

Supplementary information

Synthesis of temporin L hydroxamate-based peptides and evaluation of their coordination properties of iron (III)

Rosa Bellavita,^a Linda Leone,^b Angela Maione,^c Lucia Falcigno,^a Gabriella D'Auria,^a Francesco Merlino,^a Paolo Grieco,^a Flavia Nastri,^b Emilia Galdiero,^c Angela Lombardi,^b Stefania Galdiero,^{a} Annarita Falanga^{d*}*

^aDepartment of Pharmacy, University of Naples "Federico II", Via Domenico Montesano 49, 80138 Naples, Italy

^bDepartment of Chemical Sciences, University of Napoli "Federico II", Napoli, Italy.

^cDepartment of Biology, University of Naples Federico II, Via Cinthia, 80126 Naples, Italy.

^dDepartment of Agricultural Science, University of Naples "Federico II", via Università 100, 80055, Portici, Italy

Table of contents

1. HPLC chromatograms and HRMS of peptides Pep-cyc1, Pep-cyc2, and Pep-cyc3 (Figures S1-S3)	1-2
2. UV-Vis spectra of peptide Pep-cyc (Figure S4)	3
3. UV-Vis spectra of peptide Pep-cyc and its linear analogue acquired during the titration of Fe ³⁺ (Figure S5)	4

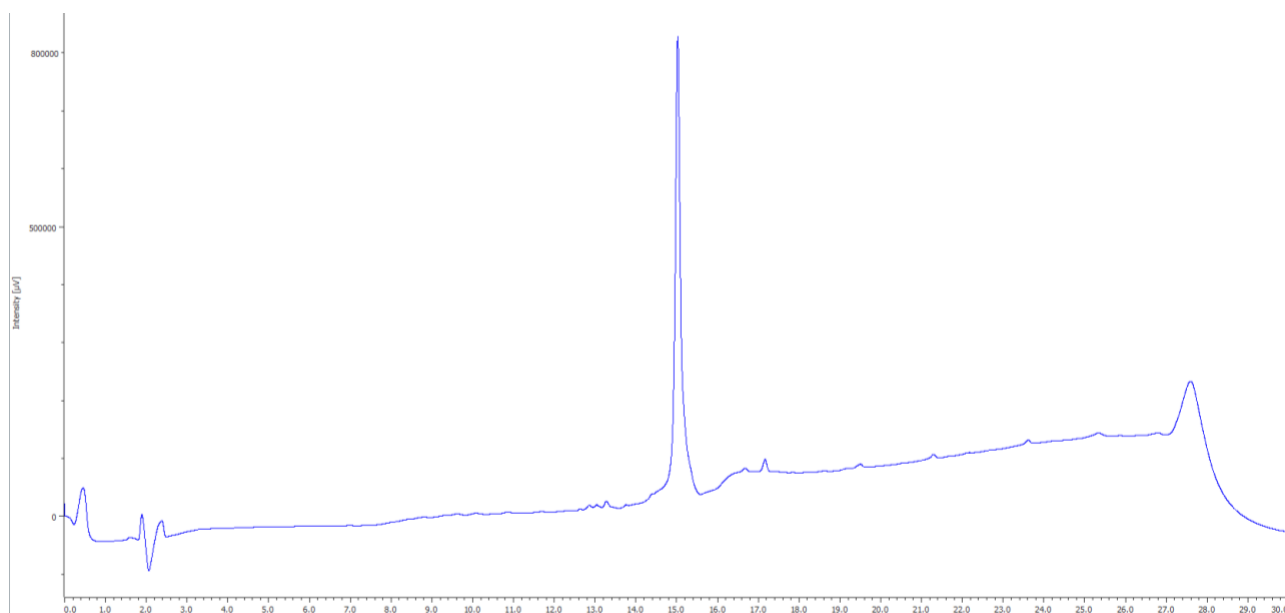


Figure S1. Chromatogram of peptide **Pep-cyc1** obtained by an analytical HPLC (Jasco LC-NetII/ADC) equipped with a Phenomenex Kinetex C18 column (150 mm × 4.6 mm, 5 μm, 100 Å), and monitored by UV detection at 220 nm. [linear gradient 10-90% MeCN (0.1% TFA) in H₂O (0.1% TFA) over 20 min, flow rate of 1 mL/min]. Calculated mass: 1833.2671, Found mass: $[M+2H]^+/2=917.5502$, $[M+3H]^+/3=612.0363$.

