

Dynamic Self-Assembly of Surfactant-like Peptides A₆K and A₉K

Jing Wang^a, Shuyi Han^a, Gang Meng^a, Hai Xu^{a,*}, Daohong Xia^a, Xiubo Zhao^b, Ralf
Schweins^c, Jian R. Lu^{b,*}

^a *Centre for Bioengineering and Biotechnology, China University of Petroleum
(East China), 66 Changjiang West Road, Qingdao Economic Development Zone,
Qingdao 266555, P.R. China*

^b *Biological Physics Group, School of Physics and Astronomy, University of
Manchester, Schuster Building, Manchester M13 9PL, United Kingdom*

^c *Institut Laue Langevin, DS/LSS Group, 6 Rue Jules Horowitz, BP 156, 38042
Grenoble Cedex 9, France*

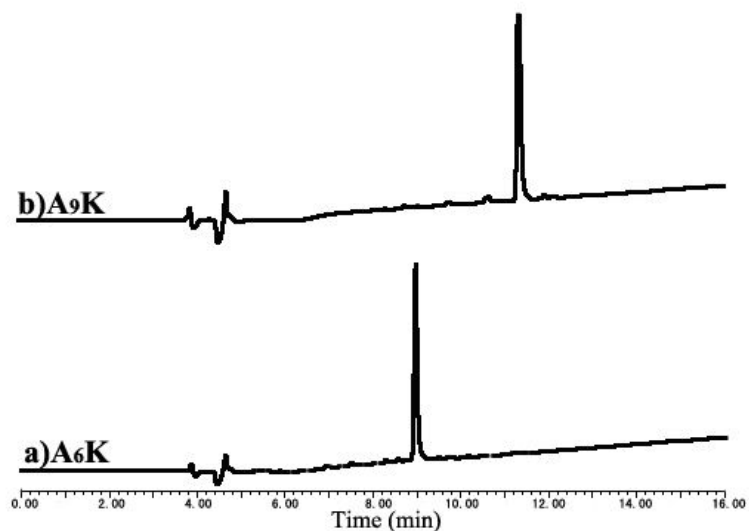


Figure SI-1 HPLC profiles of a)A₆K and b)A₉K. The experimental conditions for this HPLC analysis of two peptides are as follows: eluent A, 0.1% trifluoroacetic acid in water, 0→3min, 95% (A%), 3→5min, 95→40% (A%); eluent B, 0.1% acetonitrile in water; UV, 214nm; flow rate, 0.8mL/min; column, RP-18, 4.6mm×150mm. The measurements were performed on a Waters 2695 Alliance HPLC system at the temperature of 25 °C

