



The McGill-Montreal Chapter

Sigma Xi :: The Scientific Research Society ::





Dr. Chris Williams

PhD. McGill (1996)

Principal Scientist, Chemical Computing Group

PUBLIC LECTURE

when:

Monday **11 December** 2006 **6:00** P.M.

where:

McGill University
Otto Maass Chemistry
room 10

RECEPTION

all welcome 7:00 P.M.

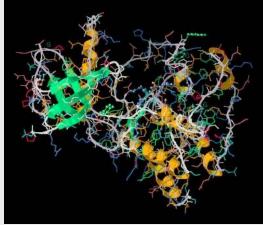


Molecular Modeling and Computer-Aided Drug Design:

An overview of methods with application to tyrosine kinase inhibitors

The use of computers to aid the drug design process has become increasingly widespread over the past decades. These computational methods, often referred to as 'in silico' approaches, are attractive to pharmaceutical and biotechnology companies because they are generally less expensive than experiments and can often access quantities inaccessible by other means. Furthermore, the sheer volume of data generated in the drug development industry, potentially millions of molecules and hundreds of millions of data points, necessitates the use of computers as data storage and data manipulation devices. As a result, there now exists, within pharmaceutical and biotechnology companies, established computational chemistry/molecular modeling groups that employ a range of computational techniques in their drug optimization efforts. This talk will overview some of the major areas of computer aided drug design. Practical examples of computer aided drug design taken from the speakers current research projects will also be presented.

Chris Williams graduated from McGill in 1996 from the Chemistry Department. He quickly got a foot in industry by doing consulting work in computational chemistry for the firm he currently works for: Chemical Computing Group.







JOIN US FOR THE RECEPTION AFTER THE LECTURE come enjoy the food and have a good time TIME: 7:00 P.M.