Mesoscale simulation of mucin-type proteins adsorption to model surfaces

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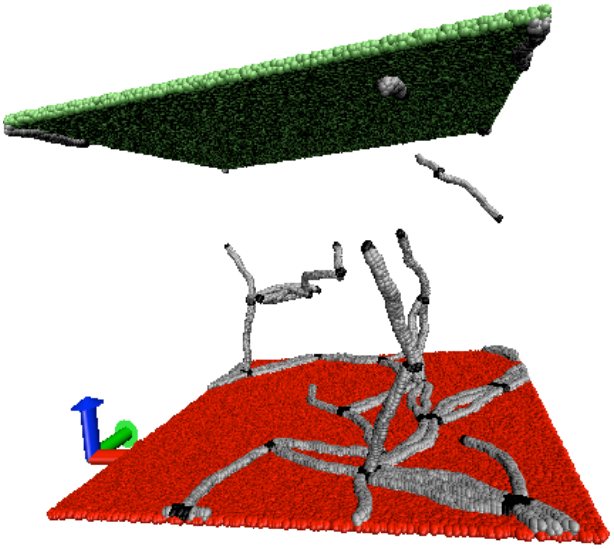
Behaviour of mucin-type glycoproteins is a key aspect on the study of several health disorders as well as in biomedical devices design where protein adsorption must be promoted or avoided according to the purpose [1–3]. This work presents and *in silico* study of mucin-type proteins adsorption supported by simulation tests of a water protein solution at the solid-liquid interphase with different hydrophobic levels of the surface and different protein concentrations. Behaviour is simulated using the Dissipative Particle Dynamics (DPD) to calculate status of a simplified representation of the system where multiple atoms are modelled in a single spherical particle (bead) applying a mesoscale coarse-graining approach to represent proteins, water and the model surface [4]. Relation between aggregation and adsorption dynamics is highlighted by simulation results and the powerful ability of the technique to study this phenomenon at the nanometer scale [5,6].



Keywords: Glycoproteins, Mucins, Molecular Simulation, Adsorption, Mucoadhesion, Bioahdhesion, Dissipative Particle Dynamics

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