

A New Synthesis of Cystamine Modified Eu³⁺ DOTAM-Gly-Phe-OH: A Conjugation Ready Temperature Sensitive MRI Contrast Agent

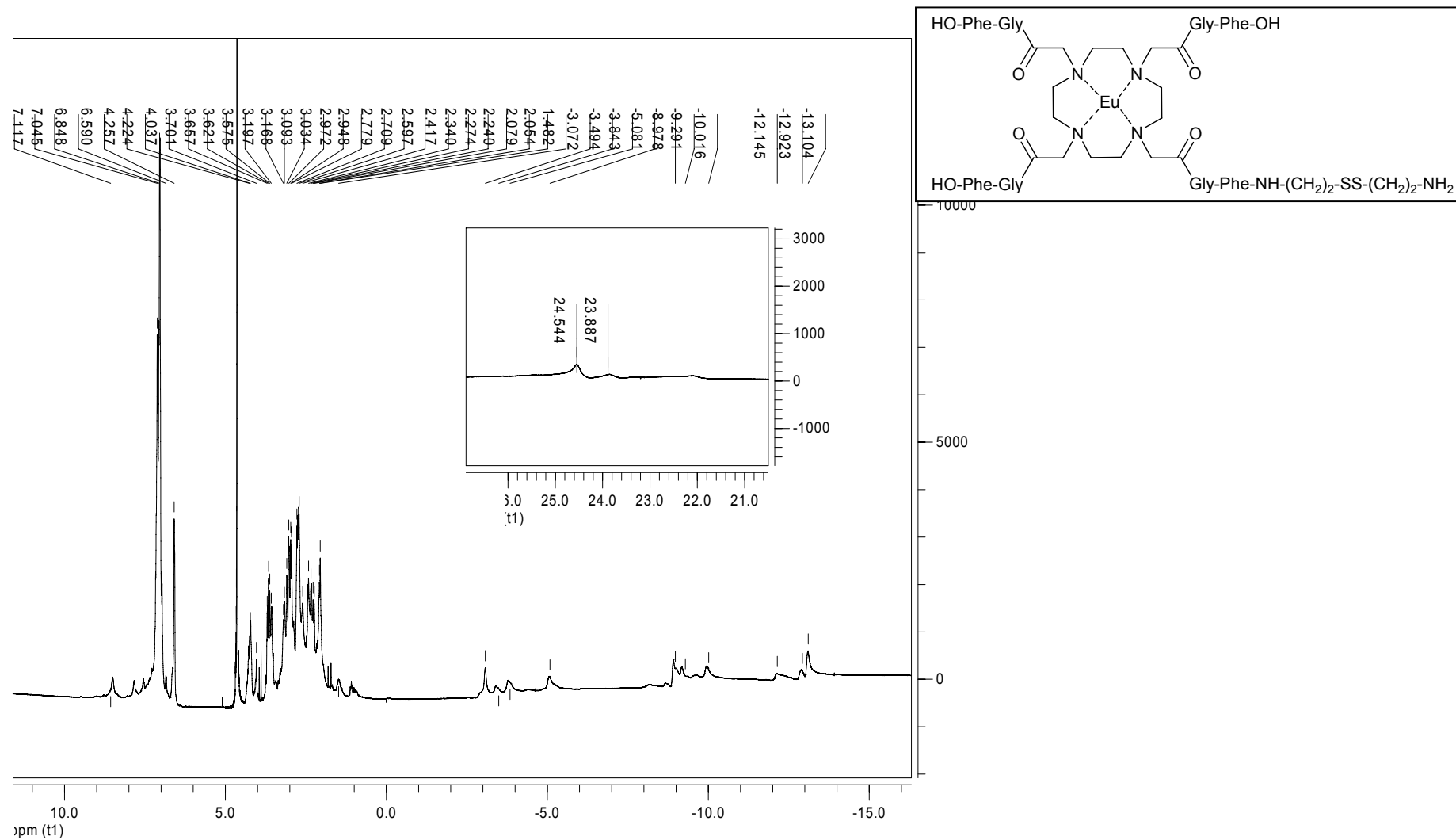
Mojmír Suchý, Alex X. Li, Robert Bartha and Robert H. E. Hudson

(Electronic supplementary information)

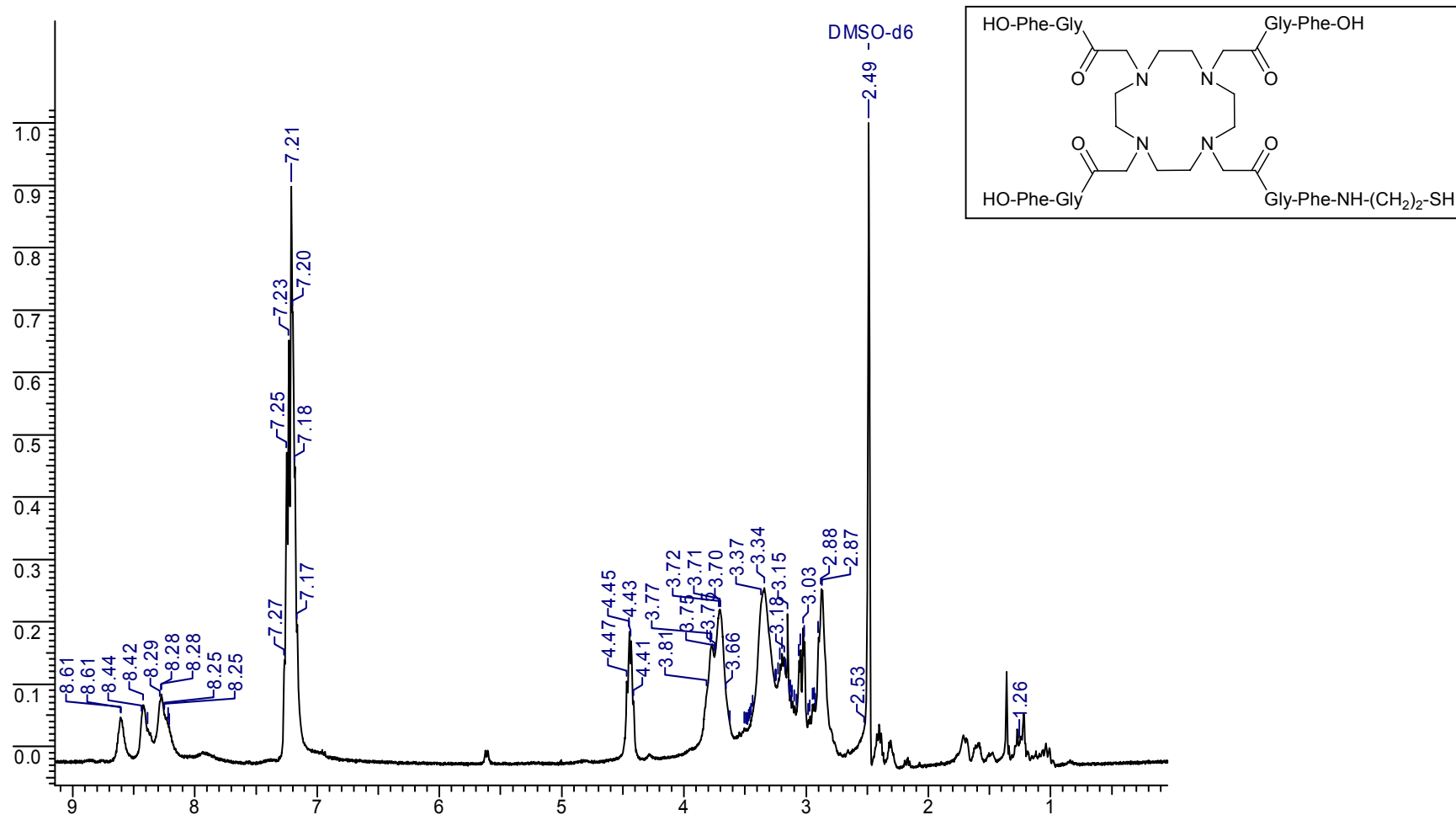
¹H NMR spectra of compounds **4a**, **5a**, **5b**, **8**, **11**, **12a**, **12b** and **18-22**

