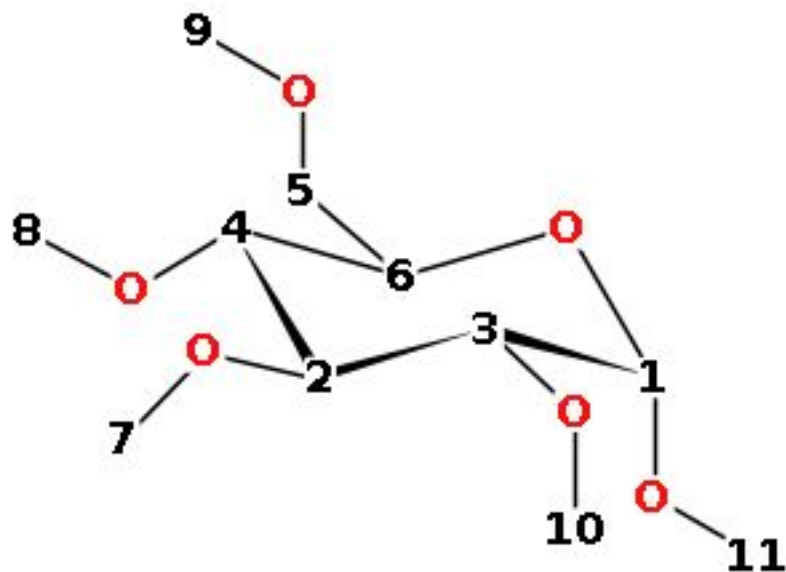


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	4.64	0.18
10	3.4	0.04
11	3.32	0.06
2	3.44	0.04
3	3.05	0.34
4	3.08	0.10
5a	3.57	0.07, calculated from average of shifts
5b	3.44	0.36, calculated from average of shifts
6	3.51	0.09
7	3.55	0.04
8	3.49	0.03
9	3.34	0.04

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

Mean deviation from prediction: 0.12 ppm -> 0.06 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 Thu Dec 07 21:11:00 CET 2017