

72 mannose_6_threo

XYZ file generated by Avogadro.

H	-0.10910	-5.12040	-0.53320
O	-0.54020	-5.18640	-1.39750
C	-1.52800	-4.20160	-1.45670
H	-2.15200	-4.41260	-2.33090
O	-0.87440	-2.95340	-1.63260
C	-1.78190	-1.86230	-1.77740
H	-2.45820	-2.05180	-2.62300
C	-0.97260	-0.62280	-2.08590
H	-1.65920	0.22230	-2.20540
H	-0.42070	-0.75780	-3.02200
O	-0.06360	-0.39150	-1.02070
C	-2.61440	-1.72280	-0.49800
H	-1.94980	-1.51680	0.34620
O	-3.59070	-0.69770	-0.62020
H	-3.18240	0.14840	-0.39050
C	-3.35830	-3.02070	-0.23910
H	-4.06790	-3.18600	-1.06060
O	-4.04350	-2.98680	1.00290
H	-4.51930	-2.14750	1.05370
C	-2.38710	-4.19200	-0.19580
H	-2.94880	-5.13090	-0.15270
O	-1.50220	-4.09590	0.90860
H	-2.03350	-4.04220	1.71280
C	0.29870	0.97370	-0.85440
H	0.56930	1.40700	-1.82460
C	1.53320	0.96370	0.03940
H	1.31950	0.35180	0.92380
C	1.99460	2.34100	0.48840
H	2.85100	2.22730	1.16170
H	1.19420	2.83230	1.04340
C	-0.84390	1.76230	-0.25040
C	-2.97640	3.16690	0.85380
C	-1.25280	2.95960	-0.82710
C	-1.48320	1.26220	0.88450
C	-2.55690	1.96300	1.42550
C	-2.31840	3.66920	-0.26890
H	-0.74750	3.32630	-1.71170
H	-1.14850	0.33360	1.32940
O	-4.03700	3.86230	1.36460
H	-4.40650	3.35830	2.10370
O	-3.28640	1.56420	2.50560
C	-3.02800	0.25510	3.01280
H	-3.16290	-0.49250	2.22570
H	-3.75400	0.09390	3.80600
H	-2.01640	0.19210	3.41950
O	2.56570	0.33000	-0.74310
C	3.61420	-0.17840	-0.01380
C	5.75290	-1.23260	1.38720
C	4.81340	0.53360	0.06310
C	3.49300	-1.42870	0.60220
C	4.56950	-1.96060	1.31300
C	5.89440	0.00590	0.77080

H	4.49290	-2.92430	1.79720
H	6.82840	0.54580	0.84220
H	6.59000	-1.64440	1.93800
O	4.82790	1.72760	-0.59100
C	5.98040	2.55360	-0.43260
H	6.86230	2.07270	-0.86080
H	6.15000	2.77840	0.62270
H	5.76280	3.47080	-0.97550
O	2.33620	3.17330	-0.61020
H	3.16770	2.82290	-0.96150
O	-2.80770	4.84350	-0.75420
O	2.29020	-2.03810	0.44290
C	-2.17310	5.38240	-1.91130
H	-2.25970	4.69500	-2.75590
H	-1.12070	5.59660	-1.71110
H	-2.70000	6.30700	-2.13510
C	2.11230	-3.31400	1.05280
H	2.23800	-3.24650	2.13600
H	1.09190	-3.61060	0.82010
H	2.81460	-4.04180	0.64000

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H	3.27300	-1.84230	-2.14440
O	4.14130	-1.39730	-2.13230
C	4.42210	-1.12020	-0.79400
H	4.53210	-2.04330	-0.20720
O	3.33090	-0.37940	-0.27900
C	3.46380	-0.11280	1.11090
H	3.64240	-1.05570	1.64880
C	2.14850	0.47360	1.57960
H	1.91300	1.38200	1.01410
H	2.21800	0.72830	2.63780
O	1.11540	-0.49400	1.43490
C	4.66140	0.81060	1.31490
H	4.47770	1.75750	0.79140
O	4.81700	1.04030	2.70620
H	5.62700	1.55120	2.82820
C	5.91150	0.14020	0.74090
H	6.12230	-0.74830	1.34280
O	7.04230	0.98660	0.86910
H	6.94170	1.70790	0.23350
C	5.70080	-0.29450	-0.70640
H	6.54770	-0.90630	-1.03350
O	5.60470	0.88350	-1.49100
H	5.51890	0.62770	-2.41720
C	0.33400	-0.37550	0.24140
C	-0.13270	-1.81150	-0.04540
H	-0.60850	-2.20970	0.85330
C	1.01730	-2.73110	-0.43050
H	0.65600	-3.76330	-0.43340
H	1.82770	-2.63970	0.29240
C	-0.78770	0.61670	0.45490
C	-2.89830	2.39520	0.79740

C	-1.75430	0.36780	1.43160
C	-0.84930	1.76670	-0.32360
C	-1.90710	2.65770	-0.14520
C	-2.81960	1.24560	1.59080
H	-1.69070	-0.52920	2.03530
H	-0.09350	1.94910	-1.07750
O	-3.95620	3.24480	0.97290
H	-3.84760	3.99430	0.37020
O	-2.08710	3.81710	-0.84680
C	-1.02170	4.23570	-1.69740
H	-1.32370	5.19920	-2.10140
H	-0.87210	3.52550	-2.51340
H	-0.09770	4.34570	-1.12500
O	-1.03690	-1.88700	-1.16290
C	-2.35090	-1.52180	-0.98500
C	-4.98600	-0.71440	-0.67680
C	-3.19090	-2.20470	-0.09970
C	-2.85820	-0.47720	-1.76570
C	-4.18080	-0.06200	-1.60420
C	-4.51260	-1.78790	0.06930
H	-4.57870	0.75750	-2.18660
H	-5.16590	-2.29250	0.76760
H	-6.01060	-0.38850	-0.54350
O	-2.62800	-3.25270	0.56330
C	-3.45160	-3.96700	1.48140
H	-2.82230	-4.75210	1.89440
H	-4.30730	-4.41230	0.96880
H	-3.79770	-3.31220	2.28470
O	1.55810	-2.40470	-1.70820
H	0.85730	-2.49390	-2.36580
H	0.96210	-0.03430	-0.58530
O	-1.98470	0.07150	-2.65160
O	-3.84160	1.07960	2.47970
C	-3.78700	-0.07400	3.31420
H	-2.89500	-0.05310	3.94500
H	-3.79740	-0.98820	2.71460
H	-4.67810	-0.03400	3.93660
C	-2.42990	1.21230	-3.37810
H	-1.57830	1.53880	-3.97120
H	-2.73920	2.01130	-2.69890
H	-3.25900	0.95070	-4.04030

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H	2.28850	-2.28830	-0.91010
O	2.41450	-3.02070	-0.28070
C	2.45530	-2.48120	1.00980
H	2.72540	-3.29510	1.69250
O	1.15480	-2.00730	1.30270
C	0.98320	-1.31820	2.53680
H	1.11790	-2.01500	3.37620
C	-0.44820	-0.80120	2.55690
H	-0.64400	-0.34180	3.52640
H	-1.14330	-1.63630	2.42300

O	-0.66880	0.19610	1.56730
C	1.99550	-0.18040	2.68470
H	1.78540	0.59500	1.93880
O	1.84330	0.34400	3.99470
H	2.48560	1.05600	4.10220
C	3.40580	-0.69110	2.46040
H	3.65610	-1.42490	3.23850
O	4.28060	0.42400	2.54620
H	5.18610	0.10310	2.45750
C	3.48330	-1.35610	1.10150
H	3.26080	-0.61290	0.32420
O	4.79560	-1.86440	0.93590
H	4.90150	-2.14120	0.01770
C	-2.62570	-0.16620	0.18580
C	-5.38100	0.07100	-0.09600
C	-3.24330	1.04830	0.48300
C	-3.37210	-1.25690	-0.25020
C	-4.75530	-1.13790	-0.39500
C	-4.62250	1.15870	0.34420
H	-2.65100	1.88790	0.82410
H	-2.87130	-2.18980	-0.47580
O	-6.73940	0.16470	-0.23330
H	-7.00950	1.05950	0.01700
O	-5.58290	-2.13850	-0.81100
C	-4.97800	-3.38940	-1.12800
H	-4.48160	-3.81320	-0.25200
H	-5.79050	-4.04130	-1.44030
H	-4.26060	-3.27720	-1.94440
C	-1.12280	-0.28950	0.30370
H	-0.84030	-1.33710	0.19110
C	-0.40370	0.51090	-0.78190
H	-0.61300	1.57880	-0.65710
C	-0.78830	0.08280	-2.19010
H	-0.22880	0.68710	-2.91260
H	-1.85150	0.26740	-2.34970
O	-0.55260	-1.30050	-2.41390
H	0.40740	-1.43190	-2.38650
O	0.99720	0.26220	-0.55640
C	1.90050	0.98550	-1.28330
C	3.86650	2.34750	-2.67650
C	2.16480	2.32560	-0.98010
C	2.64840	0.32730	-2.26350
C	3.63850	1.00710	-2.97060
C	3.14750	3.01610	-1.69140
H	4.22020	0.50960	-3.73410
H	3.35950	4.05430	-1.47650
O	1.42310	2.85220	0.02860
C	1.67830	4.20770	0.38980
H	1.47240	4.87740	-0.44820
H	2.71180	4.33080	0.72160
H	1.00010	4.42770	1.21100
H	4.63140	2.88390	-3.22510
O	-5.35490	2.27980	0.60630
O	2.33940	-0.99140	-2.44150

C	3.05120	-1.70810	-3.45380
H	2.88740	-1.25130	-4.43150
H	2.64240	-2.71620	-3.44220
H	4.11770	-1.73640	-3.22220
C	-4.64670	3.42980	1.06300
H	-3.92400	3.75880	0.31300
H	-4.13680	3.21760	2.00540
H	-5.39730	4.20160	1.21510

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H	-3.31900	-1.70310	2.15840
O	-4.14190	-1.18020	2.15650
C	-4.40870	-0.87760	0.82140
H	-4.51920	-1.79360	0.22240
O	-3.31530	-0.12900	0.32200
C	-3.43620	0.14810	-1.06730
H	-3.62230	-0.78860	-1.61280
C	-2.11210	0.72000	-1.52820
H	-1.84600	1.59870	-0.93030
H	-2.18800	1.01800	-2.57440
O	-1.10350	-0.27900	-1.43920
C	-4.62340	1.08510	-1.26960
H	-4.43520	2.02450	-0.73370
O	-4.76950	1.32900	-2.65860
H	-5.55640	1.87430	-2.78090
C	-5.87590	0.42790	-0.70250
H	-6.10620	-0.45500	-1.31380
O	-6.93330	1.36980	-0.80190
H	-7.75950	0.92250	-0.58320
C	-5.66550	-0.02290	0.73680
H	-5.52280	0.85450	1.37920
O	-6.81890	-0.74810	1.12720
H	-6.78750	-0.88000	2.08200
C	0.85760	0.68210	-0.41570
C	3.07280	2.34240	-0.67830
C	0.99230	1.78370	0.42150
C	1.80290	0.42720	-1.41170
C	2.91970	1.24510	-1.53200
C	2.10300	2.61530	0.28350
H	0.25170	1.97290	1.18880
H	1.68190	-0.43110	-2.06110
O	4.18330	3.13030	-0.81140
H	4.11940	3.85480	-0.17290
O	3.92560	1.06440	-2.43620
C	3.79060	-0.03170	-3.33650
H	2.89770	0.08500	-3.95560
H	4.67850	-0.01280	-3.96450
H	3.74450	-0.97870	-2.79210
C	-0.31710	-0.25500	-0.24320
C	0.07080	-1.72660	-0.02470
H	0.51430	-2.10860	-0.94660
C	-1.12830	-2.59430	0.33070
H	-0.83300	-3.64560	0.27170

