Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information for:

Switching of Self-Assembly in a Peptide Nanostructure with a Specific Enzyme

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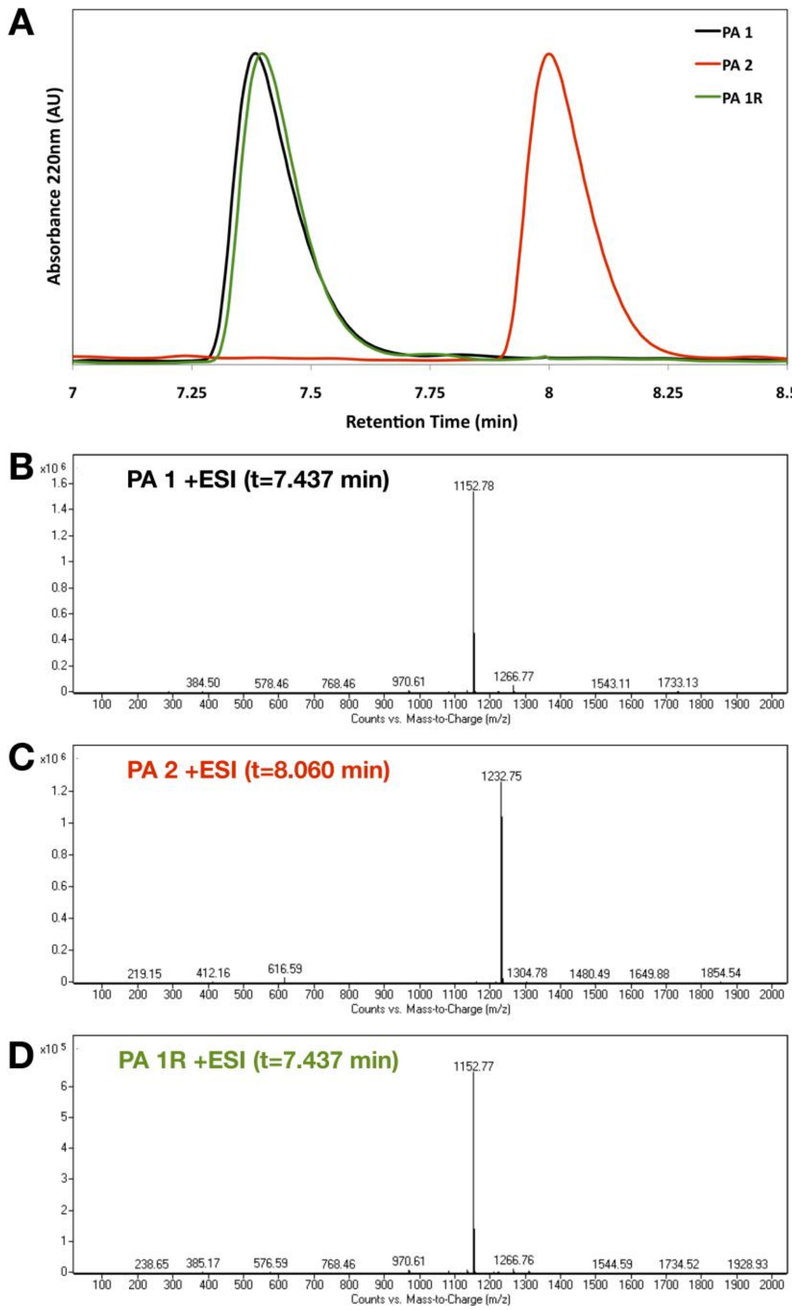

Figure S1: Treatment of PA **1** with PKA to form PA **2** and then subsequent dephosphorylation with AP to recover PA **1R**. LC traces (**A**) indicate reaction goes to completion in each direction, while MS results (**B-D**) confirm the identity of each peak to correspond to the addition and removal of a phosphate.

