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Molecular dynamics of structures and dynamics of A β oligomers

Phuong Nguyen

CNRS, Paris

Small soluble oligomers of amyloid-beta protein play a central role in the Alzheimer's disease. Unraveling their structure, dynamics is one of the major research objectives because this is probably the first step in the fight against the disease. In the first part, I will present some molecular dynamics simulation results on the structure and growth mechanism of amyloid-beta oligomers. If these results depend on the employed force field in the simulation are then discussed. In the second part, a multiscale simulation approach is presented to study the interaction of drugs that were recently suggested by experiments which seem to be the potential candidates for inhibiting amyloid-beta oligomerization.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15