

Macintosh computers will be used. However, the skills learned and all the software used is available and readily transferable to the Windows platform.

D. PREDICTION OF PHYSICAL AND CHEMICAL PROPERTIES BY COMPUTATIONAL CHEMISTRY

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This workshop will be a hands-on session aimed at demonstrating and testing computational chemistry methods for the prediction of molecular properties. A survey of various force field, semiempirical molecular orbital, and ab initio molecular orbital methods will be made with consideration of their capabilities of predicting specific properties. Case studies will be carried out to evaluate properties such as: molecular geometry, conformational analysis, vibrational spectroscopy, UV-vis spectroscopy, dipole moments, and chemical reactivity. Time will be allotted for free-format labs when workshop attendees focus on problems of their own specific interest. Problems both of educational and research interest are encouraged. Extrapolation from molecular to macromolecular properties will be briefly considered, but generally will be outside the scope of this workshop.

Because of the applied nature of this workshop, some previous experience with computational modeling techniques will be expected. A brief overview of the methods used in the workshop will be given to orient workshop attendees sufficiently to proceed with the specific exercises given.



Pharmaceuticals, Their Discovery, Regulation and Manufacture OLCC-3

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This is an invitation to register your school for the On-Line Chemistry Course for Upper Division Chemistry Students (Prerequisite - one year of organic chemistry) to be held during the Fall term of 1998. The on-line activities will be scheduled for September 14 to November 25, 1998. The title of the course will be "Pharmaceuticals, Their Discovery, Regulation and Manufacture." The course is sponsored by the American Chemical Society, Division of Chemical Education's Committee on Computers in Chemical Education (CCCE). In this course, the Internet will be used for discussions among students (student Listserv and WebBoard), faculty (faculty Listserv and WebBoard) and experts, all from around the world.

TOPICS MAY INCLUDE BUT ARE NOT NECESSARILY LIMITED TO:

1. Drug discovery including computer-aided design, combinatorial chemistry and other, earlier strategies
2. Development of clinically useable drugs including optimization of novel lead structures and assessment of pharmacodynamics, safety and efficacy of promising drug candidates
3. "Case studies" of the development and use of certain classes of widely used drugs including analgesics, antidepressants, anti-inflammatory drugs, antibiotics, AIDS and anti-cancer compounds
4. The FDA approval and FDA regulated testing process

PROCESS AND CONTENT RELATED GOALS OF THE PHARMACEUTICALS COURSE:

1. To provide an opportunity for students to investigate frequently used processes for discovery and manufacture of pharmaceuticals used as drugs for man and other animals
2. To provide the opportunity for students to gain an understanding of the general procedures for drug testing, its limitations, analysis, use and regulation
3. To provide an electronic forum which permits students to interact with professionals who are involved with the processes in 1 and 2
4. To provide an environment in which students will

interact locally and at a distance to do brain-storming, data-gathering, data analysis and problem-solving

tor, Dr. James Beard, e-mail: jbeard@catawba.edu to obtain the form.

5. To provide a forum for discovery of and discussion of industry's interaction with its regulatory, client and physical environment including such items as government inspections, user complaints and hazardous waste handling)

RESPONSIBILITIES OF PARTICIPANTS:

Students will participate in collaborative learning assignments where they can practice division of labor, teamwork, and individual responsibility. The Listservs and WebBoards will be used for the discussion of concepts and processes.



Instructors at local sites will guide "traditional" literature searches as well as on-line data-gathering. On-line, students will be guided by faculty and each other in their exploration of the content of this course. On-line questions from faculty will sometimes require critical thinking about industrial procedures in terms of a personal values framework.

It is the responsibility of each participating institution to register students and to provide college credit for the course. The role of the OLCC organizing committee and the CCCE is limited to assistance in organizing and administering electronic aspects of the course. The American Chemical Society will neither provide credit nor assess any fees. It is suggested that students receive three semester hours of credit for the course. It is the responsibility of each local faculty member to assign grades to their students. It is anticipated that a national evaluation will be administered.

SWITCHING STUDENTS ON TO SCIENCE An On-Line Conference in September and October 1998

For further information about previous on-line courses like this, see the Web Pages for OLCC-1 at <http://www.py.iup.edu/college/chemistry/chem-course/webpage.html> and additional information and evaluations of OLCC-1 at <http://www.clarkson.edu/~rosen2/olcc.html>.

Further information can also be obtained by contacting the course coordinator:

Dr. Lindy Harrison
Department of Chemistry
York College of Pennsylvania
York, PA 17405-7199
717-846-7788 X1210
aharriso@eagle.ycp.edu

In the fall of 1998 a CHEMCONF on-line conference will take place on the topic "Switching Students on to Science". The session has been organized and will be chaired by:

Dr. Hugh Cartwright
Physical and Theoretical Chemistry Laboratory
Oxford University, England
(Hugh.Cartwright@chemistry.oxford.ac.uk - <http://physchem.ox.ac.uk/~hmc>).

The focus of the conference will be: "How do we develop and maintain interest in science among students?"

Those interested in participating in this OLCC-3 course during the Fall of 1998 should complete a pre-registration form. Contact the OLCC-3 registration coordina-

It is a common observation that science is one of the most popular subjects with young school children.