A Cyclic Peptide Mimetic of Damaged Collagen

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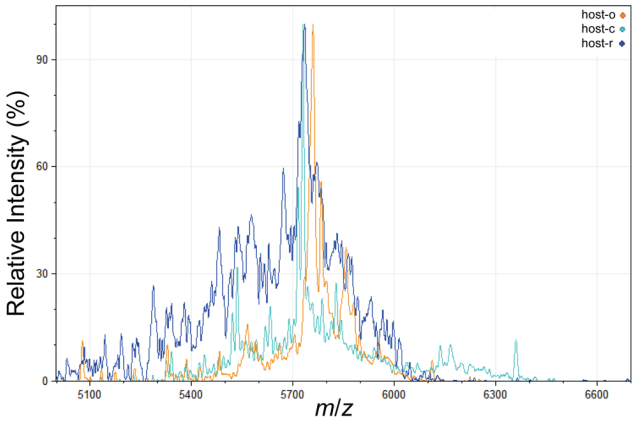


Figure S1. MALDI–TOF mass spectra of host-o (5757.07), host-c (5728.55), and host-r (5731.67).

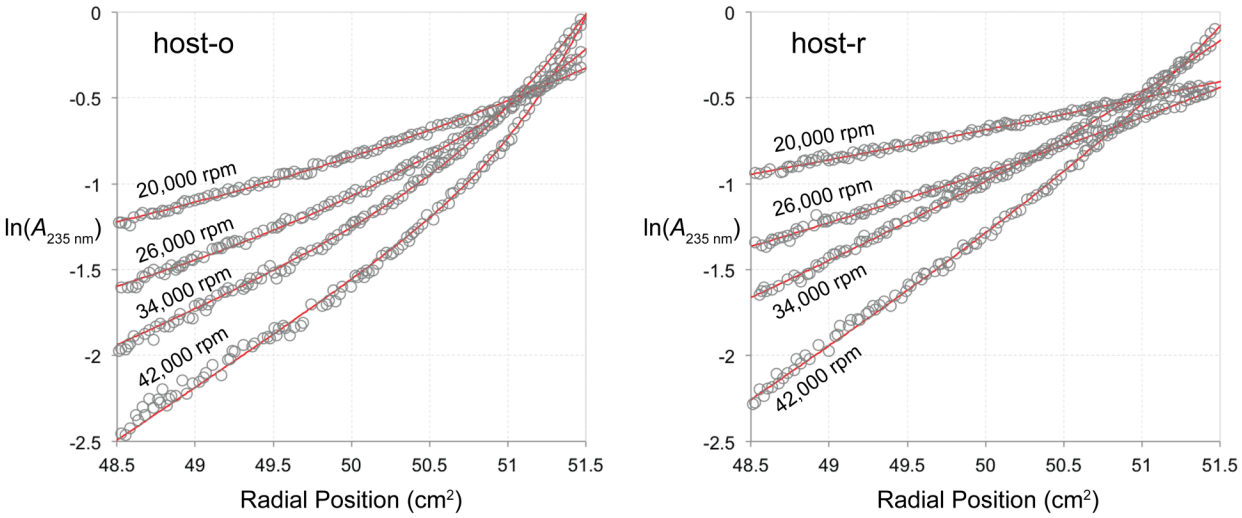


Figure S2. Sedimentation equilibrium analysis. Equilibrium gradients (gray circles) for host-o and host-r are shown at four different speeds (20, 26, 34, and 42 k rpm) with models that provide optimal fits (red lines). The host-o data are modeled best as a mixture of monomers and pentamers, whereas the host-r data are modeled best as a mixture of monomers and trimers. The gradients for host-r are mostly linear, due to a near-uniform composition dominated by monomers. In contrast, non-linear behavior seen in host-o gradients indicate appreciable levels of high-molecular weight species present in solution. These trends are apparent at all speeds.

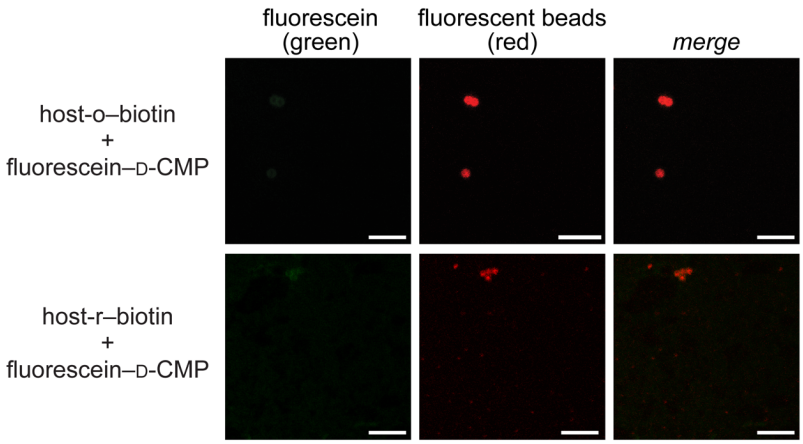


Figure S3. Binding of immobilized host-o and host-r to a fluorescent D-CMP, which iss (D-Pro-D-Pro-Gly)$_7$. Representative confocal microscopy images are shown. Streptavidin-coated fluorescent beads (red) were treated with host-o or host-r and then incubated with D-CMP–fluorescein (green), as in Figure 4. Scale bar: 10 μm.

