

Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year (New format)	AY2026-2027
Semester/Trimester/Others (specify approx. Start/End date)	Semester 2
Course Author * Faculty proposing/revising the course	Basuri Pallab, Zhang Zhengyang
Course Author Email	zhang.zy@ntu.edu.sg; pallab.basuri@ntu.edu.sg
Course Title	Advanced Analytical Chemistry
Course Code	CM4011
Academic Units	3
Contact Hours	39
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	(CM2011 and CM2062 and CM3062)
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

The lectures provide an advanced account of modern analytical methods and instruments that are used to quantify chemical and biological samples and to monitor the progress of reactions. Students will understand the principles of advanced chromatography and mass spectrometry applied to chemical analysis. The students will be able to use their in-depth knowledge of analytical chemistry to devise experiments that can quantify a range of diverse chemical components. The students will learn problem solving skills where they apply their theoretical knowledge to real life problems in the environment.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Capillary Electrophoresis a. Explain how ions are separated in capillary zone electrophoresis. b. Describe how charge is related to electrophoretic mobility. c. Explain how the solution is transported from anode to cathode. d. Describe the arrival of species in the detector. e. Describe what is apparent mobility. f. Explain how zone dispersion arises in capillary zone electrophoresis. g. Describe how stacking of solute ions in the capillary occurs. h. Describe electroosmotic flow under low pH. i. Explain how covalent coatings reduces electroosmosis and wall adsorption. j. Describe hydrodynamic and electrokinetic sample injection. k. Describe common detection methods in capillary electrophoresis. l. Explain how micellar electrophoretic chromatography separates neutral molecules and ions. m. Explain how capillary gel electrophoresis separates macromolecules and discuss the speed of separation with molecular exclusion chromatography. n. Discuss how microfluidic devices function.
ILO 2	

Mass spectrometry

- a. Explain how ions are created in mass spectrometer.
- b. Describe how magnetic sector mass spectrometer separates gaseous ions.
- c. Describe how ions are detected.
- d. Explain the high resolution obtained by double-focusing mass spectrometer.
- e. Explain the operations of transmission quadrupole and time-of-flight mass spectrometer.
- f. Describe how resolving power is defined.
- g. Describe how to determine molecular ion from the mass spectrum.
- h. Explain how to predict the relative intensities of isotopic peaks for a given composition.
- i. Interpret the fragment ions arising from bond cleavage to determine the molecular structure.
- j. Calculate the molecular composition from the rings + double bonds equation.
- k. Explain how electrospray ionization creates ions in liquid chromatography.
- l. Describe how atmospheric pressure chemical ionization create gaseous ions.
- m. Explain how collisionally activated dissociation produce fragmented ions.
- n. Describe the working principle of matrix-assisted laser desorption/ionization.
- o. Describe the peaks obtained in reconstructed total ion chromatogram and extracted ion chromatogram.
- p. Describe the working principle in selected ion monitoring.
- q. Explain how molecules can be ionized from the surface of an object in ambient atmosphere.
- r. Explain how ion mobility spectrometer separates gas-phase ions.

ILO 3

Advanced mass spectrometry and instrumentation

- a. Discuss the functional building blocks of a modern mass spectrometer.
- b. Explain the electrodynamic physics of RF multipoles and ion guides in achieving collisional cooling and beam focusing.
- c. Explain the ionization mechanisms of Electrospray Ionization.
- d. Describe the physical and chemical ionization processes of MALDI.
- e. Formulate the principles of ion trapping and stability in quadrupoles and 2D/3D ion traps using the Mathieu stability equation.
- f. Explain mass separation in linear and reflectron Time-of-Flight (TOF) instruments.
- g. Model ion motion in an Orbitrap analyzer.
- h. Elucidate the biophysical mechanism of Collision-Induced Dissociation (CID/HCD).
- i. Evaluate the mechanism and energy deposition kinetics of Surface-Induced Dissociation (SID).
- j. Compare radical- and photon-driven activation mechanisms, such as Electron Capture Dissociation (ECD), Electron Transfer Dissociation (ETD), and Ultraviolet Photodissociation (UVPD).
- k. Formulate the physics of gas-phase ion transport under low electric fields, defining the relationship between ion mobility, drift velocity, and electric field.
- l. Differentiate mass-to-charge separation from mobility separation based on ion charge, geometric cross-section, polarizability, and buffer gas interactions.
- m. Explain the operational mechanism of Drift Tube Ion Mobility Spectrometry (DTIMS) for primary, calibration-free CCS measurements.
- n. Describe the mechanism of Traveling Wave Ion Mobility Spectrometry (TWIMS) and explain why empirical CCS calibration is required.
- o. Explain the principles of multipass Cyclic Ion Mobility Spectrometry (cIMS), detailing how scalable path length enhances mobility resolution.