H	-1.94130	-2.41320	-0.37230
O	-1.62950	-2.30520	1.63320
H	-0.93490	-2.49980	2.27430
O	0.97930	-1.90690	1.07650
C	2.31060	-1.60950	0.90300
C	4.98690	-0.94120	0.61480
C	2.88310	-0.63950	1.73320
C	3.10400	-2.29130	-0.02530
C	4.44650	-1.94240	-0.18410
C	4.22720	-0.29450	1.58360
H	5.06440	-2.44560	-0.91490
H	4.67600	0.46740	2.20600
O	2.04810	-0.08850	2.65410
C	2.56520	0.98040	3.43970
H	3.37750	0.63120	4.08200
H	1.73700	1.32630	4.05460
H	2.92290	1.79490	2.80400
H	6.02820	-0.66910	0.48990
H	-0.92570	0.08140	0.59980
O	2.47840	-3.26840	-0.73840
O	2.35830	3.72200	1.04420
C	1.33040	4.15250	1.93400
H	0.40820	4.35200	1.38310
H	1.69530	5.07020	2.38940
H	1.14720	3.40520	2.70910
C	3.26040	-3.99030	-1.68660
H	3.64550	-3.32370	-2.46190
H	2.58710	-4.71930	-2.13160
H	4.08800	-4.50530	-1.19350

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H	4.93620	-0.55470	-1.35330
O	4.70030	-1.19410	-2.03950
C	3.56770	-1.89500	-1.62190
H	3.42730	-2.71860	-2.33190
O	2.45570	-1.01770	-1.68920
C	1.23070	-1.68380	-1.39120
H	1.14240	-2.57110	-2.03310
C	0.07370	-0.77080	-1.73480
H	-0.84220	-1.36990	-1.75390
H	0.22900	-0.32230	-2.72290
O	-0.02100	0.24490	-0.74830
C	1.23630	-2.16910	0.06470
H	0.29720	-2.70240	0.25900
O	1.41980	-1.12420	1.01440
H	0.85340	-0.38350	0.74300
C	2.41590	-3.11600	0.24370
H	2.25620	-4.00720	-0.36890
O	2.53630	-3.56630	1.58420
H	2.54390	-2.78410	2.15260
C	3.71080	-2.43840	-0.20460
H	3.92970	-1.59180	0.46160
O	4.78850	-3.35860	-0.20560

H	4.81990	-3.77190	0.66620
C	-2.41680	0.10980	-0.41560
C	-4.59460	-1.47470	0.26560
C	-3.61120	0.24700	-1.11420
C	-2.29460	-0.81440	0.62070
C	-3.38590	-1.60900	0.95290
C	-4.70730	-0.54530	-0.76830
H	-3.68020	0.96700	-1.91970
H	-1.35240	-0.91740	1.14530
O	-5.67800	-2.24900	0.57910
H	-5.43300	-2.83520	1.30900
O	-3.39560	-2.55880	1.93170
C	-2.19220	-2.73540	2.67700
H	-2.39680	-3.53010	3.39030
H	-1.93210	-1.81720	3.20870
H	-1.37130	-3.03070	2.01870
C	-1.22970	0.98920	-0.74770
C	-1.03110	2.05550	0.33170
H	-0.83180	1.54620	1.27940
C	-2.22630	2.97020	0.51320
H	-1.98450	3.70290	1.28850
H	-3.08880	2.38960	0.84110
O	-2.60080	3.62230	-0.69390
H	-1.87230	4.19400	-0.96340
O	0.08300	2.90280	-0.00540
C	1.33250	2.47640	0.38020
C	3.89180	1.70520	1.11740
C	2.28700	2.19560	-0.60290
C	1.67650	2.39850	1.73430
C	2.95790	1.98720	2.10780
C	3.57880	1.81940	-0.23310
H	3.23110	1.90720	3.15070
H	4.32940	1.61540	-0.98430
O	1.85910	2.30900	-1.88810
C	2.82830	2.13370	-2.91900
H	3.62490	2.87620	-2.82840
H	2.29390	2.28210	-3.85490
H	3.25060	1.12750	-2.89230
H	-1.37060	1.46410	-1.72560
H	4.89100	1.39950	1.40440
O	-5.92380	-0.49830	-1.38080
C	-6.08140	0.44430	-2.43810
H	-7.10650	0.33380	-2.78400
H	-5.39100	0.22790	-3.25660
H	-5.92210	1.46270	-2.07580
O	0.69880	2.75760	2.61120
C	0.98700	2.62840	4.00100
H	0.08260	2.93510	4.52140
H	1.81570	3.27950	4.28830
H	1.22330	1.59150	4.25130

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H	-3.22600	1.84530	-1.67160
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O	-3.99390	1.26320	-1.60110
C	-3.72600	0.27760	-0.64800
H	-3.20950	0.70560	0.22410
O	-2.90130	-0.70800	-1.24180
C	-2.53490	-1.70950	-0.29750
H	-2.15240	-1.22760	0.61050
C	-1.43870	-2.55150	-0.92040
H	-1.80120	-3.02450	-1.83380
H	-1.13620	-3.32830	-0.20870
O	-0.31280	-1.77560	-1.30870
C	-3.76370	-2.50910	0.11460
H	-3.48060	-3.23060	0.88920
O	-4.28120	-3.18390	-1.02190
H	-5.16520	-3.49990	-0.79570
C	-4.78710	-1.53730	0.69780
H	-4.38280	-1.14070	1.63800
O	-5.98010	-2.26430	0.94590
H	-6.66660	-1.63580	1.20190
C	-5.04580	-0.36670	-0.24180
H	-5.54030	-0.72550	-1.15200
O	-5.88010	0.54570	0.45220
H	-6.19170	1.21020	-0.17350
C	-0.08740	0.18990	0.13060
C	-1.02680	2.72200	0.79740
C	-0.32270	1.12620	-0.87290
C	-0.30720	0.51160	1.46700
C	-0.78000	1.78050	1.79600
C	-0.79340	2.39340	-0.53870
H	-0.14540	0.85820	-1.90680
H	-0.12560	-0.22900	2.23600
O	-1.49160	3.97420	1.09820
H	-1.59690	4.03640	2.05790
O	-1.04710	2.21940	3.06100
C	-0.85820	1.29060	4.12560
H	0.18580	0.97430	4.17970
H	-1.50630	0.42080	3.99550
H	-1.12990	1.82020	5.03570
C	0.42230	-1.19070	-0.24080
C	1.87290	-1.13660	-0.72690
H	1.92590	-0.51640	-1.62920
C	2.44800	-2.51110	-1.03240
H	3.47750	-2.40030	-1.39140
H	1.86200	-2.97230	-1.82680
O	2.40580	-3.37560	0.09330
H	3.06680	-3.04120	0.71710
O	2.61280	-0.50300	0.33380
C	3.87750	-0.09250	-0.00900
C	6.44970	0.74110	-0.64950
C	4.98360	-0.85570	0.39520
C	4.07750	1.08690	-0.72220
C	5.36430	1.50830	-1.04670
C	6.27220	-0.43730	0.07410
H	5.49050	2.42970	-1.60260
H	7.13250	-1.01860	0.37690

O	4.69190	-1.98660	1.09480
C	5.77380	-2.85870	1.42200
H	6.28920	-3.18610	0.51640
H	6.47590	-2.36480	2.09660
H	5.32270	-3.71340	1.92100
H	0.37260	-1.84000	0.64110
H	7.45440	1.05950	-0.89970
O	2.98880	1.82920	-1.12190
O	-1.05010	3.38800	-1.43730
C	2.52170	2.72570	-0.10310
H	1.76800	3.36060	-0.56590
H	3.34970	3.34180	0.25690
H	2.08090	2.16580	0.72690
C	-0.73950	3.11680	-2.80200
H	-0.97620	4.02720	-3.34780
H	-1.34670	2.29110	-3.18230
H	0.32180	2.88100	-2.91610

72 mannose_2_threo

XYZ file generated by Avogadro.

H	1.62480	2.51050	0.13050
O	1.59140	3.23770	-0.51000
C	0.40520	3.11060	-1.23310
H	0.48590	3.74880	-2.11880
O	-0.65370	3.58080	-0.40940
C	-1.91850	3.58930	-1.07050
H	-1.85540	4.20260	-1.98070
C	-2.90970	4.23350	-0.12160
H	-3.88120	4.31110	-0.60910
H	-2.55890	5.24100	0.12140
O	-3.09830	3.47050	1.06250
H	-2.24640	3.39940	1.50950
C	-2.29780	2.16220	-1.45690
H	-2.39710	1.55720	-0.54680
O	-3.53590	2.21280	-2.14870
H	-3.72350	1.32170	-2.46960
C	-1.21080	1.55540	-2.33610
H	-1.16850	2.11500	-3.27600
O	-1.53450	0.21720	-2.67630
H	-1.58260	-0.30190	-1.85450
C	0.14780	1.66380	-1.64590
H	0.94780	1.34390	-2.32110
O	0.16020	0.88470	-0.45780
C	0.77810	-0.40030	-0.55680
C	-0.04720	-1.32750	0.32890
H	-0.07550	-0.92540	1.34690
C	0.45690	-2.76120	0.36260
H	1.48240	-2.77460	0.73490
H	-0.16110	-3.34110	1.05600
O	0.44980	-3.35990	-0.92460
H	-0.47860	-3.54180	-1.13630
O	-1.37550	-1.28810	-0.23910
H	0.71770	-0.76120	-1.58760
C	2.22550	-0.33720	-0.13050

C	4.87840	-0.23620	0.68910
C	3.20520	-0.93610	-0.91480
C	2.55650	0.30680	1.06180
C	3.88750	0.36740	1.46710
C	4.53360	-0.88800	-0.49480
H	2.93130	-1.43080	-1.83810
H	1.77550	0.75930	1.66080
C	-2.38590	-1.77700	0.54770
C	-4.48750	-2.76720	2.06170
C	-2.86610	-1.03430	1.63760
C	-2.96420	-3.00210	0.23130
C	-4.02370	-3.50370	0.98050
C	-3.91930	-1.53900	2.39810
H	-4.45750	-4.45910	0.71130
H	-4.30310	-0.98200	3.24200
H	-5.30760	-3.14800	2.65820
O	-2.24400	0.14980	1.86140
C	-2.61380	0.87060	3.03540
H	-3.65190	1.20420	2.97570
H	-2.47000	0.25280	3.92480
H	-1.94950	1.73090	3.07830
O	6.17820	-0.16410	1.10770
H	6.73650	-0.60790	0.45350
O	4.32700	0.98510	2.59830
C	3.34980	1.66230	3.38480
H	2.60620	0.96020	3.76890
H	3.89350	2.11030	4.21320
H	2.85780	2.44350	2.79970
O	5.58960	-1.43010	-1.16570
C	5.30700	-2.11550	-2.38390
H	6.26480	-2.47450	-2.75280
H	4.63910	-2.96060	-2.20270
H	4.86090	-1.43520	-3.11270
O	-2.44960	-3.72360	-0.82600
C	-2.99270	-3.32180	-2.09440
H	-2.78940	-2.26400	-2.27670
H	-2.49970	-3.93100	-2.84990
H	-4.06960	-3.50420	-2.11150

72 mannose_2_erythro

XYZ file generated by Avogadro.

