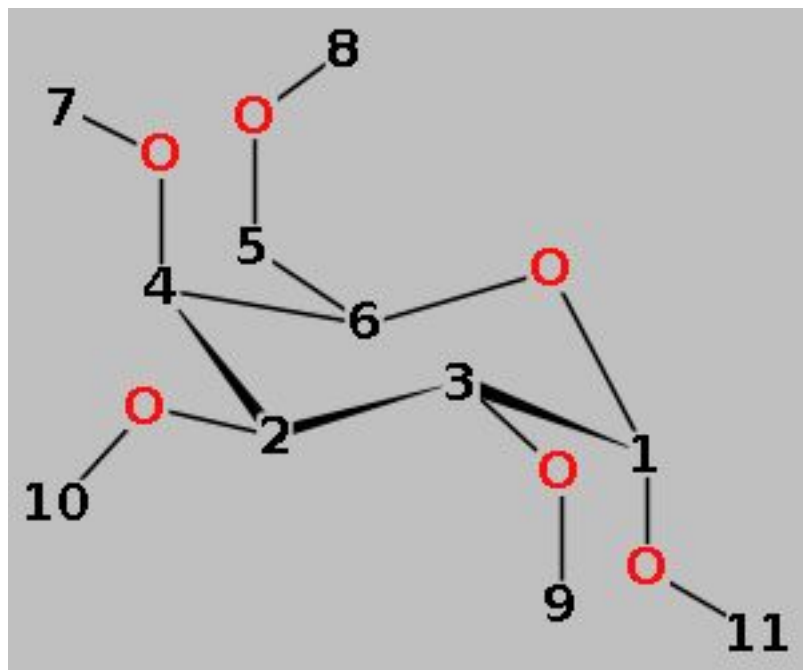


nmrshiftdb2 quality report

Created Sun Nov 12 11:20:33 CET 2017



Atom number	Shift	Deviation from prediction
1	97.87	1.10
10	58.01	2.35
11	55.43	0.07
2	80.4	3.73, prediction not reliable (only 2.0 spheres used, Range > 10 ppm)
3	77.96	3.92
4	76.15	4.65, prediction not reliable (only 2.0 spheres used, Range > 10 ppm)
5	71.17	0.40
6	68.94	1.23
7	61.32	1.46
8	59.35	1.49
9	58.95	0.03

Overall mark 9 (out of 1 to 10, 10 being best), reliability good, recommendation: accept

Mean deviation from prediction: 1.86 ppm -> 0.93 Points

No. of red or missing shifts: 0.0 -> 0.0 Points

No. of yellow shifts: 0.0 -> 0.0 Points

Result: 9/accept