Supplementary Information (SI) for Faraday Discussions.
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64 mannose_6_threo
XYZ file generated by Avogadro.
H      4.84130    2.04710    0.82490
O      5.34020    1.81540    0.02780
C      4.85460    0.59510   -0.44160
H      5.55920    0.22200   -1.19110
O      3.59500    0.84940   -1.04940
C      2.98900   -0.28530   -1.67100
H      3.61290   -0.63530   -2.50280
C      1.65540    0.21300   -2.18840
H      1.11280   -0.59120   -2.69390
H      1.80940    1.04070   -2.88900
O      0.96420    0.67130   -1.03870
C      2.80480   -1.42570   -0.66210
H      2.03160   -1.13940    0.06160
O      2.37300   -2.56390   -1.39160
H      2.12450   -3.24530   -0.75490
C      4.09760   -1.70890    0.09240
H      4.83050   -2.12560   -0.60480
O      3.88900   -2.69250    1.09280
H      3.32390   -2.30490    1.77520
C      4.66790   -0.42110    0.67960
H      5.63320   -0.62620    1.14490
O      3.83870    0.11660    1.70240
H      3.00950    0.43400    1.31490
C     -0.30430    1.25670   -1.23550
H     -0.31020    1.82640   -2.17500
C     -0.46960    2.29270   -0.11050
H     -1.42490    2.80780   -0.24990
C      0.62920    3.35280   -0.13780
H      0.33950    4.16790    0.52660
H      0.69850    3.74740   -1.15740
C     -1.40380    0.20610   -1.27490
C     -3.47390   -1.66410   -1.16270
C     -1.12410   -1.14700   -1.14440
C     -2.73630    0.62510   -1.38850
C     -3.76620   -0.29730   -1.30790
C     -2.15970   -2.08350   -1.10130
H     -0.10250   -1.48990   -1.03500
H     -2.96200    1.67960   -1.49510
H     -1.95200   -3.14170   -0.98950
O     -4.49040   -2.57840   -1.07130
H     -5.33520   -2.10810   -1.10820
O     -5.09850    0.00000   -1.34520
C     -5.45400    1.37900   -1.39870
H     -5.05270    1.91140   -0.53220
H     -6.54090    1.40940   -1.38040
H     -5.08700    1.83590   -2.32060
O     -0.41810    1.69100    1.18930
C     -1.54900    1.04250    1.63740
C     -3.76880   -0.35640    2.54050
C     -1.42690   -0.31980    1.95760
C     -2.75640    1.69920    1.80640
C     -3.87710    0.99740    2.25140
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C     -2.54630   -1.01770    2.40320
H     -2.82030    2.75480    1.56510
H     -4.82330    1.51140    2.36940
H     -2.47720   -2.07270    2.63500
H     -4.63350   -0.91280    2.88240
O     -0.19190   -0.86200    1.78220
C     -0.06480   -2.27090    1.94030
H     -0.26250   -2.56610    2.97390
H      0.96710   -2.50860    1.68450
H     -0.74430   -2.80030    1.26730
O      1.89570    2.90050    0.32050
H      2.15600    2.12210   -0.19710

64 mannose_6_erythro
XYZ file generated by Avogadro.
H     -0.58810   -3.88320   -1.57340
O     -0.82380   -4.34490   -0.75600
C      0.07060   -3.93710    0.23360
H      0.00080   -4.65140    1.06000
O     -0.33860   -2.65380    0.68730
C      0.44810   -2.19200    1.78600
H      0.42090   -2.93810    2.59270
C     -0.17700   -0.91730    2.30550
H      0.25570   -0.65770    3.27770
H     -1.25150   -1.08420    2.43440
O      0.06020    0.13520    1.38000
C      1.89650   -2.00710    1.32280
H      1.93030   -1.25440    0.53050
O      2.74050   -1.62550    2.40070
H      2.68280   -0.67000    2.51650
C      2.42510   -3.32400    0.78140
H      2.46590   -4.04710    1.60710
O      3.71030   -3.16990    0.20000
H      4.27490   -2.72340    0.84350
C      1.50010   -3.88020   -0.29260
H      1.81690   -4.89400   -0.55740
O      1.47010   -3.05640   -1.44810
H      2.36140   -3.01840   -1.81530
C     -0.86570    1.20350    1.49970
C     -0.22090    2.41960    0.82880
H      0.72240    2.62620    1.34350
C     -1.12480    3.63660    0.89070
H     -1.53940    3.73320    1.89660
H     -1.95370    3.49570    0.18830
C     -2.21320    0.83610    0.91350
C     -4.67770    0.21520   -0.23380
C     -3.39280    1.26030    1.51150
C     -2.26640    0.08390   -0.26450
C     -3.48920   -0.22650   -0.83730
C     -4.62660    0.95310    0.93510
H     -3.35800    1.83200    2.43270
H     -1.34570   -0.26080   -0.71420
H     -5.55540    1.27530    1.39140
O     -5.88960   -0.09350   -0.79220
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H     -5.73890   -0.59570   -1.60530
O     -3.65850   -0.95300   -1.98070
C     -2.47600   -1.37070   -2.65940
H     -1.87050   -2.01230   -2.01520
H     -1.89030   -0.50380   -2.97570
H     -2.81050   -1.93000   -3.52980
O      0.04600    2.16510   -0.56560
C      1.32060    1.77040   -0.91430
C      3.87280    1.02990   -1.73340
C      2.37850    2.69340   -0.83510
C      1.54340    0.50590   -1.43390
C      2.82170    0.13120   -1.84870
C      3.65750    2.31310   -1.22960
H      0.70990   -0.18520   -1.50110
H      2.98950   -0.85950   -2.25240
H      4.48080    3.01230   -1.16500
H      4.87120    0.74570   -2.04400
O      2.05280    3.93490   -0.38330
C      3.10150    4.88970   -0.23290
H      2.62850    5.78690    0.16080
H      3.56510    5.10840   -1.19720
H      3.85270    4.52670    0.47170
O     -0.42790    4.83890    0.59400
H      0.29940    4.62220   -0.00840
H     -0.99530    1.46540    2.55790

64 glucose_6_threo
XYZ file generated by Avogadro.
H      3.73010   -4.47950   -1.69030
O      3.38720   -4.72860   -0.82100
C      3.13350   -3.56820   -0.08920
H      2.90410   -3.88240    0.93490
O      2.00550   -2.92940   -0.66300
C      1.54390   -1.80370    0.07870
H      1.27160   -2.11230    1.09720
C      0.31550   -1.32200   -0.67730
H     -0.48160   -2.06840   -0.59350
H      0.57050   -1.18860   -1.73620
O     -0.09670   -0.08320   -0.12490
C      2.64540   -0.74000    0.15980
H      2.82060   -0.33230   -0.84480
O      2.31350    0.29850    1.06790
H      1.52210    0.74110    0.72740
C      3.93650   -1.35120    0.67720
H      3.79150   -1.62920    1.72990
O      5.02050   -0.44010    0.56350
H      4.81160    0.34230    1.08920
C      4.30810   -2.59850   -0.10330
H      4.51820   -2.32980   -1.14790
O      5.42210   -3.25280    0.47610
H      6.13880   -2.60980    0.54500
C     -2.47750   -0.43250    0.14560
C     -4.55490   -1.73830    1.46370
C     -2.40670   -0.65700    1.51550
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C     -3.59040   -0.87390   -0.57590
C     -4.62930   -1.52030    0.07900
C     -3.44570   -1.31390    2.17410
H     -1.54050   -0.32330    2.07570
H     -3.63470   -0.70450   -1.64490
H     -3.40700   -1.49830    3.24150
O     -5.57560   -2.37780    2.11460
H     -6.27020   -2.58630    1.47400
O     -5.76430   -1.99260   -0.51210
C     -5.91400   -1.76650   -1.91140
H     -5.11880   -2.26680   -2.46860
H     -6.87710   -2.19240   -2.18190
H     -5.90680   -0.69600   -2.12990
C     -1.38360    0.33710   -0.56230
H     -1.46820    0.18810   -1.64540
C     -1.44480    1.83800   -0.26770
H     -1.10400    2.00360    0.75890
C     -2.82300    2.44870   -0.43320
H     -2.75580    3.51660   -0.20660
H     -3.52220    1.98800    0.26460
O     -3.34540    2.24710   -1.74110
H     -2.76760    2.70380   -2.36410
O     -0.59240    2.53640   -1.19610
C      0.73230    2.71380   -0.86750
C      3.41650    3.18140   -0.32560
C      1.08940    3.54530    0.20980
C      1.71150    2.15180   -1.67020
C      3.06050    2.38920   -1.40790
C      2.43800    3.75950    0.48520
H      1.39790    1.52320   -2.49670
H      3.82000    1.94260   -2.03820
H      2.73260    4.38760    1.31540
O      0.06000    4.10690    0.89980
C      0.39200    4.93540    2.01080
H      0.97870    5.79900    1.68900
H      0.94510    4.36920    2.76390
H     -0.55610    5.27000    2.42550
H      4.46100    3.36350   -0.10150

64 glucose_6_erythro
XYZ file generated by Avogadro.
