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88 - Multi-seeded MD simulation to effectively sample the conformation space of short peptide

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We propose a method–multi-seeded MD (molecular dynamics) simulation–to effectively sample the conformational space of short peptides. Multi-seeded simulations prepare an exhaustive set of distinct initial conformations by assigning uniformly-distributed phi/psi angles for each amino acid. These distinct conformations act as seeds for subsequent short relaxation simulations. We apply this method to several short cyclic peptides, including scaffolded epitopes of Abeta and Tau protein. The results show that CPU requirements and simulation time are reduced, but sampling the phase space is comparable, when comparing to REMD (replica exchange molecular dynamics). The multi-seeded method can sample structures rarely explored in REMD and normal MD simulation.

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