

Supporting Information

for

Synthesis of Ureido-Muraymycidine Derivatives for Structure Activity Relationship

Studies of Muraymycins

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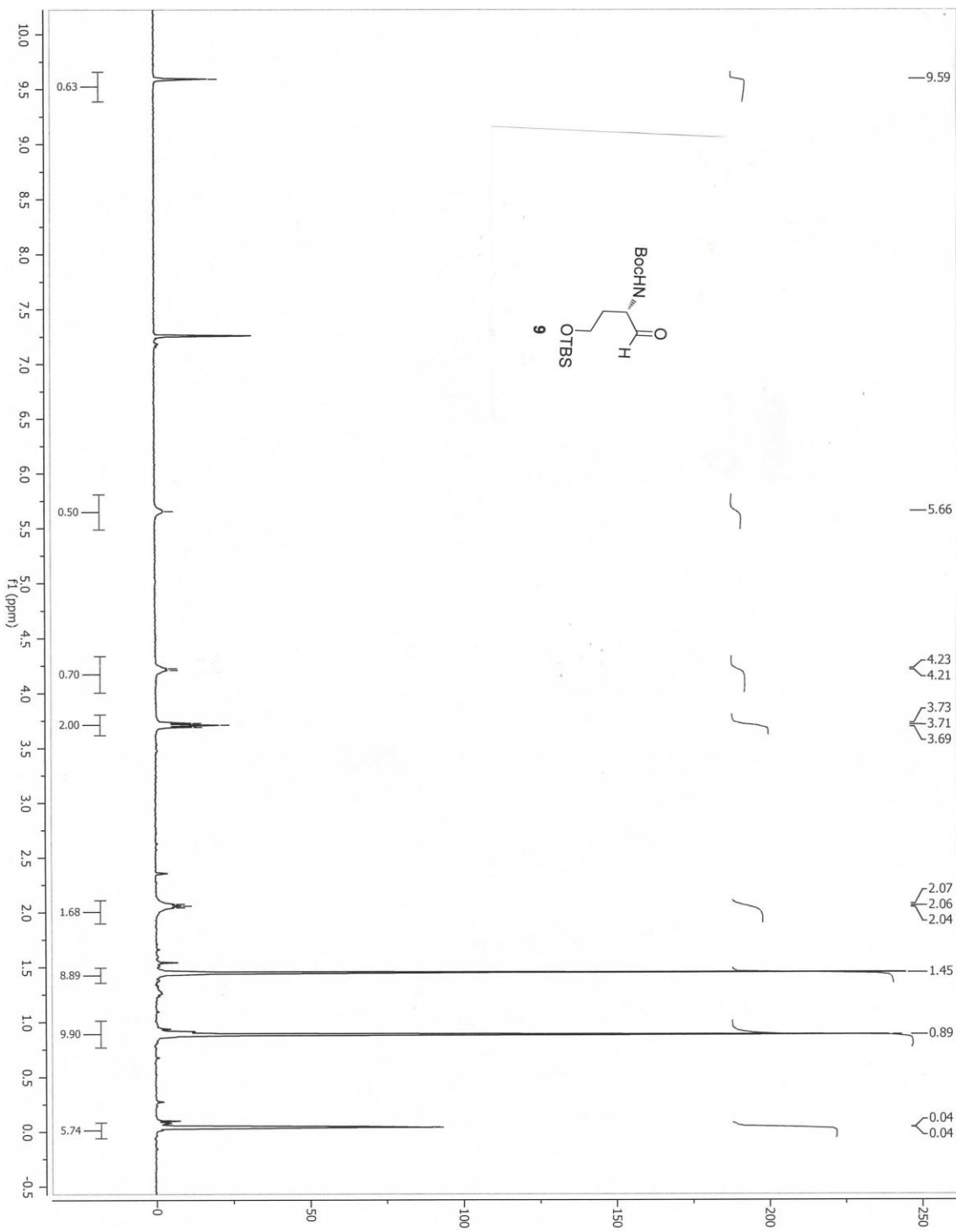
mkurosu@uthsc.edu