H      4.01030   -0.48770   -0.88040
O      3.98140    0.45190   -1.10690
C      2.96740    1.07670   -0.37780
H      2.84740    0.60620    0.60890
O      1.75300    0.96340   -1.10100
C      0.66160    1.49260   -0.35770
H      0.67490    1.07280    0.65760
C     -0.63080    1.10910   -1.05080
H     -0.63420    1.49130   -2.07430
H     -1.46640    1.55280   -0.50010
O     -0.81180   -0.29760   -1.15300
C      0.83980    3.00510   -0.24820
H      0.84940    3.43970   -1.25620
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O     -0.23990    3.53090    0.50620
H     -0.07310    4.47160    0.64400
C      2.16860    3.29460    0.43700
H      2.09860    2.95080    1.47760
O      2.36570    4.70030    0.40660
H      3.10750    4.91730    0.98340
C      3.31310    2.55460   -0.24040
H      3.46560    2.95960   -1.24860
O      4.46960    2.74210    0.55580
H      5.22720    2.38140    0.07970
C      0.37210   -1.49820    0.60990
C      2.85450   -2.35570    1.54960
C      0.63350   -1.53580    1.97390
C      1.35490   -1.91150   -0.29330
C      2.59370   -2.32040    0.17140
C      1.87160   -1.97310    2.44610
H     -0.12250   -1.20280    2.67740
H      1.15760   -1.86690   -1.35670
H      2.09010   -2.00180    3.50720
O      4.08100   -2.75220    2.00940
H      4.62580   -3.01330    1.25340
O      3.65470   -2.65830   -0.62760
C      3.37680   -2.91350   -2.00680
H      3.07080   -1.99690   -2.51670
H      4.30740   -3.27780   -2.43530
H      2.59700   -3.67240   -2.10160
C     -0.95170   -0.96540    0.09330
C     -1.99350   -2.07720   -0.07220
H     -2.13250   -2.56150    0.90040
C     -1.62680   -3.12500   -1.10700
H     -0.71330   -3.63600   -0.80460
H     -1.46300   -2.64750   -2.07810
O     -2.63910   -4.11810   -1.20400
H     -3.45650   -3.67590   -1.46310
O     -3.24420   -1.52940   -0.52230
C     -3.82320   -0.57810    0.28800
C     -4.99430    1.40640    1.83810
C     -4.08340    0.68270   -0.27660
C     -4.16130   -0.83850    1.60640
C     -4.74670    0.15670    2.38880
C     -4.66920    1.67340    0.50770
H     -3.96150   -1.82110    2.01840
H     -5.00560   -0.05190    3.41950
H     -4.87160    2.65140    0.09150
O     -3.73270    0.84080   -1.58140
C     -3.82790    2.15270   -2.12720
H     -3.23270    2.85950   -1.54240
H     -4.86790    2.48540   -2.16450
H     -3.42990    2.08430   -3.13730
H     -5.44720    2.18730    2.43710
H     -1.34690   -0.26060    0.83590

64 galactose_6_threo
XYZ file generated by Avogadro.
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H	4.68880	-0.23340	-2.37030
O	4.57520	-0.58910	-1.48000
C	3.42000	-1.36970	-1.45690
H	3.37670	-2.03090	-2.33360
O	2.29610	-0.50180	-1.48030
C	1.06910	-1.22930	-1.48990
H	1.09040	-1.95830	-2.31170
C	-0.07440	-0.28100	-1.77550
H	-0.96490	-0.87720	-2.00010
H	0.16210	0.34630	-2.64230
O	-0.29920	0.53220	-0.63400
C	0.91470	-2.01800	-0.18320
H	-0.01580	-2.59730	-0.23510
O	0.92500	-1.20110	0.98220
H	0.39930	-0.40730	0.79080
C	2.10270	-2.96300	-0.04980
H	2.05710	-3.70990	-0.84680
O	2.07120	-3.67980	1.17450
H	1.98420	-3.03220	1.88720
C	3.41680	-2.19180	-0.17720
H	3.52200	-1.50090	0.66970
O	4.51930	-3.08090	-0.23510
H	4.48160	-3.64400	0.54780
C	-2.72190	0.42620	-0.64470
C	-4.99050	-1.18300	-0.51110
C	-3.83460	0.72280	-1.41730
C	-2.73590	-0.69040	0.20100
C	-3.86050	-1.49690	0.26390
C	-4.97440	-0.08100	-1.34610
H	-3.82130	1.58330	-2.07740
H	-1.85710	-0.92480	0.79090
H	-5.85370	0.13740	-1.94080
O	-6.10690	-1.97250	-0.44840
H	-5.95270	-2.68060	0.19270
O	-3.98710	-2.61450	1.03500
C	-2.87280	-2.97150	1.85010
H	-3.16480	-3.87690	2.37660
H	-2.65390	-2.17830	2.56880
H	-1.99240	-3.16890	1.23320
C	-1.49020	1.30490	-0.66570
C	-1.42750	2.18450	0.58750
H	-1.46470	1.53510	1.46850
C	-2.56270	3.18650	0.68020
H	-2.43760	3.76510	1.59990
H	-3.51500	2.65810	0.72950
O	-2.62450	4.04840	-0.44840
H	-1.81840	4.57780	-0.46550
O	-0.20480	2.93510	0.58720
C	0.90270	2.34500	1.15600
C	3.21330	1.24650	2.24230
C	2.06760	2.25950	0.37420
C	0.90720	1.89540	2.46690
C	2.06360	1.33640	3.01340
C	3.22160	1.71130	0.92550

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H      0.00570    1.98850    3.06200
H      2.05770    0.98340    4.03730
H      4.12350    1.62980    0.33330
O      1.96590    2.72000   -0.90250
C      3.16660    2.79440   -1.66690
H      3.90170    3.42960   -1.16620
H      2.88480    3.23930   -2.61880
H      3.58590    1.80080   -1.83530
H     -1.49090    1.93570   -1.56210
H      4.11730    0.81470    2.65520
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64 galactose_6_erythro
XYZ file generated by Avogadro.
H     -4.55580   -2.92180    0.63140
O     -5.07510   -2.15280    0.89900
C     -4.84460   -1.12080   -0.01200
H     -4.86520   -1.49360   -1.04470
O     -3.56400   -0.57450    0.26180
C     -3.21450    0.47970   -0.63840
H     -3.27830    0.10590   -1.66870
C     -1.78130    0.84560   -0.32710
H     -1.69040    1.14420    0.72180
H     -1.45380    1.67280   -0.96600
O     -1.01520   -0.32380   -0.56860
C     -4.17990    1.64770   -0.49580
H     -3.94970    2.39080   -1.26740
O     -4.02250    2.21520    0.79590
H     -4.75100    2.83420    0.93270
C     -5.60460    1.14400   -0.70520
H     -5.70660    0.82270   -1.74940
O     -6.48320    2.22450   -0.43580
H     -7.38870    1.89150   -0.46560
C     -5.90360   -0.04650    0.19520
H     -5.87600    0.26390    1.24590
O     -7.19280   -0.52250   -0.15200
H     -7.47470   -1.15630    0.51810
C      1.27900    0.45600   -0.36730
C      3.39410    1.99330   -1.32680
C      1.75200    0.27060   -1.66400
C      1.84440    1.44420    0.44120
C      2.89900    2.21420   -0.03470
C      2.81330    1.03300   -2.14180
H      1.31240   -0.49210   -2.29800
H      1.46810    1.58930    1.44710
H      3.20620    0.88910   -3.14180
O      4.44870    2.72980   -1.79600
H      4.71550    3.36010   -1.11200
O      3.53230    3.20560    0.65970
C      2.99950    3.54950    1.93610
H      1.96030    3.87340    1.84060
H      3.61040    4.37050    2.30420
H      3.06310    2.70480    2.62550
C      0.18350   -0.42630    0.18780
C      0.52270   -1.92340    0.18110
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H      0.61040   -2.27430   -0.85100
C     -0.52260   -2.76530    0.91560
H     -0.69400   -2.33660    1.91000
H     -0.11230   -3.76830    1.04040
O     -1.74390   -2.90640    0.20900
H     -2.17280   -2.03720    0.15630
O      1.74620   -2.13640    0.89720
C      2.92460   -2.03660    0.18830
C      5.32070   -1.71810   -1.18320
C      3.93240   -1.21830    0.72830
C      3.14460   -2.72750   -0.99190
C      4.34270   -2.56380   -1.68710
C      5.12440   -1.05210    0.02790
H      2.36910   -3.37770   -1.37980
H      4.50120   -3.09690   -2.61660
H      5.90070   -0.40590    0.41600
O      3.65340   -0.63470    1.92490
C      4.61090    0.28690    2.43480
H      4.76960    1.11070    1.73270
H      4.19340    0.66740    3.36450
H      5.56120   -0.21290    2.63910
H     -0.01570   -0.13300    1.22680
H      6.25120   -1.57550   -1.71950


64 mannose_2_threo
XYZ file generated by Avogadro.