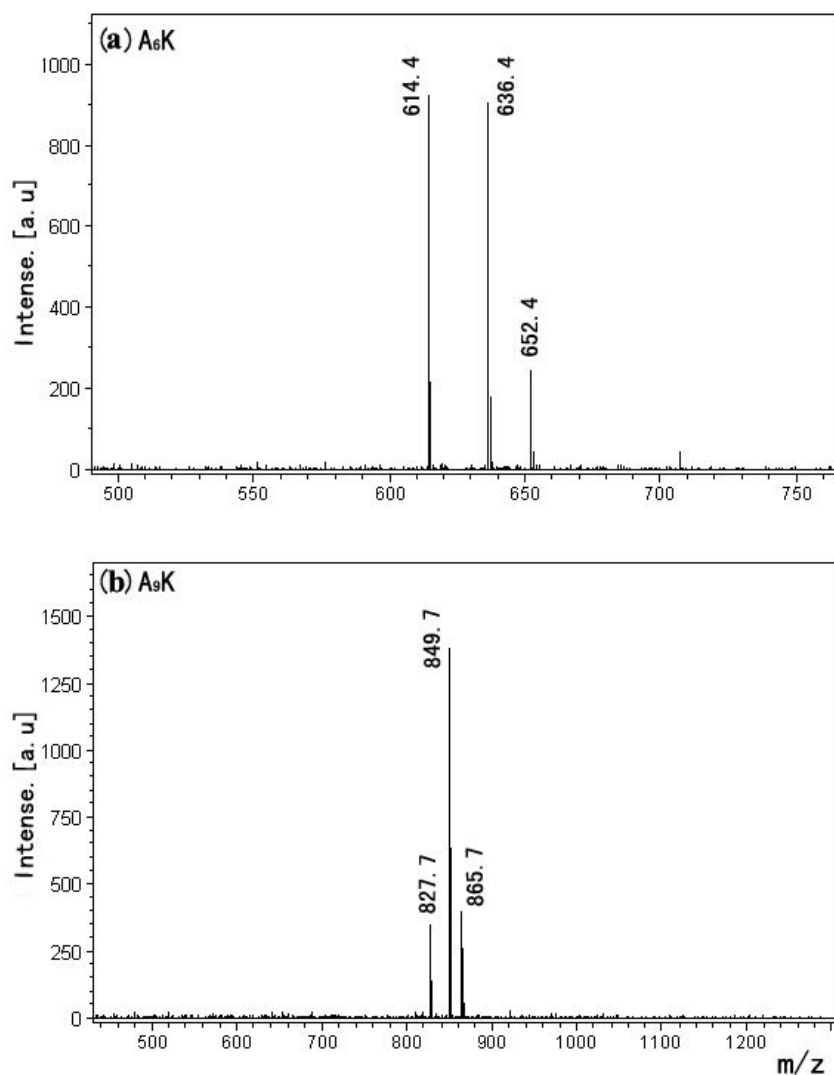


Figure SI-2. MALDI-TOF mass spectra of a) A₆K and b) A₉K. The measurements were performed on Bruker Biflex III matrix assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometer equipped with a 337 nm nitrogen laser, and 4-hydroxy- α -cyanocinnamic acid was used as the matrix. The samples were dissolved with the matrix in 1:1 (v/v) acetonitrile : water with 1% trifluoroacetic acid. Around 0.5 μ l of the sample solution was placed on a metal sample plate and then allowed to air-dry at ambient temperature. Mass spectra were acquired in positive linear mode and using an acceleration voltage of 19 kV. External mass calibration was performed using a standard peptide mixture. Spectra were obtained by setting the laser power close to the threshold of ionization and generally 100 pulses were acquired and averaged.

The calculated molecular masses for the two peptides are all well consistent with the observed as follows:

A₆K: expected masses $[M+H]^+=614.7$, $[M+Na]^+=636.7$, $[M+K]^+=652.7$; observed masses $[M+H]^+=614.4$, $[M+Na]^+=636.4$, $[M+K]^+=652.4$.

A₉K: expected masses $[M+H]^+=827.9$, $[M+Na]^+=849.9$, $[M+K]^+=865.9$; observed masses $[M+H]^+=827.7$, $[M+Na]^+=849.7$, $[M+K]^+=865.7$.

It is important to note that besides the singly charged molecular ion peaks, no other peak as well as fragmental ion peak was observed, indicating the high purity of our peptide samples.

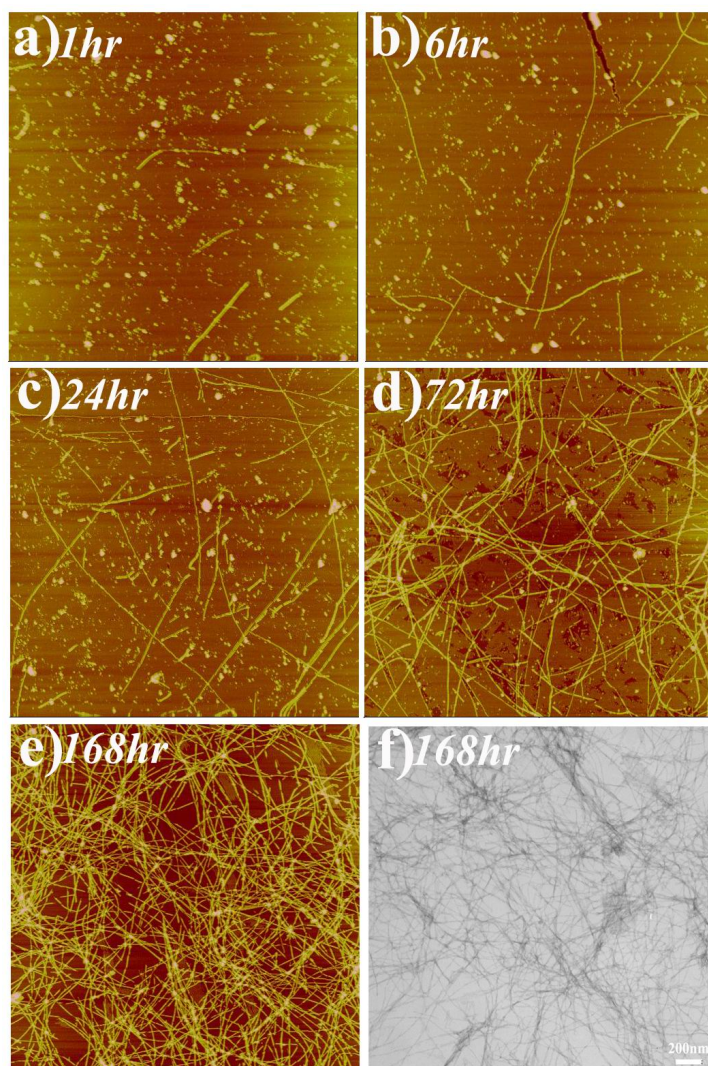


Figure SI-3 Low magnification height AFM images of A_6K assemblies (2mM at pH 6.0) at different time points: a) 1h, b) 6h, c) 24h, d) 72h and e) 168h and the low magnification TEM micrograph at 168h. These AFM images were scanned using the tapping mode, and the scan size is $5 \times 5 \mu\text{m}^2$ and the Z scales are 15 nm. For TEM, the sample was negatively stained with uranyl acetate, and the scale bar is 200 nm