

## SUPPORTING INFORMATION - part B

# Synthesis, Conformational Analysis and GalNAc-Lectin Interactions of constrained C-glycoside analogue of T<sub>N</sub> antigen

Juliette Dourdan, Florian Rouzier, Thanh Thao Huynh, Sullivan Bricaud, Arnaud Nourry,\* Stéphane Guillarme\*

*Institut des Molécules et des Matériaux du Mans, UMR 6283 CNRS and Le Mans Université,  
Avenue O. Messiaen, 72085 Le Mans, France.*

### DFT calculation data

A complete conformational search was first undertaken at Molecular Mechanics (MM) level using Spartan Software<sup>1</sup> with MMFF Force Field. The 100 most stable conformers of **1** and **2** were selected for geometry optimization by increasing level of theory from semi-empirical (PM6) to DFT (B3LYP/3-21G). The geometries of the most stable conformers were then optimized by DFT calculations carried out with Gaussian 16<sup>2</sup> at M06-2X/6-311+G(d,p) level.<sup>3</sup> The SMD model<sup>4</sup> was used for the description of water as solvent during the optimization process as well as in the final frequency calculations. For the 20 most stable conformers, the Electronic energy (E), zero-point energy (ZPE), enthalpy (H), Gibbs free energy (G) were calculated at 298 K or 353 K and the Boltzmann distribution was computed from the  $\Delta G$  according to  $\frac{e(-\frac{\Delta G}{RT})}{\sum e(-\frac{\Delta G}{RT})}$ . The results of the 10 most stable conformers are presented in the following tables.

### Summary

- 1) Table of energies (E, Ezpe, H and G) in Hartree and Boltzmann distribution for the conformers of **1** at 298 K
- 2) Table of energies (E, Ezpe, H and G) in Hartree and Boltzmann distribution for the conformers of **2** at 298 K and 353 K.
- 3) Geometries of the conformers of **1**
- 4) Geometries of the conformers of **2**
- 1) Table of energies (E, Ezpe, H and G) in Hartree and Boltzmann distribution for the conformers of **1** at 298 K

<sup>1</sup> Spartan'10, Wavefunction, INC., Irvine, CA.

<sup>2</sup> M.e. Frisch, G. Trucks, H.B. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, G. Petersson, H. Nakatsuji, Gaussian 16, Gaussian, Inc. Wallingford, CT2016.

<sup>3</sup> Zhao, Y., Truhlar, D. G., *Theor.Chem.Acc.* **2007**, *120*, 215–241.

<sup>4</sup> A. V. Marenich, C.J. Cramer, D. G. Truhlar, *J. Phys. Chem.* **2009**, *113(18)*, 6378-6396.

T = 298 K							
1-Conf-x	E	ZPE energy	H	G	$\Delta G$	Boltzmann Distribution	Conformation
1-Conf-2	-1314,133889	-1341,16162	-1314,132945	-1314,221937	0	66,9%	<sup>4</sup> C <sub>1</sub>
1-Conf-8	-1314,135507	-1314,162638	-1314,134563	-1314,220438	0,001499	13,7%	<sup>4</sup> C <sub>1</sub>
1-Conf-20	-1314,133992	-1314,161251	-1314,133048	-1314,220173	0,001764	10,3%	<sup>4</sup> C <sub>1</sub>
1-Conf-1	-1314,132245	-1314,159556	-1314,131301	-1314,219212	0,002725	3,7%	<sup>4</sup> C <sub>1</sub>
1-Conf-5	-1314,132577	-1314,159752	-1314,131633	-1314,218316	0,003621	1,4%	<sup>4</sup> C <sub>1</sub>
1-Conf-6	-1314,129972	-1314,157412	-1314,129028	-1314,218124	0,003813	1,2%	<sup>4</sup> C <sub>1</sub>
1-Conf-12	-1314,131898	-1314,159104	-1314,130954	-1314,217765	0,004172	0,8%	<sup>4</sup> C <sub>1</sub>
1-Conf-9	-1314,132066	-1314,159087	-1314,131121	-1314,217718	0,004219	0,8%	<sup>4</sup> C <sub>1</sub>
1-Conf-7	-1314,132223	-1314,159449	-1314,131279	-1314,217558	0,004379	0,6%	<sup>4</sup> C <sub>1</sub>
1-Conf-10	-1314,13403	-1314,160841	-1314,133086	-1314,217509	0,004428	0,6%	<sup>4</sup> C <sub>1</sub>

100,0%
--------

100,0%	<sup>4</sup> C <sub>1</sub>
0,0%	Twist Boat
0,0%	<sup>1</sup> C <sub>4</sub>

2) Table of energies (E, Ezpe, H and G) in Hartree and Boltzmann distribution for the conformers of **2** at 298 K and 353 K.

T = 298 K							
2-Conf-x	E	ZPE energy	H	G	$\Delta G$	Boltzmann Distribution	Conformation
2-Conf-15	-1352,157303	-1352,184809	-1352,156359	-1352,244302	0	59,1%	Pseudo $^4C_1$
2-Conf-7	-1352,155903	-1352,183312	-1352,154958	-1352,243104	0,001198	16,6%	Pseudo $^4C_1$
2-Conf-9	-1352,157007	-1352,18403	-1352,156062	-1352,241972	0,00233	5,0%	Twist Boat
2-Conf-18	-1352,156611	-1352,183643	-1352,155667	-1352,241948	0,002354	4,9%	Twist Boat
2-Conf-17	-1352,156104	-1352,182998	-1352,155159	-1352,241733	0,002569	3,9%	Pseudo $^1C_4$
2-Conf-3	-1352,157376	-1352,184086	-1352,156432	-1352,24151	0,002792	3,1%	Twist Boat
2-Conf-6	-1352,155749	-1352,182711	-1352,158405	-1352,241249	0,003053	2,3%	Twist Boat
2-Conf-14	-1352,15784	-1352,184568	-1352,156896	-1352,241248	0,003054	2,3%	Pseudo $^1C_4$
2-Conf-11	-1352,157102	-1352,183989	-1352,156158	-1352,24101	0,003292	1,8%	Twist Boat
2-Conf-8	-1352,156503	-1352,183275	-1352,155559	-1352,240541	0,003761	1,1%	Twist Boat
						100,0%	

<b>75,7%</b>	Pseudo $^4C_1$
<b>18,1%</b>	Twist Boat
<b>6,2%</b>	Pseudo $^1C_4$

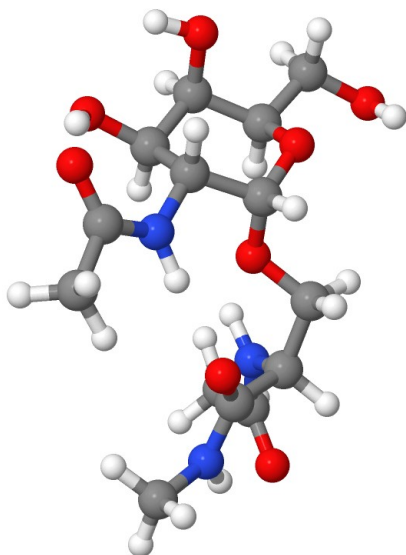
T = 353 K							
2-Conf-x	E	ZPE energy	H	G	$\Delta G$	Boltzmann Distribution	Conformation
2-Conf-15	-1352,147809	-1352,184809	-1352,146691	-1352,2613	0	55,5%	Pseudo $^4C_1$
2-Conf-7	-1352,146435	-1352,183312	-1352,145317	-1352,260137	0,001163	19,6%	Pseudo $^4C_1$
2-Conf-18	-1352,147181	-1352,183643	-1352,146063	-1352,258634	0,002666	5,1%	Twist Boat
2-Conf-9	-1352,147576	-1352,18403	-1352,146458	-1352,258589	0,002711	4,9%	Twist Boat
2-Conf-17	-1352,146704	-1352,182998	-1352,145586	-1352,25847	0,00283	4,4%	Pseudo $^1C_4$
2-Conf-3	-1352,147981	-1352,184086	-1352,146863	-1352,257971	0,003329	2,8%	Twist Boat
2-Conf-6	-1352,146321	-1352,182711	-1352,145204	-1352,257965	0,003335	2,8%	Twist Boat
2-Conf-14	-1352,148458	-1352,184568	-1352,14734	-1352,257575	0,003725	2,0%	Pseudo $^1C_4$
2-Conf-11	-1352,14767	-1352,183989	-1352,146552	-1352,257434	0,003866	1,7%	Twist Boat
2-Conf-8	-1352,147097	-1352,183275	-1352,145979	-1352,256986	0,004314	1,2%	Twist Boat
						100,0%	

<b>75,1%</b>	Pseudo $^4C_1$
<b>18,5%</b>	Twist Boat
<b>6,4%</b>	Pseudo $^1C_4$

### 3) Geometries of the conformers of **1**

The geometries of the conformers of the molecule **1** are given in XYZ format.

