

## **Research Associate in Artificial Intelligence and Decision Making (Fixed Term – 30 months)**

***Project Title: Innovative Health Initiative***

***PHARMECO***

**Job Ref: REQ250783**

**As part of the University's ongoing commitment to redeployment, please note that this vacancy may be withdrawn at any stage of the recruitment process if a suitable redeployee is identified.**

### **Project Description**

This project is part of the Innovative Health Initiative (IHI) - PHARMECO, a large research consortium involving more than 30 industrial and academic partners from 14 countries. The intended research will be based in the Department of Chemical Engineering in the School of Aeronautical, Automotive, Chemical and Materials Engineering (AACME). Following a recent £25 million refurbishment, the department houses a range of state-of-the-art laboratory facilities and a modern office environment.

The consortium aims to address the urgent need for sustainability in the healthcare industry by integrating environmentally friendly technologies, innovative processes, and standardized sustainability assessment methods.

### **Job Description**

**Job Grade:** Specialist and Supporting Academic Grade 6

### **Job Purpose**

The ultimate objective of this research position is to develop pathways for safe and sustainable synthetic routes and manufacturing processes by design. The researcher will leverage state-of-the-art computer-assisted retrosynthesis tools and advanced process simulation technologies to design and optimise total synthetic routes for complex active pharmaceutical ingredients (APIs). They will also develop systematic decision-making frameworks to evaluate and rank alternative routes based on multiple criteria, including environmental impacts, economic feasibility, and regulatory compliance. In addition, the researcher will generate process and inventory data to support prospective life cycle assessments (LCA) and contribute to early-stage experimentation and simulation activities. Furthermore, the research associate will develop new retrosynthesis methods/tools based on artificial intelligence and data-driven approaches for both small API molecules and large and complex molecules such as peptides, oligonucleotides, and natural products.

### **Job Duties**

- To leverage and develop computer-assisted retrosynthesis methods.
- To develop multicriteria decision frameworks for the synthetic route design.
- To generate inventory data for prospective life cycle assessments (LCA).
- To support experimentation and process simulation activities
- To work collaboratively with the other researchers and relevant work packages across the research consortium

- To generate, analyse, interpret and present research data.
- To work collaboratively with the research team particularly the research associate in process optimisation and control
- To liaise with academic and industrial project partners, and coordinate activities across the research centre
- Be responsible for conducting the day to day running of the project.
- To formulate detailed plans for the project based on broad guidance from the project team.
- To feed back to the project team on progress, to make recommendations for next steps.
- Write up regular progress reports and present outcomes to all Investigators and Collaborators.
- Travel to attend meetings and make presentations both within the project partners working group and to external stakeholders.
- To support the project team by enhancing relationships with existing collaborators and by assisting the establishment of relationships with new collaborators.
- To write research papers suitable for publication in high quality academic journals.
- To attend and contribute to conferences.
- To contribute to project promotion and public engagement events.
- Contribute ideas for new research and enterprise directions.

- Maintain confidentiality at all times and ensure that intellectual property (IPR) agreements are not violated.
- To assist the academic staff in the project team with the supervision of undergraduate MSc and PhD project work and day-to-day supervision and support of other researchers.
- Where appropriate, to deliver teaching, tutorial and laboratory sessions to students.
- Engage in training programmes in the University (or elsewhere) that are consistent with the needs and aspirations of the project and those of the Department.
- Undertake other duties as may be reasonably requested and that are commensurate with the nature and grade of the post.

### **Points To Note**

The purpose of this job description is to indicate the general level of duties and responsibility of the post. The detailed duties may vary from time to time without changing the general character or level of responsibility entailed.

### **Special Conditions**

All staff have a statutory responsibility to take reasonable care of themselves, others and the environment and to prevent harm by their acts or omissions. All staff are therefore required to adhere to the University's Health, Safety and Environmental Policy & Procedures.

All staff should hold a duty and commitment to observing the University's Equity, Diversity & Inclusion policy and procedures at all times. Duties must be carried out in accordance with relevant Equity, Diversity & Inclusion legislation and University policies/procedures.

