

CHEM 577 Mass Spectrometry

Spring 2023 TTh 9:30-10:45 1801 Gilman

Instructor: Young-Jin Lee

Email: yjlee@iastate.edu

Office: 3759 Gilman

Phone: 294-1235

Office Hour: Right after class or make appointment.

Learning Outcome: Understand the fundamentals and instrumental aspects of mass spectrometry as well as mass spectral interpretation and various biological applications.

Pre-requirement: None. Basic knowledge in chemistry and physics is strongly recommended.

Grading

- 1st & 2nd Exam – 35% each.
- Homework– 10%
- Final term report– 20%

Homework: Due in 1 week on Canvas after the corresponding lecture.

Final term report: There is no final exam but final term report is due in the Final week. There are three topics students can choose from for the final report: 1) new mass spectrometry instrumentation, 2) new mass spectrometry application, or 3) most recent novel publications in either instrumentation or application. Details will be discussed in the class.

Textbook: The course is not following any formal textbook but students may download the following free e-books from the library as reading materials.

Optional Textbook 1: Mass Spectrometry: An Applied Approach, 2nd Ed, Ed. by Smoluch, Grasso, Suder, Silberring, Publisher: John Wiley & Sons, published in Jun 24, 2019
FREE ON-LINE VERSION IS AVAIALBLE THROUGH UNIVERSITY LIBRARY:
<https://onlinelibrary.wiley.com/doi/book/10.1002/9781119377368>

Optional Textbook 2: Mass Spectrometry, 2nd ed. By Jürgen H. Gross
Publisher: Springer, Published on Apr 6, 2011.

FREE ON-LINE VERSION IS AVAIALBLE THROUGH UNIVERSITY:
<https://link.springer.com/book/10.1007%2F978-3-642-10711-5>

Academic Dishonesty.

The class will follow Iowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the [Dean of Students Office](#).

Accessibility Statement.

Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility

Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294-7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Discrimination and Harassment

Iowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex, marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011, Tel. 515-294-7612, Hotline 515-294-1222, email eooffice@iastate.edu

Religious Accommodation

Iowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request the reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the [Dean of Students Office](#) at 515-294-1020 or the [Office of Equal Opportunity](#) at 515-294-7612.

Contact Information for Academic Issues

If you are experiencing, or have experienced, a problem with any of the above statements, email academicissues@iastate.edu

Freedom of Speech

Iowa State University supports and upholds the First Amendment protection of freedom of speech and the principle of academic freedom in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Course contents and schedule (tentative)

Watch the video content BEFORE the corresponding class. Homework is due in one week.

There will be a class discussion regarding the video content.

Videos are mostly from *ASMS resources for teaching MS remotely*,

<https://asms.org/about-mass-spectrometry/resources-for-teaching-ms-remotely>

, particularly ASMS vimeo channels: <https://vimeo.com/channels/asms>

You can use the link of each presentation title. The link is also available at Canvas.

0. Overview	Jan 17
HW1: Calculate Mass	
1. History of MS	Jan 16
2. Vacuum Systems	Jan 24
HW 2: Calculate leak rate	
Ion Formation -	
3. Electron Ionization (EI)	Jan 27
<u>Ionization Methods</u> by David C. Muddiman (North Carolina State University)	
<u>EIMS and CIMS</u> by Burnaby Munson (University of Delaware)	
4. Chemical Ionization (CI)	Jan 26
HW 3: Pressure in CI source	
5. Electrospray ionization (ESI)	Jan 31/Feb 2
<u>Mechanism of Electrospray Ionization (ESI)</u> by Lars Konermann (University of Western Ontario)	
HW 4: MW of protein in ESI mass spectrum	
6. Atmospheric pressure chemical ionization and photoionization (APCI, APPI)	Feb 7
7. Ambient ionization (DESI, LAESI, DART)	Feb 7
<u>Ambient Mass Spectrometry</u> by Jentaie Shiea (National Sun Yat-Sen University)	
8. Matrix-Assisted Laser Desorption/Ionization (MALDI)	Feb 9/14
<u>MALDI: Past and Future</u> by Kermit Murray (Louisiana State University)	
<u>Imaging Mass Spectrometry</u> by Ron M.A. Heeren (FOM-AMOLF)	
9. Secondary ion mass spectrometry (SIMS)	Feb 14
HW 5: Ionization summary	
10. Ion fragmentations in EI-MS	Feb 21/23
HW 6: EI fragmentation reaction	
11. EI spectral interpretation	Feb 28
HW 7: Elemental composition	
1st Exam (Overview to Ionization): 9-10:50am	Mar 2
Mass Analyzers	
<u>Mass Analyzers</u> by Richard Vachet (University of Massachusetts Amherst)	
12. Magnetic sector	Mar 7
13. Quadrupole, Triple Quadrupole, Quadrupole Trap	Mar 9/21

