Symposium on Biomolecular Simulations

Stockholm University – Magneli Hall

Wednesday 14 June 2017

09.30 – 09.40 Fahmi Himo - Symposium Opening

09.40 – 10.10 Per Siegbahn *(Stockholm University)*
How Cluster Model Calculations Should be Done for Enzymes

10.10 – 10.40 Iñaki Tuñon *(University of Valencia)*
Enzymatic Transition States - Quantifying the Limits of Transition State Theory in Enzymatic Catalysis

10.40 – 11.00 Coffee Break

11.00 – 11.30 Maria Ramos *(University of Porto)*
S-S Bond Studies within the Thioredoxin Family of Enzymes

11.30 – 12.00 Margareta Blomberg *(Stockholm University)*
Reaction Mechanisms of Heme-Copper Oxidases - How to Combine Computational and Experimental Data to Solve Fundamental Problems in Bioenergetics

12.00 – 12.30 Nino Russo *(University of Calabria)*
Contributions of Quantum Chemistry to Cancer Therapy

12.30 – 14.30 Lunch

14.30 – 15.00 Ivan Rivalta *(École Normale Supérieure de Lyon)*
Towards Accurate Simulations of 2D Electronic Spectroscopy

15.00 – 15.30 Edina Rosta *(King's College London)*
Mg-Dependent Catalytic Mechanism of Phosphate Cleavage Reactions

15.30 – 16.00 Hugo Gutierrez de Teran *(Uppsala University)*
Understanding the Effects of Single-Point Mutations on Ligand Binding through Free Energy Simulations

16.00 – 16.30 Pedro Fernandes *(University of Porto)*
Nanosecond Timescale Conformational Changes Strongly Influence Enzyme Reaction Rates

16.30 – Symposium Closing