



Structure of Biological Molecules

Workshop @ German Conference on Bioinformatics 2026

A decade after AlphaGo's landmark success, AlphaFold has transformed structural bioinformatics from a search for static coordinates of protein atoms to a foundation for generative design. In some way, one could say that the "folding problem" has been solved. Others may say it has evolved. As the field moves beyond predictions of three-dimensional structures for isolated protein chains, the frontier now lies in capturing the dynamic, multi-component reality of the cellular environment.

This workshop aims to connect ML researchers and structural biologists to discuss the current state and perspectives of structural biology. Our main focus areas include, but are not limited to:

- **Conformational landscapes:** Modeling protein dynamics and Boltzmann distributions.
- **Genotype-to-phenotype relationships:** Predicting the effect of mutations on protein structure, dynamics, and function
- **The non-folding frontier:** Predicting intrinsically disordered regions (IDRs) and transient states.
- **Inter-molecular logic:** Protein-RNA interactions, ligand binding, and complex assemblies.
- **Protein generation and design:** Models for de novo protein generation and targeted design.

The workshop will be held on **Tuesday, September 22nd**, during the GCB Workshops time slots (**12:30 to 16:50, with a coffee break**). The workshop language is **English**. We plan to have 1 - 3 **invited talks**, 5 - 8 **contributed talks**, and a **poster session**.

We encourage relevant work submitted to GCB to be submitted to this workshop as well for discussion with a more specialized audience.

For submission instructions, please visit the conference website: old-shatterhand.github.io/workshop_sbm2026.html. The deadline for submissions is **06.08.2026 anywhere on earth**.