The Biomaterials Store

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Statement of Purpose: The Biomaterials Store is an integrated, user-based, password-protected environment for computational modeling of new polymeric biomaterials for biomedical research. It will be a unique resource for the biomaterials research community by providing the capability to model bioresponse to polymeric biomaterials without the need to know the technical intricacies of computational modeling.

Methods: The Biomaterials Store is a Graphical User Interface (GUI) written in Java Swing. Access is username and password protected. An authenticated user will be able to draw a polymer of his choice and then model the descriptors using Molecular Operating Environment (MOE™). After the polymers and the molecular descriptors are generated and a database of experimental bioresponse data is uploaded (as required), the modeling of the bioresponse is performed using the Artificial Neural Network and the Decision Tree. The Decision tree is used for the pre-screening of descriptor data before the modeling is done by the ANN. Modeling can also be done without using the Decision Tree for preselection of the descriptor data. The Artificial Neural Network (ANN) is written in the C programming language and models the bioresponse to the biomaterials using the information contributed by collaborators. The current experimental dataset includes, for example, protein adsorption, gene expression of pro- and anti-inflammatory cytokines of macrophages in contact with specific polymeric substrata and cell attachment, growth, migration, and differentiation for a library of tyrosine-derived polyarylates synthesized at the NJ Center for Biomaterials. All data is stored in a MySQL database (including all structural and biological response data). The current database contains nearly 850 molecular descriptors computed for each of the 112 members of the polyarylate library, as well as other details concerning the structure of each monomer.

Results / Discussion: Version 1.0 of The Biomaterials Store integrates the Artificial Neural Network and the Decision Tree in a Graphical User Interface to create models for fibrinogen and fibronectin adsorption, and cellular proliferation for the polyarylate library. A screen shot of the interface banner is shown in Fig. 1.

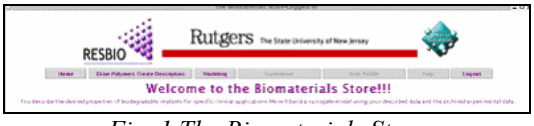

Fig. 1 The Biomaterials Store

A graph of experimental fibrinogen adsorption *vs* predicted fibrinogen adsorption is shown in Fig. 2.

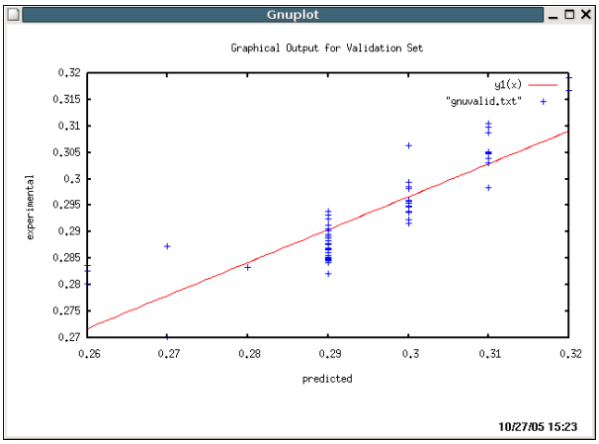

Fig. 2 Prediction vs. Experiment of fibrinogen adsorption

Conclusions: Version 1.0 of The Biomaterials Store has been completed and has successfully modeled the adsorption of fibrinogen and fibronectin to polymers in the polyarylate library. Future plans include integration of Polynomial Neural Networks into the Biomaterials Store for modeling the bioresponse of biomaterials and expansion of the experimental database to other polymer libraries. This work was supported by seed funds provided by Rutgers University, by NIH grant R01 EB00286, and by RESBIO-The National Resource for Polymeric Biomaterials funded under NIH grant P41 EB001046-01A1. Financial support was also provided by NIH Grant HL-60416 and the New Jersey Center for Biomaterials.

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