Elimination of branching in self-assembled beta hairpin peptide fibrils

SAMEER SATHAYE, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware, POCHAN GROUP TEAM — Hydrophobic collapse of amphiphilic -hairpin peptides (e.g. MAX1 VKVKVKVKVDPTKVKVKVKV-NH$_2$) into fibrils and their hierarchical assembly into branched, hydrogel networks has been extensively studied. A physically crosslinked hydrogel network is formed due to fibrillar entanglement and branched defects in hydrophobic collapse during fibril formation. Alternating valine residues with side chains of the same size are responsible for the hydrophobic collapse of the molecule into a β-hairpin and fibril nanostructure with branching. In a new sequence LNK1 (LNK1 (Nal)K(Nal)KAKAKVDPTKAKAK(Nal)K(Nal)-NH$_2$) the non-beta turn valines were replaced with Napthylalanine and alanine amino acid residues, with hydrophobic side chains of larger and smaller volume, respectively, than valine. Thus, formation of a “lock and key” type structure was attempted in the hydrophobic core of the peptide fibrils that would eliminate fibril branching. The folding and network formation of LNK1 has been studied by Circular Dichroism spectroscopy (CD), Transmission Electron Microscopy (TEM) and Oscillatory Rheology. Preliminary rheological characterization suggests the elimination of branching in the fibrils and also a possibility that LNK1 networks, unlike MAX1, are just nanofibrillar suspensions rather than permanently physically crosslinked hydrogels.

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