ILO 4

Ambient ionization and mass spectrometry imaging

- a. Classify ambient ionization techniques by their working mechanism, comparing liquid extraction, laser ablation, plasma ionization, variants of electrospray, and acoustic spray methods.
- b. Illustrate the mechanism of Desorption Electrospray Ionization (DESI), showing how charged solvent droplets hit a surface, dissolve molecules, and splash off into the mass spectrometer.
- c. Describe how nano-ESI works at very low flow rates, producing tiny droplets that improve sensitivity and reduce ion suppression.
- d. Explain how nano-DESI uses a tiny liquid bridge between two capillaries to gently sample surface molecules.
- e. Explain how Atmospheric Pressure Chemical Ionization uses a corona discharge needle to ionize volatile and less polar compounds.
- f. Select the most suitable ambient ionization technique for a given sample type (e.g., dry pill, fresh plant leaf, liquid droplet, or tissue section).
- g. Explain the basic concept of Mass Spectrometry Imaging (MSI): recording a mass spectrum at every grid position (pixel) to map where molecules reside.
- h. Define spatial resolution, step size (pitch), and spot size, and explain how they determine image sharpness and total acquisition time.
- i. Identify proper sample handling steps for tissue imaging, including freezing, cryosectioning, and thaw-mounting to prevent molecular smearing.
- j. Contrast the working principles of MALDI-MSI (laser + chemical matrix in vacuum/air) with DESI-MSI (solvent spray in open air without matrix).
- k. Describe how Nano-DESI MSI achieves high-resolution mapping on soft, untreated surfaces using localized liquid extraction.
- l. Explain how LAESI-MSI enables open-air imaging of living plant leaves and provides 3D molecular depth profiling through layer-by-layer laser ablation.

ILO 5

	Quality assurance and calibration methods - Explain the steps in Quality Assurance (Use objectives, Specifications and Assessment). - Describe how method validation is performed. - Calculate the limit of detection (LOD) and limit of quantification (LOQ) and understand how they differ. - Explain how and why standard additions are performed and how to calculate the concentration. - Describe the principles of internal standards.
ILO 6	Modern applications of mass spectrometry - Distinguish between "bottom-up" (peptide-based) and "top-down" (intact protein) proteomics workflows for protein identification and sequence verification. - Explain how tandem mass spectrometry is used to locate post-translational modifications (PTMs) such as phosphorylation and glycosylation on proteins. - Preparative mass spectrometry, accelerated reactions, and surface modification. - Mass spec pen for online diagnostics.

Course Content

No.	Course Content	Approx. Lecture Hours
1	Capillary Electrophoresis	8
2	Fundamentals of Mass spectrometry	8
3	Advanced Mass spectrometry and instrumentation	8
4	Ambient ionization and mass spectrometry imaging	5
5	Quality Assurance and Calibration Methods	3
6	Modern applications of mass spectrometry	3

Reading and References (if applicable)

D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch "Fundamentals of Analytical Chemistry (9th Edition)", Brooks/Cole, Cengage Learning, 2014.

Reference textbook: D. C. Harris and C. A. Lucy "Quantitative Chemical Analysis (9th Edition)", W. H. Freeman and Company, 2016.

Gross, J. H. (2004). *Mass spectrometry: a textbook*. Springer.