H	-1.71500	-2.39270	1.48340
O	-2.44710	-2.16920	2.09240
C	-3.28550	-1.22400	1.50510
H	-4.07950	-0.99560	2.22440
O	-3.85460	-1.81850	0.34600
C	-4.82960	-0.99380	-0.28880
H	-5.61470	-0.73480	0.43600
C	-5.42210	-1.81430	-1.41490
H	-4.62330	-2.09640	-2.11020
H	-6.16310	-1.22170	-1.95020
O	-6.08940	-2.96830	-0.92330
H	-5.44390	-3.49560	-0.43790
C	-4.16400	0.28460	-0.78880

H	-3.40060	0.02280	-1.53400
O	-5.16280	1.10260	-1.37730
H	-4.75930	1.95790	-1.57280
C	-3.50070	1.00330	0.38120
H	-4.28480	1.32540	1.07300
O	-2.84070	2.17810	-0.05760
H	-2.08000	1.91600	-0.60250
C	-2.55250	0.06400	1.12080
H	-2.18240	0.55410	2.02700
O	-1.47860	-0.25060	0.24830
C	-0.18100	-0.19950	0.82760
C	0.75160	-1.00050	-0.08610
H	1.02910	-0.41650	-0.96960
C	0.15960	-2.32280	-0.53960
H	-0.71830	-2.13580	-1.15690
H	0.89500	-2.86420	-1.14290
O	-0.25580	-3.11870	0.56450
H	0.55000	-3.40450	1.02020
O	1.91640	-1.22090	0.73090
H	-0.19590	-0.70700	1.79830
C	0.34050	1.20270	1.04120
C	1.51730	3.71460	1.40980
C	0.90070	1.56430	2.26320
C	0.37850	2.12530	-0.01180
C	0.94230	3.38570	0.17850
C	1.50150	2.80350	2.45650
H	0.88300	0.84760	3.07730
H	1.94410	3.07590	3.40670
C	3.04820	-1.56420	0.03270
C	5.35330	-2.25780	-1.31890
C	3.43150	-2.90480	-0.03750
C	3.82870	-0.56680	-0.56010
C	4.99150	-0.91580	-1.24790
C	4.59530	-3.25960	-0.72160
H	5.60800	-0.16090	-1.71640
H	4.90720	-4.29260	-0.79000
H	6.25630	-2.53030	-1.85220
O	2.60510	-3.78020	0.59730
C	2.87540	-5.17170	0.43950
H	3.83730	-5.43210	0.88620
H	2.07520	-5.68960	0.96360
H	2.86600	-5.44750	-0.61750
O	2.07680	4.94560	1.58820
H	1.98990	5.44420	0.76170
O	0.96940	4.33630	-0.81380
C	-0.31680	4.92810	-1.06290
H	-0.68060	5.41950	-0.15750
H	-1.03260	4.16840	-1.38600
H	-0.17130	5.66170	-1.85340
O	3.36590	0.70000	-0.40270
O	-0.19710	1.77710	-1.20440
C	0.56380	1.98880	-2.40490
H	1.63140	1.90120	-2.19580
H	0.25920	1.20420	-3.09620

H	0.34550	2.96590	-2.83650
C	4.12370	1.75520	-0.98930
H	4.18440	1.63340	-2.07350
H	5.12830	1.79200	-0.56170
H	3.58910	2.67320	-0.74950

72 glucose_2_threo

XYZ file generated by Avogadro.

H	-1.73210	0.40970	-2.29340
O	-1.45200	1.32690	-2.14430
C	-1.71610	1.62130	-0.79980
H	-2.61830	1.09020	-0.45990
O	-1.93720	3.01410	-0.75780
C	-2.32050	3.47160	0.53790
H	-3.21520	2.92370	0.86480
C	-2.64190	4.94430	0.39790
H	-1.74980	5.47460	0.04620
H	-2.93360	5.34820	1.36660
O	-3.73220	5.15500	-0.48740
H	-3.48250	4.80070	-1.34920
C	-1.18280	3.21730	1.52220
H	-0.30310	3.79540	1.20920
O	-1.61480	3.63320	2.80690
H	-0.91920	3.40980	3.43770
C	-0.82370	1.73990	1.52050
H	-1.67760	1.17140	1.91450
O	0.29890	1.57980	2.37300
H	0.49410	0.63730	2.44630
C	-0.53700	1.26400	0.10350
H	0.36540	1.75690	-0.27880
O	-0.36530	-0.14470	0.15080
C	0.42610	-2.20570	-0.69110
C	0.58970	-0.68810	-0.76750
H	0.36090	-0.35550	-1.78280
C	1.45280	-2.95980	-1.51590
H	2.45340	-2.76590	-1.13000
C	1.99690	-0.26610	-0.40710
C	4.58830	0.48080	0.26400
C	2.47090	-0.49660	0.88360
C	2.80580	0.33260	-1.36700
C	4.10620	0.70110	-1.02600
C	3.76570	-0.11440	1.22340
H	1.82950	-0.97410	1.61360
H	2.41970	0.50960	-2.36300
O	1.45090	-2.56120	-2.88120
O	5.85760	0.84630	0.61930
H	6.29000	1.23670	-0.15340
O	5.00050	1.29960	-1.86450
C	4.56950	1.56340	-3.19790
H	4.31020	0.63330	-3.70870
H	5.41290	2.03530	-3.69610
H	3.71280	2.24100	-3.19720
H	0.58600	-2.77240	-3.25230
H	0.51530	-2.51910	0.35130

H	1.24600	-4.03030	-1.42680
O	-0.85530	-2.60920	-1.21730
C	-1.95800	-2.50330	-0.40670
C	-4.24320	-2.29200	1.15630
C	-2.05990	-3.22630	0.78870
C	-3.03830	-1.72990	-0.84170
C	-4.18470	-1.61520	-0.05660
C	-3.19850	-3.10150	1.58610
H	-5.01800	-1.00670	-0.37930
H	-3.27930	-3.64040	2.51980
H	-5.12890	-2.19830	1.77290
O	-2.88340	-1.11640	-2.05400
C	-4.03970	-0.48660	-2.61400
H	-4.86130	-1.20070	-2.69380
H	-3.74210	-0.15180	-3.60540
H	-4.34340	0.37200	-2.00980
O	4.32380	-0.27410	2.45600
O	-1.00690	-4.03800	1.08070
C	-1.05030	-4.75330	2.31280
H	-1.10650	-4.06390	3.15840
H	-0.12180	-5.31770	2.35990
H	-1.89960	-5.43980	2.33390
C	3.48680	-0.80990	3.47790
H	2.60640	-0.17890	3.62600
H	4.09030	-0.81800	4.38250
H	3.17760	-1.82870	3.23250

72 glucose_2_erythro

XYZ file generated by Avogadro.

H	-2.64250	2.05760	-0.78390
O	-2.95710	1.66640	-1.61070
C	-3.42970	0.37860	-1.36030
H	-3.46580	-0.14050	-2.32480
O	-4.74360	0.48280	-0.83350
C	-5.38700	-0.78120	-0.67260
H	-5.40380	-1.31280	-1.63410
C	-6.81590	-0.49720	-0.25370
H	-7.35130	-1.43840	-0.13030
H	-7.30370	0.08190	-1.04350
O	-6.88900	0.19120	0.98720
H	-6.43820	1.03770	0.88290
C	-4.61110	-1.61670	0.34290
H	-4.62610	-1.10940	1.31540
O	-5.24240	-2.88310	0.43920
H	-4.69250	-3.43860	1.00620
C	-3.16720	-1.76310	-0.10770
H	-3.14620	-2.33160	-1.04760
O	-2.47230	-2.47500	0.90210
H	-1.60820	-2.77360	0.56350
C	-2.55980	-0.38750	-0.36880
H	-2.51790	0.19120	0.56420
O	-1.26460	-0.52910	-0.92580
C	0.99620	-1.12340	-0.57550
C	-0.20190	-0.37330	0.00740

H	-0.46430	-0.84810	0.95760
C	0.67430	-2.54900	-0.99130
H	-0.05910	-2.53510	-1.79630
C	0.13010	1.08100	0.25730
C	0.94100	3.70350	0.69020
C	0.32710	1.93170	-0.82980
C	0.31780	1.53280	1.55900
C	0.72550	2.84930	1.77050
C	0.74070	3.24240	-0.61360
H	0.18460	1.55670	-1.83520
H	0.16320	0.85730	2.39090
O	0.11760	-3.30540	0.07820
O	1.35400	4.99490	0.87500
H	1.45430	5.15060	1.82470
O	0.95280	3.41750	2.99080
C	0.80700	2.58100	4.13610
H	1.49950	1.73770	4.08600
H	1.04640	3.20480	4.99400
H	-0.21960	2.21740	4.21840
H	0.82590	-3.43790	0.72550
H	1.38870	-0.58260	-1.44430
H	1.58260	-3.03280	-1.36400
O	1.97090	-1.11280	0.48270
C	3.25660	-1.37730	0.07590
C	5.85350	-1.90400	-0.70260
C	4.03460	-0.35540	-0.47790
C	3.78630	-2.65630	0.25540
C	5.09820	-2.92650	-0.13780
C	5.34450	-0.62070	-0.87790
H	5.52530	-3.91160	-0.01040
H	5.95900	0.15510	-1.31380
H	6.87100	-2.11220	-1.01110
O	2.94270	-3.56190	0.82190
C	3.37720	-4.91950	0.87830
H	2.54330	-5.47980	1.29540
H	4.24980	-5.02010	1.52700
H	3.60950	-5.28970	-0.12280
O	3.41820	0.84970	-0.57600
O	0.99680	4.14910	-1.59910
C	0.94150	3.67120	-2.94060
H	1.64720	2.84860	-3.08550
H	1.22310	4.51340	-3.56850
H	-0.06930	3.34440	-3.19600
C	4.13300	1.91190	-1.20150
H	4.38110	1.65530	-2.23420
H	5.04390	2.14650	-0.64590
H	3.46390	2.77100	-1.18410

72 galactose_2_threo

XYZ file generated by Avogadro.