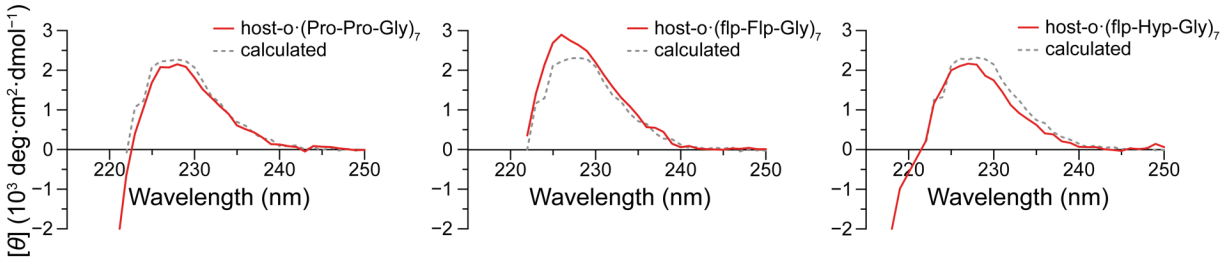


Figure S4. Circular dichroism spectra of host-o·CMP complexes. Calculated spectra for non-interacting mixtures of host-o and CMPs are shown (dashed gray lines) together with acquired spectra for host-o·CMP complexes (red lines). Spectra were obtained in 50 mM HOAc at 4 °C.

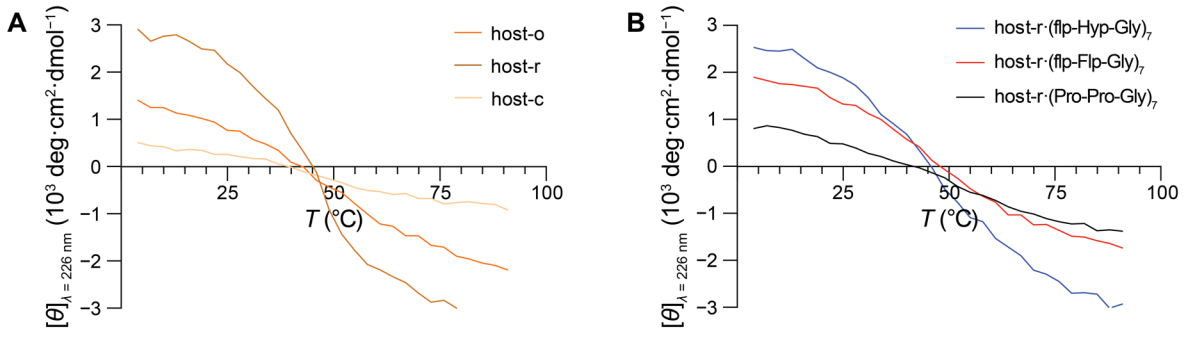


Figure S5. Circular dichroism temperature-denaturation experiments for all three hosts alone (A) and host-r·CMP complexes (B).

