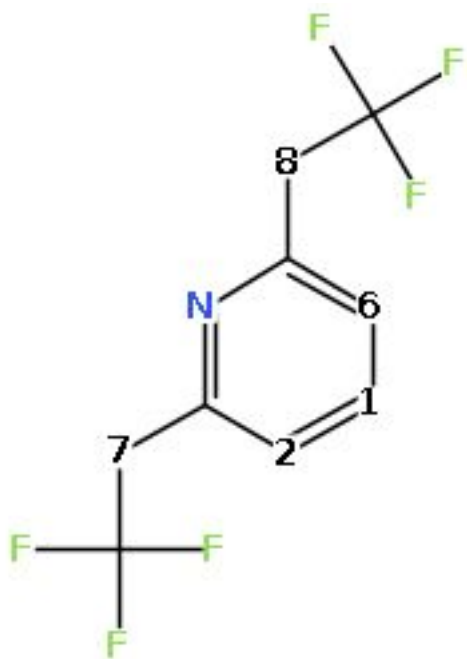


nmrshiftdb2 Quality Report - ^1H



Atom	δ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
1	7.72	0.19	4.0	11.0	<u>2D</u>
2	7.33	0.01	4.0	5.0	<u>2D</u>
6	7.33	Symmetric to atom 2	4.0	5.0	<u>2D</u>
7a	3.63	1.52 ³ 1, 2	2.0	15150.0	<u>2D</u>
7b	3.63	1.52 ³ 1, 2	2.0	15150.0	<u>2D</u>
8a	3.63	Symmetric to atom 7	2.0	15150.0	<u>2D</u>
8b	3.63	Symmetric to atom 7	2.0	15150.0	<u>2D</u>

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

Mean deviation from prediction: 0.76 ppm \rightarrow 0.38 Points

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

No. of yellow shifts: 0.0 \rightarrow 0.0 Points

Result: 10/accept

2 yellow shift(s) not taken into account because the underlying prediction was unreliable.

Created Sun Mar 07 18:31:15 CET 2021