SORS:Exploring mechanistic details in enzyme catalysis through mutiscale hybrid QM/MM simulations.

Speaker: Suwipa Saen-Oon

Abstract: The origin of many diseases responsible for the death of many thousands of people in the world reside in the malfunctioning of certain proteins. Enzymes are proteins that catalyze all chemical reactions necessary for life. Understanding the principles of mechanistic details in enzymatic reaction is crucial as it is a foundamental and important for further development in drug design, drug metabolism, overcoming drug resistance as well as enzyme engineering. During the past decades, hybrid quantum mechanical/molecular mechanical (QM/MM) simulations have demonstrated its abilities and accomplishments to elucidate the enzymatic catalytic reaction mechanisms at an electronic and atomic level. This talk will present an application of hybrid QM/MM method in studying the reaction mechanism in enzyme *Plasmodium falciparum* Phosphoethanolamine Methyltransferase, an attractive target for anti-malarial drug development.

Short Bio: Suwipa Saen-Oon received her PhD in Computational Chemistry (October-2003) from Kasetsart University (Thailand). She spent her post-doctoral research training at Chulalongkorn University (Thailand), Emory University (Atlanta) and Albert Einstein College of Medicine (New York). She is currently a researcher with Prof. Victor Guallar at the Barcelona Supercomputing Center. Her research interests involve computer simulations of chemical reactions and dynamics in enzymes as well as electron transfer process in proteins.

Severo Ochoa Mobility Grant funded visit: The school of Chemistry, University of Bristol , United Kingdom. The visit was to collaborate on topics linked with a SO Personalized Medicine application research and development.