

# PROTON TRANSFER IN BIOLOGY WORKSHOP

Organizers: Robert Gennis and Peter Brzezinski

Monday, July 16 - 20, 2012

TSRC @ Telluride Intermediate School

725 W. Colorado

Telluride CO 81435

TSRC Contacts: Rory 970-708-4542, Nana 970-708-0004

## Monday, July 16 (morning session)

time	name	title
7.30	TSRC Catered Breakfast, at meeting site	
8.30	Bertrand Garcia-Moreno	Determinants of $pK_a$ values of buried ionizable groups in proteins
9.00	Susan Smith	Structural themes in proton selective transport
9.30	Gerhard Hummer	Water -- all wired up
10.00-10.30	Discussion Break	
10.30-11	Coffee Break	
11.00	Klaus Gerwert	Proton transfer via protein-bound water molecules
11.30	Noam Agmon	Proton Diffusion on Membranes
12.00	Discussion Break	
12.30	TSRC Catered Lunch, at meeting site	

## Tuesday, July 17 (afternoon session)

<b>time</b>	<b>name</b>	<b>title</b>
13.00	Bob Gennis	Introduction Pumping channels and the heme-copper superfamily
13.30	Shelagh Ferguson-Miller	The Conformation / Regulation Questions - what controls proton pathways in Cytochrome Oxidase?
14.00	Marilyn Gunner	A new view of the CoC pumping site
14.30	Break	
15.00	Pia Ädelroth	Proton transfer in NO-reducing heme-copper oxidases
15.30	Qiang Cui	QM/MM analysis of proton transfers in bulk water and in cytochrome c oxidase
16.00	Discussion Break	
16.30	Arieh Warshel	Gaining deeper physical insight on proton transport in CcO and related systems
17.00 -	Discussion Break	
18.00-19.15	Town Talk, Palm Theatre	

## Wednesday, July 18 (morning session)

time	name	title
7.30	TSRC Catered Breakfast, at meeting site	
8.30	Tom DeCoursey	Attempts to Understand How Proton Selectivity Works
9.00	Claudio Grosman	Dissecting the mechanism of cation-transport catalysis by glutamate side chains in nicotinic receptors. Protonation–deprotonation or side-chain conformational flexibility?
9.30	Rob Burnap	The role of amino acids in the second ligation sphere of the water-oxidizing $Mn_4Ca$ cluster of photosystem II
10.00-10.30	Discussion Break	
10.30-11	Break	
11.00	Bridgette Barry	Proton coupled electron transfer and redox active tyrosine residues
11.30	Hemi Gutman	Single molecule mapping of protein in a cluster on the inner leaflet of the plasma membrane
12.00	Discussion Break	
12.30	TSRC Catered Lunch, at meeting site	

## Thursday, July 19 (afternoon session)

<b>time</b>	<b>name</b>	<b>title</b>
13.00	Uli Brandt	What we do know and what we don't know about the proton pump of respiratory complex I
13.30	Leo Sazanov	Structure and coupling mechanism of respiratory complex I
14.00	Discussion Break	
14.30	Tim Cross	The Influence of Membrane Mimetic Environments on Membrane Protein Structures: The M2 Proton Transporter
15.00	Coffee Break	
15.30	Jana Shen	Constant pH molecular dynamics simulations provide new insights into proton-coupled conformational phenomena
16.00	Eti Nachliel/ Yossi Tsfadia	Molecular dynamics simulations of MRP1 multidrug resistant proteins (all Atom) with clarification of the reaction mechanism of a specific blockage of the channel by specific drug
16.30	Regis Pomes	TBA
17.00	Discussion Break	
18.00- dark	TSRC picnic (families welcome)	

## Friday, July 20 (morning session)

time	name	title
7.30	TSRC Catered Breakfast, at the meeting site	
8.30	David Silverman	Proton Transfer through Intervening Water Molecules in Catalysis by Carbonic Anhydrase
9.00	Ali Ahmed Hassanali	On the Recombination of $H_3O^+$ and $OH^-$ in water
10.00	Dan Huppert	Excited -State Proton Transfer as a research tool for Biological and Chemical systems
10.30-11	Coffee Break	
11.30	Peter Brzezinski	Proton selectivity in cytochrome c oxidase
11.50	Discussion Break	
12.30	The End	