

**Mechanistic insights into water-catalysed formation of
levoglucosenone from anhydrosugar intermediates by means of
high-level theoretical procedures**

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Supplementary Material

(Figure S1, Tables S1–S4)

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Figure S1. Competing reaction mechanism proposed by Shafizadeh *et al.* [1].

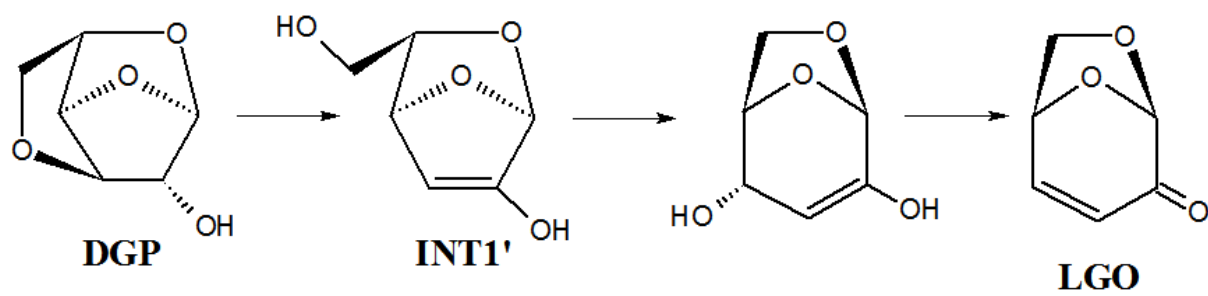


Table S1. G4(MP2) Gibbs free energies (ΔG_{298} , kcal mol⁻¹) for the first step in the competing reaction mechanism proposed by Shafizadeh et al.^[1] (shown in Figure S1).

Structure	ΔG_{298}
DGP	0.0
TS1'	73.6
WTS1'	71.1
INT1'	15.6

Table S2. Reaction profile (G4(MP2), kcal mol⁻¹) on the electronic (ΔE_e), enthalpic (ΔH_{298}) and Gibbs-free energy (ΔG_{298}) surfaces for the uncatalysed and water-catalysed conversion of DGP to LGO.

Structure	ΔE_e	ZPVE ^a	$H_{298}-H_0^b$	$T \times \Delta S^c$	ΔH_{298}	ΔG_{298}
DGP	0.0	0.0	0.0	0.0	0.0	0.0
TS1	48.9	-0.1	-0.8	-10.2	48.0	58.1
INT1	-12.7	3.5	-0.9	-10.2	0.0	0.0
TS2	36.5	-1.1	-0.7	-9.6	34.8	44.4
STS2	26.8	-1.3	-1.5	-11.6	24.0	35.5
WTS2	17.6	1.1	-2.0	-20.3	16.7	37.0
INT2	-5.6	2.1	-0.3	-8.6	4.8	4.8
TS3	54.0	-1.7	-0.5	-9.6	51.8	61.4
WTS3	38.2	0.4	-1.8	-20.6	37.7	57.3
INT3	2.9	0.7	0.5	-6.9	11.1	11.1
TS4	64.6	-3.5	0.4	-7.0	61.6	68.6
WTS4	37.8	-1.3	-0.8	-17.8	35.7	53.5
INT4	-5.8	0.9	0.3	-7.3	2.7	2.7
TS5	57.6	-2.9	0.3	-7.2	54.9	62.1
WTS5	37.8	-0.9	-1.0	-18.2	49.0	54.1
INT5	11.1	-4.1	2.2	5.4	3.8	3.8
TS6	47.6	-6.5	1.4	3.8	42.5	38.8
WTS6	24.5	-3.8	-0.1	-7.9	20.7	28.6
INT6	-3.5	-2.1	1.3	3.2	-4.3	-7.5
TS7	51.3	-4.9	1.0	2.0	47.4	45.5
LGO	3.9	-4.9	1.9	12.4	-0.9	-11.6

^aZero-point vibrational energy corrections

^bHeat content function (aka enthalpy function) corrections.

^c $T \times \Delta S$ entropic corrections at 298 K.

Table S3. Absolute energies needed for the calculation the G4(MP2) reaction profiles (in Hartree) for all the species considered in the present work.

