

**CECAM Workshop**  
**Membrane Protein Assembly: Theory and Experiment**  
**Lausanne, September 3-6, 2008**

**Schedule of the meeting**

Organizers:

Ana-Nicoleta Bondar, University of California at Irvine

Stephen H. White, University of California at Irvine

Gunnar von Heijne, University of Stockholm

Jeremy C. Smith, University of Heidelberg, and the Oak Ridge National Laboratory

Each talk should be limited to 30 minutes, followed by 10 minutes of discussions.

The posters should be available during the entire workshop. The workshop includes a round-table discussion of the posters, with 5 minutes oral presentation followed by 5 minutes of discussion for each poster. The short presentations of the posters should be limited to 2-3 slides summarizing the most important result.

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**September 3**

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**Session 1. Membrane protein assembly I**

Chairman: Stephen H. White

14:00 – 14:20 Introduction from Stephen White

14:20 – 15:00 Doug Tobias 'Helices in motion in membranes: molecular dynamics simulation studies of the SecY and LacY transporters'

15:00 – 15:40 Jan Gumbart „Membrane protein insertion in the translocon“

15:40 - 16:20 Frank Duong “Studying translocon function in a membranous puck”

16:20 – 16:40 coffee

## **Session 2. Membrane protein assembly II**

Chairman: Mark Sansom

16:40 – 17:20 Martin Ulmschneider “Folding proteins into membranes”

17:20 – 18:00 Jochen Zimmer “Crystal structure of the protein-translocation complex formed by the SecY channel and the SecA ATPase”

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## **September 4**

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## **Session 3. Peptides in membranes**

Chairman: Douglas J. Tobias

09:00 – 09:40 Matthias Ullmann „The energetics of proteins in membranes investigated by continuum electrostatics”

09:40 – 10:20 Martin Spiess “Orientation of signal-anchor sequences at the Sec61 translocon”

10:20 – 10:40 coffee

## **Session 4. Dynamics of protein/lipid interactions**

Chairman: Bert de Groot

10:40 – 11:20 Helmut Grubmueller

11:20 - 12:00 Toby W. Allen „Aromatic and ionizable protein side chain interactions with membranes”

12:00 – 13:30 Lunch

## **Session 5. Lipid/protein interactions and the hydrophobic mismatch**

Chairman: Berend Smit

13:30 – 14:10 Patrick Fuchs “Orientation of a transmembrane peptide under positive mismatch by computer simulations

14:10 – 14:50 Eitan Bibi „Intra-membrane proteolysis: specificity and structure of the rhomboid-like integral membrane serine protease GlpG“

14:50 – 15:30 Frederick de Meyer “Free energy of specific and selective lipid mediated protein-protein interactions induced by hydrophobic mismatch”

15:30 – 15:50 Coffee

## **Session 6. Cholesterol and protein/lipid membrane interactions**

Chairman: Eitan Bibi

15:50 – 16:30 Berend Smit 'Understanding the effect of cholesterol'

16:30 – 17:10 Grace Brannigan "Cholesterol and the structural integrity of the Acetyl Choline Receptor"

17:10 – 17:30 coffee

## **Session 6. Protein/protein interactions in lipid bilayers**

Chairman: Antoinette Killian

17:30 – 18:10 Andreas Engel

18:10 – 18:50 Durba Sengupta "Self-association of membrane proteins: A molecular dynamics study"

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## **September 5**

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## **Session 7. Membrane protein dynamics**

Chairman: Mounir Tarek

08:20 – 09:00 Mark Sansom 'Coarse-Grained Simulations of Membrane Proteins and Peptides'

09:00 – 09:40 Matteo dal Peraro , Proton gating mechanism of M2 protein from influenza A virus: a new perspective from molecular dynamics'

09:40 – 10:00 Coffee

## **Session 8. Round-table discussion of the posters**

Chairman: Ana-Nicoleta Bondar

8.1 Energetics of membrane/lipid interactions

10:00 – 10:10 Jerome Henin 'Insertion of an antimicrobial peptide mimetic in a mixed bilayer'

