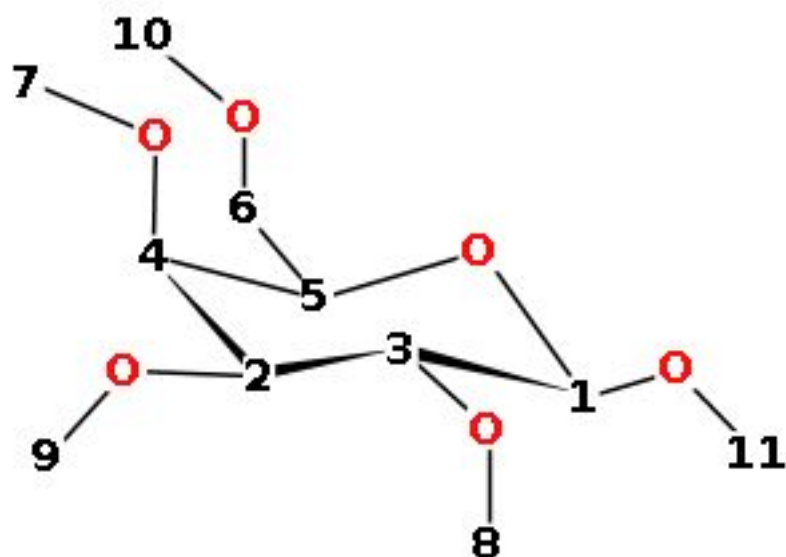


nmrshiftdb2 Quality report



| Atom number | Shift | Deviation from prediction |
|-------------|-------|---|
| 1 | 4.17 | 0.00 |
| 10 | 3.43 | 0.04 |
| 11 | 3.53 | 0.03 |
| 2 | 3.16 | 0.04 |
| 3 | 3.33 | 0.07 |
| 4 | 3.67 | 0.03 |
| 5 | 3.5 | 0.05 |
| 6a | 3.65 | 0.03, calculated from average of shifts |
| 6b | 3.56 | 0.26, calculated from average of shifts |
| 7 | 3.58 | 0.05 |
| 8 | 3.61 | 0.06 |
| 9 | 3.54 | 0.03 |

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 Fri Dec 08 09:56:16 CET 2017