Electronic Supplementary Material (ESI) for Chemical Communications

Fabrication of Artifical Toroid Nanostructures by Modified β-sheet Peptide

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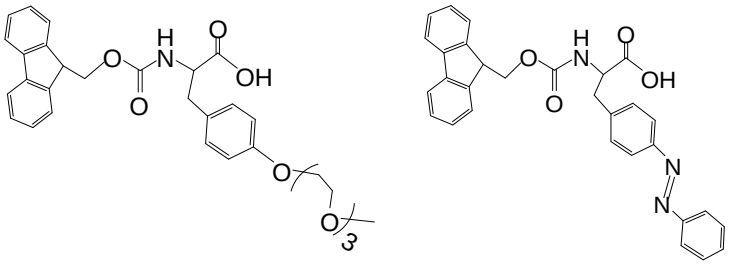
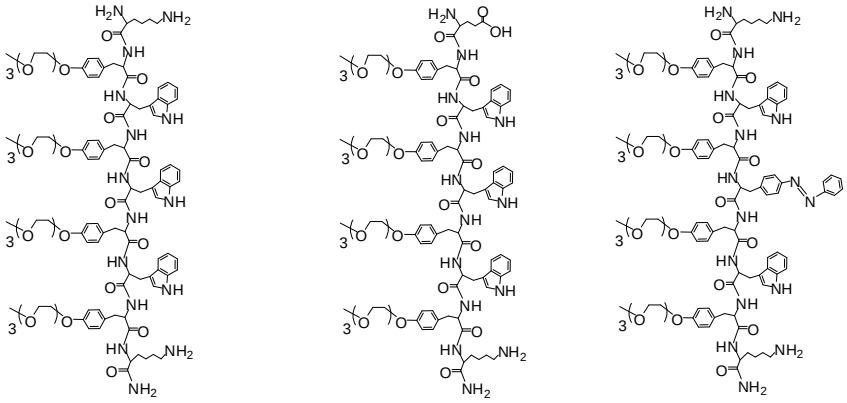
1. Peptide synthesis:



Fmoc-tyrosine derivative with tri(ethylene glycol) monomethyl ether and Fmoc-L-Phenylalanine-4'-azobenzene (Fmoc-Phe-Azo) were synthesized according to previous method. [1]



P1 P2 P3

All the peptides were synthesized with a microwave-equipped liberty peptide synthesizer (CEM). Rink amide resin was utilized and loaded using standard methods HBTU activation. Peptide synthesis was carried out using standard Fmoc methods.

2. Measurements:

Circular Dichroism Spectroscopy. Peptide solutions were analyzed by CD spectroscopy to characterize secondary structure. Spectra were recorded on a JASCO model J-810 spectropolarimeter. CD spectra were obtained from 260-190 nm with a 1.0 nm step, 1.0 nm bandwidth, and a 3 s collection time per step at 25 ^{o}C in a 0.1 cm path length quartz cuvette (Hellma). Scans were repeated five times and averaged. The JASCO software was used for background subtraction, conversion to molar ellipticity per amino acid residue.

Fourier Transform Infrared Spectroscopy. FT-IR spectra were obtained using a Bruker Equinox 55 FT-IR spectrophotometer. The aqueous solution of the peptide samples was cast onto gold plate. Absorbance spectra were obtained from 1750 to 1550 cm^{-1} with a 4 cm^{-1} resolution. 502 scans were acquired and background spectra were also collected and subtracted.

Dynamic Light Scattering (DLS). DLS experiment was performed at room-temperature with LV/CGS-3 Compact Goniometer System equipped with He-Ne laser operating at 632.8 nm. The scattering angle was 90^{o}. Bbefore measurement, the sample was centrifuged at 16,110×g for 20 min to sediment and dust particles. The size distribution was determined by using a constrained regularization method.