H      1.63920    1.93880    0.19460
O      1.46300    2.65760   -0.43060
C      0.18300    2.47280   -0.95210
H      0.06620    3.17280   -1.78580
O     -0.74920    2.79140    0.06990
C     -2.10150    2.77000   -0.38370
H     -2.21650    3.48440   -1.21290
C     -2.95310    3.20190    0.79150
H     -2.79490    2.50220    1.62080
H     -4.00520    3.18130    0.51000
O     -2.65500    4.53180    1.19340
H     -1.72560    4.55860    1.45000
C     -2.47270    1.36510   -0.86800
H     -2.42420    0.68010   -0.01630
O     -3.81070    1.32070   -1.33500
H     -3.87610    1.86400   -2.13150
C     -1.48780    0.90920   -1.94290
H     -1.60230    1.56480   -2.81360
O     -1.76610   -0.40100   -2.40470
H     -1.76900   -1.01500   -1.65630
C     -0.05210    1.04340   -1.43650
H      0.65130    0.82660   -2.24640
O      0.16240    0.16250   -0.33950
C      0.97010   -0.98570   -0.62170
C      0.63450   -2.01710    0.45270
H      0.82850   -1.60920    1.44650
C      1.43500   -3.29790    0.27580
```

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H      1.28010   -3.68870   -0.73650
H      2.49590   -3.09230    0.41450
O      1.06850   -4.26310    1.24860
H      0.12810   -4.44820    1.13520
O     -0.73610   -2.40690    0.31770
H      0.68090   -1.40170   -1.59300
C      2.43830   -0.63610   -0.64320
C      5.14130    0.03510   -0.66480
C      3.21410   -0.89380   -1.76330
C      3.01860   -0.04110    0.48640
C      4.36000    0.30410    0.47410
C      4.57100   -0.56210   -1.77270
H      2.76430   -1.35120   -2.63750
H      2.41040    0.15700    1.36260
H      5.19000   -0.75300   -2.64140
C     -1.73690   -1.74470    0.97730
C     -3.95410   -0.50620    2.13200
C     -3.01140   -1.87840    0.39070
C     -1.58950   -0.99780    2.13670
C     -2.70050   -0.37360    2.70910
C     -4.11400   -1.26490    0.97080
H     -0.61820   -0.87700    2.59710
H     -2.56970    0.21670    3.60790
H     -5.09160   -1.35770    0.51650
H     -4.81630   -0.02090    2.57310
O     -3.04590   -2.59800   -0.76910
C     -4.27070   -2.59360   -1.49840
H     -4.57370   -1.57020   -1.73410
H     -4.07120   -3.14060   -2.41710
H     -5.06020   -3.09630   -0.93520
O      6.46610    0.37200   -0.68070
H      6.68870    0.80550    0.15530
O      5.03040    0.90550    1.49590
C      4.26350    1.30210    2.63090
H      3.47080    1.99290    2.33230
H      4.95810    1.80190    3.30170
H      3.83220    0.43000    3.12720


64 mannose_2_erythro
XYZ file generated by Avogadro.
H     -1.92730   -0.72700   -4.09930
O     -1.26870   -0.61610   -3.40220
C     -1.59710   -1.46860   -2.34750
H     -1.79930   -2.48670   -2.70450
O     -2.76950   -0.95570   -1.73280
C     -3.25440   -1.78760   -0.68130
H     -3.45980   -2.79290   -1.07550
C     -4.53550   -1.14990   -0.18520
H     -4.31040   -0.13900    0.17700
H     -4.94240   -1.73670    0.63780
O     -5.52840   -1.11070   -1.19980
H     -5.17940   -0.58780   -1.93120
C     -2.20430   -1.87800    0.42150
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H	-2.07130	-0.88000	0.86020
O	-2.67930	-2.78400	1.40480
H	-1.97940	-2.89700	2.06060
C	-0.86770	-2.34830	-0.14600
H	-0.97480	-3.38550	-0.47600
O	0.12420	-2.34250	0.86650
H	0.27230	-1.41530	1.11100
C	-0.44970	-1.49310	-1.34160
H	0.44210	-1.92350	-1.80900
O	-0.18510	-0.18730	-0.86030
C	0.88650	0.51050	-1.49410
C	0.65340	1.98190	-1.14140
H	-0.26610	2.29900	-1.64010
C	1.79280	2.86720	-1.58650
H	2.66650	2.68930	-0.95180
H	2.05420	2.62150	-2.62160
O	1.36070	4.21820	-1.47880
H	2.12140	4.79010	-1.62510
O	0.49770	2.13200	0.27820
H	0.79670	0.42570	-2.58080
C	2.24190	-0.01590	-1.08030
C	4.77630	-0.90870	-0.33150
C	3.21140	-0.27130	-2.04160
C	2.54310	-0.20930	0.27350
C	3.79770	-0.66270	0.64610
C	4.48260	-0.71150	-1.66790
H	2.98000	-0.12920	-3.09180
H	1.79350	0.00840	1.02310
H	5.24640	-0.91760	-2.40850
C	-0.78500	2.20520	0.76700
C	-3.33210	2.35550	1.87870
C	-1.13400	1.35370	1.82960
C	-1.70480	3.12380	0.28360
C	-2.98520	3.19630	0.83160
C	-2.40900	1.43860	2.38320
H	-1.41130	3.78810	-0.52110
H	-3.69570	3.91540	0.44280
H	-2.69580	0.78730	3.19800
H	-4.32250	2.40250	2.31550
O	-0.17970	0.47080	2.24270
C	-0.49520	-0.32780	3.38270
H	0.38320	-0.93920	3.57650
H	-0.70260	0.30450	4.24910
H	-1.35430	-0.97250	3.17940
O	6.01700	-1.35460	0.03540
H	6.03460	-1.46770	0.99620
O	4.19400	-0.90380	1.93010
C	3.17520	-0.88410	2.92750
H	2.38660	-1.59660	2.67060
H	3.65650	-1.18060	3.85650
H	2.75380	0.11870	3.03330

64 glucose_2_threo
XYZ file generated by Avogadro.

H	-2.29300	-0.39230	-1.53290
O	-1.97870	0.48860	-1.79970
C	-1.83680	1.25000	-0.63560
H	-2.43130	0.81490	0.18090
O	-2.31870	2.54340	-0.94220
C	-2.30100	3.41850	0.18440
H	-2.88970	2.97240	0.99790
C	-2.94650	4.71250	-0.26520
H	-2.36790	5.13300	-1.09520
H	-2.95120	5.42480	0.55880
O	-4.29930	4.51090	-0.64840
H	-4.30540	3.88770	-1.38460
C	-0.86270	3.62440	0.65750
H	-0.28690	4.10570	-0.14400
O	-0.89870	4.45560	1.80650
H	0.00510	4.54960	2.13190
C	-0.23340	2.27800	0.97620
H	-0.76050	1.84030	1.83470
O	1.12850	2.50230	1.30730
H	1.53180	1.65000	1.52070
C	-0.37350	1.34350	-0.21290
H	0.21870	1.72640	-1.05340
O	0.07970	0.05860	0.17760
C	0.57580	-2.12790	-0.52830
C	0.82390	-0.65000	-0.81620
H	0.42510	-0.42170	-1.80760
C	1.36920	-3.07060	-1.41570
H	2.43670	-2.93190	-1.24000
C	2.28370	-0.27040	-0.76230
C	4.97440	0.43670	-0.63480
C	2.97080	0.07900	-1.91540
C	2.94670	-0.27180	0.47220
C	4.28340	0.08730	0.53940
C	4.32140	0.42890	-1.85270
H	2.45540	0.08700	-2.86940
H	2.40430	-0.54480	1.37060
H	4.87100	0.71090	-2.74320
O	1.13710	-2.82280	-2.79600
O	6.29390	0.79390	-0.57220
H	6.57530	0.78480	0.35360
O	5.03180	0.14190	1.67750
C	4.35850	-0.10310	2.91000
H	3.54360	0.61240	3.04790
H	5.10390	0.02940	3.69040
H	3.96880	-1.12300	2.93930
H	0.19980	-2.97170	-2.97030
H	0.81690	-2.32300	0.52120
H	1.10550	-4.10150	-1.16110
O	-0.82680	-2.33170	-0.75990
C	-1.56540	-2.98090	0.18840
C	-3.24100	-4.20490	2.04640
C	-1.07050	-3.97060	1.02470
C	-2.92000	-2.60680	0.27060
C	-3.75130	-3.21820	1.19920

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C     -1.91010   -4.58020    1.95980
H     -0.03350   -4.27360    0.94860
H     -4.79170   -2.93030    1.27320
H     -1.51210   -5.34960    2.61000
H     -3.89790   -4.67340    2.76900
O     -3.32330   -1.63790   -0.60190
C     -4.63880   -1.10780   -0.43890
H     -5.39080   -1.87200   -0.64530
H     -4.72450   -0.30180   -1.16540
H     -4.77000   -0.71380    0.57140

64 glucose_2_erythro
XYZ file generated by Avogadro.
H     -2.64350    1.89050    0.07780
O     -2.91300    1.63610   -0.81650
C     -3.14830    0.26180   -0.84890
H     -3.16750   -0.03460   -1.90340
O     -4.41870    0.01760   -0.26430
C     -4.83060   -1.34480   -0.36760
H     -4.81170   -1.65090   -1.42280
C     -6.24810   -1.40850    0.16040
H     -6.25820   -1.07020    1.20260
H     -6.60850   -2.43560    0.11940
O     -7.13160   -0.62570   -0.62970
H     -6.81310    0.28460   -0.60890
C     -3.87130   -2.22090    0.43210
H     -3.91700   -1.92700    1.48940
O     -4.27340   -3.57230    0.27960
H     -3.60930   -4.12400    0.71200
C     -2.45270   -2.01610   -0.07460
H     -2.39410   -2.38780   -1.10680
O     -1.58710   -2.76500    0.76110
H     -0.69000   -2.78680    0.37800
C     -2.09730   -0.53250   -0.07980
H     -2.07730   -0.15210    0.95040
O     -0.83680   -0.35350   -0.70410
C      1.51990   -0.47570   -0.53430
C      0.23750   -0.07710    0.19380
H      0.14930   -0.71580    1.07860
C      1.45780   -1.87710   -1.12150
H      0.71530   -1.90080   -1.91770
C      0.22970    1.36920    0.63060
C      0.14130    4.04270    1.40910
C      0.12880    1.70630    1.97240
C      0.28520    2.38020   -0.33880
C      0.23790    3.70930    0.04560
C      0.08880    3.04670    2.36490
H      0.07720    0.92420    2.72200
H      0.34500    2.11520   -1.38780
H      0.00920    3.32520    3.40920
O      1.07810   -2.85170   -0.15640
O      0.09500    5.35670    1.78840
H      0.11930    5.90880    0.99390
O      0.27400    4.78110   -0.79760
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C      0.31010    4.50900   -2.19640
H     -0.57200    3.93900   -2.49790
H      0.31130    5.47790   -2.68990
H      1.21720    3.95900   -2.45750
H      1.81390   -2.92840    0.47000
H      1.74040    0.23200   -1.34220
H      2.42950   -2.13420   -1.55570
O      2.53690   -0.38210    0.47650
C      3.83350   -0.47520    0.01640
C      6.46480   -0.69210   -0.82060
C      4.46070    0.61170   -0.56770
C      4.51630   -1.68910    0.18730
C      5.83950   -1.79270   -0.23270
C      5.78490    0.50670   -0.99190
H      3.89980    1.53330   -0.68300
H      6.38430   -2.71930   -0.10950
H      6.27630    1.35730   -1.44760
H      7.49470   -0.78450   -1.14430
O      3.80430   -2.69690    0.76450
C      4.42390   -3.98000    0.83920
H      3.67870   -4.64370    1.27210
H      5.30550   -3.94650    1.48260
H      4.69970   -4.33140   -0.15760

64 galactose_2_threo
XYZ file generated by Avogadro.
