INTER AMERICAN UNIVERSITY OF PUERTO RICO
_____ CAMPUS
_____DEPARTAMENT
CHEMISTRY PROGRAM

SYLLABUS

I. GENERAL INFORMATION

Course Title	**:**	Laboratory of Computer and its Application to Chemistry
Code and Number	**:**	CHEM 3400
Credits	**:**	2 credits
Academic Term	**:**	
Professor	**:**	
Office Hours	**:**	
Office Phone Number	**:**	
Email	**:**	

II. DESCRIPTION

Use and handling of the computer in the chemistry field aimed at solving problems and conducting experiments. Includes writing of technical reports and search, access, and management of scientific information and chemical compounds data. Requires 60 hours of presential closed lab. Requirement: CHEM 2221.

III. OBJECTIVES

1. **Use of computers to perform written works and presentations:** Provide basic knowledge in the field of computers and their relationship to chemistry.

   a. Use computer programs for the preparation of text, integrating figures, tables, and indexes.
   b. Develop skills to properly use computer programs to prepare presentations.

2. **Use of computers to perform mathematical calculations related to chemistry.** Use computer to do calculations, obtain results, and analyze problems related to the field of chemistry.

   a. Use of computer programs, such as Microsoft Excel, to perform complex mathematical calculations.
   b. Use of spreadsheets to solve chemistry problems.
   c. Use of computer programs to manipulate and graph data properly.

3. **Chemistry experiments using computers:** Integrate the effective use of modern computer-based technology to conduct experiments in chemistry.

   a. Know the basis of computer programs that integrate theory and experiments into the study of chemical systems.
   b. Know the basis of computer programs that allow to build, visualize models, calculate properties of chemical structures and/or verify established theories.
   c. Design simple chemistry experiments to re-evaluate chemical principles, using computer programs.

4. **Scientific information search:** Use of electronic access to obtain information from scientific literature.

    a. Perform information proper searches over the Internet, such as, physical constants, chemical characteristics, safety data sheet (SDS), and chemical problems, among others.
    b. Perform bibliographic searches of scientific literature on the Internet.
    c. Analyze the information searched to study the chemical behavior of molecules in different environments.
    d. Propose theories about the behavior of molecules based on information obtained either from the Internet or computer programs.

5. **Information analysis:** Develop scientific and critical thinking of the student.

    a. Analyze data obtained from computer programs.
    b. Collect, organize, and interpret experimental information obtained.
    c. Prepare reports that include results of a bibliographic search, results of experiments or calculations, and analysis of these.
    d. Summarize experimental works through an oral presentation.
    e. Use ethical conduct in data analysis.

6. **Chemistry Research:** Study chemistry problems using chemistry computer programs.

    a. Use of computer programs to determine constants and characteristics of chemical molecules.
    b. Compare results obtained with computer programs with those reported in the literature.
    c. Identify characteristics and behavior trends of related molecules and explain them based on what was studied in previous chemistry courses.
    d. Propose and test theories using physical and chemical properties determined using data from the Internet or computer programs.
    e. Develop steps of the scientific process using ethical and moral principles.

IV. CONTENT

1. INTRODUCTION TO THE USE OF COMPUTERS IN CHEMISTRY

2. INFORMATION ACCESS RESOURCES AVAILABLE IN THE LIBRARY.

3. USING WORD PROCESSING PROGRAM – MICROSOFT WORD

    3.1 Introduction to Microsoft Word
    3.2 Tables in Microsoft Word
    3.3 Tables and graphs in texts
    3.4 Using mathematical formula editors in Microsoft Word.

4. USING SPREADSHEET PROGRAM– MICROSOFT EXCEL

    4.1 Introduction: Basic elements of a spreadsheet.
    4.2 Graphs and tables in Excel
    4.3 Simple calculations with Excel
    4.4 Mathematical and statistical calculations
    4.5 Programming elements with Excel
    4.6 Complex functions and two or more variables
    4.7 Exponential equation to linear regression
    4.8 Titration curves in Excel.

5. SIMPLE PROGRAMMING

5.1 Basic elements of programming
5.2 Forms and simple programs
5.3 Graphics

6. USE AND APPLICATION OF MOLECULAR MODELING PROGRAM

6.1 Basic principles of molecular modeling.
6.2 Drawing and ways of representing molecules with computer programs.
6.3 Molecular modeling data in word processing and spreadsheets programs.