H	2.28030	-0.33800	-2.87720
O	2.68890	0.51850	-2.68810
C	3.19350	0.49540	-1.38730
H	3.54650	1.51100	-1.16950

O	4.28390	-0.40970	-1.36150
C	4.99390	-0.39280	-0.12170
H	5.33680	0.63130	0.07710
C	6.19710	-1.29680	-0.28900
H	5.87040	-2.30280	-0.56590
H	6.73820	-1.34930	0.65670
O	7.10070	-0.78370	-1.25900
H	6.64520	-0.77280	-2.10900
C	4.08810	-0.81570	1.02570
H	4.62690	-0.67360	1.96900
O	3.73700	-2.18370	0.86180
H	3.03960	-2.38490	1.49940
C	2.84320	0.06120	1.03500
H	3.14640	1.09390	1.25290
O	1.98760	-0.41950	2.05450
H	1.30200	0.25120	2.22580
C	2.16810	0.05370	-0.33850
H	1.81460	-0.95180	-0.59500
O	1.08130	0.96300	-0.23710
C	-0.76680	2.17470	-1.09310
H	-1.67630	2.06170	-1.68650
C	0.00040	0.84320	-1.15840
H	0.38350	0.78240	-2.18110
C	0.01950	3.32930	-1.69430
H	0.26380	3.06320	-2.72850
H	-0.61370	4.21780	-1.70830
O	1.19490	3.67450	-0.97160
H	1.60560	2.85240	-0.66900
C	-0.88570	-0.37110	-0.92160
C	-2.66660	-2.47060	-0.49500
C	-0.72240	-1.19780	0.18220
C	-1.91130	-0.61150	-1.83750
C	-2.80990	-1.65270	-1.61740
C	-1.61400	-2.24550	0.38960
H	0.06330	-1.00490	0.89710
H	-2.01780	0.02760	-2.70550
O	-3.56790	-3.48170	-0.28980
H	-3.32210	-3.94610	0.52280
O	-1.56530	-3.10710	1.44880
C	-0.43310	-3.00700	2.31140
H	-0.54350	-3.80470	3.04230
H	-0.41760	-2.03980	2.81950
H	0.49240	-3.14560	1.74560
O	-1.09920	2.58000	0.24620
C	-1.79770	1.71590	1.05620
C	-3.18130	-0.06160	2.70150
C	-1.22270	1.25470	2.23930
C	-3.10580	1.31240	0.72810
C	-3.78830	0.40840	1.53720
C	-1.91620	0.36860	3.06420
H	-4.78350	0.07640	1.27440
H	-1.43450	0.02130	3.97020
H	-3.71510	-0.76110	3.33370
O	0.06370	1.55460	2.61030

C	0.51630	2.91520	2.52980
H	0.97210	3.11330	1.56130
H	-0.31710	3.59910	2.69840
H	1.25340	3.03290	3.32330
O	-3.86380	-1.95480	-2.42980
O	-3.61080	1.84490	-0.41580
C	-4.86620	1.34590	-0.86990
H	-5.66060	1.59400	-0.16210
H	-5.05640	1.83960	-1.82040
H	-4.82260	0.26260	-1.01410
C	-4.02970	-1.15760	-3.59900
H	-4.19570	-0.10970	-3.33720
H	-4.90760	-1.55220	-4.10550
H	-3.15790	-1.24310	-4.25200

72 galactose_2_erythro

XYZ file generated by Avogadro.

H	-2.68080	1.78140	-0.86500
O	-2.96800	1.39030	-1.70200
C	-3.38630	0.07850	-1.47600
H	-3.39120	-0.42540	-2.44960
O	-4.70610	0.11850	-0.95760
C	-5.28600	-1.17750	-0.81430
H	-5.27360	-1.69160	-1.78500
C	-6.74060	-0.99770	-0.41040
H	-7.17840	-1.99130	-0.26560
H	-7.27480	-0.50010	-1.22060
O	-6.91450	-0.19030	0.74610
H	-6.32460	-0.53890	1.42870
C	-4.48150	-2.03400	0.15880
H	-4.88990	-3.05010	0.14550
O	-4.60060	-1.48070	1.46710
H	-4.02570	-1.98290	2.05820
C	-3.02100	-2.07850	-0.27370
H	-2.96010	-2.61330	-1.22990
O	-2.29750	-2.77360	0.72700
H	-1.39100	-2.95840	0.41920
C	-2.49060	-0.66230	-0.48760
H	-2.50160	-0.10580	0.45830
O	-1.17550	-0.71640	-1.01550
C	1.12420	-1.10090	-0.60480
H	1.50270	-0.52270	-1.45520
C	-0.15210	-0.46210	-0.05860
H	-0.39510	-0.96050	0.88510
C	0.93680	-2.54450	-1.03860
H	0.24210	-2.58380	-1.87650
H	1.89650	-2.95250	-1.37080
O	0.39320	-3.34790	0.00310
H	1.08140	-3.43250	0.67950
C	0.03350	1.01630	0.20290
C	0.52830	3.70960	0.67870
C	0.05510	1.48750	1.51100
C	0.24150	1.88110	-0.87100
C	0.49760	3.22760	-0.63280

C	0.30300	2.83960	1.74430
H	-0.10740	0.80230	2.33340
H	0.22570	1.49370	-1.88180
O	0.78220	5.03780	0.88720
H	0.78560	5.20080	1.84110
O	0.35300	3.43040	2.97380
C	0.15010	2.59230	4.10930
H	0.91570	1.81450	4.15480
H	0.23190	3.24150	4.97770
H	-0.84300	2.13840	4.07930
O	2.05450	-1.01700	0.48980
C	3.37120	-1.18080	0.13180
C	6.02880	-1.50440	-0.54610
C	3.98960	-2.41670	0.32920
C	4.08970	-0.09980	-0.38920
C	5.43070	-0.26260	-0.73820
C	5.33230	-2.58440	-0.01350
H	6.00150	0.55950	-1.14790
H	5.82770	-3.53510	0.12760
H	7.07040	-1.63280	-0.81530
O	3.19650	-3.38660	0.86070
C	3.73700	-4.70390	0.94640
H	4.58860	-4.72910	1.62940
H	2.93540	-5.32770	1.33570
H	4.03810	-5.06030	-0.04130
O	0.74550	4.15430	-1.60160
O	3.38620	1.05460	-0.50790
C	4.03890	2.17410	-1.10030
H	3.30380	2.97780	-1.10560
H	4.90590	2.47580	-0.50810
H	4.34670	1.94520	-2.12350
C	0.81140	3.67820	-2.94310
H	-0.14970	3.26210	-3.25520
H	1.59540	2.92310	-3.04690
H	1.05140	4.54470	-3.55490

68 arabinose_2_threo

XYZ file generated by Avogadro.

O	-3.70550	-0.85110	-3.10850
C	-3.23590	-1.18010	-1.81840
H	-2.86380	-2.20440	-1.78080
O	-4.25870	-1.06550	-0.85740
C	-4.37560	0.30470	-0.42780
H	-5.27980	0.74520	-0.86020
C	-4.53140	0.33050	1.08340
H	-5.43750	-0.21810	1.34580
H	-4.65880	1.37120	1.39930
O	-3.47170	-0.29070	1.79790
C	-3.14870	1.04360	-1.01030
H	-2.65330	1.66810	-0.26500
O	-3.49170	1.89460	-2.09090
H	-3.88410	1.34850	-2.78620
C	-2.22400	-0.10140	-1.43810
H	-1.57030	0.17100	-2.26990

O	-1.50080	-0.46700	-0.28370
C	-0.39570	-1.32670	-0.47400
H	-0.63740	-2.11460	-1.19930
C	0.82990	-0.56670	-0.96710
C	3.16090	0.78890	-1.65740
C	0.82340	0.82160	-1.05570
C	1.98560	-1.28940	-1.25970
C	3.15010	-0.60580	-1.59440
C	1.99050	1.50100	-1.40010
H	-0.07260	1.37330	-0.80330
H	1.98030	-2.37100	-1.19610
C	-0.14480	-2.03900	0.86690
H	0.84270	-2.49900	0.82780
C	-1.13150	-3.15510	1.16520
H	-0.96410	-3.47620	2.19930
H	-0.89150	-3.99370	0.50820
O	-2.49910	-2.85210	0.94790
H	-2.71390	-1.95770	1.26600
O	-0.20290	-1.13120	1.98820
C	0.68740	-0.08090	2.02980
C	2.41360	2.09910	2.11710
C	0.17950	1.21890	2.13450
C	2.07530	-0.27900	2.02520
C	2.94110	0.81570	2.04190
C	1.04250	2.31370	2.18250
H	4.01210	0.67090	2.01150
H	0.65560	3.32050	2.25410
H	3.08550	2.94890	2.13720
O	4.30420	1.47780	-1.96660
H	5.01620	0.83720	-2.10350
O	4.35280	-1.18890	-1.87440
C	4.40760	-2.61320	-1.85360
H	4.16180	-2.99550	-0.86010
H	5.43220	-2.87620	-2.10600
H	3.72400	-3.03360	-2.59480
O	-1.17850	1.33140	2.16730
C	-1.72890	2.64650	2.22430
H	-1.43130	3.22830	1.34800
H	-1.41650	3.15730	3.13750
H	-2.80940	2.51480	2.23140
H	-2.64560	0.20820	1.68200
H	-4.37680	-1.49750	-3.36100
O	2.09700	2.85910	-1.48600
O	2.49420	-1.57260	1.99950
C	0.89800	3.61390	-1.32840
H	0.48800	3.49180	-0.32260
H	0.15410	3.31630	-2.07190
H	1.17880	4.65320	-1.48440
C	3.88960	-1.80760	1.82920
H	4.00220	-2.88720	1.75690
H	4.45300	-1.43690	2.68890
H	4.25400	-1.33280	0.91380

68 arabinose_2_erythro

XYZ file generated by Avogadro.

O	3.67160	-2.95820	-0.77030
C	3.77910	-1.61750	-1.17240
H	3.48800	-1.51410	-2.21970
O	5.11730	-1.14530	-1.04460
C	5.19040	-0.18020	0.00860
H	5.33570	-0.67610	0.97710
C	6.34080	0.76770	-0.26510
H	6.16690	1.28030	-1.21780
H	7.27740	0.21240	-0.33080
O	6.48140	1.70060	0.79920
C	3.81610	0.47660	-0.02770
H	3.75180	1.12930	-0.90880
O	3.56760	1.21190	1.15310
H	2.79390	1.78330	0.98660
C	2.92810	-0.74390	-0.25270
H	2.78220	-1.27050	0.69840
O	1.68390	-0.46860	-0.86260
C	0.64490	-0.13850	0.05700
H	1.07120	0.19170	1.00900
C	-0.26570	-1.32120	0.29950
C	-2.12320	-3.35060	0.69280
C	-0.72250	-2.06140	-0.79030
C	-0.71310	-1.59890	1.58670
C	-1.64360	-2.61880	1.77820
C	-1.66070	-3.07020	-0.59470
H	-0.37030	-1.82210	-1.78530
H	-0.35140	-1.01270	2.42200
C	-0.12360	1.03920	-0.54900
H	-0.61580	0.71570	-1.47380
C	0.75550	2.24220	-0.85190
H	0.14900	3.02730	-1.31440
H	1.53690	1.95450	-1.55460
O	1.39440	2.74570	0.31660
H	0.69990	3.14440	0.86260
O	-1.11530	1.38560	0.43380
C	-2.17080	2.12460	-0.04610
C	-4.31960	3.60670	-0.95610
C	-2.19480	3.50650	0.15330
C	-3.23790	1.48170	-0.68310
C	-4.31980	2.22900	-1.14980
C	-3.27660	4.25870	-0.30700
H	-5.14980	1.74920	-1.65000
H	-3.30960	5.32990	-0.16430
H	-5.15950	4.18860	-1.31660
O	-3.05050	-4.34350	0.86000
H	-3.26840	-4.40050	1.80120
O	-2.16860	-2.99120	2.98210
C	-1.75090	-2.25760	4.13080
H	-2.28080	-2.69560	4.97330
H	-0.67350	-2.35740	4.27990
H	-2.01910	-1.20330	4.03200
O	-1.12030	4.02100	0.81220

C	-1.03910	5.44020	0.93520
H	-1.86470	5.82320	1.53850
H	-0.09460	5.63940	1.43670
H	-1.04280	5.91180	-0.04990
H	5.61230	2.08420	0.97820
H	4.01980	-3.51880	-1.47430
O	-3.12070	0.13440	-0.78850
O	-2.20570	-3.82840	-1.58890
C	-1.87790	-3.46420	-2.92690
H	-2.16520	-2.42790	-3.12530
H	-0.81010	-3.59650	-3.11620
H	-2.44860	-4.13380	-3.56630
C	-4.16390	-0.57370	-1.45270
H	-3.88110	-1.62460	-1.41400
H	-4.25020	-0.25040	-2.49280
H	-5.11670	-0.43190	-0.93730

68 xylose_2_threo

XYZ file generated by Avogadro.

