SKILL COURSE
ON
'COMPUTER APPLICATIONS IN CHEMISTRY'

Open for Third Year Graduate Student w.e.f. 2022-23

Approved by the Board of Studies in Chemistry
and
Finalized by the Academic Council

Devrukh Shikshan Prasarak Mandal's

Nya. Tatyasaheb Athalye Arts, Ved. S. R. Sapre Commerce, and Vid. Dadasaheb Pitre Science College (Autonomous), Devrukh. Tal.Sangmeshwar, Dist. Ratnagiri-415804, Maharashtra, India

Academic Council Item No: _____

Name of the Implementing Institute	:	Nya. Tatyasaheb Athalye Arts, Ved. S. R. Sapre Commerce, and Vid. Dadasaheb Pitre Science College (Autonomous), Devrukh. Tal. Sangmeshwar, Dist. Ratnagiri-415804,
Name of the Parent University	:	University of Mumbai
Name of the Programme	:	Bachelor of Science
Name of the Class to Which the course is Open	:	Third Year, Semester six
No. of Credits	:	03
Title of the Course	:	Computer Application in Chemistry
Course Code	:	UCHSK61
Passing Marks		40%
Nature of Course	:	Skill Course
Level	:	UG/ PG
Pattern	:	70:30
Status	:	Multidisciplinary- Open to all in the Third Year Science students
To be implemented from Academic Year	:	2022-2023

Syllabus for Skill Course on "Computer Application in Chemistry"

(With effect from the academic year 2022-2023)

Title of the Course: Computer Application in Chemistry

COURSE CODE: UCHSK61 **Credits - 03**

COURSE CONTENT			
Module No.	**Content**	**Theory Lectures**	**Practical**
1	**Introduction to Computer Fundamentals:** Introduction to Computer, Computer System Hardware Computer Memory, Input and Output Devices, Interaction between User and Computer, Introduction to Free and Open-Source Software's, Definition of Computer Virus, Types of Viruses, Use of Antivirus software. **Basics of Operating System:** Definition of Operating System, Objectives, types, and functions of Operating Systems, Working with Windows Operating System: Introduction, The Desktop, Structure of Windows, Windows Explorer, File and Folder Operations, The Search, The Recycle Bin, Configuring the Screen, Adding or Removing New Programs using Control Panel, Applications in windows (Paint, Notepad, WordPad, Calculator)	03	09
2	**Applications of Word, Excel PowerPoint:** MS-Word: Introduction to MS-Word, Working with MS-**Word:** Use of shapes, SmartArt, charts, links, Insertion of Header, Footer and Page numbers, Tables, Pictures, equations, symbols, Page setting, Text formatting, use of referencing tools. **MS-Excel:** Introduction, Starting MS-Excel, Basics of Spreadsheet, working with MS-Excel: Drawing different types of charts with excel, use of equations and mathematical calculations, data processing using excel sheet. **MS-PowerPoint:** Introduction, Basics of PowerPoint, Preparation of good PPT presentation using various tools like Slide design, drawing tools, animation tools, transitions to slides, add voice backgrounds to slides.	03	09

3	**Internet and Internet application:** Introduction, Internet evolution, Working of Internet, Use of Internet, Overview of World Wide Web (Web Server and Client), Introduction to Search engine (Google Scholar, ChemSpider, ChemIndustry, Chemicalbook, Wiki-databases, SciFinder, Scopus, etc.) and Searching the Web, Internet resources for Chemistry, downloading files, Introduction to Web Browsers, Working with E-mail (creation and use)	03	09
4	**Computer programs in chemistry:** Introduction to various drawing tools: Chemdraw and Chemsketch (Installation and handling) Computer-aided techniques used in drug design and discovery: Introduction to Molecular Docking, Introduction to PDB, free tools for docking (AutoDock, Dock, etc.) ADME prediction Tools: Bioclipse Programs for molecular visualization: Jmol, chimera	03	09
	Total	15	60

Practical Record: A journal comprising one exercise each needs to be submitted by the student at the end of the semester.

After completing the course, the learner will be able to…		
Course Learning Outcome No.	Blooms Taxonomy	Course Learning Outcome
CLO-01	Remember	Remember the fundamentals of computers
CLO-02	Understand	Understand the elements of MS Office, www
CLO-03	Apply	Apply the knowledge to create and design word document, excel sheet, ppt presentation
CLO-04	Analyze	Analyze the data with the help of computer programs
CLO-05	Evaluate	Evaluate the infographics provided through Maps
CLO-06	Create	Create 2D and 3D structures of chemical compounds

Required Previous Knowledge

No previous knowledge is necessary to start learning the course.

Detail Assessment Scheme

The assessment will be in the form of a Continuous Assessment.

A) Theory Component- 30 marks

a) Continuous Internal Assessment (CIA)- 10 marks
One 30 marks test shall be conducted for given semester and the marks obtained shall be converted to 10 marks. The duration for the test shall be of 1 hrs.

b) Semester End Assessment (SEA)- 20 marks
The semester End Examination of 50 marks and 2 hrs duration shall be conducted for each semester and the marks obtained shall be converted to 20 marks.

B) Practical Component- 70 marks

a) Continuous Internal Assessment (CIA)- 40 marks
1) Attendance- 10 marks
2) Journal/ workbook/assignment book- 20 marks
3) Viva- 10 marks

c) Semester End Assessment (SEA)- 30 marks
Semester End Examination comprises one practical/ project/presentation shall be conducted for each semester for 30 marks.

Eligibility for the Course: Candidates pass in TYBSc level with Biology/ Physics/ Chemistry/ Biochemistry/ Microbiology/ Agriculture
Grading Scale

References:-

1. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
2. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).

3. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
4. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).
5. Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).