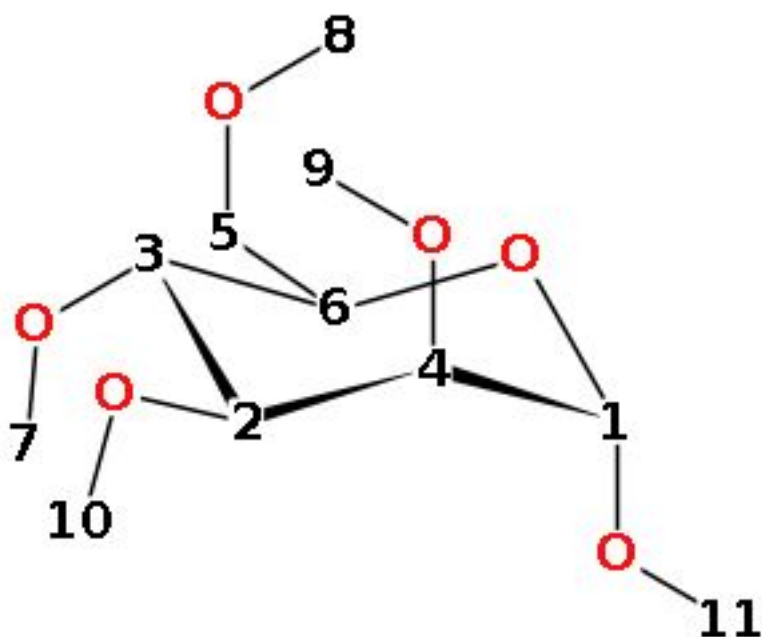


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	4.59	0.16
10	3.4	0.03
11	3.28	0.05
2	3.41	0.06
3	3.38	0.02
4	3.44	0.05
5a	3.55	0.06, calculated from average of shifts
5b	3.47	0.35, calculated from average of shifts
6	3.4	0.13
7	3.45	0.02
8	3.34	0.04
9	3.42	0.02

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

Mean deviation from prediction: 0.08 ppm -> 0.04 Points

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

No. of yellow shifts: 0.0 -> 0.0 Points

Result: 10/accept

Created Fri Dec 01 10:46:26 CET 2017