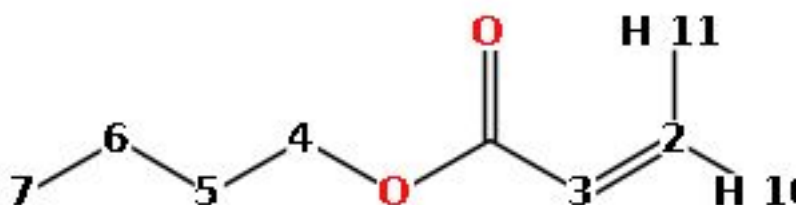


nmrshiftdb2 Quality Report -  $^1\text{H}$



Atom	$\delta$ [ppm]	Deviation from prediction	Prediction		HOSE Code
			No. Spheres	No. shift values	
2a	6.32	0.07, calculated from average of shifts	6.0	2.0	<u>3D</u>
2b	5.74	Not possible	-	-	-
3	6.05	0.01	6.0	1.0	<u>3D</u>
4a	4.09	0.18	4.0	3.0	<u>2D</u>
5a	1.59	0.17	5.0	1.0	<u>2D</u>
6a	1.34	0.17	6.0	1.0	<u>2D</u>
7	0.88	0.08	6.0	3.0	<u>2D</u>

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

Mean deviation from prediction: 0.11 ppm  $\rightarrow$  0.06 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**

Created Wed Jun 05 07:58:03 CEST 2019