

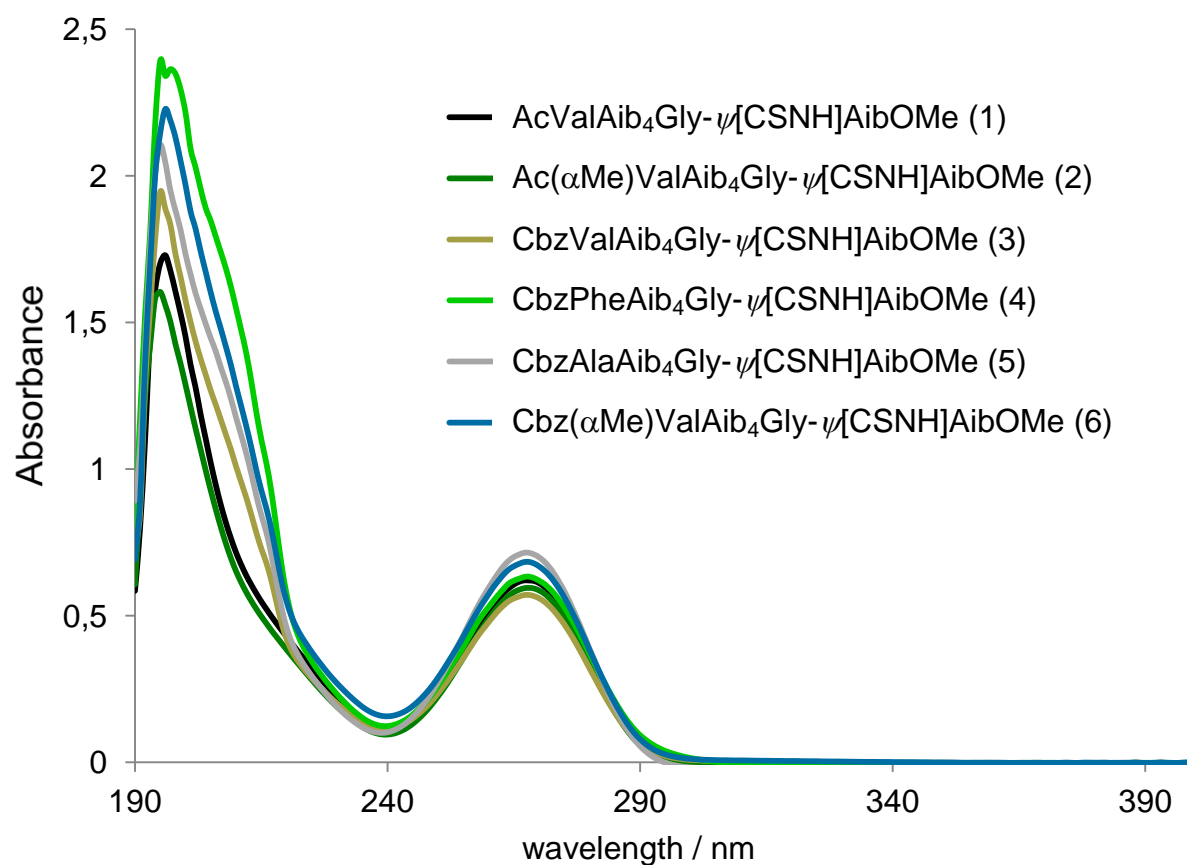
Thionoglycine as a multifunctional spectroscopic reporter: CD validation of an NMR method for analysing screw-sense preference in helical foldamers

Matteo De Poli and Jonathan Clayden*

Supporting Information

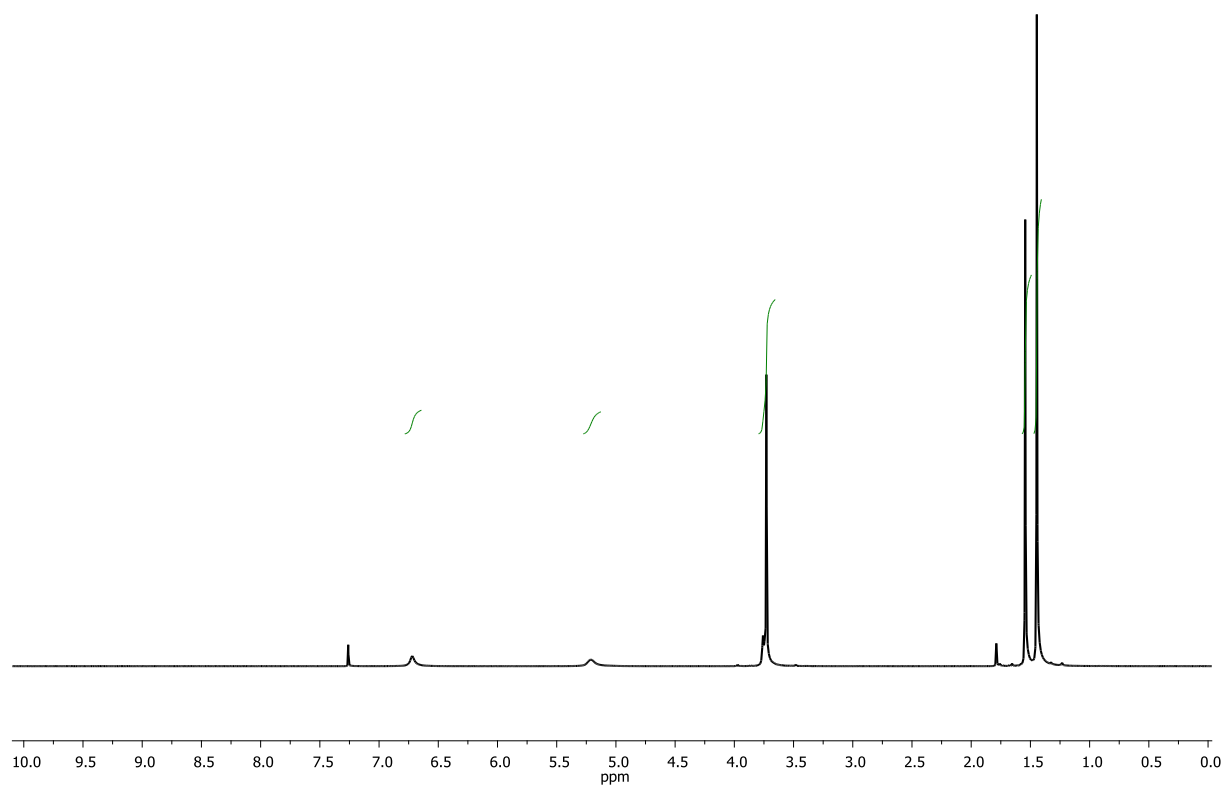
UV spectra of compounds 1-6 in MeOH

concentration $\sim 6.5 \cdot 10^{-4}$ M

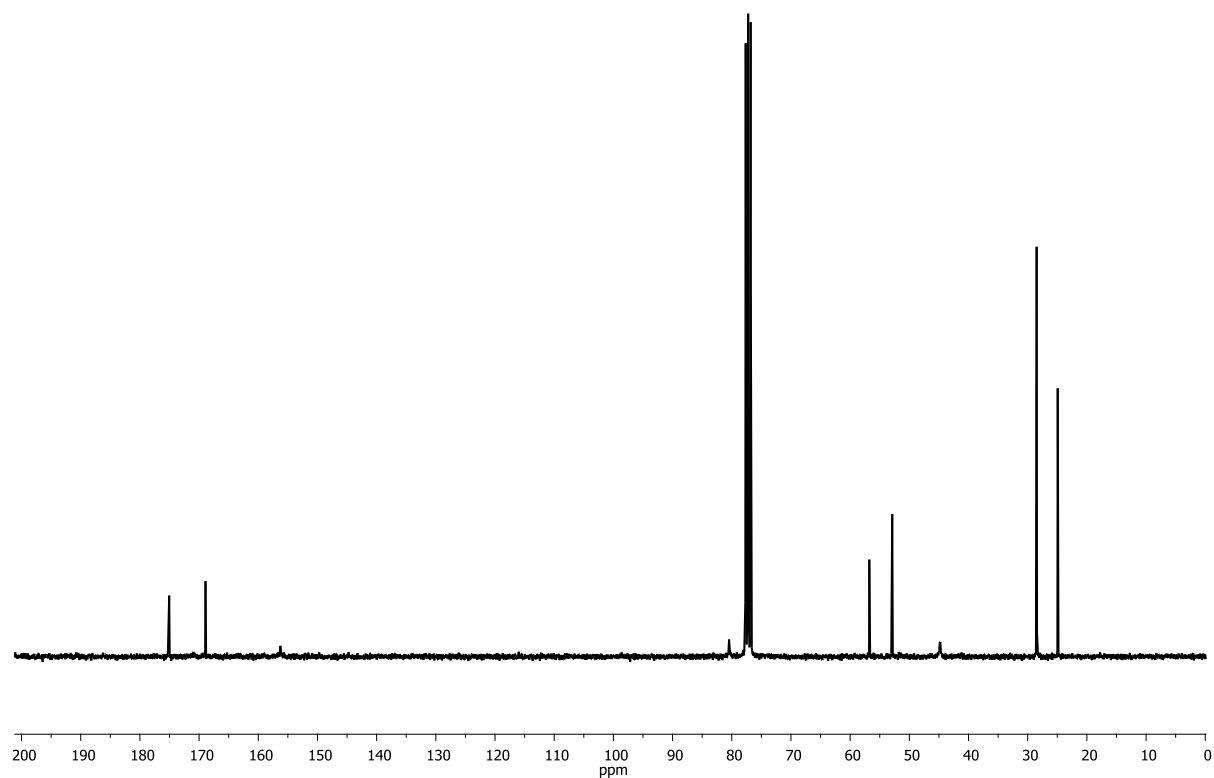


Copies of NMR spectra

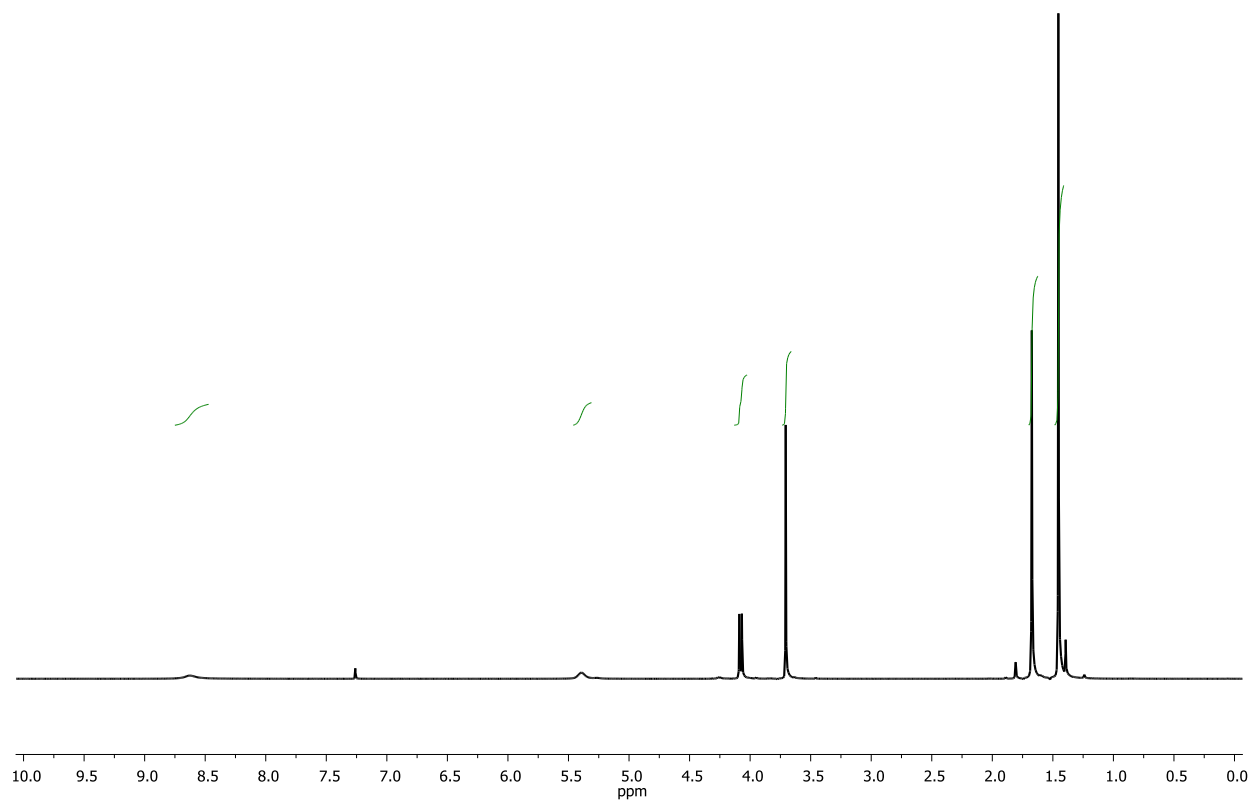
^1H NMR spectrum of Boc-Gly-Aib-OMe (CDCl_3 , 300 MHz)



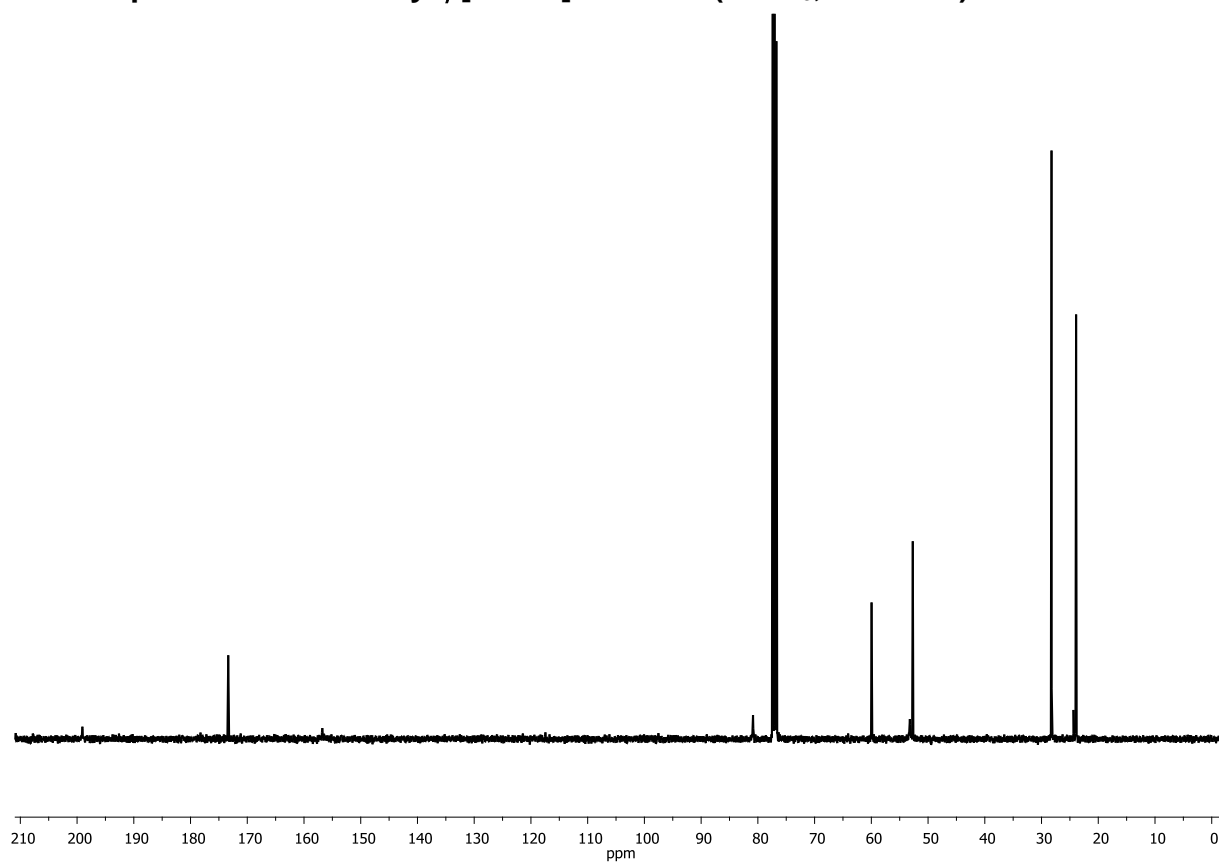
^{13}C NMR spectrum of Boc-Gly-Aib-OMe (CDCl_3 , 125 MHz)



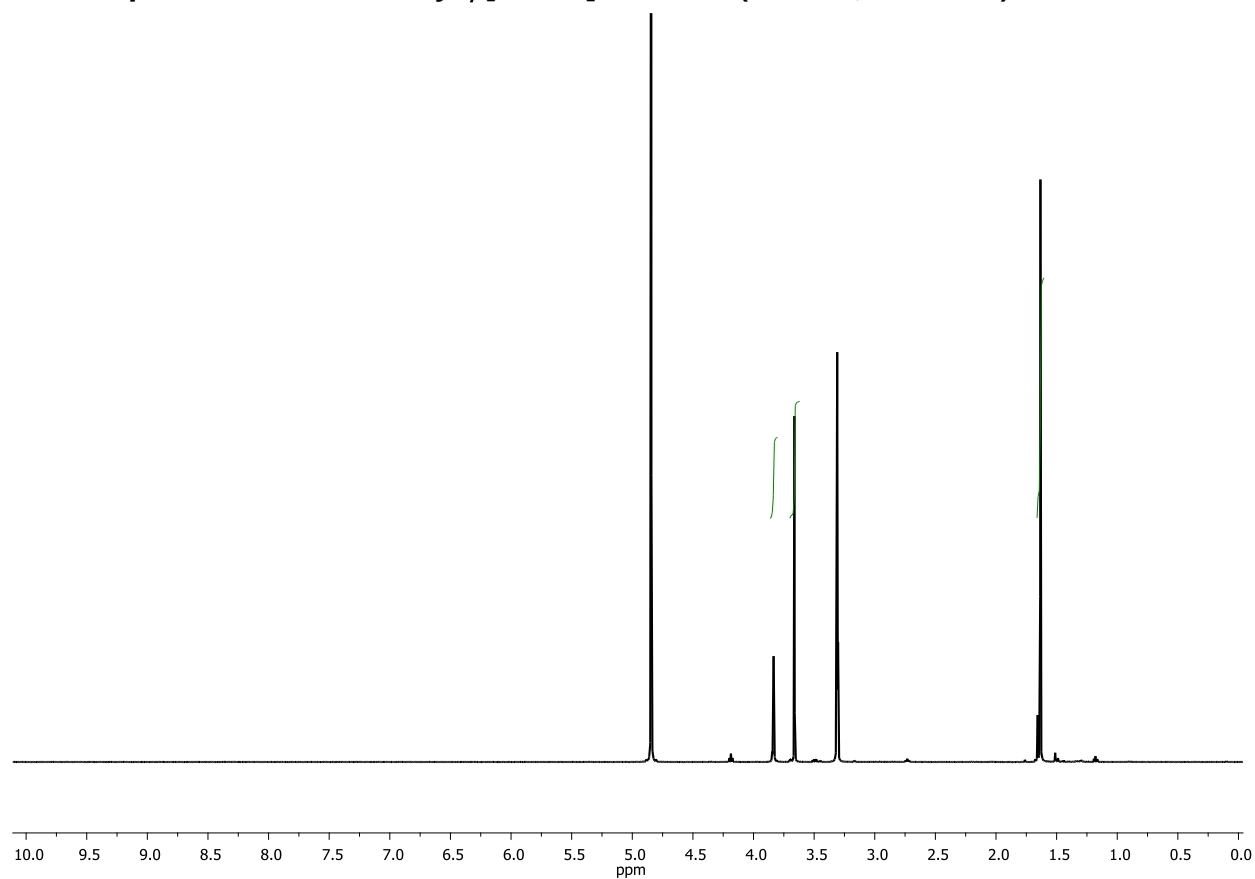
^1H NMR spectrum of Boc-Gly- ψ [CSNH]Aib-OMe (CDCl_3 , 300 MHz)



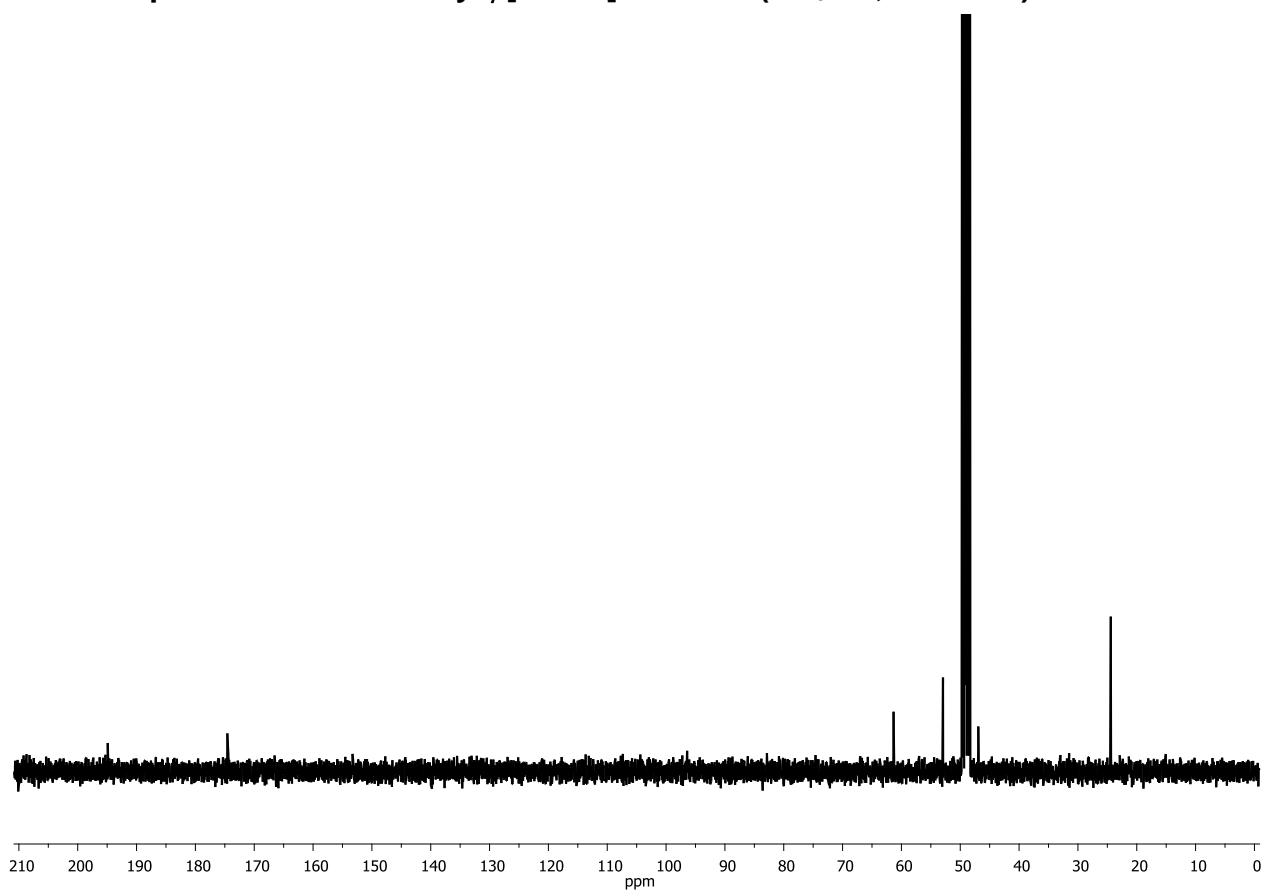
^{13}C NMR spectrum of Boc-Gly- ψ [CSNH]Aib-OMe (CDCl_3 , 300 MHz)



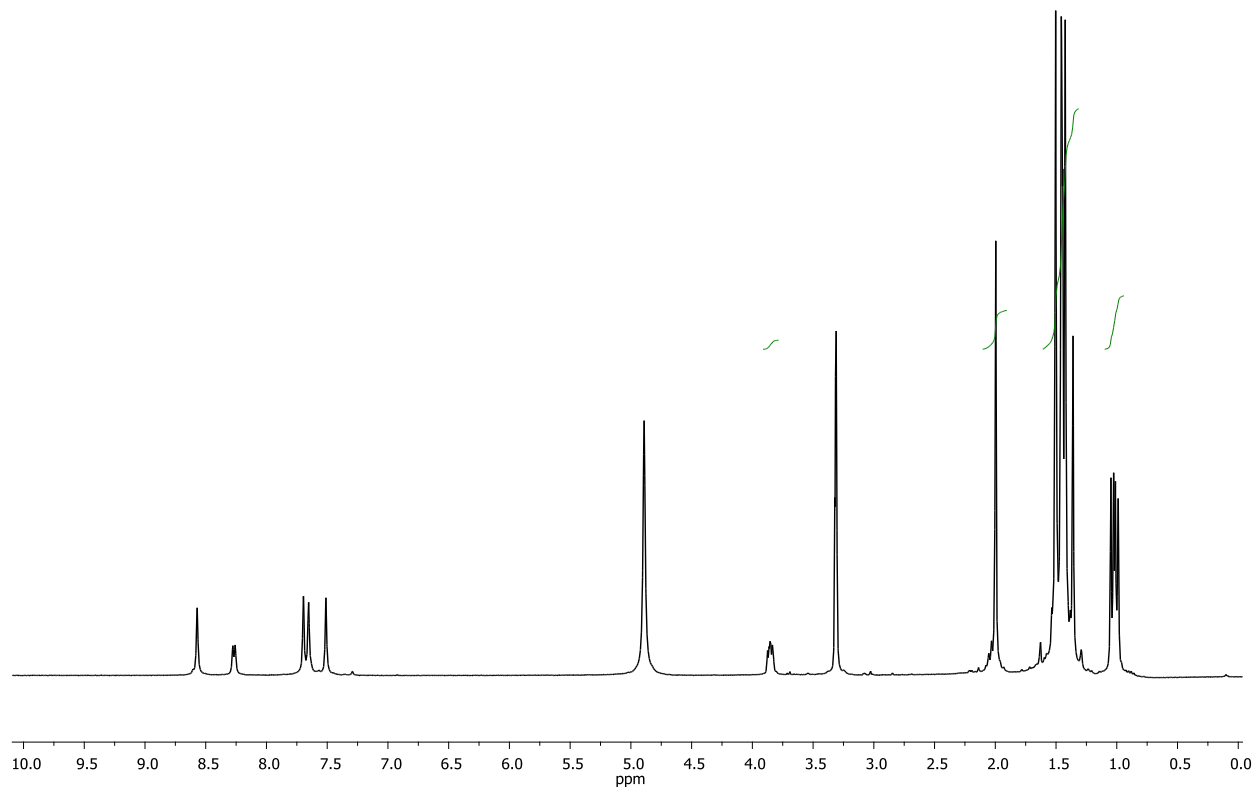
¹H NMR spectrum of HCl·H-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 500 MHz)



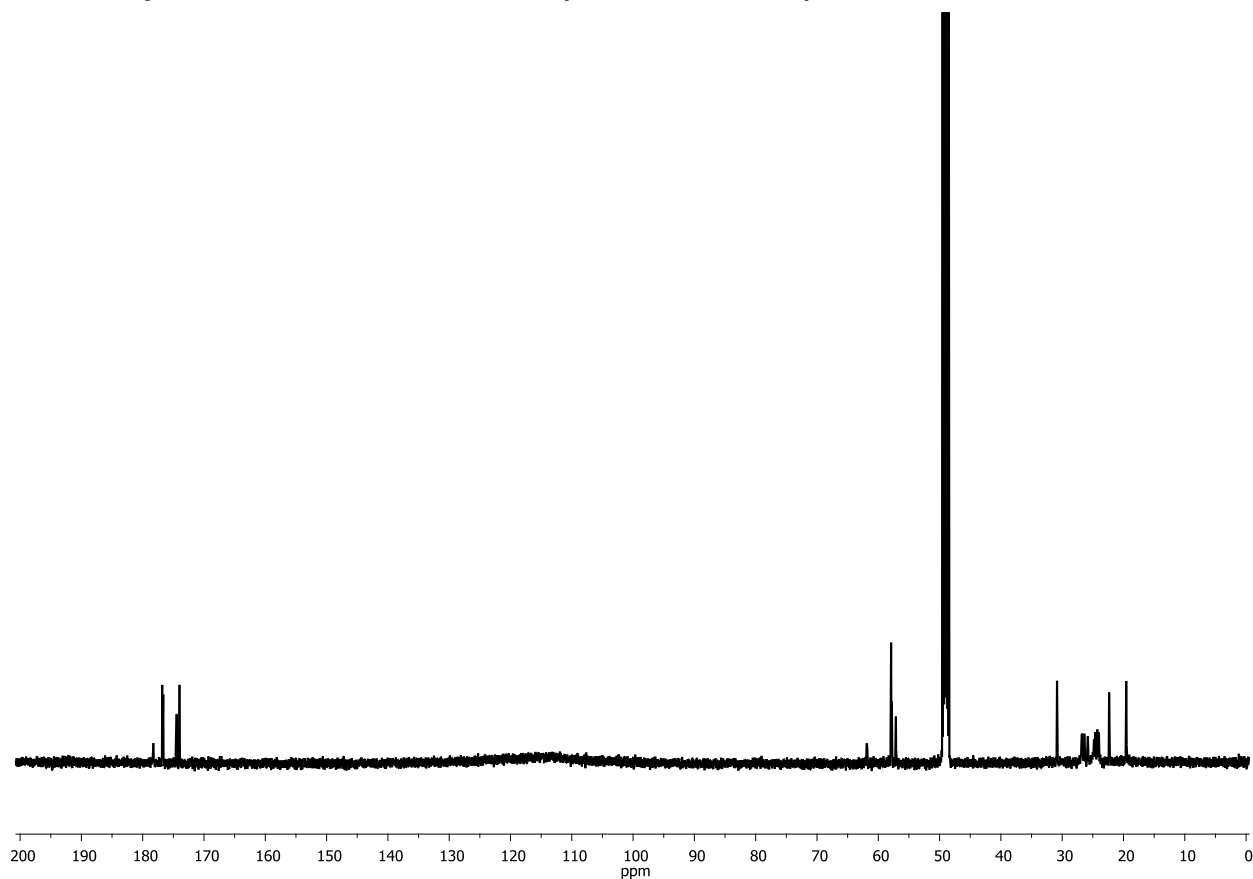
¹³C NMR spectrum of HCl·H-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 101 MHz)



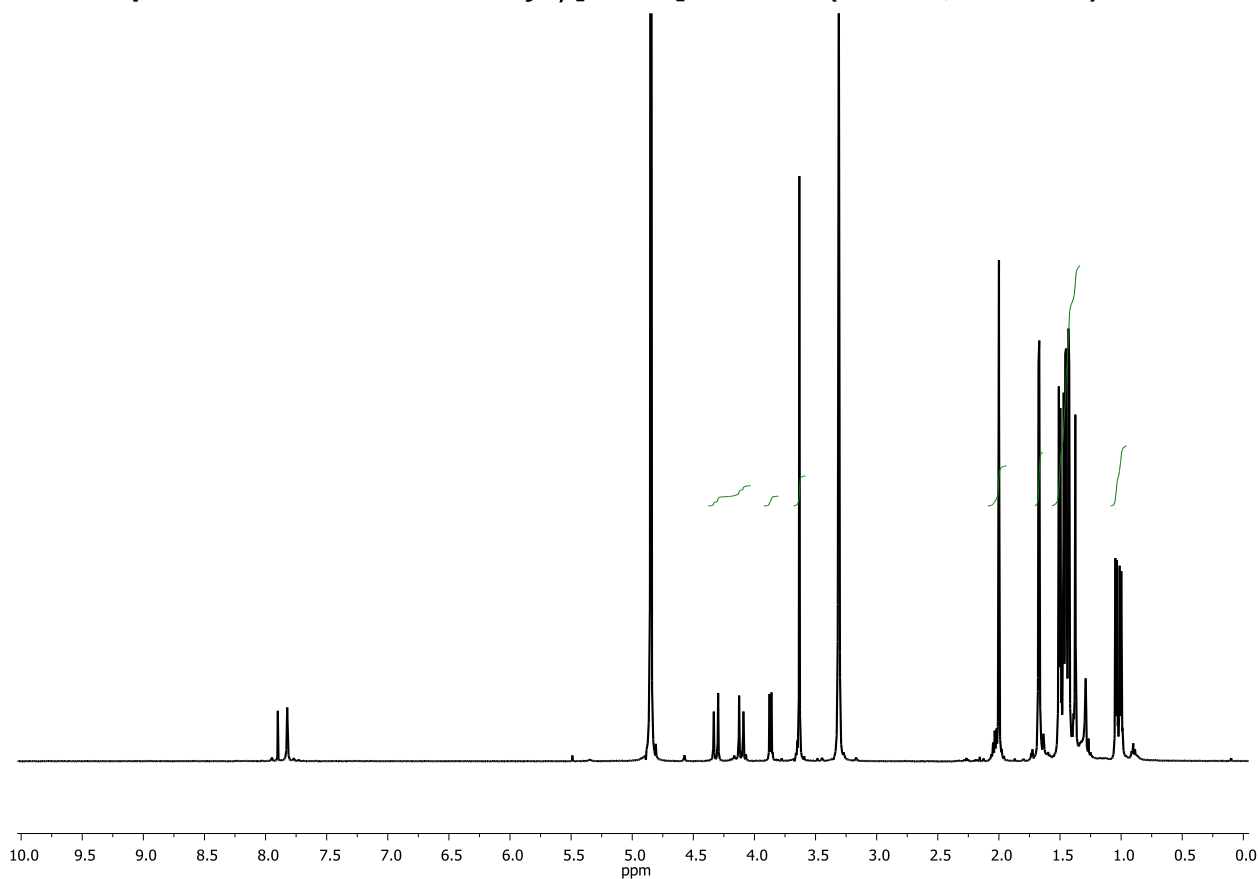
^1H NMR spectrum of Ac-Val-Aib₄-OH (CD₃OD, 300 MHz)



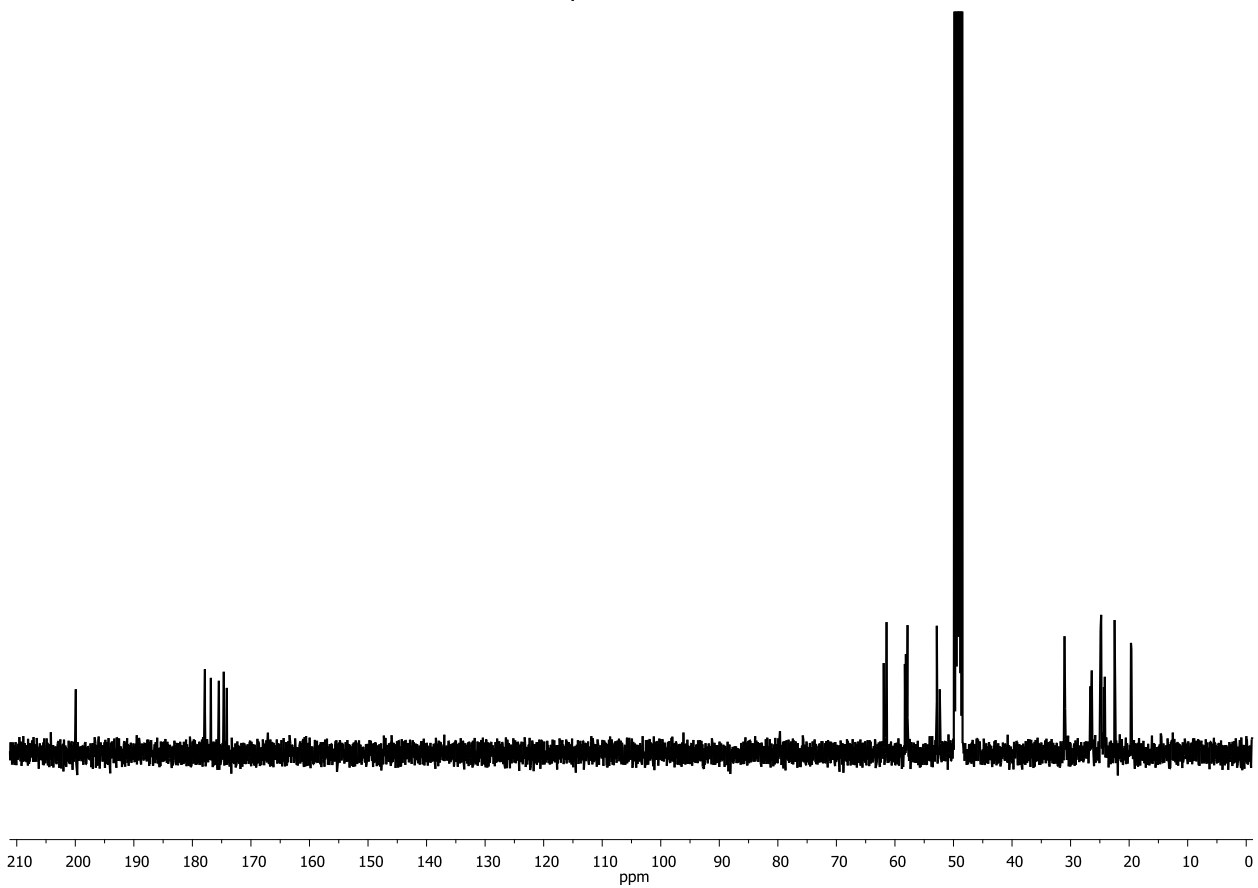
^{13}C NMR spectrum of Ac-Val-Aib₄-OH (CD₃OD, 75 MHz)



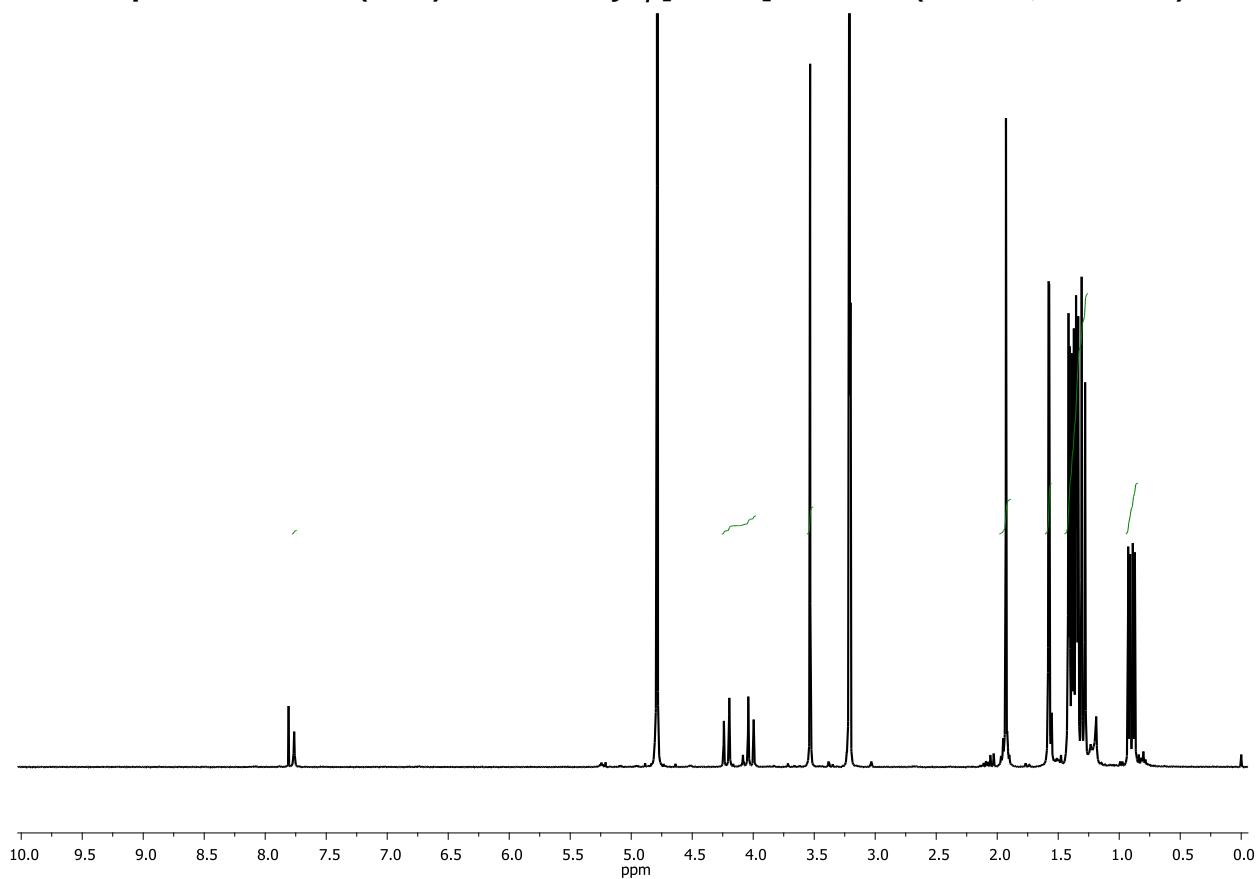
^1H NMR spectrum of Ac-Val-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 500 MHz)



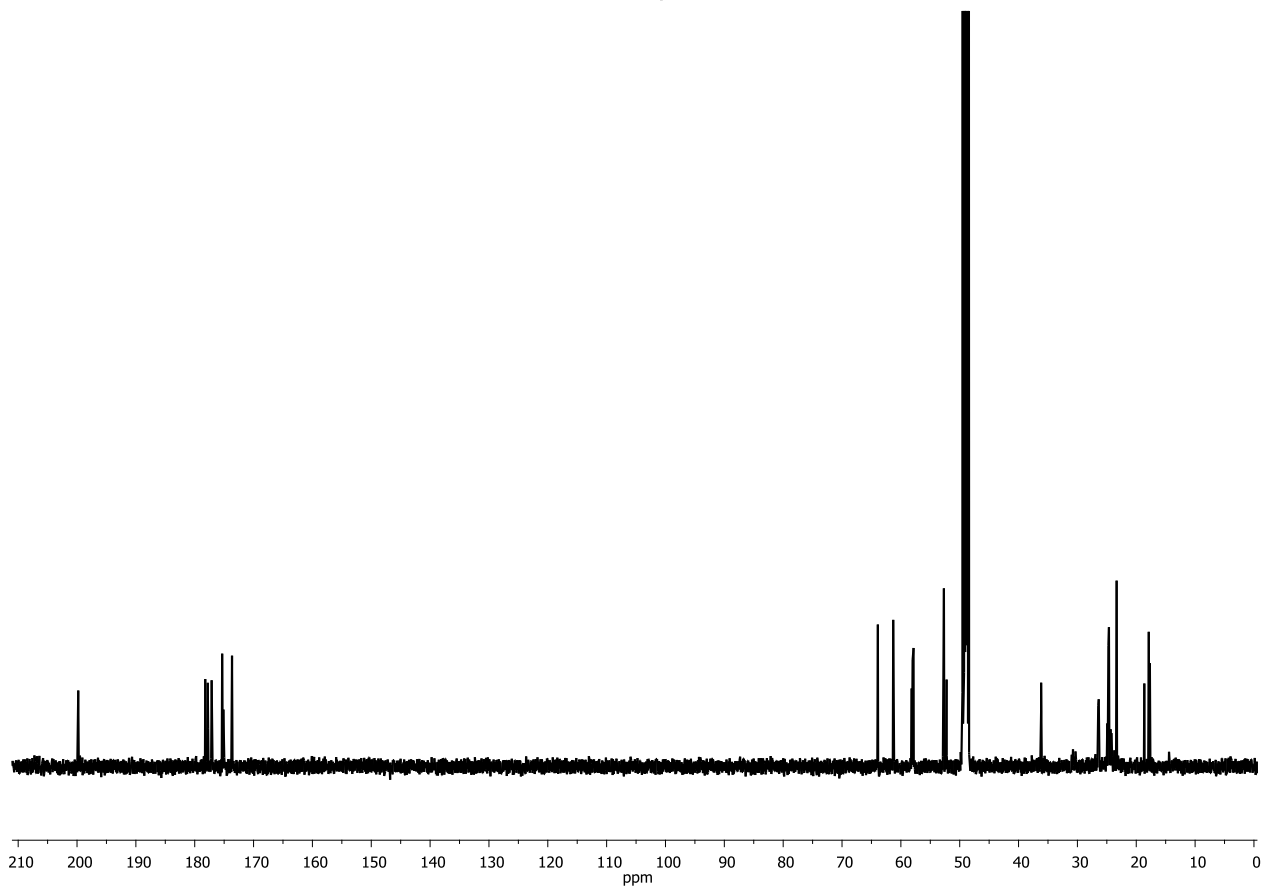
^{13}C NMR spectrum of Ac-Val-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 125 MHz)



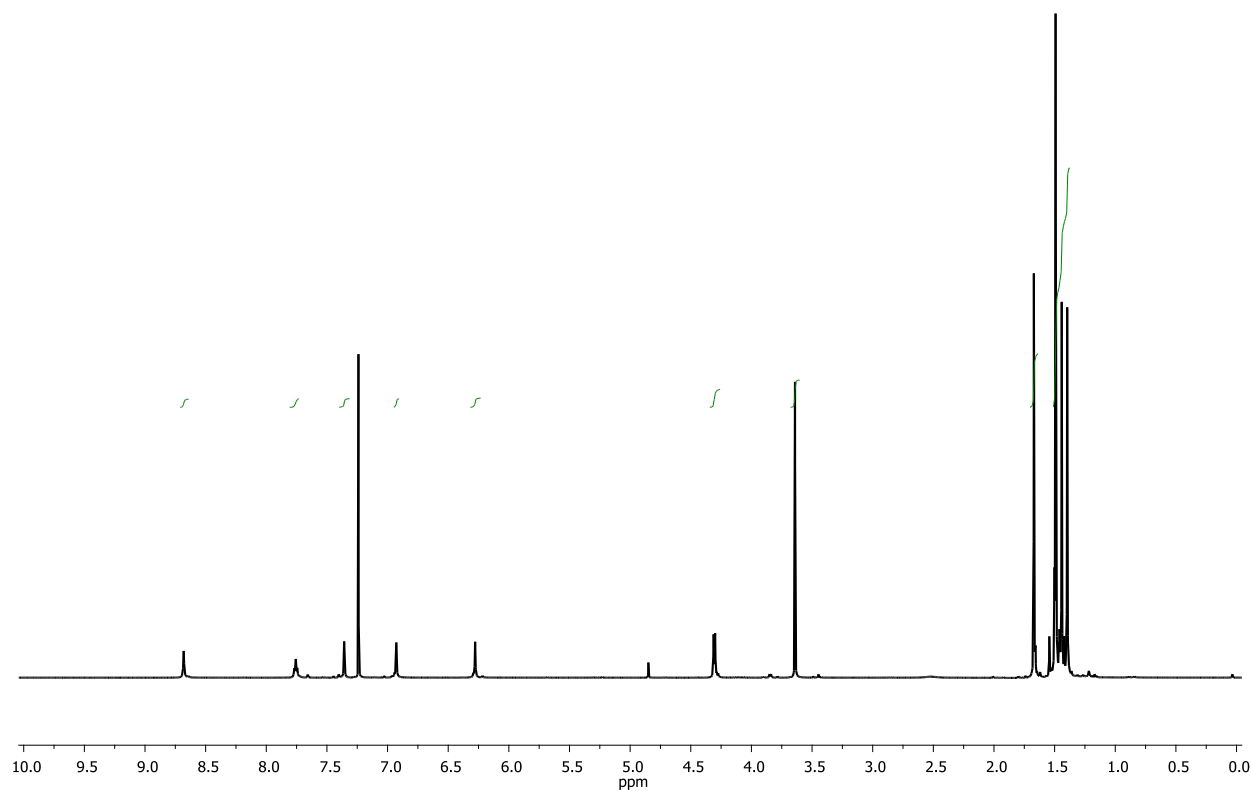
¹H NMR spectrum of Ac-(αMe)Val-Aib₄-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 500 MHz)



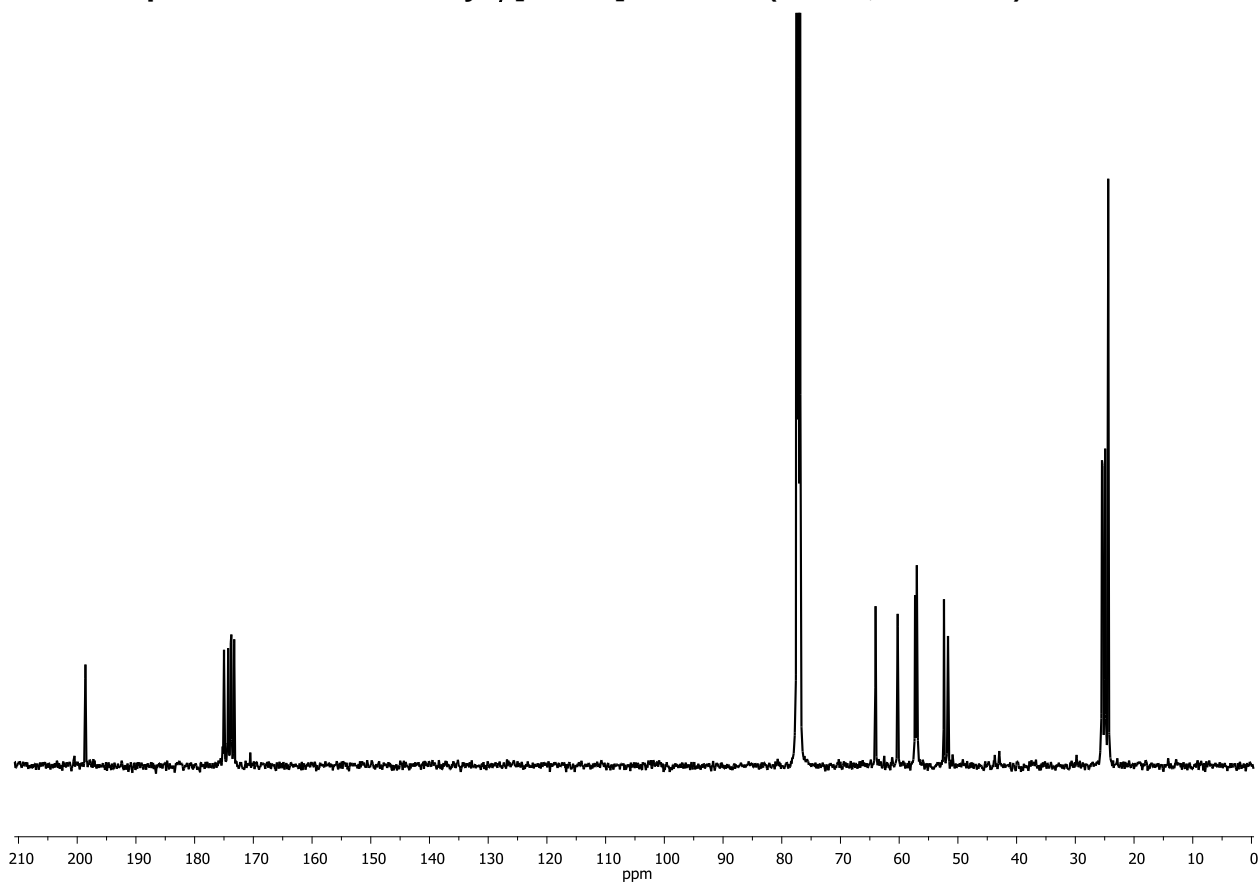
¹³C NMR spectrum of Ac-(αMe)Val-Aib₄-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 125 MHz)



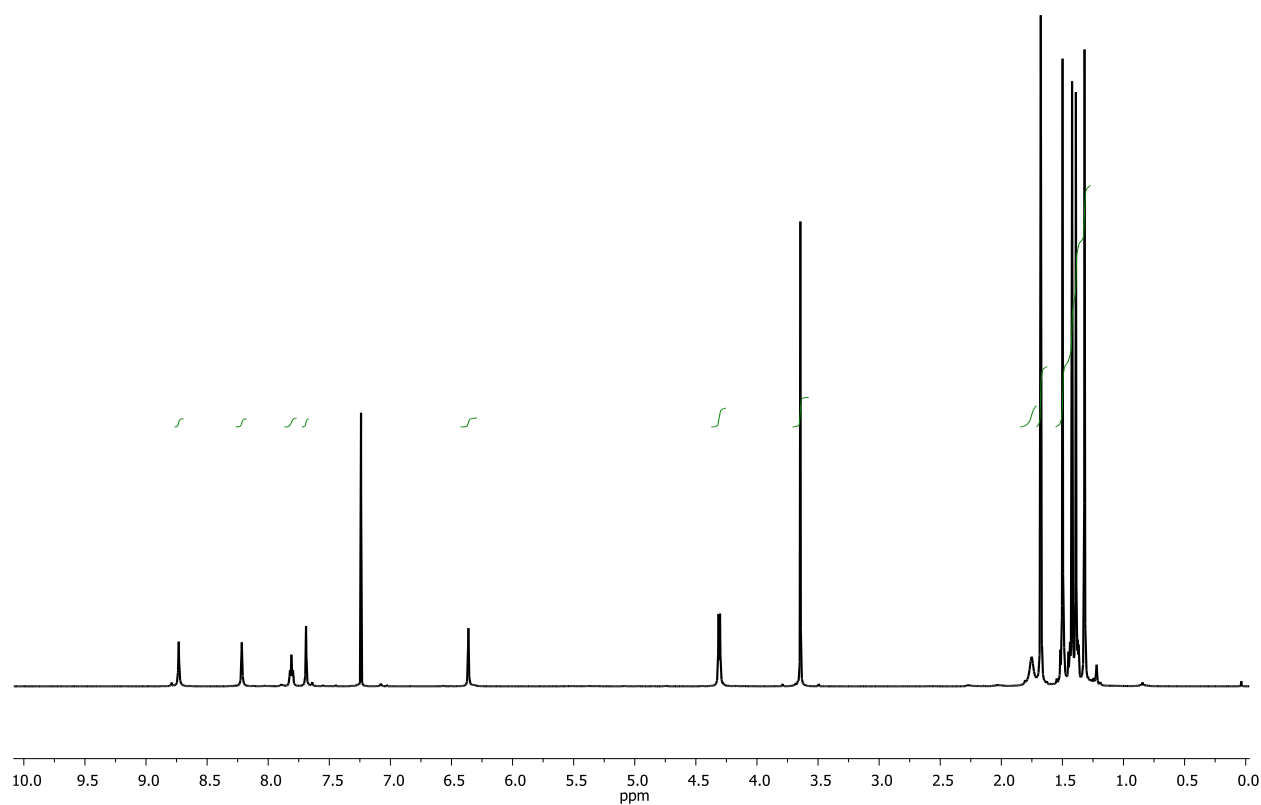
^1H NMR spectrum of $\text{N}_3\text{Aib}_4\text{-Gly-}\psi[\text{CSNH}]\text{Aib-OMe}$ (CDCl_3 , 500 MHz)



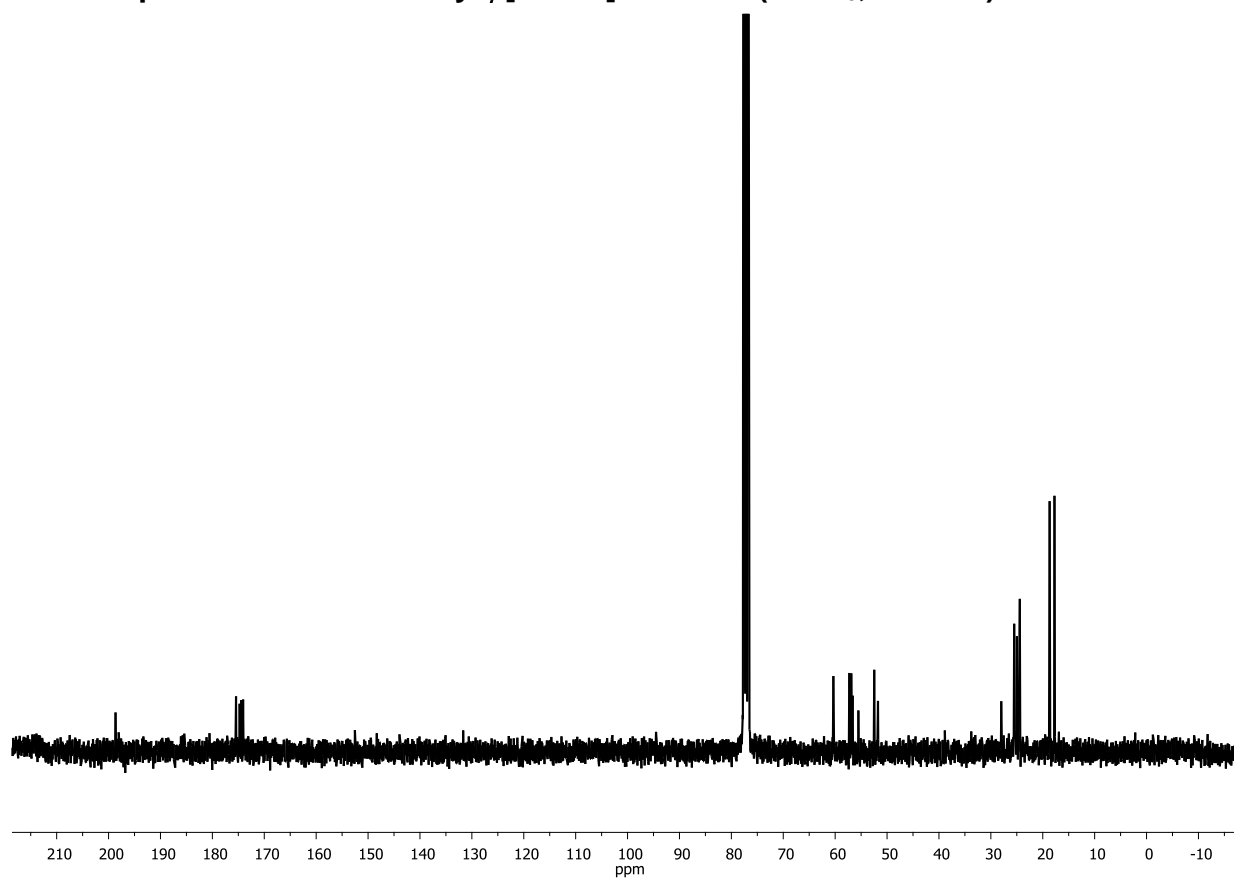
^{13}C NMR spectrum of $\text{N}_3\text{Aib}_4\text{-Gly-}\psi[\text{CSNH}]\text{Aib-OMe}$ (CDCl_3 , 125 MHz)



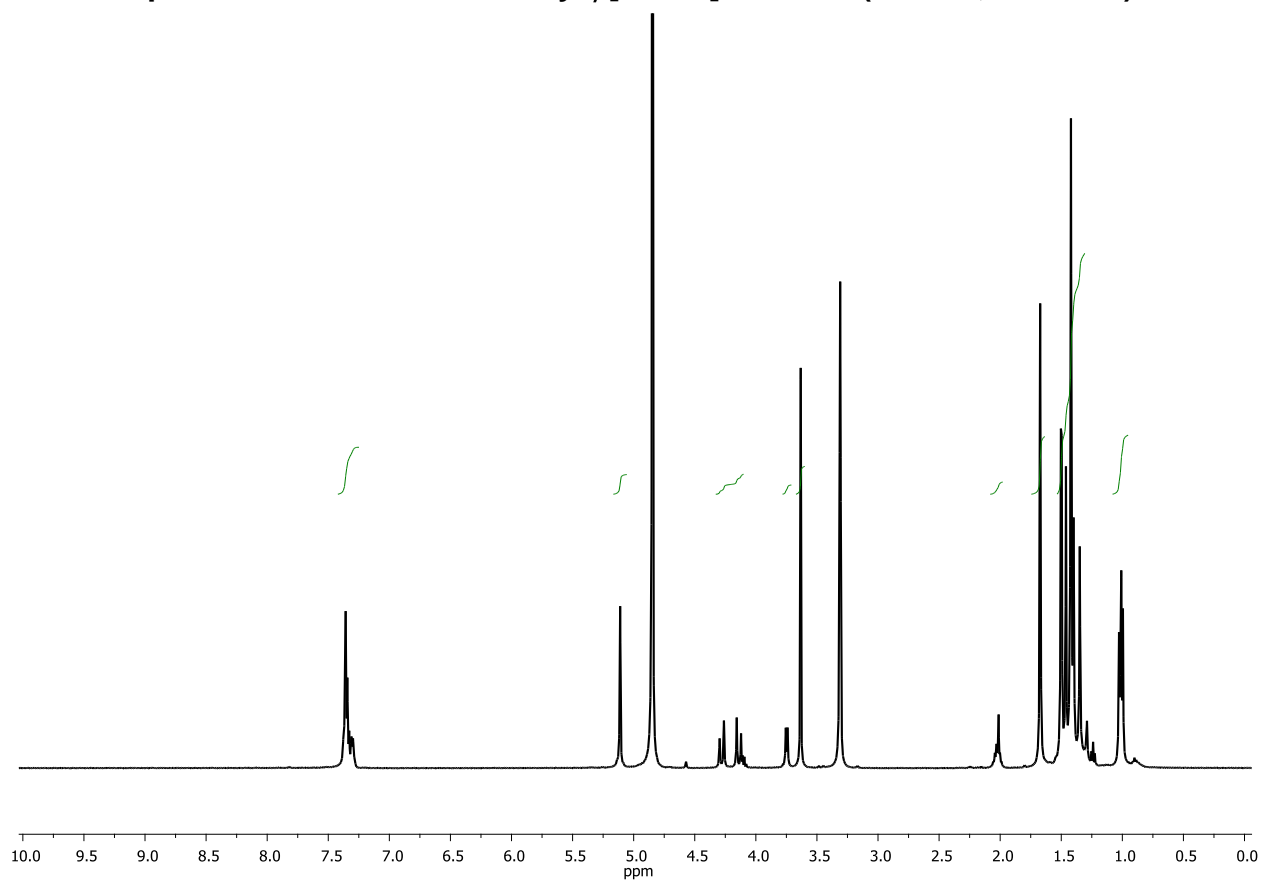
^1H NMR spectrum of H-Aib₄-Gly- ψ [CSNH]Aib-OMe (CDCl₃, 500 MHz)



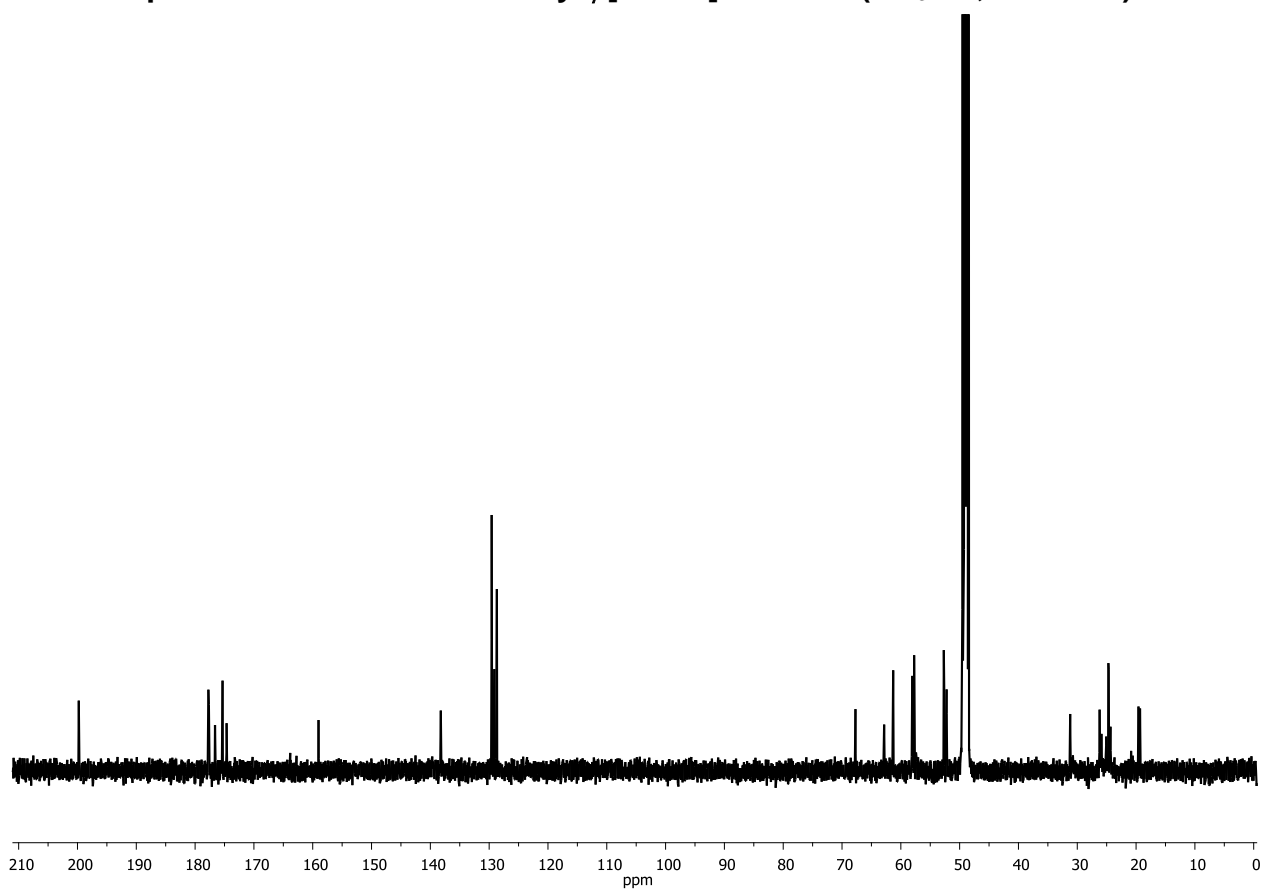
^{13}C NMR spectrum of H-Aib₄-Gly- ψ [CSNH]Aib-OMe (CDCl₃, 75 MHz)



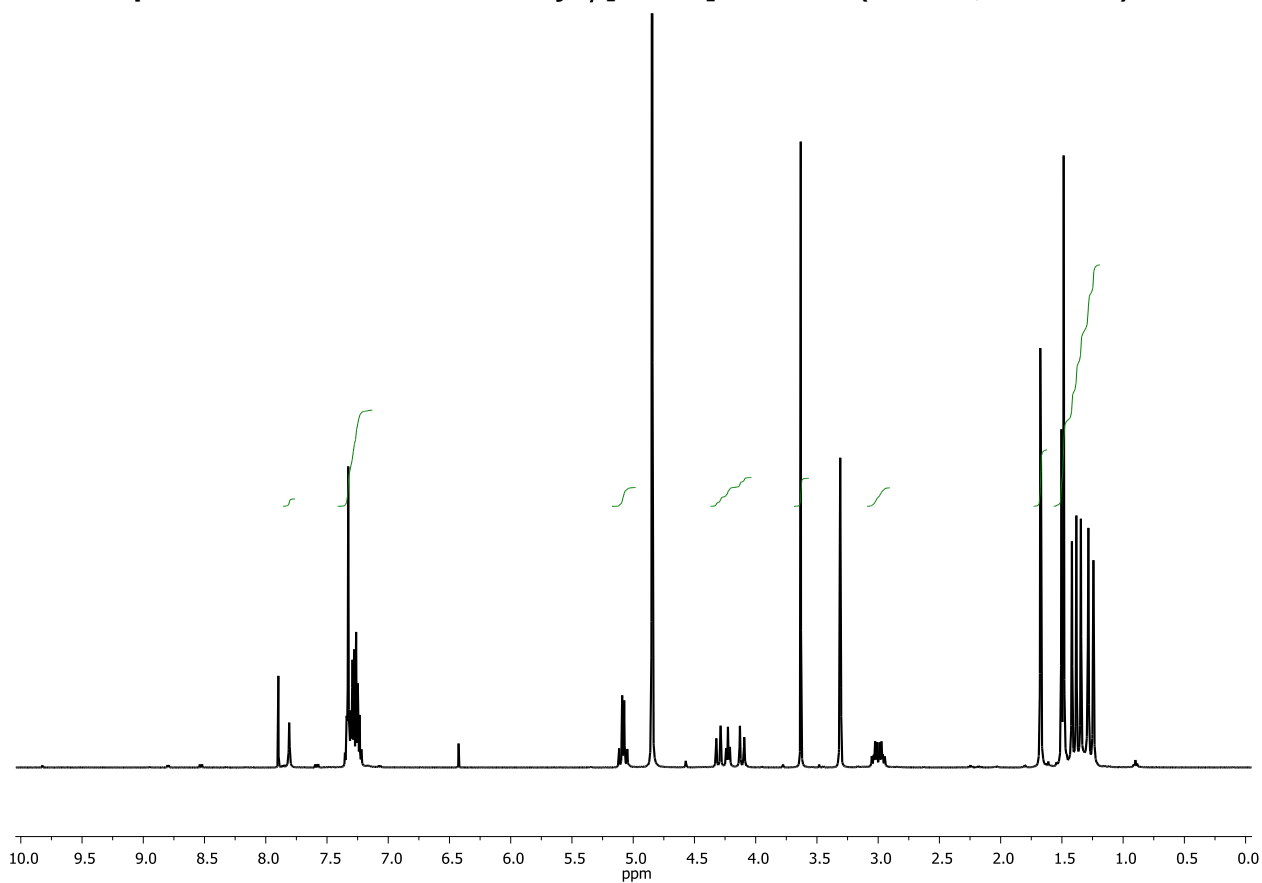
^1H NMR spectrum of Cbz-Val-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 500 MHz)



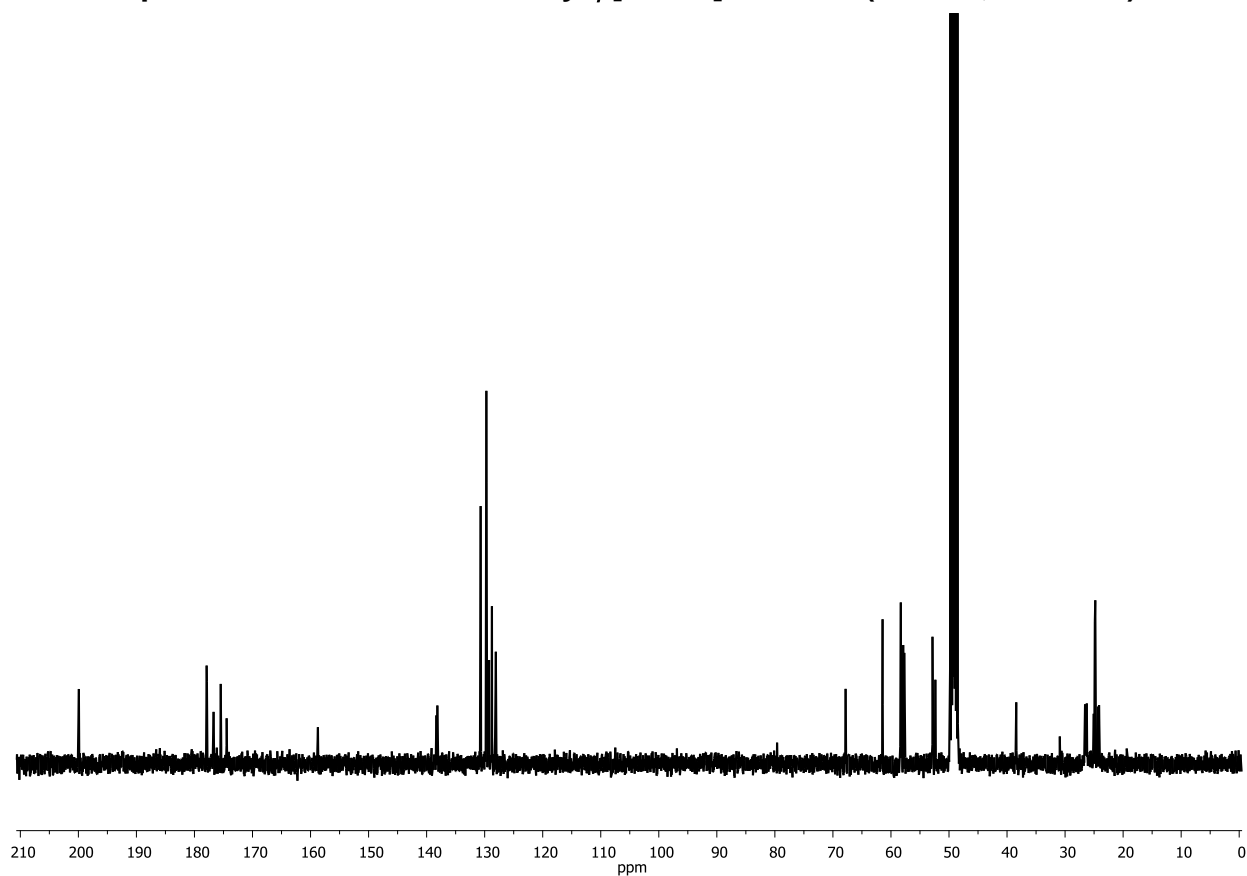
^{13}C NMR spectrum of Cbz-Val-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 125 MHz)



