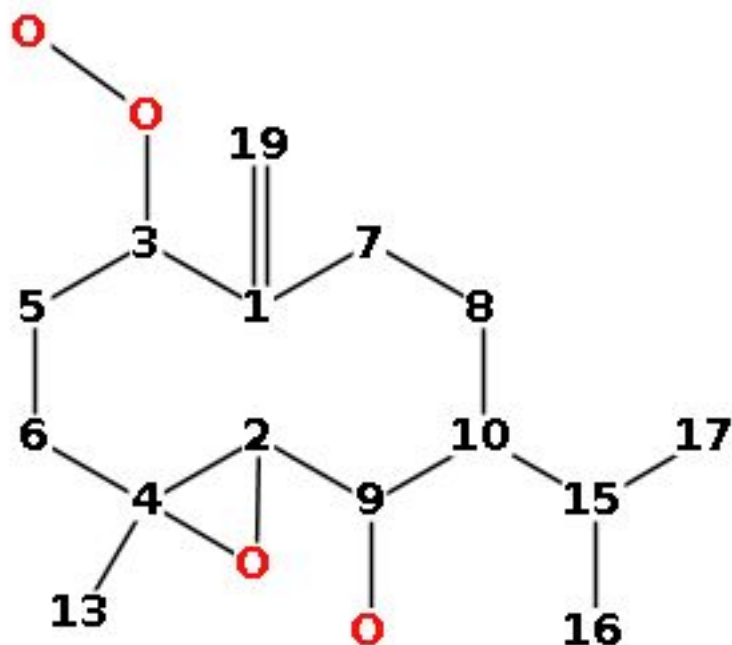


nmrshiftdb2 Quality Report -  $^{13}\text{C}$ 

Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	145.0	2.92 <sup>1, 2</sup>	2.0	18.0	<u>2D</u>
2	67.9	1.40	4.0	1.0	<u>2D</u>
3	86.2	0.45 <sup>1</sup>	2.0	4.0	<u>2D</u>
4	59.3	1.20	3.0	7.0	<u>2D</u>
5	25.3	0.70	3.0	1.0	<u>2D</u>
6	33.9	0.47	3.0	3.0	<u>2D</u>
7	34.2	3.30	3.0	5.0	<u>2D</u>
8	27.3	0.70	3.0	3.0	<u>2D</u>
9	70.9	0.80	5.0	1.0	<u>2D</u>
10	47.2	0.90	4.0	1.0	<u>2D</u>
13	16.9	2.26 <sup>2</sup>	4.0	8.0	<u>2D</u>
15	31.6	0.80	5.0	1.0	<u>2D</u>
16	20.8	0.55	6.0	2.0	<u>2D</u>
17	21.1	Symmetric to atom 16	6.0	2.0	<u>2D</u>
19	116.5	6.98 <sup>2</sup>	3.0	6.0	<u>2D</u>

Overall mark 9 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 1.67 ppm  $\rightarrow$  0.84 Points

No. of red or missing shifts: 0.0  $\rightarrow$  0.0 Points

No. of yellow shifts: 0.0  $\rightarrow$  0.0 Points

**Result: 9/accept**

1 yellow shift(s) not taken into account because the underlying prediction was unreliable.

