UNIVERSITI TEKNOLOGI MARA
CMT400: APPLICATIONS OF COMPUTER IN CHEMISTRY

Course Name (English)	APPLICATIONS OF COMPUTER IN CHEMISTRY `APPROVED`
Course Code	CMT400

MQF Credit	3

Course Description	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.

Transferable Skills	Computer and visual basic programming

Teaching Methodologies	Lectures, Lab Work

CLO	CLO1	Explain concepts related to computers including types of computers, operating systems and the application of computer in society and chemistry
	CLO2	Apply the basic features of the following softwares or their equivalence: spreadsheet software (Excel), chemical drawing software
	CLO3	Develop simple applications using Microsoft Access and Visual Basic for Application (VBA)

Pre-Requisite Courses	No course recommendations

Topics
1. Introduction 1.1) Components of computer 1.2) Types of Computers 1.3) System and application software 1.4) Operating systems and Utility programs 1.5) Examples of computer applications in society and chemistry
2. Spreadsheet Applications in Chemistry 2.1) Examples of different spreadsheets e.g Excel 2.2) Calculations and Solving equations 2.3) Plotting of graphs 2.4) Built-in functions: Logical and Lookup 2.5) Statistical analysis and Linear Regression 2.6) Interactive worksheet
3. Chemical Drawing Applications 3.1) Drawing packages e.g IsisDraw or ChemDraw 3.2) Drawing simple and complex structures 3.3) Using templates 3.4) Creating reports 3.5) Searching chemical information using Chemspider
4. Database Management using Microsoft Access 4.1) Database concepts 4.2) Common data types 4.3) Types of Objects 4.4) Types of relationship 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

Reading List	Reference Book Resources	• Sime, RJ, *Physical Chemistry Calculations with Excel*, Pearson Benjamin Cummings, • *Excel for Chemists* • Kumari, R. 2005, *Computers and their applications to chemistry*, 2 Ed., Alpha Science International, Oxford, UK • Barrante, James R. 2004, *Applied mathematics for Physical Chemistry*, Pearson Prentice Hall
Article/Paper List	This Course does not have any article/paper resources	
Other References	This Course does not have any other resources	