Hydrophobic Region Induced Transitions in Self-assembled Peptide Nanostructures

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1. HPLC Analysis

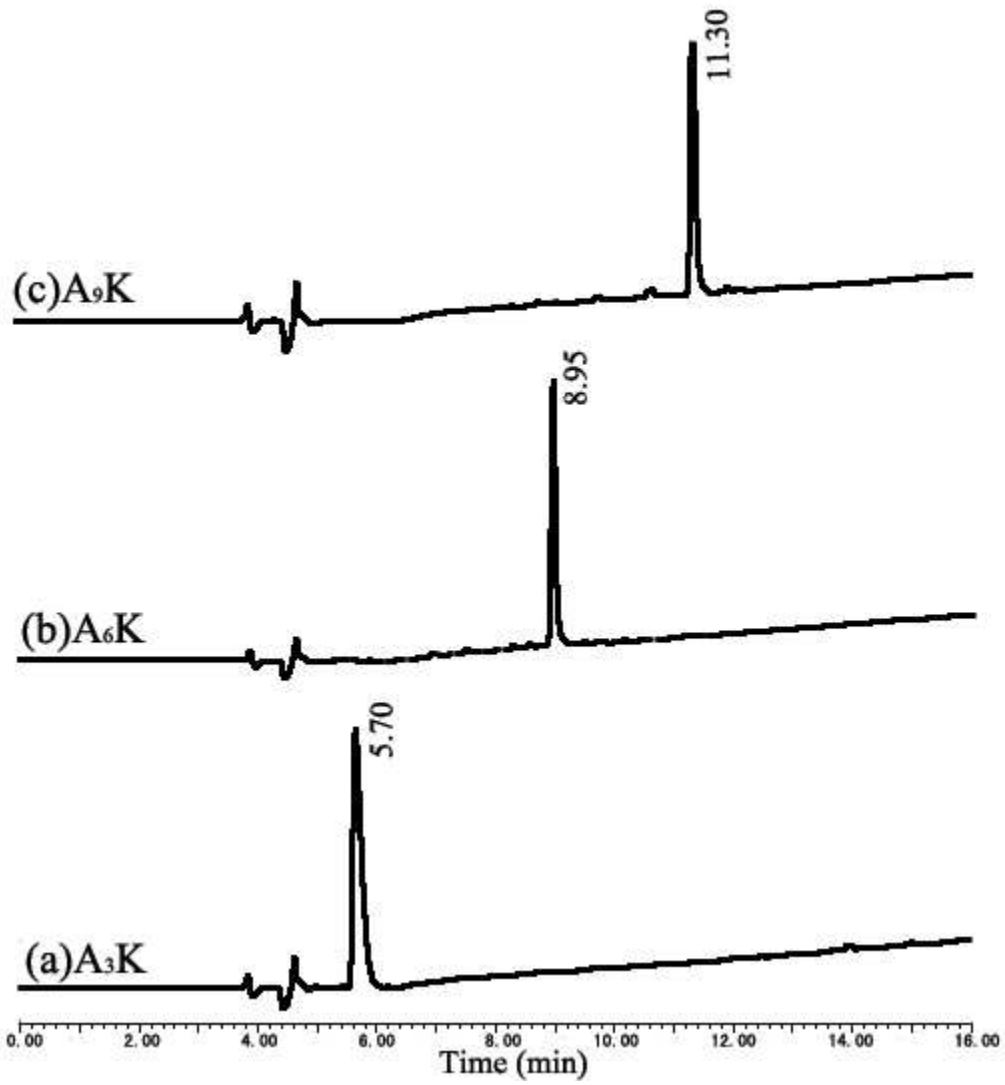

Figure SI-1. HPLC profiles of (a)A_3K, (b)A_6K, and (c)A_9K. The conditions for HPLC analysis of the three peptides are as follows: eluent A, 0.1% trifluoroacetic acid in water, 0→3min, 95% (A%), 3→5min, 95→40% (A%); eluent B, 0.1% acetonitrile in water; UV, 214nm; flow rate, 0.8mL/min; column, RP-18, 4.6mm×150mm. The measurements were performed on a Waters 2695 Alliance HPLC system at 25 ^oC

