.090520
11	8	0	3.959628	-0.932533	0.231266
12	7	0	-2.455967	-0.606157	-0.454190
13	8	0	-4.698128	-0.876071	-0.368756
14	6	0	-3.663717	-0.572608	0.209371
15	6	0	-3.642711	-0.137941	1.667878
16	8	0	1.423230	2.381240	-0.603225
17	6	0	1.328799	3.610732	0.101318
18	1	0	0.838548	1.415844	1.143480
19	1	0	-0.580338	1.055071	-1.521482
20	1	0	-1.161037	-0.312392	1.145862
21	1	0	1.920211	-0.002116	-1.349819
22	1	0	3.589928	1.100507	0.054000
23	1	0	2.925934	0.351453	1.515382
24	1	0	0.417515	-2.245938	-2.029028
25	1	0	-2.239027	2.060052	-0.402356
26	1	0	-2.517228	-0.922370	-1.416049
27	1	0	-3.110596	0.809555	1.798351
28	1	0	-4.676572	-0.033291	1.998669
29	1	0	-3.148396	-0.889190	2.296270

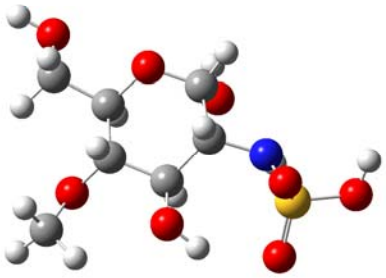
```
   30          1             0        1.850362    4.353889   -0.508125
   31          1             0        0.286997    3.918080    0.244273
   32          1             0        1.824659    3.547866    1.081758
   33         11             0        2.894796   -2.610576    0.718099
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1021.25485034

Zero-point correction=                           0.264095 (Hartree/Particle)
 Thermal correction to Energy=                    0.282995
 Thermal correction to Enthalpy=                  0.283939
 Thermal correction to Gibbs Free Energy=         0.216143

Frequencies --    35.3626               40.2706               53.5824
 Frequencies --    60.4894               71.1775               82.7570
 Frequencies --   124.2996              138.5765              160.6376
 Frequencies --   162.8664              170.4149              192.2096
 Frequencies --   196.1111              235.2143              256.2106
 Frequencies --   267.6140              285.0724              310.9016
 Frequencies --   319.8971              345.4277              377.3958
 Frequencies --   379.4030              421.3695              441.5132
 Frequencies --   468.1949              491.8403              496.9169
 Frequencies --   550.0866              558.8910              604.5390
 Frequencies --   618.9181              633.3220              663.0011
 Frequencies --   775.8291              816.1318              848.8971
 Frequencies --   936.3685              965.4817              993.4987
 Frequencies --  1029.0238             1046.4977             1057.9015
 Frequencies --  1069.7780             1079.1140             1103.4041
 Frequencies --  1113.8655             1129.2759             1144.6317
 Frequencies --  1156.7429             1167.7838             1179.3867
 Frequencies --  1187.7577             1211.5217             1227.0406
 Frequencies --  1228.9894             1282.2469             1296.0063
 Frequencies --  1308.8322             1340.7508             1348.6708
 Frequencies --  1354.6304             1375.0251             1384.9976
 Frequencies --  1403.9963             1404.5836             1418.8462
 Frequencies --  1424.3939             1447.5980             1451.6614
 Frequencies --  1499.3958             1503.4263             1511.0269
 Frequencies --  1514.4167             1520.9360             1529.9449
 Frequencies --  1544.0388             1794.1875             2726.4555
 Frequencies --  2906.8266             2997.4957             3012.3372
 Frequencies --  3016.0855             3052.2820             3057.9695
 Frequencies --  3084.9485             3094.9641             3121.8341
 Frequencies --  3125.4610             3139.9556             3179.5677
 Frequencies --  3582.0488             3739.1906             3743.7466
```

GlcNHSO3H, 4-OMe, alpha anomer



Standard orientation:

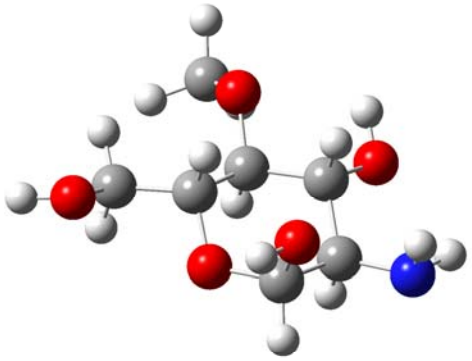
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.650047	0.863658	0.148590
2	6	0	0.182937	0.712194	-0.290430
3	6	0	-0.455603	-0.547798	0.341587
4	6	0	0.441669	-1.781082	0.161578
5	8	0	1.742833	-1.531370	0.613692
6	6	0	2.419099	-0.452951	-0.055874
7	8	0	-0.504537	1.887532	0.111454
8	8	0	0.391716	-2.119720	-1.213547
9	1	0	0.077180	-2.609164	0.780951
10	6	0	3.831109	-0.402480	0.498935
11	8	0	4.529526	-1.548255	0.026532
12	8	0	2.317102	1.851306	-0.619952
13	6	0	2.262100	3.176616	-0.104396
14	7	0	-1.782456	-0.906680	-0.201771
15	16	0	-3.103560	0.064635	0.136445
16	8	0	-4.272521	-0.921919	-0.428525
17	8	0	-3.198410	0.187593	1.581810
18	8	0	-3.194383	1.234709	-0.736035
19	1	0	1.663295	1.130410	1.218073
20	1	0	0.179250	0.608064	-1.385181
21	1	0	-0.581079	-0.372859	1.413511
22	1	0	2.478832	-0.663012	-1.130698
23	1	0	-1.329521	1.969126	-0.400322
24	1	0	0.961313	-2.895617	-1.343741
25	1	0	4.296780	0.529499	0.152076
26	1	0	3.780306	-0.384493	1.599227
27	1	0	5.428099	-1.514192	0.386752
28	1	0	2.884585	3.786497	-0.764880
29	1	0	1.239642	3.564124	-0.091785
30	1	0	2.674601	3.222903	0.915378
31	1	0	-1.739966	-1.118591	-1.199011
32	1	0	-4.357923	-1.668034	0.195555

```
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1330.71846378
Zero-point correction=                           0.253289 (Hartree/Particle)
 Thermal correction to Energy=                    0.271477
 Thermal correction to Enthalpy=                  0.272421
 Thermal correction to Gibbs Free Energy=         0.206980

Frequencies --    37.9452                48.9864                66.0169
 Frequencies --    72.4344                95.5281               108.1438
 Frequencies --   121.3913               150.0574               165.5489
 Frequencies --   191.4367               211.6998               213.4664
 Frequencies --   231.5167               255.7332               265.3778
 Frequencies --   310.3056               323.0254               338.1829
 Frequencies --   369.1302               378.3030               385.2558
 Frequencies --   407.8104               433.0025               448.8851
 Frequencies --   471.9110               479.5451               524.6643
 Frequencies --   542.1178               553.4537               597.2921
 Frequencies --   619.3122               629.7432               704.0570
 Frequencies --   785.0386               814.0682               862.2324
 Frequencies --   884.7169               935.5741               983.7116
 Frequencies --  1018.1372              1061.3011              1061.9765
 Frequencies --  1084.8327              1099.8714              1102.8159
 Frequencies --  1108.8885              1133.9889              1148.0523
 Frequencies --  1152.1196              1160.2189              1162.7874
 Frequencies --  1187.1525              1192.6630              1214.7352
 Frequencies --  1226.4860              1230.5881              1270.9153
 Frequencies --  1277.4129              1294.2736              1329.7667
 Frequencies --  1336.7114              1361.1130              1372.8846
 Frequencies --  1387.3790              1391.2555              1404.0508
 Frequencies --  1417.6492              1447.1769              1456.8410
 Frequencies --  1466.9691              1483.5346              1498.7632
 Frequencies --  1510.9643              1543.6764              1546.8180
 Frequencies --  2998.9202              3005.4146              3012.6053
 Frequencies --  3032.4309              3062.0848              3070.6732
 Frequencies --  3074.9638              3108.1847              3121.9990
 Frequencies --  3149.4603              3510.4696              3678.0198
 Frequencies --  3694.7198              3739.4346              3760.3224
```

GlcNH2, 4-OMe, alpha anomer



Standard orientation:

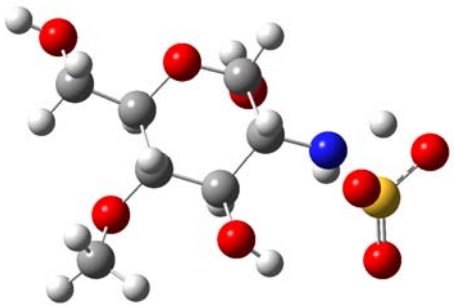
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470173	0.825487	-0.140609
2	6	0	1.007089	0.939712	0.245322
3	6	0	1.853833	-0.084318	-0.524493
4	6	0	1.249898	-1.481514	-0.341270
5	8	0	-0.127233	-1.506912	-0.665109
6	6	0	-0.947345	-0.616330	0.107117
7	8	0	1.511205	2.237284	-0.052205
8	8	0	1.485554	-1.872963	0.997253
9	1	0	1.712132	-2.186495	-1.041562
10	6	0	-2.388421	-0.873521	-0.293958
11	8	0	-2.760016	-2.156464	0.193218
12	8	0	-1.195166	1.776680	0.647340
13	6	0	-2.054120	2.634762	-0.086321
14	7	0	3.274889	-0.102566	-0.192227
15	1	0	-0.572545	1.064654	-1.209191
16	1	0	1.092254	0.737758	1.324569
17	1	0	1.765078	0.158541	-1.591582
18	1	0	-0.845138	-0.845841	1.175746
19	1	0	0.969144	2.853049	0.467526
20	1	0	1.131611	-2.771211	1.100338
21	1	0	-3.015984	-0.084406	0.146476
22	1	0	-2.471112	-0.816494	-1.390804
23	1	0	-3.653454	-2.347497	-0.128706
24	1	0	-2.500764	3.324051	0.635712
25	1	0	-1.501033	3.213047	-0.840602
26	1	0	-2.861009	2.084306	-0.591311
27	1	0	3.379568	-0.403873	0.775873
28	1	0	3.627704	0.851707	-0.245592

SCF Done: E(RB+HF-LYP) = -706.830273838
Zero-point correction=   0.238765 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.252911
 Thermal correction to Enthalpy=                0.253855
 Thermal correction to Gibbs Free Energy=       0.198735

Frequencies --    63.4147               76.4659              100.6662
 Frequencies --   117.2495              144.4539              168.9687
 Frequencies --   192.2864              216.8371              240.3341
 Frequencies --   256.9860              259.2395              286.8414
 Frequencies --   319.0264              342.3093              359.3106
 Frequencies --   383.9786              403.2799              417.3989
 Frequencies --   446.1732              462.6008              509.1895
 Frequencies --   570.6251              603.5597              634.3601
 Frequencies --   770.9028              855.6511              885.4925
 Frequencies --   930.0255              985.4352             1019.1606
 Frequencies --  1042.9389             1062.1863             1078.2867
 Frequencies --  1091.8780             1106.9635             1120.0612
 Frequencies --  1123.2245             1152.2732             1160.8880
 Frequencies --  1179.9908             1190.4082             1204.3052
 Frequencies --  1215.5741             1227.5807             1242.8087
 Frequencies --  1280.3741             1298.3063             1302.1010
 Frequencies --  1351.6078             1369.4427             1385.9908
 Frequencies --  1393.9773             1405.1627             1424.2648
 Frequencies --  1430.6096             1443.6951             1471.1066
 Frequencies --  1486.7132             1504.1364             1520.0156
 Frequencies --  1538.0886             1542.2573             1689.6336
 Frequencies --  3001.3198             3008.6048             3011.8056
 Frequencies --  3030.2904             3039.5781             3054.9677
 Frequencies --  3063.1156             3063.8300             3078.4598
 Frequencies --  3134.7755             3470.7805             3558.4911
 Frequencies --  3732.6674             3738.5413             3759.3344
```

GlcNHSO3H, 4-OMe, alpha anomer, TS to lose N-sulfate



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622315	0.877333	0.131318
2	6	0	0.186551	0.680992	-0.383363
3	6	0	-0.444506	-0.580772	0.246896
4	6	0	0.474731	-1.799642	0.080073
5	8	0	1.749712	-1.526180	0.589119
6	6	0	2.432289	-0.422936	-0.033596
7	8	0	-0.560190	1.845443	-0.061812
8	8	0	0.477455	-2.117680	-1.297542
9	1	0	0.106772	-2.643212	0.677590
10	6	0	3.809870	-0.341591	0.599264
11	8	0	4.560369	-1.464089	0.154479
12	8	0	2.298004	1.877155	-0.610053
13	6	0	2.199631	3.200732	-0.093598
14	7	0	-1.762872	-0.874661	-0.344411
15	16	0	-3.255115	0.081206	0.187733
16	8	0	-3.949455	-1.306679	0.103692
17	8	0	-3.028154	0.556150	1.542934
18	8	0	-3.599133	1.026905	-0.873886
19	1	0	1.574582	1.147827	1.198610
20	1	0	0.250406	0.544433	-1.472939
21	1	0	-0.600796	-0.406950	1.314918
22	1	0	2.557444	-0.622057	-1.104881
23	1	0	-1.330406	1.922885	-0.649368
24	1	0	1.071886	-2.875973	-1.422457
25	1	0	4.269757	0.605585	0.287147
26	1	0	3.697849	-0.336416	1.695050
27	1	0	5.434279	-1.418817	0.569972
28	1	0	2.828039	3.824613	-0.734617
29	1	0	1.169236	3.566688	-0.111954
30	1	0	2.580542	3.252934	0.937702
31	1	0	-1.708559	-0.841368	-1.367089

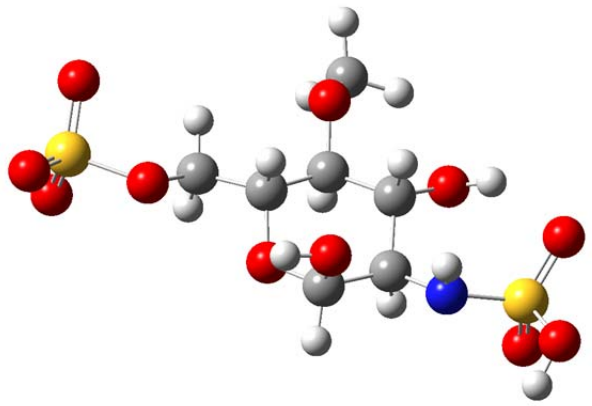
```
   32          1             0       -2.753240   -1.709716   -0.067951
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1330.67133745

Zero-point correction=                           0.249138 (Hartree/Particle)
 Thermal correction to Energy=                    0.267037
 Thermal correction to Enthalpy=                  0.267981
 Thermal correction to Gibbs Free Energy=         0.202733

