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Computational approach for the assessment of inhibitory potency against beta-amyloid aggregation

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Abstract

Beta-amyloid (Aβ) plaques are one of the hallmarks of Alzheimer's disease. Their presence in the brain leads to neurodegeneration and memory decline. Therefore, search for new drugs able to decrease formation of such deposits is of great interest. Our previously developed multifunctional compounds inhibited transformation of monomers into fibrils. Herein, we describe the computational approach for the assessment of inhibitory activity against Aβ aggregation. The influence of novel inhibitors on amyloid $A\beta_{17-42}$ was studied by employing of molecular docking and all-atom molecular dynamics simulations. We found that the number of intermolecular backbone hydrogen bonds at the end of 100 ns MD simulation was correlated with the level of anti-aggregation potency of studied compounds. Such data may be successfully applied to *in silico* design of novel inhibitors of Aβ aggregation.

Keywords

Beta-amyloid, aggregation, inhibitors, molecular dynamics, simulations