CH168-15 Data Science for Chemists

26/27

Department
Chemistry
Level
Undergraduate Level 1
Module leader
Daniel Murdock
Credit value
15
Module duration
20 weeks
Assessment
100% coursework
Study location
University of Warwick main campus, Coventry

Description

Introductory description

A module focused on equipping students with fundamental quantitative skills required for their degree and their professional careers.

Module web page

Module aims

To develop the skills of Y1 chemists in mathematics, coding and IT skills (both generic and chemistry-specific), preparing them for their chemistry modules and starting their skills development for their future careers.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

- This module will develop fundamental maths skills of student, and the syllabus may include elements from the following :
  Understand the basis of differential calculus, be able to differentiate and, find maxima and

minima.
Integrate functions and solve simple differential equations.
Determine the limits of simple functions.
Introduction to error propagation.
Introduction to linear algebra.

- An introduction to basic coding in python and its use in data science.
- An introduction to the use of general IT software for example spreadsheets and graph-drawing software packages.
- An introduction to the use of specific chemistry software for example the use of chemistry drawing software packages.

Learning outcomes

By the end of the module, students should be able to:

- Be able to evaluate functions and determine their limiting values.
- Be able to differentiate functions and find maxima and minima. Integrate functions and solve simple differential equations
- Have become familiar with the use of a range of general IT software packages
- Be able to write and debug simple programs using the Python coding language, and use these to solve simple problems typical to data science

Indicative reading list

Reading lists can be found in Talis

Subject specific skills

Numeracy and IT competency

Transferable skills

Numeracy and IT competency

Study

Study time

Type	Required
Lectures	11 sessions of 1 hour (10%)
Seminars	27 sessions of 1 hour (25%)
Practical classes	(0%)
Total	110 hours

Type	Required
Work-based learning	(0%)
Private study	72 hours (65%)
Total	110 hours

Private study description

N/A

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group A1

	Weighting	Study time	Eligible for self-certification
Assessment component			
In-class maths test	35%	10 hours	No
In-class maths test covering differentiation, integration, differential equations, and functions			
Reassessment component is the same			
Assessment component			
Excel Assessment	20%	5 hours	Yes (extension)
Using Excel for data analysis and graph plotting			
Reassessment component is the same			
Assessment component			
ChemDraw Assessment	10%	5 hours	Yes (extension)

	Weighting	Study time	Eligible for self-certification

Covering practical usage of Chemdraw, Chem3D, and other physical modelling software

Reassessment component is the same

Assessment component

Python coding project	35%	20 hours	Yes (extension)

Short project applying the Python programming language to a simple data-science type problem

Reassessment component is the same

Feedback on assessment

Marked scripts for IT and Python coding assessments are returned to the student with appropriate feedback. Detailed breakdown of student marks for maths test is available on request (but scripts are not returned)

Availability

Post-requisite modules

If you pass this module, you can take:

- CH280-15 Chemistry for Sustainability

Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 1 of F101 Chemistry (with Intercalated Year)
  - Year 1 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 1 of F100 Chemistry
  - Year 1 of F121 Chemistry with Medicinal Chemistry
- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 1 of F100 Chemistry
  - Year 1 of F110 MChem Chemistry (with Industrial Placement)
  - Year 1 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement
- Year 1 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)

- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
    - Year 1 of F109 MChem Chemistry (with International Placement)
    - Year 1 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
    - Year 1 of F100 Chemistry
    - Year 1 of F105 Chemistry
    - Year 1 of F110 MChem Chemistry (with Industrial Placement)
    - Year 1 of F109 MChem Chemistry (with International Placement)
    - Year 1 of F125 MChem Chemistry with Medicinal Chemistry
- Year 1 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)