CHEM 6344
Computer Assisted Drug Design, Fundamentals and Application

Class location:	TBD
Lectures, time and location:	TBD
Lab times and location:	TBD
Instructor:	Elfi Kraka, 231 FOSC, ext 8-2480, ekraka@smu.edu http://smu.edu/catco/
Office Hours:	By appointment
Units:	3
Grading:	ABC Letter Grade
Class number	

1. Rationale:

When a student enters pharmaceutical industry, sooner or later he/she will be involved in drug design. The student will realize that pharmaceutical industry is willing to do anything to cut down and simplify the long and very expensive process of drug design (more than 10 years and hundreds of million dollars costly). Drug development can be best accelerated by computer-assisted approaches. It is a constant (and actually justified) claim of pharmaceutical industry that not enough is done at the universities to prepare students for this work.

The course fills this gap and presents a thorough and in-depth going overview over methods and techniques in computer assisted drug design (CADD) where especially the needs of pharmaceutical industry are considered. Its contents includes topics such as famous examples of drug discovery and drug design, molecular recognition and docking, ligand-receptor interactions, pharmacophore searching, virtual screening, *de novo* design, molecular graphics, chemometrics, etc.

2. Course Recommendations:

The course is designed for all graduate students from chemistry, biochemistry, medicinal chemistry, biology, and engineering who want to obtain a thorough and in-depth overview over methods and techniques applied in computer assisted drug design (CADD). Basic chemical knowledge is required, however no special skills in pharmacy, mathematics or computer science. Since the course addresses a broad audience, it is designed as an interdisciplinary course taking care of the special needs of students with different background.

3. Texts:

a) Textbook: Molecular Modelling: Principles and Applications (Paperback), by Andrew R. Leach, Pearson Higher Education, USA, 2001 (ISBN 0582382106).
b) Handouts and notes for the computer labs

4. Course Aims and Objectives:

For a compound to become a drug many factors come into play beyond its fit to a receptor. From hundred thousands of substances tested every year, maybe 40-45 turn out to be a useful drug. Therefore, in order to keep the development costs for a drug at a reasonable level, pharmaceutical industry has to replace more and more costly experiments by modeling chemical properties, especially biological activities of a compound on the computer.
Molecular modeling (MM) has seen in the last years a rapid development which is far beyond its original goal to easily assess conformation and dynamics of larger molecules essentially provided by molecular mechanics and computer graphics. The same holds for computer assisted drug design (CADD). From its in infants in the late 70s it has become a powerful tool ranging now from graphical drug design (De novo design) to application of neural network and artificial intelligence. However, most of these developments have been done at pharmaceutical companies rather than at universities. Therefore, the course will bridge the gap how MM and CADD is performed by industry and used as a money making tool and how it is trained in academics.
The aim of this course is to present the appropriate tools for such a modeling ranging from molecular mechanics, molecular dynamics over computer graphics, data visualization, De Novo Design and chemometrics to computer assisted synthesis design based on artificial intelligence. Among various applications modeling of antigenic complexes, determination of recognition forces in pharmacological processes, computer assisted synthesis of pharmacophors and the design of new anticancer drugs will be discussed. The lectures will be accompanied by computer labs to complete the dedicated knowledge by practical experience

Specific Learning Objectives:
At the end of the course the student

will have an in-depth overview over the state-of-the art methods and techniques nowadays applied in CADD.

will be able to choose the appropriate method (in terms of applicability, accuracy, and economy) for a given problem like, lead optimization, structure based design, investigation of ligand receptor interaction.

will be able to perform, understand, and interpret the results of the calculations and bring them in a publication ready form.

At the end of the course each student will meet the expectations of pharmaceutical industry in this area.

5. Course Outline:

The course is divided into the following 14 chapters:

The lectures are complemented by a series of computer labs using the TRIPOS-SYBYL software, the state-of-the-art-modeling software used in pharmaceutical industry.

6. Student Responsibilities:

We are planning to have a quiz after every second chapter. Therefore, it is recommended that each student actively participate in the lectures. The student has to hand in a lab report for each computer lab along the lines described in the lab instructions. Each quiz and lab report will count toward the final grade. Questions regarding grades should be brought to the instructor's attention within one week after receiving back the exam.

7. Final Examination: TBD

8. Grading Procedures:

Final grades will be calculated according to the following scheme:
Final exam 40%
Quizzes 30%
Lab reports 30%

Grading Table	A	100 – 90 %
	B	89 – 80 %
	C	79 – 70 %
	D	69 - 60 %
	F	59% and below

9. Statement of Honor Code:
All SMU Dedman College students are bound by the honor code. The applicable section of the code reads: "All academic work undertaken at the University shall be subject to the guidelines of the Honor Code. Any giving or receiving of aid on academic work submitted for evaluation, without the express consent of the instructor, or the toleration of such action shall constitute a breach of the Honor Code." A violation of the Code can result in an F for the course and an Honor Code Violation recorded on a student's transcript. Academic dishonesty includes plagiarism, cheating, academic sabotage, facilitating academic dishonesty and fabrication. Plagiarism is prohibited in all papers, projects, take-home exams or any other assignments in which the student submits another's work as being his or her own. Cheating is defined as intentionally using or attempting to use unauthorized materials, information or study aids in any academic exercise. Academic sabotage is defined as intentionally taking any action, which negatively affects the academic work of another student. Facilitating academic dishonesty is defined as intentionally or knowingly helping or attempting to help another to violate any provision of the Honor Code. Fabrication is defined as intentional and unauthorized falsification or invention of any information or citation in an academic exercise.

10. Disability Accommodations:
Students needing academic accommodations for a disability must first contact Ms. Rebecca Marin, Director, Services for Students with Disabilities (214-768-4557) to verify the disability and establish eligibility for accommodations. They should then schedule an appointment with the professor to make appropriate arrangements.

11. Religious Observance:
Religiously observant students wishing to be absent on holidays that require missing class should notify their professors in writing at the beginning of the semester, and should discuss with them, in advance, acceptable ways of making up any work missed because of the absence.

12. Excused Absences for University Extracurricular Activities:
Students participating in an officially sanctioned, scheduled University extracurricular activity should be given the opportunity to make up class assignments or other graded assignments missed as a result of their participation. It is the responsibility of the student to make arrangements with the instructor prior to any missed scheduled examination or other missed assignment for making up the work.

13. Assessment:
In accordance with University regulations copies of student work may be retained to asses how the learning objectives of the course are being met.

14. Course Schedule:
Will be discussed in the first meeting worked out to accommodate best to the student needs.