



UNIVERSITI TEKNOLOGI MARA
CMT625: LCMS AND NMR FOR NATURAL PRODUCT ANALYSIS

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| 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) ¹ H 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) ¹³ C 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 |

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| Reading List | This Course does not have any book resources | | |
| Article/Paper List | Recommended Article/Paper Resources | <ul style="list-style-type: none"> • Wolfender JL1, Glauser G, Boccard J, Rudaz S. 2009, MS-based plant metabolomic approaches for biomarker discovery., <i>Natural Product Communication</i>, 4 | |
| Other References | <ul style="list-style-type: none"> • Textbook Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce 2014, <i>Spectrometric Identification of Organic Compounds, 8th Edition</i> , Wiley, United States | | |