Thesis Project Offer

Joint Research and Education Programme "Palestinian-German Science Bridge PGSB"
Forschungszentrum Jülich GmbH & Palestine Academy for Science and Technology

Thesis type*

☐ BSc	☒ MSc	☐ PhD	Intended starting date (approx.): July 2023

Contact details of supervisor/responsible host at Forschungszentrum Jülich

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Project description*

Title: Molecular Modeling and NMR Investigation of Protein Corona Formation and Its Interactions with Liposome In medical applications, the entry of nanoparticles such as liposomes into a living organism is a challenging process involving complex interactions with biological fluids, most commonly blood. Blood proteins are the first biological barrier to targeted drug delivery; they tend to coat the liposome in a shell-like fashion, often referred to as the protein corona. The protein corona has, until recently, received little attention in the study of drug delivery mechanisms. This started to change, as it has been recently shown that such a protein corona influences the behavior of the liposome and thus its fate. Consequently, the interaction of blood proteins with liposomes now receives more attention, and it is now believed that protein corona formation plays an important role in influencing liposome targeting *in vivo*. Serum albumin is the most abundant (~50%) and important carrier protein in blood plasma. It is conceivable that serum albumin is an important component of the liposome protein corona. However, there is still a lack of knowledge about its binding affinity to liposomes and the dynamics of the binding process. This project will focus on the liposome protein corona effect for targeted drug delivery, in particular the use of molecular dynamics simulations to understand the role of serum protein in the nanoparticle delivery process. This project will benefit from the expertise of both **Prof. Birgit Strodel** and **Dr. Hebah Fatafta** in computer-aided drug discovery and molecular dynamics simulation of membrane proteins. The knowledge gained will be used to develop a generalized model for predicting protein-nanoparticle binding. Theoretical models will be complemented and validated by NMR experiments on the interaction of serum albumin with liposomes performed in the group of **Dr. Nils-Alexander Lakomek**. To achieve our goals, the project is divided into two work packages, which can be manifested via integrating two master students into it: The 1st master's student will be assigned to perform the task of building the liposome structure and simualting its interaction with serum albumin. The 2nd master's student will be assigned to perform solution and solid-state NMR measurements on the interaction between serum albumin and liposomes.

Date*	**Signature***
Jan 31th, 2023	Dr. Hebah Fatafta Hiba Fatafta

* required field

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