

SUPPORTING INFORMATION

A concise stereoselective synthesis of orthogonally protected lanthionine and β -methyllanthionine derivatives

Steven L. Cobb and John C. Vederas*

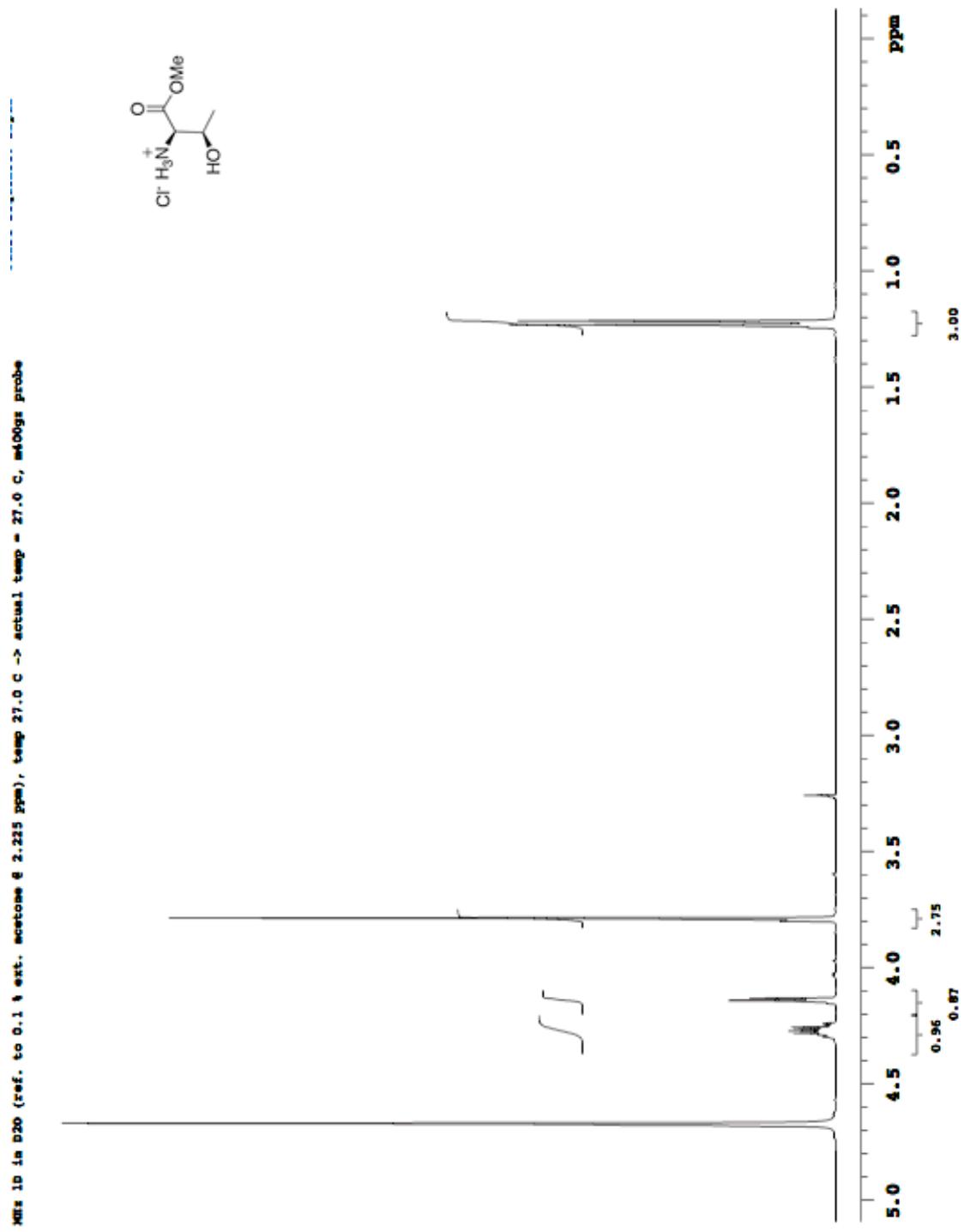
Department of Chemistry, University of Alberta, Edmonton, AB, Canada, T6G 2N8

^1H NMR and ^{13}C NMR spectra for compounds reported.

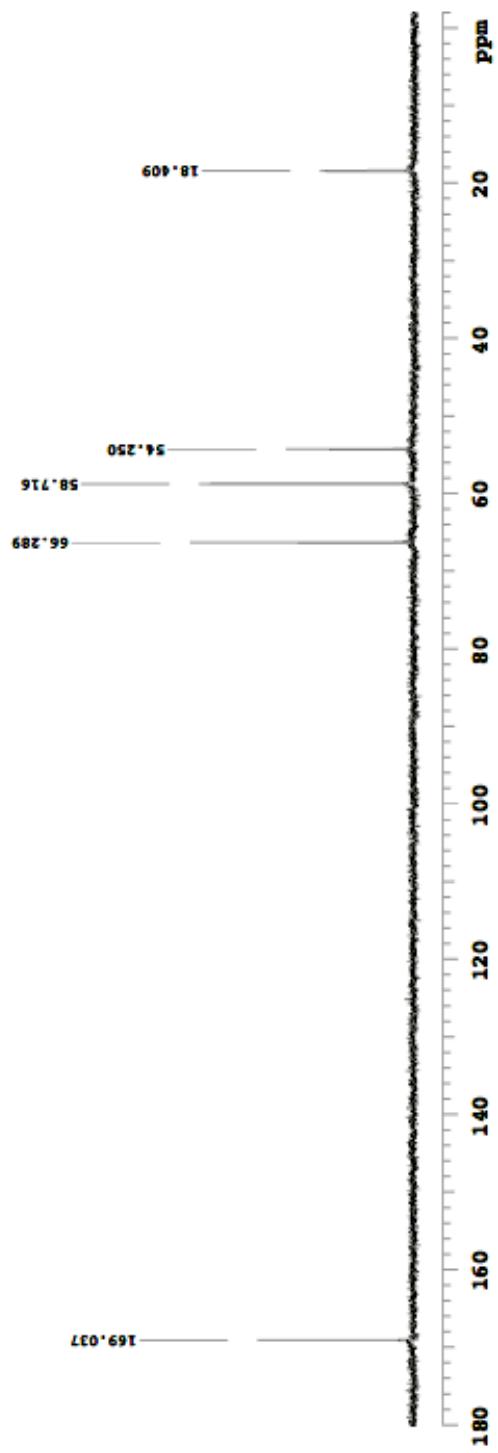
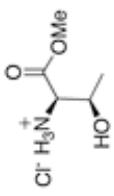
^1H NMR purity determination of **19a** and **19b**.

^1H NMR purity determination of **20a** and **20b**.

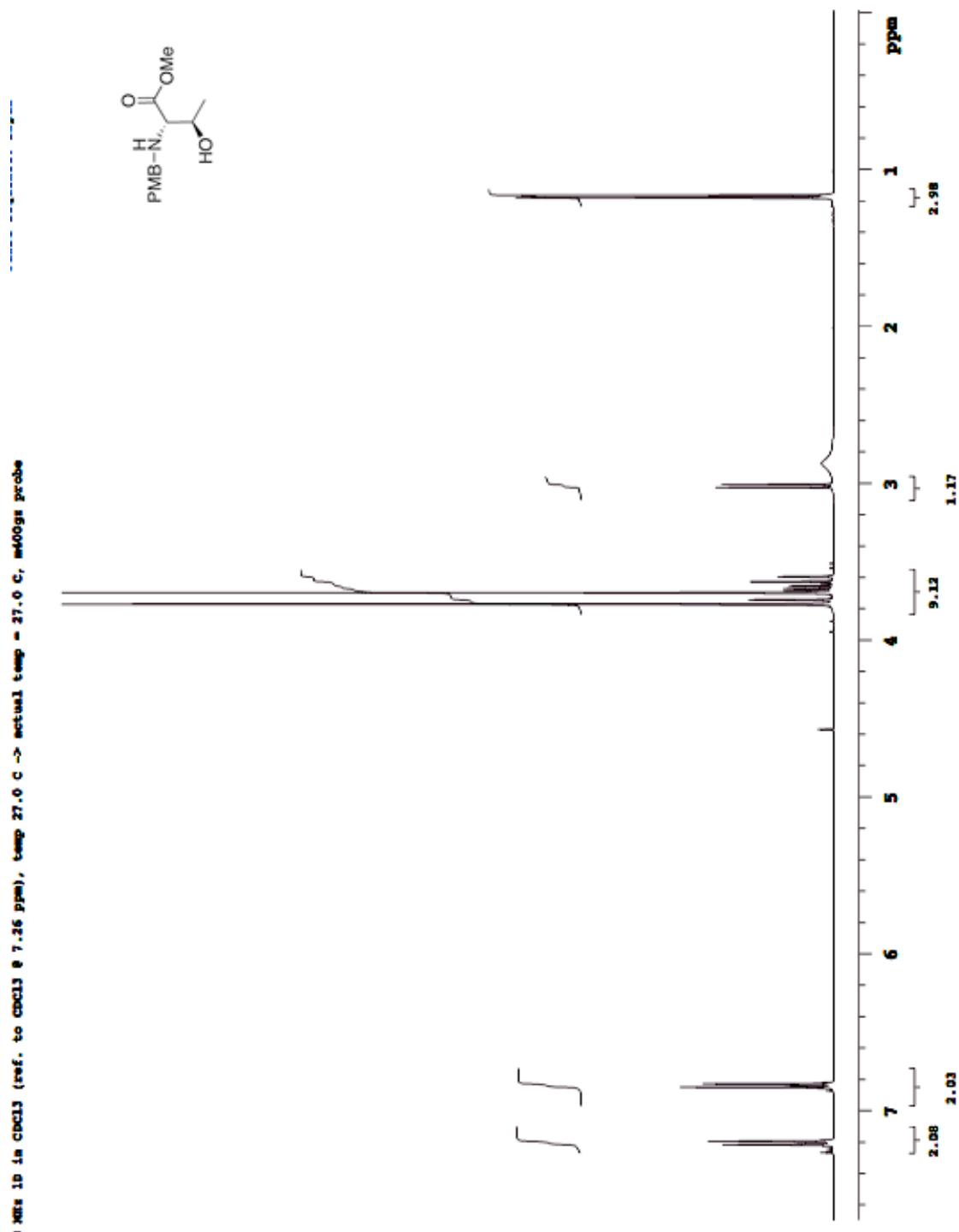
400 MHz 1H NMR in D2O (ref. to D2O), ext. acetone @ 2.225 ppm, temp 27.0 C -> actual temp = 27.0 C, 3000gs probe



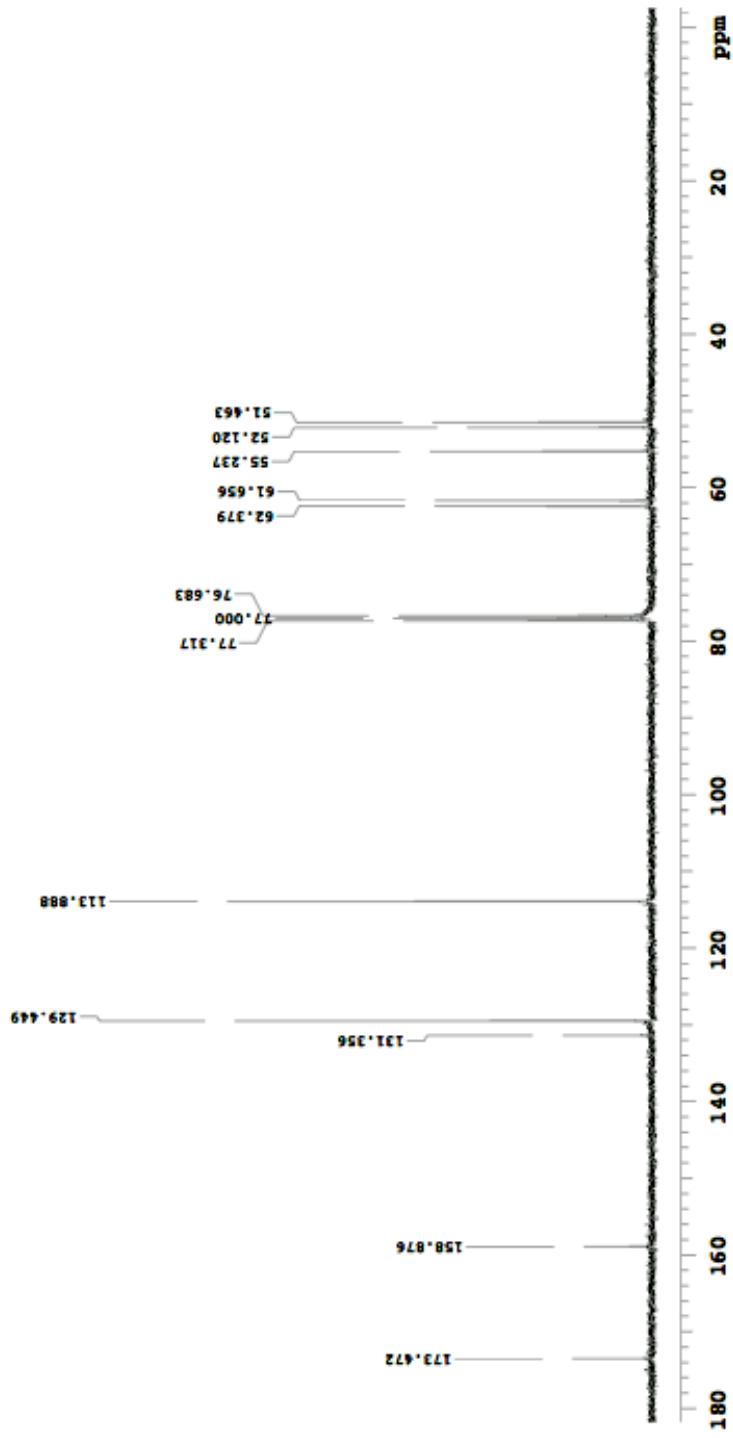
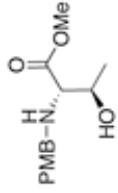
100 MHz 1D C13 in D2O (ref. to 1t acetone @ 31.07 ppm), temp 27.0 C → actual temp = 27.0 C, 3600gs probe



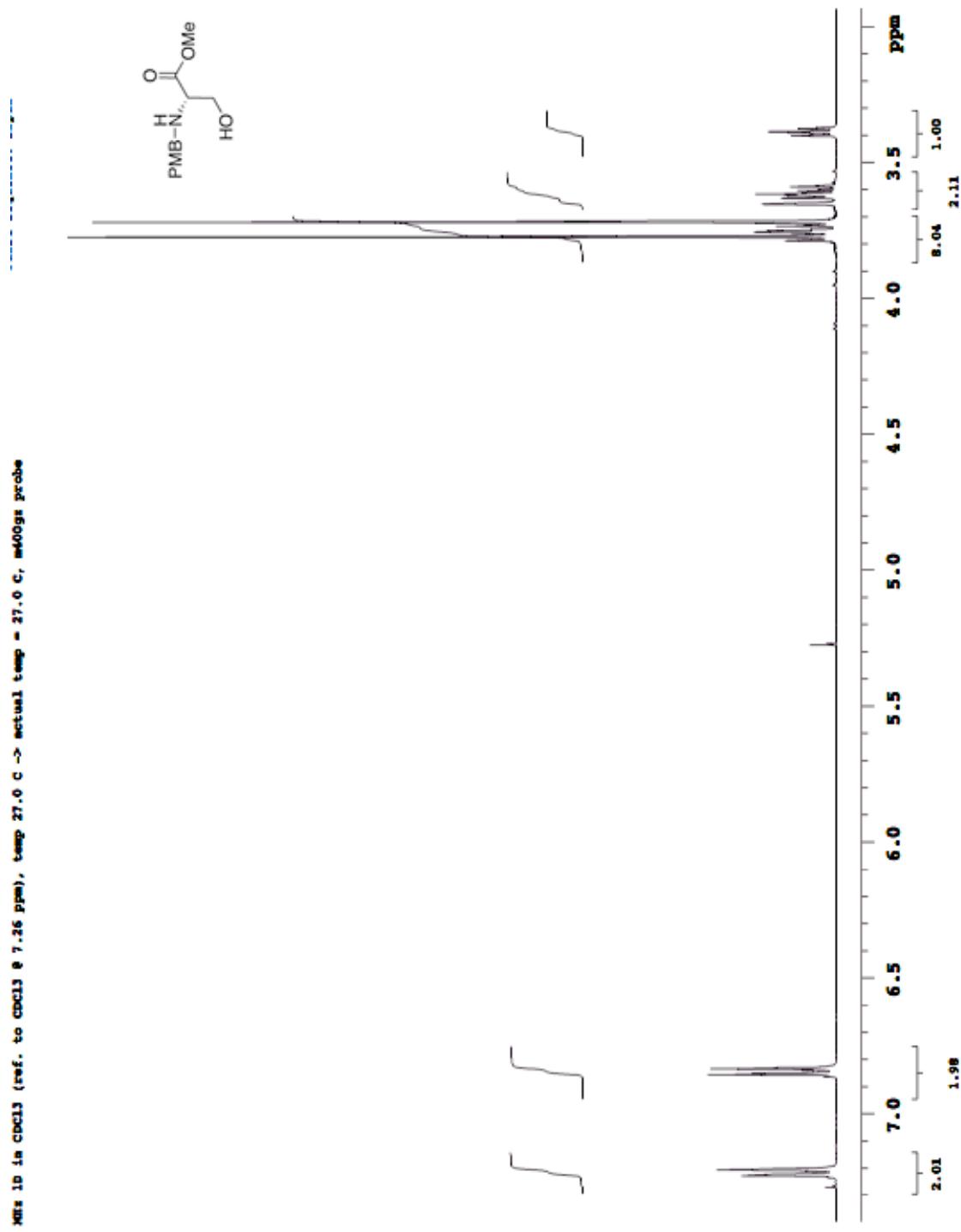
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 C → actual temp = 27.0 C, minisq probe