Frequencies -- -1684.8604               38.8979               50.9342
 Frequencies --    63.0867               73.9874               75.8300
 Frequencies --    95.7319              128.0763              145.3714
 Frequencies --   164.8369              169.8888              205.5139
 Frequencies --   223.5120              243.0024              258.0533
 Frequencies --   265.5291              306.4465              315.4015
 Frequencies --   367.7181              374.1715              389.6911
 Frequencies --   414.3109              425.9616              437.6093
 Frequencies --   451.6477              471.4453              490.4629
 Frequencies --   514.1189              554.2029              611.1363
 Frequencies --   617.5251              649.3924              731.9905
 Frequencies --   789.2314              864.6467              908.0164
 Frequencies --   932.2042              953.0696              987.8614
 Frequencies --  1018.9500             1059.7154             1063.2355
 Frequencies --  1083.4409             1101.9265             1107.8853
 Frequencies --  1114.9699             1135.1779             1146.8470
 Frequencies --  1159.0065             1162.9465             1187.6140
 Frequencies --  1194.1386             1211.9103             1217.6777
 Frequencies --  1225.9001             1234.1319             1271.7522
 Frequencies --  1288.3608             1326.3376             1328.8146
 Frequencies --  1344.4121             1358.1574             1374.5636
 Frequencies --  1388.0093             1389.9730             1408.3449
 Frequencies --  1419.8774             1448.3537             1452.6805
 Frequencies --  1484.2075             1485.7033             1499.8092
 Frequencies --  1512.2034             1542.6092             1545.9534
 Frequencies --  1979.3780             3002.0894             3007.4413
 Frequencies --  3016.5453             3029.3829             3060.9497
 Frequencies --  3061.3480             3074.7916             3110.2574
 Frequencies --  3124.7306             3151.4805             3464.7850
 Frequencies --  3721.6996             3737.0034             3761.0276
```

GlcNHSO3H, 6-OSO3 anion, 4-OMe, alpha anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.086163	1.253517	0.115370
2	6	0	-1.350178	0.861605	-0.270263
3	6	0	-1.759508	-0.482618	0.370098
4	6	0	-0.667392	-1.550591	0.186987
5	8	0	0.575408	-1.076806	0.583120
6	6	0	1.053234	0.085811	-0.136302
7	8	0	-2.223058	1.906265	0.150754
8	8	0	-0.704769	-1.940444	-1.181456
9	1	0	-0.873112	-2.413119	0.834410
10	6	0	2.478576	0.340626	0.320837
11	8	0	3.273526	-0.720601	-0.164966
12	8	0	0.504413	2.353263	-0.679028
13	6	0	0.422528	3.619943	-0.048491
14	7	0	-3.012000	-1.060112	-0.171228
15	16	0	-4.477561	-0.327878	0.138239
16	8	0	-5.448469	-1.531219	-0.405009
17	8	0	-4.613748	-0.190228	1.579992
18	8	0	-4.793301	0.783932	-0.758819
19	1	0	0.106423	1.514092	1.184669
20	1	0	-1.368709	0.758893	-1.364566
21	1	0	-1.909072	-0.328393	1.441889
22	1	0	1.072598	-0.133086	-1.210147
23	1	0	-3.028089	1.883226	-0.394304
24	1	0	0.104872	-2.455017	-1.341238
25	1	0	2.814205	1.300723	-0.091395
26	1	0	2.516330	0.393275	1.419151
27	1	0	0.816751	4.346854	-0.764849

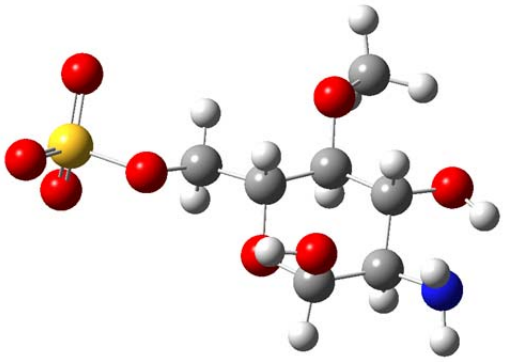
```
   28          1             0       -0.611627    3.879278    0.207686
   29          1             0        1.040586    3.655730    0.861573
   30          1             0       -2.921354   -1.278646   -1.164026
   31          1             0       -5.306361   -2.297768    0.182204
   32         16             0        4.966280   -0.466758    0.051463
   33          8             0        5.112317   -0.324631    1.517047
   34          8             0        5.489181   -1.712447   -0.533021
   35          8             0        5.232314    0.770311   -0.717001
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1954.10618642

Zero-point correction=                           0.256212 (Hartree/Particle)
 Thermal correction to Energy=                    0.278010
 Thermal correction to Enthalpy=                  0.278954
 Thermal correction to Gibbs Free Energy=         0.201927


Frequencies --     7.0774               26.1089               31.6093
 Frequencies --    52.1429               54.6742               69.2009
 Frequencies --    84.4672              110.5686              116.5655
 Frequencies --   130.8122              144.6856              165.7590
 Frequencies --   179.7668              205.1773              224.4273
 Frequencies --   235.3621              249.2620              283.8069
 Frequencies --   306.3363              328.2859              353.5207
 Frequencies --   366.3821              371.9406              374.6765
 Frequencies --   402.8133              426.1430              445.7096
 Frequencies --   449.3779              471.3005              473.0161
 Frequencies --   506.3831              525.4162              532.7907
 Frequencies --   540.0181              542.3385              567.0098
 Frequencies --   587.3523              619.4067              629.2446
 Frequencies --   705.6536              718.7139              783.6977
 Frequencies --   808.5594              857.7687              887.2773
 Frequencies --   929.3318              990.2686              999.7897
 Frequencies --  1024.6101             1060.5806             1071.6757
 Frequencies --  1088.9716             1094.0836             1106.6958
 Frequencies --  1116.5182             1130.3723             1148.4765
 Frequencies --  1159.5831             1160.6474             1169.3022
 Frequencies --  1188.4625             1201.3310             1224.4471
 Frequencies --  1229.3829             1235.5793             1241.6598
 Frequencies --  1271.2691             1273.0064             1279.4124
 Frequencies --  1324.2685             1332.2631             1356.5385
 Frequencies --  1365.9040             1377.3218             1386.4983
 Frequencies --  1403.2386             1412.4828             1432.9552
 Frequencies --  1448.4548             1454.3456             1462.2259
 Frequencies --  1499.6462             1514.8514             1537.6941
 Frequencies --  1544.5378             3009.4589             3016.6969
 Frequencies --  3021.3156             3036.4627             3049.8604
 Frequencies --  3071.3031             3081.9170             3084.2635
 Frequencies --  3123.5198             3130.6388             3507.1085
 Frequencies --  3698.2942             3706.3992             3725.4074
```

GlcNH2, 6-OSO3 anion, 4-OMe, alpha anomer



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.370227	1.003006	0.164469
2	6	0	-2.742873	0.410480	-0.172922
3	6	0	-2.957755	-0.945591	0.515676
4	6	0	-1.769795	-1.882958	0.267975
5	8	0	-0.561496	-1.262113	0.588315
6	6	0	-0.273704	-0.039772	-0.129578
7	6	0	1.121783	0.397630	0.283201
8	8	0	-1.832756	-2.308935	-1.087393
9	1	0	-1.820130	-2.755458	0.937997
10	7	0	-4.274551	-1.458916	0.102272
11	8	0	2.037378	-0.547429	-0.234054
12	8	0	-3.787350	1.295147	0.223596
13	16	0	3.685223	-0.120825	0.022051
14	8	0	3.801150	-0.032595	1.495246
15	8	0	4.352037	-1.272651	-0.608350
16	8	0	3.827264	1.172842	-0.684275
17	8	0	-1.094807	2.144691	-0.635566
18	6	0	-1.527234	3.378947	-0.092704
19	1	0	-1.343720	1.268663	1.233902
20	1	0	-2.767938	0.262194	-1.264673
21	1	0	-2.998545	-0.757078	1.595540
22	1	0	-0.266956	-0.243206	-1.207391
23	1	0	1.317457	1.395636	-0.127585
24	1	0	1.186042	0.446370	1.380294
25	1	0	-0.966156	-2.704366	-1.282810
26	1	0	-4.171137	-1.867191	-0.827476
27	1	0	-4.561040	-2.220474	0.715921
28	1	0	-4.585863	0.734362	0.183795
29	1	0	-1.164933	4.158137	-0.770434
30	1	0	-2.619599	3.433416	-0.016904
31	1	0	-1.091724	3.552493	0.904245

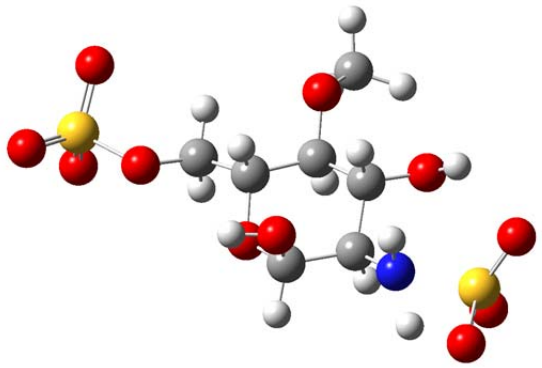
```
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1330.21579430

Zero-point correction=                           0.241997 (Hartree/Particle)
 Thermal correction to Energy=                    0.259576
 Thermal correction to Enthalpy=                  0.260520
 Thermal correction to Gibbs Free Energy=         0.194299

