



MBIB COVID-19 Related Research

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# Engagement in DOE NVBL Working Groups



### Testing

Structural biology to aid in the design of new diagnostics

### Molecular Design of Therapeutics

- Computation for prioritizing viral and host targets
- Computational design of new anti-viral small molecules
- Structural biology assisted drug design
- Biochemical validation

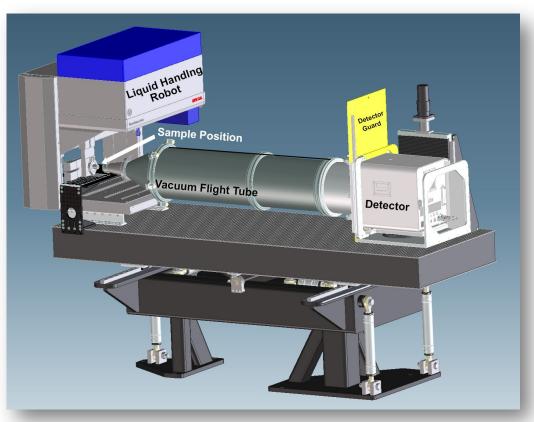
### Biodesign of Host-Directed and Combination Therapeutics (proposed)

- Production of reagents
- Impact of viral proteins on host cells
- Structural biology of viral/host protein interactions

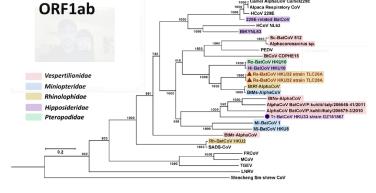
# Small Angle X-ray Scattering (SAXS) at the ALS



• Liquid handling robotics + Synchrotron High Flux beams = High-throughput structural analysis of viral proteins and target complexes in solution

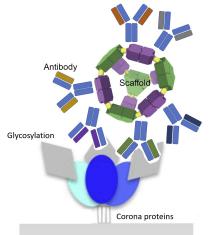


 Rapid characterization of viral proteins and their many interactions under various contexts



 Ideal for testing designed engineered structures for viral detection and vaccination

Greg Hura, Beamline 12.3.1





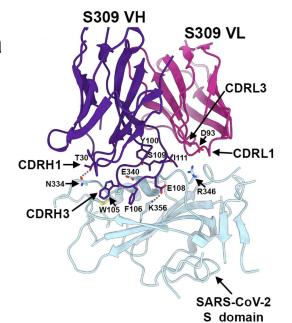
#### MBIB ALS Beamline Activities

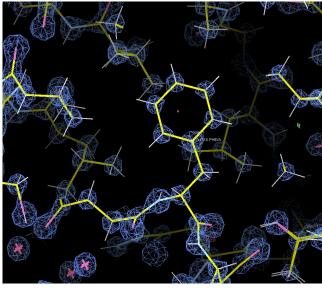


- The ALS is operating in a limited capacity supporting COVID-19- related research and proprietary research (all remote operation)
- MX/SAXS beamlines from the ALS-ENABLE program are accepting research proposals: <a href="http://als-enable.lbl.gov/">http://als-enable.lbl.gov/</a>



- Soft X-ray Tomography beamline also available for COVID-19 research
- MX data collection on crystals from academia and industry
  - Vir Biotechnology, Novartis, IniXium
  - University of Washington, UCSF
- Structures have been solved by the Veesler Group (U. Washington) and combined with cryo-EM data to understand how an antibody binds to and neutralizes SARS-CoV-2





Jaime Fraser (UCSF), Beamline 8.3.1





## Safety



- No work with live virus
  - MX/SAXS work is on isolated viral proteins or viral proteins in complex with antibodies, antigens or host proteins
  - SXT work is on fixed cryo-cooled host cells and virus
- Lab work with viral protein gene constructs requires approval by the Lab's institutional biosafety committee (IBC)
- ALS beamline use is either performed remotely or by trained beamline staff
- Social distancing requirements are integrated into revised WPC activities at each work location