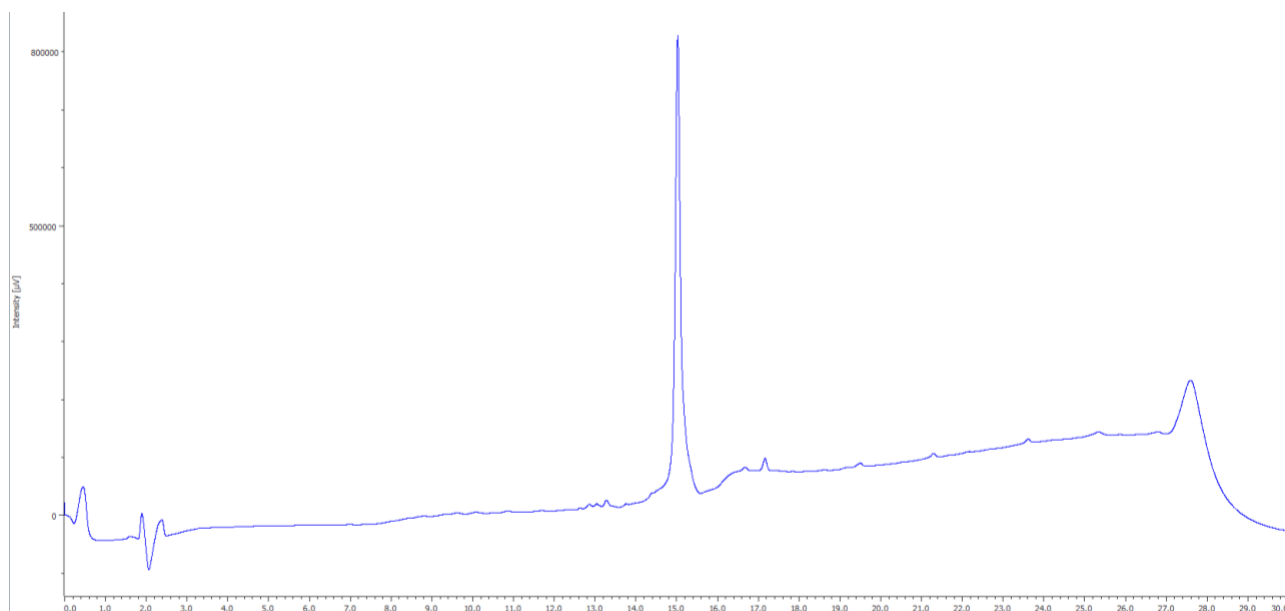


Figure S2. Chromatogram of peptide **Pep-cyc2** obtained by an analytical HPLC (Jasco LC-NetII/ADC) equipped with a Phenomenex Kinetex C18 column (150 mm × 4.6 mm, 5 μm, 100 Å), and monitored by UV detection at 220 nm. [linear gradient 10-90% MeCN (0.1% TFA) in H₂O (0.1% TFA) over 20 min, flow rate of 1 mL/min]. Calculated mass: 1918.3716. Found mass: $[M+2H]^+/2=960.0773$, $[M+3H]^+/3=640.3872$.