Transmission Electron Microscopy. Samples (2 μL) were spotted directly onto a carbon-coated copper grid and dried completely. Then 2 % (w/v) uranyl acetate solution (2 μL) was added and allowed to stand for 1 min. Then, the excess amount of solution was carefully removed by capillary action (filter paper). The cryogenic transmission electron microscopy experiments (cryo-TEM) were performed with a thin film of solution of the peptide (5μL) transferred to a lacey-supported grid. The thin aqueous films were prepared under controlled temperature and humidity conditions (97-99 %) within a custom-built environment chamber to prevent evaporation of water from sample solution. The excess amount of liquid was blotted with filter paper for 2-3 s, and the thin aqueous films were rapidly vitrified by plunging them into liquid ethane (cooled by liquid nitrogen) at its freezing point. The grid was transferred onto a Gatan 626 cryoholder using a cryotransfer device. After that they were transferred to a JEOL-JEM 2100 TEM instrument. Direct imaging was carried out at a temperature of approximately -175 ^{o}C and with a 120 kV accelerating voltage, while acquiring the images with a SC 1000 CCD camera (Gatan, Inc., USA). The data were analyzed with Digital Micrograph software.

Peptide self-assembly. Peptides were dissolved in unbuffered filtered water (Millipore 0.22 μm filter, 18 Ω) by the addition of water to the lyophilized powder followed by sonication (3 min) to obtain homogeneous and optically transparent solutions.

3. Peptide Characterization.

The molecular weights of the peptides were confirmed by MALDI-TOF mass spectrometry.

Peptide **P1** (MALDI-TOF-MS) m/z 2070.08 (2070.43 calcd for [M+H^+]), 2092.17 (2092.42 calcd for [M+Na^+]), 2108.21 (2108.53 calcd for [M+K^+]).

Peptide **P2** (MALDI-TOF-MS) m/z 2071.24 (2071.38 calcd for [M+H^+]), 2093.01 (2093.37 calcd for [M+Na^+]), 2109.18 (2109.48 calcd for [M+K^+]).

Peptide **P3** (MALDI-TOF-MS) m/z 2135.82 (2135.51 calcd for [M+H^+]), 2157.79 (2157.5 calcd for [M+Na^+]), 2173.85 (2173.61 calcd for [M+K^+]).