Frequencies --    14.3766               34.1452               37.4234
 Frequencies --    63.0430               88.7963               98.2128
 Frequencies --   123.9139              151.8480              168.7938
 Frequencies --   183.1243              232.7465              237.1363
 Frequencies --   250.7605              282.7220              307.9188
 Frequencies --   328.6557              363.0579              368.8753
 Frequencies --   374.6283              393.7026              428.4670
 Frequencies --   443.4080              450.2598              495.3522
 Frequencies --   522.8568              541.4615              559.5812
 Frequencies --   567.3188              571.0629              617.5633
 Frequencies --   636.8671              719.6654              779.3246
 Frequencies --   857.1058              890.4803              955.5813
 Frequencies --   985.2011              999.3820             1025.6760
 Frequencies --  1026.8298             1075.9868             1084.2296
 Frequencies --  1102.1348             1113.1857             1120.2085
 Frequencies --  1141.5706             1157.2806             1162.3295
 Frequencies --  1172.1208             1191.7254             1205.4809
 Frequencies --  1224.0782             1232.2296             1236.2932
 Frequencies --  1258.8076             1269.9857             1283.7108
 Frequencies --  1328.0666             1349.8787             1363.6591
 Frequencies --  1369.8763             1392.6181             1395.4829
 Frequencies --  1413.6209             1420.5019             1432.8602
 Frequencies --  1458.3194             1472.5278             1501.6529
 Frequencies --  1513.3160             1540.1135             1546.2199
 Frequencies --  1696.1120             2994.0784             3001.7955
 Frequencies --  3004.9640             3008.0164             3022.2280
 Frequencies --  3064.9429             3069.2942             3082.4120
 Frequencies --  3085.4762             3126.6169             3458.9877
 Frequencies --  3542.7211             3635.8856             3723.6526
```

GlcNHSO3H, 6-OSO3 anion, 4-OMe, alpha anomer, TS to lose N-sulfate



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.083129	1.217876	0.085284
2	6	0	-1.335048	0.821574	-0.354774
3	6	0	-1.758761	-0.517478	0.282690
4	6	0	-0.669783	-1.589479	0.095876
5	8	0	0.562353	-1.125089	0.532850
6	6	0	1.061793	0.053839	-0.146724
7	8	0	-2.233874	1.865498	0.008755
8	8	0	-0.685841	-1.945016	-1.279296
9	1	0	-0.889293	-2.465626	0.721451
10	6	0	2.467116	0.307638	0.368992
11	8	0	3.286145	-0.740862	-0.100220
12	8	0	0.517542	2.324110	-0.688297
13	6	0	0.446261	3.581593	-0.036476
14	7	0	-3.024763	-1.013732	-0.296843
15	16	0	-4.641356	-0.295294	0.194775
16	8	0	-5.118645	-1.779048	0.136980
17	8	0	-4.530753	0.235743	1.544452
18	8	0	-5.134288	0.558244	-0.888006
19	1	0	0.065314	1.469504	1.156481
20	1	0	-1.303357	0.702827	-1.447511
21	1	0	-1.925960	-0.370579	1.352804
22	1	0	1.124064	-0.145574	-1.222593
23	1	0	-2.981391	1.881116	-0.610002
24	1	0	0.124388	-2.458915	-1.439813
25	1	0	2.810899	1.275105	-0.018901
26	1	0	2.461097	0.347765	1.468740
27	1	0	0.843629	4.316808	-0.742067
28	1	0	-0.585958	3.844082	0.225345
29	1	0	1.066473	3.597774	0.872135

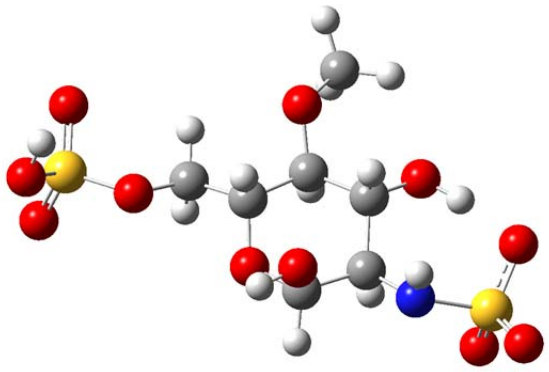
```
   30          1             0       -2.964964   -0.993292   -1.319785
   31         16             0        4.975064   -0.423599    0.083058
   32          8             0        5.132669   -0.226906    1.540757
   33          8             0        5.530795   -1.669716   -0.467987
   34          8             0        5.186416    0.795472   -0.729796
   35          1             0       -3.879333   -1.995404   -0.014451
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1954.06250568

Zero-point correction=                           0.252054 (Hartree/Particle)
 Thermal correction to Energy=                    0.273569
 Thermal correction to Enthalpy=                  0.274513
 Thermal correction to Gibbs Free Energy=         0.198081

Frequencies -- -1672.0866               11.8654               26.2444
 Frequencies --    31.7916               52.7747               53.6670
 Frequencies --    61.4778               76.3023               91.3741
 Frequencies --   120.7752              129.4516              143.7002
 Frequencies --   167.1189              175.3353              198.5371
 Frequencies --   229.1910              238.1646              258.4382
 Frequencies --   267.9940              300.9045              349.7993
 Frequencies --   360.2794              366.0046              372.2933
 Frequencies --   382.3212              413.4842              427.0080
 Frequencies --   449.5271              452.9708              467.5815
 Frequencies --   485.8780              504.2004              526.3405
 Frequencies --   540.2739              547.5142              576.6867
 Frequencies --   607.3126              623.8512              652.0427
 Frequencies --   714.5521              738.6900              793.2866
 Frequencies --   859.4472              910.6472              926.6945
 Frequencies --   950.5201              995.2020             1000.4921
 Frequencies --  1026.6437             1061.3463             1069.7171
 Frequencies --  1090.5898             1102.6264             1109.4254
 Frequencies --  1118.2603             1130.1081             1158.1705
 Frequencies --  1159.2554             1168.6829             1187.7133
 Frequencies --  1188.4509             1219.9463             1224.4075
 Frequencies --  1231.4411             1235.3113             1241.1438
 Frequencies --  1274.1645             1276.4128             1320.1923
 Frequencies --  1326.6705             1340.5101             1348.6476
 Frequencies --  1365.7036             1378.1760             1386.1695
 Frequencies --  1405.3711             1412.9569             1432.5879
 Frequencies --  1449.2620             1450.9041             1484.7204
 Frequencies --  1500.8037             1516.2684             1535.3309
 Frequencies --  1542.8435             1990.9775             3013.1301
 Frequencies --  3015.4830             3022.2471             3033.6493
 Frequencies --  3041.3047             3071.5200             3082.3206
 Frequencies --  3084.4345             3126.7731             3134.0411
 Frequencies --  3461.9973             3723.0172             3736.9977
```

GlcNHSO3 anion, 6-sulfate, 4-OMe, alpha anomer



Standard orientation:

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1	6	0	0.036600	1.193374	0.056882
2	6	0	-1.405657	0.867413	-0.379353
3	6	0	-1.846070	-0.528425	0.151992
4	6	0	-0.765329	-1.584557	-0.103827
5	8	0	0.507298	-1.180145	0.391153
6	6	0	0.989072	0.015242	-0.212570
7	6	0	2.357445	0.297077	0.369693
8	8	0	-0.706073	-1.839569	-1.494577
9	1	0	-1.001220	-2.497382	0.452852
10	7	0	-3.102129	-1.060137	-0.361973
11	8	0	3.286626	-0.714171	-0.153250
12	8	0	-2.214357	1.909706	0.111983
13	16	0	-4.607275	-0.443898	0.258609
14	8	0	-5.599767	-1.309802	-0.402034
15	8	0	-4.450920	-0.578050	1.720928
16	8	0	-4.689826	0.988833	-0.207548
17	16	0	4.833361	-0.542822	0.205382
18	8	0	5.009997	-0.140855	1.596481
19	8	0	5.503642	-1.688148	-0.365076
20	8	0	5.232509	0.769115	-0.702034
21	8	0	0.600773	2.303617	-0.640470
22	6	0	0.171422	3.586479	-0.203228
23	1	0	0.012147	1.403364	1.139642
24	1	0	-1.411201	0.835365	-1.484099
25	1	0	-1.965473	-0.446918	1.237887
26	1	0	1.083338	-0.114104	-1.298219
27	1	0	2.689718	1.284511	0.044903
28	1	0	2.348208	0.219779	1.459076
29	1	0	-0.095522	-2.583253	-1.620557
30	1	0	-3.138319	-1.052818	-1.379188

```
   31          1             0       -3.174508    1.659639   -0.015187
   32          1             0        5.451413    1.480251   -0.072673
   33          1             0        0.766140    4.314890   -0.765208
   34          1             0       -0.894878    3.737731   -0.384683
   35          1             0        0.363582    3.723555    0.873431
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1954.11348550

Zero-point correction=                           0.256010 (Hartree/Particle)
 Thermal correction to Energy=                    0.277641
 Thermal correction to Enthalpy=                  0.278585
 Thermal correction to Gibbs Free Energy=         0.202694