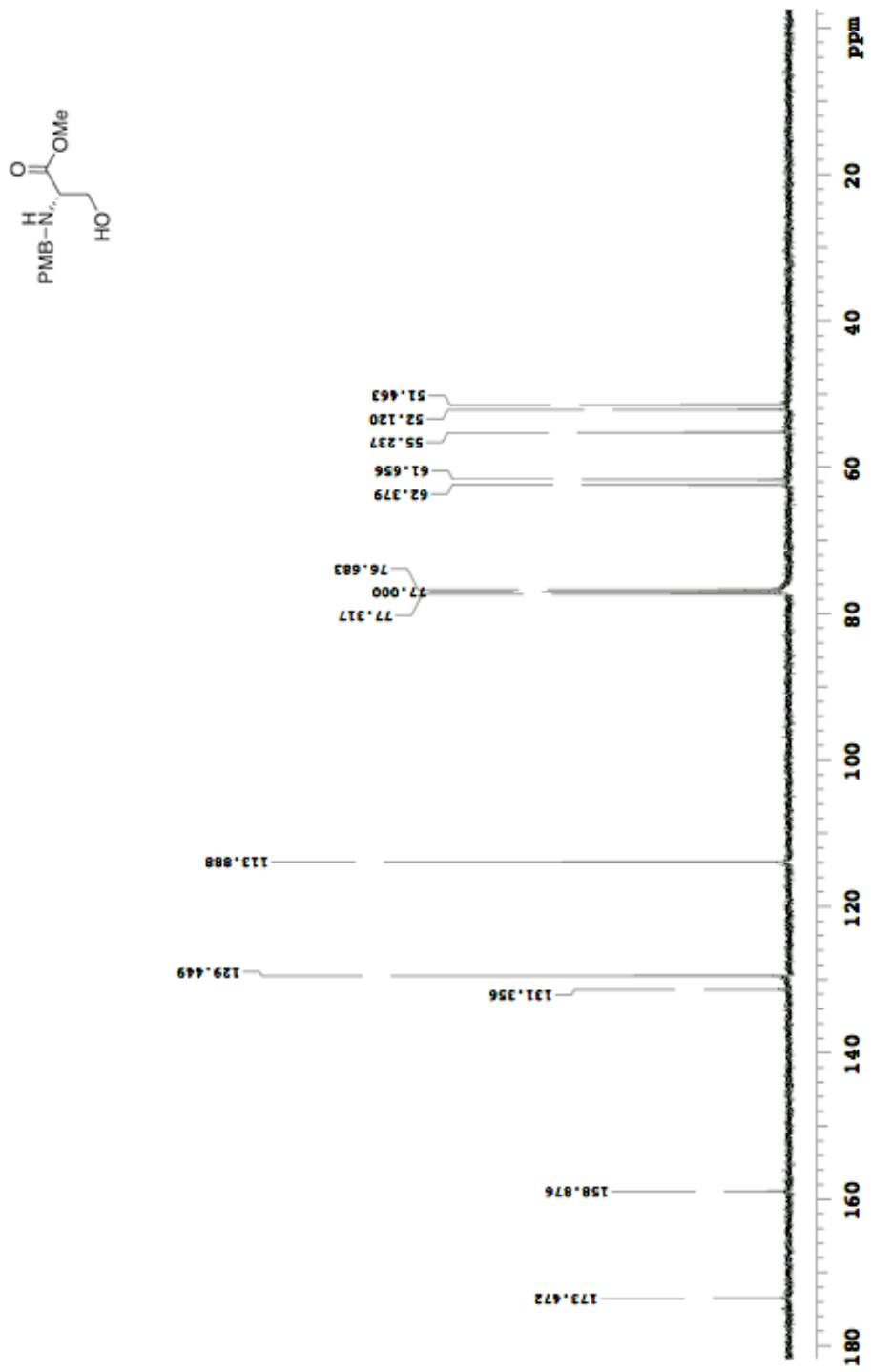
100 MHz 1D Cl3 in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, 3400gs probe



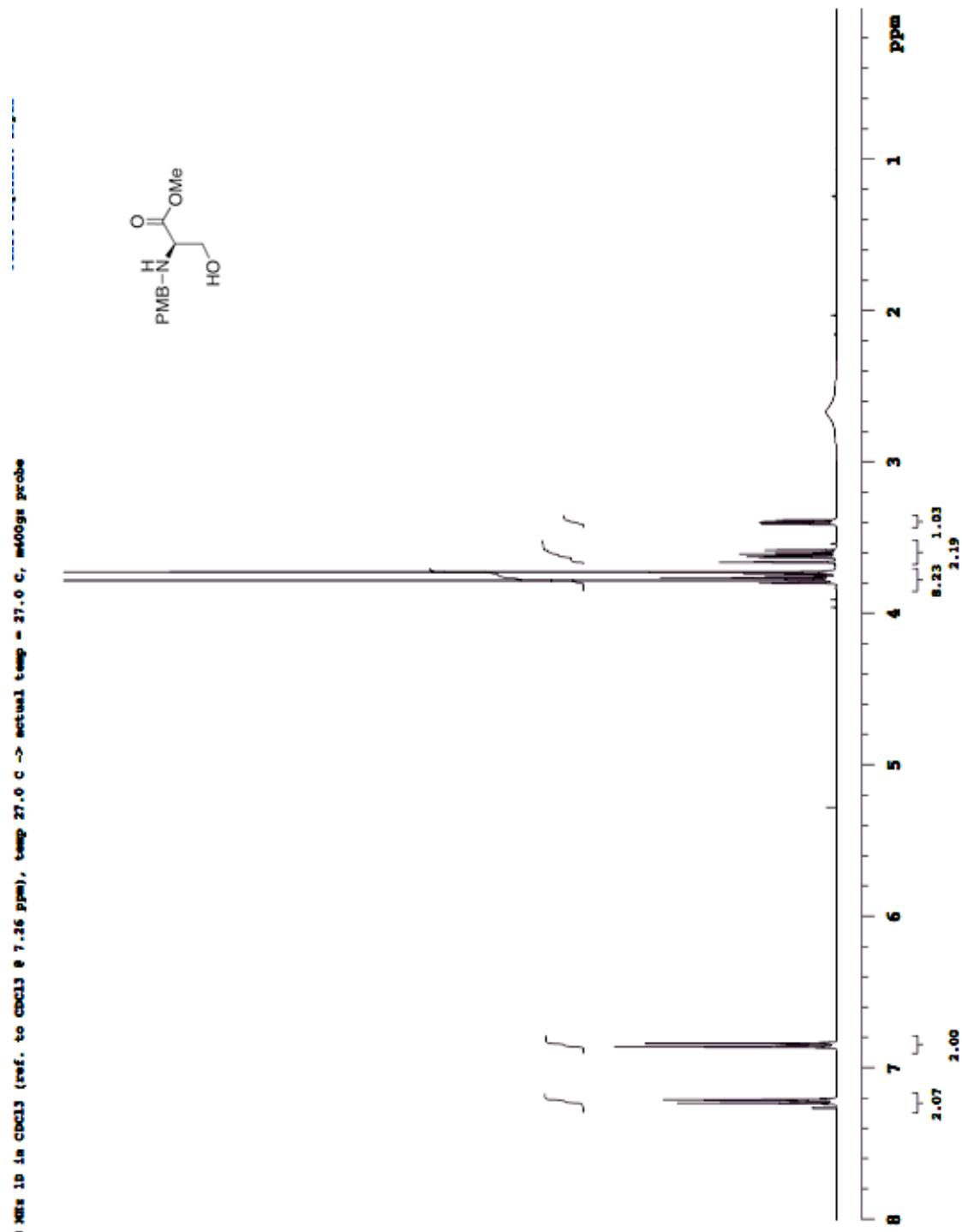
400 MHz 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 C → actual temp = 27.0 C, 6400gs probe



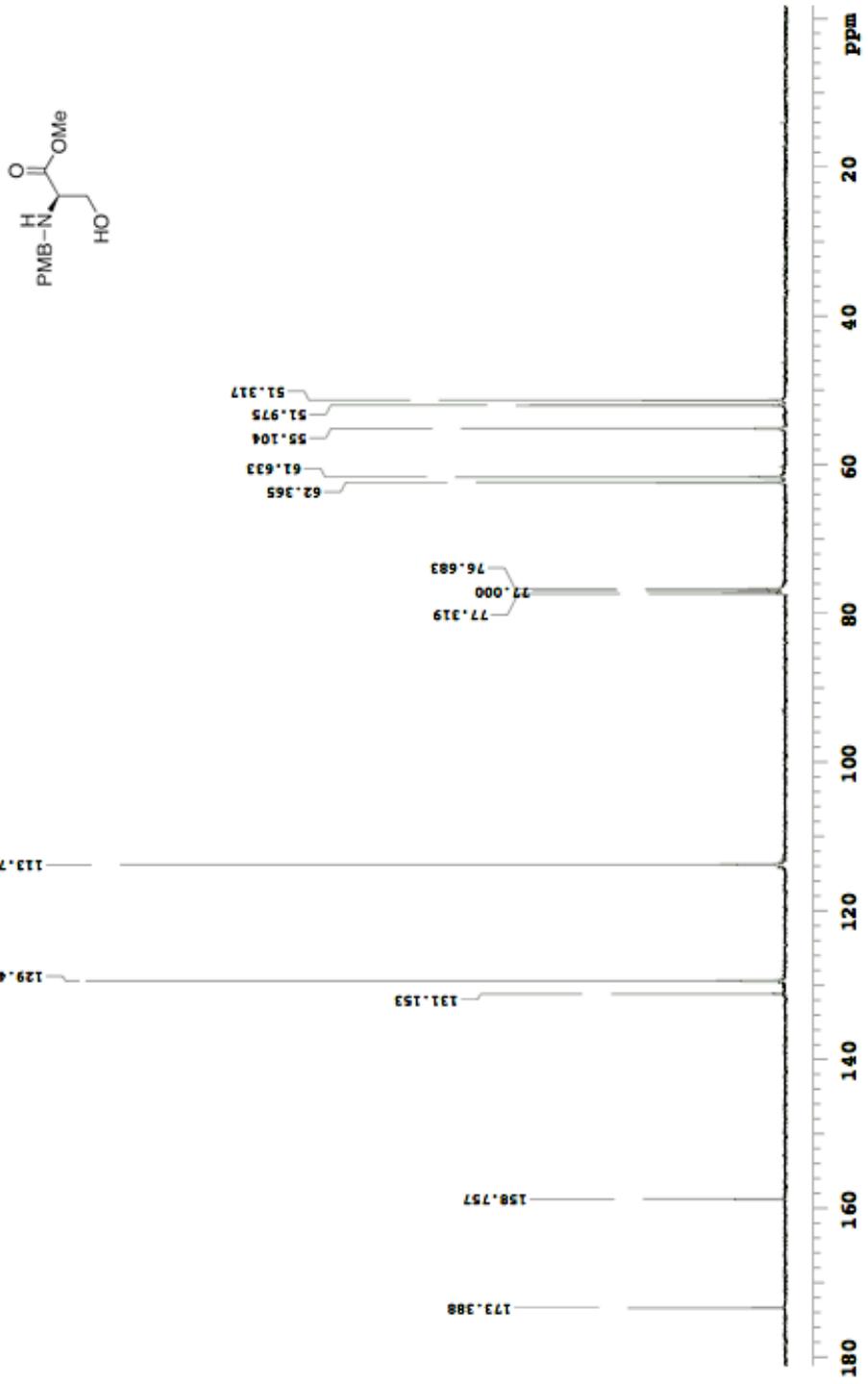
100 MHz 1D C13 in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3400gs probe

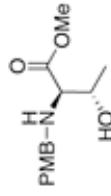


400 MHz 1H in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 C → actual temp = 27.0 C, 400Gz probe

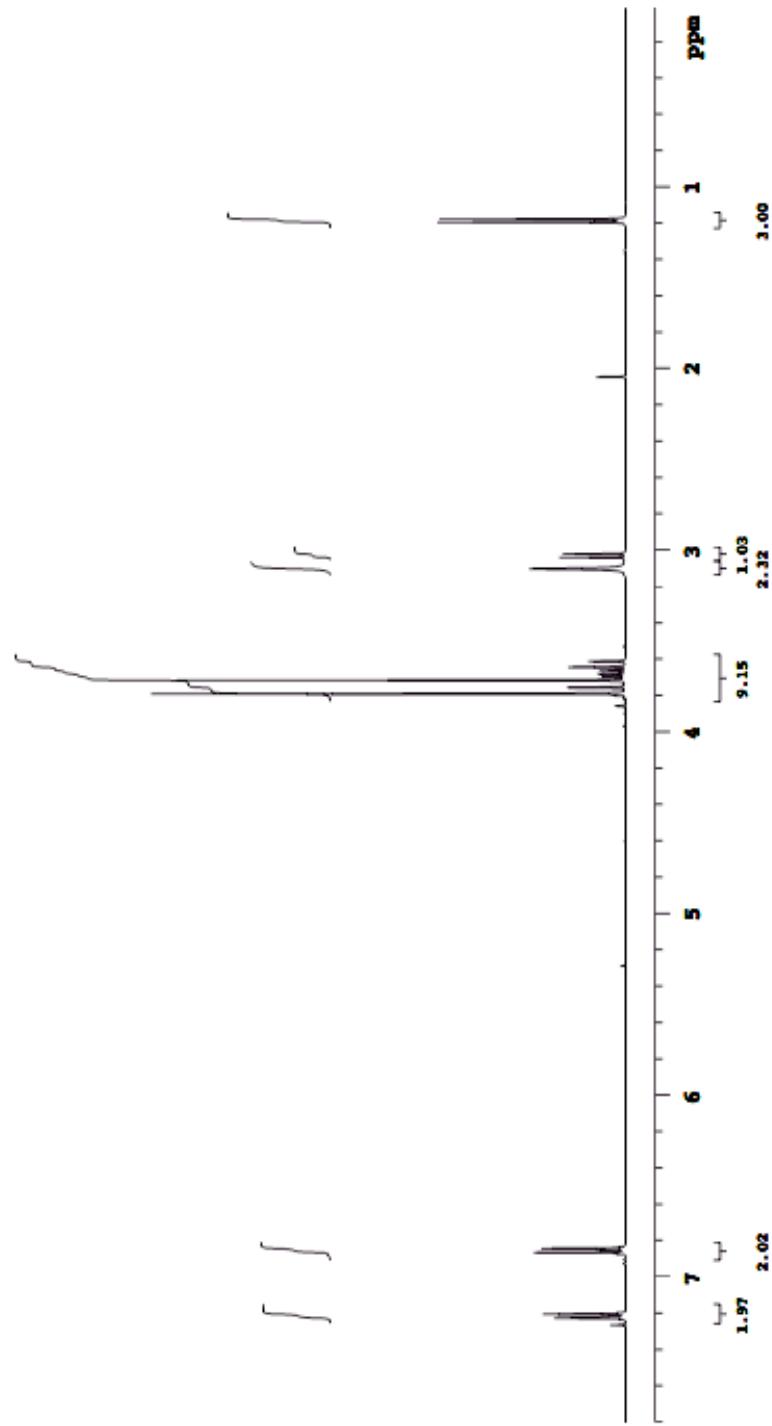


100 MHz 1D Cl3 in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, 3600gs probe

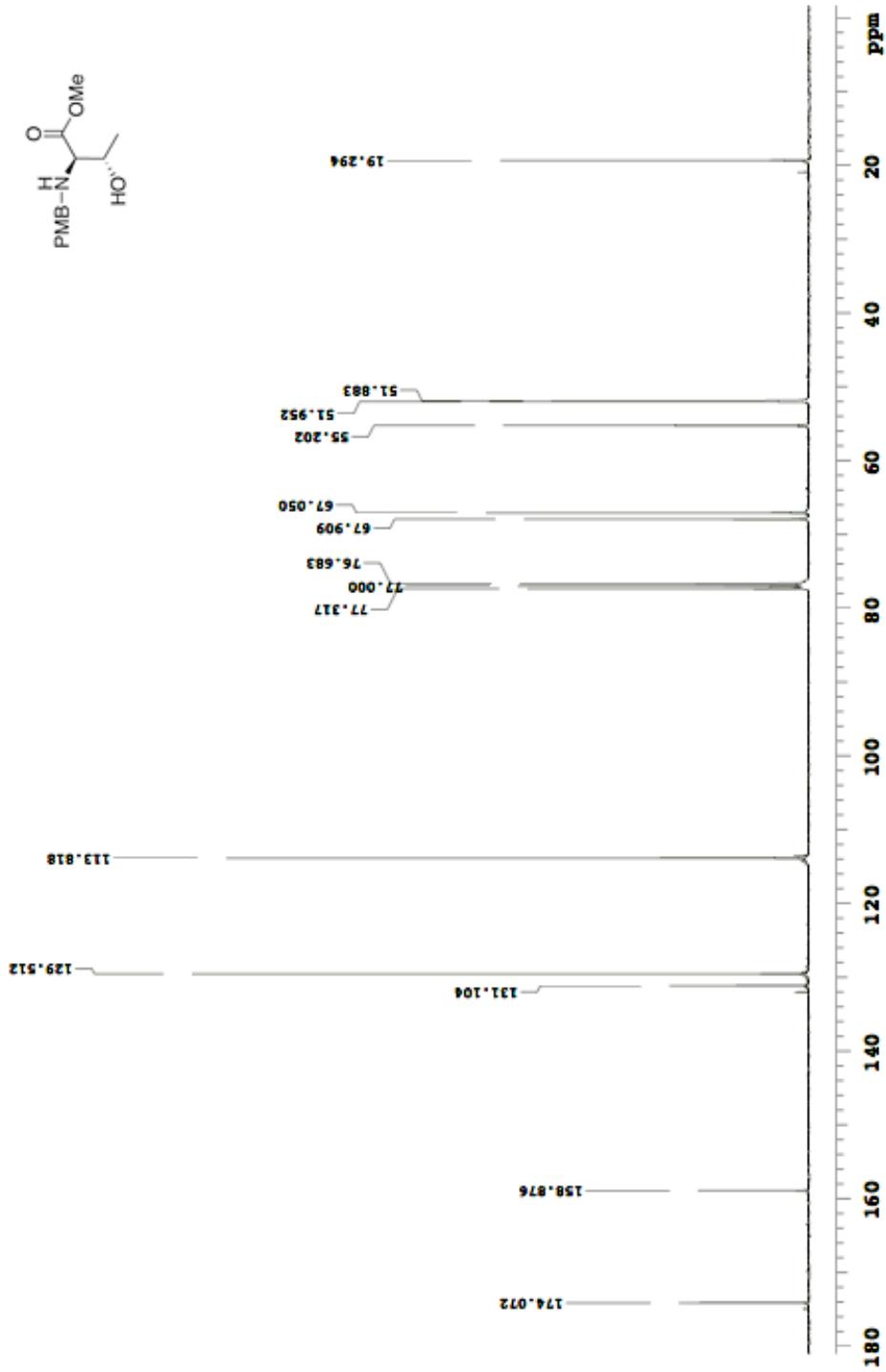
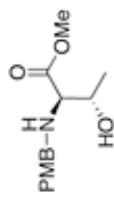




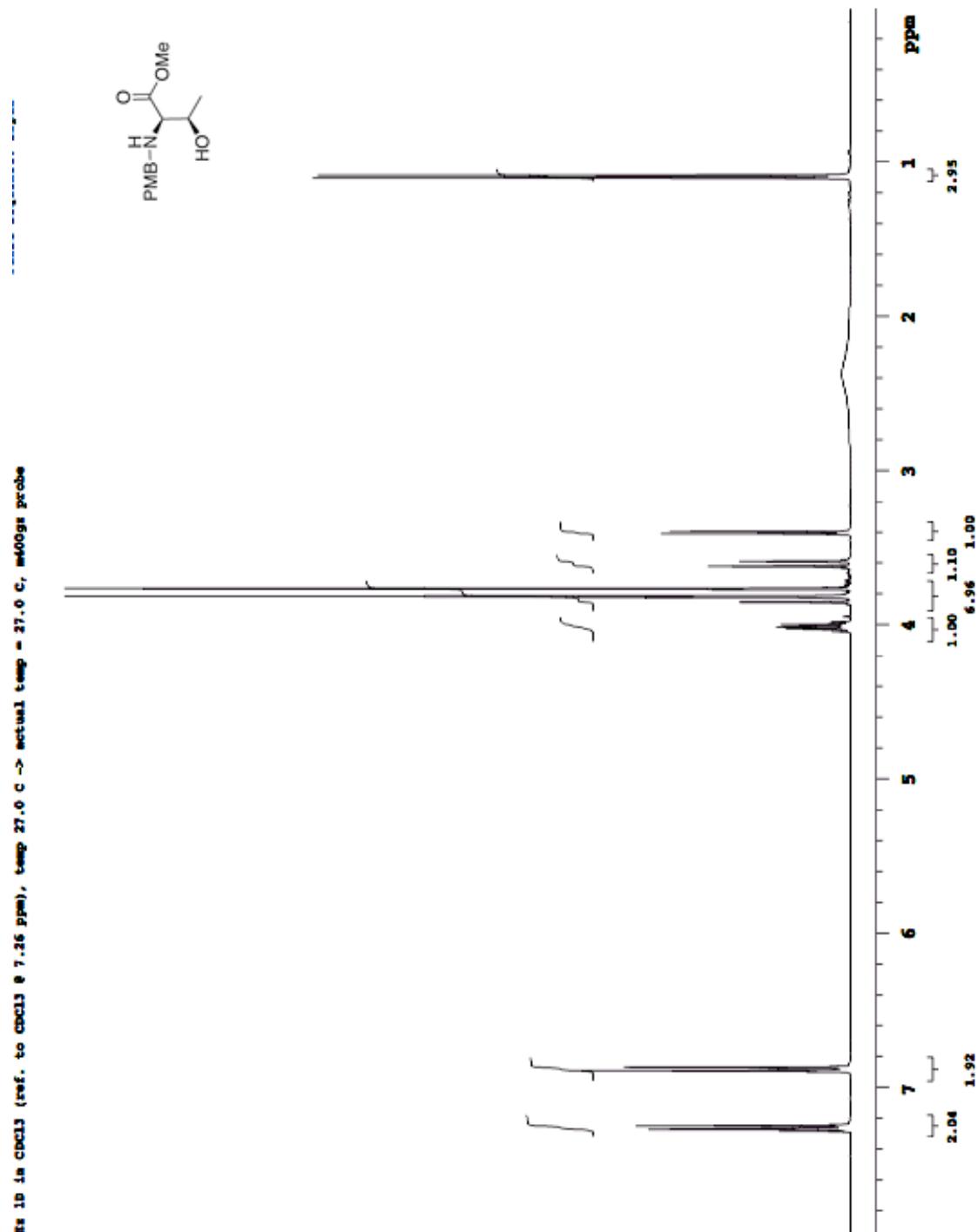
400 MHz 1D in C6C13 (ref. to CDCl₃ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, no sig. probe



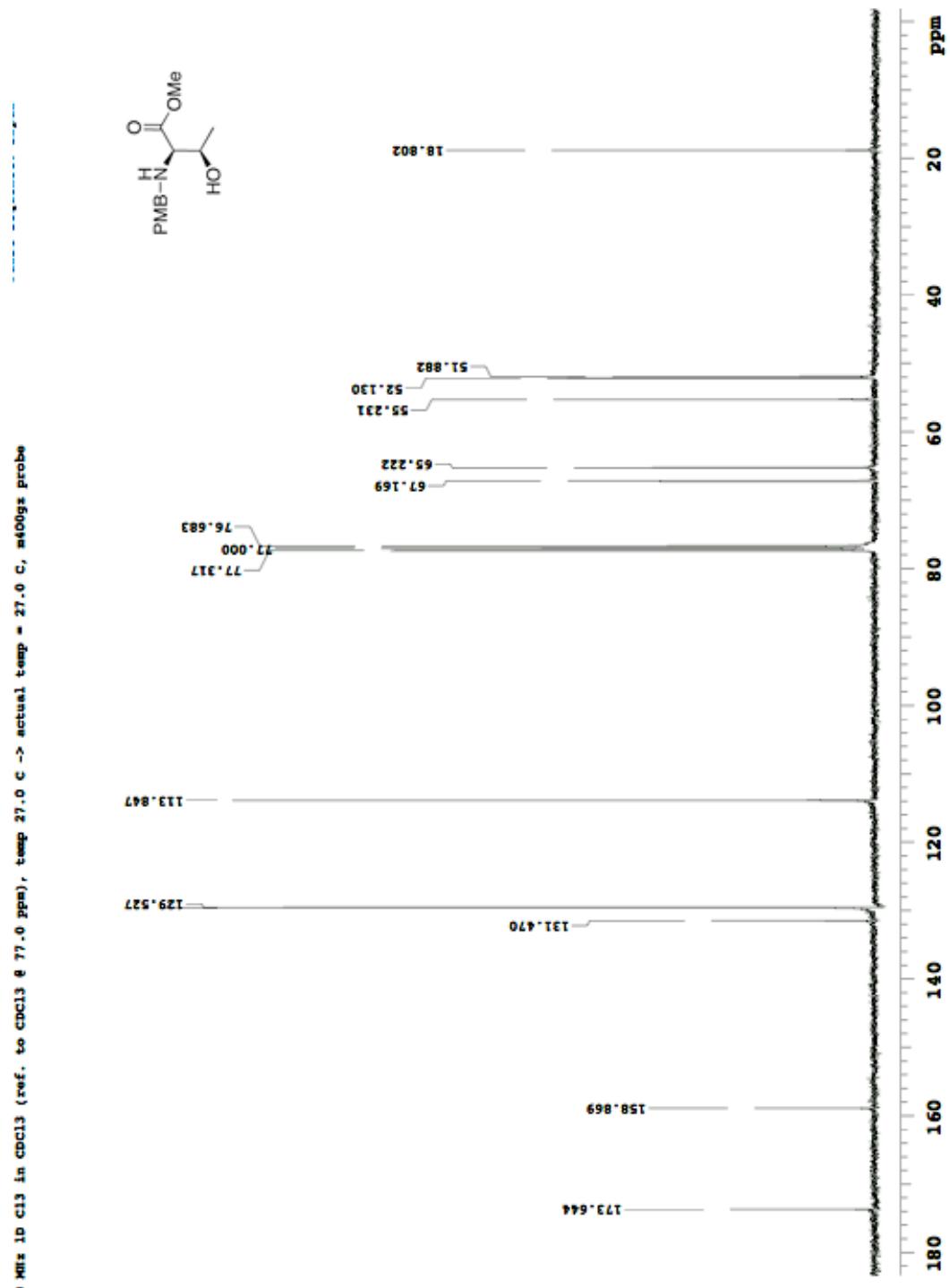
100 MHz ¹D NMR in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3600gz probe



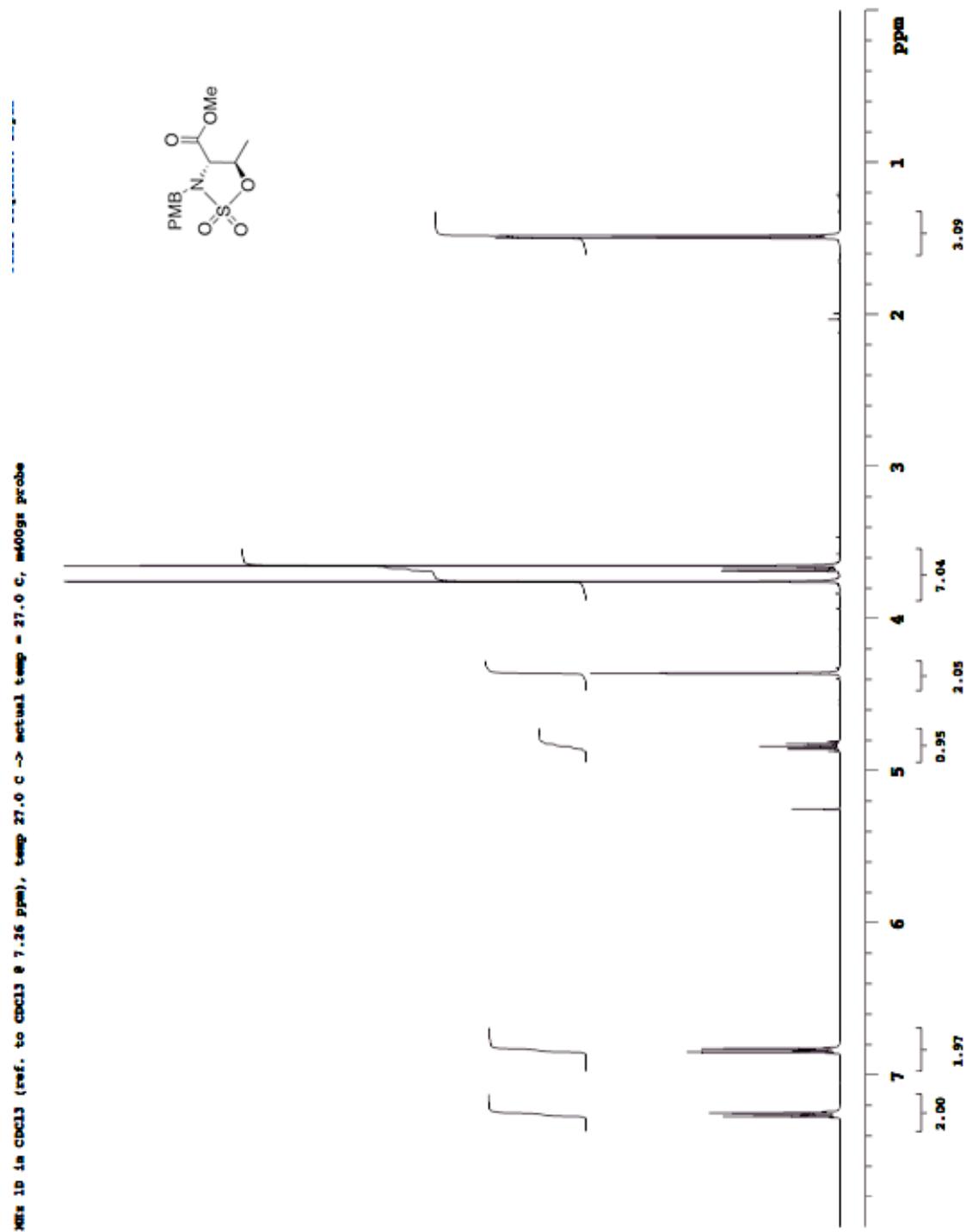
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 1H NMR probe



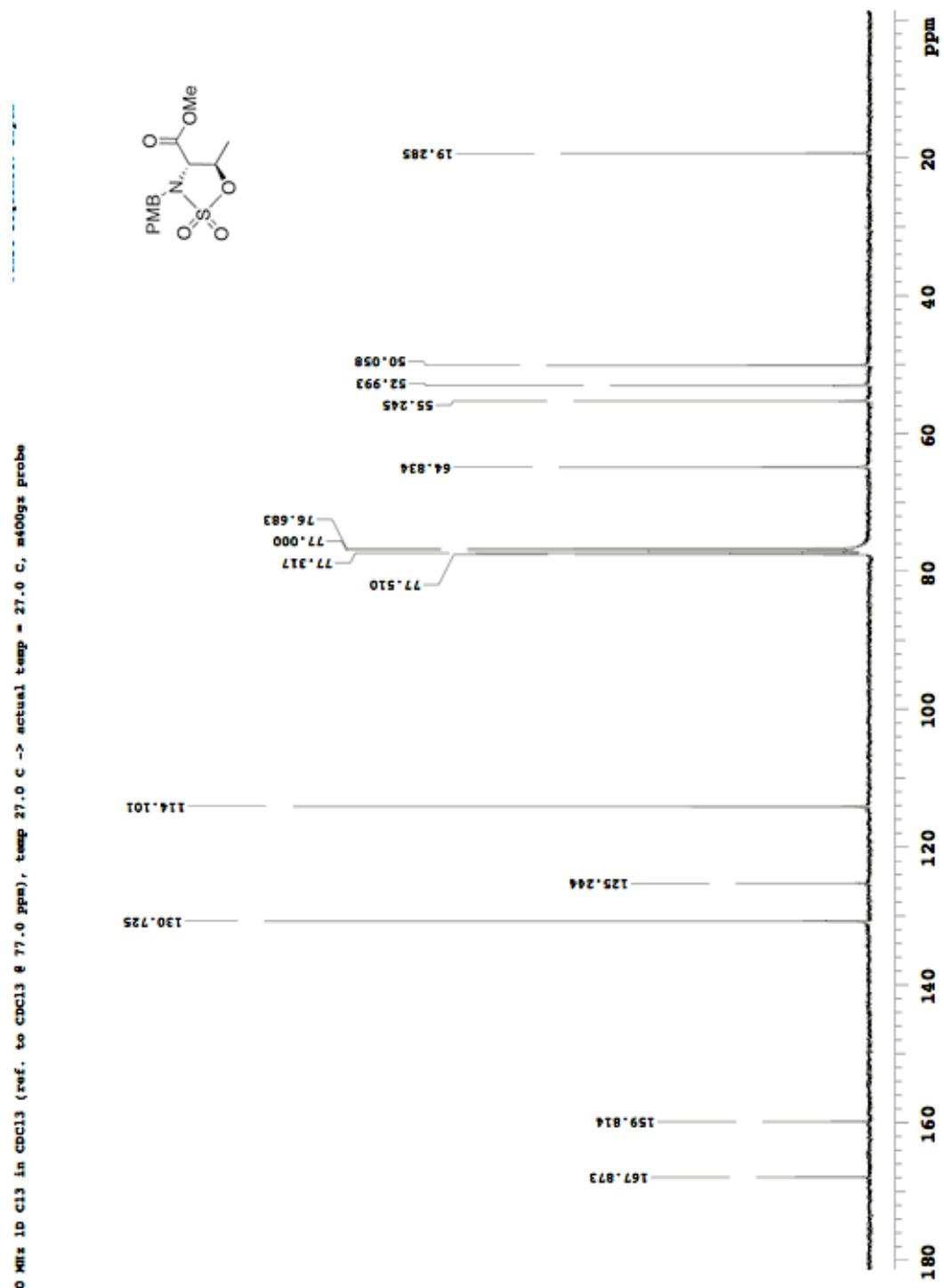
100 MHz 1D C13 in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 300gs probe



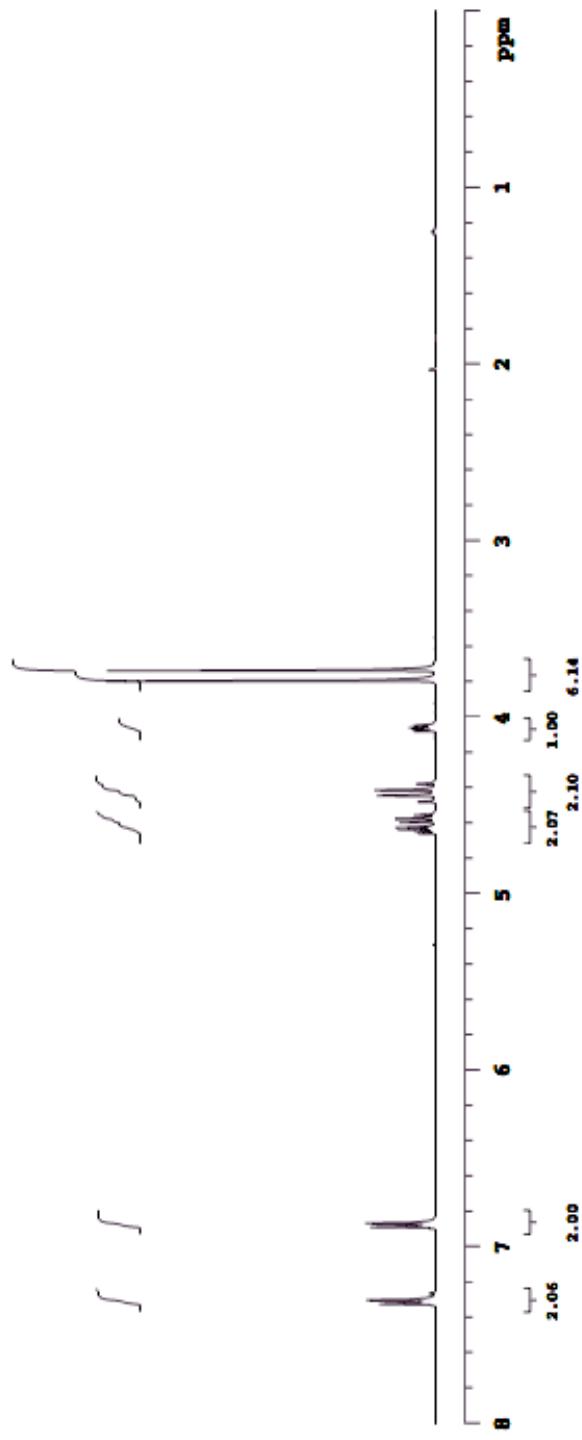
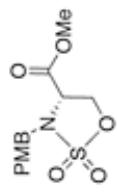
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 5000g probe



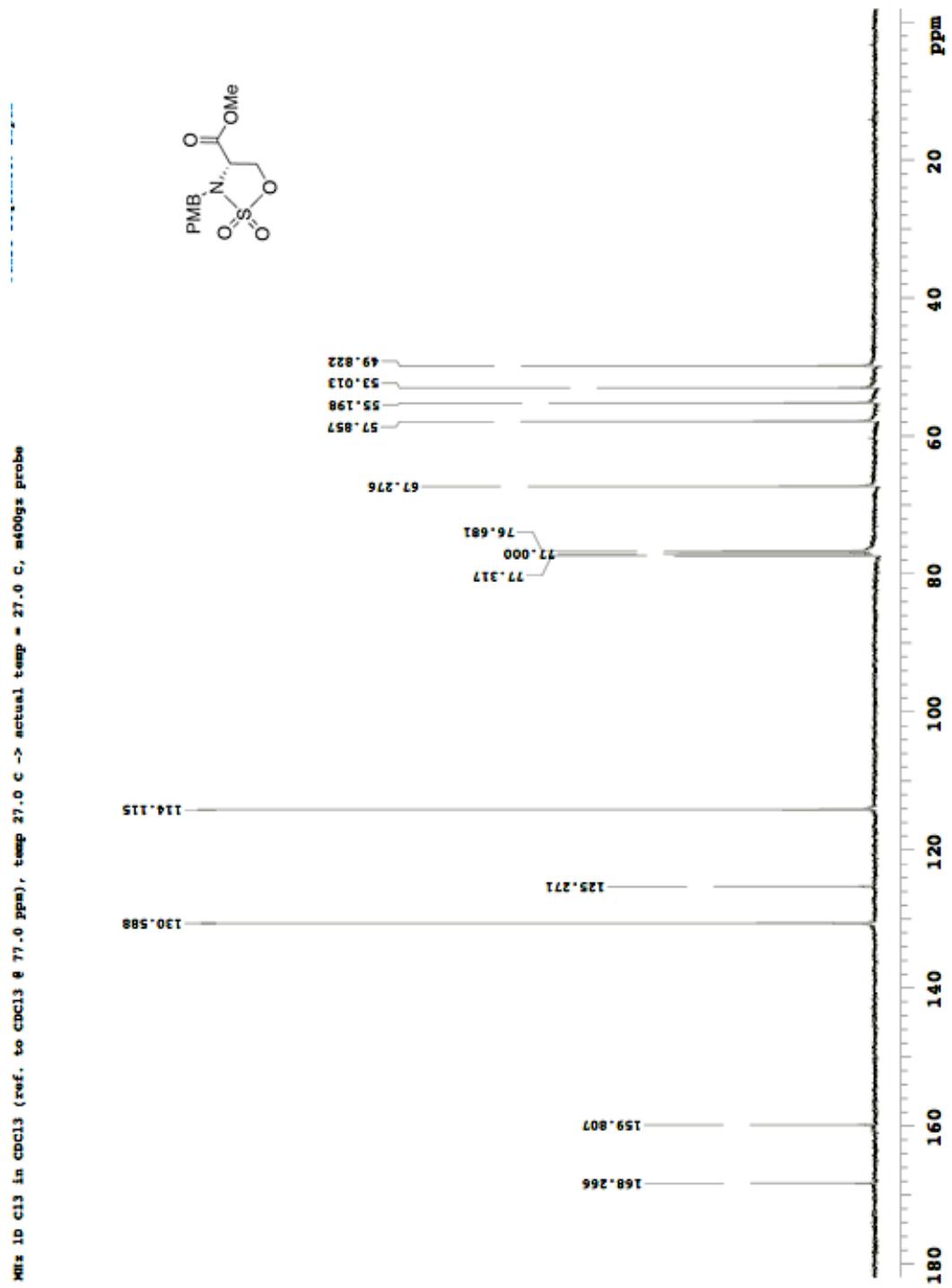
100 MHz 1D Cl₃ in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3400g3 probe



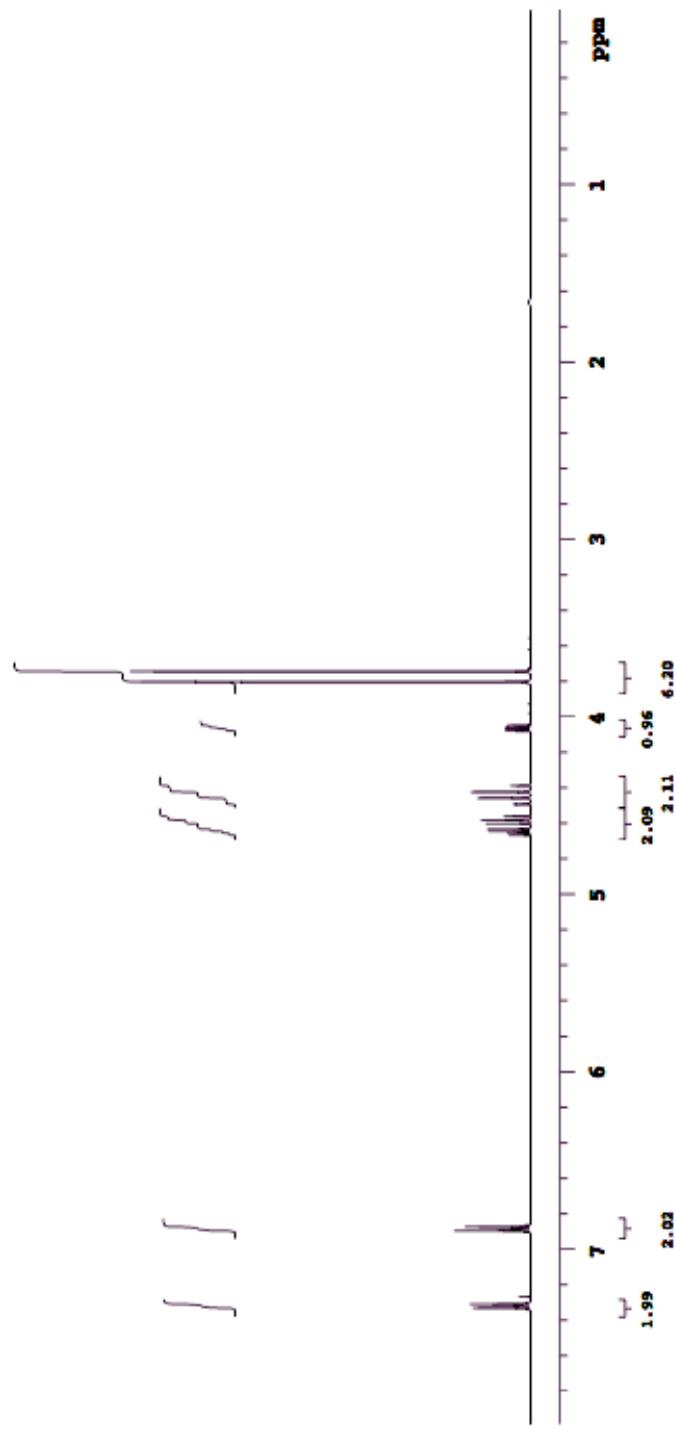
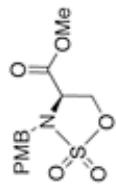
400 MHz 1H in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 400Gz probe



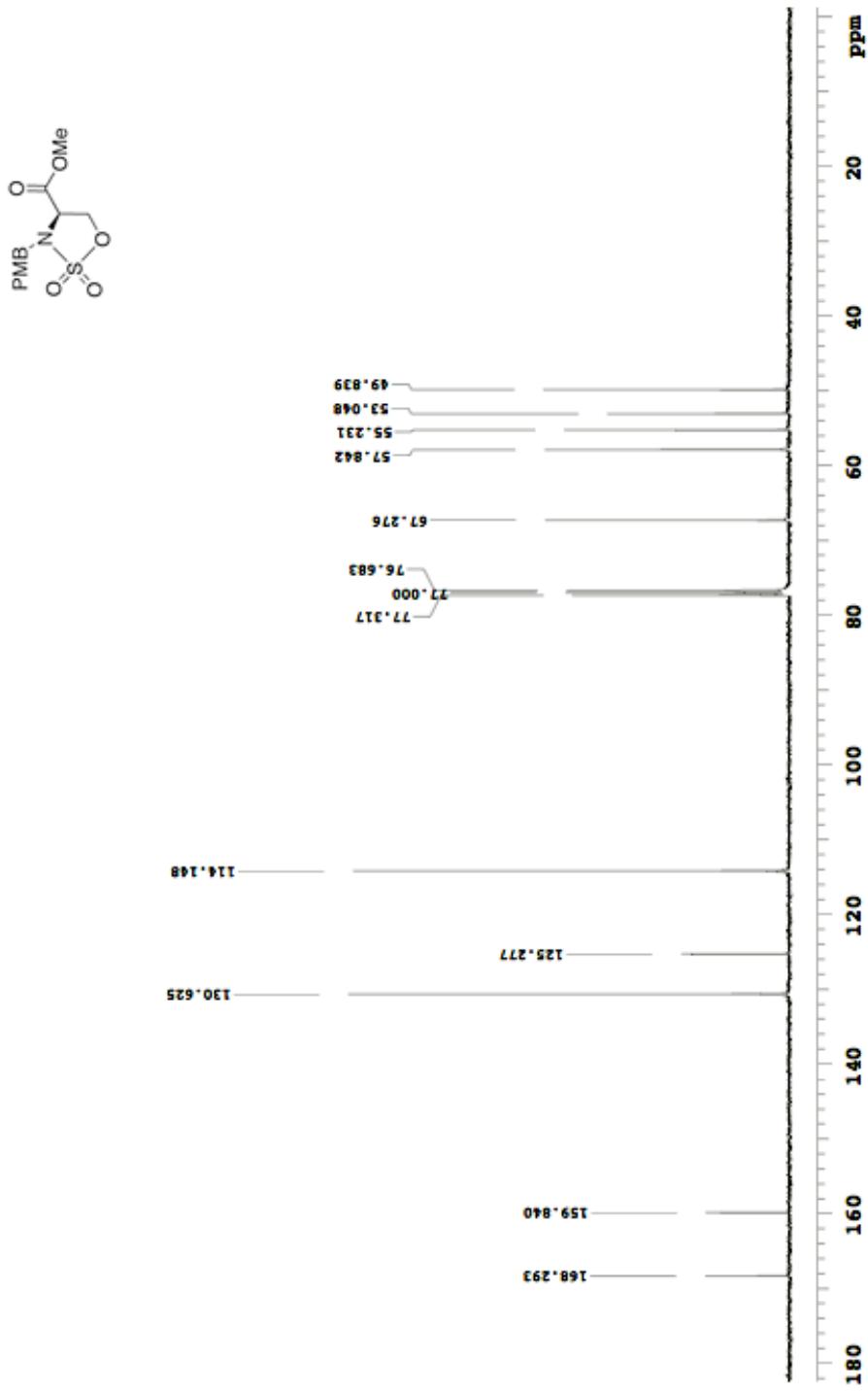
100 MHz 1D Cl₃ in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3600gs probe



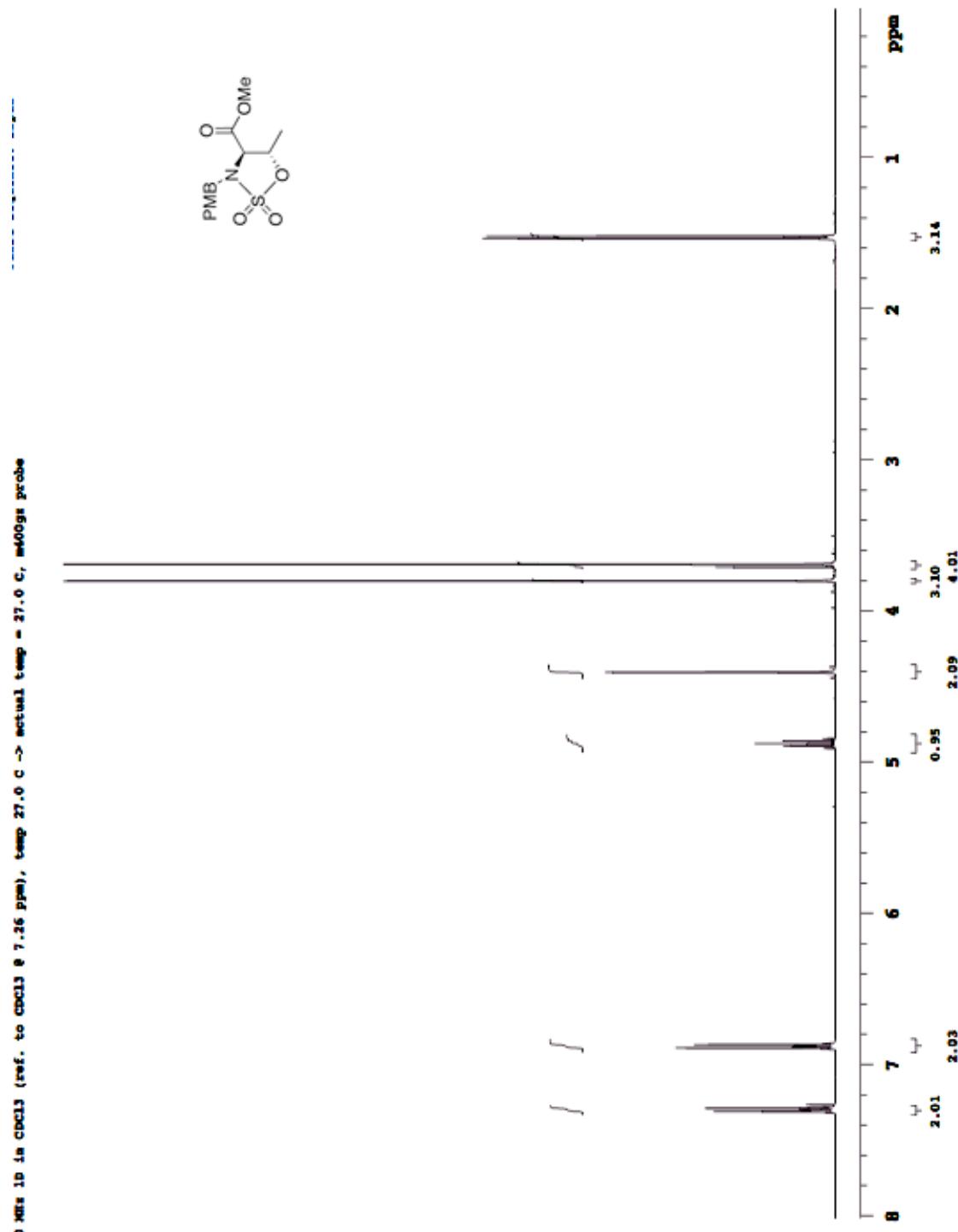
400 MHz 1H in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 C → actual temp = 27.0 C, 1H09g probe



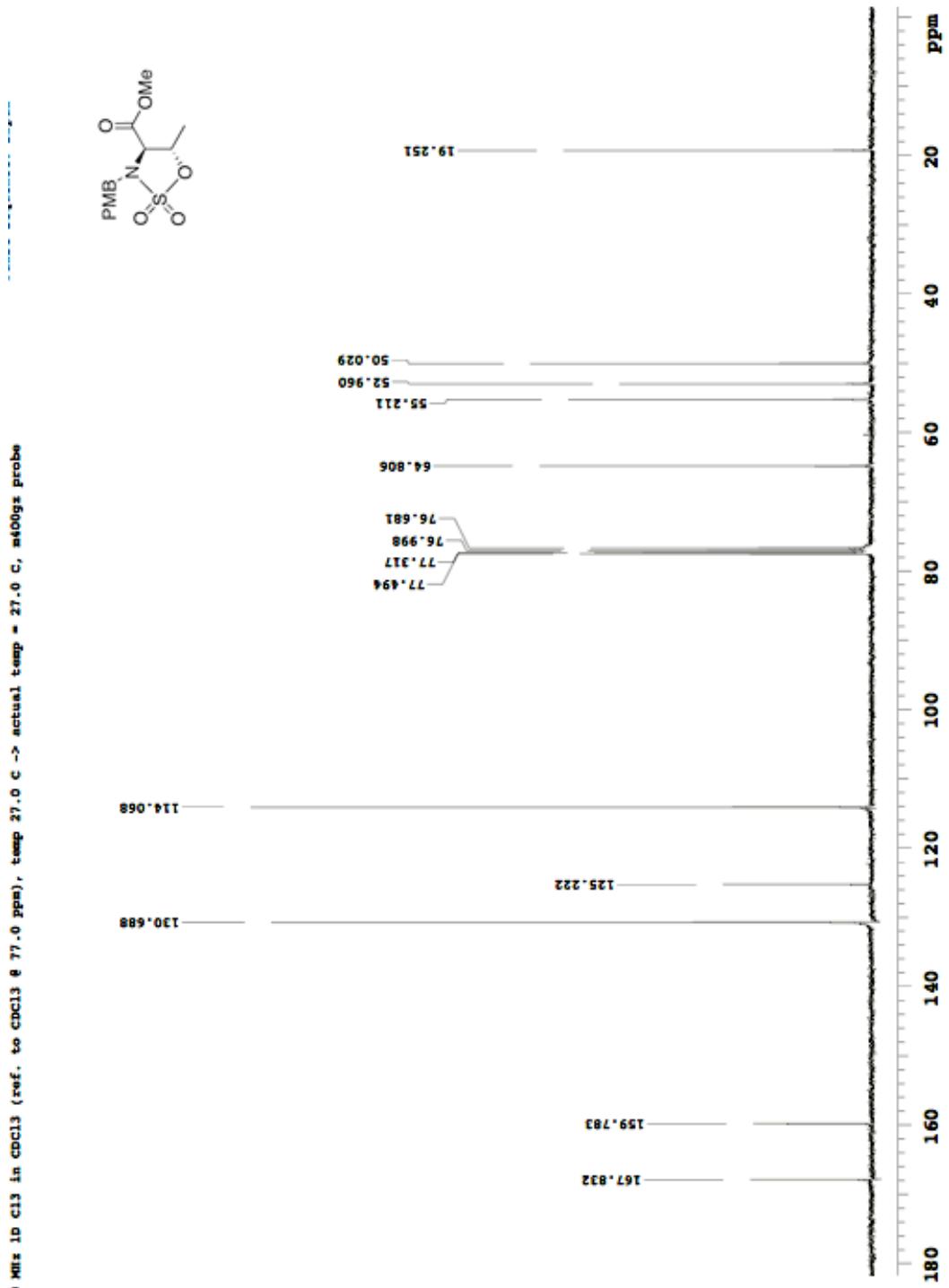
100 MHz 1D CDCl_3 in CDCl_3 (ref. to CDCl_3 at 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3400gs probe



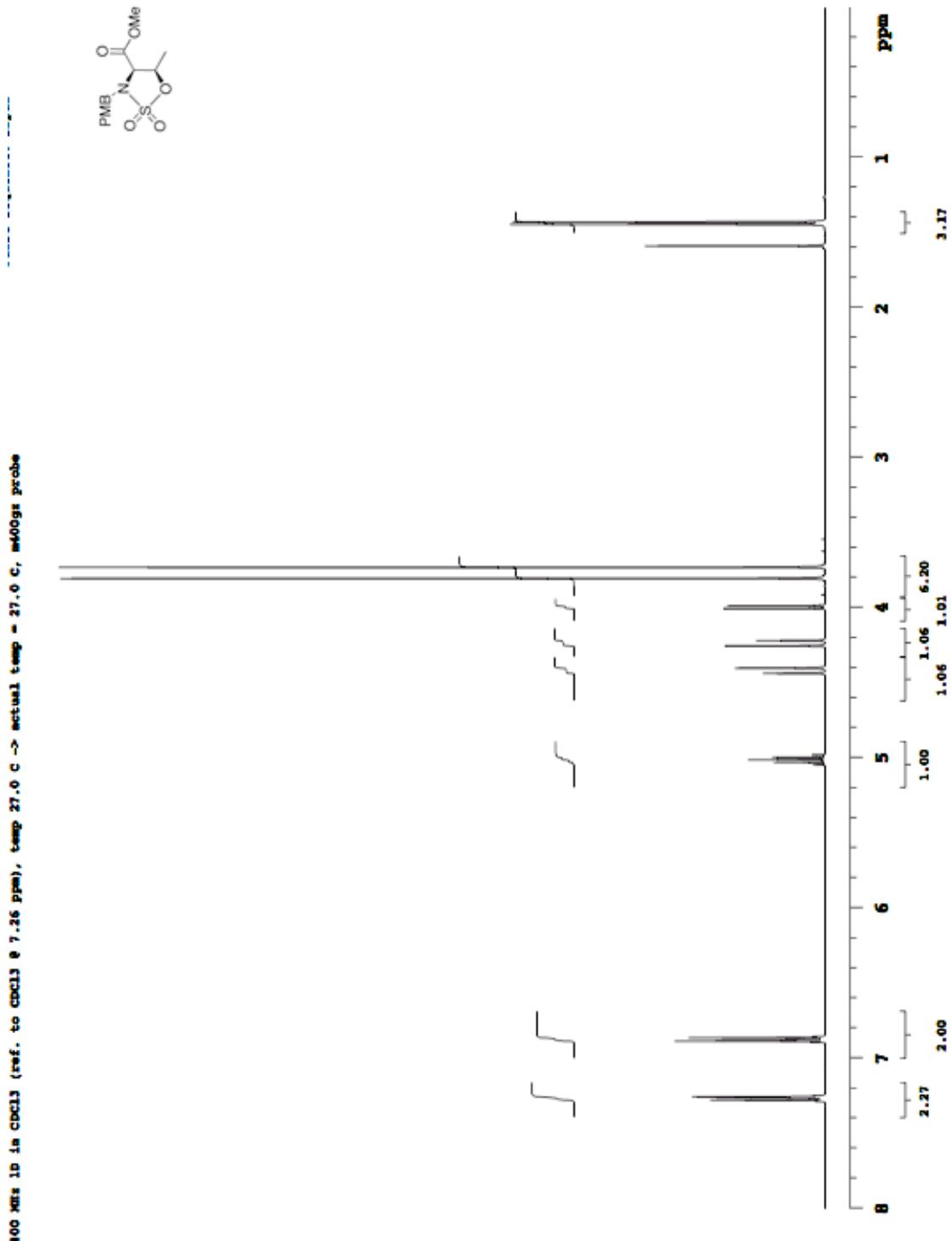
400 MHz 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 C → actual temp = 27.0 C, 400GS probe



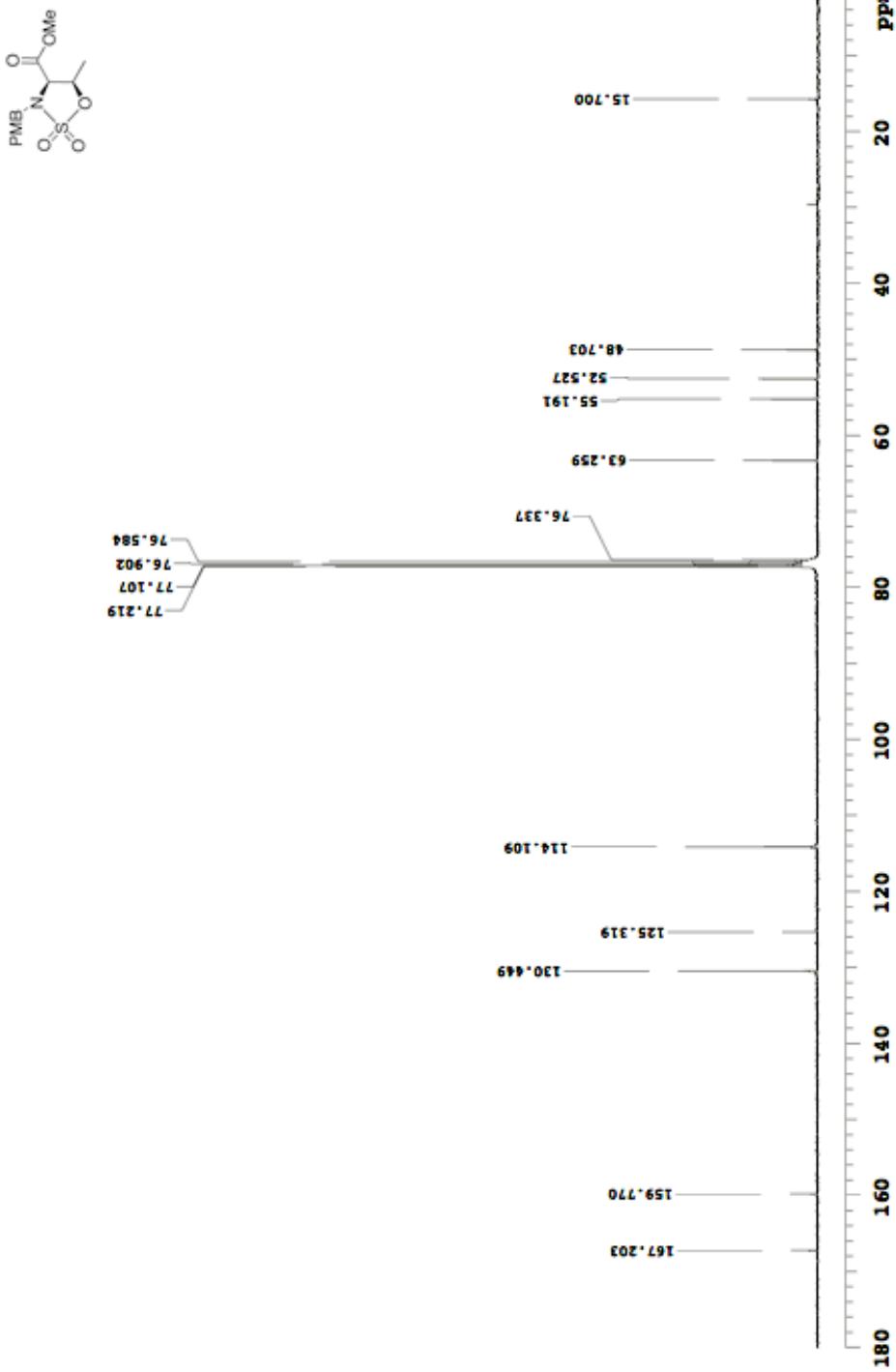
100 MHz 1D C13 in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3600gs probe



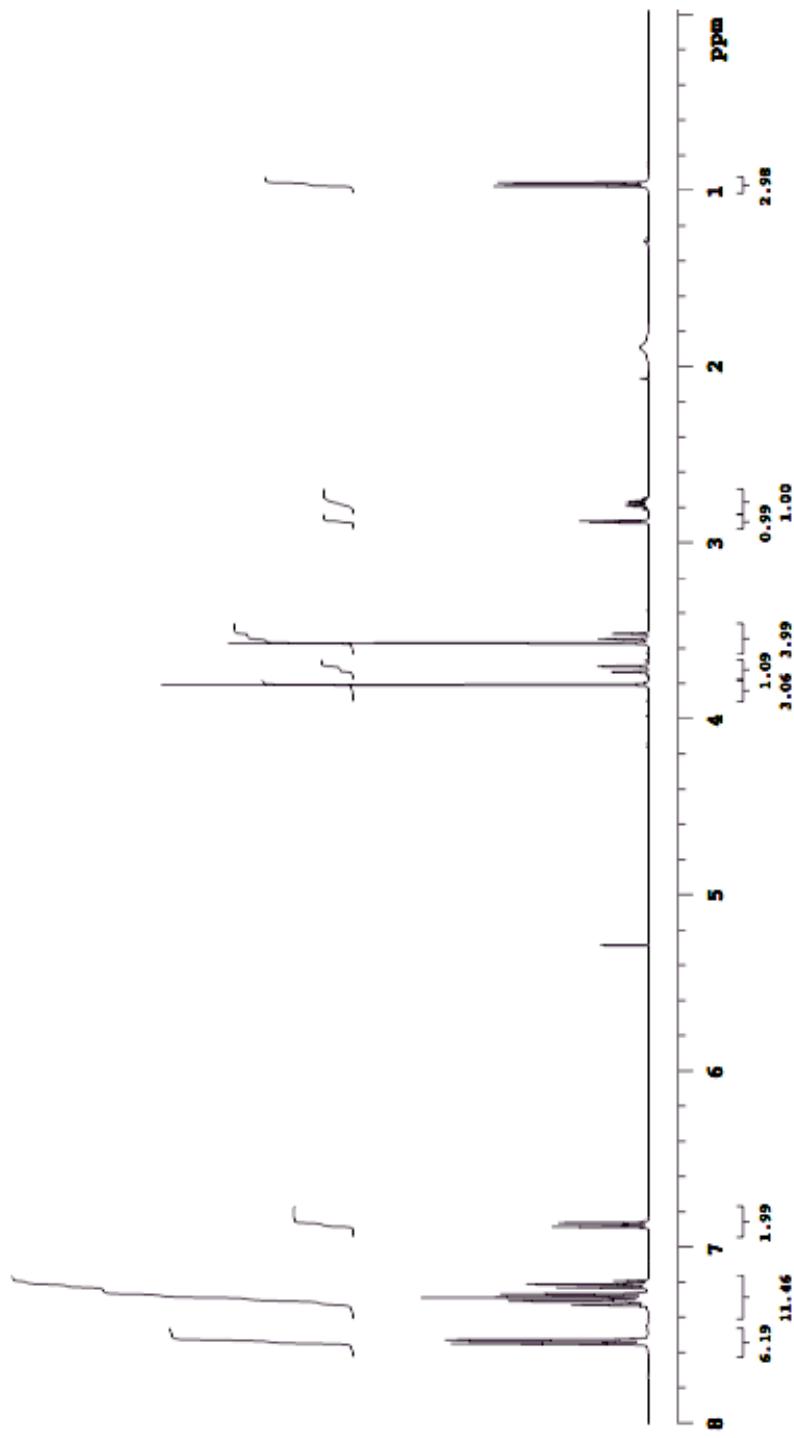
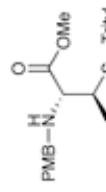
400 MHz 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 4000gs probe



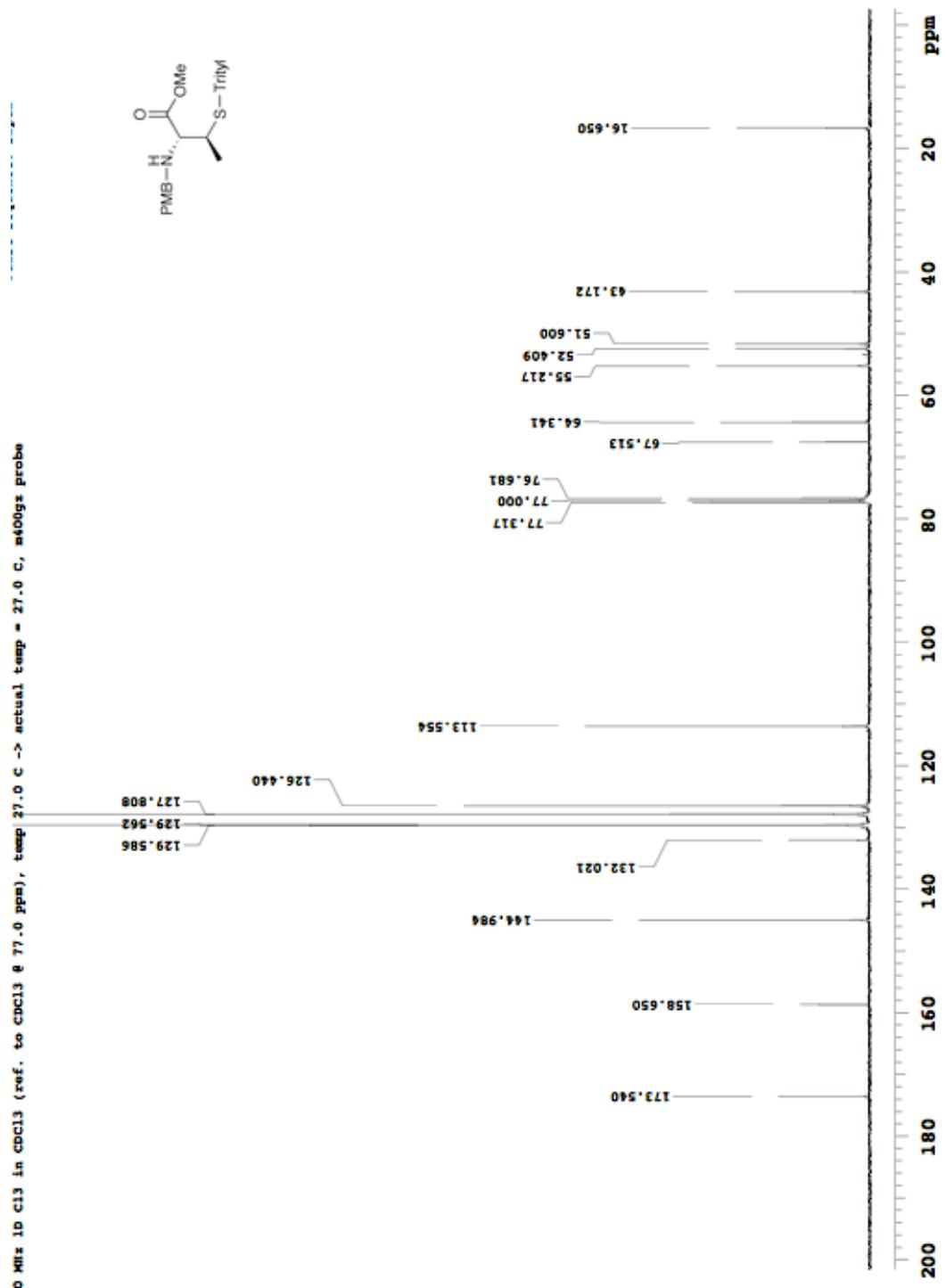
100 MHz 1D Cl^3 in CDCl_3 (ref. to CDCl_3 at 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3400gs probe



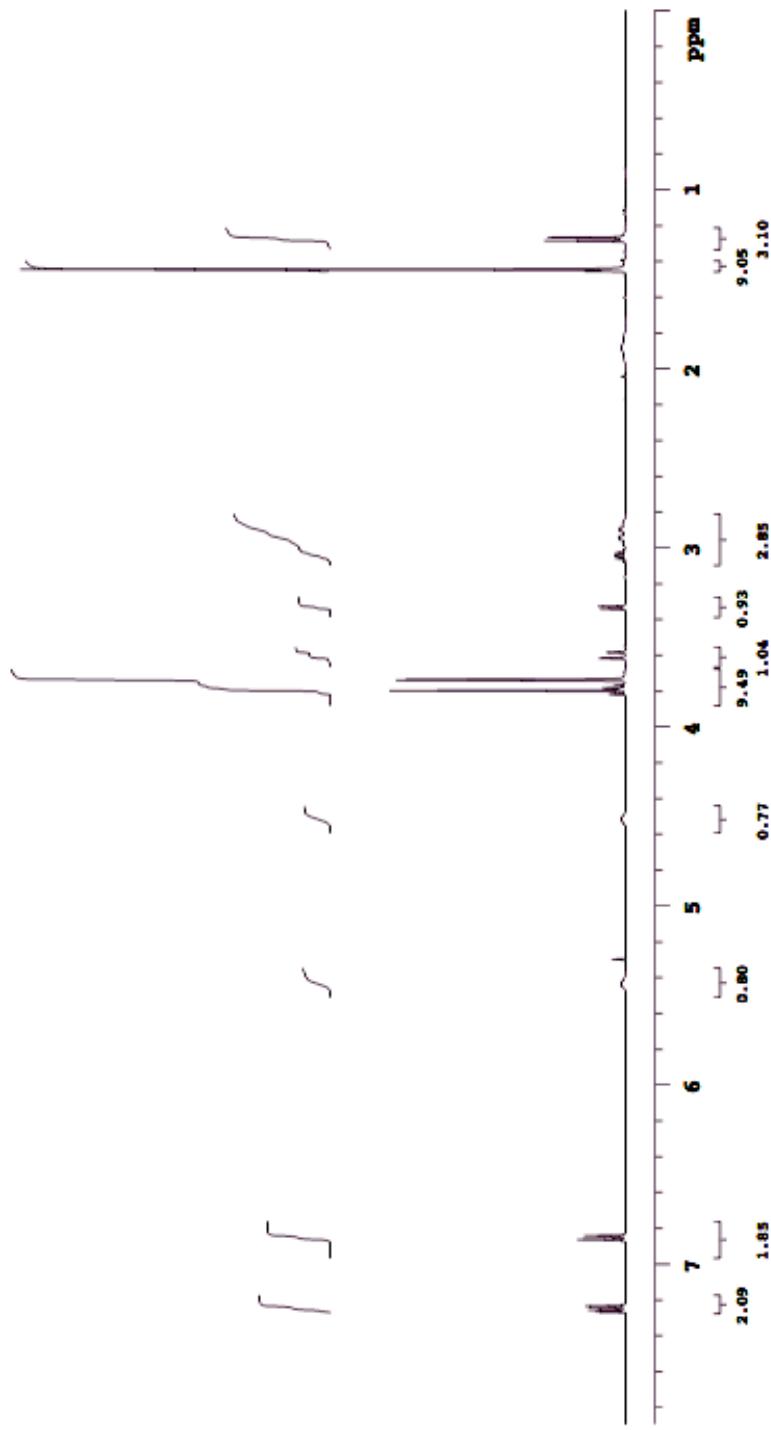
400 MHz 1H in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 1H0D9S probe

