COURSE IMPLEMENTATION DATE:
COURSE REVISED IMPLEMENTATION DATE: September 2007
COURSE TO BE REVIEWED: March 2011
(Four years after UPAC final approval date) (MONTH YEAR)

OFFICIAL COURSE OUTLINE INFORMATION

Students are advised to keep course outlines in personal files for future use.
Shaded headings are subject to change at the discretion of the department and the material will vary - see course syllabus available from instructor

FACULTY/DEPARTMENT: **Faculty of Science, Health & Human Services/Chemistry**

CHEM 422		4
COURSE NAME/NUMBER	FORMER COURSE NUMBER	UCFV CREDITS

Conformations of Molecules and Introduction to Computer-Aided Drug Design
COURSE DESCRIPTIVE TITLE

CALENDAR DESCRIPTION:

This course covers modern computational techniques currently used in the conformational analysis of organic and biological molecules and includes an introduction to computer-aided drug design. This lecture course is accompanied by a computer lab where students will obtain practical experience in applying these techniques.

PREREQUISITES: CHEM 213, MATH 111, MATH 112, and one of PHYS 105 or PHYS 111 (CHEM 224 and MATH 211 are recommended)
COREQUISITES:

SYNONYMOUS COURSE(S)
(a) Replaces: **n/a** *(Course #)*
(b) Cannot take: **n/a** *(Course #)* for further credit.

SERVICE COURSE TO: *(Department/Program)* *(Department/Program)*

TOTAL HOURS PER TERM: **72**
STRUCTURE OF HOURS:

Lectures:	**39**	Hrs
Seminar:		Hrs
Laboratory:	33	Hrs
Field Experience:		Hrs
Student Directed Learning:		Hrs
Other (Specify):		Hrs

TRAINING DAY-BASED INSTRUCTION
LENGTH OF COURSE:
HOURS PER DAY:

MAXIMUM ENROLLMENT: **24**
EXPECTED FREQUENCY OF COURSE OFFERINGS: **Every other year**
WILL TRANSFER CREDIT BE REQUESTED? (lower-level courses only) ☐ Yes ☐ No
WILL TRANSFER CREDIT BE REQUESTED? (upper-level requested by department) ☐ Yes ☒ No
TRANSFER CREDIT EXISTS IN BCCAT TRANSFER GUIDE: ☐ Yes ☒ No

AUTHORIZATION SIGNATURES:

Course Designer(s): Noham Weinberg
Chairperson: Art Last *(Science Curriculum Committee)*
Department Head: Art Last
Dean: Wanda Gordon
UPAC Approval in Principle Date:
UPAC Final Approval Date: Mar. 30, 2007

LEARNING OBJECTIVES / GOALS / OUTCOMES / LEARNING OUTCOMES:

Upon successful completion of this course, students will:
- be familiar with molecular mechanics, molecular dynamics, and Monte Carlo techniques in their application to the conformational analysis, and
- will be able to perform molecular mechanics calculations.

METHODS:

Lectures, computer lab, problem solving.

PRIOR LEARNING ASSESSMENT RECOGNITION (PLAR):

Credit can be awarded for this course through PLAR (Please check:) ☒ Yes ☐ No

METHODS OF OBTAINING PLAR:

Examination

TEXTBOOKS, REFERENCES, MATERIALS:

[Textbook selection varies by instructor. An example of texts for this course might be:]

A. Leach, Molecular Modeling, 2nd ed., Pearson, Singapore, 2001

SUPPLIES / MATERIALS:

STUDENT EVALUATION:

[An example of student evaluation for this course might be:]

Assignments	10%
Midterms (2)	30%
Final	30%
Lab	30%

COURSE CONTENT:

[Course content varies by instructor. An example of course content might be:]

Introduction
Molecular geometry. Internal and Cartesian coordinates. Bond length. Bond angle. Torsion angle.

Conformational analysis of simple systems
Ethane, butane, ethylene, butene, cyclohexane.

Force fields
Stretching and bending energy. Harmonic approximation. Anharmonicity. Torsion energy. Rotation around single and double bond. Van-der-Waals interactions. Exp-6 and Lennard-Jones potentials. Parametrization.

Energy minimization
Potential energy surface. Stationary points: minima, maxima, saddle points. Minimization procedures.

Computer program packages
ECEPP, MM2/MM3, AMBER, CHARMm.

Conformations of large molecules
Multiple minima problem. Global minimum. Relative importance of conformations. Experimental sources of the molecular conformation data.

Molecular dynamics and Monte Carlo techniques
Introduction to techniques.

Proteins
Primary, secondary, tertiary, and quaternary structures. Protein conformations. Protein data base (PDB).

Introduction to computer-aided drug design
Basics of the molecular mechanism of drug action. Guest-host interactions. Specific and nonspecific interactions. Hydrophobic interactions. Docking. Rigid-molecules approximation. Conformational change upon complexation.

COMPUTER LABS

1. Introduction to UNIX environment.
2. Input files: internal and Cartesian coordinates.
3. Simple MM3 calculations.
4-5. Conformational analysis of medium-sized rings.
6-7. Effect of solvent on molecular conformations.
8. Comparative analysis of the potential functions in MM3 and AMBER.
9-10. Protein Data Base.
11-12. Docking.

SELECTED REFERENCES:

1. U. Burkert, N.L. Allinger, Molecular Mechanics, ACS, Washington, 1982.
2. Molecular Modelling and Drug Design, J.G. Vinter and M. Gardner, eds., CRC Press, Boca Raton, FL, 1994.
3. T. Clark, A Handbook of Computational Chemistry, Wiley, N.Y., 1985.
4. P. Comba, T.W. Hambley, Molecular Modeling of Inorganic Compounds, VCH, Weinheim, FRG, 1995.
5. K. Rasmussen, Potential Energy Functions in Conformational Analysis; Lectures Notes in Chemistry; Springer-Verlag: Berlin, Heidelberg, New York, 1985, Vol. 37.
6. J.M. Haile, Molecular Dynamics Simulations: Elementary Methods, Wiley, N.Y., 1992.
7. A.C. Norris, Computational Chemistry. An Introduction to Numerical Methods, Wiley, N.Y., 1981.
8. W.H. Press et al., Numerical Recipes. The Art of Scientific Computing, Cambridge University Press, Cambridge, 1989.
9. Prediction of Protein Structure and the Principles of Protein Conformation, G.D. Fasman, ed., Plenum Press, N.Y., 1989.
10. C. Branden, J. Tooze, Introduction to Protein Structure, Garland Publishing, N.Y., 1991.
11. Applications of NMR Spectroscopy to Problems in Stereochemistry and Conformational Analysis, Y. Takeuchi and A.P. Marchand, eds., VCH Publishers, Deerfield Beach, FL, 1986.