



## UNIVERSITI TEKNOLOGI MARA

### CMT400: APPLICATIONS OF COMPUTER IN CHEMISTRY

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| <b>Course Name (English)</b>   | APPLICATIONS OF COMPUTER IN CHEMISTRY <b>APPROVED</b>  |
| <b>Course Code</b>   | CMT400   |
| <b>MQF Credit</b>  | 3  |
| <b>Course Description</b>  | This course is aimed at providing students with knowledge on the use and application of computer in chemistry. The topics in this course include introduction to computers, use of spreadsheet in chemistry, chemical structure drawing packages, database management and visual basic for applications.   |
| <b>Transferable Skills</b>   | Computer and visual basic programming  |
| <b>Teaching Methodologies</b>  | Lectures, Lab Work   |
| <b>CLO</b>   | CLO1 Explain concepts related to computers including types of computers, operating systems and the application of computer in society and chemistry<br>CLO2 Apply the basic features of the following softwares or their equivalence: spreadsheet software (Excel), chemical drawing software<br>CLO3 Develop simple applications using Microsoft Access and Visual Basic for Application (VBA ) |
| <b>Pre-Requisite Courses</b>   | No course recommendations  |
| <b>Topics</b>  |  |
| <b>1. Introduction</b><br>1.1) Components of computer<br>1.2) Types of Computers<br>1.3) System and application software<br>1.4) Operating systems and Utility programs<br>1.5) Examples of computer applications in society and chemistry   |  |
| <b>2. Spreadsheet Applications in Chemistry</b><br>2.1) Examples of different spreadsheets e.g Excel<br>2.2) Calculations and Solving equations<br>2.3) Plotting of graphs<br>2.4) Built-in functions: Logical and Lookup<br>2.5) Statistical analysis and Linear Regression<br>2.6) Interactive worksheet |  |
| <b>3. Chemical Drawing Applications</b><br>3.1) Drawing packages e.g IsisDraw or ChemDraw<br>3.2) Drawing simple and complex structures<br>3.3) Using templates<br>3.4) Creating reports<br>3.5) Searching chemical information using Chemspider   |  |
| <b>4. Database Management using Microsoft Access</b><br>4.1) Database concepts<br>4.2) Common data types<br>4.3) Types of Objects<br>4.4) Types of relationship<br>4.5) Creating Chemical inventory using MS Access  |  |

## **5. Visual Basic for Applications (VBA)**

- 5.1) Excel VBA
- 5.2) Data types
- 5.3) Visual basic controls and properties
- 5.4) Basic commands
- 5.5) Writing a Visual Basic program
- 5.6) Designing simple application using VBA e.g pH Calculator

| Assessment Breakdown  | %      |
|-----------------------|--------|
| Continuous Assessment | 60.00% |
| Final Assessment      | 40.00% |

| Details of Continuous Assessment | Assessment Type | Assessment Description         | % of Total Mark | CLO  |
|----------------------------------|-----------------|--------------------------------|-----------------|------|
|                                  | Assignment      | Assignment 1 - Excel           | 5%              | CLO2 |
|                                  | Assignment      | Assignment 2 -Chem Draw        | 5%              | CLO2 |
|                                  | Assignment      | Assignment 3 -Access Database  | 5%              | CLO3 |
|                                  | Group Project   | Project - Visual Basic Program | 15%             | CLO3 |
|                                  | Test            | Test1 -Topic 1 and 2           | 10%             | CLO1 |
|                                  | Test            | Test2 -Topic 3 and 4           | 10%             | CLO2 |
|                                  | Test            | Test3 -Topic 5                 | 10%             | CLO3 |

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| Reading List       | <p><b>Reference Book Resources</b></p> <ul style="list-style-type: none"> <li>• Sime, RJ, <i>Physical Chemistry Calculations with Excel</i>, Pearson Benjamin Cummings,</li> <li>• <i>Excel for Chemists</i></li> <li>• Kumari, R. 2005, <i>Computers and their applications to chemistry</i>, 2 Ed., Alpha Science International, Oxford, UK</li> <li>• Barrante, James R. 2004, <i>Applied mathematics for Physical Chemistry</i>, Pearson Prentice Hall</li> </ul> |
| Article/Paper List | This Course does not have any article/paper resources   |
| Other References   | This Course does not have any other resources   |