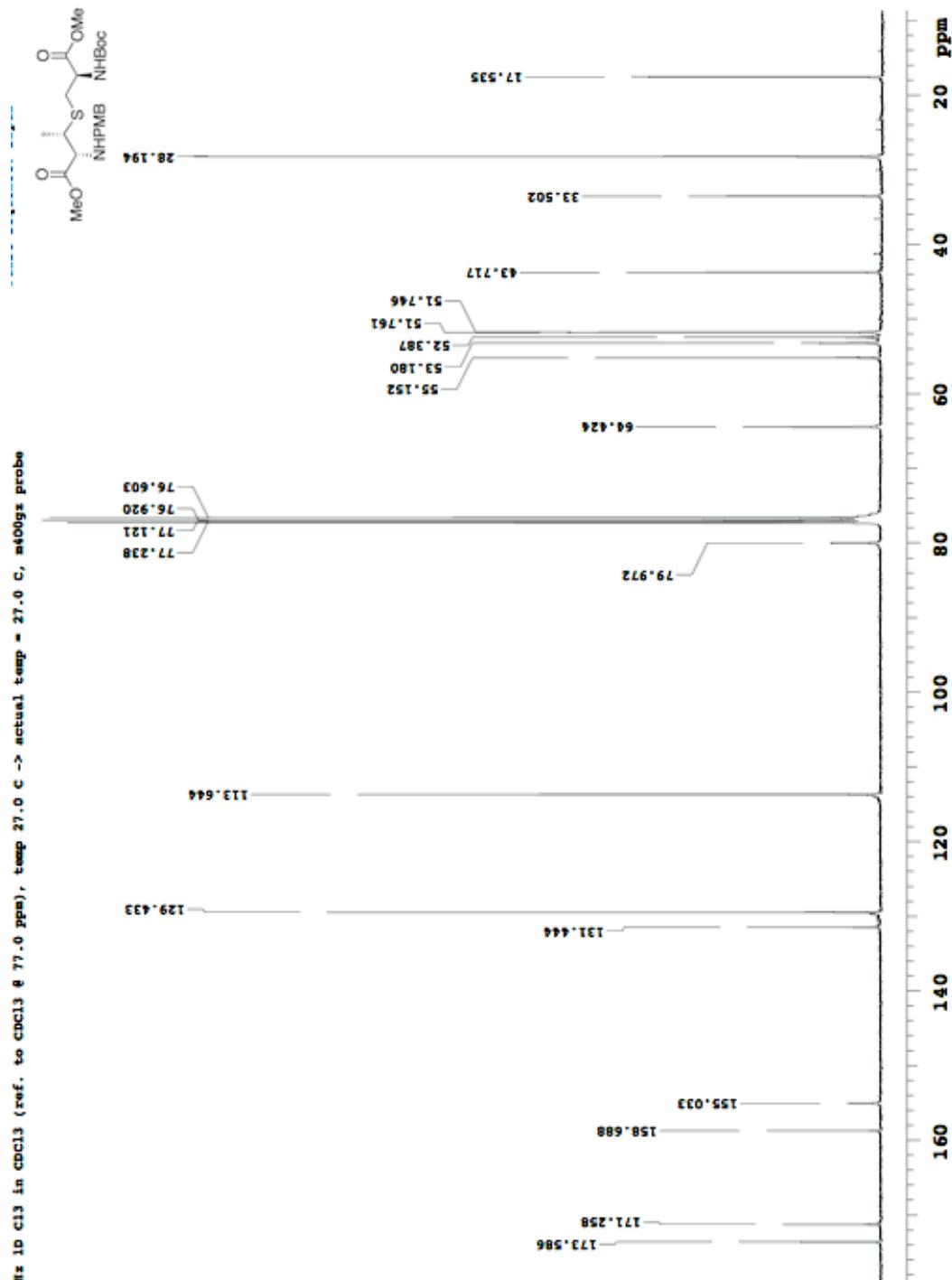


100 MHz 1D C13 in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 3400gz probe

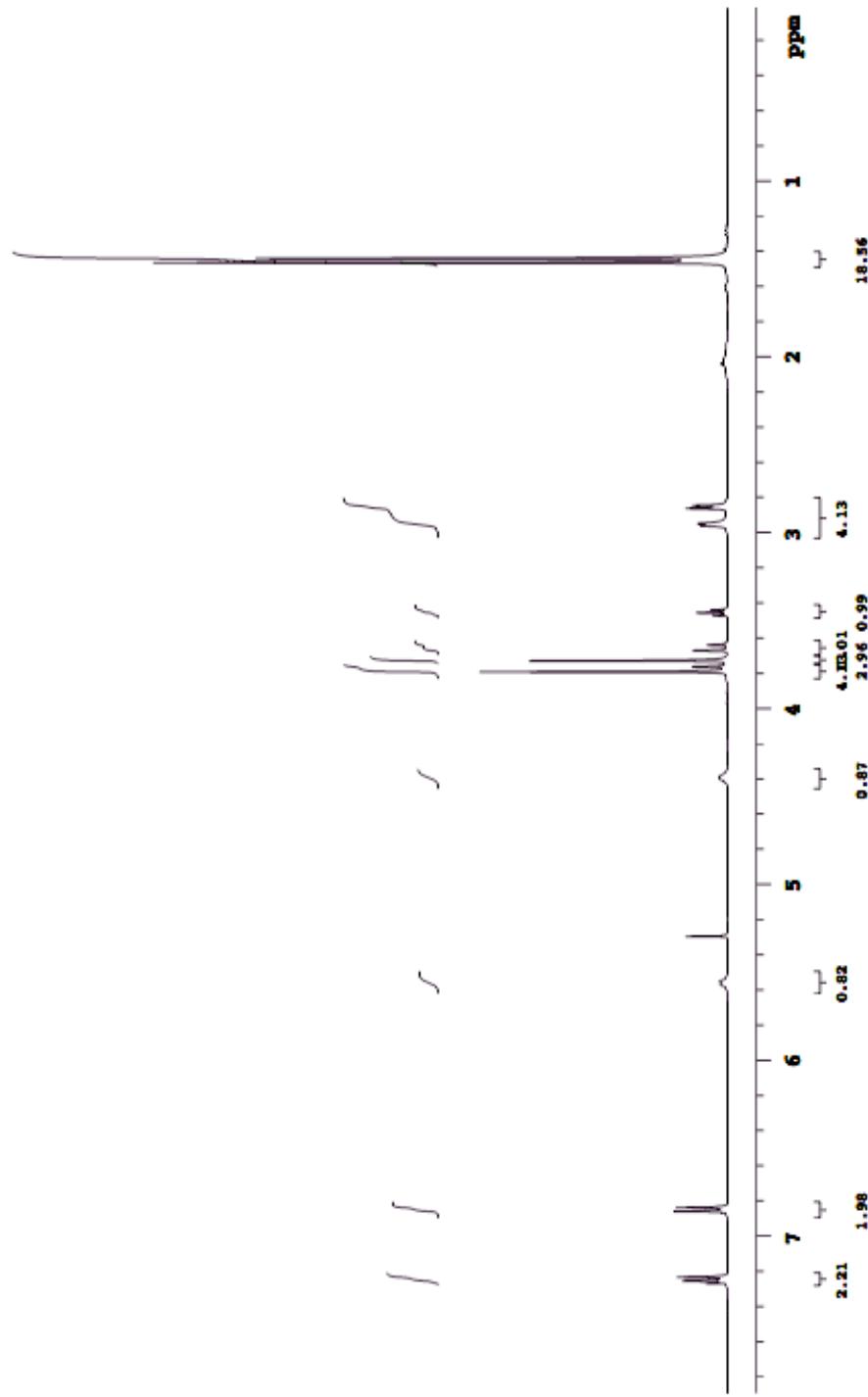


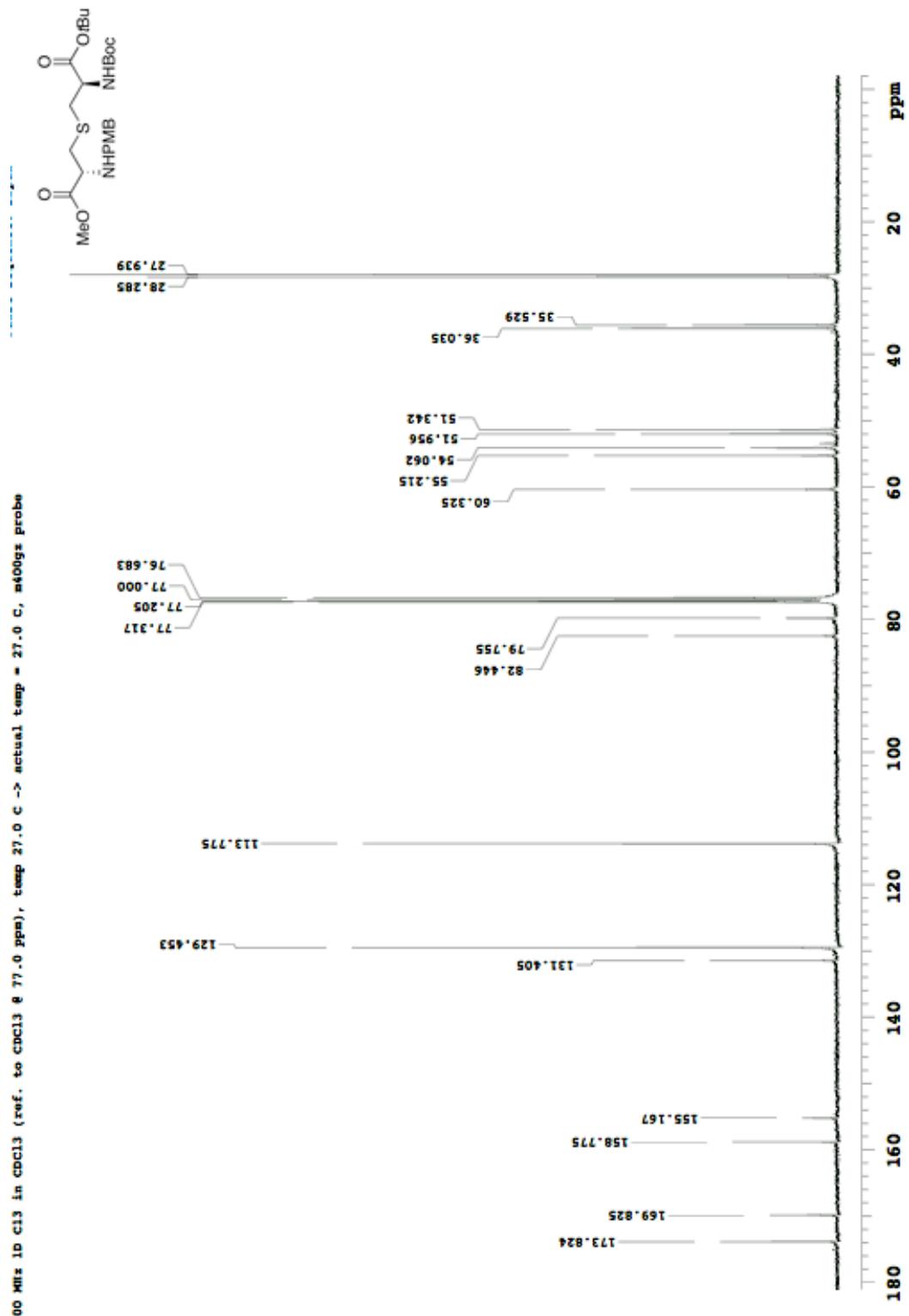
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 4000ggs probe

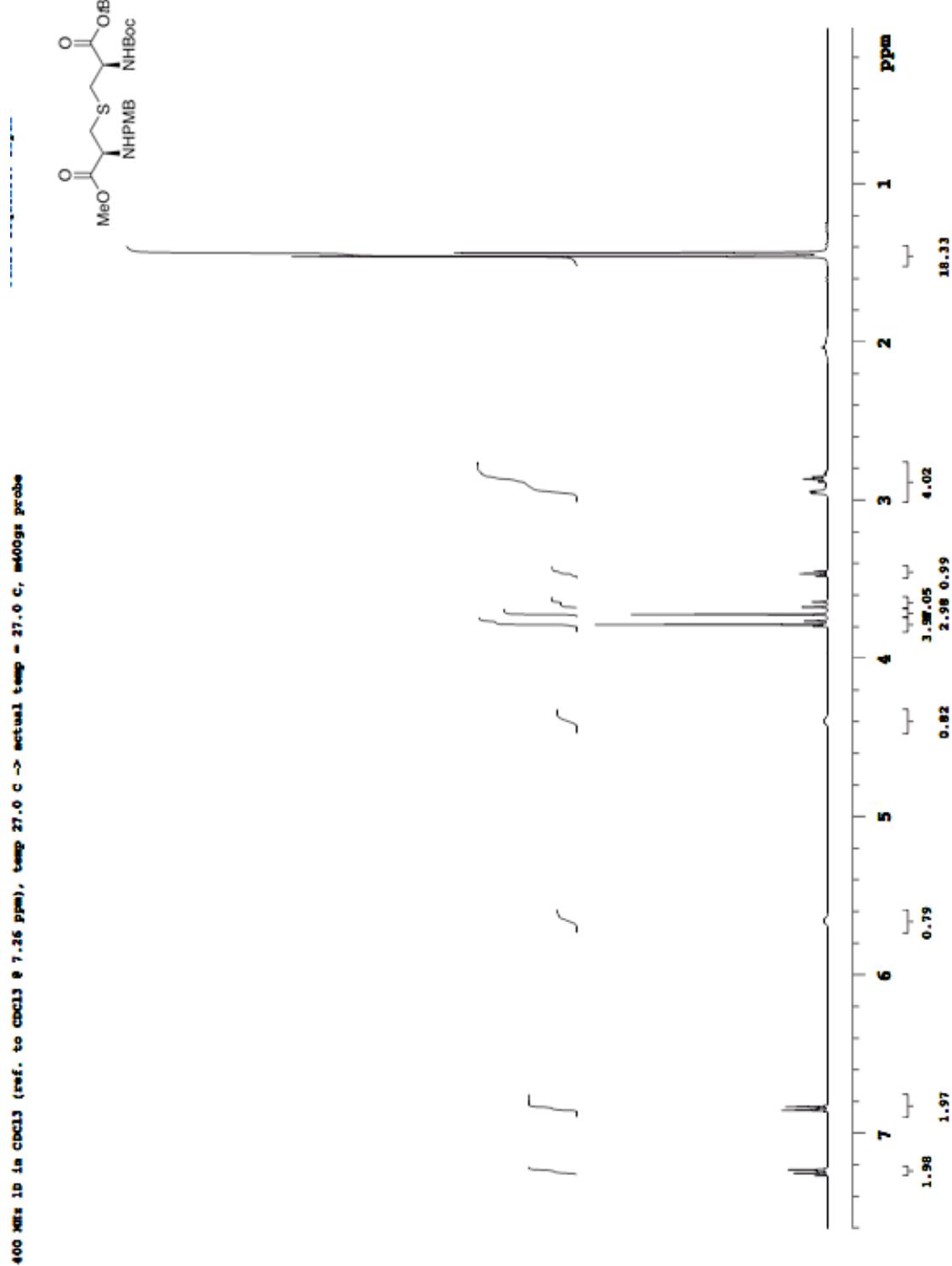




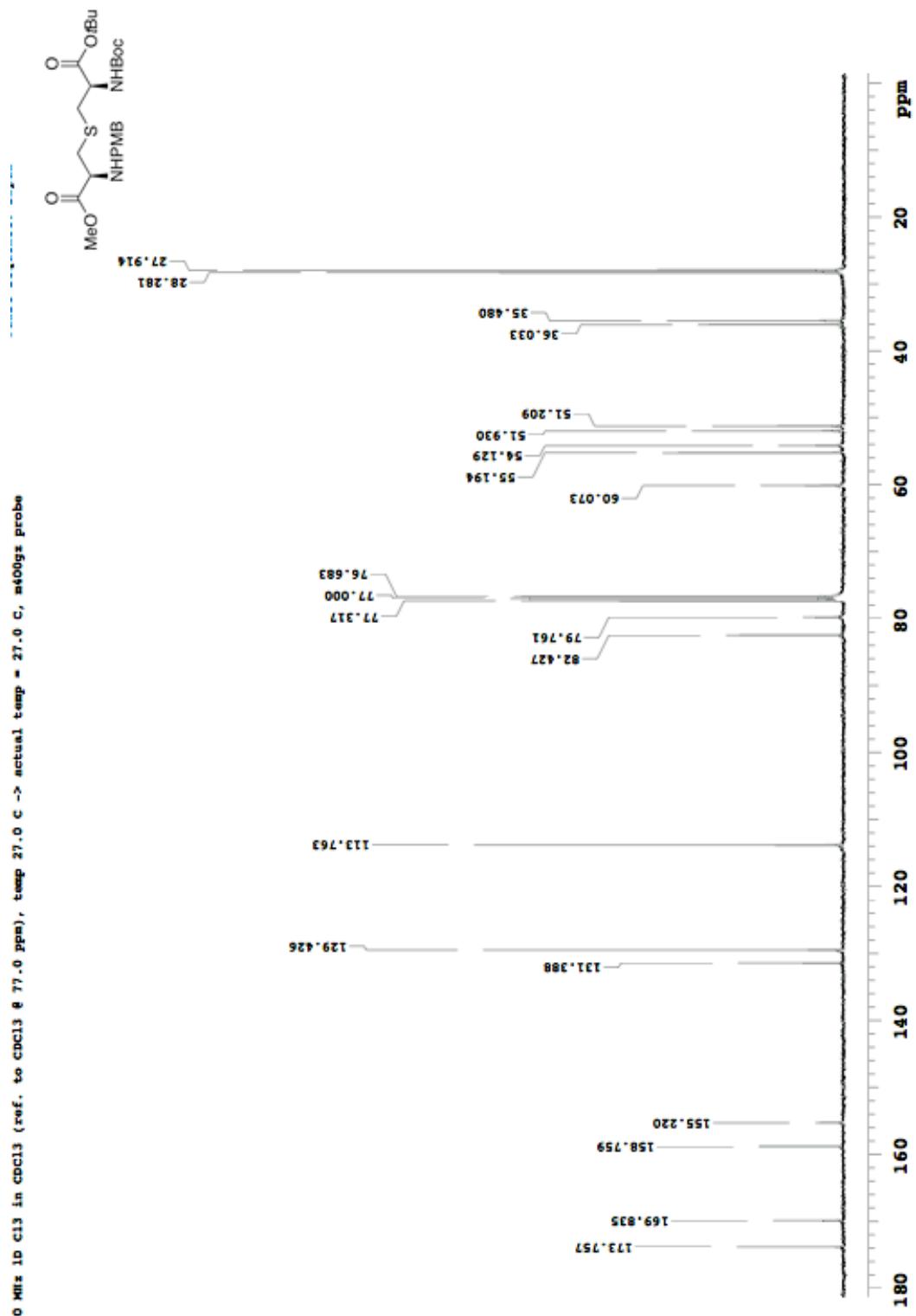
400 MHz 1D in C6C13 (ref. to C6C13 @ 7-26 ppm), temp 27.0 °C → actual temp = 27.0 °C, δ 600 Hz probe