2. MALDI-TOF MS Analysis

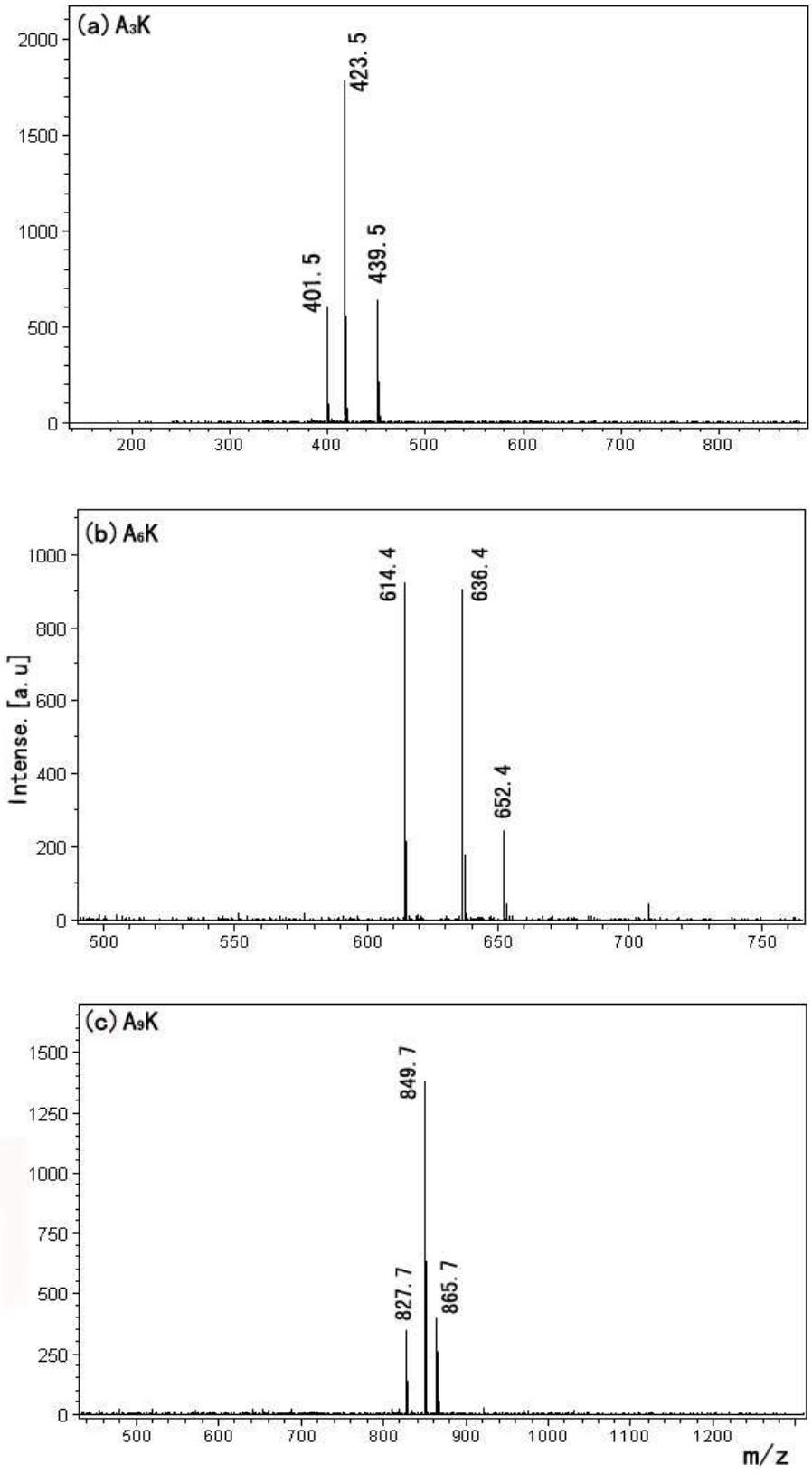

Figure SI-2. MALDI-TOF mass spectra of (a)A_3K, (b)A_6K, and (c)A_9K. The measurements were

performed on Bruker Biflex III matrix assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometer equipped with a 337nm 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 μl 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 three peptides are all well consistent with the observed as follows:

A_3K: expected masses $[M+H]^+$=401.4, $[M+Na]^+$=423.4, $[M+K]^+$=439.4; observed masses $[M+H]^+$=401.5, $[M+Na]^+$=423.5, $[M+K]^+$=439.5.

A_6K: 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.

A_9K: 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 distinguished singly charged molecular ion peaks, no other peak as well as fragmental ion peaks was observed, indicating the high purities of our peptide samples.