

Supporting information

Structures, Stability and Hydrogen Bonding in Inositol Conformers

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Table S1: The C-C-C-C Torsional Angles (degree) in various MP2/6-311+G(d,p) optimized inositols.

Angles	6e	5e/1a	4e/2a			3e/3a			2e/4a			1e/5a	6a
	Scyllo	myo	neo	epi	dl	allo	cis	muco	1,2eq	1,3eq	1,4eq		
C ₅ C ₆ C ₁ C ₂	57.6	56.9	55.7	61.2	54.1	46.5	48.3	53.2	53.1	46.7	48.9	56.2	53.1
C ₆ C ₁ C ₂ C ₃	57.6	-59.6	-55.1	-61.4	-51.8	-46.5	-48.3	-53.5	-52.6	-46.5	-50.1	-50.9	53.1
C ₁ C ₂ C ₃ C ₄	57.6	59.3	55.3	53.1	53.9	52.5	48.3	55.1	53.1	50.6	-50.1	46.7	53.1
C ₂ C ₃ C ₄ C ₅	57.6	-56.4	-55.7	-45.8	-58.2	-59.4	-48.4	-57.2	-54.8	-55.1	-49.0	-46.0	53.1
C ₃ C ₄ C ₅ C ₆	57.6	53.1	55.1	45.1	60.0	58.8	48.3	57.0	56.1	55.4	50.1	50.1	53.1
C ₄ C ₅ C ₆	57.6	-53.5	-55.3	-52.4	-58.1	-51.9	-48.4	-54.6	-54.8	-51.2	-50.1	-56.2	53.1
C ₄ C ₅ C ₆ C ₁	57.6	56.4	55.3	53.1	56.0	52.6	48.3	55.1	54.0	50.9	49.7	51.0	53.1

Table S2. Thermodynamic quantities^a of Inositols relative to the *scyllo* isomer

quantities	5e/1a	4e/2a			3e/3a			2e/4a			1e/5a	6a
	Myo	neo	epi	dl	allo	cis	muco	1,2eq	1,3eq	1,4eq		
Δ ZPE ^b	0.40	0.82	0.60	0.04	0.48	0.32	0.85	1.17	0.85	0.18	1.04	0.69
Δ E ^c	-0.15	-0.32	-0.25	0.006	-0.20	-0.13	-0.37	-0.53	-0.37	-0.04	-0.51	-0.25
-T Δ S ^d	-0.36	-0.74	-0.59	-0.04	-0.46	-0.27	-0.90	-1.32	-0.91	0.01	-1.27	-0.77
Δ G ^e	0.60	1.23	0.94	0.08	0.74	0.47	1.38	1.95	1.39	0.12	1.80	1.20

^aCalculated at 298.15 K using the B3LYP/6-311+G** method, in kcal/mol. ^bFor *scyllo*, ZPE= 124.02 kcal/mol. ^cSum of rotational, translational, and thermal vibrational energies (excluding ZPE). For *scyllo*, E_t= 7.77 kcal/mol. ^dFor *scyllo*, TS= 31.67 kcal/mol. ^eFor *scyllo*, G= 100.71 kcal/mol.

Table S3: Free energies of Inositols relative to the *scyllo* isomer in solvent phase at B3LYP/6-311+G** level

quantities	5e/1a	4e/2a			3e/3a			2e/4a			1e/5a	6a
	<i>Myo</i>	<i>neo</i>	<i>epi</i>	<i>dl</i>	<i>allo</i>	<i>cis</i>	<i>muco</i>	<i>1,2eq</i>	<i>1,3eq</i>	<i>1,4eq</i>		
$\Delta G_{\text{B3LYP}}(\text{Water})^{\text{a,d}}$	0.94	2.61	5.38	17.13	5.54	10.21	3.41	6.71	7.76	6.76	11.13	20.03
$\Delta G_{\text{B3LYP}}(\text{DMSO})^{\text{b,d}}$	1.56	2.05	5.41	15.18	5.51	9.04	3.55	6.32	7.38	7.10	10.53	17.86
$\Delta G_{\text{B3LYP}}(\text{Ethanol})^{\text{c,d}}$	1.51	2.41	4.94	15.01	4.44	9.68	3.29	6.25	7.48	7.37	10.65	17.70

^aFor *scyllo*, E(Water)= -687.24748Hatrees, TS= 23.48 kcal/mol and G(Water)=-687.28396 Hatrees.