H     -1.03260   -1.85570    0.61580
O     -0.38330   -2.47880    0.98960
C      0.64690   -2.64640    0.05170
H      0.24980   -3.06720   -0.88450
O      1.53940   -3.56500    0.63930
C      2.63590   -3.87320   -0.22350
H      2.25190   -4.24950   -1.18130
C      3.42080   -4.99720    0.42690
H      4.25920   -5.26180   -0.21830
H      2.77240   -5.86960    0.53920
O      3.97240   -4.62740    1.69000
H      3.24680   -4.53250    2.31950
C      3.46630   -2.61780   -0.51670
H      4.25550   -2.89100   -1.22670
O      4.03370   -2.04920    0.65620
H      4.32300   -2.77890    1.22440
C      2.55560   -1.57690   -1.15390
H      2.19380   -1.98040   -2.10790
O      3.28880   -0.38390   -1.37660
H      2.67140    0.28900   -1.69560
C      1.36030   -1.32980   -0.24700
H      1.69620   -0.88100    0.69310
O      0.44340   -0.47320   -0.91160
C     -1.52130    0.77290   -0.50750
H     -1.63090    0.81360   -1.59770
C     -0.04510    0.63580   -0.15420
H      0.02450    0.40920    0.91380
C     -2.19550    1.98500    0.11420
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H     -1.71720    2.89340   -0.25480
H     -3.24630    2.00850   -0.19450
O     -2.09370    1.98340    1.53020
H     -2.67090    1.27070    1.84260
C      0.75140    1.88230   -0.45800
C      2.20110    4.19370   -1.01430
C      1.22030    2.67720    0.59150
C      1.01170    2.24710   -1.77530
C      1.74120    3.40220   -2.05260
C      1.94130    3.83170    0.31670
H      1.01970    2.38210    1.61450
H      0.65140    1.62980   -2.59120
H      1.95680    3.69960   -3.07210
O      2.91720    5.32630   -1.29110
H      3.15490    5.75650   -0.45750
O      2.45450    4.68390    1.24870
C      2.21310    4.37610    2.61960
H      2.68500    5.17100    3.19190
H      1.14040    4.35690    2.82490
H      2.66120    3.41480    2.88130
O     -2.13160   -0.43870   -0.01230
C     -3.39700   -0.71120   -0.48830
C     -5.95220   -1.31070   -1.36860
C     -4.49030   -0.49150    0.36300
C     -3.58240   -1.22250   -1.76100
C     -4.86760   -1.52380   -2.20930
C     -5.77290   -0.79710   -0.08360
H     -2.71200   -1.37980   -2.38900
H     -5.01350   -1.92480   -3.20460
H     -6.63070   -0.63720    0.55620
H     -6.95550   -1.54360   -1.70520
O     -4.19730    0.01630    1.59230
C     -5.29140    0.34510    2.44760
H     -5.85720   -0.55110    2.71030
H     -5.94670    1.07650    1.96930
H     -4.84760    0.77570    3.34230

64 galactose_2_erythro
XYZ file generated by Avogadro.
H     -2.52200    1.87560   -0.06530
O     -2.73390    1.69440   -0.99240
C     -3.10910    0.35730   -1.12310
H     -3.06750    0.11790   -2.19200
O     -4.44600    0.22860   -0.66450
C     -4.96880   -1.08410   -0.86390
H     -4.86700   -1.36140   -1.92230
C     -6.45130   -1.04320   -0.54320
H     -6.87670   -2.03230   -0.71670
H     -6.94320   -0.32610   -1.20480
O     -6.71310   -0.71590    0.82140
H     -6.50160    0.21610    0.95590
C     -4.18070   -2.10520   -0.04170
H     -4.56260   -3.10570   -0.27420
O     -4.24970   -1.86470    1.35920
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H     -5.15400   -1.58350    1.56670
C     -2.71040   -2.02310   -0.43150
H     -2.59770   -2.35680   -1.46630
O     -1.91450   -2.89710    0.35740
H     -2.06900   -2.68270    1.28820
C     -2.20690   -0.58490   -0.32770
H     -2.22560   -0.25890    0.72010
O     -0.89050   -0.51260   -0.84760
C      1.42460   -0.79530   -0.51170
H      1.68530   -0.13300   -1.34450
C      0.12730   -0.32190    0.13710
H     -0.07820   -0.96330    1.00120
C      1.34290   -2.22050   -1.04000
H      0.70190   -2.23650   -1.92530
H      2.34480   -2.53570   -1.34300
O      0.88610   -3.14540   -0.06580
H     -0.07490   -3.03390    0.04130
C      0.18530    1.11500    0.60080
C      0.20900    3.77660    1.42840
C      0.48530    2.12960   -0.31890
C     -0.10250    1.44430    1.91740
C     -0.08950    2.77770    2.33460
C      0.49800    3.45210    0.09020
H      0.68810    1.87860   -1.35320
H     -0.34050    0.66070    2.62850
H     -0.31160    3.04870    3.36010
O      0.22090    5.08330    1.83350
H      0.45830    5.64120    1.07940
O      0.77320    4.52460   -0.70660
C      1.09270    4.25600   -2.06940
H      0.25210    3.77270   -2.57270
H      1.29080    5.22230   -2.52690
H      1.98200    3.62430   -2.13670
O      2.42110   -0.68910    0.51530
C      3.71510   -0.55320    0.05900
C      6.34830   -0.28570   -0.76650
C      4.61000   -1.61790    0.24890
C      4.13700    0.62530   -0.53510
C      5.45880    0.76410   -0.95500
C      5.93290   -1.47440   -0.16590
H      3.41730    1.42880   -0.66050
H      5.78570    1.68680   -1.41810
H      6.64080   -2.28080   -0.02840
H      7.37940   -0.19030   -1.08530
O      4.10050   -2.73210    0.83920
C      4.98080   -3.83900    1.01220
H      4.38600   -4.62110    1.47840
H      5.35830   -4.18820    0.04820
H      5.81570   -3.57320    1.66470

60 arabinose_2_threo
XYZ file generated by Avogadro.
O     -4.58200   -0.43440   -1.78260
C     -3.31040   -0.94950   -1.45720
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H	-2.71480	-1.14740	-2.34940
O	-3.41160	-2.15840	-0.74110
C	-3.77980	-1.85520	0.62180
H	-4.85840	-1.99440	0.74330
C	-3.05390	-2.82100	1.53400
H	-3.28330	-3.84380	1.21560
H	-3.42500	-2.68770	2.55190
O	-1.65280	-2.60680	1.56850
C	-3.43640	-0.36150	0.83160
H	-2.79790	-0.21000	1.70130
O	-4.59220	0.43710	1.02670
H	-5.15540	0.33530	0.24710
C	-2.68660	0.01640	-0.45310
H	-2.82780	1.06740	-0.71820
O	-1.32270	-0.30550	-0.27700
C	-0.45910	0.26880	-1.24340
H	-0.91920	0.22950	-2.23840
C	-0.12240	1.71100	-0.91260
C	0.64740	4.31930	-0.30340
C	0.40210	2.53760	-1.89890
C	-0.27270	2.19370	0.39010
C	0.10580	3.49420	0.69370
C	0.79150	3.84140	-1.59390
H	0.51390	2.16710	-2.91260
H	-0.68450	1.54810	1.15520
H	1.20280	4.49730	-2.35240
C	0.80050	-0.58670	-1.32170
H	1.44700	-0.12470	-2.07540
C	0.56580	-2.04270	-1.73050
H	1.51300	-2.45910	-2.09040
H	-0.15400	-2.07420	-2.55100
O	0.06390	-2.85590	-0.67930
H	0.77590	-2.92640	-0.02210
O	1.44560	-0.53690	-0.04140
C	2.81610	-0.67690	-0.06450
C	5.57030	-0.97510	-0.01650
C	3.37500	-1.87190	0.41240
C	3.62800	0.35330	-0.50900
C	5.01410	0.20640	-0.48950
C	4.75930	-2.01650	0.43640
H	3.15810	1.26500	-0.86620
H	5.64850	1.01270	-0.83630
H	5.20950	-2.93010	0.80130
H	6.64630	-1.09980	0.00570
O	1.02620	5.60220	-0.00630
H	0.87030	5.76220	0.93510
O	0.00160	4.07830	1.92310
C	-0.53210	3.28440	2.97970
H	-1.55420	2.97410	2.74930
H	-0.53040	3.92030	3.86170
H	0.09360	2.40620	3.15460
O	2.48930	-2.82150	0.82770
C	3.01680	-4.07630	1.25620
H	3.58830	-4.54760	0.45370

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H      3.64560   -3.94670    2.13930
H      2.15360   -4.68950    1.50530
H     -1.30140   -2.59970    0.66130
H     -5.01850   -1.04930   -2.38560

60 arabinose_2_erythro
XYZ file generated by Avogadro.