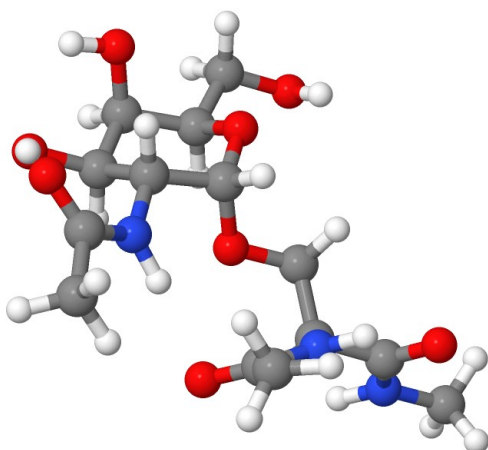
#### a) **1-Conf-1**



```
C 2.61821 -0.47097 -0.92078
C 1.43462 -2.52132 -0.13768
O 0.94880 -1.78730 0.99484
C 1.98832 0.27321 0.26045
H 1.97218 -0.36784 -1.80199
H 0.71484 -2.43258 -0.96253
C 2.76883 -1.95990 -0.60167
H 3.07550 -2.48733 -1.51556
H 2.69495 0.26362 1.09750
C 0.71430 -0.42403 0.74208
H 0.37736 -0.00267 1.69618
C 1.50459 -3.97122 0.29750
H 1.91536 -4.57362 -0.51657
H 2.15234 -4.07081 1.17578
O 0.20744 -4.48505 0.57720
H -0.15976 -3.97841 1.32025
O 3.73411 -2.15208 0.42214
H 4.50585 -1.60831 0.18353
O 3.90935 0.04514 -1.22543
H 4.08586 0.83170 -0.66938
N 1.67912 1.66047 -0.05367
H 0.73763 1.88606 -0.37910
C 2.58811 2.64359 0.04321
O 3.78083 2.40527 0.32578
C 2.10804 4.04793 -0.18808
H 1.08538 4.08470 -0.56794
H 2.15737 4.58688 0.76370
H 2.78386 4.54079 -0.89134
O -0.26637 -0.23410 -0.24358
```

C	-1.55364	-0.72823	0.10177
H	-1.73967	-1.66760	-0.43129
H	-1.61554	-0.91388	1.18092
C	-2.58973	0.32754	-0.29584
H	-2.47307	0.56771	-1.35613
C	-3.98343	-0.22558	-0.01725
O	-4.47953	-0.12949	1.11649
N	-4.59711	-0.83624	-1.03071
H	-4.14038	-0.86879	-1.93516
C	-5.89163	-1.47750	-0.86101
H	-5.83551	-2.25614	-0.09588
H	-6.64619	-0.74423	-0.56497
H	-6.17864	-1.92577	-1.81087
N	-2.41928	1.54167	0.47785
H	-2.87001	1.57099	1.38787
C	-1.66062	2.57925	0.08751
O	-1.06835	2.59672	-1.00766
C	-1.53463	3.72303	1.05648
H	-1.67180	4.66227	0.51528
H	-0.51759	3.71357	1.46418
H	-2.24773	3.66069	1.88071

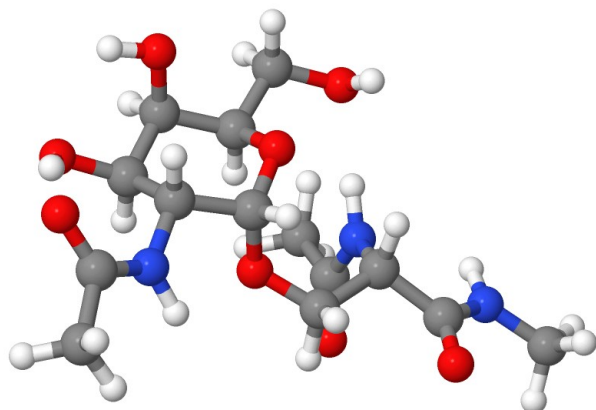
**b) 1-Conf-2**



C	2.61821	-0.47097	-0.92078
C	1.43462	-2.52132	-0.13768
O	0.94880	-1.78730	0.99484
C	1.98832	0.27321	0.26045
H	1.97218	-0.36784	-1.80199
H	0.71484	-2.43258	-0.96253
C	2.76883	-1.95990	-0.60167
H	3.07550	-2.48733	-1.51556
H	2.69495	0.26362	1.09750
C	0.71430	-0.42403	0.74208
H	0.37736	-0.00267	1.69618
C	1.50459	-3.97122	0.29750
H	1.91536	-4.57362	-0.51657
H	2.15234	-4.07081	1.17578

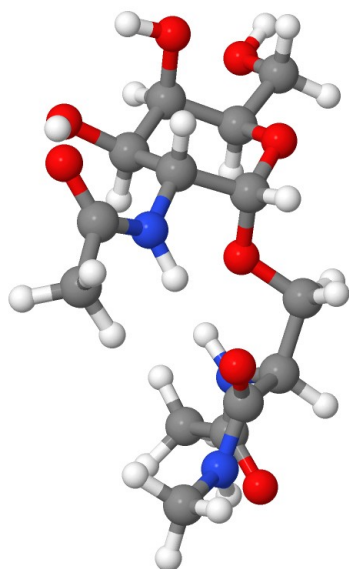
O	0.20744	-4.48505	0.57720
H	-0.15976	-3.97841	1.32025
O	3.73411	-2.15208	0.42214
H	4.50585	-1.60831	0.18353
O	3.90935	0.04514	-1.22543
H	4.08586	0.83170	-0.66938
N	1.67912	1.66047	-0.05367
H	0.73763	1.88606	-0.37910
C	2.58811	2.64359	0.04321
O	3.78083	2.40527	0.32578
C	2.10804	4.04793	-0.18808
H	1.08538	4.08470	-0.56794
H	2.15737	4.58688	0.76370
H	2.78386	4.54079	-0.89134
O	-0.26637	-0.23410	-0.24358
C	-1.55364	-0.72823	0.10177
H	-1.73967	-1.66760	-0.43129
H	-1.61554	-0.91388	1.18092
C	-2.58973	0.32754	-0.29584
H	-2.47307	0.56771	-1.35613
C	-3.98343	-0.22558	-0.01725
O	-4.47953	-0.12949	1.11649
N	-4.59711	-0.83624	-1.03071
H	-4.14038	-0.86879	-1.93516
C	-5.89163	-1.47750	-0.86101
H	-5.83551	-2.25614	-0.09588
H	-6.64619	-0.74423	-0.56497
H	-6.17864	-1.92577	-1.81087
N	-2.41928	1.54167	0.47785
H	-2.87001	1.57099	1.38787
C	-1.66062	2.57925	0.08751
O	-1.06835	2.59672	-1.00766
C	-1.53463	3.72303	1.05648
H	-1.67180	4.66227	0.51528
H	-0.51759	3.71357	1.46418
H	-2.24773	3.66069	1.88071

c) **1-Conf-5**



C	2.66369	0.75780	0.67137
C	0.65372	1.96072	-0.18364
O	0.46649	0.93054	-1.16051
C	2.36741	-0.33550	-0.35888
H	2.17382	0.50744	1.62129
H	0.10315	1.69791	0.73037
C	2.12208	2.10321	0.18378
H	2.21104	2.83580	0.99807
H	2.93993	-0.12380	-1.26883
C	0.88503	-0.34874	-0.74831
H	0.72817	-1.00379	-1.61252
C	0.06573	3.22761	-0.77674
H	0.13200	4.03050	-0.03768
H	0.61769	3.52280	-1.67422
O	-1.31530	3.05588	-1.09032
H	-1.37581	2.60820	-1.94999
O	2.84801	2.54478	-0.95397
H	3.79206	2.43441	-0.74251
O	4.06207	0.90457	0.88859
H	4.54254	0.19811	0.40837
N	2.72907	-1.66745	0.10469
H	1.98618	-2.25316	0.47444
C	3.97659	-2.15767	0.03418
O	4.93308	-1.45151	-0.34585
C	4.17402	-3.59434	0.42269
H	4.47427	-4.15170	-0.47007
H	4.98825	-3.65482	1.14897
H	3.27189	-4.04440	0.84067
O	0.15168	-0.81943	0.35373
C	-1.03361	-1.53968	0.03715
H	-1.34469	-2.01782	0.96589
H	-0.80749	-2.31210	-0.70440
C	-2.14862	-0.62952	-0.50739
H	-1.88097	-0.32060	-1.52447
C	-3.44110	-1.43600	-0.64345
O	-3.39161	-2.65499	-0.87728
N	-4.59268	-0.76571	-0.56736
H	-4.57057	0.21411	-0.31067
C	-5.87160	-1.44165	-0.71053
H	-5.94468	-1.91737	-1.69178
H	-6.66407	-0.70107	-0.61152
H	-5.99440	-2.20632	0.06175
N	-2.31390	0.59513	0.25117
H	-1.99381	1.46280	-0.18143
C	-2.56938	0.60390	1.57593
O	-2.86258	-0.43159	2.19411
C	-2.48932	1.93955	2.26528
H	-1.67250	1.90082	2.99290
H	-3.42045	2.11344	2.81125
H	-2.31169	2.76270	1.56995

