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Unravelling the spontaneous self-assembly of α-helical Aβ-peptides in lipid membranes by analytical and multiscale approach

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Abstract

The mechanisms underlying the neurotoxicity in Alzheimer's disease are still under intense debate. As experimentally shown, Aβ peptide, primary component of amyloid plaques, self assembles to aggregate that permeabilize membranes. By a combination of multi scale simulations and analytical theory, we unveiled the early steps of the spontaneous self-assembly of membrane-embedded α-helical Aβ (1–40) peptides. The presence of distorted structures called ''frustrated helices'' was predicted and confirmed by large scale Coarse Grained simulations while the stability of these helical structures has been validated by fully atomistic simulations. In addition, CG simulations clearly evidenced mechanical stress on the membrane structure induced by the presence of the growing assemblies. We believe that these findings will provide an alternative view to the traditional models that consider a conformational transition towards b-sheet rich structures as a prerequisite for triggering membrane damage, suggesting new potential targets for the drug treatment.

Biography

Martina Pannuzzo has completed her Ph.D. in Chemical Science in 2012 from University of Catania (Italy), and she has been awarded for the best Italian Ph.D. thesis in Theoretical Biophysics, 2010-2012. She got several fellowships to visit important research groups in the field of Computational Biophysics in the Netherlands and Canada. She is currently postdoctoral researcher in Computational Biology at the University of Erlangen-Nuremberg, working in the field of membrane biophysics. She is the author of 9 papers published in well reputed chemical-physics journals.

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