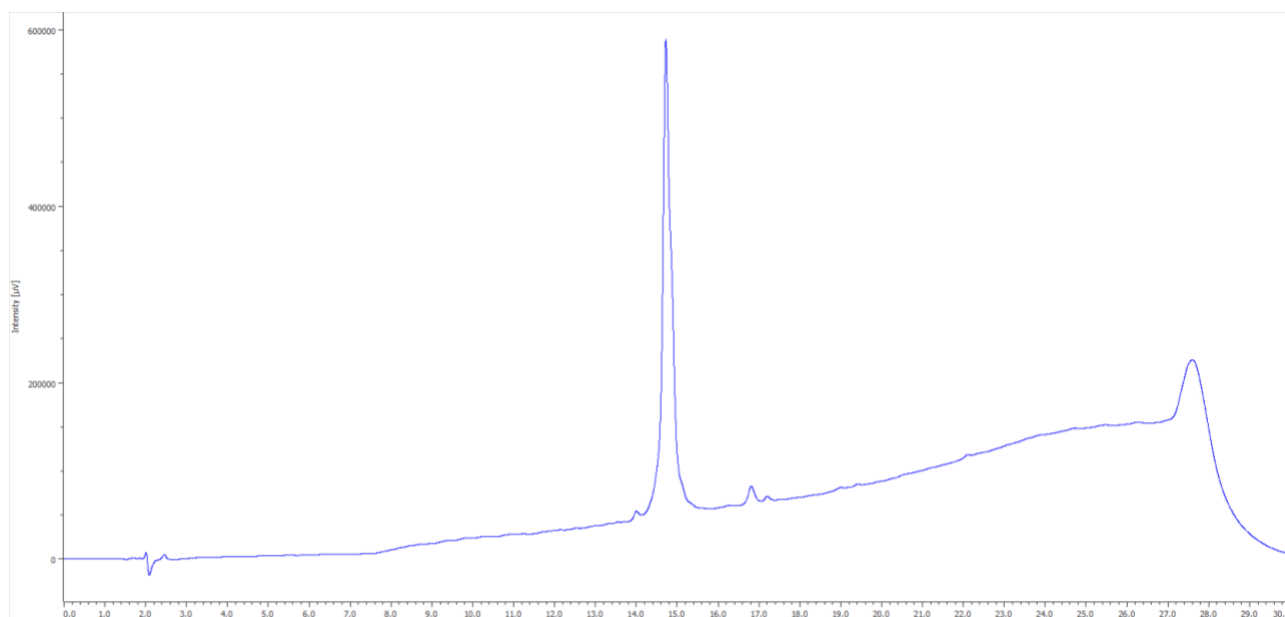


Figure S3. Chromatogram of peptide **Pep-cyc3** obtained by an analytical HPLC (Jasco LC-NetII/ADC) equipped with a Phenomenex Kinetex C18 column (150 mm × 4.6 mm, 5 μm, 100 Å), and monitored by UV detection at 220 nm. [linear gradient 10-90% MeCN (0.1% TFA) in H₂O (0.1% TFA) over 20 min, flow rate of 1 mL/min]. Calculated mass: Found mass: 1978.1719. $[M+2H]^+/2=990.0878$, $[M+3H]^+/3=660.3942$.

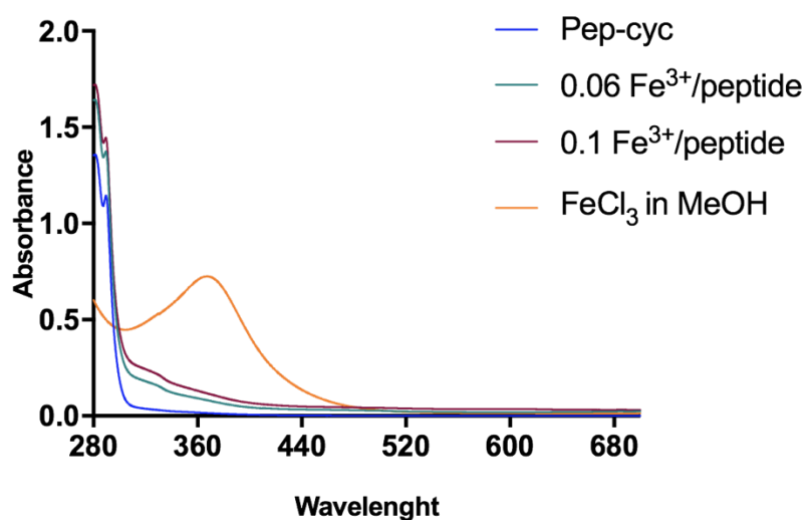


Figure S4. UV-vis spectra of Pep-cyc (blue trace), Fe³⁺ (orange trace) and Fe³⁺/ligand complex at the ratios of 0.06 and 0.1 (green and purple traces).

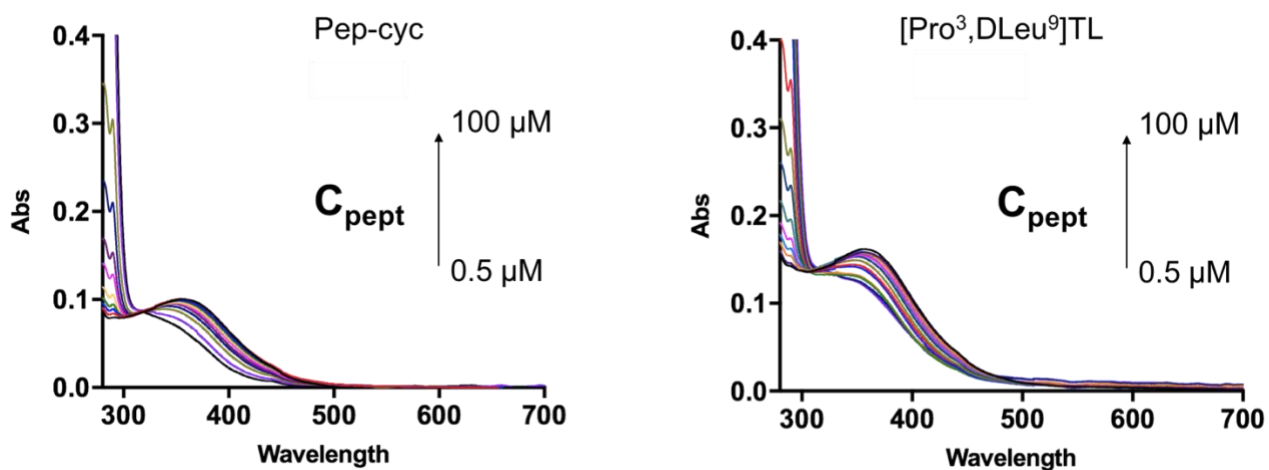


Figure S5. UV-vis spectra of Pep-cyc (on the left) and its analogue [Pro³,DLeu⁹]TL (on the right) acquired during the titration of Fe³⁺ (black line) with increasing peptide concentrations ranging from 0.5 μM to 100 μM.