

## Carbohydrates in the gas phase: conformational preference of D-ribose and 2-deoxy-D-ribose

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**Cartesian coordinates of the most stable minima in gas phase (less than 5 kJ mol<sup>-1</sup>) for the open-chain, furanose and pyranose forms of 2-deoxy-D-ribose and D-ribose calculated with the M06-2X hybrid functional and the 6-311++G(d,p) Pople's basis set.**

### Open-chain 2-deoxy-D-ribose (3)

#### dDR01

C, 0.3703581687, 0.5205658108, -0.2277400174  
C, 0.2838714808, 0.7883709243, 1.247419969  
C, 0.9960534272, -0.2599081094, 2.0915967338  
C, 0.8750096738, 0.0538891974, 3.5843187531  
C, 1.4109942837, -1.0916006362, 4.4490018252  
O, 0.4723000963, -2.1469312071, 4.5256028852  
H, -0.0308835286, 1.3094164291, -0.8915963377  
H, 0.6865992099, 1.789585479, 1.4412296866  
H, -0.7751922119, 0.8312473555, 1.5289454566  
H, 2.0645597299, -0.2703497807, 1.8343558709  
H, 1.4696951836, 0.953955969, 3.7766192063  
H, 1.5552268286, -0.7371533442, 5.4704921545  
H, 2.3753309468, -1.4368101936, 4.0576662095  
O, 0.8326753938, -0.4866891062, -0.7040460285  
O, 0.4480005648, -1.5539435164, 1.8656731521  
O, -0.4558661835, 0.3492737684, 3.9462891508  
H, 0.360113697, -2.4833309064, 3.6269219625  
H, 0.5832455149, -1.7663550523, 0.93450451  
H, -0.856603517, -0.4837094199, 4.2264434435

#### dDR02

C, -0.24197666, -0.4421010354, 0.0084068105  
C, -0.1138279231, 0.0166107496, 1.4319360174  
C, 1.2965399481, -0.0066274098, 2.0026118194  
C, 2.0980209127, 1.2736661475, 1.7485862128  
C, 2.3548068572, 1.5943539564, 0.2827458314  
O, 3.1795324178, 0.6081147177, -0.305862995  
H, -1.2754447882, -0.4941018052, -0.3824609048  
H, -0.573460514, 1.0105268487, 1.5175187629  
H, -0.7449878102, -0.6433149429, 2.0391452782  
H, 1.8451643895, -0.8534405762, 1.5681136518  
H, 1.5599804575, 2.104570946, 2.2192672404  
H, 2.9024501755, 2.5374859418, 0.2295867192  
H, 1.415231038, 1.7165954171, -0.2661719989  
O, 0.6797130215, -0.7566752468, -0.7027202256  
O, 1.1622709388, -0.1877962373, 3.3999578429  
O, 3.3364052088, 1.1550755198, 2.432405301  
H, 2.6077816032, -0.1184815784, -0.583710522  
H, 2.030210616, -0.0138252645, 3.7835655714  
H, 3.9417276389, 0.7060057955, 1.8277191951

#### dDR03

C, -0.7302598619, -0.9663272561, 0.9346358973  
C, 0.1057177478, 0.2865328061, 0.9352990864  
C, 1.4868508694, 0.0729490519, 1.5395739622  
C, 2.299989944, 1.3598796756, 1.6381886941  
C, 2.6158899822, 1.996204646, 0.2957329437  
O, 3.2898035827, 1.0961380658, -0.5578829314  
H, -1.7246970617, -0.8849796071, 0.456344839  
H, 0.1778214595, 0.6274112982, -0.1039770732

H, -0.4499773836, 1.0581846541, 1.4841052012  
H, 2.0433880513, -0.6428644827, 0.9241745998  
H, 1.7381656424, 2.0758022006, 2.25653604  
H, 3.2185126207, 2.89304098, 0.4791104724  
H, 1.702651524, 2.3033761612, -0.2170034484  
O, -0.3762633072, -2.0133307546, 1.4129153123  
O, 1.3982423712, -0.4020614768, 2.8765531845  
O, 3.5515220449, 1.0736313845, 2.23545708  
H, 4.0645419156, 0.7861496362, -0.0762890195  
H, 1.0334138606, -1.2934916739, 2.8454410737  
H, 3.3798695351, 0.4920812838, 2.9851234007

### Open-chain D-ribose (9)

#### DR01

C, 0.5515145235, -0.1399113931, -0.238420086  
C, 0.2558266857, 0.4361146325, 1.1332888567  
C, 0.9515610825, -0.4268290475, 2.1896117783  
C, 0.595764477, 0.0042582832, 3.6217099152  
C, 1.390569506, -0.7777281842, 4.6622194395  
O, 1.0100200664, -2.1455240536, 4.6502933449  
H, 1.6147695405, -0.2931873383, -0.4921164474  
H, 0.6854723796, 1.4474290699, 1.1713855249  
H, 2.0359631398, -0.2643888753, 2.0686069499  
H, 0.8524188931, 1.0706211212, 3.7163630655  
H, 1.2131526385, -0.3399374027, 5.6498065566  
H, 2.4602980753, -0.7397189082, 4.4482713249  
O, -0.331310007, -0.4146968546, -1.0027623125  
O, -1.1322781256, 0.513596686, 1.3343709389  
O, 0.61178316, -1.7605494296, 1.9000326059  
O, -0.7570787821, -0.225271683, 3.9476772268  
H, 0.0621527784, -2.1588155815, 4.8323835354  
H, -1.5569615092, 0.100009981, 0.568180695  
H, 0.8019667567, -2.3000138646, 2.6799202207  
H, -1.2963071747, -0.006478042, 3.1753964561

#### DR02

C, 0.357982287, 0.0534715104, -0.1622680678  
C, 0.1787688368, 0.4604907399, 1.2854254725  
C, 0.9922221415, -0.4736576115, 2.1896013018  
C, 0.6713520014, -0.2265322829, 3.6701621094  
C, 1.6892045991, -0.8739537211, 4.5940111523  
O, 1.3404884551, -0.6733701231, 5.943424008  
H, 1.3951292373, -0.0468208449, -0.5260682221  
H, 0.5707987956, 1.4837279928, 1.394142116  
H, 2.0551599433, -0.2723644209, 2.0112647039  
H, 0.6425168433, 0.8523010865, 3.8698818774  
H, 2.6693373272, -0.4168663143, 4.4440244151  
H, 1.7614219986, -1.9417150189, 4.3525560829  
O, -0.5879655296, -0.144347745, -0.8743472642  
O, -1.1857081601, 0.4322266097, 1.6279037782  
O, 0.7613669669, -1.8187865448, 1.8423535398  
O, -0.5784658164, -0.8195260228, 3.9978225525  
H, 0.4239177261, -0.9533153256, 6.0392848714  
H, -1.6833406848, 0.2496051786, 0.8169589163  
H, -0.0126064713, -2.1112479214, 2.3407119509  
H, -1.2634177419, -0.3636468135, 3.4914438471

### DR03

C, -0.0072531202, 0.0817068943, -0.0176876571  
C, -0.0993196428, -0.099610935, 1.4815640709  
C, 1.298185399, -0.0678773503, 2.1071648195  
C, 1.3003470755, 0.091801177, 3.6387079159  
C, 0.5795353515, -1.006400138, 4.4247325849  
O, -0.8209678507, -0.7939297761, 4.4370294735  
H, 0.5341917737, 0.9739799861, -0.3761803991  
H, -0.6846831463, 0.7391156148, 1.8851310328  
H, 1.8160152175, 0.8140069581, 1.7164365941  
H, 2.3553447869, 0.0810882819, 3.9308723095  
H, 0.905682502, -0.9549179397, 5.4649877856  
H, 0.8365509384, -1.9973165271, 4.0367166596  
O, -0.5037858186, -0.7085766369, -0.7735751176  
O, -0.7250854717, -1.334774909, 1.7617600725  
O, 2.0350897783, -1.1943727675, 1.6935395364  
O, 0.7595829439, 1.3517582554, 3.9708622761  
H, -1.1817718659, -1.1560541574, 3.6179401156  
H, -1.0683684924, -1.6829115822, 0.9245911734  
H, 1.4703323098, -1.9682957056, 1.7994457664  
H, -0.1378121849, 1.1943062167, 4.2921805767

### DR04

C, 0.5531329334, -1.0633659498, 0.052919564  
C, -0.189322025, -0.3373630273, 1.1489618848  
C, 0.7698096588, 0.44216304, 2.0591329095  
C, 1.6145320486, 1.4698011475, 1.3038460853  
C, 2.2195104863, 2.5139870239, 2.2466808288  
O, 1.2523249914, 3.4816397165, 2.6020419632  
H, 1.0675834572, -0.4388129807, -0.6967164191  
H, -0.8629852713, 0.3891433339, 0.680857464  
H, 1.4458763782, -0.2773604066, 2.5437649401  
H, 2.4316181193, 0.9258208601, 0.816348127  
H, 3.0129177744, 3.0512082732, 1.7254138896  
H, 2.6459544937, 2.02346116, 3.1286894458  
O, 0.575152072, -2.2655317199, 0.0068834621  
O, -0.9284581449, -1.2293136624, 1.9455744135  
O, -0.0013729356, 1.0993621387, 3.0526404343  
O, 0.875662533, 2.1076251777, 0.2835459712  
H, 0.5865636795, 3.0288767893, 3.1346199407  
H, -0.6886835511, -2.127185972, 1.6771714297  
H, -0.6186128253, 0.4532208336, 3.4162659061  
H, 0.5298229938, 2.9275616548, 0.6609360779

