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Supporting Information

for

pH- and concentration-dependent supramolecular self-assembly of a naturally occurring octapeptide

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Materials and methods as well as additional figures

Materials and methods

Rink amide resin (Rink amide 4-methylbenzhydrylamine, polymer-bound), Fmoc-protected amino acids, *O*-(benzotriazol-1-yl)-*N*,*N*,*N*',*N*'-tetramethyluronium hexafluorophosphate (HBTU), triisopropylsilane (TIPS), trifluoroacetic acid (TFA), and *N*-methylmorpholine (NMM), were purchased from Sigma-Aldrich. Ninhydrin, dimethylformamide (DMF), dichloromethane (DCM), phenol, piperidine, and pyridine were purchased from Merck. All solvents were distilled and dried following standard protocols before use. [1] Reversed-phase high-performance liquid chromatography (RP-HPLC) was done with a Waters HPLC (2489 UV–vis detector) system. An applied Biosystems 4700 Proteomics Analyzer 170 MALDI-TOF mass spectrometer was used to determine the molecular mass of the peptide. Circular dichroism (CD) experiments were performed on a J1500 spectrophotometer from JASCO. FTIR spectra were recorded by using a PerkinElmer Spectrum 100FTIR spectrometer.

Additional figures

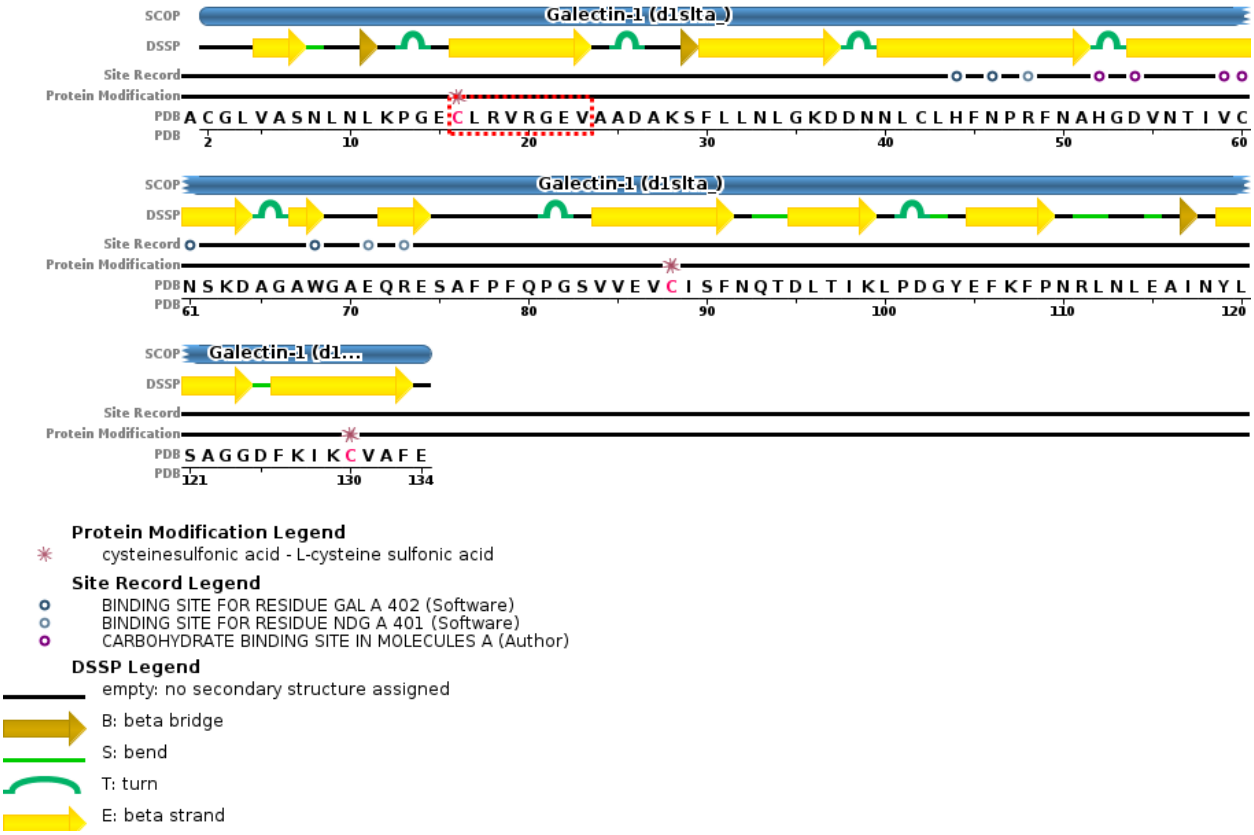

Figure S1: Amino acid sequence of galectin-1 from the crystal structure (the red dotted box indicates the PEP-1 sequence). Image from the RCSB PDB (rcsb.org); PDB ID: 1SLT.

