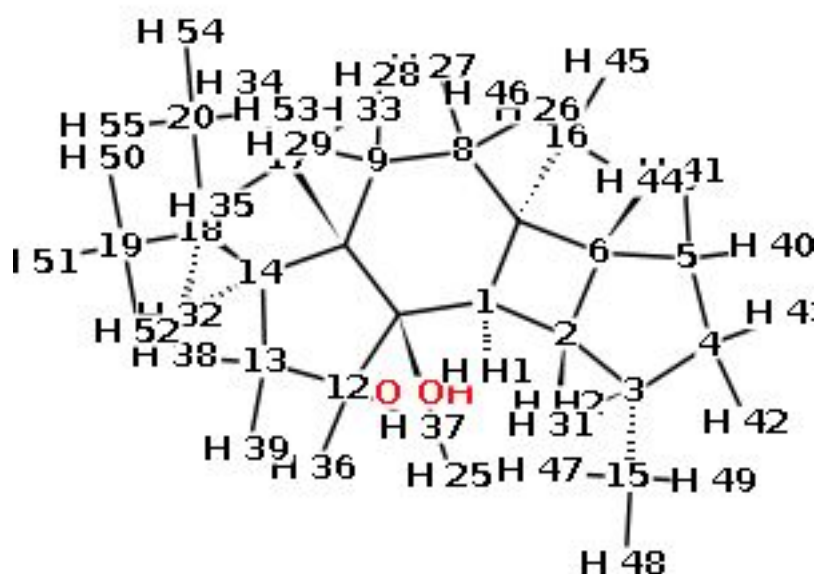





nmrshiftdb2 Quality Report - ^1H 

Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	1.7	0.45  ¹	2.0	54.0	<u>3D</u>
12a	1.31	0.76, calculated from average of shifts	4.0	3.0	<u>2D</u>
12b	1.44	0.52, calculated from average of shifts  ¹	2.0	314.0	<u>2D</u>
13a	1.35	0.01, calculated from average of shifts	4.0	8.0	<u>2D</u>
13b	1.58	0.05, calculated from average of shifts	3.0	12.0	<u>2D</u>
14	1.46	0.14	3.0	143.0	<u>2D</u>
15	0.95	0.02	4.0	110.0	<u>2D</u>
16	0.87	0.06	3.0	55.0	<u>3D</u>
17	1.07	0.02	4.0	57.0	<u>2D</u>
18	1.65	0.20	3.0	47.0	<u>2D</u>
19	0.96	0.03	5.0	12.0	<u>2D</u>
2	2.38	0.23  ¹	2.0	54.0	<u>3D</u>
20	0.89	Symmetric to atom 19	5.0	12.0	<u>2D</u>
3	1.81	0.13	3.0	53.0	<u>2D</u>
4a	1.3	0.07, calculated from average of shifts	4.0	2.0	<u>2D</u>
4b	1.67	0.03, calculated from average of shifts	3.0	12.0	<u>2D</u>
5a	1.44	0.02, calculated from average of shifts	3.0	7.0	<u>3D</u>
5b	1.65	0.03, calculated from average of shifts	3.0	12.0	<u>2D</u>
6	2.2	0.56	3.0	1.0	<u>2D</u>

8a	1.17	0.13, calculated from average of shifts	3.0	81.0	<u>3D</u>
8b	1.53	0.42, calculated from average of shifts	3.0	2.0	<u>2D</u>
9a	1.58	0.21, calculated from average of shifts	3.0	81.0	<u>3D</u>
9b	1.81	0.08, calculated from average of shifts	3.0	2.0	<u>2D</u>

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

Mean deviation from prediction: 0.19 ppm → 0.09 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 Mon Oct 22 23:23:09 CEST 2018



¹ Less than 3 spheres used