identification number, first choice of due date, and second choice of due date. This information is sent to a CGI-script (written in the Perl scripting language) that checks to see if the maximum number of registrants for the first due date choice has been reached. If the maximum enrollment has not been reached, the student is given their first due date choice. Otherwise the script checks their second choice. If their second choice already has maximum enrollment, the student is unfortunately given their least preferred due date. This possibility does provide some incentive for registering early. The web-based form and the CGI-script will be provided via email to anyone interested in them.

Group Projects in Large Classrooms: Online Group Discussion Pages

One common student gripe about group projects is their inability to find common meeting times. The use of computer-based discussion pages can assist students to hold asynchronous meetings and discussions. Several mechanisms exist for implementing online discussions among groups of students. Electronic mail can be used, either through the use of group mailing lists or listservs. A newsgroup-like system would also provide a discussion mechanism, with the added benefit of maintaining an archive of postings. I have utilized the group functionality designed into the *LectureOnline* course development and delivery system developed at Michigan State University by Gerd Kortemeyer (kortemeyer@nscl.msu.edu). This system allows course instructors to design web-based courses or course supplements, to develop semi-individualized homework assignments, and (most important to this topic) to organize students into groups. Each group can access group pages for any group to which they are assigned and post notes to other members of their group. Instructors can access the group pages for all groups. Instructor access to project discussions can assist in the evaluation of contributions by various group members. This provides instructors a good mechanism for dealing with another common student concern, distribution of work in group projects.

The two examples in this article should demonstrate that computer use in instruction need not be limited to educational tools for students. Computers also provide capabilities to facilitate classroom activities and assessment.

A Sunscreen Experiment Using the World Wide Web and Molecular Modeling

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Recently Dick Cornelius and coworkers[1] published an experiment in which students measure the UV spectra of commercial sunscreens and use molecular modeling to predict the electronic spectra of compounds used in sunscreens. We have incorporated Cornelius's experiment into a longer discovery-based laboratory project that introduces students to organic chemistry and spectroscopy, molecular modeling, and search engines available on the World Wide Web. One of the aims of this project is to give students experience with the computational and information-gathering tools that are now available with powerful desktop computers and modern networks. At the same time, we want them to realize that the results of computations or Web searches should not be blindly accepted just because they appear on the computer screen. Some sort of evaluation always is necessary.

The four-week long project begins by introducing the students to organic compounds and functional groups in a short lecture at the beginning of the first laboratory period. After the introduction, groups of three or four students are given infrared spectra of several simple organic compounds and discover the IR peaks that are characteristic of different functional groups. They also measure the visible-UV spectra of six organic compounds and discover the characteristics of the structures of compounds that absorb visible and ultraviolet radiation. In the last part of this experiment they use this information to help them identify compounds. They record the IR spectrum of an unknown and choose the most likely structure for the unknown from a list which we supply. They also match structures of three compounds, one of which is aromatic and one of which is conjugated, with their real-world applications as components of sunscreens, lipstick, and perfume (the latter by default when the other two have been identified).

In the second week of the project, the groups measure the UV spectra of commercial sunscreens with different SPF values, which we use to construct a standard curve so that the SPF of an unknown sunscreen can be estimated[1]. The groups then design a new compound that they expect to be a good sunscreen. As they work on their new compound we ask them to think about the structures of known sunscreens, the general rules they have learned for constructing organic structures, and the relationship between polarity and water solubility.

One of the objectives of this project is to have students write individual formal reports based on their own experiments and on information accumulated by the class as a whole. This information is shared by posting it on a Sunscreen and Ultraviolet Radiation Web site that I maintain (http://www.wofford.edu/~whisnantdm/sun_uv98.htm). At the end of the second week's laboratory, the groups turn in their experimental spectra and the structures of their proposed sunscreens, which I incorporate into pages on the project Web site. During the third week, in lieu of their regularly scheduled laboratory, individual students search the Web for information on sunscreens, ultraviolet radiation, stratospheric ozone depletion, and related topics. Most students have had experience with the WWW, but few have used search engines with a Boolean search structure. To help students who haven't had experience with advanced searches, we distribute a handout describing how to use HotBot and Alta Vista. Because Web sites are not peer-reviewed, the quality of information on the Web is variable, to say the least. This handout also suggests strategies that students can use to help evaluate information from the Web for credibility and reliability[2] http://www.sccu.edu/faculty/R_Harris/evalu8it.htm. Each student is asked to turn in the titles and URLs of three good web sites by the end of the week. After testing, links to these URLs are posted to the project Web site.

During the final week of the project, the students use Quantum CAChe, running on 266 MHz Pentium II computers, to model their compound. They optimize the structures of their proposed sunscreens using molecular mechanics and then predict the electronic spectra using ZINDO. Each group copies their predicted spectrum to a paint program and then saves it as a .jpg file suitable for posting on the WWW. I add the spectra to the project Web pages that already contain names of the students in the groups and the structures of their proposed sunscreen. I also post ZINDO spectra from CAChe calculations for four common components of sunscreens along with wavelengths of peaks from experimental spectra [1]. These can be compared to give the students an idea of the reliability of the ZINDO predictions.

At the end of the project the students write formal laboratory reports. To put the experiments in a larger context, the students are asked to include a discussion of ultraviolet radiation, health effects, the ozone layer, and classes of sunscreen in their introduction. Other then some leading questions in the project handout, we give the class no written information on these topics. The URLs found by the class and linked to the project Web page furnish more than enough information to write this introduction. In their report the students also discuss their experimental work, the expected quality of the CAChe UV spectrum predictions, how good a sunscreen their proposed compound would appear to be based on the molecular modeling results, and which of the compounds proposed by the class they would expect to be the best sunscreen.

[1]C. Walters, A. Keeney, C. T. Wigal, C. R. Johnson, and R. D. Cornelius, *J. Chem. Educ.* **1997**, *74*, 99.
[2]Harris, R. (1997). *Evaluating Internet Research Sources*, [Online]. Available:

Integrating Computational Chemistry and Molecular Modeling into the Undergraduate Chemistry Curriculum.

A Symposium Report

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At the spring, 1998 meeting of the American Chemical Society in Dallas, Texas, the Committee on Computers in Chemical Education sponsored a symposium entitled, "Integrating Computational Chemistry and Molecular Modeling into the Undergraduate Chemistry Curriculum." The following description is intended to briefly review that symposium(with apologies to the various presenters for compressing their papers so much).

Molecular modeling and computational chemistry have become standard tools for many industrial and synthetic chemists. The decrease in the price of computer hardware and software has made it increasingly possible to include this type of material in the undergraduate program, but it is not yet clear how this material can best be integrated into an already crowded curriculum. Thus, it was not surprising that