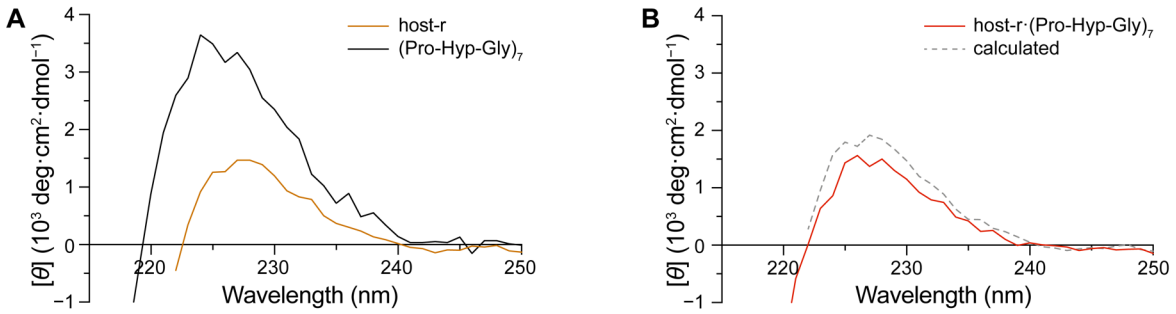
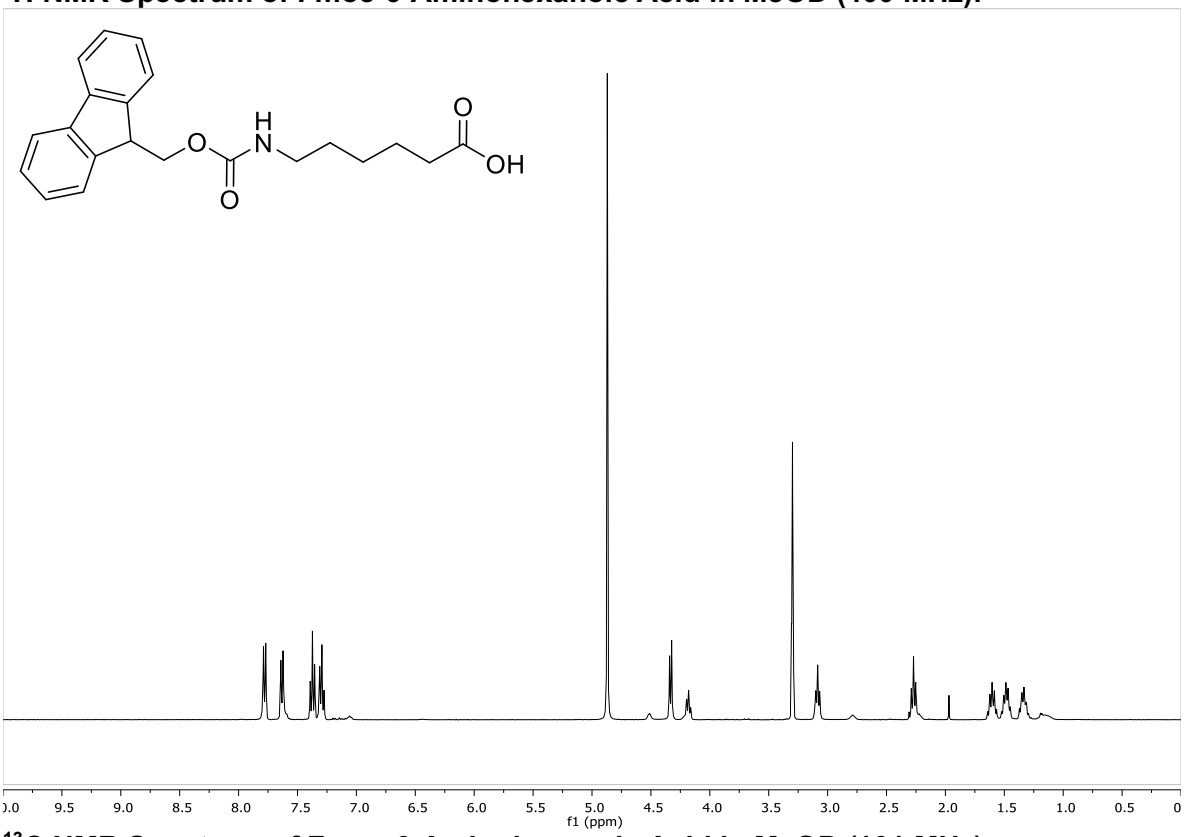
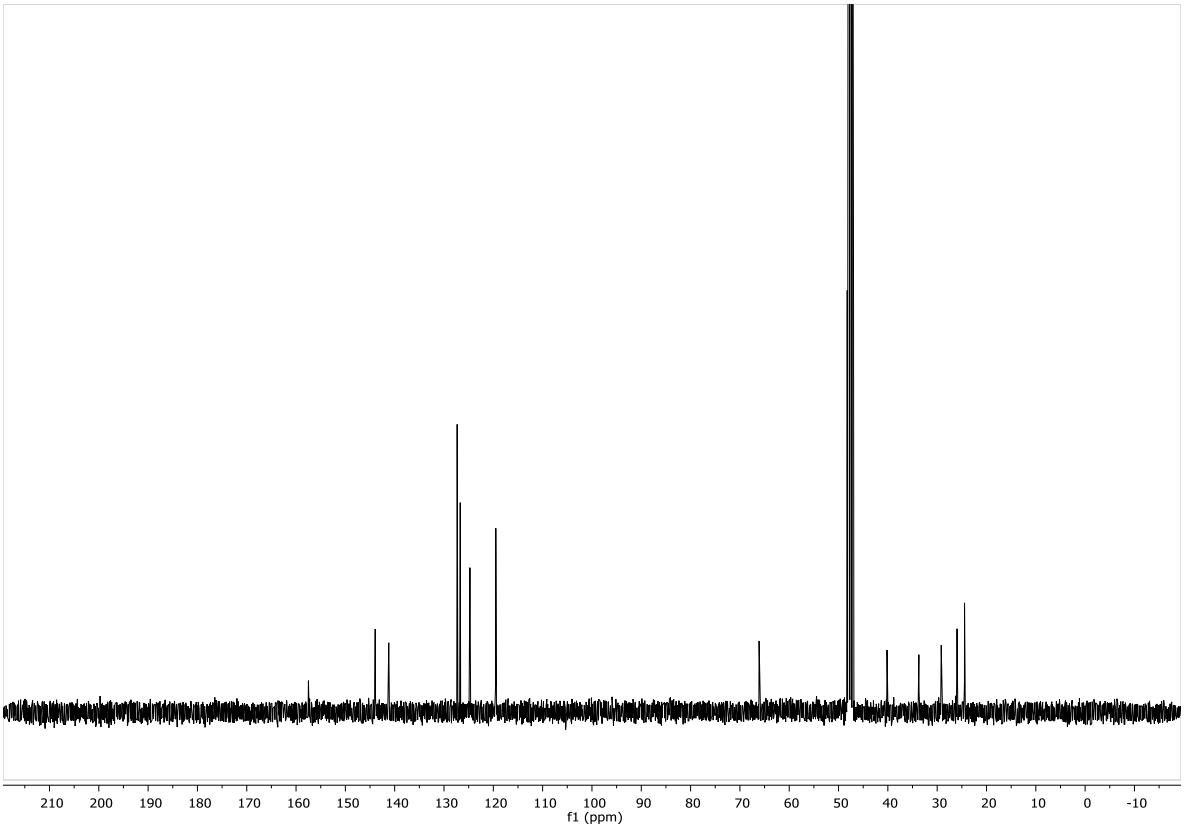


Figure S6. Circular dichroism spectra of host-r and $(Pro\text{-}Hyp\text{-}Gly)_7$ alone (A), and their complex (B). A spectrum calculated assuming a mixture of non-interacting species is shown as a comparison (dashed gray line). Spectra were obtained in 50 mM HOAc at 4 °C.

