Programme: M. Sc. Part-II (Analytical Chemistry)
Course Code: ACO-503
Title of the Course: Advanced Mass Spectrometry
Number of Credits: 3 **Effective from AY**: 2019-20

Prerequisites for the course:	Should have studied the spectroscopy topics at T. Y. B. Sc. (Chemistry) and M. Sc. part-I (Chemistry) levels.	
Course Objectives:	1. Study of various theoretical concepts related to mass spectroscopic techniques. 2. Introduction of tandem mass spectrometry techniques. 3. Learning interpretational aspects of spectral data obtained from hyphenated techniques	
Course Outcomes:	1. Students should be in a position to understand principle behind different ionizations sources. 2. Students should be in a position to select mass analysers and ionization sources for analysis of particular type of analyte. 3. Students should be in a position to deduce structures of simple to moderately complex molecules/biomolecules by combining the spectral data obtained from hyphenated techniques.	
Content:	**1. Introduction** Mass spectrometry principle, general instrumentation, general interpretation procedure for mass spectra; **2. Ionization methods:** 2.1. Gas Phase ionization: electron ionization (EI), chemical ionization (CI), Field ionization and field desorption (FI, FD) 2.2. Particle Bomabardment: Fast atom bombardment (FAB); Secondary ion mass spectrometry (SIMS) 2.3. Atmospheric pressure Ionization: electrospray ionization (ESI), atmospheric pressure ionization (APCI) 2.4. Laser Desorprtion: MALDI 2.5. Inorganic ionization sources: thermal ionization; Spark source; Glow discharge, Inductively couple plasma (ICP) **3. Mass analyzers:** 3.1. Characteristics of analysers: nominal mass, mass accuracy, resolving power, resolutions, numericals to calculate nominal and accurate mass 3.2. Magnetic, electromagnetic and double focusing 3.3. Single Quadrupole and triple quadrupole 3.4. Time of flight analyser 3.5. Ion cyclotron resonance analyzer, 3.6. hybrid instrumentation 3.7. Detectors: electron multiplier, photon multiplier, Faraday cup (Note: instrumentation, working principles, characteristic features, advantages, practical consideration shall be discuss). **3. Hyphenated Techniques:** 3.1. Coupled techniques; Interface and their characteristic features; Importance of hyphenation of two analytical techniques; 3.2. Introduction and instrumentation of following techniques: GC-FTIR, GC-MS, LC-MS, MS-MS (tandem) mass spectrometry (use of	2 hrs 10 hrs 8 hrs 8 hrs

	stable isotopes), ICP-MS, TG-MS. 3.3. Analysis of chromatogram obtained from hyphenated techniques: Total ion chromatogram (TIC), Extracted Ion chromatogram (XIC). 4. **Tandem Mass spectrometry applications:** 4.1. Pharmacokinetic studies: Fate of drug in living organisms, metabolite identification, biotransformation of ziprasidone 4.2. Tandem MS and fragmentation pattern of following drugs: Paracetamol, 2-mercaptonicotinic acid, Sulfasalazine, Narcotics-amphetaine, 4.3. Analysis of biomolecules-Protein and peptides: structure and sequence determination using fragmentation, solve problems based on MS/MS data.	8 hrs
Pedagogy:	Lectures/ tutorials/ seminars/ term papers/assignments/ presentations/ self-study or a combination of some of these. Sessions shall be interactive in nature to enable peer group learning.	
References/ Readings	1. H. Jürgen, *Mass Spectrometry: A Textbook Gross*, Springer publisher, 2011, 2nd Ed. 2. E. De Hoffmann, V. *Stroobant, Mass Spectrometry: Principles and Applications*, J. Wiley publisher, 2007, 2nd Ed. 3. R. B. Cole, *Electrospray and MALDI Mass Spectrometry: Fundamentals, Instrumentations, Practicalities and Biological Applications*, J. Wiley publishers, 2010, 2nd Ed. 4. J. T. Watson, O. D. Sparkman, *Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation*, J. Wiley, 2007, 4th Ed. 5. K. Wanner, G. Höfner (editors.), *Mass Spectrometry in Medicinal Chemistry Applications in Drug Discovery*, Wiley-VCH, 2007, 1st Ed. 6. M. Kinter, N. E. Sherman, *Protein Sequencing and Identification Using Tandem Mass Spectrometry*, J. Wiley publisher, 2000, 1st Ed. 7. P. James, *Proteome Research: Mass Spectrometry (Principles and Practice)*, Springer publisher, 2000, 1st Ed.	