SUPPORTING INFORMATION

A supramolecular peptide polymer from hydrogen-bond and coordination-driven self-assembly

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1. HPLC and M-TOF analysis of peptide 1

The Peptide 1 was purified by Reverse-phase HPLC (AKTA purifier 100, GE Healthcare, USA) with a RPC18 HPLC column and UV detector. A gradient of 35-100% of acetonitrile aqueous solution containing 0.1% TFA as mobile phase was used at a total flow rate of 1 mL/min. The UV absorption peaked at 530 nm was recorded for analysis. Purity HPLC: 95%.

The mass spectra of peptide **1** was confirmed by a 4800 Plus MALDI TOF/TOF Analyzer (AB SCIEX, USA). Firstly, a volume of 0.5 μL of peptide **1** solution was spotted on a MALDI plate before droplet of 0.5 μL matrix solution (CHCA), and then allowed to air-dry at room temperature. All MALDI-TOF-MS measurement was performed in positive ion mode. MALDI-TOF (m/z): calcd. for 967.3878, found $[M+H]^+$ 968.3280.

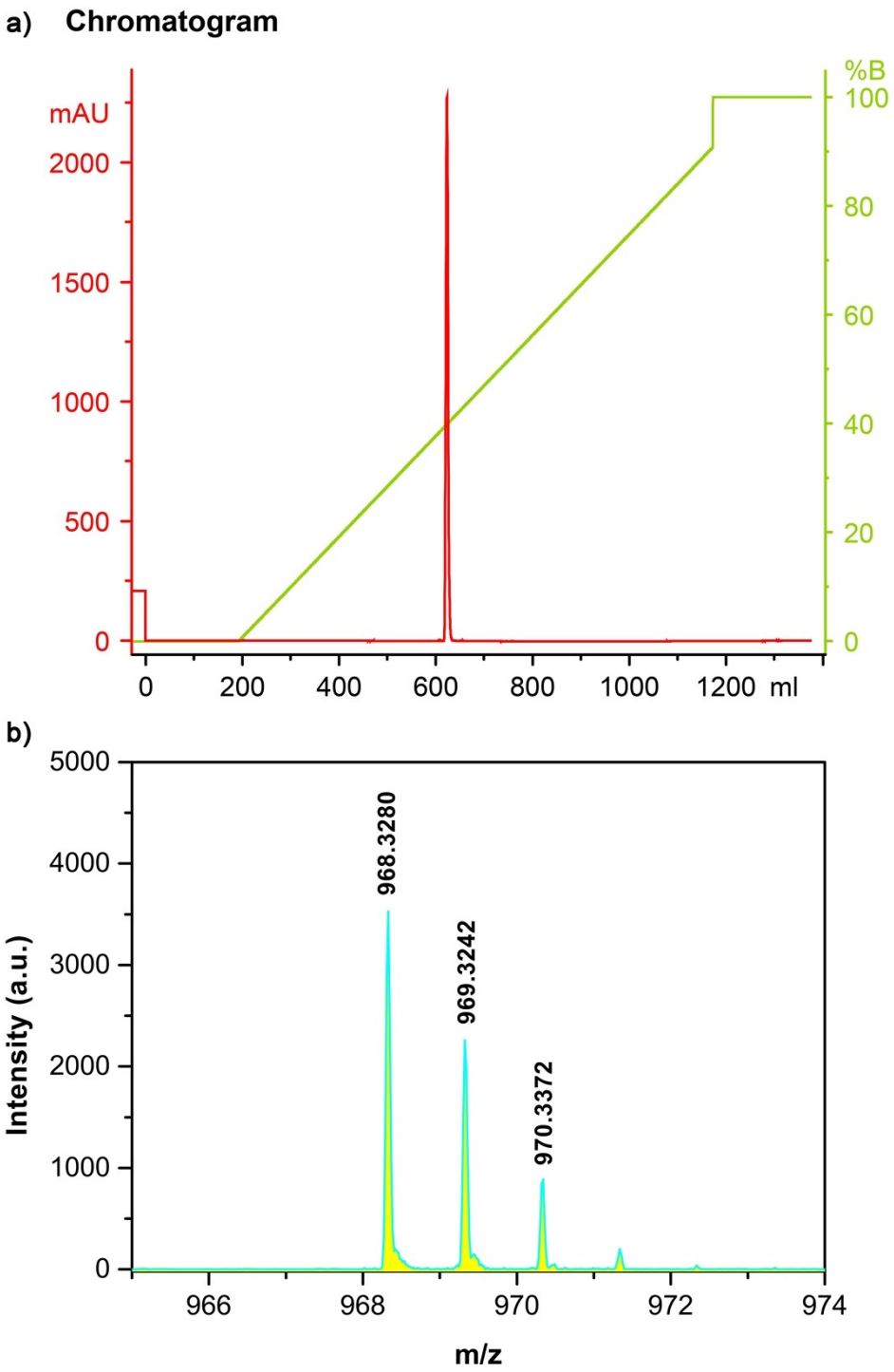

Fig. S1. a) HPLC and b) MALDI-TOF analysis of peptide 1.