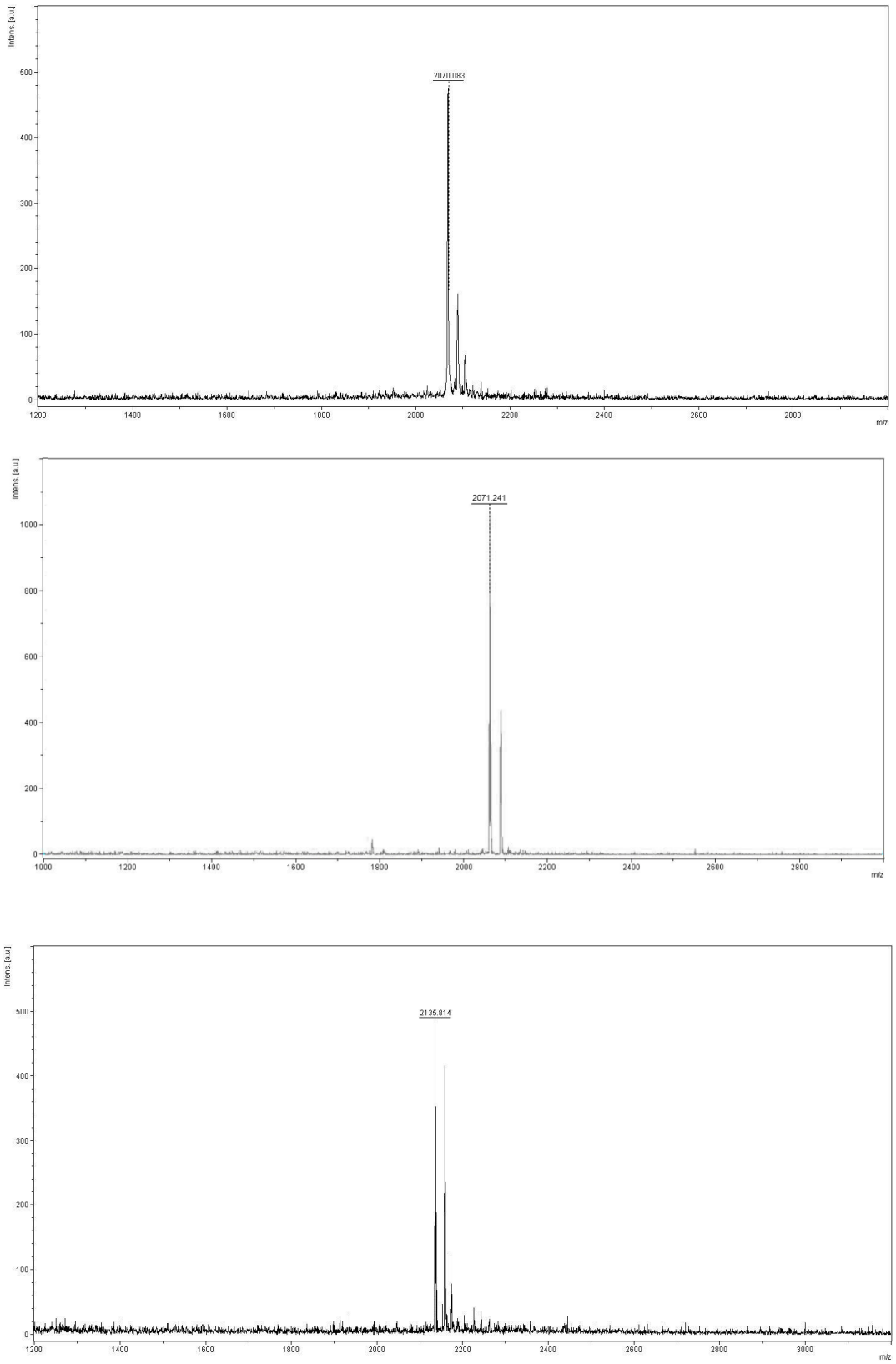


Fig. S1 MS spectra of peptides P1 (top), P2 (middle) and P3 (bottom).

