Programme Specification (PG)

Awarding body / institution:	Queen Mary University of London
Teaching institution:	Queen Mary University of London
Name of final award and title:	Master of Science in Artificial Intelligence for Drug Discovery
Name of interim award(s):	PG Cert/PG Dip
Duration of study / period of registration:	1 calendar year (FT)
Queen Mary programme code(s):	PFQM-I4F1-09
QAA Benchmark Group:	Chemistry
FHEQ Level of Award:	Level 7
Programme accredited by:	
Date Programme Specification approved:	
Responsible School / Institute:	School of Physical and Chemical Sciences

Schools / Institutes which will also be involved in teaching part of the programme:

Collaborative institution(s) / organisation(s) involved in delivering the programme:

Programme outline

Drug discovery in industry and academia is increasingly reliant on computational methods. Artificial Intelligence (AI) is creating a revolution in the field, thanks to the advancements in computational power and the increased availability both of efficient algorithms and of high-quality data. Machine learning and advanced data analysis techniques are not part of the traditional training in undergraduate Chemistry, Pharmaceutical Chemistry or related degrees. Consequently, there is a shortage of professionals with the breadth of knowledge and skills required to effectively apply computational methods to drug discovery pipelines.

The MSc programme in Artificial Intelligence for Drug Discovery will cover:
- Principles of drug discovery and lead optimisation
- Scientific programming
- Supervised and unsupervised machine learning methods
- Deep learning methods
- Modelling and simulation techniques applied to biomolecular systems

Taught by experts from the School, delivery of the programme will involve a combination of face-to-face teaching and interactive workshops to cover the theoretical aspects of the programme. Students will have the opportunity to develop

practical coding skills and use state-of-the-art software in extensive computer lab sessions. Students will also acquire valuable research experience by carrying out a research-based project where they will apply the concepts and tools learnt in the taught modules to complex problems.

Highlights:
- New programme with a unique and comprehensive combination of topics in Artificial Intelligence for drug discovery
- Emphasis on practical skills
- No previous knowledge of coding or machine learning is assumed

Aims of the programme

The aim of the MSc programme in AI for Drug Discovery is to provide students with the breadth and depth of knowledge required to apply state-of-the art computational techniques to drug discovery and development pipelines, interpret the resulting predictions and assess their quality. The wide range of competences required for the delivery of the programme will be provided by academic staff in the newly formed School of Physical and Chemical Sciences.

More specifically, the programme aims to:

* Provide students with an in-depth understanding of a range of topics including principles of drug discovery and design, machine learning, deep learning, chemoinformatics, and biomolecular modelling and simulation.

* Develop practical coding skills essential to apply artificial intelligence to the field of drug discovery.

* Enable students to acquire substantial research experience through a final research-based project.

This programme will equip students with the knowledge, skills and competencies to contribute to the future of drug discovery. Specifically, it will generate highly skilled graduates better prepared for a career in research or in the pharmaceutical and other chemical industries.

What will you be expected to achieve?

Students who successfully complete the programme are expected to possess the following knowledge/skills/attributes:

Academic Content:	
A 1	In depth knowledge of practical aspects and key theory concepts of artificial intelligence methods applied to drug discovery
A 2	In depth knowledge of practical aspects and key theory concepts of molecular modelling tools applied to drug discovery
A 3	Understanding of key concepts of Pharmaceutical Chemistry and Pharmacology and ability to use them to design computational pipelines for the analysis, interpretation and prediction of data in the context of drug discovery
A 4	Ability to engage critically and reflectively with different sources of scientific literature in drug discovery

Disciplinary Skills - able to:

B 1	Independently identify, select, combine and use computational tools to solve complex problems in drug discovery
B 2	Critically assess and reflect on the performance and reliability of machine learning and molecular modelling methods applied to drug discovery
B 3	Write, test and document scientific code to perform a range of tasks in drug discovery, including searching and extracting information from databases, performing predictions, analysing and visualising data, and automating pipelines.
B 4	Conduct and report on a significant piece of research work related to the problems and challenges in drug discovery.