Successful completion of probation will be dependent on attendance at the University's mandatory courses which include Belonging and Inclusion, Health & Safety, etc.

### **Organisational Responsibility**

Reports to Professor Brahim Benyahia, Department of Chemical Engineering.

## Person Specification

Your application will be reviewed with respect to meeting the essential and desirable criteria listed below. Your application will be reviewed against the essential and desirable criteria listed below. Applicants are strongly advised to explicitly state and evidence how they meet each of the essential (and desirable) criteria in their application. Stages of assessment are as follows:

- 1 – Application
- 2 – Test/Assessment Centre/Presentation
- 3 – Interview

### Essential Criteria

Area	Criteria	Stage
Experience	Experience in computer assisted retrosynthesis	1,3
	Experience in machine learning including supervised and unsupervised techniques as well as deep and transfer learning	1,3
	Programming with Python	1,3
	Experience in sustainability assessment including life cycle assessment (LCA) and green chemistry	1,3
	Experience in process modelling	1,3
	Relevant experience in conducting original research that can be, or has been published in high quality journals	1,3
	Relevant experience in an academic research environment or equivalent industrial experience	1,3
	Record of high quality publications or other forms of research outputs.	1,3
	Experience of presenting research findings at all levels, adapted to specific audience needs, ranging from academic experts to general public	1,3
Skills and abilities	Ability to coordinate project activities, manage project tasks, prioritise and meet deadlines	1,3
	Ability to work independently and as part of a team	1,3
	Excellent written and oral communication skills	1,3
	Self-motivated with ability to meet deadlines	1,3
	Excellent interpersonal, and organisational skills	1,3
	Ability to write project reports and make technical presentations to industrial and academic research groups	1,3
	Skills in finding information in the scientific literature and proposing original ideas	1,3
	Knowledge of relevant Health & Safety issues	1,3
Training	Demonstrate evidence of having undertaken further training	1,3
Qualifications	PhD (or near completion)	1,3
Other	Commitment to observing the University's Equal Opportunities policy at all times.	1,3

### Desirable Criteria

Area	Criteria	Stage
Experience	Experience in supervising junior members (e.g. PhD, MSc or final year project students)	1,3
	Writing research proposals for funding from internal/external sources	1,3
	Mathematical modelling and simulation of chemical or pharmaceutical processes	1,3

	Multi-objective optimisation and multicriteria decision aiding	1,3
	Experience with Synthia or equivalent software	1,3
	Reinforcement learning	1,3
Skills and abilities	Authoring original work, in the highest quality refereed academic journals	1,3
	A strong publication track record	1,3
Qualifications	PhD (or near completion) in Chemical Engineering, Computational Chemistry and related areas	1,3
Other	Travel / Able to travel Independently / Working patterns	1,3

## Conditions of Service

The position is FULL TIME and FIXED TERM for 30 months. Salary will be on Specialist and Supporting Academic Research, Grade 6, Salary Band £35,116 - £45,413 per annum, at a starting salary to be confirmed on offer of appointment

The appointment will be subject to the University's Terms and Conditions of Employment for STAFF GRADES 6 AND ABOVE, details of which can be found [here](#).

The University is committed to enabling staff to maintain a healthy work-home balance and has a number of family-friendly policies which can be found [here](#).

The University offers a wide range of employee benefits which can be found [here](#).

We also offer an on-campus nursery with subsidised places, subsidised places at local holiday clubs and a childcare voucher scheme (further details are available at: <http://www.lboro.ac.uk/services/hr/a-z/childcare-information---page.html>)

In addition, the University is supportive, wherever possible, of flexible working arrangements.

We also strive to create a culture that supports equality and celebrates diversity throughout the campus. The University holds a Bronze Athena SWAN award which recognises the importance of support for women at all stages of their academic career. For further information on Athena SWAN see <http://www.lboro.ac.uk/services/hr/athena-swan/>

## Applications

The closing date for receipt of applications is 10/10/2025. Interviews will be held during the week commencing 13/10/2025.