Frequencies --    14.4419               29.3920               33.8765
 Frequencies --    46.0196               56.6402               67.9941
 Frequencies --    93.8494              118.9066              119.0029
 Frequencies --   143.2881              160.5924              168.8377
 Frequencies --   180.6092              187.4569              216.7285
 Frequencies --   237.0429              238.7221              274.6237
 Frequencies --   300.1115              340.5900              345.8438
 Frequencies --   360.6574              370.5683              380.9378
 Frequencies --   394.0651              421.6384              433.4616
 Frequencies --   456.5459              480.9347              490.3021
 Frequencies --   508.8226              518.4961              527.6677
 Frequencies --   550.6990              572.0114              581.1825
 Frequencies --   622.9578              639.4726              675.2152
 Frequencies --   766.5513              788.9624              817.5670
 Frequencies --   828.2766              846.6570              883.5482
 Frequencies --   930.0239              969.8855              977.5174
 Frequencies --   980.6443             1041.1962             1051.5657
 Frequencies --  1076.0992             1096.0512             1108.0262
 Frequencies --  1133.6948             1139.8344             1141.5570
 Frequencies --  1153.9862             1160.0604             1167.0154
 Frequencies --  1178.4209             1192.4159             1193.5934
 Frequencies --  1226.5237             1231.1759             1243.0854
 Frequencies --  1266.0003             1282.5868             1297.8759
 Frequencies --  1334.0650             1344.7840             1365.5074
 Frequencies --  1374.5511             1392.4021             1400.9062
 Frequencies --  1406.0728             1417.7552             1435.5139
 Frequencies --  1448.1448             1454.9458             1497.0436
 Frequencies --  1505.3782             1519.2238             1520.3885
 Frequencies --  1549.7913             2959.5315             2989.5913
 Frequencies --  2999.4863             3062.0134             3085.6469
 Frequencies --  3091.2652             3096.7604             3103.4156
 Frequencies --  3152.4986             3173.1575             3181.8725
 Frequencies --  3525.7304             3719.2020             3738.2914
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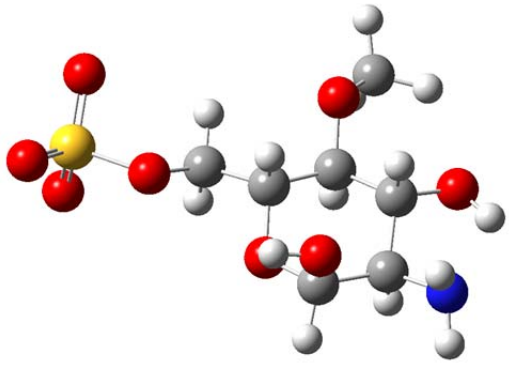
GlcNHSO3 anion, 4-OMe, alpha anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.611209	0.857617	0.138374
2	6	0	0.156398	0.735386	-0.355759
3	6	0	-0.515008	-0.552941	0.198849
4	6	0	0.405680	-1.766058	0.030618
5	8	0	1.694963	-1.543850	0.573809
6	6	0	2.396414	-0.453502	-0.030856
7	6	0	3.766274	-0.388322	0.620124
8	8	0	0.483262	-2.081187	-1.350835
9	1	0	0.004230	-2.613244	0.598355
10	7	0	-1.815165	-0.911430	-0.357711
11	8	0	4.545433	-1.501670	0.175956
12	8	0	-0.509329	1.908309	0.056633
13	16	0	-3.237108	-0.059974	0.166757
14	8	0	-4.317626	-0.800861	-0.510120
15	8	0	-3.168518	-0.155748	1.639518
16	8	0	-3.094242	1.349919	-0.350390
17	8	0	2.354183	1.846447	-0.577757
18	6	0	2.125802	3.189623	-0.181642
19	1	0	1.573515	1.123110	1.208683
20	1	0	0.193166	0.658895	-1.457551
21	1	0	-0.666890	-0.412210	1.274463
22	1	0	2.531309	-0.642684	-1.103785
23	1	0	4.233905	0.563372	0.335447
24	1	0	3.635899	-0.407596	1.713792
25	1	0	1.052047	-2.864565	-1.421129
26	1	0	-1.805376	-0.938872	-1.375176
27	1	0	5.391645	-1.460462	0.645337
28	1	0	-1.486763	1.799334	-0.114216
29	1	0	2.835926	3.802095	-0.749107
30	1	0	1.099546	3.503931	-0.386996

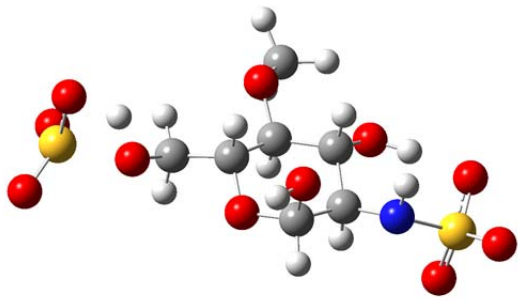
```
   31          1             0        2.322106    3.326809    0.894974
 -------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1330.22082745

Zero-point correction=                           0.241206 (Hartree/Particle)
 Thermal correction to Energy=                    0.258661
 Thermal correction to Enthalpy=                  0.259606
 Thermal correction to Gibbs Free Energy=         0.195399

Frequencies --    35.6348               45.7795               60.2293
 Frequencies --    84.2893               92.8330              114.2604
 Frequencies --   128.9038              165.0461              177.0967
 Frequencies --   187.7751              206.0350              228.9745
 Frequencies --   244.1561              257.1081              272.7376
 Frequencies --   332.6098              344.1440              358.3845
 Frequencies --   376.4321              393.8438              410.0133
 Frequencies --   436.2691              457.7069              487.1951
 Frequencies --   523.1181              527.5280              565.7467
 Frequencies --   575.0991              625.3585              636.3530
 Frequencies --   673.7205              786.9871              816.4023
 Frequencies --   824.6439              872.1916              929.3508
 Frequencies --   975.6124              981.2374             1020.0898
 Frequencies --  1048.7782             1062.6801             1085.7094
 Frequencies --  1097.3071             1107.1589             1131.1612
 Frequencies --  1134.9869             1144.2166             1156.5424
 Frequencies --  1163.7485             1176.6152             1194.3552
 Frequencies --  1217.7036             1229.5442             1237.0874
 Frequencies --  1258.8212             1272.8251             1282.0401
 Frequencies --  1305.7347             1336.8140             1344.4702
 Frequencies --  1368.4961             1382.6162             1394.6831
 Frequencies --  1409.6853             1419.8177             1446.2426
 Frequencies --  1456.2056             1477.1044             1498.1483
 Frequencies --  1503.3778             1520.6439             1541.1492
 Frequencies --  1551.4414             2960.3396             2985.8956
 Frequencies --  2991.6191             3003.1353             3053.3716
 Frequencies --  3067.0677             3071.4626             3082.9285
 Frequencies --  3095.7065             3143.6870             3220.9339
 Frequencies --  3525.0573             3734.3150             3752.7709
```

