

Computational Chemist, Modeling and Drug Design

[New Equilibrium Biosciences](#) discovers drugs that target intrinsically disordered proteins through its integrated computational-experimental platform, with the mission of creating transformative medicines for patients with cancers and neurodegenerative disorders. We are seeking a PhD-level scientist with a background in computational chemistry or biology to join our growing team starting in March 2021. You should have experience in molecular dynamics simulations of proteins and computer-aided drug design, and you should be passionate about using and building interdisciplinary, novel technologies to facilitate drug discovery for currently undrugged targets.

Required Qualifications:

- Ph.D. in Computational Chemistry, Computational Biology, or a related field
- Experience with:
 - Running and analyzing enhanced sampling molecular dynamics simulations
 - Intrinsically Disordered Proteins
 - Structure-based drug design
- Positive attitude and passion for New Equilibrium's goals
- Out-of-box thinker committed to rigorous scientific work

Desirable Qualifications (any combination of these):

- Postdoc/Industry experience related to Computational Chemistry, Computational Biology, Drug Discovery, Biophysics, or a related field
- Experience with:
 - Developing algorithms related to molecular dynamics simulations, in silico screening, or structure-based drug design
 - Fragment-based drug discovery
 - Free Energy Perturbation
 - Force field parameterization
 - AI-powered drug discovery
 - Developing machine learning algorithms
 - Building and configuring cloud-based and/or local HPC clusters
- Strong theoretical background in statistical mechanics, thermodynamics, quantum chemistry, and/or machine learning
- Interest in application-specific hardware and quantum computing
- Excellent oral and written communication skills

Responsibilities:

- Initiate, monitor, and analyze protein simulations

- Model the conformational ensemble of intrinsically disordered proteins
- Develop new methodologies for modeling intrinsically disordered proteins and their interactions with ligands
- Work closely with experimentalists and medicinal chemists to design and test drug molecules
- Prepare figures/slides/documents for external presentations
- Help shape the culture of New Equilibrium Biosciences

If interested, please apply via [our google form](#) by March 15th, 2021. We will be reviewing applications as they come in, so apply now and join us in our mission of creating new medicines for life-threatening diseases!