Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Diethylammonium Iodide as Catalyst for the Metal-Free Synthesis of 5-Aryl-2-Oxazolidinones from Aziridines and Carbon Dioxide

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Supporting Information

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Figure S1. Comparative view of the ^{1}H NMR spectra (CD_3CN, N_2 atmosphere) of: 1-methyl-2-phenylaziridine (top); 1-methyl-2-phenylaziridine/$[NBu_4]I$ 1:1 molar mixture (middle); 1-methyl-2-phenylaziridine/$[NBu_4]I$ 1:1 molar mixture after 4 days (bottom).

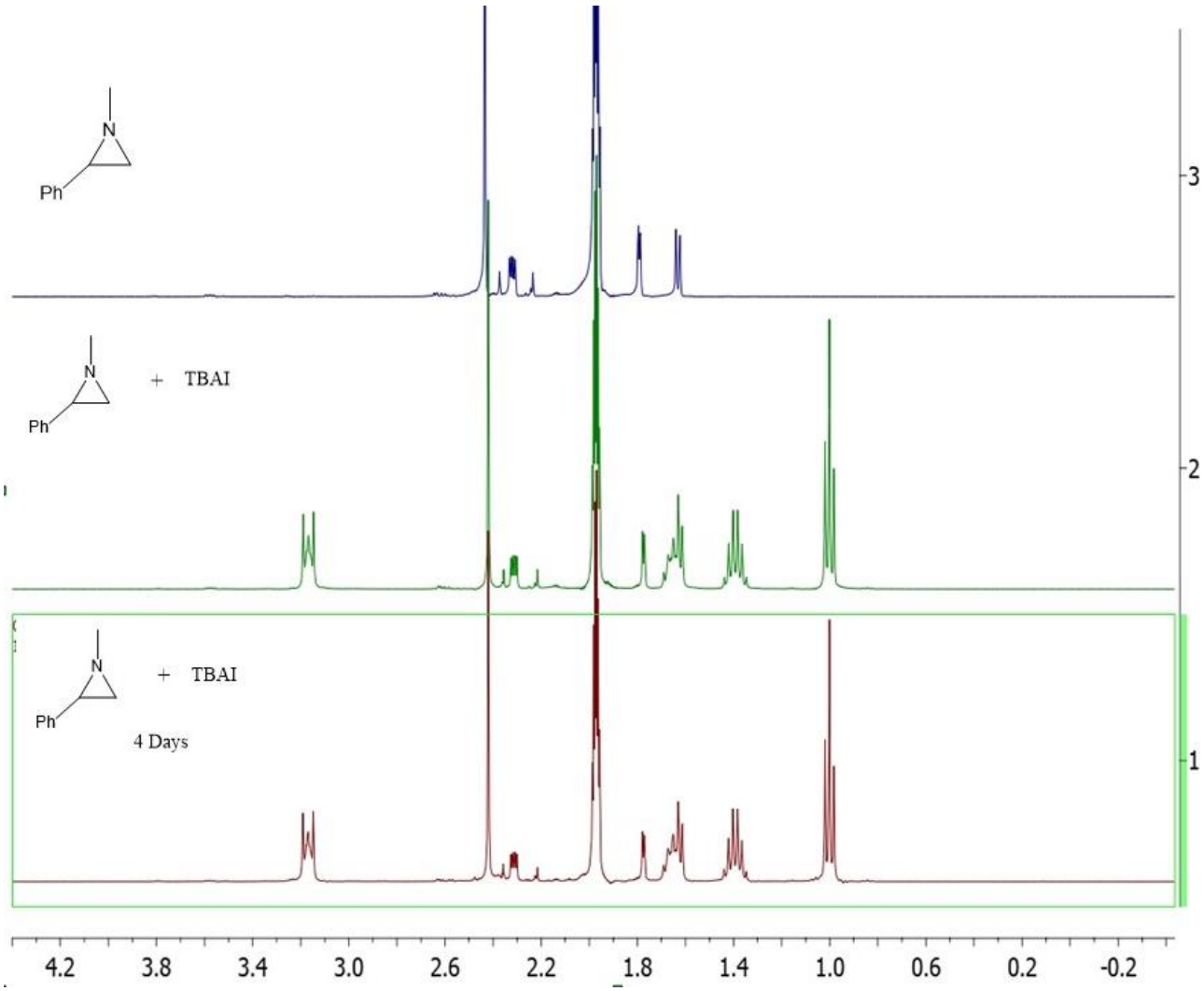


Figure S2. Comparative view of the ^{1}H NMR spectra (CD_3CN, N_2 atmosphere) of: 1-methyl-2-phenylaziridine (top); $[NH_2Et_2]I$ (middle); 1-methyl-2-phenylaziridine/$[NH_2Et_2]I$ 1:1 molar mixture after 2 hours (bottom).

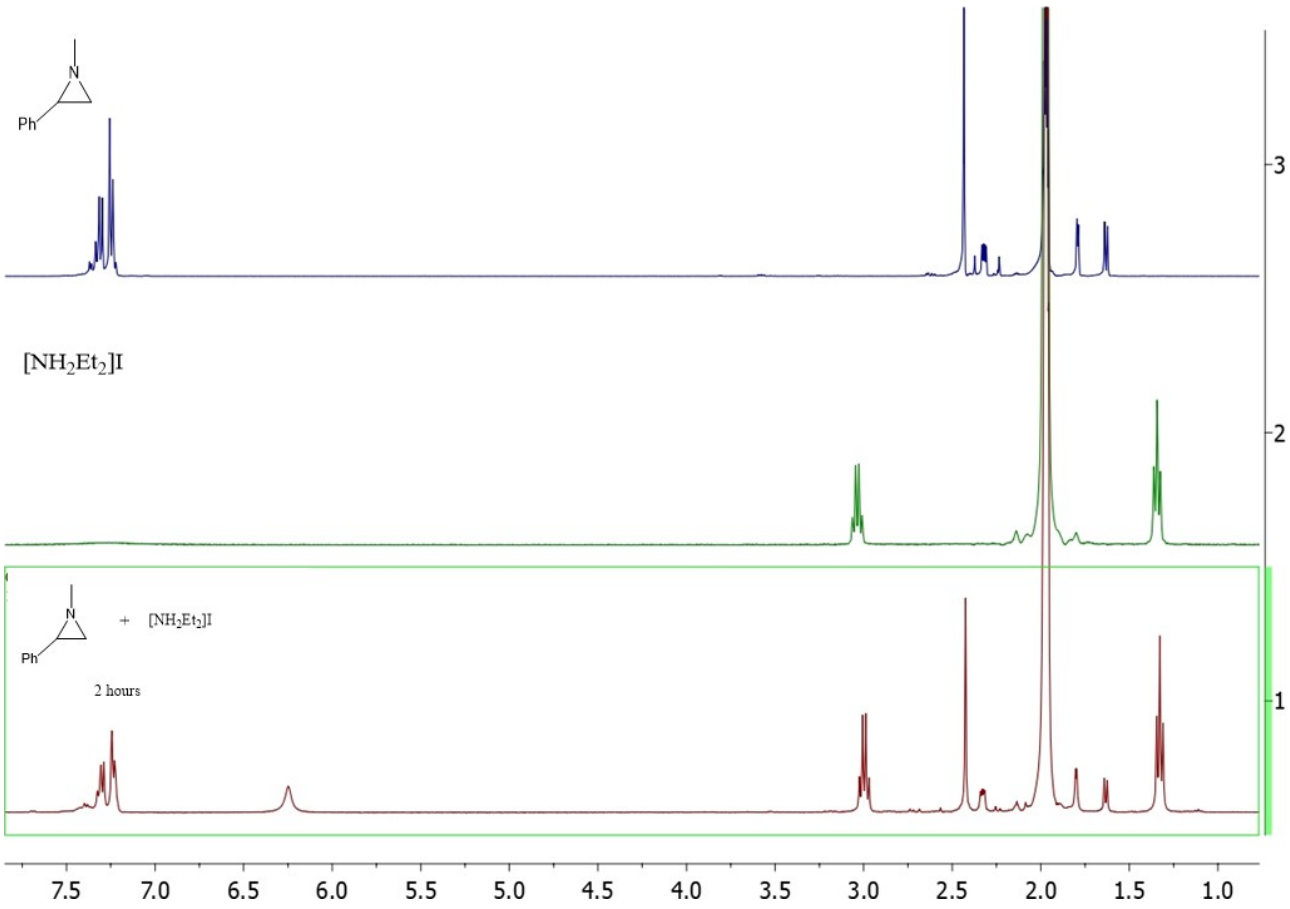


Figure S3. Transition state geometry for the reaction between 1-methyl-2-phenylaziridine and iodide in the presence of CO_2. C-PCM/B3PW91/def2-SVP calculations, ε = 8.9. Imaginary frequency i259.89 cm^{-1}.

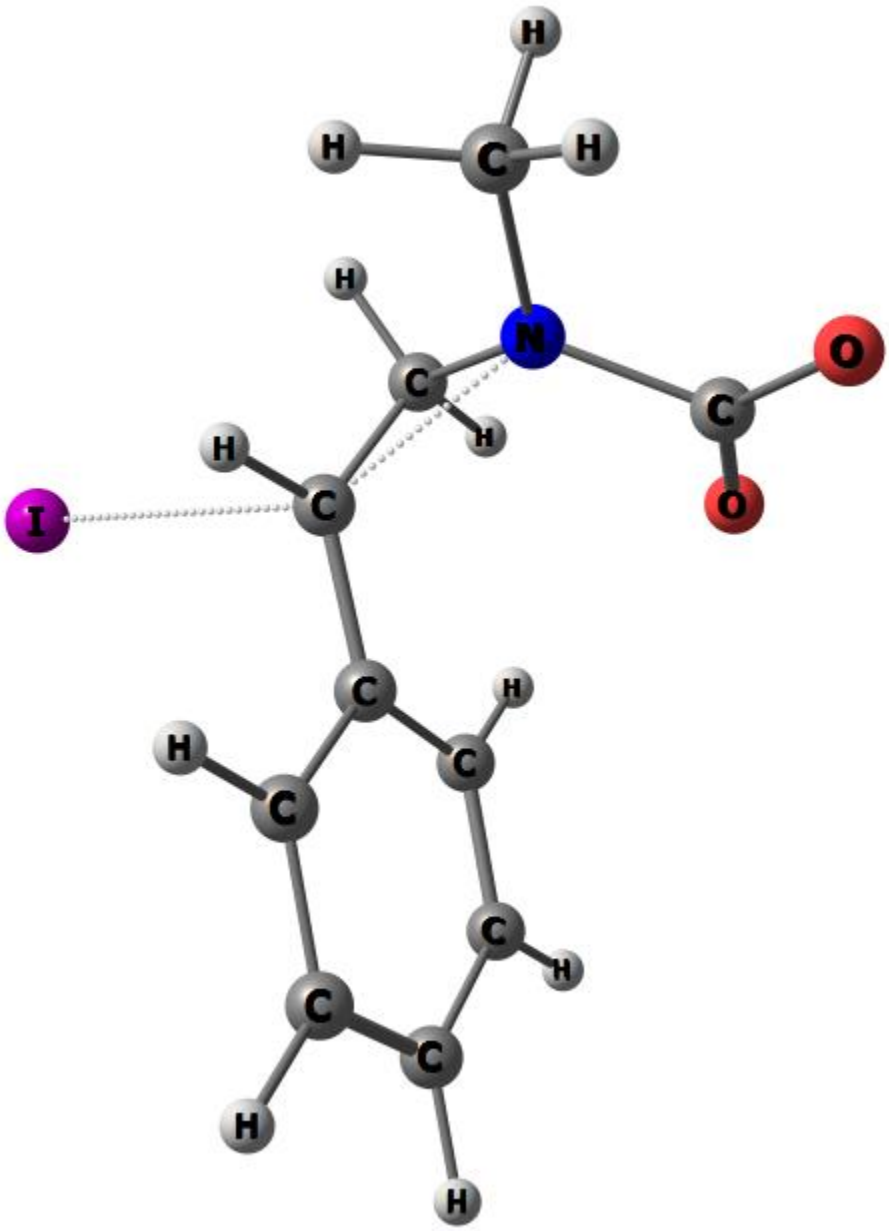


Figure S4. Hydrogen bond interaction between 1-methyl-2-phenylaziridine and $[NH_2Et_2]^+$ (step **a** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9.

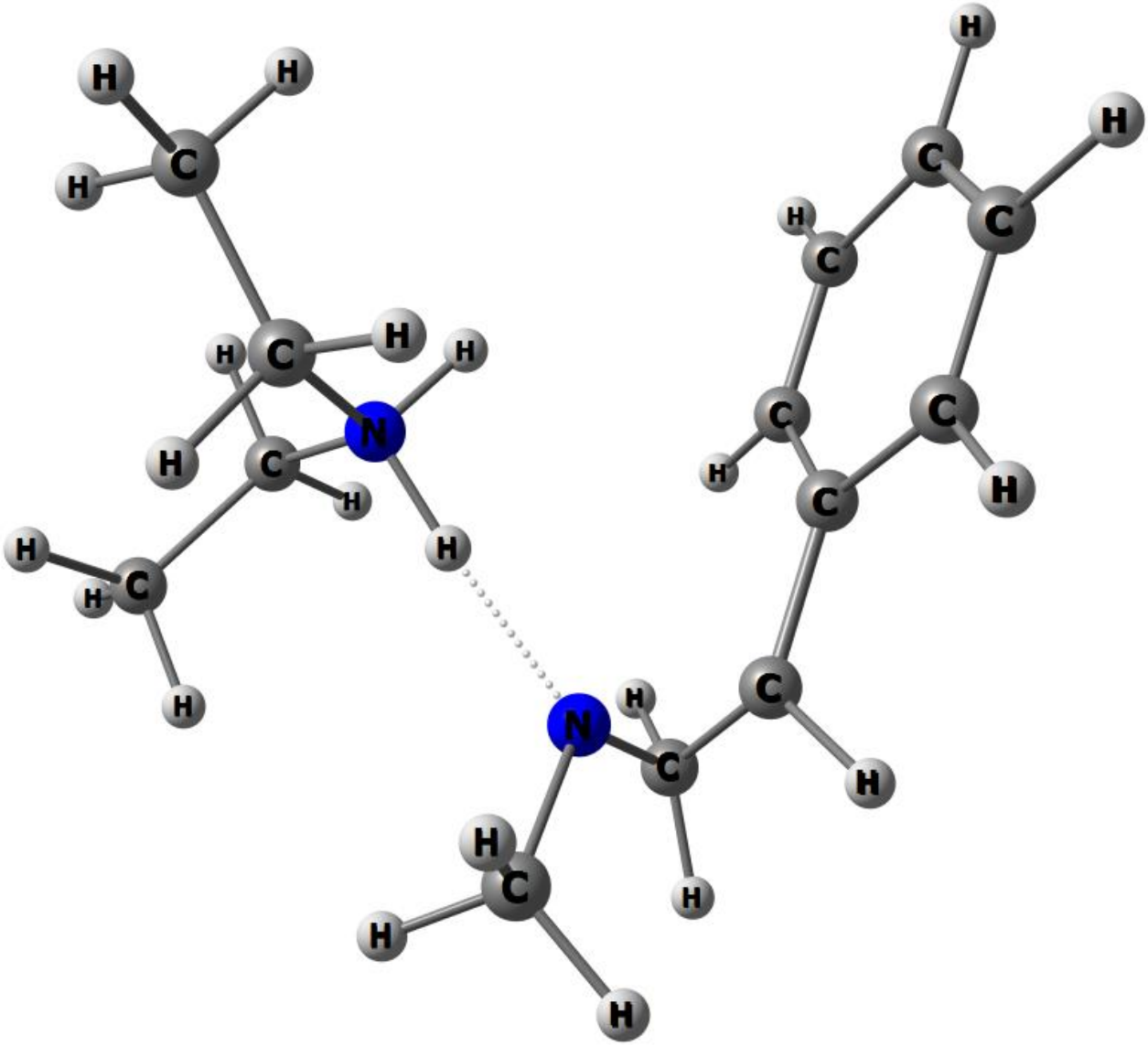


Figure S5. Transition state geometries for the nucleophilic attack of X^- (X = Br, I) to 1-methyl-2-phenylaziridine in the presence of $[NH_2Et_2]^+$ (step **b** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9. Imaginary frequencies i359.23 cm^{-1} (X = Br), i323.36 cm^{-1} (X = I).