Hoffmann, E. de, & Stroobant, V. (2007). *Mass spectrometry: principles and applications*. (3rd ed. / Edmond de Hoffmann, Vincent Stroobant.). J. Wiley.

NOTE: The above listing comprises the foundational readings for the course and more up-to-date relevant readings will be provided when they become available.

Planned Schedule

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
1	Capillary Electrophoresis	1	In-person	Lecture and online	
2	Capillary Electrophoresis	1	In-person	Lecture and online	
3	Capillary Electrophoresis	1	In-person	Lecture and online	
4	Fundamentals of Mass Spectrometry	2	In-person	Lecture and online	
5	Fundamentals of Mass Spectrometry	2	In-person	Lecture and online	
6	Fundamentals of Mass Spectrometry	2	In-person	Lecture and online	
7	Advanced Mass spectrometry and instrumentation	3	In-person	Lecture and online	
8	Advanced Mass spectrometry and instrumentation	3	In-person	Lecture and online	
9	Advanced Mass spectrometry and instrumentation	3	In-person	Lecture and online	
10	Ambient ionization and mass spectrometry imaging	4	In-person	Lecture and online	
11	Ambient ionization and mass spectrometry imaging	4	In-person	Lecture and online	
12	Quality Assurance and Calibration Methods	5	In-person	Lecture and online	

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
13	Modern applications of mass spectrometry	6	In-person	Lecture and online	

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Blend of online and face-to-face lectures.	The bulk of the content will be delivered online. This allows (a) extensive use of animations and laboratory videos and (b) use of interactive questions so that students may immediately test their learning. Face to face lectures and experimental demonstrations will be employed for selected topics.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(Mid-term 1)			25		Individual	Analytic	Multistructural
2	Continuous Assessment (CA): Test/Quiz(Midterm 2)			25		Individual	Analytic	Multistructural
3	Continuous Assessment (CA): Class Participation()			10		Individual	Analytic	Multistructural
4	Continuous Assessment (CA): Presentation(Team Application Exercises + Peer Evaluation)			40		Individual and Team	Analytic	Multistructural

Description of Assessment Components (if applicable)

Formative Feedback

You will be given feedback in four ways:

1. By response to postings on the course discussion board.
2. Through the marking of the mid-terms.
3. Through one-on-one discussions via appointment with the course instructor
4. General feedback will be provided to the students following the final exam.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Communication	Basic
Learning Agility	Basic
Critical Thinking	Basic

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to complete all activities in good time.

Policy (Absenteeism)

If you miss a lecture, you are expected to make up for the lost learning activities. If you miss one of the mid-term tests with a valid reason and approval (such as a medical certificate), then the total CA will come from the other mid-term test. If you miss both mid-term tests with a valid reason then an additional make-up test will be set to obtain the total CA mark.

Policy (Others, if applicable)

Diversity and Inclusion Policy

Integrating a diverse set of experiences is important for a more comprehensive understanding of science and engineering.

It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences. That honours your identities; including ethnicity, gender, socioeconomic status, sexual orientation, religion or ability.

To help accomplish this:

- If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety disorder or social phobia;
- If you feel your performance in the course is being impacted by your experiences outside of class;
- If something was said in the course (by anyone, including instructor/supervisor) that made you uncomfortable.

Please e-mail to your Associate Chair (Undergraduate) at ac-cceb-ug@ntu.edu.sg about how we can help facilitate your learning experience.

As a participant in course discussions you should also strive to honour the diversity of your classmates. You can do this by; using preferred pronouns and names; being respectful of others opinions and actively making sure all voices are being heard; and refraining from the use of derogatory or demeaning speech or actions. All members of the course are expected to strictly adhere to the student code of conduct (<https://www.ntu.edu.sg/life-at->

ntu/student-life/student-conduct) . If you witness something that goes against this or have any other concerns, please speak to your instructors or a faculty member.

Technical Skills To Be Developed

All skills to be developed for this course:

Chromatography Equipment Operation and Control
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Analytical Method Validation

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Last Updated By: Natasha Bhatia (Dr)