



Postdoctoral Training Fellow In Silico Medicinal Chemistry Candidate Information

March 2023

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 component of the Division of Cancer Therapeutics and is 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.

In Silico Medicinal Chemistry

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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 approaches including, structure-based and ligand-based computational techniques, molecular dynamics simulations, ab-initio calculations, QSAR/QSPR, ADME-Tox modelling, compound library design and HTS analyses. 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.



Our values set out how each of us at the ICR, works together to meet our mission – to make the discoveries that defeat cancer. They summarise our desired behaviours, attitudes and culture – how we value one another and how we take pride in the work we do, to deliver impact for people with cancer and their loved ones.”

Professor Kristian Helin
Chief Executive

In Silico Medicinal Chemistry

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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, Principal 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 capable of modulating the activity of protein targets involved in cancer development and progression by applying computational methods aiding the optimisation of potency, selectivity, permeability and ADMET properties.

Guide medicinal chemistry efforts through knowledge of SAR, effective data analysis and visualization.

Provide data-driven insights enabling progress of drug discovery projects via the development and application of appropriate predictive models.

Develop new computational chemistry methods and implement state-of-the-art procedures to expand the capabilities of the In Silico Medicinal Chemistry group and consolidate the impact of computational drug design.

Collaborate with interdisciplinary project teams and communicate effectively with colleagues and senior staff both in formal and informal contexts.

Publish or present original work at conferences and/or in peer-reviewed journals.

Maintain an up to date knowledge of literature and recent developments within the field of computational chemistry.

Guide scientists from different disciplines in the appropriate and effective use of computational tools.

Maintain 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 a number of different structure- and ligand-based methods to accelerate drug discovery projects. This may include for example docking, molecular dynamics, virtual screening, QSAR, homology modelling, free energy calculations and/or QM approaches.	Essential
Ability to apply cheminformatics and machine learning toolkits for the development of predictive models.	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 and 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 small molecules with improved properties (e.g., enhanced affinity for a given protein target).	Essential
Experience using state-of-the-art molecular modelling software packages (e.g., Schrödinger, MOE, OpenEye).	Essential
Familiarity with scientific programming (e.g., Python, UNIX) and/or data analytics platforms (KNIME).	Essential
Familiarity with data visualization, machine learning and statistical analysis.	Desirable
Track record of publication in the field of computational chemistry in peer-reviewed journals.	Desirable

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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.