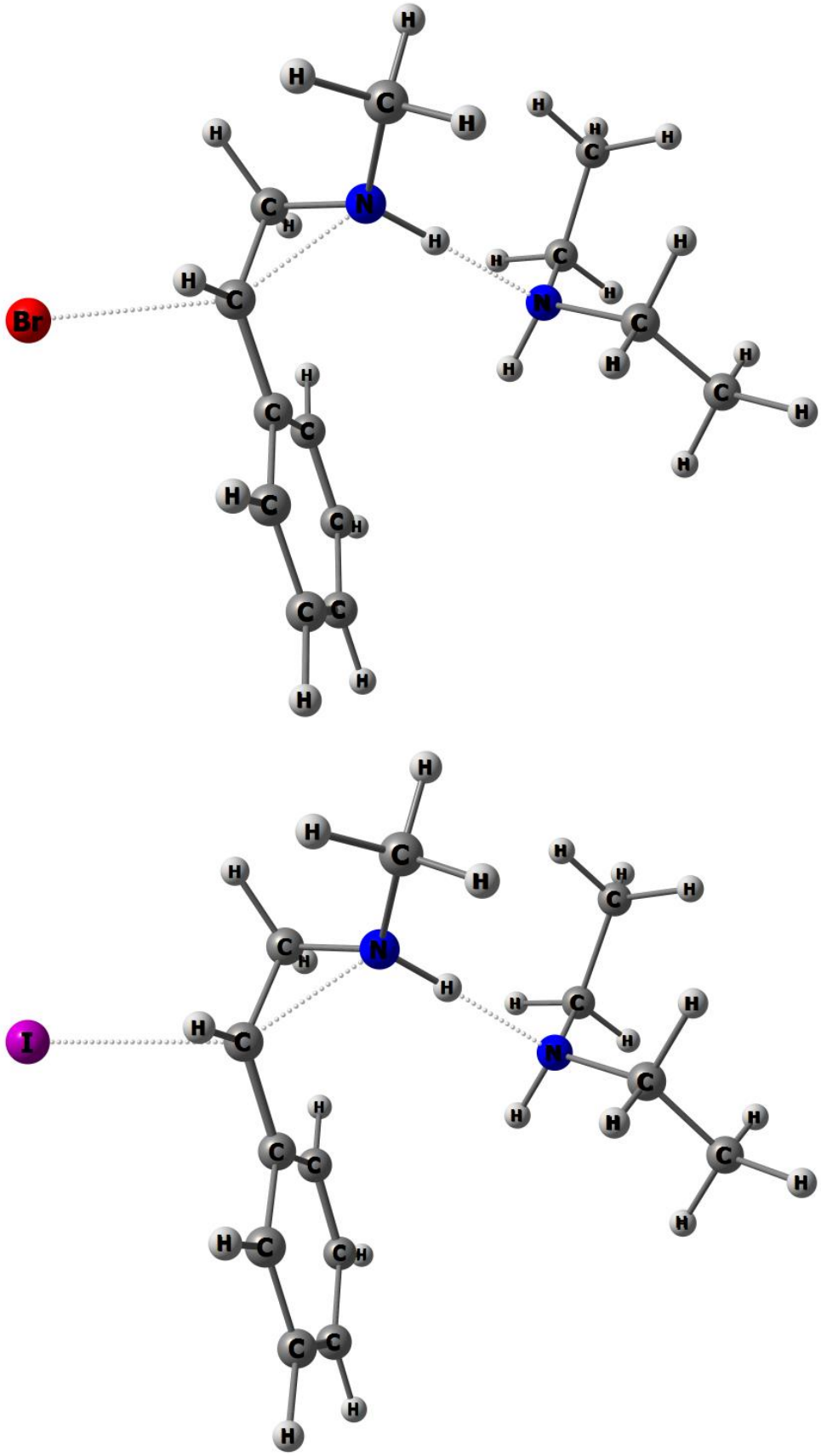


Figure S6. Intermediate species after the nucleophilic attack of X^- (X = Br, I) to 1-methyl-2-phenylaziridine in the presence of $[NH_2Et_2]^+$ (step **c** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9.

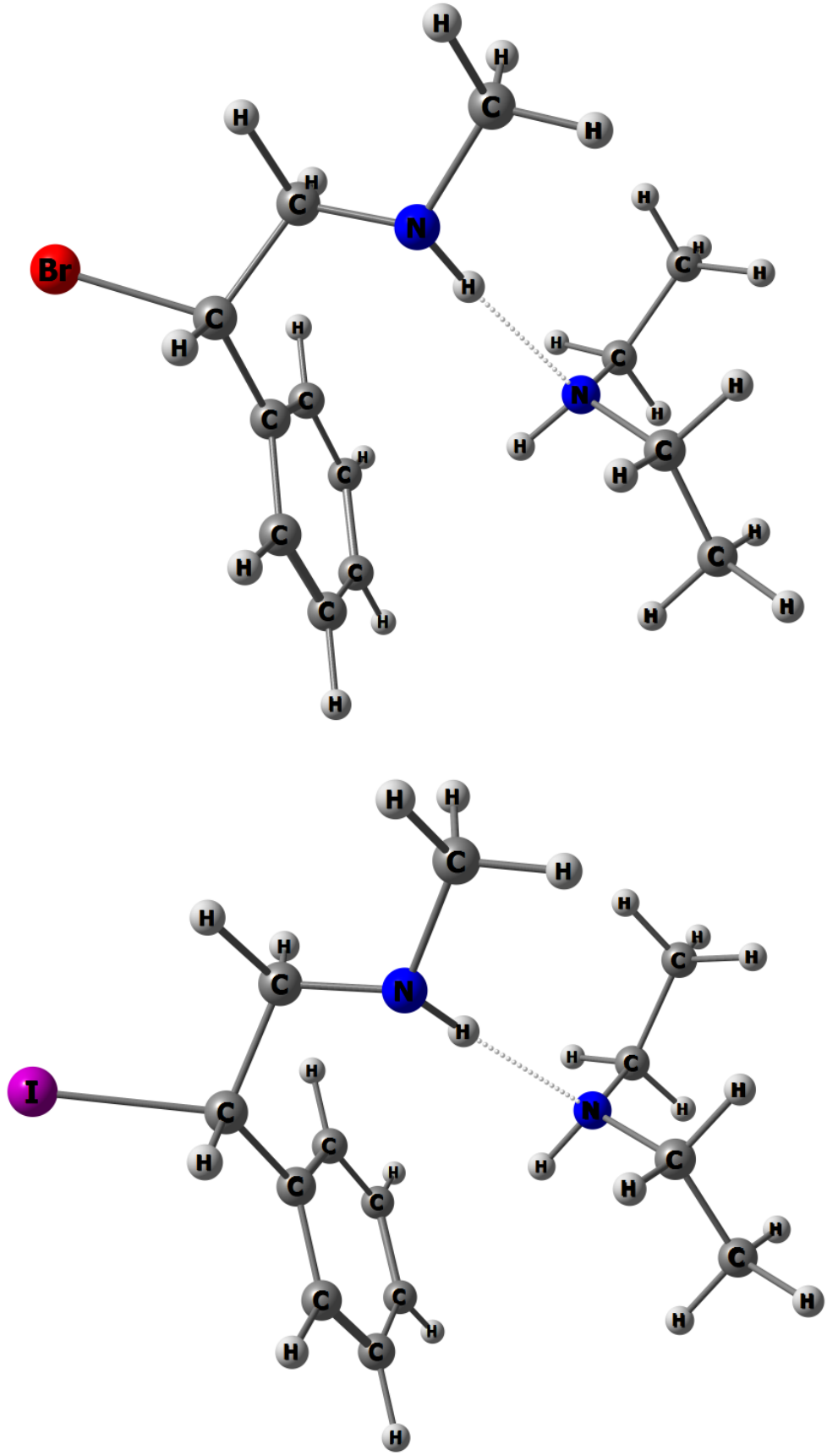
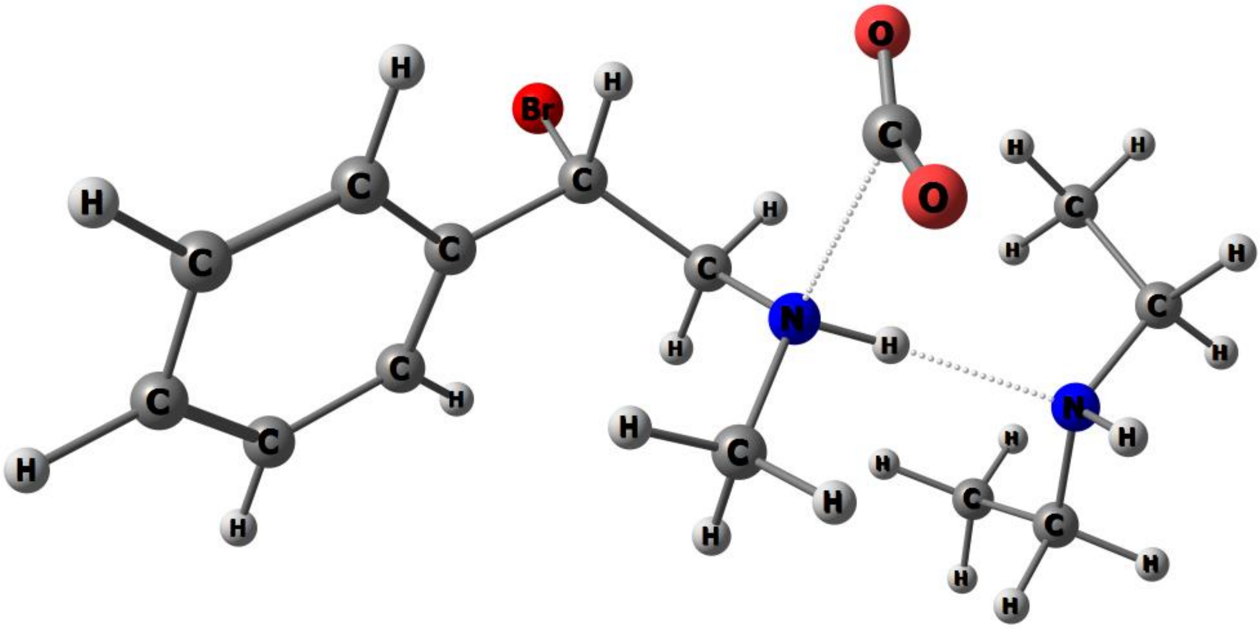


Figure S7. Transition state geometries for the interaction of the amines with CO_2 in the presence of $[NH_2Et_2]^+$ (step **d** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9. Imaginary frequencies i149.58 cm^{-1} (X = Br), i150.95 cm^{-1} (X = I).



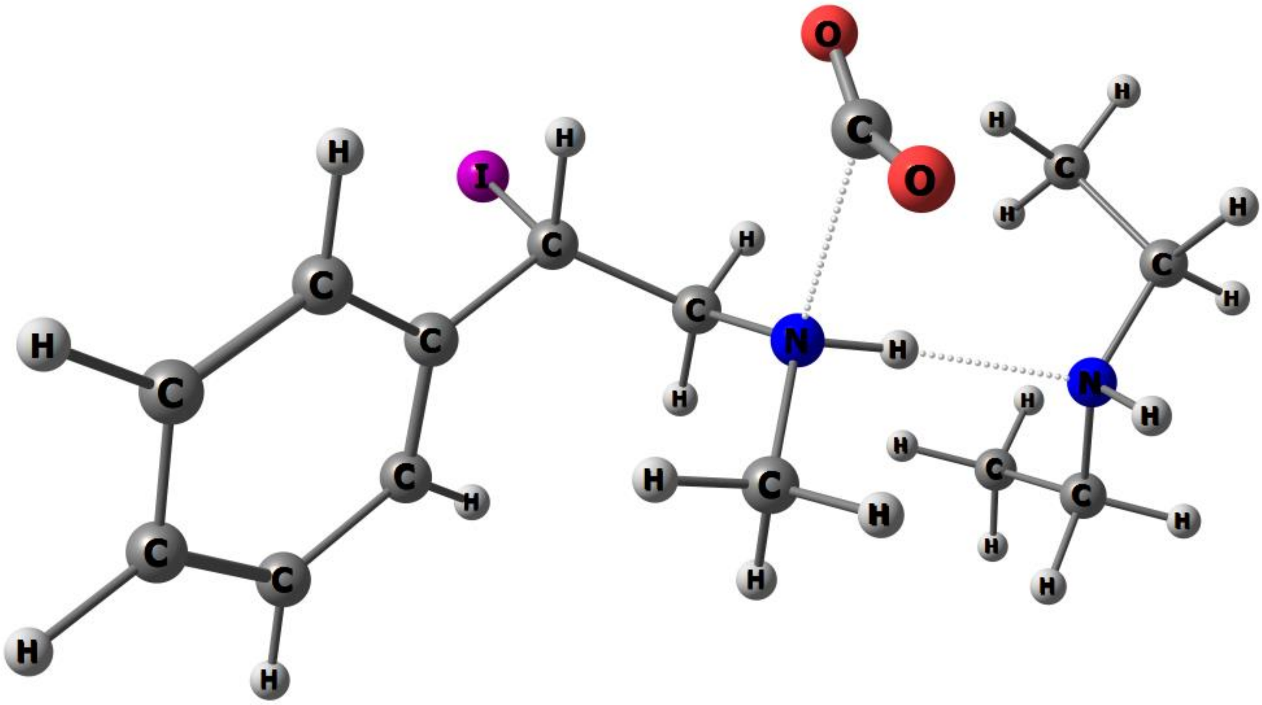


Figure S8. Intermediate carbamic acids after the interaction of the amines with CO_2 in the presence of $[NH_2Et_2]^+$ (step **e** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9.

