



Computational Structural Scientist, Molecular Modelling

Remote, full/part-time, Postdoc-to-senior

About us

We are an early stage, science driven startup building at the intersection of biology, data, and innovation. We are creating something ambitious from the ground up and are looking for people who enjoy working closely with the founder, taking ownership early, and helping build strong internal structures from day one.

The role

Multi-protein complexes populate distributions of states, and a method that outputs one confident answer is misrepresenting the biology. You will build sampling and scoring that produce an honest distribution across a large, flexible assembly, benchmark it properly against experimental structures, and then stake a prospective prediction on a system with nothing published.

Few computational structural biologists get a test this clean. Most of us have to settle for retrospective benchmarks and hope.

What you will do

- Develop restrained sampling and scoring for large flexible protein assemblies
- Design the filtering and ranking strategy, and defend every choice in it
- Benchmark rigorously against curated experimental structures, including honest treatment of where the method fails
- Deliver the sealed prospective prediction that is scored blind

What you will bring

- PhD in computational structural biology, biophysics or a closely related field
- Hands-on protein-protein docking experience, including familiarity with how it fails: near-native poses buried among decoys, scoring functions that rank the wrong cluster first
- Real understanding of pose-quality metrics and their limitations
- Strong Python and comfort running large sampling campaigns on HPC or cloud

Bonus: Multi-state or ensemble modelling, experience with cryo-EM conformational heterogeneity, distance-restraint methods from crosslinking or related data

What we offer

- The opportunity to join early and help build the company from the ground up
- Meaningful ownership and real responsibility from day one
- A fun, ambitious, and supportive startup environment
- Close collaboration with the founder and direct exposure to key business topics
- The chance to shape processes, ways of working, and how the company grows
- A fair share in the upside of what we are building together

How to apply

Please send your CV and a short motivation letter to contact@mithryon.com.