Job description and selection criteria

<table>
<thead>
<tr>
<th>Job title</th>
<th>Postdoctoral computational chemistry engineer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Division</td>
<td>Medical Sciences</td>
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<tr>
<td>Department</td>
<td>Nuffield Department of Medicine (NDM)</td>
</tr>
<tr>
<td>Location</td>
<td>Structural Genomics Consortium, Old Road Campus Research Building, Headington, Oxford</td>
</tr>
<tr>
<td>Grade and salary</td>
<td>Grade 7: £31,604 - £38,833 per annum</td>
</tr>
<tr>
<td>Hours</td>
<td>Full time</td>
</tr>
<tr>
<td>Contract type</td>
<td>Fixed Term until 31st December 2018 in the first instance</td>
</tr>
<tr>
<td>Reporting to</td>
<td>Frank von Delft</td>
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<tr>
<td>Vacancy reference</td>
<td>132678</td>
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Job description

Overview of the role

XChem is a collaborative project between the University of Oxford's Department of Chemistry and Structural Genomics Consortium (SGC), and Diamond Light Source (DLS) [www.diamond.ac.uk/Beamlines/Mx/Fragment-Screening.html](http://www.diamond.ac.uk/Beamlines/Mx/Fragment-Screening.html). It enables high-throughput generation of protein-ligand structures using X-ray crystallography. Most recently, the XChem project has begun to work on automated synthesis techniques to improve the throughput of follow-up chemistry for fragment-based discovery.

The role will be tasked with adapting and hardening open-source computational approaches to ensure they effectively drive the robotic and parallel synthesis approaches being used to target a range of disease targets (Cancer, Alzheimers, AMR).

This will thereby produce vital infrastructure for the vast amount of small molecule discovery work within the XChem project, and result in assemblies of tools that enable the generation of unique datasets and novel approaches to validating extant algorithms.
The role requires a range of skills, ranging from high-level integration of tools to low-level engineering of prototype approaches.

The work will entail significant collaboration: internally, working closely with experimental synthetic chemists to help turn their methods into routine protocols; and externally, interfacing with collaborators to adapt published algorithms for deployment in the XChem compute infrastructure.

This project falls within the framework of the Rosalind Franklin Institute (RFI), a new £100M UK government investment for transforming the impact of physical sciences on biological research. The work will integrate closely with the nascent CCP-CompMedChem effort (http://www.ccp-cmc.org/), thereby ensuring methods serve an industrial unmet need and achieve broad exposure. The output software tools and data generated will be made freely available and will have a global impact due to Diamond and XChem’s broad appeal.

You will have a background in computational chemistry or synthetic chemistry.

**Responsibilities/duties**

1. Develop research questions within a specific context, conduct individual research, analysing detailed and complex qualitative and/or quantitative data from a variety of sources, and generate original ideas by building on existing concepts

2. Work with chemists in Oxford Chemistry to computationally analyse novel syntheses and chemotypes to extend XChem fragment libraries

3. Generate computational tools to streamline the design and synthesis of follow-up compounds for FBDD programmes

4. Work with a synthetic chemist at the RFI in developing automated synthesis protocols

5. Present results on a regular basis to the supervisor and other project members at regular project and group meetings.

6. Communicate frequently and effectively with the XChem team to report data and discuss the requirements of projects

7. Take a formal or informal role (as required) in the supervision of research students and other group members (e.g. PhD and Masters students), as well as training of group members and visitors on the specific tools and approaches being developed.

**Hazard-specific/Safety-critical duties**

*See:* [www.admin.ox.ac.uk/personnel/recruit/preempcheck/compulsorychecks/medical](http://www.admin.ox.ac.uk/personnel/recruit/preempcheck/compulsorychecks/medical)

This job includes the following hazards or safety-critical activities which will require successful pre-employment health screening through our Occupational Health Service before the successful candidate will be allowed to start work:

- Lone Working
- Regular manual handling
Selection criteria

Essential

1. Hold a PhD (or equivalent experience) in computational or medicinal chemistry or have submitted a PhD thesis prior to taking up the appointment
2. Demonstrable ability to draft section of manuscripts for publication and present statistical results at conferences
3. Extensive computational chemistry and/or synthetic organic chemistry experience
4. Experience of working within a small molecule drug discovery or medicinal chemistry programme
5. Well-organised, with the ability to work as part of a team and to collaborate with colleagues on a range of diverse projects.
6. Good communication skills with experience of working effectively with scientists from varied backgrounds
7. Ability to work on multiple projects in parallel with rapidly priorities
8. Demonstrable experience of significant programming (C/C++, Python) and knowledge of chemoinformatics APIs

Desirable

1. Experience of small molecule synthesis
2. Experience of fragment- based drug discovery
3. Experience of automated synthesis methodologies
4. Working knowledge of protein crystallography
5. Experience of having worked in an integrated discovery group
6. A good recent publication record in scientific journals

About the University of Oxford

Welcome to the University of Oxford. We aim to lead the world in research and education for the benefit of society both in the UK and globally. Oxford’s researchers engage with academic, commercial and cultural partners across the world to stimulate high-quality research and enable innovation through a broad range of social, policy and economic impacts.

