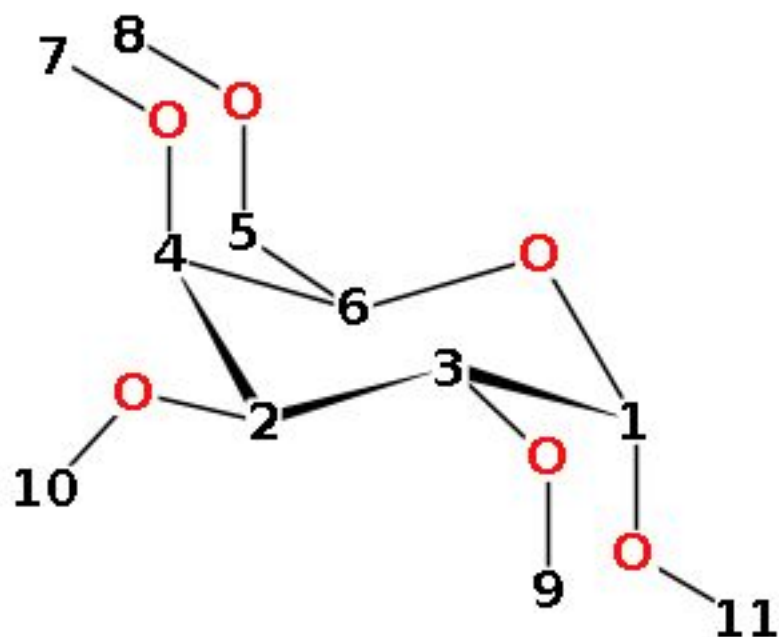


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	4.89	0.02
10	3.54	0.04
11	3.44	0.06
2	3.56	0.00
3	3.66	0.07
4	3.71	0.04
5a	3.58	0.00, calculated from average of shifts
5b	3.54	0.30, calculated from average of shifts
6	3.87	0.01
7	3.59	0.06
8	3.43	0.04
9	3.54	0.07

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

Mean deviation from prediction: 0.06 ppm -> 0.03 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 Wed Dec 06 13:27:43 CET 2017