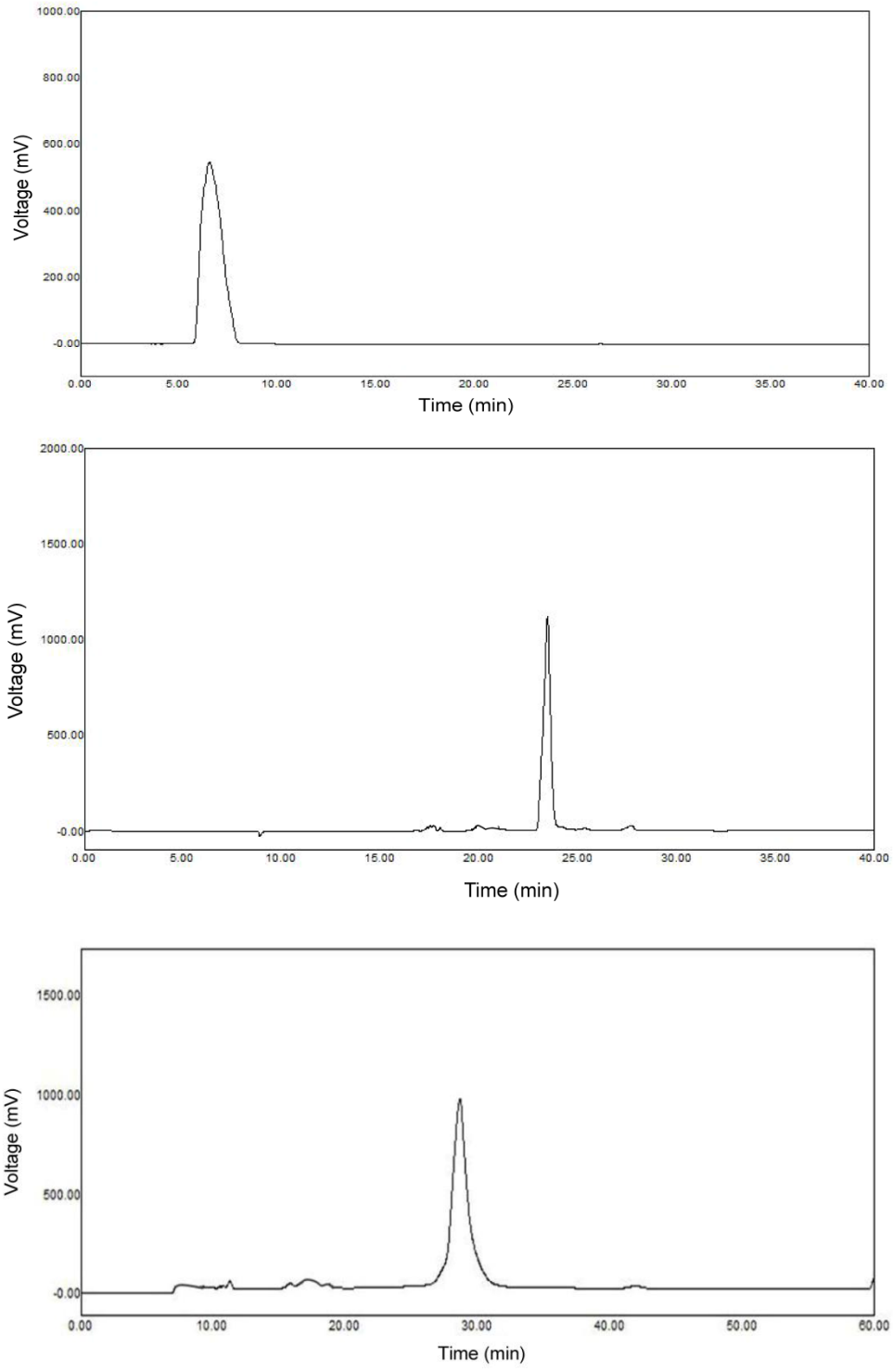


Fig. S2 HPLC spectra of peptides P1 (top), P2 (middle) and P3 (bottom).

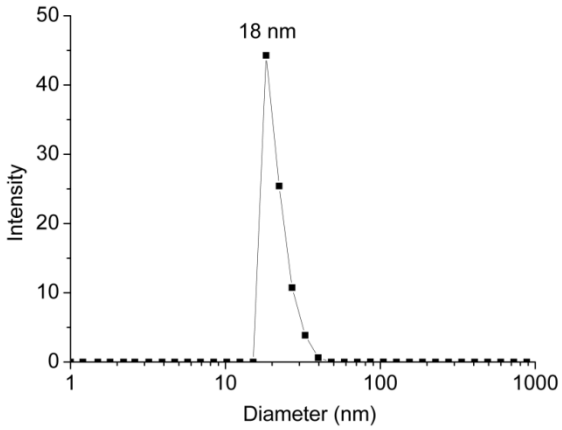


Fig. S3 DLS spectra of peptide P1 obtained from 40 μM aqueous solution.

