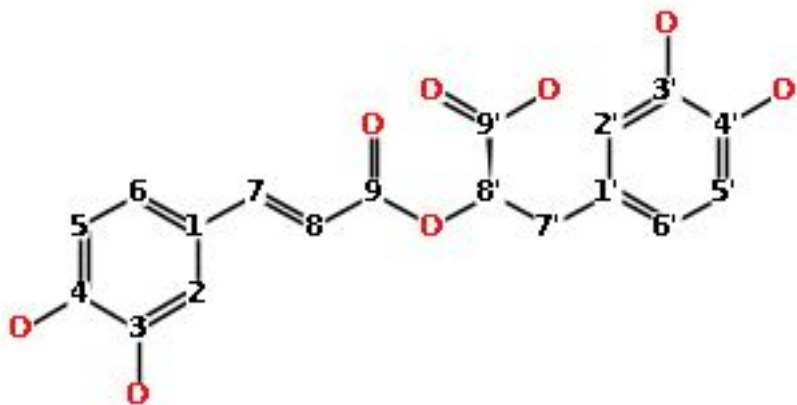


nmrshiftdb2 Quality Report - ^{13}C



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	127.8	1.15	6.0	2.0	<u>3D</u>
2	115.2	0.06	6.0	14.0	<u>3D</u>
3	146.9	0.01	6.0	16.0	<u>3D</u>
4	149.7	1.20	6.0	21.0	<u>3D</u>
5	117.0	0.59	6.0	16.0	<u>3D</u>
6	123.1	0.38	6.0	14.0	<u>3D</u>
7	147.7	1.15	6.0	2.0	<u>3D</u>
8	114.3	0.40	6.0	2.0	<u>3D</u>
9	168.6	1.90	6.0	2.0	<u>3D</u>
1'	129.4	0.75	6.0	2.0	<u>3D</u>
2'	117.7	0.35	6.0	2.0	<u>3D</u>
3'	146.3	0.75	6.0	2.0	<u>3D</u>
4'	145.3	0.60	6.0	2.0	<u>3D</u>
5'	115.9	0.20	6.0	2.0	<u>3D</u>
6'	121.9	0.75	6.0	2.0	<u>3D</u>
7'	31.0	6.10	6.0	2.0	<u>3D</u>
8'	74.6	0.45	6.0	2.0	<u>3D</u>
9'	173.6	1.55	6.0	2.0	<u>3D</u>

Overall mark 7 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 1.02 ppm \rightarrow 0.51 Points

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

No. of yellow shifts: 1.0 \rightarrow 2.5 Points

Result: 7/accept

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