

# ACS Teaching with Technology Fellowship Proposal

Interactive Web-Based Medicinal Chemistry Exercises

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## 1. Background

In response to student interests, chemistry departments have started to offer more upper-level courses in relatively new sub-specialties such as environmental chemistry, forensics, and medicinal chemistry. Unfortunately, teaching materials for these new courses are generally not available, and appropriate textbook options are very limited. A lack of resources suitable for advanced undergraduates is a significant barrier to teaching speciality courses.

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 usage. To date, three working examples of medicinal chemistry exercises have been prepared using the Java tools of Christian and Belloni. 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. The three prototype examples are fully functional except they do not have proper error checking in the input fields. The three working exercises 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)

With regard to medicinal chemistry, the types of problems that seem most amenable to online exercises fall under three categories. First are the concepts that relate the plasma concentration of a drug relative to time. The three preliminary exercises that have already been developed fall under this category. Second are receptor theory problems that plot response percentage against drug concentration. Michaelis-Menten and Lineweaver-Burk enzyme activity plots may also be placed under this second classification. The final group comprises quantitative structure-activity relationships (QSAR) in which a molecular property, such as electron density or size, is correlated with the activity of a drug. All three categories may be incorporated into an interactive web

page using the DataGraph and DataTable applets already developed by Christian and Belloni. Examples of possible exercises are shown in the table below.

<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)	$\log(\text{dose})$ -response (with inhibitors)	
$C_p$ vs time (iv infusion)	Michaelis-Menten (with inhibitors)	
$C_p$ vs time (infusion with loading dose)	Lineweaver-Burk (with inhibitors)	
$C_p$ 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 summer of 2005 I propose to write approximately 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.

## 3. Timeline

June-August 2005	Write approximately five exercises
Fall 2005 or Spring 2006	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.

## **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 will next be taught during either the fall semester of 2005 or spring 2006. Feedback will also be solicited from other ACS faculty and through feedback links on the pages of the exercises themselves.

## **9. Collaboration and Dissemination**

Medicinal chemistry is actively taught at least three other ACS institutions, Washington and Lee, Richmond, and Southwestern, and Spelman teaches a course on toxicology. The relevant faculty at these institutions will be notified of the online exercises. 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 and will be included in the notification. Finally, the exercises will be openly posted on my web page at Davidson and will be available to any interested person with internet access.