HW 8: Quadrupole and ion trap

Spring break (Mar 14-18)

- | | |
|------------------------------------------|--------|
| 14. Time-of-Flight (TOF) | Mar 23 |
| 15. Fourier-transform MS (ICR, Orbitrap) | Mar 28 |
| 16. MS detector | Mar 30 |

HW 9: Mass analyzer summary

MS/MS

Tandem Mass Spectrometry or MS/MS by Scott A. McLuckey (Purdue University)

- | | |
|------------------------------------|-------|
| 17. Collision-Induced Dissociation | Apr 4 |
|------------------------------------|-------|

Collision Induced Dissociation by Peter B. Armentrout (University of Utah)

- | | |
|-----------------------------------------------|-------|
| 18. Photodissociation | Apr 6 |
| 19. Electron capture or transfer dissociation | Apr 6 |

HW 10: MS/MS summary

- | | |
|----------------------|--------|
| 20. Innovation in MS | Apr 11 |
|----------------------|--------|

- | | |
|---------------------------------------------------------|--------|
| 21. Connection with Chromatography: GC-MS, LC-MS, CE-MS | Apr 11 |
|---------------------------------------------------------|--------|

CE/MS - Ready for Prime Time? by Norman Dovichi (University of Notre Dame)

LC and MS: A Match Made in Heaven by James Jorgenson (UNC at Chapel Hill)

- | | |
|-------------------------------|--------|
| 22. Ion Mobility Spectrometry | Apr 13 |
|-------------------------------|--------|

Ion Mobility Spectrometry - Analyzing Molecules as They Tumble Through Life by Erin S. Baker (Pacific Northwest National Laboratory, not at North Carolina State University)

Combining Ion Mobility Spectrometry with MS presented by David E. Clemmer (Indiana University)

- | | |
|---------------------------------------|--------|
| 23. High-Resolution Mass Spectrometry | Apr 18 |
|---------------------------------------|--------|

- | | |
|-------------------------------|--------|
| 24. MS for structural biology | Apr 20 |
|-------------------------------|--------|

Native Mass Spectrometry presented by Michal Sharon (Weizmann Institute)

- | | |
|--------------------|--------|
| 25. ID of unknowns | Apr 20 |
|--------------------|--------|

- | | |
|--------------------------------------------------------------------|--------|
| 2 nd Exam (Mass analyzers to ID of unknowns): 9-10:50am | Apr 25 |
|--------------------------------------------------------------------|--------|

- | | |
|----------------------------------|--------|
| 26. Applications to Metabolomics | Apr 27 |
|----------------------------------|--------|

Metabolite Profiling at the 'Omic' Scale by Gary Patti (Washington University, St. Louis)

- | | |
|--------------------------------|---------|
| 27. Applications to Proteomics | May 2/4 |
|--------------------------------|---------|

UC Davis proteomics online short course: https://video.ucdavis.edu/playlist/details/0_4jkc4swu

Particularly, Intro to Proteomics Brett Phinney

Peptide Spectrum Matching using Data Dependent Acquisition (DDA)

LCMS for Proteomics- part1

NO Final Exam. Term report due by May 11th (Thursday)

(Optional topics) Mass spectrometry and isotope. Hands-on proteomics data analysis.