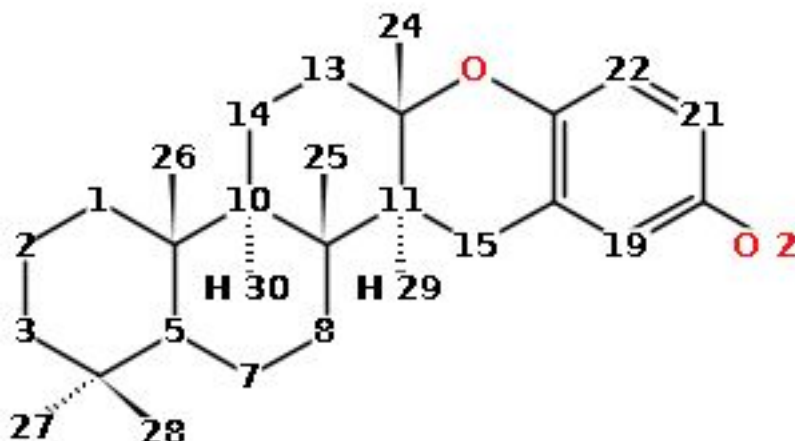


nmrshiftdb2 Quality Report - <sup>1</sup>H

Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1b	0.85	Not possible	-	-	-
1a	1.07	0.61, calculated from average of shifts	3.0	381.0	<u>3D</u>
2b	1.41	Not possible	-	-	-
2a	1.67	0.01, calculated from average of shifts	4.0	12.0	<u>2D</u>
3b	1.17	Not possible	-	-	-
3a	1.34	0.06, calculated from average of shifts	6.0	10.0	<u>2D</u>
5	0.84	0.05	5.0	1.0	<u>2D</u>
7b	1.38	Not possible	-	-	-
7a	1.57	0.02, calculated from average of shifts	5.0	2.0	<u>2D</u>
8b	1.05	Not possible	-	-	-
8a	1.77	0.07, calculated from average of shifts	4.0	4.0	<u>2D</u>
10	0.99	0.58	3.0	13.0	<u>3D</u>
11	1.63	0.19	3.0	7.0	<u>2D</u>
13b	1.65	Not possible	-	-	-
13a	2.02	0.34, calculated from average of shifts	3.0	4.0	<u>3D</u>
14b	1.32	Not possible	-	-	-
14a	1.71	0.02, calculated from average of shifts	3.0	215.0	<u>3D</u>
15b	2.56	Not possible	-	-	-
15a	2.56	0.26, calculated from average of shifts	3.0	7.0	<u>3D</u>
19	6.55	0.34	3.0	354.0	<u>2D</u>

21	6.56	0.74	5.0	2.0	<u>2D</u>
22	6.62	0.23	4.0	27.0	<u>2D</u>
24	1.16	0.30	4.0	8.0	<u>2D</u>
25	0.88	0.04	5.0	2.0	<u>2D</u>
26	0.85	0.02	5.0	2.0	<u>2D</u>
27	0.86	0.02	6.0	10.0	<u>2D</u>
28	0.82	Symmetric to atom 27	6.0	10.0	<u>2D</u>

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

Mean deviation from prediction: 0.22 ppm → 0.11 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 06 13:52:14 CET 2019