We believe our strengths lie in both empowering individuals and teams to address fundamental questions of global significance, and in providing all of our staff with a welcoming and inclusive workplace that supports everyone to develop and do their best work. Recognising that diversity is a great strength, and vital for innovation and creativity, we aspire to build a truly diverse community, which values and respects every individual’s unique contribution.
While we have long traditions of scholarship, we are also forward-looking, creative and cutting-edge. Oxford is one of Europe's most entrepreneurial universities. Income from external research contracts in 2014/15 exceeded £522.9m and ranked first in the UK for university spin-outs, with more than 130 spin-off companies created to date. We are also recognised as leaders in support for social enterprise.

Join us and you will find a unique, democratic and international community, a great range of staff benefits and access to a vibrant array of cultural activities in the beautiful city of Oxford.

For more information please visit www.ox.ac.uk/about/organisation

**Medical Sciences**

The Medical Sciences Division is an internationally recognized centre of excellence for biomedical and clinical research and teaching.

We are the largest academic division in the University of Oxford World-leading programmes, housed in state-of-the-art facilities, cover the full range of scientific endeavour from the molecule to the population. With our NHS partners we also foster the highest possible standards in patient care.

For more information please visit: www.medsci.ox.ac.uk

**Nuffield Department of Clinical Medicine (NDM)**

The Nuffield Department of Clinical Medicine (NDM) is one of the largest departments of the University of Oxford and is part of the Medical Sciences Division, with responsibility for a significant part of the teaching of clinical students within the Medical School. The Department also has a substantial research programme which requires high quality administrative management.

NDM has significant financial turnover and complexity, resulting from its diverse research portfolio, its geographical spread and its close links with NHS funding and strategic teams involved in the development and delivery of increasingly integrated clinical research platforms.

For more information please visit: www.ndm.ox.ac.uk/home

The University of Oxford is a member of the Athena SWAN Charter and holds an institutional Bronze Athena SWAN award. The Nuffield Department of Medicine holds a Silver Athena SWAN award to recognise advancement of gender equality: representation, progression and success for all.

For more information please visit: www.ndm.ox.ac.uk/athena-swan

**Structural Genomics Consortium (SGC)**

The Structural Genomics Consortium (SGC), a not-for-profit, public-private partnership funds pre-competitive research that contributes to new hypotheses in understanding and treating human disease, and the subsequent identification of new targets for drug discovery. The SGC supports pioneering research at the University of Oxford (UK), University of Toronto (Canada), University of Campinas (Brazil), and University of North Carolina (USA). The reagents and knowledge related to human proteins that the SGC supports are made openly
accessible to researchers around the world to accelerate the discovery of new medicines in order to bring potentially life-saving drugs to market faster and at a lower cost.

SGC Oxford, a part of the Nuffield Department of Clinical Medicine, receives funding from public, charitable and private sector organisations such as the European Commission, UK Research Councils, Wellcome Trust, and pharmaceutical companies. Research in SGC Oxford is focused on the production and characterisation of the 3-dimensional structures of soluble and of integral membrane proteins, the discovery of selective chemical probes that can modulate protein function, and the development of target enabling packages that transform genetic hits into starting points for drug discovery. SGC Oxford shares its research outputs through collaborations with researchers worldwide.

For more information please visit: http://www.thesgc.org/scientists/groups/oxford/

**How to apply**

Before submitting an application, you may find it helpful to read the ‘Tips on applying for a job at the University of Oxford’ document, at www.ox.ac.uk/about/jobs/supportandtechnical/.

If you would like to apply, click on the **Apply Now** button on the ‘Job Details’ page and follow the on-screen instructions to register as a new user or log-in if you have applied previously. Please provide details of two referees and indicate whether we can contact them now.

You will also be asked to upload a CV and a supporting statement. The supporting statement should explain how you meet the selection criteria for the post using examples of your skills and experience. This may include experience gained in employment, education, or during career breaks (such as time out to care for dependants).

Your application will be judged solely on the basis of how you demonstrate that you meet the selection criteria stated in the job description.

