Daily Program

Saturday, July 26, 2003	
5:00pm-8:00pm	**Registration** Main Lobby of the Department of Chemistry, 80 St. George Street
Sunday, July 27, 2003	
	Morning Session: 8:45am-12:35pm *Computational Biophysics: Protein Hydration, Dynamics, and Folding* Session Chair: Hue Sun Chan (University of Toronto, Biochemistry, Canada) **Rm 1160, Bahen Centre for Information Technology, 40 St. George Street**
8:45am-9:00am	Opening Comments: Régis Pomès (Hospital for Sick Children, Canada)
9:00am-9:45am	**Angel Garcia** (Los Alamos National Laboratory, USA) *Folding a Protein in the Computer – All Atom Stimulation of the Folding/Unfolding Thermodynamics of Protein A*
9:45am-10:30am	**Gordon M. Crippen** (University of Michigan, USA) *Progress in Predicting Human Metabolic Site of Metabolism 'In Silico'*
10:30am-10:45am	Coffee Break
10:45am-11:30am	**Wonpil Im** (The Scripps Research Institute, USA) *An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins*
11:30am-12:00pm	**Stuart Rothstein** (Brock University, Canada) *Efficient Generation of Low-Energy Folded States of Model Protein: Automated Histogram Filtering*
12:00pm-12:30pm	**Yaoqi Zhou** (University of Buffalo SUNY, USA) *Learning Folding and Domain Swapping from All-Atom Structures and Simple Parameters*
12:30pm-2:00pm	Lunch: Pay Your Own Way Dim Sum
2:00pm-4:00pm	**MDIT Workshop:** Régis Pomès and Lakshmi Kotra **Faculty of Pharmacy, 19 Russell Street**
	Afternoon Session: 4:00pm-6:15pm *Computational Biophysics: Self-Assembly, Membranes, and Transport* Session Chair: Régis Pomès (Hospital for Sick Children, Canada) **Rm 1160, Bahen Centre for Information Technology, 40 St. George Street**
4:00pm-4:45pm	**Shekhar Garde** (Rensselaer Polytechnic Institute, USA) *Proteins Under Stress: Molecular Simulation Studies of Pressure Effects on Proteins*
4:45pm-5:30pm	**Peter Tieleman** (University of Calgary, Canada) *Non-Equilibrium Simulations of Lipid Bilayers*
5:30pm-6:15pm	**Volkhard Helms** (Max Planck Institute of Biophysics, Germany) *Proton Transfer Reactions in Biological Systems Simulated with Q-HOP Molecular Dynamics*
6:30pm-8:00pm	Welcome Reception and BBQ Hart House Quadrangle

Monday, July 28, 2003	
	Morning Session: 9:00am-12:15pm *Reaction Pathways and Rough Energy Landscapes* Session Chair: Jeremy Schofield (University of Toronto, Chemistry, Canada) **Isabel Bader Theatre, 93 Charles Street**
9:00am-9:45am	**Hannes Jonsson** (University of Washington, USA)
9:45am-10:30am	**Phillip Geissler** (University of California, Berkeley, USA) *Statistical Mechanics of Reactive Trajectories: In and Out of Equilibrium*
10:30am-10:45am	Coffee Break
10:45am-11:30am	**David Reichman** (Harvard University, USA) *Models of Slow Dynamics in Glassy Media*
11:30am-12:15pm	**Tom Woolf** (Johns Hopkins University, USA) *Tools for Channels: Moving Towards Molecular Calculations of Gating and Permeation in Ion Channel Biophysics*
12:15pm-2:00pm	Lunch Hart House Quadrangle
2:00pm-4:00pm	**Poster Session I** **East Common Room of Hart House**
	Afternoon Session: 4:00pm-6:00pm *Advances in Computational Methods in Material Science* Session Chair: John Tse (National Research Council of Canada, Canada) **Isabel Bader Theatre, 93 Charles Street**
4:00pm-4:45pm	**Julian Gale** (Imperial College, United Kingdom) *The SIESTA Method and it's Application to Nanostructures*
4:45pm-5:30pm	**Michiel Sprik** (University of Cambridge, United Kingdom) *Electronic States in Aqueous Solution: Redox Reactions and Spectroscopy*
5:30pm-6:00pm	**M.A. (Tony) Whitehead** (McGill University, Canada) *Molecularly Self-Assembled Thin Films: Theory and Experiment*
Tuesday, July 29, 2003	
	Morning Session: 9:00am-12:30pm *Drug Design I: Advances in Structure-Based Design* Session Chair: Alan Cameron (ProMetic BioSciences Inc., Canada) **Isabel Bader Theatre, 93 Charles Street**
9:00am-9:40am	**Ajay Jain** (UCSF Cancer Research Institute, USA) *Molecular Surface Representation: Applications in Structure-Based Drug Design*
9:40am-10:20am	**Christopher Bayly** (Merck Frosst Center for Therapeutic Research, Canada) *Structure-Based Design of COX-2 Selectivity into Flurbiprofen*
10:20am-10:30am	Coffee Break
10:30am-11:10am	**Enrico Purisima** (National Research Council of Canada, Canada) *Issues in Parametrizing Emperical Binding Free Energy Functions*
11:10am-11:50am	**Maria Zavodszky** (Michigan State University, USA) *Modeling Protein Flexibility in Docking*
11:50am-12:30pm	**Shaomeng Wang** (University of Michigan, USA) *Structure-Based Discovery and Optimization of Novel, Potent and Selective*