### DR05

C, -0.2405859931, -0.222815316, -0.1328664116  
C, -0.1598894679, -0.5217501109, 1.3565808077  
C, 0.6241627085, 0.57371614, 2.089964146  
C, 0.4081819108, 0.5038177894, 3.6027863813  
C, 1.2939724394, 1.4931210018, 4.3618017137  
O, 2.625555335, 1.019327292, 4.4328091848  
H, 0.0701025658, -1.0548128089, -0.7927408956  
H, -1.1901061268, -0.5430552043, 1.7380876088  
H, 0.2794988441, 1.5458632789, 1.7240193939  
H, -0.6433949282, 0.7340115649, 3.8060200589  
H, 0.9458971995, 1.5786014844, 5.3924306684  
H, 1.2387193308, 2.4812806108, 3.8920215869  
O, -0.6240413856, 0.8290730182, -0.5581423951  
O, 0.4706136066, -1.7772143507, 1.4936274693

O, 2.0033959773, 0.460495861, 1.7626624222  
O, 0.6571297053, -0.8148973314, 4.0803120028  
H, 2.9576533586, 0.9876886309, 3.5262698998  
H, 0.484634425, -1.9786126202, 2.4403404157  
H, 2.1811905005, -0.4770894751, 1.609777399  
H, 1.544413511, -0.8055980386, 4.4655364596

#### DR06

C, -0.1329542435, -0.0637588862, 0.1050952528  
C, -0.0711514111, 0.1855686968, 1.5952479972  
C, 1.3612862725, 0.0981858081, 2.1282766956  
C, 2.1390369247, -1.1593226168, 1.7267188819  
C, 1.4405231571, -2.4699379355, 2.058206062  
O, 1.0873821932, -2.5256294258, 3.4265769345  
H, 0.5237271154, 0.5594367799, -0.524136239  
H, -0.396680688, 1.2235044449, 1.7566724365  
H, 1.2903161772, 0.1208226924, 3.2241533079  
H, 2.3435378018, -1.1181336751, 0.6505531659  
H, 2.1435959942, -3.285060403, 1.8743728255  
H, 0.570808136, -2.6155413209, 1.4102113025  
O, -0.869748412, -0.895017405, -0.3590130206  
O, -0.8975997417, -0.7120732779, 2.2937369518  
O, 2.0325040778, 1.2448487696, 1.6507271883  
O, 3.40573892, -1.0835293954, 2.3663843076  
H, 0.2655579831, -2.0284021151, 3.5216784603  
H, -1.4698170528, -1.1430527152, 1.6428264307  
H, 2.9664263073, 1.1323766124, 1.8629041199  
H, 3.2851208835, -1.4052392049, 3.2685033159

#### DR07

C, -0.4030765361, -1.3614450532, 0.8515289919  
C, 0.1633758678, 0.0244713989, 1.0845111532  
C, 1.5923023498, -0.077695611, 1.6057902518  
C, 2.2466634838, 1.2833209375, 1.8469206282  
C, 2.3467993153, 2.1395017446, 0.5979225472  
O, 2.9854085168, 1.4428584215, -0.4535864034  
H, 0.1950372462, -2.0403999369, 0.2186889158  
H, 0.1748193269, 0.5301285347, 0.1069018332  
H, 2.2000807681, -0.6307325265, 0.8850232861  
H, 1.666688963, 1.8230619326, 2.6077081243  
H, 2.8898150248, 3.0563010522, 0.85244015  
H, 1.3541876976, 2.4225741875, 0.2438510884  
O, -1.4570180209, -1.6924010323, 1.3220287279  
O, -0.6161390427, 0.7236310587, 2.0195799593  
O, 1.6172083935, -0.827748909, 2.8107022137  
O, 3.5778679185, 1.0712082874, 2.288320071  
H, 3.8590014857, 1.194015151, -0.1333595038  
H, -1.45628916, 0.2510940125, 2.1054410226  
H, 0.9426884857, -0.4538747735, 3.392100627  
H, 3.5605913424, 0.3630483283, 2.9417700568

#### DR08

C, -0.1204921959, -0.0905516187, 0.018246681  
C, -0.117764684, 0.0821275026, 1.5215134545  
C, 1.3100316246, -0.0723840526, 2.0548431113  
C, 1.3309112955, -0.0893728125, 3.5900733596  
C, 2.7386273886, 0.1084334139, 4.1219310386  
O, 3.1415590348, 1.4155914468, 3.7487534406  
H, 0.5869951942, 0.5349041848, -0.5531138061

H, -0.4622765458, 1.1048889975, 1.7392410616  
H, 1.9016215499, 0.7811870267, 1.7097003206  
H, 0.6981898394, 0.7240377295, 3.9676756274  
H, 3.3943757757, -0.6541024825, 3.6873957233  
H, 2.7181658291, -0.014694073, 5.2091891733  
O, -0.8590014625, -0.8696212326, -0.5200165324  
O, -0.9884843965, -0.8523218752, 2.1156547791  
O, 1.9076606039, -1.2397171468, 1.5362194284  
O, 0.8956122761, -1.3463841853, 4.0728166975  
H, 4.0581397215, 1.5461722563, 3.997933573  
H, -1.4394168805, -1.3231610326, 1.3994530211  
H, 1.6526968987, -1.9693377671, 2.1151878317  
H, -0.0154863117, -1.4679803714, 3.7760979918

#### DR09

C, -0.2068738626, -0.1317076313, 0.0288707705  
C, -0.0992202735, -0.0069484279, 1.5381951404  
C, 1.3464386865, 0.0979527865, 2.0280732582  
C, 2.1849906701, -1.1085347641, 1.584742649  
C, 3.4880114091, -1.2102985941, 2.3591388865  
O, 4.169048549, 0.0394252004, 2.2308610137  
H, 0.3213896424, 0.6224108953, -0.5735838337  
H, -0.5854359973, 0.9469012283, 1.795598041  
H, 1.312947285, 0.1294265764, 3.1245265486  
H, 1.6056720963, -2.0164324162, 1.7727456922  
H, 4.088634882, -2.0195878111, 1.9343892459  
H, 3.2777037444, -1.4243255226, 3.4129848028  
O, -0.8939085025, -0.9872800767, -0.4654236361  
O, -0.732299277, -1.081782927, 2.1700066067  
O, 1.8570857377, 1.3059006746, 1.4953128597  
O, 2.4166183551, -1.0538179003, 0.1924314896  
H, 5.0630659964, -0.0359880157, 2.5698283478  
H, -1.2107991713, -1.5670969784, 1.4825751443  
H, 2.754431866, 1.4154136552, 1.8334036627  
H, 2.8300065543, -0.2026155795, 0.0055640657

### $\alpha$ -2-deoxy-D-ribofuranose (2)

#### dDR $\alpha$ f01

C, 0.2334666827, -0.0748958686, 0.150797356  
C, 0.2796572986, -0.4210008218, 1.6275052868  
C, 1.5787672237, 0.271346623, 2.0544405423  
C, 2.4464764454, 0.1902636757, 0.775254484  
O, 1.559982676, -0.2069587385, -0.2911311759  
C, 3.5556879374, -0.8420021393, 0.8353598081  
H, -0.3813608448, -0.7258829371, -0.4741714153  
H, 0.3671304516, -1.5023923371, 1.7425304129  
H, -0.5841857691, -0.0543548575, 2.1800130104  
H, 2.0628642461, -0.2411249062, 2.8852294421  
H, 2.8608042613, 1.1798604225, 0.5592753779  
H, 4.2449847002, -0.5943757535, 1.6447116701  
H, 4.1128129531, -0.8349538704, -0.1085808993  
O, -0.1982370508, 1.2692889665, 0.0467886343  
O, 1.3705336891, 1.6037638114, 2.4754497218  
O, 3.0399967715, -2.1294452966, 1.1088211349  
H, -0.0948074732, 1.5496557671, -0.8680523496  
H, 0.8204595462, 2.0336735838, 1.8096757341  
H, 2.4627794415, -2.3585660357, 0.3737136826

#### dDR $\alpha$ f02

C, 0.1391569805, -0.0567871833, 0.0480219656  
C, 0.2166654347, -0.408658317, 1.5229487485  
C, 1.5142060117, 0.3036204299, 1.9295927059  
C, 2.3729976526, 0.165152354, 0.6587089575  
O, 1.4604441293, -0.1462978995, -0.4185462824  
C, 3.3783721401, -0.9696352686, 0.7253401797  
H, -0.4687841604, -0.7225189651, -0.5678490751  
H, 0.3133770285, -1.4906980024, 1.6307055921  
H, -0.6424328424, -0.0571473545, 2.0922203005  
H, 2.0000294259, -0.1749122252, 2.7819117942  
H, 2.8758500349, 1.1082262159, 0.4311520346  
H, 2.8676695838, -1.8822489388, 1.0670445745  
H, 4.1636322031, -0.7256179703, 1.4436774047  
O, -0.3342754579, 1.2740648575, -0.0421841143  
O, 1.2997069482, 1.6454458491, 2.3059849104  
O, 4.0024548137, -1.1787500359, -0.5197032674  
H, -0.2491329814, 1.5616696905, -0.9566678897  
H, 0.7429013515, 2.049550171, 1.6292700001  
H, 3.3019359259, -1.2435080432, -1.1773842558

#### $\beta$ -2-deoxy-D-ribofuranose (4)

#### dDR $\beta$ f01

C, 0.2822151291, -0.0989292771, 0.0513236014  
C, 0.2227015138, -0.2964376989, 1.5719029296  
C, 1.5483078602, 0.2848799876, 2.0849983185  
C, 2.4376302983, 0.2537695169, 0.8376812245  
O, 1.5129617785, 0.5233881435, -0.2296441882  
C, 3.2100000508, -1.0452065422, 0.6428440271  
H, -0.4970155139, 0.5515263017, -0.3518542278  
H, 0.1413238832, -1.3595736738, 1.7946120826  
H, -0.6198124963, 0.2262444955, 2.024051905  
H, 1.9667611238, -0.2997197073, 2.9030385792  
H, 3.1477728234, 1.0839120812, 0.8468750795  
H, 4.0433384922, -1.052143646, 1.3499554121  
H, 3.6254202358, -1.05028745, -0.3725187709  
O, 0.1972183528, -1.3677026384, -0.5726315209  
O, 1.4007404571, 1.6065405126, 2.5753090079  
O, 2.4611555701, -2.2119275635, 0.9016413111  
H, 0.2078391586, -1.2357946786, -1.5258963352  
H, 1.118963468, 2.1691722189, 1.846889405  
H, 1.7405349965, -2.2601313382, 0.259347873

