Course Name (English)	LCMS AND NMR FOR NATURAL PRODUCT ANALYSIS APPROVED
Course Code	CMT625

MQF Credit	3

Course Description	This course will expose the students to the application of Nuclear Magnetic Resonance and Mass Spectrometry in the structural determination of natural products. The students will learn the metabolomics approach of natural products analysis especially in the herbal standardization and quality control. The outcomes shall be assessed through a variety of tools which include the traditional paper examination (tests and final examination), and case study report.

Transferable Skills	The students should be able to elucidate chemical structures using NMR and MS spectrum and understand the use NMR and MS as natural products analysis and herbal quality control tool.

Teaching Methodologies	Lectures, Case Study

CLO		
	CLO1	Explain the concepts of one dimensional and two dimensional nuclear magnetic resonance, and mass spectrometry for characterization of natural products, and plant metabolomics as an approach for natural products analysis (PLO1, C2)
	CLO2	Interpret the NMR and LCMS data for characterization of natural products and for natural products analysis using plant metabolomics approach (PLO3, C6)

Pre-Requisite Courses	No course recommendations

Topics
1. One Dimensional Nuclear Magnetic Resonance 1.1) 1H Nuclear Magnetic Resonance 1.2) Chemical Shift 1.3) Shielding and deshielding effect 1.4) Integration 1.5) Spin-spin coupling 1.6) Proton Coupling 1.7) Proton equivalence 1.8) 13C NMR 1.9) Proton-decoupled experiment 1.10) APT 1.11) DEPT
2. Two dimensional Nuclear Magnetic Resonance 2.1) COSY 2.2) HSQC/HMQC 2.3) HMBC 2.4) NOESY
3. Case Study: Structural characterization of secondary Metabolites 3.1) Flavonoids 3.2) Alkaloids 3.3) Terpenes 3.4) Other compounds

4. Mass Spectrometry for Identification of Secondary metabolites
4.1) Introduction to mass spectrometry
4.2) Ionisation techniques
4.3) Mass analyzers
4.4) Characterization of mass spectrum
4.5) Tandem mass spectrometry

5. Metabolomics
5.1) Introduction to metabolomics
5.2) Multi variate data analysis (MVDA) for discrimination of samples and bioactivity correlation model

6. Plant metabolomics workflow
6.1) Sample preparation (Harvesting, extraction and sample preparation for analysis)
6.2) Data acquisition, data pre-processing, data pre-treatment
6.3) Data analysis using MVDA
6.4) Biomarker identification

Assessment Breakdown	%
Continuous Assessment	60.00%
Final Assessment	40.00%

Details of Continuous Assessment	Assessment Type	Assessment Description	% of Total Mark	CLO
	Case Study	Case Study 1: Structural elucidation of real example of natural products	10%	CLO2
	Case Study	Case Study 2: Metabolomic analysis of selected medicinal plants.	10%	CLO2
	Test	n/a	40%	CLO2

Reading List	This Course does not have any book resources
Article/Paper List	**Recommended Article/Paper Resources** • **Wolfender JL1, Glauser G, Boccard J, Rudaz S. 2009, MS-based plant metabolomic approaches for biomarker discovery.,** *Natural Product Communication***, 4**
Other References	• **Textbook Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce 2014,** *Spectrometric Identification of Organic Compounds, 8th Edition* **, Wiley, United States**