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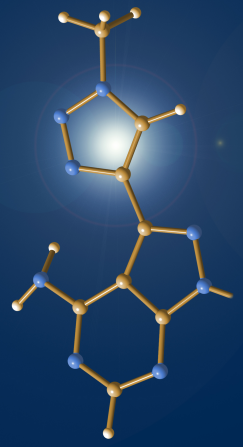
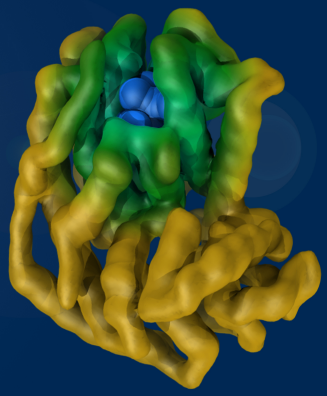
CHEMICAL BIOLOGY PROGRAM





2015

Inaugural UC Davis

CBP Retreat

September 11, 2015
Student Community Center

Schedule of Events

8:30am – 9:00am **Breakfast and Registration**

9:00am – 9:10am **Welcome and Introduction**
Dr. Pete Beal

Session I
Chair: Heesung Shim

9:10am – 9:35am **Gabby Nepomuceno (Shaw)**
Targeting FtsZ and its Effects on Bacterial Cell Division.

9:35am – 10:00am **Matthew Blain-Hartung (Lagarias)**
Understanding and Exploiting Second Messenger Signaling via Light Responsive CBCRs.

10:00am – 10:25am **Muhammad Hagras (Stuchebrukhov)**
Theory of Electron Transfer in bc_1 Complex (Respiratory Complex III).

Coffee Break and Posters
10:25am – 10:45am

Session II
Chair: Tyler Mix

10:45am – 11:10am **Brandon Tautges (Louie)**
Activatable MRI Contrast Agents for Imaging Bioluminescence.

11:10am – 11:35am **Melissa Matthews (Fisher)**
Structural Basis for RNA Editing by Human Adenosine Deaminase Acting on RNA.

11:35am – 12:00pm **Sean Kodani (Hammock)**
Applied Polypharmacology: Design and Synthesis of Multi-Target Inhibitors for sEH and FAAH.

Lunch
12:00pm – 1:00pm

Poster Session
1:00pm – 2:00pm

Session III
Chair: Julia Jennings

2:00pm – 2:25pm **Dong hee Chung (Toney)**
New Library Generation Methods for Protein Engineering.

2:25pm – 2:50pm **Simon Park (Gervay-Hague)**
The Synthesis of Unique Sialoglycoconjugates: Building Blocks to Explore Sialic Acid Biochemistry.

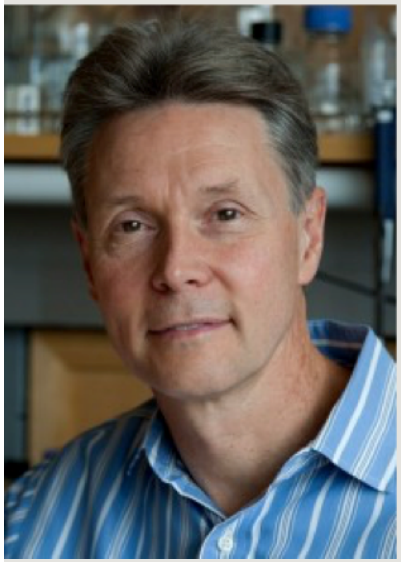
2:50pm – 3:15pm **Rachel Valenzuela (Beal)**
Modulating siRNA Off-Target Effects through Nucleobase Modifications.

Coffee Break and Posters
3:15pm – 3:30pm

Keynote Talk
3:30m – 4:30pm **Dr. Charles S. Craik (UCSF)**
Global Analysis and Visualization of Proteolysis in Disease.

Join us for a brief reception from 5:00pm to 5:30pm in the Chemistry Courtyard following Dr. Craik's talk!

Keynote Speaker



Dr. Craik received his BS in Chemistry from Allegheny College in Meadville, PA. He attended Columbia University (New York, NY) where he earned his Masters and PhD in Chemistry. After his PhD, Dr. Craik moved to UCSF in the Department of Biochemistry and Biophysics for his postdoctoral work on proteases in the laboratory of William Rutter. Dr. Craik was hired as Assistant Professor at UCSF in 1985, where his current position is Professor in the Departments of Biochemistry and Biophysics and Pharmaceutical Chemistry. Dr. Craik is currently the Director of Chemistry and Chemical Biology Graduate Program at UCSF and Director of Quantitative Biosciences Consortium of Graduate Programs.

