

# Mass Spectrometry

**Instructor:** Alena Kubatova, Abbott Hall (301), 777-0348

Lecture: T, Th 12:00- 1:30 PM Abbott Hall 138

Since this course is more intensive than others, it will occur within 25 lecture meetings

Office hours: T 2:30-3:30 PM Abbott Hall 138

This course will cover mass spectrometry instrumentation and applications currently applied in industrial as well as research laboratories. Although this course is a graduate level, fundamentals will be reviewed. However, students will be expected to be familiar with those topics and thus quick in understanding of quantitative chemistry. To enhance interaction and active learning there will be special assignments within this class including a presentation of a peer reviewed article. There will also be home work/lab assignments, in which students will individually demonstrate their understanding on applied examples.

## The topics covered

- MS Introduction (history, and review of basics)
- Instrumentation
- MS ionization methods
  - EI, PICI, NICI
  - API (ESI, APCI)
  - LD, MALDI, FAB
  - ICP
- MS analyzers
  - Magnetic sector,
  - Quadrupole & Ion Trap
  - TOF
  - FTMS, Orbitrap
- Applications
  - GC/MS (EI interpretation)
  - LC/MS
  - Tandem MS
  - MS of polymers
  - MS of inorganics

## Grading

Components	No.	Points each	Total Points
Article presentations	1	70	70
Lab assignments/Home works			100
Exams	2	100	200
Final Exam	1	150	150
<b>Total</b>			<b>~520</b>

**Letter Grades:** A ( $\geq 90\%$ ), B (89-80%), C (79-70%), D (69-55%), F (<55%)

### **Academic integrity**

Students are expected to display academic honesty as defined in the code of Student Life and the Dictionary of Academic Integrity. Academic dishonesty will result in failing the course.

### **Supporting Materials**

*No single text really covers all of the mass spectrometry, but some texts are better than others.* One problem is that published material becomes old within about 5 years of publication. Another problem is that most books are shallow in key areas. They are good surveys, but do not cover the details of the field in adequate depth for this course.

*The resources used within this course will be recently published peer reviewed papers (the references will be provided during the course available in the reading room with links on the balckboard) and the following books. The books can be borrowed from the instructor for the period of three hours.*

- E. De Hoffmann & V. Stroobant, *Mass Spectrometry: Principles and Applications*, 2<sup>nd</sup> ed., John Wiley, 2002 (currently new edition is available) ISBN-10: 0-471-48565-9
- K. Downard, *Mass Spectrometry a foundation course*, 1<sup>st</sup> ed., The Royal Society of Chemistry, 2004, ISBN 0-85404-609-7
- F.W. Mc Lafferty & F. Tureček, *Interpretation of Mass Spectra*, 4<sup>th</sup> ed., University science Books, 1993, ISBN 0-935702-25-3
- T.A. Lee. *A Beginner's Guide to Mass Spectral Intepretation*, John Wiley & Sons, Ltd, 1998, ISBN 0-471-92628-8
- C.G. Herbert & R.A. Herbert, *Mass Spectrometry basics*, CRC Press LLC 2003, ISBN 0-8493-1354-6
- R. Willoughby, E. Sheehan & S. Mitrovich, *A Global View of LC/MS*, 2<sup>nd</sup> Ed. Global View Publishing 2002, ISBN 0-9660813-5-8
- Editors G. Montaudo & R. P. Lattimer, *Mass Spectrometry of Polymers*, CRC Press 2001, ISBN 0-8493-3127-7
- W. Henderson, J.S. McIndoe, *Mass Spectrometry of Inorganic and Organometallic Compounds*, John Wiley & Sons, Ltd, 2005, ISBN 0-470-85015-9
- R. E. Ardrey, *Liquid Chromatography-Mass Spectrometry an Introduction*, John Wiley & Sons, Ltd, 2003, ISBN 10:0471-49801-7
- M.C. McMaster, *LC/MS a Practical User's Guide*, John Wiley & Sons, Inc, 2005 ISBN-13-978-0471-65531-2
- H.-J. Hübschmann, *Handbook of GC/MS Fundamentals and Applications*, Wiley-VCH Verlag GmbH, 2001, ISBN 3-527-30170-4
- M. Kinter & N.E. Sherman, *Protein Sequencing and Identification using Tandem Mass Spectrometry*, Willey Interscience Series on Mass spectrometry, John Wiley & Sons, Inc, 2000, ISBN 0-471-32249-07

### **Presentations**

The topic of the presentation will be selected by students and approved by the instructor. The topic has to be related to Mass Spectrometry fundamentals or application published within the last 3 years from the peer reviewed journals such as Journal of Mass Spectrometry, Rapid Communications in Mass spectrometry, Analytical Chemistry etc. In order to obtain approval from the instructor students have to prepare short summary (100-200 words) describing the topic of the presentation. [The topic, summary and preferred date \(January – March\) of presentation must be submitted via E-mail by January 13<sup>th</sup>.](#)

The presentation should be presented in a clear comprehensive manner so other students can learn from it. The questions regarding the presentation may appear on exams. Each student should show understanding of the material covered. Students need to deliver PowerPoint presentation to the instructor one day prior to in the class presentation. The presentation will be posted on the blackboard in the form of PDF file. The students also need to provide one copy of the original paper to be placed in the binder in the reading room.

The grading presentation will be evaluated in class by the instructor and classmates based using the following criteria.

- 1) Timely delivery of summary, hardcopy of the paper, and presentation.
- 2) Was the summary clear?
- 3) Was the goal of the presentation stated clearly and early enough?
- 4) Was the introduction sufficient yet not too general (supplementary materials and review/textbook were used as appropriate)?
- 5) Was the introduction presented within reasonable amount of time (5-10 min)?
- 6) Was the presentation comprehensive (organized in logical sequence)?
- 7) What was the delivery of the presentation (voice modulation, eye contact, reading of the presentation)?
- 8) What was the quality of slides (figures, clarity, transitions, numbering)?
- 9) Was the text on slides limited?
- 10) Has attention been paid to a grammar and sentence structure? Were typographical and spelling errors minimized?
- 11) Were the references used appropriately?
- 12) Was the presentation presented within reasonable amount of time (30-40 min)?
- 13) Were the conclusions presented clearly?
- 14) Based on the discussion, did the presenter understand the topic of the presentation?

Each item will be graded on a scale from 1-5.

5=excellent, 4=good, 3 acceptable, 2 weak, 1 terrible

The points from the class will be averaged and total presented as the final grade for the presentation. The outliers in grading will be eliminated prior to the calculation.