Job title	Computational Chemistry KTP Associate	Job family and level	Off scale – KTP Associate £45,000 to £50,000
School/ Department	School of Chemistry	Location	Colorifix Limited Innovation Centre Colney Lane Norwich NR4 7GJ

Purpose of role

To develop novel computational chemistry tools to improve the rate of production of sustainable pigments and dyes for the textile industry.

	Main responsibilities (Primary accountabilities and responsibilities expected to fulfil the role)	% time
1	Gain an understanding of Colorifix's science and technology, current products and the gaps relating to data analysis.	10%
2	Generate colourant datasets to provide data for use in establishing the best data-science skills for Colorifix to optimise productivity.	15%
3	Use ML to predict colourant properties for improved productivity.	25%
4	Use ML to accelerate the discovery of new colourants with improved properties	25%
5	Fully document new software and write research papers for peer-reviewed publication	20%
6	Ensure that knowledge developed through the project is transferred to existing staff and stored in an accessible format so that future staff can access knowledge.	5%

Person specification

	Essential	Desirable
Personal skills	- Have an excellent command of the English language with written and verbal communication that is clear and easy to understand. - Be able to clearly communicate complex information. - Be able to build strong alliances with colleagues and stakeholders and engage effectively with personnel in a wide range of roles. - Be self-starting and pro-active, and have the ability to work in a team to meet deadlines and to prioritise tasks. - Be enthusiastic and self-motivated with the drive to embed new knowledge and take full ownership of the project and the results. - Have the ability to plan a project, execute the plan and make adjustments according to delays and technical issues.	- Have an awareness and understanding of commercial drivers. - Demonstrate a high level of competence using word processing and presentation software, MS Office, etc.
Knowledge and experience	- Strong programming skills including Python. - Familiarity with data science Python libraries including pandas, scikit-learn, pytorch, and numpy - Experience in developing QSAR models. - Familiarity with version control systems such as git. - Familiarity with a Unix operating system. - Experience in building predictive software tools and database management. - Familiarity with common Cheminformatics libraries including Rdkit. - Experience of writing reports and conducting effective bibliographic research.	- Relevant industrial experience (including industrial placements). - An interest in applying organic and quantum chemistry to new and sustainable technologies. - Demonstrate awareness of operating in a laboratory environment under appropriate H&S regulations.
Qualifications, certification and training (relevant to role)	Hold or be close to completion of a PhD in Chemistry, Statistics, Mathematics, Computer Science	

	or a closely related discipline with a significant cheminformatics component.	
Other	- Have a commitment to continuing professional development. - Be willing to undertake appropriate further training and to adopt new procedures as and when required. - Be committed to maintaining confidentiality at all times. - Have a commitment to observing Equality & Diversity policies at all times.	Be willing to travel.

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.

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	Line Manager, School of Chemistry
Role holder	**Computational Chemistry KTP Associate**
Key stakeholder relationships	Colorifix / Academic Team / UoN KTP Team / KT Adviser