Please upload all documents as PDF files with your name and the document type in the filename.

All applications must be received by **midday** on the closing date stated in the online advertisement.

<table>
<thead>
<tr>
<th>Information for priority candidates</th>
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<tr>
<td>A priority candidate is a University employee who is seeking redeployment because they have been advised that they are at risk of redundancy, or on grounds of ill-health/disability. Priority candidates are issued with a redeployment letter by their employing departments.</td>
</tr>
</tbody>
</table>

If you are a priority candidate, please ensure that you attach your redeployment letter to your application (or email it to the contact address on the advert if the application form used for the vacancy does not allow attachments)

Should you experience any difficulties using the online application system, please email recruitment.support@admin.ox.ac.uk. Further help and support is available from www.ox.ac.uk/about_the_university/jobs/support/. To return to the online application at any stage, please go to: www.recruit.ox.ac.uk.

Please note that you will be notified of the progress of your application by automatic emails from our e-recruitment system. **Please check your spam/junk mail** regularly to ensure that you receive all emails.
Important information for candidates

Pre-employment screening
Please note that the appointment of the successful candidate will be subject to standard pre-employment screening, as applicable to the post. This will include right-to-work, proof of identity and references. We advise all applicants to read the candidate notes on the University’s pre-employment screening procedures, found at:
www.ox.ac.uk/about/jobs/preemploymentscreening/.

The University's policy on retirement
The University operates an Employer Justified Retirement Age (EJRA) for all academic posts and some academic-related posts. From 1 October 2017, the University has adopted an EJRA of 30 September before the 69th birthday for all academic and academic-related staff in posts at grade 8 and above. The justification for this is explained at:
www.admin.ox.ac.uk/personnel/end/retirement/revisedejra/revaim/.

For existing employees, any employment beyond the retirement age is subject to approval through the procedures: www.admin.ox.ac.uk/personnel/end/retirement/revisedejra/revproc/

Form 1 October 2017, there is no normal or fixed age at which staff in posts at grades 1–7 have to retire. Staff at these grades may elect to retire in accordance with the rules of the applicable pension scheme, as may be amended from time to time.

Equality of Opportunity
Entry into employment with the University and progression within employment will be determined only by personal merit and the application of criteria which are related to the duties of each particular post and the relevant salary structure. In all cases, ability to perform the job will be the primary consideration. No applicant or member of staff shall be discriminated against because of age, disability, gender reassignment, marriage or civil partnership, pregnancy or maternity, race, religion or belief, sex, or sexual orientation.
Benefits of working at the University

University Club and sports facilities

The University Club provides social, sporting and hospitality facilities. It incorporates a bar, café and sporting facilities, including a gym. Staff can also use the University Sports Centre on Iffley Road at discounted rates, including a fitness centre, powerlifting room, and swimming pool. See: www.club.ox.ac.uk and www.sport.ox.ac.uk/oxford-university-sports-facilities.

Information for international staff (or those relocating from another part of the UK)

If you are relocating to Oxfordshire from overseas, or elsewhere in the UK, the University’s International Staff website includes practical information related to moving to and settling in Oxford such as advice on immigration, relocation, accommodation, or registering with a doctor. See: www.internationalstaffwelcome.admin.ox.ac.uk/

The University of Oxford Newcomers’ Club

The University of Oxford Newcomers’ Club is an organisation run by volunteers that aims to assist the partners of new staff to settle into Oxford and to provide them with an opportunity to meet people in the area. See www.newcomers.ox.ac.uk/

Childcare

The University has excellent childcare services with five University nurseries, as well as University-supported places at many other private nurseries. For full details including how to apply and the costs, see www.admin.ox.ac.uk/childcare.

Family-friendly benefits

The University subscribes to My Family Care (www.admin.ox.ac.uk/personnel/staffinfo/benefits/family/mfc/) and staff are eligible to register for emergency back-up childcare and adultcare services, a ‘speak to an expert’ phone line and a wide range of guides and webinars through a website called the Work + Family space.

Disabled staff

We are committed to supporting members of staff with disabilities or long-term health conditions. Please visit www.admin.ox.ac.uk/eop/disab/staff for further details including information about how to make contact, in confidence, with the University’s Staff Disability Advisor.

Staff networks

The University has a number of staff networks including the Oxford Research Staff Society, BME staff network, LGBT+ staff network and a disabled staff network. You can find more information at www.admin.ox.ac.uk/eop/inpractice/networks/

Other benefits

Staff can enjoy a range of other benefits such as free visitor access to the University’s colleges and the Botanic Gardens as well as a range of discounts. See www.admin.ox.ac.uk/personnel/staffinfo/benefits