**Workshop on Computational Modeling of Proteins for Infectious Disease Researchers**

**Day 1: [--]**

**Session 1. Foundations and Introduction to Computational Tools (Bart Staker)**

**1:00 PM - 1:30 PM**: Registration

**1:30 PM - 2:00 PM**: Welcome and Workshop Overview (**Peter Myler**)

**2:00 PM - 3:00 PM**: Basics of Protein Structure (**Dominika Borek**)

-Review of protein structure and structure determination methods.

**3:00 PM - 3:15 PM**: Coffee Break

**3:15 PM - 5:15 PM**: Hands-On Session: Basic Protein Modeling **(Craig Smith)**

- From sequence to predicted structure using Chimera graphical user interface.

**5:15 PM - 5:30 PM**: Q&A and Wrap-Up of Day 1

**Day 2: [-]**

**Session 2: Analysis of Protein Models (Adam Godzik)**

**8:30 AM - 9:00 AM**: Coffee and Networking

**9:00 AM - 10:30 AM**: Presentation (**Adam Godzik**)

**10:30 AM - 10:45 AM**: Coffee Break

**10:45 AM - 12:00 PM**: Hands-On Session (**Adam Godzik**)

**12:00 PM - 1:00 PM**: Lunch Break

**Session 3: Protein Complexes (Rocco Moretti)**

**1:00-1:45: Application talk.** Protein complex prediction and validation usingalphafold **(Alexei Savchenko)**

**1:45 PM - 2:30 PM**: Presentation (**Rocco Moretti**)

**2:30 PM - 2:45 PM**: Coffee Break

**2:45 PM - 4:00 PM**: Hands-On Session (**Rocco Moretti**)

**4:00 PM - 4:30 PM**: Q&A and Wrap-Up of Day 2

**Day 3: [-]**

**Session 4: Ligand Docking (Rocco Moretti)**

**8:30 AM - 9:00 AM**: Coffee and Networking

**9:00 AM – 9:45 AM: Application talk:** Modeling selective binding in parasite targets. **(Bart Staker)**

**9:45-10:30 AM**: Presentation (**Rocco Moretti**)

**10:30 AM - 10:45 AM**: Coffee Break

**10:45 AM - 12:00 PM**: Hands-On Session (**Rocco Moretti**)

**12:00 PM - 1:00 PM**: Lunch Break

**Session 5: Future Trends in Computational Protein Modeling (Isabelle Phan)**

**1:00-1:45:** Introduction to Protein Designwith Paul T Kim, Baker Lab, Institute of Protein Design

Paul will provide an introduction and overview of the latest advances at the IPD, aimed at providing attendees with an understanding of what tools exist, what is currently possible with these tools, and what outstanding challenges remain. The talk will also aim to facilitate collaboration between the Baker Lab and attending researchers by introducing the various subgroups in the lab and corresponding graduate students and postdocs, so that attendees will know who best to partner with for their specific goals.

**1:45 PM - 2:15 PM:** Applied Protein design at SSGCID **(Sophia Groustra)**

**2:15 PM - 2:45 PM: Coffee Break**

**2:45 PM - 3:45 PM: Future Developments in Protein Modeling and Design (Isabelle Phan)**

- Latest algorithms and tools in protein structure modeling and design

**3:45 PM - 4:30 PM:** Integrating structural tools into undergraduate education **(Craig Smith)**

**4:30 PM - 5:00 PM:** Q&A and Wrap-Up of Day 3 **(Karla Satchell)**

**5:00 END**