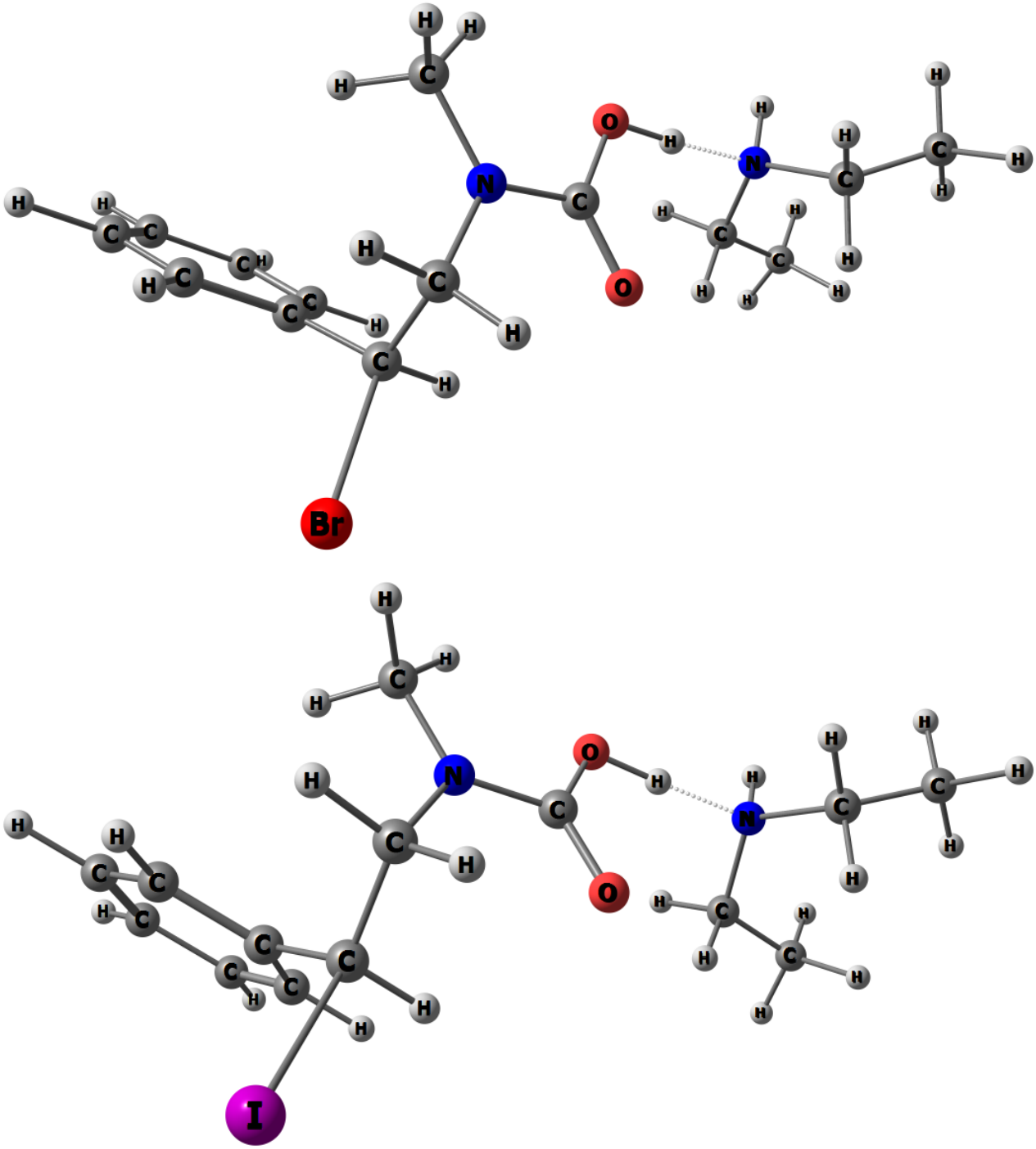


Figure S9. Transition state geometries for the intramolecular cyclization reactions in the presence of $[NH_2Et_2]^+$ (step **f** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9. Imaginary frequencies i344.54 cm^{-1} (X = Br), i300.35 cm^{-1} (X = I).

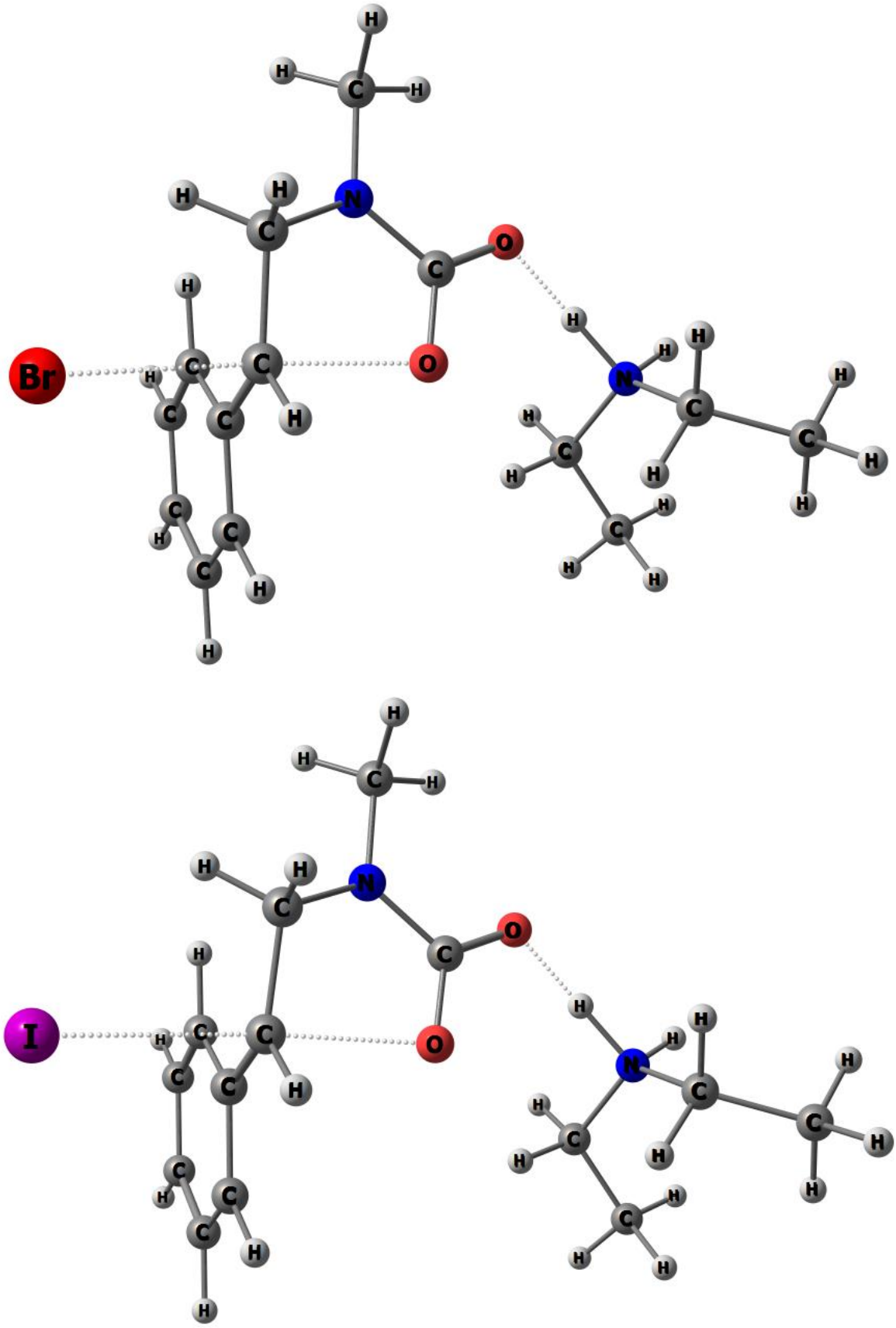
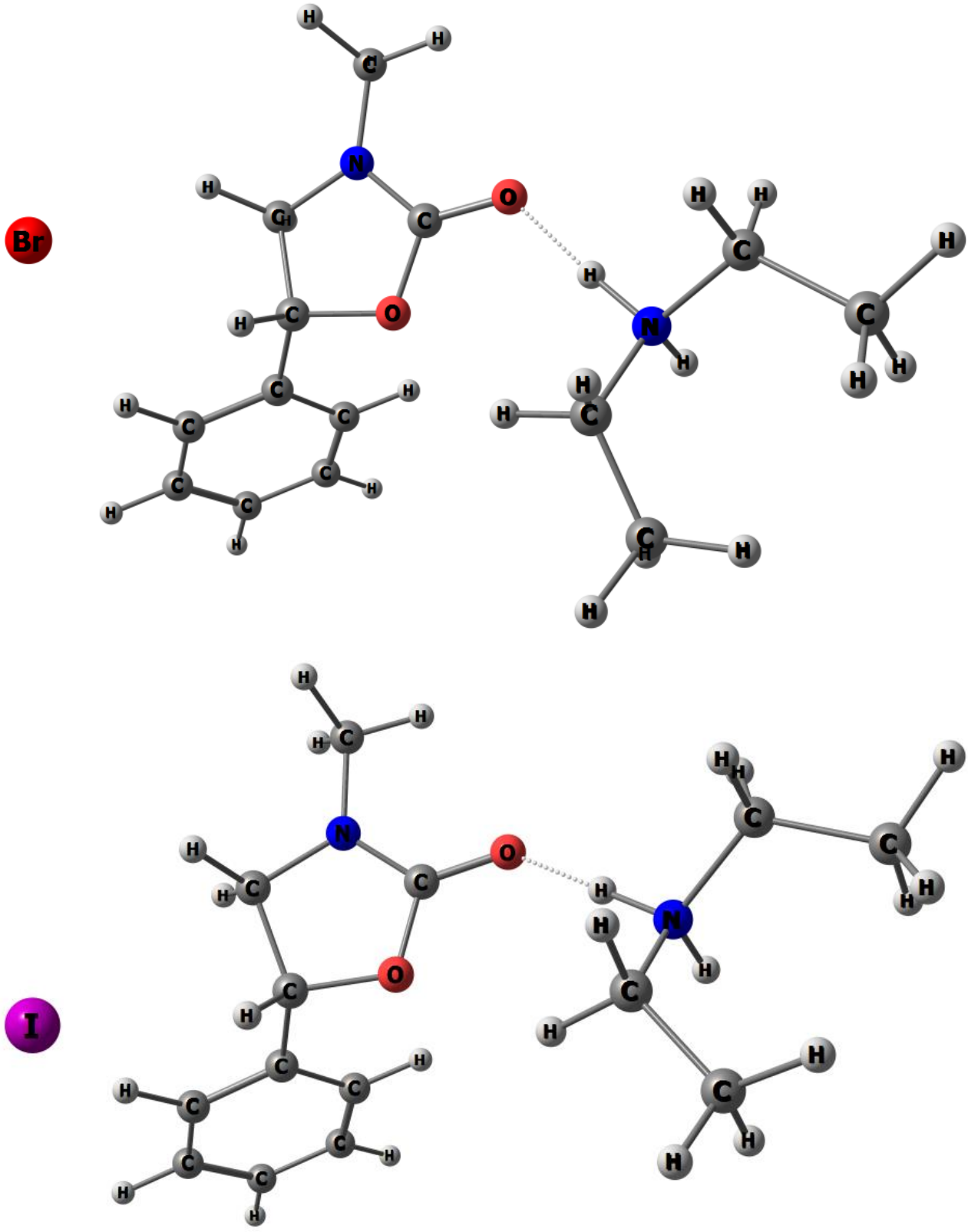
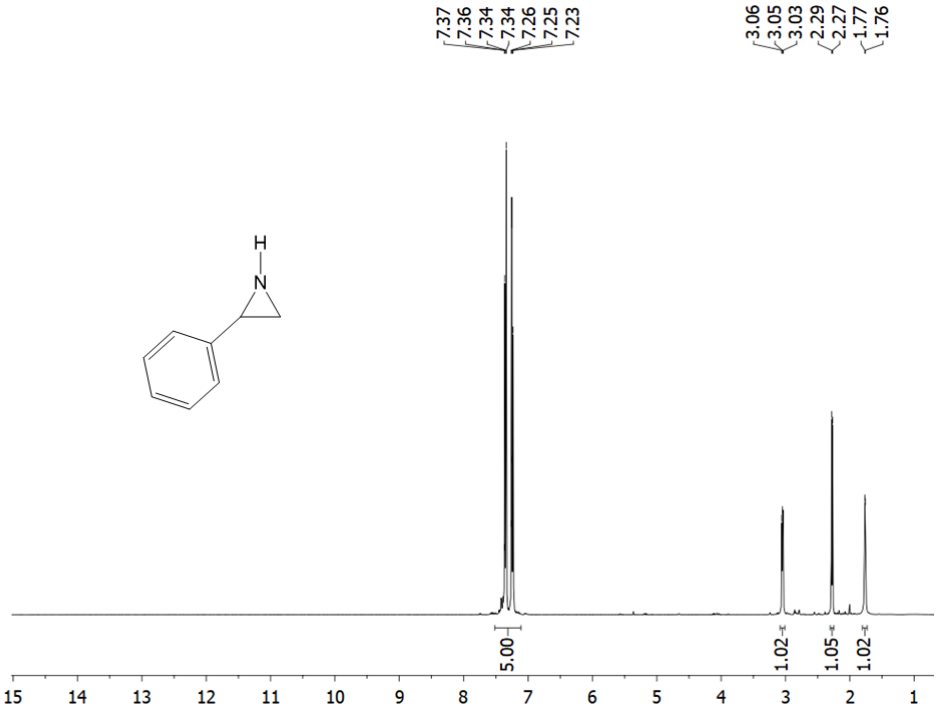
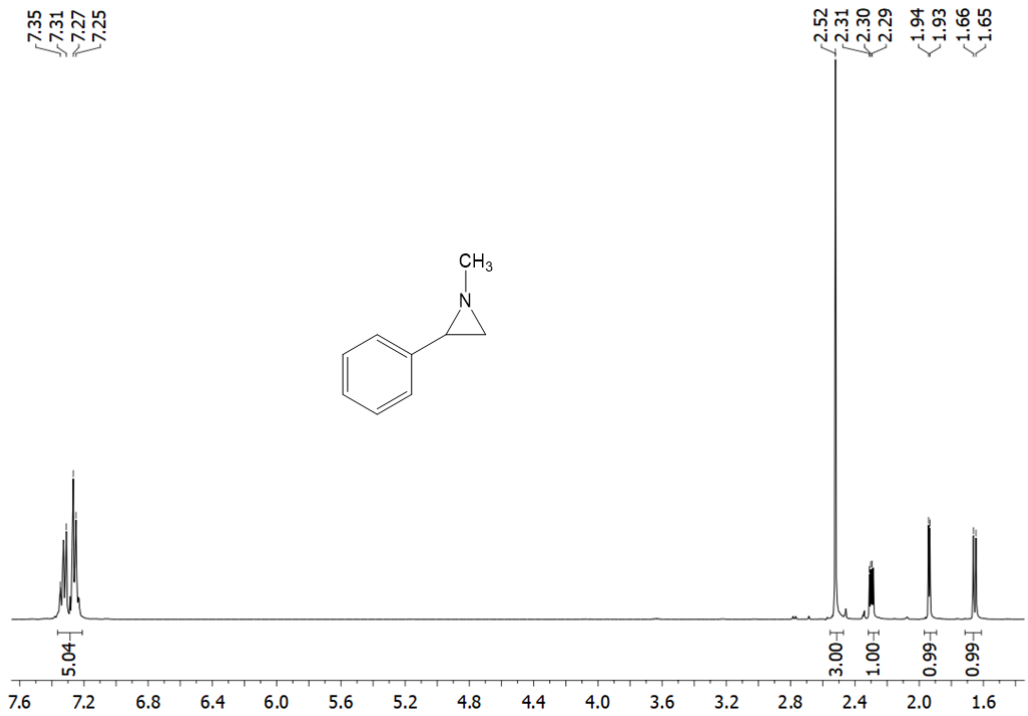


