

COGRIMEN – Coarse-Grained Method for Modeling of Biological Systems in Implicit Environments

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The COGRIMEN (Coarse-Grained Implicit Environments) method combines coarse-grained (CG) representations of proteins with dynamics in implicit environments including water and membrane. In COGRIMEN we implemented the most frequently used the coarse-grained force fields MARTINI and RB-CG as well as the membrane potential employed in IMM1 method. Usage of CG representations in implicit environments allows to increase time of molecular dynamics simulations of membrane protein system by at least one order of magnitude or to increase number of proteins in the system by one order of magnitude, depending on size of protein. The method may be used for study of formation of protein oligomers and their dynamics in cell membranes. The COGRIMEN method facilitates using of large number of proteins in a single simulation which enables estimation of kinetic parameters of processes linked to protein-protein interactions and binding of peptide ligands by proteins. This method may be used to study processes of cellular signaling and formation of large protein complexes in cell membranes.