PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

Unraveling the Role of Protein Corona in the Interaction between Silver Nanoparticles and Bacteria: A Computational Approach

1 Master research project (6-9 month)

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Summary:

The interaction between silver nanoparticles (AgNPs) and bacteria is influenced by the formation of a protein corona, which plays a critical role in modulating the biological responses and behavior of nanoparticles. Understanding the dynamic interplay between the protein corona and the AgNP-bacteria interaction is of paramount importance in elucidating the underlying mechanisms and optimizing the design of nanomaterials for biomedical and environmental applications. In this study, we present a comprehensive computational approach to investigate the role of the protein corona in the interaction between silver nanoparticles and bacteria. Our primary objective is to employ molecular dynamics simulations and advanced computational techniques to unravel the intricate interplay between AgNPs, bacterial surfaces, and the protein corona. By incorporating realistic models of proteins, bacterial membranes, and AgNPs, we aim to elucidate the binding dynamics, structural changes, and functional implications of the protein corona on the AgNP-bacteria interface. All these changes will be correlated through microbiology test to validate the *in silico* results: Study and synthetize modified AgNP with different range of studied biomolecules and how this contributes to its adhesion to bacteria. The AgNP release kinetic under different biological media and the characterization of the formed protein corona will be also studied. The outcomes of this research will contribute to a deeper understanding of the complex interplay between silver nanoparticles, bacteria, and the protein corona, providing crucial insights into the mechanisms governing their interactions.