d) 1-Conf-6

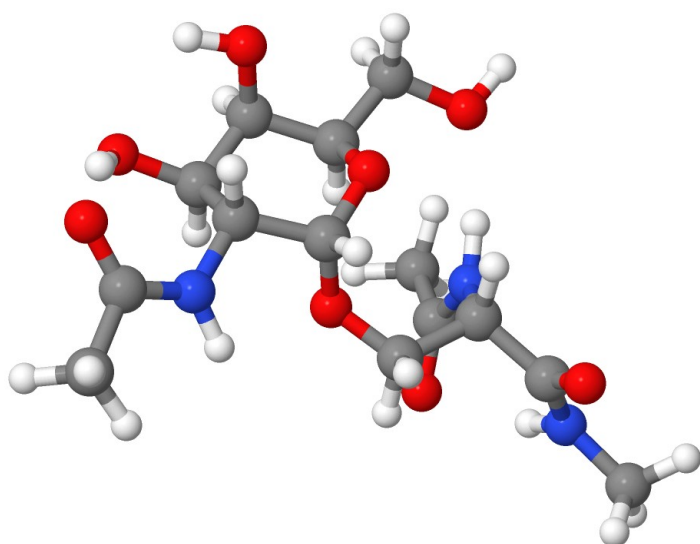


C	-2.14709	0.50348	1.00125
C	-2.51746	-1.59711	-0.31819
O	-2.05972	-0.91903	-1.49280
C	-1.62371	1.14660	-0.28558
H	-1.30695	0.07112	1.56004
H	-1.66979	-2.08986	0.17629
C	-3.13818	-0.61423	0.66498
H	-3.38389	-1.14975	1.59148
H	-2.45152	1.66171	-0.78609
C	-1.09504	0.07334	-1.23990
H	-0.86036	0.51259	-2.21567
C	-3.49177	-2.65128	-0.81490
H	-4.32113	-2.17026	-1.34526
H	-2.96727	-3.31791	-1.50898
O	-3.96316	-3.36919	0.31818
H	-4.59832	-4.03619	0.01438
O	-4.31583	-0.06834	0.08860
H	-4.56276	0.69784	0.63653
O	-2.83229	1.44197	1.82208
H	-2.65121	2.34900	1.49384
N	-0.54267	2.10249	-0.07009
H	0.39963	1.81551	-0.34458
C	-0.74964	3.36695	0.32109
O	-1.88078	3.77153	0.66689
C	0.43874	4.28528	0.33118
H	0.53634	4.72393	1.32774
H	1.36515	3.77458	0.06133
H	0.25270	5.09701	-0.37853
O	0.06192	-0.45394	-0.65379
C	0.97520	-1.07683	-1.54979
H	0.98607	-0.54833	-2.50853
H	0.69193	-2.12202	-1.71503
C	2.34684	-1.00750	-0.90951



H	3.05628	-1.55071	-1.54373
C	2.83827	0.44787	-0.80205
O	2.16964	1.40299	-1.23215
N	4.03597	0.61281	-0.23741
H	4.55510	-0.21201	0.05363
C	4.61793	1.93451	-0.06789
H	3.96511	2.56542	0.54142
H	4.76943	2.41774	-1.03703
H	5.57888	1.82425	0.43267
N	2.30938	-1.66748	0.38869
H	1.42959	-1.65287	0.89573
C	3.37141	-2.28504	0.93698
O	4.48707	-2.27187	0.38586
C	3.15221	-2.98632	2.24765
H	3.84720	-2.57310	2.98373
H	2.12953	-2.88800	2.61555
H	3.39061	-4.04567	2.11585

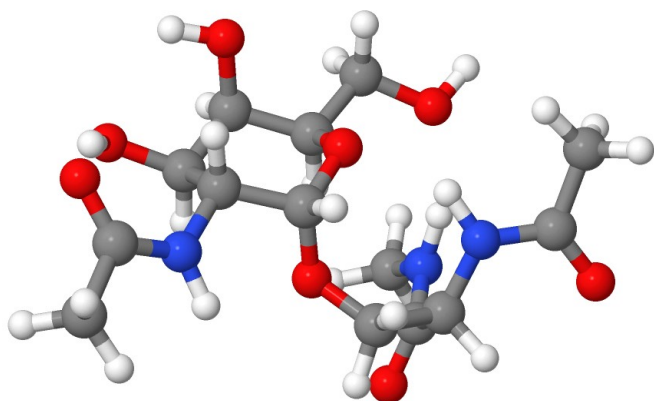
e) **1-Conf-7**



C	2.64114	0.67222	0.68753
C	0.71917	1.97029	-0.22752
O	0.49995	0.93833	-1.19633
C	2.31643	-0.41469	-0.34039
H	2.11380	0.45770	1.62614
H	0.13449	1.75129	0.67669
C	2.18388	2.03846	0.17369
H	2.29193	2.77326	0.98345
H	2.92119	-0.23967	-1.23710
C	0.84636	-0.35661	-0.76954
H	0.68030	-1.00629	-1.63596
C	0.22331	3.26071	-0.84158
H	0.43488	4.08559	-0.15109
H	0.73469	3.44671	-1.79198
O	-1.18026	3.13182	-1.05678
H	-1.51344	3.94590	-1.46564

O	2.95690	2.43103	-0.95045
H	3.88948	2.27930	-0.71550
O	4.03882	0.74787	0.94277
H	4.49632	0.02213	0.46929
N	2.60149	-1.75791	0.14278
H	1.82482	-2.30018	0.50950
C	3.82521	-2.30837	0.10460
O	4.82177	-1.65523	-0.26694
C	3.94654	-3.74489	0.52339
H	3.00383	-4.15781	0.88597
H	4.70724	-3.82045	1.30467
H	4.28830	-4.32573	-0.33861
O	0.06082	-0.79138	0.31322
C	-1.16145	-1.42438	-0.03782
H	-1.52268	-1.89605	0.87589
H	-0.97997	-2.19799	-0.79355
C	-2.20271	-0.43681	-0.59758
H	-1.85105	-0.08265	-1.56892
C	-3.48313	-1.21637	-0.90299
O	-3.57878	-1.81367	-1.98906
N	-4.44060	-1.25132	0.02553
H	-4.24098	-0.86096	0.94260
C	-5.65596	-2.02315	-0.17824
H	-6.18155	-1.67448	-1.07046
H	-5.42851	-3.08650	-0.29747
H	-6.29823	-1.88776	0.69076
N	-2.36075	0.76024	0.21744
H	-2.07318	1.63014	-0.23242
C	-2.50280	0.78498	1.55599
O	-2.77603	-0.23467	2.21542
C	-2.34170	2.12121	2.22976
H	-3.24922	2.33937	2.79951
H	-1.50959	2.04711	2.93688
H	-2.14525	2.93268	1.52654

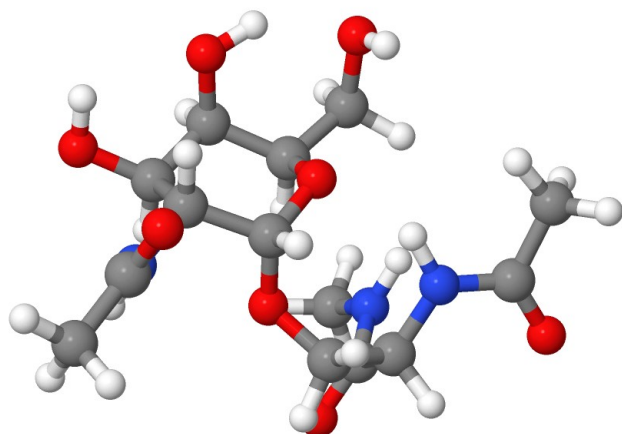
f) **1-Conf-8**



C	2.31502	0.96336	0.78680
C	-0.00860	1.65342	0.19881

O	0.04166	0.78875	-0.94748
C	2.27785	0.02689	-0.42246
H	1.97914	0.42219	1.68083
H	-0.39949	1.09168	1.05812
C	1.38121	2.15272	0.55843
H	1.31348	2.73188	1.48953
H	2.69666	0.55419	-1.28661
C	0.84140	-0.36101	-0.78588
H	0.82204	-0.86857	-1.75582
C	-0.96083	2.77899	-0.13766
H	-0.64980	3.27008	-1.06575
H	-0.94475	3.51066	0.67906
O	-2.26360	2.22013	-0.28950
H	-2.86660	2.90844	-0.61243
O	1.86563	2.97143	-0.49501
H	2.81305	3.11821	-0.32570
O	3.62438	1.47071	1.01471
H	4.25033	1.05870	0.38424
N	3.04734	-1.19136	-0.22080
H	2.54455	-2.02441	0.07091
C	4.37344	-1.26007	-0.42136
O	5.04113	-0.24524	-0.70703
C	5.02175	-2.60782	-0.29049
H	5.84353	-2.53346	0.42638
H	4.32246	-3.38162	0.03011
H	5.44424	-2.88104	-1.26208
O	0.35348	-1.21523	0.21737
C	-0.58705	-2.21431	-0.17634
H	-0.39212	-2.53111	-1.20663
H	-0.42270	-3.06008	0.49316
C	-2.04161	-1.76576	-0.04084
H	-2.66210	-2.65653	-0.18128
C	-2.28115	-1.28951	1.39526
O	-2.08435	-2.07649	2.33741
N	-2.67983	-0.03024	1.57342
H	-2.70322	0.60380	0.77605
C	-2.76065	0.54932	2.90372
H	-3.52889	0.04763	3.49771
H	-3.02024	1.60319	2.80165
H	-1.80141	0.46135	3.42358
N	-2.41027	-0.79845	-1.05220
H	-1.74342	-0.05731	-1.27042
C	-3.68348	-0.66144	-1.48119
O	-4.59009	-1.42052	-1.10397
C	-3.95044	0.46445	-2.44284
H	-4.53976	0.07998	-3.27915
H	-3.03452	0.92552	-2.81705
H	-4.54822	1.22317	-1.92712

