

Job Title: Computational Chemist

Job Type: Full Time

Location: Cambridge, UK

Astex Pharmaceuticals is a world leader in innovative drug discovery and development. The company has successfully applied its proprietary Fragment-Based Drug Discovery platform to generate multiple new drug candidates that are progressing in clinical development. Successful collaborations have led to three launched oncology drugs (Kisqali® partnered with Novartis, Balversa® partnered with Janssen and Truqap™ partnered with AstraZeneca). Astex continues to grow and focuses on Neurological Disorders and Oncology.

The Role

Astex Pharmaceuticals is making a strategic investment in advanced molecular simulation and free energy methods as a key component of our structure-based drug discovery platform. We are now recruiting computational chemists, both permanent and fixed-term, at seniorities ranging from experienced research scientist to Director level, to help shape, develop and apply these capabilities across our internal discovery portfolio.

Astex offers a distinctive environment for computational chemists: world-class structure-based drug discovery, close integration with medicinal chemistry and structural biology, frequent access to high-quality protein–ligand structures from X-ray crystallography and cryo-EM, and a proprietary historical dataset of more than 20,000 structures across diverse target classes. This creates an unusually rich setting for both method development and prospective application on active drug discovery programmes. Our focus on scientific rigour and impact for patients has led to numerous clinical candidates and 3 marketed drugs.

Successful candidates will contribute to the development and application of Astex's internal simulation platform, with a particular focus on free energy and related molecular simulation approaches for prediction of affinity, including combining such methods with ML. Depending on seniority, responsibilities may include applying simulation methods to guide compound design, developing robust workflows, validating novel methods against high-quality experimental datasets, influencing project strategy, and providing scientific leadership across multidisciplinary teams.

This is an opportunity to join Astex at a time of deliberate growth in simulation science, helping to define how advanced computational methods are used to drive the next generation of structure-based drug discovery.

Skills and Experience

- PhD in Computational Chemistry or a related field
- Ability to work collaboratively in multidisciplinary project teams

- Excellent communication skills, in particular the ability to communicate effectively with scientists from different disciplines
- Several years' experience developing and/or applying modern simulation methods (in particular FEP/TI or similar) in a drug discovery context
- Strong programming / scripting skills, ideally in Python, with an interest in developing robust, scalable workflows

At director level:

- 10+ years of experience in industrial drug discovery and a proven track record of successful application / development of computational approaches
- Evidence of scientific leadership and strategic influence

Why Astex

We offer excellent training and career development opportunities as well as highly competitive salary and benefits package including hybrid working options to promote a flexible and inclusive work environment.

At Astex we embrace diversity and equality of opportunity. We are committed to building an inclusive and diverse Company representing all backgrounds, harnessing industry-leading scientific innovation and behaviours.

Astex is situated 2.5 miles from Cambridge City centre on the Cambridge Science Park. The Park has onsite sports facilities and excellent transport links to London.

How to Apply

All applicants should apply by email to recruitment.uk@astx.com, attaching their CV and covering letter as PDF documents. The subject line of the email should clearly state the reference (COMP/0726). When submitting your application, please indicate which position you are applying for.

Please note that Astex holds a UK sponsor licence; if you require sponsorship, please state this in your application email.

The closing date for applications is midnight on 30th September 2026