Electronic Supplementary Infromation on

Stability and growth mechanism of self-assembling putative anti-freeze cyclic peptides

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Straightforward MD and nanotube sequences

This Supplementary Information details some of the settings and outcome of the straightforward MD simulation discussed in the Main Text. Table 1 reports the literature values for the dihedral angles for beta strands [1]. Table 2 gives the composition of the system for each of the MD simulations. Table 3 and 4 summarize the outcome of the MD simulations of the original and altered CPNT systems, respectively. Fig. 1 plots the radial distribution function of water around the hydroxyl oxygen of THR of AFCP. Table 5 and 6 list the sequence and the orientation of the original and altered CPNT systems, respectively. Finally, Table 7 and 8 report the measured average and standard deviation of backbone ϕ and ψ angles for each aminoacid of the different size nanotubes of the original and altered CP sequence, respectivly.

Amino acid	Φ_{aver}	σ_Φ	Ψ_{aver}	σ_Ψ
L-ALA	-130.2	21.4	143.8	14.6
L-LEU	-115.2	15.8	131.8	13.5
L-LYS	-118.9	17.5	134.2	15.3
L-THR	-123.9	14.0	138.1	14.3
D-ALA	130.2	-	-143.8	-

Table 1 Average values for the dihedral angles Φ, Ψ and their estimated standard deviations $\sigma_{\phi,\psi}$ for anti-parallel β-strands [1].

Original CP sequence					
System	**#CP**	**#AA**	**#H_20**	**#atoms**	**V (nm^3)**
CPNT2	2	16	4093	12519	127.48
CPNT3	3	24	4519	13917	139.09
CPNT4	4	32	4847	15021	151.47
CPNT5	5	40	5549	17247	174.34
CPNT6	6	48	6280	19560	197.25
AFCP sequence					
System	**#CP**	**#AA**	**#H_20**	**#atoms**	**V (nm^3)**
CPNT2	2	16	4035	12325	122.57
CPNT3	3	24	4100	12630	131.07
CPNT4	4	32	4662	14426	144.55
CPNT5	5	40	5417	16801	169.58
CPNT6	6	48	6267	19317	195.47

Table 2 Original CP sequence: Composition of systems containing CPNTs of sequence cyclo-[(L-LYS-D-ALA-L-LEU- D-ALA)$_2$]. AFCP sequence: Composition of systems containing nanotubes of AFCP sequence cyclo-[(L-LYS-D-ALA)$_2$-(L- THR-D-ALA)$_2$].

System	Run 1	Run 2	Run 3	Run 4	Run 5
CPNT2	B	B	B	B	B
CPNT3	B	B	B	B	B
CPNT4	B	B	B	B	B
CPNT5	B	B	B	B	B
CPNT6	B	B	B	B	B $\rightarrow$ I

Table 3 Original sequence: Visiting states of different size CPNTs in the course of a 100 ns NPT simulations. B denotes the bound state and I the area of phase space which does not belong neither to B nor U.

System	Run 1	Run 2	Run 3	Run 4	Run 5
CPNT2	B $\rightarrow$I$\rightarrow$U$\rightarrow$ I$\rightarrow$U$\rightarrow$I	B	B$\rightarrow$I$\rightarrow$U$\rightarrow$I	B	B$\rightarrow$I$\rightarrow$B
CPNT3	B	B	B	B	B
CPNT4	B	B	B	B	B
CPNT5	B	B	B	B	B
CPNT6	B	B	B	B	B

Table 4 AFCP sequence: Visiting states of different size CPNTs in the course of a 100 ns NPT simulations. B denotes the bound state and U the unbound state. I denotes the area of phase space which does not belong neither to B nor U.

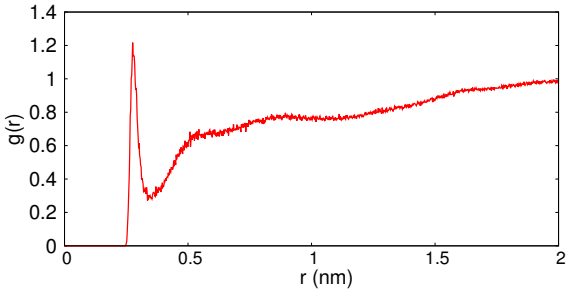

Figure 1 Radial distribution function of the water oxygen around the side chain oxygen of the THR residue in the AFCP sequence hexamer.

