Capstone Project Progress Report
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BioFitWeb: A Comprehensive On-Line Resource for Enzyme Kinetics Researchers

a progress report

1. Completed Work

The BioFitWeb site is currently available at http://156.56.92.83/BioFitWeb.htm. Presently the site consists of more than a dozen pages and cgi scripts. Three of the proposed tools have been implemented – this involves the ability to upload data, parse and store it, process the data, and return results. Much of the supporting material for these tools is in place as well, including background, technical documentation, and some references.

The working tools calculate several parameters from time-course enzyme reaction data, including initial reaction velocity, maximum reaction velocity, initial substrate concentration, and the Michaelis-Menten constant for the enzyme, along with the standard errors for each parameter and the chi-square error for the fitting. Supporting materials include a derivation for the Michaelis-Menten equation, and a discussion of the quasi-steady-state assumption along with the conditions under which its use is justified. Each tool page also includes extensive background material on the methods used by the tool, and recommendations for the best methodologies to be used in collecting data to be analyzed by the tool. Links to several relevant references are also included.

2. Current Activities

BioFitWeb is undergoing some structural redesign at this time to make the web interface easier and more flexible to use. I am reviewing a set of related software applications to determine features and usability requirements that BioFitWeb may need to include or change. The site will be getting a cosmetic make-over during the semester break, as well.

The tool for reaction pathway prediction is still under development at this time.

The data storage and retrieval system is being re-implemented using SQL instead of flat files. This should improve cross-tool flexibility as well as allowing for multi-session use and voluntary archiving of results for review by other users.

3. Future Work

Several tools remain to be implemented. The reaction pathway prediction tool should become available next, followed by a suite of diagnostic/graphics tools that will aid the user in

selecting the best model for their situation. Emphasis will be placed on producing a few mature, useable tools rather than a wide selection of poorly-implemented ones.

Much more background, technical, and reference material will be added to the site as new tools are brought on-line.

A bibliography management system will also be implemented at some point, based either on SQL or LaTeX technology.