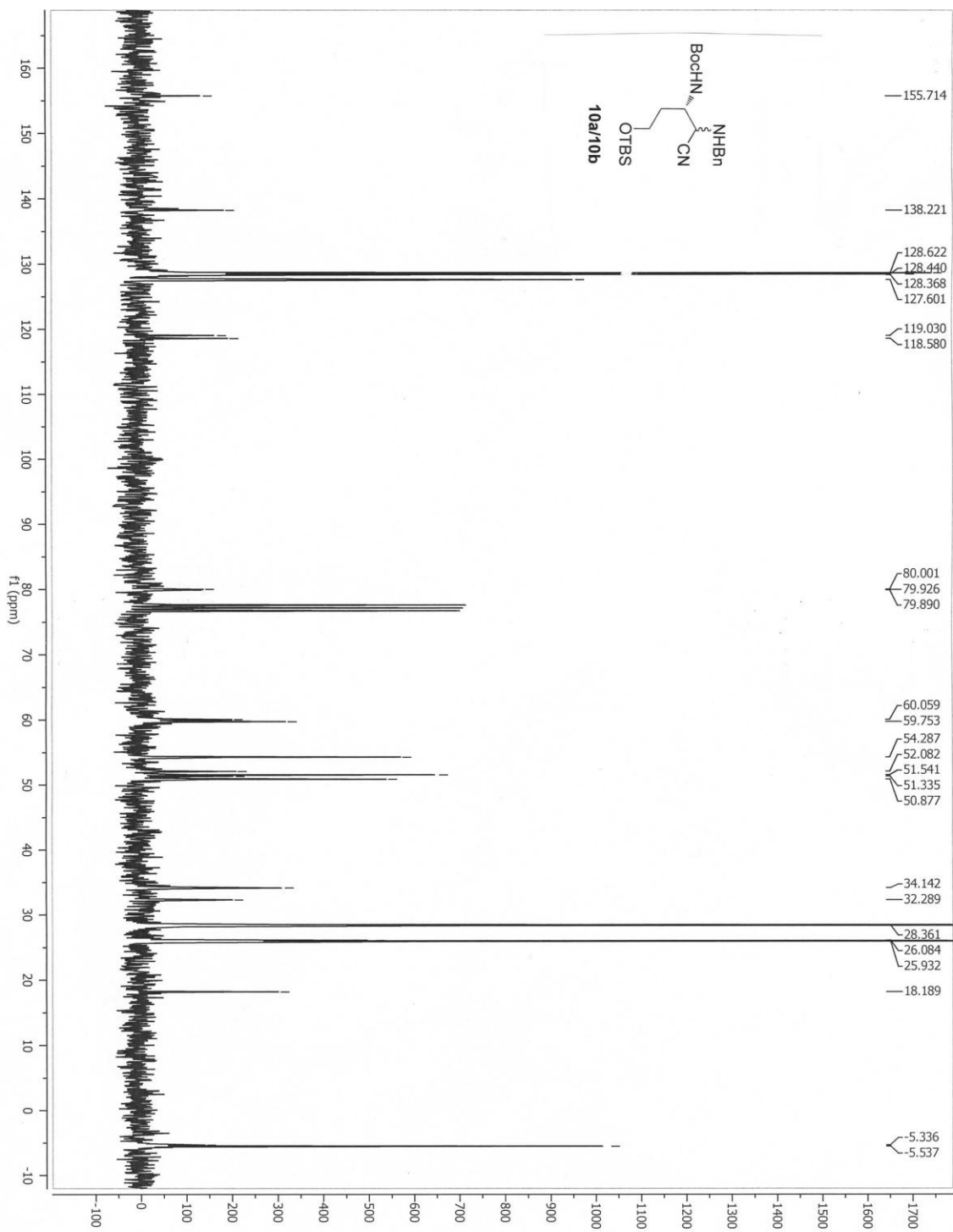
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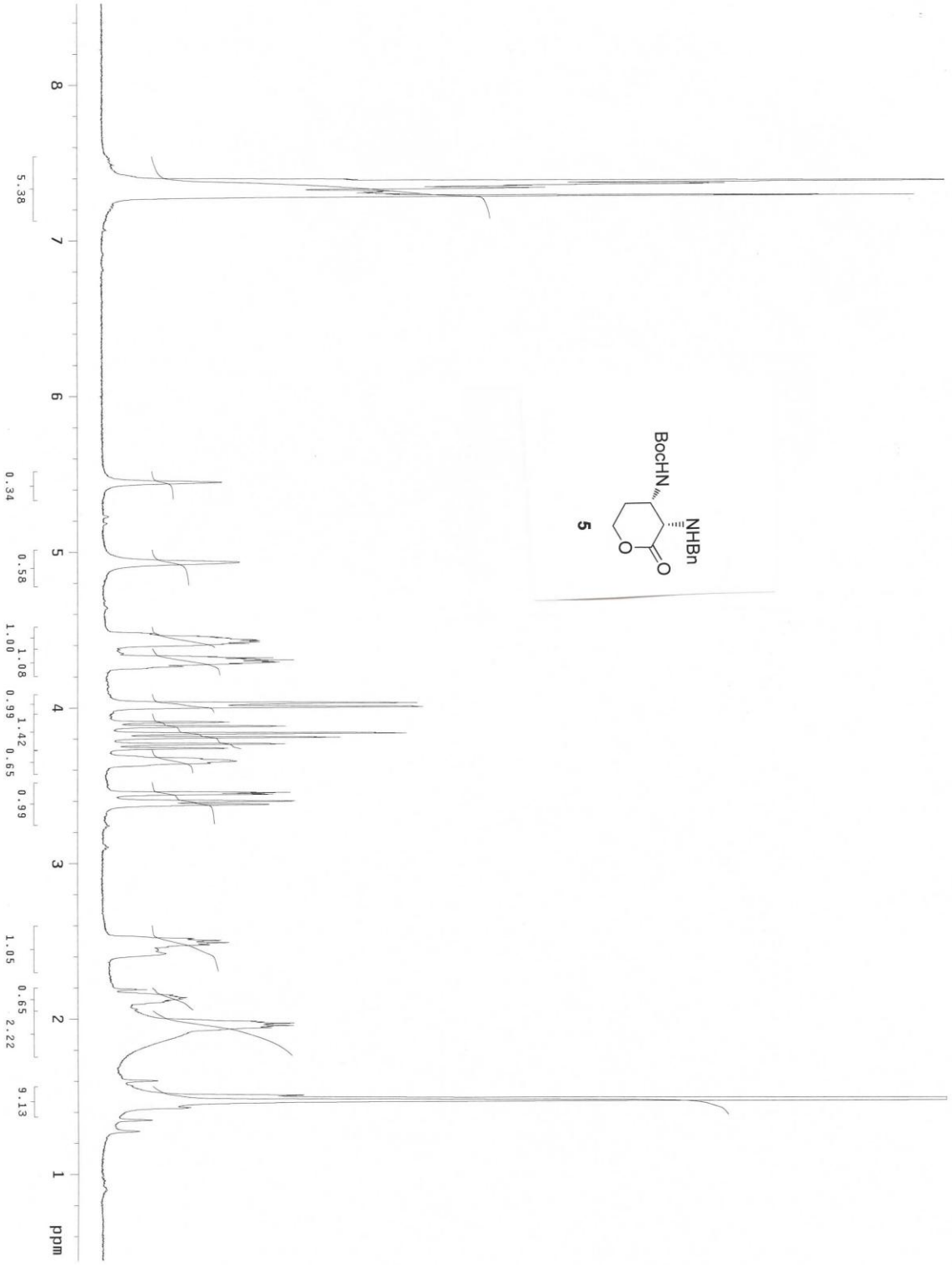
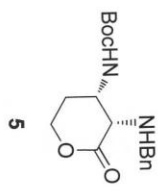
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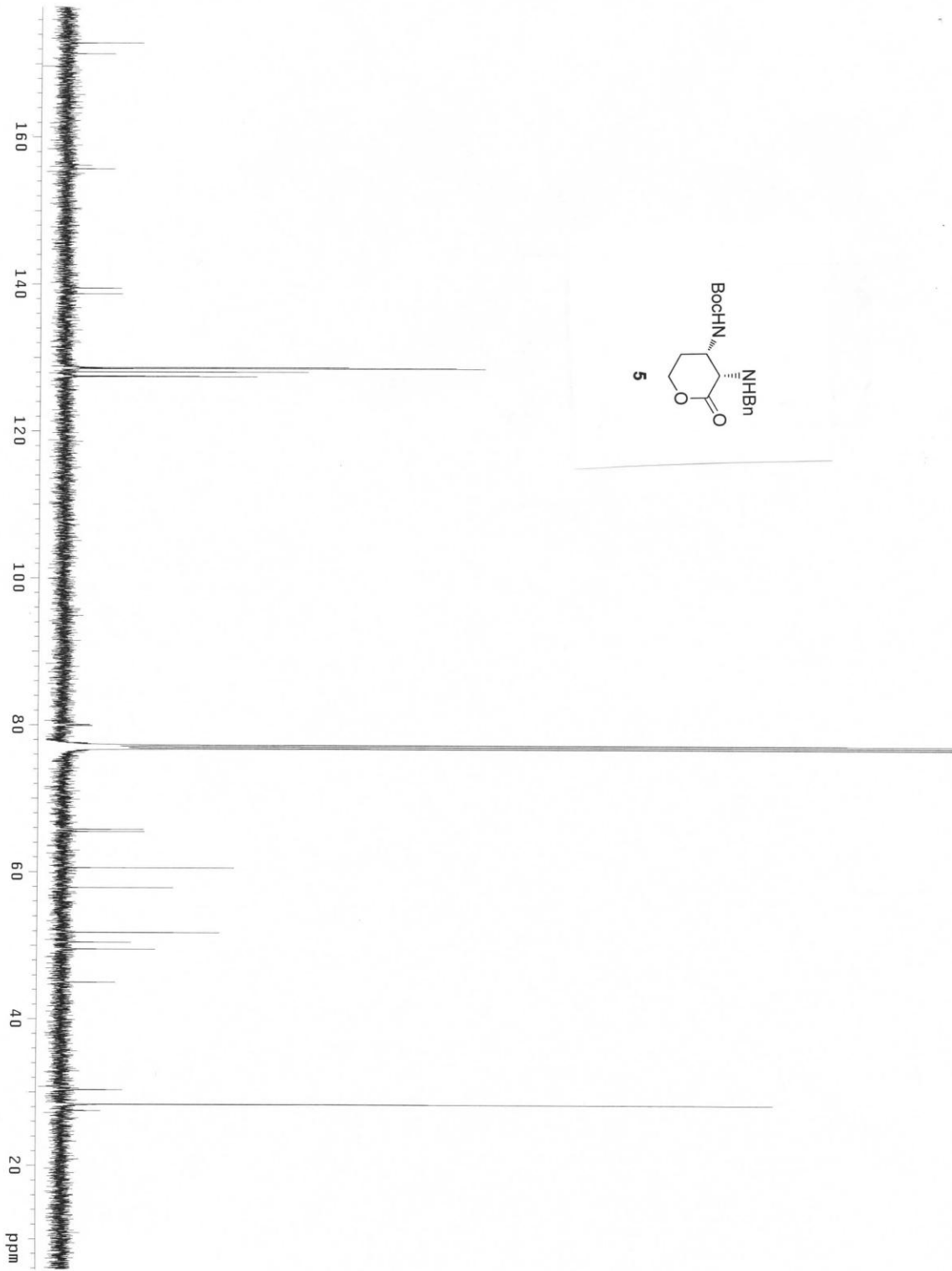
General

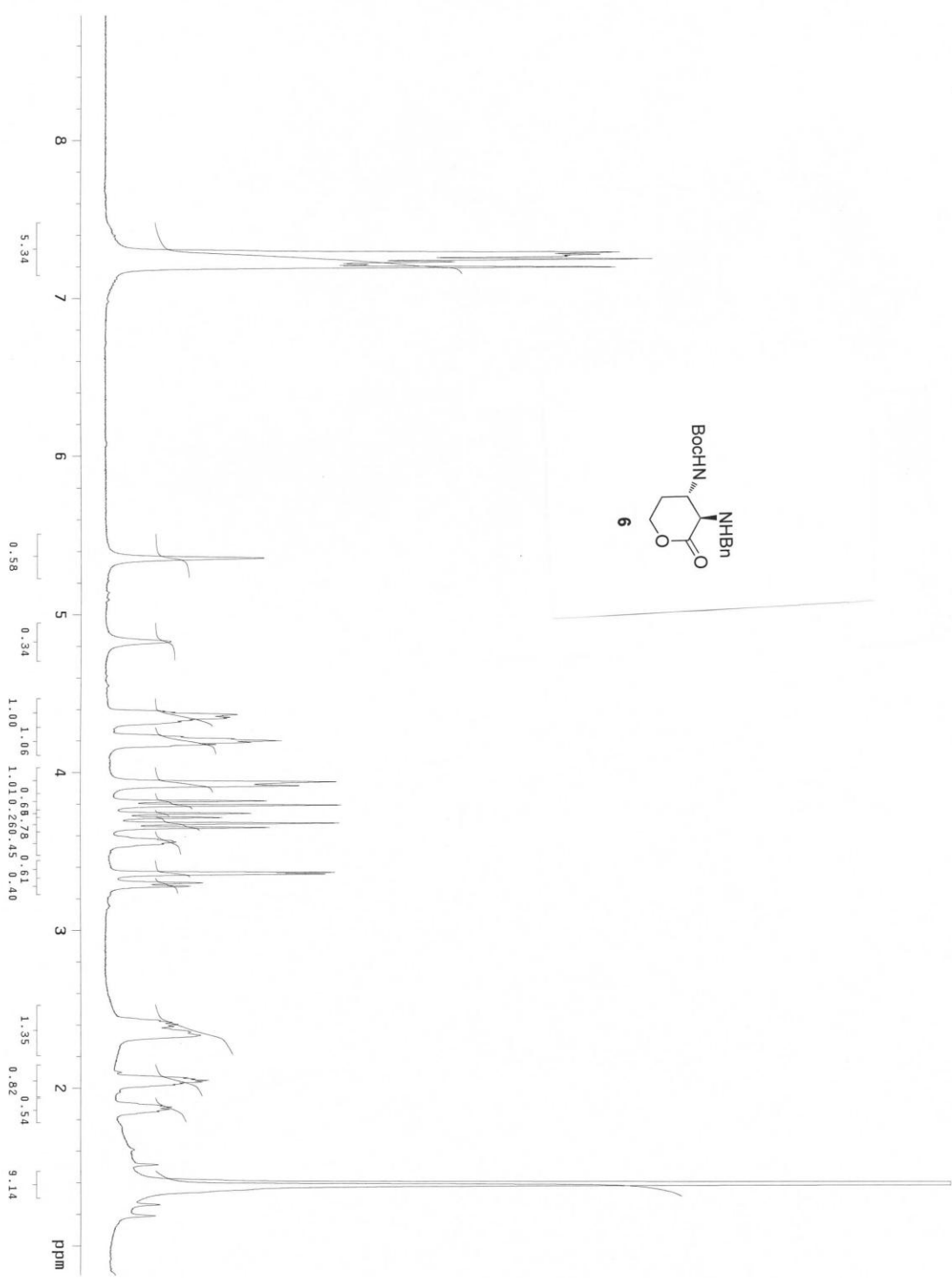
All reactions were carried out using oven-dried glassware, assembled hot and cooled under a stream of nitrogen before use. Reactions with air sensitive materials were carried out by standard syringe techniques. Commercially available reagents were used as received without further purification. Analytical thin-layer chromatography was performed with 0.25 mm coated commercial silica gel plates (EMD, Silica Gel 60F₂₅₄) visualizing at 254 nm, or developed with ceric ammonium molybdate or anisaldehyde solutions by heating on a hot plate. Specified products were purified by flash column chromatography using silica gel 60 (230-400 mesh, Merck). IR absorptions on NaCl plates were run on a FT-IR 1600 spectrometer. ¹H-NMR spectral data were obtained using 300, 400, and 500 MHz instruments. ¹³C NMR spectral data were obtained using a 100, 125 MHz spectrometer. For all NMR spectra, δ values are given in ppm and *J* values in Hz.

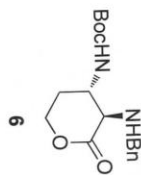
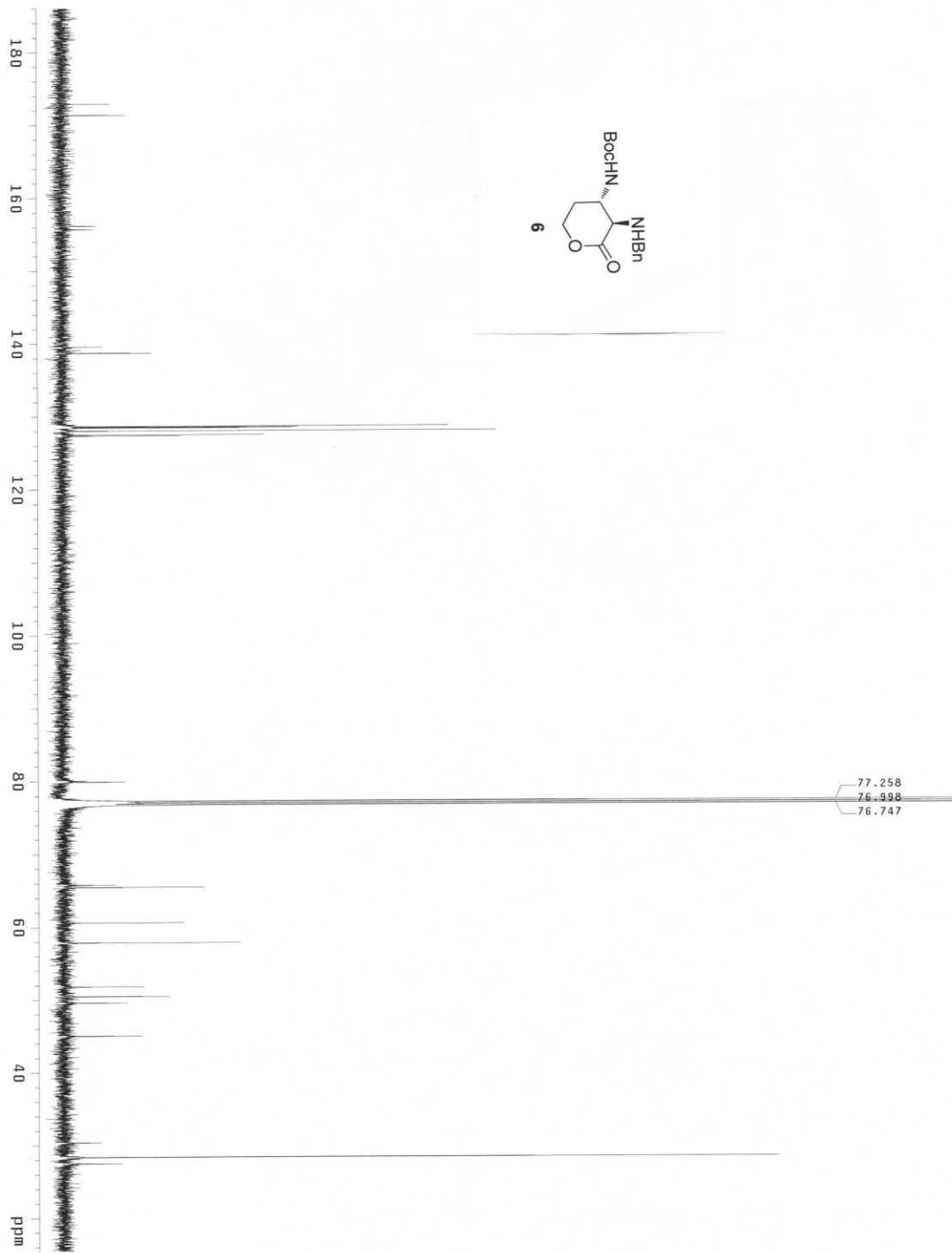


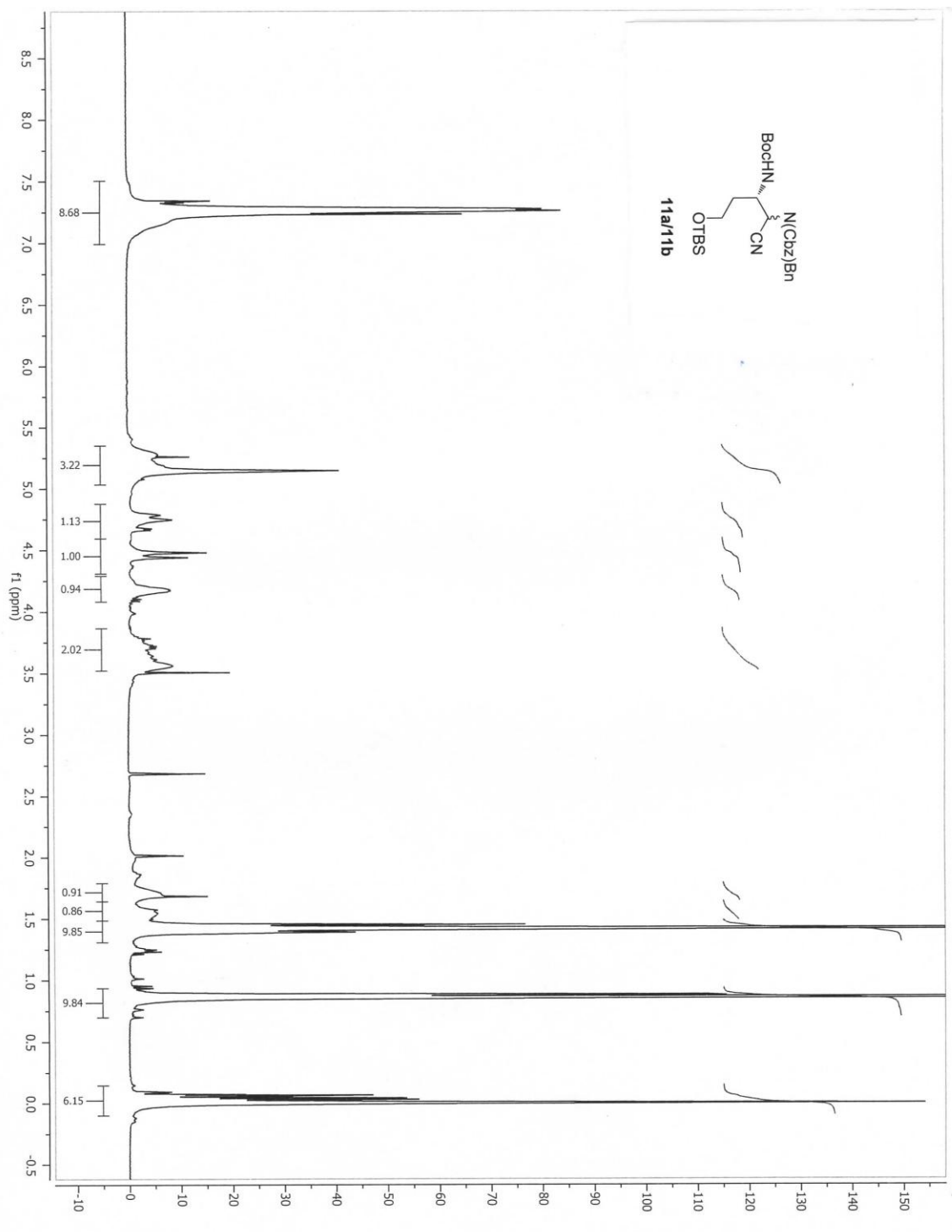


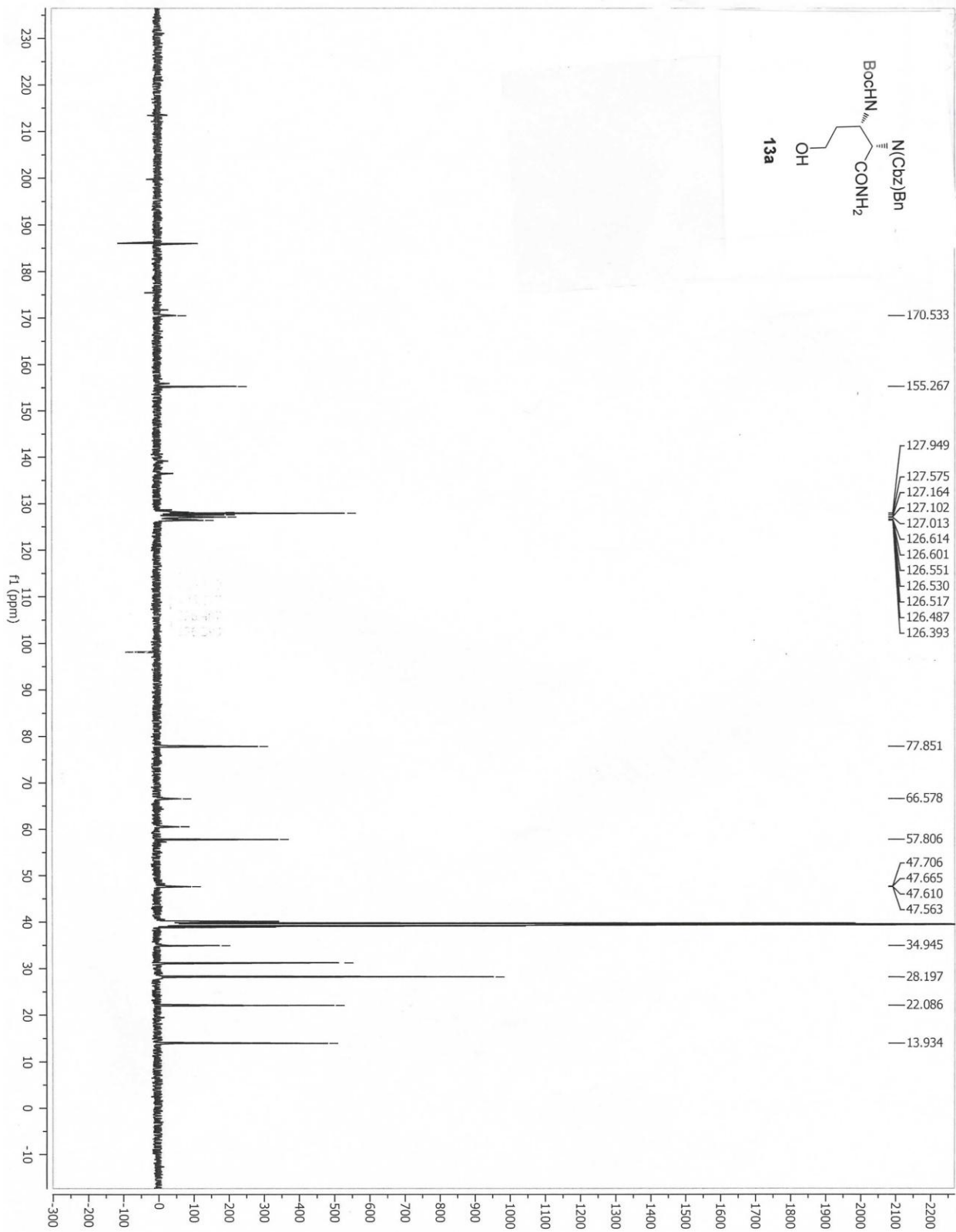


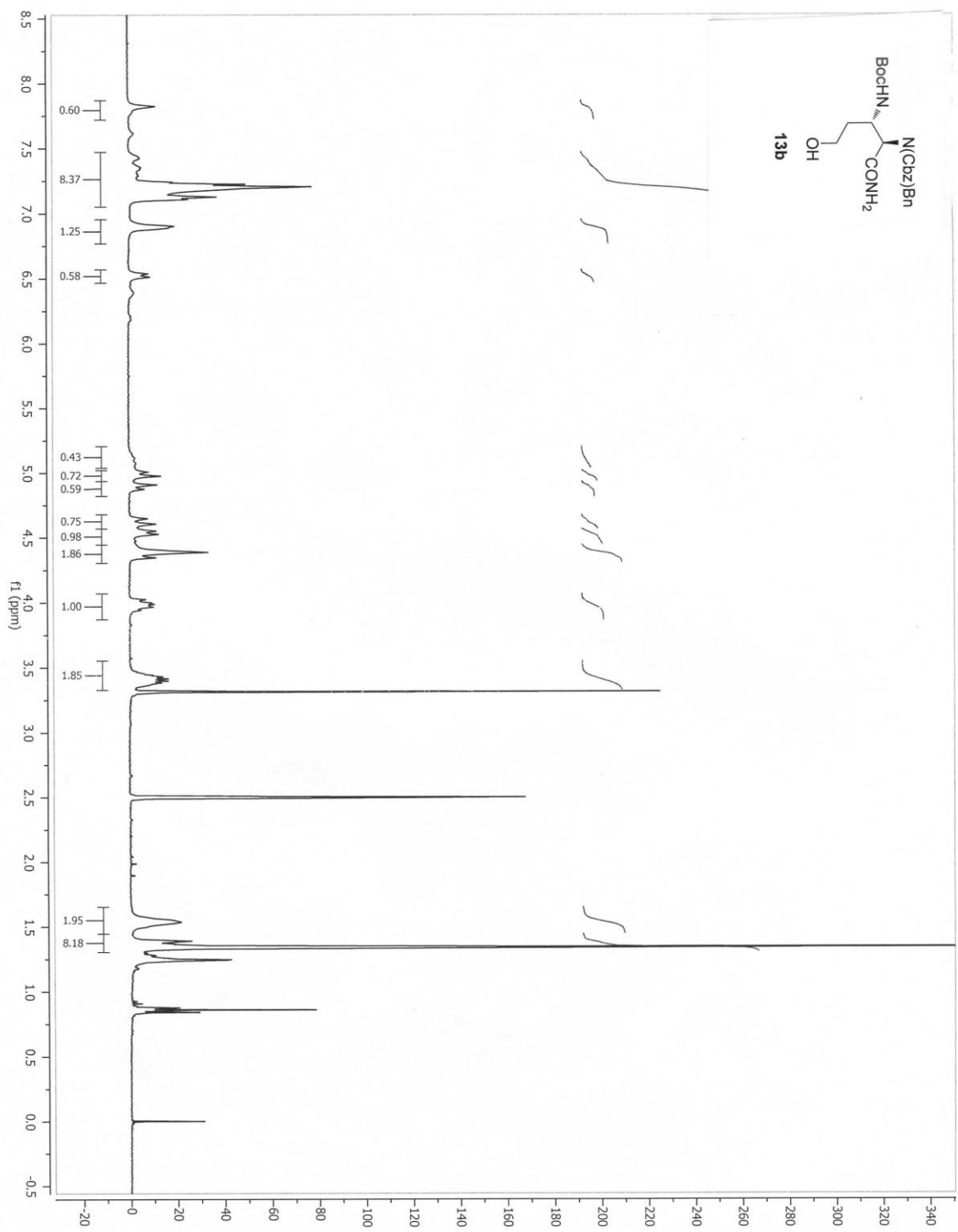