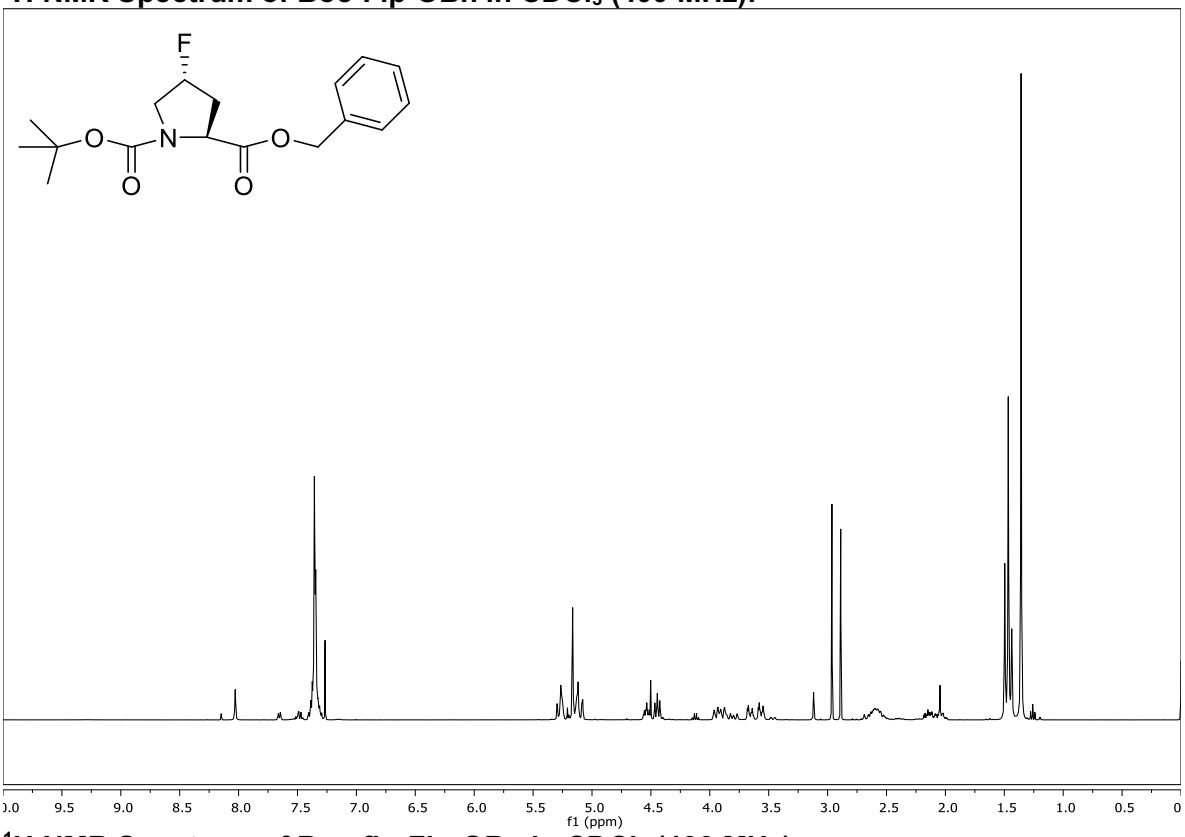
^{1}H NMR Spectrum of Fmoc-6-Aminohexanoic Acid in MeOD (400 MHz):



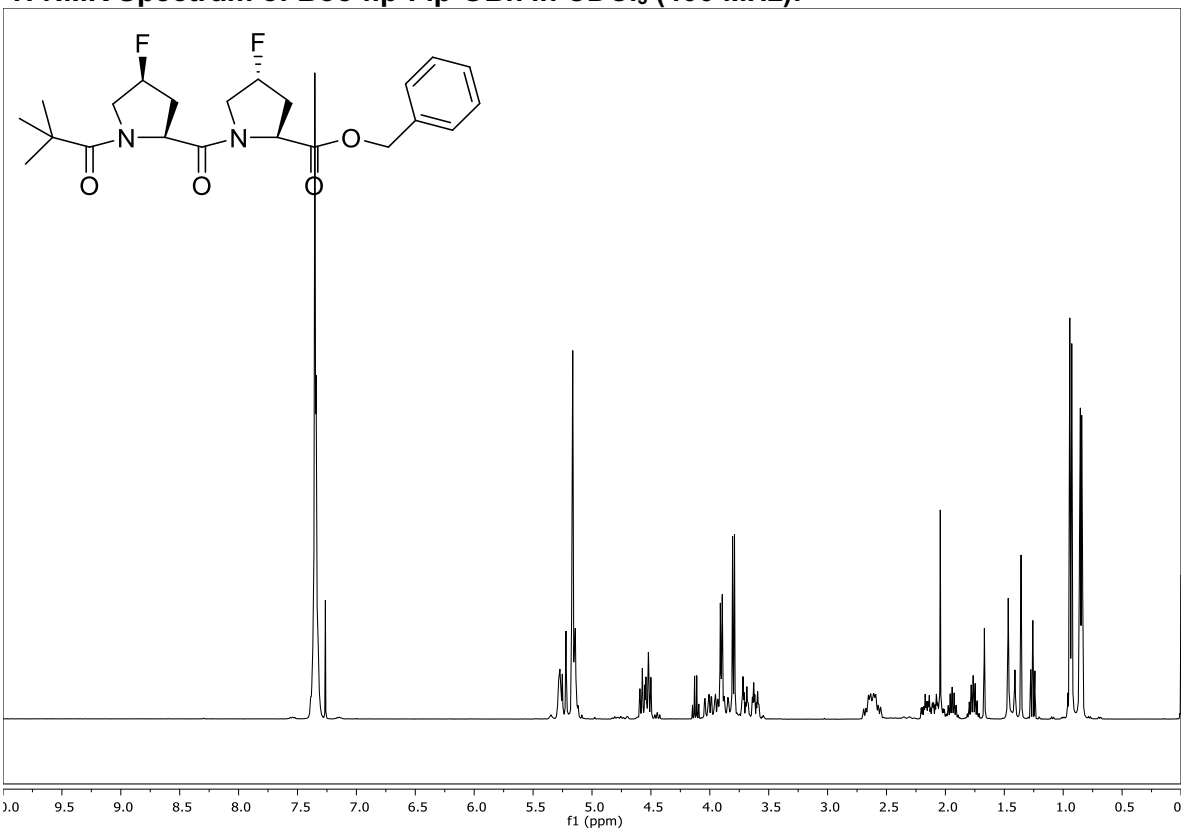
^{13}C NMR Spectrum of Fmoc-6-Aminohexanoic Acid in MeOD (101 MHz):