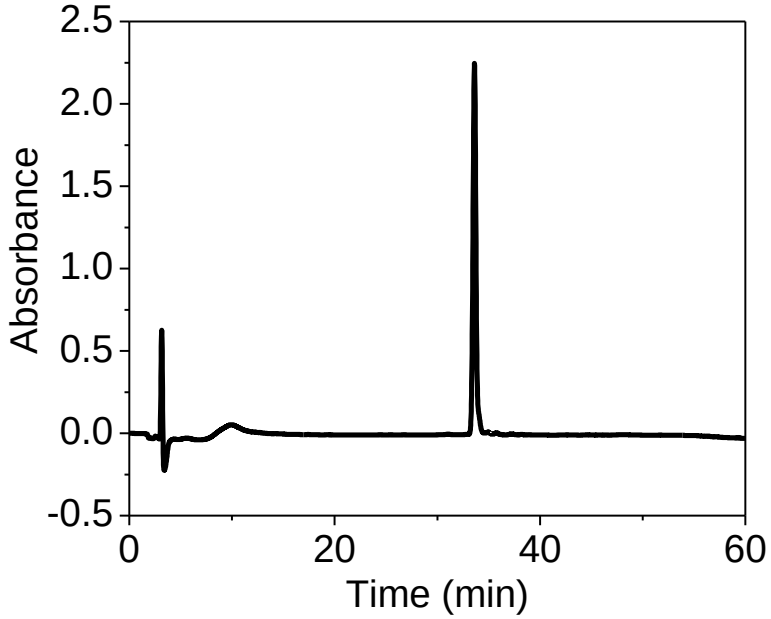

Figure S2: Reversed-phase HPLC chromatogram of purified PEP-1.

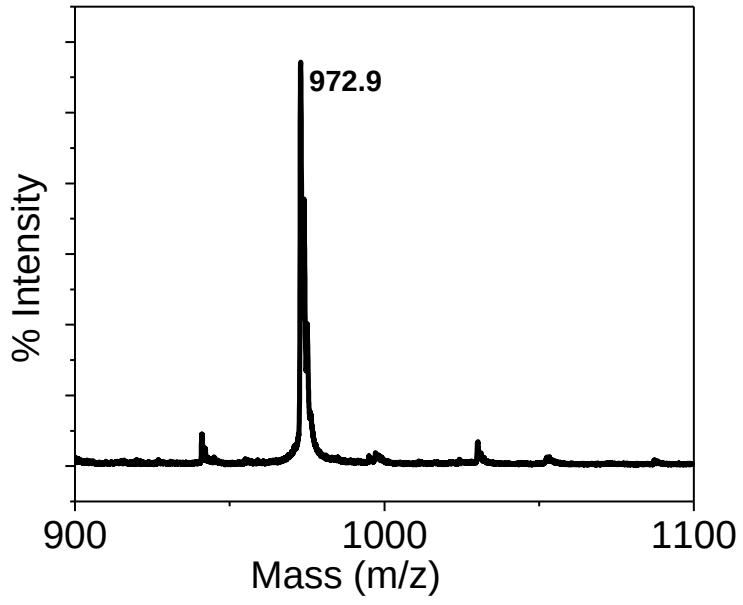

Figure S3: MALDI-TOF mass spectrum of purified PEP-1.

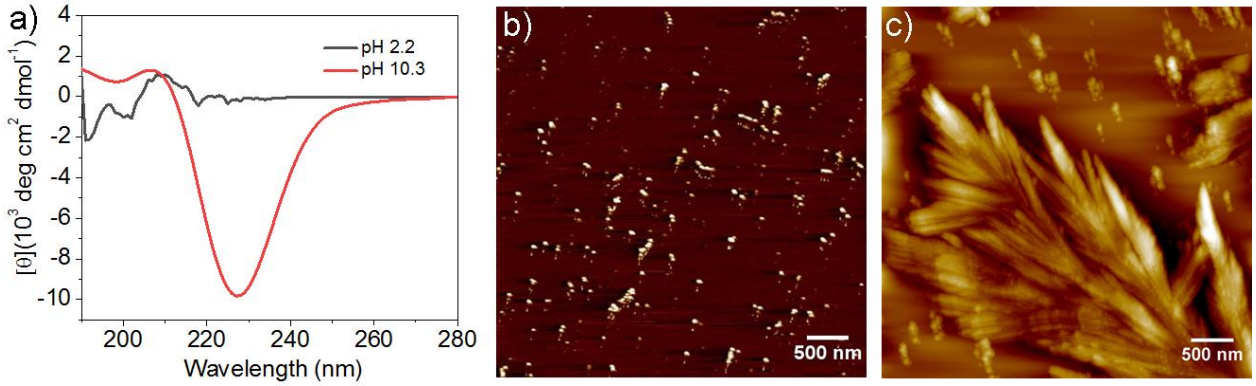

Figure S4: a) CD spectra at pH 2.2 and 10.3, respectively. b) AFM images of PEP-1 at pH 2.2 and c) pH 10.3 (c = 5 × 10^{-4} M, T = 25 °C).