	Ligands for the Dopamine 3 (D3) Receptor
12:30pm-2:00pm	Lunch Hart House Quadrangle
2:00pm-4:00pm	**Poster Session II** **East Common Room of Hart House**
	Afternoon Session: 4:00pm-6:30pm *Quantum Dynamics in Complex Systems I* Session Chair: Ray Kapral (University of Toronto, Chemistry, Canada) **Isabel Bader Theatre, 93 Charles Street**
4:00pm-4:45pm	**Emily Carter** (UCLA, USA) *Linking Quantum and Continuum Mechanics to Study Mechanical Response of Materials: Shocked, Stressed, and Embrittled Iron*
4:45pm-5:30pm	**Pierre-Nicholas Roy** (University of Alberta, Canada) *Rotational Solute Dynamics in Quantum Clusters*
5:30pm-6:00pm	**Alessandro Sergi** (University of Toronto, Canada) *Quantum-Classical Dynamics of Nonadiabatic Chemical Reactions*
6:00pm-6:30pm	**Yossi Elran** (University of Toronto, Canada) *Semiclassical IVR (Intial Value Representation) Treatment of the S-matrix*
6:30pm-6:45pm	Organizational Meeting for CCCC6
7:00pm-9:00pm	Banquet Great Hall of Hart House
Wednesday, July 30, 2003	
	Morning Session: 9:00am-12:15pm *Quantum Dynamics in Complex Systems II* Session Chair: Styliani Consta (University of Western Ontario, Canada) **Isabel Bader Theatre, 93 Charles Street**
9:00am-9:45am	**Glenn Martyna** (IBM, USA) *Manybody Polarization and Disperison Effects on Condensed Phase Systems*
9:45am-10:05am	**Victor Batista** (Yale University, USA) *Coherent Control of Cis/Trans Photoisomerization in Rhodopsin*
10:05am-10:35am	**Alexander Wang** (University of British Columbia, Canada) *Theoretical Studies of the Catalytic Mechanisms of the Periplasmic Nitrate Reductase*
10:35am-10:45am	Coffee Break
10:45am-11:30am	**Gilles Peslherbe** (Concordia University, Canada) *Ab Initio Excited-State Molecular Dynamics Simulations: Application to Cluster Photochemistry*
11:30am-12:15pm	**Zsolt Zsoldos** (SimBioSys Inc., Canada) *eHiTS: electronic High Throughout Screening*
12:15pm-2:00pm	Lunch Hart House Quadrangle
	Afternoon Session: 2:00pm-5:15pm *Drug Design II: In-Silico ADME/Tox in Drug Discovery* Session Chair: Sanjay Srivastava (AstraZeneca, Canada) **Isabel Bader Theatre, 93 Charles Street**

2:00pm-2:45pm 2:45pm-3:30pm	**Peter Grootenhuis** (Vertex Pharmaceuticals Inc., USA) *Enhancing Drug Discovery Through Computational ADME* **Gabriele Cruciani** (University of Perugia, Italy) *Process in Predicting Human Metabolic Site Metabolism 'In Silico'*
3:30pm-3:45pm	Coffee Break
3:45pm-4:30pm	**Gilles Klopman** (Case Western Reserve University, USA) *MCASE; A Computational Tool for the Rational Evaluation of the Hazard Potential of New Pharmaceuticals*
4:30pm-5:15pm	**Ulf Norinder** (AstraZeneca R&D Sodertalje, Sweden) *Rapid 'In Silico' Predictions of ADMET Properties Using Machine-Learning Techniques*