Structure	E_e^a	H_0^b	H_{298}^c	G_{298}^d
H2O	-76.376916	-76.355854	-76.352074	-76.373502
DGP	-533.794024	-533.651986	-533.643708	-533.683837
TS1	-610.092944	-609.930042	-609.919337	-609.964690
INT1	-610.191199	-610.022513	-610.011925	-610.057306
TS2	-610.112716	-609.951342	-609.940354	-609.986631
STS2	-610.128268	-609.967254	-609.957555	-610.000694
WTS2	-686.519862	-686.333942	-686.321219	-686.371802
INT2	-610.179850	-610.013420	-610.001906	-610.049710
TS3	-610.084813	-609.924379	-609.913118	-609.959454
WTS3	-686.487047	-686.302215	-686.289270	-686.339479
INT3	-610.166277	-610.002042	-609.989184	-610.039666
TS4	-610.067970	-609.910419	-609.897649	-609.947972
WTS4	-686.487645	-686.305532	-686.290944	-686.345573
INT4	-610.180106	-610.015605	-610.003010	-610.052975
TS5	-610.079149	-609.920745	-609.908242	-609.958335
WTS5	-686.487572	-686.304884	-686.290634	-686.344632
INT5	-533.776285	-533.640858	-533.629084	-533.677853
TS6	-533.718215	-533.586467	-533.575959	-533.622076
WTS6	-610.131843	-609.974785	-609.962845	-610.011844
INT6	-533.799637	-533.661022	-533.650594	-533.695854
TS7	-533.712218	-533.577918	-533.568115	-533.611362
LGO	-457.410952	-457.297781	-457.290219	-457.328753

^aElectronic energy.

^bZero-point inclusive energy (or enthalpy at 0 K).

^cEnthalpy at 298 K.

^dGibbs-free energy at 298 K.

Table S4. B3LYP/6-31G(2df,p) optimised geometries for all the local minima and transition structures

• Transition structures:

1.1 Uncatalysed reactions:

TS1:

O	-0.24297300	-1.46166400	-0.72513300
C	1.44229800	0.13037000	0.45793300
O	0.75684000	-0.27964500	1.46199100
C	-0.65411800	-0.10092700	1.18616400
C	-0.72099900	1.11249600	0.24504800
O	-1.81990400	0.92388400	-0.60610300
C	-2.34508600	-0.40757900	-0.41010700
C	-1.18384400	-1.21788700	0.20103600
C	0.68005300	1.07903600	-0.44697500
O	1.29732200	2.35667900	-0.36024500
H	2.51410700	0.12623400	0.58416600
H	-1.14948400	-0.01811000	2.15194000
H	-0.81355000	2.07467900	0.76121500
H	-3.23422200	-0.35867400	0.23771100
H	-2.62151000	-0.81687800	-1.38344100
H	-1.55381000	-2.09187600	0.77307400
H	0.58553500	0.70358900	-1.46362500
H	1.88166200	2.47244300	-1.11569900
O	2.19073700	-1.80090600	-0.51363200
H	2.46397000	-1.69854700	-1.43235200
H	1.16130200	-1.87269600	-0.56661100

TS2:

O	-2.76736600	-0.73542000	-0.61870300
C	1.78056800	0.75288200	-0.21016800
O	0.43112500	0.78262500	-1.27496300
C	-0.48446300	-0.25313900	-0.89197900
C	0.04618700	-0.90209400	0.40751700
O	-0.67943500	-0.33172900	1.48831300
C	-1.56748800	0.67045600	1.00859200
C	-1.83837900	0.32339300	-0.46039900
C	1.55189300	-0.59503300	0.47723500
O	2.19940300	-1.64811100	-0.21593000
H	2.63695500	0.74800700	-0.90841700
H	-0.09087900	-1.98717100	0.42124000
H	-2.47888000	0.64747900	1.61696900
H	-1.11267500	1.66582900	1.10179500
H	1.86475800	-0.51768900	1.52662500
H	3.14829000	-1.48812700	-0.20212100
O	1.42696700	1.87245500	0.35793600
H	-3.56721700	-0.51476300	-0.13165400
H	-0.58759700	-0.95218700	-1.72207100
H	-2.11633700	1.20266500	-1.05724100
H	0.48812800	1.69859900	-0.52313300

TS3:

O	1.44211800	0.85966100	-1.24986200
C	-1.74350200	0.90791300	-0.58542300
O	0.52516200	1.47975000	1.52465900
C	0.90903600	0.21215400	1.10367400
C	-0.26005900	-0.75682700	0.76987000
O	0.39996600	-1.71716000	-0.29065500
C	1.81032000	-1.34726400	-0.46992900
C	1.86264500	0.13413900	-0.12389000
C	-1.44972600	-0.38646200	-0.06619900
O	-2.60467100	-1.15435000	0.21637300
H	-2.76710100	0.96803800	-0.99807700
H	1.45758100	-0.23209000	1.94360600
H	-0.54175500	-1.39849100	1.60259000
H	2.39387200	-1.98048400	0.20452200
H	2.07232500	-1.54985700	-1.50766500
H	2.87581500	0.43699700	0.17320800
H	-0.41043300	-1.15484700	-0.92876300
H	-2.59595400	-1.94846100	-0.32443500
O	-1.00106600	1.90470100	-0.66504900
H	0.67415100	1.42239200	-1.03446100
H	-0.02286200	1.87406400	0.81712800

TS4:

O	-0.61741300	-0.55909500	-1.42056800
C	2.26855800	0.43449600	-0.51143000
O	0.45136000	-2.13653000	0.77403200
C	-0.42048900	-1.02138100	0.96814600
C	0.27594400	0.28777600	1.23767100
O	-2.03591200	1.46426200	-0.28724300
C	-2.48324000	0.12670100	-0.14467500
C	-1.35980800	-0.91000200	-0.25511800
C	1.16674300	0.94729500	0.34949400
O	0.96674400	2.21683100	0.37967100
H	3.00608700	1.21021500	-0.79241600
H	-1.03767200	-1.27533500	1.83772400
H	0.48071000	0.54327700	2.27797000
H	-2.96251200	0.05247700	0.83681600
H	-3.24314500	-0.10564500	-0.90555600
H	-1.81839600	-1.90232400	-0.38182900
H	-1.51621600	1.48839900	-1.09946500
H	-0.04531400	1.73217100	1.03498600
O	2.38080900	-0.71892100	-0.87090700
H	0.05870700	-1.23348000	-1.55416000
H	1.22680200	-1.83144600	0.28152700

TS5:

O	-0.80826200	-0.45788600	-1.46559300
C	1.97225400	-0.05259700	-0.87086800
O	0.44390400	-1.70541600	1.30177900

C	-0.50954900	-0.49760900	1.01188800
C	0.49673700	0.59924000	1.15370600
O	-2.34634600	1.49839900	-0.09962200
C	-2.65486400	0.12370700	-0.13893800
C	-1.40111400	-0.75906000	-0.21339900
C	1.47596800	0.95723500	0.17041000
O	2.12415500	2.00475500	0.13022400
H	2.57208100	0.44602500	-1.65392800
H	-1.15266300	-0.51989300	1.89246300
H	1.04788500	-0.79414400	1.69237600
H	-3.22018000	-0.10125400	0.77111000
H	-3.28557100	-0.13259700	-1.00299000
H	-1.72722600	-1.80996900	-0.17484200
H	-1.77797300	1.68409300	-0.85613000
H	0.23300400	1.40626100	1.82838300
O	1.86447200	-1.27186200	-0.85965300
H	-0.14887700	-1.12376600	-1.68187500
H	0.95954100	-1.82417600	0.45155700

TS6:

O	-0.39875500	1.27705900	-0.02703300
C	1.21841400	0.80286300	0.50674400
C	-0.56641000	-0.79644600	-1.31926100
C	0.61479000	-1.27370500	-0.91430100
O	-1.91515600	-0.60629600	1.37748200
C	-2.40989700	-0.00613300	0.20368900
C	-1.26492200	0.40170300	-0.75183600
C	1.41196200	-0.66958200	0.16352300
O	2.28069900	-1.26590800	0.76580700
H	1.17889400	0.99478400	1.59033800
H	-1.12976400	-1.33647500	-2.07733200
H	-3.06154600	-0.73869600	-0.28303800
H	-3.00581700	0.89141000	0.42130100
H	-1.70462600	0.98616200	-1.57214600
H	-1.46251900	0.08068500	1.87842100
H	1.01237000	-2.20102200	-1.31560200
O	1.73769300	1.68746400	-0.29075300
H	0.51354800	1.83240600	-0.57731700

TS7:

C	0.54016000	1.26358900	-0.04048800
C	0.68193700	0.15378300	0.96824900
C	-0.86057600	1.62684300	-0.29941800
O	-0.32787900	-0.53128300	1.37685000
O	0.07297900	-0.90414900	-1.29599600
C	-1.84368200	0.77856900	0.03570600
C	-1.48961300	-0.56885300	0.51069200
C	-0.99584300	-1.47183700	-0.75240100
H	1.51871500	0.18257300	1.65380900
H	-2.89123500	0.99660500	-0.14150300

H	-2.25945000	-1.07493900	1.09085300
H	-0.84001700	-2.47804500	-0.30945200
H	-1.88511200	-1.52852900	-1.40977200
O	1.51760700	1.88545800	-0.40079900
H	-1.03487900	2.60806500	-0.72607800
O	2.19064400	-1.21353300	0.00818500
H	1.42949200	-1.23236100	-0.66949700
H	2.14137200	-2.05787700	0.47168900

1.2 Catalysed reactions:

WTS2:

O	-2.71096200	0.10167700	-0.85637000
C	1.60239300	0.83542600	-0.35128500
O	0.00110200	0.59210600	-1.05504900
C	-0.36739400	-0.76218600	-0.85780500
C	0.41959200	-1.24579600	0.36196100
O	-0.32064700	-0.75534200	1.47093100
C	-1.71157500	-0.79356200	1.15530200
C	-1.83291900	-0.90061000	-0.38329900
C	1.77719300	-0.55898200	0.30926100
O	2.61312900	-1.39720800	-0.47495200
H	2.15493400	0.88194000	-1.30684600
H	-0.15220300	-1.33355400	-1.76719900
H	0.53923800	-2.33814800	0.39973800
H	-2.18797700	-1.64850500	1.65234600
H	-2.17351800	0.13198600	1.50668100
H	2.16651900	-0.40974600	1.32373800
H	3.47294800	-0.97260400	-0.55627900
O	1.57495200	1.89803400	0.36193700
H	-2.73978200	0.04773000	-1.81744200
H	0.34415000	2.21801200	0.62955200
O	-0.77208700	2.23459500	0.48720100
H	-0.61449300	1.41280100	-0.34843800
H	-1.02205400	3.07180600	0.08007600
H	-2.19539900	-1.89835200	-0.67031700

STS2:

O	1.68174900	1.30557300	0.04974500
C	-1.13393100	1.05327900	-0.41864000
O	-0.33437200	1.01181100	1.12012700
C	0.31372200	-0.26789800	1.16889300
C	-0.33137500	-1.19607600	0.11525200
O	0.62023100	-1.39826300	-0.92102800
C	1.92296400	-1.11617300	-0.42820600
C	1.76039300	0.00128400	0.59575800
C	-1.53374500	-0.42860000	-0.43685900
O	-2.62136900	-0.70378300	0.42364000
H	-1.96119200	1.72996000	-0.14906400
H	0.27942100	-0.64886500	2.18887400
H	-0.65529900	-2.15307100	0.54144000

H	2.36222900	-2.00413900	0.05499000
H	2.55264400	-0.82570200	-1.27224500
H	2.53611600	-0.01765700	1.36649000
H	-1.72337100	-0.72861200	-1.47543100
H	-3.37314700	-0.16863900	0.15034100
O	-0.28033000	1.49038900	-1.28578300
H	0.84212700	1.33932500	-0.82435200
H	0.62502900	1.55669600	0.74816300

WTS3:

C	1.53942300	-1.42088000	-0.69310600
O	-1.14341900	-1.89877700	0.68071900
C	-1.10627200	-0.51312400	0.80088300
C	0.28226700	0.15239500	0.96084700
O	-0.06765400	1.62526700	0.52086300
C	-1.39003100	1.67841400	-0.08906200
C	-1.75344900	0.23208900	-0.37812600
C	1.49231900	-0.34912700	0.23981400
H	-1.69756100	-0.25975800	1.69108100
H	-2.09276400	2.11095900	0.62917600
H	-1.32742300	2.31900800	-0.97127400
H	0.80494500	1.95677300	-0.27675000
O	0.59841400	-1.97088600	-1.28926100
H	-0.61027500	-2.11270400	-0.12325400
H	0.53852100	0.30941600	2.00924800
O	2.71486600	-0.04009600	0.90816700
O	-3.15063200	0.07152000	-0.42195400
H	-3.31050300	-0.87949500	-0.37390600
H	-1.27840200	-0.11219900	-1.30882700
O	1.66609400	1.88081300	-1.08067500
H	1.71340100	0.80068800	-0.81204300
H	2.58298900	-1.72084900	-0.92463900
H	2.48148500	2.26207100	-0.72738300
H	2.86870100	-0.69525000	1.59818800