H	-1.87190	1.25550	-1.27400
O	-1.72860	2.07370	-1.78430
C	-0.80640	2.86570	-1.08530
H	-1.24250	3.22530	-0.14060
O	-0.53830	3.96250	-1.92940
C	0.33260	4.90040	-1.30610
H	0.44770	5.73290	-1.99810
H	-0.11350	5.26660	-0.37300
C	1.68710	4.26630	-1.01030
H	2.16160	3.96350	-1.95150
O	2.47200	5.25050	-0.35700
H	3.34250	4.87260	-0.18360
C	1.49660	3.03420	-0.14090
H	1.10640	3.34940	0.83640
O	2.75800	2.40380	0.01950
H	2.64160	1.63060	0.58920
C	0.48640	2.10620	-0.79640
H	0.89300	1.72220	-1.73910
O	0.18070	1.04490	0.09170
C	0.28940	-0.28490	-0.41490
H	0.18310	-0.27880	-1.50430
C	1.62240	-0.89000	-0.04310
C	4.05790	-2.02510	0.66580
C	2.33050	-1.62970	-0.98400
C	2.11740	-0.71200	1.24910
C	3.34400	-1.27250	1.60060
C	3.54800	-2.20250	-0.62010
H	1.93620	-1.75050	-1.98500
H	1.54900	-0.13330	1.96620
C	-0.90140	-1.03920	0.17080
H	-0.96700	-0.81770	1.24220
C	-0.87050	-2.54430	-0.02850
H	-1.73780	-2.98900	0.47060
H	0.02920	-2.95200	0.43490
O	-0.85270	-2.89850	-1.40250

H	-1.73980	-2.70630	-1.73850
O	-2.05260	-0.47830	-0.50520
C	-3.25240	-0.61940	0.15390
C	-5.69100	-0.84670	1.42960
C	-4.12650	-1.64710	-0.20440
C	-3.61100	0.31140	1.13410
C	-4.84060	0.19630	1.78300
C	-5.35670	-1.76890	0.44380
H	-5.13510	0.90420	2.54550
H	-6.04360	-2.56260	0.18480
H	-6.64570	-0.93970	1.93330
O	5.25930	-2.56530	1.03380
H	5.63030	-3.03240	0.27160
O	4.34360	-2.94630	-1.44010
C	3.88700	-3.16310	-2.77380
H	2.93460	-3.69780	-2.77100
H	3.78160	-2.21320	-3.30250
H	4.64980	-3.77040	-3.25480
O	-3.69410	-2.46590	-1.20050
C	-4.48580	-3.61470	-1.50030
H	-4.60210	-4.24190	-0.61370
H	-3.93920	-4.15730	-2.26840
H	-5.46490	-3.31980	-1.88290
O	-2.69380	1.28210	1.36830
O	3.93330	-1.14690	2.82160
C	3.26900	-0.32480	3.77780
H	2.28940	-0.73700	4.03020
H	3.15850	0.69440	3.39870
H	3.90440	-0.32250	4.66030
C	-3.02150	2.28090	2.33060
H	-2.16710	2.95390	2.36110
H	-3.91540	2.83070	2.02730
H	-3.17390	1.83430	3.31570

68 xylose_2_erytho

XYZ file generated by Avogadro.

H	-3.47140	3.43740	0.81390
O	-2.91580	2.92020	0.21830
C	-1.64720	3.49410	0.17080
H	-1.33200	3.84210	1.16350
O	-1.70860	4.60340	-0.71260
C	-0.46370	5.28260	-0.82090
H	-0.63080	6.15550	-1.45030
H	-0.12180	5.61220	0.16830
C	0.57210	4.35900	-1.44210
H	0.24540	4.06890	-2.44840
O	1.79920	5.06710	-1.50790
H	2.47640	4.45140	-1.81450
C	0.70380	3.11070	-0.58780
H	1.10240	3.40200	0.39350
O	1.61220	2.23360	-1.23480
H	1.84740	1.52130	-0.61720
C	-0.66260	2.46180	-0.36910
H	-1.05950	2.07560	-1.31600

O	-0.54540	1.41700	0.58520
C	-0.38410	0.10820	0.05080
H	-0.02390	0.17360	-0.97790
C	-1.67410	-0.68730	0.05030
C	-3.96870	-2.25560	0.01520
C	-1.73910	-1.80330	-0.78280
C	-2.74260	-0.34770	0.87060
C	-3.89200	-1.13570	0.84270
C	-2.88600	-2.59140	-0.80020
H	-0.89220	-2.04590	-1.41330
H	-2.67760	0.51980	1.51220
C	0.70360	-0.60780	0.85060
H	0.73560	-1.65490	0.54000
C	0.51270	-0.52740	2.35450
H	-0.45490	-0.95690	2.62060
H	0.53380	0.51790	2.67410
O	1.50820	-1.27590	3.03850
H	2.36850	-0.86420	2.86160
O	1.97950	0.00630	0.53330
C	2.96780	-0.85160	0.10450
C	4.99590	-2.52720	-0.75110
C	2.86160	-1.49760	-1.13200
C	4.09370	-1.04690	0.90730
C	5.12120	-1.88620	0.47660
C	3.87920	-2.34980	-1.56080
H	5.99830	-2.04770	1.08770
H	3.80770	-2.86140	-2.51080
H	5.78990	-3.18420	-1.08520
O	-5.09370	-3.03510	-0.02450
H	-5.74780	-2.65460	0.57850
O	-3.05470	-3.69640	-1.58070
C	-1.96970	-4.05330	-2.43410
H	-1.07430	-4.27820	-1.84940
H	-1.75750	-3.25230	-3.14660
H	-2.29240	-4.94390	-2.96830
O	1.73070	-1.22660	-1.83050
C	1.49090	-1.97240	-3.02200
H	1.44500	-3.04220	-2.80320
H	2.26470	-1.77550	-3.76720
H	0.52880	-1.62840	-3.39680
O	-5.01660	-0.90600	1.58260
O	4.08390	-0.38410	2.09870
C	-5.02690	0.25600	2.40930
H	-4.24770	0.19250	3.17210
H	-6.00530	0.27600	2.88330
H	-4.88750	1.15730	1.80720
C	5.18170	-0.60660	2.98470
H	4.96680	-0.01780	3.87320
H	6.11480	-0.26620	2.53180
H	5.25460	-1.66390	3.24800

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XYZ file generated by Avogadro.

H	4.59770	-2.76510	0.74010
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O	4.96700	-2.59670	-0.13930
C	4.48430	-1.35770	-0.55960
H	4.64800	-1.28160	-1.63890
O	5.23930	-0.35220	0.10390
C	4.91240	0.96580	-0.33430
H	5.03920	1.02740	-1.42440
C	5.88520	1.90350	0.34800
H	5.76770	1.81340	1.43390
H	5.67140	2.93050	0.05410
O	7.22620	1.63090	-0.03460
H	7.41990	0.71860	0.21230
C	3.46090	1.27840	0.02080
H	3.34740	1.25770	1.11230
O	3.13950	2.55970	-0.48970
H	2.16750	2.65590	-0.51820
C	2.55970	0.22210	-0.59670
H	2.61410	0.32900	-1.68900
O	1.24460	0.51300	-0.15610
C	3.00250	-1.19460	-0.23100
H	2.43520	-1.92450	-0.81800
O	2.85930	-1.46020	1.15580
H	1.94070	-1.70770	1.32420
C	0.19720	0.01520	-0.97300
H	0.57280	-0.16620	-1.98680
C	-0.88200	1.09000	-1.10780
H	-1.66110	0.67610	-1.75730
C	-0.40030	2.39670	-1.73640
H	0.17030	2.16680	-2.63840
H	-1.27610	2.98640	-2.02880
C	-0.38140	-1.27410	-0.42640
C	-1.63840	-3.54550	0.57290
C	-0.98670	-2.16590	-1.30750
C	-0.39640	-1.50910	0.94600
C	-1.01200	-2.65680	1.44600
C	-1.62660	-3.29330	-0.79990
H	-0.97410	-1.96630	-2.37200
H	0.04030	-0.78150	1.61770
O	-1.43180	1.33960	0.19810
O	0.43130	3.17690	-0.88760
H	-0.12570	3.46930	-0.14900
C	-2.70950	1.85010	0.19900
C	-5.27870	2.88220	0.26150
C	-3.80600	1.00610	-0.01750
C	-2.91120	3.20670	0.46600
C	-4.20360	3.73140	0.49780
C	-5.10040	1.52690	0.00560
H	-4.37230	4.77990	0.70020
H	-5.95640	0.88890	-0.16560
H	-6.28360	3.28650	0.28210
O	-3.50410	-0.29850	-0.23460
C	-4.57820	-1.18560	-0.53590
H	-4.12160	-2.16020	-0.70000
H	-5.10180	-0.86560	-1.43990
H	-5.27830	-1.24460	0.30050

O	-2.25510	-4.65490	1.08550
H	-2.64740	-5.15050	0.35270
O	-1.06960	-2.99080	2.76560
C	-0.38220	-2.13690	3.67670
H	-0.82070	-1.13630	3.67790
H	0.67960	-2.07770	3.42250
H	-0.50170	-2.59080	4.65760
O	-1.78200	3.93600	0.68840
O	-2.27970	-4.22970	-1.54620
C	-2.44210	-3.95570	-2.93610
H	-3.03500	-4.77520	-3.33510
H	-1.47310	-3.92270	-3.43860
H	-2.97050	-3.00960	-3.07900
C	-1.92710	5.34480	0.86760
H	-0.91680	5.73290	0.97730
H	-2.50530	5.56020	1.76820
H	-2.40560	5.79560	-0.00430

72 mannose_3_erythro

XYZ file generated by Avogadro.

