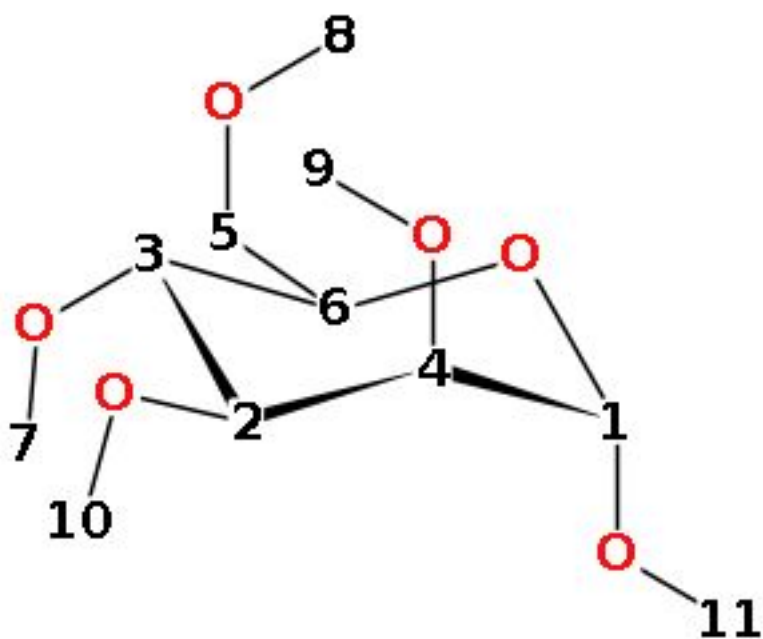


nmrshiftdb2 Quality report



Atom number	Shift	Deviation from prediction
1	97.42	1.40
10	56.75	0.02
11	54.88	1.41
2	79.51	2.99
3	76.2	0.09
4	75.77	1.45
5	71.04	0.59
6	69.82	6.22
7	60.07	0.51
8	58.33	0.06
9	58.22	0.09

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

Mean deviation from prediction: 1.35 ppm -> 0.67 Points

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

No. of yellow shifts: 1.0 -> 2.5 Points

Result: 7/accept

Created Thu Nov 23 08:40:32 CET 2017