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Aggregation of alpha-synuclein by a coarse-grained Monte Carlo simulation BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Alpha-synuclein, an intrinsic protein abundant in neurons, is believed to be a major cause of neurodegenerative diseases (e.g. Alzheimer, Parkinson's disease). Abnormal aggregation of ASN leads to Lewy bodies with specific morphologies. We investigate the self-organizing structures in a crowded environment of ASN proteins by a coarse-grained Monte Carlo simulation. ASN is a chain of 140 residues. Structure detail of residues is neglected but its specificity is captured via unique knowledge-based residue-residue interactions. Large-scale simulations are performed to analyze a number local and global physical quantities (e.g. mobility profile, contact map, radius of gyration, structure factor) as a function of temperature and protein concentration. Trend in multi-scale structural variations of the protein in a crowded environment is compared with that of a free protein chain.

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