#### dDR $\beta$ f02

C, -0.4217950963, -1.360023339, 0.3103411065  
C, 0.4668227735, -1.0288991345, -0.8945729941  
C, 1.2400427743, 0.2182369701, -0.4731729093  
C, 0.3883024374, 0.7850031027, 0.6701481278  
O, -0.1961740187, -0.3677932226, 1.2793373833  
C, -0.664830451, 1.7864975835, 0.2102221392  
H, -0.2018333548, -2.3196934105, 0.7815414281  
H, -0.1617772944, -0.8320723476, -1.7617887342  
H, 1.1625313584, -1.8346947126, -1.1238417964  
H, 1.33991988, 0.9368132917, -1.2922260769  
H, 1.0113256387, 1.2578471694, 1.436031388  
H, -0.1639148495, 2.7170697223, -0.0706947261



H, -1.3309081493, 2.0003122733, 1.0551849276  
O, -1.7737946274, -1.3470839857, -0.1196097558  
O, 2.5131473223, -0.2149727297, -0.0173450655  
O, -1.3889923492, 1.3666110247, -0.9245917827  
H, -2.3281057985, -1.6024428605, 0.6243492135  
H, 3.0060072329, 0.5427968366, 0.3069545033  
H, -1.8507034284, 0.5440897683, -0.7104263762

#### dDRβf03

C, -1.3861296199, -0.1361900859, -0.2078676892  
C, -0.7549465129, 0.8331168508, 0.8000599703  
C, 0.5803632425, 1.2368859878, 0.1632102209  
C, 0.8333844891, 0.1220323839, -0.8509809022  
O, -0.4746632986, -0.2911545379, -1.2614876149  
C, 1.6433502783, -1.0385385051, -0.2900094756  
H, -2.3227336946, 0.2157315059, -0.6450807926  
H, -0.598204133, 0.3128564275, 1.7447794559  
H, -1.3907884941, 1.7018297846, 0.9744196468  
H, 1.3852046345, 1.2904173488, 0.9022994356  
H, 1.3303114127, 0.5236719277, -1.7365650277  
H, 2.6793728644, -0.7141428575, -0.1636886065  
H, 1.6279611119, -1.8568250328, -1.0199308353  
O, -1.6139180419, -1.3709949891, 0.4534914854  
O, 0.4858409471, 2.4473121687, -0.5723810726  
O, 1.2029962119, -1.4717633015, 0.9796249575  
H, -2.0444565832, -1.9673756694, -0.1671461202  
H, 0.2680553415, 3.1605007015, 0.0326782749  
H, 0.2887248445, -1.7770051082, 0.9024286895

#### dDRβf04

C, 0.1507529661, -0.2523126561, -0.0374712213  
C, -0.0224716933, 0.2305640344, 1.3905562482  
C, 1.3748942073, 0.0044999443, 1.9717148742  
C, 2.2888296507, 0.2450818693, 0.7626694466  
O, 1.460347131, 0.1115222758, -0.4033340501  
C, 3.4481589083, -0.7287328676, 0.6659388733  
H, -0.527464151, 0.2081561535, -0.7586565047  
H, -0.8184199117, -0.3018248188, 1.9091713604  
H, -0.2290166135, 1.3035126012, 1.3924337156  
H, 1.4874540395, -1.0285755363, 2.3131583401  
H, 2.6637874675, 1.2727721294, 0.8041530318  
H, 4.112536053, -0.5751091119, 1.5200623702  
H, 4.0084910201, -0.5206393499, -0.2531286983  
O, 0.0010047139, -1.6575786957, -0.0559297892  
O, 1.7431669993, 0.9122857877, 2.9931332501  
O, 3.019688624, -2.0724378437, 0.7070388561  
H, -0.0350108363, -1.9483237203, -0.9719646592  
H, 1.4221485724, 0.5847514618, 3.8357698101  
H, 2.2310548525, -2.1532806569, 0.1570067463

### α-D-ribofuranose (5)

#### DRαf01

C, 0.168371348, 0.0557133195, 0.1056833807  
C, 0.2518579387, -0.2833965228, 1.6025861043  
C, 1.6182996655, 0.319640304, 1.9689692275  
C, 2.4311892692, 0.1449216759, 0.6841523162  
O, 1.4761559278, -0.1264253099, -0.3616639645



C, 3.4043446588, -1.0182894361, 0.7158920658  
H, -0.491921855, -0.5938853096, -0.467539026  
H, 0.2829020002, -1.3661600867, 1.7399055422  
H, 2.0827510298, -0.1808822977, 2.8223833476  
H, 2.9611528507, 1.0762691217, 0.4609103592  
H, 4.1400739339, -0.8633765579, 1.5072733733  
H, 3.9314807567, -1.070817284, -0.2429512781  
O, -0.3133737725, 1.3597547701, -0.0858696071  
O, -0.7990404828, 0.2560438735, 2.3631396493  
O, 1.4772927863, 1.7126095516, 2.2095920471  
O, 2.7387580212, -2.2321110247, 0.9983396202  
H, 0.2896625655, 1.9707480431, 0.3612576383  
H, -1.2634400916, 0.8900189514, 1.8028909837  
H, 0.8137873391, 1.80928142, 2.9034113161  
H, 2.1567775747, -2.4120858936, 0.2534501182

#### DRcf02

C, 0.0919571654, -0.0815974017, 0.1417911476  
C, 0.1995271541, -0.4033130937, 1.6356365915  
C, 1.5479721924, 0.266227574, 1.9656983408  
C, 2.3394196318, 0.0994941499, 0.6548111762  
O, 1.3843026061, -0.3275928334, -0.3425281752  
C, 3.4261746337, -0.9565035506, 0.7084470258  
H, -0.6017486905, -0.7062602428, -0.4228077321  
H, 0.30089183, -1.4859630992, 1.7371863092  
H, 2.046029746, -0.2149638858, 2.8062250525  
H, 2.7691682704, 1.0626123775, 0.3587242263  
H, 4.1691853311, -0.679729507, 1.4586902739  
H, 3.9224600582, -1.014788184, -0.2670108584  
O, -0.2461972626, 1.2838989844, 0.03146429  
O, -0.8686935413, 0.0142397068, 2.4232744918  
O, 1.3585334353, 1.6205985034, 2.3330640761  
O, 2.9016267542, -2.211675505, 1.0876178614  
H, -0.3348344479, 1.5130461636, -0.8980111978  
H, -0.7233622757, 0.9419400739, 2.6431353581  
H, 0.9821169189, 2.0798600393, 1.5713286907  
H, 2.2923955365, -2.4830056593, 0.394107478

#### DRcf03

C, 0.0381750517, -0.1280677475, 0.1793502689  
C, 0.0388668519, 0.2400868436, 1.6765764648  
C, 1.4560238429, -0.1586291288, 2.1083524974  
C, 2.2566029378, 0.1453543499, 0.8388390694  
O, 1.3843727801, -0.2784413387, -0.2156939739  
C, 3.5569973211, -0.6214499435, 0.7103181358  
H, -0.4709719846, -1.0759694707, -0.017781382  
H, -0.7476631268, -0.2836914026, 2.2249031947  
H, 1.5125573667, -1.2302454881, 2.3148721517  
H, 2.4429091124, 1.2249177634, 0.7718971319  
H, 4.176711831, -0.4042989402, 1.5826473347  
H, 4.0916593424, -0.2933785732, -0.1887655262  
O, -0.5872704953, 0.9119744379, -0.5240457756  
O, -0.0733394083, 1.6322754712, 1.8820482499  
O, 1.9109272297, 0.5242698183, 3.2399802046  
O, 3.3364761454, -2.0150225001, 0.6877864464  
H, -0.4271651119, 0.7902753102, -1.4642467083  
H, -0.4789489692, 2.023540189, 1.099013495  
H, 1.5667372586, 1.4244062477, 3.1786599528  
H, 2.7415472576, -2.1930861862, -0.0472949739

#### DR $\alpha$ f04

C,0.205275402,0.1449980838,0.0714321199  
C,0.2795261688,-0.2797653892,1.5484257991  
C,1.6205958634,0.3411030691,1.9742402119  
C,2.4633985643,0.1929064604,0.7154395204  
O,1.5297468545,0.0814026643,-0.3818699337  
C,3.3293496113,-1.0553376098,0.7024715344  
H,-0.4078050902,-0.5082350711,-0.5482118988  
H,0.3331766175,-1.3697150279,1.6162849037  
H,2.0687433436,-0.1644455228,2.8357071602  
H,3.0779586546,1.0813454861,0.5523224984  
H,2.7165446077,-1.9289444173,0.9704333192  
H,4.1295510109,-0.9589762667,1.4393797565  
O,-0.3527358079,1.4255879378,-0.0537944495  
O,-0.7977029772,0.1796932973,2.3208097082  
O,1.443506448,1.7231074665,2.2357299789  
O,3.9368430005,-1.2314772432,-0.553588308  
H,0.2398018284,2.0500928343,0.388610154  
H,-1.2786536458,0.8229479162,1.7845026874  
H,0.7694900788,1.7952734178,2.9223037303  
H,3.2438439859,-1.1476595568,-1.2175767315

