Supplementary Information 1

Coarse-grained molecular dynamics studies of the structure and stability of peptide-drug amphiphile filaments for drug delivery

Myungshim Kang, Honggang Cui, and Sharon M. Loverde

S1-1. Coarse-grained molecular model

CG representation (mapping)

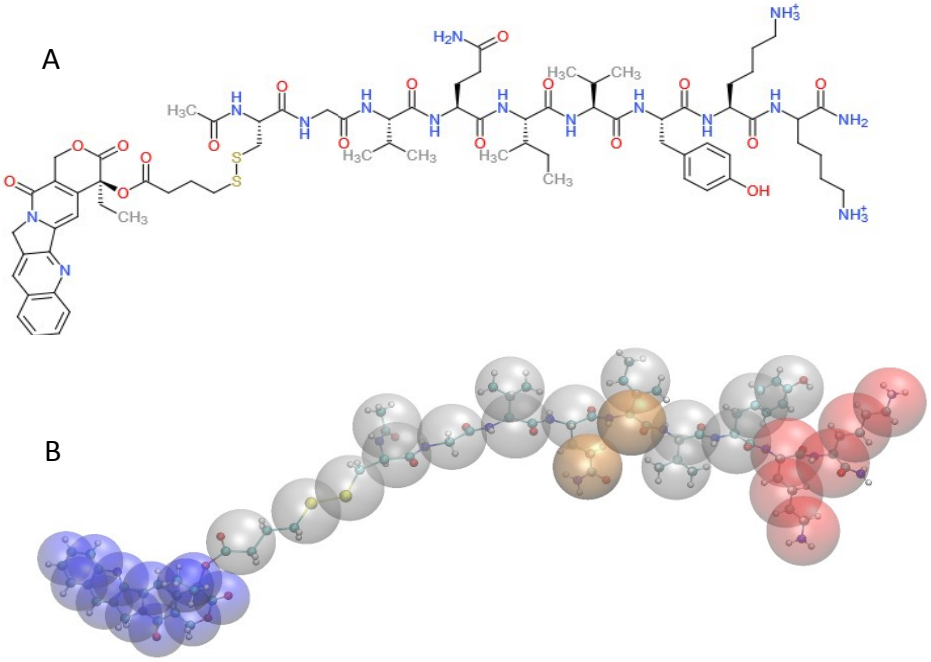

Fig. S1-1. Structure of DA. A. mCPT-buSS-Tau in 2D structure. B. mCPT-buSS-Tau in CG beads, overlapped on its atomistic structure. CPT, LYS, GLU, and the rest are in blue, red, orange, and gray.

Table S1-1. Simulation systems.

System	mCPT-buSS-Tau	Cl^-	[Cl-], mM	Water	Simulation box at equilibrium, $Å^3$	Simulation time, μs
random, 16 mM	96	192	31	112,132	211 x 244 x 199	1
random, 200 mM	960	1,920	398	68,105	187 x 213 x 201	1
Pre-assembled, infinite filament	84	168	252	10,432	140 x 149 x 53	1
Pre-assembled, finite filament	840	1,680	250	129,148	120 x 122 x 762	1.515

