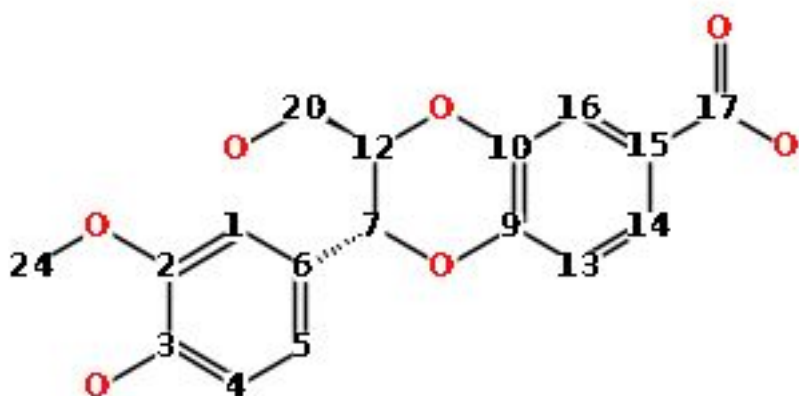


nmrshiftdb2 Quality Report - ^{13}C 

Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	112.2	0.50	5.0	1.0	<u>3D</u>
2	149.4	1.60	6.0	1.0	<u>3D</u>
3	148.6	1.30	6.0	1.0	<u>3D</u>
4	116.4	1.00	6.0	1.0	<u>3D</u>
5	121.9	1.20	5.0	1.0	<u>3D</u>
6	129.3	2.60	4.0	1.0	<u>3D</u>
7	77.7	0.00	4.0	1.0	<u>3D</u>
9	149.0	4.00	4.0	1.0	<u>3D</u>
10	145.0	0.15	3.0	2.0	<u>3D</u>
12	80.5	0.75	5.0	2.0	<u>2D</u>
13	117.8	6.80  ²	3.0	277.0	<u>2D</u>
14	124.6	0.83	4.0	6.0	<u>2D</u>
15	124.7	2.55	4.0	6.0	<u>2D</u>
16	119.8	8.85  ²	3.0	31.0	<u>2D</u>
17	169.5	0.12	5.0	6.0	<u>2D</u>
20	62.1	0.00	6.0	1.0	<u>3D</u>
24	56.6	0.90	6.0	1.0	<u>3D</u>

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

Mean deviation from prediction: 1.95 ppm $\rightarrow$ 0.98 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

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

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