O      3.39690    2.66300    1.02870
C      3.61310    1.28820    1.22060
H      3.34180    1.00510    2.23970
O      4.97900    0.94630    1.02440
C      5.11950    0.17630   -0.17830
H      5.22030    0.84590   -1.04240
C      6.33580   -0.70790   -0.06100
H      6.37270   -1.37400   -0.92460
H      6.25530   -1.31260    0.84880
O      7.54640    0.03810   -0.06280
C      3.80220   -0.58220   -0.26860
H      3.79550   -1.39630    0.46810
O      3.59800   -1.08280   -1.57280
H      2.87930   -1.74000   -1.53560
C      2.82150    0.50260    0.17740
H      2.60810    1.16320   -0.67210
O      1.61830    0.02540    0.74600
C      0.59810   -0.27530   -0.21450
H      1.04910   -0.41950   -1.19950
C     -0.41650    0.83710   -0.32590
C     -2.42120    2.74740   -0.64770
C     -0.45960    1.62770   -1.46680
C     -1.37140    1.02430    0.68150
C     -2.38400    1.95380    0.51170
C     -1.45480    2.59400   -1.62380
H      0.27000    1.47600   -2.25480
H     -1.34650    0.41030    1.57330
H     -1.50600    3.21030   -2.51390
C     -0.02680   -1.60100    0.23160
H     -0.34870   -1.51430    1.27320
C      0.93580   -2.77130    0.13800
H      0.41000   -3.68540    0.42730
H      1.76870   -2.61230    0.82330
O      1.50220   -2.91950   -1.16180
H      0.78960   -3.05930   -1.79830
O     -1.15880   -1.85120   -0.61620
C     -2.39600   -1.91380   -0.01790
C     -4.94520   -2.00520    1.09150
C     -3.44350   -1.18840   -0.61640
C     -2.63450   -2.67420    1.11610
C     -3.91110   -2.71830    1.67900
C     -4.71640   -1.24140   -0.05460
H     -1.81770   -3.23450    1.55750
H     -4.08630   -3.31470    2.56590
H     -5.53210   -0.68720   -0.49960
H     -5.94120   -2.03310    1.51710
O     -3.42910    3.65550   -0.82540
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H     -4.03110    3.60440   -0.06940
O     -3.41360    2.16360    1.38290
C     -3.48840    1.29970    2.51550
H     -4.39950    1.57420    3.04220
H     -3.54280    0.25400    2.19860
H     -2.62480    1.44770    3.16800
O     -3.12290   -0.46640   -1.72280
C     -4.13440    0.37840   -2.26350
H     -3.66100    0.93050   -3.07300
H     -4.96450   -0.21370   -2.65710
H     -4.50290    1.07700   -1.50720
H      7.56300    0.58310    0.73230
H      3.71680    3.13450    1.80760
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60 xylose_2_threo
XYZ file generated by Avogadro.
H     -3.77500    2.09060   -0.21000
O     -3.02280    2.10780   -0.81430
C     -1.91040    2.60200   -0.13380
H     -1.90400    2.26290    0.91030
O     -1.98390    4.02140   -0.15060
C     -0.89120    4.63100    0.52690
H     -1.07680    5.70400    0.52790
H     -0.83950    4.27460    1.56360
C      0.41470    4.31300   -0.18830
H      0.37990    4.71050   -1.20980
O      1.46060    4.92850    0.54570
H      2.29670    4.69920    0.12210
C      0.58950    2.80590   -0.24840
H      0.71760    2.44800    0.78120
O      1.75020    2.50300   -1.00360
H      1.92630    1.55790   -0.86980
C     -0.64860    2.17010   -0.88030
H     -0.74120    2.53410   -1.90840
O     -0.51060    0.76390   -1.00380
C     -0.47710   -0.00530    0.20320
H     -0.23100    0.62550    1.06120
C     -1.81100   -0.66800    0.45490
C     -4.27100   -1.89220    0.90500
C     -2.40250   -1.43340   -0.55800
C     -2.45070   -0.52540    1.67730
C     -3.68450   -1.13900    1.90420
C     -3.62670   -2.04310   -0.33600
H     -1.90400   -1.53620   -1.51430
H     -1.99420    0.07190    2.45930
H     -4.20000   -1.03270    2.85160
C      0.65210   -1.01560    0.02470
H      0.50350   -1.55650   -0.91750
C      0.77540   -2.01240    1.16640
H      1.59380   -2.70750    0.94940
H     -0.14500   -2.59250    1.24340
O      0.98960   -1.36780    2.41310
H      1.89620   -1.02800    2.38960
O      1.85810   -0.22670   -0.06840
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C      2.95560   -0.88200   -0.58940
C      5.21400   -2.12110   -1.60210
C      3.96140   -1.30890    0.29010
C      3.08170   -1.07030   -1.95500
C      4.21640   -1.69580   -2.46950
C      5.09560   -1.93090   -0.22480
H      2.28340   -0.72070   -2.60150
H      4.31650   -1.84290   -3.53770
H      5.88460   -2.26790    0.43430
H      6.10140   -2.60650   -1.99030
O     -5.48260   -2.48940    1.12510
H     -5.74910   -2.95940    0.32220
O     -4.30500   -2.80950   -1.23750
C     -3.70510   -2.99700   -2.51700
H     -3.57890   -2.03860   -3.02580
H     -4.39080   -3.62610   -3.07940
H     -2.73920   -3.49770   -2.41790
O      3.74040   -1.06980    1.61200
C      4.69660   -1.57660    2.54270
H      4.31290   -1.32250    3.52820
H      5.66890   -1.10340    2.39130
H      4.78740   -2.66090    2.44760

60 xylose_2_erythro
XYZ file generated by Avogadro.
H      0.98410    4.05910   -0.31840
O      0.67750    3.69820    0.52770
C      0.81110    2.29830    0.49880
H      0.13970    1.89030    1.25600
O      2.10530    1.88160    0.88600
C      3.13780    2.27180   -0.02420
H      3.19560    3.36320   -0.08320
H      4.06940    1.89340    0.39570
C      2.91400    1.68350   -1.40800
H      3.65520    2.10940   -2.08960
O      3.11200    0.27540   -1.42060
H      2.36760   -0.13260   -0.95170
C      1.51120    2.04940   -1.92380
H      1.30320    1.48310   -2.83730
O      1.41230    3.44970   -2.15960
H      2.10330    3.71580   -2.77900
C      0.45030    1.71440   -0.87120
H     -0.52730    2.09990   -1.17660
O      0.41730    0.30880   -0.69380
C     -0.56700   -0.39550   -1.44440
H     -0.51830   -0.10300   -2.49950
C     -1.96050   -0.13110   -0.92230
C     -4.54580    0.27160    0.03690
C     -2.18120   -0.01650    0.45540
C     -3.02970   -0.03160   -1.80360
C     -4.32540    0.16400   -1.32380
C     -3.46750    0.18670    0.93230
H     -1.34050   -0.08410    1.13500
H     -2.85760   -0.10280   -2.87170
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H     -5.16850    0.24750   -1.99960
C     -0.11930   -1.86240   -1.35130
H      0.81780   -1.94790   -1.90820
C     -1.12450   -2.85290   -1.90350
H     -2.05440   -2.79890   -1.32740
H     -0.70730   -3.85940   -1.80650
O     -1.34870   -2.52260   -3.26740
H     -2.01280   -3.12560   -3.61840
O      0.10350   -2.21850    0.01940
C      1.40970   -2.15770    0.45800
C      4.02400   -2.00370    1.39140
C      1.69480   -1.39010    1.60130
C      2.42120   -2.85930   -0.18090
C      3.73500   -2.78120    0.27940
C      3.00960   -1.31390    2.05640
H      2.17300   -3.46510   -1.04560
H      4.51800   -3.32770   -0.23160
H      3.25210   -0.71430    2.92350
H      5.04080   -1.92810    1.75770
O     -5.81540    0.47600    0.50760
H     -5.77880    0.56130    1.47060
O     -3.80670    0.32110    2.24770
C     -2.73420    0.36140    3.18470
H     -2.06610    1.19630    2.95680
H     -2.17640   -0.57860    3.17300
H     -3.19080    0.50790    4.16080
O      0.64400   -0.75980    2.18850
C      0.91590   -0.00560    3.36760
H      1.32580   -0.64890    4.15010
H     -0.03870    0.39940    3.69390
H      1.60800    0.81210    3.15560


64 mannose_3_threo
XYZ file generated by Avogadro.
