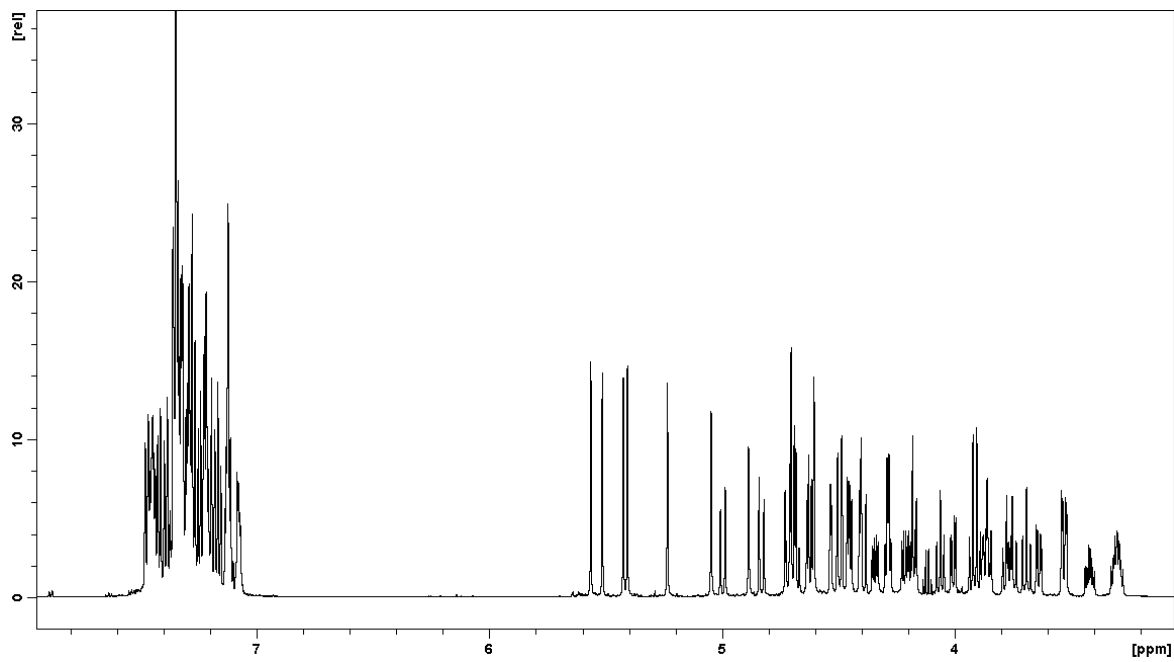


**Fully Deprotected β -(1 \rightarrow 2)-Mannotetraose Forms a Contorted α -Helix
in Solution: Convergent Synthesis and Conformational
Characterization by NMR and DFT**

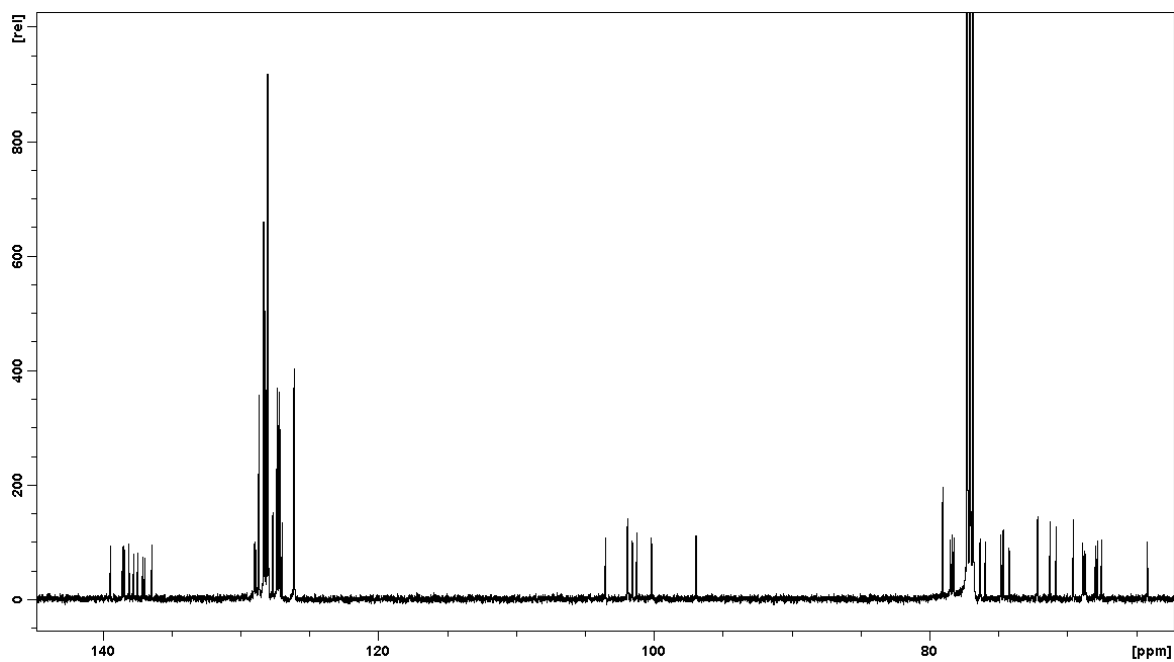
Filip S. Ekholm, Jari Sinkkonen and Reko Leino*