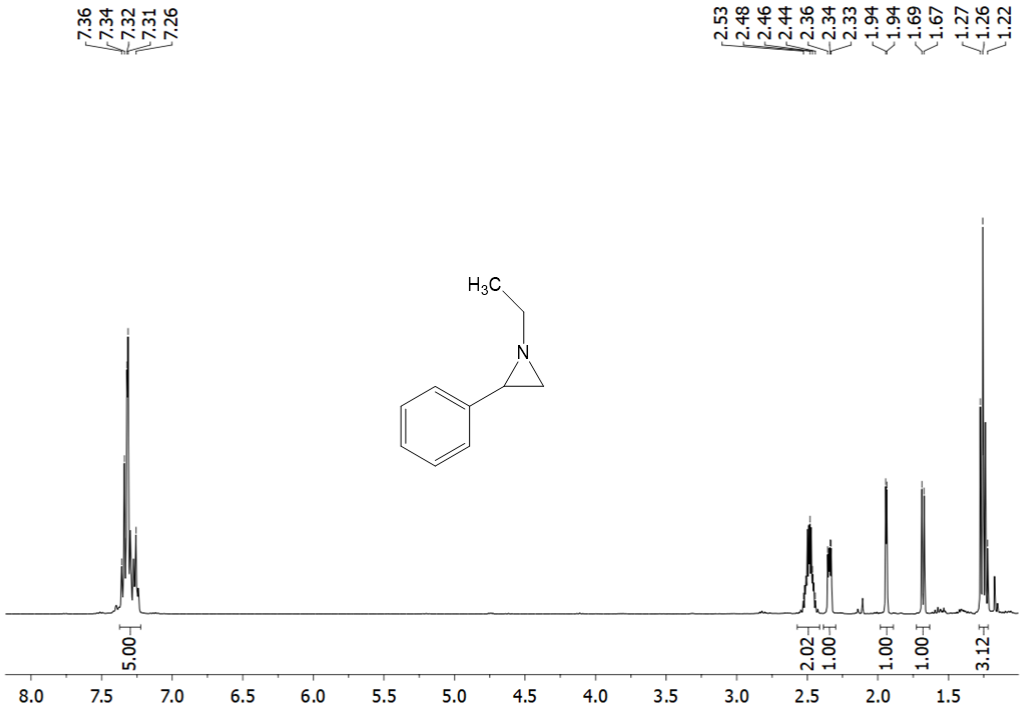
Figure S10. 3-methyl-5-phenyloxazolidin-2-one, $[NH_2Et_2]^+$ and X^- formed after the intramolecular cyclization reaction of the carbamic acids (step **g** in Figure 1). C-PCM/B3PW91/def2-SVP calculations, ε = 8.9.