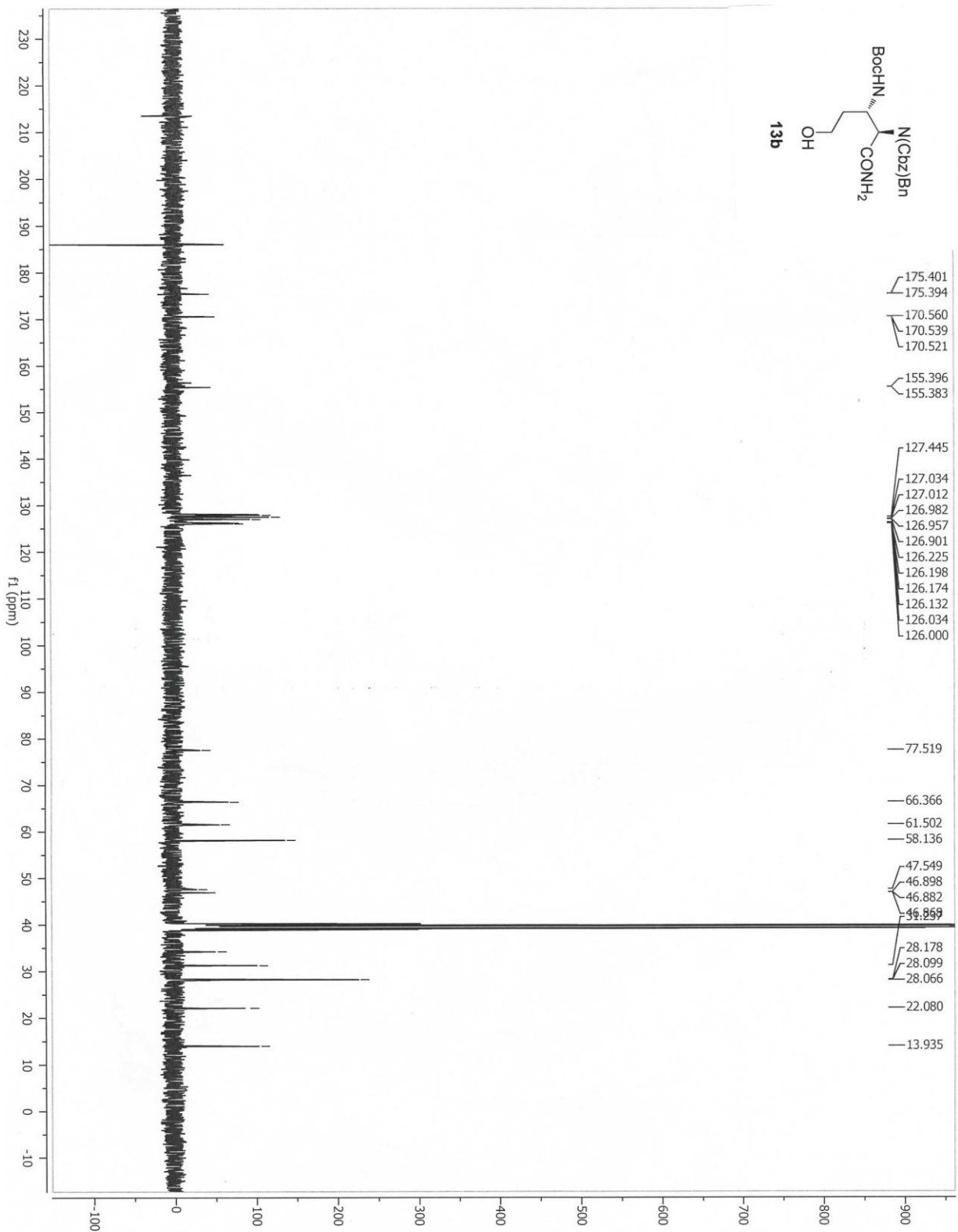


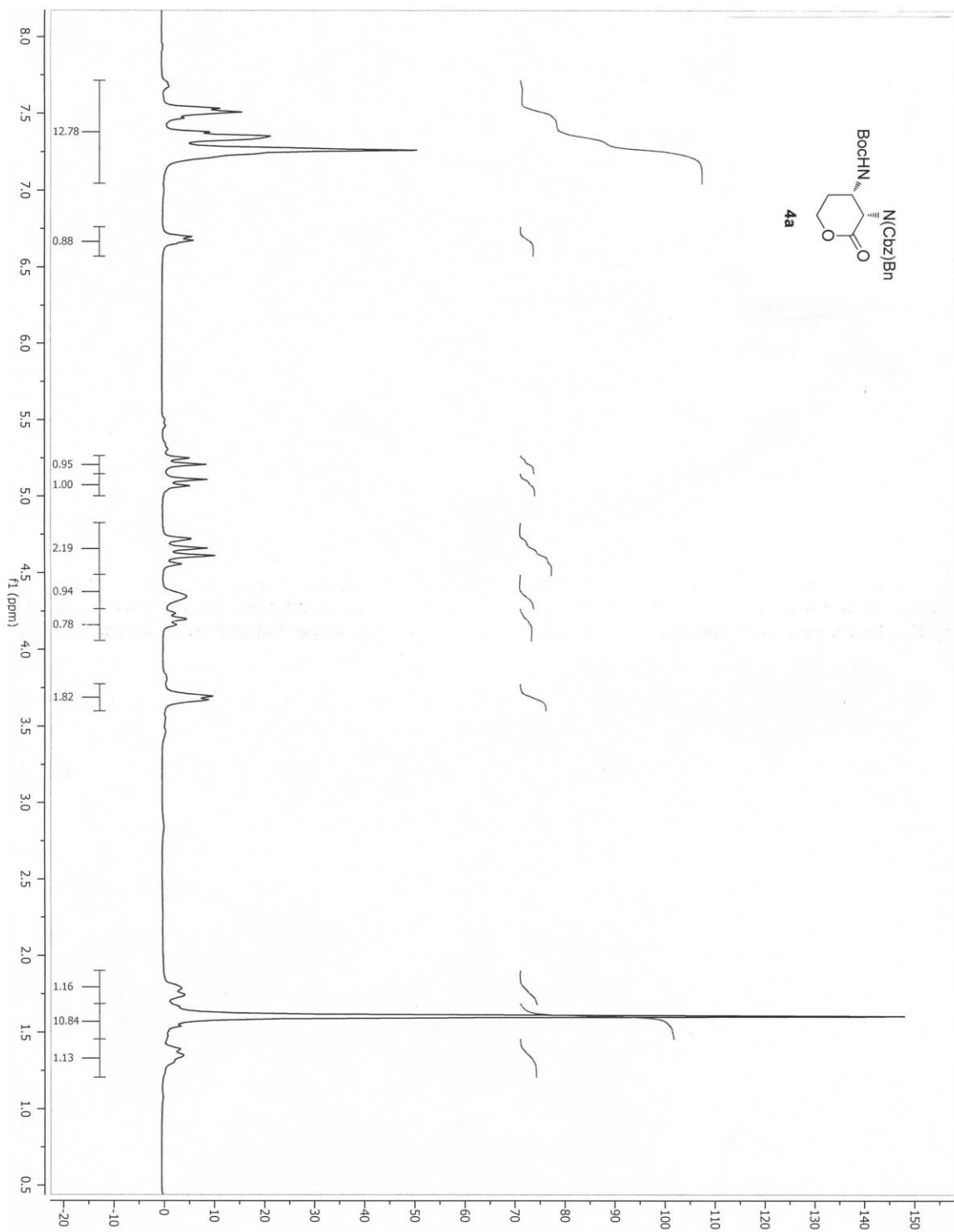


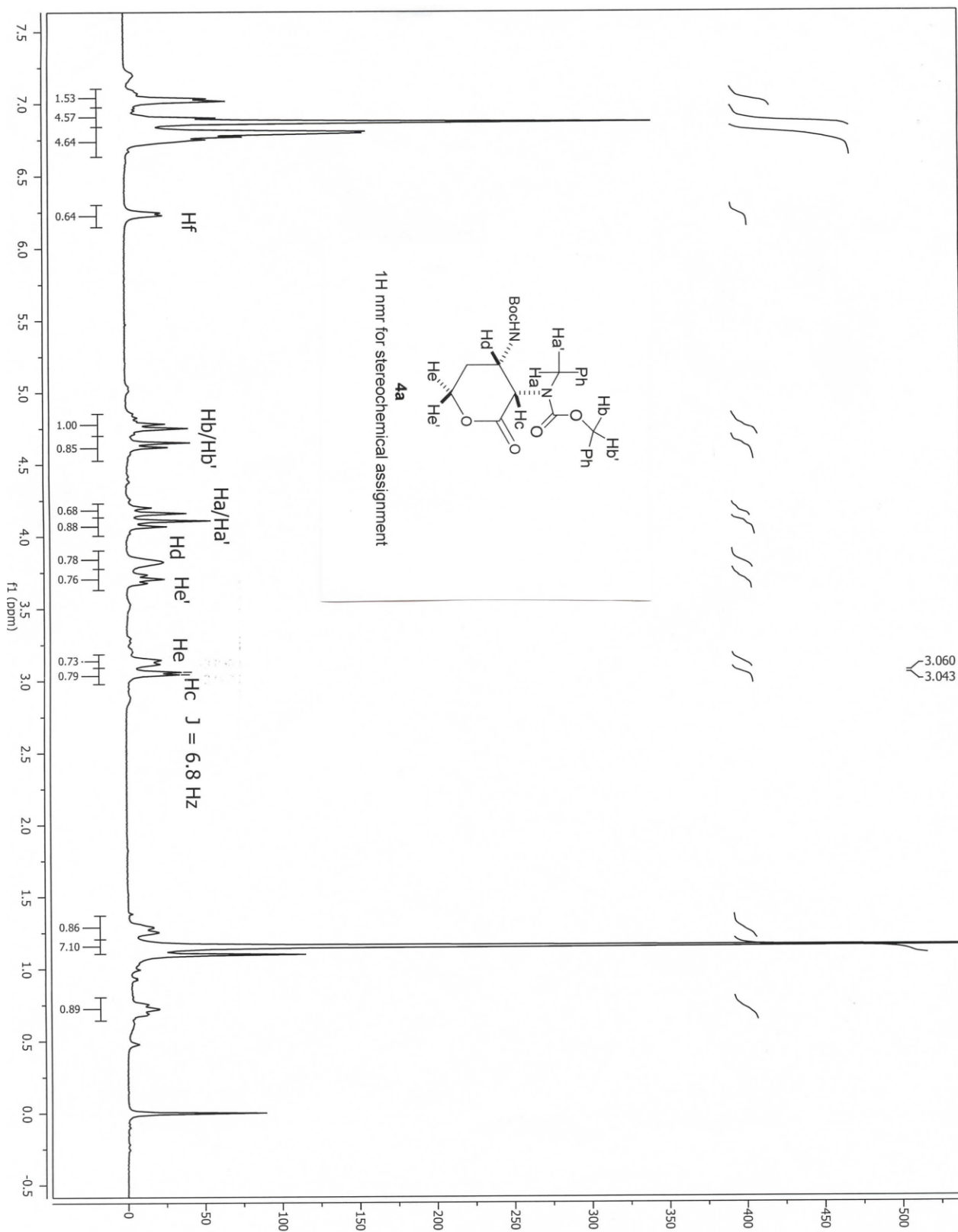


