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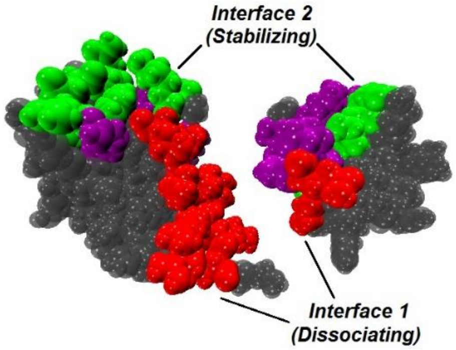
Modelling protein-protein interactions in confining environment



Protein-protein interactions play a pivotal role in all biological processes such as signal transduction, enzymatic catalysis as well as the formation of protein quaternary structures. Therefore, finding the protein complex association constant is important to unveil the fundamental principles underlying biochemical pathways in cells. In this project, the student will model protein interfaces and understand their stability using a collection of computational methodologies among which are methodologies that we have developed in our lab as described in the references 1 and 2. Via the modelling of the protein complexes we will analyze the role of the solvent (water) and boundaries such as confinement and compartmentalization in the stability of the protein interfaces. An example of a protein complex where we have identified the interfaces that lead to dissociation and others that are stable are shown in the illustration. The project combines knowledge of molecular and mathematical modelling, statistical analysis, computer science and biochemistry. The project can be divided between two students if there are two interested individuals.

Knowledge of a programming language such as Python, C++, C is a desirable skill but not necessary as long as the student is willing to dedicate the time to learn a programming language in a timely fashion.

References

1. Myong In Oh and S. Consta ``Stability of a Transient Protein Complex in a Charged Aqueous Droplet with Variable pH'', Journal of Physical Chemistry Letters, vol. 8: 80-85 (2017).

2. M. In Oh and S. Consta ``What Factors Determine the Stability of a Weak Protein-Protein Interaction in a Charged Aqueous Droplet?'' Physical Chemistry Chemical Physics vol. 19: 31965--3198 (2017).