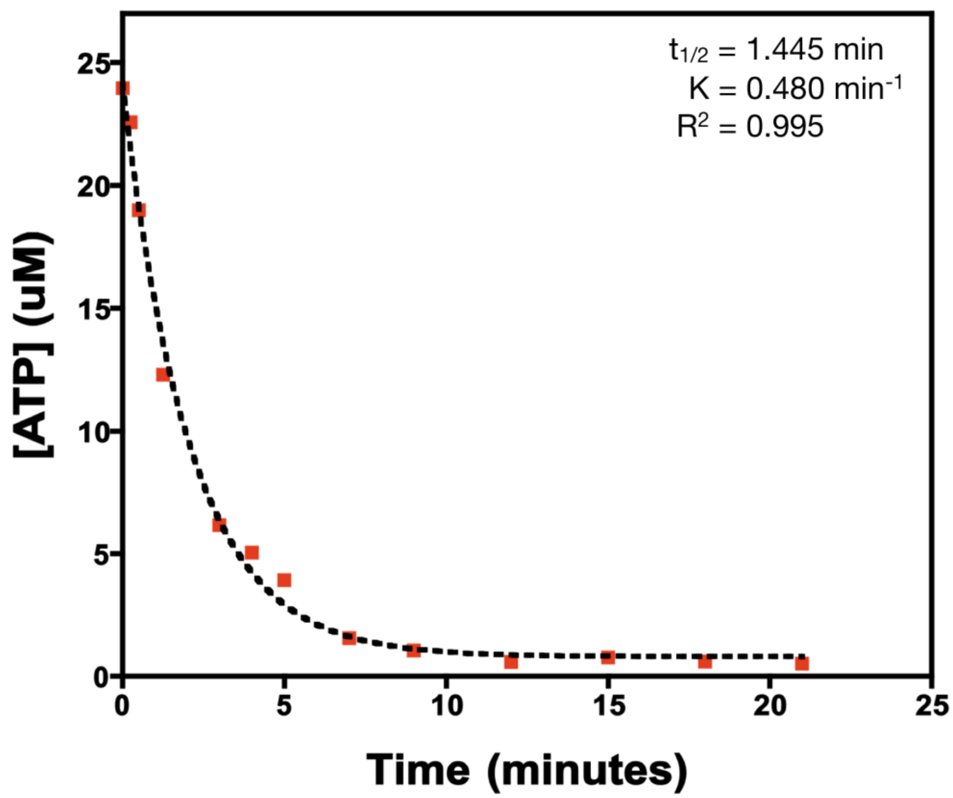

Figure S2: Monitoring reaction rate through ATP concentration over time and fitting this data to a 1-phase exponential decay model where $[ATP]=(\Delta C)*e^{-Kt} + C_f$ results in a half-life (0.69/K) of approximately 1.445 minutes for phosphorylation of PA **1** to form PA **2**.