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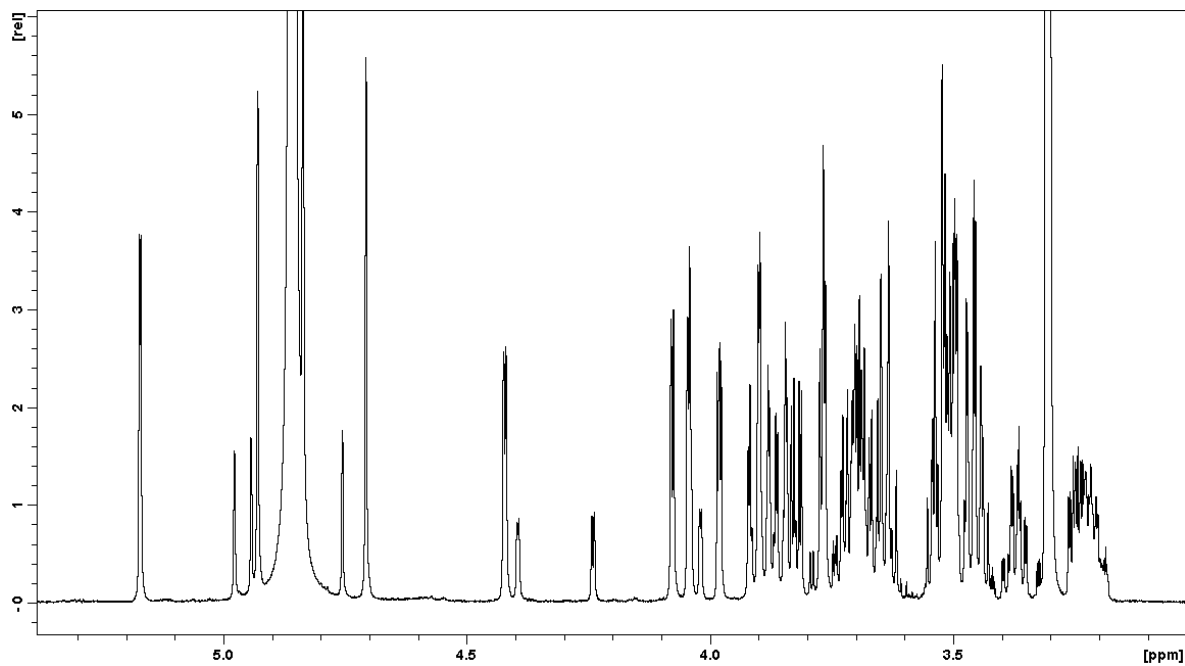
^1H spectrum of compound 3 in CDCl_3S2
^{13}C spectrum of compound 3 in CDCl_3S2
^1H spectrum of compound 4 in MeODS3
^{13}C spectrum of compound 4 in MeODS3
2D-NOESY spectrum of compound 4 in MeODS4
^1H spectrum of compound 4 in D_2OS4
^{13}C spectrum of compound 4 in D_2OS5
2D-NOESY spectrum of compound 4 in D_2OS5
The B3LYP/6-61G(d,p) optimized structure of 4S6



