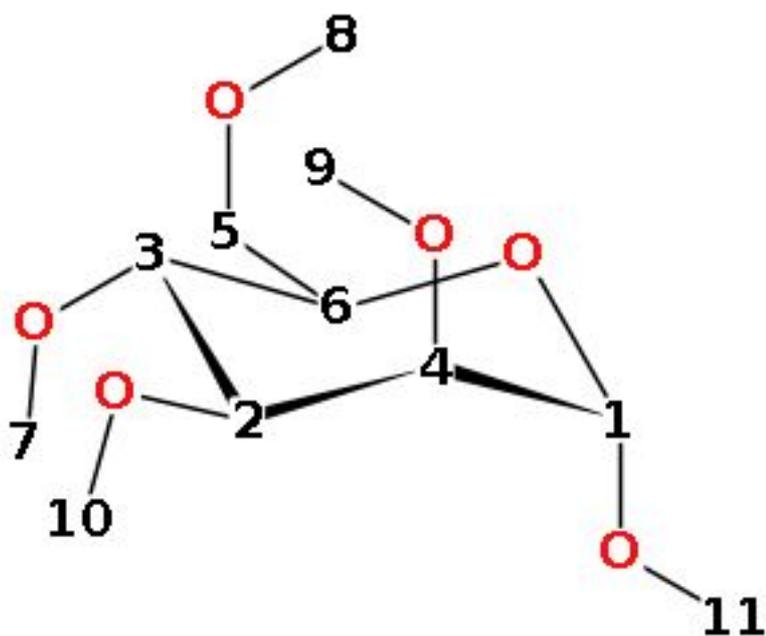


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	4.84	0.09
10	3.39	0.04
11	3.33	0.00
2	3.5	0.03
3	3.28	0.08
4	3.73	0.34
5a	3.63	0.03, calculated from average of shifts
5b	3.58	0.26, calculated from average of shifts
6	3.61	0.08
7	3.42	0.05
8	3.33	0.05
9	3.38	0.06

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

Mean deviation from prediction: 0.09 ppm -> 0.05 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 10:31:21 CET 2017