

Telluride Workshop on Proton Transfers in Biology

Telluride Intermediate School

735 W. Colorado Avenue

July 12-July 16, 2016

Organizers: Pia Ädelroth (+46-73-8000370), Mark Maupin (720-775-8161)

Local TSRC Host: Mark Kozak (970-708-4426)

of Participants [23]

July 11th Monday

18-20 Informal reception and Early registration in the tent at the Telluride Elementary School at 447 W Columbia Ave. Complimentary beer and wine.

Tuesday July 12th

7:30-8:00 Breakfast at Telluride Intermediate School
Registration, Outside on Basketball Court by TSRC entrance
Meeting on the second floor

8:00-8:30 Introduction **Mark Kozak**, TSRC director+**Pia/Mark**

8:30-9:15 **Tom de Coursey**: 'The Proton Selectivity Mechanism of the Voltage-Gated Proton Channel May Be Replicated in Other Molecules'

9:15-10:00 **Qiang Cui**: 'Water dynamics and proton transfers in soluble and membrane proteins'

10:00-10:30 **Coffee Break**

10:30-11:15 **Jon Hosler**: 'Membrane-bound cyclic peptides that appear to stimulate/inhibit proton uptake/release'

11:15-12:00 **Petra Hellwig**: 'The diversity of the redox potentials in terminal oxidases'

12:00-12:45	Noam Agmon: 'Water wires in GFP dynamics'
12:45-13:15	Conclusions/General Discussion
18:00	Town talk at the Telluride Conference Center in Mountain Village: Featured Speaker: Greg Beran , PhD, Professor of Chemistry, University of California, Riverside: 'Drug Recalls, Patent Fights, and Chocolate: Adventures in Crystal Packing'

Wednesday July 13th

7:30-8:00	Breakfast at Telluride Intermediate School
8:00-8:45	Susan Smith: 'Tryptophan and the mystery of proton selectivity in the voltage gated proton channel, Hv1TBA'
8:45-9:30	Pia Ädelroth: 'Proton transfer in the B, C and NOR heme-copper oxidases'
9:30-10:00	Coffee Break
10:00-10:45	Bertrand Garcia-Moreno: 'Buried ion pairs and hydrogen bonds in proteins'
10:45-11:30	Alexei Stuchebrukhov: 'Coupled surface-bulk diffusion mechanism of proton transport along the membranes'
11:30-12:15	Peter Pohl: 'Proton mobility at the membrane water interface'
12:15-12:45	General discussion
18-21	TSRC Picnic at the Telluride Elementary School at 447 W Columbia Ave

Thursday July 14th

7:30-8:00	Breakfast
8:00-8:45	Marilyn Gunner: 'Proton transfer pathways in cytochrome c oxidase'
8:45-9:30	Hai Lin: 'Adaptive Multiscale Simulations of Proton Transfer'

9:30-10:00	Coffe Break
10:00-10:45	Elena Pohl: 'Dinitrophenol and membrane proton leak'
10:45-11:30	Peter Brzezinski: 'Electron and proton transfer in respiratory oxidases'
11:30-12:15	Ana Nicoleta Bondar: 'Dynamic protein/water hydrogen-bond networks in proton transfers'
12:15-12:45	General Discussion
12:45-14:00	CATERED LUNCH at TSRC
14:00-14:45	Ehud Pines: 'Controlling reactivity by remote protonation of a basic side group in a bifunctional photoacid'
14:45-15:30	Philip Kiefer: 'Computer Simulations of Proton Transfer in Water Bridged Systems: Acid-Base Effects'
15:30-16:00	Coffee Break
16:00-16:45	Tom Haines: 'The Chlorosulfolipids and Unique Hydrogen Bonds of <i>Ochromonas danica</i> '

Friday July 15th

7:30-8:00	Breakfast
8:00-8:45	Joachim Heberle: 'Proton transfer reactions in channelrhodopsin-2 - direct detection by time-resolved IR spectroscopy'
8:45-9:30	Ramona Schlesinger: 'Structural changes and protonation dynamics in channelrhodopsins after light activation'
9:30-10:00	Coffee Break
10:00-10:45	Régis Pomès: 'Molecular simulations of ion channels'
10:45-11:30	Mark Maupin: 'Impact of pH, residue pKa, and charge coupling on <i>Melanocarpus albomyces</i> cellobiohydrolase Cel7B'
11:30-12:15	Robert Gennis: 'Coupling hydride transfer to proton pumping: The Nicotinamide Nucleotide Transhydrogenase'
12:15-13:00	Final discussion and conclusions, end of scheduled talks

Lunch break in town

14:30-17

Group Hike (Mark Maupin)

Saturday July 16th

Free time