#### DR $\alpha$ f05

C,0.2463141746,0.0601137008,0.0290429684  
C,0.3376409641,-0.2223373694,1.5401030505  
C,1.6698479841,0.4556559026,1.8936882693  
C,2.5029339689,0.2253345421,0.6358215544  
O,1.5659627518,0.0243730136,-0.4326014828  
C,3.4249120891,-0.9720281668,0.7231451349  
H,-0.3385658615,-0.674427934,-0.5232269364  
H,0.4166466955,-1.2955813725,1.7133588661  
H,2.1374279951,0.0324932018,2.7863822491  
H,3.0959925061,1.1187799536,0.4200858265  
H,4.2605314574,-0.7306987036,1.391761742  
H,3.815390605,-1.1776329217,-0.2786312576  
O,-0.373379545,1.3008930669,-0.2111201427  
O,-0.7427240089,0.3059097245,2.2692392692  
O,1.4712232831,1.8549767337,2.0345579109  
O,2.6812310843,-2.0720441502,1.2203371847  
H,0.2095663103,1.9878128969,0.1405903232  
H,-1.2396207727,0.8739164244,1.6665829623  
H,0.7708134583,1.9678092272,2.6884477276  
H,3.1808750035,-2.8805108659,1.0934632546

### **$\beta$ -D-ribofuranose (10)**

#### DR $\beta$ f01

C,0.0824541825,-0.3062045389,-0.0199007333  
C,-0.0832375253,0.2013786185,1.4048332049  
C,1.3215916588,-0.046861442,1.9671792398  
C,2.2167764083,0.2541497123,0.761670548  
O,1.4059517101,0.0088176965,-0.3930059918  
C,3.4526151784,-0.6214544002,0.6839404421  
H,-0.5907634657,0.1878119433,-0.7226903123  
H,-0.8699774921,-0.3460383202,1.9317453774  
H,1.4316253329,-1.0927922214,2.2639726409  
H,2.5004041102,1.3117015873,0.7803935081

H, 4.0882472682, -0.426386682, 1.5509765135  
H, 4.0135448289, -0.3667846613, -0.2225306677  
O, -0.1128796863, -1.6985503319, -0.0030048835  
O, -0.3523777686, 1.5806301032, 1.3523189145  
O, 1.6409737609, 0.8361790417, 3.0287836859  
O, 3.120472509, -1.9924058307, 0.7100978758  
H, -0.1378170931, -2.0163629634, -0.9096572168  
H, 0.075891303, 1.9850494889, 2.1165572564  
H, 1.5188787387, 0.386606611, 3.8676349459  
H, 2.4161607035, -2.1317745927, 0.0664063376

#### DRβf02

C, 0.0595381086, -0.257439645, 0.0167827921  
C, -0.1312855537, 0.2030910886, 1.4641236734  
C, 1.2659507169, -0.0385022214, 2.0411566387  
C, 2.1737879295, 0.2590880907, 0.8224941013  
O, 1.3413905763, 0.2053393071, -0.3357178351  
C, 3.3127498706, -0.7283903802, 0.6738218158  
H, -0.6621664436, 0.1856108446, -0.6727984887  
H, -0.9176252831, -0.358873986, 1.9722325865  
H, 1.3655181017, -1.084236925, 2.3361194159  
H, 2.5814521688, 1.2703120626, 0.9135946672  
H, 3.9804848212, -0.6389003461, 1.5382532225  
H, 3.8660582817, -0.5050935775, -0.2428548252  
O, -0.044154433, -1.6472785709, -0.0892673524  
O, -0.3389954457, 1.6031437439, 1.5502732187  
O, 1.5667402161, 0.7390673178, 3.1677086832  
O, 2.7456522957, -2.0347707185, 0.6107683721  
H, 0.8343755708, -2.0206523765, 0.0795474574  
H, -1.217647163, 1.8252934478, 1.2346680092  
H, 1.1568870989, 1.6019639737, 3.0303311112  
H, 3.4063495881, -2.6640756976, 0.3156501332

#### DRβf03

C, -0.0311855317, -0.4042464353, 0.0373217902  
C, -0.0978891362, 0.1999073223, 1.4331014595  
C, 1.3505933772, 0.0241015099, 1.8842171637  
C, 2.1126595145, 0.3130222528, 0.5851162283  
O, 1.2508499593, -0.0876328592, -0.4729315474  
C, 3.426163561, -0.4360463171, 0.5179521353  
H, -0.7711583168, 0.0194345588, -0.6449764963  
H, -0.8140650342, -0.3340333529, 2.0626673724  
H, 1.5121848765, -1.01415552, 2.1961633373  
H, 2.2972950574, 1.3909784046, 0.5159895963  
H, 3.974319823, -0.1804000043, -0.3937843355  
H, 3.2252661759, -1.5135826753, 0.5303708782  
O, -0.1825695693, -1.7924629627, 0.176056947  
O, -0.4174642439, 1.5647192492, 1.3131868343  
O, 1.6471898371, 0.9234477789, 2.9260013532  
O, 4.1374829878, -0.0298924547, 1.6843526128  
H, -0.024806663, -2.1947785572, -0.6827136626  
H, -0.003111855, 2.0180245556, 2.0569385304  
H, 2.603354166, 0.9101439741, 3.0494135791  
H, 4.9976280203, -0.4530623154, 1.7089582801

#### DRβf04

C, 0.0612939225, -0.1963772713, 0.054158449  
C, -0.1128087046, 0.2745070321, 1.4955992249  
C, 1.2787431536, -0.0112206891, 2.0772466124

C, 2.1923284034, 0.2851341156, 0.8592314568  
O, 1.3371928489, 0.3220339666, -0.2917616823  
C, 3.2987119784, -0.7300475896, 0.6618968017  
H, -0.6712701511, 0.2431476747, -0.6245396535  
H, -0.9236013677, -0.2318136596, 2.0150433908  
H, 1.3610404911, -1.0607833169, 2.3656100538  
H, 2.6467652028, 1.273220904, 0.9810016085  
H, 3.9908049971, -0.6683513073, 1.5092329505  
H, 3.8326054609, -0.5046797155, -0.2656203528  
O, -0.0105866325, -1.5783764912, -0.0725946666  
O, -0.3634933804, 1.6711963962, 1.5513262328  
O, 1.5882168932, 0.7604942614, 3.2062591045  
O, 2.7050279211, -2.0235031889, 0.5966941453  
H, 0.8588959941, -1.9538458898, 0.1383477814  
H, 0.0647342816, 2.0873130451, 0.7943755708  
H, 1.1017361772, 1.5900975795, 3.1177933709  
H, 3.3372587003, -2.6600913334, 0.2575869982

#### DRβf05

C, 0.2766632296, -0.139135711, 0.1450461164  
C, 0.2716277881, -0.2086708486, 1.683085205  
C, 1.5850519209, 0.4782670887, 2.0842844346  
C, 2.4599743398, 0.2830187879, 0.8482525393  
O, 1.5401607917, 0.3146049233, -0.2535163556  
C, 3.2614431628, -1.0084569878, 0.8425942587  
H, -0.4737536054, 0.5598191195, -0.2332971634  
H, 0.2908596496, -1.2559754518, 1.9893111078  
H, 2.0238426467, 0.0145449062, 2.9740571389  
H, 3.1300613032, 1.1373801386, 0.7315542317  
H, 4.017347603, -0.9657954575, 1.6302438021  
H, 3.7749711997, -1.0942407164, -0.1220057669  
O, 0.0252600735, -1.4409606274, -0.3508740635  
O, -0.8128142302, 0.481423243, 2.2728931933  
O, 1.3944108033, 1.8613266251, 2.2704581115  
O, 2.4676484429, -2.1480902706, 1.1043020832  
H, -0.0246097769, -1.3931215852, -1.310513369  
H, -1.5740216607, -0.0993159456, 2.3293800503  
H, 0.5359393716, 1.9847344784, 2.6916063398  
H, 1.8068742005, -2.2339086809, 0.4044224587

#### DRβf06

C, 0.0979197874, -0.3010534655, 0.118142502  
C, 0.0213909783, 0.2519334424, 1.5430339426  
C, 1.4385135332, -0.0300760832, 2.0457649181  
C, 2.2815645554, 0.18908215, 0.7719588616  
O, 1.3853243902, 0.0543916849, -0.3355659929  
C, 3.394501314, -0.8358890086, 0.6170936713  
H, -0.6352466777, 0.1396554066, -0.558349503  
H, -0.7607359787, -0.2339650908, 2.1304728706  
H, 1.5193107433, -1.071325674, 2.3692930753  
H, 2.6887330907, 1.2048887085, 0.7764429394  
H, 3.9904617308, -0.8714525602, 1.5315737818  
H, 4.0487964169, -0.5638897924, -0.2164218282  
O, -0.115098429, -1.6835626663, 0.0838803361  
O, -0.1063613811, 1.6627884343, 1.5550401166  
O, 1.8356413569, 0.7612955123, 3.1297509663  
O, 2.8454153829, -2.1299817328, 0.4180507164  
H, 0.605826477, -2.1212382305, 0.5560601196  
H, -0.9972515346, 1.9162134974, 1.3034779777

H, 1.4839653369, 1.6467019615, 2.9759079256  
H, 2.5075434697, -2.1523529373, -0.4836497138

#### DRβf07

C, 0.0713838164, -0.3476019189, 0.0226113879  
C, -0.0468073566, 0.1226662837, 1.4693946033  
C, 1.3643060832, -0.1573816375, 1.9911912052  
C, 2.2250955887, 0.1936493718, 0.768088013  
O, 1.391713916, -0.0596780955, -0.3752504264  
C, 3.48760564, -0.6355293395, 0.6417715037  
H, -0.6026517684, 0.1775683087, -0.6607587455  
H, -0.829554699, -0.4108907583, 2.0111483912  
H, 1.4678366327, -1.2195556925, 2.2177473558  
H, 2.4755488447, 1.2602748838, 0.7903532125  
H, 4.1114827213, -0.4667117661, 1.5224799291  
H, 4.043560882, -0.3151457707, -0.247269309  
O, -0.1743886106, -1.7295942781, 0.0128324989  
O, -0.2113098752, 1.528899417, 1.5408554084  
O, 1.7030496828, 0.5632446343, 3.1426966528  
O, 3.2001058893, -2.0153723341, 0.591064779  
H, -0.1319273179, -2.0432792088, -0.8948811125  
H, -1.1327103608, 1.7621501501, 1.410588599  
H, 1.3466197608, 1.4531951641, 3.0351669347  
H, 2.5191637945, -2.1403092829, -0.078507152