NMR spectra of aziridines



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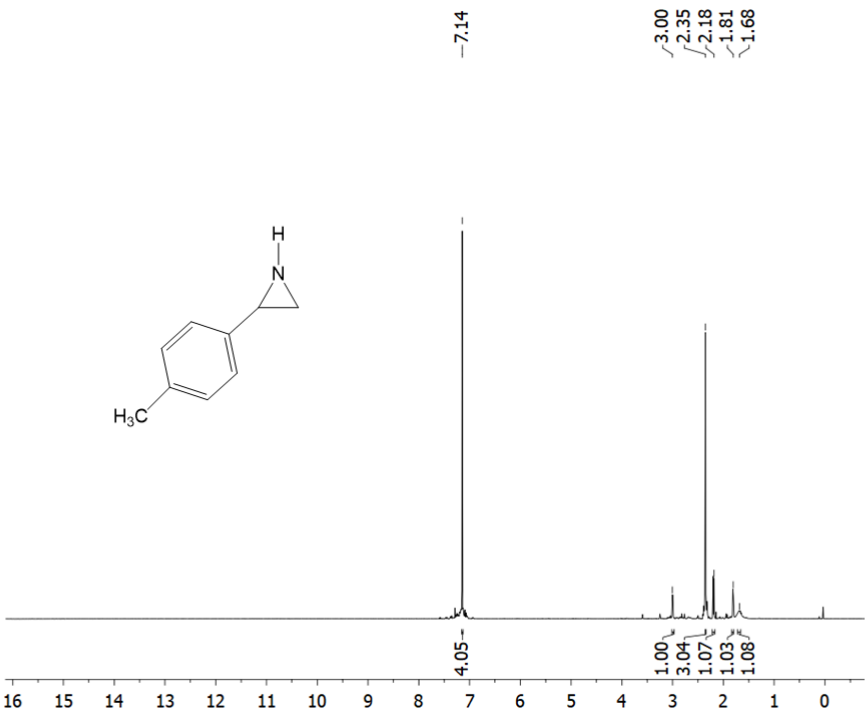
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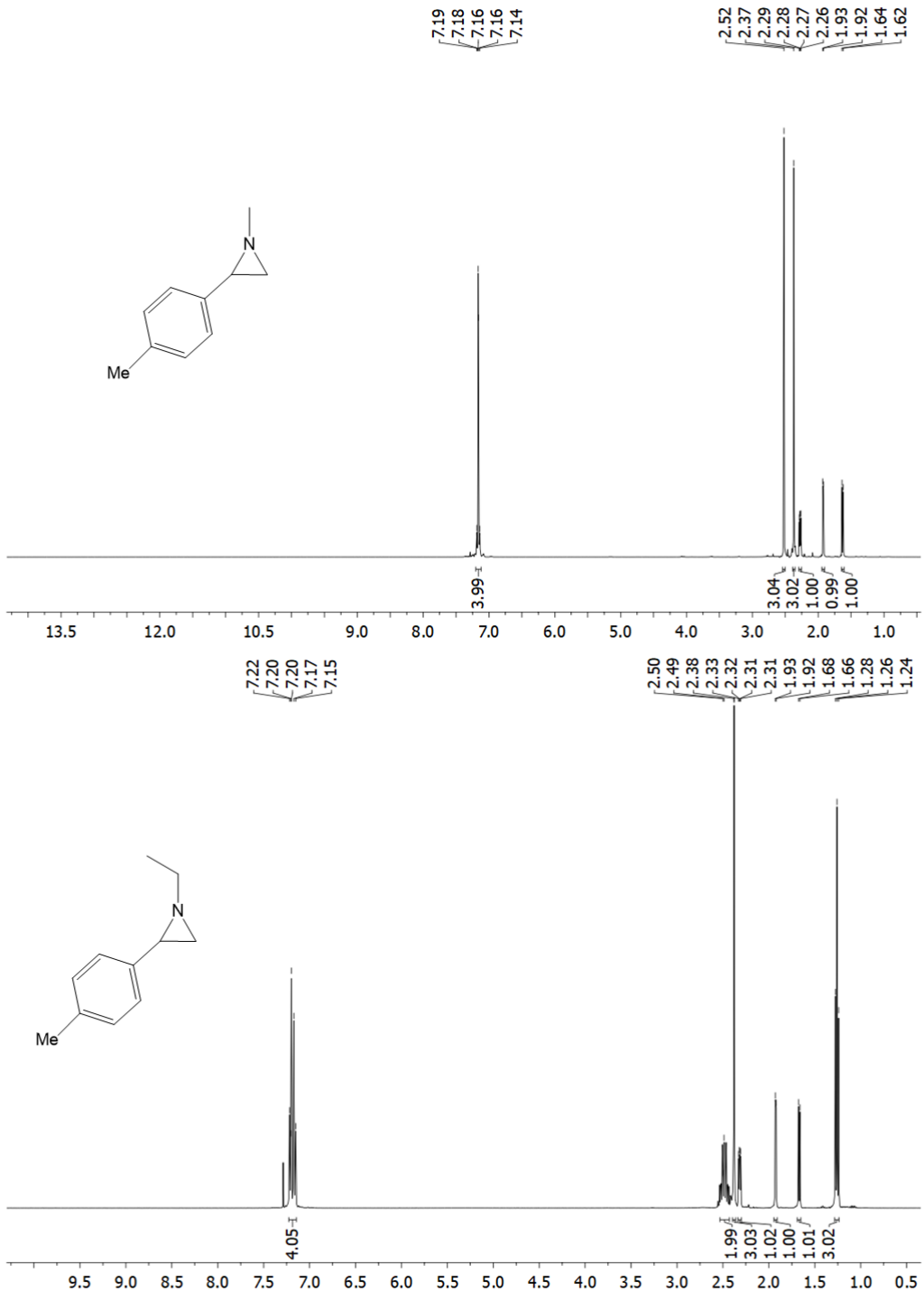
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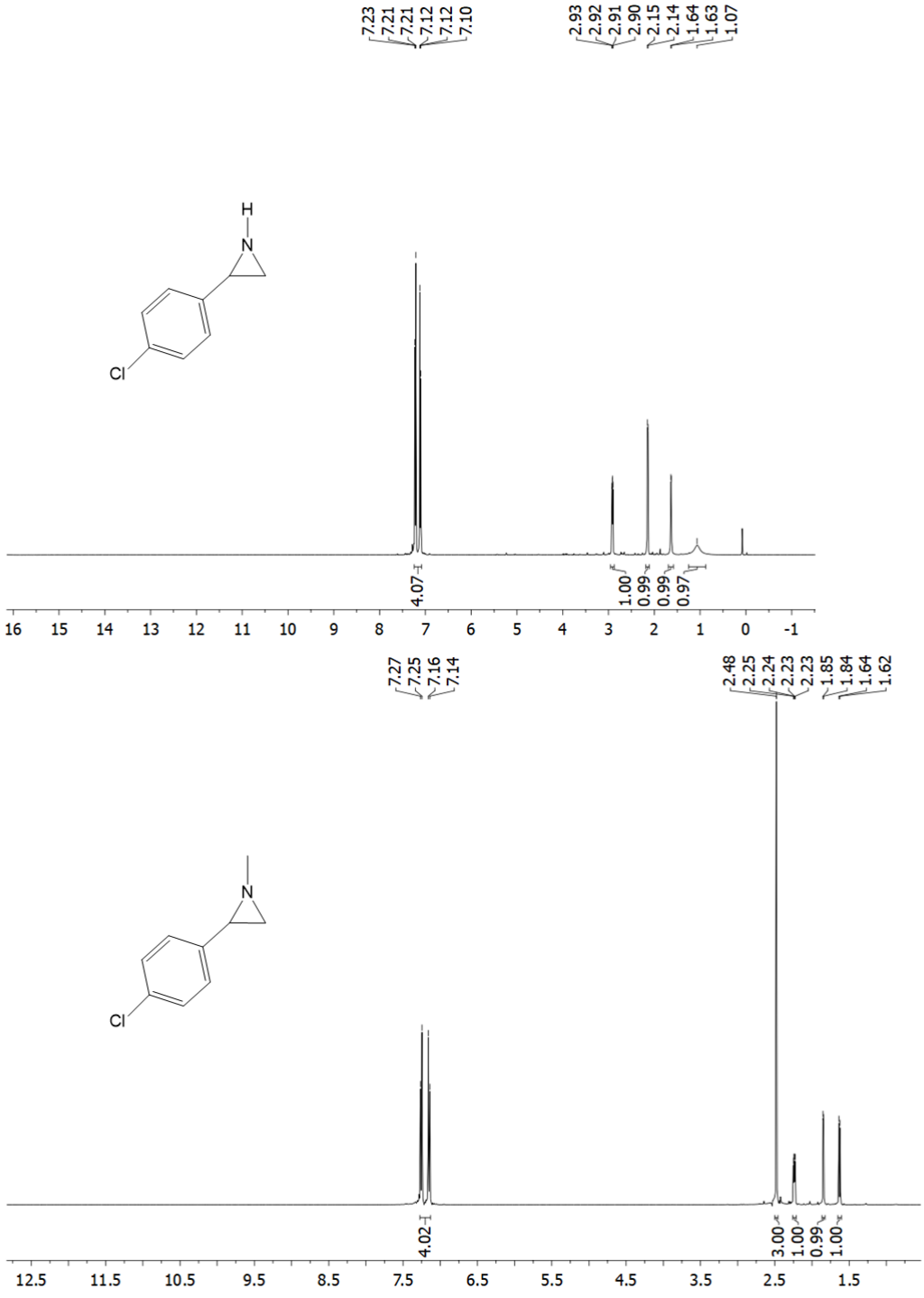
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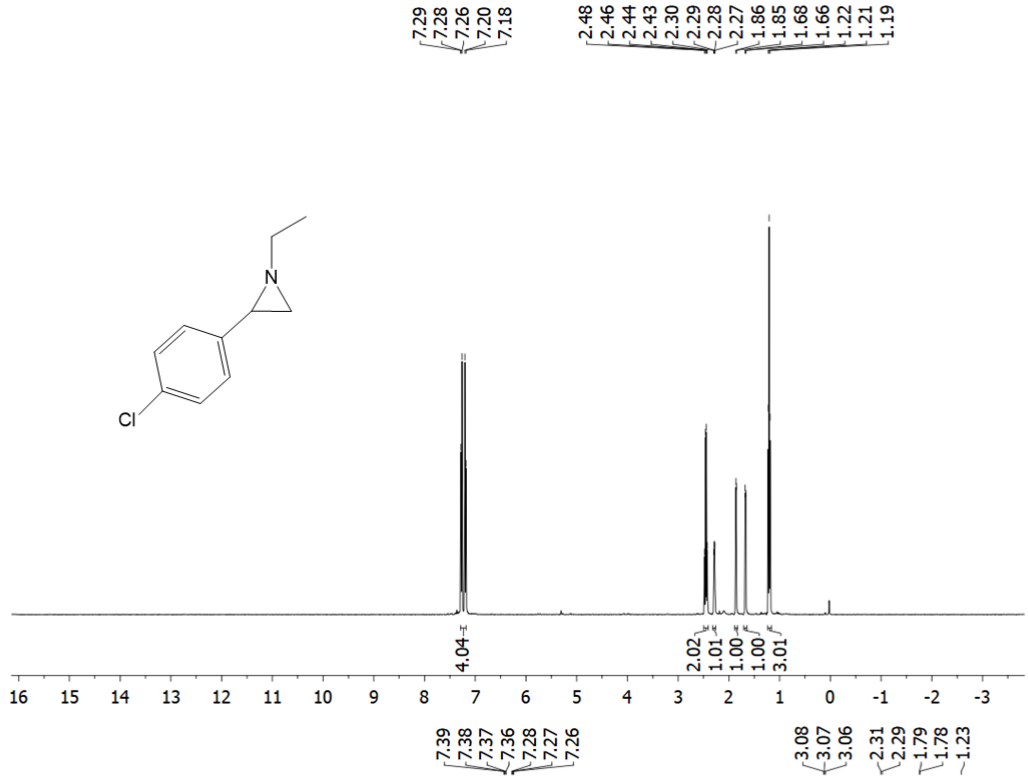
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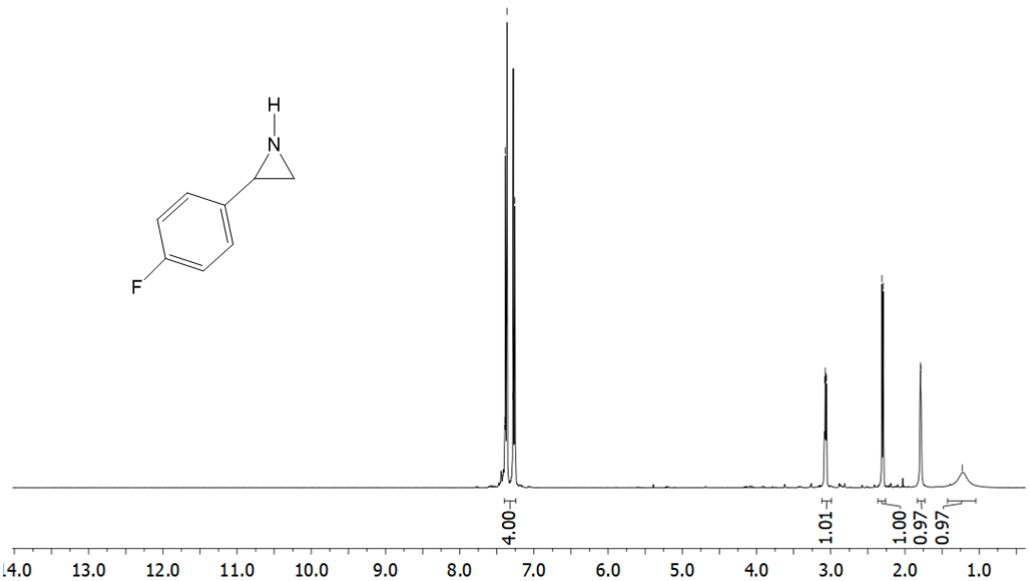
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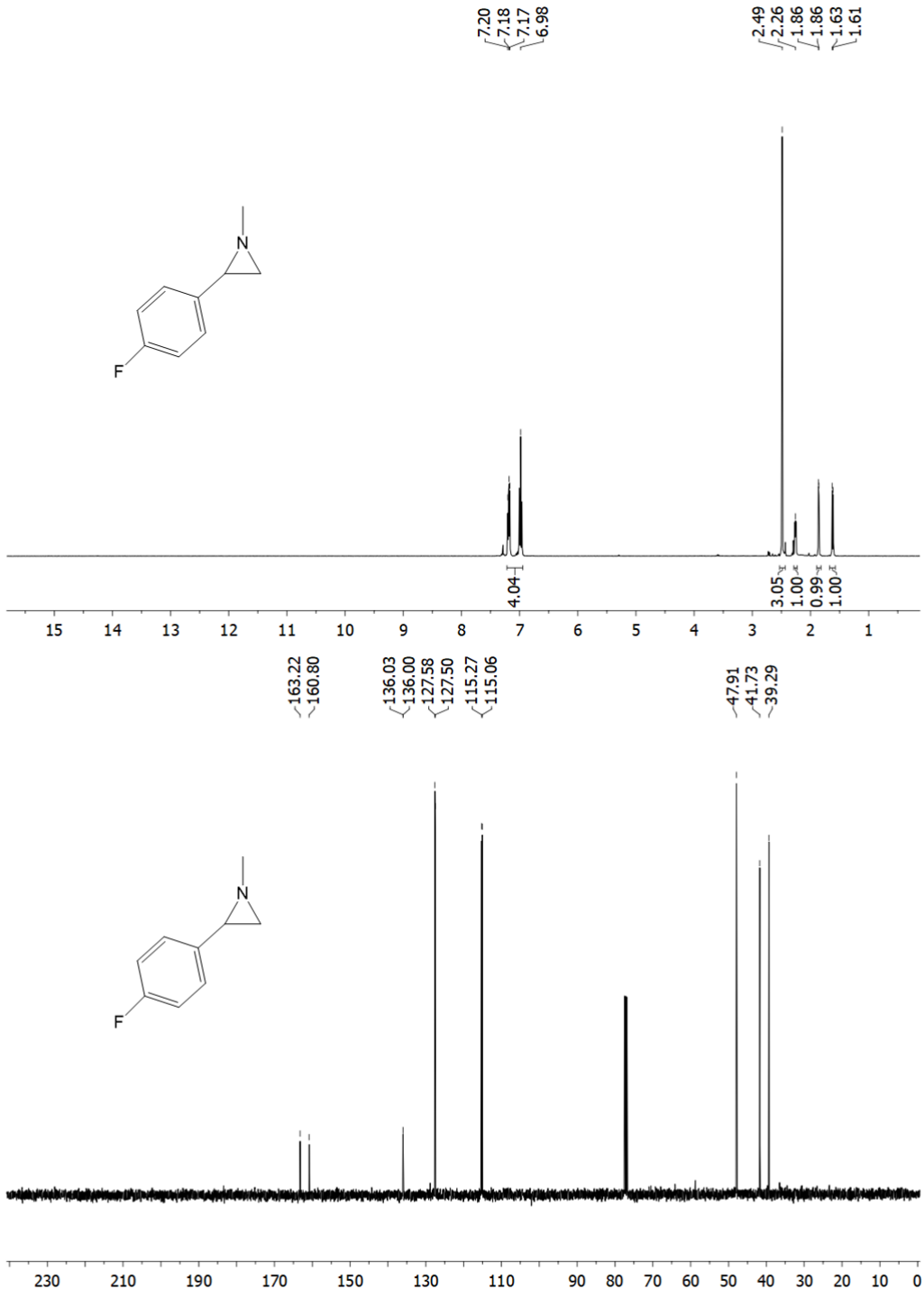
