



Computational Chemist, Cheminformatics & Molecular Dynamics

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

A dual remit spanning small-molecule design space and simulation. On one side, the chemistry engine for a structurally constrained compound class and its developability assessment. On the other, conformational sampling of a large flexible biological assembly, and physical descriptors that must reproduce experimental measurements on systems the model has never seen.

You will also own the company's largest compute line and the simulation protocols that make a sealed, pre-registered result reproducible a year and a half later.

What you will do

- Build the cheminformatics engine for a structurally constrained compound class, including geometric feasibility screening and developability assessment
- Generate and validate conformational ensembles of a large, flexible multi-subunit assembly
- Develop physical descriptors from simulation that are calibrated against experimental measurement
- Investigate mechanistic approaches to a known developability bottleneck in this compound class
- Own simulation protocols, reproducibility and compute planning

What you will bring

- PhD in computational chemistry, biophysics or cheminformatics, with post-PhD experience
- Production-level MD: GROMACS, AMBER, OpenMM or NAMD, including enhanced sampling and system preparation you would defend in review

- Strong RDKit and cheminformatics engineering
- Sound judgement about convergence, and the willingness to say a simulation is not converged before a deadline rather than after

Bonus: Free-energy or unbinding methods, permeability modelling for difficult chemical space, experience owning a substantial compute budget

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.