Programme Information		
Programme Title	Programme Code	HECoS Code
Digital Chemistry with AI and Automation	F1H6O F1H6OC	100417

Award	Length of Study	Mode of Study	Entry Point(s)	Total Credits	
				ECTS	CATS
MSc (F1H6O)	1 Calendar Year (12 months)	Full-Time	Annually in October	90	180
PG Certificate (F1H6OC)	6 months	Full-Time	Annually in October	30	60

Ownership			
Awarding Institution	Imperial College London	Faculty	Faculty of Natural Sciences
Teaching Institution	Imperial College London	Department	Chemistry
Associateship	Diploma of Imperial College (DIC) (MSc only)	Main Location(s) of Study	White City Campus
External Reference			
Relevant QAA Benchmark Statement(s) and/or other external reference points		Subject Benchmark Statement - Chemistry	
FHEQ Level		Level 7 - Masters	
EHEA Level		2nd Cycle	
External Accreditor(s) (if applicable)			
External Accreditor 1:	N/A		
Accreditation received:	N/A	Accreditation renewal:	N/A
Collaborative Provision			
Collaborative partner	Collaboration type	Agreement effective date	Agreement expiry date
N/A	N/A	N/A	N/A
Specification Details			
Programme Leads		Alex Ganose, Becky Greenaway and João Pedro Malhado	
Student cohorts covered by specification		2025-26 entry	

Date of introduction of programme	October 21
Date of programme specification/revision	March 25

Programme Overview

The practice of Chemistry in academia and industry is being revolutionised by advances in automation, artificial intelligence (AI), and big data. The new era of digital molecular design will transform synthesis and fabrication from small molecules to materials and vaccines. Computational modelling can now allow predictive insights into the behaviour of complex molecules and systems, parallel experiments can be monitored in real-time to give spectroscopic data readouts that allow rapid analysis of kinetics and yield optimisation. AI and machine learning (ML) are revolutionising our ability to predict reaction outcomes, plan complex multistep syntheses and understand small-molecule-macromolecule interactions to name just a few advances. Automation and robotic techniques are enabling the more rapid translation of ideas into practice *via* multiple parallel experimentation methods and the collection of huge and rich datasets relating to *in situ* monitoring of reaction parameters ranging from physical characteristics of reaction media (*e.g.,* viscosity data) to spectroscopic profiles of transient reaction intermediates [*e.g.,* infra red (IR) fingerprints]. This Master's programme will equip you to navigate and contribute to this future of chemistry and join the next generation of scientists that are in great need and currently in short supply.
This one-year programme will comprise a series of modules to provide training in the area and application of Data Science, Machine Learning and Automation in a diverse range of areas in the chemical sciences. The taught modules will be delivered in terms 1 and 2 (Spring and Autumn) on campus (i.e., 'face-to-face' delivery) followed by a one term 'practical project' module that is also undertaken on campus but may have elements that can be undertaken off campus. You will be able to choose from a broad range of projects and areas within the Digital Chemistry, AI and Automation remit. It may be possible for projects to be carried out partly or wholly at an external organisation and requests will be considered on a case by case basis.

Learning Outcomes

Upon completion of the MSc in Digital Chemistry with AI and Automation, you will be able to:

- Select appropriate machine learning methodology to solve a problem in chemistry, drug discovery or material sciences
- Implement a machine learning strategy using the main algorithms, libraries and Applications programming interfaces (APIs)
- Select appropriate representations of chemical information suitable for algorithmic processing
- Use automated facilities to optimise chemical reaction conditions
- Create curated chemical information datasets using automated experiments or computation
- Articulate the relevance of digital chemistry technologies in addressing contemporary industrial and research challenges
- Work in groups
- Be aware of ethical issues in data science
- Design and carry out research in an unfamiliar topic in a short time
- Communicate research findings for experts and non-experts

Upon completion of the PG Certificate in Digital Chemistry with AI and Automation, you will be able to:

- Select appropriate machine learning methodology to solve a problem in chemistry, drug discovery or material sciences
- Evaluate a machine learning strategy using the main algorithms, libraries and Applications programming interfaces (APIs)
- Select appropriate representations of chemical information suitable for algorithmic processing
- Use automated facilities to optimise chemical reaction conditions
- Create curated chemical information datasets using automated experiments or computation
- Articulate the relevance of digital chemistry technologies in addressing contemporary industrial and research challenges
- Work in groups

The Imperial Graduate Attributes are a set of core competencies which we expect students to achieve through completion of any Imperial degree programme. The Graduate Attributes are available at:

https://www.imperial.ac.uk/about/education/our-graduates/

Entry Requirements	
Academic Requirement	The minimum requirement is normally a 2:1 UK Bachelor's Degree with Honours in Chemistry, Biochemistry, Chemical Engineering (or a comparable qualification recognised by the university). Applicants with a 2:1 UK Bachelor's degree in a data science related area (computing, applied mathematics, statistics) will be considered on a case by case basis. For further information on entry requirements, please go to www.imperial.ac.uk/study/pg/apply/requirements/pgacademic
Non-academic Requirements	N/A
English Language Requirement	Higher requirement (PG) Please check for other Accepted English Qualifications
Admissions Test/Interview	Online interviews for shortlisted candidates

The programme's competency standards documents can be found at: www.imperial.ac.uk/chemistry/postgraduate/mres/

Learning & Teaching Approach

Learning and Teaching Delivery Methods

The Digital Chemistry with AI and Automation programme will be delivered by departmental academic staff as well as some staff from aligned departments within Imperial using a range of methods including: a blend of on campus and pre-recorded lectures, face-to-face workshops and tutorials, coding exercises and lab experiments. You will learn as part of a cohort and *via* interactions with your peers through discussions, group projects and peer assessed exercises. Staff will be available on campus to support you in your learning and facilitate ways in which you can work most effectively.