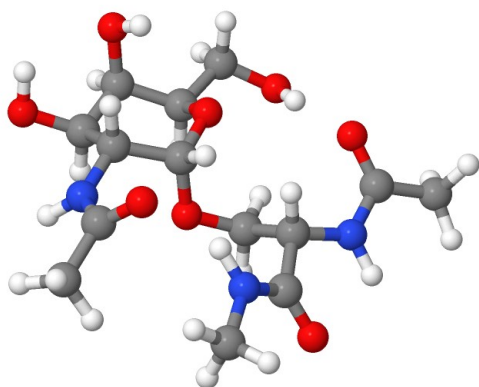
g) 1-Conf-9



C	2.15911	1.02289	1.17208
C	-0.11315	1.60474	0.31606
O	0.13957	0.83297	-0.86784
C	2.33780	0.16636	-0.08507
H	1.74766	0.41369	1.98423
H	-0.55682	0.96005	1.08765
C	1.19176	2.16709	0.87432
H	0.96604	2.69548	1.81074
H	2.81940	0.77407	-0.85674
C	0.98183	-0.28447	-0.65047
H	1.11520	-0.74629	-1.63416
C	-1.14357	2.66085	-0.04360
H	-2.06512	2.17680	-0.39010
H	-1.37258	3.24654	0.85053
O	-0.67345	3.58114	-1.02729
H	-0.63577	3.12301	-1.88363
O	1.85322	3.03937	-0.03474
H	1.17143	3.56700	-0.49384
O	3.40117	1.51843	1.64002
H	3.73714	2.14886	0.97891
N	3.18991	-0.97352	0.17749
H	3.10193	-1.43701	1.07582
C	3.97286	-1.53262	-0.76521
O	4.05391	-1.06714	-1.91454
C	4.76213	-2.74764	-0.35844
H	4.58232	-3.04550	0.67621
H	5.82568	-2.53141	-0.49434
H	4.49819	-3.57310	-1.02530
O	0.40806	-1.20098	0.24381
C	-0.47593	-2.17749	-0.30373
H	-0.30579	-3.09619	0.25993
H	-0.23754	-2.35668	-1.35761
C	-1.94968	-1.79366	-0.16990
H	-2.53811	-2.67723	-0.44075
C	-2.25650	-1.50715	1.30398
O	-2.00192	-2.37336	2.15696
N	-2.78929	-0.32469	1.61517

H	-2.90577	0.36535	0.88178
C	-2.99079	0.07544	2.99815
H	-3.68835	-0.60340	3.49500
H	-2.04177	0.06760	3.54287
H	-3.40392	1.08335	3.00719
N	-2.30327	-0.71683	-1.06970
H	-1.58984	-0.01763	-1.27552
C	-3.55026	-0.54274	-1.55570
O	-4.47735	-1.31950	-1.27934
C	-3.76137	0.65808	-2.43820
H	-2.82930	1.17155	-2.68597
H	-4.42761	1.35388	-1.91842
H	-4.25911	0.33696	-3.35690

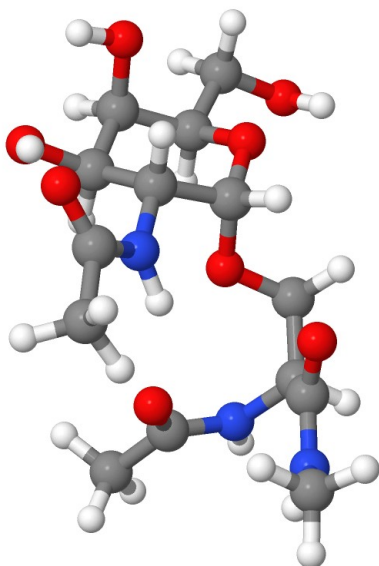
**h) 1-Conf-10**



C	3.05427	-0.57707	-0.66096
C	1.25948	-2.27568	-0.41360
O	0.64219	-1.43824	0.57328
C	2.26608	0.34137	0.28317
H	2.76399	-0.36421	-1.69608
H	0.89296	-2.00427	-1.41298
C	2.76362	-2.05310	-0.37343
H	3.24957	-2.66075	-1.14249
H	2.65879	0.22347	1.30250
C	0.78129	-0.05789	0.34653
H	0.30655	0.41152	1.20908
C	0.81224	-3.68683	-0.09213
H	1.32270	-4.39017	-0.75530
H	1.06820	-3.93104	0.94628
O	-0.58258	-3.84345	-0.31409
H	-1.07588	-3.19326	0.22504
O	3.33967	-2.44693	0.86620
H	2.77604	-2.12962	1.59385
O	4.44258	-0.30991	-0.57319
H	4.75178	-0.66650	0.27907
N	2.45534	1.71749	-0.14557
H	2.99681	1.87761	-0.98880
C	1.87756	2.77366	0.44783
O	1.17732	2.65007	1.47057

C	2.08168	4.11170	-0.20799
H	2.20552	4.87392	0.56406
H	2.93982	4.12056	-0.88319
H	1.17973	4.34948	-0.78324
O	0.16577	0.35187	-0.85448
C	-1.16552	-0.10686	-1.03528
H	-1.19817	-1.20121	-1.02585
H	-1.47046	0.24508	-2.02439
C	-2.15893	0.40915	0.02752
H	-1.75369	0.25822	1.03213
C	-2.46314	1.88366	-0.20041
O	-3.44771	2.22711	-0.87625
N	-1.60430	2.75646	0.32658
H	-0.78449	2.42584	0.83247
C	-1.72157	4.18431	0.07601
H	-0.92968	4.69192	0.62666
H	-1.62061	4.40367	-0.99097
H	-2.69068	4.55294	0.42162
N	-3.39303	-0.34014	-0.08529
H	-4.16684	0.10082	-0.57369
C	-3.50365	-1.59956	0.36838
O	-2.55999	-2.17033	0.94801
C	-4.82175	-2.28870	0.15423
H	-5.21661	-2.59566	1.12670
H	-5.55148	-1.65481	-0.35271
H	-4.64789	-3.19083	-0.43931

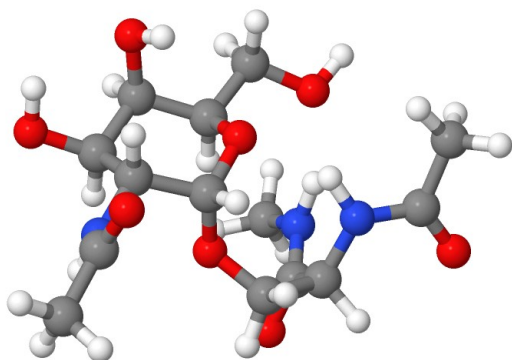
i) **1-Conf-12**



C	-2.06688	1.10505	0.83003
C	-2.91348	-1.15336	0.18497
O	-2.16446	-1.07046	-1.03452
C	-1.22839	1.09242	-0.45050
H	-1.46947	0.70426	1.65949
H	-2.29239	-1.62240	0.95992