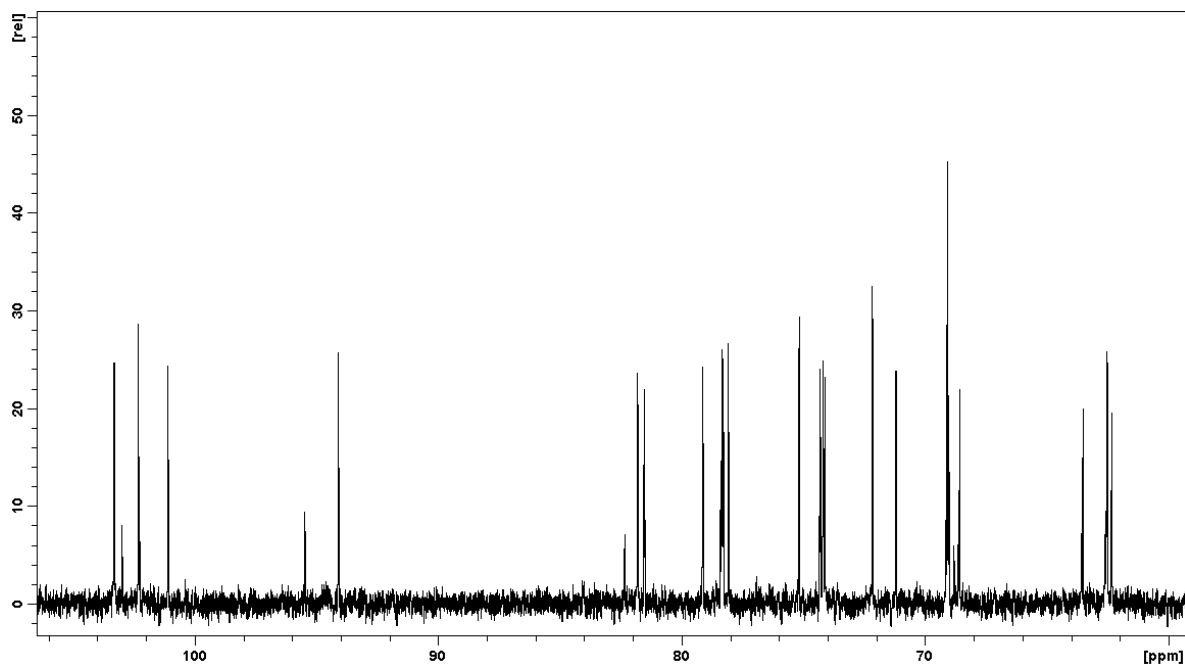
^1H NMR spectrum of compound **3** in CDCl_3 recorded at $25\text{ }^\circ\text{C}$.



