ICR The Institute of Cancer Research

Postdoctoral Training Fellow *In Silico* Medicinal Chemistry

Candidate Information

August 2025

The Institute of Cancer Research

About our organisation

We are one of the world's most influential cancer research institutes with an outstanding record of achievement dating back more than 100 years. We are world leaders in identifying cancer genes, discovering cancer drugs and developing precision radiotherapy. Together with our hospital partner The Royal Marsden, we are rated in the top four centres for cancer research and treatment worldwide.

As well as being a world-class institute, we are a college of the University of London. We came top in the league table of university research quality compiled from the Research Excellence Framework (REF 2014).

We have charitable status and rely on support from partner organisations, charities, donors and the general public.

We have more than 1000 staff and postgraduate students across three sites – in Chelsea and Sutton.

Division of Cancer Therapeutics

The Centre for Cancer Drug Discovery is a major hub within the Division of Cancer Therapeutics and a multidisciplinary 'bench to bedside' centre, comprising approximately 160 chemistry and biology scientists dedicated to the discovery and development of novel therapeutics for the treatment of cancer. We implement innovative drug discovery technologies, discover novel mechanism-based drugs, and develop these as rapidly as possible from the laboratory through to hypothesis-testing early clinical trials. These activities are carried out in highly focused multi-disciplinary project teams analogous to those in a biotechnology company, with patient benefit as the primary driver. We publish our work extensively and have a large network of collaborations with academia, biotechnology companies, and the pharmaceutical industry.

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***In Silico* Medicinal Chemistry, Medicinal Chemistry Team 3**

The *In Silico* Medicinal Chemistry group comprises 4-6 postdoctoral and staff grade in silico scientists focussed on the application of cutting edge computational chemistry techniques and data analysis to accelerate our drug discovery. Group members work in close collaboration with chemists and biologists on projects at all stages of drug discovery, from early target validation and chemical hit finding, through to lead optimisation and candidate selection. To achieve this, the *In Silico* Medicinal Chemistry group applies a wide range of computational approaches including structure-based and ligand-based virtual screening, molecular dynamics, generative chemistry, property modelling, library design and data analysis. All necessary technologies, including high-performance computing and an integrated data-platform, are in place to make this possible. The group works closely with in-house experts in structural chemistry, structural biology, biological assays, DMPK and bioinformatics to inform their research. Many projects also involve scientific collaborations with external academic and commercial partners.

Our mission is to make the discoveries that defeat cancer.

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Our values

The ICR has a highly skilled and committed workforce, with a wide variety of roles, each requiring different skills. But whether you work as a researcher, or work as part of our corporate team, your work and behaviour is underpinned by these six values. They are what bring us together as one team - as 'One ICR'.

Pursuing excellence

We aspire to excellence in everything we do, and aim to be leaders in our field.

Acting with Integrity

We promote an open and honest environment that gives credit and acknowledges mistakes, so that our actions stand up to scrutiny.

Valuing all our people

We value the contribution of all our people, help them reach their full potential, and treat everyone with kindness and respect.

Working together

We collaborate with colleagues and partners to bring together different skills, resources and perspectives.

Leading innovation

We do things differently in ways that no one else has done before, and share the expertise and learning we gain.

Making a difference

We all play our part, doing a little bit more, a little bit better, to help improve the lives of people with cancer.

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Job description

Department / division:	Division of Cancer Therapeutics, Centre for Cancer Drug Discovery
Pay grade / staff group:	PDTF / Academic
Hours / duration:	Full time (35 hours per week), Monday to Friday. Fixed-term contract (2 years)
Reports to:	Dr Andrea Scarpino, Lead Computational Chemist, *In Silico* Medicinal Chemistry
Main purpose of the job:	To support drug discovery projects in the Division of Cancer Therapeutics by applying innovative computational methods.