SI-2. Starting structures for the preassembled filament system

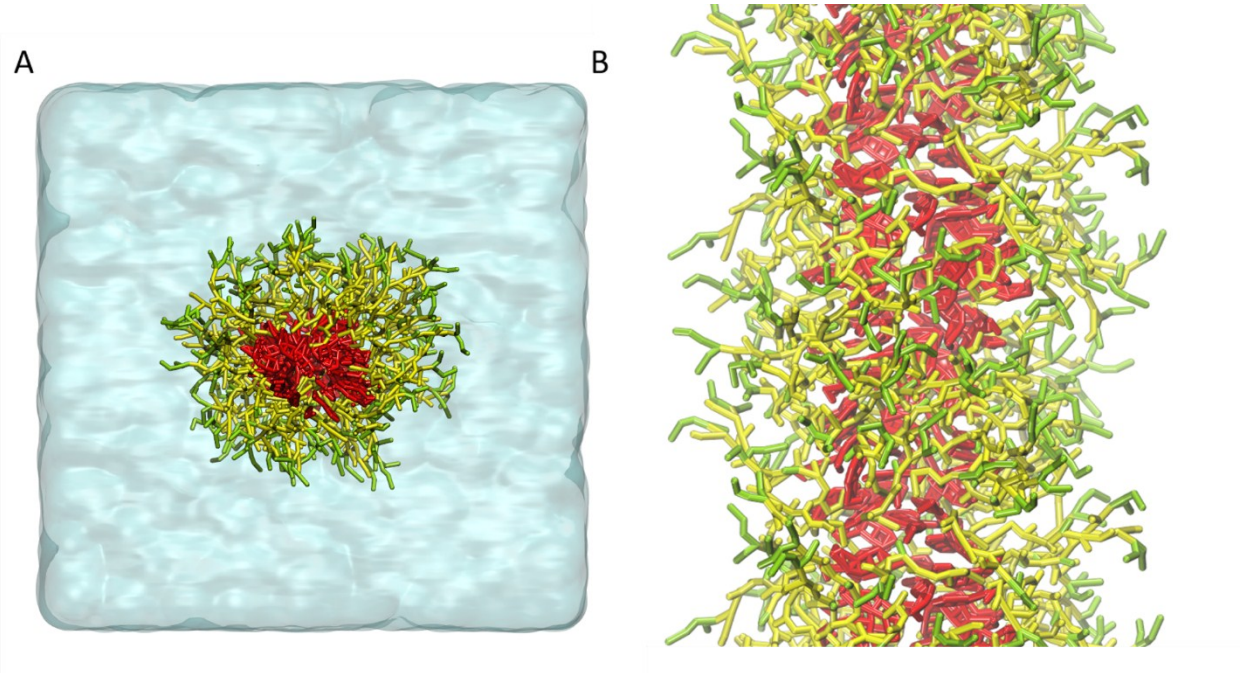

Fig. S1-2. Starting structure of the preassembled system. A. Top view. The CPT, charged LYS, polar GLN, and the rest of the DA are displayed in red, light green, light green and yellow, respectively. Water box is shown in transparent cyan. The periodic boundary conditions are used in x, y and z. B. Side view.

