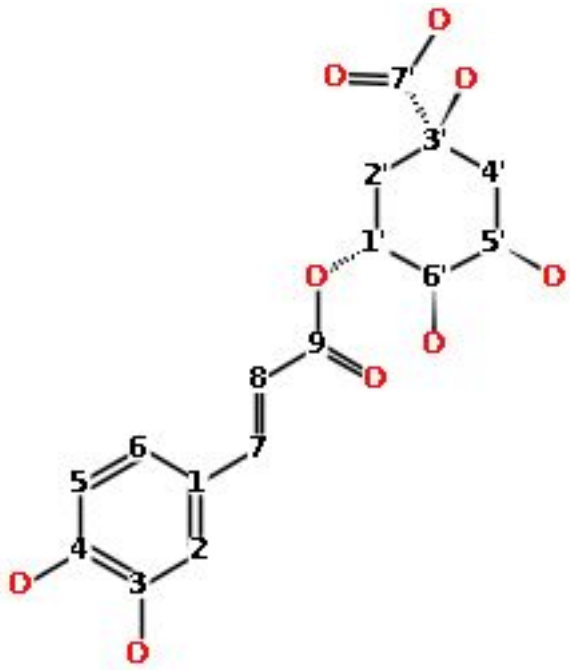
nmrshiftdb2 Quality Report - ^{13}C



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE
			No. Spheres	No. shift values	Code
1	127.74	0.11	6.0	3.0	3D
2	115.12	0.02	6.0	13.0	3D
3	149.58	2.88	6.0	14.0	3D
4	147.08	1.43	6.0	19.0	3D
5	116.43	0.07	6.0	14.0	3D
6	123.0	0.30	6.0	13.0	3D
7	146.79	0.01	6.0	1.0	3D
8	115.19	0.11	5.0	1.0	3D
9	168.62	0.08	4.0	1.0	3D
2'	38.17	0.23	3.0	1.0	3D
3'	73.38	1.48	4.0	1.0	2D
4'	38.69	0.31	4.0	4.0	2D
5'	71.22	2.42	3.0	4.0	2D
6'	76.09	0.61 [1]	2.0	1.0	3D
7'	177.03	3.57	5.0	1.0	2D

[D@122c78a

Result: 10/accept

Created Sat Nov 23 19:49:53 CET 2019

/ prediction unreliable

[1] Less than 3 spheres used

[2] Range > 10 ppm