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Role of Acetylcholinesterase in β -Amyloid Aggregation Studied by Accelerated Molecular Dynamics

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Abstract

© 2016, Springer Science+Business Media New York. Mechanisms of Alzheimer's disease development are still under investigation. It was shown that acetylcholinesterase promotes aggregation of β -amyloid. Accelerated molecular dynamics simulations were performed to investigate molecular mechanisms of this process. Results showed that A β is strongly attracted to the surface of acetylcholinesterase and forms stable complexes. It was hypothesized that acetylcholinesterase serves as a nucleation center for propagation of β -amyloid aggregation.

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Keywords

Accelerated molecular dynamics, Acetylcholinesterase, β -amyloid

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