TUESDAY, MARCH 14
Arrival and Registration

WEDNESDAY, MARCH 15
Welcome and Keynote Address
David Baker, University of Washington, USA
De novo Design of Function

Computational de novo Design of Biomolecules
Possu Huang†, Stanford University, USA
Talk Title to be Announced
William F. DeGrado, University of California, San Francisco, USA
de novo Design of Binding Proteins and Catalysts
Tanja Kortemme, University of California, San Francisco, USA
Computational Design of New Molecular Geometries and Ligand-Controlled Functions

Short Talks Chosen from Abstracts

Repurposing Proteins for Binding, Catalysis, and Sensing
Timothy Whitehead, University of Colorado Boulder, USA
One-Shot Design and Engineering of Portable in vitro and in vivo Biosensors
Birte Höcker, University of Bayreuth, Germany
Evolution and Design of Proteins
Dek Woolfson, University of Bristol, UK
Exploring the Dark Space of Protein Structure and Function through Rational and Computational Design
Neil P. King, University of Washington, USA
Computational Design of Self-Assembling Protein Nanomaterials for Medical Applications

Short Talks Chosen from Abstracts

Poster Session 1

THURSDAY, MARCH 16
Energy Landscape Search for Affinity and Specificity
Amy E. Keating, Massachusetts Institute of Technology, USA
Mapping Peptide Binding Specificity Space
Roberto A. Chica, University of Ottawa, Canada
Computational Design of Protein Energy Landscapes
Bruce Donald, Duke University, USA
Algorithms for Ensemble-Based Computational Protein Design
Sophie Barbe, Toulouse Biotechnology Institute, France
Search Algorithms in Protein Design

Short Talks Chosen from Abstracts

Machine Learning for Design of Enhanced Therapeutics and Biocatalysts
Joanna Slusky, University of Kansas, USA
Machine Learning for Accelerating the Design of Metalloenzymes
Bruno Emanuel Correia, École Polytechnique Fédérale de Lausanne, Switzerland
Deciphering Interaction Fingerprints from Protein Molecular Surfaces using Geometric Deep Learning
Daniela Grabs, Arzeda Corp, USA
Designer Enzymes to Deliver Performance Chemicals and Materials
Arvind Sivasubramanian, Adimab LLC, USA
Talk Title to be Announced

Short Talks Chosen from Abstracts

Poster Session 2

FRIDAY, MARCH 17
Early Career Protein Designers
Anum Glasgow, Columbia University, USA
Biophysical Requirements for Affinity and Stability in Engineered Anti-SARS-CoV-2 Receptor Traps
Anastassia A. Vorobieva, VIB-VUB, Belgium
De Novo Design of Pore-Forming Transmembrane beta-barrels
Nicholas F. Polizzi, Dana-Farber Cancer Institute, USA
A COMBS approach for Designing Functional Proteins

Short Talks Chosen from Abstracts

Prediction and Design of Protein Ligand Interactions
Brian K. Shoichet, University of California, San Francisco, USA
Ultra-Large Library Docking for Discovering New Chemotypes
Nir London, Weizmann Institute of Science, Israel
Designing Covalent Inhibitors
Xavier Barril, University of Barcelona, Spain
High-Throughput Virtual Dissociation Experiments: Application to Fragment Screening
Ora Furman, Hebrew University, Hadassah Medical School, Israel
Peptides as Far as the Eye Can See

Short Talks Chosen from Abstracts

Meeting Wrap-Up: Outcomes and Future Directions (Organizers)

SATURDAY, MARCH 18
Departure

* Session Chair  † Invited but not yet accepted     Program current as of November 17, 2022 Meal formats are based on meeting venue.
For the most up-to-date details, visit https://www.keystonesymposia.org.