^bFor *scyllo*, E(DMSO)= -687.244182Hatrees, TS= 25.50 kcal/mol and G(DMSO)=-687.283881 Hatrees.

^cFor *scyllo*, E(Ethanol)= -687.243472Hatrees, TS= 24.48 kcal/mol and G(Ethanol)=-687.281539 Hatrees.

^dIn solvent medium the Gibbs Free energies were calculated wherein the translational entropy was corrected with the method developed by Whitesides et al.(Mammen, M; Shakhnovich, E. I.; Deutch, J. M.; Whitesides, G. M. *J. Org. Chem.* **1998**, *63*, 3821)

Cartesian coordinates of 13 inositol isomers

Scyllo

C	-0.384141000	-1.387549000	-0.241478000
C	1.009578000	-1.026451000	0.241511000
C	1.393732000	0.361094000	-0.241467000
C	0.384141000	1.387552000	0.241477000
C	-1.009576000	1.026448000	-0.241518000
C	-1.393726000	-0.361091000	0.241475000
H	1.023361000	-1.037971000	1.341773000
H	-0.387213000	-1.405268000	-1.341739000
H	0.387206000	1.405274000	1.341738000
H	-1.023349000	1.037955000	-1.341781000
H	-1.410616000	-0.367257000	1.341737000
H	1.410635000	0.367267000	-1.341728000
O	-0.804960000	-2.648255000	0.264474000
H	-0.107995000	-3.277533000	0.043572000
O	1.890986000	-2.021245000	-0.264420000
H	2.784433000	-1.732319000	-0.043459000
O	2.695935000	0.627023000	0.264506000
H	2.892438000	1.545242000	0.043573000
O	0.804957000	2.648259000	-0.264475000
H	0.107988000	3.277539000	-0.043588000
O	-1.890991000	2.021244000	0.264392000
H	-2.784439000	1.732294000	0.043469000
O	-2.695937000	-0.627025000	-0.264476000
H	-2.892417000	-1.545256000	-0.043574000

Myo

C	0.020370000	-1.550941000	-0.247799000
C	-1.243578000	-0.754161000	-0.544310000
C	-1.244686000	0.582024000	0.179117000
C	-0.015328000	1.387121000	-0.194987000
C	1.233201000	0.613501000	0.182582000
C	1.271036000	-0.730989000	-0.538532000
H	-1.301283000	-0.563343000	-1.626663000
H	0.027048000	-2.457497000	-0.867744000
H	-0.013375000	1.570719000	-1.280811000
H	1.229976000	0.444303000	1.268517000
H	1.342935000	-0.542901000	-1.615943000
H	-1.234292000	0.407389000	1.263421000
O	0.089810000	-1.906152000	1.131125000
H	-0.748965000	-2.335752000	1.340134000
O	-2.340117000	-1.560114000	-0.129250000
H	-3.113941000	-0.983250000	-0.131351000
O	-2.448654000	1.241928000	-0.197860000

H	-2.402572000	2.128771000	0.178965000
O	-0.104043000	2.623338000	0.503080000
H	0.738849000	3.072967000	0.369336000
O	2.348141000	1.417737000	-0.185965000
H	3.129683000	0.864041000	-0.068116000
O	2.450538000	-1.444203000	-0.184765000
H	2.254461000	-1.865053000	0.662918000

Neo

C	-0.015562000	1.421686000	0.402425000
C	-1.259567000	0.554871000	0.509391000
C	-1.241168000	-0.572867000	-0.520178000
C	0.015561000	-1.421688000	-0.402419000
C	1.259567000	-0.554876000	-0.509390000
C	1.241170000	0.572867000	0.520173000
H	-1.304050000	0.112794000	1.509039000
H	-0.024340000	2.171599000	1.204746000
H	0.024339000	-2.171610000	-1.204732000
H	1.304051000	-0.112804000	-1.509041000
H	1.277617000	0.136762000	1.528052000
H	-1.277599000	-0.136758000	-1.528055000
O	-0.082122000	2.069271000	-0.867861000
H	0.748291000	2.551446000	-0.965717000
O	0.082122000	-2.069260000	0.867874000
H	-0.748264000	-2.551483000	0.965713000
O	-2.450141000	1.323644000	0.362758000
H	-2.284004000	1.925328000	-0.374896000
O	2.450140000	-1.323649000	-0.362751000
H	2.283995000	-1.925339000	0.374897000
O	2.347553000	1.445920000	0.315204000
H	3.113240000	0.874628000	0.175100000
O	-2.347558000	-1.445914000	-0.315228000
H	-3.113234000	-0.874617000	-0.175088000

