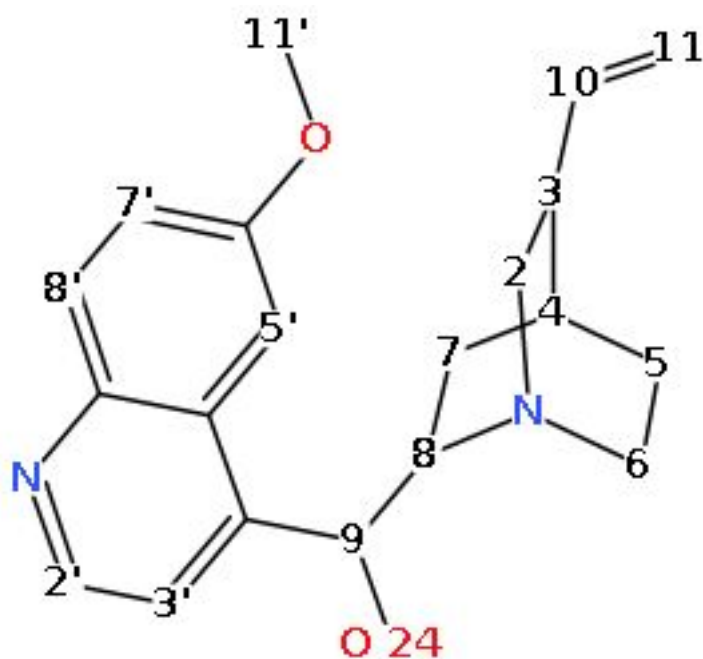


nmrshiftdb2 Quality Report - <sup>1</sup>H

Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
10	6.03	0.08	6.0	3.0	<u>2D</u>
11'	3.85	0.05	6.0	38.0	<u>2D</u>
11a	5.03	0.03, calculated from average of shifts	6.0	6.0	<u>2D</u>
11b	5.03	0.10, calculated from average of shifts	4.0	2.0	<u>2D</u>
2'	8.54	0.03	6.0	3.0	<u>2D</u>
2a	3.31	0.11, calculated from average of shifts	6.0	4.0	<u>2D</u>
2b	2.88	0.85, calculated from average of shifts	3.0	2.0	<u>2D</u>
3	2.21	0.01	6.0	2.0	<u>2D</u>
3'	7.49	0.02	6.0	2.0	<u>2D</u>
4	1.74	0.00	6.0	2.0	<u>2D</u>
5'	7.17	0.00	6.0	2.0	<u>2D</u>
5a	1.49	0.12, calculated from average of shifts	6.0	2.0	<u>2D</u>
5b	1.49	0.40, calculated from average of shifts ⚠ <sup>1</sup>	2.0	314.0	<u>2D</u>
6a	2.85	0.11, calculated from average of shifts	6.0	4.0	<u>2D</u>
6b	2.73	0.24, calculated from average of shifts	3.0	6.0	<u>2D</u>
7'	7.28	0.05	6.0	2.0	<u>2D</u>
7a	2.03	0.02, calculated from average of shifts	6.0	2.0	<u>2D</u>
7b	1.13	0.31, calculated from average of shifts	3.0	2.0	<u>2D</u>

8	3.03	0.09	6.0	3.0	<u>2D</u>
8'	7.93	0.06	6.0	2.0	<u>2D</u>
9	5.55	0.01	6.0	2.0	<u>2D</u>

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

Mean deviation from prediction: 0.13 ppm → 0.06 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 Sep 28 13:04:08 CEST 2018



<sup>1</sup> Less than 3 spheres used