¹³C NMR spectra of compounds **8**, **11**, **12a**, **12b** and **20**

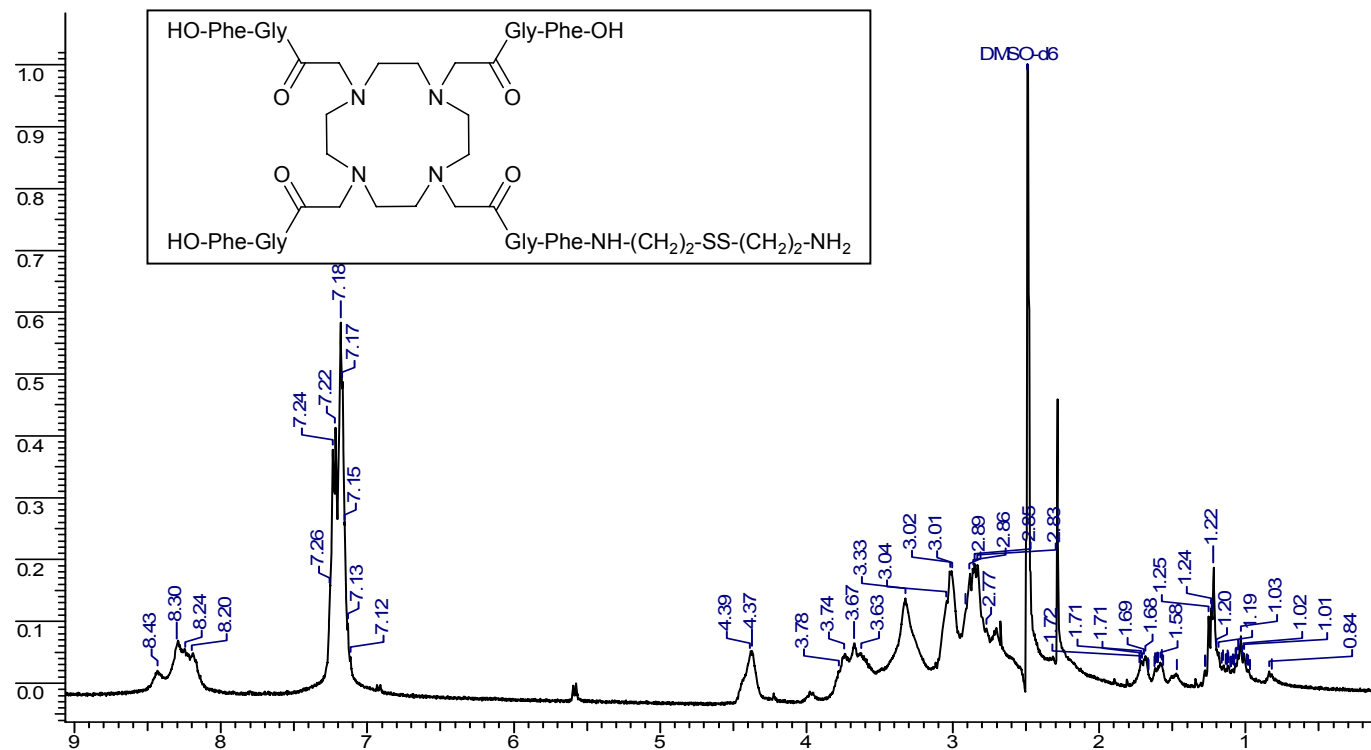
Eu³⁺ monoacetyl-Gly-Phe-cystamine-triacetyl-Gly-Phe-OH cyclen (**4a**) ¹H NMR spectrum in D₂O



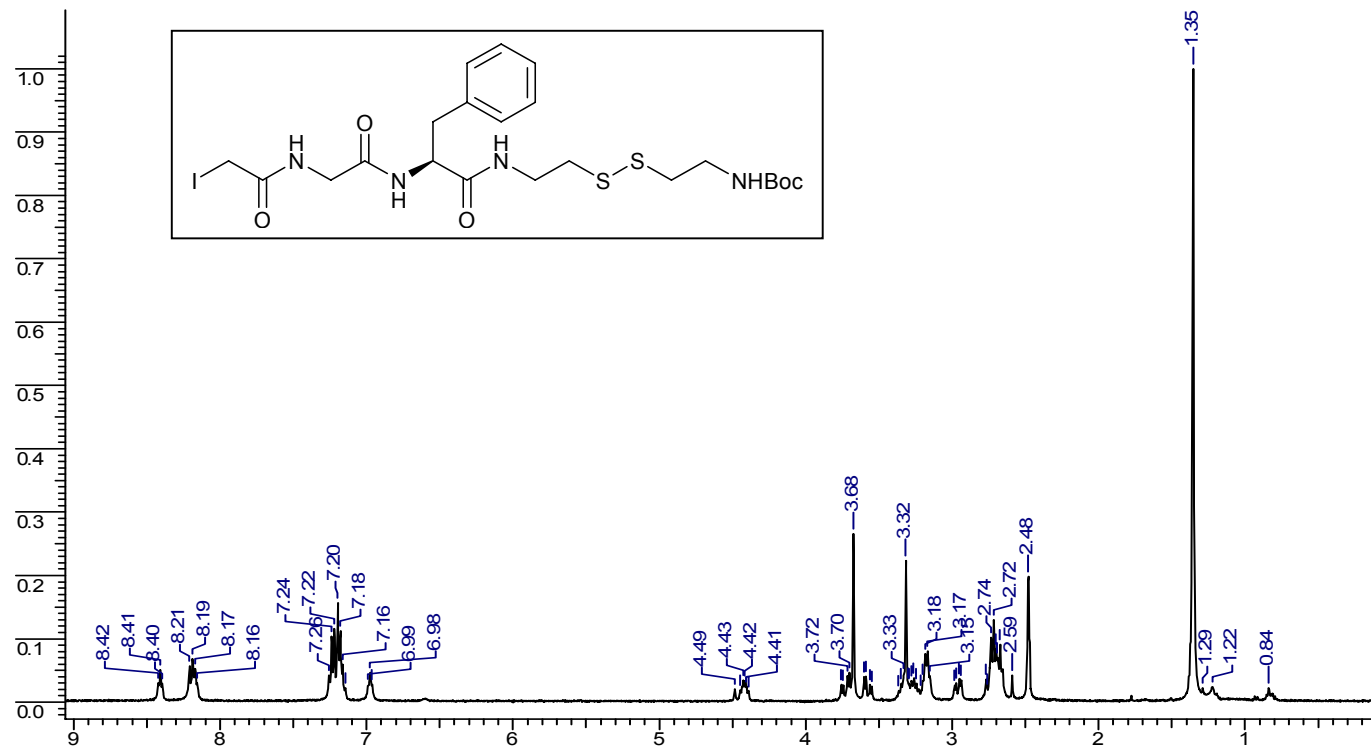
Monoacetyl-Gly-Phe-NH(CH₂)₂SH-triacetyl-Gly-Phe-OH cyclen (**5a**) ¹H NMR spectrum in DMSO-D₆



