

On the synthesis of α -amino sulfoxides

Peter J. Rayner,^a Giacomo Gelardi,^a Peter O'Brien,^{*a} Richard A. J. Horan^b and David C. Blakemore^c

^aDepartment of Chemistry, University of York, Heslington, York YO10 5DD, U.K.,

^bGlaxoSmithKline Pharmaceuticals, Medicines Research Centre, Gunnels Wood Road, Stevenage SG1 2NY, U.K.

^cNeusentis Chemistry, Pfizer Worldwide Research and Development, The Portway Building, Granta Park, Cambridge, CB21 6GS, U.K.

peter.obrien@york.ac.uk

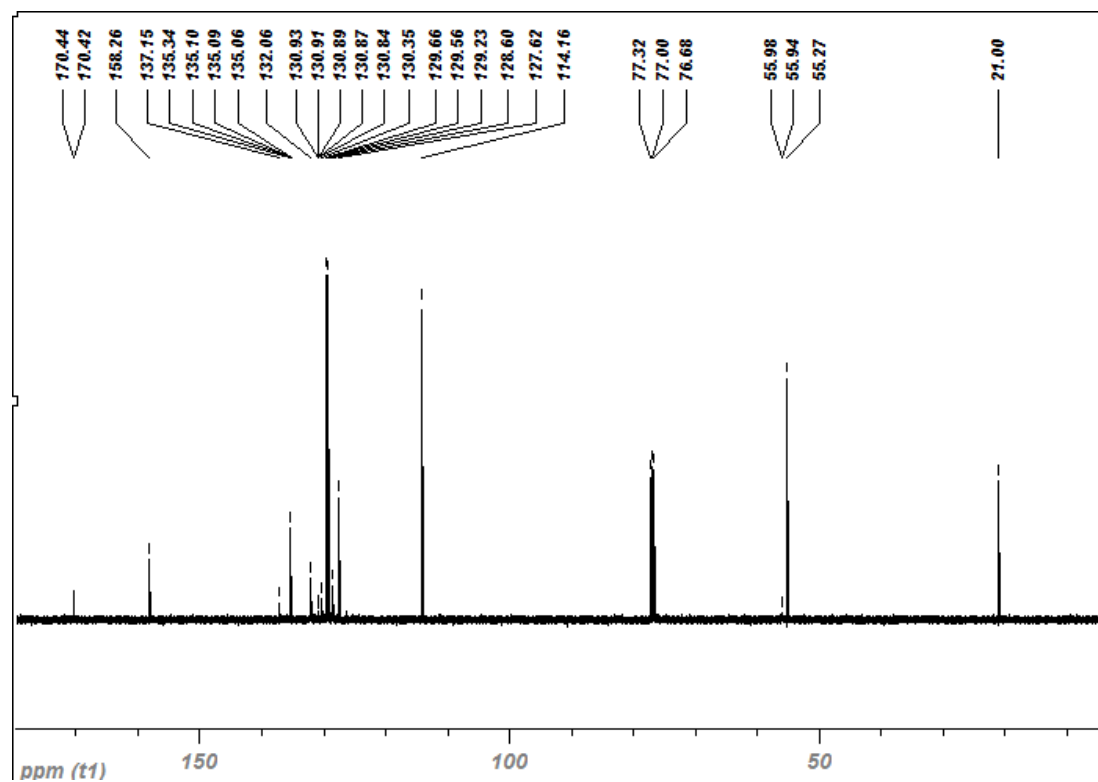
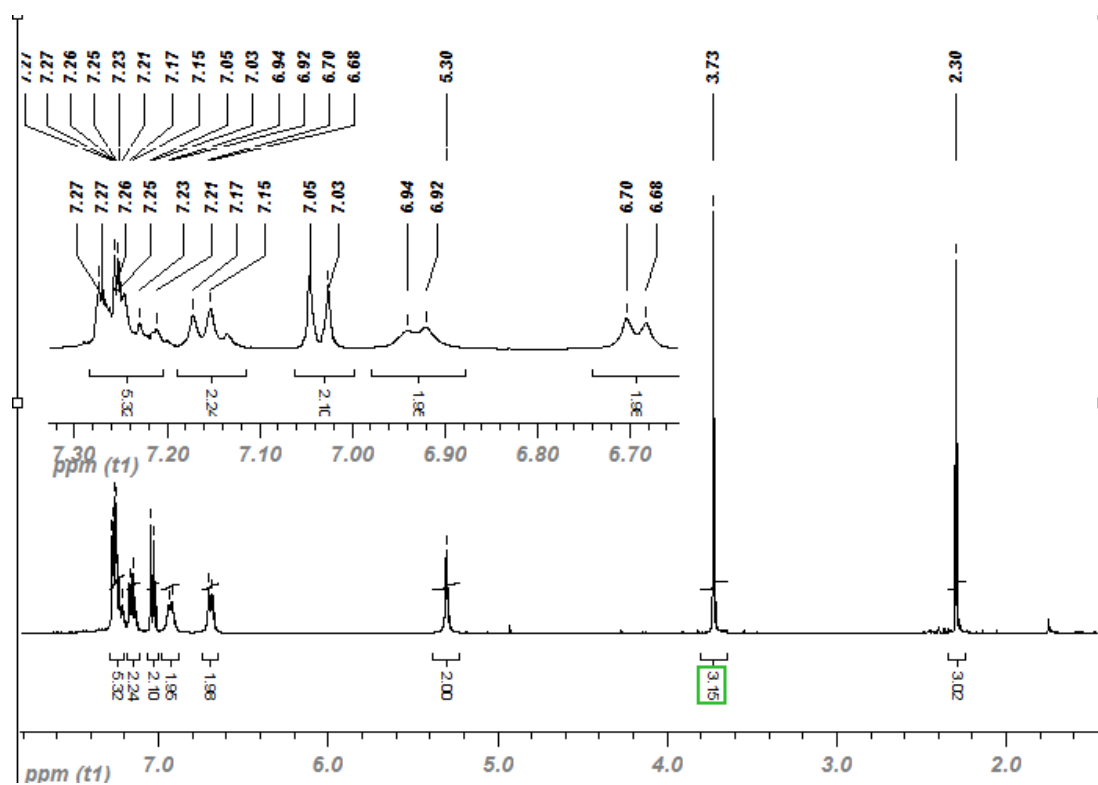
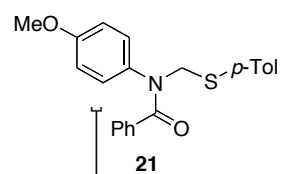
Electronic Supplementary Information (ESI): Copies of ¹H NMR and ¹³C NMR spectra.

Chemical structure of 18: CC(C)(C)N(C)CC[S+](C)(C)C(=O)[O-] (Boc-protected p-toluenesulfonamide derivative).

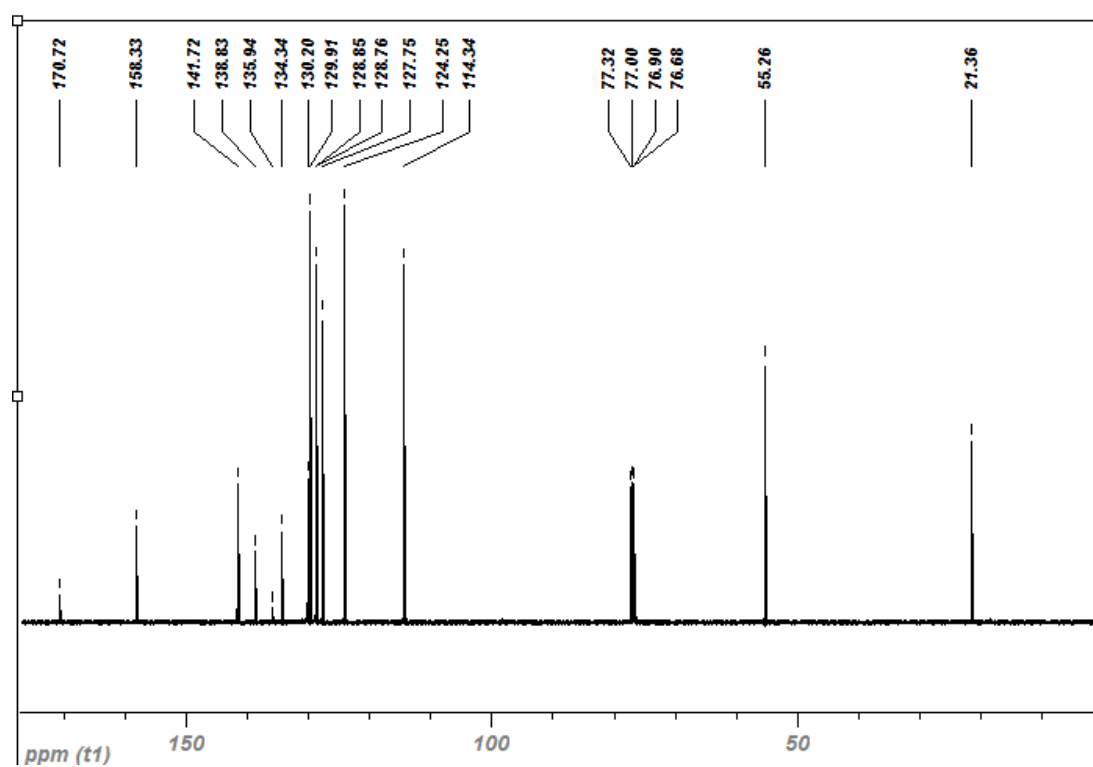
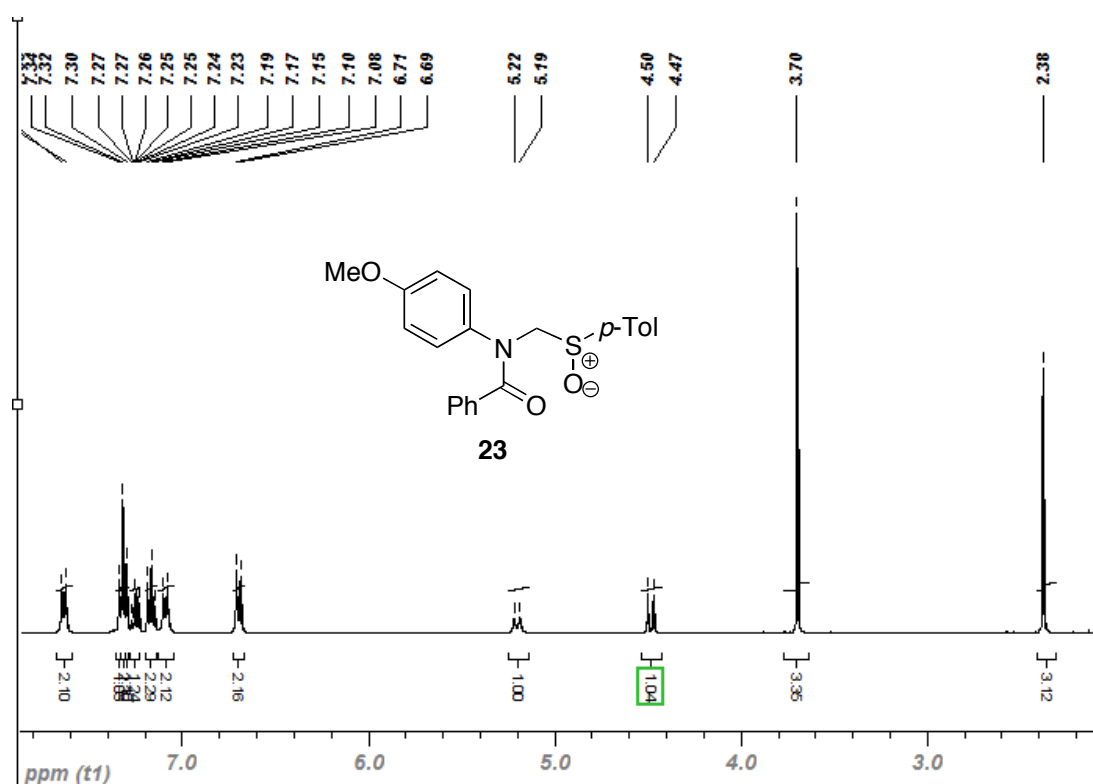
¹H NMR spectrum (top): The x-axis is labeled "ppm (t1)" and ranges from 1.0 to 8.0. The spectrum shows several multiplets and doublets. Key peaks are labeled with their chemical shifts: 7.56, 7.54, 7.52, 7.50, 7.36, 7.34, 7.32, 4.60, 4.56, 4.39, 4.36, 4.32, 4.28, 4.13, 4.09, 3.06, 2.94, 2.42, 2.41, 1.44, and 1.39. Integrations are provided below the peaks: 2.80, 2.80, 0.88, 0.88, 0.80, 0.80, 1.48, 1.48, 1.64, and 4.88. A green box highlights the peak at 4.32 ppm with an integration of 0.80.

¹³C NMR spectrum (bottom): The x-axis is labeled "ppm (t1⁵⁰)" and ranges from 0 to 160. The spectrum shows several sharp peaks. Key peaks are labeled with their chemical shifts: 155.20, 154.16, 142.03, 141.66, 138.74, 138.43, 138.47, 130.07, 129.88, 125.55, 125.34, 124.30, 124.20, 81.20, 81.02, 74.65, 74.47, 37.08, 36.32, 28.16, 28.03, and 21.39.

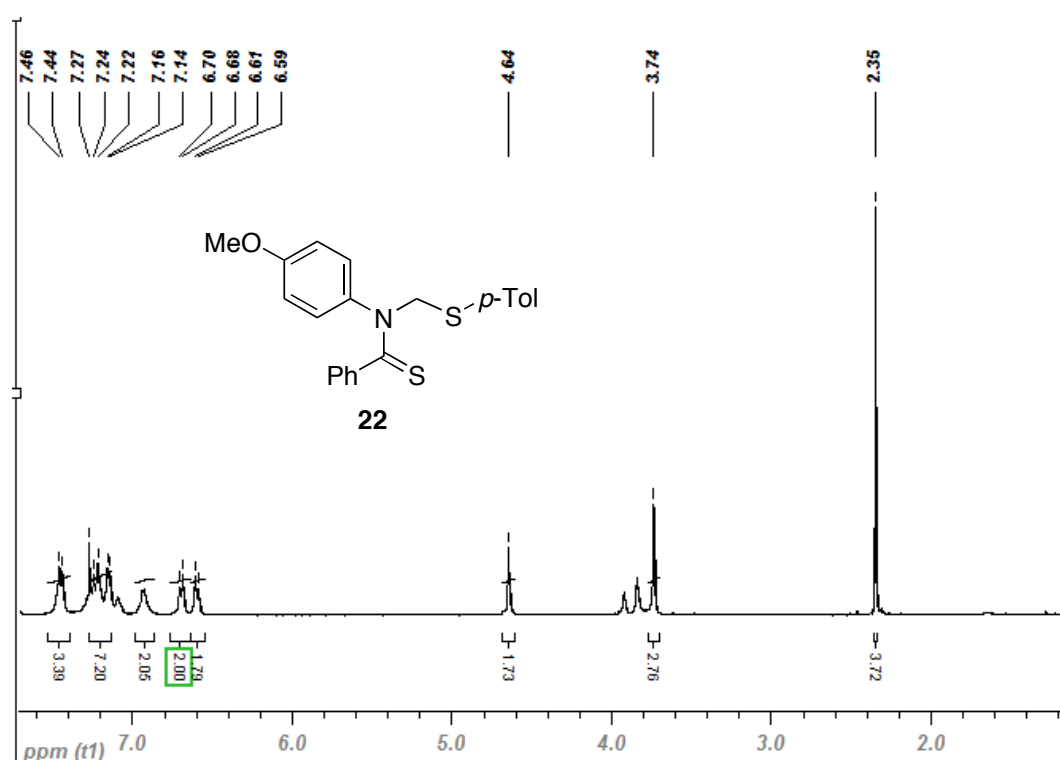
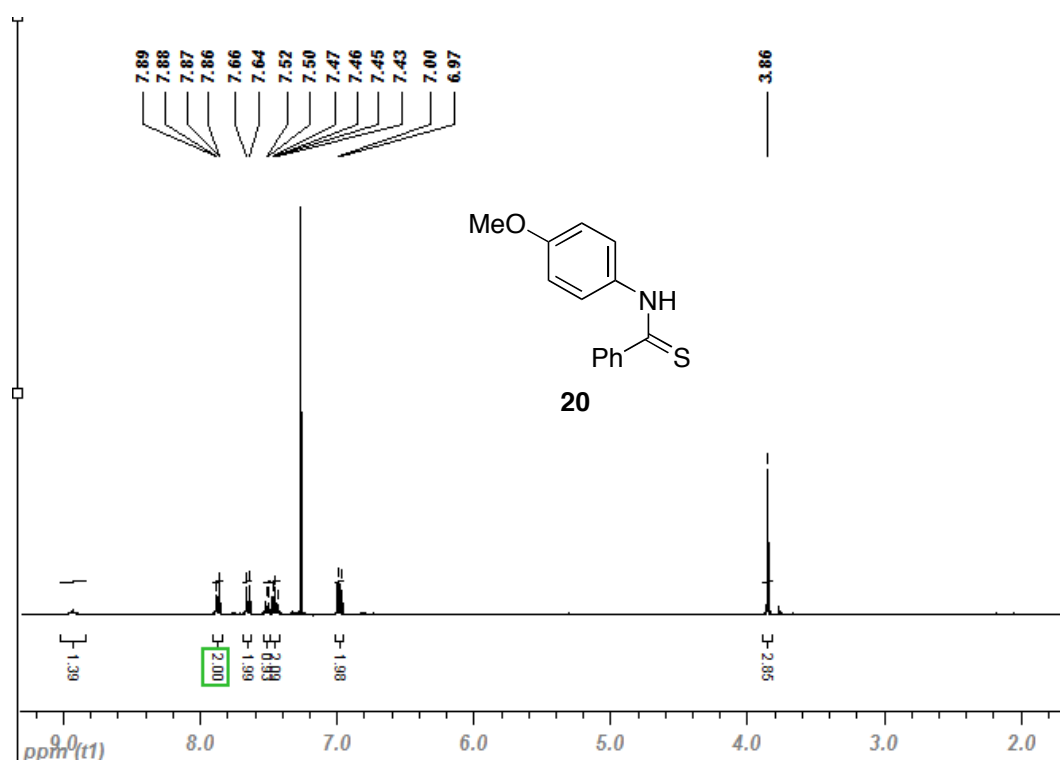
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



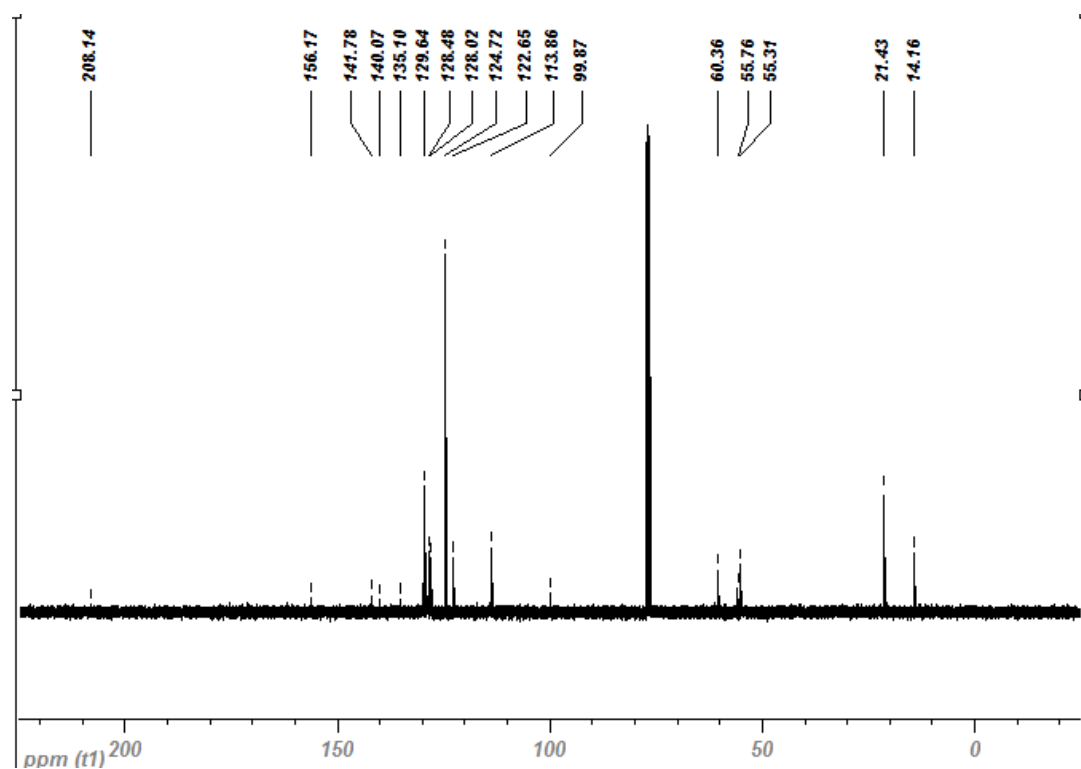
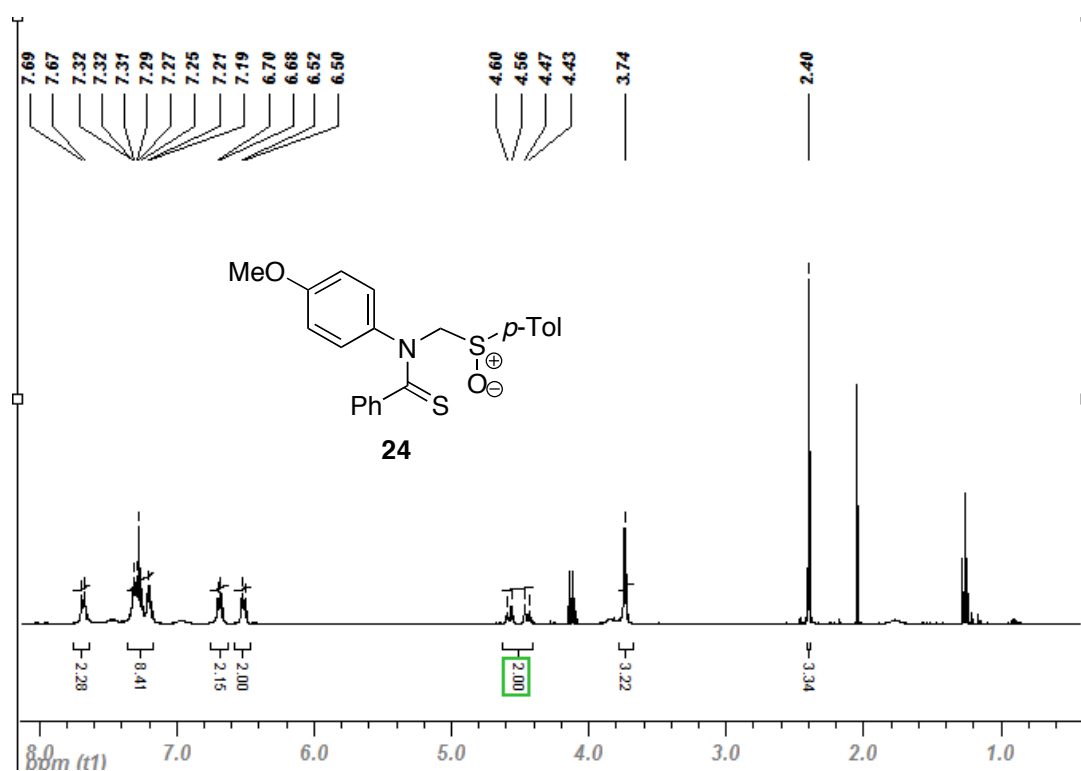
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



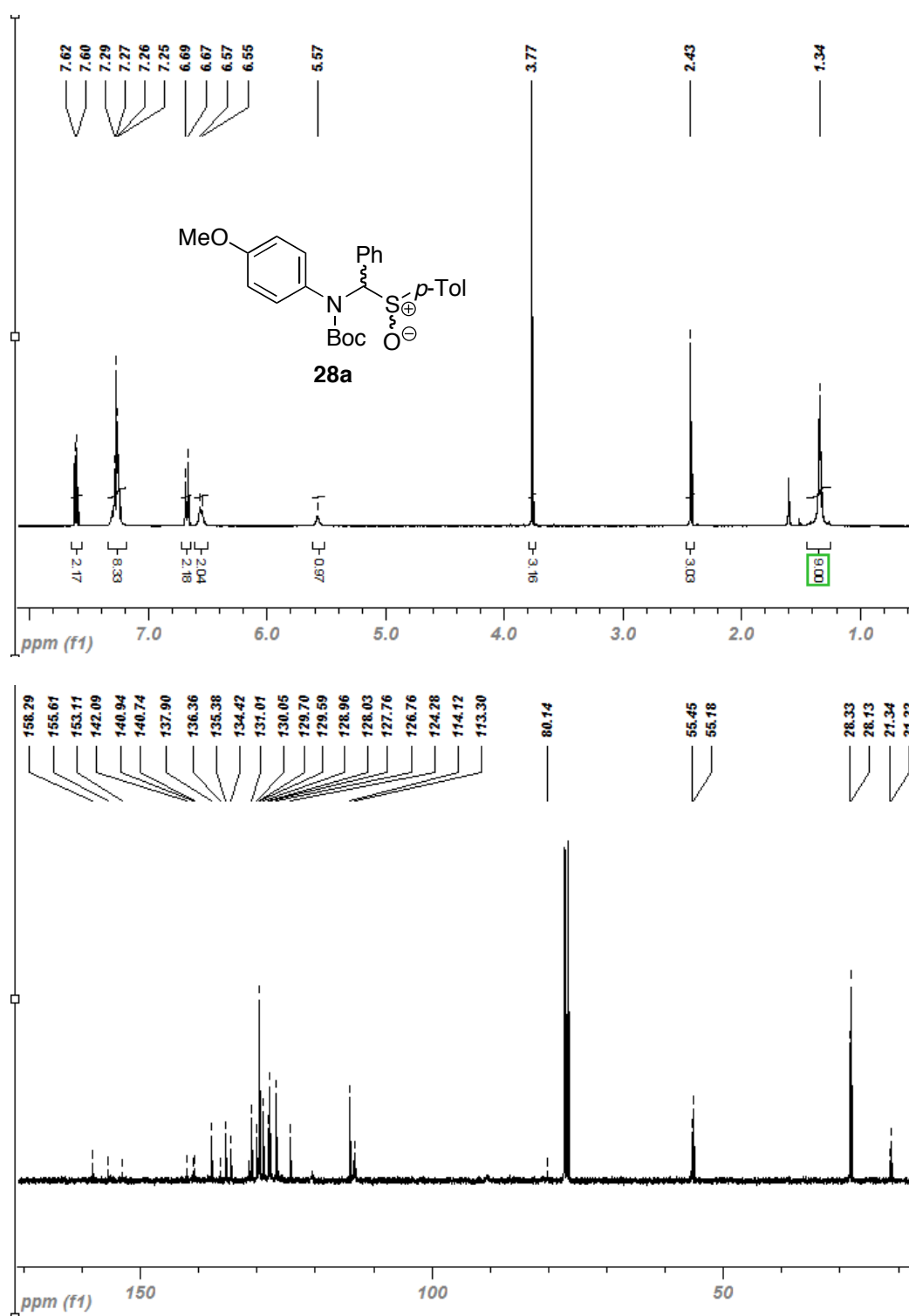
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



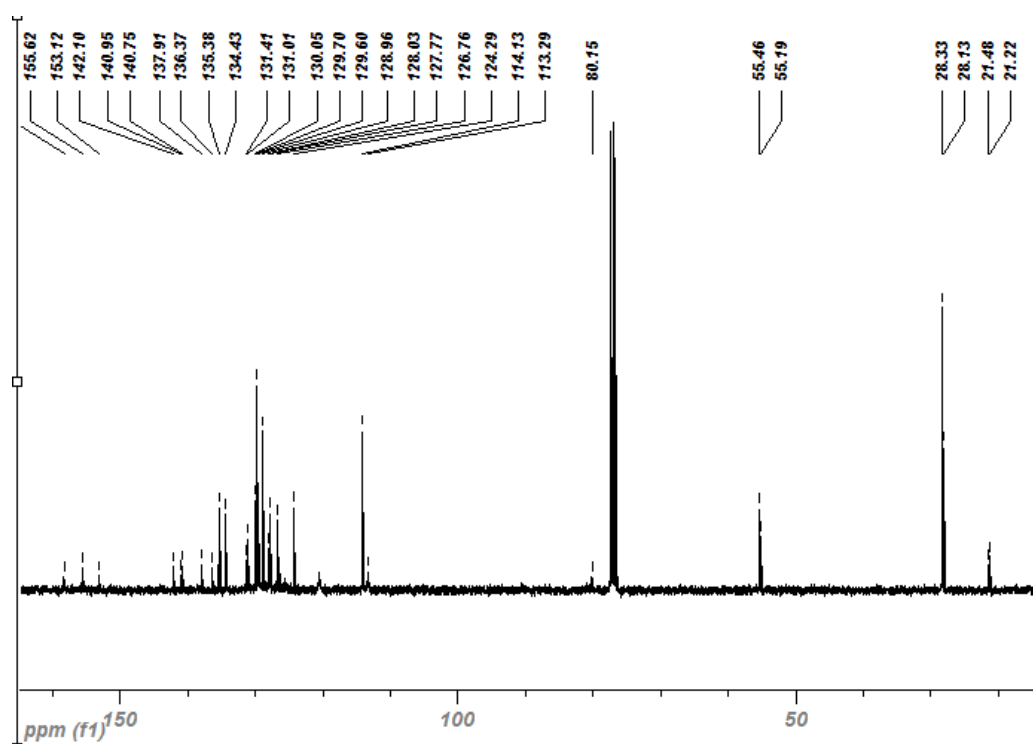
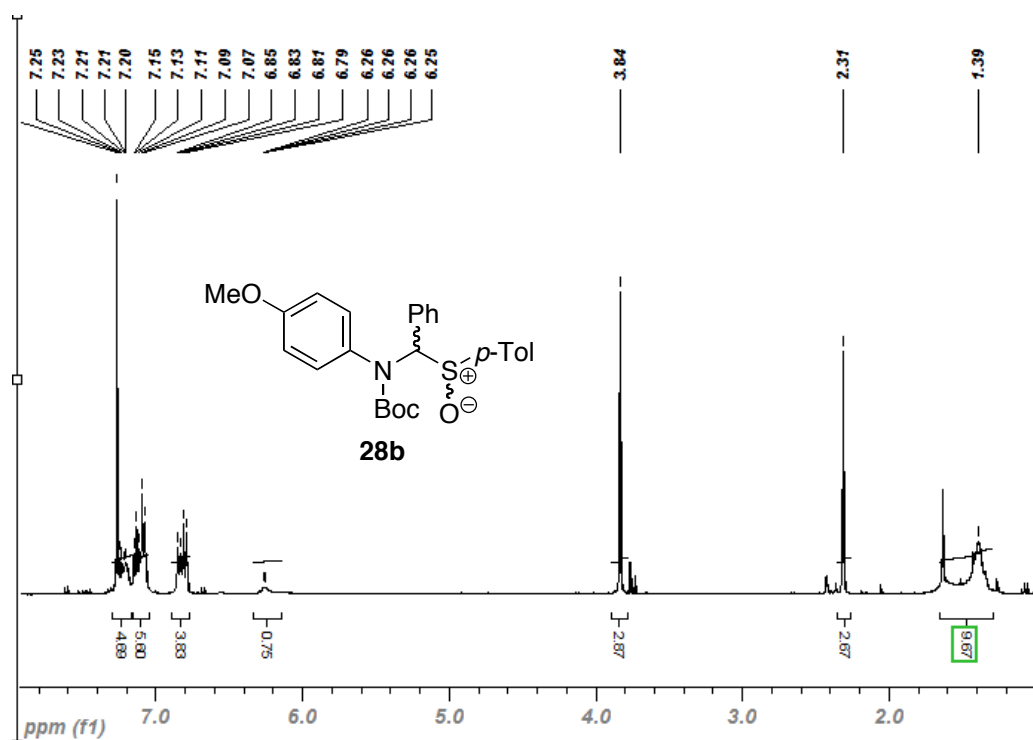
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



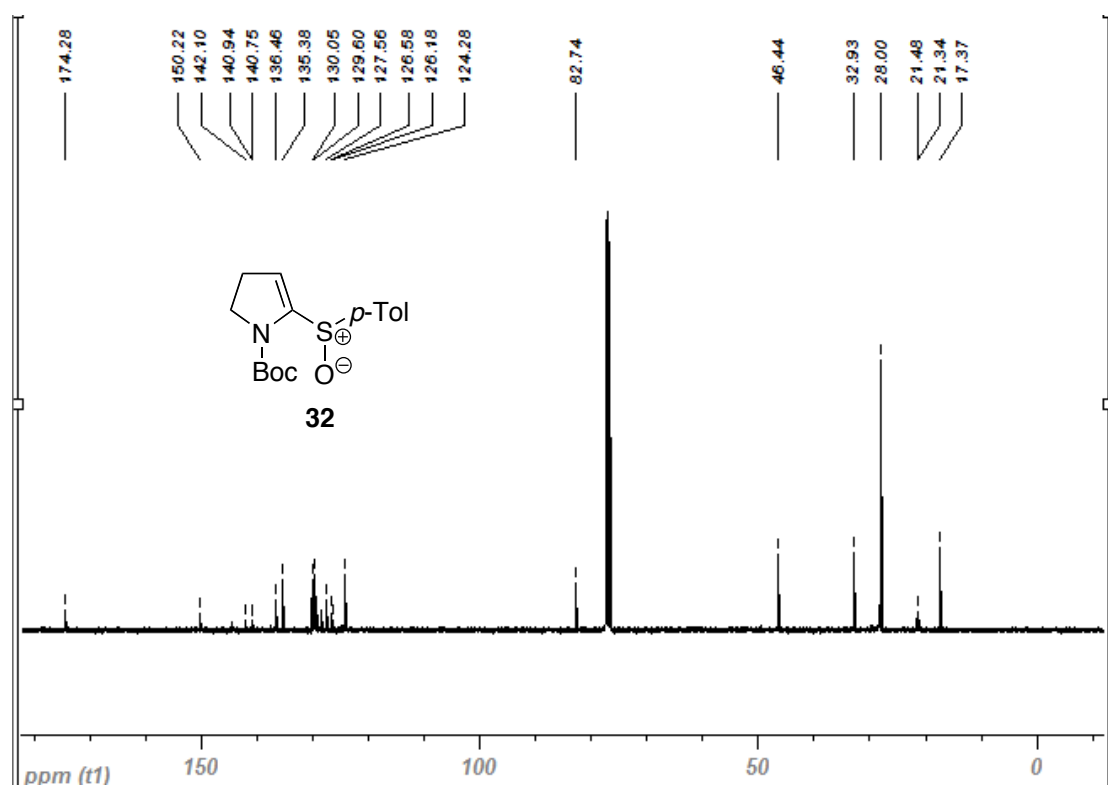
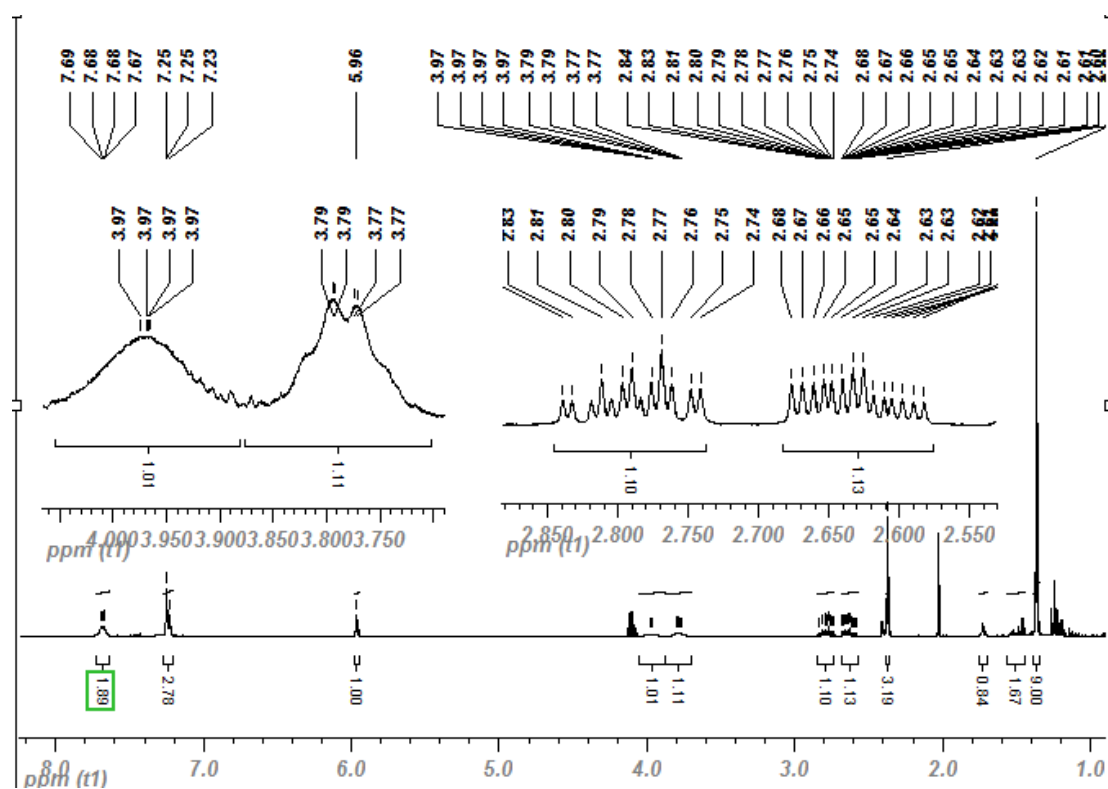
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



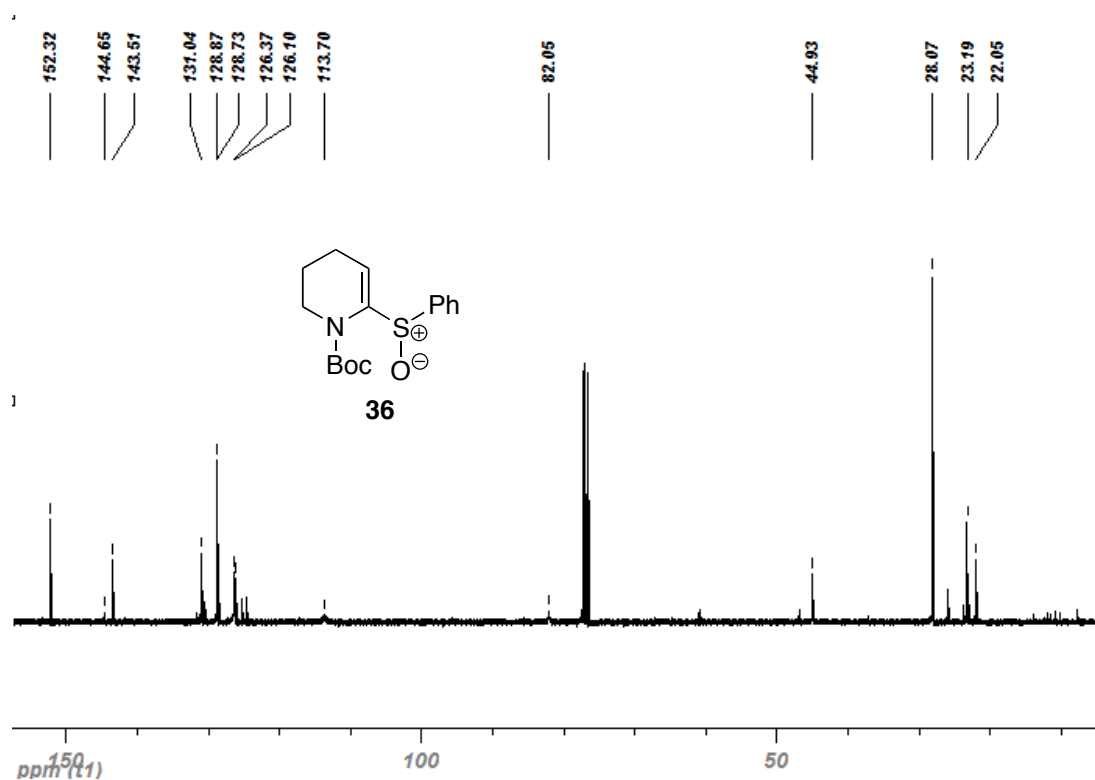
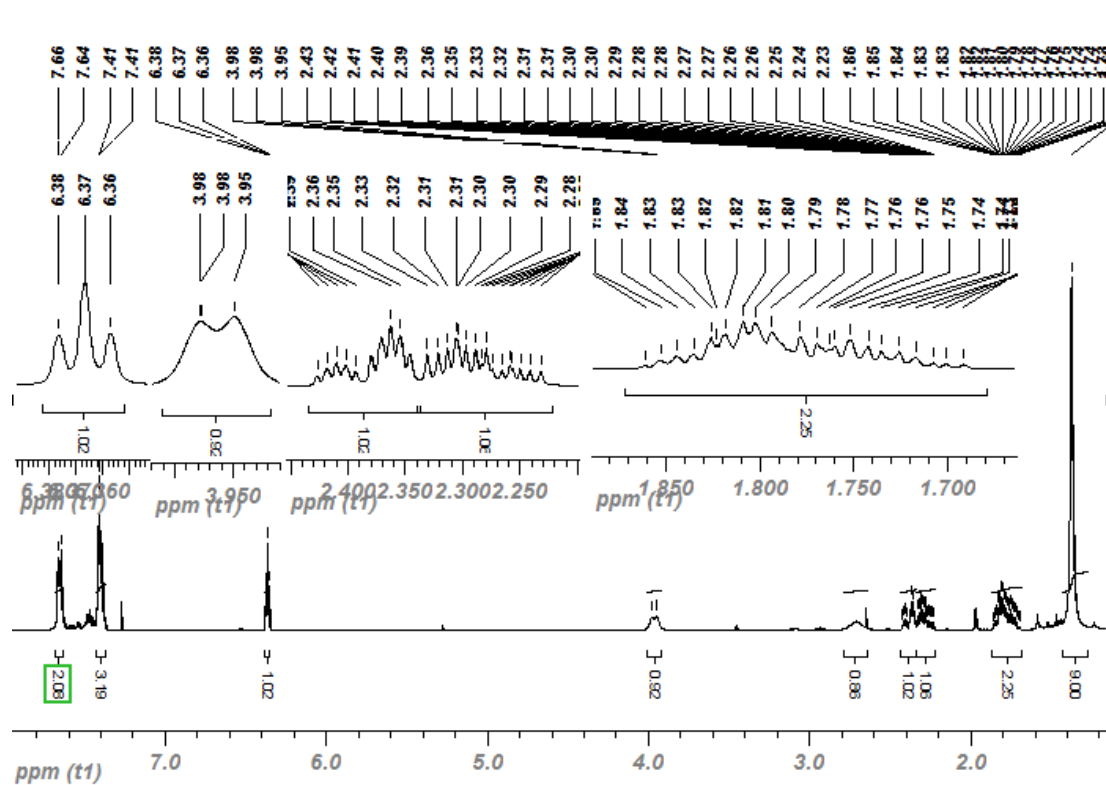
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



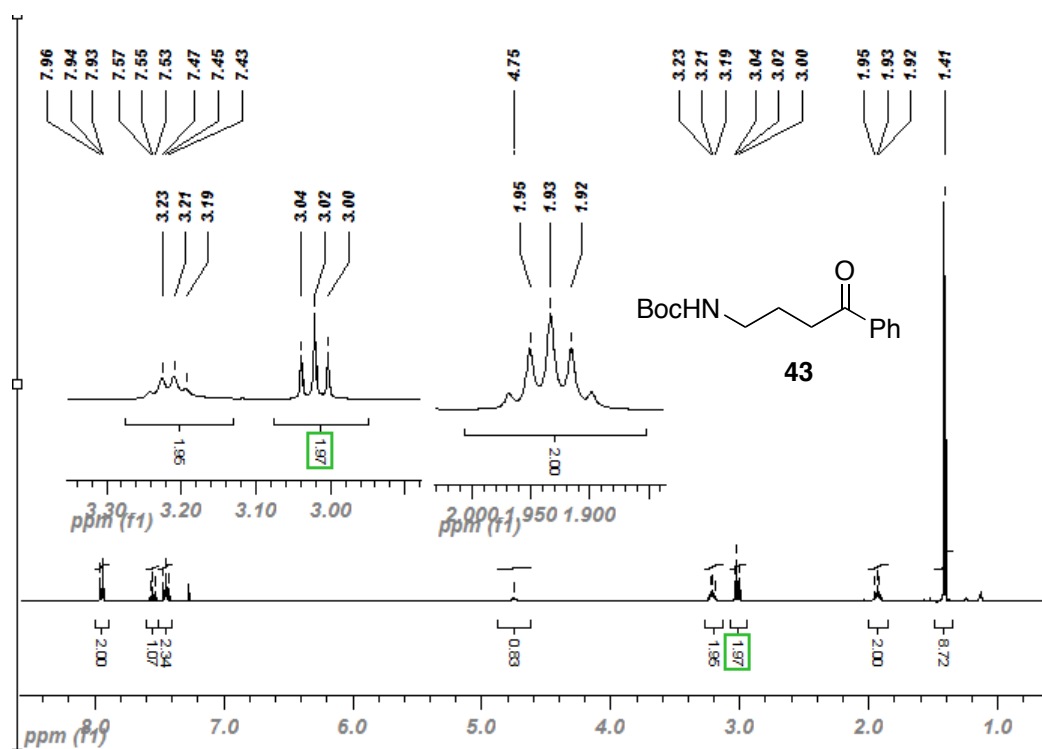
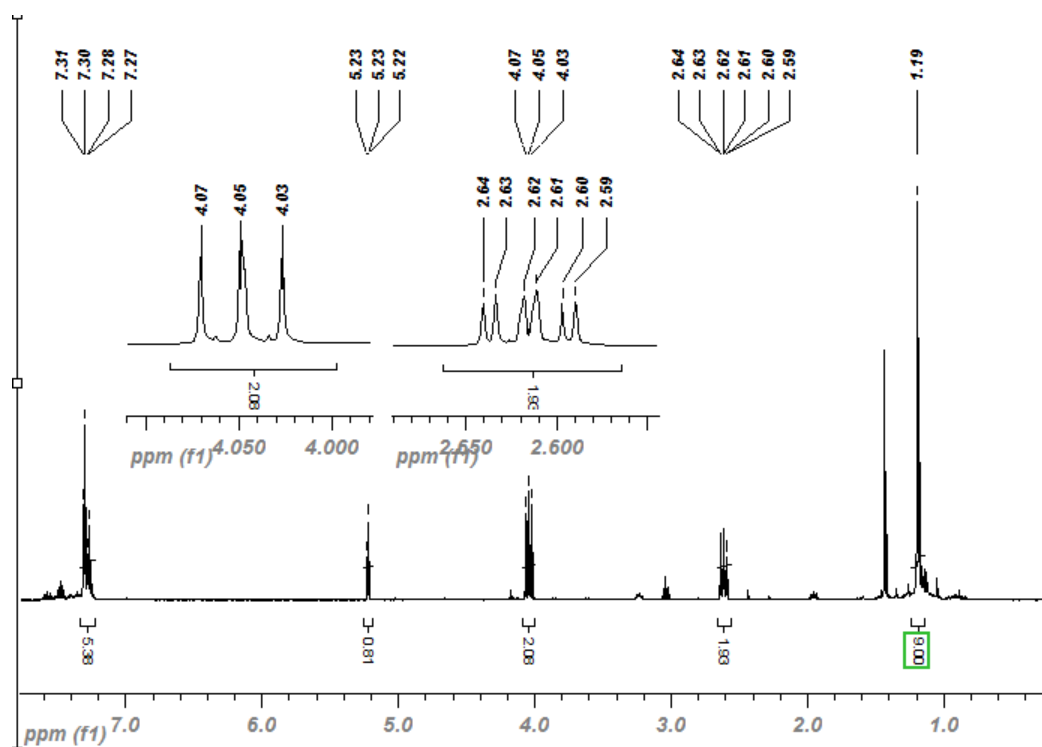
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



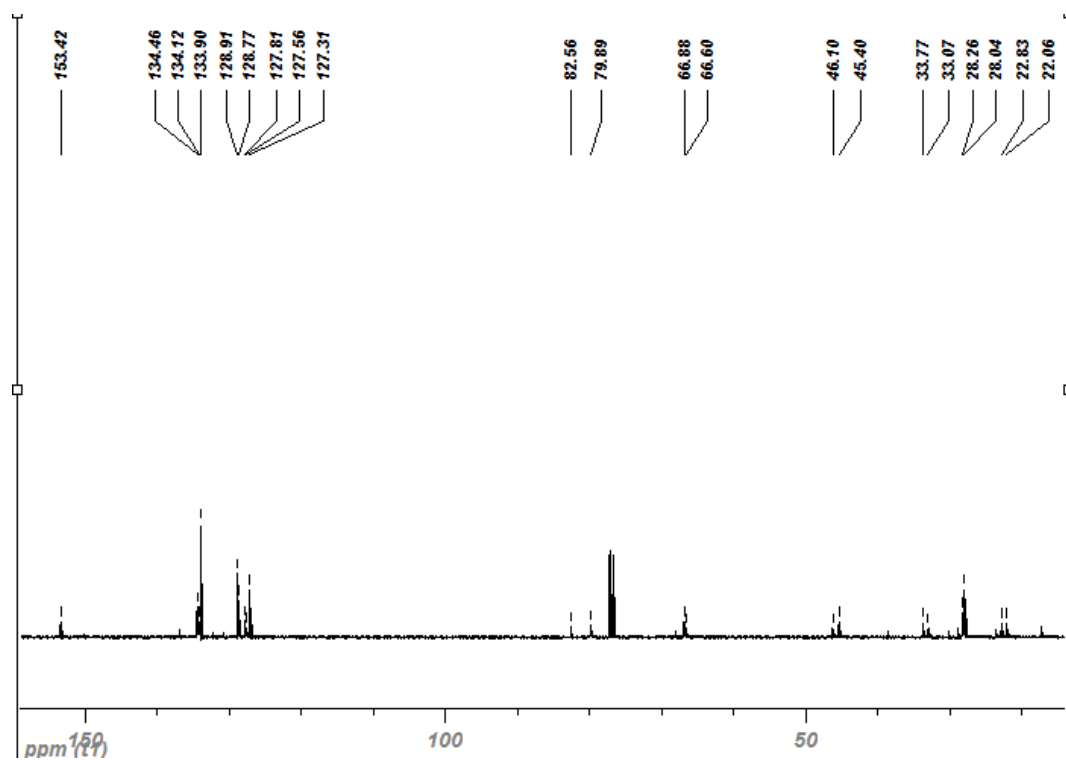
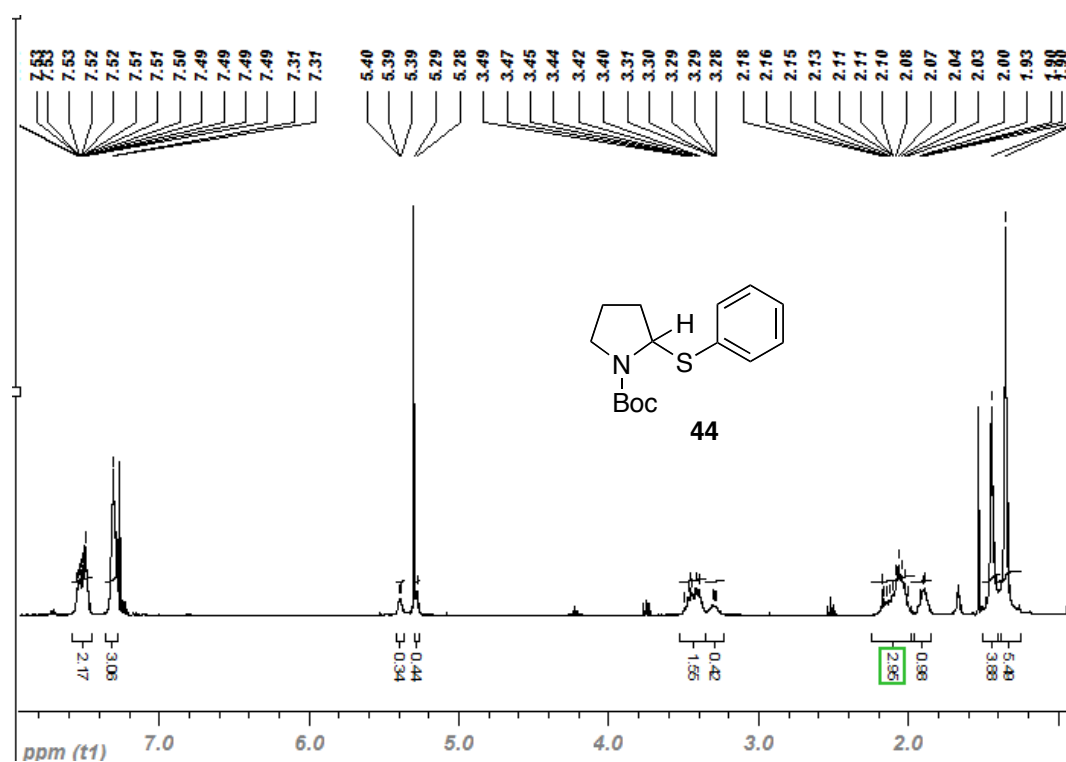
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



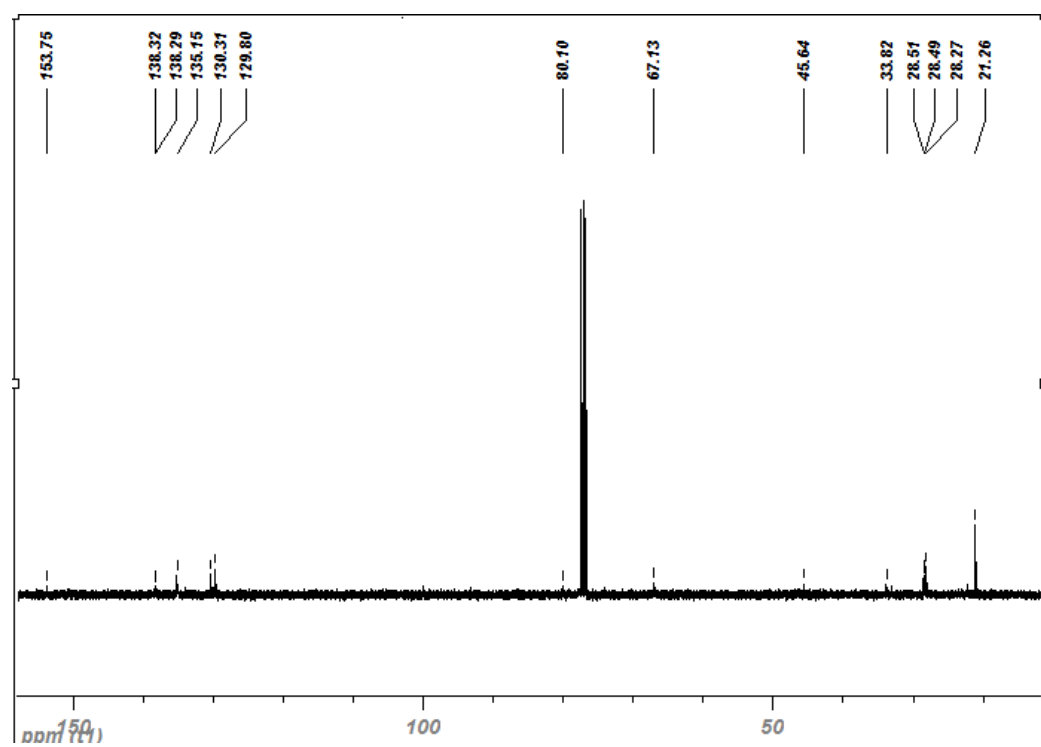
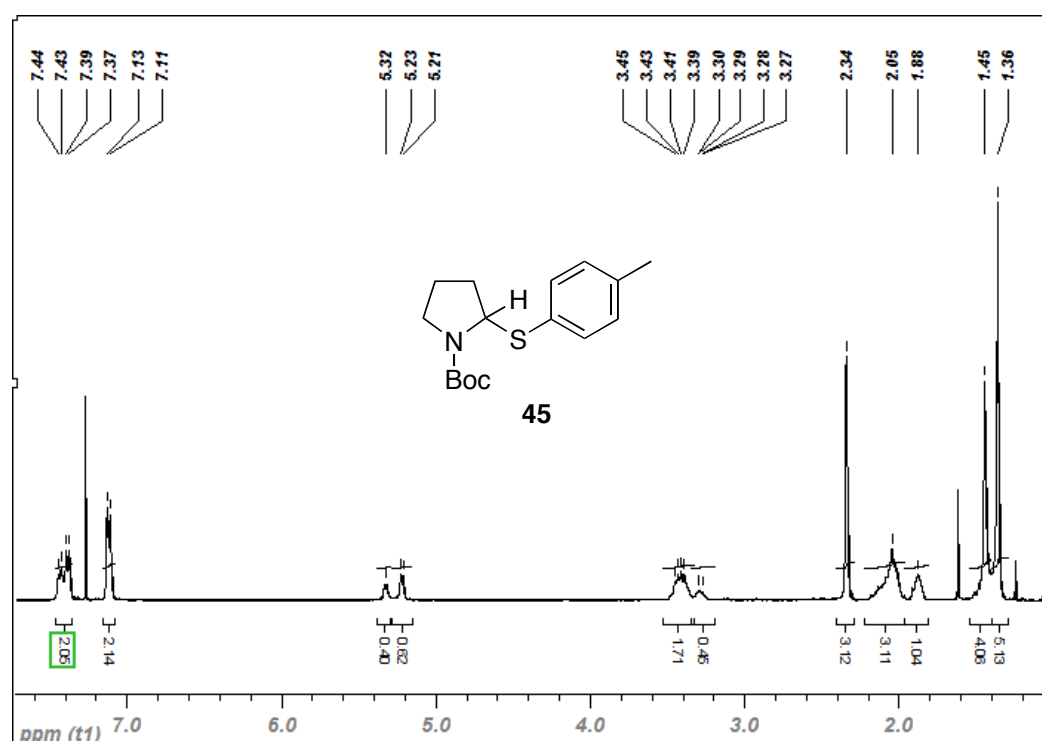
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



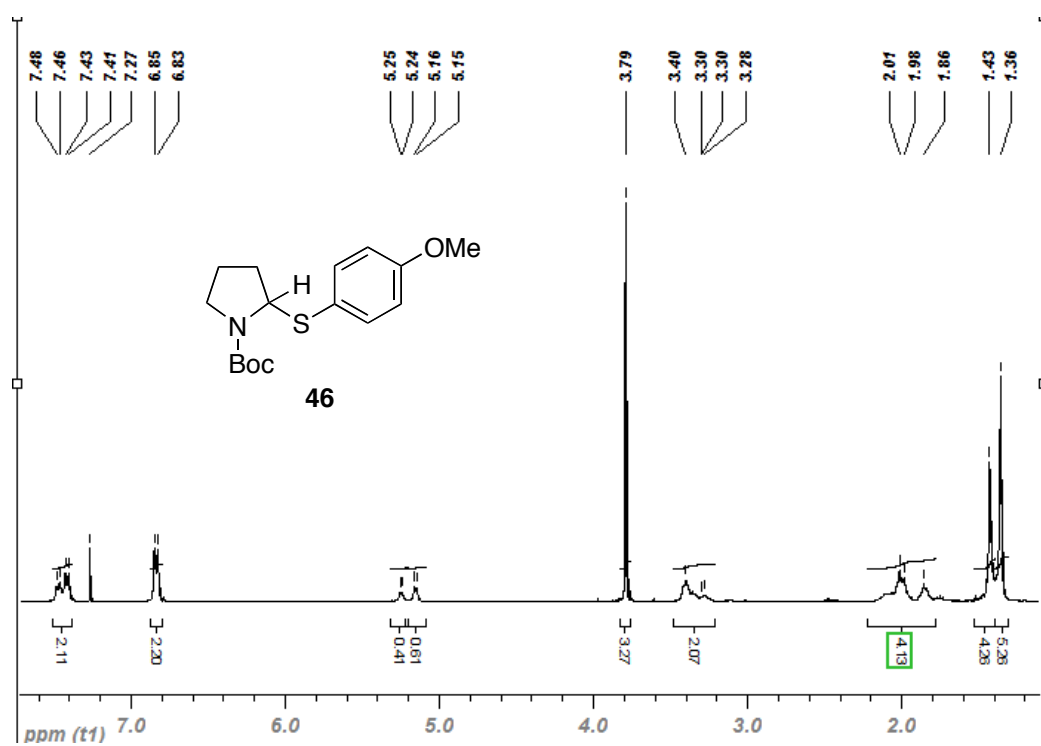
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



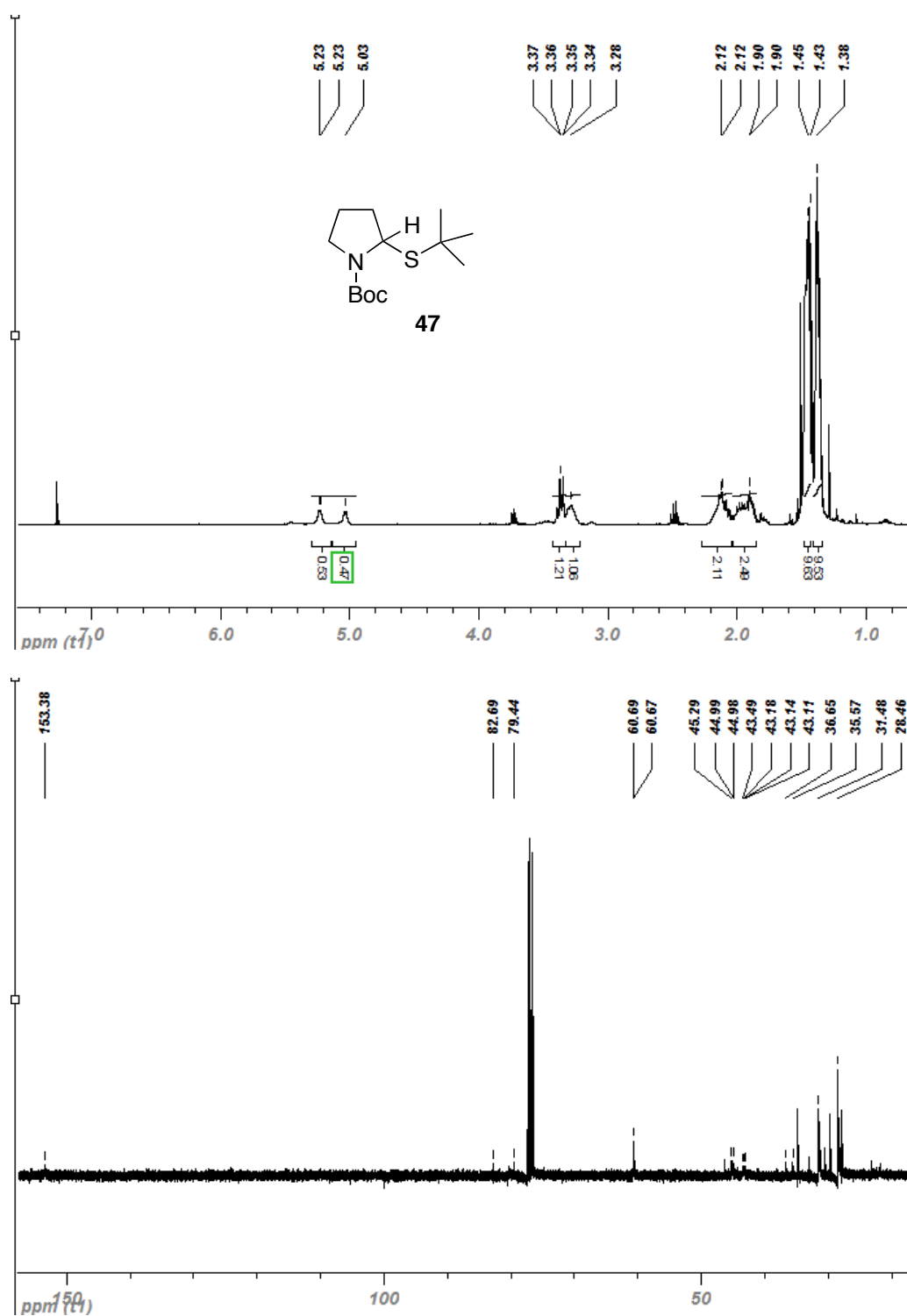
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



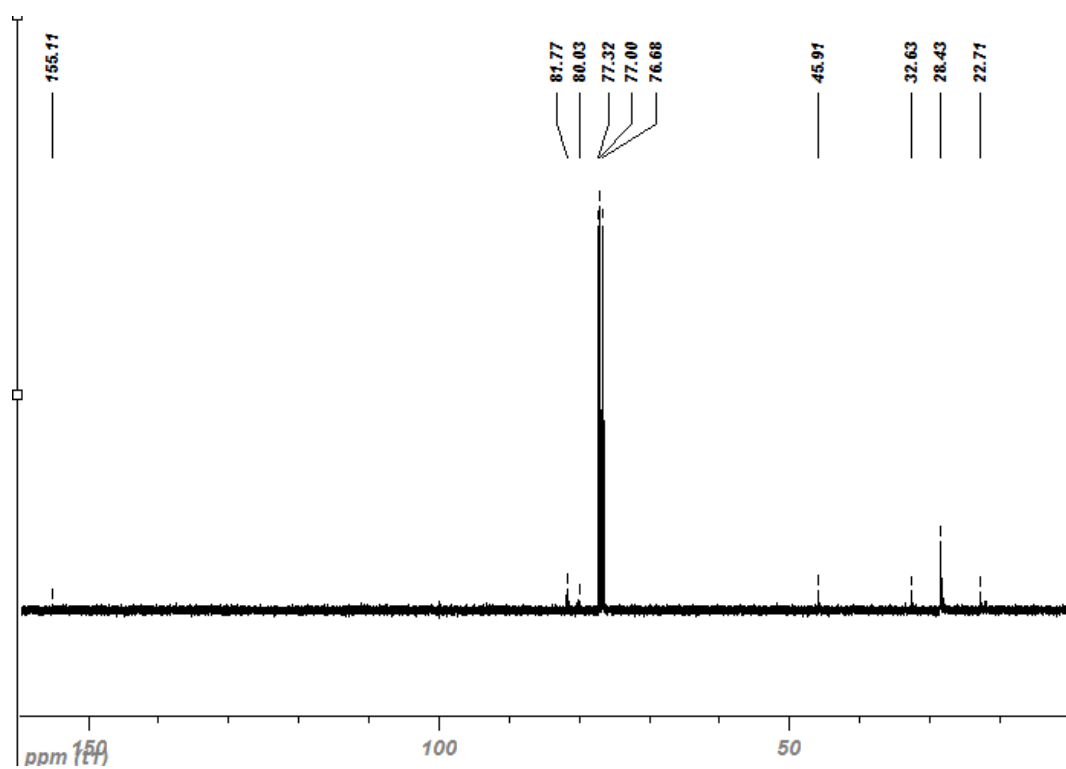
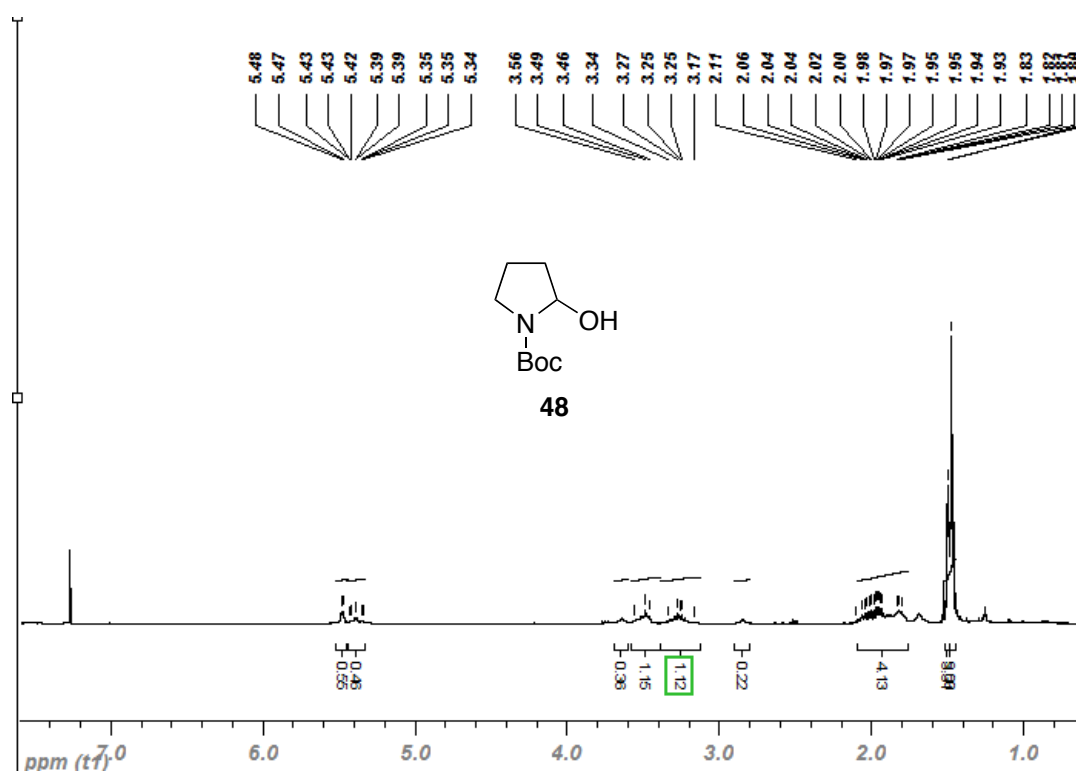
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



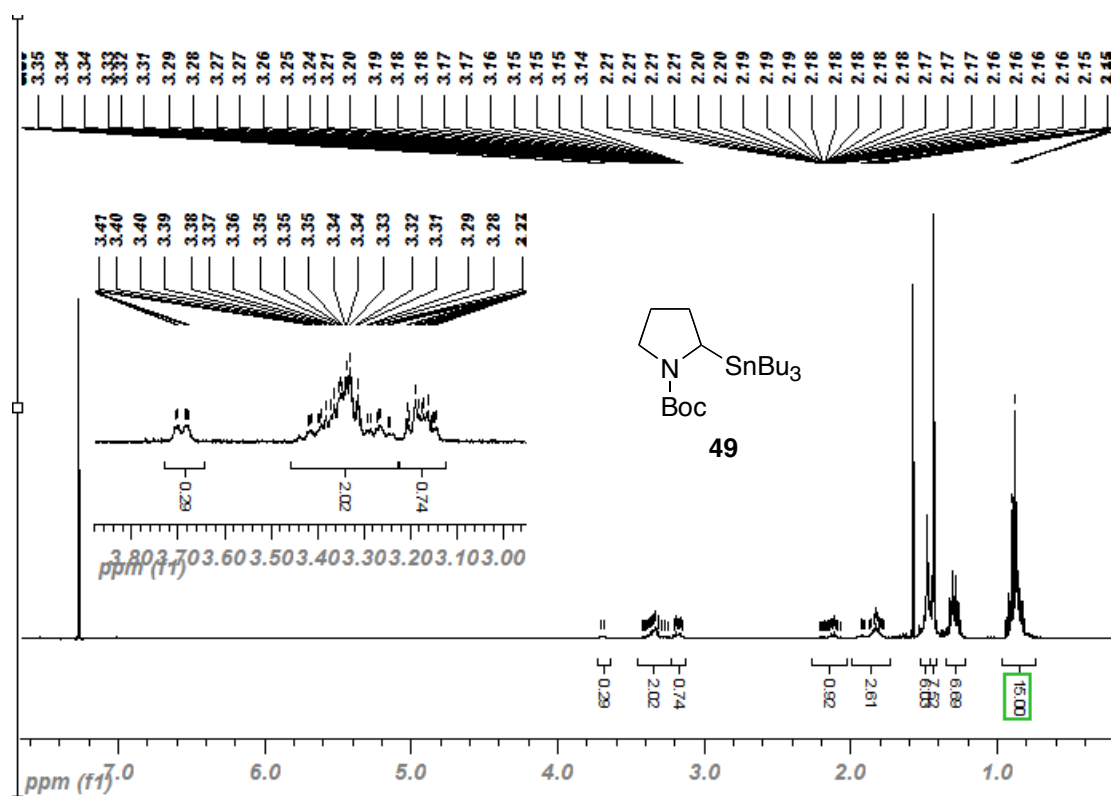
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



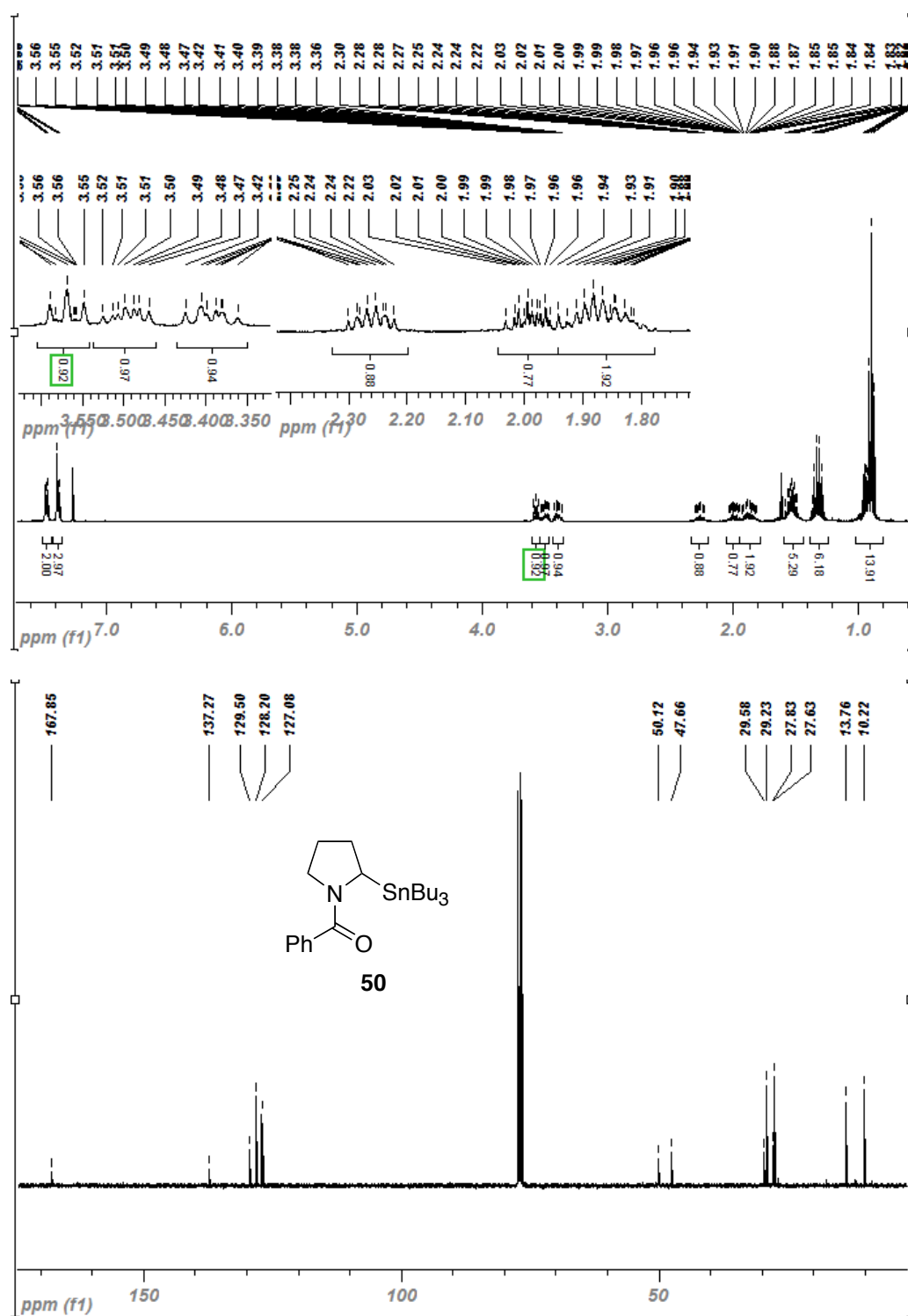
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



