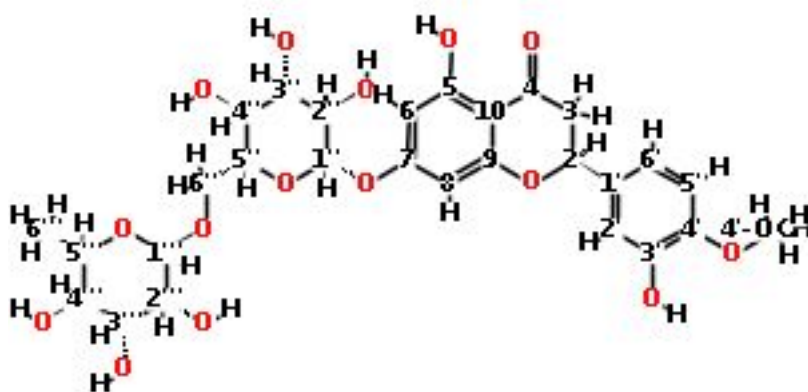



nmrshiftdb2 Quality Report - ¹³C



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1'	131.0	1.50	4.0	1.0	<u>2D</u>
1''	100.9	0.80	5.0	1.0	<u>3D</u>
1'''	99.8	1.48	6.0	6.0	<u>2D</u>
10	103.6	0.20	4.0	1.0	<u>3D</u>
2	78.8	0.90	3.0	3.0	<u>2D</u>
2'	114.2	4.00	4.0	1.0	<u>2D</u>
2''	73.3	0.40	6.0	1.0	<u>3D</u>
2'''	70.6	0.73	6.0	6.0	<u>2D</u>
3	42.3	1.80	4.0	1.0	<u>3D</u>
3'	146.1	0.00	5.0	1.0	<u>2D</u>
3''	76.6	0.45	5.0	4.0	<u>3D</u>
3'''	71.1	0.35	6.0	6.0	<u>2D</u>
4	197.4	0.30	5.0	1.0	<u>3D</u>
4'	148.0	0.90	6.0	1.0	<u>2D</u>
4''	69.9	1.05	6.0	6.0	<u>2D</u>
4'''	72.5	1.49	5.0	7.0	<u>3D</u>
4'-OCH3	56.0	0.20	6.0	14.0	<u>2D</u>
5	165.4	1.50	4.0	1.0	<u>2D</u>
5'	112.0	0.80	5.0	1.0	<u>2D</u>
5''	75.7	1.15	5.0	6.0	<u>2D</u>
5'''	68.7	0.68	6.0	6.0	<u>2D</u>
6	96.8	1.81	4.0	12.0	<u>2D</u>
6'	118.0	3.80  2	4.0	2.0	<u>2D</u>
6''	66.4	2.10	6.0	1.0	<u>2D</u>
6'''	18.2	0.40	6.0	6.0	<u>2D</u>

7	163.3	2.70	5.0	1.0	<u>2D</u>
8	95.9	0.20	4.0	1.0	<u>2D</u>
9	162.8	0.29	3.0	9.0	<u>3D</u>

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

Mean deviation from prediction: 1.14 ppm → 0.57 Points

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

No. of yellow shifts: 0.0 → 0.0 Points

Result: 9/accept

Created Mon Oct 22 13:43:54 CEST 2018



² Range > 10 ppm