10:10 – 10:20 Walter Ash

10:20 – 10:30 Christian Schwieger 'Non-electrostatic contributions to the interaction of positively charged polypeptides with negatively charged bilayers'

- 10:30 – 10:40 Anna Johansson 'Amino acid solvation on membranes as function of protonation state and lipid bilayer properties'
- 10:40 – 10:50 Jesus Salgado 'Free-energy landscape of peptides in membranes: understanding orientation and dynamics'
- 10:50 – 11:00 Santiago Esteban 'How does dynamics affect the orientation of membrane peptides determined from NMR data'
- 11:00 – 11:10 Anirban Mudi 'Insights into helix-helix interactions using alchemical free energy calculations for a transmembrane dimer'

## 8.2. Protein-induced perturbations of lipid membranes

- 11:10 – 11:20 Daniel Parton 'Investigating the membrane lysing action of the antimicrobial peptide maculatin 1.1'
- 11:20 – 11:30 Jen Hsin 'Purple bacteria LH1-RC-PufX dimer curves chromatophore membrane'
- 11:30 – 11:40 Catherine Etchebest 'Insights into the mechanical sensitivity of MscL: from membrane influence to sequence specificities'

## 8.3 New developments in computer simulations of membrane proteins and lipid/protein interactions

- 11:40 – 11:50 Jakob Ulmschneider
- 11:50 – 12:00 Lucie Delemotte 'Auto-assembly, reorganization and folding of small peptides in interaction with membranes: a CG study'
- 12:00 – 12:10 Maria Sperotto 'A guided tour through the landscape of coarse-grain biomembrane models'
- 12:10 – 12:20 Dan Mihailescu 'Molecular dynamics simulation of a LPS/DPPE bilayer'
- 12:20 – 12:30 Alfredo Freitas 'Describing the protein-membrane interface by a Voronoi tessellation analysis of molecular dynamics simulations'

12:30 – 14:00 Lunch

## **Session 9. Protein-protein and protein-lipid interactions**

Chairman: Toby Allen

- 14:00 – 14:40 Bert de Groot 'Permeation mechanisms across membranes'
- 14:40 – 14:20 Siewert-Jan Marrink 'Membrane proteins under stress'

14:20 – 15:00 Antoinette Killian

15:00 – 15:20 Coffee

### **Session 10. Proteins in membranes: dynamics and conformational changes**

Chairman: Frank Duong

15:20 – 16:00 Yves-Henri Sanejouand “Conformational changes of membrane proteins:  
elastic network model studies

16:00 – 16:40 Daniel Mueller

16:40 – 17:00 coffee

### **Session 11. Posters, 17:00 – 19:00**

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**September 6**

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### **Session 12. Ion transfer across lipid bilayers**

Chairman: Rebecca Wade

08:20 – 09:00 Himanshu Khandelia “Simulations of pumps and lipid gymnastics”

09:00 – 09:40 Erik Lindahl “Microsecond simulations of voltage-gated ion channels”

09:40 – 10:00 coffee

### **Session 13. Protein translocation and proteins in membranes**

Chairman: Matthias Ullmann

10:00 – 10:40 Ioan Andricioaei “Kinetics and mechanisms for protein passages through  
pores”

10:40 – 11:20 Paolo de los Rios “Protein translocation into mitochondria: the role of  
Hsp70 chaperones

11:20 – 12:00 Carol Deutch „Tunnel vision“

12:00 – 13:30 Lunch

**Session 14. Challenges in computer simulations of membrane proteins and lipid membranes**

Chairman: Ioan Andricioaei

13:30 – 14:10 Rebecca Wade

14:10 – 14:50 Mounir Tarek 'Charge gating in membrane proteins: on the activation of voltage gated K channels'

14:50 – 15:10 coffee

**Session 15. Perspectives in membrane protein assembly research**

Chairman: Gunnar von Heijne

15:10 – 15:30 Gunnar von Heijne

15:30 – 16:30 Panel discussions, conclusions and outlook