Epi

C	0.770113000	-1.219553000	-0.491498000
C	1.292457000	0.049339000	0.168651000
C	0.665909000	1.265373000	-0.483657000
C	-0.846971000	1.258376000	-0.321688000
C	-1.465473000	-0.059414000	-0.790742000
C	-0.738730000	-1.327015000	-0.314764000
H	1.037386000	0.035805000	1.235925000
H	1.020816000	-1.189647000	-1.558714000
H	-1.269546000	2.074009000	-0.926064000
H	-1.438496000	-0.066420000	-1.888295000
H	-1.113288000	-2.172885000	-0.908898000

H	0.914162000	1.252242000	-1.556503000
O	-1.218837000	1.439222000	1.039835000
H	-0.723359000	2.208036000	1.349224000
O	-0.943807000	-1.591908000	1.067387000
H	-1.897486000	-1.605197000	1.206213000
O	1.435864000	-2.360908000	0.037242000
H	0.965776000	-2.574094000	0.854902000
O	2.700606000	0.175338000	-0.006602000
H	3.076481000	-0.679784000	0.236931000
O	1.130775000	2.473268000	0.108033000
H	2.085599000	2.372376000	0.208057000
O	-2.832083000	-0.121782000	-0.400399000
H	-2.902012000	0.437080000	0.385449000

DI

C	-0.793109000	-1.428777000	-0.054441000
C	0.727845000	-1.464931000	0.090239000
C	1.375673000	-0.210540000	-0.487204000
C	0.773425000	1.047047000	0.113395000
C	-0.719010000	1.082084000	-0.140332000
C	-1.383512000	-0.134880000	0.494787000
H	1.119848000	-2.337686000	-0.454678000
H	-1.223817000	-2.274226000	0.495796000
H	0.947294000	1.054738000	1.198139000
H	-0.900871000	1.081334000	-1.224978000
H	-1.219744000	-0.098027000	1.575481000
H	1.219429000	-0.188652000	-1.573827000
O	-1.175783000	-1.475497000	-1.434085000
H	-1.080300000	-2.382515000	-1.740460000
O	1.002212000	-1.586340000	1.477252000
H	1.948368000	-1.413532000	1.568870000
O	2.765594000	-0.301949000	-0.186448000
H	3.134025000	0.572960000	-0.360747000
O	1.446770000	2.146578000	-0.493718000
H	0.998813000	2.943558000	-0.186212000
O	-1.211399000	2.287059000	0.435373000
H	-2.173316000	2.208785000	0.438579000
O	-2.792704000	-0.084973000	0.298401000
H	-2.935116000	-0.385777000	-0.608821000

Allo

C	0.588164000	1.188587000	-0.539896000
C	1.379649000	-0.099555000	-0.753605000
C	0.950295000	-1.279089000	0.136481000
C	-0.565519000	-1.457655000	0.165827000
C	-1.262424000	-0.153455000	0.516588000

C	-0.909285000	0.930330000	-0.494391000
H	1.406257000	-2.187837000	-0.289670000
H	1.236123000	-0.408211000	-1.795124000
H	0.803968000	1.871394000	-1.374765000
H	-0.819983000	-2.209043000	0.923323000
H	-0.939507000	0.162890000	1.511093000
H	-1.243763000	0.614644000	-1.492376000
O	-1.071079000	-1.842882000	-1.119285000
H	-0.873083000	-2.775521000	-1.248631000
O	1.349003000	-1.125872000	1.485563000
H	2.266045000	-0.828584000	1.459803000
O	1.047195000	1.772587000	0.675131000
H	0.445723000	2.505644000	0.857863000
O	2.770356000	0.148993000	-0.564430000
H	2.820890000	0.922731000	0.012609000
O	-2.678199000	-0.313581000	0.576042000
H	-2.914479000	-0.820876000	-0.211555000
O	-1.524112000	2.165424000	-0.138729000
H	-2.418788000	1.940441000	0.147069000

