

CHEM 577 Mass Spectrometry

Spring 2021 TTh 9:30-10:45 1222 Hach

Instructor: Young-Jin Lee

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Office Hour: Right after class or make appointment.

Course Description: The course is designed to provide understanding of mass spectrometry and current research performed in the field.

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

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

Grading

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

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

Class participation: Graded each week except 1st and two exam weeks.

Final term report: There is no final exam but final term report is due by the end of 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.

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>

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.

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](#).

Free Speech Statement: *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.*

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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 issues, email academicissues@iastate.edu

COVID-19 health and safety requirements: Students are responsible for abiding by the university's COVID-19 health and safety expectations. All students attending this class in-person are required to:

- properly wear a face covering and/or face shield, covering the nose and mouth, while in classrooms, laboratories, studios, offices, and other learning spaces. It is important to remember that a face covering and/or face shield is required to be worn whenever you are on campus, in the presence of others, and unable to maintain physical distance.
- practice physical distancing to the extent possible;
- assist in maintaining a clean and sanitary environment;
- not attend class if you are sick or experiencing symptoms of COVID-19;
- not attend class if you have been told to self-isolate or quarantine by a health official.
- follow the faculty member's guidance with respect to these requirements.

Failure to comply constitutes disruptive classroom conduct. Faculty and teaching assistants have the authority to deny a non-compliant student entry into a classroom, laboratory, studio, conference room, office, or other learning space. These requirements extend outside of scheduled class time, including coursework in laboratories, studios, and other learning spaces, and to field trips. These requirements may be revised by the university at any time during the semester.

Course contents and schedule (tentative)

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

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 26
HW1: Calculate Mass	
1. History of MS	Jan 28
2. Vacuum Systems	Feb 2
HW 2: Calculate leak rate	
Ion Formation -	
3. Electron Ionization (EI)	Feb 4
<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)	Feb 4
HW 3: Pressure in CI source	
5. Electrospray ionization (ESI)	Feb 9
<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 11
7. Ambient ionization (DESI, LAESI, DART)	Feb 11
<u>Ambient Mass Spectrometry</u> by Jentaie Shiea (National Sun Yat-Sen University)	
8. Inductively coupled plasma (ICP) (AAFS)	Feb 16
9. Matrix-Assisted Laser Desorption/Ionization (MALDI)	Feb 18
<u>MALDI: Past and Future</u> by Kermit Murray (Louisiana State University)	
<u>Imaging Mass Spectrometry</u> by Ron M.A. Heeren (FOM-AMOLF)	
10. Secondary ion mass spectrometry (SIMS)	Feb 23
HW 5: Ionization summary	
11. Ion fragmentations in EI-MS	Feb 23/25
12. EI spectral interpretation	Mar 2/4
HW 6: EI fragmentation reaction	
1st Exam (Overview to Ionization): 9-10:50am (Pittcon)	Mar 9
Mass Analyzers	
<u>Mass Analyzers</u> by Richard Vachet (University of Massachusetts Amherst)	
13. Magnetic sector	Mar 4
14. Quadrupole, Triple Quadrupole, Quadrupole Trap	Mar 11/16
HW 7: Quadrupole and ion trap	

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| 15. Time-of-Flight (TOF) | Mar 18 |
| 16. Fourier-transform MS (ICR, Orbitrap) | Mar 23/25 |
| 17. MS detector | Mar 25 |

HW 8: [Mass analyzer summary](#)

MS/MS

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

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| 18. Collision-Induced Dissociation | Mar 30 |
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Collision Induced Dissociation by Peter B. Armentrout (University of Utah)

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| 19. Photodissociation | Apr 1 |
| 20. Electron capture or transfer dissociation | Apr 1 |

HW 9: [MS/MS summary](#)

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| 21. Connection with Chromatography: GC-MS, LC-MS, CE-MS | Apr 6 |
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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)

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| 22. Ion Mobility Spectrometry | Apr 8 |
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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)

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| 23. High-Resolution Mass Spectrometry | Apr 13 |
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HW 10: [Elemental composition](#)

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| 24. MS for structural biology | Apr 13 |
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Native Mass Spectrometry presented by Michal Sharon (Weizmann Institute)

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| 25. Innovation in MS | Apr 15 |
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| 26. ID of unknowns | Apr 15 |
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| 2 nd Exam (Mass analyzers to MS for structural biology): 9-10:50am | Apr 20 |
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| 27. Applications to Metabolomics | Apr 22 |
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Metabolite Profiling at the 'Omic' Scale by Gary Patti (Washington University, St. Louis)

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| 28. Applications to Proteomics | Apr 27/29 |
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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 6th (Thursday)