

# Structure elucidation

## CH 314

**Part 1 : Mass spectrometry**

*Principles and instrumentation*

*8 -> 29 September 2025 (4 weeks)*

*Dr Pascal Miéville*

**EPFL**

# Structure elucidation – 1<sup>st</sup> part Mass spectrometry

## CH – 314 – Monday from 2pm to 6 pm

### Course goal and organization

This course is designed to give students an understanding of mass spectrometry fundamentals, methodology and instrumentation. It is meant to be complementary with the spectral analysis lecture given by Dr. Patiny in Bachelor 2<sup>nd</sup> year.

It is organized partly with reversed teaching strategy and combine autonomous readings, classical teaching and exercises sessions.

### Course content

- Masses of elements and molecules
- Isotopes and isotope distributions
- Mass spectrometry instrumentation: Ion sources, mass analyzers, and detectors
- Mass accuracy and resolution
- Tandem MS
- Coupling with separation technics (chromatography) and quantification
- Ion mobility MS

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### Main reference book

- J. S. O. McCullagh, N. J. Oldham, **Mass Spectrometry, Oxford Chemistry Primers, 2019**

Password for chapters : MSE\_2025\*

Password for corrections : corrMSE\_2025\*

### Secondary reference books

- K. Downard Mass Spectrometry: A Foundation Course, Royal Society of Chemistry, 2004
- H. Gross "Mass Spectrometry – A Textbook", 3rd edition, 2017, associated Exercises: <https://ms-textbook.com/concept-of-exercises-and-website/>

### Useful online tools

<https://www.leskoff.com/s01810-0> (series of SMILES, names and structure converters)

<https://ms.epfl.ch/applications/theoretical-calculations/> (various mass and fragmentation calculation tools from EPFL Dr L. Patiny)

### EPFL trained chatbot

For this lecture, students have access to an EPFL specifically MS trained chatbot. It is dedicated to support students during lectures and exercises. It is developed in collaboration with the **EPFL - CEDE - Center for Digital Education**. **It is still a prototype and can't and must not be considered as an official source of information.** Students feedbacks are more than welcome.

### Disclaimers

- Only information written in the main reference book (J. S. O. McCullagh, N. J. Oldham, **Mass Spectrometry**) and in the official lecture slides are considered valid for the examination.
- No claims based on data extracted from the EPFL trained chatbot or any other artificial intelligence tool will be accepted.

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### Time table

Week	Date	Slot	Topics
1	<b>8.9.25</b>	2.15 pm – 3.45 pm	Structure elucidation – general introduction & algorithmics
		4.15 pm - 5.45 pm	Introduction to mass spectrometry (chapter 1 of McCullagh & Oldham Mass Spectrometry)
		For next week	Autonomous study of chapter 2 up to 2.3 included – Ionization technics
2	<b>15.9.25</b>	2.15 pm – 3.45 pm	Desorption and atmospheric ionization technics (chapters 2.4 and 2.5)
		4.15 pm – 5.45 pm	Exercise session covering chapter 1 to 2 (up to chapter 2.5 included) Corrections available on 16.9.25 at 7am
		For next week	Autonomous study of chapter 4 – Resolution, accurate mass and sensitivity
3	<b>22.9.25</b>	2.15 pm - 3.45 pm	Methods of mass analysis – mass analysers (chapter 3)
		4.15 pm - 5.45 pm	Exercise session covering chapter 3 and 4 Corrections available on 22.9.25 at 7am
		For next week	Autonomous study of chapter 5 – Tandem mass spectrometry
4	<b>29.9.25</b>	2.15 pm – 3.45 pm	Separation techniques and quantification (chapter 7)
		4.15 pm – 5.45 pm	Exercise session covering chapter 5 and 7 Corrections available on 29.9.25 at 7am