Cis

C	0.566786000	-1.374644000	-0.326265000
C	-0.897399000	-1.158961000	-0.722336000
C	-1.473898000	0.196600000	-0.326206000
C	-0.554960000	1.356635000	-0.722179000
C	0.907185000	1.178226000	-0.325994000
C	1.452450000	-0.197583000	-0.722254000
H	-2.422889000	0.332996000	-0.867119000
H	-0.949445000	-1.237613000	-1.816652000
H	0.923293000	-2.264590000	-0.867306000
H	-0.597032000	1.440892000	-1.816515000
H	1.499589000	1.932033000	-0.866989000
H	1.546549000	-0.203137000	-1.816570000
O	0.747864000	-1.576458000	1.067398000
H	0.162323000	-2.300246000	1.316485000
O	0.991313000	1.435768000	1.067657000
H	1.910990000	1.291226000	1.316779000
O	-1.739141000	0.140423000	1.067543000
H	-2.075446000	1.008567000	1.316403000
O	-1.694596000	-2.208429000	-0.185905000
H	-2.106860000	-1.834300000	0.604898000
O	2.759962000	-0.363441000	-0.185925000
H	2.642131000	-0.906935000	0.605286000
O	-1.065127000	2.571943000	-0.186146000
H	-0.536374000	2.741021000	0.605735000

Muco

C	-0.386888000	1.159339000	-0.069212000
C	-1.354566000	0.095902000	0.416371000
C	-0.912607000	-1.289251000	-0.036985000
C	0.517360000	-1.590291000	0.404783000
C	1.500829000	-0.500282000	-0.037905000
C	1.029247000	0.882431000	0.414397000
H	-1.583690000	-2.041294000	0.394756000
H	-1.397154000	0.121526000	1.512408000
H	-0.394504000	1.171698000	-1.168459000
H	0.820110000	-2.545220000	-0.044742000
H	2.479455000	-0.695292000	0.417999000
H	1.045068000	0.943283000	1.506960000
O	-0.930735000	-1.372776000	-1.465030000
H	-1.778964000	-0.995088000	-1.735246000
O	0.469664000	-1.672682000	1.826564000
H	1.305227000	-2.044482000	2.126373000
O	1.716380000	-0.511429000	-1.446998000
H	0.868484000	-0.748062000	-1.854097000
O	-0.867808000	2.407733000	0.419991000
H	-0.174828000	3.052355000	0.230208000
O	-2.651760000	0.300924000	-0.141595000
H	-2.852020000	1.236933000	-0.018685000
O	1.909951000	1.894677000	-0.062046000
H	2.137031000	1.624969000	-0.963258000

1,2eq

C	1.073265000	0.529551000	-0.545565000
C	-0.181423000	1.397702000	-0.504270000
C	-1.453062000	0.539610000	-0.559999000
C	-1.456041000	-0.549804000	0.519022000
C	-0.182131000	-1.397350000	0.491991000
C	1.062830000	-0.523249000	0.557125000
H	-2.312170000	1.194000000	-0.378029000
H	-0.179798000	2.054975000	-1.378892000
H	1.138577000	0.026022000	-1.515020000
H	-2.323107000	-1.199866000	0.349831000
H	-0.180952000	-2.084777000	1.352173000
H	1.099027000	-0.022811000	1.533777000
O	2.251322000	1.321087000	-0.431449000
H	2.032848000	2.003097000	0.219542000
O	2.176691000	-1.401962000	0.417364000
H	2.935979000	-0.834309000	0.231656000
O	-0.136669000	2.250543000	0.642147000
H	-0.565016000	1.777210000	1.368581000
O	-1.623885000	-0.026577000	-1.848877000

H	-1.122032000	-0.853994000	-1.863267000
O	-1.562338000	0.129465000	1.776185000
H	-1.642466000	-0.528473000	2.475078000
O	-0.199677000	-2.148334000	-0.721226000
H	0.694936000	-2.503610000	-0.818401000

1,3eq

C	0.102826000	-1.175183000	-0.717553000
C	-1.235559000	-0.429402000	-0.764321000
C	-1.323358000	0.750049000	0.209644000
C	-0.114643000	1.679350000	0.072996000
C	1.202814000	0.932760000	0.243431000
C	1.311774000	-0.241492000	-0.733091000
H	-2.229509000	1.316405000	-0.040864000
H	-1.370351000	-0.049351000	-1.782283000
H	0.161426000	-1.828883000	-1.599723000
H	-0.174404000	2.456432000	0.845664000
H	2.027977000	1.625949000	0.035179000
H	1.403943000	0.180192000	-1.739407000
O	-2.294195000	-1.342280000	-0.499785000
H	-2.480602000	-1.232196000	0.444264000
O	2.501928000	-0.976063000	-0.454054000
H	2.212768000	-1.777043000	0.002654000
O	0.217430000	-1.980310000	0.458897000
H	-0.514718000	-2.607055000	0.421315000
O	1.251922000	0.507071000	1.603380000
H	2.000635000	-0.098572000	1.665748000
O	-1.516795000	0.296468000	1.543288000
H	-0.639934000	0.039816000	1.871697000
O	-0.070698000	2.243138000	-1.237993000
H	-0.777090000	2.893626000	-1.300751000

