



Job Title: Postdoctoral Research Associate, Sustaining Innovation (Ref SI-CC005)

Project: Artificial Intelligence and Computational Chemistry

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 and the company is a recognised world expert in structural biology and crystallography. The sustaining innovation Postdoctoral research program aims to enhance the Company's excellent scientific culture by fostering basic research in the drug discovery field, whilst working with scientists in the biotech sector and with academic experts in the areas of research interest.

University of Cambridge and Astex Pharmaceuticals have partnered to create an exciting new postdoctoral position in AI-based Computational Chemistry. The successful candidate will join Dr. Lucy Colwell's group at the Chemistry Department, leaders in the innovative application of modelling and AI-based approaches to unsolved problems in chemistry, biochemistry and structural biology.

Project title: Development and application of Artificial Intelligence technologies to data from fragment screening campaigns to generate deeper understanding and more accurate predictive models.

Artificial Intelligence (AI) techniques are now widespread in society, where they have become hugely successful in fields ranging from voice recognition to clinical diagnostics. A recurring question in Fragment-Based Drug Discovery is why certain fragments bind to a target, while other fragments do not? AI methods, trained on data from fragment screening campaigns, may well be able to identify rules about what dictates fragment binding that would otherwise not be detected. This project will apply AI methodologies to data from Astex's fragment screening campaigns to help understand and predict what drives fragment binding. The successful candidate will be based in the chemistry department, and will also spend time embedded at the Astex headquarters in Cambridge.

Candidate Requirements

- A PhD in a chemistry or in a relevant theoretical science
- Thorough understanding of chemistry and non-bonded interactions
- Significant, relevant and demonstrable programming experience
- Excellent communication skills
- Good data management skills

Desirable skills

- Hands-on experience with large data sets and machine learning technologies
- Experience of relational databases

To apply please send your CV and a cover letter, quoting the job reference **SI-CC005** to HR.UK@astx.com