According to estimates from the UNAIDS 2008 Report on the global AIDS epidemic, around 30.8 million adults and 2 million children were living with the human immunodeficiency virus (HIV) at the end of 2007. During 2007, some 2.7 million people became infected with HIV, which causes AIDS. The year also saw two million deaths from AIDS (www.avert.org/worldstatinfo.htm).

Needless to say, it is of great importance to fight this disease. Associate Professors Hiroshi Matsuo and Reuben S. Harris, Department of Biochemistry, Molecular Biology, and Biophysics, and their research groups, including post-doctoral associate Dr. Elena Harjes, are investigating the human APOBEC3G (A3G) protein. A3G is capable of altering the HIV genome by deaminating cytosines to uracils. (Cytosine is one of the bases in DNA; uracil is a base in RNA.) DNA deamination can genetically inactivate HIV and recent studies have shown that this activity is as potent as any current anti-

Solution Structure of the Catalytic Domain of APOBEC3G

Also in This Issue

Using Data-Mining Techniques to Assess Changes in Land Cover ........................................... 4
2009 Undergraduate Summer Internships .......................... 6
MSI Open House 2009 ............ 7
Bioinformatics: Building Bridges 2009 ..................... 7
Research Reports .................. 8

continued on page 3

Figure 1a. Superimposition of ten NMR structures showing α-helices in red, β-sheets in yellow and Zn$^{2+}$ in purple.  
1b, 1c. Ribbon diagrams of the NMR structure shown in 1a from the same (b) and 180° (c) angles, respectively. The β3-to-β2 and β4-to-α3 loops are colored blue in 1b, and the β2-bulge-β2’ is colored orange in 1c. This figure was generated by modifying Figure 2 in Chen et al., Nature, 452, 116–119 (2008).
retroviral drug (Haché et al., Current Biology, 18, 819–24 (2008)). However, as a counter-defense, HIV uses an auxiliary protein called Vif (virion infectivity factor) to degrade A3G. Structural information is valuable for understanding protein function including enzymatic activity and interactions with other molecules.

In the case of A3G the interaction with DNA and Vif are of the greatest interest. Understanding the A3G-DNA or A3G-Vif interaction provides fundamental knowledge of the mechanisms by which A3G catalyzes single-strand DNA (ssDNA) cytosine deamination or Vif degrades A3G, respectively.

A3G consists of two domains, containing the N-terminal Vif interacting domain (NTD) and the C-terminal catalytic domain (CTD). The researchers have calculated the structure of the A3G catalytic domain using NMR data and proposed model for DNA binding (Chen et al., Nature, 452, 116–119 (2008)). Five helices are arranged over five strands (Figure 1). The structure of A3G-CTD shares some attributes with previously known structures of cytosine deaminases. The α-β-α Zn²⁺-binding motif, α1-β3-α2 in A3G-CTD, is the clearest characteristic trait in structures of this deaminase superfamily. The unique β2 strand, which is interrupted with a loop-like bulge of six residues (Figure 1c) is a remarkable feature of A3G-CTD. The only other available APOBEC structure, the crystal structure of APOBEC2, has a continuous 11-residue β2 strand, which mediates dimerization through the β2 strand of another molecule (Prochnow, et al., Nature, 445, 447–451 (2007)). The presence of β2-bulge-β2’ suggests that different contacts will connect N- and C-terminal domains of A3G. It is possible that the β2-bulge-β2’ mediates interactions with RNA and/or other proteins, although the researchers have not yet found any specific sequence or molecules. Since amino acid residues located in the β2-bulge region are not important for the deamination activity, the interactions involving this region may not affect A3G’s catalytic activity.

A fundamental question is how A3G binds ssDNA. To bind DNA, proteins usually need positive charges on their surfaces. The electrostatic potential of the active-site face of A3G-CTD was
largely negative. Only a few positively charged residues were arranged on an apparent brim surrounding the concave catalytic site (Figure 2a). To test directly whether any of these residues interacted with DNA, NMR chemical shift perturbation experiments were conducted by titration of 21-base ssDNA oligonucleotide, which contained an A3G deamination hotspot. Significant chemical shift perturbations occurred predominantly on the active-site face of A3G-CTD (Figure 2b), including catalytically key residue glutamic acid E259. Additional chemical shift perturbations were detected for conserved arginines R215 and R313. Residues adjacent to R313 (located in the β4-to-α3 loop) and to E259 also showed strong chemical shift perturbations. Unfortunately, NMR signals of R213 and R320 could not be detected with this technique.

The NMR titration data and a computational method were used to find the lowest energy A3G-ssDNA binding model (Figures 2b and 2c). This model predicted that the 5´ nucleotide C1 would interact with the conserved R313, the phosphate of the 3´ nucleotide T3 would contact both R215 and R213, and the C2 phosphate would interact with R320.