2. 2D COSY, 2D TOCSY and 2D NOESY NMR analysis of peptide 1 and peptide 1–Fe^{2+} complex

The NMR spectra were recorded at room temperature with a *Bruker* Avance 800 NMR spectrometer at 800 MHz. The peptide 1 (5.8 mg, 6 µmol) was dissolved in DMSO-d_6. The peptide 1–Fe^{2+} complex was prepared by addition of 0.5 eq. Fe^{2+} (0.38 mg, 3 µmol) into peptide 1

(5.8 mg, 6 µmol) in DMSO-d_6 (0.5 ml) for 20 min. Immediately the colorless solution turned to dark purple.

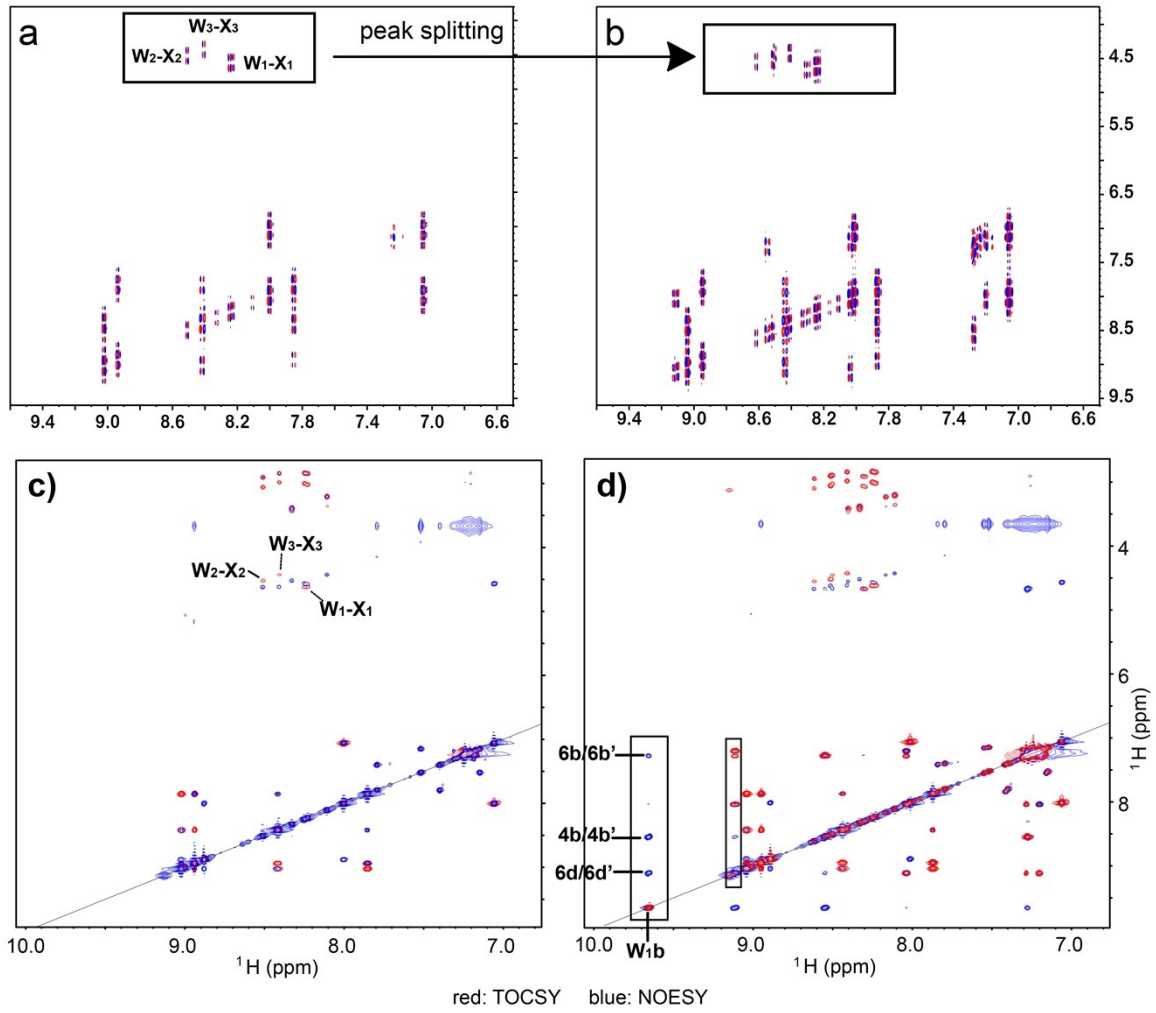

Fig. S2. 2D COSY NMR analysis of a) peptide 1 and b) the peptide 1–Fe^{2+} complex. 2D TOCSY and 2D NOESY NMR analysis of c) peptide 1 and d) the peptide 1–Fe^{2+} complex.