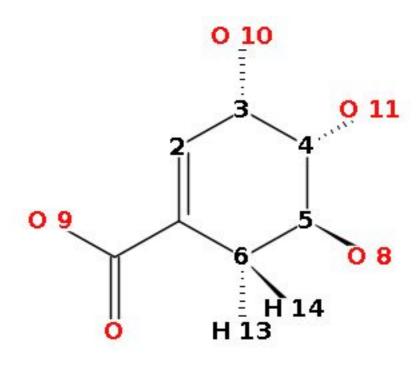
## nmrshiftdb2 Quality Report - <sup>1</sup>H



			Prediction		HOSE
Atom	δ [ppm]	Deviation from prediction	No. Spheres	No. shift values	Code
2	6.81	0.00	6.0	1.0	<u>2D</u>
3	4.44	0.03	6.0	1.0	<u>2D</u>
4	3.76	0.04	6.0	1.0	<u>2D</u>
5	4.02	0.01	6.0	1.0	<u>2D</u>
6b	2.22	Not possible	-	-	-
6a	2.73	0.01, calculated from average of shifts	6.0	2.0	<u>2D</u>

Overall mark 10 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 0.02 ppm  $\rightarrow$  0.01 Points

No. of red or missing shifts:  $0.0 \rightarrow 0.0$  Points

No. of yellow shifts:  $0.0 \rightarrow 0.0$  Points

Result: 10/accept

Created Mon Dec 23 16:30:54 CET 2019