To test this DNA binding model, the researchers tried to determine whether residues, mentioned above, would be important for catalytic activity. The model predicted that R215 and R313 would promote DNA binding and that W285 would help to form the hydrophobic active site. E259 is predicted to be important for exchanging protons during the catalytic reaction. All of these residues proved essential for the catalytic activity using *Escherichia coli*-based activity assay. R213 and R320 were predicted to interact with the phosphate backbone of ssDNA. Therefore, an alanine substitution at these positions might be tolerated, but a negatively charged substitution might kill the catalytic activity by repelling the phosphate backbone. Indeed, R213A and R320A derivatives still retained 20% of wild-type activity, whereas R213E and R320E derivatives were nearly dead.

The catalytic domain of the HIV-1 restriction factor A3G represents the first high-resolution ssDNA cytosine deaminase structure and provides insights into the A3G-DNA interaction. Future research directions include deciphering the catalytic mechanism of full-length A3G, the interaction between A3G and Vif, and small molecules that work by disrupting this axis.
Using Data-Mining Techniques to Assess Changes in Land Cover

Professor Vipin Kumar, Department of Computer Science and Engineering and MSI Fellow, and his team have developed scalable algorithms to detect changes in land cover using data from NASA’s Earth Observing System (EOS) satellites, and have shown their effectiveness in detecting changes in forest cover due to fires, logging, and other events. The need to assess the state of the forest ecosystem and how it is changing has become increasingly urgent. In particular, detecting changes in the forest ecosystem and their recovery periods is critical for sustainable management of forest resources, monitoring the impacts of climate change on forests, documenting a nation’s compliance with United Nations protocols, and carbon trading.

Even though changes in forests account for as much as 20% of the greenhouse gas emissions into the atmosphere (second only to fossil fuel emissions), the lack of technology to reliably determine changes in the global forest cover has prevented forests from becoming part of the carbon trading system.

The land cover change detection problem is essentially one of detecting when the land cover at a given location has been converted from one type to another. Examples of this include the conversion of forested land to barren land or farmland (possibly due to logging or a fire) or farmland being converted to land used for housing developments. The general change detection problem has been extensively studied in the fields of statistics, signal processing, and control theory. However, most techniques from these fields are not well-suited for earth science data due to their inability to take advantage of seasonality and spatio-temporal autocorrelation inherent in the data and their inability to

Figure 1: Vegetation time series (left) identified by the change detection algorithm shows a sustained decrease in vegetation. The corresponding satellite image from Google Earth (right) shows that logging has indeed occurred in this forested area located in Northern California.
handle massive global datasets.

Professor Kumar’s work addresses these challenges with new change-detection techniques that are based on novel data-mining approaches. Specifically, these techniques take advantage of some of the inherent characteristics of spatio-temporal data and are scalable so that they can be applied to increasingly high-resolution earth science datasets.

Application of the new algorithm to EOS data (specifically MODIS (moderate-resolution imaging spectroradiometer) EVI (enhanced vegetation index) and FPAR (fraction of photosynthetically active radiation) products) has detected a number of interesting land cover changes in California, including logging (Figure 1), conversion from desert to farmland, and large-scale forest fires worldwide (Figure 2). This work is unique because it is among the first time series-based schemes for land cover change detection and because of the high quality of the changes detected. The ability to reliably detect forest cover changes across the globe in a timely fashion will have a significant impact on conservation efforts and carbon-trading markets. The collaborators on this project (funded by NSF and NASA) are graduate student Shyam Boriah, Dr. Michael Steinbach and Professor Joe Knight of the University of Minnesota, Dr. Chris Potter of NASA Ames Research Center, Steve Klooster of California State University, and Professor Pang-Ning Tan of Michigan State University.

More details about this project can be found in “Land Cover Change Detection: A Case Study” (S. Boriah, V. Kumar, M. Steinbach, C. Potter, and S. Klooster, in KDD ’08: Proceedings of the 14th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 857–865, 2008).

Figure 2: The collection of time series (left) identified by the change detection algorithm show a dramatic drop in the vegetation index (FPAR) around the summer of 2002. Satellite imagery (right) for this location (a forested area near Phoenix) from June 2002 shows a large-scale forest fire in progress—the well-documented Rodeo Fire.
Summer 2009
Undergraduate Internship Program

The Supercomputing Institute is pleased to announce its Undergraduate Internship Program for Summer 2009. Appointments are for full-time, 10-week internships, and will run from June 1 through August 9, 2009. A student interested in becoming an intern must still be an undergraduate in August 2009 and must be a citizen or permanent resident of the United States or its possessions. Interns will be paid a stipend of $5,000 and are responsible for their own travel and housing costs.

All applications are evaluated competitively based on the qualifications of the applicant and the availability of a suitable project. Prospective applicants should review the research projects list and indicate projects in which they are interested, although they may be offered other projects due to availability.

