Report for 2005 ACS Teaching with Technology Fellowship
Title: Interactive Web-Based Medicinal Chemistry Exercises
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Background

The developed medicinal chemistry exercises provide a means for students to learn pharmacokinetic and pharmacodynamic principles in a convenient fashion. Pharmacokinetics and pharmacodynamics consist of ideas and relationships that are best illustrated through graphical relationships. Unfortunately, dynamic interaction with graphical information is difficult or impossible with textbooks alone. The medicinal chemistry exercises allow a student to immediately see the graphical effect of changing an equation parameter. In most cases, multiple examples may be viewed at once for side-by-side comparisons. While the ideas presented in the exercises are often not overly challenging, they are frequently not intuitive. The medicinal chemistry exercises will hopefully make the underlying ideas of the field more accessible.

Pedagogy

While the exercises are intended to demonstrate selected concepts in medicinal chemistry, they are not suitable as a stand-alone tutorial. The brief introductory text for each exercise is only meant to reinforce ideas that have already been more thoroughly covered in the corresponding lecture and textbook.

In theory, the use of related exercises could be employed to emphasize any graphical concept for which the relationships can be expressed mathematically. Beyond the science applications, field that might benefit from similar exercises may include economics and accounting. Additional treatments are likely obvious to those more closely associated with other fields.

Technical Information

Development of the medicinal chemistry exercises was partially funded with an Associated Colleges of the South-Mellon Technology Fellowship. The exercises themselves utilize Java applets, called Physlets, that have been written by Professors Wolfgang Christian and Mario Belloni of the Davidson College Physics Department. The Physlets primarily provide the graphical output in the exercises. Interaction between each exercise web page and the Java Physlet is accomplished with scripts written in JavaScript. Specific information on implementing Physlets in web pages with JavaScript may be found in *Physlets: Teaching Physics with Interactive Curricular Material* by Christian and Belloni (Prentice-Hall, 2001). The full HTML and JavaScript source code for all exercises is available by selecting “View Source” from the “View” browser menu.

Assessment Methods

The effectiveness of the exercises will be evaluated based on feedback from students currently (Fall 2005) enrolled in Medicinal Chemistry (CHE 309) at Davidson College. All four areas - introduction, applet, problem information, and problems - of each exercise will be addressed with space for a numerical score and general comments. Feedback will be posted to this report as it is completed. The first exercise that will be addressed in class will be QSAR. The concentration-time cases will follow with the dose-response examples being covered last. All feedback information will be included on the website of the exercises:

http://www.chm.davidson.edu/erstevens/stevens_med.html

Future Work

The 2005 ACS Teaching with Technology Fellowship proposal described five new exercises that would be written. These exercises have been completed and are available on the website listed above. Future exercises will likely cover metabolite formation, IV infusion with a loading dose, multiple exponential distribution, dose-response plots with various types of inhibitors, Scatchard plots, and QSAR with multiple independent variables. Other ideas may be considered if they may be implemented effectively and lend themselves to the web medium.