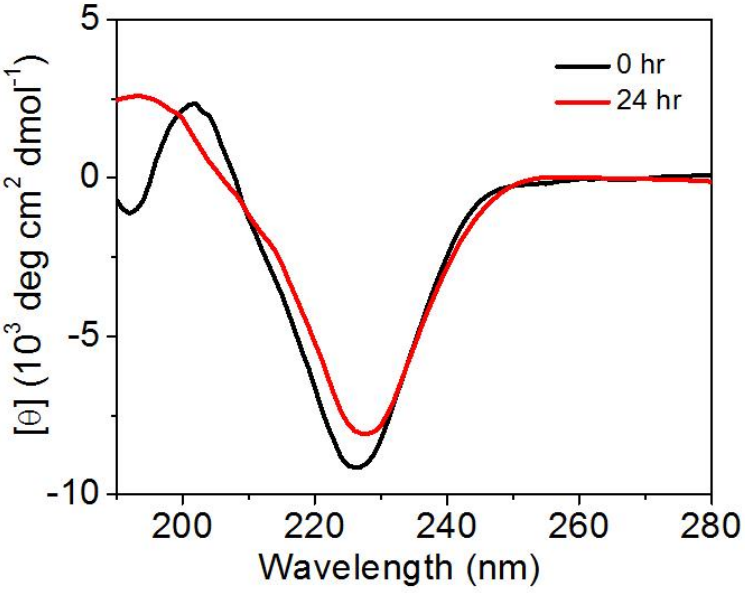

Figure S5: Time-dependent CD spectra of PEP-1 at pH 7.4 (PBS buffer; c = 5 × 10^{-4} M, T = 25 °C).

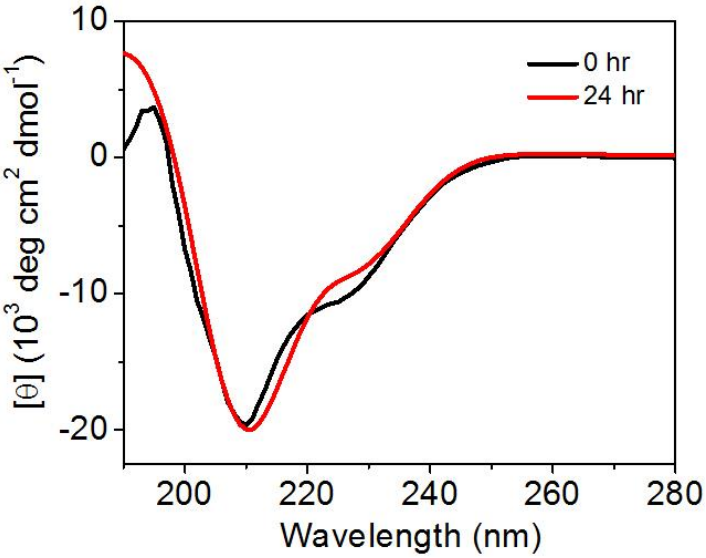

Figure S6: Time-dependent CD spectra of PEP-1 at pH 7.4 (PBS buffer; $c = 1.25 \times 10^{-4}$ M, $T = 25$ °C).

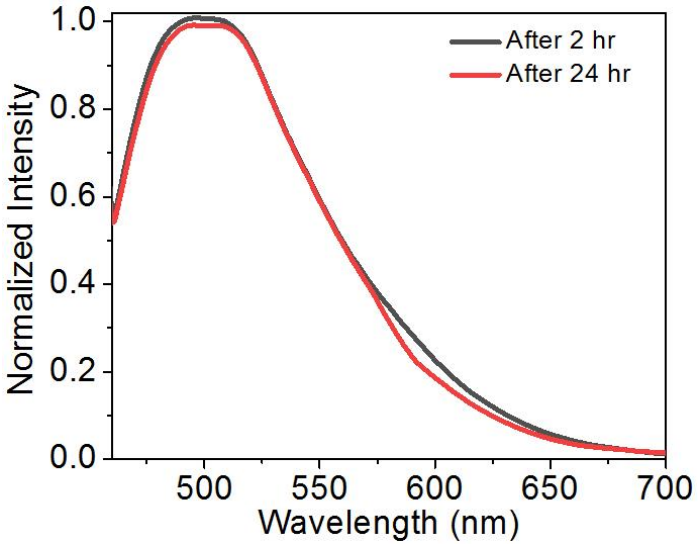

Figure S7: Time-dependent ThT assay of PEP-1 at pH 7.4 (PBS buffer; $c = 5 \times 10^{-4}$ M, $T = 25$ °C).

References

1. Perrin, D.; Armarego, W. L. F.; Perrin, D. R. Purification of Laboratory Chemicals, 2nd ed., *Pergamon, Oxford*, **1980**.