#### DRβf08

C, 0.0424404174, -0.2975785853, 0.2781998072  
C, -0.1956357304, 0.1547945224, 1.7150986955  
C, 1.2211259931, 0.0582601297, 2.2951158475  
C, 2.08367401, 0.5005228312, 1.0901601811  
O, 1.2468317865, 0.373121023, -0.0720114247  
C, 3.3374700733, -0.3377381102, 0.8981369244  
H, -0.7351190958, 0.0316223994, -0.4108187531  
H, -0.9343385799, -0.4509815349, 2.2362314137  
H, 1.4558144831, -0.9756541928, 2.564642445  
H, 2.3576771406, 1.5539401807, 1.2089740187  
H, 3.9034188509, -0.3625763028, 1.8318944083  
H, 3.9687422661, 0.0986360409, 0.1187124182  
O, 0.1342679302, -1.680685348, 0.149636547  
O, -0.6297080703, 1.5044191264, 1.7662463577  
O, 1.4189625867, 0.8360705574, 3.4427011057  
O, 2.9979412367, -1.6769048834, 0.5723421152  
H, 0.901461992, -1.9970617307, 0.6467509895  
H, -0.2474871983, 1.9791301764, 1.0191601818  
H, 0.8394189059, 1.6045111022, 3.3644427063  
H, 2.7418501691, -1.6874343722, -0.3561951255

#### DRβf09

C, -0.0357876222, -0.3297428835, -0.0000879005  
C, -0.1574097136, 0.1593107563, 1.4366410563  
C, 1.2676007533, -0.073195799, 1.9319430217  
C, 2.0874096198, 0.3221277154, 0.6978871416  
O, 1.274006746, 0.0039718786, -0.4249238696  
C, 3.4110887812, -0.4142405224, 0.6345647174  
H, -0.7379410494, 0.1614185783, -0.6772049875  
H, -0.9056730426, -0.4143761492, 1.9890313704  
H, 1.4050402582, -1.1380328391, 2.1525007365  
H, 2.260019081, 1.4055337059, 0.7248331819  
H, 3.9814748908, -0.1335869237, -0.2546088893

H, 3.2268290197, -1.4906141774, 0.6018578098  
O, -0.2116581222, -1.7209390157, 0.0175061058  
O, -0.4568221751, 1.5343702028, 1.4147761499  
O, 1.525405985, 0.7207712283, 3.0658945527  
O, 4.1346143376, -0.1374192596, 1.8338040186  
H, -0.0118189917, -2.0565965556, -0.8609789146  
H, -0.100760975, 1.9151359298, 2.2259321062  
H, 2.4613230494, 0.6205807713, 3.2730811503  
H, 4.7464965039, 0.5839738124, 1.6751065434

#### DRβf10

C, 0.281923011, -0.0902838339, 0.0410307543  
C, 0.2270029839, -0.2268886797, 1.5791499425  
C, 1.5754839344, 0.3849049276, 2.0362561586  
C, 2.4449719819, 0.2796805254, 0.785538018  
O, 1.5091833188, 0.5286220044, -0.275638531  
C, 3.1929952585, -1.0406826737, 0.6425201235  
H, -0.5200726798, 0.5437751979, -0.3404298231  
H, 0.1842306404, -1.2858332895, 1.8365018038  
H, 1.9940574776, -0.1317654101, 2.89836898  
H, 3.1767641314, 1.0913045991, 0.7483537481  
H, 4.0367841631, -1.0257440152, 1.3370456747  
H, 3.5926542867, -1.0982157662, -0.3773323655  
O, 0.2042921511, -1.3783469537, -0.5335998195  
O, -0.8841853702, 0.4230712771, 2.1353752563  
O, 1.3871503271, 1.7415842935, 2.4161392602  
O, 2.4307926433, -2.1788952557, 0.9698643588  
H, 0.1762248769, -1.2846040419, -1.4907299082  
H, -0.5611626748, 1.2271304558, 2.5611468424  
H, 1.3419174995, 2.2787565508, 1.6168772887  
H, 1.7156504705, -2.2636126905, 0.3248859669

### **α-2-deoxy-D-ribofuranose (1)**

#### dDRαp01

C, -0.0536937977, 0.0490691249, 0.1769090173  
C, 0.0370204149, -0.342836396, 1.6456118142  
C, 1.2716714223, 0.2631470137, 2.307907102  
C, 2.5154650866, -0.0502402453, 1.4721683492  
C, 2.292698075, 0.3672041226, 0.0206133  
O, 1.1225709573, -0.2374392219, -0.5282064965  
H, -0.8339470435, -0.5170963149, -0.3373928531  
H, 0.1011169362, -1.4324703811, 1.6972182338  
H, -0.868669202, -0.0253356738, 2.1664194155  
H, 1.4077945022, -0.1542367223, 3.3085372347  
H, 2.7096415924, -1.1265334083, 1.5095469457  
H, 3.125777907, 0.0426731748, -0.6004412866  
H, 2.225298369, 1.459857367, -0.0378860765  
O, -0.3513416845, 1.4356910804, 0.133836907  
O, 1.1674222827, 1.6698100373, 2.4881499208  
O, 3.6462395102, 0.6029429562, 1.996943216  
H, -0.4089841561, 1.7088117702, -0.7872830245  
H, 0.6533787797, 2.0339605899, 1.756327327  
H, 3.3457842346, 1.4706471923, 2.2963071728

### **β-2-deoxy-D-ribofuranose (3)**

#### dDRβp01

C, 0.0309480387, 0.0239717156, -0.0041478529  
C, -0.0119938125, -0.0722664726, 1.514071854  
C, 1.3939297709, -0.0377465264, 2.117964592  
C, 2.1714510951, 1.1494958621, 1.5453218786  
C, 2.1441831586, 1.1045942696, 0.0273596676  
O, 0.7959612866, 1.134584168, -0.4360261945  
H, -0.9637218536, 0.2063601517, -0.4197140787  
H, -0.5265445924, -0.9866495593, 1.8113516076  
H, -0.5873436104, 0.7749598842, 1.8999455695  
H, 1.9228078882, -0.960490821, 1.8666155787  
H, 3.201296376, 1.1198789895, 1.9090313579  
H, 2.6539252711, 0.2065515453, -0.334293238  
H, 2.6253776379, 1.9878655947, -0.3929514965  
O, 0.5645997934, -1.179117152, -0.4932192986  
O, 1.3458992176, 0.0350444379, 3.5251423473  
O, 1.6094896537, 2.3636470679, 2.0291668438  
H, 0.5333093134, -1.1573319389, -1.454410326  
H, 1.1471499237, 0.9524661808, 3.7479295233  
H, 0.8968351001, 2.6187385414, 1.4323802655

#### dDRβp02

C, 0.0509931705, 0.0530668946, 0.0062221844  
C, -0.0063466585, 0.1284697418, 1.5258131101  
C, 1.4027286911, 0.103577553, 2.1058111734  
C, 2.2368809673, 1.2144187071, 1.4743149739  
C, 2.1780037863, 1.1060589764, -0.0400695843  
O, 0.8483747206, 1.0679138071, -0.5405539509  
H, -0.937787883, 0.2144574625, -0.4313024964  
H, -0.6011412157, -0.7079550987, 1.9023041738  
H, -0.4878215214, 1.067625068, 1.8065635854  
H, 1.8801909997, -0.8592216, 1.8928169496  
H, 3.2820140564, 1.096347538, 1.7912441066  
H, 2.7260319719, 0.2117316999, -0.357740802  
H, 2.6380605942, 1.9871360515, -0.4860367878  
O, 0.5395432227, -1.2271118813, -0.3304828579  
O, 1.4080912005, 0.3604875113, 3.5050326736  
O, 1.747992884, 2.4821718774, 1.8549714888  
H, 0.5547288993, -1.2965381179, -1.2898124069  
H, 0.8004805533, -0.2413074107, 3.9420005219  
H, 1.6293818474, 2.4607369907, 2.8109716645

#### dDRβp03

C, 0.0471617399, 0.0283345489, -0.0184717643  
C, -0.0069258066, 0.0091221186, 1.5013371322  
C, 1.4008741327, -0.0118341255, 2.0950427831  
C, 2.2054328903, 1.1477535729, 1.5139704545  
C, 2.1547233887, 1.1074248377, -0.0080287706  
O, 0.8286451497, 1.0950629122, -0.5072211626  
H, -0.9430068409, 0.2001456923, -0.448526105  
H, -0.5666127176, -0.8642693992, 1.8380483158  
H, -0.5213622904, 0.9126324657, 1.8374419445  
H, 1.8972310209, -0.9479719124, 1.8302477367  
H, 3.2491044899, 1.0669391632, 1.8432597903  
H, 2.7044150009, 0.2242476372, -0.3552076639  
H, 2.6259204433, 1.9954367252, -0.4356103002  
O, 0.5650075366, -1.2117982553, -0.4402712433  
O, 1.3796799214, 0.0480123921, 3.5039377589  
O, 1.6115271846, 2.3242238663, 2.0476195866  
H, 0.5484703412, -1.2325967682, -1.4016869813