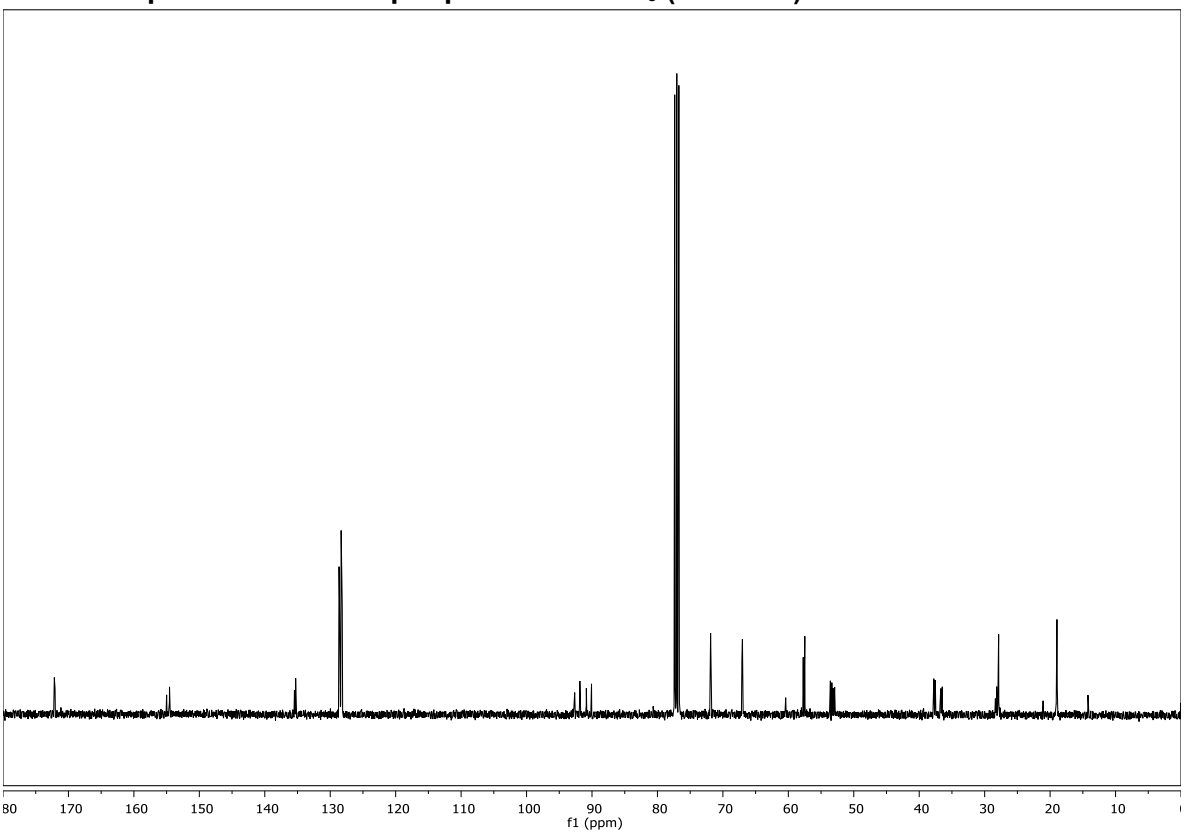
^{1}H NMR Spectrum of Boc-Flp-OBn in $CDCl_3$ (400 MHz):