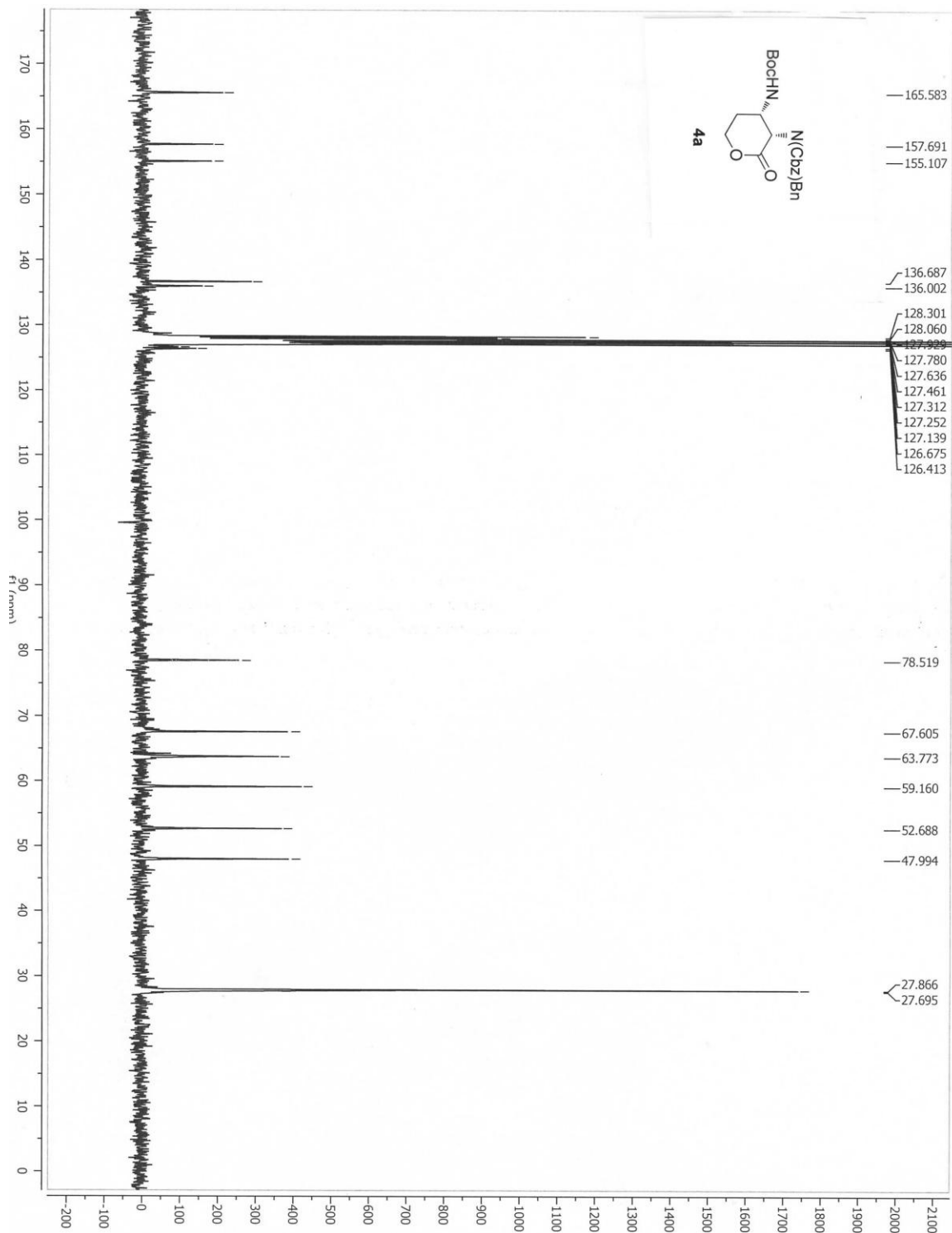


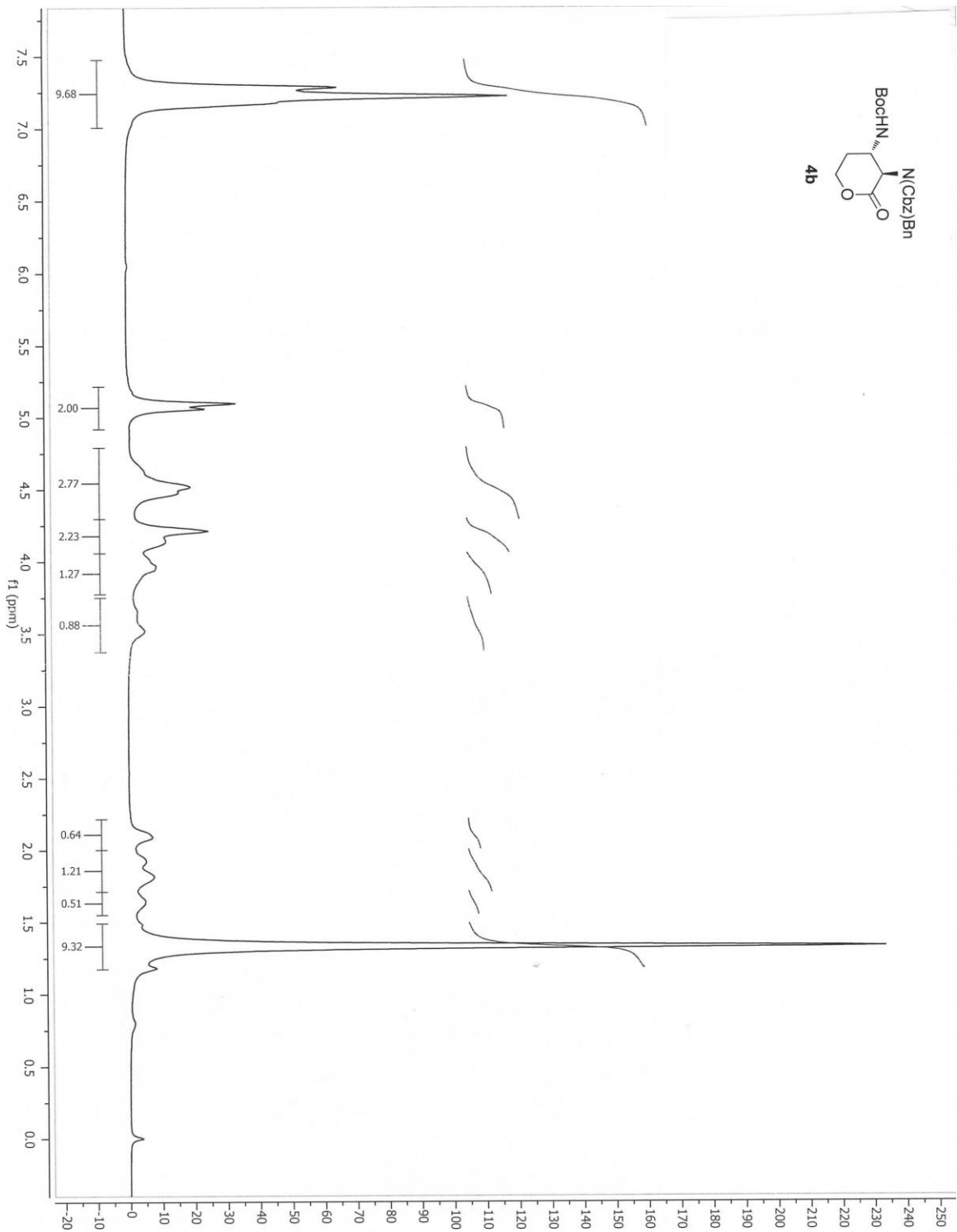
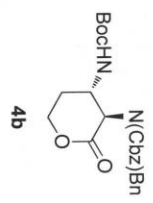