H, 1.1368778033, 0.950342, 3.7416144403  
H, 2.0515131852, 3.1021261649, 1.6977622813

### $\alpha$ -D-ribofuranose (4)

#### DR $\alpha$ p01

C, 0.0261781766, -0.0571943672, 0.1462267787  
C, 0.0354767266, 0.002319415, 1.6724248657  
C, 1.479157877, 0.0508395441, 2.1788433917  
C, 2.2585171519, 1.1685322284, 1.4704413333  
C, 2.1025430251, 1.023916894, -0.0393774772  
O, 0.7304901354, 1.0247237163, -0.4110764325  
H, 0.4782175601, -1.0015965761, -0.2008125487  
H, -0.4691717377, -0.8848549061, 2.0723019937  
H, 1.950509854, -0.9075136745, 1.9352039729  
H, 3.3158164028, 1.078928915, 1.7329409793  
H, 2.584845431, 0.0975084189, -0.3841009757  
H, 2.557089353, 1.873517794, -0.5465504641  
O, -1.3021228982, 0.0489430595, -0.2600609812  
O, -0.6205057479, 1.1808861654, 2.1048175468  
O, 1.5326064241, 0.1804053466, 3.5733264001  
O, 1.8475117188, 2.4412516786, 1.9219907154  
H, -1.3115619053, 0.2847869665, -1.1934416531  
H, -1.4596958956, 1.2332001349, 1.6326829123  
H, 1.2658427899, 1.082973792, 3.7851922424  
H, 0.8955643799, 2.5107760962, 1.7675418572

#### DR $\alpha$ p02

C, -0.0625165094, 0.0892142959, 0.1879049643  
C, 0.0320066687, -0.3122568074, 1.6641875691  
C, 1.2854223649, 0.285799116, 2.3027270229  
C, 2.5190653522, -0.0507961327, 1.4616507395  
C, 2.28730613, 0.3340925965, 0.0007958212  
O, 1.0971113299, -0.260081191, -0.5127819773  
H, -0.8812339628, -0.4438760729, -0.299466387  
H, 0.1206812554, -1.4016582725, 1.6864144602  
H, 1.4086844399, -0.1188973098, 3.3099163241  
H, 2.7017723872, -1.1280865504, 1.5187380515  
H, 3.104286879, -0.0287384367, -0.6203064699  
H, 2.2428788331, 1.4254280344, -0.094461332  
O, -0.2940334081, 1.4861589212, 0.1525764535  
O, -1.1370899511, 0.0182946111, 2.3646103014  
O, 1.1721100671, 1.6942370256, 2.4760822573  
O, 3.6601008618, 0.5985904188, 1.9674298653  
H, -0.5104155832, 1.752599567, -0.7457000544  
H, -1.1245550441, 0.968272199, 2.5262437454  
H, 0.8278576426, 2.0798912976, 1.6588672266  
H, 3.3721955331, 1.4634057044, 2.2850544405

#### DR $\alpha$ p03

C, 0.0748240444, -0.0918023553, 0.0027177798  
C, 0.0967419507, -0.2170844604, 1.5278671243  
C, 1.5184278248, -0.0960738997, 2.0911032896  
C, 2.2503131357, 1.1077615316, 1.487164889  
C, 2.1015375093, 1.0948429157, -0.0273025074  
O, 0.7349841389, 1.0980139808, -0.3898050207  
H, 0.5784139449, -0.9545792177, -0.45341183  
H, -0.3326860666, -1.1855166637, 1.8074685074

H, 2.0699885241, -1.0087806036, 1.8389028394  
H, 3.3084110886, 1.0611434967, 1.7580312523  
H, 2.6095578051, 0.2156191546, -0.4503545022  
H, 2.5414947008, 1.995994697, -0.453162913  
O, -1.2141387789, -0.0646713674, -0.4812528597  
O, -0.7267635565, 0.8364254378, 2.0110826403  
O, 1.4594706735, 0.0052312791, 3.4983931669  
O, 1.7558447777, 2.3095377372, 2.0501845285  
H, -1.7005975922, 0.5819625948, 0.0454608971  
H, -0.8160474834, 0.7234120815, 2.9627540624  
H, 1.5662862943, 0.9413855819, 3.7111572032  
H, 0.838484353, 2.4063576668, 1.7591686112

#### DR $\alpha$ p04

C, 0.073543399, -0.1540844052, 0.0283574925  
C, 0.0798656591, -0.2991326021, 1.5529094879  
C, 1.495603706, -0.1587067452, 2.1147971291  
C, 2.1702355669, 1.1090992797, 1.5739130909  
C, 1.9941720291, 1.1983294589, 0.0659678494  
O, 0.6353850715, 1.1002180422, -0.310122907  
H, 0.6538592863, -0.9580501649, -0.4444656458  
H, -0.3347729322, -1.2738107133, 1.8221136653  
H, 2.0859151748, -1.0279670437, 1.8033527777  
H, 3.2402825904, 1.0828382022, 1.8119576595  
H, 2.5817512151, 0.4042453922, -0.4175228057  
H, 2.3479767111, 2.1652439981, -0.2897069062  
O, -1.2072670035, -0.2194986726, -0.4727117956  
O, -0.7882736147, 0.6685745479, 2.1221214166  
O, 1.4730667241, -0.1265280169, 3.5280298517  
O, 1.5705752931, 2.2621658619, 2.1472849202  
H, -1.7622165188, 0.3360916573, 0.0893189714  
H, -0.3952470332, 1.5395543384, 1.9542570245  
H, 0.575936168, 0.1060937253, 3.7962665749  
H, 1.720374225, 2.2153746175, 3.0980077902

#### $\beta$ -D-ribofuranose (4)

#### DR $\beta$ p01

C, 0.1237515674, -0.0937002565, 0.1475529882  
C, 0.2178494572, -0.0045320698, 1.6685552744  
C, 1.6799394972, 0.1061342986, 2.111814878  
C, 2.3982695297, 1.2201953275, 1.3384782711  
C, 2.1601985654, 1.0758736037, -0.1537447258  
O, 0.7738699551, 0.9901682285, -0.4648716302  
H, -0.9214803118, -0.0066755308, -0.1591474893  
H, -0.2326879568, -0.8995013486, 2.1025480064  
H, 2.1834693486, -0.8434882974, 1.9113233403  
H, 3.475734365, 1.156367133, 1.5337615622  
H, 2.6865321543, 0.1895576761, -0.5221129955  
H, 2.5288359348, 1.9589753426, -0.6737887254  
O, 0.6793322804, -1.3263058979, -0.2286133511  
O, -0.5328087598, 1.0944079167, 2.1465752808  
O, 1.7525607966, 0.3690759032, 3.5003285723  
O, 1.9086869684, 2.4938969208, 1.7366024529  
H, 0.5334821159, -1.4534749217, -1.1706329538  
H, -0.1411941822, 1.8978626538, 1.7740322745  
H, 0.8964102994, 0.7268288895, 3.7657842252  
H, 2.0868817624, 2.5785827174, 2.6796337832

### DRβp02

C, 0.1456795126, 0.0049145443, 0.074832015  
C, 0.0877643059, 0.0109401354, 1.5987725344  
C, 1.4940688858, 0.0825936954, 2.2086012005  
C, 2.3173827904, 1.1952662159, 1.5503328335  
C, 2.2664927538, 1.0568860242, 0.0374381755  
O, 0.9212009483, 1.062608052, -0.4276339183  
H, -0.8553132528, 0.1739938695, -0.32900481  
H, -0.4114695051, -0.9050083921, 1.9308513024  
H, 1.9927530245, -0.8771120485, 2.0464128534  
H, 3.3556557494, 1.1203489687, 1.8854047076  
H, 2.7738100498, 0.137202718, -0.2723502307  
H, 2.7495631613, 1.9137760146, -0.430581203  
O, 0.6591553924, -1.2463302616, -0.3006461238  
O, -0.672205545, 1.152049089, 1.9623617996  
O, 1.3852947961, 0.3027849033, 3.6018723151  
O, 1.86290721, 2.4659257484, 1.983698593  
H, 0.6214675828, -1.3141966396, -1.2591798462  
H, -0.7414749623, 1.1447339662, 2.9230040146  
H, 1.5634715182, 1.2403430986, 3.7497489027  
H, 0.9508342562, 2.5664856591, 1.6766013851

### DRβp03

C, -0.0289204829, 0.1122794971, 0.144603007  
C, 0.0137613424, -0.1344985806, 1.6460387595  
C, 1.3007340959, 0.4256790834, 2.2349236139  
C, 2.5158338214, -0.0605495978, 1.4481265655  
C, 2.2969777628, 0.158229392, -0.050665574  
O, 1.0931554257, -0.4672713737, -0.4738459612  
H, -0.0396744334, 1.1941549255, -0.0599529768  
H, -0.0239327258, -1.2206339528, 1.7987639249  
H, 1.3902203022, 0.1194216029, 3.2837388231  
H, 2.6500164637, -1.1301008541, 1.6302856003  
H, 3.1085727581, -0.2927489495, -0.6190345226  
H, 2.2658544858, 1.2348180057, -0.2642038501  
O, -1.1831446078, -0.5039888828, -0.3290667307  
O, -1.0574823047, 0.516412482, 2.299073426  
O, 1.3102995806, 1.8421028066, 2.1437359663  
O, 3.686631318, 0.5867770332, 1.8853993271  
H, -1.2247549698, -0.3954402763, -1.2839907788  
H, -1.8745564458, 0.2574348679, 1.8602094675  
H, 0.4829217231, 2.1640175109, 2.5182115283  
H, 3.4686673983, 1.5194356313, 2.0007366448

### DRβp04

C, 0.0966753433, -0.0970687352, 0.1978954224  
C, 0.1817122119, -0.1547697146, 1.723229159  
C, 1.6443092214, -0.0578458874, 2.1754281453  
C, 2.3179563923, 1.1602086313, 1.5363995323  
C, 2.1190242298, 1.1208092367, 0.026057005  
O, 0.7427801672, 1.0456281317, -0.3147530963  
H, -0.9468100189, 0.0115181065, -0.1073986696  
H, -0.2354448869, -1.1051541235, 2.0603269453  
H, 2.1703473959, -0.9501055834, 1.8265952177  
H, 3.3875301536, 1.1407277852, 1.7748475445  
H, 2.6664732781, 0.2678677798, -0.390327283  
H, 2.4918642452, 2.0349265961, -0.4400651207  
O, 0.6679692269, -1.28002645, -0.2965991771

O, -0.6102705715, 0.8596274466, 2.3019978178  
O, 1.7468771139, -0.035726609, 3.5743612359  
O, 1.7095080261, 2.3165103137, 2.1082946923  
H, 0.5175012808, -1.3198059523, -1.2454693647  
H, -0.2158568003, 1.7116192371, 2.0722946859  
H, 1.1440944214, 0.6473801563, 3.8908843281  
H, 2.1747148326, 3.1063209324, 1.8221350999

**Table S1.** Relative energy in  $\text{kJ mol}^{-1}$  for the most stable minima (restricted for conformers with energies less than  $5 \text{ kJ mol}^{-1}$ ) of 2-deoxy-D-ribose and D-ribose (open-chain, furanose and pyranose forms) at M06-2X/6-311++G(d,p) and B3LYP/6-311++G(d,p) computational levels.

