# *The Future of Enzyme Modeling*

## Stockholm 28-29 Sept 2018

## Friday 28 Sept

***Session I:*** ***(Chair: Fahmi Himo)***

**08.45 – 09.00 Conference Opening**

**09.00 – 09.30 1. Arieh Warshel**
*Experiments in Computer-Aided Enzyme Design*
**09.30 – 10.00 2. Adrian Mulholland**
*Simulations to Guide Enzyme Design and Engineering?*
**10.00 – 10.30 3. Jean-Didier Maréchal**
*Challenges in Computer-Assisted Design of Artificial Metalloenzymes*

**10.30 – 11.00 Coffee**

***Session II:*** ***(Chair: Margareta Blomberg)***

**11.00 – 11.30 4. Jiri Damborsky**
*Computational Design of Protein Access Tunnels*
**11.30 – 12.00 5. Sílvia Osuna**
*Role of Conformational Heterogeneity in Enzyme Design*
**12.00 – 12.30 6. Kennie Merz**
*Role of Reaction Dynamics and Surface Topology in Enzymatic Catalysis*
**12.30 – 13.00 7. Pedro Fernandes**
*Challenges in the Prediction of Enzyme Reaction Mechanisms Using QM/MM Methods*

**13.00 – 14.30 Lunch**

***Session III:*** ***(Chair: Hugo Gutierrez de Teran)***

**14.30 – 15.00 8. Marco De Vivo**
*Metal-Aided Enzymatic Processing of DNA and RNA via Classical and Ab Initio Simulations*
**15.00 – 15.30 9. Laura Masgrau**
*Carbohydrate Active Enzymes: Reactivity, Inhibition and Ligand Migration Computational Studies*
**15.30 – 16.00 10. Katarzyna Świderek**
*Electrostatic, Dynamic or Compression Effects in Enzymatic Catalysis*
**16.00 – 16.30 11. Fahmi Himo**
*Modeling Enantioselectivity in Enzymes*

**19.00 – Dinner (Hotel C)**

## Saturday 29 Sept

***Session IV:*** ***(Chair: Bo Durbeej)***

**09.00 – 09.30** **12. Bill Jorgensen**
*Current Challenges for Modeling Organic and Enzymatic Reactions in Solution*
**09.30 – 10.00** **13. Jan Jensen**
*Can We Automate Computational Studies of Enzymes? Lessons from Small-Molecule Studies*
**10.00 – 10.30** **14. Edina Rosta**
*Coarse Graining and Molecular Kinetics from Biased Simulations*

**10.30 – 11.00 Coffee**

***Session V:*** ***(Chair: Susanna Monti)***

**11.00 – 11.30** **15. Johan Åqvist**
*Entropy and Enzyme Catalysis*
**11.30 – 12.00** **16. Iñaki Tuñón**
*Enzymatic Reaction Pathways and Transition States. Methodological and Theoretical Insights*
**12.00 – 12.30** **17. Adrian Roitberg**
*Protonation and Redox effects on Enzyme Catalysis*
**12.30 – 13.00** **18. Matthias Ullmann**
*Free Energy of pH-dependent Enzymatic Reactions*

**13.00 – 14.30 Lunch**

***Session VI:*** ***(Chair: Jan-Erling Bäckvall)***

**14.30 – 15.00** **19. Sam De Visser**
*QM Cluster vs. QM/MM: Applications on Nonheme Iron Hydroxylases and Halogenases*
**15.00 – 15.30** **20. Tiziana Marino**
*Artificial Enzymes: Insights from Theoretical Investigations*
**15.30 – 16.00** **21. Rongzhen Liao**
*Summary of Size Convergence in QM and QM/MM Studies of Enzyme Reactions*
**16.00 – 16.30** **22. Per Siegbahn**
*Modeling Redox-Active Enzymes*

**16.30 – Conference Closing**

**20.00 – Dinner (Restaurant Tabbouli)**