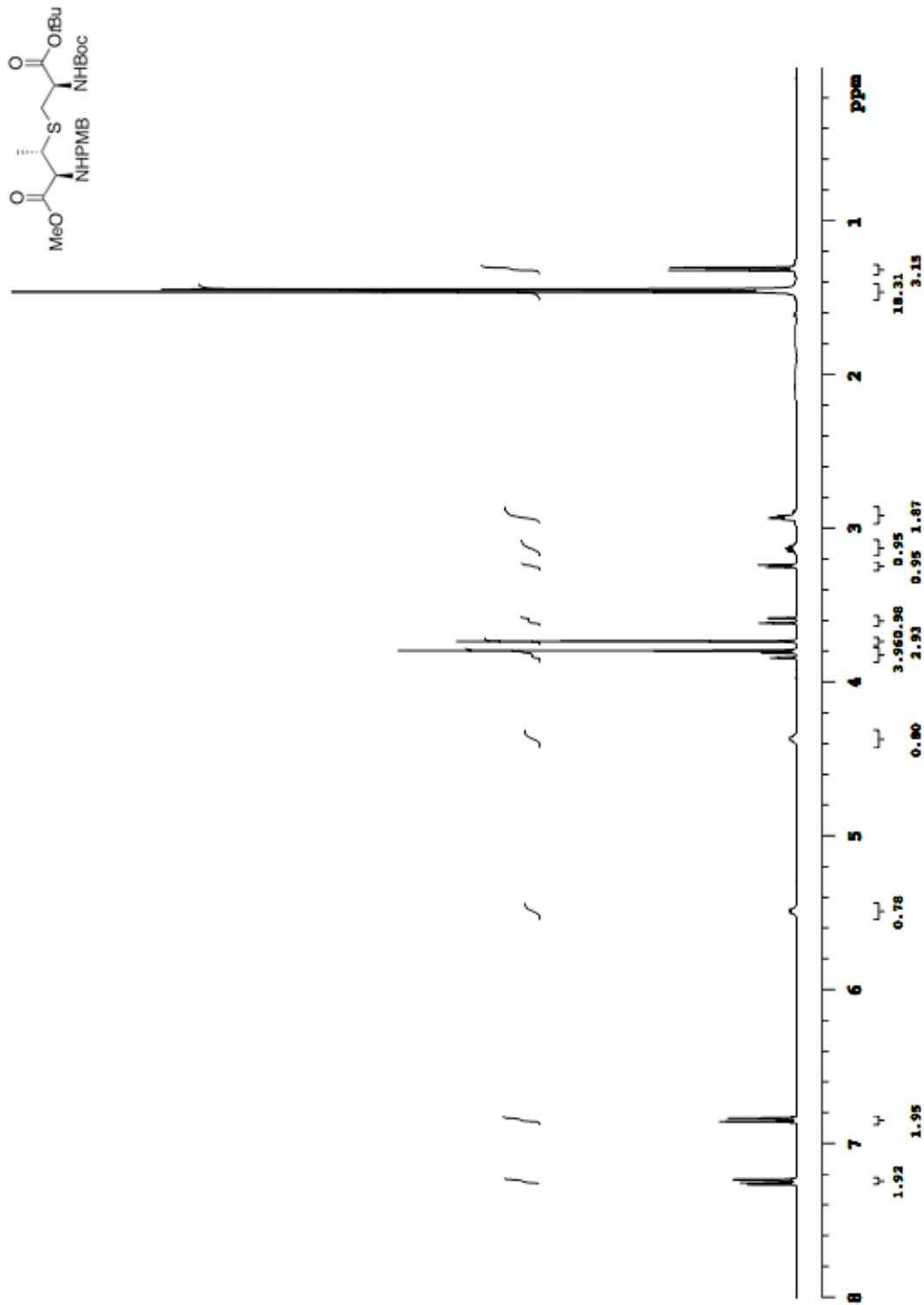


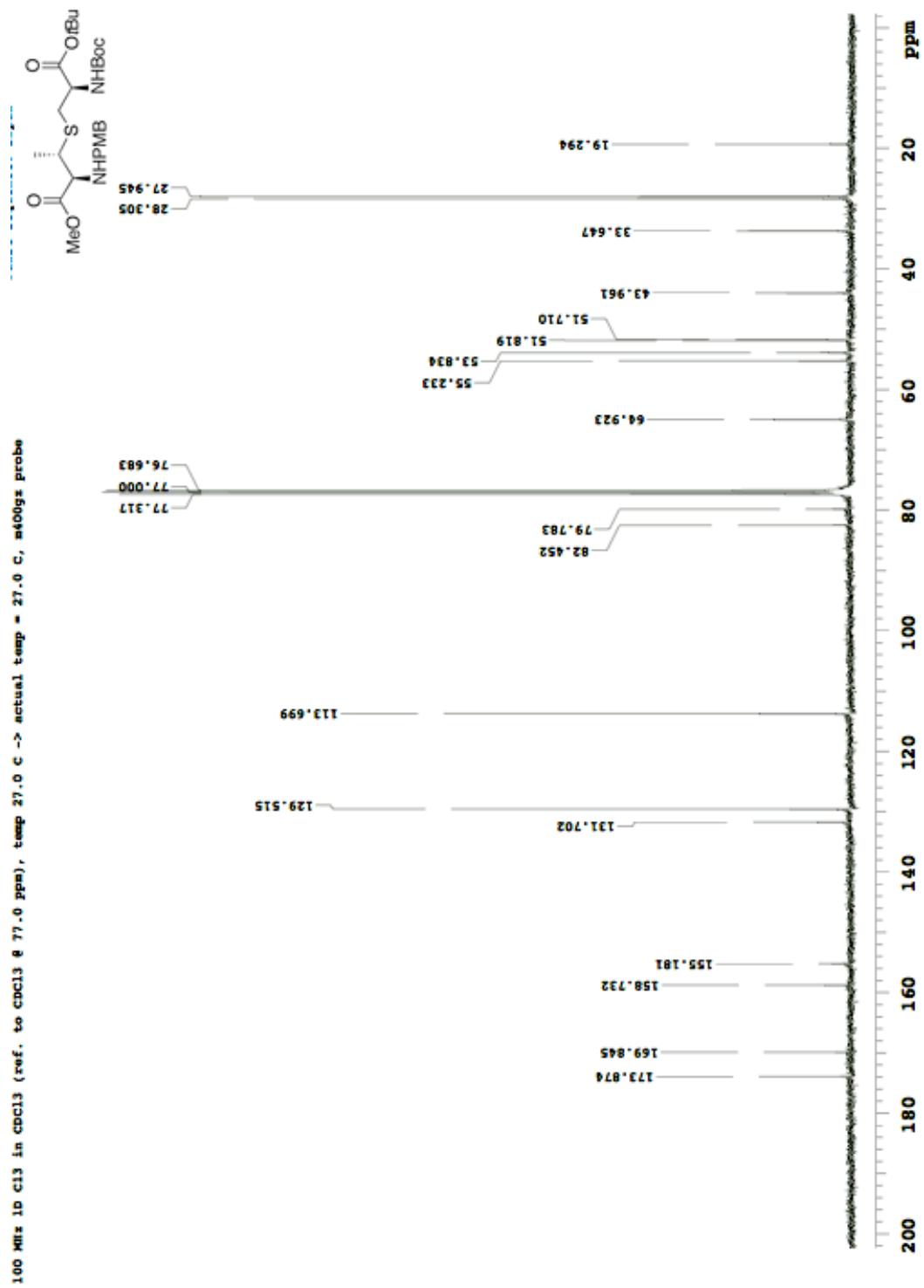


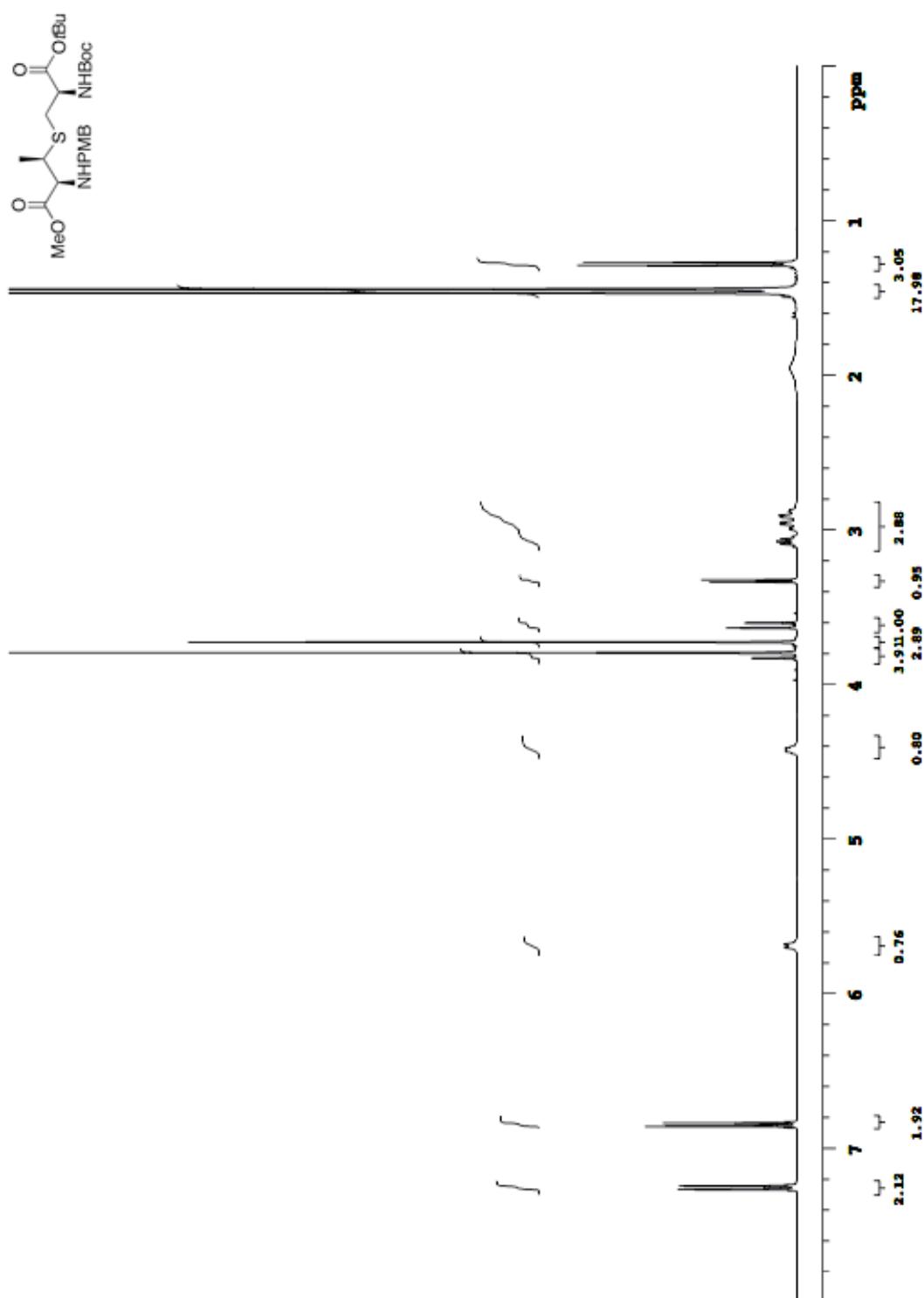


100 MHz 1D C13 (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C → actual temp = 27.0 °C, 360QZ probe

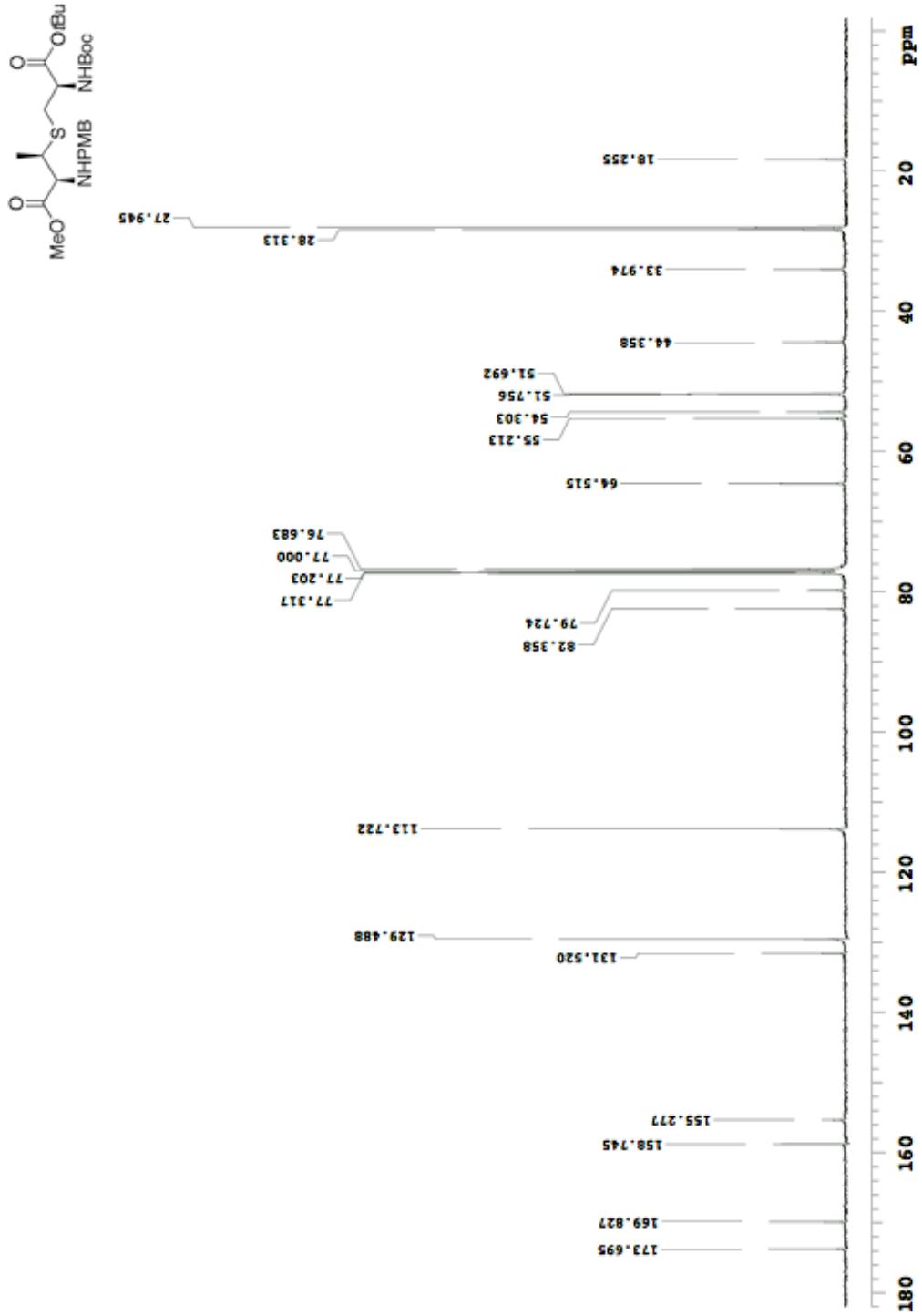




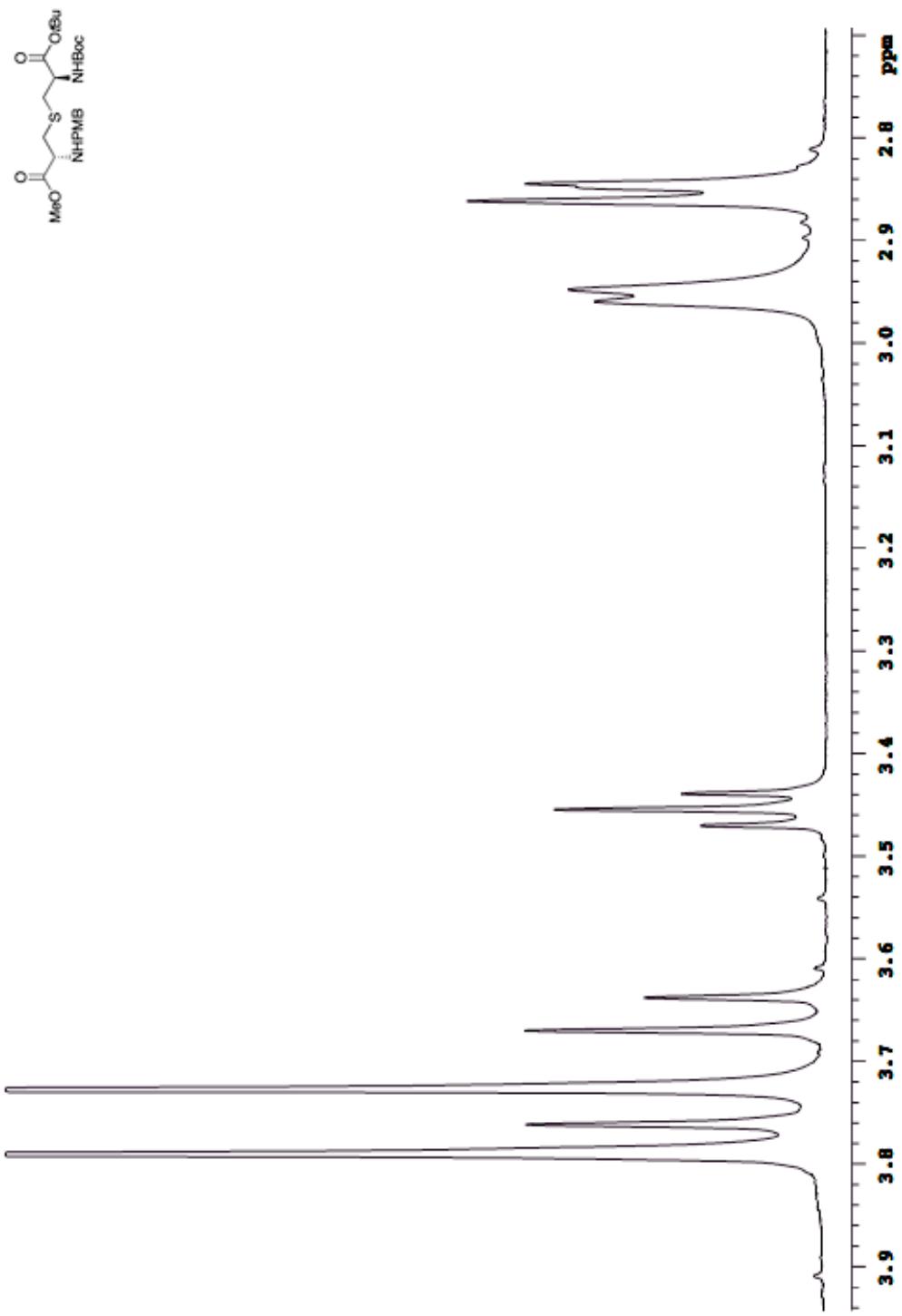




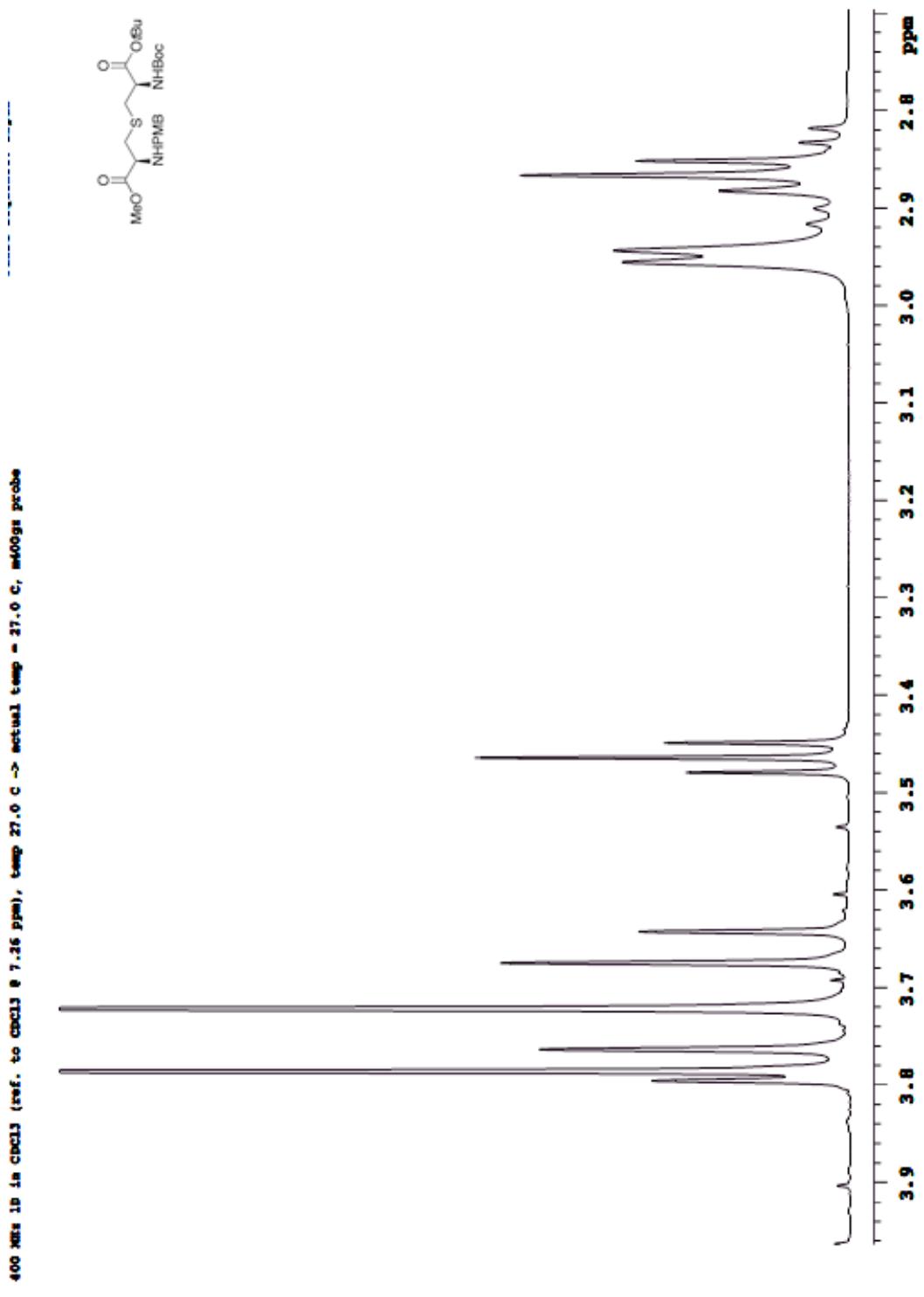
100 MHz 1D C13 in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp 27.0 °C -> actual temp = 27.0 °C, 800g3 probe



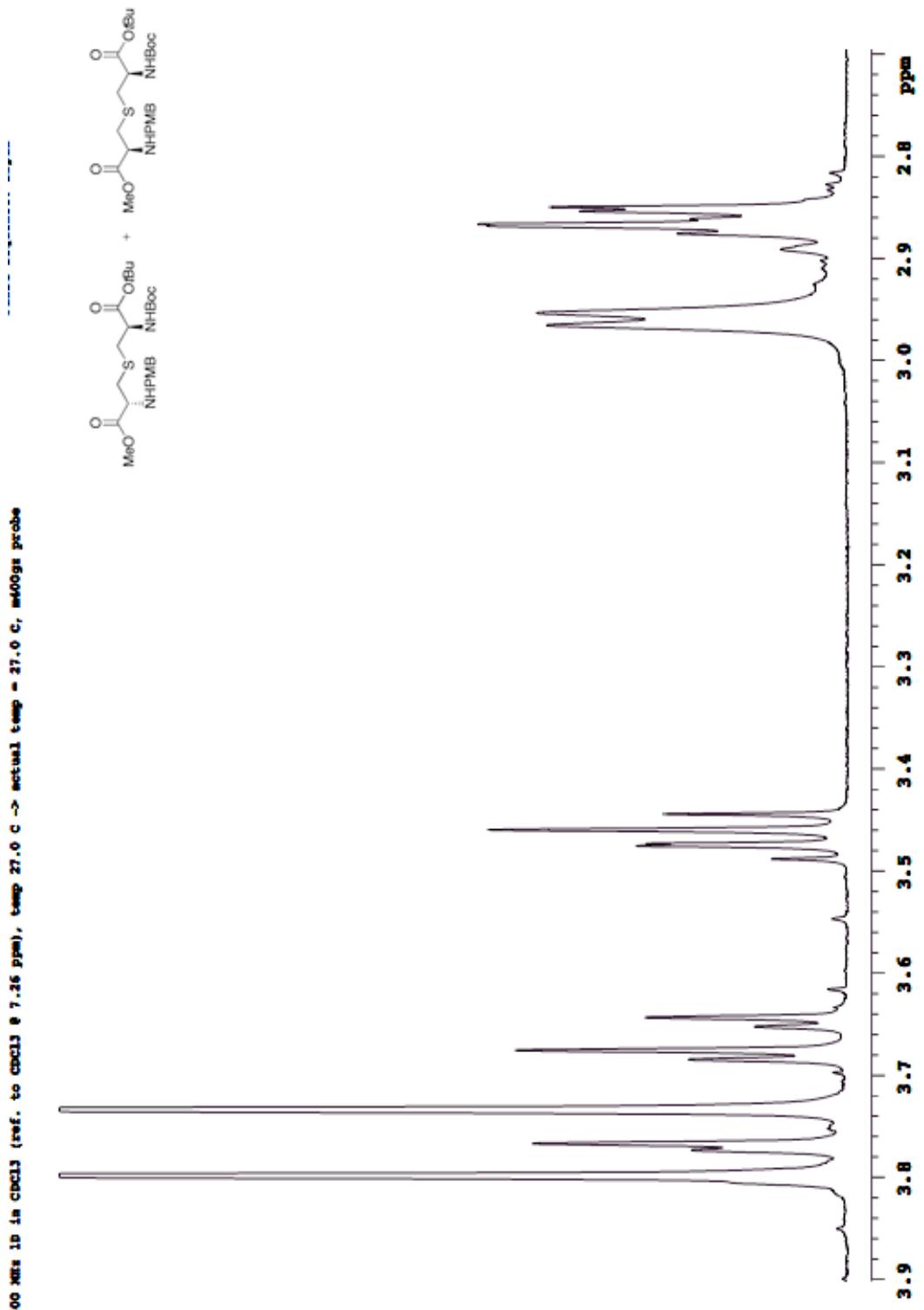
