Coarse-Grained Modeling of Insulin for Dissipative Particle Dynamics

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To simulate a drug carrier system (i.e. PIBCA (poly-isobutyl cyanoacrylate) capsule) for insulin, a coarse grained (CG) model of insulin is required. We suggest plausible CG models for insulin to be applied to dissipative particle dynamics (DPD) simulation. Insulin consists of 51 amino acid residues and has disulfide bonds connecting A and B chains. N and C-terminals of A and B-chains and side chains of residues affect the conformation of insulin. To confirm the conformational effect in CG modeling, we make the two models. First, each residue is lumped to single bead. Secondly, residues are separated by two beads, which become constituent beads for backbone and side chain. To check their reliabilities, the constant temperature molecular dynamics (MD) was performed with insulin in two solutions, which are pure water and 20% acetic acid solution. Insulin models show large differences in RMSF and RMSD since those made for DPD has much more flexibility than all-atom models. However, such flexibilities have much less effects than interactions among chemical species on the self-assembly of the drug carrier system. Instead, we found that hydrophobic side chains play an important role for insulin to go inside the PIBCA capsule with centered oil.