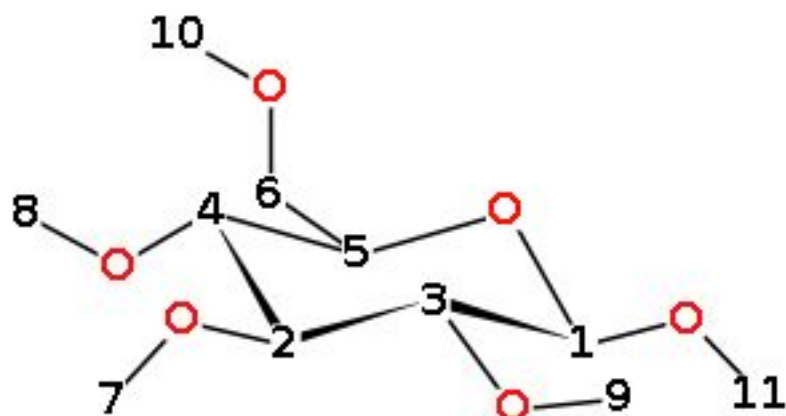


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	4.01	0.26
10	3.35	0.04
11	3.42	0.10
2	3.03	0.26
3	2.87	0.16
4	3.07	0.13
5	3.14	0.26
6a	3.56	0.12, calculated from average of shifts
6b	3.51	0.33, calculated from average of shifts
7	3.57	0.07
8	3.48	0.05
9	3.49	0.09

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

Mean deviation from prediction: 0.15 ppm -> 0.08 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 Tue Dec 05 18:25:41 CET 2017