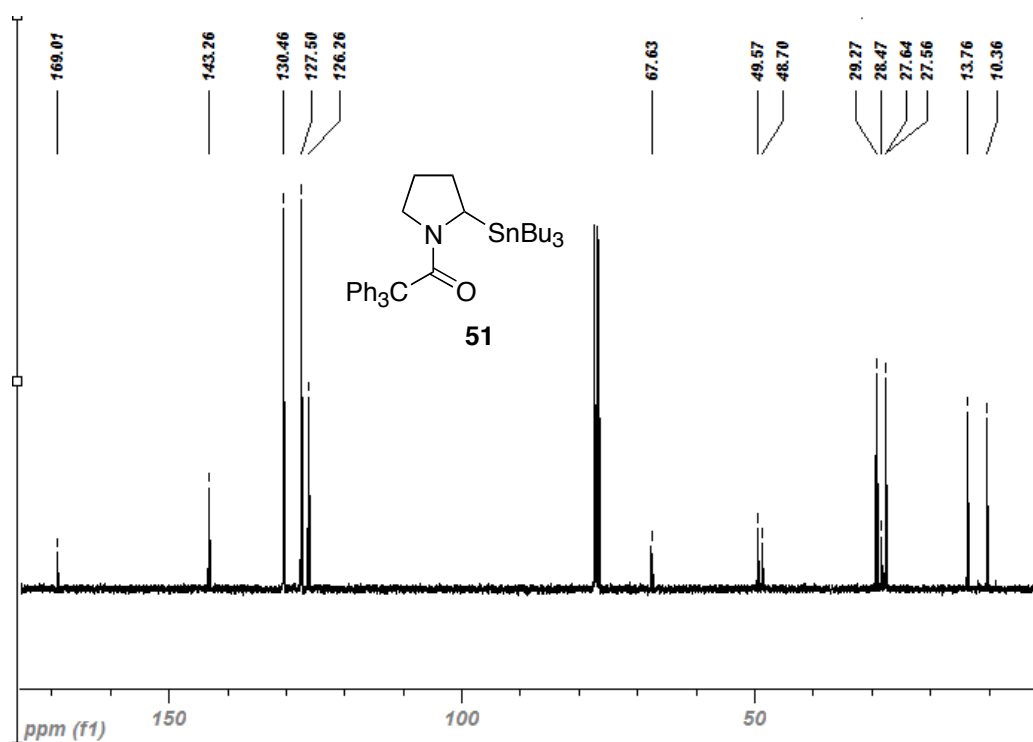
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3

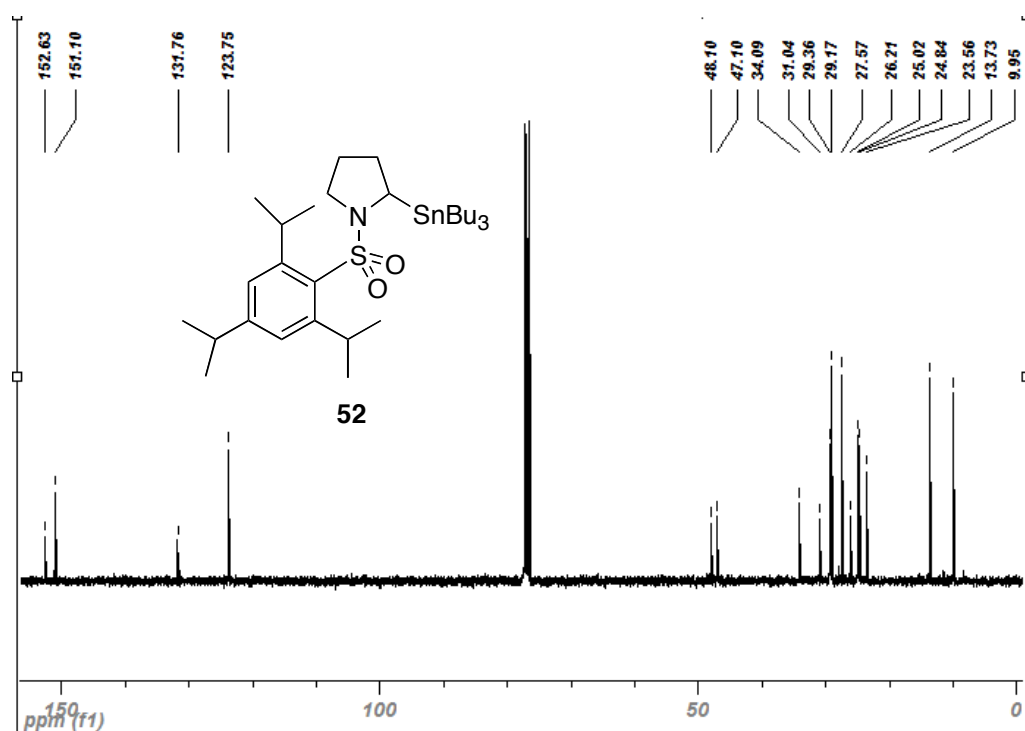


The figure displays a ^1H NMR spectrum of compound **6d**. The spectrum shows several distinct signals:

- A triplet at approximately 7.2 ppm with an integration of 1.00.
- A multiplet between 4.5 and 5.5 ppm with an integration of 0.96.
- A multiplet at approximately 2.3 ppm with an integration of 0.98.
- A complex multiplet between 1.8 and 2.3 ppm with an integration of 0.96.
- A sharp singlet at approximately 1.2 ppm with an integration of 13.26.

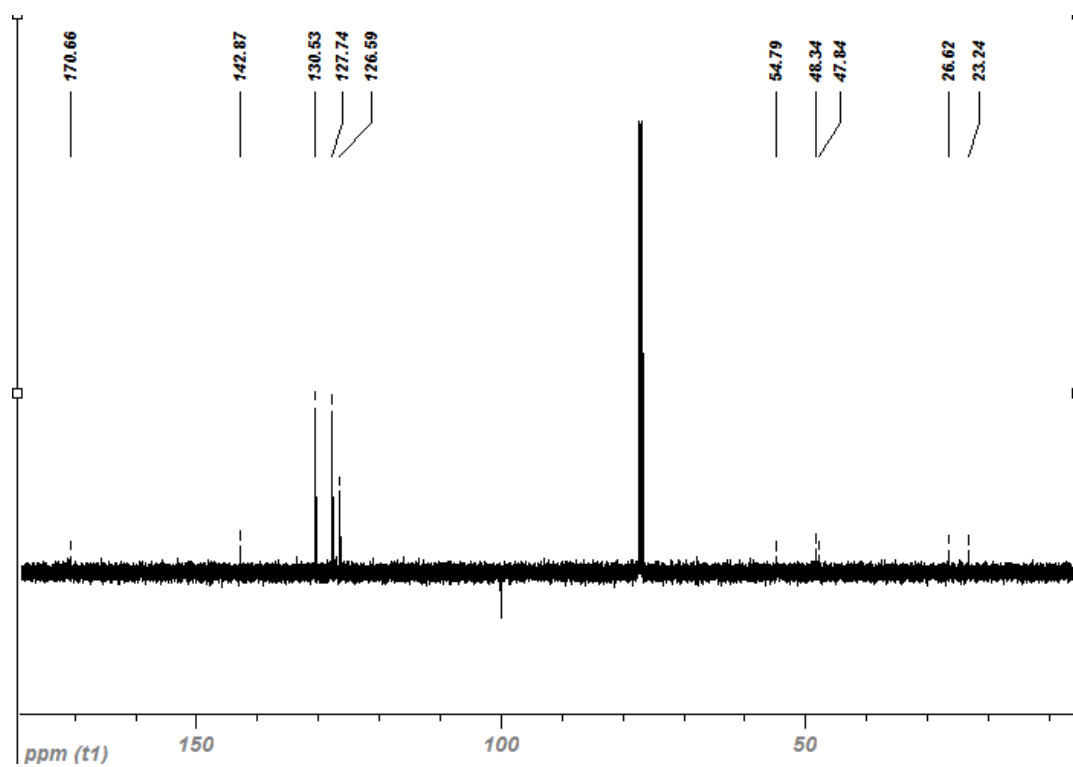
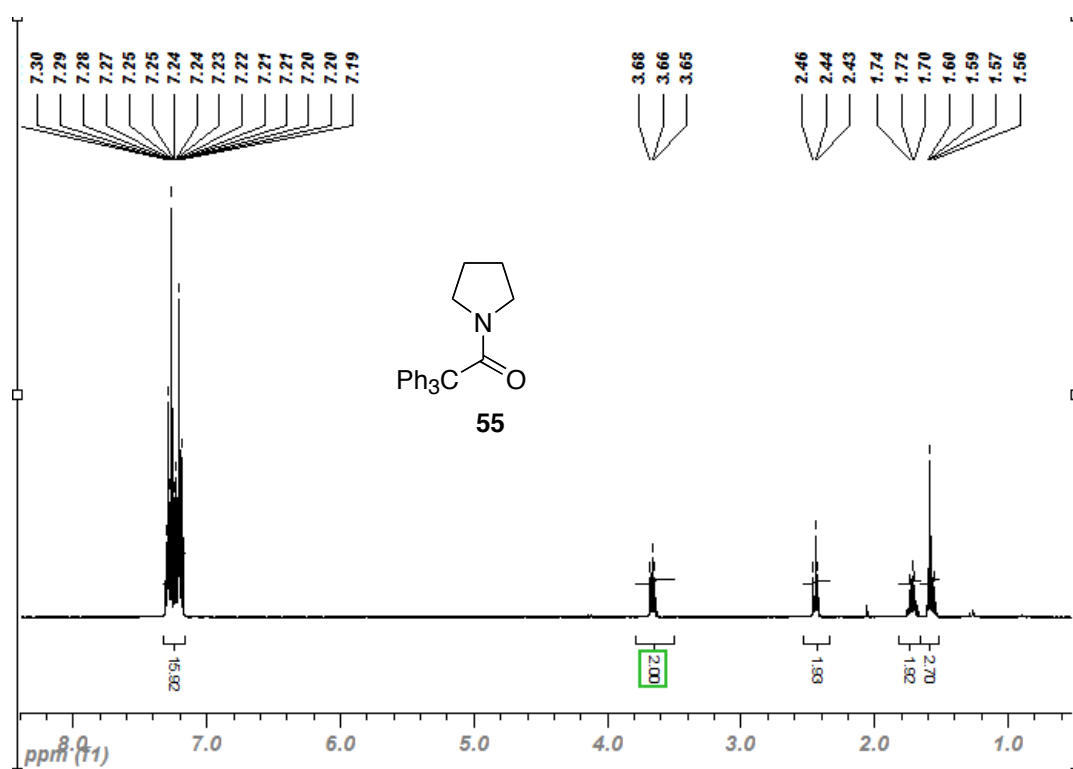
An inset provides a magnified view of the 1.8–2.3 ppm region, showing individual peaks with their chemical shifts labeled on the right side of the plot.