SI-3. Water in the DA filaments

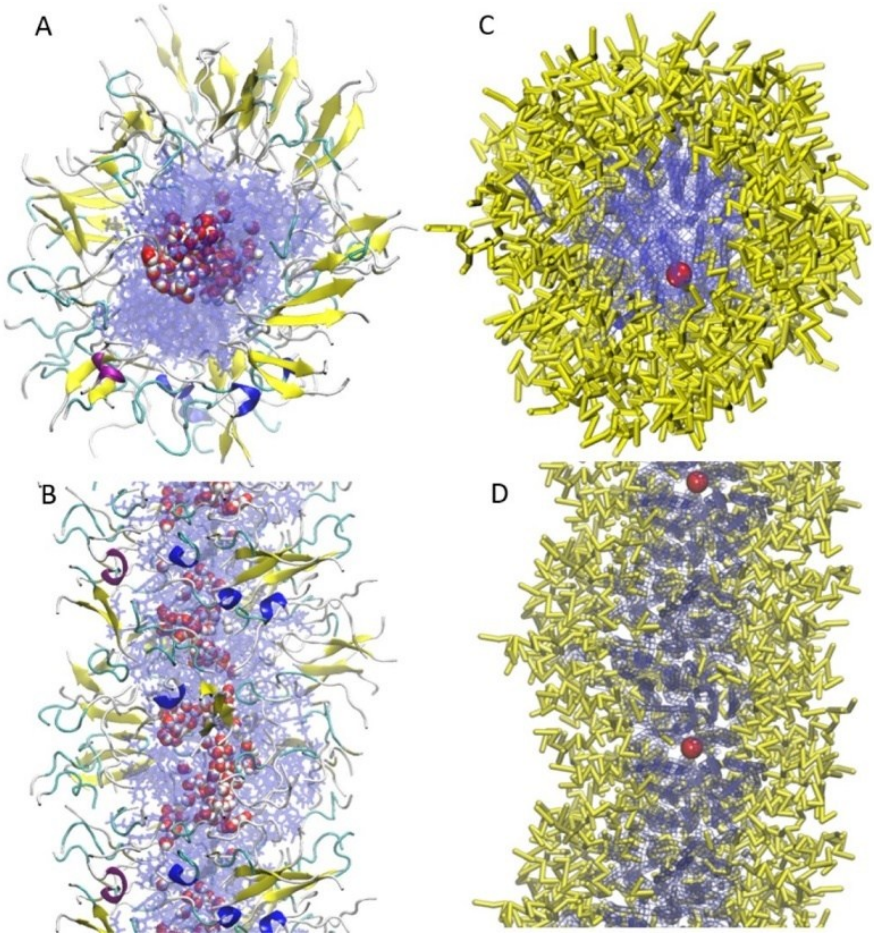

Fig S1-3 . DA filaments. A and B. Top and side views of the atomistic filament with water within 10 Å from the core highlighted in red and white. Adapted with permission from the reference 39. Copyright 2016 American Chemical Society. C and D. Top and side views of the CGed filament with water within 10 Å from the core highlighted in red.

SI-4. Simulation of the random system at the concentration of 200 mM

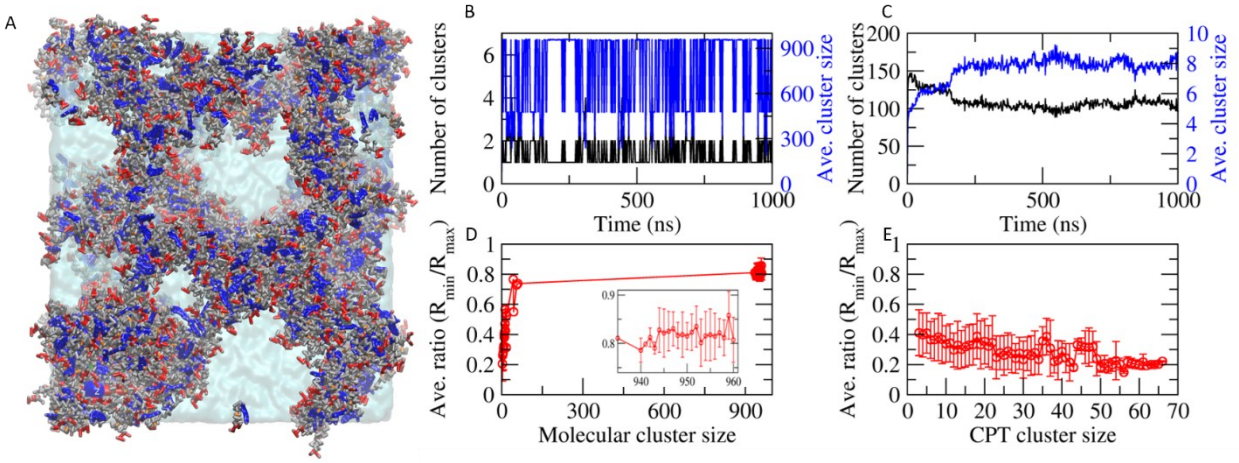

Fig. S1-4. Cluster growth in the random 200 mM system. A. Snapshot of the random 200 mM system at 1 μs. The CPT, charged LYS residue, polar GLN residue, and the rest part of mCPT-Tau are in blue, red, orange, and grey, respectively. Water box is shown in transparent cyan B. The number (black) and the size (blue) of molecular clusters over time. C. The number (black) and the size (blue) of CPT clusters over time. D. The average ratio of the shortest principle axes (R_{min}) to the longest (R_{max}) of molecular clusters. The distribution of the bigger clusters (n>900) are zoomed in the inset. E. The average ratio of R_{min}/R_{max} of CPT clusters.