Attributes:	
C 1	Ability to use problem-solving skills and computational tools to solve unfamiliar problems
C 2	Ability to communicate complex ideas and concepts in a clear, concise and informative way that is appropriate for the audience
C 3	Ability to work with information that may be incomplete or uncertain
C 4	Ability to work effectively as part of a team
C 5	Ability to manage time, prioritise workload and work to deadlines

How will you learn?

Acquisition of knowledge and understanding in taught modules will generally be achieved by on campus face-to-face teaching and interactive workshops. These will be complemented and supported by extensive online content (videos, slides, practice questions etc...) that will be made available before each session.

The programme has a strong emphasis on the development of practical skills, including coding, independent use of a range of drug discovery tools and report writing, which will be achieved through extensive computer lab sessions. Individual support will be provided during these sessions by academic and research staff to reinforce theory and concepts covered in face-to-face teaching sessions.

The ability to design pipelines, independently evaluate and compare method performance will be also developed through coursework based on the critical assessment of case studies. The project module will give the students the opportunity to develop research, communication and reporting skills through weekly support provided by the supervisory team. Additional taught sessions in this module will provide support for the development of writing and oral communication skills, and for the understanding of plagiarism and academic conduct matters.

How will you be assessed?

The assessment of the taught modules will involve a combination of coursework and written examination, with the exact proportion of the two types of assessment depending on the specific module. Coursework will vary from module to module and it may include in-class tests, problem sheets, lab reports and code writing. The project will be assessed through a written dissertation, the supervisor evaluation of practical work and an oral presentation.

Programme Title: Artificial Intelligence for Drug Discovery

How is the programme structured?

Please specify the structure of the programme diets for all variants of the programme (e.g. full-time, part-time - if applicable). The description should be sufficiently detailed to fully define the structure of the diet.

The duration of the programme is 1 calendar year.

The programme consists of 6 15-credit taught modules (3 for each of the first two semesters), a 30-credit taught module running in semesters 1 and 2, and a 60-credit project module running in semesters 2 and 3. All taught modules are compulsory and the project module is core. The bulk of the project will be carried out in the third semester, with some preliminary work performed in the second semester. Supervision of the projects will be provided by individual members of the academic staff or by a team of academics covering the necessary range of expertise.

Semester 1
Fundamentals of Medicinal Chemistry (15 credits)
Scientific programming for drug discovery (15 credits)
Molecular modelling for drug discovery (15 credits)

Semester 2
Computational ligand-based drug discovery (15 credits)
Data-driven drug discovery (15 credits)
Fine-tuning lead compounds (15 credits)

Semesters 1 and 2
Machine and Deep Learning (30 credits)

Semesters 2 and 3
Project - Artificial Intelligence for Drug Discovery (60 credits)

Academic Year of Study FT - Year 1

Module Title	Module Code	Credits	Level	Module Selection Status	Academic Year of Study	Semester
Fundamentals of Medicinal Chemistry	CHE706P	15	7	Compulsory	1	Semester 1
Scientific programming for drug discovery	CHE709P	15	7	Compulsory	1	Semester 1
Molecular modelling for drug discovery	CHE705P	15	7	Compulsory	1	Semester 1
Machine and Deep Learning	SPC707P	30	7	Compulsory	1	Semesters 1 & 2
Computational ligand-based drug discovery	CHE703P	15	7	Compulsory	1	Semester 2
Data-driven drug discovery	CHE704P	15	7	Compulsory	1	Semester 2

Programme Title: Artificial Intelligence for Drug Discovery

Module Title	Module Code	Credits	Level	Module Selection Status	Academic Year of Study	Semester
Fine-tuning lead compounds	CHE702P	15	7	Compulsory	1	Semester 2
Project - Artificial Intelligence for Drug Discovery	CHE701P	60	7	Core	1	Semesters 2 & 3

What are the entry requirements?

UK: a 2:1 or above at undergraduate level in Chemistry, Pharmaceutical Chemistry, Medicinal Chemistry, Biochemistry, Pharmacy, Biomedical Sciences or a related discipline.

International:

* an international qualification of similar standing to the above.
* English language entry requirements (IELTS scores): overall >= 6.5, reading >= 5.5, writing >= 6.0, listening >= 5.5, speaking >= 5.5.

How will the quality of the programme be managed and enhanced? How do we listen to and act on your feedback?

