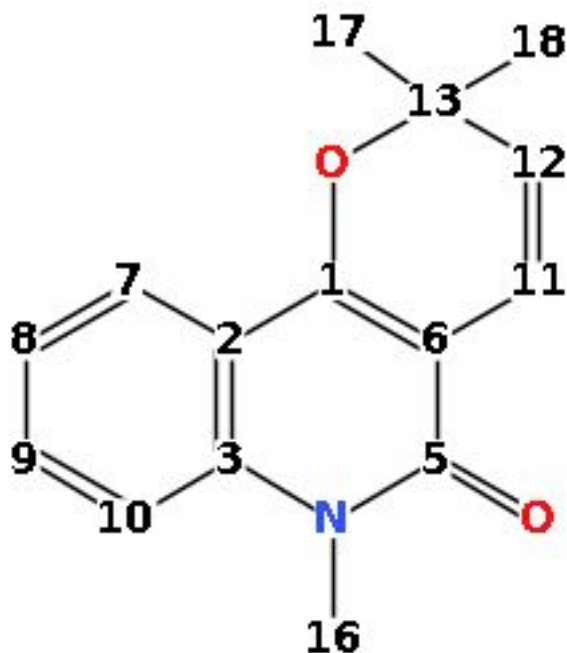


nmrshiftdb2 Quality Report -  $^{13}\text{C}$



Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	155.0	0.90	3.0	2.0	<u>2D</u>
10	114.0	0.70	5.0	6.0	<u>3D</u>
11	117.9	0.50	4.0	1.0	<u>3D</u>
12	125.5	1.00	5.0	1.0	<u>3D</u>
13	78.8	0.60	5.0	2.0	<u>3D</u>
16	28.2	1.25	4.0	15.0	<u>2D</u>
17	29.2	0.70	6.0	2.0	<u>3D</u>
18	29.2	Symmetric to atom 17	6.0	2.0	<u>3D</u>
2	116.2	0.73 <sup>2</sup>	3.0	7.0	<u>3D</u>
3	139.5	0.15	4.0	6.0	<u>3D</u>
5	161.0	0.88 <sup>1,2</sup>	2.0	79.0	<u>2D</u>
6	106.2	0.70	3.0	1.0	<u>3D</u>
7	123.0	0.03	4.0	7.0	<u>3D</u>
8	122.0	0.59	5.0	7.0	<u>3D</u>
9	131.0	0.02	6.0	6.0	<u>3D</u>



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

Mean deviation from prediction: 0.62 ppm  $\rightarrow$  0.31 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

 /  prediction unreliable

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

<sup>2</sup> Range > 10 ppm