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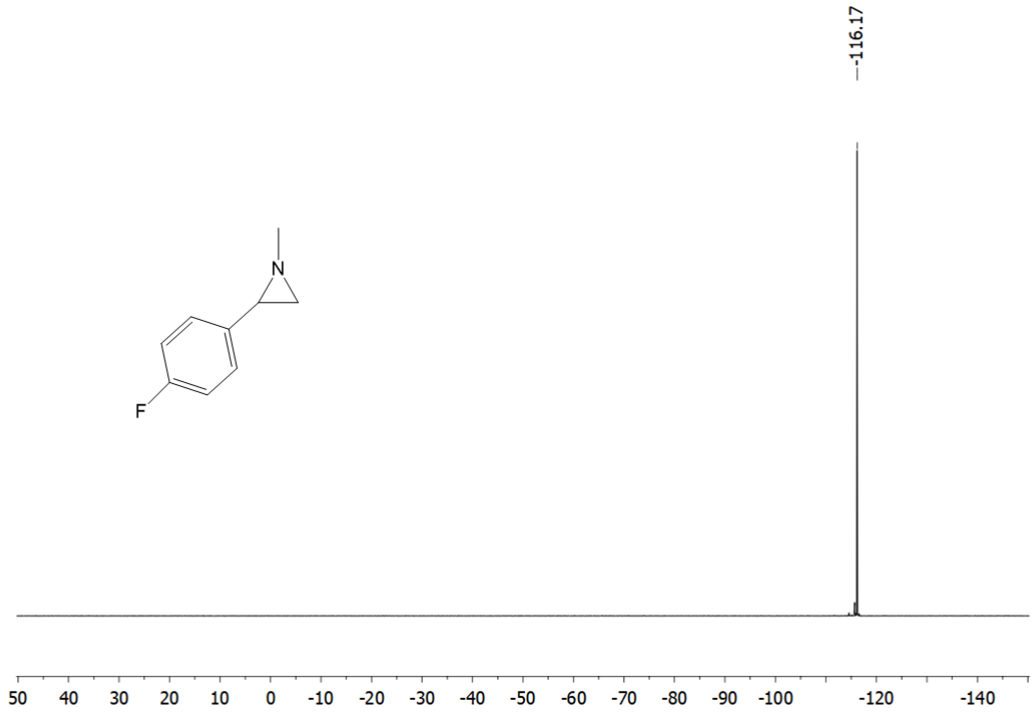
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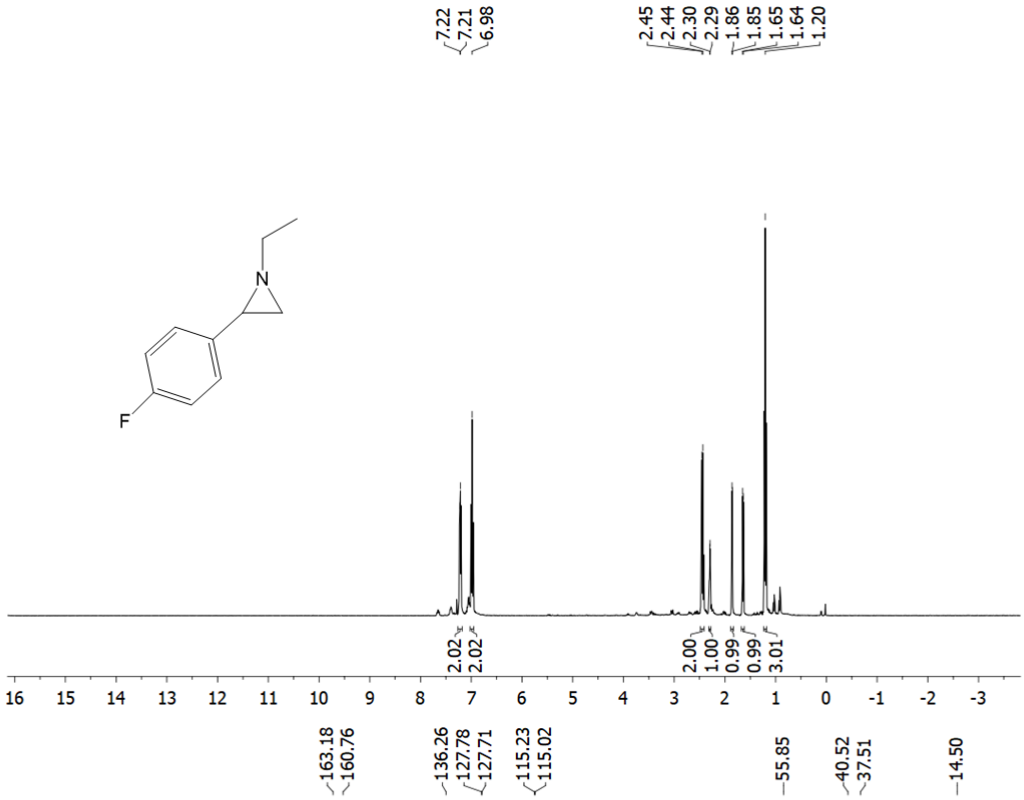
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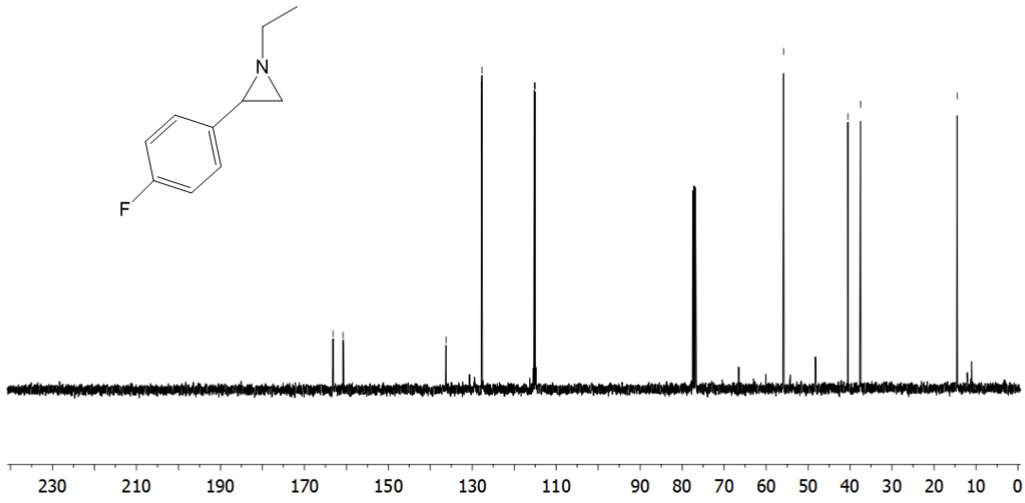
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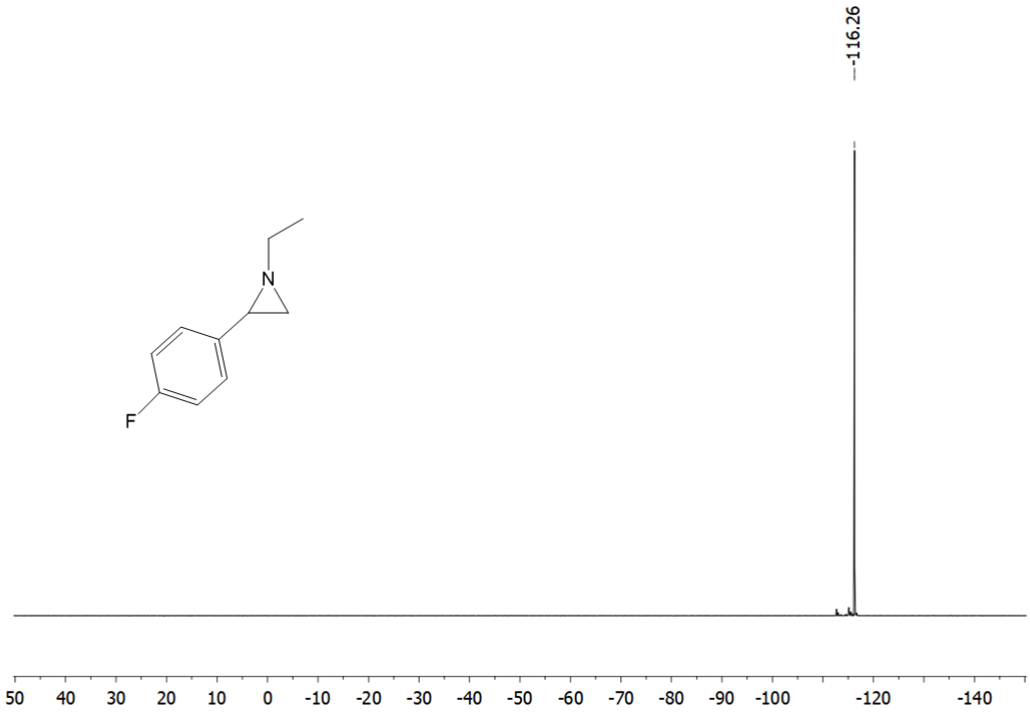
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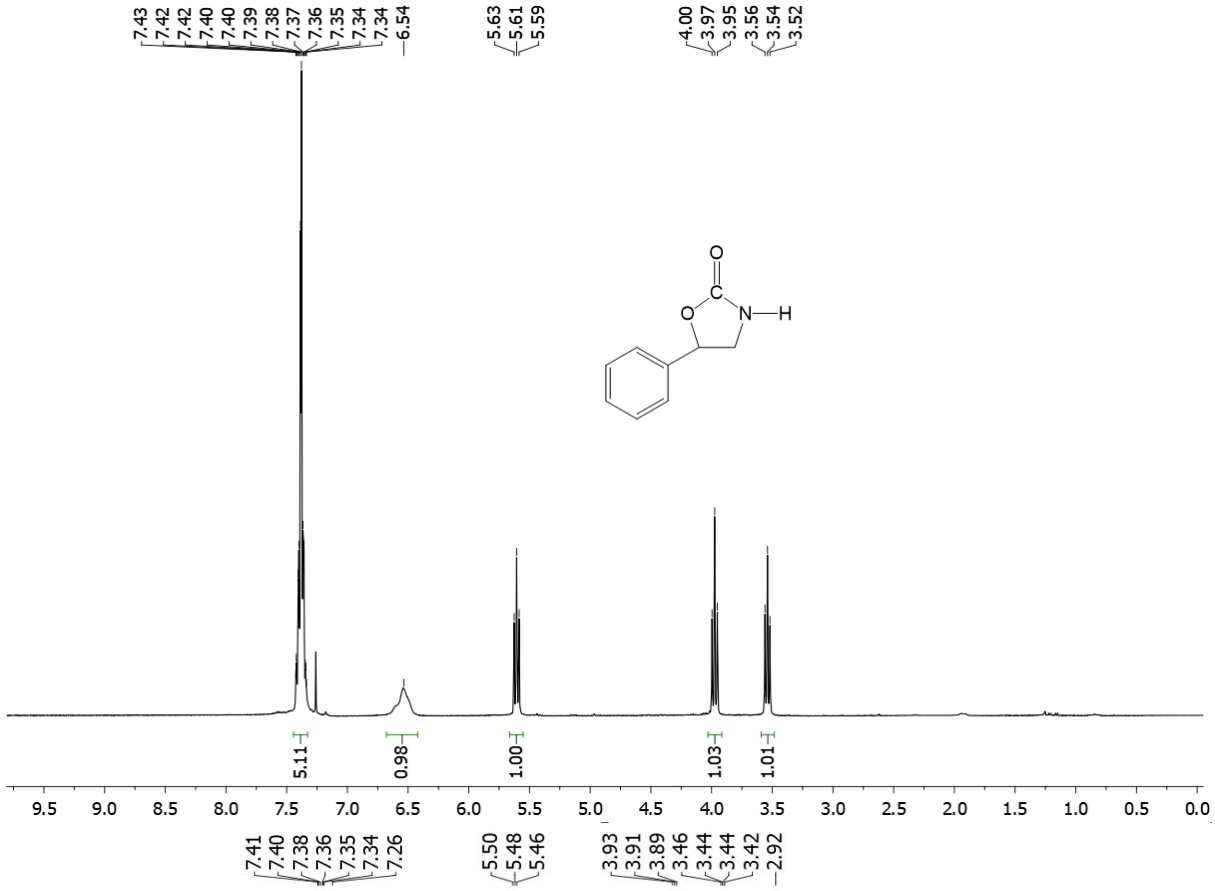
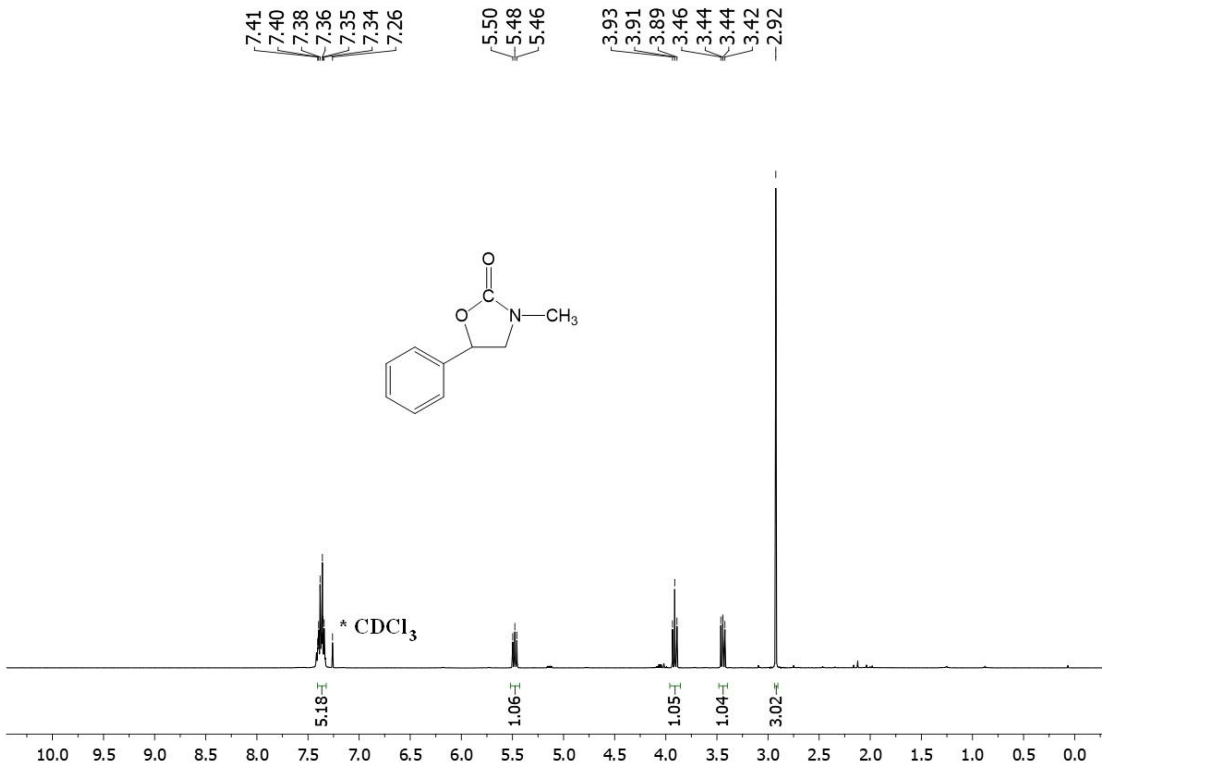
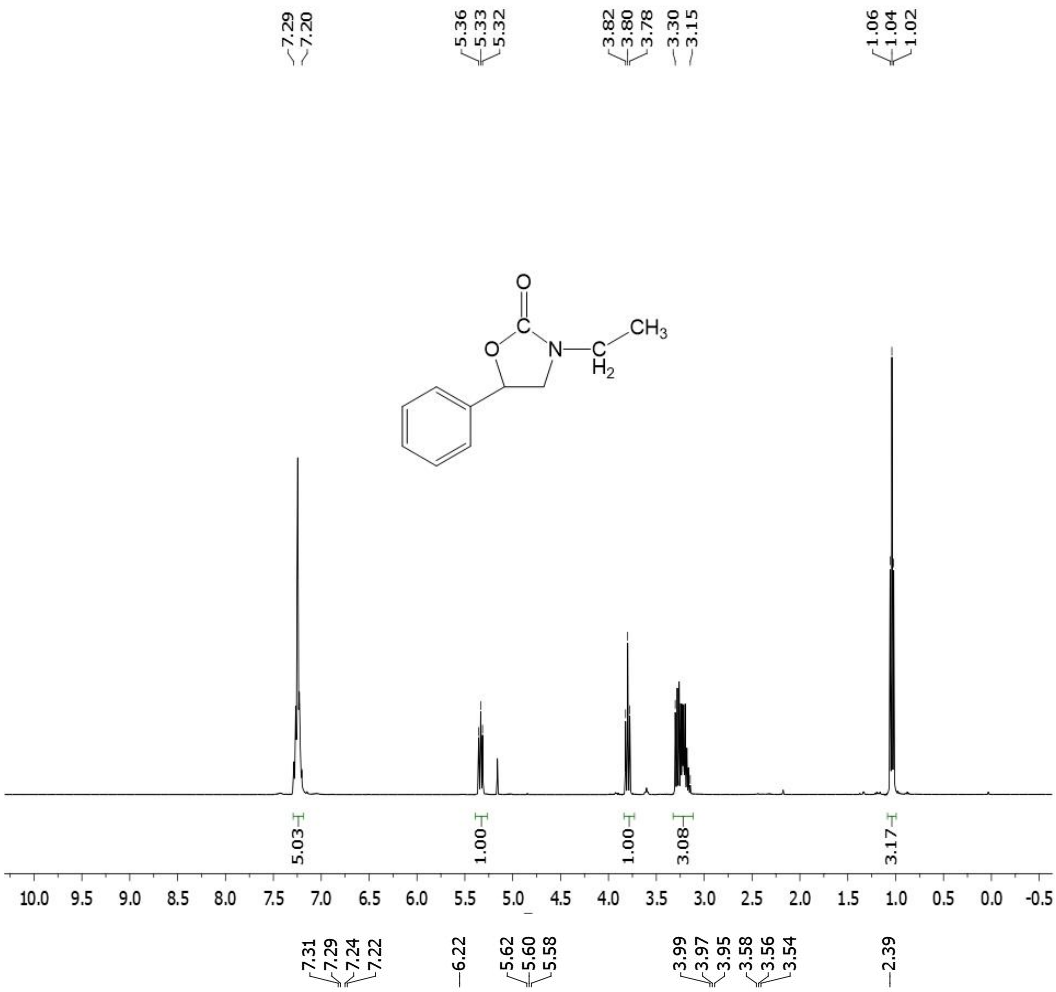
NMR spectra of 5-aryl-2-oxazolidinones