GlcNHSO3 anion, 6-sulfate, 4-OMe, alpha anomer, TS to lose 6-sulfate



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.006032	1.196354	-0.074301
2	6	0	1.432342	0.864252	0.371267
3	6	0	1.875796	-0.527933	-0.165118
4	6	0	0.794272	-1.585542	0.078194
5	8	0	-0.475522	-1.181577	-0.427780
6	6	0	-0.961976	0.014452	0.166695
7	6	0	-2.323637	0.299775	-0.438146
8	8	0	0.720470	-1.845413	1.467732
9	1	0	1.036749	-2.496093	-0.478630
10	7	0	3.127494	-1.063456	0.354937
11	8	0	-3.281244	-0.684834	0.068391
12	8	0	2.244893	1.909855	-0.104421
13	16	0	4.636285	-0.449408	-0.262142
14	8	0	5.624998	-1.318778	0.399108
15	8	0	4.481180	-0.581520	-1.724693
16	8	0	4.719250	0.981950	0.207081
17	16	0	-5.073812	-0.395596	-0.209819
18	8	0	-5.214258	0.902649	-0.850331
19	8	0	-5.626333	-1.583106	-0.835250
20	8	0	-5.088050	-0.388028	1.336388
21	8	0	-0.578309	2.289176	0.640450
22	6	0	-0.157073	3.583267	0.226026
23	1	0	0.028697	1.426040	-1.152564
24	1	0	1.427173	0.823886	1.475957
25	1	0	2.002743	-0.441355	-1.249798
26	1	0	-1.069753	-0.114754	1.253173
27	1	0	-2.655229	1.303304	-0.169052
28	1	0	-2.298209	0.175754	-1.523014
29	1	0	0.158502	-2.627754	1.582247
30	1	0	3.160161	-1.051951	1.372280

```
   31          1             0        3.204467    1.656559    0.021424
   32          1             0       -0.755655    4.296856    0.801850
   33          1             0        0.908617    3.736504    0.409834
   34          1             0       -0.352488    3.738109   -0.847170
   35          1             0       -3.826537   -0.531596    1.169192
 ---------------------------------------------------------------------

SCF Done:  E(RB+HF-LYP) =  -1954.06513760

Zero-point correction=                           0.251908 (Hartree/Particle)
 Thermal correction to Energy=                    0.272973
 Thermal correction to Enthalpy=                  0.273917
 Thermal correction to Gibbs Free Energy=         0.199164

Frequencies -- -1623.6079               19.8528                25.2582
 Frequencies --    34.3305               45.5840                55.8502
 Frequencies --    67.6739               95.6588               115.2384
 Frequencies --   125.0306              140.1609               154.4892
 Frequencies --   171.9169              185.9037               215.4018
 Frequencies --   233.6743              239.1875               267.0662
 Frequencies --   286.6483              313.4431               331.9748
 Frequencies --   346.3692              373.1781               392.8848
 Frequencies --   402.9627              433.5214               435.8780
 Frequencies --   458.2349              478.3020               487.2618
 Frequencies --   503.8558              525.0778               534.8309
 Frequencies --   569.8826              575.3024               608.0314
 Frequencies --   629.0347              639.5864               676.7177
 Frequencies --   721.8632              788.1071               817.2141
 Frequencies --   825.4831              874.9235               928.7329
 Frequencies --   942.6218              975.9543               980.6629
 Frequencies --   999.2590             1039.0547              1051.6675
 Frequencies --  1066.1680             1088.9201              1104.8152
 Frequencies --  1125.4211             1134.8419              1143.9548
 Frequencies --  1153.1092             1161.7655              1173.0516
 Frequencies --  1181.1896             1193.9985              1215.2809
 Frequencies --  1228.8536             1232.1801              1246.1660
 Frequencies --  1271.1445             1291.7052              1301.1255
 Frequencies --  1334.5614             1344.6737              1361.1945
 Frequencies --  1367.7381             1375.8440              1391.7275
 Frequencies --  1404.1188             1417.5958              1430.8370
 Frequencies --  1447.7970             1454.3950              1497.2872
 Frequencies --  1505.7900             1519.8075              1523.4500
 Frequencies --  1549.1756             2030.8168              2957.1422
 Frequencies --  2992.3639             3004.2360              3035.5222
 Frequencies --  3088.9761             3096.5556              3097.8874
 Frequencies --  3109.4473             3153.2010              3180.3062
 Frequencies --  3181.1262             3524.8414              3742.1396
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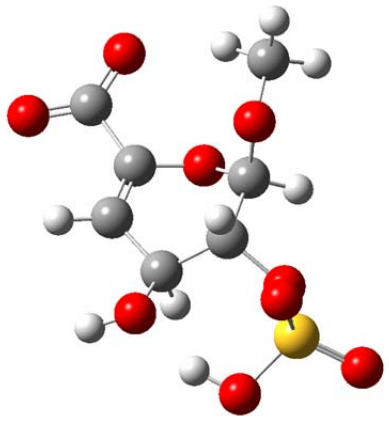
4,5-ΔHexA, 2S, 1-OMe, carboxylic anion, beta-anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.385767	-1.526071	0.085131
2	6	0	0.060757	-1.312130	-0.238041
3	6	0	0.446344	0.139045	0.058100
4	6	0	-0.650121	1.126127	-0.418606
5	8	0	-1.768913	0.494207	-1.007691
6	6	0	-2.271540	-0.606825	-0.316710
7	6	0	-3.796445	-0.651754	-0.040927
8	8	0	1.672635	0.517648	-0.654208
9	8	0	0.934077	-2.165126	0.555270
10	8	0	-4.208284	-1.781323	0.304198
11	8	0	-4.389772	0.445718	-0.165743
12	16	0	3.120831	0.205439	0.021564
13	8	0	4.089945	0.899212	-0.799630
14	8	0	3.038708	0.429336	1.458566
15	8	0	3.303637	-1.364452	-0.274793
16	1	0	2.501744	-1.839560	0.106949
17	8	0	-1.001269	1.881243	0.705463
18	6	0	-2.101111	2.769813	0.468997
19	1	0	-1.731876	-2.407430	0.613717
20	1	0	0.273124	-1.501868	-1.303451
21	1	0	0.603457	0.274350	1.129179
22	1	0	-0.247661	1.765911	-1.217038
23	1	0	0.588376	-3.069253	0.489248
24	1	0	-2.226169	3.335026	1.396721
25	1	0	-1.863666	3.470311	-0.348509
26	1	0	-3.009447	2.204556	0.229047

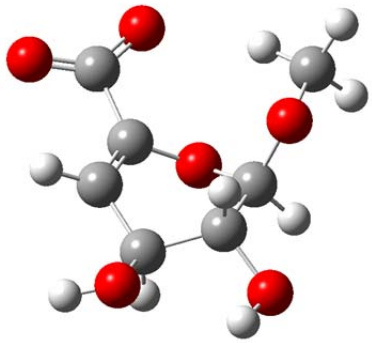
SCF Done: E(RB+HF-LYP) = -1347.65423100

Zero-point correction= 0.180731 (Hartree/Particle)
Thermal correction to Energy= 0.196756
Thermal correction to Enthalpy= 0.197700

Thermal correction to Gibbs Free Energy= 0.136526

Frequencies --	30.5886	51.3470	62.8940
Frequencies --	104.2490	109.0587	126.4606
Frequencies --	145.1449	191.4263	214.2141
Frequencies --	216.0835	238.1890	239.9993
Frequencies --	275.5343	324.9131	339.9678
Frequencies --	360.9807	379.5859	391.7612
Frequencies --	418.0555	435.0370	473.4239
Frequencies --	501.0509	521.4774	544.2259
Frequencies --	552.2969	600.5563	641.1236
Frequencies --	691.1787	747.6673	762.3095
Frequencies --	793.2993	805.3072	815.6359
Frequencies --	846.2753	881.5896	946.5161
Frequencies --	960.7544	1004.9695	1028.8690
Frequencies --	1066.7410	1083.3732	1100.8836
Frequencies --	1122.2260	1143.0971	1170.2708
Frequencies --	1211.4879	1231.5645	1243.4432
Frequencies --	1264.6643	1305.6301	1332.2492
Frequencies --	1342.2274	1357.4355	1361.8224
Frequencies --	1384.1272	1406.9963	1432.6510
Frequencies --	1474.8929	1502.2095	1525.7995
Frequencies --	1560.5008	1704.3638	1767.1107
Frequencies --	2980.6254	2988.3389	3032.1685
Frequencies --	3083.7118	3112.2643	3138.4702
Frequencies --	3147.5610	3227.7107	3751.0900

4,5-ΔHexA, 1-OMe, carboxylic anion, beta-anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.104370	-1.549137	-0.085382
2	6	0	-1.518225	-1.154382	0.223817
3	6	0	-1.732784	0.300933	-0.192341
4	6	0	-0.600787	1.188877	0.362619
5	8	0	0.461415	0.457696	0.953136
6	6	0	0.864034	-0.700710	0.284454
7	6	0	2.378619	-0.878133	0.020460
8	8	0	-2.990816	0.795789	0.274190
9	8	0	-2.530326	-1.914647	-0.464571
10	8	0	2.700928	-2.041156	-0.315658
11	8	0	3.072336	0.161178	0.146135
12	8	0	-0.150150	1.991698	-0.699256
13	6	0	1.014606	2.754336	-0.375462
14	1	0	0.148558	-2.468746	-0.601272
15	1	0	-1.711787	-1.209570	1.311558
16	1	0	-1.685299	0.341970	-1.288733
17	1	0	-0.988740	1.813895	1.181544
18	1	0	-2.352728	-2.847478	-0.270732
19	1	0	1.221238	3.370463	-1.256521
20	1	0	0.822825	3.418598	0.485104
21	1	0	1.861715	2.093886	-0.154211
22	1	0	-3.629443	0.111823	0.012449

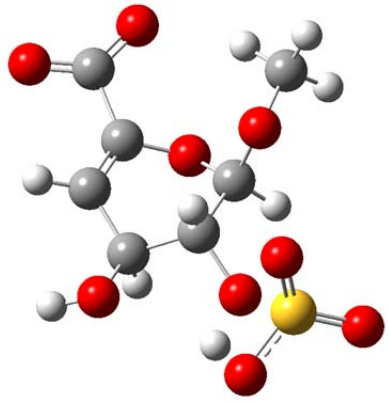
SCF Done: E(RB+HF-LYP) = -723.751899756

Zero-point correction= 0.165245 (Hartree/Particle)
Thermal correction to Energy= 0.177830
Thermal correction to Enthalpy= 0.178774
Thermal correction to Gibbs Free Energy= 0.126273

Frequencies -- 55.8545 64.4889 98.0823
Frequencies -- 132.6200 164.9057 192.6520
Frequencies -- 212.0326 227.1761 262.7802
Frequencies -- 280.0941 308.1701 349.6675