The research interests of the Craik lab focus on defining the roles and mechanisms of enzymes in complex biological processes and on developing technologies to facilitate these studies. Information on the lab can be found at the following website: http://www.craiklab.ucsf.edu. The primary emphasis of Dr. Craik's work has been on enzymes, with a particular emphasis on macromolecular recognition.

Global Analysis and Visualization of Proteolysis in Disease

Abstract

Proteases represent the largest class of post-translational modifying enzymes in the human proteome. An estimated 2% of human genes encode 687 proteases or protease-like homologs. With every protein having a cradle to grave relationship with proteolysis, uncovering the substrate specificity of these proteases is central to understanding their physiological role in homeostasis and disease. We have developed methods to functionally "profile" a given protease and identify sequences of its preferred substrate. These sequences provide a pharmacophore of the active site of the enzyme and can also be used to identify inhibitors as well as potential natural substrates. We recently extended our technology to globally detect the activity and reveal the substrate specificity of any endo or exo protease in a complex biological sample. We have applied this methodology to simultaneously detect all protease activity in indications of infectious disease and cancer. The resulting proteolytic signatures are proving beneficial for monitoring disease progression and for defining the biological role of the proteases involved.

Our understanding of the molecular recognition properties of proteases and the tools that we developed to study them in complex biological samples led us to develop methods that can visualize their enzymatic activity in vivo. Conformationally selective, recombinant antibody-based probes that are highly selective for a given enzyme permit non-invasive imaging of the protease as a biomarker for early detection and prognosis of cancer and for validating the protease as a potential therapeutic target. The approach that we are developing for identifying these probes is proving to be a general method for identification of antibody based probes for extracellular enzymes and receptors. Our studies are providing a better understanding of both the chemical make-up and the biological importance of these critical proteins.

Poster Presentations

#	Name & Title
1	**Katherine Beglinger (Fraser)** *Investigating Translation Initiation Factor Phosphorylation in Response to Cell Stress.*
2	**Muhammad Hagras (Stuchebrukov)** *Computational Studies of Electron Tunneling in Respiratory Complex III.*
3	**Amelia Manlove (David)** *New Insights into Substrate Recognition by BER Glycosylase MutY.*
4	**Andrea Faulkner (Shaw)** *Development of Molecular Photoswitches as MRI Contrast Agents.*
5	**Jan Maly (Leal)** *Structural characterization of a pheromone degrading enzyme.*
6	**Elisha Goonatilleke (Lebrilla)** *Quantitation of proteins and their glycoforms in human milk and their implications on infant health.*
7	**Nick Hurlburt (Fisher)** *Structural and mutational studies of the chitin-binding fungal effector protein, PfAvr4.*
8	**Julia Jennings (Franz)** *Multi-component synthesis of substituted malonamides, their fluorescent properties and potential applications.*
9	**David Marchiori (Britt)** *Acetate Binding at the Oxygen Evolving Complex of Photosystem II.*
10	**Julia Kirpich (Larsen)** *Characterizing the photo-induced Activity of Red/Green and Violet/Blue Bilin-binding Cyanobacteriochrome Photoreceptors.*

#	Name & Title
11	**Tyler Mix (Larsen)** *Bifurcation of the Ultrafast Dynamics of the Photoactive Yellow Proteins from Leptospira biflexa and Halorhodopspira halaphila.*
12	**Christina McCulley (Tantillo)** *An Examination of the Molecular Switches Spiropyrans.*
13	**Cody Palumbo (Beal)** *RNA Tethering to Enhance Binding to Adenosine Deaminase Acting on RNA (ADAR2).*
14	**Lucas Moore (Shaw)** *Progress Towards the Total Synthesis of Chrysophaentin E.*
15	**Gabby Nepomuceno (Shaw)** *Targeting FtsZ and its Effects on Bacterial Cell Division.*
~~16~~	~~**Edward Balmond (Shaw)**~~ ~~*Development of Light Activated MRI Contrast Agents for In Vivo Imaging.*~~
17	**Heesung Shim (Wulff)** *Rational Design of KCa channel modulators.*
18	**Derek Revels (Fisher)** *Crystallography, Kinetics, and Screening of Inhibitors to the Sulfate Assimilation Pathway of M. tuberculosis.*
19	**Matthew Turner (Ames)** *Calmodulin Triggers Release of PSD-95 from the Postsynapse.*
20	**Simon Park (Gervay-Hague)** *Using ReSET and Sialosyl Iodide Glycosylation to Develop Chemical Probes to Study Sialic Acid (Neu5Ac) Biochemistry.*