Orientation	Sequence								Name
N → C	L-LYS-1	D-ALA-2	L-LEU-3	D-ALA-4	L-LYS-5	D-ALA-6	L-LEU-7	D-ALA-8	**CP1**
C ← N	L-LYS-9	D-ALA-10	L-LEU-11	D-ALA-12	L-LYS-13	D-ALA-14	L-LEU-15	D-ALA-16	**CP2**
N → C	L-LYS-17	D-ALA-18	L-LEU-19	D-ALA-20	L-LYS-21	D-ALA-22	L-LEU-23	D-ALA- 24	**CP3**
C ← N	L-LYS-25	D-ALA-26	L-LEU-27	D-ALA-28	L-LYS-29	D-ALA-30	L-LEU-31	D-ALA-32	**CP4**
N → C	L-LYS-33	D-ALA-34	L-LEU-35	D-ALA-36	L-LYS-37	D-ALA-38	L-LEU-39	D-ALA-40	**CP5**
C ← N	L-LYS-41	D-ALA-42	L-LEU-43	D-ALA-44	L-LYS-45	D-ALA-46	L-LEU-47	D-ALA-48	**CP6**

Table 5 Original CP sequence: schematic representation of the arrangement and chirality of the amino acids in the CP chains of sequence cyclo-[(L-LYS-D-ALA-L-LEU-D-ALA)$_2$] within various CPNTs. The sequential chains are named as CP1 to CP6. The terminals are assumed to be bonded in order to form the cyclic structure.

Orientation	Sequence								Name
N → C	L-LYS-1	D-ALA-2	L-THR-3	D-ALA-4	L-THR-5	D-ALA-6	L-LYS-7	D-ALA-8	**CP1**
C ← N	L-LYS-9	D-ALA-10	L-THR-11	D-ALA-12	L-THR-13	D-ALA-14	L-LYS-15	D-ALA-16	**CP2**
N → C	L-LYS-17	D-ALA-18	L-THR-19	D-ALA-20	L-THR-21	D-ALA-22	L-LYS-23	D-ALA-24	**CP3**
C ← N	L-LYS-25	D-ALA-26	L-THR-27	D-ALA-28	L-THR-29	D-ALA-30	L-LYS-31	D-ALA-32	**CP4**
N → C	L-LYS-33	D-ALA-34	L-THR-35	D-ALA-36	L–THR-37	D-ALA-38	L-LYS-39	D-ALA-40	**CP5**
C ← N	L–LYS-41	D-ALA-42	L-THR-43	D-ALA-44	L-THR-45	D-ALA-46	L-LYS-47	D-ALA-48	**CP6**

Table 6 AFCP sequence: schematic representation of the arrangement and chirality of the amino acids in the CP Chains of sequence cyclo-[(L-LYS-D-ALA-)$_2$-(L-THR-D-ALA)$_2$] within various CPNTs. The sequential chains are named as CP1 to CP6. The terminals are assumed to be bonded in order to form the cyclic structure

	CPNT2			CPNT3			CPNT4			CPNT5			CPNT6		
angles	**LYS**	**LEU**	**ALA**	**LYS**	**LEU**	**ALA**	**LYS**	**LEU**	**ALA**	**LYS**	**LEU**	**ALA**	**LYS**	**LEU**	**ALA**
Φ	-116_{27}	-102_{18}	130_{21}	-119_{24}	-116_{19}	135_{17}	-116_{27}	-113_{19}	136_{17}	-119_{26}	-119_{18}	137_{15}	118_{27}	-116_{19}	138_{15}
Ψ	138_{23}	130_{11}	-129_{47}	137_{16}	129_{14}	-127_{45}	138_{17}	128_{13}	-123_{47}	138_{16}	127_{13}	-117_{57}	138_{16}	127_{12}	-116_{56}

Table 7 Average and standard deviation of backbone ϕ and ψ angles for each aminoacid of the different size nanotubes of the original CP sequence.

	CPNT2			CPNT3			CPNT4			CPNT5			CPNT6		
angles	**LYS**	**THR**	**ALA**	**LYS**	**THR**	**ALA**	**LYS**	**THR**	**ALA**	**LYS**	**THR**	**ALA**	**LYS**	**THR**	**ALA**
Φ	-92_{50}	-111_{29}	114_{29}	-126_{17}	-124_{18}	134_{18}	-130_{13}	-128_{14}	136_{15}	-128_{14}	-127_{15}	137_{14}	-132_{14}	-129_{14}	138_{14}
Ψ	131_{44}	116_{60}	-110_{69}	137_{18}	137_{14}	-125_{53}	137_{14}	136_{13}	-127_{47}	137_{13}	134_{13}	-122_{54}	136_{14}	134_{15}	-130_{39}

Table 8 Average and standard deviation of backbone ϕ and ψ angles for each aminoacid of the different size nanotubes of the AFCP sequence.

References

[1] S. Hovmo, *Acta. Crystallogr. D.*, 2002, **58**, 768.