

Chemistry and Data Sciences



En bref

- **Langue(s) d'enseignement:** Anglais
- **Forme d'enseignement :** Cours magistral & Travaux pratiques
- **Ouvert aux étudiants en échange:** Non

Présentation

DESCRIPTION

The objective of this lecture is to learn how to use numerical tools for the treatment of chemical data or the analysis of problems belonging to physics and chemistry. The students will learn how to analyze and plot data, how to use graphical tools, numerical analysis and scientific programming. The first part of the course (lecture 8h) will be dedicated to the introduction of different concepts related to programming and more particularly those related to the Python language (variables, data types, input/output, conditions, loops, lists, open/ write files, functions, introduction to modules), and to the presentation of the statistical tools in use in chemistry from basics to the opening of AI world. The second part of the lecture will be dedicated to practicals (16h) with a series of hands-on problem. The students will particularly use the Numpy, Pandas et Matplotlib libraries to get familiar with the chemometric tools necessary for the statistical exploitation of experimental results. The following concepts will thus be addressed via examples based on analytical chemistry: basic statistics (median, standard deviation,

variance, normal distribution, confidence interval, confidence limit), metrology (experimental errors, error propagation), estimation of variance components by analysis of variance (repeatability, reproducibility), calibration curves, statistical tests (Fisher, Student), multivariate statistical methods in chemistry (multilinear regression, Principal Component Analysis (PCA), Principal Component Regression PCR).

HEURES D'ENSEIGNEMENT

Chemistry and Data Sciences	Cours Magistral	8h
Chemistry and Data Sciences	Travaux Pratiques	16h

PRÉ-REQUIS NÉCESSAIRES

Basis in Python Programming

En bref

CONTACTS

Responsable pédagogique

Aurélie Perrier-Pineau

✉ aurelie.perrier-pineau@u-paris.fr

Responsable pédagogique

Eric Bremond

✉ eric.bremond@u-paris.fr

Pour en savoir plus, rendez-vous sur > u-paris.fr/choisir-sa-formation