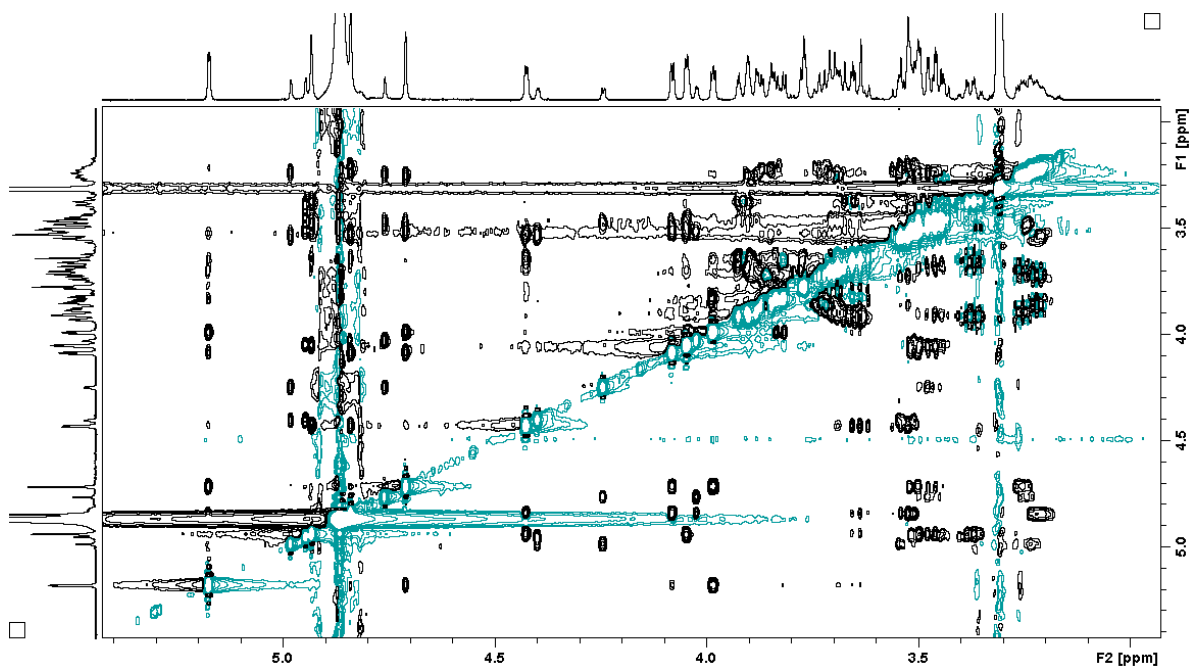
^{13}C NMR spectrum of compound **3** in CDCl_3 recorded at $25\text{ }^\circ\text{C}$.



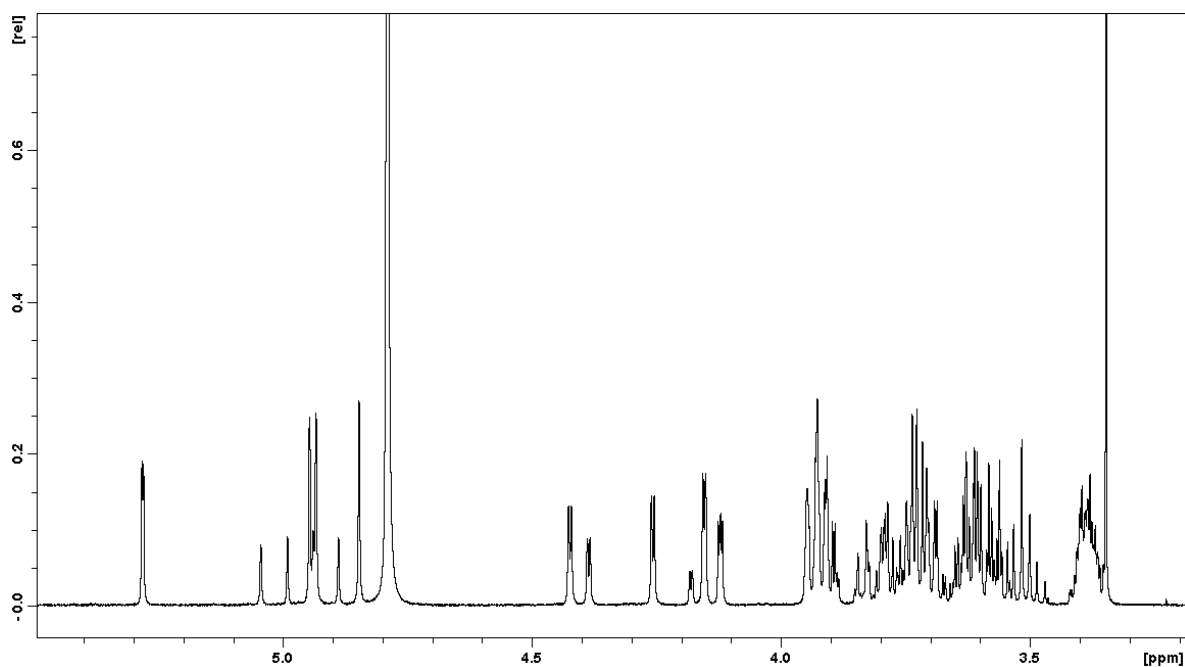
^1H NMR spectrum of compound 4 in MeOD recorded at 25 °C.