C	-3.31345	0.23385	0.66398
H	-3.81159	0.13940	1.63893
H	-1.78265	1.60917	-1.24140
C	-0.96706	-0.33684	-0.93043
H	-0.53973	-0.33184	-1.93848
C	-4.09970	-2.05134	-0.10468
H	-4.73232	-2.11139	0.78450
H	-4.68900	-1.64176	-0.93278
O	-3.68156	-3.37795	-0.40387
H	-3.16120	-3.34863	-1.22336
O	-4.19877	0.81358	-0.28352
H	-4.26513	1.75930	-0.06115
O	-2.49489	2.42393	1.15291
H	-2.05242	3.06369	0.55744
N	0.05736	1.75360	-0.28324
H	0.85441	1.17303	-0.01236
C	0.21337	3.08066	-0.38198
O	-0.75861	3.84487	-0.56609
C	1.61162	3.61608	-0.26101
H	2.35562	2.82564	-0.14568
H	1.83639	4.19966	-1.15838
H	1.65582	4.29004	0.59940
O	-0.07030	-0.91459	-0.02433
C	0.55171	-2.11434	-0.46611
H	0.39983	-2.25558	-1.54125
H	0.10992	-2.96395	0.06544
C	2.04280	-2.05645	-0.16636
H	2.45615	-3.04124	-0.41208
C	2.77552	-1.04149	-1.05386
O	2.19199	-0.44254	-1.96715
N	4.08989	-0.91233	-0.83453
H	4.48623	-1.34530	-0.00789
C	4.86026	0.11218	-1.52028
H	4.85031	-0.06046	-2.59892
H	5.88791	0.06786	-1.16190
H	4.44879	1.10681	-1.31762
N	2.32168	-1.83436	1.24688
H	2.42161	-2.65562	1.83263
C	2.38662	-0.62417	1.83965
O	2.26883	0.43713	1.20626
C	2.63572	-0.61956	3.32340
H	2.76860	-1.62140	3.73531
H	1.78514	-0.13617	3.81279
H	3.52704	-0.01939	3.52530

j) **1-Conf-20**

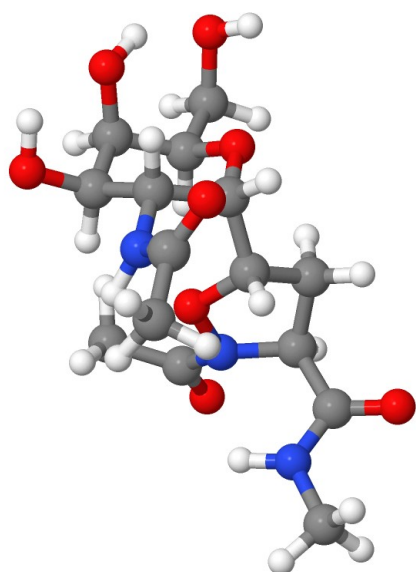


C	2.29364	1.34154	0.84756
C	-0.02763	1.74976	0.00176
O	0.17594	0.72343	-0.98396
C	2.40172	0.20881	-0.17787
H	1.93881	0.94037	1.80364
H	-0.44567	1.29898	0.91152
C	1.30084	2.40324	0.36028
H	1.13937	3.12561	1.16587
H	2.84979	0.60219	-1.09671
C	1.01338	-0.33372	-0.55086
H	1.08963	-1.01488	-1.40512
C	-1.02333	2.73079	-0.57602
H	-1.12750	3.57703	0.11368
H	-0.67099	3.10007	-1.54536
O	-2.26444	2.04813	-0.73243
H	-2.88621	2.62428	-1.20414
O	1.85494	3.14378	-0.72184
H	1.78525	2.62330	-1.54119
O	3.55670	1.92855	1.10168
H	3.79258	2.45509	0.31652
N	3.25811	-0.85155	0.30636
H	3.19693	-1.10057	1.28826
C	3.99563	-1.62931	-0.50984
O	4.04046	-1.44209	-1.73721
C	4.78059	-2.73528	0.14185
H	5.84199	-2.58109	-0.07255
H	4.63147	-2.78014	1.22210
H	4.48060	-3.68626	-0.30696
O	0.47956	-1.00185	0.56119
C	-0.36038	-2.12673	0.30943
H	-0.20112	-2.81467	1.14157
H	-0.06303	-2.62052	-0.62198
C	-1.84637	-1.77466	0.25318
H	-2.39569	-2.72126	0.22934
C	-2.24018	-1.07556	1.55782
O	-2.09517	-1.67630	2.63697
N	-2.70942	0.16906	1.47725
H	-2.69362	0.65191	0.57962
C	-2.93315	0.96621	2.67157



H	-2.02096	1.02629	3.27361
H	-3.72896	0.53305	3.28303
H	-3.22726	1.96933	2.36213
N	-2.18180	-1.02800	-0.94033
H	-1.53951	-0.29486	-1.24326
C	-3.42457	-1.04845	-1.46831
O	-4.31805	-1.78171	-1.01596
C	-3.67498	-0.13458	-2.63710
H	-4.18068	-0.70091	-3.42328
H	-2.75784	0.30687	-3.03093
H	-4.34646	0.66633	-2.31061

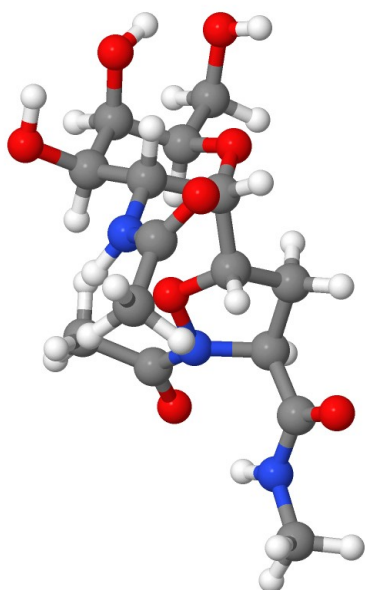
4) Geometries of the conformers of **2**  
a) **2-Conf-15**



C	-2.87674	-0.87104	0.64459
H	-3.04281	-1.57293	1.47035
C	-1.74300	1.29205	0.04514
C	-0.97279	0.53305	-1.06405
H	-0.96995	1.16439	-1.95520
O	-1.67687	-0.63679	-1.44787
C	-1.96858	-1.54129	-0.38386
H	-1.04591	-1.84474	0.12609
C	-2.55912	-2.79098	-1.01114
H	-2.78070	-3.51079	-0.22218
H	-1.82682	-3.22955	-1.69400
H	-2.63639	1.71144	-0.42406
C	-2.20720	0.38574	1.19320
H	-1.35565	0.08913	1.80706
C	0.50295	0.28902	-0.74641
H	1.03487	1.24149	-0.83972
N	-0.95870	2.39354	0.57553
H	-0.40196	2.22350	1.40436
C	-0.77787	3.54686	-0.09450

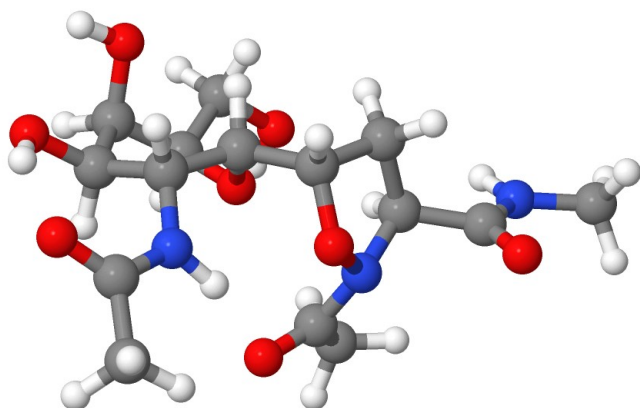
O	-1.34211	3.77342	-1.17103
C	0.14134	4.55617	0.53469
H	0.97220	4.73535	-0.15036
H	0.52884	4.23318	1.49982
H	-0.40452	5.49343	0.65341
O	-3.78517	-2.54142	-1.69859
H	-3.58394	-2.05876	-2.50943
O	-4.12402	-0.46288	0.09161
H	-4.40029	-1.13887	-0.54608
O	-3.09018	1.08627	2.05445
H	-3.90850	1.24544	1.56506
O	0.65918	-0.16133	0.62067
N	1.77502	-1.02148	0.64873
C	1.78606	-1.97368	1.62231
O	2.64831	-2.85032	1.60299
C	0.75362	-1.83729	2.70021
H	0.94375	-2.59100	3.46056
H	-0.24310	-1.97686	2.27453
H	0.78966	-0.83935	3.14029
C	1.18490	-0.77974	-1.58699
H	1.51871	-0.39773	-2.54925
H	0.52596	-1.63487	-1.73735
C	2.34829	-1.18677	-0.68093
H	2.63362	-2.23084	-0.81678
C	3.60161	-0.34653	-0.91693
O	4.09302	-0.30396	-2.04923
N	4.12641	0.28566	0.13066
H	3.67646	0.19056	1.03058
C	5.34568	1.06831	0.00570
H	5.57938	1.49924	0.97575
H	5.21079	1.87058	-0.72073
H	6.17497	0.43730	-0.31734