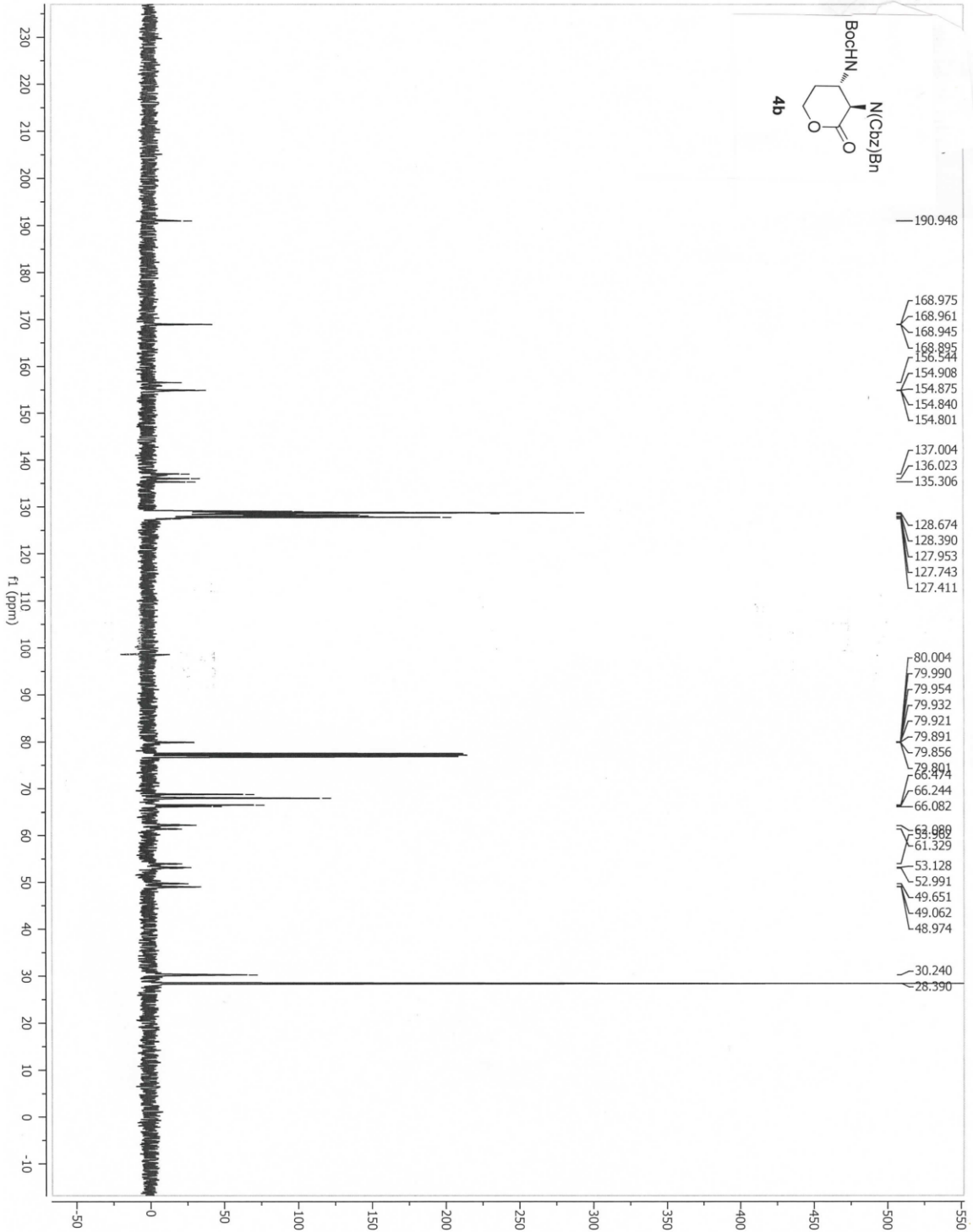


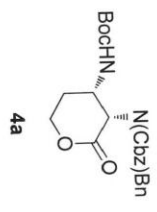




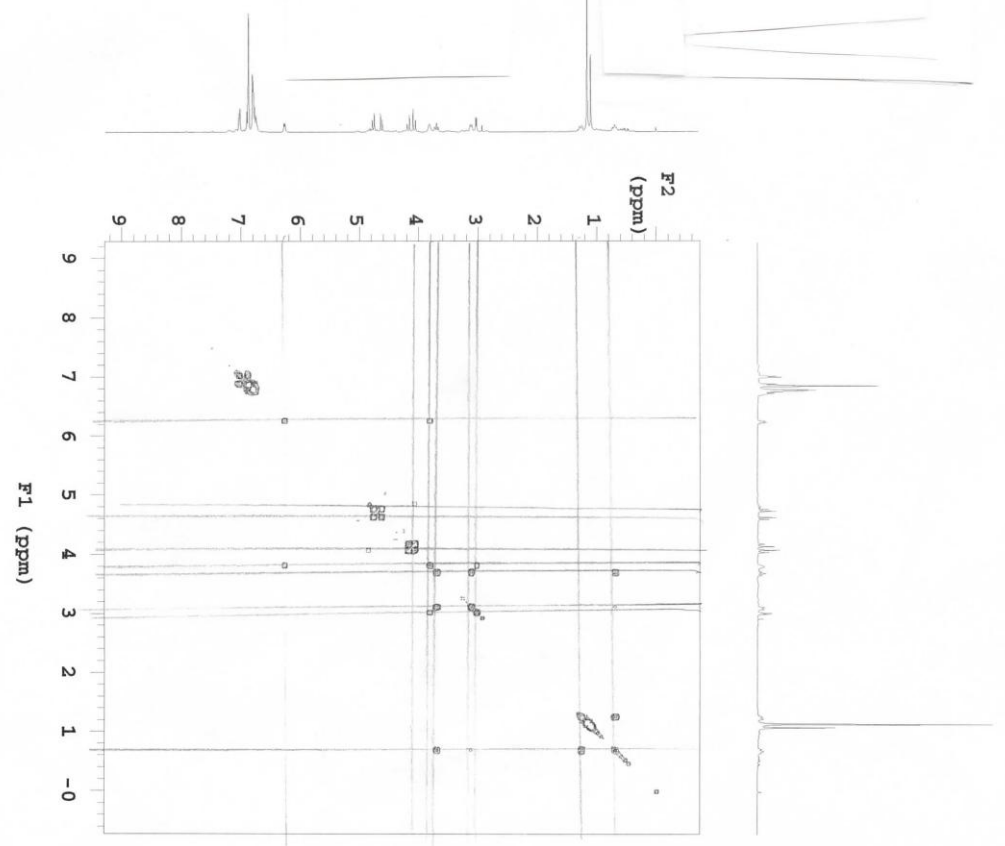


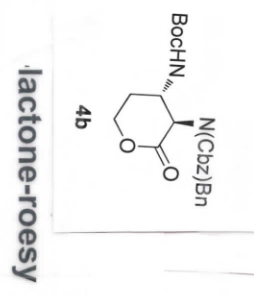
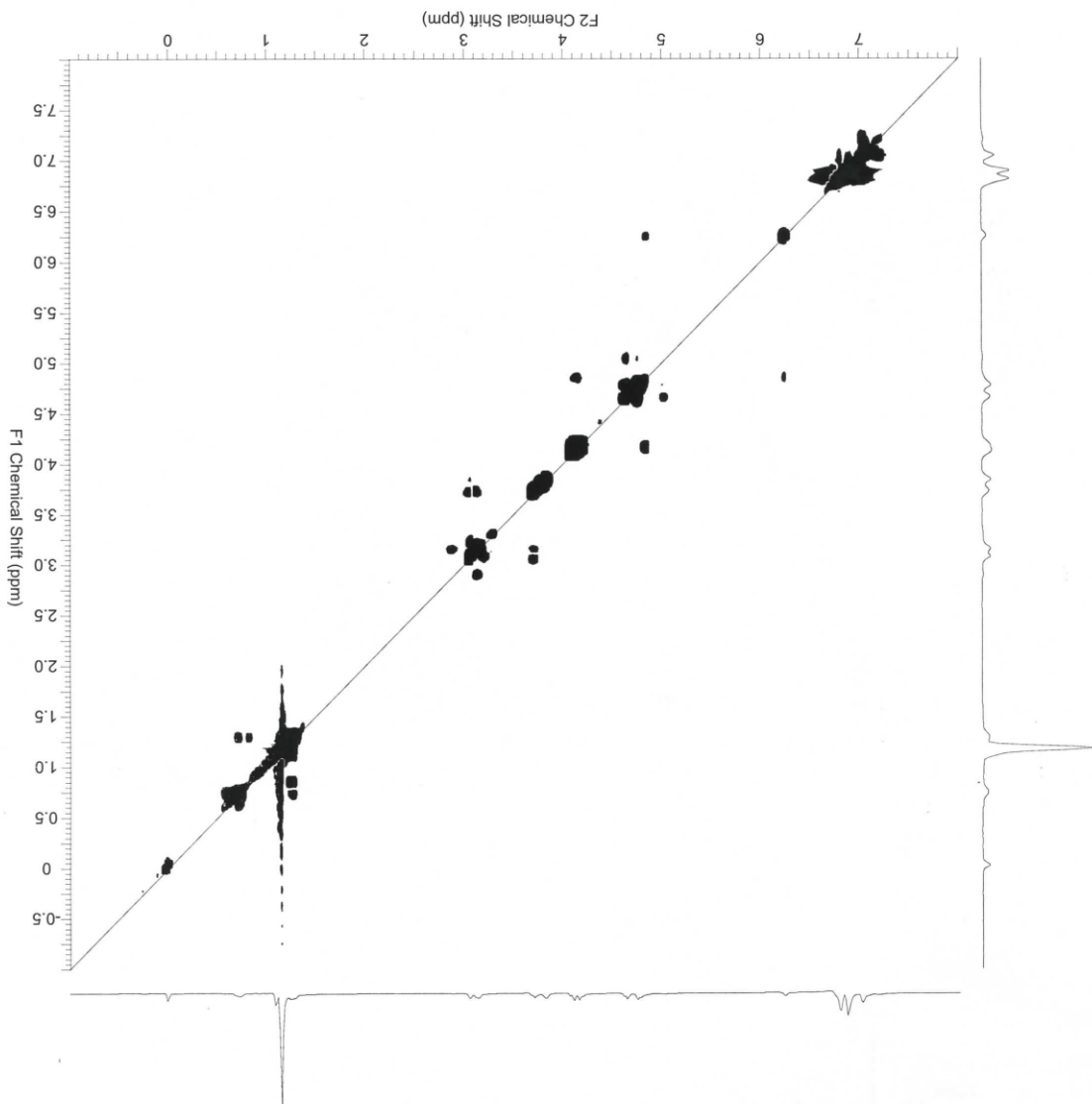


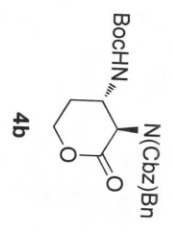
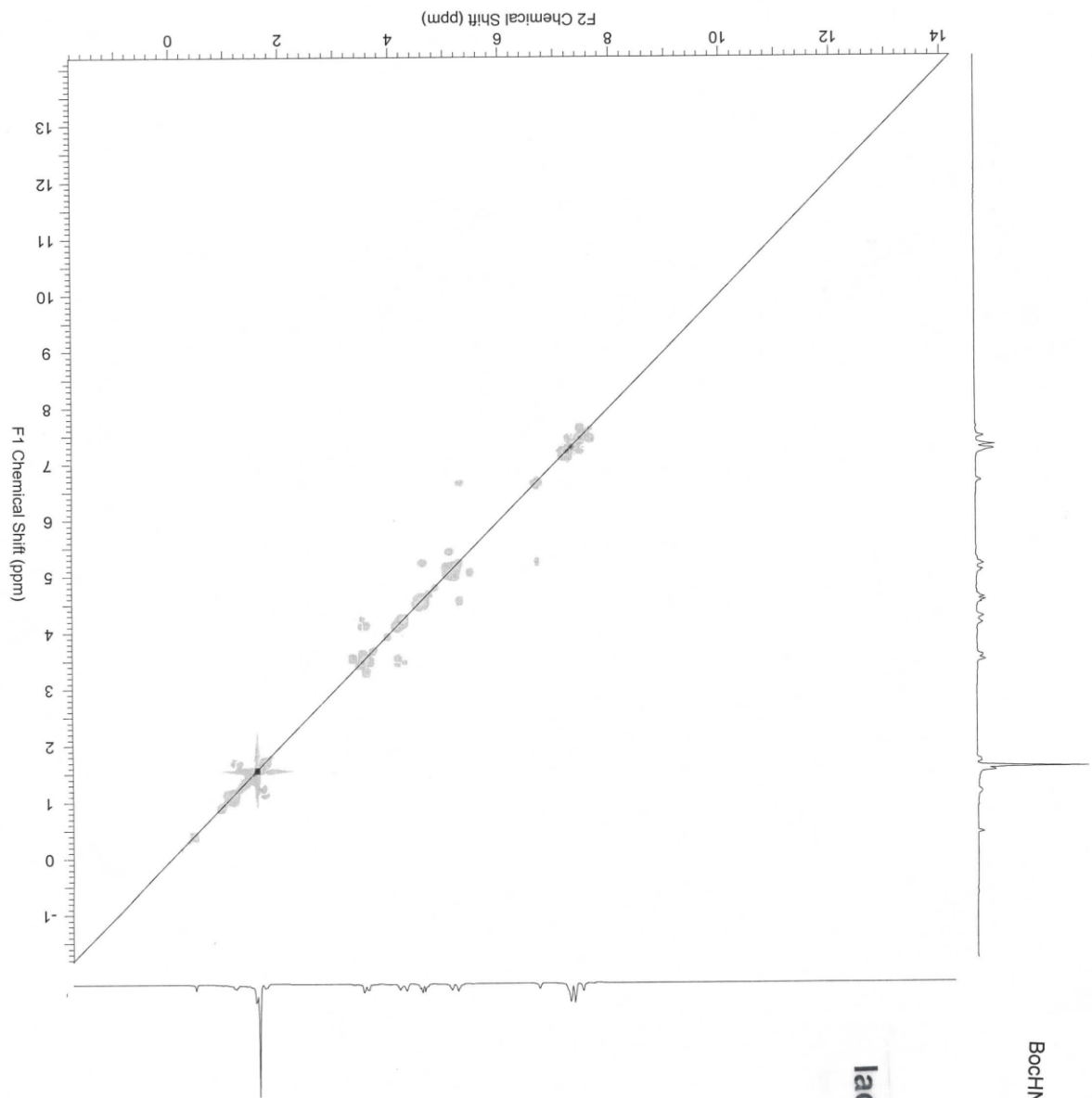




lactone COSY

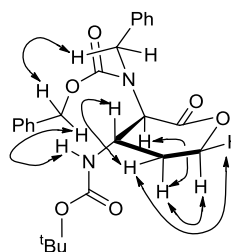
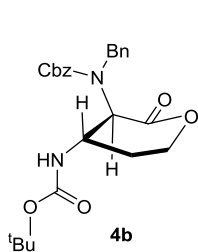




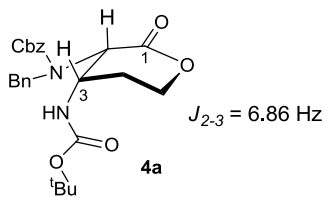


lactone-noesy