H	2.59240	3.29930	-3.46460
O	1.83530	3.88940	-3.34140
C	1.18630	3.50890	-2.16560
H	0.20760	3.99850	-2.15350
O	1.96340	3.98000	-1.07410
C	1.35260	3.73760	0.19220
H	0.34790	4.18360	0.20330
C	2.22490	4.41320	1.22900
H	3.22840	3.97410	1.19440
H	1.80420	4.25510	2.22130
O	2.28430	5.81680	1.01890
H	2.62990	5.96370	0.13010
C	1.24260	2.23370	0.41600
H	2.25040	1.79900	0.42810
O	0.59500	2.00610	1.65620
H	0.55180	1.04490	1.77330
C	0.44240	1.61370	-0.71910
H	-0.59410	1.96820	-0.64820
O	0.50010	0.20910	-0.52900
C	1.01340	1.99610	-2.08330
H	0.32650	1.68970	-2.87940
O	2.29130	1.41480	-2.28610
H	2.21930	0.47050	-2.09310
C	-0.55790	-0.53280	-1.12360
H	-0.66230	-0.26030	-2.18040
C	-0.08830	-1.98840	-1.10500
H	0.78470	-2.05800	-1.75870
C	-1.17280	-2.93510	-1.57850
H	-1.93420	-3.01800	-0.79470
H	-1.64650	-2.52440	-2.47340
C	-1.88400	-0.30070	-0.43330
C	-4.34980	0.03550	0.80860
C	-3.02930	-0.12150	-1.20550

C	-1.95710	-0.30630	0.95740
C	-3.19220	-0.12950	1.57140
C	-4.26790	0.03920	-0.58350
H	-2.94840	-0.10810	-2.28500
H	-1.05980	-0.45530	1.54180
O	0.28700	-2.40350	0.22770
O	-0.66220	-4.22040	-1.90580
H	0.15730	-4.35350	-1.40690
C	1.62330	-2.34730	0.54880
C	4.31400	-2.30520	1.25110
C	2.54640	-3.16260	-0.12160
C	2.05520	-1.56470	1.62590
C	3.40740	-1.53910	1.97220
C	3.89940	-3.12560	0.20920
H	3.75260	-0.92870	2.79480
H	4.61470	-3.73950	-0.32020
H	5.36350	-2.27470	1.51740
O	2.01940	-3.98340	-1.07030
C	2.91350	-4.80260	-1.82180
H	2.28950	-5.34600	-2.52810
H	3.63570	-4.18700	-2.36190
H	3.43270	-5.50660	-1.16840
O	-5.57090	0.20810	1.40130
H	-5.44860	0.18790	2.36110
O	-3.39680	-0.10390	2.92080
C	-2.23230	-0.10760	3.74380
H	-1.59640	0.74740	3.49910
H	-1.67340	-1.03860	3.61980
H	-2.58730	-0.02500	4.76840
O	-5.44940	0.22000	-1.23920
O	1.09700	-0.86620	2.30270
C	-5.40600	0.22310	-2.66360
H	-4.78320	1.04210	-3.03070
H	-6.43270	0.36760	-2.99180
H	-5.02890	-0.73010	-3.04150
C	1.46020	-0.37220	3.59650
H	2.20620	0.42100	3.51680
H	1.83960	-1.18430	4.21990
H	0.54790	0.03160	4.02980

72 glucose_3_threo

XYZ file generated by Avogadro.

H	1.27730	6.17660	-0.47250
O	1.19310	5.40890	0.10600
C	0.59900	4.37240	-0.61530
H	1.03090	4.29350	-1.62170
O	-0.78630	4.66030	-0.72570
C	-1.51200	3.68520	-1.47510
H	-1.06550	3.57620	-2.47340
C	-2.92680	4.20430	-1.63550
H	-3.50150	3.50030	-2.23710
H	-2.89170	5.16430	-2.15920
O	-3.60350	4.33770	-0.39290
H	-3.12640	4.98580	0.13890

C	-1.43530	2.35070	-0.74020
H	-1.89700	2.46110	0.24890
O	-2.12510	1.37450	-1.49960
H	-2.01990	0.51750	-1.05150
C	0.02400	1.96210	-0.54950
H	0.48400	1.77270	-1.52770
O	0.08070	0.78930	0.25070
C	0.79410	3.07230	0.15050
H	0.39600	3.21020	1.16400
O	2.18170	2.79150	0.19130
H	2.30280	1.93580	0.62710
C	0.53800	-0.41250	-0.36680
H	0.38920	-0.35500	-1.44970
C	-0.36790	-1.51630	0.17600
H	-0.46490	-1.38930	1.26040
C	0.09070	-2.93350	-0.12190
H	1.08550	-3.08800	0.29870
H	-0.59270	-3.63900	0.36170
C	2.00190	-0.64490	-0.07270
C	4.68330	-1.10930	0.49550
C	2.48290	-0.42710	1.21860
C	2.84660	-1.09270	-1.08280
C	4.18830	-1.33070	-0.79000
C	3.82950	-0.65020	1.50060
H	1.80750	-0.08060	1.99060
H	2.45870	-1.24950	-2.08130
O	-1.65020	-1.27260	-0.45040
C	-2.74430	-1.78300	0.20950
C	-5.00330	-2.74410	1.47470
C	-3.29570	-3.00150	-0.19160
C	-3.34190	-1.03170	1.22650
C	-4.48080	-1.51670	1.86980
C	-4.43240	-3.49380	0.45190
H	-4.95530	-0.95090	2.65970
H	-4.87070	-4.43810	0.15980
H	-5.88670	-3.12420	1.97370
O	0.16140	-3.18780	-1.51650
H	-0.75500	-3.25720	-1.82090
O	-2.73730	0.15110	1.49840
C	-3.36010	1.00660	2.45330
H	-3.39330	0.53210	3.43660
H	-4.36980	1.27230	2.13140
H	-2.74050	1.90000	2.49860
O	6.00020	-1.32270	0.79640
H	6.44880	-1.64240	0.00070
O	4.40960	-0.45520	2.71660
C	3.57900	0.06210	3.75320
H	3.17110	1.03580	3.47020
H	2.76560	-0.63070	3.98090
H	4.22250	0.17100	4.62290
O	5.12100	-1.76960	-1.68210
C	4.67820	-2.04290	-3.01000
H	4.29100	-1.13640	-3.48010
H	3.91010	-2.81980	-3.00550

H	5.55450	-2.39290	-3.55010
O	-2.66410	-3.62040	-1.22490
C	-3.11460	-4.92470	-1.58810
H	-4.14140	-4.88940	-1.95740
H	-3.04470	-5.60570	-0.73710
H	-2.44940	-5.25580	-2.38250

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XYZ file generated by Avogadro.

H	-5.45320	-3.77280	1.40570
O	-4.68410	-3.69920	0.82770
C	-4.28230	-2.36320	0.79160
H	-4.32150	-1.91330	1.79260
O	-5.17400	-1.66660	-0.06470
C	-4.89190	-0.27170	-0.15370
H	-4.88130	0.17010	0.85260
C	-6.01600	0.36700	-0.94500
H	-5.85620	1.44410	-0.99010
H	-6.96070	0.17530	-0.42750
O	-6.07650	-0.09990	-2.28570
H	-6.26920	-1.04450	-2.26570
C	-3.51810	-0.08820	-0.79280
H	-3.53560	-0.50270	-1.80760
O	-3.23800	1.30180	-0.82970
H	-2.32070	1.41680	-1.11470
C	-2.47590	-0.83340	0.02570
H	-2.38060	-0.34090	1.00230
O	-1.23540	-0.76790	-0.67210
C	-2.86760	-2.29350	0.23520
H	-2.85760	-2.81000	-0.73330
O	-2.01100	-2.93790	1.15860
H	-1.11690	-3.02720	0.77980
C	-0.10330	-0.44450	0.12940
H	-0.18190	-0.93970	1.10210
C	1.11260	-1.02160	-0.59230
H	1.28980	-0.48620	-1.53160
C	0.97470	-2.50410	-0.89790
H	0.17370	-2.64540	-1.62270
H	1.90440	-2.87460	-1.34190
C	0.01650	1.04720	0.34550
C	0.26510	3.79000	0.72320
C	0.05610	1.55860	1.63750
C	0.09200	1.89450	-0.76110
C	0.21990	3.26750	-0.57170
C	0.18070	2.93570	1.82140
H	-0.00510	0.88830	2.48550
H	0.06810	1.47740	-1.76060
O	2.20310	-0.77540	0.31420
C	3.45480	-0.97990	-0.21010
C	6.01020	-1.39940	-1.20650
C	4.05850	-0.01850	-1.01590
C	4.14100	-2.16280	0.10210
C	5.42400	-2.37200	-0.39710
C	5.34080	-0.22440	-1.51810

H	5.96470	-3.27980	-0.16650
H	5.78960	0.53830	-2.14300
H	7.00750	-1.56830	-1.59410
O	0.64080	-3.26760	0.25520
H	1.41280	-3.25000	0.84030
O	3.46350	-3.03820	0.89310
C	4.07680	-4.30030	1.15390
H	3.36310	-4.85610	1.75790
H	4.26840	-4.83400	0.22020
H	5.00780	-4.16880	1.70910
O	0.40600	5.14110	0.88400
H	0.45110	5.33220	1.83180
O	0.23270	3.56620	3.02960
C	0.16900	2.74880	4.19660
H	1.01060	2.05310	4.22440
H	-0.77360	2.19810	4.22860
H	0.22620	3.43080	5.04150
O	0.33980	4.18160	-1.57380
O	3.36820	1.12880	-1.33520
C	3.42250	2.12820	-0.30630
H	2.86640	1.80180	0.57690
H	2.96820	3.02690	-0.72070
H	4.46350	2.33140	-0.04170
C	0.39820	3.67370	-2.90470
H	1.24820	2.99640	-3.02110
H	0.52630	4.54050	-3.54870
H	-0.52880	3.15610	-3.16300

72 galactose_3_threo

XYZ file generated by Avogadro.

H	-0.53180	5.63510	-0.40780
O	-0.87010	5.36320	-1.27220
C	-1.31170	4.04030	-1.18050
H	-1.56620	3.72180	-2.19800
O	-2.46910	4.01430	-0.36400
C	-3.07080	2.71830	-0.32270
H	-3.28460	2.39480	-1.35030
C	-4.37470	2.86000	0.43390
H	-4.18280	3.26240	1.43230
H	-4.83910	1.87780	0.53290
O	-5.29310	3.68820	-0.26730
H	-4.90290	4.56770	-0.33380
C	-2.13180	1.69770	0.30380
H	-2.58140	0.70480	0.20480
O	-1.94980	2.01340	1.67730
H	-1.32710	1.36500	2.03130
C	-0.79550	1.70820	-0.43790
H	-0.95560	1.29270	-1.43850
O	0.14460	0.92200	0.28060
C	-0.24980	3.12150	-0.58090
H	0.01830	3.51290	0.40890
O	0.89220	3.05350	-1.41780
H	1.35570	3.89810	-1.37450
C	0.84340	-0.08440	-0.45550

H	0.74990	0.11650	-1.52590
C	0.20440	-1.43670	-0.14820
H	0.24940	-1.61620	0.93170
C	0.84530	-2.60600	-0.87930
H	1.89840	-2.67820	-0.60250
H	0.35100	-3.53420	-0.57170
O	0.77620	-2.45390	-2.28970
H	-0.15590	-2.56920	-2.52690
C	2.30260	-0.06330	-0.07290
C	4.99280	-0.08870	0.62400
C	2.66100	-0.12740	1.27310
C	3.27370	-0.01390	-1.06830
C	4.62500	-0.03110	-0.71940
C	4.00900	-0.13230	1.61490
H	1.89610	-0.16710	2.03810
H	2.97200	0.03610	-2.10660
O	-1.17080	-1.29830	-0.55340
O	6.32280	-0.09820	0.94540
H	6.40510	-0.16150	1.90750
O	5.65780	0.01020	-1.60810
C	5.32050	0.04380	-2.99240
H	4.74650	0.94240	-3.23020
H	6.26650	0.06060	-3.52840
H	4.75240	-0.84600	-3.27390
C	-2.03480	-2.23010	-0.03630
C	-3.85890	-4.06700	0.94040
C	-2.50000	-3.25820	-0.86110
C	-2.48740	-2.12460	1.28410
C	-3.40700	-3.05220	1.77700
C	-3.42080	-4.18580	-0.37400
H	-3.76970	-2.98790	2.79330
H	-3.78980	-4.98590	-1.00060
H	-4.57360	-4.78530	1.32400
O	-1.99460	-3.26350	-2.12630
C	-2.36670	-4.34440	-2.98050
H	-2.07530	-5.30040	-2.54030
H	-1.82510	-4.18530	-3.91030
H	-3.44150	-4.33130	-3.17300
O	4.49890	-0.18320	2.88720
O	-1.97340	-1.09170	2.00090
C	3.55060	-0.26100	3.94920
H	2.90870	0.62270	3.95690
H	4.13300	-0.30130	4.86640
H	2.94290	-1.16380	3.85540
C	-2.42510	-0.94020	3.34520
H	-3.49980	-0.74590	3.37110
H	-1.88650	-0.08510	3.74840
H	-2.19060	-1.82900	3.93510

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XYZ file generated by Avogadro.