H     -0.27780    4.01950    2.48700
O     -0.03560    4.48900    1.67560
C     -0.29210    3.63680    0.60240
H      0.23720    4.02870   -0.27150
O     -1.69440    3.66060    0.35690
C     -2.06850    2.94030   -0.81840
H     -1.52050    3.34450   -1.68120
C     -3.55600    3.15520   -1.00270
H     -4.08400    2.76970   -0.12240
H     -3.89690    2.61190   -1.88360
O     -3.86460    4.52560   -1.21230
H     -3.55850    5.01580   -0.43990
C     -1.72510    1.46470   -0.63970
H     -2.34480    1.05540    0.17020
O     -2.00010    0.77840   -1.84910
H     -2.16020   -0.14960   -1.61670
C     -0.25310    1.31110   -0.27300
H      0.34640    1.62330   -1.13750
O     -0.00040   -0.05000    0.03580
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C      0.13980    2.20120    0.90300
H      1.22320    2.17360    1.03580
O     -0.41830    1.77460    2.13660
H     -1.38240    1.79860    2.07610
C      0.79300   -0.74790   -0.91960
H      0.43650   -0.52230   -1.92990
C      0.54360   -2.22730   -0.63400
H      0.79300   -2.42290    0.41340
C      1.33040   -3.17670   -1.51830
H      2.39960   -3.03070   -1.36130
H      1.07460   -4.20350   -1.24030
C      2.25350   -0.37320   -0.80430
C      4.95380    0.26540   -0.56540
C      3.04030   -0.22220   -1.93790
C      2.81840   -0.20040    0.46510
C      4.16010    0.12630    0.58580
C      4.39500    0.09150   -1.81840
H      2.60050   -0.34700   -2.92140
H      2.19570   -0.30670    1.34510
H      5.02270    0.21590   -2.69300
O     -0.85970   -2.45190   -0.85680
O      1.07720   -2.95570   -2.89960
H      0.14160   -3.12780   -3.06130
C     -1.61040   -2.90990    0.19370
C     -3.25730   -3.78150    2.26030
C     -2.88300   -2.33620    0.36460
C     -1.18400   -3.91780    1.04570
C     -2.00550   -4.35210    2.08650
C     -3.70100   -2.77610    1.39940
H     -0.20900   -4.36600    0.89150
H     -1.66140   -5.13760    2.74790
H     -4.68020   -2.33970    1.54430
H     -3.90380   -4.11240    3.06400
O     -3.22910   -1.36460   -0.52710
C     -4.46240   -0.68010   -0.30820
H     -4.47360   -0.21390    0.68010
H     -5.30670   -1.36550   -0.40880
H     -4.51740    0.08550   -1.08010
O      6.27980    0.58550   -0.45060
H      6.49620    0.68360    0.48740
O      4.81750    0.34230    1.76150
C      4.04330    0.29170    2.95750
H      3.24130    1.03370    2.92590
H      4.72950    0.52280    3.76860
H      3.62240   -0.70590    3.10140

64 mannose_3_erythro
XYZ file generated by Avogadro.
H     -5.49390   -1.50330    2.68980
O     -4.83990   -1.77130    2.03230
C     -4.13950   -0.64210    1.60430
H     -3.79130   -0.03930    2.45260
O     -5.01940    0.14080    0.81480
C     -4.41190    1.34630    0.35370
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H	-4.03390	1.92310	1.20950
C	-5.49200	2.15740	-0.33420
H	-5.07480	3.10910	-0.66270
H	-6.29160	2.35610	0.38570
O	-6.00780	1.50950	-1.48870
H	-6.41120	0.67840	-1.21140
C	-3.24650	0.99200	-0.56500
H	-3.63030	0.46140	-1.44320
O	-2.61410	2.20090	-0.95560
H	-1.80860	1.96460	-1.43400
C	-2.25720	0.09370	0.16310
H	-1.78650	0.67670	0.96620
O	-1.29340	-0.27880	-0.80600
C	-2.94190	-1.11920	0.78990
H	-2.26000	-1.63150	1.47690
O	-3.33790	-1.99980	-0.25190
H	-3.87370	-2.70430	0.13700
C	-0.08780	-0.83980	-0.28470
H	-0.32210	-1.62280	0.44400
C	0.57340	-1.51660	-1.49200
H	0.83620	-0.76640	-2.24320
C	-0.35360	-2.52750	-2.15450
H	-1.09400	-1.98950	-2.75020
H	0.24450	-3.14570	-2.82630
C	0.76950	0.20370	0.39210
C	2.46360	2.04860	1.61150
C	1.05970	0.10410	1.74490
C	1.29960	1.26480	-0.35580
C	2.15700	2.17100	0.24340
C	1.90500	1.03050	2.36000
H	0.64680	-0.71440	2.32520
H	1.06640	1.35100	-1.41070
H	2.14640	0.96080	3.41440
O	1.75660	-2.20800	-1.06170
O	-0.99670	-3.39480	-1.23190
H	-1.77880	-2.93480	-0.88250
C	2.90850	-1.45270	-0.96930
C	5.19190	0.09970	-0.66260
C	3.58290	-1.44460	0.26300
C	3.40670	-0.73380	-2.04360
C	4.54880	0.05300	-1.89170
C	4.71970	-0.65440	0.41350
H	2.88450	-0.77090	-2.99310
H	4.92480	0.62350	-2.73220
H	5.23750	-0.61670	1.36300
H	6.07440	0.71420	-0.52960
O	3.04740	-2.22260	1.24120
C	3.64490	-2.15010	2.53100
H	3.04840	-2.79510	3.17260
H	4.67560	-2.51230	2.50250
H	3.62250	-1.12630	2.91280
O	3.32020	2.93800	2.20050
H	3.60260	3.58340	1.53700
O	2.77500	3.21360	-0.38470

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C      2.51950    3.37610   -1.77730
H      2.83760    2.48960   -2.33200
H      3.10440    4.23760   -2.09070
H      1.45770    3.56540   -1.95270

64 glucose_3_threo
XYZ file generated by Avogadro.
H     -2.29300   -0.39230   -1.53290
O     -1.97870    0.48860   -1.79970
C     -1.83680    1.25000   -0.63560
H     -2.43130    0.81490    0.18090
O     -2.31870    2.54340   -0.94220
C     -2.30100    3.41850    0.18440
H     -2.88970    2.97240    0.99790
C     -2.94650    4.71250   -0.26520
H     -2.36790    5.13300   -1.09520
H     -2.95120    5.42480    0.55880
O     -4.29930    4.51090   -0.64840
H     -4.30540    3.88770   -1.38460
C     -0.86270    3.62440    0.65750
H     -0.28690    4.10570   -0.14400
O     -0.89870    4.45560    1.80650
H      0.00510    4.54960    2.13190
C     -0.23340    2.27800    0.97620
H     -0.76050    1.84030    1.83470
O      1.12850    2.50230    1.30730
H      1.53180    1.65000    1.52070
C     -0.37350    1.34350   -0.21290
H      0.21870    1.72640   -1.05340
O      0.07970    0.05860    0.17760
C      0.57580   -2.12790   -0.52830
C      0.82390   -0.65000   -0.81620
H      0.42510   -0.42170   -1.80760
C      1.36920   -3.07060   -1.41570
H      2.43670   -2.93190   -1.24000
C      2.28370   -0.27040   -0.76230
C      4.97440    0.43670   -0.63480
C      2.97080    0.07900   -1.91540
C      2.94670   -0.27180    0.47220
C      4.28340    0.08730    0.53940
C      4.32140    0.42890   -1.85270
H      2.45540    0.08700   -2.86940
H      2.40430   -0.54480    1.37060
H      4.87100    0.71090   -2.74320
O      1.13710   -2.82280   -2.79600
O      6.29390    0.79390   -0.57220
H      6.57530    0.78480    0.35360
O      5.03180    0.14190    1.67750
C      4.35850   -0.10310    2.91000
H      3.54360    0.61240    3.04790
H      5.10390    0.02940    3.69040
H      3.96880   -1.12300    2.93930
H      0.19980   -2.97170   -2.97030
H      0.81690   -2.32300    0.52120
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H      1.10550   -4.10150   -1.16110
O     -0.82680   -2.33170   -0.75990
C     -1.56540   -2.98090    0.18840
C     -3.24100   -4.20490    2.04640
C     -1.07050   -3.97060    1.02470
C     -2.92000   -2.60680    0.27060
C     -3.75130   -3.21820    1.19920
C     -1.91010   -4.58020    1.95980
H     -0.03350   -4.27360    0.94860
H     -4.79170   -2.93030    1.27320
H     -1.51210   -5.34960    2.61000
H     -3.89790   -4.67340    2.76900
O     -3.32330   -1.63790   -0.60190
C     -4.63880   -1.10780   -0.43890
H     -5.39080   -1.87200   -0.64530
H     -4.72450   -0.30180   -1.16540
H     -4.77000   -0.71380    0.57140


64 glucose_3_erythro
XYZ file generated by Avogadro.
