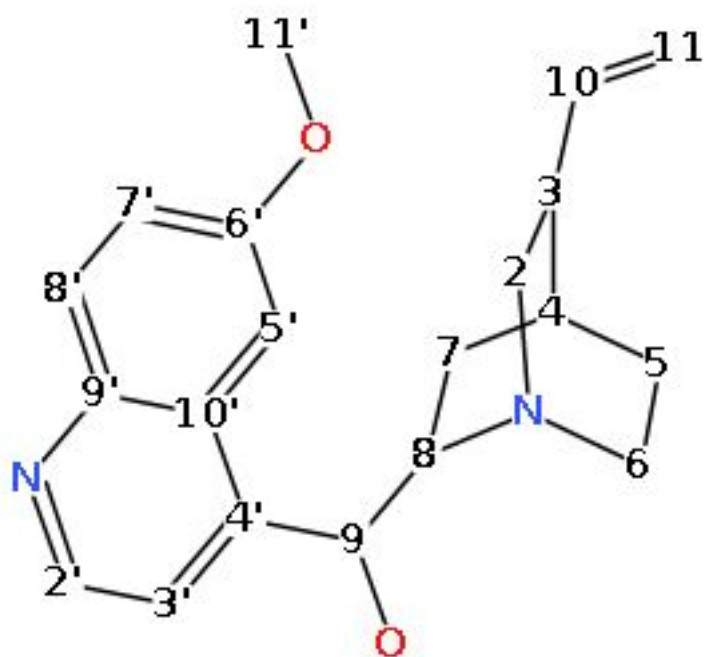


nmrshiftdb2 Quality Report - ¹³C



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
10	140.55	0.89	6.0	5.0	<u>2D</u>
10'	126.45	0.18	6.0	6.0	<u>2D</u>
11	114.61	0.41	6.0	5.0	<u>2D</u>
11'	55.69	0.10	6.0	21.0	<u>2D</u>
2	49.75	5.40	6.0	4.0	<u>3D</u>
2'	147.62	0.08	6.0	7.0	<u>2D</u>
3	40.22	0.34	6.0	4.0	<u>3D</u>
3'	118.51	2.16	6.0	6.0	<u>2D</u>
4	28.33	0.48	6.0	4.0	<u>3D</u>
4'	147.87	0.13	6.0	4.0	<u>2D</u>
5	26.58	0.93	6.0	4.0	<u>3D</u>
5'	101.33	0.07	6.0	6.0	<u>2D</u>
6	50.32	5.64	6.0	4.0	<u>3D</u>
6'	157.36	0.07	6.0	6.0	<u>2D</u>
7	21.36	1.44	6.0	4.0	<u>3D</u>
7'	121.48	2.61	6.0	6.0	<u>2D</u>
8	59.9	0.02	6.0	4.0	<u>3D</u>
8'	131.51	0.56	6.0	6.0	<u>2D</u>
9	71.97	0.47	6.0	4.0	<u>2D</u>
9'	144.03	0.31	6.0	6.0	<u>2D</u>

Overall mark 4 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 1.12 ppm → 0.56 Points

No. of red or missing shifts: 0.0 → 0.0 Points

No. of yellow shifts: 2.0 → 5.0 Points

Result: 4/revision

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