1,4eq

C	1.224198000	-0.066223000	-0.805329000
C	0.814392000	1.247663000	-0.145948000
C	-0.686883000	1.322599000	0.112181000
C	-1.224290000	0.065908000	0.805341000
C	-0.814363000	-1.247865000	0.145755000
C	0.686976000	-1.322692000	-0.111816000
H	-0.884763000	2.173214000	0.784275000
H	1.077951000	2.062105000	-0.833720000
H	0.822242000	-0.056473000	-1.823096000
H	-0.822745000	0.055929000	1.823244000
H	-1.078332000	-2.062483000	0.833148000
H	0.885430000	-2.173602000	-0.783340000
O	-2.645739000	0.141807000	0.892541000

H	-2.974101000	-0.394639000	0.159065000
O	2.645574000	-0.142087000	-0.892968000
H	2.974215000	0.394605000	-0.159811000
O	1.282787000	-1.556781000	1.153519000
H	2.232659000	-1.452908000	1.027814000
O	-1.569315000	-1.365559000	-1.064994000
H	-1.528726000	-2.285900000	-1.343310000
O	-1.283196000	1.557400000	-1.152666000
H	-2.233017000	1.453319000	-1.026624000
O	1.569908000	1.365776000	1.064371000
H	1.528863000	2.286050000	1.342828000

1e/5a

C	-0.890614000	1.282582000	0.186228000
C	-1.283335000	-0.023645000	0.881614000
C	-0.995187000	-1.250849000	0.007693000
C	0.477726000	-1.296859000	-0.410516000
C	0.967678000	0.020928000	-1.021579000
C	0.579955000	1.286010000	-0.238675000
H	-1.191116000	-2.147499000	0.607606000
H	-2.357552000	0.004764000	1.095230000
H	-1.055264000	2.110031000	0.887919000
H	0.595364000	-2.090248000	-1.158730000
H	0.533187000	0.095683000	-2.024823000
H	0.750652000	2.143464000	-0.903286000
O	2.383621000	-0.021694000	-1.166841000
H	2.725487000	0.504324000	-0.429247000
O	1.218794000	-1.632780000	0.768539000
H	2.151488000	-1.588283000	0.523919000
O	-1.850876000	-1.321113000	-1.119262000
H	-1.990492000	-0.416783000	-1.430715000
O	-0.566145000	-0.078765000	2.119985000
H	0.057699000	-0.817696000	2.058190000
O	-1.743944000	1.410100000	-0.957521000
H	-1.561876000	2.255195000	-1.381893000
O	1.451825000	1.495707000	0.868599000
H	1.058879000	1.026416000	1.619249000

6a

C	-1.113081000	-0.599359000	-0.778236000
C	-1.142004000	-0.574681000	0.754540000
C	0.268204000	-0.542499000	1.355494000
C	1.113081000	0.599359000	0.778236000
C	1.142004000	0.574681000	-0.754540000
C	-0.268204000	0.542499000	-1.355494000
H	0.182557000	-0.379855000	2.437528000

H	-1.634649000	-1.489210000	1.108826000
H	-2.145148000	-0.483328000	-1.133132000
H	2.145148000	0.483328000	1.133132000
H	1.634649000	1.489210000	-1.108826000
H	-0.182557000	0.379855000	-2.437528000
O	-0.594447000	-1.829184000	-1.293014000
H	-0.285970000	-2.344836000	-0.535216000
O	-1.931173000	0.548344000	1.157741000
H	-1.350184000	1.136205000	1.659901000
O	0.594447000	1.829184000	1.293014000
H	0.285970000	2.344836000	0.535216000
O	0.864487000	-1.824488000	1.137652000
H	1.641974000	-1.683276000	0.580070000
O	1.931173000	-0.548344000	-1.157741000
H	1.350184000	-1.136205000	-1.659901000
O	-0.864487000	1.824488000	-1.137652000
H	-1.641974000	1.683276000	-0.580070000