Duties and responsibilities:

Key Roles and Responsibilities

Work collaboratively within multidisciplinary project teams to design compounds modulating targets involved in cancer development and progression.
Apply computational chemistry methods to support the identification and optimisation of chemical series.
Guide medicinal chemistry efforts through knowledge of SAR, effective data analysis and visualisation.
Perform cheminformatics tasks for the design, processing and querying of molecular libraries or databases.
Contribute to the development and implementation of innovative computational methods for drug discovery.
Communicate effectively with interdisciplinary teams by providing clear summaries and actionable insights.
Publish and present original work at conferences and in peer-reviewed journals.
Maintain up-to-date knowledge on the latest developments in computational chemistry and related fields.
Provide guidance to scientists from different disciplines on the appropriate use of computational tools.
Keep accurate electronic records enabling the work to be followed and reproduced by others.

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General

All staff must ensure that they familiarise themselves with and adhere to any ICR policies that are relevant to their work and that all personal and sensitive personal data is treated with the utmost confidentiality and in line with the General Data Protection Regulations
Any other duties that are consistent with the nature and grade of the post that may be required.
To work in accordance with the ICR's Values.
To promote a safe, healthy and fair environment for people to work, where bullying and harassment will not be tolerated.
This job description is a reflection of the present position and is subject to review and alteration in detail and emphasis in the light of future changes or development.

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Person specification

Education and Knowledge

PhD in computational chemistry, or a related field.	Essential*
Wide-ranging knowledge and experience in the use of computational chemistry methods.	Essential
Familiarity with concepts in medicinal chemistry and drug discovery.	Desirable

**as a minimum requirement candidates must have submitted their thesis by the start date of their employment and awarded their PhD within the six month probationary period.*

Skills

Ability to apply structure- and ligand-based methods to accelerate drug discovery projects. This may include for example docking, virtual screening, molecular dynamics, binding free energy and QM calculations.	Essential
Familiarity with molecular modelling software packages (e.g., Schrödinger, MOE, OpenEye).	Essential
Proficiency with scientific programming (Python, bash) and/or data analytics platforms (e.g., KNIME).	Essential
Ability to use data visualisation tools and statistical analysis methods.	Desirable
Familiarity with cheminformatics packages (e.g., RDKit), AI/ML frameworks (e.g., PyTorch), public databases and APIs to develop advanced computational pipelines for drug discovery.	Desirable
Proactive approach with excellent time management skills and ability to work on different projects simultaneously.	Essential
Strong written and oral communication skills.	Essential
Highly motivated with strong desire to achieve scientific excellence.	Essential
Team player: proven ability to collaborate with others.	Essential

Experience

Evidence for creative problem solving using a wide variety of computational methods.	Essential
Experience applying computational techniques to design and optimise bioactive molecules.	Essential
Hands-on experience with relative binding free energy calculations (e.g., FEP) for drug discovery applications.	Desirable
Application of generative AI models to design and optimise chemical series.	Desirable
Experience working with HPC clusters and job scheduling managers (e.g., SLURM).	Essential
Track record of computational chemistry publications in peer-reviewed journals.	Desirable

Benefits

We offer a fantastic working environment, great opportunities for career development and the chance to make a real difference to defeat cancer. We aim to recruit and develop the best – the most outstanding scientists and clinicians, and the most talented professional and administrative staff.

The annual leave entitlement for full time employees is 28 days per annum on joining. This will increase by a further day after 2 years' and 5 years' service.

Staff membership to the Universities Superannuation Scheme (USS) is available. The USS is a defined benefit scheme and provides a highly competitive pension scheme with robust benefits. The rate of contributions is determined by USS and details of the costs and benefits of this scheme can be found on their website. If staff are transferring from the NHS, they can opt to remain members of the NHS Pension Scheme.

We offer a range of family friendly benefits such as flexible working, a parents' group, and a maternity mentoring scheme. Other great benefits include interest free loans for discounted season tickets for travel and bicycle purchases, access to the NHS discounts website, a free and confidential Employee Assistance Programme which offers a range of well-being, financial and legal advice services, two staff restaurants, and access to a gym and sporting facilities at our Sutton site.

Further information

You may contact Dr Andrea Scarpino for further information by emailing andrea.scarpino@icr.ac.uk. This job description is a reflection of the current position and is subject to review and alteration in detail and emphasis in the light of future changes or development.