Atomic-level three-dimensional models of amyloid-like self-assembling peptides derived by molecular dynamics

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Molecular self-assembly in ordered supramolecular structures represents an attractive tool for the fabrication of novel nanomaterials. In this field, self-assembled peptides have received significant interest as their physicochemical properties make them suitable for several applications in biology, nanomedicine, nanofabrication in both academia and industry[1]. A deep knowledge of their structural organization is essential for understanding their physicochemical properties and for the ad-hoc engineering of new materials with enhanced properties.
In recent years, we have studied novel self-assembled PEGylated peptide-based systems (F6, dinaphthylalanine, $(FY)_3$, W4, Y4) which are also endowed with interesting photoluminescent properties. Using molecular modeling and molecular dynamics (MD) techniques we were able to provide the first atomic-level model for the peptide moiety of these assemblies (Figure 1)[2-7]. We showed that the steric zipper association exhibited by amyloid-like peptides is highly compatible with the structure of the peptide-based spine of these materials. Our models well agree with the experimental characterization performed on these systems using spectroscopic and X-ray scattering techniques. Moreover, Replica Exchange MD simulations performed on aggregates of rather limited dimensions indicated that the antiparallel β-structure of the final assemblies is likely dictated by the preferred association modes of the individual chains in the very early stages of fiber formation[3]. Altogether, the determination of the fine structural features of these systems and the identification of the physicochemical basis of their stability will have significant implications for the design and the development of new peptide-based nanomaterials.

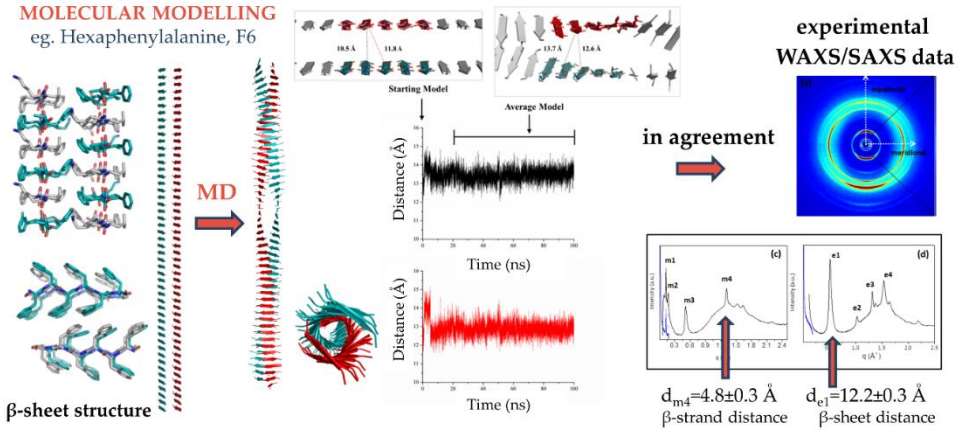

Figure 1. Atomic level model of the peptide moiety of the self-assembling F6 peptide emerged from the MD data.

References

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