H     -4.54670   -4.33070    1.20680
O     -3.82480   -4.06760    0.62320
C     -3.63520   -2.68970    0.74050
H     -3.71170   -2.37020    1.78830
O     -4.65090   -2.04850   -0.01520
C     -4.58910   -0.62560    0.04920
H     -4.62100   -0.29790    1.09770
C     -5.82020   -0.09480   -0.65810
H     -5.82360    0.99390   -0.61070
H     -6.70900   -0.47000   -0.14200
O     -5.85350   -0.45230   -2.03300
H     -5.88980   -1.41450   -2.08920
C     -3.27790   -0.15970   -0.57810
H     -3.25730   -0.45790   -1.63300
O     -3.21880    1.25270   -0.46180
H     -2.34890    1.54200   -0.76940
C     -2.11080   -0.81640    0.14290
H     -2.07270   -0.43210    1.17080
O     -0.91570   -0.46780   -0.54850
C     -2.26680   -2.33530    0.17630
H     -2.21130   -2.72350   -0.84900
O     -1.29190   -2.94660    0.99860
H     -0.41630   -2.88740    0.57250
C      0.19020   -0.12150    0.28240
H      0.21150   -0.76750    1.16520
C      1.44740   -0.40960   -0.53790
H      1.52890    0.30090   -1.36950
C      1.47970   -1.82230   -1.09950
H      0.67710   -1.94010   -1.82600
H      2.43170   -1.98920   -1.61440
C      0.10890    1.31900    0.73080
C     -0.07680    3.98300    1.52690
C     -0.05180    2.32590   -0.23160
```

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C      0.17530    1.65500    2.07440
C      0.08900    2.99100    2.47400
C     -0.15570    3.65000    0.16240
H     -0.10350    2.06120   -1.28220
H      0.29340    0.87630    2.81980
H      0.13960    3.26910    3.52020
O      2.52710   -0.19720    0.38550
C      3.78950   -0.20250   -0.16940
C      6.36400   -0.24010   -1.19030
C      4.26690    0.89150   -0.87010
C      4.59560   -1.33410    0.02690
C      5.89010   -1.34720   -0.48480
C      5.56180    0.87610   -1.38750
H      3.61480    1.74870   -1.00120
H      6.52960   -2.20830   -0.34300
H      5.93630    1.73270   -1.93420
H      7.37280   -0.26150   -1.58480
O      1.28870   -2.80790   -0.09080
H      2.07500   -2.78880    0.47640
O      4.02420   -2.35880    0.72020
C      4.78550   -3.55620    0.87120
H      4.14390   -4.24860    1.41150
H      5.04320   -3.97360   -0.10480
H      5.69240   -3.36510    1.44880
O     -0.17100    5.29070    1.91890
H     -0.28570    5.84380    1.13330
O     -0.33410    4.71200   -0.67320
C     -0.52590    4.42580   -2.05640
H     -1.39460    3.77710   -2.19440
H      0.36380    3.95380   -2.47920
H     -0.69900    5.38440   -2.53960

64 galactose_3_threo
XYZ file generated by Avogadro.
H      3.80700   -1.70950    2.27200
O      3.13740   -2.33140    2.59000
C      2.10120   -2.38540    1.65400
H      1.32010   -3.02290    2.08380
O      2.60500   -2.97070    0.46840
C      1.58520   -3.16690   -0.51230
H      0.77430   -3.76200   -0.07100
C      2.21090   -3.94670   -1.64950
H      3.06100   -3.39210   -2.05630
H      1.46990   -4.08570   -2.43790
O      2.61880   -5.24130   -1.22720
H      3.29680   -5.12910   -0.55050
C      1.00600   -1.83040   -0.96230
H      0.17090   -2.04050   -1.64150
O      2.00560   -1.08320   -1.63670
H      1.90070   -0.13850   -1.43430
C      0.48170   -1.07990    0.26430
H     -0.38820   -1.62280    0.65670
O      0.13750    0.26010   -0.04030
C      1.54390   -0.99600    1.34950
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```
H      2.37130   -0.36290    0.99740
O      0.94630   -0.43450    2.50390
H      1.64200   -0.25950    3.14900
C     -0.83790    0.45730   -1.06110
H     -0.45840    0.08070   -2.01940
C     -0.98090    1.97480   -1.16320
H     -1.37940    2.36400   -0.22180
C     -1.87270    2.40150   -2.31230
H     -1.46250    2.02120   -3.25480
H     -2.87450    1.99420   -2.17590
O     -2.00010    3.81480   -2.35370
H     -1.11180    4.18420   -2.43450
C     -2.15090   -0.21380   -0.73630
C     -4.58240   -1.41800   -0.11610
C     -2.78950   -1.01880   -1.66780
C     -2.72720   -0.00860    0.52440
C     -3.93590   -0.60930    0.83590
C     -4.01230   -1.61850   -1.35920
H     -2.33680   -1.18380   -2.63960
H     -2.21350    0.60780    1.25300
H     -4.52490   -2.25090   -2.07450
O      0.30960    2.55720   -1.41300
O     -5.77550   -2.01380    0.18830
H     -6.01250   -1.79090    1.09950
O     -4.59270   -0.49420    2.02500
C     -3.97340    0.29610    3.03730
H     -3.86290    1.33010    2.70270
H     -2.99730   -0.11710    3.30230
H     -4.63800    0.25540    3.89690
C      1.03110    2.97340   -0.31620
C      2.57120    3.79880    1.84530
C      2.33510    2.47450   -0.15860
C      0.52270    3.89110    0.58850
C      1.29030    4.30340    1.67820
C      3.09960    2.88900    0.92720
H     -0.47690    4.28280    0.43550
H      0.88340    5.01880    2.38220
H      4.10250    2.50870    1.06850
H      3.17700    4.10990    2.68780
O      2.76430    1.59480   -1.10850
C      4.11280    1.13510   -1.01160
H      4.26040    0.55560   -0.09660
H      4.80690    1.97790   -1.03740
H      4.27340    0.49990   -1.87960

64 galactose_3_erythro
XYZ file generated by Avogadro.
H     -4.22650   -3.82040    0.96490
O     -4.32380   -3.21000    1.70860
C     -3.91730   -1.93860    1.29830
H     -3.88490   -1.31280    2.19800
O     -4.89490   -1.43750    0.40170
C     -4.66130   -0.08410    0.01630
H     -4.59670    0.54450    0.91500
```

C	-5.85990	0.38960	-0.78950
H	-5.66700	1.41830	-1.11260
H	-6.74200	0.38890	-0.14820
O	-6.16410	-0.44480	-1.89910
H	-5.34520	-0.56240	-2.40000
C	-3.33340	0.05210	-0.72140
H	-3.13160	1.11710	-0.87930
O	-3.42340	-0.61410	-1.97790
H	-2.57090	-0.52330	-2.42310
C	-2.21700	-0.54530	0.12710
H	-2.06580	0.09910	1.00130
O	-1.02730	-0.60890	-0.64960
C	-2.55890	-1.95210	0.60710
H	-2.62760	-2.62440	-0.25870
O	-1.59930	-2.42550	1.53300
H	-0.73630	-2.52140	1.08860
C	0.11750	-0.03690	-0.03400
H	0.16120	-0.34320	1.01670
C	1.33220	-0.64590	-0.73680
H	1.43550	-0.23100	-1.74660
C	1.25480	-2.16170	-0.83120
H	0.44280	-2.43910	-1.50160
H	2.18890	-2.55090	-1.24930
O	0.99050	-2.76620	0.42980
H	1.78580	-2.64630	0.97050
C	0.10380	1.47410	-0.11100
C	0.13060	4.25530	-0.26190
C	-0.31190	2.11770	-1.27130
C	0.53520	2.22630	0.98520
C	0.55560	3.61250	0.91050
C	-0.30130	3.50950	-1.34540
H	-0.65370	1.53590	-2.12060
H	0.85110	1.71890	1.88900
H	-0.62720	4.02780	-2.23980
O	2.44620	-0.23240	0.07040
O	0.13420	5.62300	-0.33650
H	0.45490	5.97900	0.50410
O	0.95580	4.45300	1.90830
C	1.41050	3.85690	3.12060
H	2.27940	3.22180	2.93320
H	1.68930	4.68100	3.77280
H	0.61310	3.27150	3.58380
C	3.69080	-0.48420	-0.46590
C	6.23060	-0.98950	-1.44920
C	4.41670	-1.58120	0.02240
C	4.23080	0.34510	-1.43370
C	5.50850	0.09370	-1.93260
C	5.69350	-1.83020	-0.47310
H	3.64000	1.18420	-1.78590
H	5.93190	0.74360	-2.68830
H	6.27030	-2.67020	-0.10950
H	7.22530	-1.19290	-1.82770
O	3.79110	-2.33620	0.96820
C	4.45310	-3.52190	1.40610

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H      3.77350   -3.99730    2.10990
H      5.39170   -3.27690    1.90770
H      4.64160   -4.19010    0.56270

60 arabinose_3_threo
XYZ file generated by Avogadro.
O      3.67630    3.70940    0.79480
C      3.08480    3.33090   -0.42390
H      3.75670    3.53640   -1.25800
O      1.88900    4.06190   -0.65660
C      0.80020    3.27840   -0.17270
H      0.75410    3.31730    0.92360
C     -0.50490    3.78140   -0.76030
H     -0.47910    3.66950   -1.84990
H     -0.63220    4.83820   -0.52100
O     -1.61700    3.09480   -0.20070
C      1.18380    1.87330   -0.61790
H      1.01120    1.77330   -1.69770
O      0.40260    0.94150    0.09620
C      2.69180    1.84660   -0.34250
H      2.86380    1.48230    0.67590
O      3.46760    1.11650   -1.27620
C      0.14590   -0.28860   -0.57400
H     -0.07970   -0.08710   -1.62710
C      1.32850   -1.22340   -0.48990
C      3.54680   -2.89930   -0.33330
C      1.77910   -1.89640   -1.61800
C      1.98840   -1.39050    0.73540
C      3.09650   -2.21950    0.81300
C      2.88900   -2.74010   -1.53880
H      1.27410   -1.75660   -2.56750
H      1.63960   -0.85320    1.60870
H      3.25870   -3.26590   -2.41120
C     -1.11420   -0.83220    0.08630
H     -0.96300   -0.86830    1.17200
C     -1.53550   -2.20560   -0.40800
H     -2.43620   -2.51860    0.13160
H     -0.74590   -2.92620   -0.18970
O     -1.76520   -2.22280   -1.80880
H     -2.58450   -1.72680   -1.95390
O     -2.13030    0.14410   -0.22230
C     -3.27210    0.07590    0.54670
C     -5.61280   -0.00460    2.02510
C     -4.42660   -0.48860   -0.01630
C     -3.29240    0.59180    1.83150
C     -4.46760    0.55140    2.58030
C     -5.60120   -0.52440    0.73010
H     -2.38000    1.02260    2.23060
H     -4.48370    0.95570    3.58480
H     -6.50350   -0.95310    0.31450
H     -6.53270   -0.03910    2.59650
O      4.64330   -3.71210   -0.26010
H      4.99720   -3.67890    0.64010
O      3.83350   -2.45030    1.93510
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C      3.47880   -1.72110    3.10810
H      3.55250   -0.64620    2.92560
H      4.19350   -2.01740    3.87190
H      2.46660   -1.97760    3.42830
O     -4.30030   -0.96740   -1.28520
C     -5.42390   -1.64270   -1.84930
H     -5.70940   -2.49650   -1.23060
H     -6.26850   -0.95940   -1.95870
H     -5.10030   -1.98740   -2.82880
H     -1.50480    2.13750   -0.31480
H      4.02170    4.60540    0.69520
H      3.24500    0.17960   -1.19080

60 arabinose_3_erythro
XYZ file generated by Avogadro.
