

“Theoretical Biochemistry – Methods and Applications”

Wenner-Gren Center, Stockholm

May 14-17, 2008

Organizing committee: Fahmi Himo (chairman), Per Siegbahn & Hans Ågren

Secretariat: Maria Helgöstm (maria.helgostam@swgc.org)

Wednesday, May 14

16.00 – Registration

Session I: (Chairman Fahmi Himo)

17.00 – 17.10 Welcome

17.10 – 17.50 Lecture 1: Keiji Morokuma

“Effects of protein environment on the reaction mechanism of metalloenzymes: ONIOM QM:MM studies”

17.50 – 18.30 Lecture 2: Arieh Warshel

“Computer simulations of biological functions”

18.30 – 20.30 Welcome buffet at the Wenner-Gren Center, 23rd floor

Thursday, May 15

Session II: (Chairman Björn Roos)

9.00 – 9.40 Lecture 3: Edward I. Solomon

“Reduction of Dioxygen to Water by the Multicopper Oxidases”

9.40 – 10.20 Lecture 4: Per Siegbahn

“Large DFT models for enzymatic reactions”

10.20 – 10.50 Coffee Break

10.50 – 11.30 Lecture 5: Louis Noodleman

“Redox Energetics and Physical Properties of Iron-Sulfur Clusters from Simple Electron Transfer Proteins to the MoFe cofactor of Nitrogenase”

11.30 – 12.10 Lecture 6: Michael B. Hall

“Modelling Metalloenzymes: Hydrogenases”

12.10 – 13.30 Lunch

Session III: (Chairman *Margareta Blomberg*)

13.30 – 14.10 Lecture 7: Walter Thiel
"QM/MM Studies of Enzymes"

14.10 – 14.50 Lecture 8: Richard Friesner
"Quantum Chemical and QM/MM Modeling of Enzyme Reactions"

14.50 – 15.20 Coffee Break

(Chairman *Hans Ågren*)

15.20 – 16.00 Lecture 9: Weitao Yang
"Free energy of chemical reactions in solution and in enzymes with ab initio QM/MM-Minimum Free Energy Path method"

16.00 – 16.40 Lecture 10: Ulf Ryde
"Accurate calculations of energies in proteins"

16.40 – 17.20 Lecture 11: Jeremy Harvey
"QM/MM methods for Understanding Structure and Reactivity in Metalloproteins"

18.00 Dinner at "Haga Forum"
(Walking distance from the Wenner-Gren Center and Elite Palace Hotel)

Friday, May 16

Session IV: (Chairman *Sven Larsson*)

9.00 – 9.40 Lecture 12: Massimo Olivucci
"Ab initio Multiconfigurational Quantum Chemistry in Photobiology"

9.40 – 11.00 Poster Session + Coffee Break

11.00 – 11.40 Lecture 13: Leif A. Eriksson
"Molecular photochemistry in medicine - the photodegradation of non-steroid anti-inflammatory drugs"

11.40 – 12.20 Lecture 14: Sason Shaik
"Bonding in oxy myoglobin and haemoglobin: Is it Pauling, Weiss, or McClure-Goddard? None? All?"

12.20 – 13.30 Lunch

Session V: (Chairman Lennart Nilsson)

13.30 – 14.10 Lecture 15: Richard B. Silverman
"Design of Selective Neuronal Nitric Oxide Synthase Inhibitors for the Treatment of Neurodegenerative Diseases"

14.10 – 14.50 Lecture 16: William L. Jorgensen
"Drug-Lead Optimization Guided by Free Energy Calculations"

14.50 – 15.30 Lecture 17: Johan Åqvist
"Entropy Calculations in Biomolecular Systems"

15.30 – 16.00 Coffee Break

Session VI: (Chairman Aatto Laaksonen)

16.00 – 16.40 Lecture 18: Wilfred F. van Gunsteren
"Methodological advances in biomolecular simulation"

16.40 – 17.20 Lecture 19: David A. Case
"Vibrational probes of active sites of metalloenzymes"

17.20 – 18.00 Lecture 20: Ilpo Vattulainen
"Diffusion of lipids in membranes and lipoproteins: Insight through atomistic and coarse grained modelling"

18.30 Dinner: Boat Trip

Saturday, May 17

Session VII: (Chairman Yi Luo)

9.00 – 9.40 Lecture 21: Ian Hillier
"How do enzymes reduce metals?"

9.40 – 10.20 Lecture 22: Nino Russo
"Metal-ligand interaction in cancer therapy"

10.20 – 10.50 Coffee Break

10.50 – 11.30 Lecture 23: Ursula Röthlisberger
"Photostability through solvation"

11.30 – 12.10 Lecture 24: Michele Parrinello
"Large scale motions in proteins"

12.10 – 13.00 Lunch