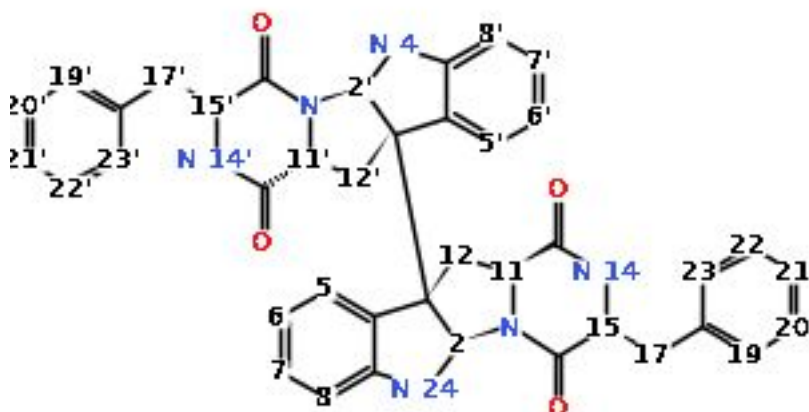


nmrshiftdb2 Quality Report - <sup>1</sup>H



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
11	4.03	Symmetric to atom 11'	4.0	1.0	<u>2D</u>
11'	1.83	2.28	4.0	1.0	<u>2D</u>
12'a	2.15	0.34, calculated from average of shifts	4.0	2.0	<u>2D</u>
12'b	2.25	0.31, calculated from average of shifts ⚠ <sup>1</sup>	2.0	314.0	<u>2D</u>
12a	2.23	Symmetric to atom 12'	4.0	2.0	<u>2D</u>
12b	2.82	Symmetric atom	2.0	314.0	<u>2D</u>
15	4.21	Symmetric to atom 15'	4.0	3.0	<u>2D</u>
15'	3.99	0.32	4.0	3.0	<u>2D</u>
17'a	2.74	Symmetric to atom 17	5.0	5.0	<u>2D</u>
17'b	3.01	0.98, calculated from average of shifts ⚠ <sup>1</sup>	2.0	314.0	<u>2D</u>
17a	2.97	0.10	5.0	5.0	<u>2D</u>
19	7.13	0.13	6.0	7.0	<u>2D</u>
19'	7.01	Symmetric to atom 19	6.0	7.0	<u>2D</u>
2	4.83	0.84	4.0	1.0	<u>2D</u>
2'	4.83	Symmetric to atom 2	4.0	1.0	<u>2D</u>
20	7.06	Symmetric to atom 20'	6.0	15.0	<u>2D</u>
20'	6.85	0.43	6.0	15.0	<u>2D</u>
21	7.06	Symmetric to atom 21'	6.0	95.0	<u>2D</u>
21'	6.84	0.38	6.0	95.0	<u>2D</u>
22	7.06	Symmetric to atom 20'	6.0	15.0	<u>2D</u>
22'	6.85	Symmetric to atom 20'	6.0	15.0	<u>2D</u>
23	7.13	Symmetric to atom 19	6.0	7.0	<u>2D</u>
23'	7.01	Symmetric to atom 19	6.0	7.0	<u>2D</u>

5	7.06	Symmetric to atom 5'	5.0	1.0	<u>2D</u>
5'	7.21	0.03	5.0	1.0	<u>2D</u>
6	6.59	0.21	6.0	1.0	<u>2D</u>
6'	6.63	Symmetric to atom 6	6.0	1.0	<u>2D</u>
7	7.0	Symmetric to atom 7'	6.0	1.0	<u>2D</u>
7'	7.13	0.00	6.0	1.0	<u>2D</u>
8	6.65	0.02	6.0	1.0	<u>2D</u>
8'	6.74	Symmetric to atom 8	6.0	1.0	<u>2D</u>

Overall mark 5 (out of 1 to 10, 10 being best)

Mean deviation from prediction: 0.45 ppm → 0.23 Points

No. of red or missing shifts: 1.0 → 5.0 Points

No. of yellow shifts: 0.0 → 0.0 Points

Result: 5/revision

Created Sun Apr 14 21:06:14 CEST 2019



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