H	-4.99160	-3.67640	0.32660
O	-5.05780	-3.19380	1.16180
C	-4.46850	-1.93880	0.99830

H	-4.39400	-1.49240	1.99690
O	-5.33430	-1.15450	0.19280
C	-4.88420	0.19110	0.03760
H	-4.73590	0.64440	1.02750
C	-5.98800	0.96580	-0.65770
H	-5.67190	2.00330	-0.77310
H	-6.89030	0.93820	-0.04200
O	-6.26970	0.47240	-1.96710
H	-6.69670	-0.38860	-1.87870
C	-3.53950	0.22070	-0.69290
H	-3.18580	1.25820	-0.72930
O	-3.61310	-0.32200	-2.00510
H	-4.45110	-0.02960	-2.39400
C	-2.55050	-0.61210	0.10860
H	-2.40060	-0.11980	1.07720
O	-1.31470	-0.70030	-0.58710
C	-3.08850	-2.02140	0.35190
H	-3.19260	-2.54210	-0.60870
O	-2.25150	-2.75430	1.22750
H	-1.39420	-2.92760	0.79820
C	-0.16960	-0.44710	0.21430
H	-0.27810	-0.93750	1.18740
C	1.01460	-1.09430	-0.50460
H	1.27320	-0.51640	-1.39930
C	0.75950	-2.53560	-0.91050
H	-0.04450	-2.56750	-1.64460
H	1.66110	-2.94990	-1.37250
O	0.35740	-3.33770	0.19420
H	1.12850	-3.42330	0.77380
C	0.06430	1.03260	0.42670
C	0.69880	3.71610	0.77250
C	0.06090	1.88550	-0.67650
C	0.36360	1.51210	1.69720
C	0.68080	2.86060	1.87260
C	0.38800	3.22390	-0.49800
H	-0.16500	1.49600	-1.66130
H	0.36170	0.83110	2.53870
O	2.08970	-1.01670	0.44850
O	1.02770	5.03110	0.96110
H	1.00520	5.47650	0.10240
O	0.99230	3.43700	3.06860
C	1.01320	2.58580	4.21110
H	0.02850	2.14550	4.38480
H	1.75830	1.79570	4.09180
H	1.28360	3.22170	5.05080
C	3.34280	-1.16950	-0.09360
C	5.87670	-1.47300	-1.14780
C	3.97460	-0.07970	-0.70130
C	3.98680	-2.40450	-0.00030
C	5.26730	-2.56200	-0.53300
C	5.25240	-0.23250	-1.24020
H	5.78080	-3.51170	-0.47340
H	5.75560	0.59560	-1.72020
O	3.25580	1.07180	-0.70930

C	3.80870	2.19500	-1.39000
H	3.07620	2.99450	-1.28720
H	3.96490	1.96790	-2.44730
H	4.75120	2.50130	-0.93030
O	0.45700	4.15630	-1.49250
H	6.86960	-1.59340	-1.56440
O	3.28020	-3.38380	0.62710
C	3.81210	-4.70640	0.58370
H	4.75520	-4.76360	1.13100
H	3.95890	-5.02680	-0.45030
H	3.07020	-5.33980	1.06510
C	0.34180	3.68050	-2.83200
H	0.49450	4.54670	-3.47140
H	1.10710	2.92690	-3.03550
H	-0.65140	3.26160	-3.00880

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XYZ file generated by Avogadro.

O	-0.03300	2.87210	-3.29520
C	-0.16650	3.51150	-2.04830
H	-0.57430	4.50230	-2.24110
O	1.09090	3.66940	-1.41410
C	1.31540	2.61800	-0.45190
H	2.19330	2.03530	-0.75070
C	1.57050	3.28360	0.89600
H	0.67100	3.79960	1.23320
H	2.36970	4.02090	0.77210
O	1.90290	2.33990	1.90320
C	0.06040	1.74000	-0.49900
H	-0.21270	1.36130	0.48570
O	0.19860	0.69670	-1.46070
C	-1.00120	2.69250	-1.06630
H	-1.79920	2.14440	-1.57000
O	-1.51200	3.57210	-0.08330
C	0.29720	-0.64680	-0.97730
H	0.23160	-1.24160	-1.88970
C	1.65200	-0.89170	-0.34160
C	4.24680	-1.15750	0.67270
C	2.71090	-1.22820	-1.19420
C	1.89680	-0.70040	1.01290
C	3.19090	-0.82960	1.51250
C	3.99750	-1.36080	-0.69300
H	2.51540	-1.37590	-2.24920
H	1.11500	-0.43050	1.71280
C	-0.88100	-1.03780	-0.07930
H	-0.77750	-0.63730	0.93170
C	-1.01810	-2.55310	0.02450
H	-1.83040	-2.79090	0.71980
H	-0.09470	-2.96780	0.43280
O	-1.24830	-3.16680	-1.23380
H	-2.13900	-2.90350	-1.51200
O	-2.05780	-0.46090	-0.67740
C	-3.19490	-0.53370	0.09350
C	-5.52100	-0.68330	1.59370

C	-4.20340	-1.43400	-0.26520
C	-3.36690	0.30020	1.20350
C	-4.53210	0.21950	1.96580
C	-5.37690	-1.50920	0.48390
H	-4.67030	0.85530	2.82970
H	-6.16340	-2.20120	0.21690
H	-6.42930	-0.74340	2.18100
O	5.50270	-1.27440	1.18640
H	6.11250	-1.49310	0.46710
O	3.44480	-0.59790	2.84750
C	3.45000	-1.80180	3.62690
H	2.46520	-2.27460	3.59090
H	3.68380	-1.51170	4.64960
H	4.20870	-2.49480	3.25570
O	-3.93970	-2.20000	-1.36130
C	-4.90840	-3.18260	-1.72900
H	-4.49440	-3.69400	-2.59500
H	-5.85390	-2.70710	-1.99710
H	-5.06180	-3.89460	-0.91530
H	2.69970	1.86670	1.63200
H	0.15480	1.93430	-3.13780
H	-2.00160	3.02460	0.54570
O	5.10280	-1.68440	-1.42050
O	-2.34520	1.16110	1.45900
C	4.92720	-1.88550	-2.82150
H	4.24340	-2.71700	-3.00630
H	5.91260	-2.12350	-3.21440
H	4.54810	-0.97680	-3.29410
C	-2.31450	1.79450	2.73990
H	-3.12890	2.51570	2.83790
H	-1.35680	2.31200	2.78720
H	-2.37340	1.04960	3.53610

68 arabinose_3_erythro

XYZ file generated by Avogadro.

O	-5.40000	-3.23580	-0.49050
C	-4.87020	-2.16330	0.24520
H	-5.21620	-2.21010	1.28000
O	-5.28870	-0.91400	-0.29740
C	-4.17440	-0.22840	-0.87910
H	-4.03480	-0.53440	-1.92370
C	-4.44620	1.26310	-0.80320
H	-4.55520	1.55670	0.24630
H	-5.37510	1.49070	-1.32810
O	-3.41980	2.01200	-1.43940
C	-2.99820	-0.71100	-0.03950
H	-3.00240	-0.19140	0.92790
O	-1.76860	-0.50930	-0.70700
C	-3.34790	-2.18420	0.14960
H	-3.06470	-2.71710	-0.76680
O	-2.78420	-2.81030	1.28240
C	-0.64960	-0.37540	0.16710
H	-0.86530	-0.84410	1.13200
C	-0.31210	1.08310	0.37890

C	0.43360	3.74090	0.70670
C	-0.18710	1.91080	-0.73770
C	-0.07660	1.57300	1.65830
C	0.29940	2.90700	1.81610
C	0.18980	3.24050	-0.57460
H	-0.35580	1.50350	-1.72700
H	-0.17490	0.91760	2.51450
C	0.51250	-1.13460	-0.47370
H	0.80320	-0.64200	-1.40900
C	0.19330	-2.59270	-0.76210
H	1.05930	-3.06720	-1.23490
H	-0.64750	-2.65050	-1.45280
O	-0.17060	-3.30470	0.41540
H	0.63010	-3.37530	0.95690
O	1.58420	-1.03680	0.48100
C	2.83480	-1.29430	-0.02920
C	5.37100	-1.79850	-1.00480
C	3.52880	-0.28890	-0.71080
C	3.42100	-2.54450	0.17690
C	4.70110	-2.80370	-0.31540
C	4.80660	-0.54330	-1.21000
H	5.16880	-3.76740	-0.16840
H	5.35540	0.22040	-1.74380
H	6.36380	-1.99770	-1.39020
O	0.80290	5.05120	0.84210
H	0.93500	5.23530	1.78290
O	0.56220	3.51430	3.00890
C	0.47280	2.71170	4.18410
H	0.72570	3.36790	5.01340
H	-0.54220	2.32900	4.31120
H	1.18230	1.88260	4.13740
O	2.86870	0.89060	-0.82550
C	3.49780	1.93570	-1.56190
H	2.80750	2.77750	-1.53170
H	3.66720	1.63130	-2.59750
H	4.44420	2.22180	-1.09700
H	-2.59720	1.89650	-0.94500
H	-6.32920	-3.34180	-0.25300
H	-1.84950	-3.00280	1.07870
O	0.36410	4.12790	-1.59330
O	2.66360	-3.43740	0.87150
C	3.14400	-4.77770	0.96460
H	2.36690	-5.33440	1.48390
H	4.07150	-4.81690	1.53930
H	3.30050	-5.19880	-0.03100
C	0.18610	3.62820	-2.91650
H	0.88900	2.81610	-3.12050
H	0.38800	4.46550	-3.58040
H	-0.83900	3.27900	-3.06330

68 xylose_3_threo

XYZ file generated by Avogadro.

