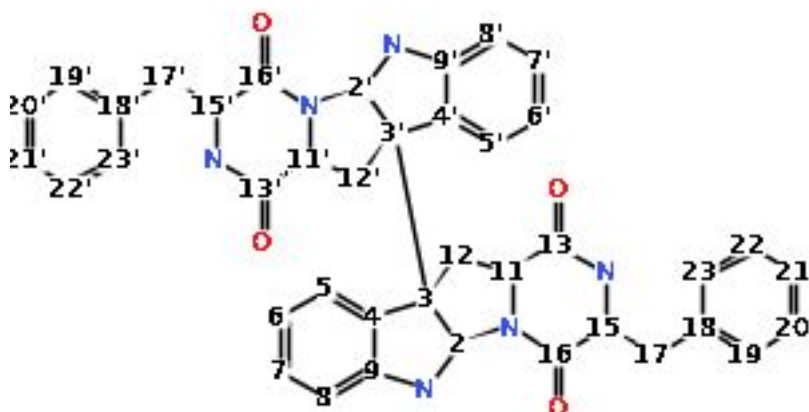



nmrshiftdb2 Quality Report - <sup>13</sup>C

Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
11	56.5	Symmetric to atom 11'	4.0	2.0	<u>2D</u>
11'	56.0	2.45	4.0	2.0	<u>2D</u>
12	34.7	Symmetric to atom 12'	3.0	3.0	<u>2D</u>
12'	36.2	0.23	3.0	3.0	<u>2D</u>
13	168.9	Symmetric to atom 13'	4.0	1.0	<u>2D</u>
13'	167.7	1.30	4.0	1.0	<u>2D</u>
15	55.8	Symmetric to atom 15'	3.0	9.0	<u>2D</u>
15'	56.9	0.18	3.0	9.0	<u>2D</u>
16	168.1	0.90	3.0	1.0	<u>2D</u>
16'	164.6	Symmetric to atom 16	3.0	1.0	<u>2D</u>
17	34.4	4.48	4.0	4.0	<u>2D</u>
17'	39.5	Symmetric to atom 17	4.0	4.0	<u>2D</u>
18	137.0	Symmetric to atom 18'	5.0	4.0	<u>2D</u>
18'	134.7	1.05	5.0	4.0	<u>2D</u>
19	129.3	0.10	6.0	4.0	<u>2D</u>
19'	130.0	Symmetric to atom 19	6.0	4.0	<u>2D</u>
2	78.9	0.03	3.0	3.0	<u>2D</u>
2'	76.9	Symmetric to atom 2	3.0	3.0	<u>2D</u>
20	127.8	Symmetric to atom 20'	6.0	6.0	<u>3D</u>
20'	128.0	0.85	6.0	6.0	<u>3D</u>
21	126.1	Symmetric to atom 21'	6.0	73.0	<u>2D</u>
21'	126.2	0.76	6.0	73.0	<u>2D</u>
22	127.8	Symmetric to atom 20'	6.0	6.0	<u>3D</u>
22'	128.0	Symmetric to atom 20'	6.0	6.0	<u>3D</u>
23	129.3	Symmetric to atom 19	6.0	4.0	<u>2D</u>
23'	130.0	Symmetric to atom 19	6.0	4.0	<u>2D</u>

3	58.7	Symmetric to atom 3'	2.0	9.0	<u>2D</u>
3'	58.3	2.31  <sup>1,2</sup>	2.0	9.0	<u>2D</u>
4	139.7	8.52	3.0	6.0	<u>2D</u>
4'	126.7	Symmetric to atom 4	3.0	6.0	<u>2D</u>
5	125.1	Symmetric to atom 5'	4.0	4.0	<u>2D</u>
5'	124.3	0.80	4.0	4.0	<u>2D</u>
6	117.7	0.85	5.0	4.0	<u>2D</u>
6'	117.7	Symmetric to atom 6	5.0	4.0	<u>2D</u>
7	128.5	Symmetric to atom 7'	6.0	4.0	<u>2D</u>
7'	129.0	0.40	6.0	4.0	<u>2D</u>
8	109.0	1.22	5.0	5.0	<u>2D</u>
8'	108.8	Symmetric to atom 8	5.0	5.0	<u>2D</u>
9	149.1	Symmetric to atom 9'	4.0	5.0	<u>2D</u>
9'	151.3	2.68	4.0	5.0	<u>2D</u>

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



Mean deviation from prediction: 1.62 ppm → 0.81 Points

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

No. of yellow shifts: 1.0 → 2.5 Points

Result: 7/accept

Created Fri Apr 12 13:05:41 CEST 2019

/  prediction unreliable

<sup>1</sup> Less than 3 spheres used

<sup>2</sup> Range > 10 ppm