



Job Title: Sustaining Innovation Postdoctoral Research Associate

Project Title: Computer Vision for Molecular Structure Determination

Job Type: 3 Year Fixed Term Contract, Full Time

Location: Cambridge, UK, with regular visits to Madrid, Spain

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. We are a member of the OpenFold consortium and are contributing structural data to the Federated OpenFold3 Initiative, underlining our commitment to developing machine learning solutions for drug discovery. Our state-of-the-art, in-house cryo-EM facility includes an extensive computing infrastructure data collection and processing workflows to facilitate the rapid generation and interpretation of cryo-EM structures (1). This resource has established a sizeable cryo-EM data lake that is highly valuable for machine learning-based method development.

IE University is a young institution investing heavily in research excellence in applied sciences with a focus on real-world impact. The group of Prof. Sanchez-Garcia has a sustained track record in deep learning for cryo-EM, including particle alignment, pose estimation and map post-processing, and has released widely used open-source tools such as DeepEMhancer (2) and MicrographCleaner (3).

The role

Astex Pharmaceuticals (Cambridge, UK) and the group of Prof. Ruben Sanchez-Garcia at IE University (Madrid, Spain) have an exciting opportunity for a joint post-doctoral position developing cutting-edge deep learning algorithms for cryo-EM single particle analysis (SPA). We are looking for outstanding candidates with expertise in either cryo-EM image processing or modern computer vision and deep learning.

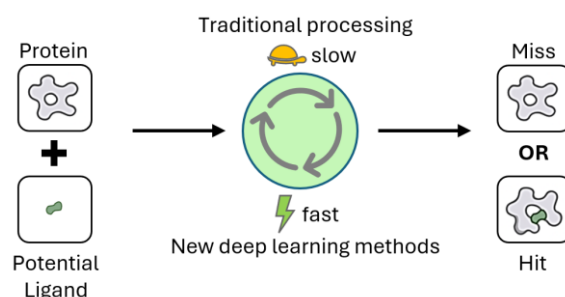
Cryo-electron microscopy (cryo-EM) is a Nobel Prize-winning imaging technology that enables the determination of near-atomic-resolution structures of biological macromolecules. From a machine learning perspective, cryo-EM presents unique challenges, including learning from extremely low signal-to-noise images or recovering accurate 3D orientations from large-scale experimental datasets.

This position will focus on pushing the boundaries of what is possible in deep learning-driven 3D pose estimation of low signal-to-noise ratio (SNR) images as present in cryo-EM, by building on our recently published software cryoPARES (4,5) and exploring self-supervised representation learning and foundation models on our Petabyte-scale cryo-EM datasets.

The position is Cambridge-based, but regular visits to Madrid will be part of this post-doctoral position.

Principle responsibilities

You would be responsible for actively advancing cutting-edge deep learning models for SPA, publishing your results in high-impact journals and making your work available to the wider machine learning and cryo-EM communities. The role will specifically focus on inferring 3D poses of particles using deep learning and improving the performance of traditional pose estimation methods by developing foundation models similar to Cryo-IEF (<https://doi.org/10.1038/s41592-025-02917-7>). You will join Astex's experienced cryo-EM and machine learning teams and benefit from Prof. Sanchez-Garcia's extensive experience in deep learning applied for cryo-EM applications (1-4).



Essential Skills

- PhD in mathematics, computer science or another relevant numerical/computational discipline, or equivalent experience in a relevant research area
- **At least, one of the following**
 - Demonstrable experience in developing computer vision algorithms using frameworks like Pytorch, JAX or Tensorflow and a strong interest of applying the technology on biological images
 - Detailed knowledge of SPA image processing theory with demonstrable experience in algorithm development for SPA
- Excellent knowledge of Python and familiarity with Git, preferably also knowledge of C/C++
- Excellent problem-solving and team working skills

Recent publications

1. Saur, Hartshorn et al. 2020: <http://doi.org/10.1016/j.drudis.2019.12.006>
2. Sanchez-Garcia et al. 2021: <https://doi.org/10.1038/s42003-021-02399-1>
3. Sanchez-Garcia et al. 2020: <https://doi.org/10.1016/j.jsb.2020.107498>
4. Sanchez-Garcia et al. 2025: <https://doi.org/10.1101/2025.03.04.641536>
5. Sanchez-Garcia et al. 2024: <https://doi.org/10.1103/PhysRevResearch.6.023245>

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.

The successful candidate will have access to proprietary Petabyte-scale cryo-EM datasets, modern GPU infrastructure, close collaborations between academia and industry, and the opportunity to publish high-impact research while developing AI methods that directly accelerate structure-based drug discovery.

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.

More information

For information on Astex Pharmaceuticals please visit: www.astx.com

For information on Otsuka Pharmaceuticals please visit: www.otsuka.co.jp

How to Apply

Eligibility

- The position is Cambridge-based, but regular visits to Madrid will be part of this post-doctoral position.
- Due to the unique nature of the role, which requires the individual to spend time in both Spain and the UK to undertake research activities, we require the candidate to already hold the right to work in Spain or be an EU national. Successful progression to interview will be subject to completion of a right-to-work check.

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 **(SIPD/0426)**.

This vacancy will remain open until a suitable candidate is appointed. Applications will be reviewed on an ongoing basis.