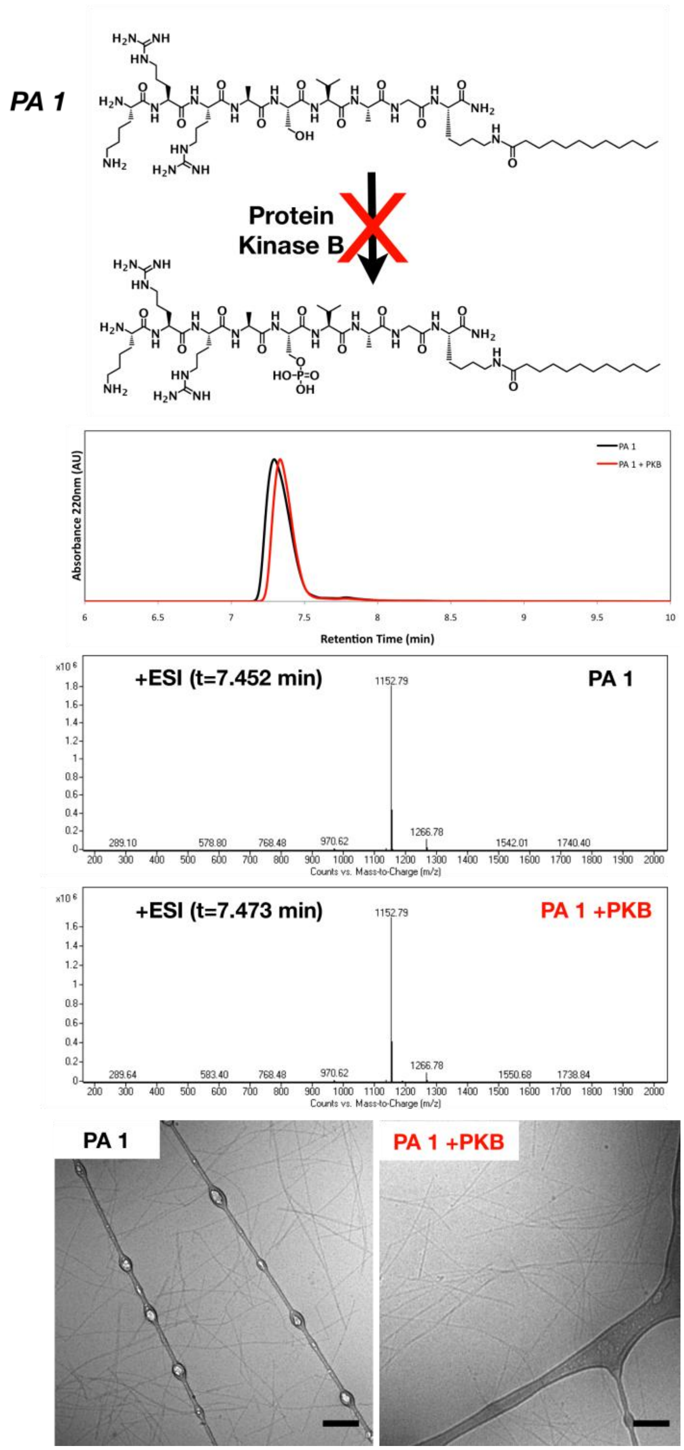

Figure S3: To evaluate sequence specificity, we treated PA **1** with protein kinase B (PKB). This resulted in no phosphorylation of the serine, detected by LC-MS, and did not lead to a loss of nanofiber morphology analyzed by cryo-TEM (scale bars of 200 nm).

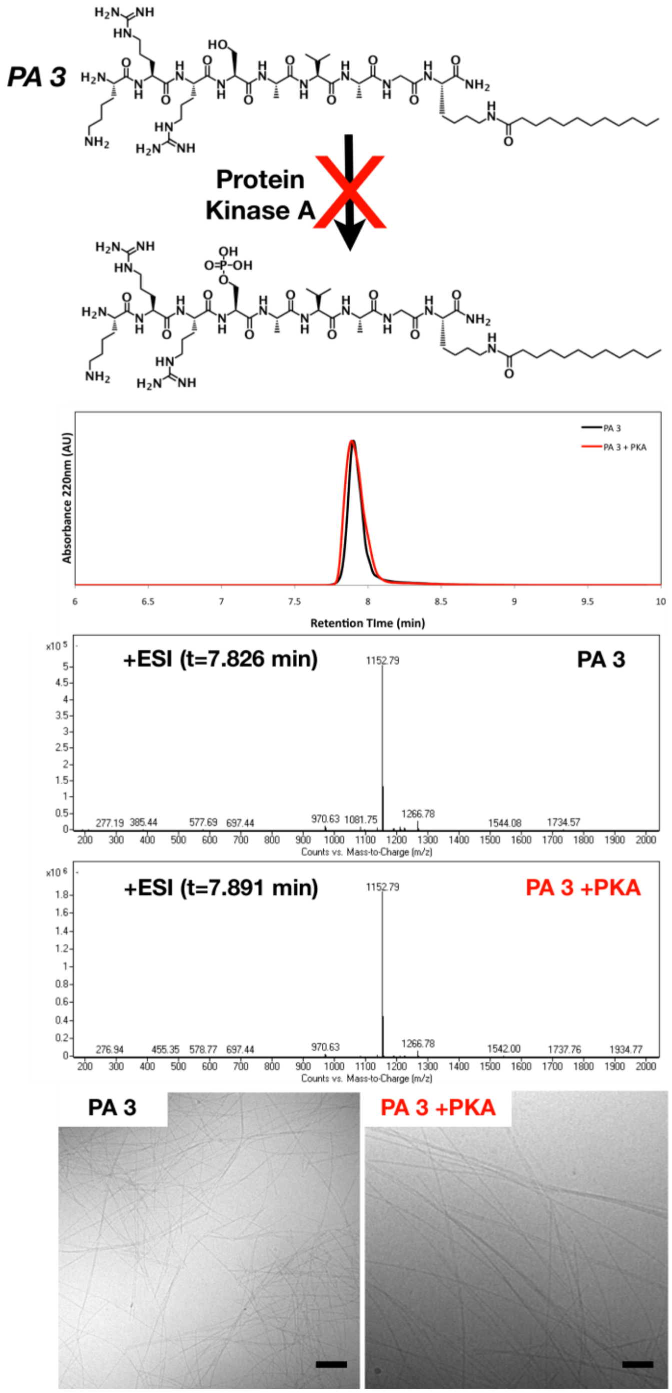

Figure S4: To further evaluate sequence specificity, we created a derivation of PA **1** with the serine residue moved (PA **3**) and treated with PKA. This resulted in no phosphorylation of the serine, detected by LC-MS, and did not lead to a loss of nanofiber morphology analyzed by cryo-TEM (scale bars of 200 nm).

