

SCHEDULE OF EVENTS

8:00 A.M.

REGISTRATION & CONTINENTAL BREAKFAST

Gallery, W.T. Young Library

8:45 A.M.

WELCOME

Dr. Lisa Cassis, Vice President for Research
Auditorium, W.T. Young Library

9:00 A.M.

ROMMIE AMARO, PH.D.

Auditorium, W.T. Young Library

"Multi-scale Dynamics: Molecules to Cells"

We are developing capabilities for multi-scale dynamic simulations that cross temporal scales from the picoseconds of macromolecular dynamics to the physiologically relevant time scales of cells (milliseconds to seconds). Our efforts are driven by gaps in current abilities to connect across scales where it is already clear that new approaches and insights will translate into biomedical research discoveries and novel therapeutic strategies.

10:00 A.M.

BREAK/REFRESHMENTS

10:30 A.M.

DAVID BAKER, PH.D.

Auditorium, W.T. Young Library

"Post-Evolutionary Biology: Design of Novel Protein Structures, Functions & Assemblies"

Proteins mediate the critical processes of life and beautifully solve the challenges faced during the evolution of modern organisms. Our goal is to design a new generation of proteins that address current

day problems not faced during evolution. In contrast to traditional protein engineering efforts, which have focused on modifying naturally occurring proteins, we design new proteins from scratch based on Anfinsen's principle that proteins fold to their global free energy minimum. We compute amino acid sequences predicted to fold into proteins with new structures and functions, produce synthetic genes encoding these sequences, and characterize them experimentally. I will describe the design of ultra-stable idealized proteins, flu neutralizing proteins, high affinity ligand binding proteins, and self-assembling protein nanomaterials. I will also describe the contributions of the general public to these efforts through the distributed computing project Rosetta@Home and the online protein folding and design game Foldit.

11:30 A.M.

LUNCH

1:30 P.M.

POSTER SESSION

Multipurpose Room, B108C, W.T. Young Library

2:30 P.M.

FRANCES ARNOLD, PH.D.

Auditorium, W.T. Young Library

**"Innovating with Evolution:
Expanding the Enzyme Universe"**

Not satisfied with nature's vast catalytic repertoire, we want to create new enzymes and expand the range of genetically encoded chemistry. I will describe how we can use the most powerful algorithm for biological design, evolution, to optimize existing enzymes and invent new ones. Mimicking nature's evolutionary tricks and using a little chemical intuition, we can generate whole new enzyme families that catalyze important reactions not (yet) known in nature, thereby expanding the chemistry of the biological world and the molecules and materials we can build.

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**PROTEIN SIGNALING
& DESIGN**

APRIL 29, 2016

CHEM.AS.UKY.EDU/NAFF-SYMPOSIUM



2016 NAAFF SYMPOSIUM

GUEST SPEAKERS



FRANCES ARNOLD, PH.D.
California Institute of Technology
B.S., Mechanical and Aerospace Engineering, Princeton University, 1979; Ph.D., Chemical Engineering, University of California, Berkeley, 1985; Postdoctoral, UC Berkeley, Chemistry, 1985; Postdoctoral, Caltech, Chemistry, 1986

Dick and Barbara Dickinson Professor of Chemical Engineering, Bioengineering and Biochemistry; Director, Donna and Benjamin M. Rosen Bioengineering Center.



DAVID BAKER, PH.D.
University of Washington
B.A., Harvard University, Ph.D. University of California, Berkeley, Postdoctoral work/ UCSF

Head of the Institute for Protein Design, Professor of Biochemistry, Adjunct Professor of Bioengineering, Adjunct Professor of Genome Sciences, Adjunct Professor of Physics, Adjunct Professor of Chemical Engineering, Adjunct Professor of Computer Science Investigator, HHMI.



ROMMIE AMARO, PH.D.
University of California, San Diego
Ph.D., Chemistry, University of Illinois at Urbana-Champaign, B.S., Chemical Engineering, University of Illinois at Urbana-Champaign

Associate Professor, Chemistry and Biochemistry
Director, National Biomedical Computation Resource
Chemical Biology & Drug Design, Senior Editor
XSEDE User Advisory Committee member
Co-Director, Drug Design Data Resource.

2016 Naff Committee Members

Professor Pete Kekeneshuskey (Chemistry, Committee Chair), pkekeneshuskey@uky.edu
Professor Jason DeRouchey (Chemistry)
Professor Marcelo Guzman (Chemistry)
Professor Chris Richards (Chemistry)

For more information, contact Dr. Pete Kekeneshuskey.