V. ACTIVITIES AND TEACHING STRATEGIES:

(a) Conferences
(b) PowerPoint presentations
(c) Whiteboard
(d) Problem Solving
(e) Practice exercises
(f) Use of computer programs like Excel, Word, Power Point
(g) Oral presentations
(h) Group work
(i) Laboratory experiences
(j) Group discussions

VI. EVALUATION (suggested)

Criteria	%
Asignaciones	50%
Informes	30%
Presentaciones	10%
Pruebas cortas (Quizes)	10%

Assignments and lab reports Will be delivered one week after each experiment is assigned or performed. Guides for lab notebook, lab reports, and research project written and oral presentations will be provided.

VII. EDUCATIONAL RESOURCES

1. Computer lab
2. Microsoft Office
3. Molecular modeling programs

VIII. BIBLIOGRAPHY

1. Richard Shepherd. ***Excel VBA Macro Programming***, 2007. McGraw – Hill
2. Gary B. Shelly, Thomas J. Cashman ***Visual Basic*** *6*, 1999. Thomson
3. Wong and J. Currie. Fujitsu ***Teaching with CAChe. Molecular Modeling in Chemistry***, 2002, CAChe Group.
4. Ebert, H. Ederer, T. L. Isenhour, ***Computer Applications in Chemistry***, VCH Publishers, New York, 1989.

Electronic Resources

1. *NIST Scientific and Technical Database*. www.nist.gov/srd (access February 20, 2021)
2. *Banco de datos de proteínas.* www.rcsb.org (access February 20, 2021)
3. *Portal del National Center for Biotechnology Information en el Instituto Nacional de Salud:* www.ncbi.nlm.nih.gov (access February 20, 2021)
4. ACD/ChemSketch for Academic and Personal Use. http://www.acdlabs.com/resources/freeware/chemsketch/ (access February 20, 2021)
5. Modelos http://www.chemeddl.org/resources/models360/models.php (access February 20, 2021)
6. UNCChem Glossary, http://www.shodor.org/unchem/glossary.html, (access February 20, 2021)
7. Explore Chemistry with ChemEd DL http://www.chemeddl.org/ (access February 20, 2021)
8. International Chemical Safety Cards (ICSC) en las páginas web de International Labour Organization http://www.ilo.org/dyn/icsc/showcard.listCards2 (access February 20, 2021)
9. Fichas Internacionales de Seguridad Química (FISQ) del Ministerio de Empleo y Seguridad www.insst.es/documentacion/colecciones-tecnicas/fisq (access February 20, 2021)

IX. SPECIAL NOTES

A. Auxiliary services or special needs. Any student who requires auxiliary services or special assistance must apply for them at the beginning of the course or as soon as he/she has knowledge that needs them, through the corresponding registration, at the Guidance Center with _____

B. Honesty, fraud, and plagiarism. Dishonesty, fraud, plagiarism, and any other inappropriate conduct in relation to academic work constitute major violations sanctioned by the General Student Guidelines. Major offences, as required by the General Student Guidelines, may result in the suspension from the university for a defined period of more than one year or the permanent expulsion from the university, among other sanctions.

C. Use of electronic devices. Cell phones and any other electronic device that could disrupt teaching and learning processes or alter the environment leading to academic excellence will be disabled. Critical situations will be addressed, as appropriate. The handling of electronic devices that allow access, storage or sending data during evaluations or exams is prohibited.

D. Compliance with the provisions of Title IX. The Federal Higher Education Act, as amended, prohibits discrimination on the grounds of sex in any academic, educational, extracurricular, athletic, or other program or employment, sponsored or controlled by a higher education institution regardless of whether it is conducted on or off the institution's premises, if the institution receives federal funds.

As provided by applicable federal regulations, our academic unit has appointed a Title IX Assistant Coordinator who will help and guidance in connection with any alleged incident constituting gender, sexual harassment, or sexual assault. You can contact the Auxiliary Coordinator _____ at extension _____, and email _____

The Normative Document entitled Standards and Procedures for Addressing Alleged Violations of the Provisions of Title IX is the document containing the institutional rules for channeling any complaint that is filed based on this type of claim. This document is available on the portal of the Inter-American University of Puerto Rico (www.inter.edu).

Revised in November 2018
Updated in February 2021