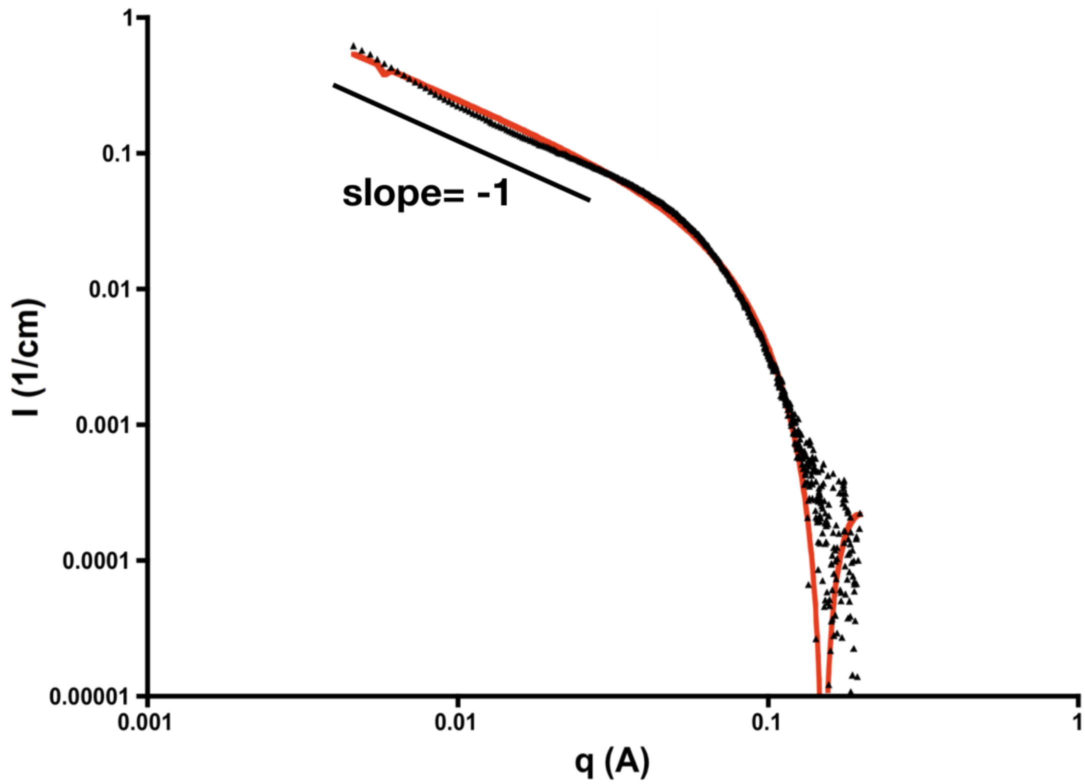

Figure S5: Solvent subtracted SAXS data of PA **1**. Initial slope of -1 is consistent with cylindrical geometry. Solid line represents a fit of this data to a cylinder model.