b) **2-Conf-7**



C	-2.87666	-1.07217	0.65692
H	-2.98592	-1.80094	1.46859
C	-1.90916	1.17645	0.09169
C	-1.09657	0.49884	-1.04064
H	-1.15031	1.14563	-1.91881
O	-1.71426	-0.71403	-1.44133
C	-1.93619	-1.65855	-0.39378
H	-0.99070	-1.90942	0.10238
C	-2.44839	-2.93158	-1.04268
H	-2.60273	-3.68402	-0.26827
H	-1.69918	-3.30011	-1.74828
H	-2.83761	1.53583	-0.35936
C	-2.28682	0.21450	1.22546
H	-1.40475	-0.03608	1.81710
C	0.39421	0.36127	-0.73922
H	0.85051	1.35625	-0.77640
N	-1.20422	2.32174	0.64042
H	-0.65308	2.18262	1.47871
C	-1.08570	3.48843	-0.01980
O	-1.64809	3.68660	-1.10295
C	-0.23216	4.54395	0.62580
H	0.63638	4.71719	-0.01311
H	0.10284	4.26356	1.62331
H	-0.80420	5.47124	0.67542
O	-3.70230	-2.75703	-1.70278
H	-3.55482	-2.23135	-2.49828
O	-4.15459	-0.73582	0.12666
H	-4.40270	-1.42666	-0.50644
O	-3.20000	0.83124	2.11850
H	-4.03727	0.94156	1.64825
O	0.57933	-0.16068	0.59359
N	1.82936	-0.80225	0.59487
C	2.08734	-1.64694	1.61902
O	3.11609	-2.32974	1.59123
C	1.10119	-1.65558	2.74628
H	1.46340	-2.32480	3.52295
H	0.12948	-1.99511	2.37812
H	0.97226	-0.64859	3.14692
C	1.16364	-0.60251	-1.62979
H	1.44953	-0.14805	-2.57542
H	0.57996	-1.50488	-1.81185
C	2.36898	-0.94229	-0.76290
H	2.70255	-1.97318	-0.89423
C	3.57537	-0.01502	-0.96319
O	3.58833	0.87277	-1.81784
N	4.60502	-0.26198	-0.15036
H	4.51202	-1.00577	0.53285
C	5.81632	0.54113	-0.19520
H	5.59397	1.58729	0.02116
H	6.28179	0.47785	-1.17981
H	6.50901	0.16118	0.55147

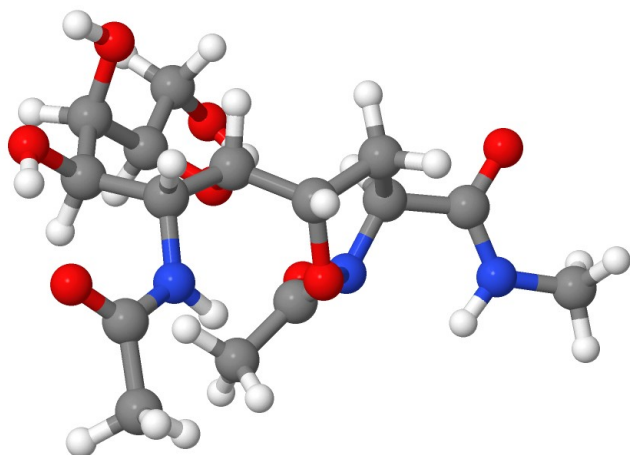
c) 2-Conf-18



C	2.36987	2.23550	0.28735
H	2.94291	2.81663	1.01632
C	2.17788	-0.09792	-0.74963
C	0.75317	0.44643	-0.88700
H	0.80650	1.29483	-1.57687
O	0.30058	0.89262	0.38562
C	0.93536	2.10521	0.81084
H	0.98792	2.02890	1.90085
C	0.06795	3.29657	0.44261
H	-0.11830	3.30865	-0.63265
H	0.58411	4.22218	0.71751
H	2.64128	-0.10683	-1.74014
C	2.99945	0.85400	0.16662
H	3.02021	0.41599	1.17171
C	-0.29658	-0.47328	-1.49655
H	0.06844	-0.84215	-2.45505
N	2.19024	-1.45959	-0.22288
H	1.35438	-1.81323	0.23622
C	3.31929	-2.17049	-0.14174
O	4.40722	-1.72851	-0.55501
C	3.21839	-3.54239	0.45988
H	3.91579	-3.60641	1.29669
H	3.52578	-4.27200	-0.29165
H	2.21041	-3.77390	0.80196
O	-1.20679	3.21834	1.06961
H	-1.07655	3.23323	2.02544
O	2.38490	2.91337	-0.96613
H	3.29748	2.90530	-1.28139
O	4.31994	1.04071	-0.31759
H	4.66013	0.15179	-0.51696
O	-0.58677	-1.64848	-0.71781
N	-1.52377	-1.25546	0.24843
C	-1.07232	-1.32563	1.53716
O	-0.03621	-1.92039	1.81583
C	-1.94737	-0.67557	2.56678
H	-1.73704	-1.12449	3.53520
H	-3.00772	-0.77121	2.33236

H	-1.69393	0.38937	2.60465
C	-1.66249	0.20448	-1.60773
H	-2.21360	-0.21976	-2.44689
H	-1.58671	1.28403	-1.72813
C	-2.34873	-0.16080	-0.27304
H	-2.31553	0.68242	0.41518
C	-3.78530	-0.60841	-0.51323
O	-4.05142	-1.74076	-0.92159
N	-4.71219	0.32921	-0.30672
H	-4.42725	1.22734	0.05986
C	-6.11838	0.07818	-0.58096
H	-6.26152	-0.18469	-1.62989
H	-6.67931	0.98214	-0.35809
H	-6.49052	-0.73772	0.04030

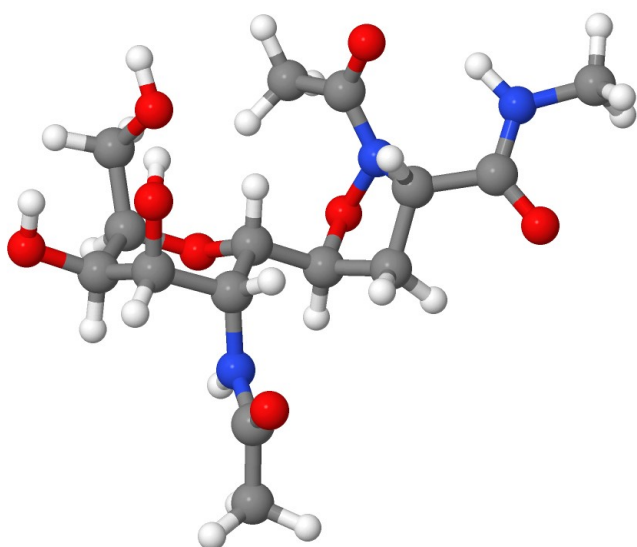
d) **2-Conf-9**



C	2.58545	2.02902	0.08694
H	3.24335	2.61155	0.73986
C	2.17263	-0.34155	-0.77422
C	0.78751	0.29734	-0.91811
H	0.86522	1.05523	-1.70250
O	0.39451	0.89966	0.30718
C	1.20477	2.00636	0.73219
H	1.35464	1.85859	1.80644
C	0.41346	3.28168	0.52319
H	0.09657	3.35022	-0.52285
H	1.02886	4.15044	0.76368
H	2.58043	-0.48311	-1.77956
C	3.12610	0.60836	0.00184
H	3.21352	0.23420	1.02909
C	-0.31881	-0.66352	-1.34846
H	0.07398	-1.35001	-2.09862
N	2.09197	-1.64936	-0.12783
H	1.22110	-1.93772	0.30177
C	3.16740	-2.43830	-0.00504
O	4.27752	-2.09665	-0.44644
C	2.97573	-3.76159	0.67767

H	1.96213	-3.89790	1.05272
H	3.68654	-3.83237	1.50232
H	3.20846	-4.55320	-0.03709
O	-0.71550	3.31969	1.39038
H	-1.19059	2.48165	1.30877
O	2.52894	2.64484	-1.19509
H	3.41557	2.59766	-1.57459
O	4.40453	0.68277	-0.60604
H	4.69235	-0.23761	-0.72490
O	-0.77767	-1.49672	-0.25995
N	-1.79263	-0.77062	0.39719
C	-1.53946	-0.40486	1.69959
O	-2.21119	0.48749	2.20432
C	-0.50486	-1.18471	2.45003
H	0.47250	-0.74133	2.24223
H	-0.48376	-2.23053	2.14597
H	-0.71525	-1.10117	3.51455
C	-1.59666	0.02048	-1.82314
H	-2.12207	-0.63337	-2.51993
H	-1.40686	0.97860	-2.30213
C	-2.40752	0.18397	-0.52661
H	-2.30169	1.19192	-0.12257
C	-3.89061	-0.03848	-0.76637
O	-4.49364	0.74000	-1.51430
N	-4.47311	-1.07387	-0.16710
H	-3.91603	-1.65297	0.44594
C	-5.88837	-1.35412	-0.35025
H	-6.49347	-0.51490	-0.00423
H	-6.14110	-2.23997	0.22662
H	-6.10851	-1.53603	-1.40290