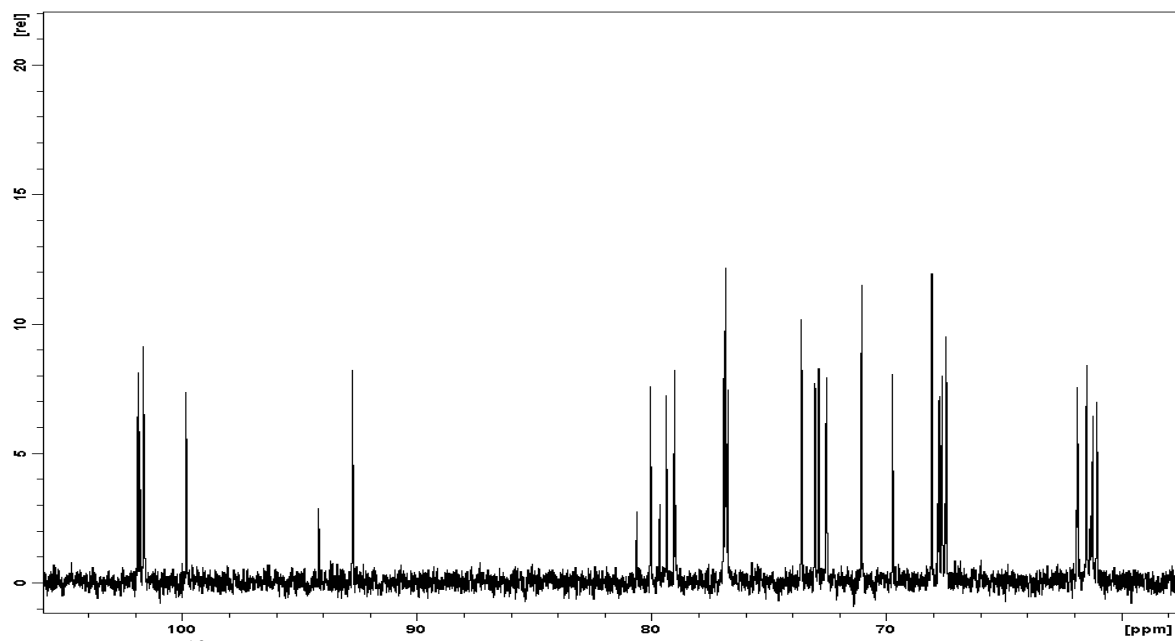
^{13}C NMR spectrum of compound 4 in MeOD recorded at 25 °C.



