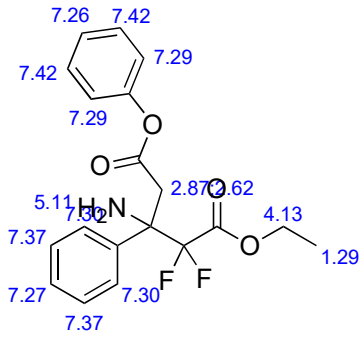
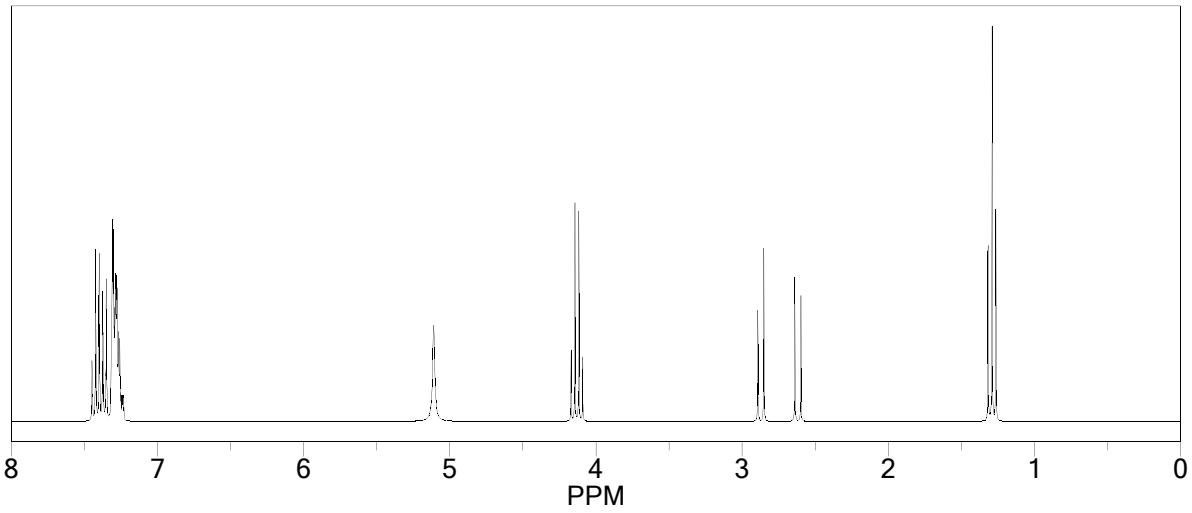
ChemNMR ^{1}H Estimation



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)
NH2	5.11	2.00	amine
		3.11	general corrections
CH	7.29	7.26	1-benzene
		-0.19	1 -OC(=O)C
		0.22	general corrections
CH	7.30	7.26	1-benzene
		-0.13	1 -C(C)C
		0.17	general corrections
CH	7.29	7.26	1-benzene
		-0.19	1 -OC(=O)C
		0.22	general corrections
CH	7.30	7.26	1-benzene
		-0.13	1 -C(C)C
		0.17	general corrections
CH	7.42	7.26	1-benzene
		-0.03	1 -OC(=O)C
		0.19	general corrections
CH	7.37	7.26	1-benzene
		-0.08	1 -C(C)C
		0.19	general corrections
CH	7.42	7.26	1-benzene
		-0.03	1 -OC(=O)C
		0.19	general corrections
CH	7.37	7.26	1-benzene
		-0.08	1 -C(C)C
		0.19	general corrections
CH	7.26	7.26	1-benzene
		-0.19	1 -OC(=O)C
		0.19	general corrections
CH	7.27	7.26	1-benzene
		-0.18	1 -C(C)C
		0.19	general corrections

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                          0.19      general corrections
CH2 4.13              1.37      methylene
                          0.00      1 alpha -C
                          2.75      1 alpha -OC(=O)-C
                          0.01      general corrections
CH2 2.87,2.615000         1.37      methylene
                          0.90      1 alpha -C(=O)O
                          0.29      1 beta -1:C*C*C*C*C*C*1
                          0.22      1 beta -N
                         -0.04      1 beta -C
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

5.11       16
7.29       22
                   23   7.5  H-C*C-H
                   26   1.5  H-C*C*C-H
                   24   1.5  H-C*CH*C-H
7.30        6
                    1   7.5  H-C*C-H
                    4   1.5  H-C*C*C-H
                    2   1.5  H-C*CH*C-H
7.29       26
                   25   7.5  H-C*C-H
                   22   1.5  H-C*C*C-H
                   24   1.5  H-C*CH*C-H
7.30        4
                    3   7.5  H-C*C-H
                    6   1.5  H-C*C*C-H
                    2   1.5  H-C*CH*C-H
7.42       25
                   26   7.5  H-C*C-H
                   24   7.5  H-C*C-H
                   23   1.5  H-C*CH*C-H
7.37        3
                    4   7.5  H-C*C-H
                    2   7.5  H-C*C-H
                    1   1.5  H-C*CH*C-H
7.42       23
                   22   7.5  H-C*C-H
                   24   7.5  H-C*C-H
                   25   1.5  H-C*CH*C-H
7.37        1
                    6   7.5  H-C*C-H
                    2   7.5  H-C*C-H
                    3   1.5  H-C*CH*C-H
7.26       24
                   25   7.5  H-C*C-H
                   23   7.5  H-C*C-H
                   26   1.5  H-C*CH*C-H
                   22   1.5  H-C*CH*C-H
7.27        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
4.13       12
                   13   8.0  H-CH-CH2-H
2.74       17 diastereotopic -12.4  H-C-H
1.29       13
                   12   8.0  H-CH2-CH-H
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