



The University of Western Ontario

Faculty of Science

Department of Applied Mathematics

APPLIED MATHEMATICS COLLOQUIUM

Date: Wednesday, February 6, 2008

Time: 2:30 pm

Location: Middlesex College Room 204

In Silico Drug Delivery

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Abstract:

The central activities of pharmaceutical research are drug design and delivery. Drug design is the design or discovery of molecular structures which fit certain receptor sites in the protein. The role of computational modelling in drug design is highly developed, dominated by a mature methodology involving techniques such as Quantitative Structure Activity Relationships (QSAR), Ligand Docking, and Molecular Dynamics. Once a drug candidate molecule has been found it must be delivered into the cell where it can interact with the receptor site of the desired protein. Drug delivery is a very wide field involving all aspects of metabolism, including absorption into the body, metabolism, delivery to the target area of the body and transfection through the cell membrane of the target cells. Computational modelling, particularly methods based on the development of structural or mechanistic understanding is not as highly developed a field for drug delivery as it is for drug discovery.

The talk will overview current work in my group relating to computational research relating to drug delivery including the development of nanotechnological drug delivery devices, gene therapy, and the activity of efflux proteins.