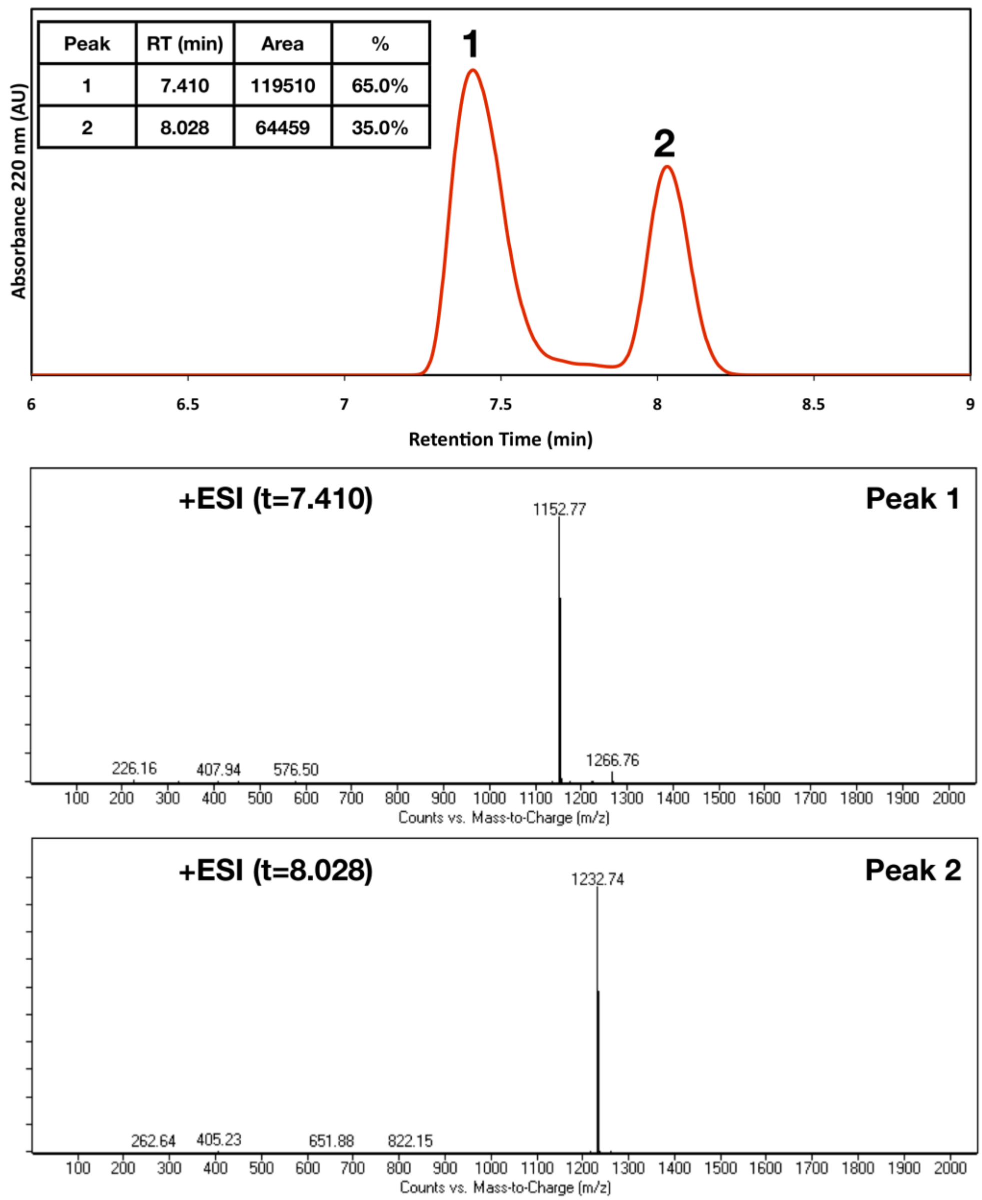

Figure S6: LC-MS from a hydrogel of PA **1** treated for 24 hours with PKA. Some (35%) of the serine residues are phosphorylated in the hydrogel state.

Small Angle X-Ray Scattering Data Fitting:

Background subtracted SAXS data was fit to a form factor for a simple cylinder. The scattering intensity of a monodispersed system of particles of identical shape can be described as (Ref. S1):

$$I(q) = NP(q)S(q)$$

where N is the number of particles per unit volume, P(q) is the form factor revealing the specific size and shape of the scaterrers and S (q) is the structure factor that accounts for the interparticle interactions In dilute solutions, where the interactions between the objects can be neglected, S(q) equals one.

A form factor for a simple cylinder given by (Ref S2):

$$P(q) = \int_0^{\pi/2} \left[\frac{\sin\left(\frac{qL\cos\alpha}{2}\right)}{\frac{qL\cos\alpha}{2}} \frac{2J_1(qR\sin\alpha)}{qR\sin\alpha} \right]^2 \sin\alpha \cdot d\alpha$$

$J_1(x)$ is the first order Bessel function and a is defined as the angle between the cylinder axis and the scattering vector, q. R and L are the cylinder radius and length, respectively.

References:

S1. O. Glatter and O. Kratky, *Small angle x-ray scattering*, Academic Press, London ; New York, 1982.

S2. J. S. Pedersen, *Advances in Colloid and Interface Science*, 1997, **70**, 171-210.