UNIVERSITY COLLEGE of the FRASER VALLEY

**PAC FORM #2**

COURSE IMPLEMENTATION DATE:[ **September 1997** ]
Revised: November 1999
COURSE TO BE REVIEWED DATE:[ **January 2003**
(Four years after implementation date)

# 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 material will vary - see course syllabus available from instructor

FACULTY/DEPARTMENT: **CHEMISTRY DEPARTMENT**

| **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. Lecture course is accompanied by a computer lab where students will obtain practical experience in applying these techniques.

**PREREQUISITES:** CHEM 211/212, MATH 111/112, and PHYS 105 or 111

**COREQUISITES:** None

**SYNONYMOUS COURSE(S)**

(a) Replaces: N/A
*(Course #)*

(b) Cannot take N/A for further credit
*(Course #)*

**SERVICE COURSE TO:**

*(Department / Program)*

*(Department / Program)*

**TOTAL HOURS PER TERM:** **78**

**STRUCTURE OF HOURS:**

| | | |
|---|---|---|
| Lectures: | 42 | hrs |
| Seminar: | | |
| Laboratory: | 36 | hrs |
| Field Experience: | | hrs |
| Student Directed Learning: | | hrs |
| Other (Specify): | | hrs |

**TRAINING DAY-BASED INSTRUCTION**

LENGTH OF COURSE:

HOURS PER DAY:

**MAXIMUM ENROLMENT:** **24**

**EXPECTED FREQUENCY OF COURSE OFFERING:**

**WILL TRANSFER CREDIT BE REQUESTED?** **YES** ____ **NO** **X**

**TRANSFER CREDIT EXISTS IN BCCAT TRANSFER GUIDE:** **YES** ____ **NO** **X**

**AUTHORIZATION SIGNATURES:**

Course designer(s): N. Weinberg

Chairperson: *(Curriculum Committee)*

Department Head: N. Weinberg

Dean: K. Wayne Welsh

PAC Approval in Principle Date:

PAC Final Approval Date: Nov. 24, 1999

**CHEM 422**

COURSE NAME / NUMBER

**LEARNING OBJECTIVES / GOALS / OUTCOMES/ LEARNING OUTCOMES:**

Students will become familiar with molecular mechanics, molecular dynamics and Monte Carlo techniques in their application to the conformational analysis, and will get practical experience with molecular mechanics calculations.

**METHODS:**

Lectures, computer lab, problem solving.

**PRIOR LEARNING ASSESSMENT RECOGNITION (PLAR):**

Credit can be awarded for this course through PLAR YES _____ NO ___X___

**METHODS OF OBTAINING PLAR:**

**TEXTBOOKS, REFERENCES, MATERIALS:**

N/A - Lecture notes and recommended reading.

**SUPPLIES / MATERIALS:**

**STUDENT EVALUATION:**

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

**COURSE CONTENT:**

**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.

**CHEM 422**

COURSE NAME / NUMBER

**COURSE CONTENT: (contd.)**

**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.
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.