Supporting Information

for

Catalytic Supramolecular Self-Assembled Peptide Nanostructures for Ester Hydrolysis

Figure S1. Mass spectra of peptides following the subtraction of water readings. a) For H-PA, [M+H]^+ (calculated) = 664.86, [M+H]^+ (observed) = 664.4967, [M/2+H]^+ (calculated) = 332.43, [M/2+H]^+ (observed) = 332.2308, [2M+H]^+ (calculated) = 1326.82, [2M+H]^+ (observed) = 1325.8982. b) For S-PA, [M-H]^− (calculated) = 612.79, [M-H]^− (observed) = 612.4022, [2M-H]^− (calculated) = 1226.58, [2M-H]^− (observed) = 1225.7999. c) For D-PA, [M-H]^− (calculated) = 639.81, [M-H]^− (observed) = 639.2788.
Figure S2. Transmission electron microscopy (TEM) images of the nanostructures of the catalytic peptide complexes.

Figure S3. Transmission electron microscopy (TEM) images of the nanostructures exhibited by peptide molecules.
Figure S4. Atomic force microscopy (AFM) images of the nanostructures of the peptide complexes.

Figure S5. FT-IR spectra of the peptide complexes for secondary structure investigation.
Figure S6. The Michaelis–Menten diagram of the catalytic activity of CT-PAs for pNPA in 1x PBS (error bars in all groups represent standard deviations of at least three independent measurements).

Figure S8. Degradation of acetylcholine in the presence of D/H/S CT-PAs, as analyzed with LC-MS. a) Relative abundance calculations used to track PA-dependent hydrolysis. b) Abundance diagram showing choline formation. c) Mass spectrum of the peptide following the subtraction of water readings. \([M]^+ \) (calculated) = 146.21, \([M]^+ \) (observed) = 146.1267, \([M]^+ \) (calculated) = 104.17, \([M]^+ \) (observed) = 104.1083.

Figure S9. Concentration dependent kinetics diagram of the catalytic activity of CT-PAs for acetylthiocholine in 1x PBS (error bars in all groups represent standard deviations of at least three independent measurements).

**Statistical Analysis.** All experiments were independently repeated at least twice, with at least four replicas for each experimental or control group in each independent assay. All quantitative results are expressed as mean ± standard error of means (SEM). Statistical analyses were performed by one-way analysis of variance (ANOVA) or Student’s test, whichever applicable. Significant differences were evaluated by the P-value; differences were considered statistically significant at P < 0.05.