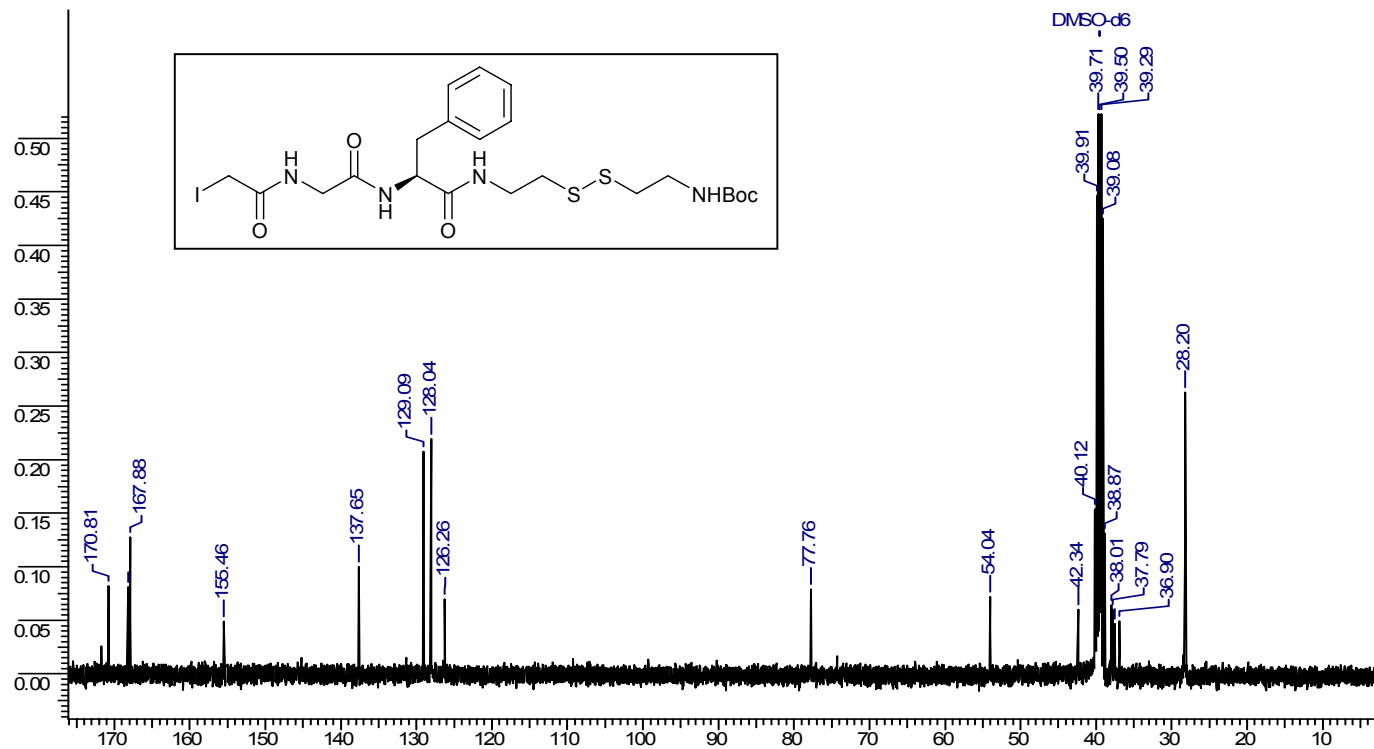
Monoacetyl-Gly-Phe-cystamine-triacetyl-Gly-Phe-OH cyclen (**5b**) ¹H NMR spectrum in DMSO-D₆



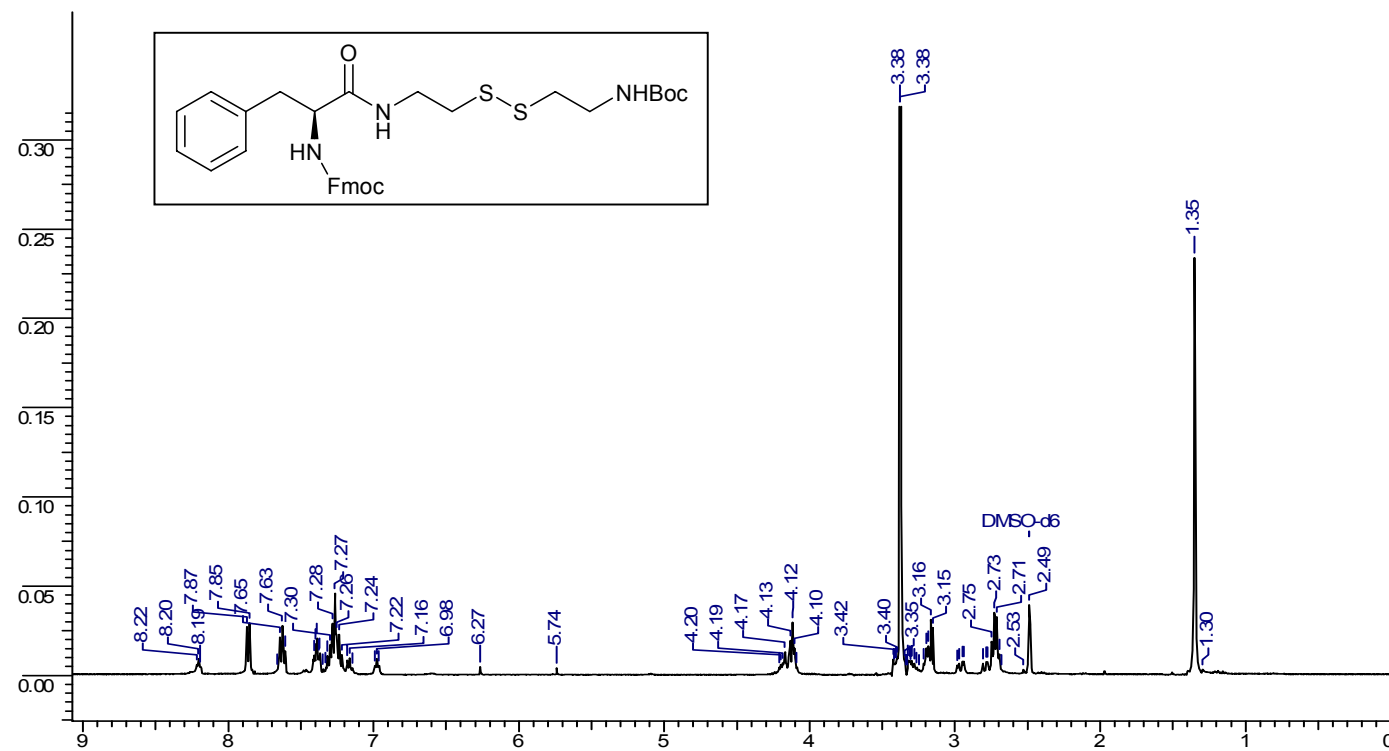
N-Iodoacetyl-Gly-Phe-cystamine(Boc) (**8**) ^1H NMR spectrum in $\text{DMSO}-\text{D}_6$



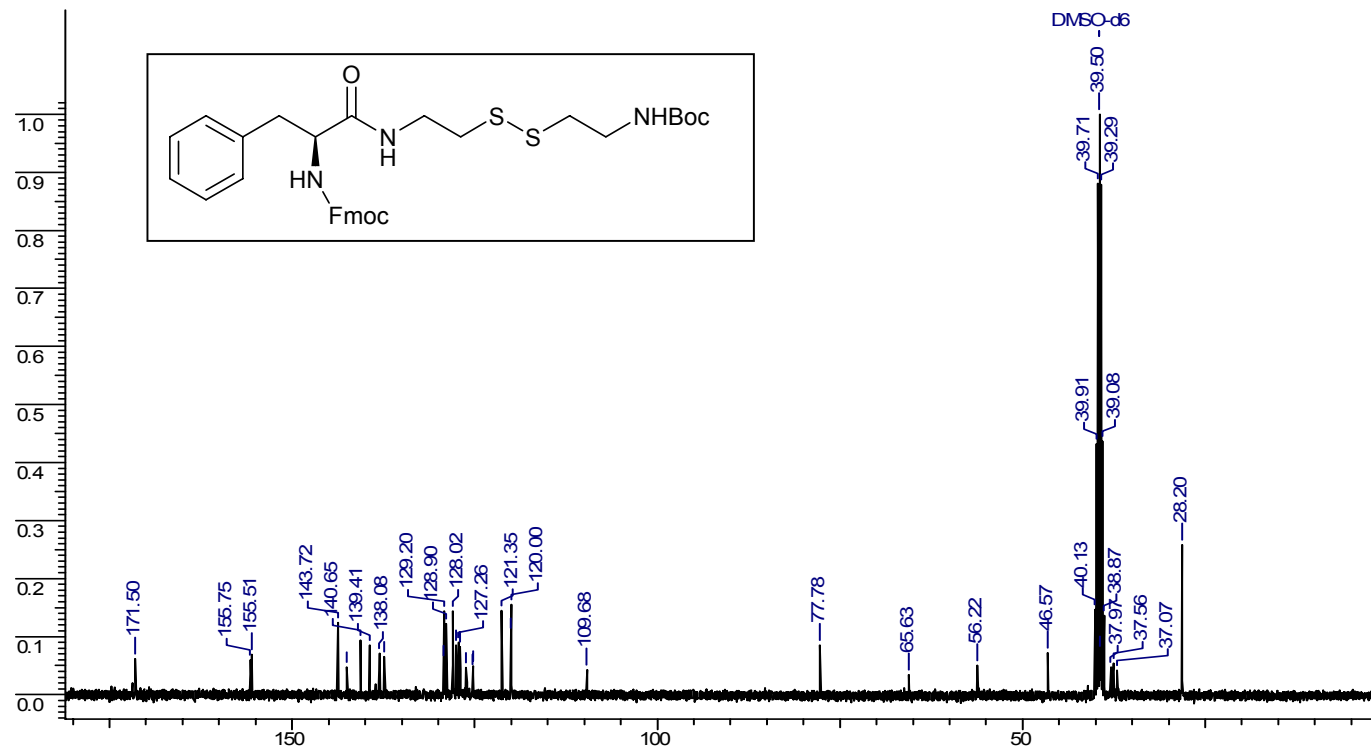
N-Iodoacetyl-Gly-Phe-cystamine(Boc) (**8**) ^{13}C NMR spectrum in $\text{DMSO-}d_6$



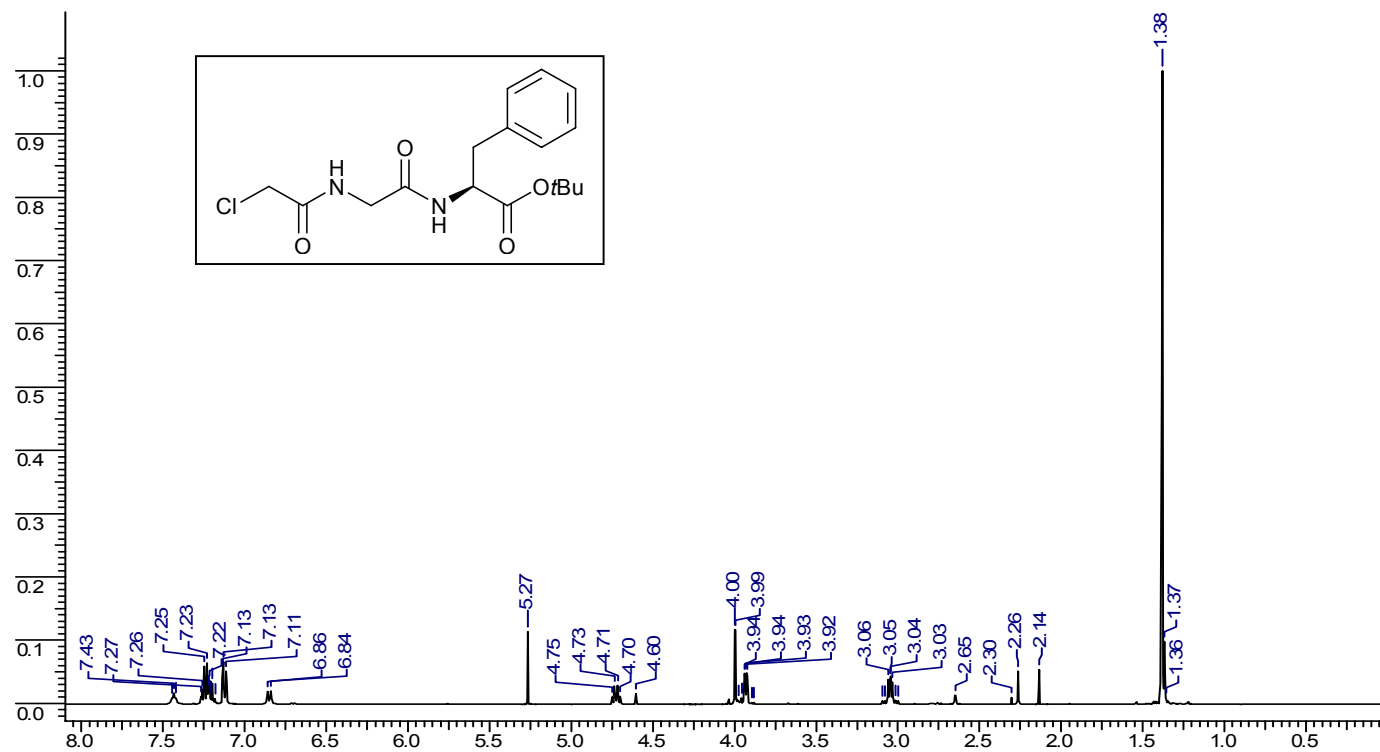
Fmoc-Phe-cystamine(Boc) (**11**) ^1H NMR spectrum in $\text{DMSO}-\text{D}_6$



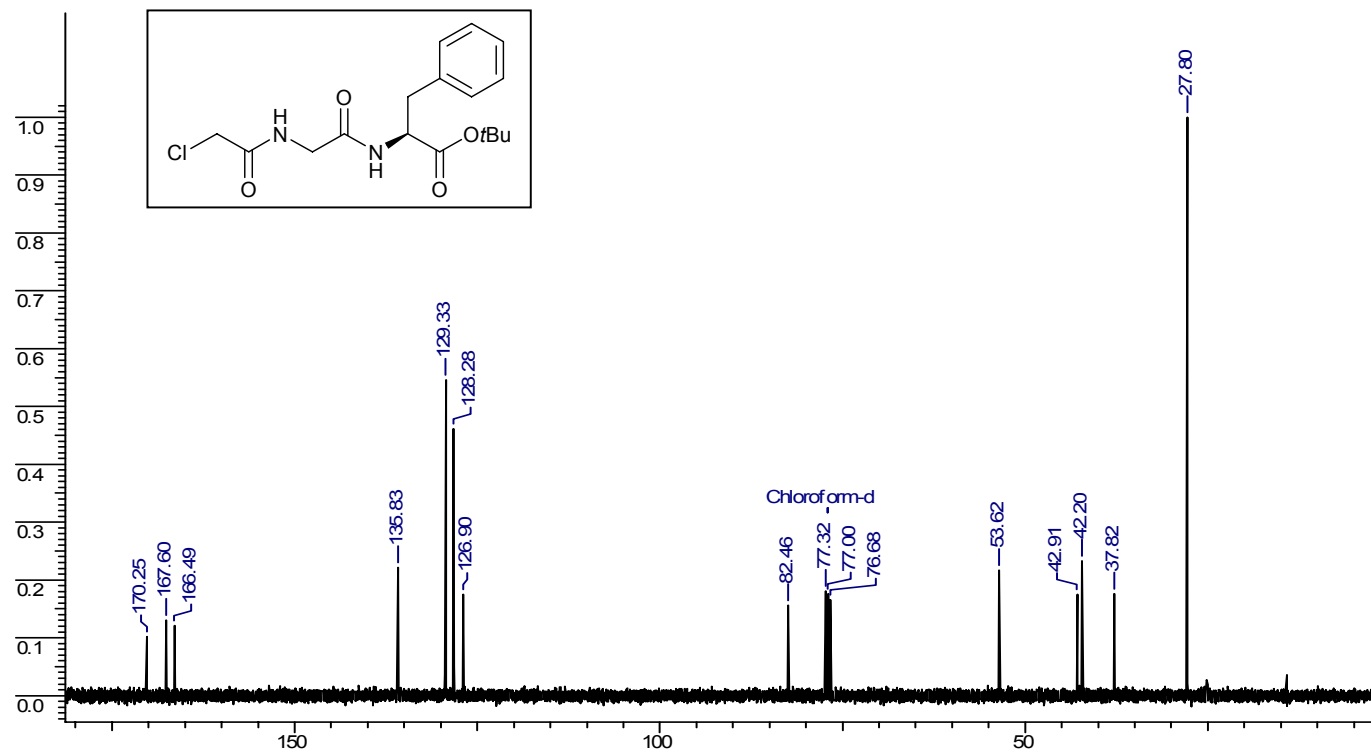
Fmoc-Phe-cystamine(Boc) (**11**) ^{13}C NMR spectrum in DMSO- D_6



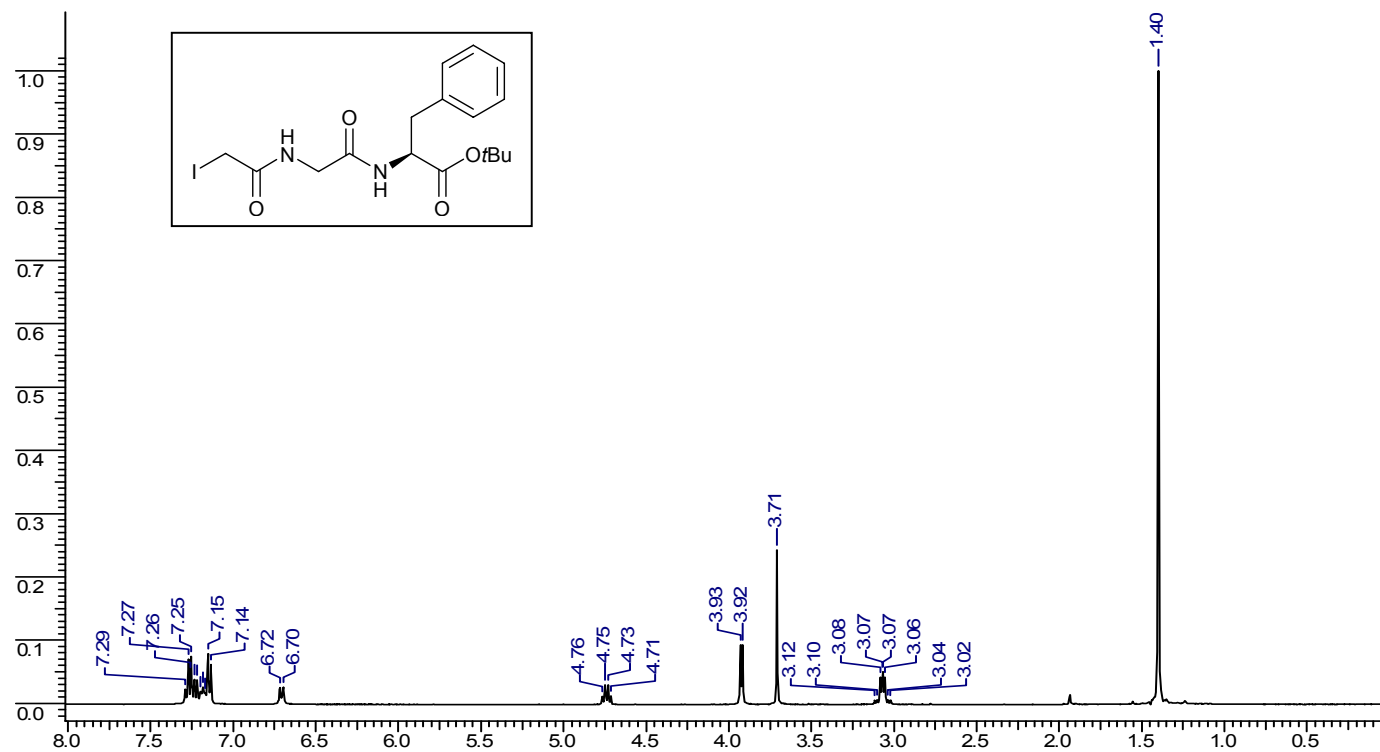
N-Chloroacetyl-Gly-Phe-*O**t*Bu (**12a**) ^1H NMR spectrum in CDCl_3



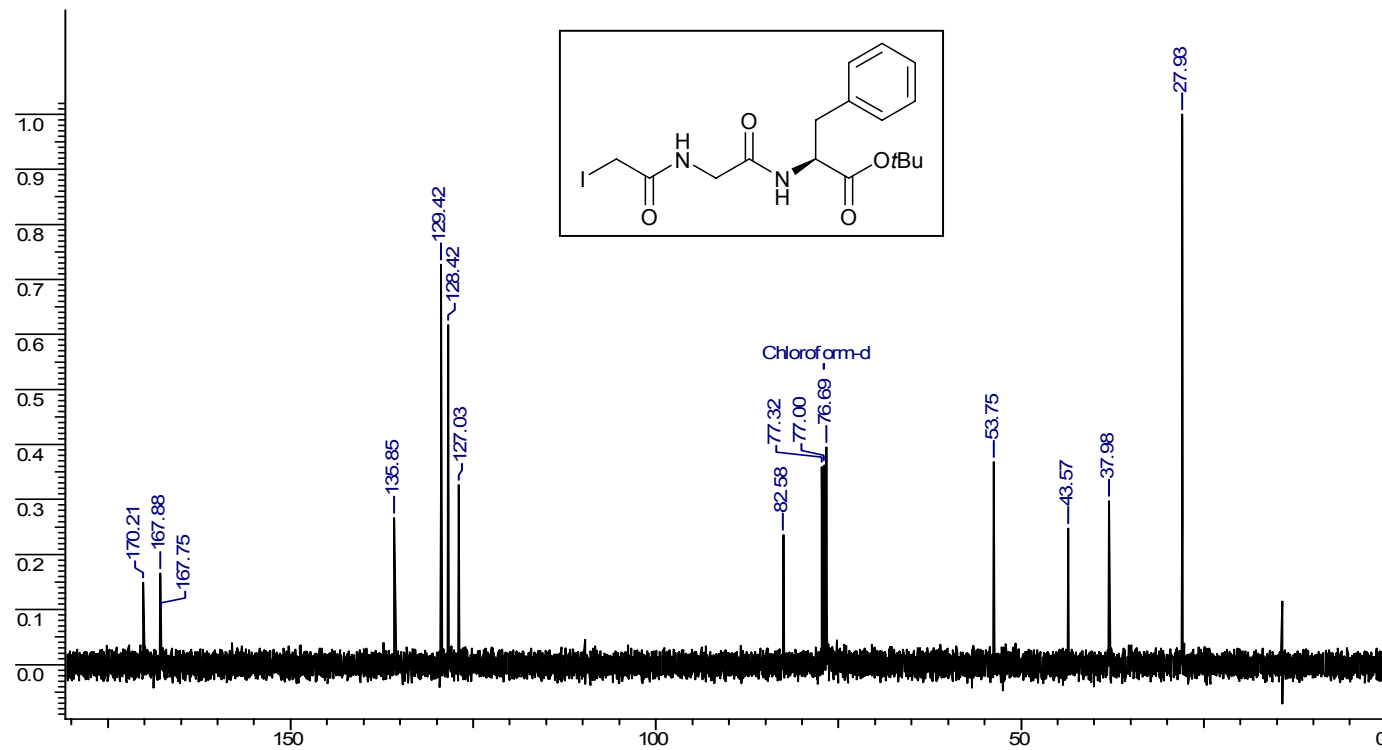
N-Chloroacetyl-Gly-Phe-*O**t*Bu (**12a**) ^{13}C NMR spectrum in CDCl_3



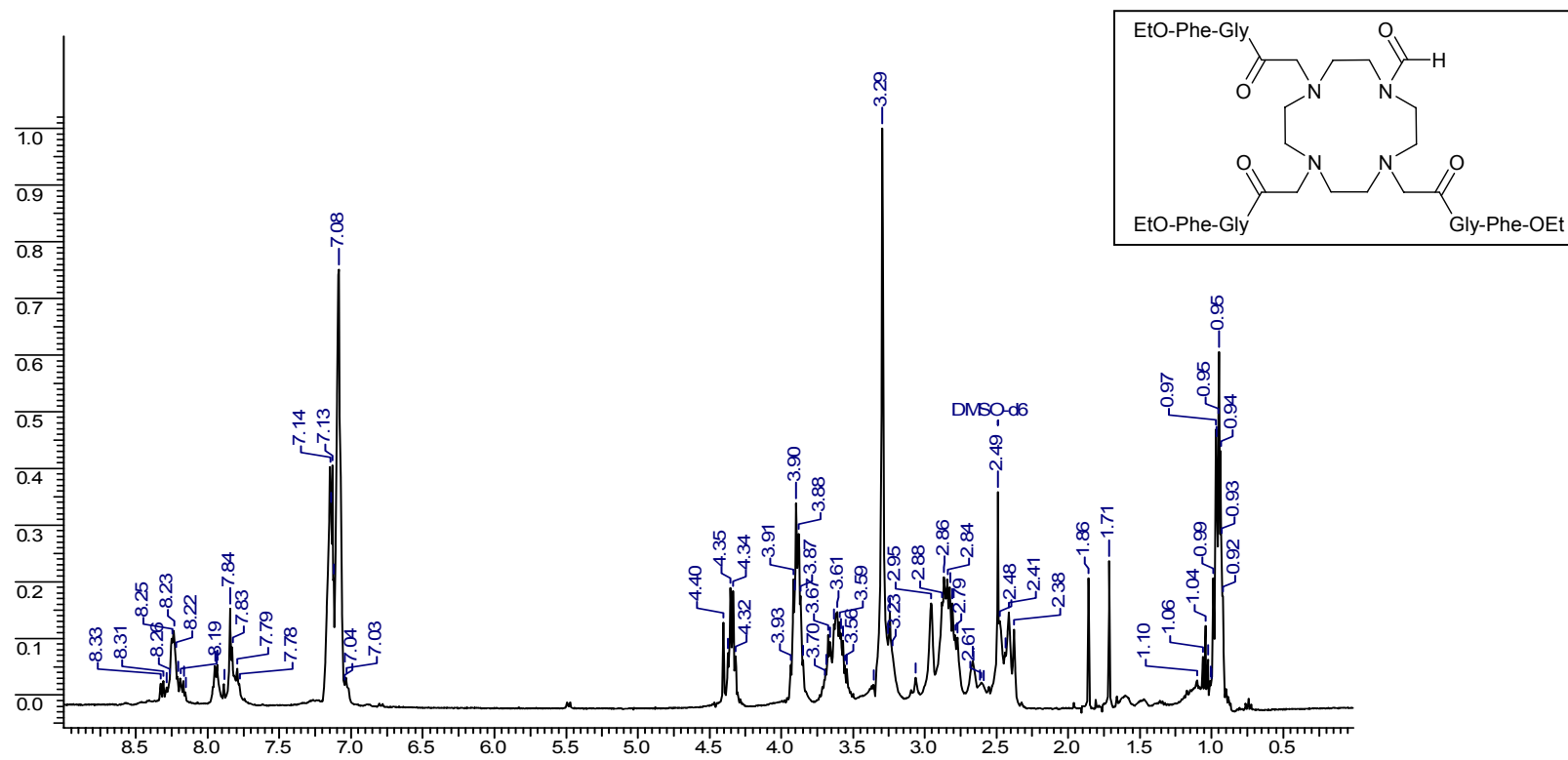
N-Iodoacetyl-Gly-Phe-*O**t*Bu (**12b**) ^1H NMR spectrum in CDCl_3



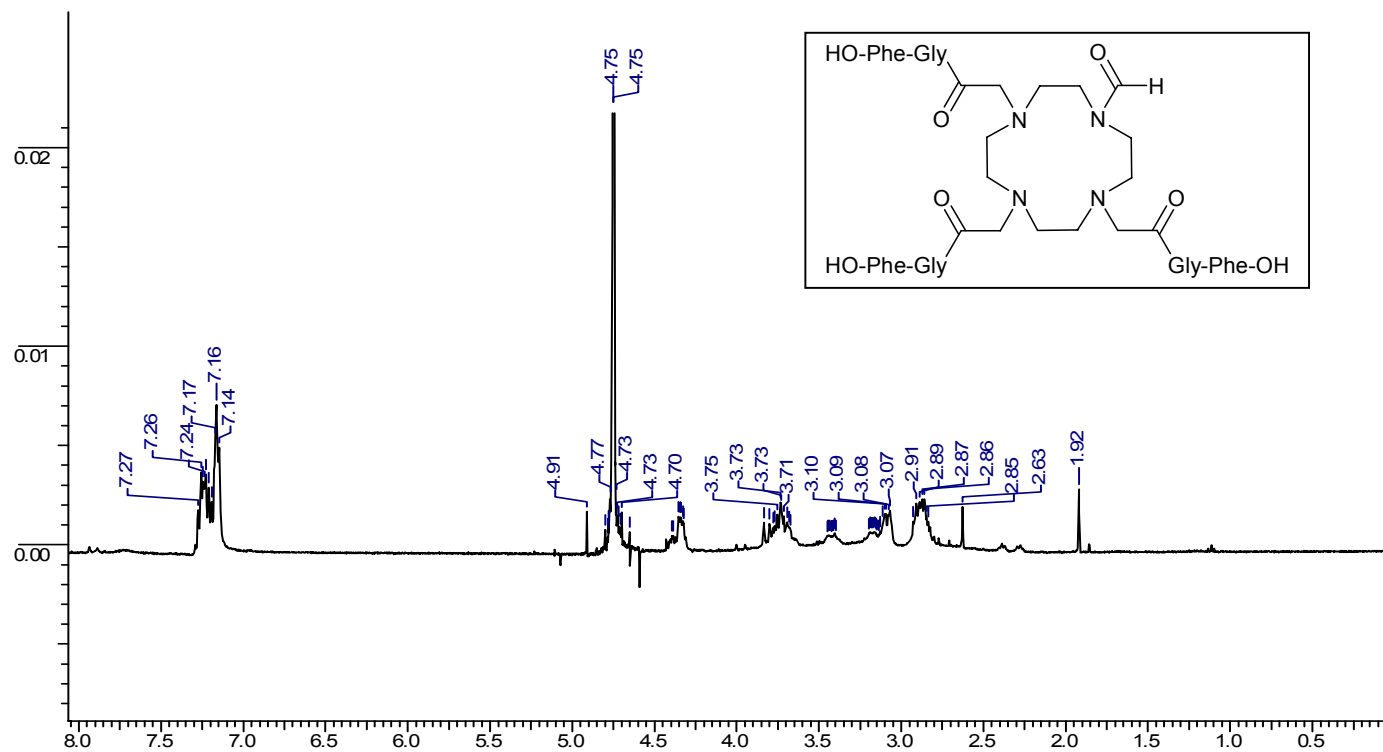
N-Iodoacetyl-Gly-Phe-*O**t*Bu (**12b**) ^{13}C NMR spectrum in CDCl_3



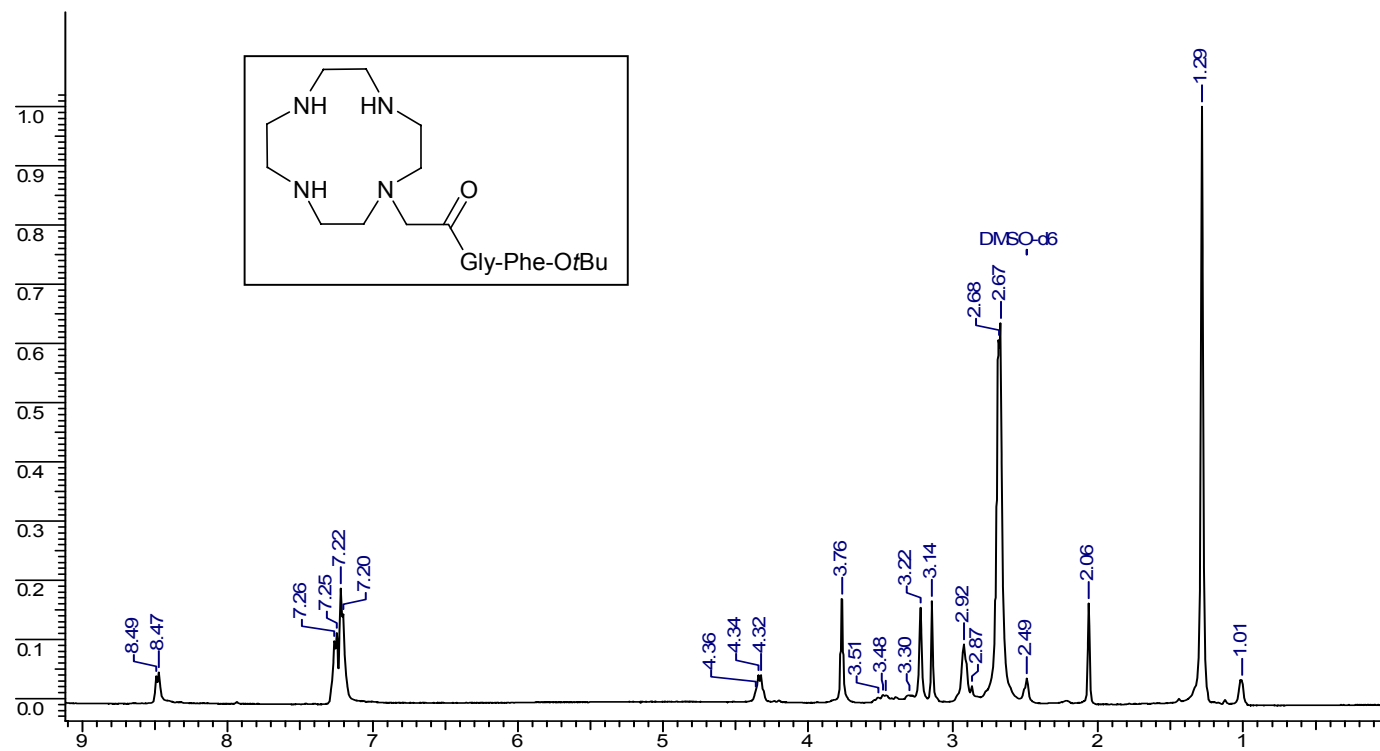
Formyl-triacetyl-Gly-Phe-OEt cyclen (**18**) ^1H NMR spectrum in $\text{DMSO-}D_6$