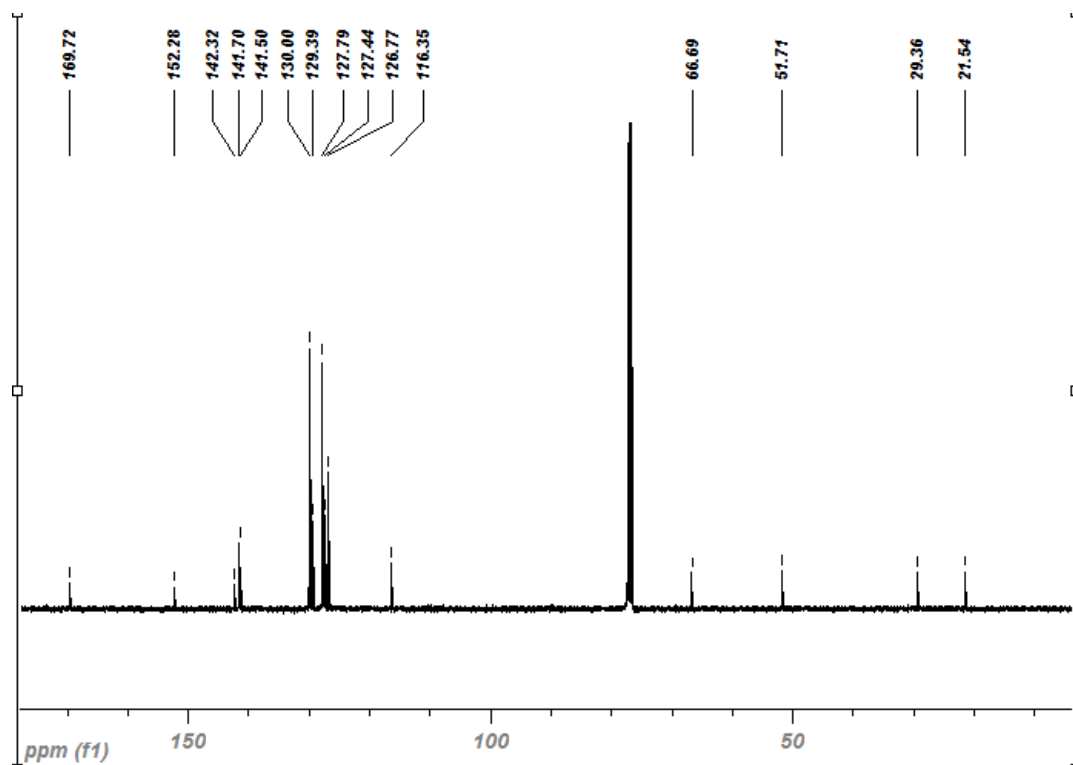
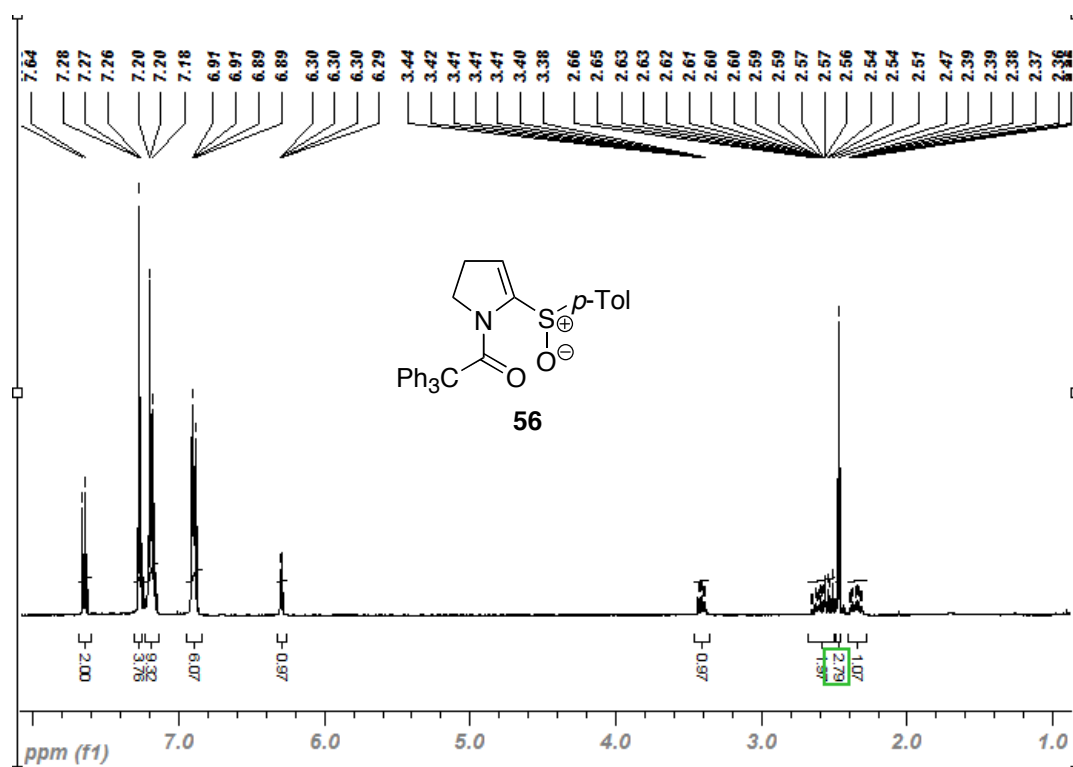


[illegible]

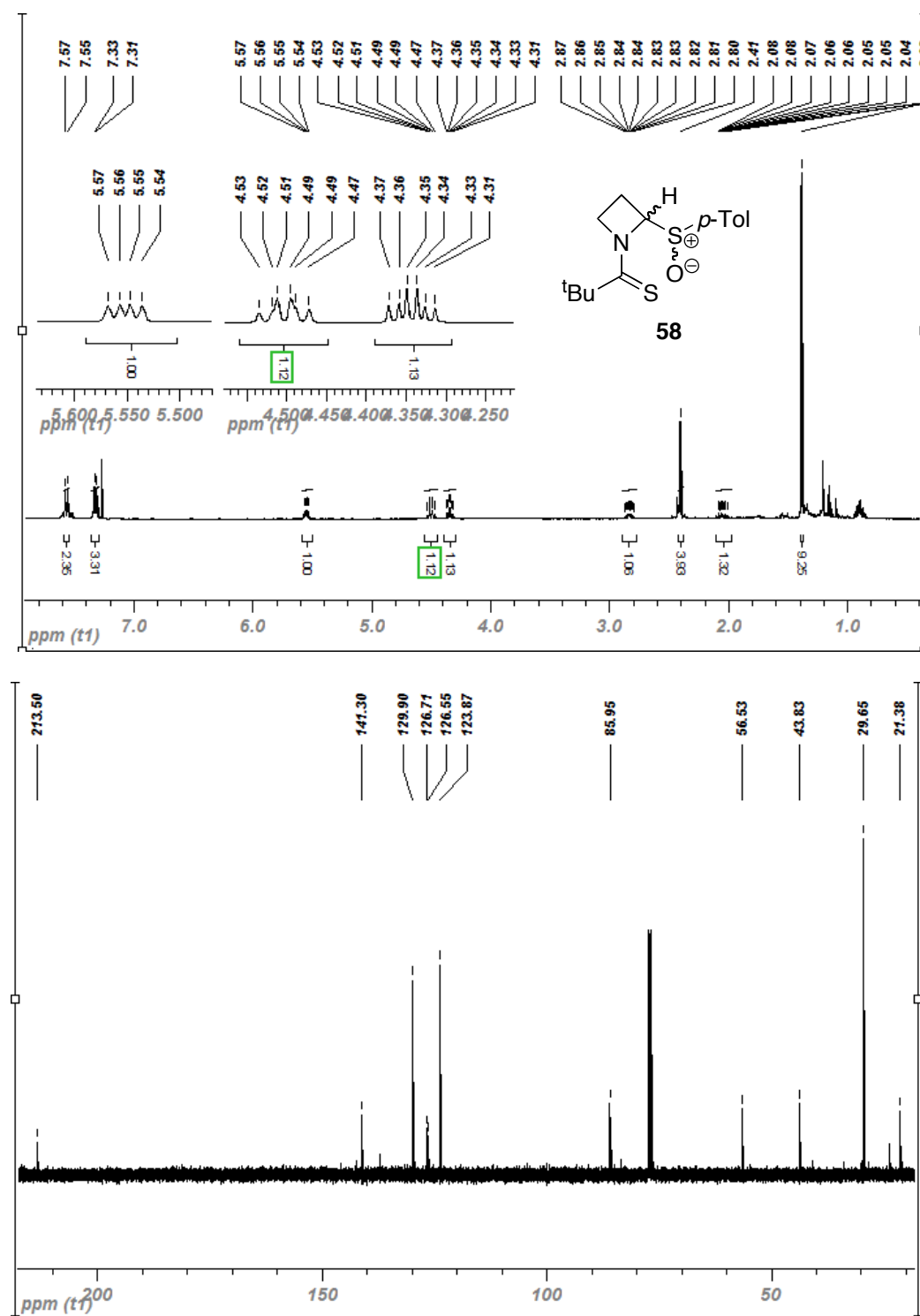
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



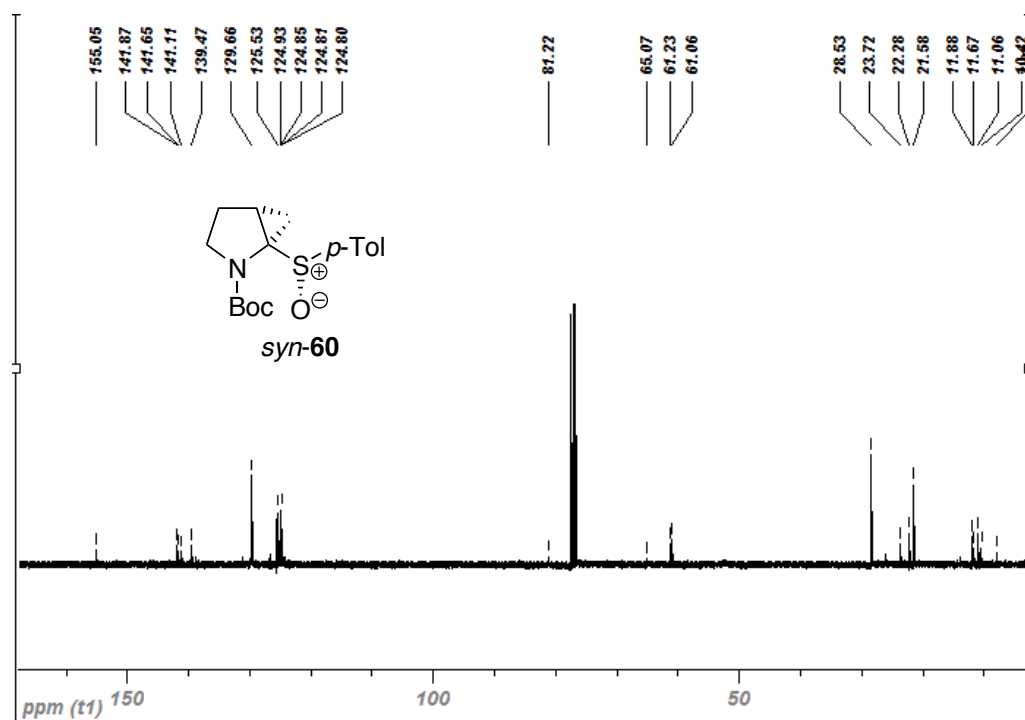
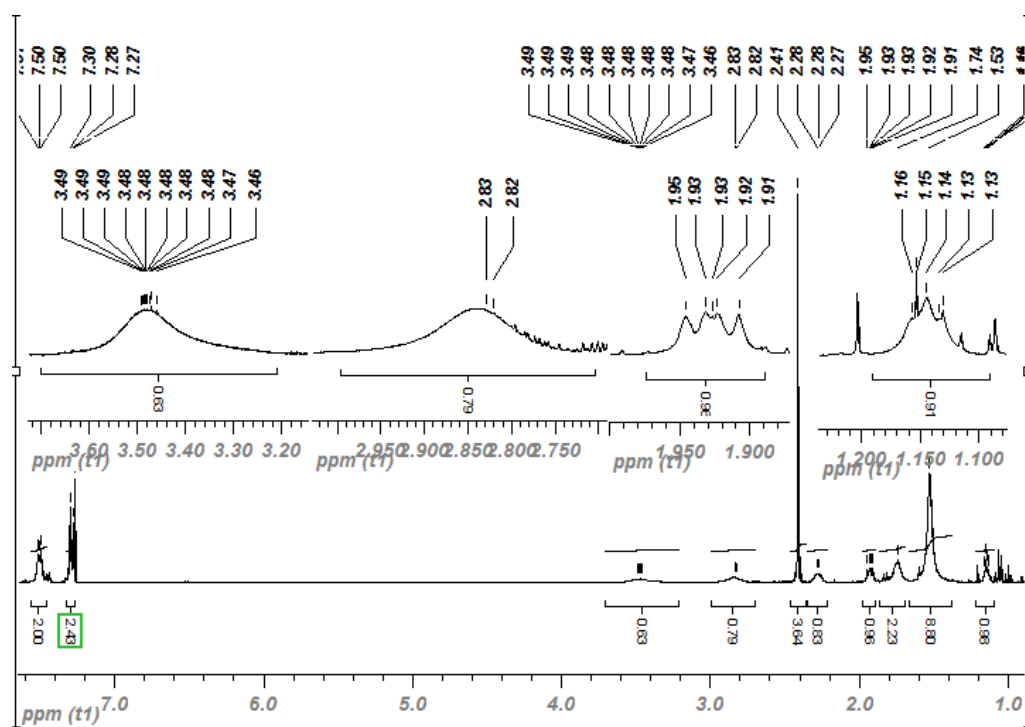
400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



400 MHz ^1H NMR spectrum; 100.6 MHz ^{13}C NMR spectrum; CDCl_3



¹H NMR spectrum of compound **1** in CDCl₃. The spectrum shows peaks from 0 to 8 ppm. Key features include a multiplet at 7.2-7.5 ppm (aromatic protons, integration 2.00), a broad peak at 7.0 ppm (NH, integration 1.00), a multiplet at 3.7-3.8 ppm (CH₂OH, integration 1.00), a multiplet at 2.2-2.3 ppm (CH₂, integration 0.88), a multiplet at 1.8-2.0 ppm (CH₂, integration 0.88), and a multiplet at 1.0-1.2 ppm (CH₃, integration 1.00). Solvent peaks for CDCl₃ are visible at 7.26, 7.27, and 7.28 ppm.