Open-chain 2-deoxy-D-ribose				Open-chain D-ribose			
Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$	Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$
dDR01	0.00	dDR01	0.00	DR01	0.00	DR01	0.00
dDR02	2.79	dDR05	6.23	DR02	0.59	DR02	0.65
dDR03	4.42	dDR02	3.44	DR03	0.61	DR04	3.15
				DR04	1.32	DR03	3.00
				DR05	2.63	DR07	4.19
				DR06	3.21	DR19	9.12
				DR07	3.42	DR06	3.49
				DR08	3.90	DR05	3.34
				DR09	3.93	DR09	6.08

$\alpha$ -2-deoxy-D-ribofuranose				$\beta$ -2-deoxy-D-ribofuranose			
Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$	Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$
dDR $\alpha$ f01	0.00	dDR $\alpha$ f01	0.00	dDR $\beta$ f01	0.00	dDR $\beta$ f01	0.00
dDR $\alpha$ f02	3.10	dDR $\alpha$ f02	1.25	dDR $\beta$ f02	1.31	dDR $\beta$ f02	0.05
				dDR $\beta$ f03	1.59	dDR $\beta$ f04	0.37
				dDR $\beta$ f04	3.11	dDR $\beta$ f03	0.28

$\alpha$ -D-ribofuranose				$\beta$ -D-ribofuranose			
Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$	Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$
DR $\alpha$ f01	0.00	DR $\alpha$ f02	0.67	DR $\beta$ f01	0.00	DR $\beta$ f01	0.00
DR $\alpha$ f02	2.49	DR $\alpha$ f06	3.00	DR $\beta$ f02	1.06	DR $\beta$ f07	3.67
DR $\alpha$ f03	4.02	DR $\alpha$ f01	0.00	DR $\beta$ f03	1.18	DR $\beta$ f02	1.17
DR $\alpha$ f04	4.33	DR $\alpha$ f04	2.85	DR $\beta$ f04	2.13	DR $\beta$ f08	4.52
DR $\alpha$ f05	4.68	DR $\alpha$ f08	4.01	DR $\beta$ f05	2.15	DR $\beta$ f04	2.67
				DR $\beta$ f06	2.99	DR $\beta$ f13	6.26
				DR $\beta$ f07	3.57	DR $\beta$ f03	2.31
				DR $\beta$ f08	3.70	---	---
				DR $\beta$ f09	4.19	DR $\beta$ f05	3.51
				DR $\beta$ f10	4.56	DR $\beta$ f12	5.97

$\alpha$ -2-deoxy-D-ribofuranose				$\beta$ -2-deoxy-D-ribofuranose			
Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$	Struc.	$\Delta E_0^{\text{M06-2X}}$	Struc.	$\Delta E_0^{\text{B3LYP}}$
dDR $\alpha$ p01	0.00	dDR $\alpha$ p01	0.00	dDR $\beta$ p01	0.00	dDR $\beta$ p01	0.00

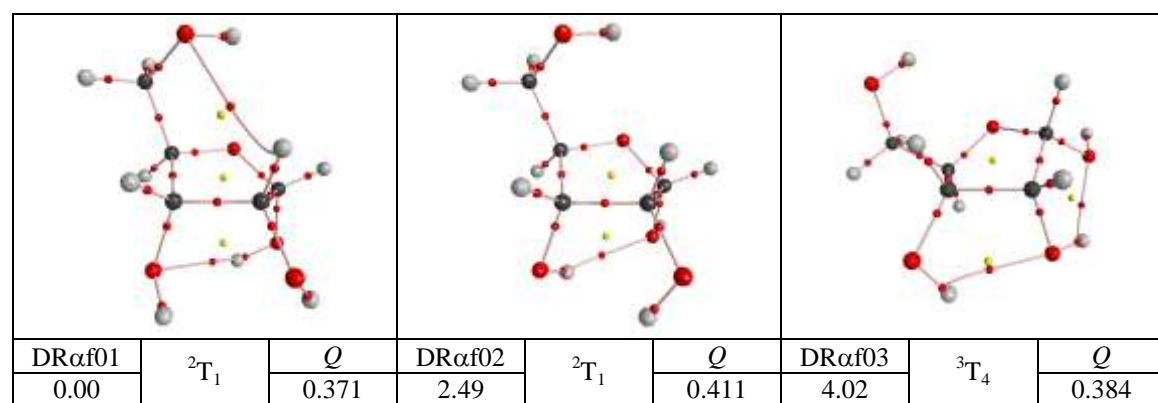
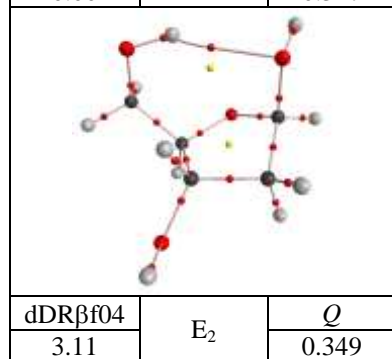
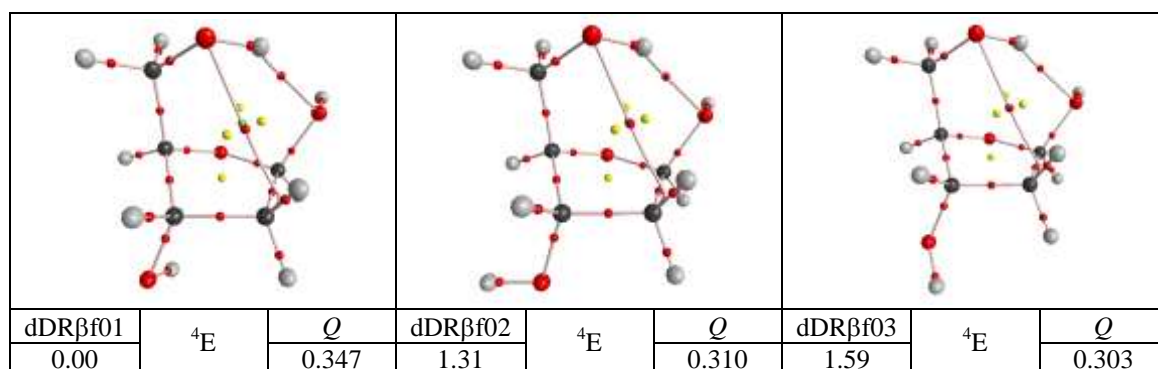
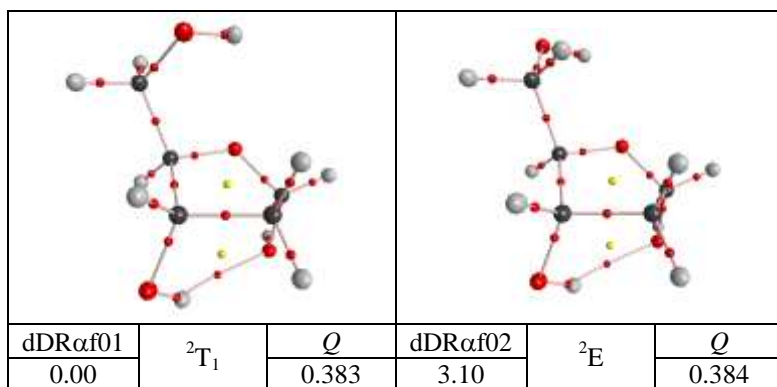
<b><math>\alpha</math>-D-ribofuranose</b>				<b><math>\beta</math>-D-ribofuranose</b>			
Struc.	$\Delta E_0^{M06-2X}$	Struc.	$\Delta E_0^{B3LYP}$	Struc.	$\Delta E_0^{M06-2X}$	Struc.	$\Delta E_0^{B3LYP}$
DR $\alpha$ p01	0.00	DR $\alpha$ p01	0.00	DR $\beta$ p01	0.00	DR $\beta$ p02	0.39
DR $\alpha$ p02	0.48	DR $\alpha$ p02	0.43	DR $\beta$ p02	0.51	DR $\beta$ p03	1.45
DR $\alpha$ p03	1.10	DR $\alpha$ p04	1.42	DR $\beta$ p03	1.92	DR $\beta$ p01	0.00
DR $\alpha$ p04	1.73	DR $\alpha$ p03	1.26	DR $\beta$ p04	4.56	DR $\beta$ p05	5.22

