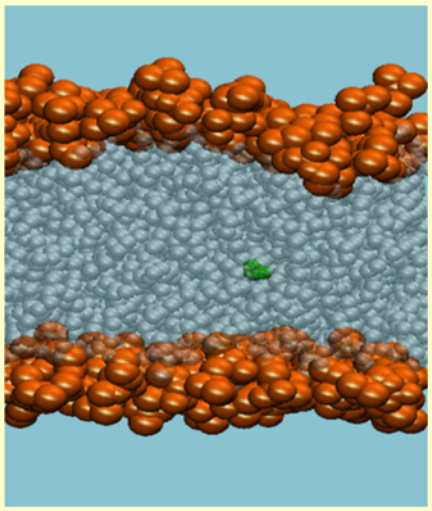
# Faculty-Undergraduate Research
# Professor Rodney Versace
# *Computational Biochemistry Research*

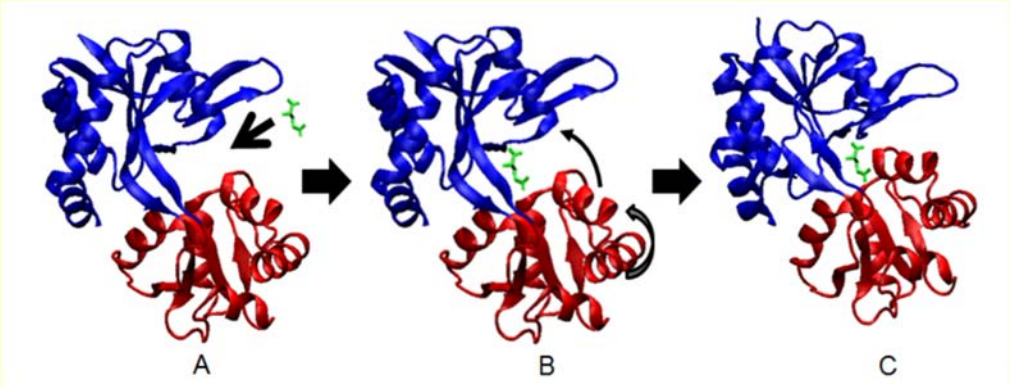
My research interests fall in the area of Computational Physical Biochemistry. My group seeks to understand and to characterize the relationship between the structure of biomolecules, such as proteins, lipids and nucleic acids, and their respective function, by analyzing the conformational changes that a molecule may suffer as a function of time due to the interactions with its aqueous or lipidic environment, and how these conformational changes affect its normal biological functions. To this end, several computational tools are used, such as molecular modeling, bioinformatics, molecular dynamics simulations, sampling algorithms, free energy calculation techniques and drug design approaches. Computational molecular simulations have proved to be an invaluable complement to experimental approaches for studying the structure, the dynamics, and the stability of several biological systems, as well as the intermolecular forces that governs its behavior.

One project currently in development is the characterization of energy landscapes for the transport of an isolated water molecule across different lipid bilayer. These free energy profiles will be compared to see the influence of the type of lipids (zwitterionic, neutral or ionic), the length of carbon chain, the number of unsaturations, the presence of other molecules inside and outside the membrane such as cholesterol, proteins, and ions. The transport of water or small solutes across the membrane has significant implications in cellular physiology, homeostasis, and drug delivery. Water plays a very important role in understanding the structural and functional properties of biological membranes; one of its main roles is to maintain organism homeostasis.



Cartoon representation of a DOPC membrane in water. The head groups of each lipid is depicted in orange, while the hydrophobic tail is in gray. A single water molecule (green) is crossing the membrane

My group is also interested in elucidating the conformational changes a receptor undergoes following the recognition of the ligand, and how these conformational changes is related to the transmission of the signal across the membrane. The objective is to obtain meaningful mechanistic hypotheses that can then be tested experimentally




*Representation of the binding of glutamate to an ionotropic glutamate receptor, a protein involved in processes of learning and memory.*

If you have any question, or wish to get more information about this research, or perhaps the probability of joining my group, please fell free to contact me at rversace@iona.edu.

1) Versace, R; Lazaridis, T. Modeling Protein – Micelle systems in implicit water. Journal of Physical Chemistry B, 2015, 119, 8037-8047

2) Lazaridis, T.; Versace, R. The treatment of solvent in multiscale biophysical modeling. Israel Journal of Chemistry, 2014, 54, 9: 1074 -1083.