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, mDQG probe



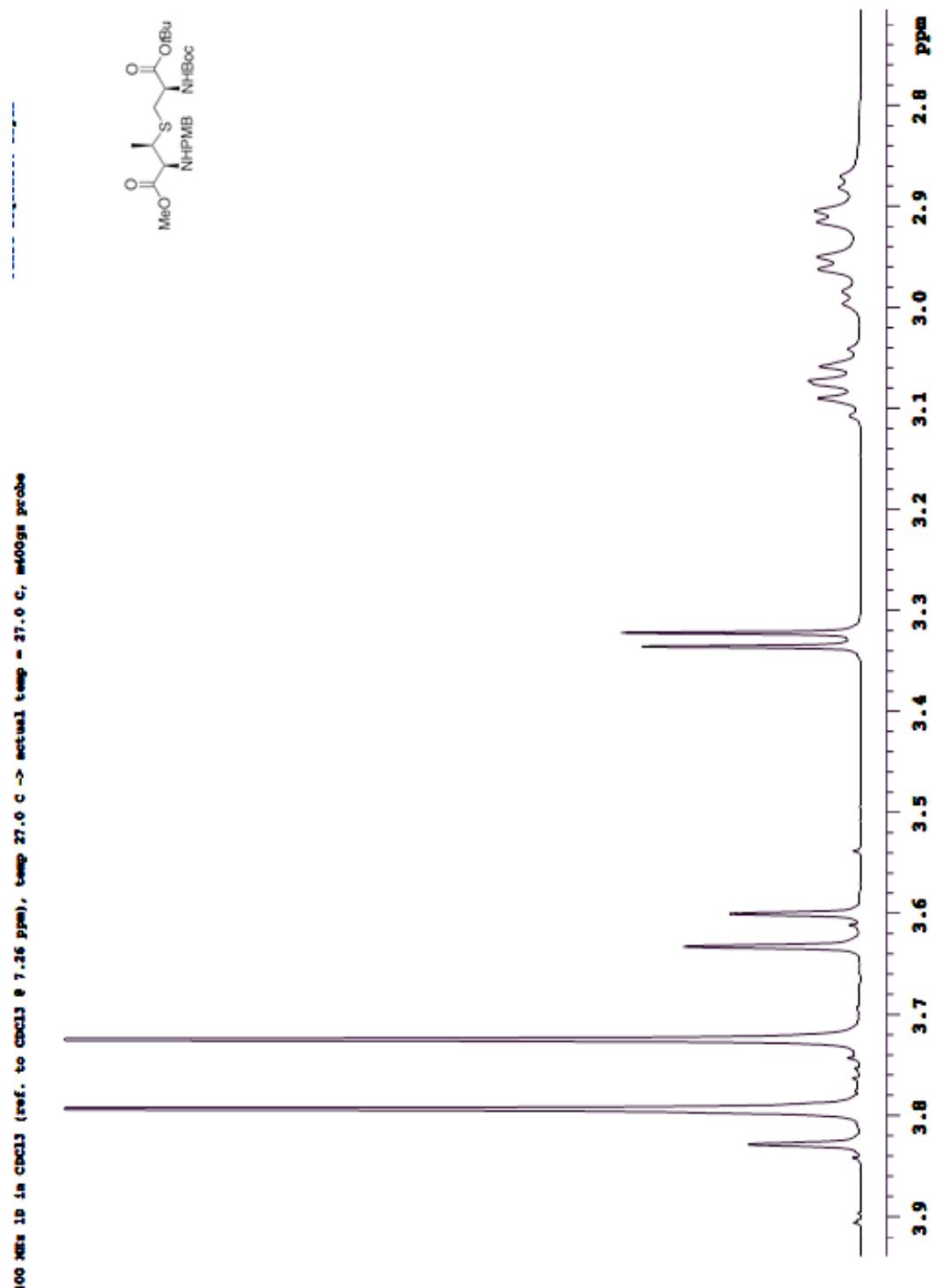
400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 4000g probe

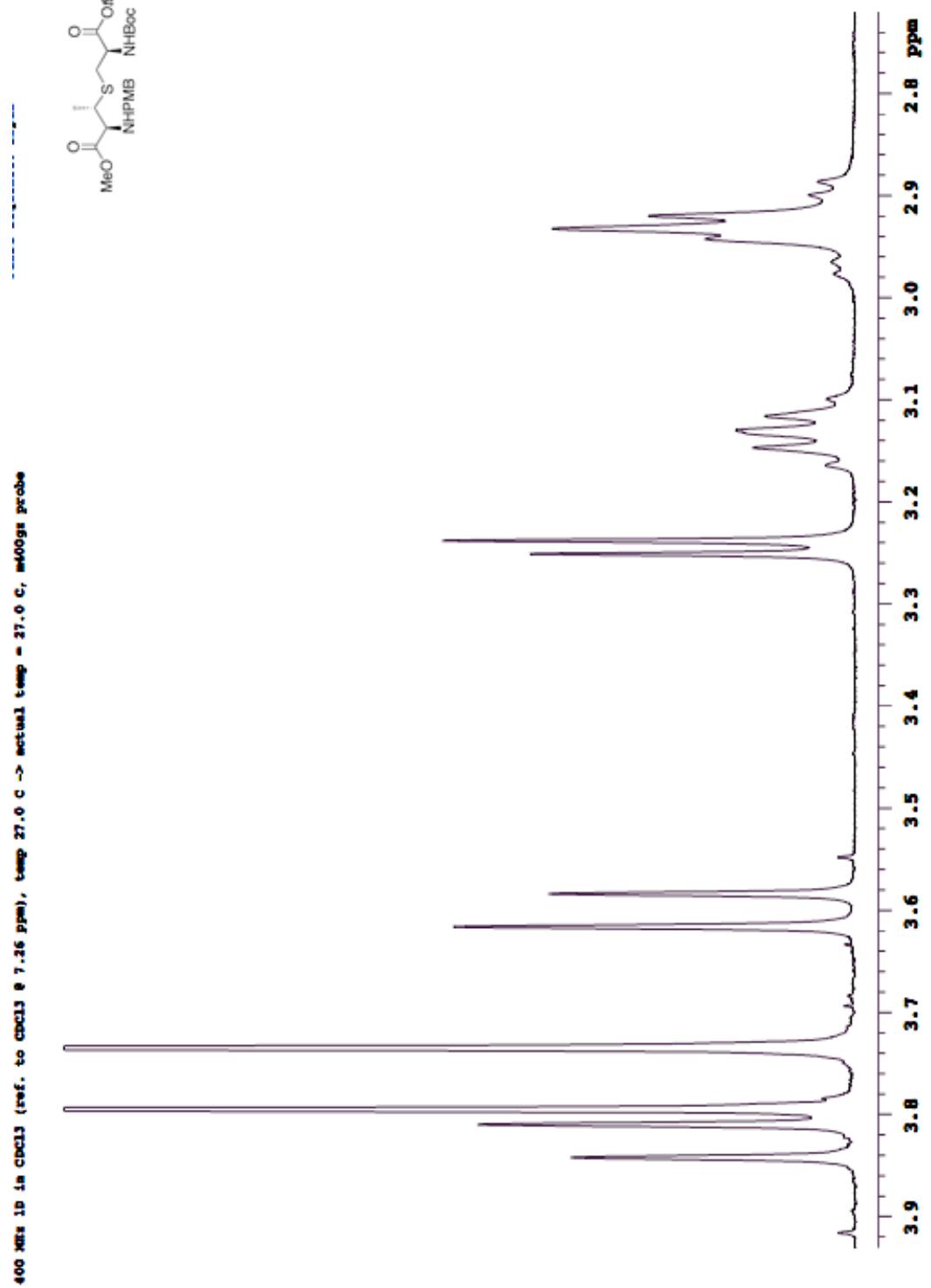


400 MHz 1H NMR (ref. to CDCl₃ at 7.26 ppm), temp. 27.0 °C → actual temp = 27.0 °C, mDQG probe



400 MHz 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 4000s probe





400 MHz 1H NMR in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.0 °C → actual temp = 27.0 °C, 1H NMR probe