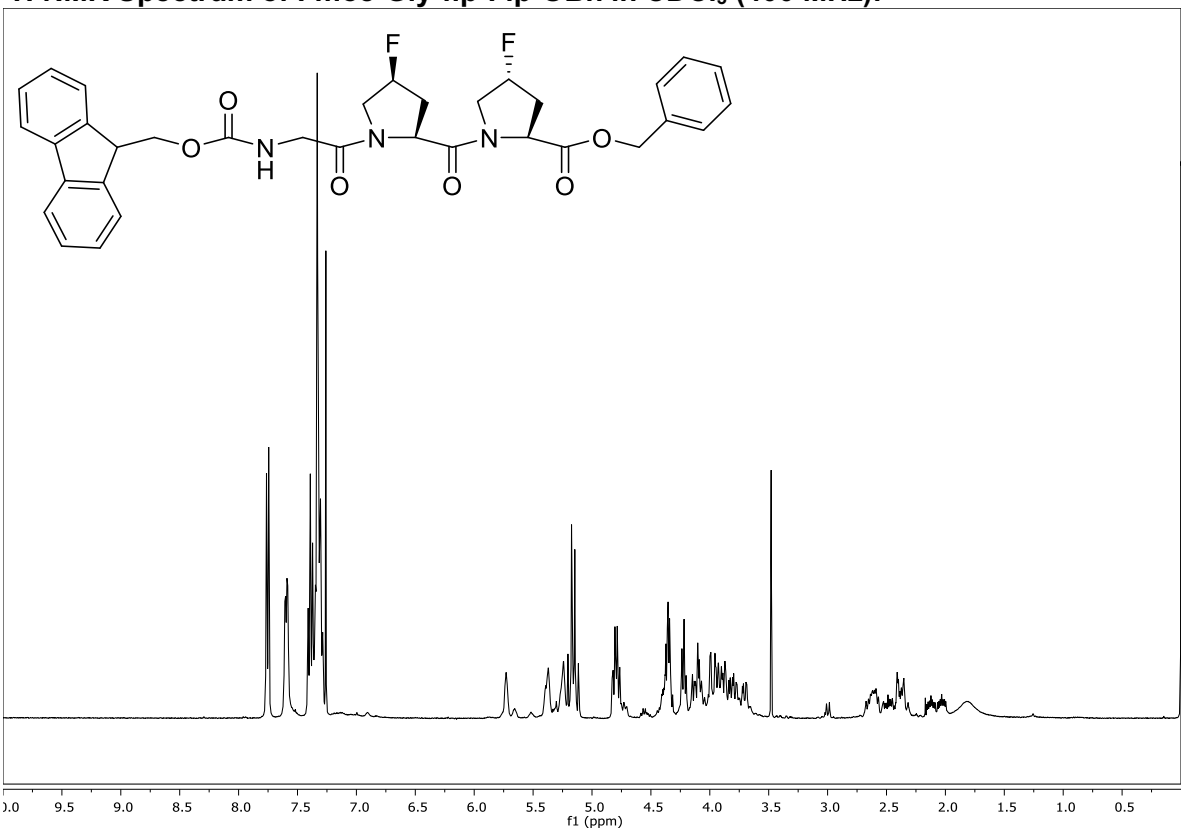
^{1}H NMR Spectrum of Boc-flp-Flp-OBn in $CDCl_3$ (400 MHz):



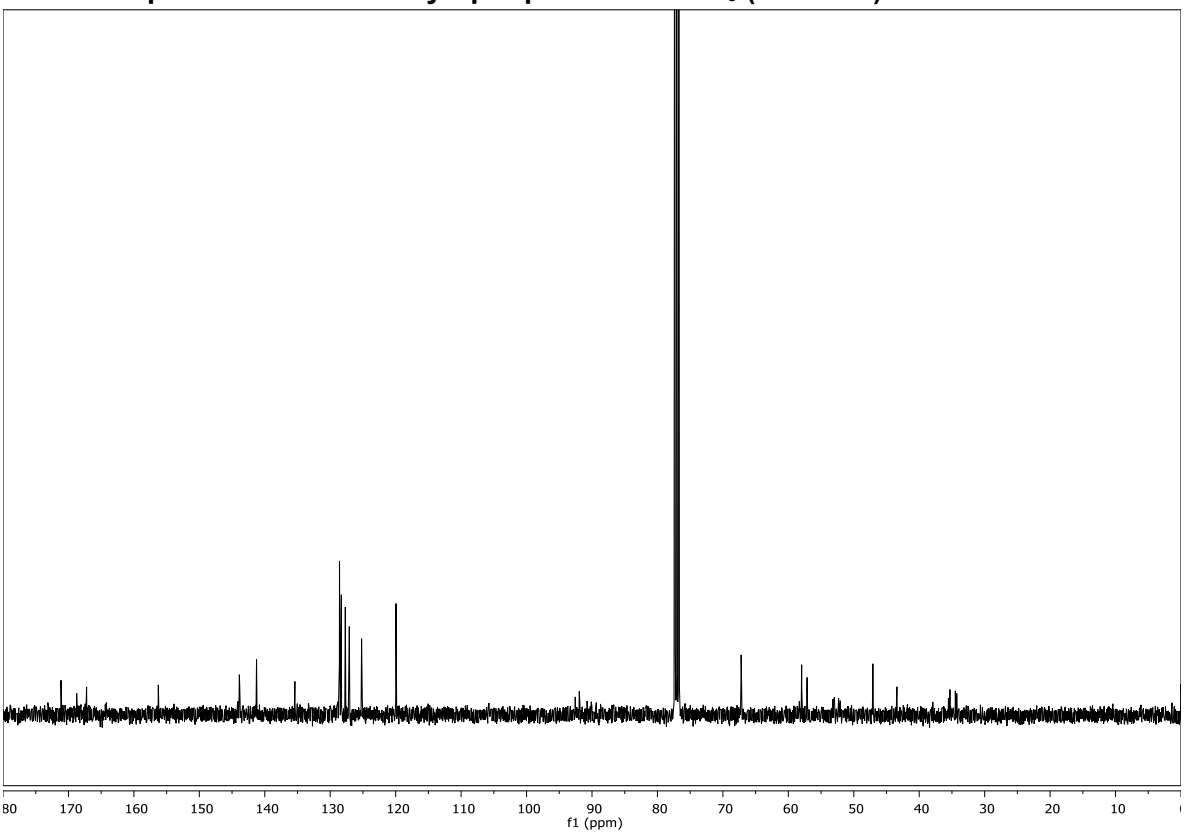
^{13}C NMR Spectrum of Boc-flp-Flp-OBn in $CDCl_3$ (101 MHz):