The whole program, ranging from live classroom sessions to team projects, allows you individually to participate in a seamless, flexible, and engaging learning experience and ensures the highest quality learning environment. The learning design allows you to have a seamless, innovative, and differentiated learning experience through:

1) rigorous assessments and targeted academic feedback;
2) collaborations with other students through applied projects;
3) participation in a vibrant and supportive social learning community through extensive high engagement on campus interactions.

Overall Workload

Your overall workload consists of face-to-face sessions and independent learning. The following gives an indication of how much time you will need to allocate to different activities at each level of the programme. At Imperial, each ECTS credit taken equates to an expected total study time of 25 hours. Therefore, the expected total study time is 2250 hours for the MSc program and 750 hours for the PG Certificate. The research project in the MSc program will amount to 1000 hours, and circa 20% of time spent on the remaining modules (250 hours for the MSc and 150 hours for the PGCert) will be spent in various structured activities (lectures, workshops and practical sessions) and 80% (1000 hours for the MSc and 600 hours for the PGCert) in independent study.

Assessment Strategy

Assessment Methods

The format of assessments will vary according to the aims, content and learning outcomes of each module. There will be short assessments for each module, some of which will be summative, followed by a final substantive summative assessment, which in most modules will take the form of a capstone project. Constructive alignment is being used throughout, moving from Intended Learning Outcomes, to assessments, to all practice material, so that all course content supports you working towards the overall achievement of the module and programme-level Learning Outcomes.

Assessment methods are module specific. These include programming assignments, critical essays, written reports, contributions to symposium-like discussions, video and poster presentations and business case development assessments. Overall, the various combinations of methods of assessment will allow a full assessment of your learning and achievements. Formative assessment opportunities will in general precede summative assessment such that you can receive feedback to improve your performance through the duration of the programme.

The final research project provides training in applied research of digital chemistry techniques. These projects will be motivated by topical research interests of members of academic staff of the Department of Chemistry and the wider Imperial community. Additionally, there will be the opportunity for industry-motivated projects. The research project provides the space for you to synthesize all the learnings from the programme into a single, coherent and novel activity. The research project is scaffolded in relation to the typical stages of a research study: literature review, underpinning learning or exploratory data analysis, study design and project proposal, conducting the research, analysing the research results and presenting and promoting these findings. Each stage is supported by a formative assessment, providing the opportunity for both feedback and direction on following stages. The final assessment involves both a written report and oral examination. In both cases, consideration will be given to both communication with a technical audience, and a lay audience.

Excluding the final research project that counts for 45% of the MSc degree, the assessment in the remaining modules is *ca.*10% exams, 60% coursework and 30% practical work.

Academic Feedback Policy

The Digital Chemistry with AI and Automation Assessment Schedule will set out the agreed submission deadlines, marking periods and feedback return dates for each academic year in advance. The individual deadlines captured in the Assessment Schedule will be discussed and confirmed by the teaching team ahead of delivery.

The program will normally provide marks/feedback on assessment to align with the university's policy – i.e., within 2 weeks of submission. This is a maximum period and much of the feedback will be provided sooner than this. For quizzes and MCQs, more immediate provisional marks are likely to be available once marks are checked by the team and depending on the nature of the assessment. With each returned coursework assignment, an individual evaluation will be provided. This will ensure that formative assessment is being implemented optimally with your learning experience being driven through the feedback received.

You will receive general feedback on the cohort examination performance. You will be provided with a percentage grade for coursework and examinations with the final numerical mark only confirmed after the Board of Examiners Meeting and will be released by Registry. Grades received during the year are deemed provisional until confirmed by the Final Board of Examiners.

Imperial's Policy on Academic Feedback and guidance on issuing provisional marks to students is available at: www.imperial.ac.uk/about/governance/academic-governance/academic-policy/exams-and-assessment/

Re-sit Policy

Imperial's Policy on Re-sits is available at: www.imperial.ac.uk/about/governance/academic-governance/academic-policy/exams-and-assessment/

Mitigating Circumstances Policy

Imperial's Policy on Mitigating Circumstances is available at: www.imperial.ac.uk/about/governance/academic-governance/academic-policy/exams-and-assessment/

Additional Programme Costs

This section should outline any additional costs relevant to this programme which are not included in students' tuition fees.