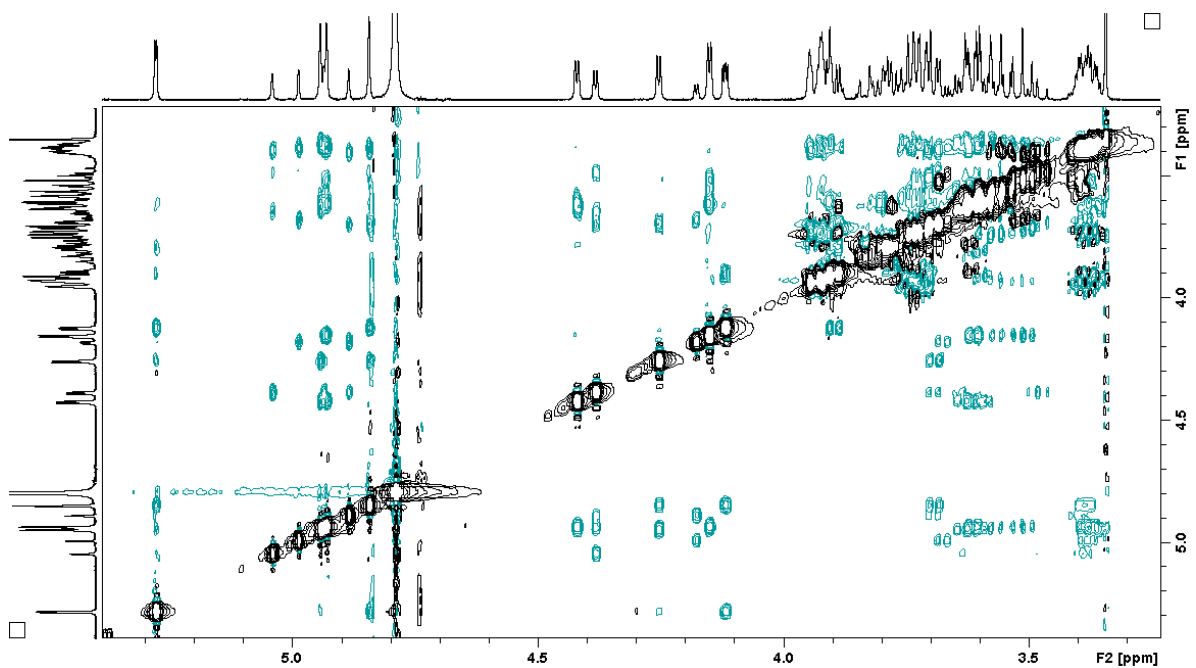
2D-NOESY spectrum of compound **4** in MeOD at 25° with a mixing time of 1 s.



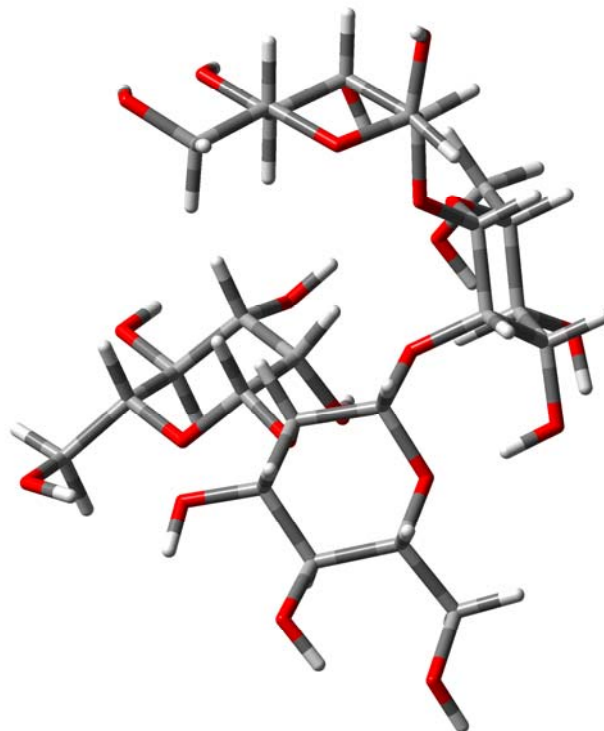
^1H NMR spectrum of compound **4** in D_2O recorded at 25 °C.



^{13}C NMR spectrum of compound 4 in D_2O recorded at 25°C .



2D-NOESY spectrum of compound 4 in D_2O at 25° with a mixing time of 1 s.



The B3LYP/6-61G(d,p) optimized structure of compound 4.

The optimized structure of compound 4 in Cartesian coordinates:

C	-1.87243600	-0.98925000	-0.84852900
C	-2.96225100	-2.77116000	-1.98632400
C	-2.95071600	-3.66590000	-0.74638500
C	-1.73692600	-3.31698800	0.11668300
H	-3.86005900	-3.45313500	-0.16309200
O	-3.01331900	-1.40208200	-1.56934600
H	-0.67684200	-1.56330300	0.82179200
H	-0.83273000	-3.61765400	-0.43434400
C	-1.67609400	-1.81143700	0.43420900
C	-4.16981000	-2.95112100	-2.89877000
O	-2.90785800	-5.02344400	-1.15598500
O	-1.86452600	-4.07183800	1.32399000
O	-2.66938300	-1.48340400	1.39287800
O	-2.05735700	0.36030200	-0.54426100
O	0.03047800	1.06787800	0.98354400
C	-0.48812400	2.03072200	0.12882300
C	-1.13682300	1.30224100	-1.05938300
C	-1.84962200	2.33152100	-1.93648700

