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GENERATION OF A COARSE-GRAINED MOLECULAR MECHANICS MODEL FOR POLOXAMER MOLECULES

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Poloxamers are amphiphilic triblock copolymers with a central hydrophobic polypropylene oxide (polyPO) block connected on either end to two hydrophilic polyethylene oxide (PolyEO) blocks. These polymers are widely used in medical applications, foaming, detergency, dispersion and stabilization. Computer simulations can provide support in characterizing, and guiding modifications to their structure. Here, a novel coarse-grained (CG) molecular mechanics model for Poloxamer molecules is presented. All-atom (AA) resolution models already exist for these molecules; however, the time and length scales afforded by AA simulations cannot capture the complex behaviour of these molecules. The proposed model aims to create general parameters for the PO bead, making the model extensible to any chain length of Poloxamer. In the study, all-atom molecular dynamics (MD) simulations were carried out using the NAMD code with CHARMM 35 force field data to obtain reference structural data for small individual units of the PPO blocks. Then the CG model was developed and parameterized to reproduce target data using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) MD code using the force field of Shinoda, DeVane and Klein. The bond stretching and bond angles of the CG model were iteratively adjusted in explicit solvent simulations to reproduce the behaviour of the Poloxamer. The non-bonded parameters were adjusted to reproduce the experimental density and surface tension of the polymer melt. After the development of the model the transferability and versatility were demonstrated, by calculating the radius of gyration (rg) of two commercially available designed Poloxamer molecules, P65 and F68 (Pluronic®□). The simulated results give close precision to the available experimental rg data of P65 and F68 proving that the CG model developed can perform *in silico* investigation of these molecules in further development and application.

Keywords: Molecular dynamics, Pluronics, Polymer simulations, SDK force field