Abstract Title: Kinetics of the protein corona assembly on nanoparticlesinetics of the protein corona assembly on nanoparticles

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Abstract:

Nanoparticles (NPs) in the extracellular matrix are immediately coated by layers of biomolecules forming a "protein corona". The protein corona gives to the NPs a "biological identity" that regulates the NP-cell interaction. Therefore, the cell uptake of the NPs is strongly affected by the protein corona. For this reason learning to predict the biological identities of NPs based on a partial experimental knowledge is essential to foresee a priori the safety implications of a NP for human health and, more in general, the environment.

To this goal we propose a multiscale approach that, adopting numerical techniques from all-atoms simulations [1] to coarse-grained models for protein-protein [2] and protein-NP interactions [3], accounts for the effect of interfaces on the hydration layer [4,5] in the description of proteins [6] and NPs in water [7]. The approach allows us to predict the protein corona assembly based on a partial experimental knowledge of the protein affinities for NPs with a specific physico-chemical composition and the size [8].

Specifically, we study, by numerical simulations, the competitive adsorption of proteins on a NP suspended in blood plasma as a function of contact time and plasma concentration. We consider the case of silica NPs in a "simplified" blood plasma made of three competing proteins: Human Serum Albumin, Transferin and Fibrinogen. These proteins are of particular interest because they have a high concentration in plasma, or because they are the most abundant in the corona of silica NPs. Our results are compared with experiments made under the same conditions showing that the approach has a predictive power [4].

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