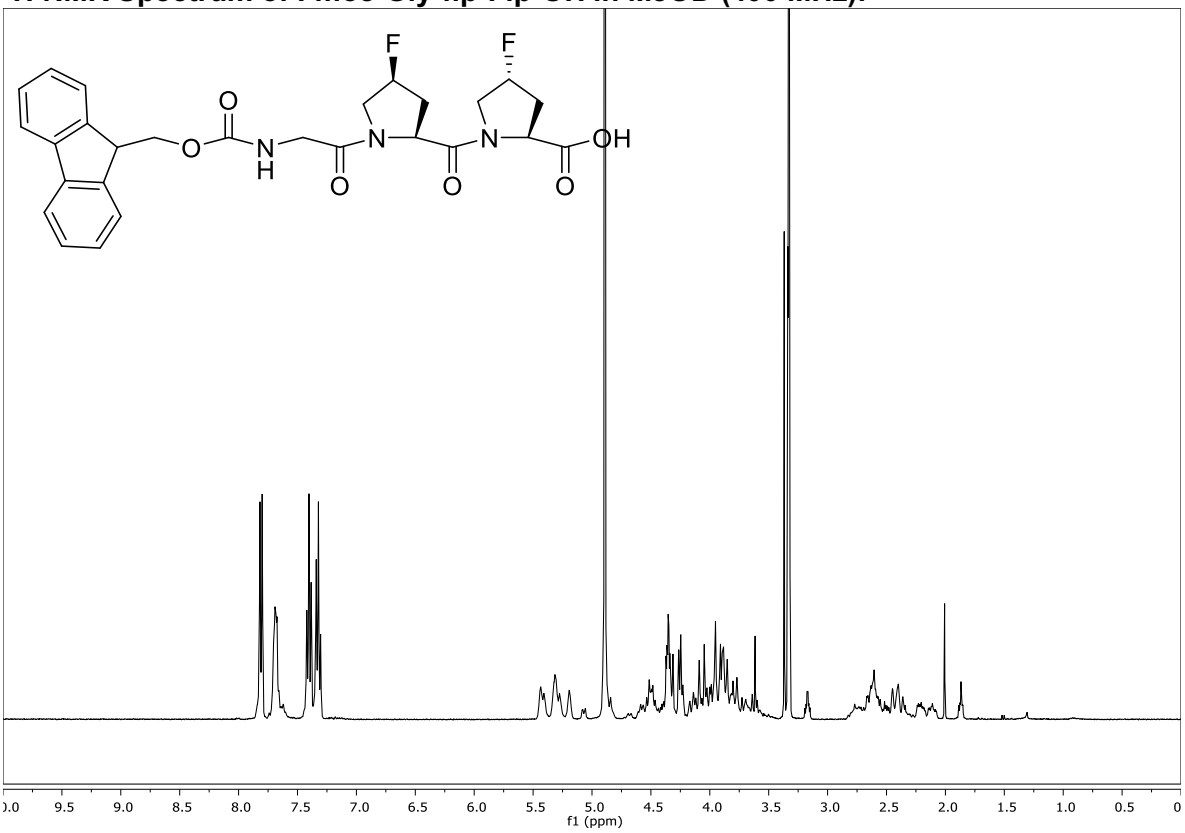
^{1}H NMR Spectrum of Fmoc-Gly-flp-Flp-OBn in $CDCl_3$ (400 MHz):



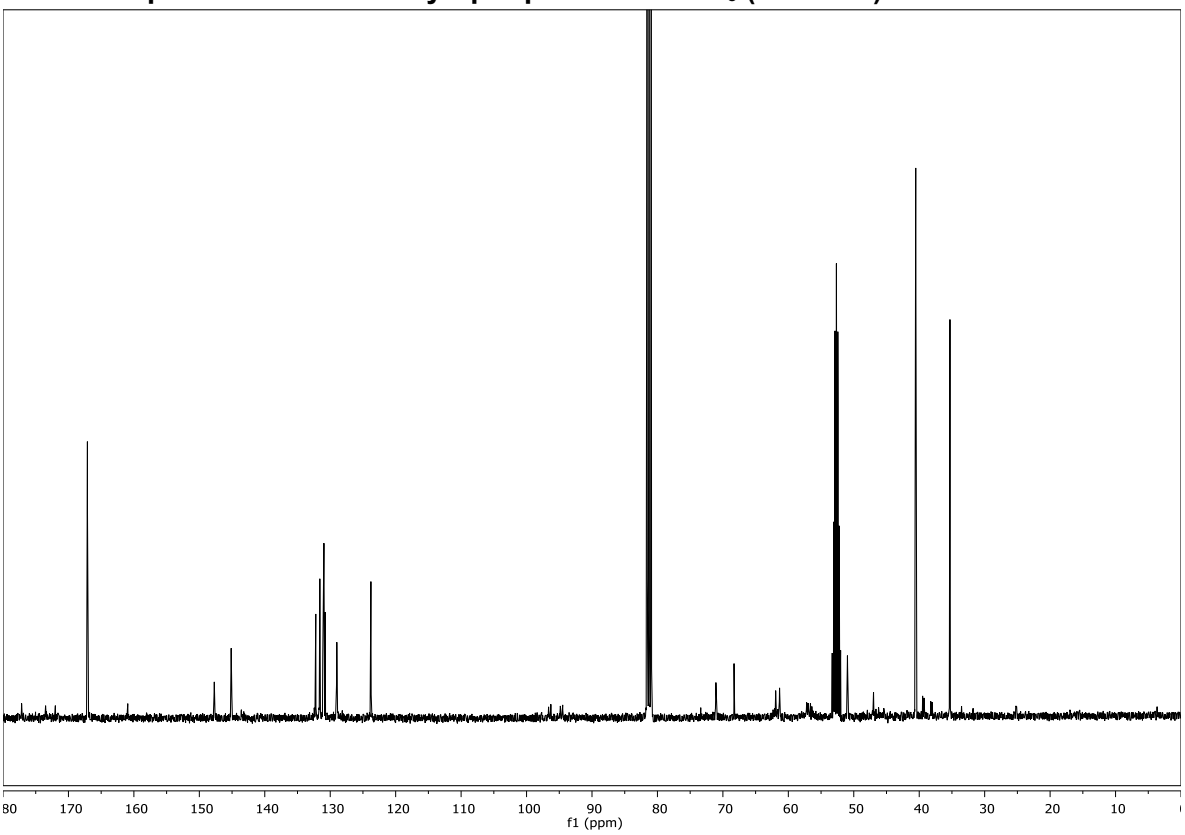
^{13}C NMR Spectrum of Fmoc-Gly-flp-Flp-OBn in $CDCl_3$ (101 MHz):



