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Inhibition of amyloid beta peptide oligomerization: Empirical and *ab initio* studies

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The primary neurodestructive agent in Alzheimer's disease is an aggregated form of the amyloid beta peptide, Aβ(1-40) and Aβ(1-42), probably acting in conjunction with redox active transition metals, copper and iron (in the form of heme). The approach in our laboratory for the past ten years has been the *in silico* development and characterization of short peptide strings which are designed to bind selectively to Aβ and prevent its oligomerization. The β-sheet-blocking peptides can interact with Aβ to form a large variety of complexes. We present here the results of a case study by molecular dynamics simulations aimed at determining the structures and relative binding affinities of one of our nano-MABs interacting with full length Aβ(1-42).

Biography

Arvi Rauk has completed his PhD from Queen's University in Kingston, Ontario and Postdoctoral studies from Princeton University, Department of Chemistry. He has published more than 200 papers in reputed journals and has been serving as an Editorial Board Member of repute.

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