Complete application information, application forms, and project lists are available on the Supercomputing Institute Web site at:

www.msi.umn.edu/programs/undergraduateinternship.html

Application forms and project lists are also available from:
Undergraduate Internship Coordinator
University of Minnesota
Supercomputing Institute
599 Walter
117 Pleasant Street SE
Minneapolis, MN 55455

Phone: (612) 624-2330
Email: uip@msi.umn.edu

All applications and letters of recommendation must be received by March 2, 2009.
MSI Open House 2009

The April 2009 Open House previously announced on this page will be combined with an event honoring MSI’s 25th anniversary. This event is tentatively scheduled for Fall 2009. Information will be posted on our Web site as it becomes available:

www.msi.umn.edu/programs/

Bioinformatics: Building Bridges 2009

The bioinformatics programs at the University of Minnesota will be sponsoring another Bioinformatics: Building Bridges conference at the Digital Technology Center on the University’s East Bank campus in Minneapolis. The conference will be held on April 16–17, 2009 and is sponsored in part by the Supercomputing Institute. As in past years, the conference will include speakers, a poster session, and tutorials presented by Supercomputing Institute User Support staff members. Some events will be available as Webcasts.

The previous Building Bridges conference was held in April 2007 (see Research Bulletin Volume 23, Number 1, Spring 2007 and www.binf.umn.edu/bisym07).

Information about the 2009 conference can be found on the conference Web site:

www.binf.umn.edu/bisymp09/

The conference organizer is MSI Principal Investigator Professor Lynda Ellis, Department of Laboratory Medicine and Pathology.
Aerospace Engineering and Mechanics

2008/100, September 2008
and CB 2008-43
A Finite Element Methodology to Determine Elastic Parameters in Biological Tissues
A. R. Aguiar and E. B. T. Prado
2008/122, October 2008
Stability and Elastic Properties of the Stress-free B2 (CsCl-type) Crystal for the Morse Pair Potential Model
V. S. Guthikonda and R. S. Elliott

Biochemistry, Molecular Biology, and Biophysics

2008/125, October 2008
Physiological and Molecular Characterization of Aluminum Resistance in Medicago truncatula
D. Chandran, N. Sharopova, K. A. VandenBosch, D. F. Garvin, and D. A. Samac
2008/130, October 2008
and CB 2008-52
Swapping Metals in Fe- and Mn-Dependent Oxigenases: Evidence for Oxygen Activation Without a Change in Metal Redox State
J. P. Emerson, E. G. Kovalcova, E. R. Farquhar, J. D. Lipscomb, and L. Que, Jr.
2008/186, October 2008
and CB 2008-64
Partially Folded Bovine Pancreatic Trypsin Inhibitor Analogues Attain Fully Native Structures When Crystallized With S195A Rat Trypsin
2008/199, November 2008
and CB 2008-70
Limited Functional Conservation of a Global Regulator Among Related Bacterial Genes: Lrp in Escherichia, Proteus, and Vibrio
2008/200, November 2008
and CB 2008-71
Overexpression of Phage HK022 Nus Protein Is Toxic for Escherichia coli
A. Uc-Mass, A. Khodursky, L. Brown, and M. E. Gottesman
2008/201, November 2008
and CB 2008-72
Gene Expression Patterns of Sulfur Starvation in Synechocystis sp.
PCC 6803
Z. Zhang, N. D. Pendse, K. N. Phillips, J. B. Cotner, and A. Khodursky
2008/202, November 2008
and CB 2008-73
A Parametric Joint Model of DNA-Protein Binding, Gene Expression, and DNA Sequence Data to Detect Target Genes of a Transcription Factor
W. Pan, P. Wei, and A. Khodursky

Agronomy and Plant Genetics

2008/103, September 2008
and CB 2008-44
L. Ma, H. B.Runesha, D. Dvorkin, J. R. Garbe, and Y. Da

Animal Science

2008/106, September 2008
Nuclear Burning and Mixing in the First Stars: Entrainment at a Convective Boundary Using the PPB Advection Scheme
P. Woodward, F. Herwig, D. Porter, T. Fuchs, A. Nowatzki, and M. Pignatari
2008/184, October 2008
Three-dimensional Magnetohydrodynamic Simulations of Buoyant Bubbles in Galaxy Clusters
S. M. O’Neill, D. S. De Young, and T. W. Jones
2008/185, October 2008
Self-similar Evolution of Cosmic-ray Modified Shocks: The Cosmic-ray Spectrum
H. Kang, D. Ryu, and T. W. Jones

Astronomy

2008/205, November 2008
and CB 2008-74
Ubiquitin Docking at the Proteasome Through a Novel Pleckstrin-Homology Domain Interaction
P. Schreiner, X. Chen, K. Husnjak, L. Randles, N. Zhang, S. Elsasser, D. Finley, I. Dikic, K. J. Walters, and M. Groll
2008/206, November 2008
and CB 2008-75
Proteasome Subunit Rpn13 Is a Novel Ubiquitin Receptor
2008/224, November 2008
and CB 2008-83
Thermodynamic and Structural Basis of Phosphorylation-induced Disorder-to-Order Transition in the Regulatory Light Chain of Smooth Muscle Myosin
L. M. Espinoza-Fonseca, D. Kast, and D. D. Thomas
2008/225, November 2008
and CB 2008-84
Structural Dynamics of the Acto-myosin Complex Probed by a Bi-functional Spin Label That Crosslinks SH1 and SH2
A. R. Thompson, N. