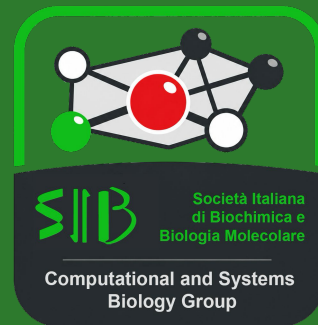


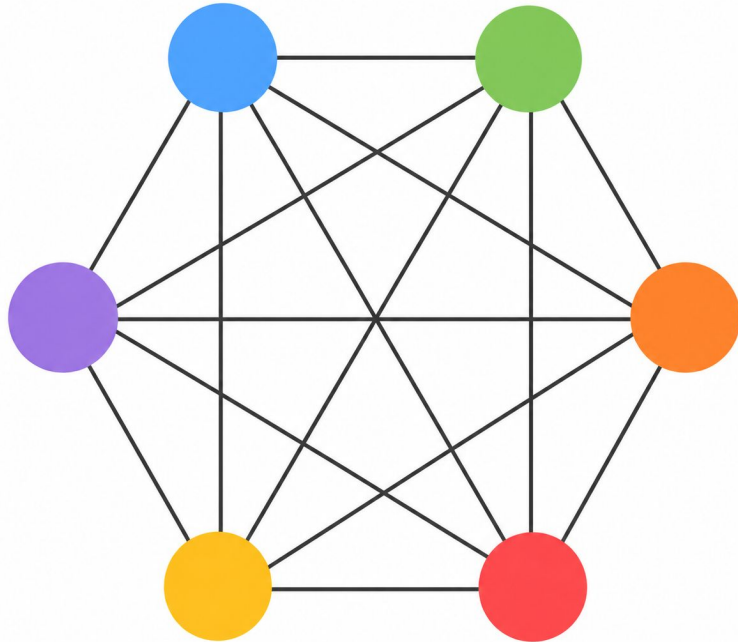
S2 · 12:25–12:40

Integrating Coevolutionary Analysis, Structural Prediction, and Molecular Dynamics for Complex Discovery

Giovanni Merici

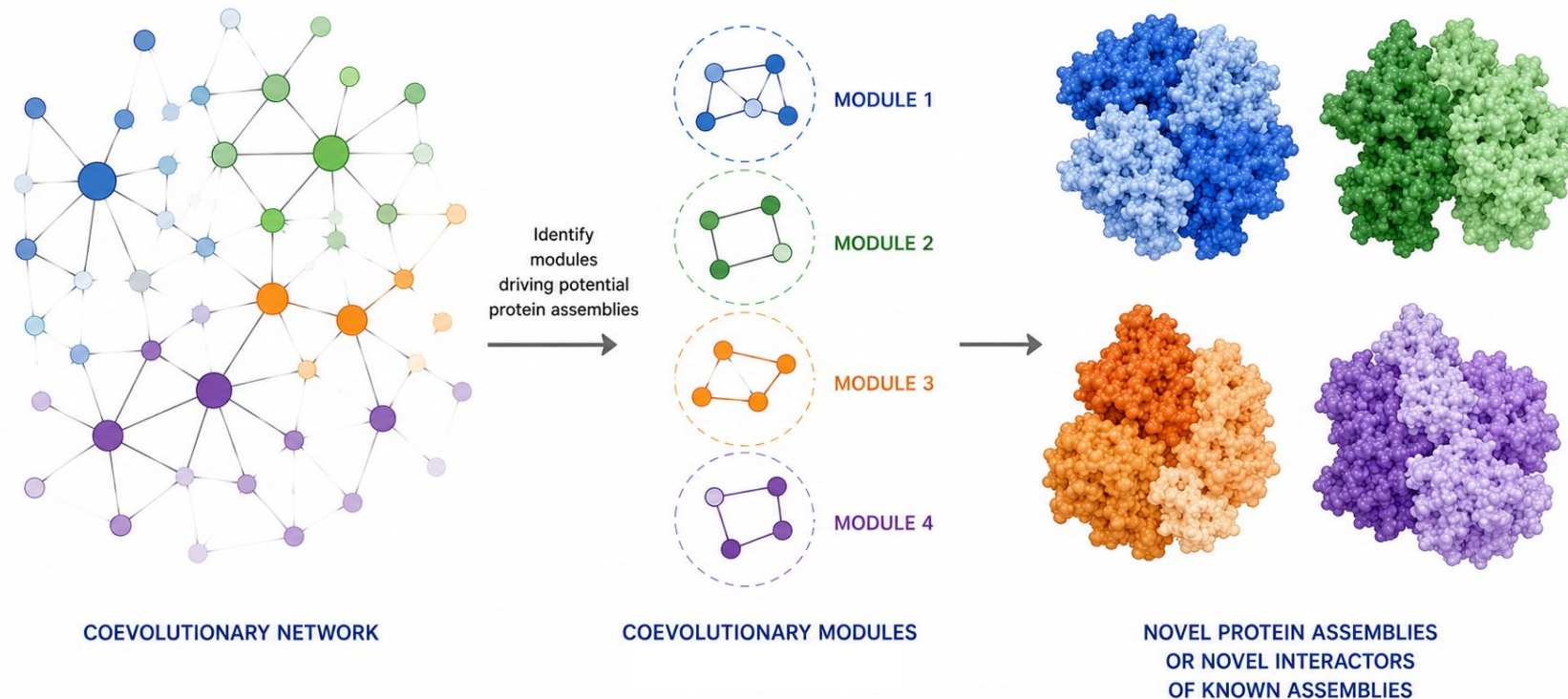
University of Parma

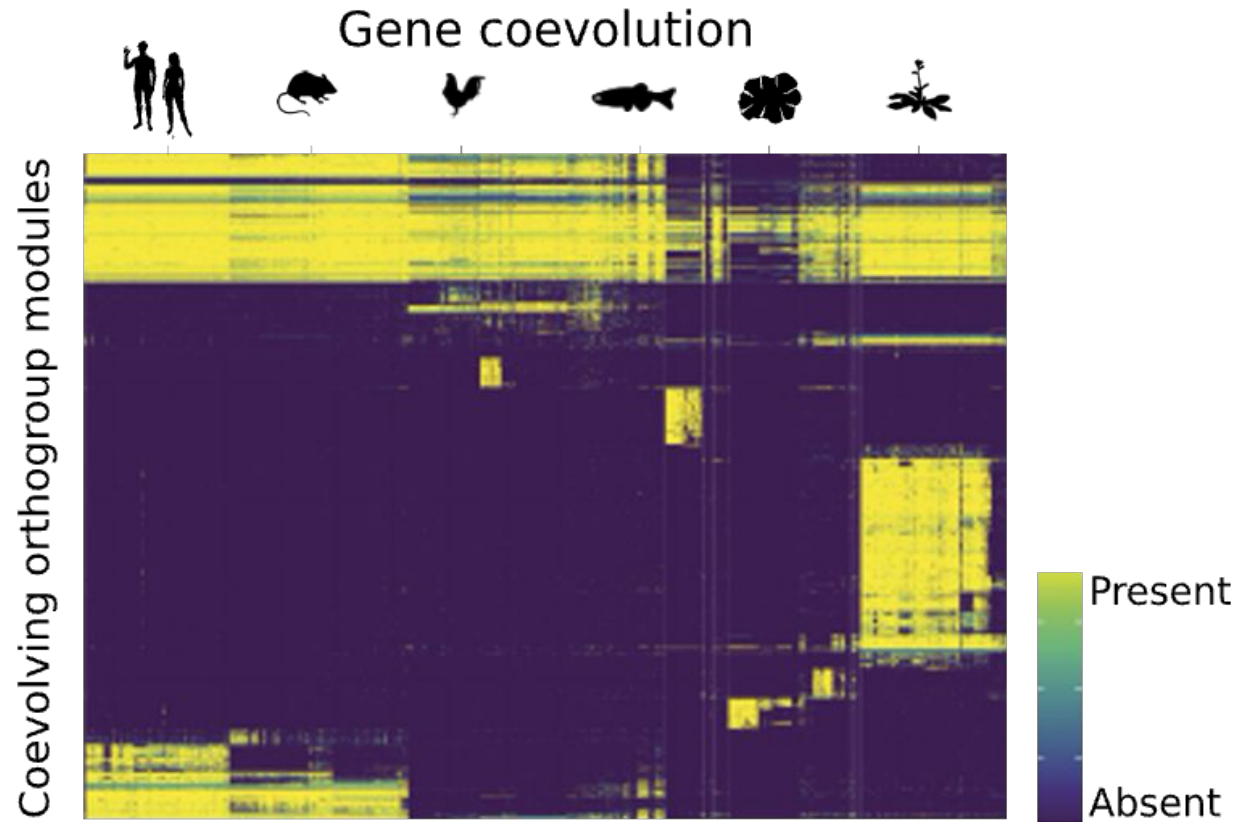


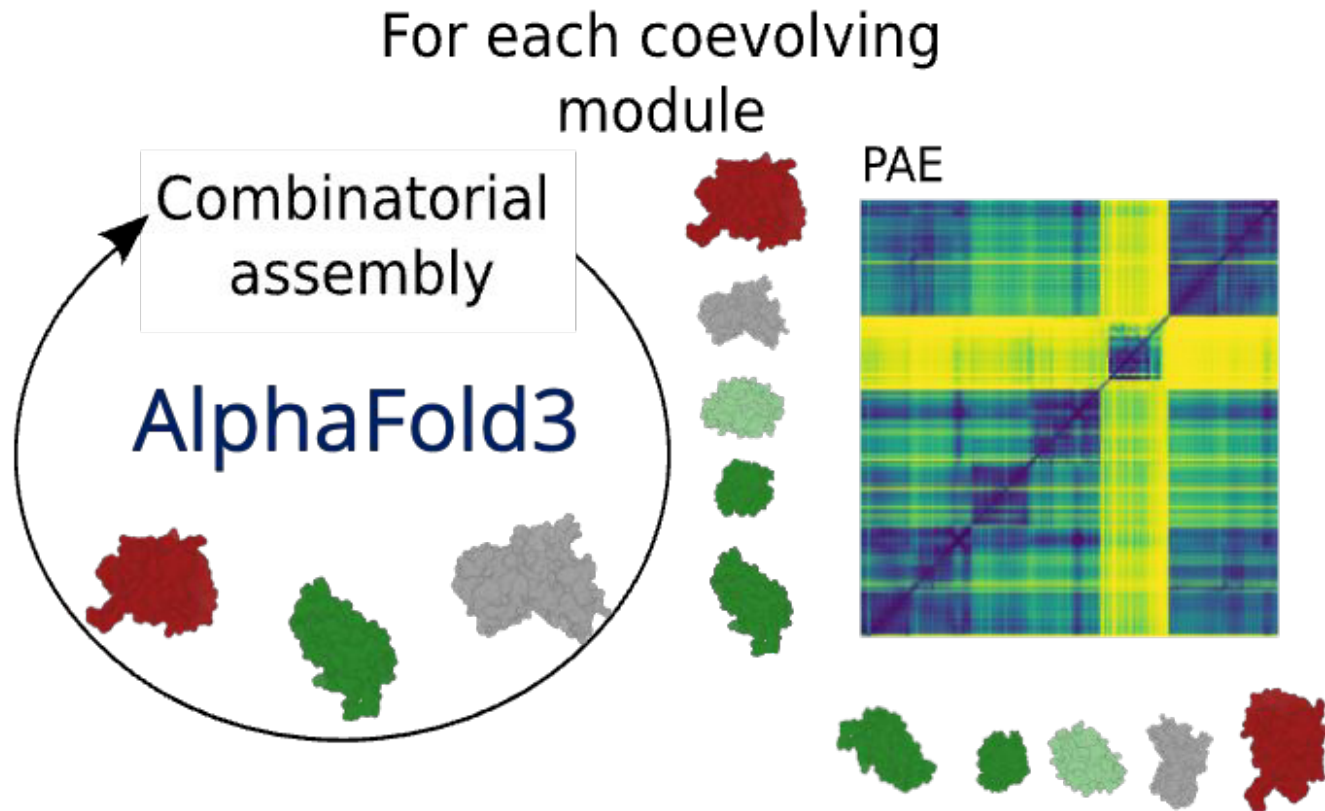


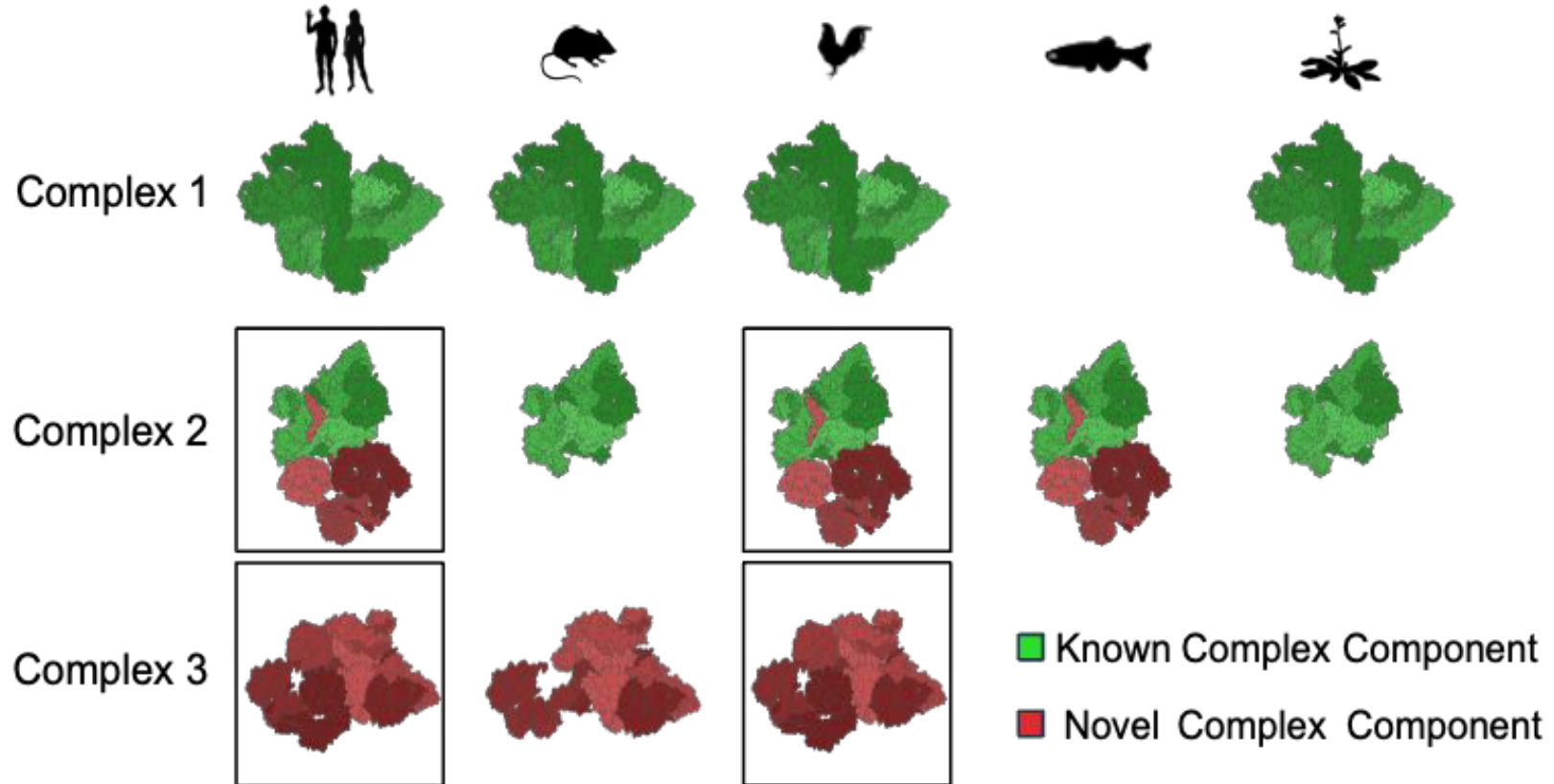
- Same Biological Pathway
- Functional Association
- Physical Association

Coevolution Analysis done by cotr: <https://doi.org/10.1073/pnas.2218329120>

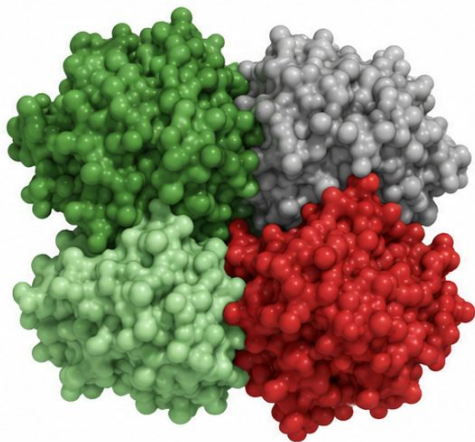




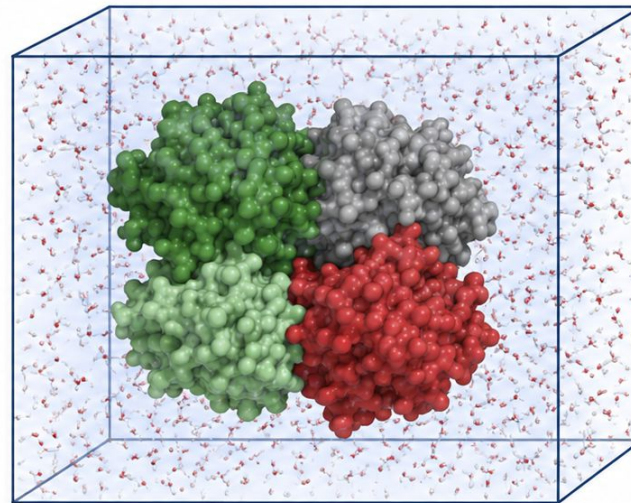




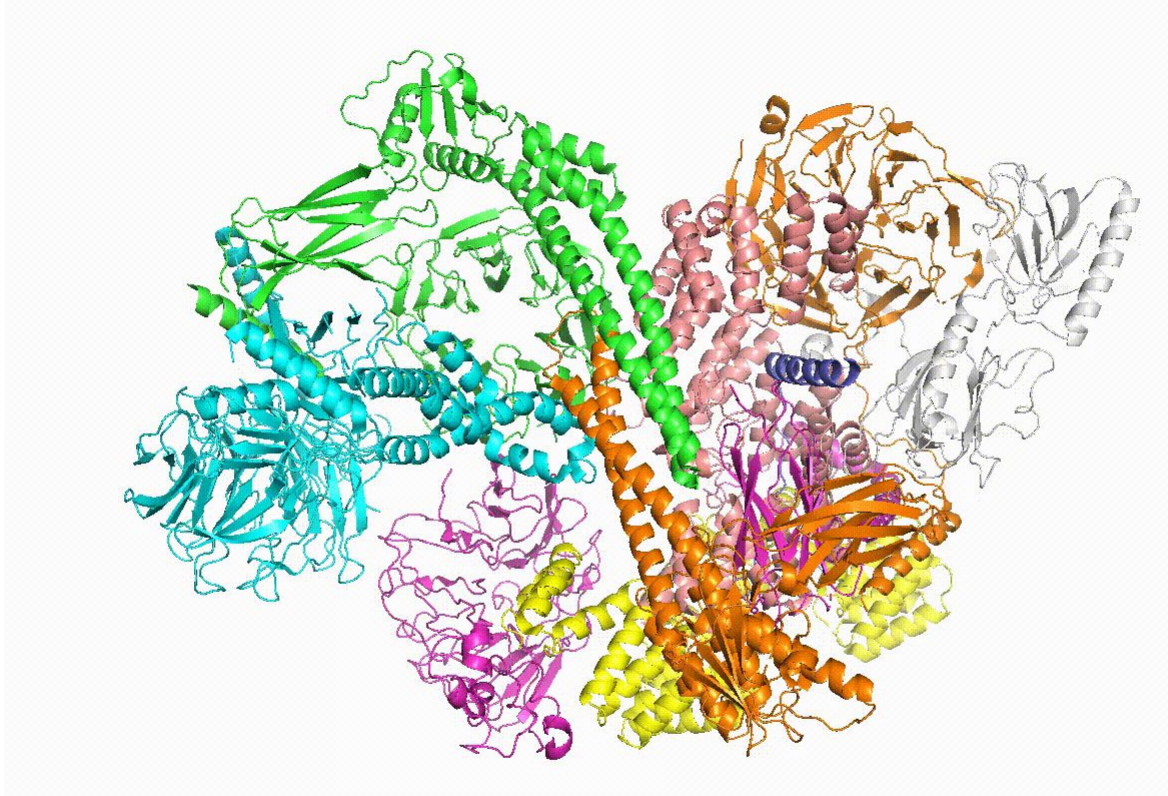
**AlphaFold validation
of putative complex**



**Molecular Dynamics
Simulation**

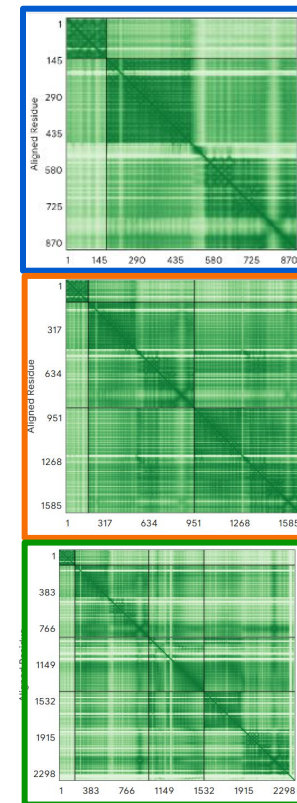
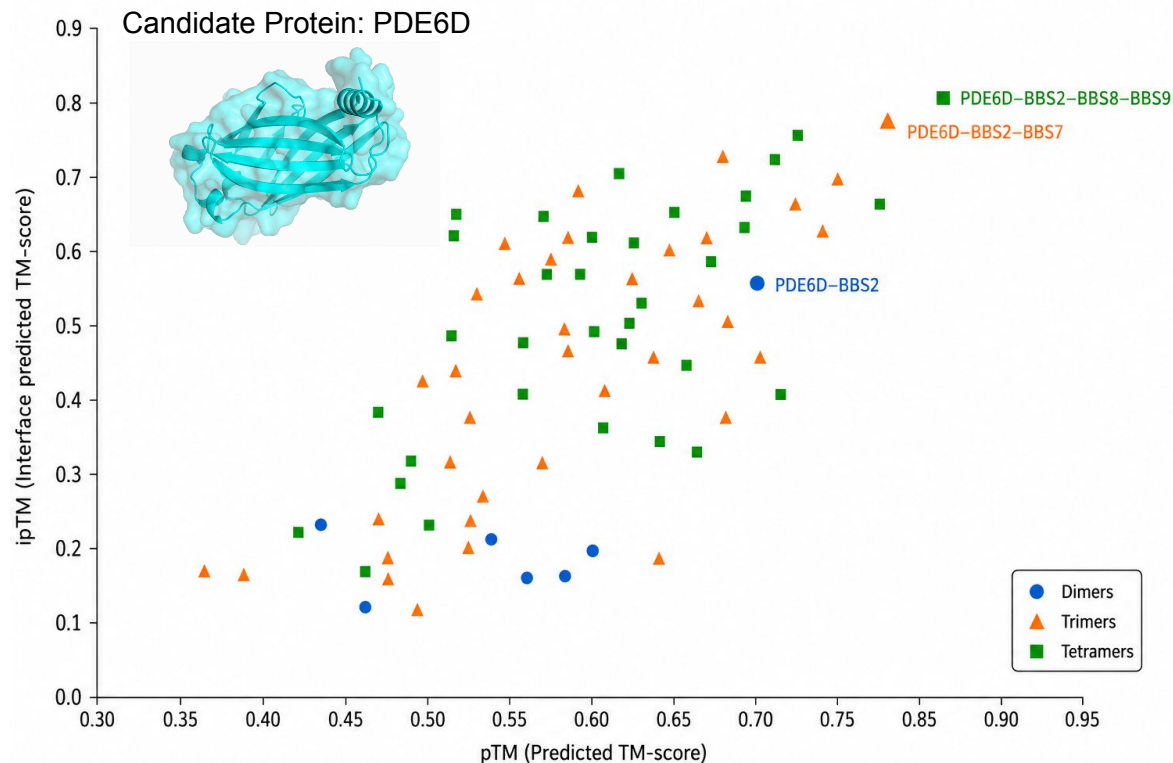


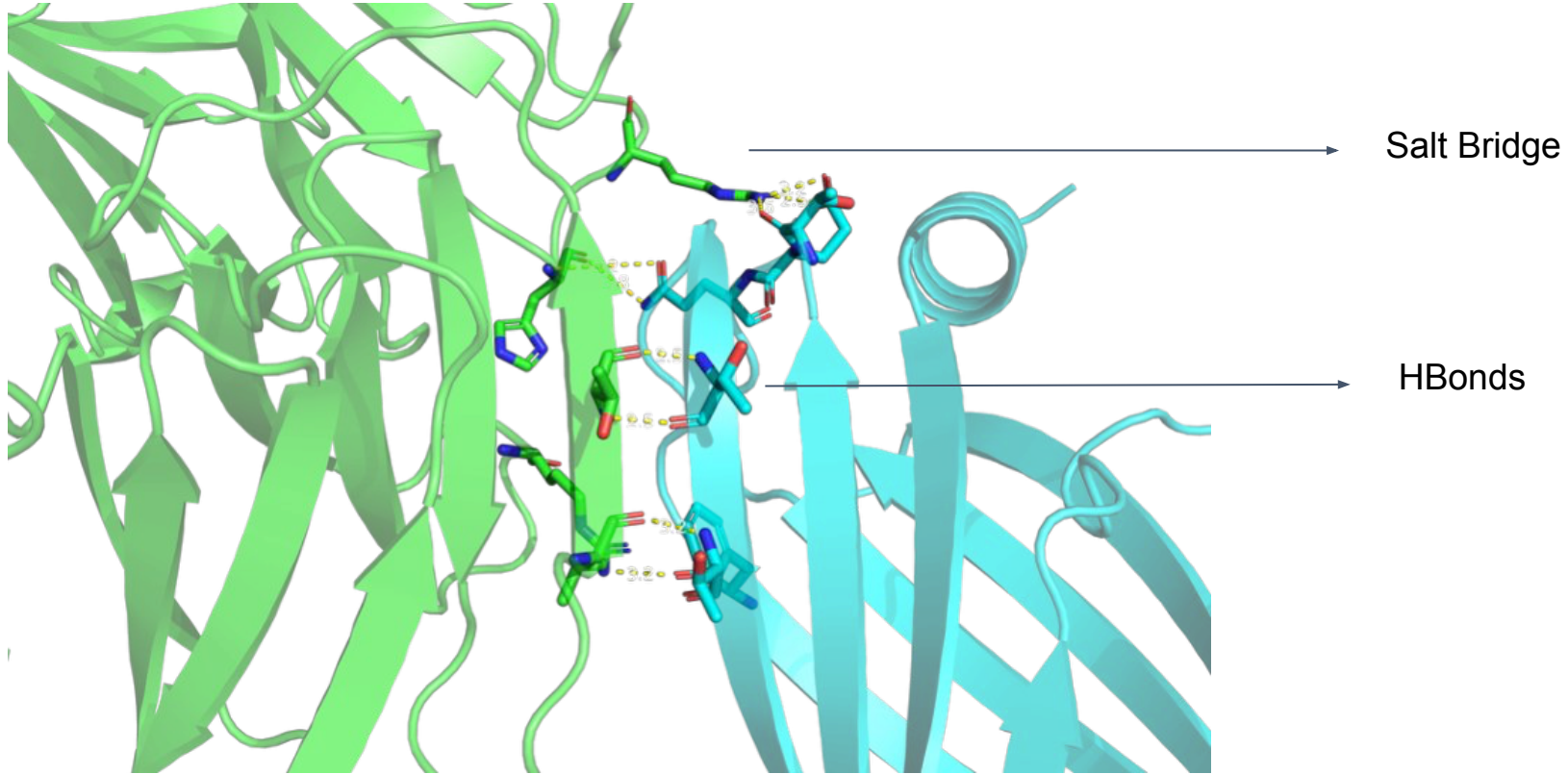
*Assess stability, flexibility and
protein-protein interactions over time*



Case Study: BBSome - AF3 Predictions

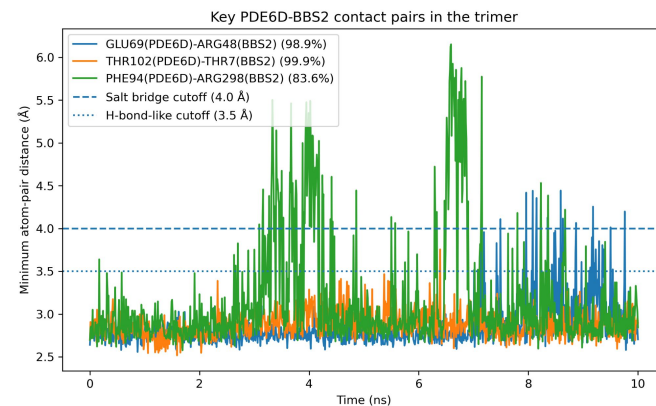
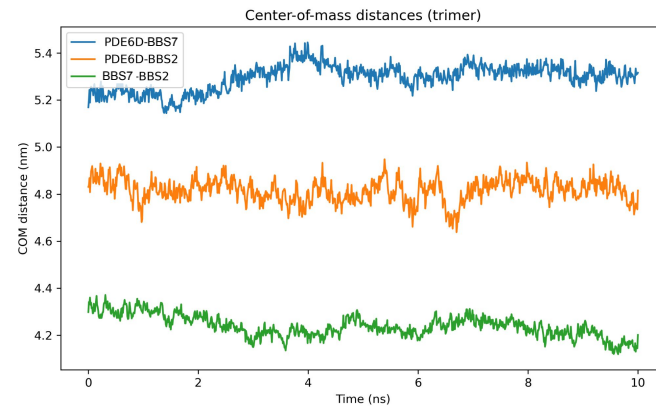
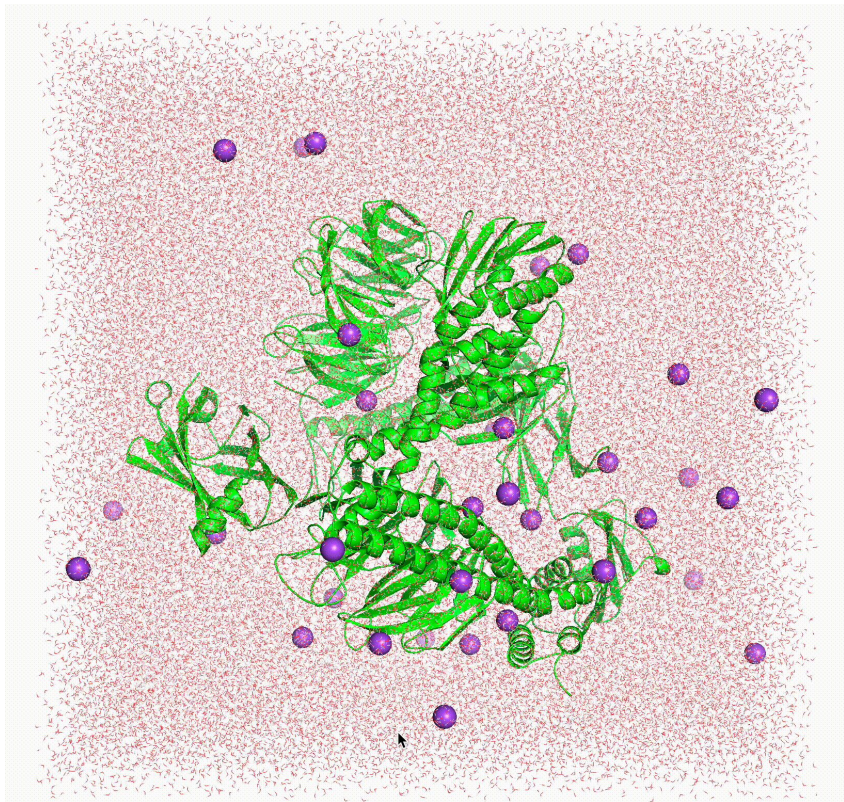
CSB Meeting 2026

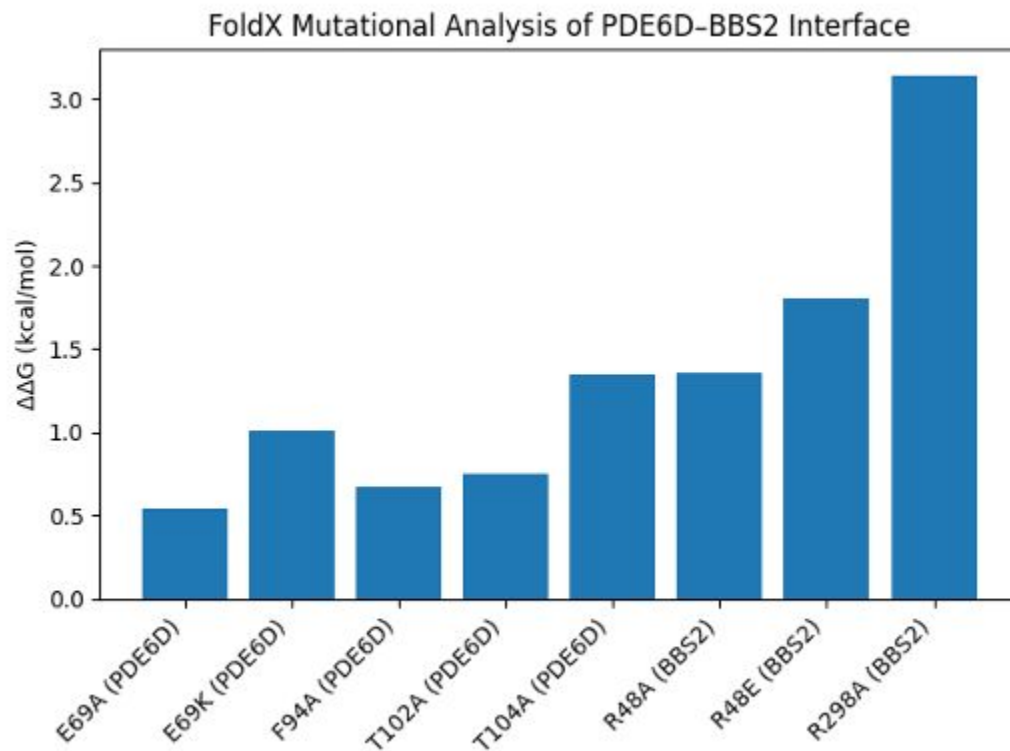




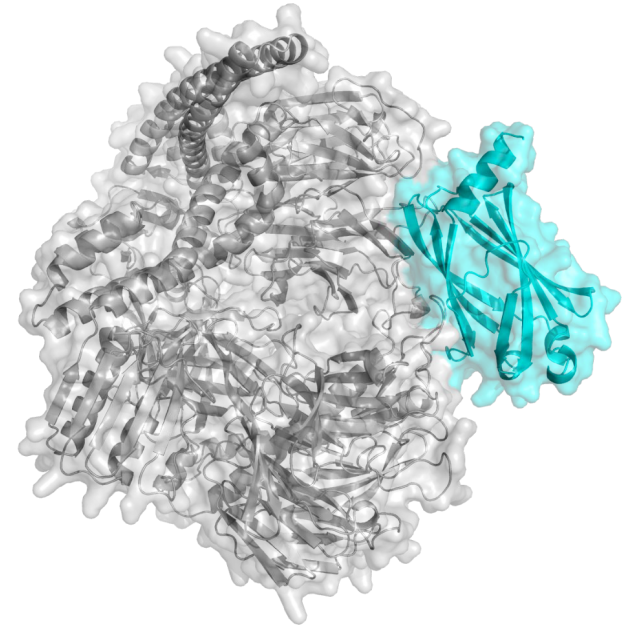
Case Study: BBSome - Molecular Dynamics

CSB Meeting 2026





- Coevolution-guided network analysis enables targeted AlphaFold 3 screening of putative protein complexes.
- Molecular dynamics simulations complement static AlphaFold 3 predictions by assessing complex stability and interaction dynamics.
- The integrated workflow generates experimentally testable hypotheses for novel protein assemblies



Acknowledgments

CSB Meeting 2026



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Thank you for the attention!