H	-6.74200	-0.03900	0.17010
O	-5.84220	0.07680	0.49880

C	-4.99760	-0.78680	-0.20140
H	-5.24340	-0.79410	-1.27220
O	-5.17850	-2.08990	0.32320
C	-4.38110	-3.04890	-0.35940
H	-4.64570	-4.02770	0.03800
H	-4.59740	-3.02770	-1.43510
C	-2.90930	-2.75490	-0.12240
H	-2.69960	-2.82490	0.95260
O	-2.15630	-3.71210	-0.84080
H	-1.20730	-3.48410	-0.77530
C	-2.58260	-1.34180	-0.58580
H	-2.65340	-1.30680	-1.68120
O	-1.23720	-1.09780	-0.18650
C	-3.55920	-0.32030	0.00150
H	-3.38130	-0.22010	1.07930
O	-3.45030	0.93940	-0.64440
C	-0.44810	-0.24940	-1.00250
H	-0.87260	-0.20680	-2.01220
C	-0.37050	1.16100	-0.44180
C	-0.18910	3.75190	0.55800
C	-0.68870	1.41230	0.89070
C	0.04140	2.19340	-1.28090
C	0.13920	3.48440	-0.77220
C	-0.60770	2.71460	1.38870
H	-1.00140	0.59650	1.52790
H	0.28410	1.98540	-2.31590
C	0.95400	-0.84050	-1.15280
H	1.51190	-0.16860	-1.81310
C	1.01140	-2.23370	-1.77370
H	2.04420	-2.44030	-2.07410
H	0.39030	-2.24090	-2.67180
O	0.54920	-3.27720	-0.92690
H	1.11190	-3.29100	-0.13510
O	1.56170	-0.83520	0.15280
C	2.92540	-0.99870	0.17240
C	5.68210	-1.35300	0.29510
C	3.78560	0.01750	-0.23800
C	3.46120	-2.20010	0.66320
C	4.83990	-2.37740	0.72500
C	5.16610	-0.15770	-0.18260
H	5.25990	-3.30090	1.09910
H	5.80950	0.65030	-0.51020
H	6.75460	-1.49730	0.34110
O	-0.09680	5.01810	1.07000
H	0.23160	5.60360	0.37300
O	-0.90380	3.07050	2.66990
C	-1.36470	2.03740	3.53730
H	-2.28270	1.58850	3.14960
H	-1.56500	2.51840	4.49180
H	-0.59950	1.26820	3.66500
O	3.26110	1.19980	-0.71050
C	3.02620	2.15780	0.33220
H	2.76340	3.09440	-0.15660
H	3.93470	2.29530	0.92410

H	2.20560	1.82620	0.97520
H	-2.71640	1.42710	-0.24880
O	0.55790	4.57510	-1.47480
O	2.54630	-3.13070	1.05840
C	1.04310	4.35090	-2.79730
H	1.38060	5.31890	-3.15940
H	0.24610	3.97300	-3.44120
H	1.87890	3.64680	-2.78280
C	3.03800	-4.39620	1.50270
H	3.61740	-4.88100	0.71430
H	2.15610	-4.98940	1.73310
H	3.64800	-4.27520	2.39980

68 xylose_3_erythro

XYZ file generated by Avogadro.

H	6.62590	-0.01110	1.28990
O	6.06080	0.19800	0.53620
C	4.86080	-0.50250	0.66920
H	4.49560	-0.46520	1.70450
O	5.10610	-1.85360	0.31160
C	3.94680	-2.66730	0.44280
H	4.24980	-3.69150	0.23070
H	3.55630	-2.61300	1.46710
C	2.87900	-2.20510	-0.53770
H	3.25400	-2.31140	-1.56260
O	1.73450	-3.02020	-0.34120
H	1.01000	-2.65760	-0.86990
C	2.56710	-0.74220	-0.27060
H	2.09530	-0.66760	0.71740
O	1.67230	-0.27410	-1.27520
C	3.83440	0.10830	-0.27630
H	4.26400	0.11070	-1.28640
O	3.57160	1.42820	0.16100
C	0.54260	0.45820	-0.78750
H	0.87090	1.12980	0.01190
C	-0.48950	-0.49500	-0.22450
C	-2.35570	-2.25560	0.84820
C	-1.20050	-1.34710	-1.06910
C	-0.67750	-0.54310	1.15430
C	-1.61820	-1.41890	1.68620
C	-2.13980	-2.22500	-0.53110
H	-1.03820	-1.31320	-2.13870
H	-0.11770	0.12640	1.79590
C	0.08420	1.30650	-1.98630
H	-0.33430	0.65960	-2.76310
C	1.23110	2.10940	-2.57580
H	0.82310	2.77480	-3.34210
H	1.96470	1.45070	-3.03630
O	1.90760	2.86740	-1.57490
H	1.23770	3.26480	-0.99280
O	-0.91050	2.30500	-1.64780
C	-1.64830	2.18780	-0.49490
C	-3.11720	1.98200	1.83810
C	-1.17480	2.77300	0.67930

C	-2.87750	1.52020	-0.50770
C	-3.61760	1.41250	0.66980
C	-1.90740	2.66670	1.86090
H	-4.56240	0.88680	0.68560
H	-1.53950	3.10120	2.78080
H	-3.68910	1.89080	2.75420
O	-3.30090	-3.10750	1.34970
H	-3.32610	-3.00110	2.31130
O	-2.91430	-3.07650	-1.26070
C	-2.75350	-3.04210	-2.67630
H	-3.46520	-3.76180	-3.07410
H	-1.73860	-3.33340	-2.95720
H	-2.97630	-2.04650	-3.06810
O	0.02770	3.41130	0.57540
C	0.78980	3.56570	1.77380
H	0.88040	2.60690	2.29140
H	0.33460	4.30660	2.43350
H	1.77240	3.91260	1.45910
H	3.01430	1.88410	-0.49960
O	-3.24400	0.99330	-1.70490
O	-1.92600	-1.53420	3.01040
C	-4.41540	0.18090	-1.72440
H	-4.51700	-0.17230	-2.74800
H	-5.29680	0.76540	-1.45020
H	-4.30800	-0.66930	-1.04460
C	-1.19900	-0.71220	3.92180
H	-1.58070	-0.95400	4.91100
H	-1.37010	0.34560	3.70700
H	-0.13120	-0.93700	3.87170

68 arabinose_5_threo

XYZ file generated by Avogadro.

H	-0.50510	5.29920	0.93810
O	-1.25650	4.69330	0.91730
C	-0.77050	3.37430	1.04120
H	-0.16770	3.25080	1.94170
O	0.03080	3.02160	-0.06450
C	-0.81890	2.62300	-1.16280
H	-0.84340	3.41760	-1.91310
C	-0.23250	1.37680	-1.78680
H	0.82040	1.55520	-2.02750
H	-0.77380	1.12640	-2.70630
O	-0.35270	0.31210	-0.85170
C	-2.23090	2.43630	-0.56210
H	-2.67720	1.49230	-0.86900
O	-3.12920	3.45930	-0.95880
H	-2.77360	4.30310	-0.64700
C	-1.97250	2.43990	0.95470
H	-2.82930	2.82060	1.50880
O	-1.65590	1.15570	1.45570
H	-1.09870	0.70060	0.79880
C	0.56570	-0.75700	-1.03830
H	0.55160	-1.07870	-2.08690
C	1.96640	-0.34440	-0.64290

C	4.54270	0.33780	0.17490
C	2.14830	0.40430	0.52400
C	3.06080	-0.74340	-1.39650
C	4.34680	-0.40540	-0.98230
C	3.43070	0.74850	0.92560
H	1.28510	0.72080	1.09760
H	2.93570	-1.31970	-2.30720
C	0.04080	-1.89840	-0.16690
H	-0.14200	-1.51260	0.84320
C	0.97860	-3.08950	-0.10600
H	1.95730	-2.77580	0.25740
H	1.09640	-3.50040	-1.11620
O	0.49140	-4.08790	0.78090
H	-0.46800	-3.98400	0.85980
O	-1.19360	-2.40020	-0.72020
C	-2.36620	-1.85650	-0.24960
C	-4.77480	-0.84430	0.66930
C	-2.80540	-2.15780	1.04310
C	-3.16120	-1.08040	-1.09770
C	-4.37570	-0.56970	-0.63420
C	-4.00850	-1.63620	1.51760
H	-4.99580	0.04360	-1.27360
H	-4.34990	-1.85030	2.52090
H	-5.71230	-0.43830	1.02990
O	5.80900	0.67600	0.55050
H	5.75870	1.20750	1.35790
O	5.44220	-0.77090	-1.73610
C	6.07010	-1.96570	-1.25190
H	6.40610	-1.83200	-0.22100
H	5.37170	-2.80460	-1.30880
H	6.92630	-2.15300	-1.89730
O	-1.98670	-2.98110	1.75110
C	-2.33410	-3.26150	3.10540
H	-1.53980	-3.89890	3.48750
H	-3.28880	-3.78900	3.15820
H	-2.38180	-2.33870	3.68760
O	-2.66560	-0.87010	-2.34520
O	3.73960	1.48550	2.02960
C	-3.45470	-0.09740	-3.24680
H	-2.88940	-0.05850	-4.17530
H	-3.60650	0.91610	-2.86640
H	-4.42090	-0.57590	-3.42320
C	2.65290	2.09220	2.72730
H	2.09450	2.74800	2.05510
H	3.10010	2.67480	3.52900
H	1.98990	1.33290	3.14790

68 arabinose_5_erythro

XYZ file generated by Avogadro.

H	4.21520	4.36270	-0.24710
O	3.57260	4.09230	0.42110
C	3.08860	2.81060	0.07940
H	3.90110	2.08950	-0.02040
O	2.39220	2.84530	-1.14690

C	1.03460	3.28320	-0.91840
H	0.91440	4.31060	-1.27130
C	0.10700	2.37640	-1.69750
H	0.28580	2.46930	-2.77410
H	-0.93080	2.65430	-1.48150
O	0.37830	1.04940	-1.28090
C	0.82420	3.23670	0.61240
H	-0.10960	2.73910	0.87470
O	0.76890	4.53480	1.18560
H	1.61600	4.97080	1.01810
C	2.03610	2.43660	1.12050
H	2.32970	2.75510	2.11970
O	1.80710	1.04340	1.16350
H	1.40110	0.75320	0.32600
C	-0.58770	0.07720	-1.65310
H	-0.84920	0.19910	-2.71110
C	-1.84320	0.18980	-0.81540
C	-4.14630	0.26710	0.74060
C	-1.74340	0.40340	0.55840
C	-3.08540	0.03320	-1.42280
C	-4.23510	0.06310	-0.63640
C	-2.89710	0.44850	1.33680
H	-0.76930	0.52510	1.01200
H	-3.14840	-0.12220	-2.49260
C	0.14930	-1.25740	-1.52660
H	0.97870	-1.23190	-2.23950
C	-0.68410	-2.50460	-1.80840
H	-0.00200	-3.34180	-1.99140
H	-1.26630	-2.33990	-2.71810
O	-1.58870	-2.83930	-0.76870
H	-1.05570	-3.12790	-0.01110
O	0.67900	-1.29270	-0.19010
C	1.74980	-2.11770	0.02390
C	3.90820	-3.76990	0.58540
C	1.57950	-3.26330	0.79590
C	3.02710	-1.78050	-0.45380
C	4.10560	-2.61840	-0.17640
C	2.65480	-4.09750	1.08350
H	5.09530	-2.37790	-0.54030
H	2.49200	-4.98310	1.68540
H	4.75450	-4.41230	0.79630
O	-5.26780	0.31260	1.52430
H	-6.03940	0.17360	0.95690
O	-5.51130	-0.08160	-1.09940
C	-5.67640	-0.31770	-2.49530
H	-5.29000	0.52290	-3.07600
H	-6.74720	-0.41560	-2.65730
H	-5.17110	-1.24000	-2.79100
O	0.31600	-3.56710	1.26270
C	-0.07820	-2.75520	2.38400
H	0.56340	-2.97430	3.24040
H	-0.01310	-1.69730	2.12330
H	-1.10960	-3.02050	2.61150
O	-2.91480	0.66330	2.68360

O	3.10180	-0.62540	-1.16040
C	-1.66160	0.92430	3.31190
H	-0.99850	0.05960	3.23240
H	-1.88840	1.11700	4.35800
H	-1.18200	1.80180	2.86970
C	4.38460	-0.22810	-1.63830
H	5.07940	-0.08370	-0.80760
H	4.22830	0.71490	-2.15790
H	4.78440	-0.96980	-2.33370

