## Role profile

<table>
<thead>
<tr>
<th>Job title</th>
<th>Research Associate/Fellow in Computational Chemistry</th>
<th>Job family and level</th>
<th>Research and Teaching Level 4 Training Grade/Level 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>School/ Department</td>
<td>School of Chemistry</td>
<td>Location</td>
<td>University Park Campus</td>
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### Purpose of role

The purpose of this role is research in computational chemistry, to improve the accuracy of computational predictions of protein-ligand binding affinity, utilising new advances in machine learning.

### Main responsibilities

(Primary accountabilities and responsibilities expected to fulfil the role) % time per year

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<th>% time per year</th>
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<tbody>
<tr>
<td>1</td>
<td>Conduct high quality computational research and provide research leadership, including expert supervision of graduate and masters students</td>
<td></td>
<td>70%</td>
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<tr>
<td>2</td>
<td>Write high quality scientific articles</td>
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<td>15%</td>
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<td>3</td>
<td>Liaise with academic collaborators as appropriate and identify and develop opportunities for research grant funding proposals</td>
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<td>10 %</td>
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<tr>
<td>4</td>
<td>Give presentations internally at group meetings and externally at conferences</td>
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<td>5%</td>
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<td>5</td>
<td>You may be asked to perform other duties occasionally which are not included in the above but appropriate to the grade and consistent with the role</td>
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<td>Person specification</td>
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<td><strong>Essential</strong></td>
<td><strong>Desirable</strong></td>
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| **Skills** | ▪ Extensive experience in computational research using cheminformatics, molecular simulations, machine learning and/or statistical methods. | ▪ Ability to play a leading role in research group in developing independent research pathways.  
▪ Research experience across a range of biological and/or medicinal chemistry. |
| **Knowledge and experience** | ▪ Excellent practical computational skills.  
▪ Proven track record in computational chemistry, as evidenced by peer-reviewed publications.  
▪ Experience in advanced computational programming. | ▪ Experience in High Performance Computing systems. |
| **Qualifications, certification and training (relevant to role)** | ▪ PhD (or near completion) in computational chemistry or a related discipline. |
| **Statutory, legal or special requirements** | ▪ To take reasonable care for the health and safety of yourself and of other persons who may be affected by your acts or omissions at work, in accordance with the Health and Safety at Work Act 1974, EC directives and the University’s Safety, Health and Environment Policies and procedures.  
▪ To cooperate with the University on any legal duties placed on it as the employer. |

The University of Nottingham is focused on embedding equality, diversity and inclusion in all that we do. As part of this, we welcome a diverse population to join our work force and therefore encourage applicants from all communities, particularly those with protected characteristics under the Equality Act 2010.

The University is a signatory of the Declaration on Research Assessment (DORA). As such we commit to focus on the scientific content of publications (where requested or provided as part of the recruitment and selection process) as a basis for review of quality, and consideration of value and impact of research conducted, rather than any proxy measures such as Journal Impact Factor.
Expectations and behaviours

The University has developed a clear set of core expectations and behaviours that our people should be demonstrating in their work, and as ambassadors of the University’s strategy, vision and values. The following are essential to the role:

**Valuing people**
Is friendly, engaging and receptive, putting others at ease. Actively listens to others and goes out of way to ensure people feel valued, developed and supported.

**Taking ownership**
Is clear on what needs to be done encouraging others to take ownership. Takes action when required, being mindful of important aspects such as Health & Safety, Equality, Diversity & Inclusion, and other considerations.

**Forward thinking**
Drives the development, sharing and implementation of new ideas and improvements to support strategic objectives. Engages others in the improvement process.

**Professional pride**
Is professional in approach and style, setting an example to others; strives to demonstrate excellence through development of self, others and effective working practices.

**Always inclusive**
Builds effective working relationships, recognising and including the contribution of others; promotes inclusion and inclusive practices within own work area.

Key relationships with others

```
           Line manager
               |
               V
          Role holder
               |
               V
  Key stakeholder relationships
               |
               V
    Colleagues

      Professor of Computational Chemistry
        \                  /  
         \                /   
          \              /     
         Research Associate/Fellow in Computational Chemistry
          \            /           
           \        /             
              \    /               
                
        Students
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