

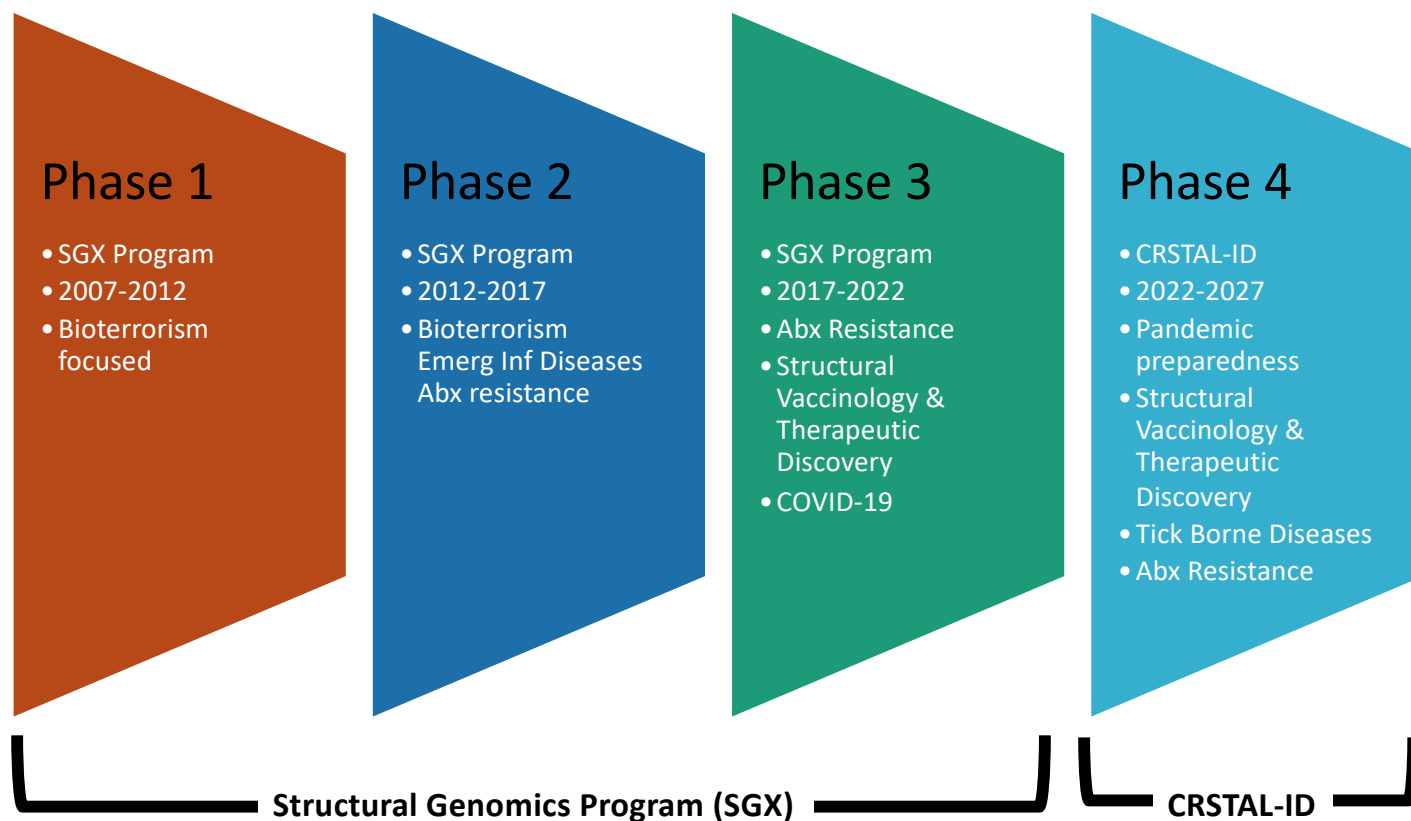
Workshop on Computational Modeling of Proteins for Infectious Disease Researchers July 20-22, 2026

Introduction

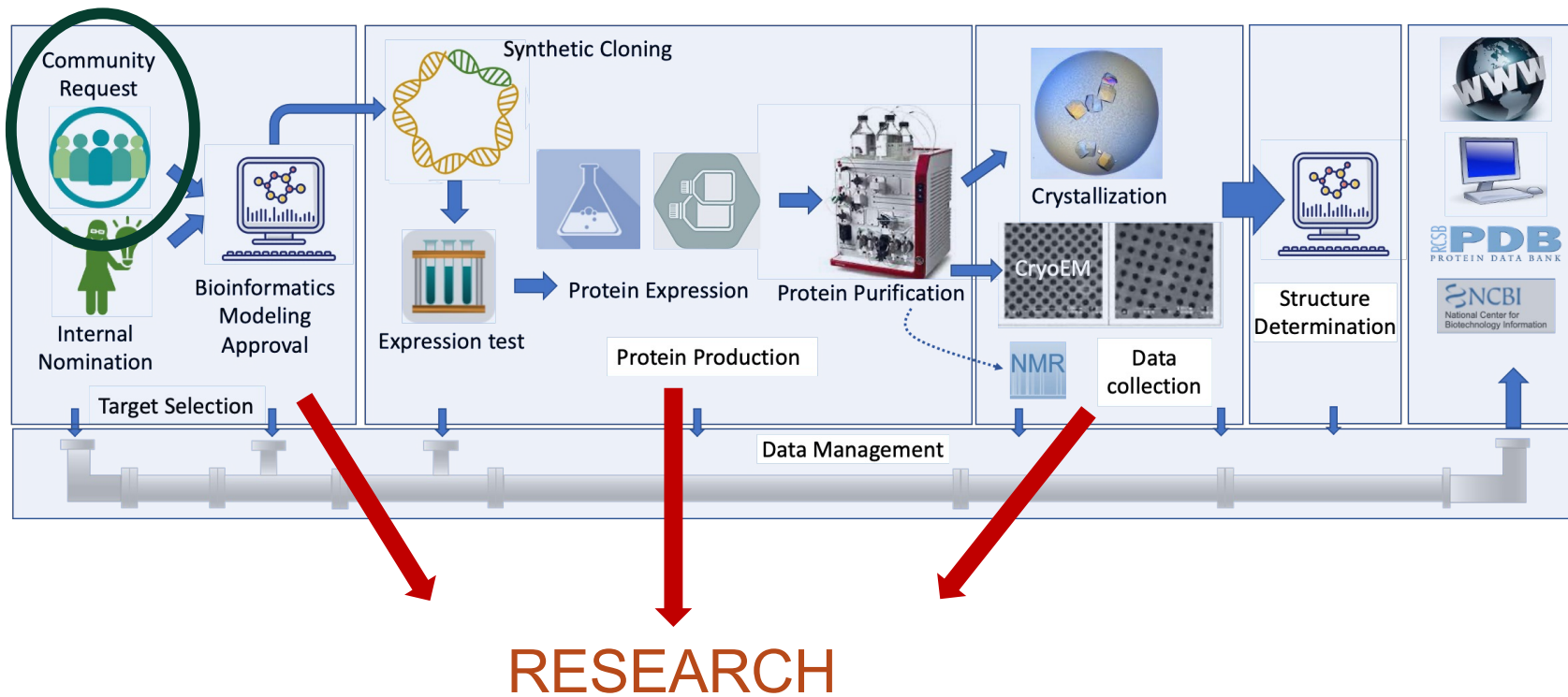
Karla Satchell, Northwestern University
Director, CSBID



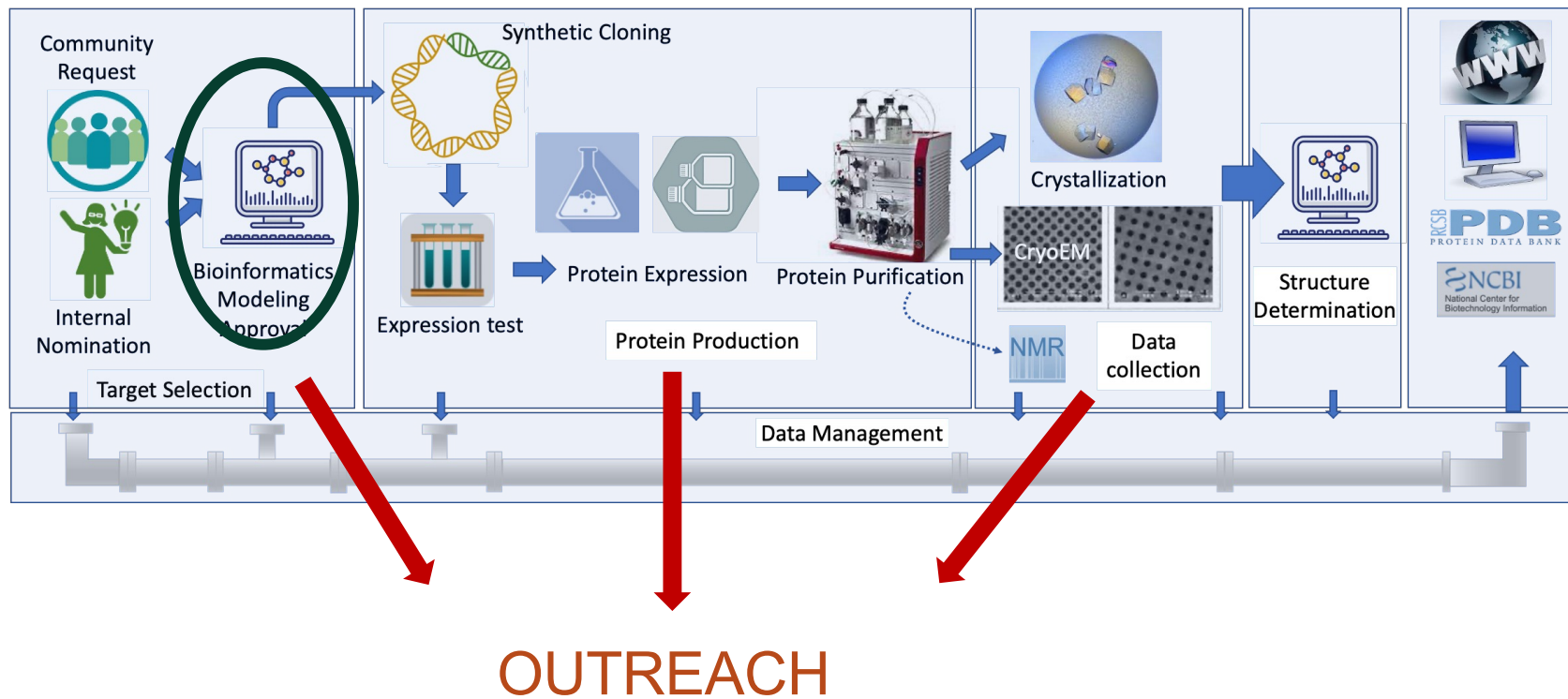
NIAID Structural Biology of Infectious Diseases Program



Structure Biology Services for Infectious Diseases



Structure Biology Services for Infectious Diseases



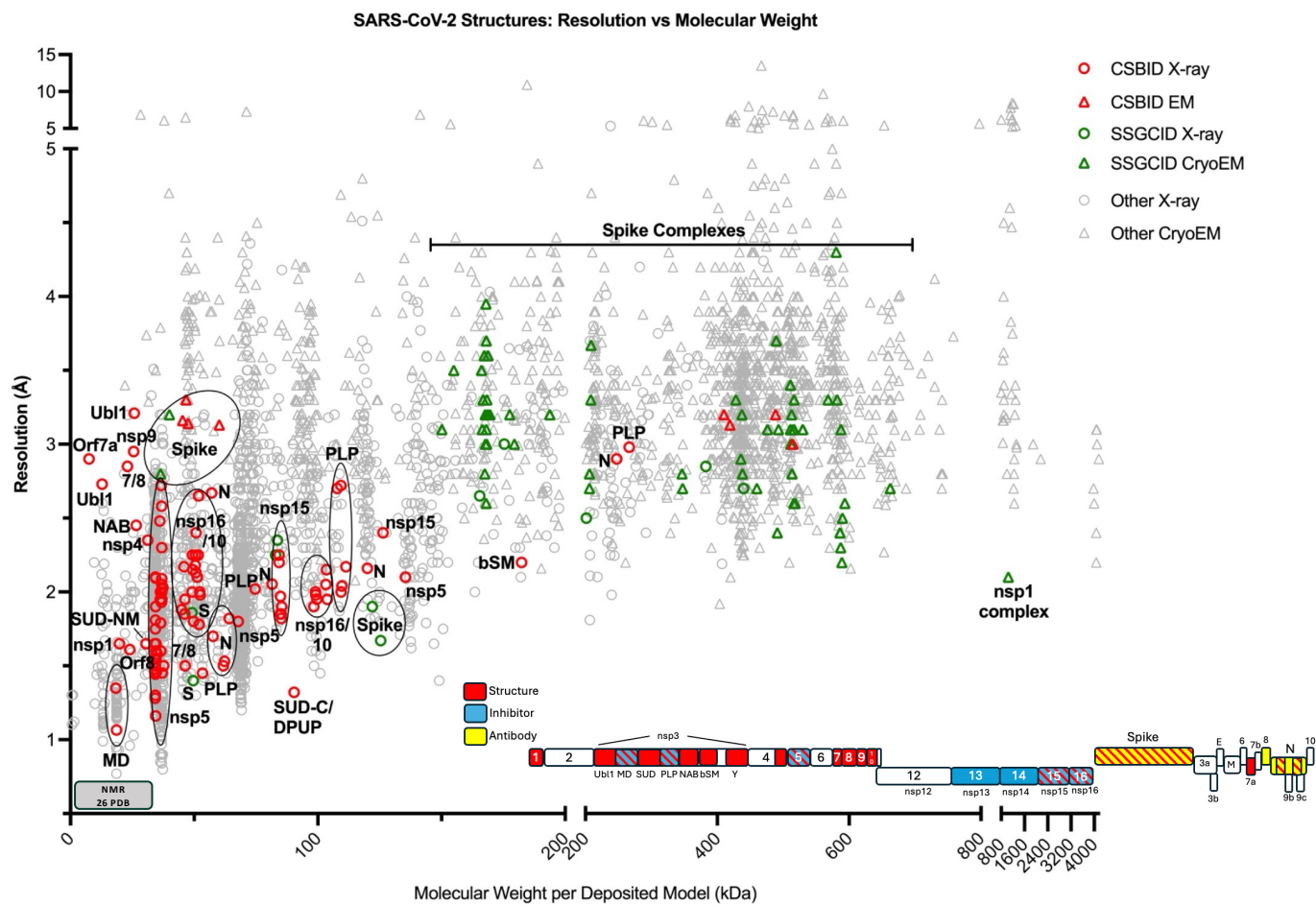
What is Structural Biology?

- Google AI says:

Structural biology is a branch of molecular biology focused on determining the 3-D shapes of biological macromolecules, primarily proteins and nucleic acids. Its core principle is that a biomolecule's 3D physical architecture directly dictates its biological function

Structural Biology Methods

- **X-ray crystallography**
Requires highly pure protein that will form a diffraction quality crystal
Can be time intensive to generate crystal
- **Cryoelectron Microscopy**
Applicable to large proteins and protein complexes
Requires less material but can be time intensive to establish proper grid conditions for data collection
- **Nuclear Magnetic Resonance**
Applicable to small proteins (<30 kD)
Requires pure material that is labelled



Modified from figure published in RCSB PDB Newsletter Education Corner July 2026

Determined structures form the training set for structural modeling

- 256,840 total structures in the PDB



- 12,212 structures come from Structural Genomics Programs

4.7%

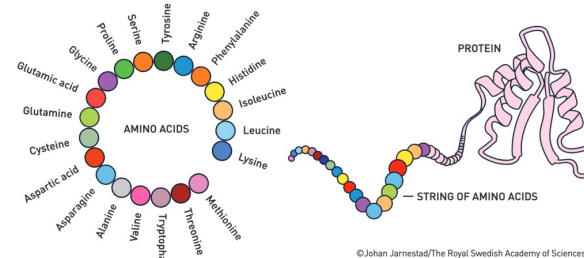
AI based structural modeling has revolutionized protein research by bringing structure to your own laptop

- Deep Mind AlphaFold (Google)
- Rosetta (David Baker)
- Meta ESMFold
- Others

 NOBELPRISET I KEMI 2024
THE NOBEL PRIZE IN CHEMISTRY 2024

 KUNGL. VETENSKAPS AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

		
David Baker University of Washington USA	Demis Hassabis Google DeepMind United Kingdom	John M. Jumper Google DeepMind United Kingdom
"för datorbaserad proteindesign" "for computational protein design"	"för proteinstrukturprediktion" "for protein structure prediction"	



NETFLIX

Why is Structural Biology important for Infectious Disease research?

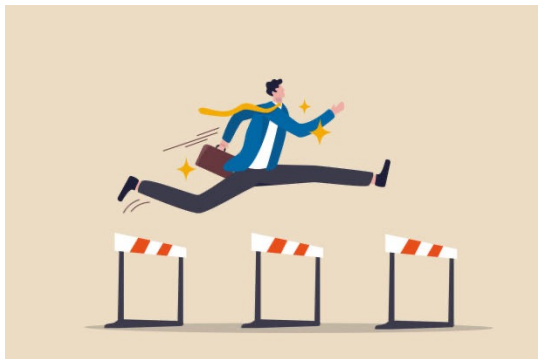
- Vaccine antigen discovery -> Vaccine development
- Antibody interactions -> Vaccines/Diagnostics
- Structure-guided drug design
- Reveal functional information for proteins
- Structural basis for protein-protein interactions
- Structural basis of protein-nucleic acid interactions
- Understand protein diversity and evolution
- Understand structural basis for genetic diseases



Barrier to implementation



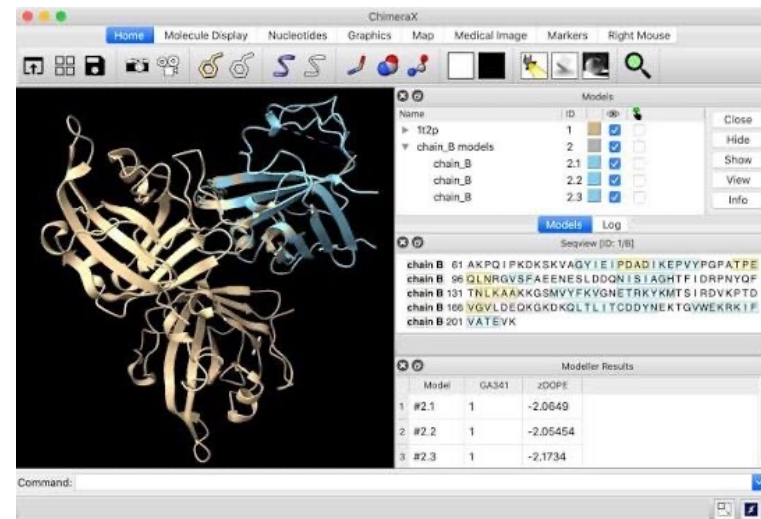
- Predominance of microbiology and infectious disease research is based on genetics, ecology, and surveillance.
- Researchers in microbiology and ID often have little or no experience in protein biochemistry or structure visualization
- Others?



Goal of
this workshop

UCSF ChimeraX

- UCSF ChimeraX is the next-generation molecular visualization program from the [Resource for Biocomputing, Visualization, and Informatics](#)(RBVI), following [UCSF Chimera](#).
- ChimeraX can be downloaded free of charge for academic, government, nonprofit, and personal use. Commercial users, please see [ChimeraX commercial licensing](#).
- ChimeraX is developed with support from [National Institutes of Health](#) R01-GM129325.
- <https://www.cgl.ucsf.edu/chimerax/>



NIAID BioViz Lab



Dr. Phil Cruz
NIAID Computational Structural Biology





Dr. Adam Godzik University of California at Riverside



Structure prediction and model analysis

Pathogens3D

HOME SARS-COV-2 BUNYAVIRALES LEGIONELLA PNEUMOPHILA PSEUDOMONAS PORINS

genomes	structures	Integrated analysis
Chromosome Plasmid	predicted experimental	MSA experiment Phylogenetic distribution Public databases COV-BRC NIH National Library of Medicine

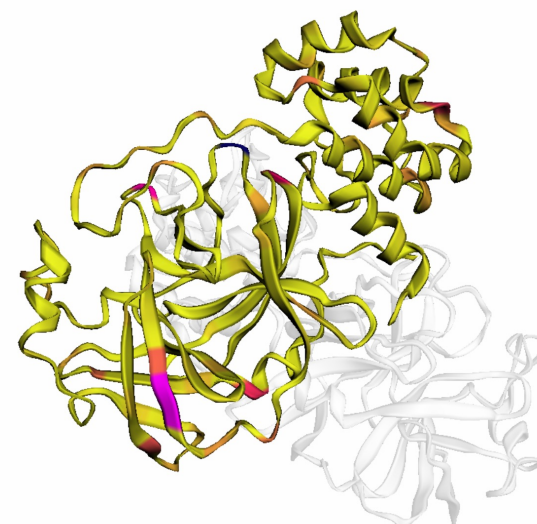
Pathogens3D

WELCOME

information on virulence factors from selected pathogens

click on the links above to see data on specific pathogens

CONTACT US



SARS-CoV-2 Main Protease



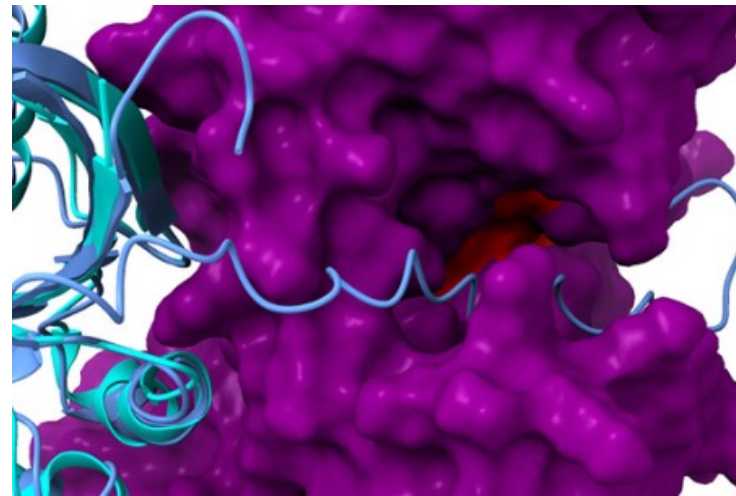
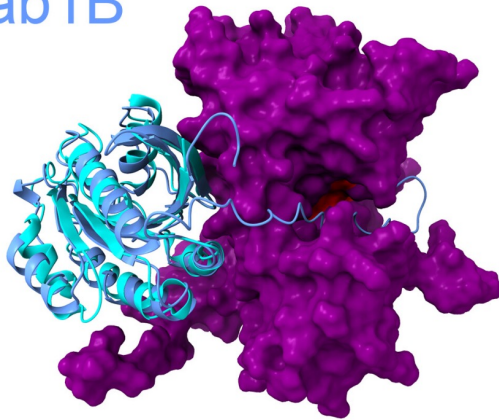
Dr. Bart Starker Seattle Children's Hospital



Protein complex prediction and validation

ARF3^{Q71L}
Rab1B

aMCF



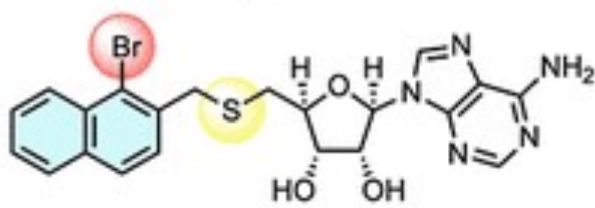
<https://doi.org/10.1073/pnas.2316143121>



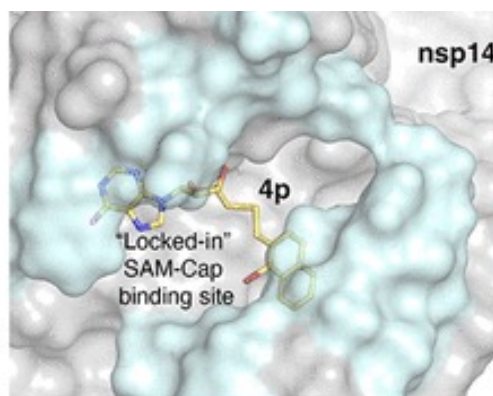
Dr. Scott Lovell Kansas University



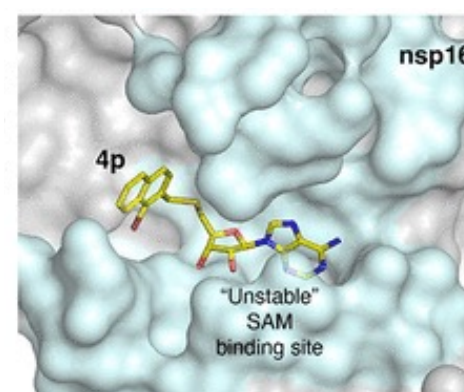
Modeling ligand binding in protein targets



SAH Analog inhibitor of
Coronavirus replication



IC₅₀ = 0.2 μ M



IC₅₀ = 87 μ M

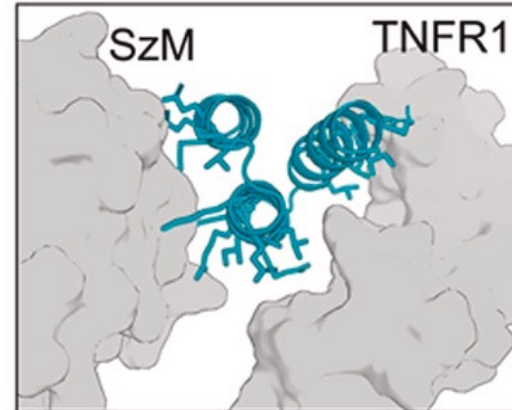
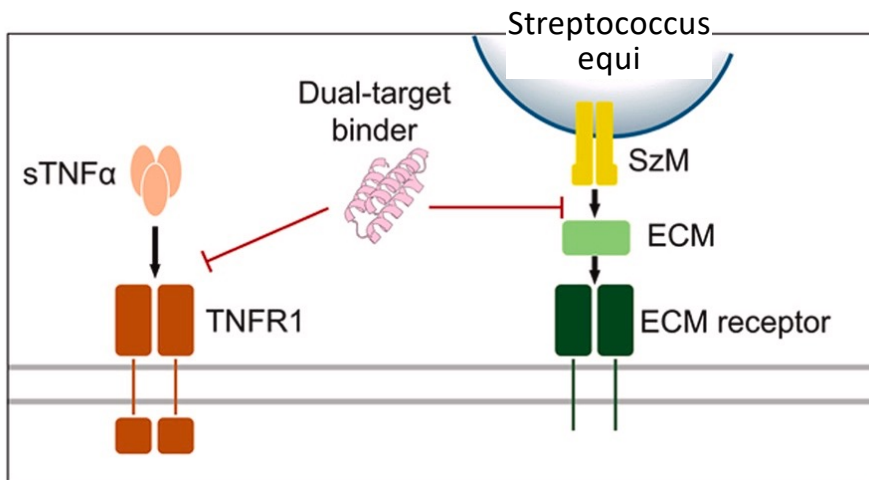
<https://doi.org/10.1021/acsmmedchemlett.5c00510>



Dr. Dominika Borek
UT Southwestern



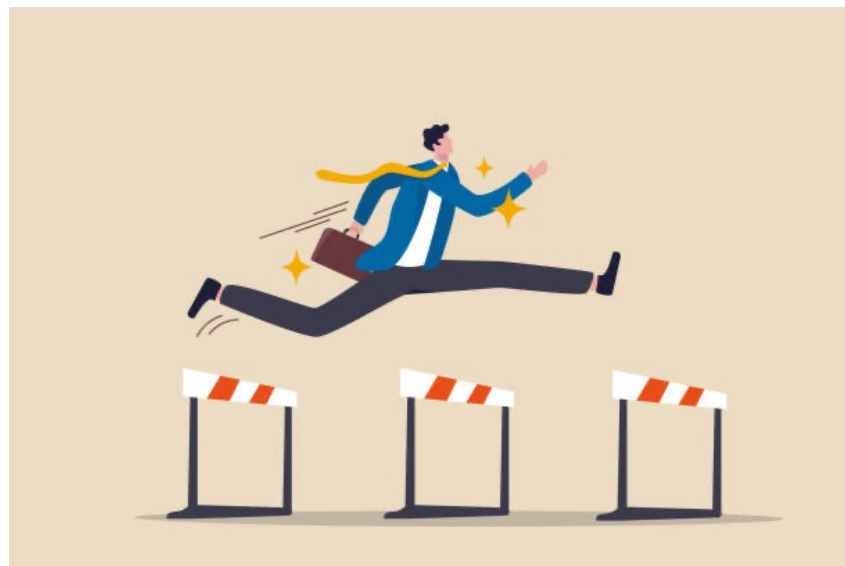
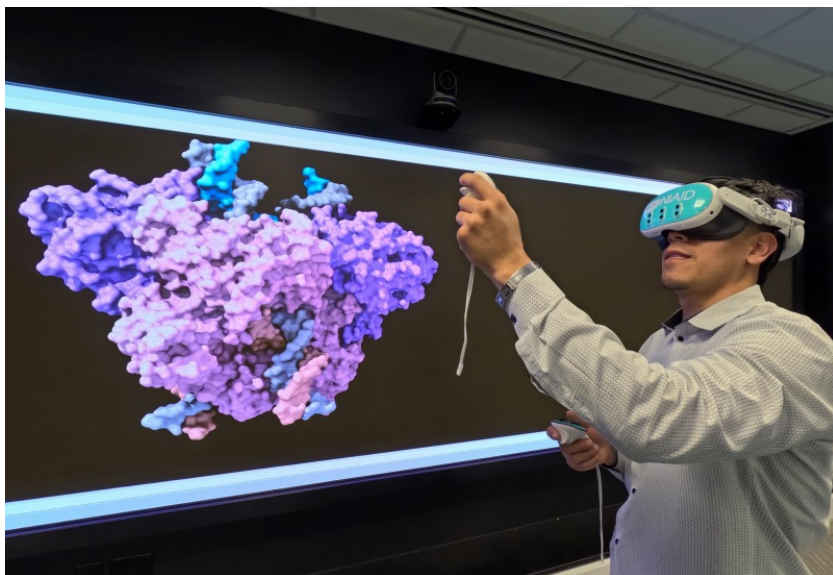
Applied Protein Design



Inhibits both
Bacterial adhesion and
TNFR1 signaling

<https://doi.org/10.1016/j.mtbio.2026.103336>

Structure is FUN!!





Thanks to---
Dr. Keewhan Kwon
NIAID Program Officer