**Senior/Principal Scientist, Computational Chemistry**

Location: Cambridge MA

We are a Cambridge-based VC-backed stealth biotech focused on discovering and developing next generation precision oncology small molecule medicines. We are advancing drug discovery programs based on a platform that combines insights in cancer biology, structural biology, biophysics and chemical biology to identify and characterize novel druggable domains of protein targets.

A unique opportunity for a motivated and experienced team player to join an early-stage company to support drug discovery programs, interface with team members on the development of unique chemical matter to solve novel biological problems. This person will work in multidisciplinary teams to develop, validate and optimize novel molecular matter, will help design and develop first of kind novel in silico drug design platform to develop a new class of novel small molecules.

**Responsibilities include**

* Work with chemists, structural biologists, data scientists and biologists to drive drug discovery programs at all stages from early target validation, hit-finding, hit-to-lead evaluation, lead optimization, and candidate delivery
* Fully embedded within the chemistry team, provide computational chemistry support for efficient lead discovery and optimization
* Perform in-depth data analyses to identify SAR trends and derive chemistry hypotheses
* Design and execute ligand- and receptor-based screening to identify hits for novel targets
* Utilize novel computational biophysics (molecular dynamics, free energy methods) and structural informatics approaches to identify cryptic pockets and novel allosteric binding mechanisms
* Contribute to the development of computational infrastructure by identification of novel tools and techniques

**Desired Skills and Experience**

* Ph.D. degree and 2+ years of computational chemistry experience (or equivalent) in pharmaceutical/biotech settings
* Experience implementing computational strategies across all stages of drug discovery, including target identification, hit finding/expansion and hit-to-lead, and lead optimization activities to drive towards program goals
* Demonstrated track record of leveraging modern computational chemistry techniques, including structure-based design, conformational analysis, molecular dynamics, free energy methods, QSAR, and cheminformatics
* Strong understanding of all aspects of modern drug discovery including medicinal chemistry, DMPK principles and multi-parameter optimization
* You are a versatile scientist and eager to dive into uncharted territories and novel modalities to tackle various challenging targets via allosteric binding mechanisms
* Open and honest communicator with strong interpersonal skills
* Self-driven, a creative thinker, and a reliable team player
* You love to dive deep into data to solve complex problems
* Experience with Schrodinger Suite and/or programming experience (Python, C++) is a plus

**Interested Candidates should forward a cover letter and CV to careers@nestedtx.com**