^{1}H NMR Spectrum of Fmoc-Gly-flp-Flp-OH in MeOD (400 MHz):

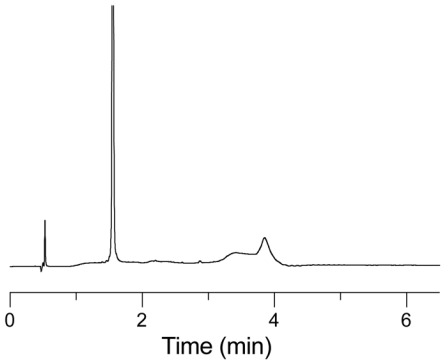


^{13}C NMR Spectrum of Fmoc-Gly-flp-Flp-OBn in $CDCl_3$ (101 MHz):

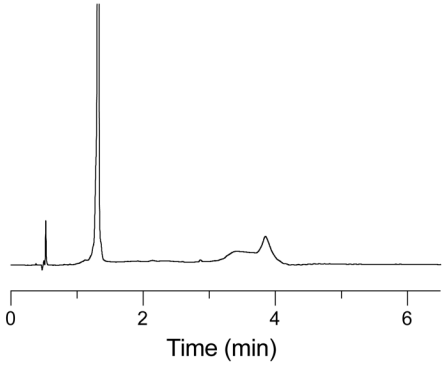


UPLC Traces of CMPs

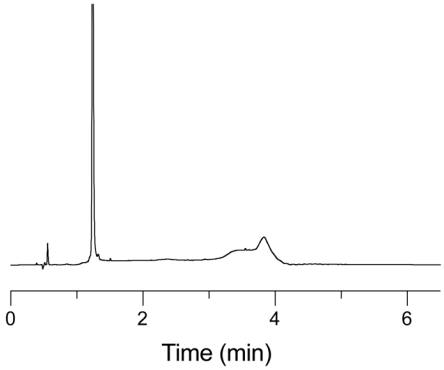
(Pro-Pro-Gly)$_7$



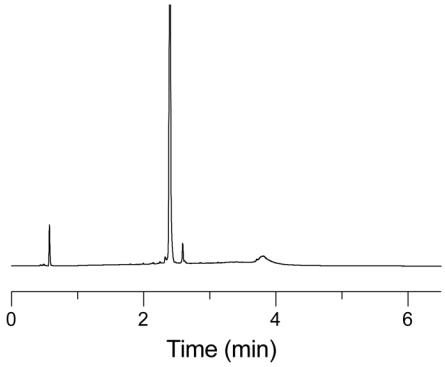
(Pro-Hyp-Gly)$_7$



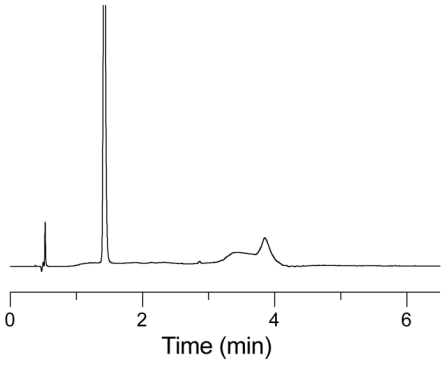
(flp-Hyp-Gly)$_7$



(Pro-Ile-Gly)$_7$

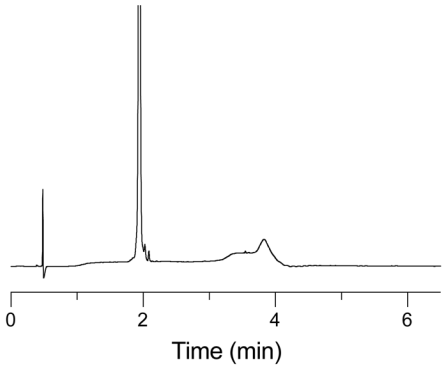


(flp-Flp-Gly)$_7$

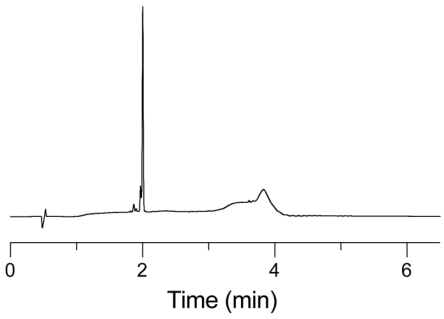


UPLC Traces of fluorescein–CMP, biotin–fluorescein, and fluorescein-D-CMP

fluorescein–CMP



biotin–fluorescein



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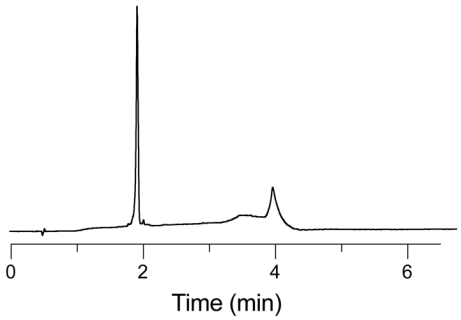

UPLC Traces of Hosts