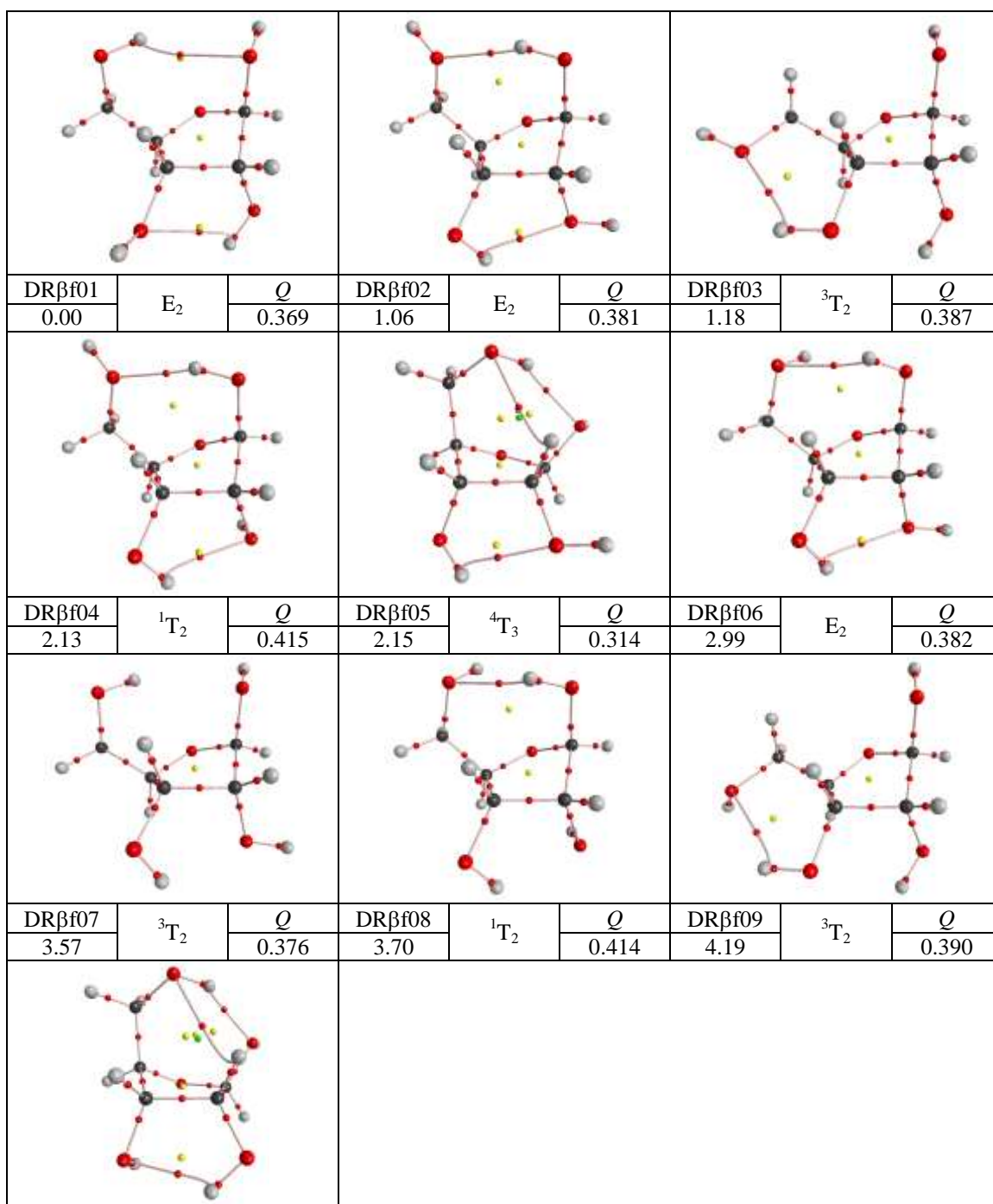
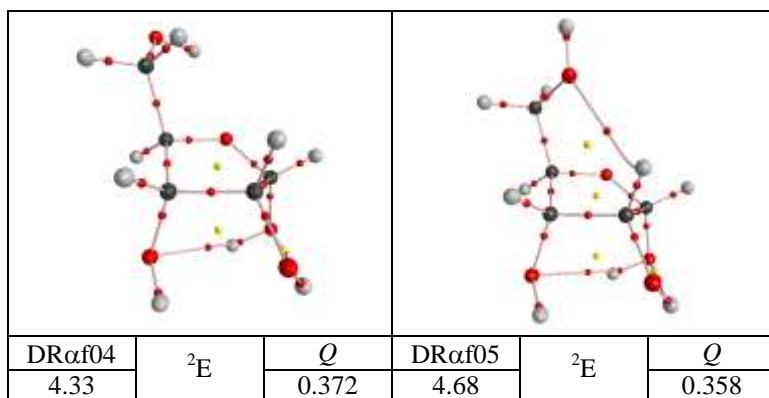
**Fig. S1.** Molecular graphs of the most stable conformers (less than 5 kJ mol<sup>-1</sup>) for 2-deoxy-D-ribose and D-ribose in gas phase calculated at M06-2X/6-311++G(d,p) computational level. For linear forms, dihedral angles  $D_{C_1C_2C_3C_4}$  ( $\varphi_1$ ) and  $D_{C_2C_3C_4C_5}$  ( $\varphi_2$ ) in deg are shown, and for cyclic ones the ring conformation,<sup>a</sup> as well as the  $Q$  parameter in Å are included. Relative energies are in kJ mol<sup>-1</sup>. Small points are BCP (red), RCP (yellow) and CCP (green).

<sup>a</sup>C=chair, H=half-chair, S=skew, B=boat, T=twist and E=envelope. Superscript at left refers to *endo* face. Subscript at right refers to *exo* face.

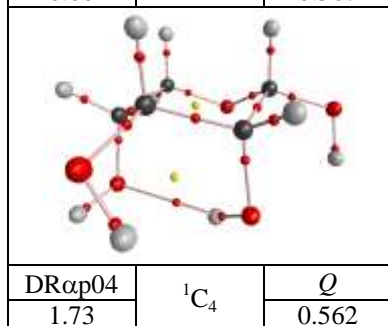
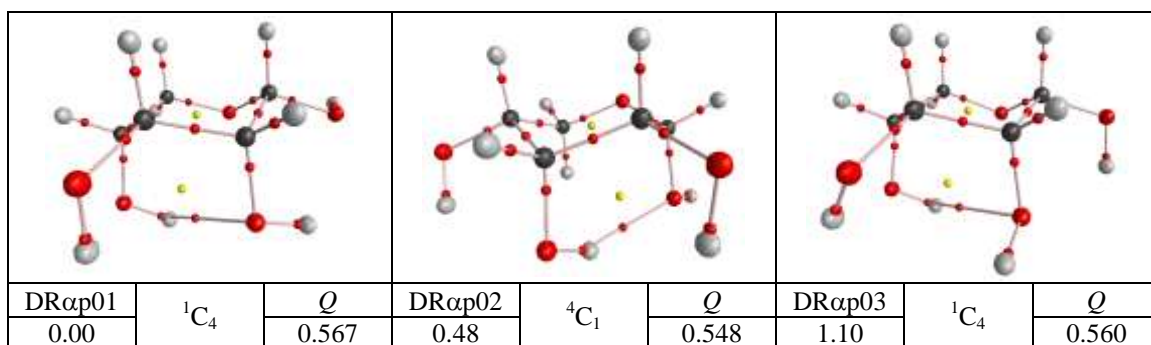
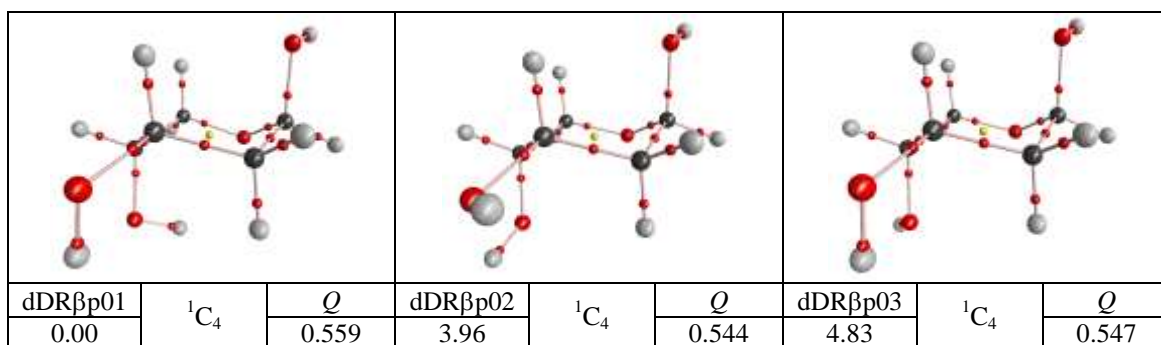
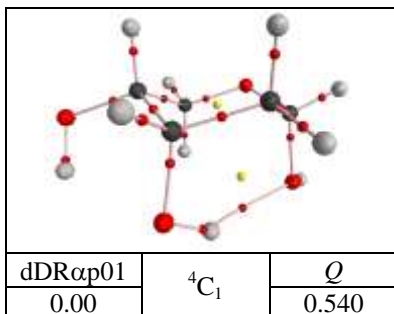
dDR01	$\varphi_1$	$\varphi_2$	dDR02	$\varphi_1$	$\varphi_2$	dDR03	$\varphi_1$	$\varphi_2$
0.00	-179.8	171.9	2.79	87.7	-62.5	4.42	-175.7	-63.1
DR01	$\varphi_1$	$\varphi_2$	DR02	$\varphi_1$	$\varphi_2$	DR03	$\varphi_1$	$\varphi_2$
0.00	-174.5	-174.8	0.59	-165.8	-171.5	0.61	166.2	59.8
DR04	$\varphi_1$	$\varphi_2$	DR05	$\varphi_1$	$\varphi_2$	DR06	$\varphi_1$	$\varphi_2$
1.32	58.1	162.0	2.63	164.9	174.0	3.21	-50.5	-53.9
DR07	$\varphi_1$	$\varphi_2$	DR08	$\varphi_1$	$\varphi_2$	DR09	$\varphi_1$	$\varphi_2$
3.42	179.1	-60.4	3.90	-172.5	-165.8	3.93	-57.6	-164.6











DRβf10	<sup>4</sup> E	$\underline{Q}$
4.56		0.363



								
DRβp01	${}^1C_4$	$Q$	DRβp02	${}^1C_4$	$Q$	DRβp03	${}^4C_1$	$Q$
0.00		0.543	0.51		0.542	1.92		0.570
								
DRβp04	${}^1C_4$	$Q$						
4.56		0.555						

**Fig. S2.** (a) Electron density at BCP in au; and (b) its Laplacian at BCP in au, both versus  $C(sp^2)\cdots HC$ ,  $H\cdots H$  or  $O\cdots HC$  distance in Å. All data are calculated at M06-2X/6-311++G(d,p) computational level.