* Each individual module including the project module will be evaluated following the existing procedures in the School of Physical and Chemical Sciences. Module evaluations will be an opportunity for students to give anonymous feedback, with numerical results indicating satisfaction and free-text fields to raise any necessary concerns.

* The Student-Staff Liaison Committee (SSLC) provides a formal means of communication and discussion between the School and its students. The committee consists of student representatives from each year together with appropriate representation from staff within the school. It is designed to respond to the needs of students, as well as act as a forum for discussing programme and module developments. The SSLC meet regularly throughout the year.

* The School operates a School Education Committee (SEC), chaired by the Director of Education (DoE), which oversees and advises on all matters relating to the delivery of taught programmes at school level including quality assurance. This includes monitoring the application of relevant QMUL policies and reviewing all proposals for module and programme approval and amendment, before submission to Taught Programmes Board. Student views are incorporated in this Committee's work in a number of ways, such as through consideration of items referred by the SSLC and by consideration of student surveys, including module evaluation questionnaires.

* An Annual Programme Review (APR) will also take place, allowing the programme lead the opportunity to evaluate and reflect on the achievements of the programme, and in particular to document the steps taken to address both student and employer feedback.

What academic support is available?

* The School has a dedicated Student Support Officer (SSO) who is available to discuss any student-related problem. Additionally, each student will be allocated an academic advisor. SSO and advisors who will provide pastoral support and academic advice to all the students on the programme.

* At the beginning of the research project module each student will be allocated a personal research supervisor who is a member of academic staff and is the primary source of guidance on all matters relating to the research project component of the degree programme.

* Each module has a module coordinator, whose role is to ensure that the module runs smoothly, and that an appropriate level of

information is provided to students of the module.

Programme-specific rules and facts

None

How inclusive is the programme for all students, including those with disabilities?

Queen Mary has a central Disability and Dyslexia Service (DDS) that offers support for all students with disabilities, specific learning difficulties and mental health issues. The DDS supports all Queen Mary students: full-time, part-time, undergraduate, postgraduate, UK and international at all campuses and all sites.
Students can access advice, guidance and support in the following areas:
* Finding out if you have a specific learning difficulty like dyslexia
* Applying for funding through the Disabled Students' Allowance (DSA)
* Arranging DSA assessments of need
* Special arrangements in examinations
* Accessing loaned equipment (e.g. digital recorders)
* Specialist one-to-one "study skills" tuition
* Ensuring access to course materials in alternative formats (e.g. Braille)
* Providing educational support workers (e.g. note-takers, readers, library assistants)
* Mentoring support for students with mental health issues and conditions on the autistic spectrum
* Reasonable adjustments will be made to the computer-based aspects of the module, for example in enabling accessible technologies, additional teaching support, and/or extra time for students with visual or motor impairments that impact routine computer use.

In addition:

* Written notes, handouts and any other asynchronous material will be provided in advance where appropriate on our digital learning platform, and in different readable formats upon request.
* Module pages on the platform will meet the baseline standard defined in the School, following the checklist for accessibility (e.g. closed captions for videos, descriptions for images etc.)
* QReview and other mixed media (e.g. Zoom) will be used in order to provide recordings of sessions.
* Microphones will be used in classrooms.
* Hard copies of all relevant books to be made available in the library, or printed copies of electronic resources provided upon request, for those that cannot read from a computer screen.
* Detailed advice from the SPCS Student Support Officer for affected students, including liaising with the QMUL disability service.

Links with employers, placement opportunities and transferable skills

Although there are no placement opportunities on the programme, academic staff involved in the programme have links with industrial drug discovery partners such as Sosei Heptares and Evotec. Graduates could also progress to careers in the AI sector not necessarily related to drug discovery or Chemistry, since the programme aims to provide them with coding skills and practical experience in the use and evaluation of AI techniques that can transferred to other fields.

Programme Specification Approval

Programme Title: Artificial Intelligence for Drug Discovery

Person completing Programme Specification:	Dr Arianna Fornili
Person responsible for management of programme:	Dr Arianna Fornili
Date Programme Specification produced / amended by School / Institute Education Committee:	29 Sep 2023
Date Programme Specification approved by Taught Programmes Board:	