```
Frequencies --   378.4525              406.0232              420.4043
Frequencies --   436.4730              503.0588              541.1918
Frequencies --   598.5269              615.6263              676.0148
Frequencies --   750.5357              783.6226              814.3819
Frequencies --   871.4788              953.2666              990.4776
Frequencies --  1023.7098             1050.0088             1069.1324
Frequencies --  1088.1003             1106.9329             1131.5591
Frequencies --  1144.4663             1209.5132             1220.2118
Frequencies --  1242.3831             1259.7707             1278.2067
Frequencies --  1339.7128             1351.7796             1362.7313
Frequencies --  1368.5641             1397.5729             1433.0279
Frequencies --  1455.9313             1502.5539             1523.4772
Frequencies --  1561.7932             1698.3735             1756.2854
Frequencies --  2937.5601             2973.6088             3014.1821
Frequencies --  3046.6213             3074.0415             3124.8102
Frequencies --  3228.0384             3721.8872             3749.3522
```

4,5-ΔHexA, 2S, 1-OMe, carboxylic anion, beta-anomer, TS to lose 2-sulfate



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.706617	-1.588275	0.091698
2	6	0	-0.283079	-1.669968	-0.384621
3	6	0	0.373240	-0.332108	-0.061735
4	6	0	-0.472541	0.845256	-0.594775
5	8	0	-1.751824	0.443266	-1.043000
6	6	0	-2.411644	-0.502554	-0.251943
7	6	0	-3.868912	-0.189279	0.169631
8	8	0	1.695677	-0.334940	-0.695140
9	8	0	0.522193	-2.674742	0.237191
10	8	0	-4.482270	-1.181689	0.621272
11	8	0	-4.216894	1.007986	0.031971
12	16	0	3.191506	0.267662	0.182141
13	8	0	3.827994	1.260212	-0.667668
14	8	0	2.817650	0.603916	1.545635
15	8	0	3.646131	-1.190039	-0.046102
16	8	0	-0.537987	1.779602	0.443878
17	6	0	-1.443149	2.859595	0.182034
18	1	0	-2.155114	-2.360035	0.706356
19	1	0	-0.248731	-1.799564	-1.482261
20	1	0	0.507765	-0.237817	1.017297
21	1	0	0.004535	1.279125	-1.487473
22	1	0	0.058641	-3.518462	0.124036
23	1	0	-1.350290	3.533822	1.037836
24	1	0	-1.149965	3.399775	-0.733282
25	1	0	-2.468838	2.484191	0.086556
26	1	0	2.448751	-1.308202	-0.509350

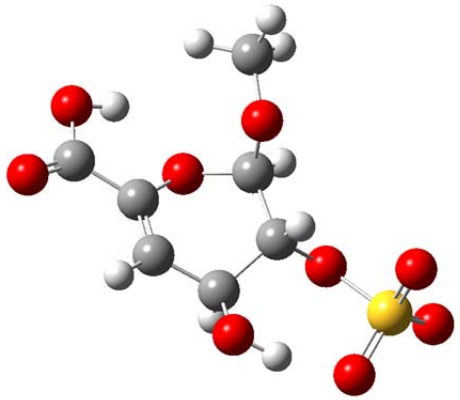
SCF Done: E(RB+HF-LYP) = -1347.59359171

Range of M.O.s used for correlation: 1 277
Zero-point correction= 0.175114 (Hartree/Particle)
Thermal correction to Energy= 0.191586

```
 Thermal correction to Enthalpy=                 0.192530
 Thermal correction to Gibbs Free Energy=        0.129382