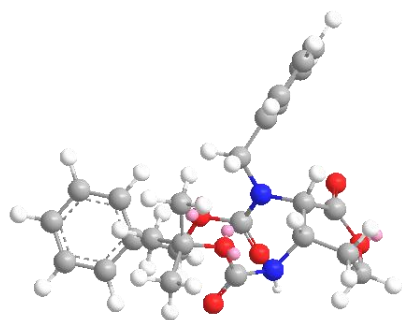
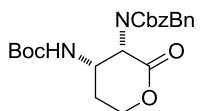
NOESY map for Compound 4b and the selected J value



NOESY map for 4b



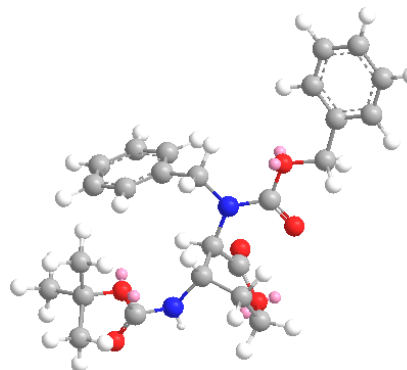
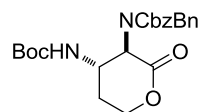
The lowest energy conformers determined by MM2 calculations and predicted coupling constant between the C2- and C3-protons



18.09 Kcal/mol

37.1°

$J = \sim 6\text{--}8$ Hz



24.9551 Kcal/mol

81.3°

$J = \sim 0.05$ Hz