WTS4:

O	-0.97783400	-1.05985000	-1.05642400
C	1.69375400	-0.94493300	-1.05419100
O	-0.02991500	-1.88243700	1.55331800
C	-0.42594900	-0.54021300	1.26849900
C	0.70949800	0.41640500	0.95547400
C	-2.15417500	0.78030400	-0.10768500
C	-1.51306000	-0.56942700	0.17239900
C	1.57711600	0.28033600	-0.15579000
O	2.36479700	1.20889800	-0.53817600
H	1.85395200	-0.70328300	-2.12092400
H	-0.91083700	-0.17747500	2.18445400
H	-2.28448900	1.32130100	0.84447500
H	-2.30531400	-1.24450200	0.52385800
H	1.77772100	2.28839200	-0.14478900

O	1.78349300	-2.07219600	-0.62586500
H	-0.76777200	-1.99005300	-0.91171400
H	0.75528400	-2.08319200	1.02445200
H	1.21399000	0.81910700	1.83743400
O	0.87800800	2.90421000	0.22330000
H	0.46744900	1.86180300	0.61505100
O	-3.40065300	0.55126200	-0.74306600
H	-3.71931000	1.38893700	-1.09057500
H	-1.48152700	1.37367700	-0.74222600
H	1.13457800	3.41135900	1.00358500

WTS5:

O	1.35851600	0.47466700	1.40372900
C	-1.37764700	1.39408800	0.91848200
O	-0.76499700	-1.71493500	0.65738800
C	0.25779900	-1.03173200	-0.24247900
C	-0.40406400	0.04819900	-1.05498300
O	2.67730500	0.56623300	-1.09936500
C	2.75575700	-0.52070200	-0.20560600
C	1.48839300	-0.71440100	0.63481400
C	-0.87674100	1.29070300	-0.52584000
O	-1.05788200	2.34215800	-1.14861200
H	-1.62943900	2.44008000	1.17372800
H	0.55190700	-1.84691700	-0.90886700
H	-1.73752500	-0.85353800	-1.33823500
H	2.94233000	-1.41569700	-0.80858800
H	3.59546300	-0.40806800	0.49730700
H	1.65521000	-1.58251600	1.29079600
H	2.38094900	1.33159400	-0.59319800
H	0.02963500	0.15416100	-2.04621100
O	-1.56697200	0.50236300	1.73604300
H	0.73165200	0.33224900	2.11891000
H	-1.12264000	-0.96634700	1.22388500
O	-2.34411900	-1.74841100	-1.13963400
H	-1.63059800	-1.90103800	-0.09244200
H	-3.24271700	-1.45748700	-0.93979800

WTS6:

O	0.40112200	0.58908100	-0.51587500
C	-1.38655400	0.47837500	-0.37684000
C	0.53307300	-1.32373100	0.97039300
C	-0.67086200	-1.78304200	0.61723200
O	2.73528200	-0.91039000	-0.96268400
C	2.57552700	-0.09029600	0.17012600
C	1.10067000	0.01181500	0.58754700
C	-1.62509200	-1.01654200	-0.19706700
O	-2.62114500	-1.50234700	-0.69073900
H	1.18461000	-1.94099800	1.58422600
H	3.16299400	-0.53513900	0.98079600
H	2.95939500	0.92857600	-0.00096000

H	1.03423000	0.67577600	1.46789200
H	2.09669500	-0.59513300	-1.61419100
O	-1.72648000	1.24553800	0.58951900
H	0.35039200	1.79883600	-0.35000000
O	-0.12690400	2.87370300	-0.06722100
H	-1.04805000	2.30396000	0.34486200
H	0.34195900	3.31096300	0.65092200
H	-0.99973600	-2.77845300	0.89950200
H	-1.53806300	0.80745800	-1.41540700

• Local minima

H₂O

O	0.00000000	0.00000000	0.11886300
H	0.00000000	0.75665500	-0.47545400
H	0.00000000	-0.75665500	-0.47545400

DGP:

O	-0.48014900	-1.24216200	-0.98444300
C	0.83081700	-1.00785000	-0.46660600
O	0.72390400	-1.25402900	0.91919000
C	-0.36114600	-0.36584400	1.14069800
C	0.07405200	0.99601000	0.52894300
O	-1.08293100	1.58737200	-0.03198600
C	-2.02784600	0.55882700	-0.35706400
C	-1.37683800	-0.76009500	0.03637700
C	1.10846400	0.51042200	-0.53018300
O	2.40227400	0.85637900	-0.08113700
H	1.54418400	-1.68397200	-0.93851300
H	-0.69238800	-0.38640000	2.17542700
H	0.53704200	1.69954100	1.22107000
H	-2.95389300	0.72690600	0.20885200
H	-2.26020500	0.58593600	-1.42694200
H	-2.08756300	-1.54825700	0.29394800
H	0.87530500	0.93012900	-1.51580100
H	3.04771800	0.50681200	-0.70402200

INT1:

O	-2.06220000	1.17945200	-0.12076400
C	1.20324000	1.05366000	0.12609800
O	0.38274500	0.99373400	-1.04671700
C	-0.31220700	-0.25340000	-1.09537000
C	0.30946200	-1.15012800	0.00197000
O	-0.62551500	-1.14481900	1.07621100
C	-1.91668400	-1.13762900	0.46508800
C	-1.81051700	-0.09967200	-0.65624000
C	1.58479200	-0.41641300	0.40195300
O	2.60059900	-0.88172600	-0.46691600
H	2.06258800	1.68169100	-0.12672900
H	-0.21407400	-0.65606400	-2.10484800
H	0.51829800	-2.17163900	-0.33743900

H	-2.15521500	-2.13481600	0.06341000
H	-2.65440300	-0.85951100	1.21908300
H	1.83094700	-0.56647300	1.45967400
H	3.39514300	-0.36115400	-0.31265100
O	0.56618700	1.67058700	1.20008500
H	-1.35610600	1.75962600	-0.44351100
H	-0.17350000	1.10740000	1.47259000
H	-2.49671300	-0.31539400	-1.48575600

INT2:

C	-1.84781800	0.52556000	1.05297000
O	-0.08251900	-1.80641700	-0.12925100
C	0.62319700	-0.67071600	-0.60813500
C	-0.23225600	0.60659500	-0.89585600
O	0.36840800	1.67606000	-0.16029400
C	1.73204200	1.34242600	0.07111600
C	1.72112900	-0.15898600	0.35229800
C	-1.71366500	0.53040700	-0.48231800
H	1.10738900	-0.99855500	-1.53211800
H	2.35696700	1.54655900	-0.81204200
H	2.09109400	1.94795000	0.90531800
O	-1.47830200	-0.38555100	1.76054700
H	-0.48650800	-1.55810600	0.72443400
H	-0.20042000	0.82899100	-1.97176400
O	-2.37398400	-0.56761200	-1.06767500
O	3.00040700	-0.70769400	0.13015000
H	2.95533000	-1.65000700	0.32278100
H	1.38437100	-0.33468100	1.38551600
H	-2.21816500	1.43250000	-0.84478700
H	-2.33890300	1.40912500	1.50656200
H	-1.81900300	-1.34578000	-0.89216900

INT3:

C	2.33918300	-0.55752600	-0.66866600
O	-0.13686000	-1.81858500	0.90019200
C	-0.52509800	-0.45957200	0.84742500
C	0.59062800	0.55116000	0.80006500
O	-1.52433800	2.19668700	-0.41237200
C	-2.33267800	1.04162300	-0.23879300
C	-1.54841200	-0.26918900	-0.31406700
C	1.78670900	0.51571200	0.18108000
H	-1.07869000	-0.28724100	1.77959200
H	-2.79366900	1.13350600	0.75016500
H	-3.14670400	0.99745800	-0.97534400
H	-1.17842400	2.18065300	-1.31068900
O	1.80802000	-1.61697700	-0.94344200
H	0.50418600	-1.96714300	0.17832900
H	0.35294900	1.47662200	1.32057700
O	2.69188200	1.54688900	0.23260500
O	-2.48997900	-1.31424600	-0.25946100

