Modeling study of drug nanoparticle with Insulin via coarse-graining method

신은혜, 주세훈, 곽상규*
울산과학기술대학교
(skkwak@unist.ac.kr*)

We suggest coarse-grained (CG) models for insulin to be applied to dissipative particle dynamics (DPD) simulation. First, each amino acid residues lumped into one beads. Second, each amino acid separated by two or three beads. Third, secondary structural information of insulin is applied to the second model. The first and second models have full flexibility but the latter, which is closer to the actual insulin structure, keeps its own secondary structure. We investigated two set of interaction parameters from Hildebrand and Hansen solubility parameters to extract the best possible parameters. To check the different models, the constant-temperature CG molecular dynamics (MD) was performed with an insulin in two solutions, which are pure water and 20% acetic acid solution. The third model show similar results of RMSF and RMSD compared to those of all-atom models in literature. We also performed CG MD simulation of three insulin models, which are loaded in oil-filled PIBCA nanocapsule and confirmed the stability of insulin in oil, which originates from good affinity of head group of oils and hydrophobic side chain outward from insulin.