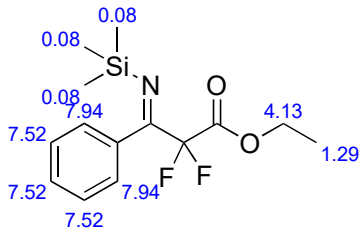
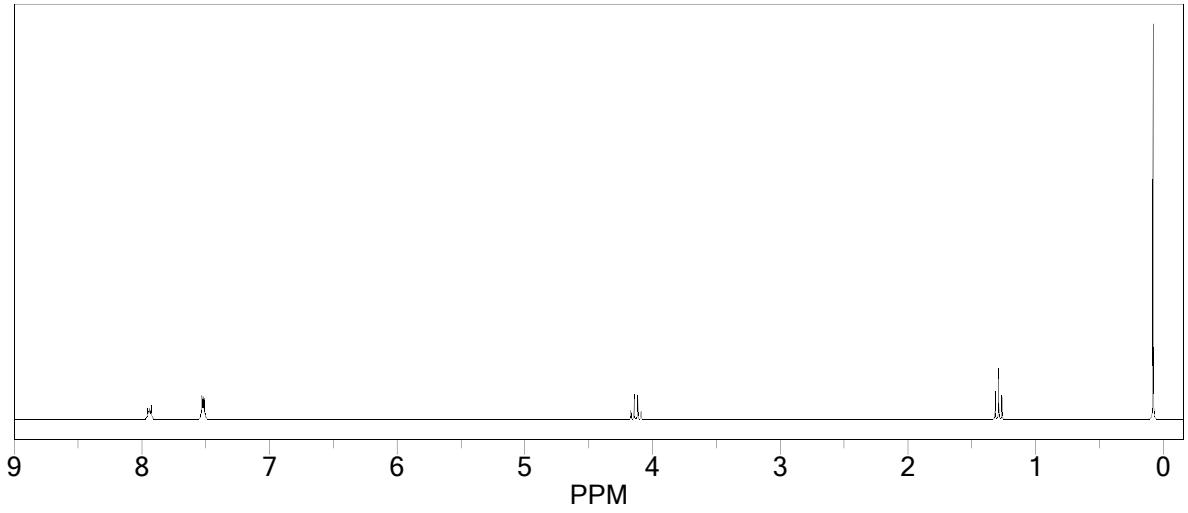
ChemNMR ^{1}H Estimation



Estimation quality is indicated by color: good, medium, rough



Protocol of the H-1 NMR Prediction:

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
CH	7.94	7.62	benzylidenimin
		?	1 unknown substituent(s)
		0.32	general corrections
CH	7.94	7.62	benzylidenimin
		?	1 unknown substituent(s)
		0.32	general corrections
CH	7.52	7.29	benzylidenimin
		?	1 unknown substituent(s)
		0.23	general corrections
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		?	1 unknown substituent(s)
		0.23	general corrections
CH3	0.08	0.86	methyl
		-0.78	1 alpha -Si(C)C
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		-0.78	1 alpha -Si(C)C
CH2	4.13	1.37	methylene
		0.00	1 alpha -C
		2.75	1 alpha -OC(=O)-C
		0.01	general corrections
CH3	1.29	0.86	methyl
		0.44	1 beta -OC(=O)C
		-0.01	general corrections

1H NMR Coupling Constant Prediction

shift	atom index	coupling partner, constant and vector
7.94	6	
		1 7.5 H-C*C-H
		4 1.5 H-C*C*C-H

		4	1.5	H-C*C*C-H
		2	1.5	H-C*CH*C-H
7.94	4			
		3	7.5	H-C*C-H
		6	1.5	H-C*C*C-H
		2	1.5	H-C*CH*C-H
7.52	3			
		4	7.5	H-C*C-H
		2	7.5	H-C*C-H
		1	1.5	H-C*CH*C-H
7.52	1			
		6	7.5	H-C*C-H
		2	7.5	H-C*C-H
		3	1.5	H-C*CH*C-H
7.52	2			
		3	7.5	H-C*C-H
		1	7.5	H-C*C-H
		4	1.5	H-C*CH*C-H
		6	1.5	H-C*CH*C-H
0.08	18			
0.08	19			
0.08	20			
4.13	13			
		14	8.0	H-CH-CH2-H
1.29	14			
		13	8.0	H-CH2-CH-H