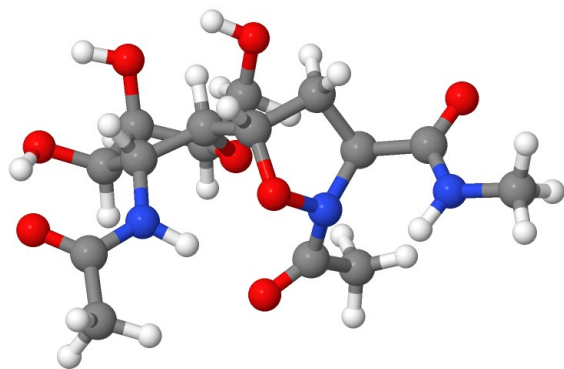
e) **2-Conf-17**



C	3.43612	-0.82501	0.03291
H	3.95922	-0.13715	-0.63582
C	1.57922	0.82961	0.40504

C	0.68648	-0.10119	-0.41139
H	0.21029	-0.80069	0.28461
O	1.45233	-0.82338	-1.37870
C	2.49727	-1.65875	-0.86738
H	3.08132	-1.93348	-1.74949
C	2.00201	-2.98752	-0.32166
H	2.87418	-3.60466	-0.08936
H	1.42963	-3.48509	-1.10935
H	0.99281	1.28492	1.20336
C	2.71760	0.03528	1.07342
H	3.43739	0.75079	1.47822
C	-0.38857	0.63442	-1.20463
H	0.05220	1.12816	-2.06982
N	2.10775	1.89118	-0.43566
H	2.33538	1.68001	-1.39956
C	2.40018	3.11517	0.04468
O	2.20150	3.41918	1.22589
C	2.97701	4.09974	-0.93323
H	2.33489	4.98175	-0.95443
H	3.06982	3.68965	-1.93778
H	3.95982	4.40737	-0.57174
O	1.18791	-2.82475	0.84082
H	1.00503	-3.69412	1.21556
O	4.43303	-1.63273	0.63111
H	4.05059	-2.05301	1.41311
O	2.25191	-0.71702	2.17999
H	1.77665	-1.50892	1.86316
O	-1.33202	-0.31372	-1.74758
N	-2.20761	-0.59683	-0.68954
C	-2.23477	-1.88009	-0.22042
O	-2.83535	-2.11466	0.82777
C	-1.59779	-2.93134	-1.07343
H	-2.16447	-3.03448	-2.00192
H	-1.60620	-3.87342	-0.52982
H	-0.58019	-2.64390	-1.33670
C	-1.29597	1.55152	-0.39249
H	-1.80303	2.23332	-1.07371
H	-0.78461	2.13361	0.37066
C	-2.30404	0.57010	0.20950
H	-2.00536	0.24683	1.21131
C	-3.72502	1.12982	0.31073
O	-3.96040	2.32691	0.13170
N	-4.66734	0.24484	0.64063
H	-4.38801	-0.71345	0.81989
C	-6.05430	0.64802	0.80715
H	-6.14904	1.38644	1.60512
H	-6.64000	-0.23142	1.06262
H	-6.44179	1.07942	-0.11685

f) 2-Conf-3

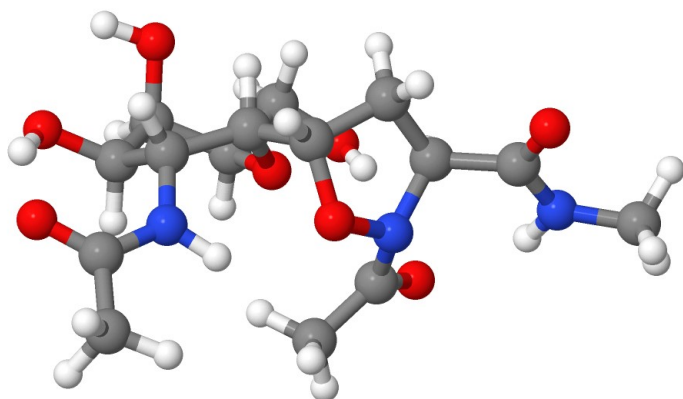


C	2.68754	1.81510	0.51600
H	3.37043	2.20517	1.27693
C	2.06176	-0.33335	-0.73166
C	0.76382	0.47580	-0.79659
H	0.96881	1.34482	-1.42831
O	0.38811	0.90843	0.50595
C	1.27389	1.86604	1.09895
H	1.36213	1.57791	2.15068
C	0.64209	3.25079	1.05507
H	1.32921	3.96806	1.51872
H	-0.28027	3.23141	1.63805
H	2.49317	-0.35721	-1.73644
C	3.07442	0.37541	0.21198
H	3.07721	-0.16476	1.16628
C	-0.43407	-0.20383	-1.44771
H	-0.13737	-0.57929	-2.42703
N	1.83189	-1.70872	-0.30018
H	0.95211	-1.94055	0.15349
C	2.82007	-2.60972	-0.30326
O	3.96041	-2.33114	-0.71648
C	2.49193	-3.98565	0.20021
H	2.63854	-4.69573	-0.61591
H	3.19124	-4.23986	0.99814
H	1.46961	-4.06102	0.56847
O	0.27937	3.66092	-0.25692
H	1.08314	3.63079	-0.79349
O	2.78161	2.63322	-0.65047
H	3.67037	2.52804	-1.01326
O	4.37972	0.40314	-0.34180
H	4.56642	-0.50897	-0.62067
O	-0.92765	-1.35273	-0.72938
N	-1.77780	-0.85248	0.26851
C	-1.32559	-1.05462	1.54930
O	-0.41465	-1.83980	1.77980
C	-2.04764	-0.29628	2.62172
H	-3.10920	-0.17360	2.40688
H	-1.59168	0.69686	2.69480
H	-1.91391	-0.81810	3.56687
C	-1.66028	0.70485	-1.51449



H	-2.27631	0.42754	-2.36991
H	-1.39801	1.75839	-1.58295
C	-2.40330	0.39141	-0.19628
H	-2.24202	1.18521	0.53299
C	-3.90043	0.28215	-0.43797
O	-4.52413	1.30053	-0.75761
N	-4.46659	-0.91669	-0.32331
H	-3.89390	-1.69319	-0.02221
C	-5.88957	-1.10498	-0.55747
H	-6.12627	-2.15582	-0.41210
H	-6.47617	-0.50443	0.13937
H	-6.14994	-0.81568	-1.57637

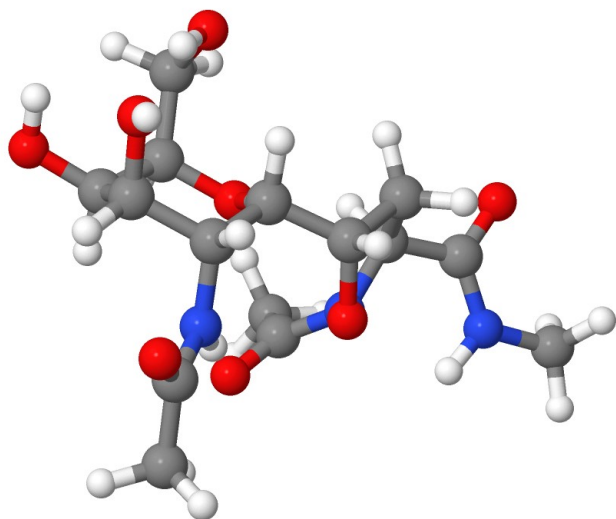
g) **2-Conf-6**



C	2.45769	2.14878	0.13917
H	3.03731	2.78088	0.81938
C	2.24210	-0.24890	-0.71109
C	0.82576	0.29507	-0.93025
H	0.89108	1.05041	-1.71858
O	0.33862	0.88200	0.26878
C	1.03692	2.06458	0.68696
H	1.11382	1.98122	1.77528
C	0.17696	3.26542	0.34876
H	-0.05444	3.26168	-0.72172
H	0.70322	4.18968	0.59356
H	2.71769	-0.35087	-1.69107
C	3.07634	0.75780	0.12728
H	3.09396	0.40069	1.16427
C	-0.19595	-0.73619	-1.40069
H	0.26989	-1.39450	-2.13395
N	2.21501	-1.56699	-0.08036
H	1.34380	-1.91287	0.30397
C	3.32789	-2.29197	0.09005
O	4.43753	-1.88205	-0.29111
C	3.18174	-3.62939	0.75616
H	3.55560	-4.39567	0.07491
H	2.15097	-3.85354	1.02748
H	3.80748	-3.63935	1.65025
O	-1.02217	3.24994	1.11745

H	-1.40417	2.36359	1.06029
O	2.46092	2.72937	-1.16073
H	3.37304	2.71463	-1.47721
O	4.39680	0.89350	-0.37138
H	4.73503	-0.01186	-0.47647
O	-0.63748	-1.60015	-0.32897
N	-1.72603	-0.95065	0.28579
C	-1.55281	-0.56312	1.59052
O	-2.31375	0.27770	2.06402
C	-0.49221	-1.25430	2.38891
H	-0.74939	-1.17772	3.44360
H	0.45619	-0.73987	2.21265
H	-0.38081	-2.29829	2.09834
C	-1.49910	-0.13685	-1.92139
H	-1.95303	-0.81720	-2.64008
H	-1.35201	0.83546	-2.38793
C	-2.37101	-0.03628	-0.67385
H	-2.34950	0.96830	-0.24906
C	-3.83641	-0.43067	-0.88874
O	-4.24529	-0.91458	-1.94593
N	-4.62907	-0.20308	0.16120
H	-4.20744	0.16098	1.00807
C	-6.03617	-0.56785	0.14103
H	-6.55645	-0.03873	-0.65848
H	-6.47728	-0.29293	1.09576
H	-6.15573	-1.64159	-0.01370

