

Materials Advances

The morphology and structure features of amyloid fibrils fibrillated by hexapeptides with antibiofilm formation activity

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Supplementary Table 1 The first 10 hexapeptides with highest Rosetta energy predicted by ZipperDB

Sequence	Rosetta energy	Antimicrobial effects (Yes or No)	Antibiofilm effects (Yes or No)
LFWLVF	-78.6	No	Yes
MTVGEE	-59.1	No	No
CKNIYS	-53.4	No	No
LKSHQR	-53.4	No	No
CVNAIA	-53.4	No	No
CVQAQY	-51.2	No	No
GMSTFI	-51	No	No
EQIQYY	-49.6	No	No
SSTLSL	-49.6	No	No
TREEKV	-49.5	No	No

Supplementary Table 2 Peak position and the corresponding secondary structure assignment

Position(cm ⁻¹)	Secondary structure assignment
1600-1640, 1670-1680	β -sheets
1640-1650	Random coils
1650-1660	α -helices
1660-1670, 1680-1700	β -turns

Supplementary Table 3 The secondary structures features of ASAPs (H5 and H12) and non-ASAPs (H18 and H21) analyzed by circular dichroism (CD)

		Helix	Sheet	Turn	Unordered
ASAPs	H5 monomers	3.7	43.7	21.2	31.4
	H5 fibrils	3.5	42.4	21.2	32.9
	H12 monomers	3.7	42.3	21.4	32.7
	H12 fibrils	3.4	42.6	21.4	32.7
non-ASAPs	H18 monomers	3.3	42.3	21.3	33.0
	H18 fibrils	3.0	43.9	20.4	32.8
	H21 monomers	3.5	41.9	21.3	33.2
	H21 fibrils	3.4	42.1	20.7	33.9