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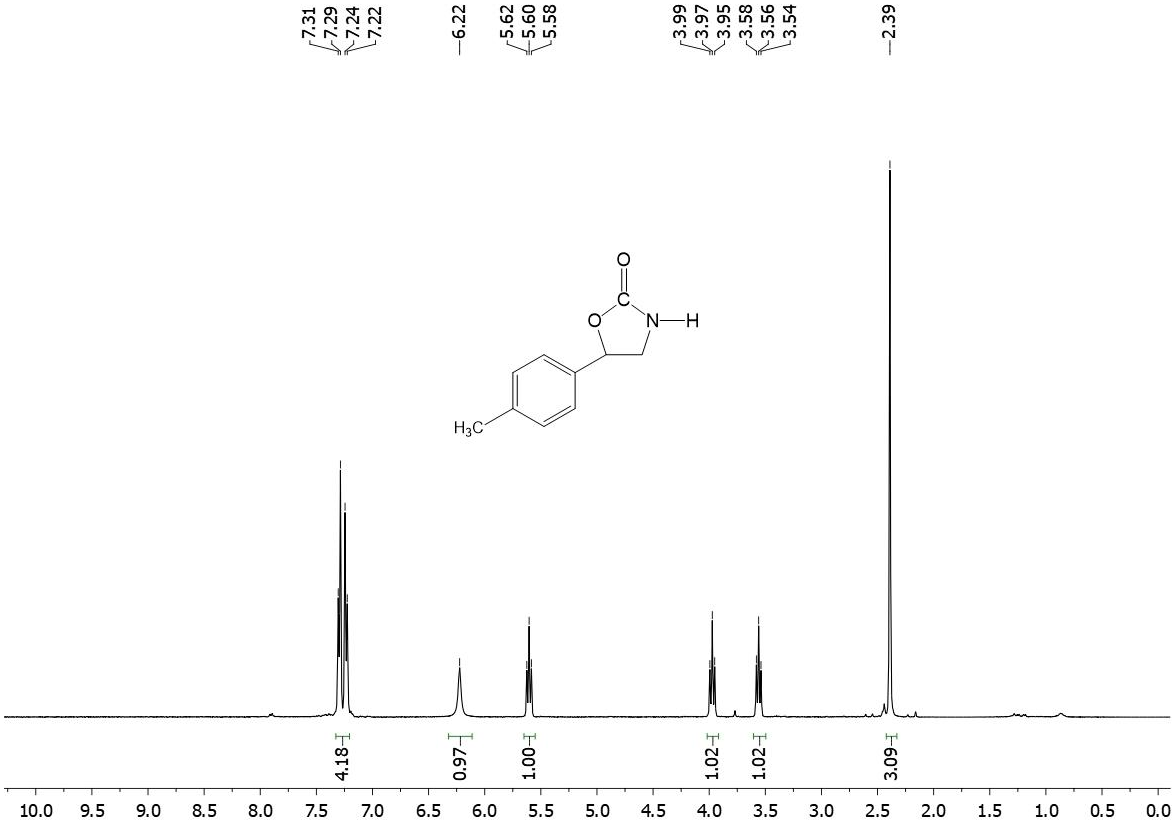
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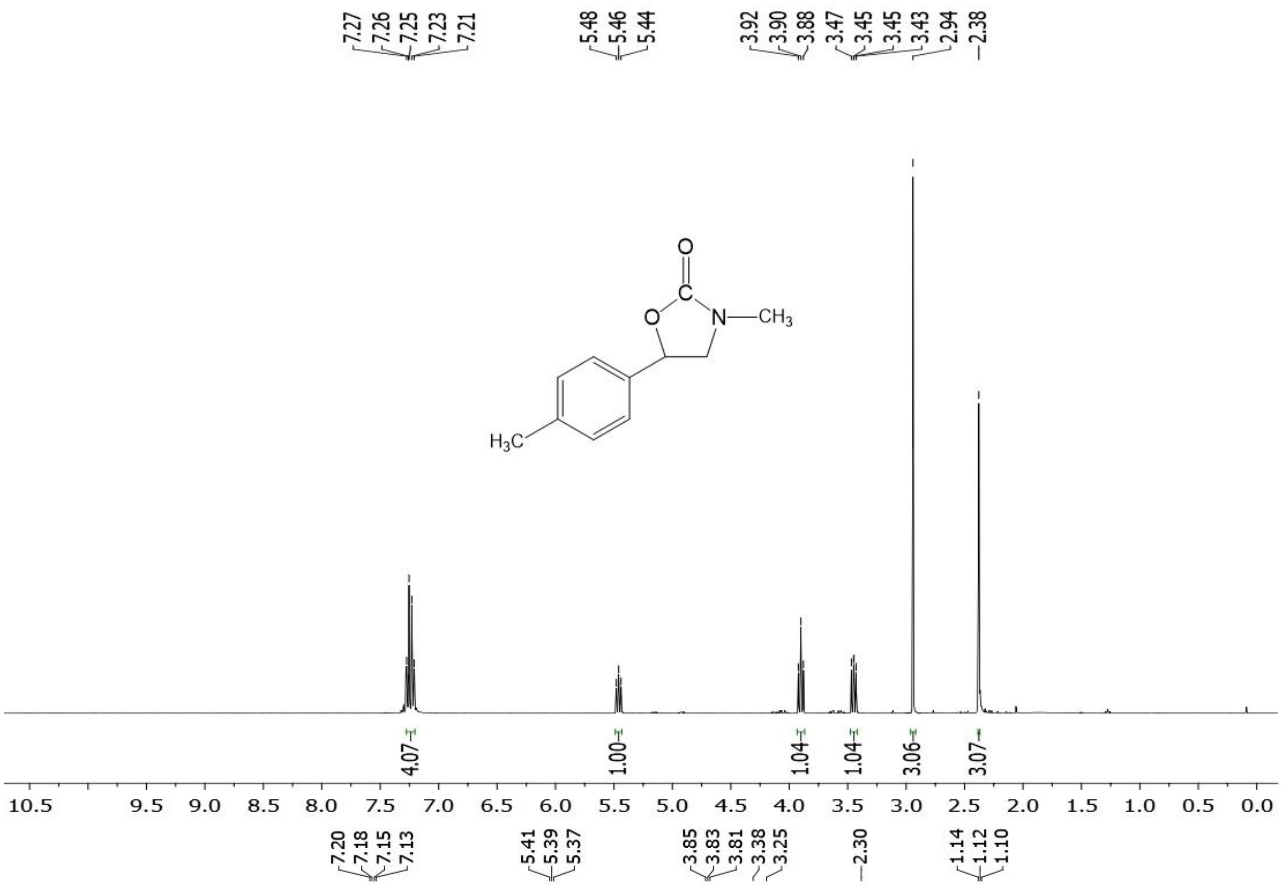
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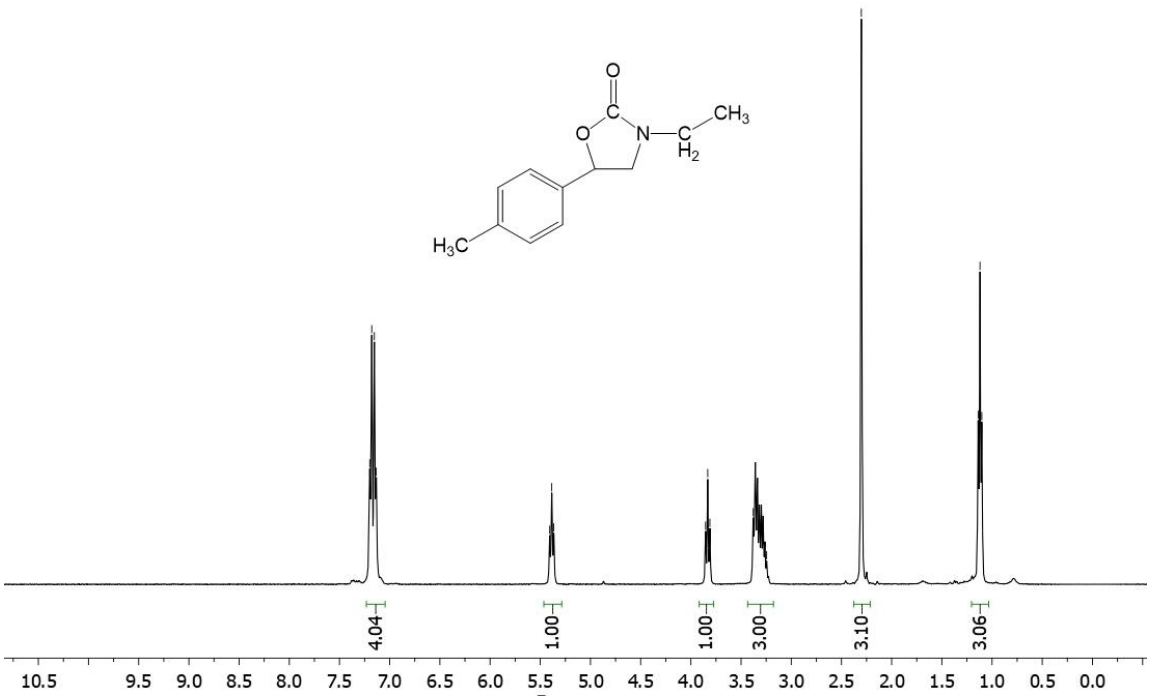
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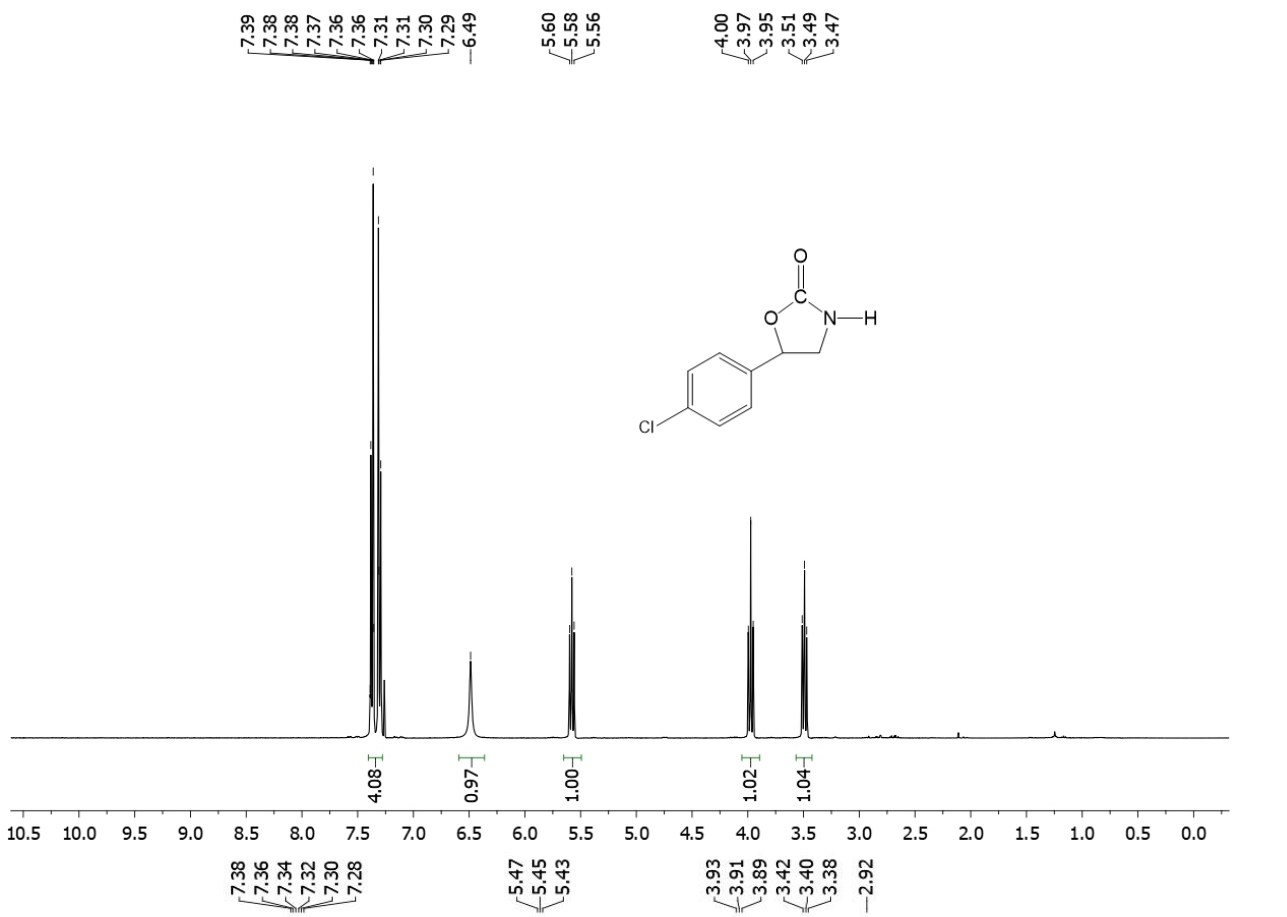
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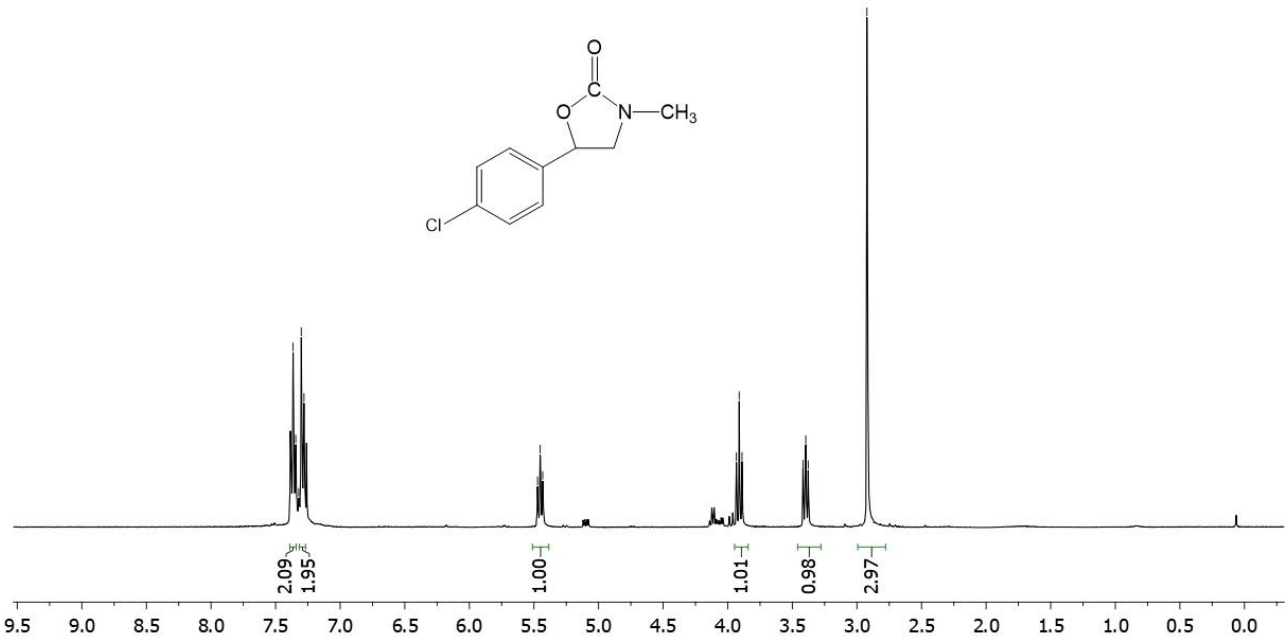
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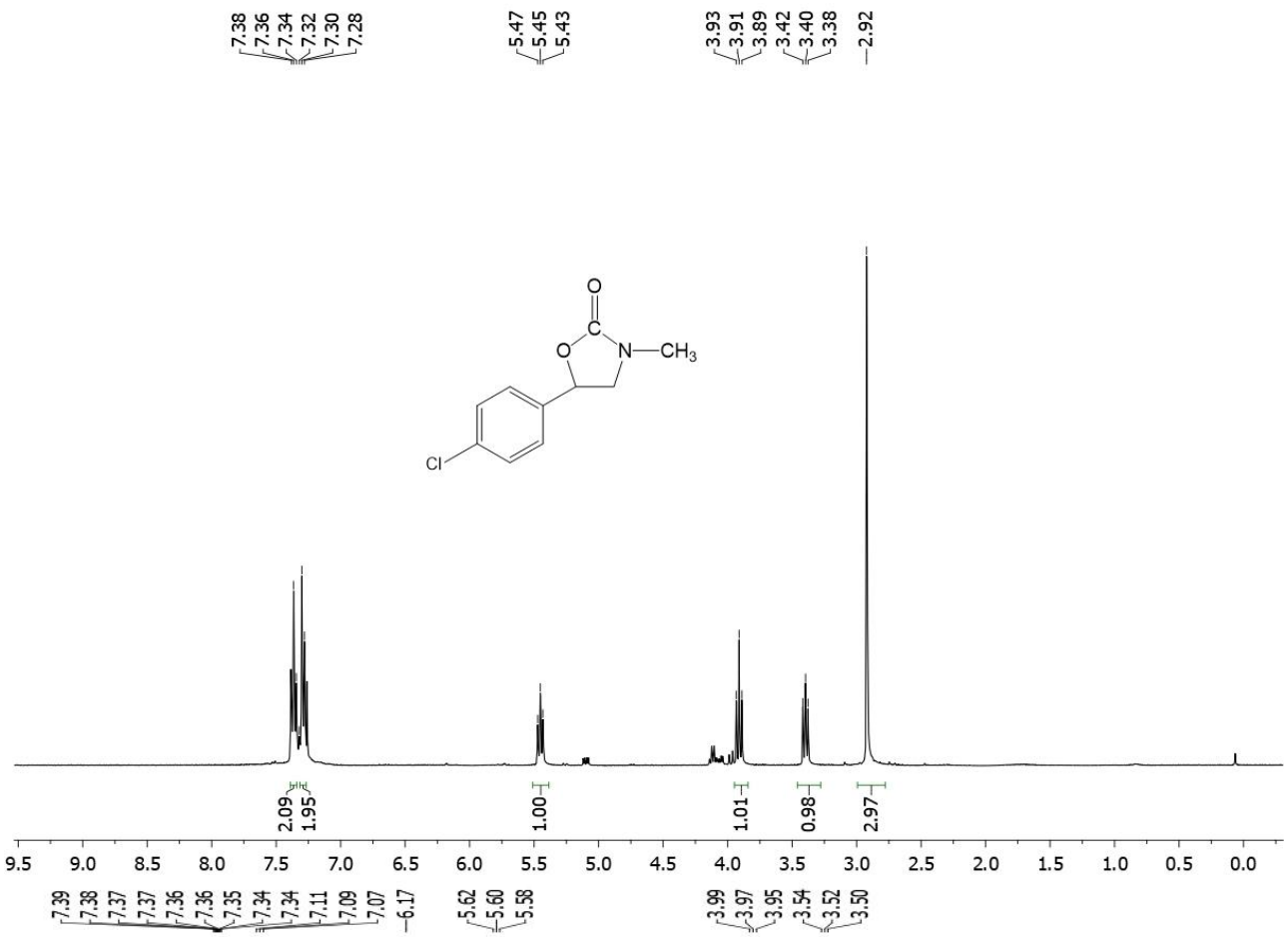