Description	Mandatory/Optional	Approximate cost
Laptop	Mandatory	£500

Important notice: Programme Specifications are the result of a large curriculum and pedagogy reform implemented by the Department and supported by the Learning and Teaching Strategy of Imperial College London. The modules, structure and assessments presented in this Programme Specification are correct at time of publication but might change as a result of student and staff feedback and the introduction of new or innovative approaches to teaching and learning. You will be consulted and notified in a timely manner of any changes to this document.

Programme Structure[1]

Year 1 – FHEQ Level 7 (Except for Key Concepts in Chemistry and Programming in Python which are at level 6)
As a student on the MSc program, you will study all compulsory modules and must choose one of the elective options from group A (this choice must be approved by the course directors). PG Certificate students will study six of the 5 ECTS modules (including up to one level 6 module). The precise choice will be made under the guidance and advice of the programme directors.

Code	Module Title	Compulsory/ Elective	Group	Term	Credits
CHEM60011	Programming in Python	Elective	A	Autumn	5
CHEM60012	Key Concepts in Chemistry	Elective	A	Autumn	5
CHEM70012	Data Analytics in Chemistry	Compulsory		Autumn	5
CHEM70013	"Hacking" for Chemists	Compulsory		Spring	5
CHEM70014	Automation and Enabling Technologies in Chemistry	Compulsory		Autumn	5
CHEM70015	Ethical Machine Learning and Data Science in Chemistry	Compulsory		Spring	5
CHEM70016	Journal Club	Compulsory		Autumn - Summer	5
CHEM70017	Artificial Intelligence in Chemistry: Drug Discovery	Compulsory		Spring	5
CHEM70018	Chemical Entrepreneurship and Sustainability Innovation in Chemistry	Compulsory		Spring	5
CHEM70020	Design of Experiments (DoE)	Compulsory		Autumn	5
CHEM70021	Artificial Intelligence in Chemistry: Materials	Compulsory		Spring	5
CHEM70019	Research Project	Core		Spring - Summer	40
				Credit Total	90

[a] Students with a Chemistry or related background will generally take the Programming in Python module; Students with a Data Science or related background will generally take the Key Concepts in Chemistry module.

[1] **Core** modules are those which serve a fundamental role within the curriculum, and for which achievement of the credits for that module is essential for the achievement of the target award. Core modules must therefore be taken and passed in order to achieve that named award. **Compulsory** modules are those which are designated as necessary to be taken as part of the programme syllabus. Compulsory modules can be compensated.
Elective modules are those which are in the same subject area as the field of study and are offered to students in order to offer an element of choice in the curriculum and from which students are able to select. Elective modules can be compensated.

Progression and Classification

Award and Classification for Postgraduate Students

Award of a Postgraduate Certificate (PG Cert)
To qualify for the award of a postgraduate certificate a student must have a minimum of 30 credits at Level 7 (this may include a maximum of 5 credits from Level 6 where this is approved as part of the award).

Award of a Postgraduate Degree (MSc)
To qualify for the award of a postgraduate degree a student must have:

1. accumulated credit to the value of no fewer than 90 credits at level 6 or above of which no more than 15 credits may be from credit level 6;
2. and no more than 15 credits as a Compensated Pass;
3. met any specific requirements for an award as outlined in the approved programme specification for that award.

Classification of Postgraduate Taught Awards

The university sets the class of Degree that may be awarded as follows:

1. Distinction: 70.00% or above
2. Merit: 60.00% and above but less than 70.00%.
3. Pass: 50.00% or above but less than 60.00%.

For a Masters, your classification will be determined through the Programme Overall Weighted Average meeting the threshold for the relevant classification band.

Your degree algorithm provides an appropriate and reliable summary of your performance against the programme learning outcomes. It reflects the design, delivery, and structure of your programme without unduly over-emphasising particular aspects.

Programme Specific Regulations

N/A

Supporting Information
The Programme Handbook is available upon enrolment.
The Module Handbooks are available upon enrolment.
Imperial's entry requirements for postgraduate programmes can be found at: www.imperial.ac.uk/study/pg/apply/requirements
Imperial's Quality & Enhancement Framework is available at: www.imperial.ac.uk/registry/proceduresandregulations/qualityassurance
Imperial's Academic and Examination Regulations can be found at: www.imperial.ac.uk/about/governance/academic-governance/regulations
Imperial College London is an independent corporation whose legal status derives from a Royal Charter granted under Letters Patent in 1907. In 2007 a Supplemental Charter and Statutes was granted by HM Queen Elizabeth II. This Supplemental Charter, which came into force on the date of Imperial's Centenary, 8th July 2007, established Imperial as a University with the name and style of "The Imperial College of Science, Technology and Medicine". www.imperial.ac.uk/admin-services/secretariat/university-governance-structure/charters/
Imperial College London is regulated by the Office for Students (OfS) www.officeforstudents.org.uk/advice-and-guidance/the-register/
This document provides a definitive record of the main features of the programme and the learning outcomes that you may reasonably be expected to achieve and demonstrate if you take full advantage of the learning opportunities provided. This programme specification is primarily intended as a reference point for prospective and current students, academic and support staff involved in delivering the programme and enabling student development and achievement, for its assessment by internal and external examiners, and in subsequent monitoring and review.