The Institute For Biomolecular Design

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Computers are playing an increasingly important role in nearly every aspect of drug discovery and development. Indeed, they have helped design and discover new treatments for many diseases including AIDS, cancer, high blood pressure, obesity and arthritis. Because of their importance many larger pharmaceutical companies are hiring dozens, if not hundreds of computer specialists every year to develop better software to visualize complex drug molecules, to perform computer-aided drug design, or to mine vast databases of biological and chemical information. Computer aided drug design has grown so fast that there is now a critical shortage of skilled individuals to perform these tasks. In response to this shortage, the University of Alberta, in cooperation with the provincial and federal governments, is putting together the Institute for Bimolecular Design (IBD).

This $25 million on-campus institute will house state-of-the-art computer and graphics facilities to start training the next generation of computational chemists and biologists. Current plans call for nearly $2 million dollars of high-end computing equipment to be purchased for this facility. This equipment will include specialized graphics terminals (SGI's and other UNIX machines) for molecular modeling and visualization, numerous multiprocessor machines (for local number crunching), high-capacity storage devices (to store 100's of gigabytes of biological, chemical and sequence data), a large screen projection device for virtual reality (i.e. molecular docking) simulations and a high-speed fibre optic link to Aurora (the University of Alberta's new *"supercomputer"*).

The IBD will also be purchasing a quarter million dollars worth of hardware upgrades for Aurora and will likely become a major user of this machine. Indeed, many simulations in computational biology are often measured in terms of central processing unit days or central processing unit weeks -- even on very fast processors. This is why access to a super computer such as Aurora will be key to the IBD's long-term success.

While many of the IBD's computer facilities will be used in computer intensive applications such as bioinformatics (biological sequence comparison and analysis), molecular modeling and computer aided drug design, they will also be used in many other research activities including protein structure determination by X-ray crystallography, NMR spectroscopy or mass spectrometry. All of the computer facilities will be extensively networked and maintained by at least two full-time system administrators.

The IBD is expected to house some 25 different principal investigators plus another 75 students, post-docs, technicians and support staff. The IBD's scientists will come from all corners of the University campus with representatives from biochemistry, chemistry, biology and pharmaceutical sciences. Many of its members are internationally known scientists with outstanding records of achievement. Over the next five years at least 10 new academic positions will have to be filled to bring the institute up to speed. At least three of these appointments will be computational biologists or chemists, with some (or perhaps all) having their primary appointment in the department of Computing Science.

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