C	-2.87358200	3.11078000	-1.11282100
C	-2.19037200	3.75081700	0.11031100
C	-3.18532400	4.34889600	1.10289400
O	-2.44765800	1.67836000	-3.03478700
O	-3.41421400	4.09034700	-1.98728500
O	-1.46529700	2.77252400	0.86541500
O	-3.95464000	5.33726600	0.41402400
O	2.73598200	0.76764700	0.67902000
C	2.17881200	0.62372600	1.93702100
C	0.91017800	1.48598900	2.02623700
C	0.23242600	1.24685400	3.38896900
C	-0.00482800	-0.25518300	3.57508100
C	1.31623600	-1.01773100	3.44926500
C	1.16235500	-2.53153300	3.66025200
O	-0.97415400	1.96267800	3.55718700
O	-0.56096000	-0.54266900	4.85473300
O	1.85517900	-0.75732500	2.14173600
O	-0.11791300	-3.04026400	3.29669500
C	4.80388400	1.49283400	-0.26822400
C	4.10842900	0.36060300	0.51104400
C	4.19683200	-0.94398900	-0.28961500
C	3.65965100	-0.70837200	-1.70422100
C	4.44347700	0.41535500	-2.38886300
C	3.91529500	0.75340700	-3.78539400
O	3.54937000	-2.05427200	0.30986200
O	3.78236600	-1.89589700	-2.47824100
O	4.33169600	1.60979000	-1.59068500
O	4.22164100	-0.25845400	-4.72219700
O	6.18531700	1.22319200	-0.20355800
H	0.29771100	2.72150800	-0.22233300
H	-0.34856700	0.80816200	-1.64158700
H	-1.09236600	3.05774700	-2.28454500
H	-3.64375200	2.40598200	-0.76617900
H	-1.50875900	4.53953600	-0.24651800
H	-3.82231600	3.53879200	1.48459200
H	-2.63735100	4.78464200	1.94897400
H	-3.03099600	2.33402200	-3.44534100
H	-3.97309700	4.67142800	-1.44578700
H	-4.67269300	5.62519600	0.99083800
H	2.88829900	0.93222400	2.72774400
H	1.17653300	2.54325300	1.91040400
H	0.90968800	1.59312500	4.18243600
H	-0.68695100	-0.58803800	2.78426700
H	2.02765200	-0.64207200	4.20328100
H	1.36680700	-2.75801100	4.71315900
H	1.90344300	-3.05352400	3.04942800

H	-1.42897700	1.98749000	2.69524400
H	-1.28297000	0.09590800	4.96785800
H	-0.75552400	-2.63329200	3.90450900
H	4.55458400	2.45705200	0.19389400
H	4.58790400	0.24687600	1.49014400
H	5.25712500	-1.20936900	-0.36873900
H	2.60371100	-0.40177400	-1.63189500
H	5.49537700	0.11481700	-2.47864400
H	2.83234400	0.95382900	-3.72143100
H	4.39722900	1.67443500	-4.12867500
H	2.74814200	-1.73347800	0.76048700
H	3.49026000	-2.61871400	-1.90088300
H	3.93299000	-1.09910300	-4.33262400
H	6.63444600	1.89874900	-0.73102600
O	-4.12009300	-2.03490600	-3.97581600
H	-0.97230200	-1.12569600	-1.47686100
H	-2.04632300	-2.94818700	-2.57498200
H	-4.16947100	-3.96176500	-3.31422500
H	-5.08611500	-2.82679200	-2.29803400
H	-2.75776100	-5.53974300	-0.35088000
H	-1.07657300	-3.91377900	1.87846000
H	-2.81296300	-2.31223700	1.87973800
H	-3.91003300	-1.17503000	-3.57864700