O     -3.75250   -4.48620   -0.61470
C     -3.53890   -3.32270    0.14060
H     -3.78770   -3.50390    1.18900
O     -4.35860   -2.25140   -0.32660
C     -3.53970   -1.20600   -0.87390
H     -3.34740   -1.38980   -1.93840
C     -4.24870    0.12110   -0.72400
H     -5.18040    0.10110   -1.29800
H     -3.60750    0.90640   -1.13130
O     -4.50410    0.45340    0.63270
C     -2.24760   -1.34390   -0.08550
H     -2.38930   -0.94290    0.92500
O     -1.17530   -0.69690   -0.73470
C     -2.09690   -2.85700   -0.03020
H     -1.73460   -3.19880   -1.00830
O     -1.27740   -3.35660    1.00490
C     -0.18490   -0.20380    0.16520
H     -0.14640   -0.83360    1.05910
C     -0.49960    1.21460    0.57810
C     -1.10470    3.83230    1.31360
C     -0.45760    1.59550    1.91130
C     -0.84830    2.15130   -0.40370
C     -1.15270    3.45290   -0.03960
C     -0.75650    2.90880    2.28080
H     -0.19560    0.86830    2.67190
H     -0.88890    1.84710   -1.44290
H     -0.73270    3.22040    3.31850
C      1.15590   -0.34800   -0.55070
H      1.18740    0.30820   -1.42920
C      1.42210   -1.78110   -0.99020
H      2.41480   -1.84550   -1.44780
H      0.68490   -2.07060   -1.73800
O      1.32090   -2.70490    0.08870
H      2.07590   -2.53700    0.67320
O      2.13180    0.08320    0.41060
C      3.41050    0.24400   -0.08010
C      6.01320    0.55610   -0.97600
C      4.36520   -0.74290    0.20880
C      3.75700    1.36900   -0.80850
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C      5.06550    1.52960   -1.26280
C      5.67250   -0.58040   -0.24120
H      2.99200    2.11120   -1.01070
H      5.33670    2.41060   -1.83110
H      6.42440   -1.32870   -0.02850
H      7.03360    0.67110   -1.32180
O     -1.41080    5.11640    1.67680
H     -1.66130    5.61300    0.88490
O     -1.51550    4.45060   -0.89640
C     -1.63030    4.11380   -2.27640
H     -1.94020    5.02490   -2.78250
H     -0.66850    3.77930   -2.67190
H     -2.38360    3.33510   -2.41890
O      3.91960   -1.81260    0.92580
C      4.83310   -2.88780    1.14030
H      4.27110   -3.65150    1.67340
H      5.67830   -2.55970    1.74890
H      5.18840   -3.28560    0.18710
H     -5.05490   -0.24420    1.00840
H     -4.57380   -4.89790   -0.32070
H     -0.35240   -3.15850    0.76650

60 xylose_3_threo
XYZ file generated by Avogadro.
H      4.31010    4.93640    0.07270
O      3.81840    4.29350    0.59780
C      2.76510    3.79480   -0.17140
H      3.07970    3.63510   -1.21140
O      1.71050    4.74120   -0.14320
C      0.60010    4.32030   -0.92890
H     -0.13330    5.12490   -0.90150
H      0.91160    4.15240   -1.96780
C      0.01650    3.04020   -0.35070
H     -0.32810    3.23260    0.67290
O     -1.07050    2.64430   -1.16880
H     -1.47780    1.85680   -0.77060
C      1.09470    1.96280   -0.29900
H      1.39890    1.70440   -1.32190
O      0.58100    0.81300    0.35770
C      2.31230    2.47560    0.44920
H      2.05190    2.66200    1.49860
O      3.33530    1.50190    0.35100
C      0.22880   -0.28230   -0.49060
H      0.00150    0.08730   -1.49510
C      1.35210   -1.28640   -0.57690
C      3.40520   -3.16140   -0.72080
C      1.93650   -1.76970    0.60140
C      1.79950   -1.74140   -1.80850
C      2.82790   -2.68370   -1.88150
C      2.96100   -2.69940    0.53140
H      1.59020   -1.40290    1.56030
H      1.34990   -1.36240   -2.71960
H      3.19160   -3.04660   -2.83570
C     -1.05250   -0.87040    0.09010
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H     -0.90710   -1.07460    1.15760
C     -1.52610   -2.13580   -0.60640
H     -2.44280   -2.48960   -0.12170
H     -0.76860   -2.91350   -0.50020
O     -1.74620   -1.92850   -1.99340
H     -2.53960   -1.37680   -2.06210
O     -2.03840    0.17330   -0.06440
C     -3.19230    0.02600    0.67510
C     -5.55590   -0.21140    2.09790
C     -4.35880   -0.38640    0.01380
C     -3.21110    0.31380    2.02900
C     -4.39840    0.19340    2.74980
C     -5.54520   -0.50160    0.73310
H     -2.28940    0.63120    2.50500
H     -4.41400    0.41930    3.80870
H     -6.45710   -0.81480    0.24240
H     -6.48510   -0.30560    2.64710
O      4.41700   -4.08050   -0.79200
H      4.71330   -4.28850    0.10530
O      3.61640   -3.23850    1.59920
C      3.23090   -2.78880    2.89560
H      3.39360   -1.71280    2.99190
H      3.86540   -3.32280    3.59880
H      2.18220   -3.02640    3.08800
O     -4.23150   -0.64530   -1.31730
C     -5.37030   -1.17120   -1.99840
H     -5.04490   -1.35450   -3.02000
H     -6.18840   -0.44810   -1.99570
H     -5.69420   -2.10720   -1.53790
H      4.07410    1.78900    0.90120

60 xylose_3_erythro
XYZ file generated by Avogadro.
H     -6.56070   -1.74200    1.35410
O     -5.80090   -1.99770    0.81720
C     -5.04370   -0.86040    0.53060
H     -4.99670   -0.18920    1.39830
O     -5.64830   -0.18190   -0.55520
C     -4.93740    1.00450   -0.88610
H     -5.49600    1.50260   -1.67690
H     -4.88000    1.66800   -0.01410
C     -3.53100    0.66530   -1.36230
H     -3.59120    0.05640   -2.27220
O     -2.88240    1.89630   -1.63010
H     -1.96470    1.71270   -1.86990
C     -2.80010   -0.13210   -0.28940
H     -2.62660    0.52070    0.57610
O     -1.55660   -0.58530   -0.81460
C     -3.64570   -1.32250    0.13700
H     -3.74110   -2.02090   -0.70380
O     -3.01020   -1.95590    1.23710
C     -0.43210   -0.39960    0.04160
H     -0.72210   -0.58940    1.08090
C      0.13060    0.99910   -0.07540
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C	1.28680	3.52360	-0.30430
C	0.47100	1.71370	1.07440
C	0.36710	1.55420	-1.32970
C	0.93520	2.82060	-1.44450
C	1.05470	2.97010	0.96330
H	0.28620	1.27630	2.04830
H	0.12270	0.99300	-2.22680
H	1.12700	3.26620	-2.41390
C	0.60940	-1.45230	-0.35380
H	1.03290	-1.20320	-1.33430
C	0.04750	-2.86430	-0.40870
H	0.86160	-3.56090	-0.61860
H	-0.66870	-2.92860	-1.23220
O	-0.54310	-3.26650	0.81650
H	-1.38560	-2.79210	0.92540
O	1.62990	-1.34600	0.65530
C	2.86120	-1.85710	0.30230
C	5.37930	-2.82870	-0.33880
C	3.75270	-1.04890	-0.42520
C	3.23780	-3.12540	0.71060
C	4.50290	-3.61920	0.39130
C	5.01310	-1.54540	-0.74790
H	2.52900	-3.71460	1.28210
H	4.79350	-4.61170	0.71270
H	5.71420	-0.93970	-1.30650
H	6.36430	-3.20060	-0.59520
O	1.86390	4.75970	-0.42170
H	2.05440	5.09950	0.46400
O	1.43880	3.75820	2.00850
C	1.25520	3.23600	3.32210
H	0.19610	3.05570	3.51940
H	1.63200	3.99670	4.00150
H	1.82220	2.31100	3.44990
O	3.30280	0.18990	-0.75090
C	4.17830	1.03380	-1.49360
H	5.09340	1.23310	-0.93100
H	4.42470	0.58300	-2.45810
H	3.63370	1.96280	-1.64940
H	-3.56290	-2.70010	1.51220