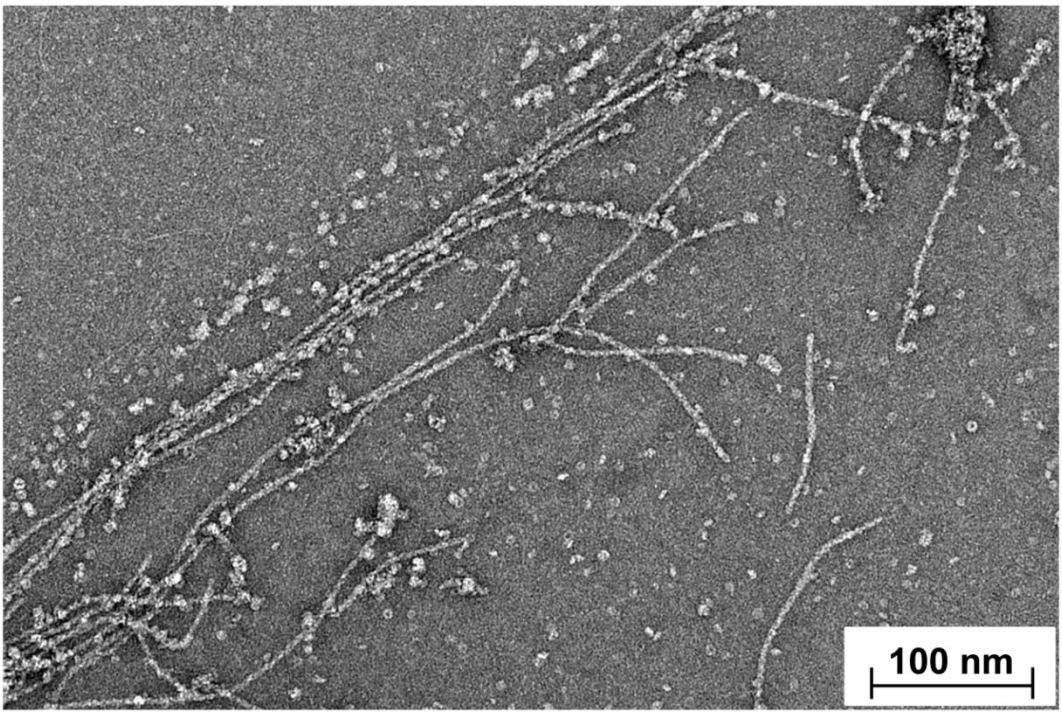


Fig. S4 TEM image of P1 obtained from 40 μM aqueous solution with NaCl concentration of 200 mM.

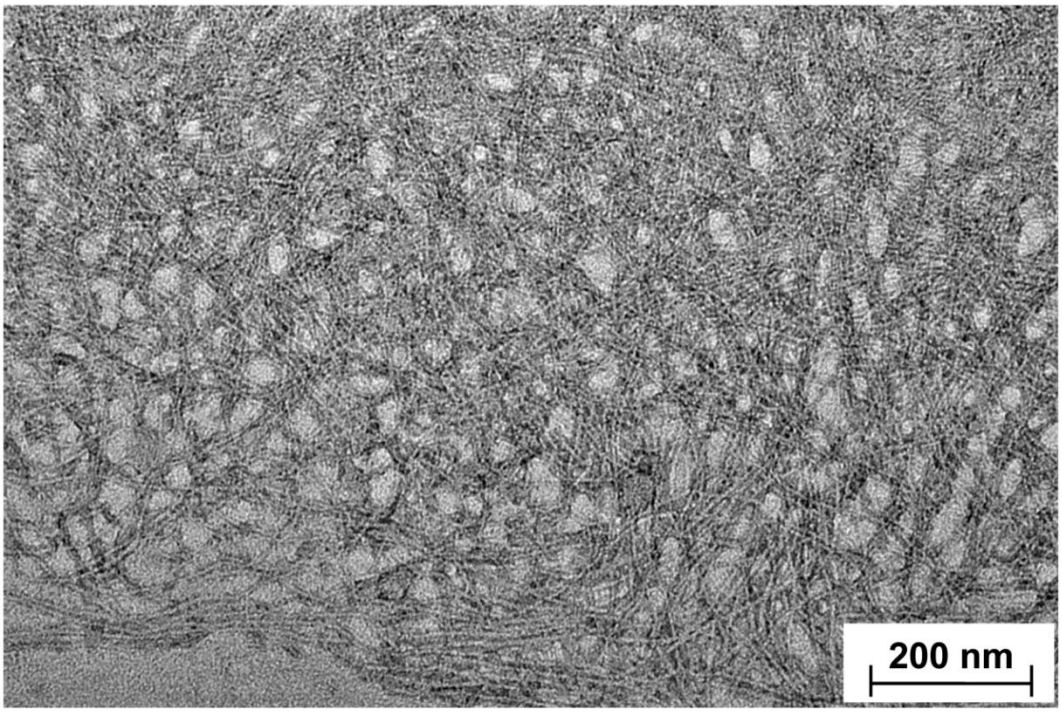


Fig. S5 TEM image of P2 obtained from 40 μM aqueous solution.