Frequencies -- -1639.6665               28.9720               38.4070
 Frequencies --    50.1654               62.3297               98.6121
 Frequencies --   113.6256              143.1581              161.8978
 Frequencies --   181.2494              195.3525              221.8245
 Frequencies --   235.7365              254.1414              271.7352
 Frequencies --   304.5152              339.9225              366.8225
 Frequencies --   405.7454              413.6420              435.8457
 Frequencies --   473.5199              481.5603              504.1982
 Frequencies --   547.7280              590.2330              608.9782
 Frequencies --   624.3612              660.8981              741.1520
 Frequencies --   751.0955              796.4666              814.6791
 Frequencies --   870.0581              935.5601              959.2196
 Frequencies --   991.4436             1017.3543             1036.2984
 Frequencies --  1064.2161             1077.8224             1089.2287
 Frequencies --  1135.9067             1148.0137             1152.8069
 Frequencies --  1211.2705             1214.2926             1230.4801
 Frequencies --  1241.6146             1263.3309             1310.4286
 Frequencies --  1338.6186             1349.2881             1362.2419
 Frequencies --  1366.9940             1399.0367             1409.9673
 Frequencies --  1440.1337             1503.0876             1523.2823
 Frequencies --  1560.0936             1696.9936             1765.0075
 Frequencies --  1983.2946             2944.1093             2987.6023
 Frequencies --  3010.4583             3084.2526             3139.5974
 Frequencies --  3142.2762             3237.7986             3754.1870
```

4,5-ΔHexA, 2S anion, 1-OMe, beta-anomer



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.375994	-1.571154	0.195203
2	6	0	0.093240	-1.403682	-0.051074
3	6	0	0.525841	0.087153	0.104609
4	6	0	-0.581945	1.097077	-0.262526
5	8	0	-1.741629	0.492899	-0.901555
6	6	0	-2.222172	-0.639586	-0.251072
7	6	0	-3.704602	-0.690954	-0.142990
8	8	0	1.628874	0.392970	-0.739771
9	8	0	0.804672	-2.264858	0.801995
10	8	0	-4.333824	-1.592693	0.364261
11	8	0	-4.322277	0.392120	-0.686807
12	16	0	3.195043	0.090064	-0.093774
13	8	0	4.033943	0.677273	-1.142631
14	8	0	3.184392	0.764322	1.217698
15	8	0	3.251995	-1.401152	-0.009803
16	8	0	-0.966320	1.761467	0.904273
17	6	0	-1.827707	2.867606	0.700839
18	1	0	-1.740700	-2.450204	0.713643
19	1	0	0.282546	-1.645636	-1.114832
20	1	0	0.790269	0.256502	1.153835
21	1	0	-0.212594	1.795326	-1.020718
22	1	0	1.762441	-2.109071	0.603606
23	1	0	-1.874784	3.405867	1.650876
24	1	0	-1.436708	3.542121	-0.076157
25	1	0	-2.842146	2.552767	0.421983
26	1	0	-3.607592	0.953756	-1.051076

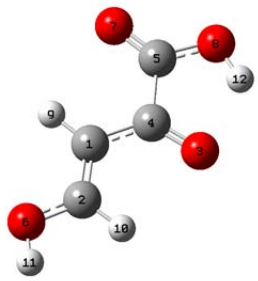
SCF Done: E(RB+HF-LYP) = -1347.69953102

Zero-point correction= 0.182517 (Hartree/Particle)
Thermal correction to Energy= 0.198328
Thermal correction to Enthalpy= 0.199272

Thermal correction to Gibbs Free Energy= 0.137652

Frequencies --	19.8216	38.7676	65.1941
Frequencies --	97.2432	109.4003	118.6177
Frequencies --	126.7883	176.5953	199.7846
Frequencies --	213.3716	227.3270	247.7777
Frequencies --	263.3926	328.9131	367.3476
Frequencies --	397.1719	410.1533	421.9522
Frequencies --	460.1050	479.5057	518.3880
Frequencies --	541.4020	548.1801	570.2078
Frequencies --	606.0927	639.7999	665.8975
Frequencies --	702.8528	714.1096	752.9890
Frequencies --	774.9959	785.2022	848.4310
Frequencies --	874.8065	939.6318	984.9832
Frequencies --	1001.6270	1017.5803	1043.2394
Frequencies --	1073.3616	1095.3446	1124.5485
Frequencies --	1139.8977	1163.1574	1190.7219
Frequencies --	1207.1783	1233.7398	1241.9640
Frequencies --	1266.2507	1291.4060	1299.7173
Frequencies --	1305.8696	1342.6349	1360.4444
Frequencies --	1400.8303	1406.0372	1424.8396
Frequencies --	1500.6891	1521.0492	1526.2693
Frequencies --	1540.7357	1730.3346	1853.9029
Frequencies --	2933.5490	3011.5818	3071.7768
Frequencies --	3090.2444	3092.2964	3139.4062
Frequencies --	3246.4456	3384.2814	3605.6200

4,5-ΔHexA, 2S anion, 1-OMe, beta-anomer, ^{0,2}A fragment



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Standard orientation:

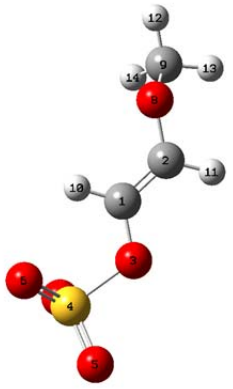
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.927907	-0.402168	0.000096
2	6	0	-2.119475	0.231347	-0.000073
3	8	0	0.368105	1.613804	-0.000077
4	6	0	0.287758	0.381754	-0.000007
5	6	0	1.618696	-0.406154	0.000009
6	8	0	-3.282773	-0.436746	0.000063
7	8	0	1.688161	-1.612199	-0.000121
8	8	0	2.675275	0.413310	0.000077
9	1	0	-0.851362	-1.482825	0.000277
10	1	0	-2.163851	1.319796	-0.000197
11	1	0	-4.025514	0.186312	-0.000100
12	1	0	2.296149	1.322687	0.000349

SCF Done: E(RB+HF-LYP) = -455.859672736

Zero-point correction= 0.082933 (Hartree/Particle)
Thermal correction to Energy= 0.090549
Thermal correction to Enthalpy= 0.091493
Thermal correction to Gibbs Free Energy= 0.050402

Frequencies --	82.6189	140.6346	142.2314
Frequencies --	238.0239	301.2150	379.4024
Frequencies --	450.0634	471.9447	483.0937
Frequencies --	556.4710	711.5331	757.1535
Frequencies --	807.7015	896.7556	907.0835
Frequencies --	1011.3317	1100.4804	1187.2493
Frequencies --	1225.4763	1308.0580	1366.2025
Frequencies --	1393.8322	1452.7178	1692.0303
Frequencies --	1754.7043	1870.8320	3184.1825
Frequencies --	3249.7718	3515.9572	3764.7145

4,5-ΔHexA, 2S anion, 1-OMe, beta-anomer, ^{0,2}X fragment



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.786752	-0.316928	0.238869
2	6	0	2.004502	-0.630220	-0.219091
3	8	0	-0.338580	-0.772604	-0.354019
4	16	0	-1.813211	0.133309	0.002239
5	8	0	-2.811566	-0.859516	-0.419405
6	8	0	-1.714225	0.380686	1.456330
7	8	0	-1.684402	1.331807	-0.847374
8	8	0	3.148018	-0.268512	0.491844
9	6	0	3.992248	0.589860	-0.246748
10	1	0	0.657396	0.277111	1.142186
11	1	0	2.169017	-1.217364	-1.123477
12	1	0	4.873308	0.793234	0.373019
13	1	0	4.324805	0.124637	-1.190810
14	1	0	3.491878	1.538277	-0.493930

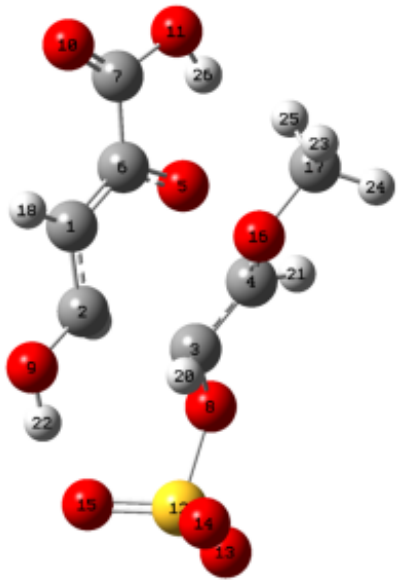
SCF Done: E(RB+HF-LYP) = -891.796051304

Zero-point correction= 0.092343 (Hartree/Particle)
Thermal correction to Energy= 0.102041
Thermal correction to Enthalpy= 0.102985
Thermal correction to Gibbs Free Energy= 0.055408

Frequencies --	32.3191	43.5620	94.8242
Frequencies --	133.5376	207.5217	214.8331
Frequencies --	289.2591	325.1208	354.3552
Frequencies --	466.9604	486.2277	535.5544
Frequencies --	575.1742	581.7677	693.5550
Frequencies --	799.8792	978.3956	1005.7914
Frequencies --	1019.8600	1154.4968	1189.2973
Frequencies --	1217.3582	1238.8130	1254.0906
Frequencies --	1281.0303	1315.8187	1324.3887
Frequencies --	1496.6455	1509.9930	1537.5822
Frequencies --	1738.8286	2977.9765	3033.8578

```
Frequencies --  3098.7279              3144.6938              3181.6247
```

4,5-ΔHexA, 2S anion, 1-OMe, beta-anomer, ^{0,2}X/A fragmentation TS



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.362140	-1.461867	-0.327724
2	6	0	-0.046332	-1.352683	-0.070719
3	6	0	-0.675411	0.459821	-0.260465
4	6	0	0.368634	1.377126	-0.015458
5	8	0	1.789242	0.196768	1.276365
6	6	0	2.211451	-0.672944	0.408375
7	6	0	3.708730	-0.690243	0.180258
8	8	0	-1.713077	0.581741	0.662863
9	8	0	-0.843104	-2.128541	-0.852699
10	8	0	4.322256	-1.388955	-0.598339
11	8	0	4.317192	0.206645	0.997270
12	16	0	-3.279504	0.076254	0.129812
13	8	0	-4.123145	0.691507	1.154755
14	8	0	-3.376705	0.604966	-1.242406
15	8	0	-3.196862	-1.414850	0.202545
16	8	0	1.205077	1.624223	-1.019605
17	6	0	2.275980	2.533315	-0.750147
18	1	0	1.729364	-2.084183	-1.135265
19	1	0	-0.325470	-1.302315	0.985824
20	1	0	-0.983442	0.374288	-1.301997
21	1	0	0.374358	2.026321	0.852237
22	1	0	-1.777012	-2.020923	-0.523986
23	1	0	2.761269	2.722608	-1.708704
24	1	0	1.884565	3.472895	-0.341188
25	1	0	2.984241	2.085377	-0.050402
26	1	0	3.546059	0.562697	1.515773

SCF Done: E(RB+HF-LYP) = -1347.65524823

Zero-point correction=   0.178555 (Hartree/Particle)
 Thermal correction to Energy=   0.194862
 Thermal correction to Enthalpy=   0.195807
 Thermal correction to Gibbs Free Energy=   0.134037

Frequencies --	-468.2720	39.6514	48.6942
Frequencies --	71.6944	94.1771	113.4335
Frequencies --	122.9956	135.5841	150.4022
Frequencies --	185.7817	196.4953	220.1478
Frequencies --	231.3266	253.8735	273.1733
Frequencies --	316.8437	370.1749	390.8781
Frequencies --	400.3731	424.3227	444.0497
Frequencies --	464.2306	505.9320	538.5102
Frequencies --	544.5026	567.2047	575.2695
Frequencies --	614.7063	621.4005	706.8620
Frequencies --	717.4999	784.9824	838.0165
Frequencies --	874.4471	882.0032	891.1928
Frequencies --	923.3116	962.1936	987.7372
Frequencies --	1030.4199	1089.8152	1117.7068
Frequencies --	1140.4518	1172.9637	1183.9881
Frequencies --	1185.6600	1203.7134	1208.2949
Frequencies --	1249.7223	1256.2467	1301.3339
Frequencies --	1306.5151	1331.7766	1354.3751
Frequencies --	1433.3026	1460.9049	1485.2506
Frequencies --	1515.9621	1532.6807	1565.5847
Frequencies --	1571.3016	1637.6010	1851.2037
Frequencies --	3052.5591	3091.7100	3144.9490
Frequencies --	3157.5786	3181.7133	3235.8396
Frequencies --	3239.4640	3272.3759	3329.5684