Name of the Programme: M.Sc. Part-II (Analytical Chemistry)

Course Code: CHA-602 **Title of the course:** Advanced Mass Spectrometry

Number of Credits: 4

Effective from AY: 2023-24

Prerequisites for the course:	Students should have studied analytical chemistry course at M.Sc. Part I.	
Course Objective:	1. To study various ionisation sources and mass analyser. 2. To introduce tandem mass spectrometry techniques. 3. To learn interpretational aspects of spectral data obtained from hyphenated techniques.	
Content	**1. Ionization methods:** a. Mass spectrometry: introduction, principle, general instrumentation, general interpretation procedure for mass spectra; b. Gas Phase ionization: electron ionization (EI), chemical ionization (CI), Field ionization and field desorption (FI, FD) c. Particle Bombardment: Fast atom bombardment (FAB), Secondary ion mass spectrometry (SIMS). d. Atmospheric pressure Ionization: electrospray ionization (ESI), atmospheric pressure ionization (APCI). e. Laser Desorption: MALDI. f. Inorganic ionization sources: thermal ionization, Spark source, Glow discharge, Inductively coupled plasma (ICP). g. Problem solving using mass spectrometry.	No of hours 15
	2. Mass analyzers: a. Characteristics of analysers: nominal mass, mass accuracy, resolving power, resolutions, isotopic composition, numericals to calculate nominal and accurate mass. b. Magnetic, electromagnetic and double focusing c. Single Quadrupole and triple quadrupole d. Time of flight analyzer e. Ion cyclotron resonance analyzer f. Hybrid instrumentation g. Detectors: electron multiplier, photon multiplier, Faraday cup *Note: instrumentation, working principles, characteristic features, advantages, practical consideration shall be discussed.*	15

	3. Hyphenated Techniques: a. Coupled techniques, Importance of hyphenation of two analytical techniques, Interface and their characteristic features. b. Introduction, principle and instrumentation of following techniques: GC-MS, LC-MS, ICP-MS, CE-MS, TG-MS. c. Tandem mass (MS-MS): Introduction, concepts of tandem mass spectrometry, Ion activation methods. d. Analysis of chromatogram: Total ion chromatogram (TIC), Extracted Ion Chromatogram (XIC). e. Analysis of chemical data of natural product, drugs, etc. Dereplication using hyphenated technique.	15
	4. Tandem Mass spectrometry applications: a. Pharmacokinetic studies: Fate of drug in living organisms, metabolite identification, biotransformation of ziprasidone. b. Tandem MS and fragmentation pattern of following drugs: Paracetamol, 2-mercaptonicotinic acid, Sulfasalazine, amphetamine, Trocade. c. Analysis of biomolecules: Proteins, Peptides, Oligonucleotides, structure and sequence determination using fragmentation, solve problems based on MS/MS data.	15
Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References / Readings	1. H. Jürgen, Mass Spectrometry: A Textbook Gross, 2nd Ed, Springer publisher, 2011. 2. E. De Hoffmann, V. Stroobant, Mass Spectrometry: Principles and Applications, 2nd Ed, Wiley, 2007. 3. R. B. Cole, Electrospray and MALDI Mass Spectrometry: Fundamentals, Instrumentations, Practicalities and Biological Applications, 2nd Ed, Wiley, 2010. 4. J. T. Watson, O. D. Sparkman, Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation, 4th Ed, Wiley, 2007. 5. K. Wanner, G. Höfner, Mass Spectrometry in Medicinal Chemistry Applications in Drug Discovery, 1st Ed, Wiley-VCH, 2007. 6. M. Kinter, N. E. Sherman, Protein Sequencing and Identification Using Tandem Mass Spectrometry, 1st Ed, Wiley, 2000. 7. P. James, Proteome Research: Mass Spectrometry (Principles and	

	Practice), 1st Ed, Springer publisher, 2000. 8. J. K. Prasain, Tandem Mass Spectrometry-Applications and Principles, InTech publisher, 2012.
Course Outcome:	1. Students will be able to explain principle behind different ionizations sources. 2. Students will be able to select mass analysers and ionization sources for analysis of particular type of analyte. 3. Students will be able to deduce structures of simple to moderately complex molecules/biomolecules by combining the spectral data obtained from hyphenated techniques. 4. Students will be able to apply tandem Mass spectrometry for biomolecule analysis.