

## ACS Teaching with Technology Fellowship Proposal

**Title:** Interactive Web-Based Medicinal Chemistry Exercises

**Applicant:** Erland Stevens, Associate Professor of Chemistry, Davidson College

### 1. Background

In response to student interests, chemistry departments are now offering more upper-level courses in new sub-specialties including environmental chemistry, forensics, and medicinal chemistry. Quality teaching resources for these subjects are scarce, and appropriate textbook options are very limited. The lack of materials is a significant barrier to teaching specialty courses. This problem is especially acute for most small college faculty members, whose training typically lies in traditional areas of chemistry. Teaching a sub-specialty requires considerable learning on the part of the faculty member.

I teach medicinal chemistry to junior- and senior-level chemistry majors and minors, and the course is offered approximately every other year. As the course has evolved, an obvious short-coming recognized by both the students and myself is an unavailability of exercises for the students to perform outside of class. While traditional, written homework sets are useful in medicinal chemistry, much of the course material is strongly dependent upon mathematical relationships that are best represented graphically. This fact makes interactive graphical web pages a very promising means of reinforcing lectures and generating homework assignments.

Interactive web pages have been extensively utilized in the physics department at Davidson College by Drs. Wolfgang Christian and Mario Belloni. In preparing their online materials, Christian and Belloni have generated a number of Java applets that are well-documented, readily available, and easily adapted to non-physics applications.

To date, eight medicinal chemistry exercises have been written using the Java tools of Christian and Belloni. Five of the eight were prepared under the support of an ACS Teaching with Technology Fellowship in the summer of 2005. All examples are characterized by some type of interactive interface through which a student can manipulate graphing parameters and observe the resulting changes. The graphical section of the page is followed by questions that require a student to compare specific data sets and interpret their significance. All examples can be viewed through the link below.

[http://www.chm.davidson.edu/erstevens/stevens\\_crs.html](http://www.chm.davidson.edu/erstevens/stevens_crs.html)

Topics that seem most amenable to online exercises are broken down into the three categories shown in the table below. Specific exercise examples are listed in each column with completed exercises being italicized. All three categories may be incorporated into an interactive web page using the DataGraph and DataTable applets already developed by Christian and Belloni.

<b>plasma conc. (<math>C_p</math>) vs time</b>	<b>response vs drug conc.</b>	<b>QSAR</b>
$C_p$ vs time (iv bolus)	dose-response (with inhibitors)	single parameter QSAR
$\ln C_p$ vs time (iv bolus)	log(dose)-response (with inhibitors)	mult-parameter QSAR
$C_p$ vs time (iv infusion)	<i>Michaelis-Menten (with inhibitors)</i>	
$C_p$ vs time (infusion with loading dose)	<i>Lineweaver-Burk (with inhibitors)</i>	
$C_p$ vs time (oral dose)	Scatchard plots	
$C_p$ vs time (multiple oral doses)	occupancy theory (intrinsic activity)	
bioavailability (iv vs oral)		
metabolite $C_p$ vs time		
clearance and half-life		
volume of distribution		
multiple exponential distribution		

## 2. Description

During the spring of 2006 I propose to write at least five additional web-based exercises. The exercises will be taken from those in the table above with likely two from the first column, two from the second, and one from the third. As they are written, the exercises will be accessible through my faculty web page on the Davidson College chemistry department site (see link above).

## 3. Timeline

January-May 2006	Write approximately five exercises
Fall 2006 or Spring 2007	Assess the exercises, primarily by student evaluation, during next offering of medicinal chemistry

## 4. Technology

At a minimum the work in this proposal requires server space for the completed exercises and supporting applets and a computer for writing the HTML and JavaScript code. Server space available in the chemistry department will be sufficient. Additionally, computers running a variety of operating systems and using a selection of web browsers are available both within the chemistry department and on the campus of Davidson College. These computers will be used to test platform compatibility of the exercises.

## 5. Other Support

Not applicable.

## **6. Learning Outcomes**

The proposed web-based exercises will enhance student learning by providing a user-friendly, graphical means of demonstrating medicinal and biochemical concepts. Students will be able to modify parameters and drug conditions and immediately see the effects of the changes. This will complement traditional lecture and textbook learning.

I am also currently in writing a text on medicinal chemistry, and the first chapter and table of contents are under review by a publisher. Computer exercises similar to those developed with this fellowship will hopefully being included with the text as ancillary materials. The text will require stand-alone applications, not web-based exercises, but much of the programming involved for the textbook will overlap with the work discussed in this fellowship application.

## **7. Curriculum**

The proposed exercises will be used as homework assignments. Students will be expected to complete the exercises and turn in written answers which will be graded and returned.

## **8. Assessment**

Evaluation of the web-based exercises will be performed primarily through questionnaires distributed to the students in medicinal chemistry. This class is currently being taught in the fall of 2005. Feedback on the QSAR applet, the first to be used in the class, is currently being solicited. I will hopefully teach medicinal chemistry again during either the fall semester of 2006 or spring 2007. Feedback will also be solicited from anyone viewing the pages through feedback links on the pages of the exercises themselves.

## **9. Collaboration and Dissemination**

Medicinal chemistry is actively taught at at least three other ACS institutions, Washington and Lee, Richmond, and Southwestern, and Spelman teaches a course on toxicology. Also, while they do not teach at ACS institutions, Drs. Phil Bowen (UNC-Greensboro), Anne Glenn (Guilford), and Gene Gooch (Elon) all teach medicinal chemistry at their respective schools in North Carolina. The applets have been made available to these faculty members for use in their respective course.