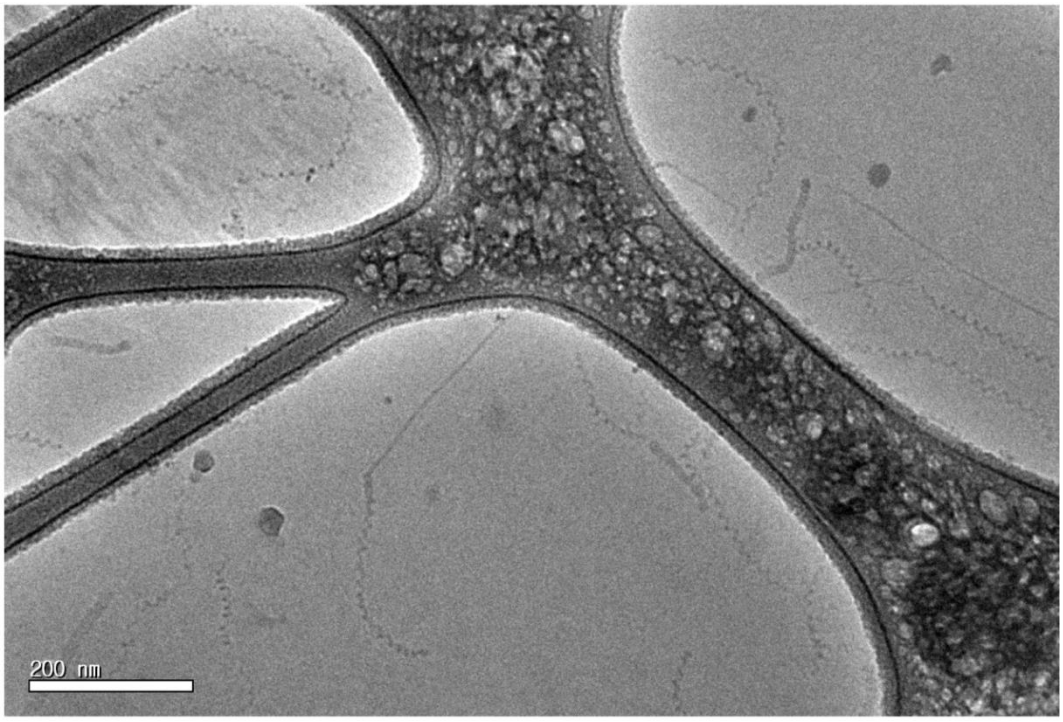


Fig. S6 cryo-TEM image of peptide P2 obtained from 40 μM aqueous solution.

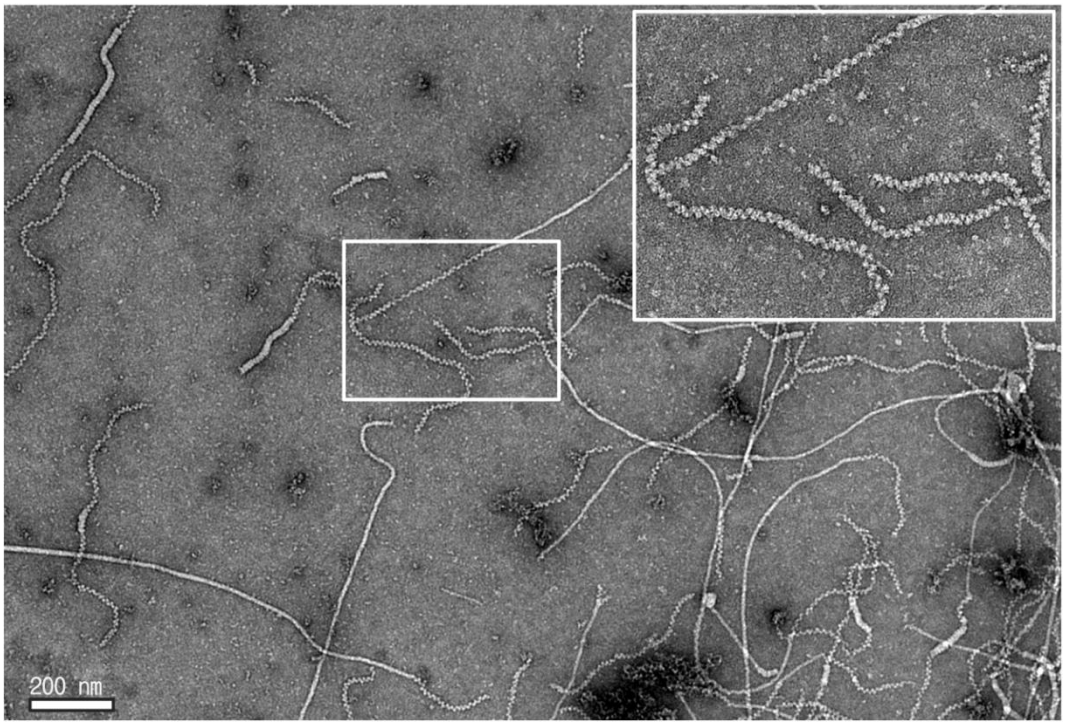


Fig. S7 TEM image of peptide P2 obtained from 40 μM aqueous solution.