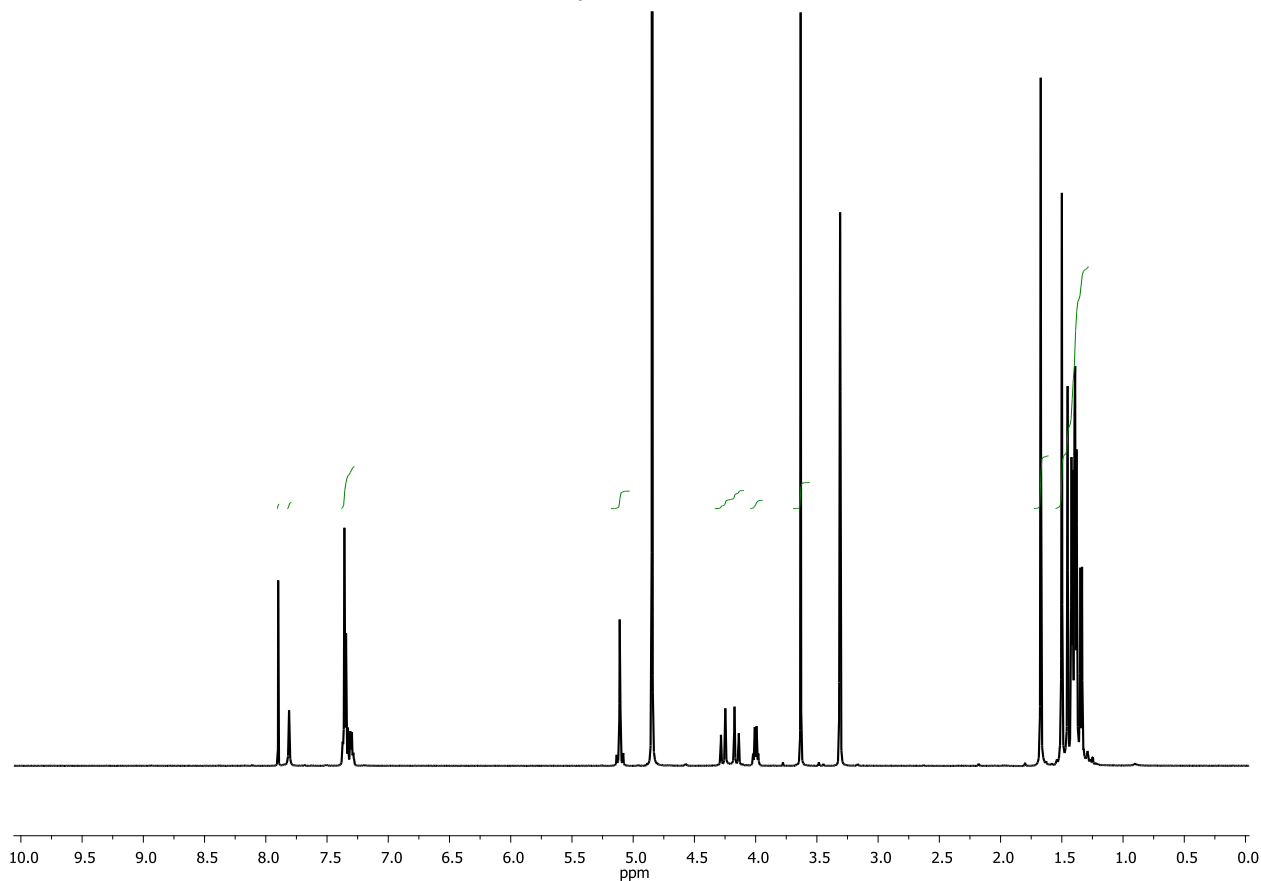
¹H NMR spectrum of Cbz-Phe-Aib₄-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 500 MHz)



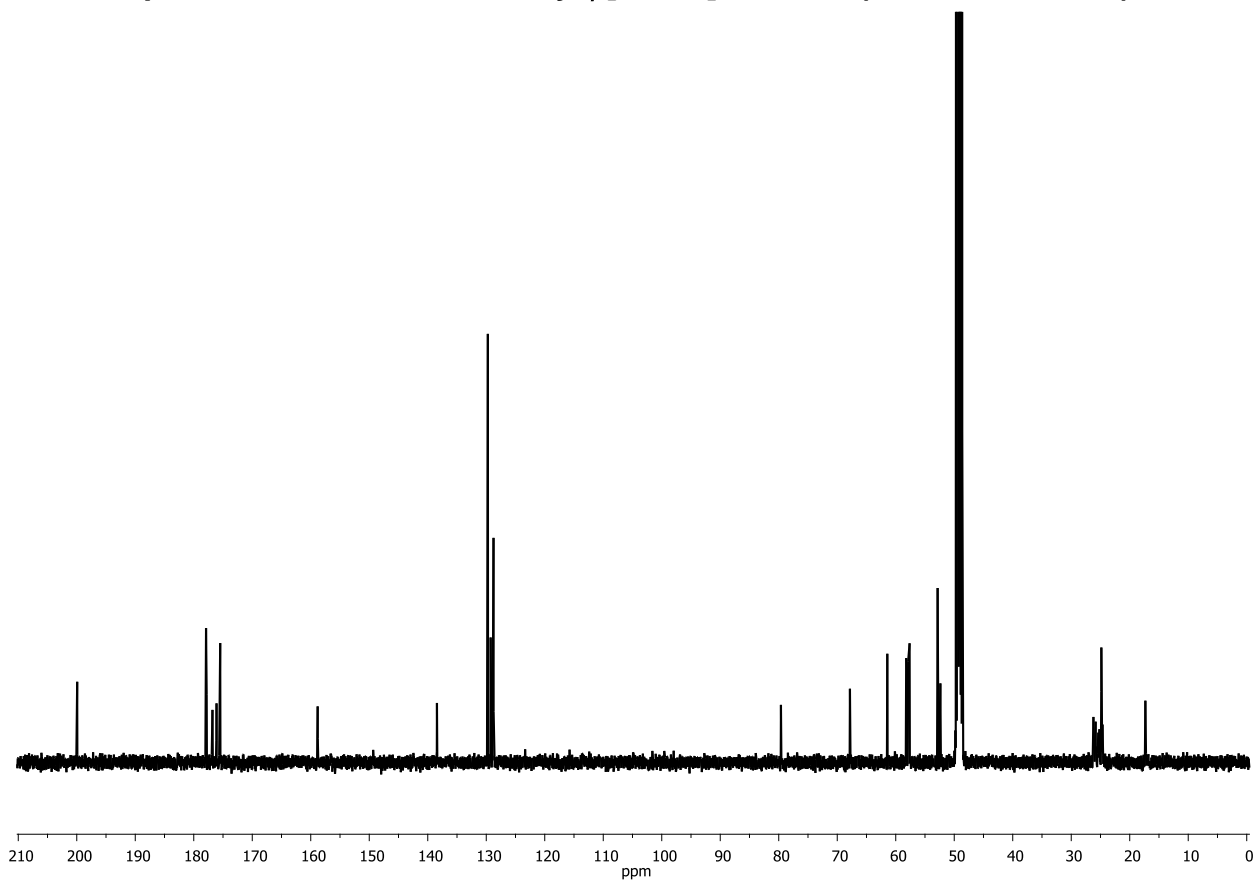
¹³C NMR spectrum of Cbz-Phe-Aib₄-Gly-ψ[CSNH]Aib-OMe (CD₃OD, 125 MHz)



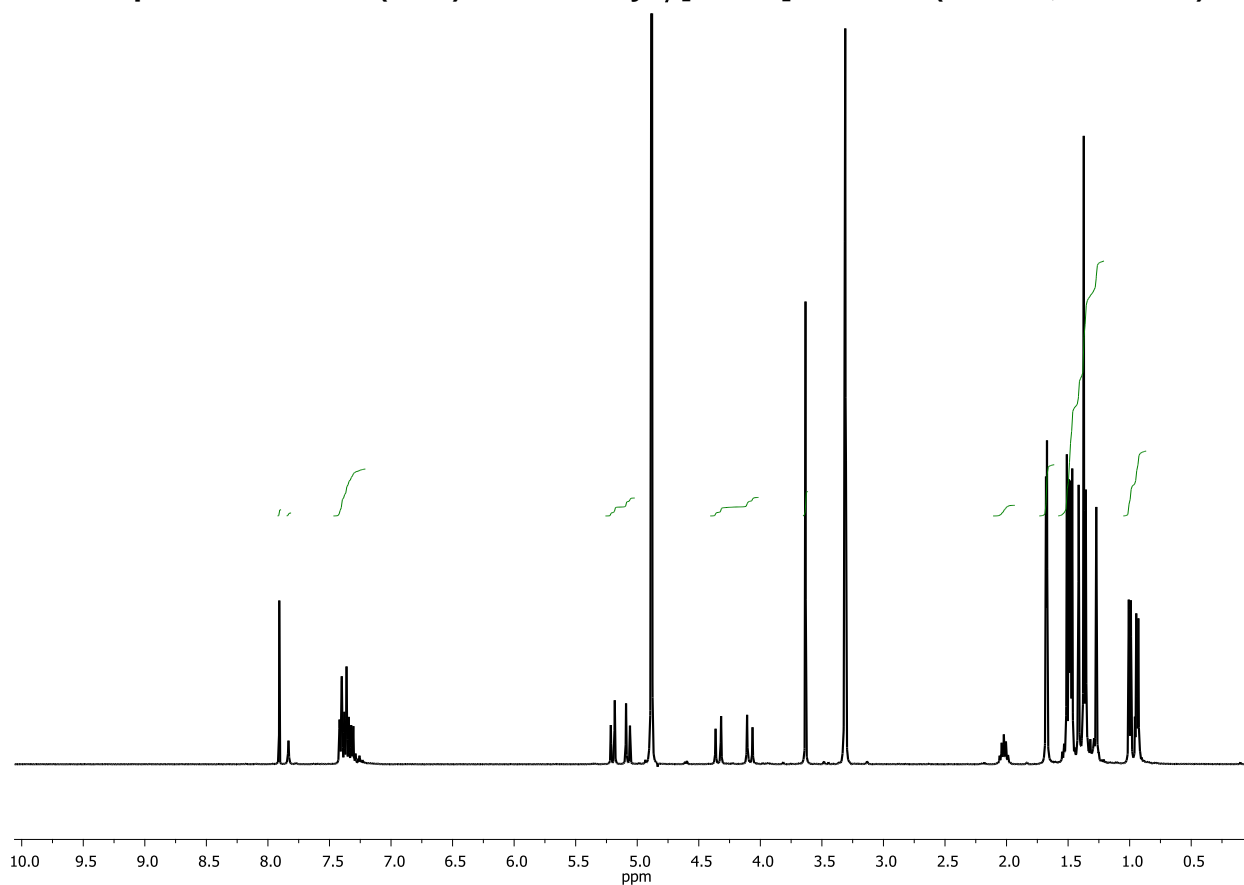
^1H NMR spectrum of Cbz-Ala-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 500 MHz)



^{13}C NMR spectrum of Cbz-Ala-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 125 MHz)



^1H NMR spectrum of Cbz-(α Me)Val-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 500 MHz)



^{13}C NMR spectrum of Cbz-(α Me)Ala-Aib₄-Gly- ψ [CSNH]Aib-OMe (CD₃OD, 125 MHz)