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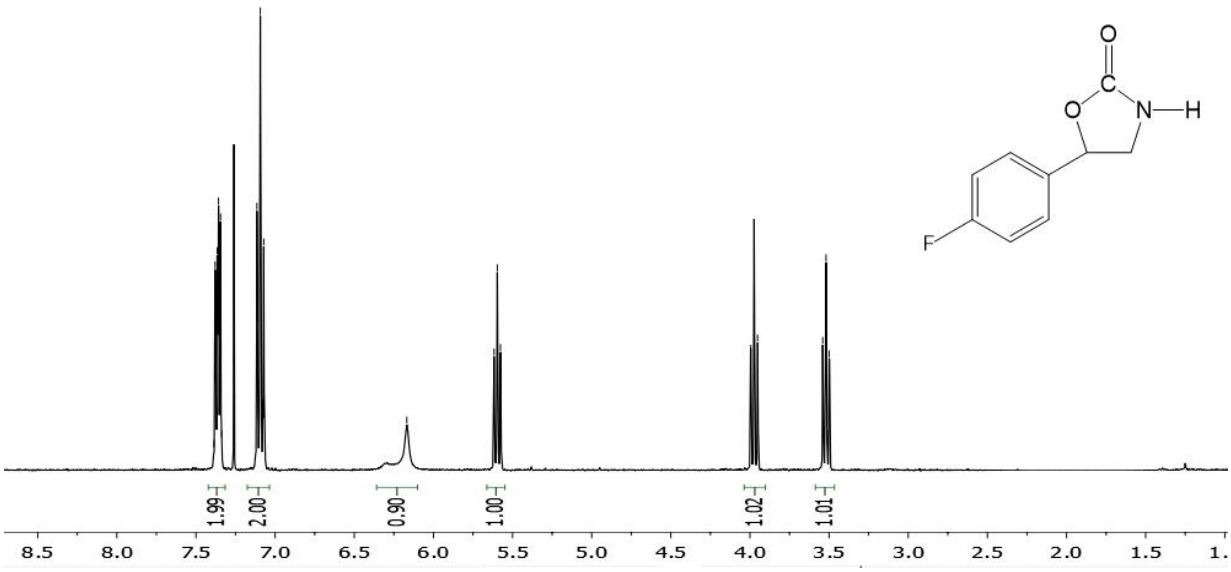
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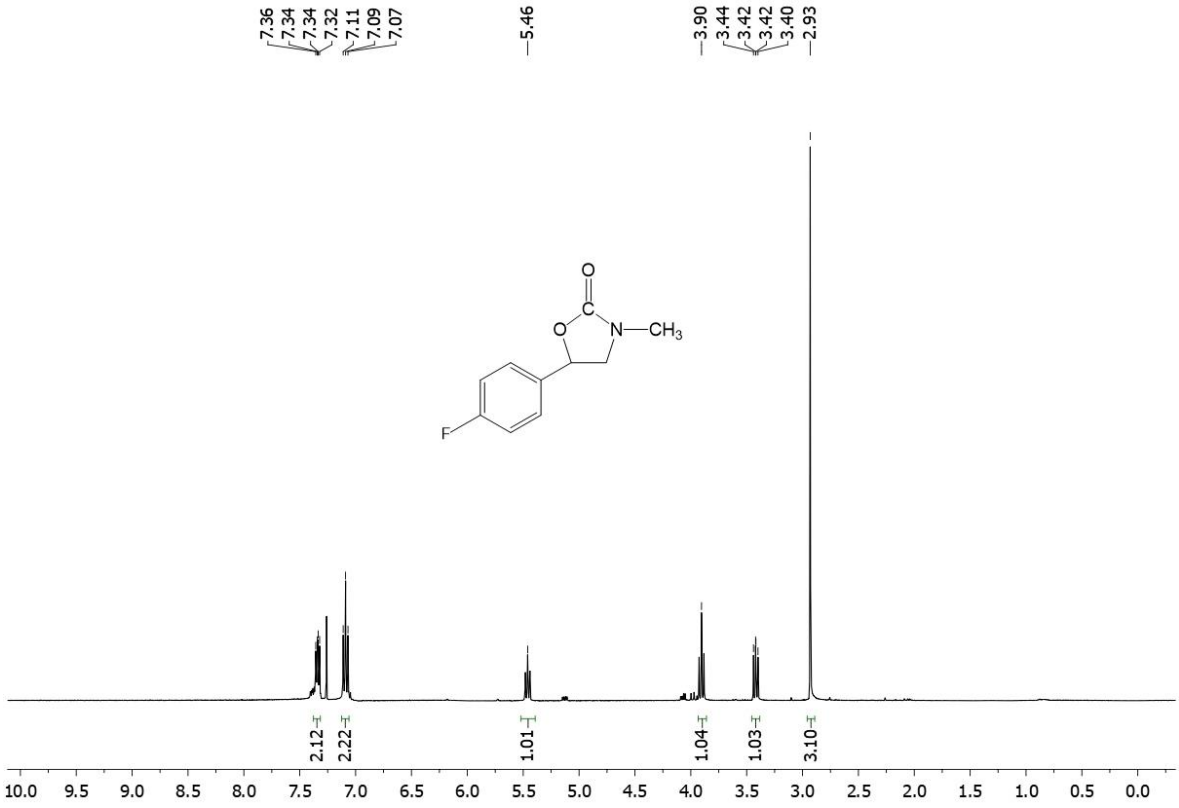
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2.12
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3.10
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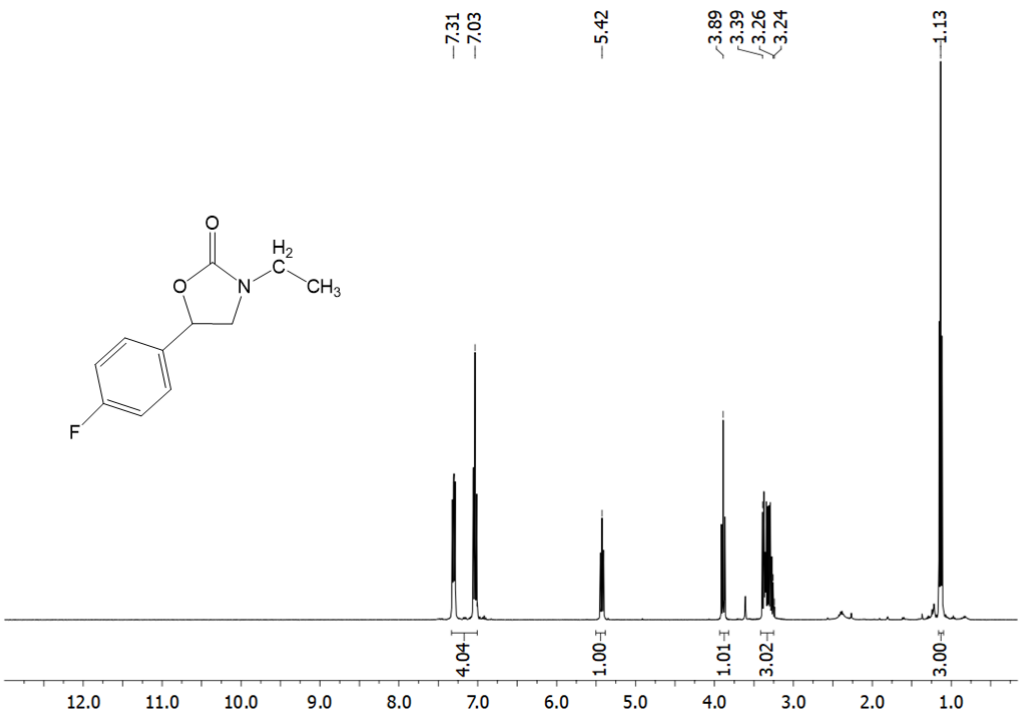
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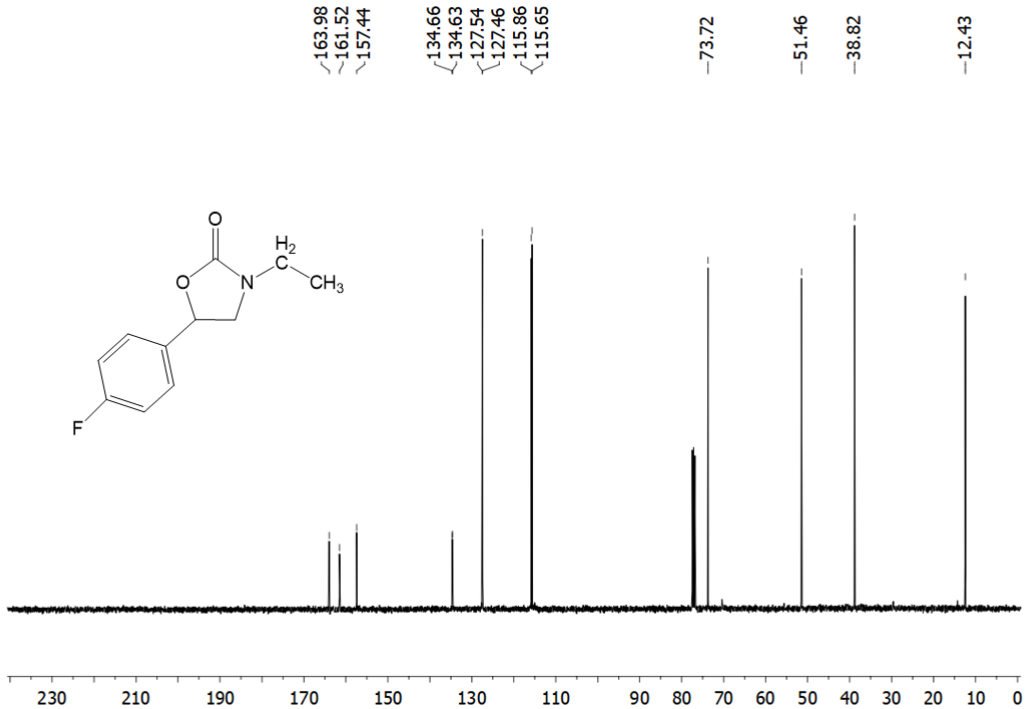
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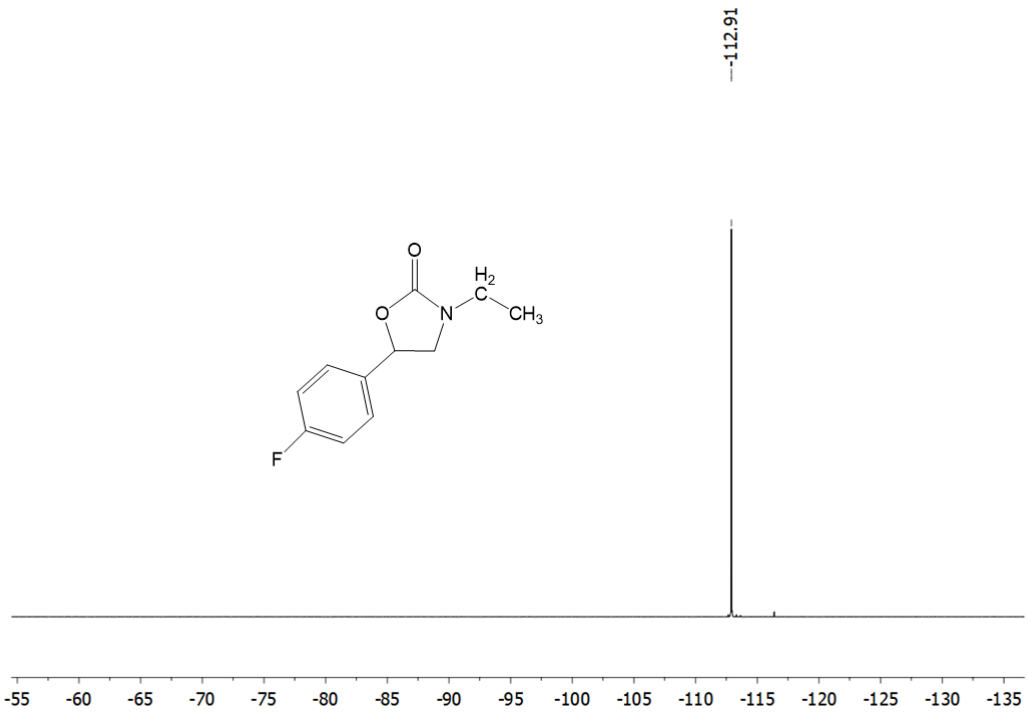
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