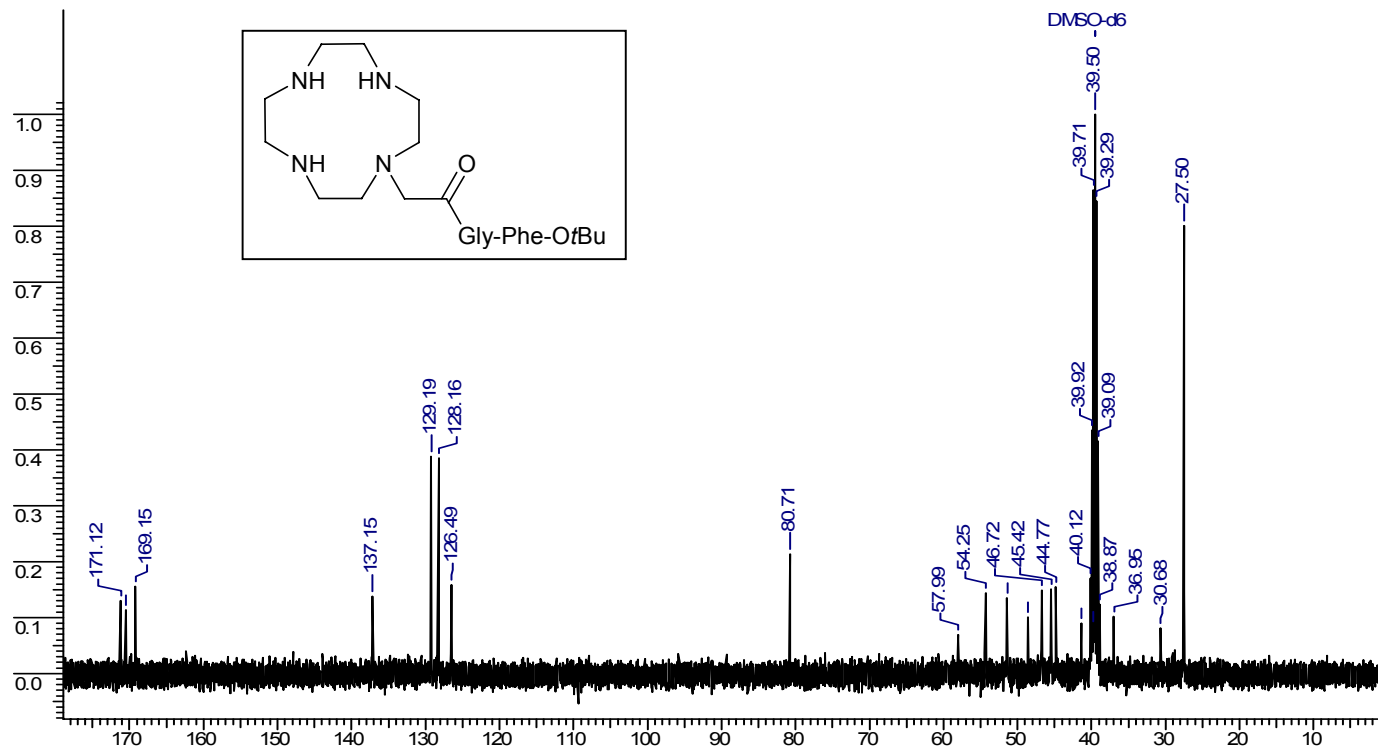
Formyl-triacetyl-Gly-Phe-OH cyclen (**19**) ^1H NMR spectrum in D_2O



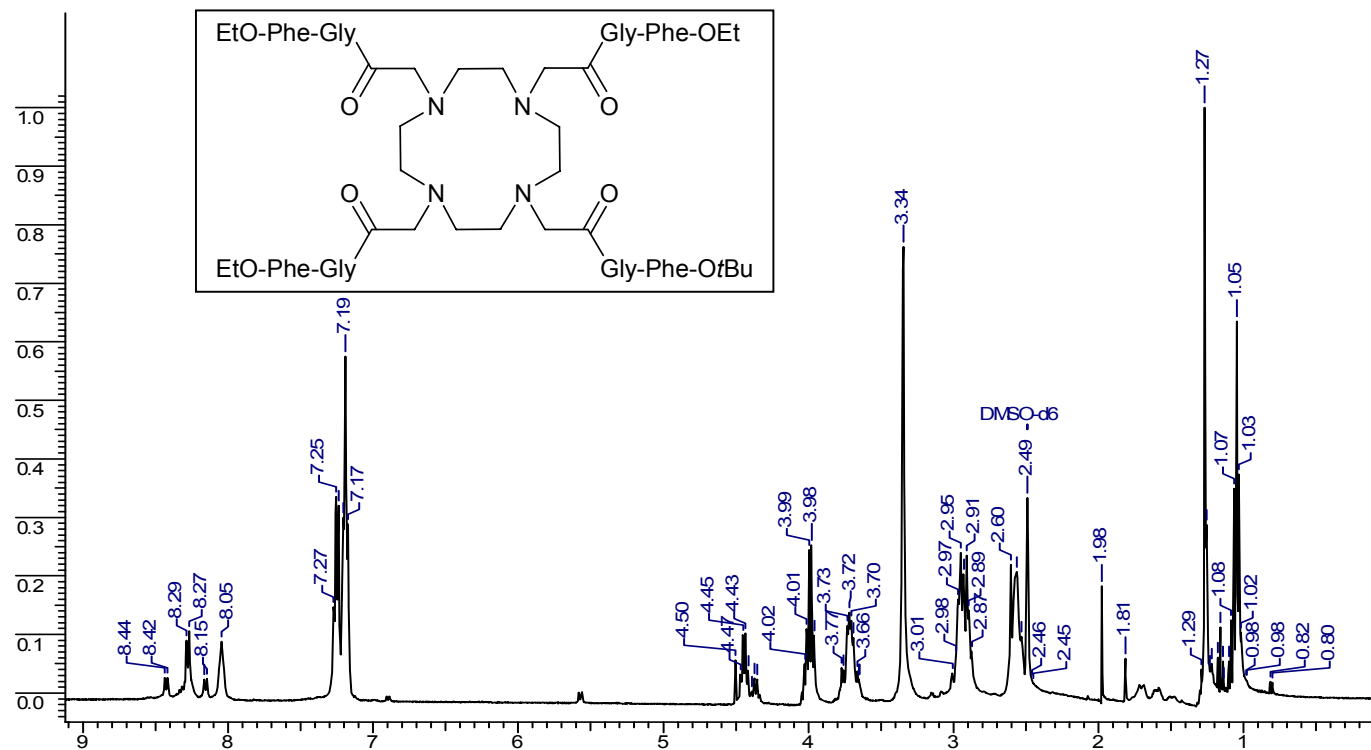
Monoacetyl-Gly-Phe-*O*tBu cyclen (**20**) ¹H NMR spectrum in DMSO-D₆



Monoacetyl-Gly-Phe-OfBu cyclen (**20**) ^{13}C NMR spectrum in DMSO- D_6



Monoacetyl-Gly-Phe-O t Bu-triacetyl-Gly-Phe-OEt cyclen (**21**) ^1H NMR spectrum in DMSO- D_6



Monoacetyl-Gly-Phe-cystamine(Boc)-triacetyl-Gly-Phe-OEt cyclen (**22**) ¹H NMR spectrum in DMSO-D₆

