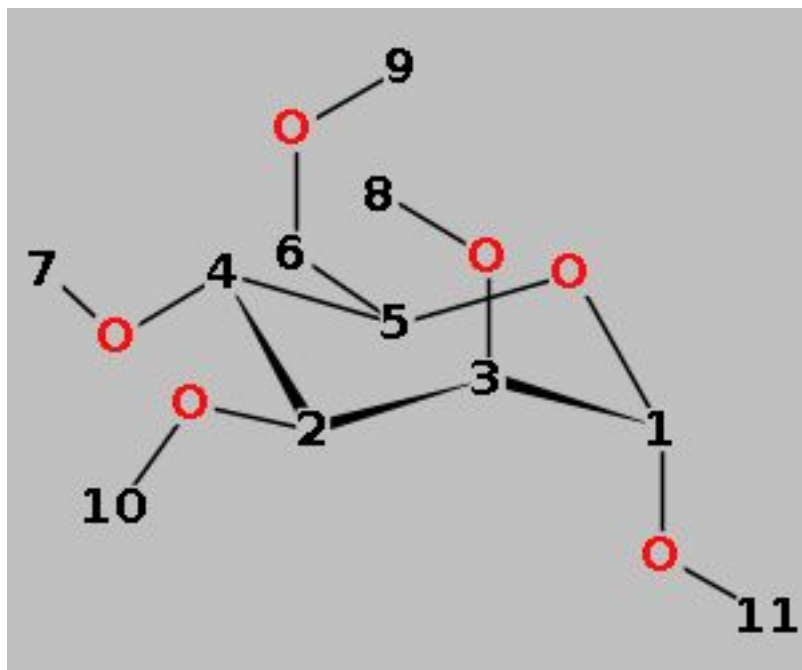


nmrshiftdb2 quality report

Created Mon Nov 13 16:11:42 CET 2017



Atom number	Shift	Deviation from prediction
1	98.82	0.95
10	56.77	1.24
11	53.47	1.96
2	82.5	2.10
3	77.22	0.74
4	76.29	0.14
5	76.04	7.10
6	71.63	0.46
7	59.56	1.76
8	58.31	0.64
9	58.27	1.82

Overall mark 7 (out of 1 to 10, 10 being best), reliability excellent, recommendation: accept

Mean deviation from prediction: 1.72 ppm -> 0.86 Points

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

No. of yellow shifts: 1.0 -> 2.5 Points

Result: 7/accept