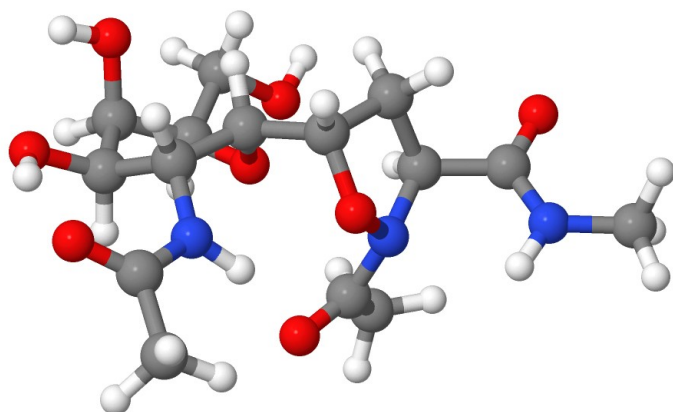
**h) 2-Conf-14**



C	-2.77348	-0.79214	1.01558
H	-2.57779	0.04551	1.68856
C	-1.89635	0.51879	-0.94211
C	-0.70742	-0.43944	-0.93524
H	-0.96947	-1.26610	-1.60241
O	-0.43449	-0.93623	0.37503
C	-1.49165	-1.65292	1.01729

H	-1.18018	-1.72400	2.06382
C	-1.59455	-3.10616	0.55985
H	-2.35173	-3.59898	1.18087
H	-0.63367	-3.57827	0.77424
H	-2.12490	0.77111	-1.98153
C	-3.12448	-0.18903	-0.33854
H	-3.92624	0.54068	-0.19665
C	0.59331	0.13240	-1.48318
H	0.40006	0.56740	-2.46369
N	-1.62514	1.74604	-0.21254
H	-0.86361	1.75916	0.46356
C	-2.32839	2.86804	-0.42776
O	-3.24383	2.92547	-1.26144
C	-1.94489	4.06660	0.39552
H	-2.81569	4.38128	0.97348
H	-1.11388	3.86254	1.06969
H	-1.67791	4.88069	-0.28049
O	-1.84918	-3.33094	-0.81910
H	-2.59247	-2.76791	-1.09045
O	-3.87255	-1.49608	1.56462
H	-4.19538	-2.11595	0.89706
O	-3.58542	-1.24105	-1.17850
H	-3.98493	-0.86914	-1.97437
O	1.13524	1.20673	-0.68847
N	1.89898	0.60675	0.32162
C	1.42490	0.79183	1.59406
O	0.54816	1.61428	1.83553
C	2.08152	-0.03286	2.66015
H	1.56289	-0.99591	2.70782
H	1.96428	0.47819	3.61343
H	3.13665	-0.21750	2.46000
C	1.72942	-0.88979	-1.51169
H	2.39632	-0.67913	-2.34739
H	1.36551	-1.91224	-1.59190
C	2.46182	-0.65547	-0.17091
H	2.24433	-1.45872	0.53234
C	3.96793	-0.62613	-0.38080
O	4.53382	-1.66136	-0.74981
N	4.60432	0.52532	-0.18280
H	4.07449	1.31442	0.16096
C	6.04229	0.63613	-0.37064
H	6.33826	1.66155	-0.16504
H	6.57148	-0.03431	0.30830
H	6.31258	0.38307	-1.39649

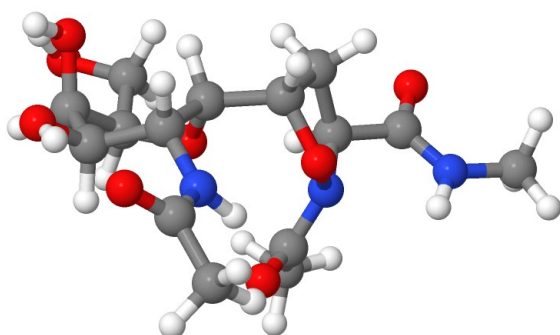
i) 2-Conf-11



C	2.65627	1.98232	0.30727
H	3.29495	2.47774	1.04488
C	2.12407	-0.29815	-0.71491
C	0.79461	0.44765	-0.87614
H	0.97765	1.26278	-1.58368
O	0.40072	0.98903	0.37892
C	1.20310	2.10794	0.77791
H	1.20268	2.07836	1.87028
C	0.55639	3.39883	0.32211
H	0.40617	3.38217	-0.76155
H	1.21109	4.23969	0.57334
H	2.60607	-0.35503	-1.69477
C	3.04583	0.51244	0.23769
H	2.93739	0.09465	1.24584
C	-0.37770	-0.31693	-1.47607
H	-0.07151	-0.74809	-2.42902
N	1.93633	-1.65929	-0.22056
H	1.06296	-1.88946	0.24635
C	2.94180	-2.53957	-0.17845
O	4.08090	-2.26028	-0.59597
C	2.63502	-3.89866	0.38109
H	3.34251	-4.11221	1.18357
H	1.61575	-3.97358	0.75794
H	2.78648	-4.63774	-0.40808
O	-0.69444	3.51076	0.99431
H	-1.16834	4.26283	0.62377
O	2.83282	2.60995	-0.95990
H	3.74186	2.43444	-1.23492
O	4.40245	0.46310	-0.17586
H	4.58469	-0.46462	-0.40609
O	-0.83393	-1.42943	-0.68134
N	-1.69818	-0.89153	0.28285
C	-1.24268	-0.99340	1.57372
O	-0.29936	-1.72252	1.85384
C	-2.00235	-0.20195	2.59474
H	-1.85112	-0.65786	3.57087
H	-3.06691	-0.14059	2.36896
H	-1.59130	0.81303	2.60717

C	-1.62809	0.55455	-1.59507
H	-2.23326	0.22139	-2.43800
H	-1.39030	1.61026	-1.71464
C	-2.36965	0.29323	-0.26414
H	-2.24641	1.13749	0.41404
C	-3.85940	0.10804	-0.50614
O	-4.51898	1.07641	-0.90077
N	-4.37959	-1.10064	-0.30851
H	-3.77933	-1.83008	0.05091
C	-5.79239	-1.36249	-0.53366
H	-6.40715	-0.73401	0.11241
H	-5.98860	-2.40766	-0.30872
H	-6.05643	-1.16284	-1.57292

j) **2-Conf-8**



C	2.75610	1.68105	0.31776
H	3.45851	2.08663	1.05171
C	1.98871	-0.51763	-0.74606
C	0.73789	0.35784	-0.86368
H	0.98977	1.17055	-1.55218
O	0.41420	0.89956	0.41318
C	1.33221	1.91180	0.84140
H	1.36709	1.83483	1.93018
C	0.76848	3.27038	0.43525
H	-0.16350	3.44123	0.97559
H	0.55112	3.27216	-0.63756
H	2.42950	-0.61927	-1.74167
C	3.02067	0.18961	0.17603
H	2.93088	-0.25088	1.17642
C	-0.50975	-0.27721	-1.46308
H	-0.25469	-0.71581	-2.42773
N	1.67675	-1.85237	-0.24404
H	0.79085	-1.99652	0.23358
C	2.59679	-2.82164	-0.20489
O	3.75000	-2.65368	-0.64228
C	2.17320	-4.13936	0.37732
H	2.86421	-4.40261	1.17950
H	2.25339	-4.90130	-0.40048
H	1.15399	-4.11709	0.76128
O	1.65386	4.32850	0.77348

H	2.41227	4.26649	0.17859
O	2.94141	2.35967	-0.92351
H	3.83686	2.16063	-1.22556
O	4.34575	0.04571	-0.30962
H	4.44942	-0.89513	-0.53319
O	-1.06182	-1.35808	-0.68550
N	-1.86665	-0.76233	0.29590
C	-1.41714	-0.93540	1.58108
O	-0.54292	-1.75375	1.83833
C	-2.09779	-0.10380	2.62589
H	-1.59601	0.86874	2.66210
H	-1.98478	-0.59650	3.58922
H	-3.15323	0.05974	2.40862
C	-1.67357	0.70927	-1.55348
H	-2.31131	0.45236	-2.39903
H	-1.33946	1.74026	-1.65322
C	-2.43077	0.48869	-0.22402
H	-2.23155	1.30410	0.47119
C	-3.93176	0.44366	-0.46378
O	-4.49785	1.46945	-0.85818
N	-4.56305	-0.71030	-0.26438
H	-4.03459	-1.49116	0.09959
C	-5.99532	-0.83616	-0.48397
H	-6.24352	-0.60143	-1.51973
H	-6.54577	-0.15990	0.17186
H	-6.28755	-1.86078	-0.26918