H	-1.99213600	-2.08225200	0.05965200
H	-0.98120700	-0.29658600	-1.26451100
H	3.33330700	-0.30344700	-1.08190900
H	2.32859200	2.26504600	0.76169800

INT4:

O	0.43943000	-0.44023500	1.52397600
C	-2.19829500	0.74400100	0.42180200
O	-0.68845900	-2.08877700	-0.37285600
C	0.30316900	-1.14751700	-0.76994200
C	-0.30489100	0.17549800	-1.29834700
O	2.30533200	1.14812100	-0.38694200
C	2.47414700	-0.09362600	0.26456500
C	1.22483400	-0.95841000	0.44781900
C	-0.86978200	1.11303300	-0.24921800
O	-0.38868800	2.18394700	0.05457300
H	-2.57155000	1.53306300	1.10315900
H	0.87767100	-1.58840400	-1.59580700
H	-1.11247500	-0.08954500	-1.99232200
H	3.18512900	-0.65654500	-0.35046500
H	2.92611900	0.02891700	1.26037000
H	1.58496800	-1.96327000	0.71873400
H	1.65407200	1.68326300	0.08595400
H	0.46633900	0.72724100	-1.83452800
O	-2.79065000	-0.29101700	0.23272000
H	-0.24404500	-1.10683900	1.67332900
H	-1.55704500	-1.66207500	-0.38026700

INT5:

O	-0.59001200	0.65062200	0.99922300
C	1.98357000	0.92683100	0.20263300
C	-0.48654500	-0.74130000	-0.93383600
C	0.75165700	-1.19843200	-0.72837500
O	-3.01288400	-0.72173500	0.55691300
C	-2.63361200	0.37130700	-0.24909400
C	-1.10966000	0.49211400	-0.33289400
C	1.80174000	-0.59433000	0.12186100
O	2.64082400	-1.26063000	0.69314200
H	2.53572800	1.22770700	1.11798700
H	-1.14687500	-1.32254900	-1.57182900
H	-3.05620700	0.20673000	-1.24654500
H	-3.04480200	1.32285600	0.12956500
H	-0.83736900	1.36231500	-0.94778900
H	-2.46934600	-0.66631400	1.35309200
H	1.04503200	-2.15173400	-1.15991600
O	1.69575500	1.69660600	-0.67704900
H	-0.73853400	1.56494700	1.26582900

INT6:

O	0.31592400	0.91085400	-0.52356500
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C	-1.09252200	0.83650700	-0.43831400
C	0.48909900	-0.96387800	1.01917400
C	-0.69473900	-1.43460900	0.61268600
O	2.65637900	-0.58036200	-0.94780900
C	2.48728100	0.29843600	0.14127400
C	1.02595100	0.37140500	0.59422100
C	-1.57050200	-0.61176000	-0.23305100
O	-2.60622100	-1.00057900	-0.72680500
H	1.12183400	-1.54265300	1.68760800
H	3.10812700	-0.07756900	0.96098800
H	2.82169800	1.31944600	-0.09779100
H	0.95843800	1.06595200	1.44797400
H	2.01134500	-0.31132500	-1.61262500
O	-1.60021800	1.57883800	0.63745600
H	-1.49318100	2.51472000	0.43307100
H	-1.06322800	-2.41526800	0.89501100
H	-1.45935000	1.20008200	-1.40440200

LGO:

C	1.36622000	-0.04935700	0.00156600
C	0.20815600	-0.97651400	0.42069800
C	0.92121400	1.33693200	-0.27695700
O	-0.65634600	-0.29022600	1.28936300
O	-0.55538500	-1.26998900	-0.75422200
C	-0.36752700	1.65633000	-0.10095000
C	-1.32724900	0.59987900	0.38816300
C	-1.67745600	-0.39010400	-0.75047300
H	-0.75481000	2.64500800	-0.32948400
H	-2.19734100	1.01598000	0.89633400
O	2.50459400	-0.44107800	-0.12106000
H	1.67077600	2.04433100	-0.61551300
H	-2.59192300	-0.94476300	-0.51016600
H	-1.77786100	0.08364300	-1.73066400
H	0.56811100	-1.89685000	0.88455400

References:

- [1] F. Shafizadeh, R. H. Furneaux, T. T. Stevenson, T. G. Cochran. *Carbohydr. Res.* **1978**, 60, 519-28.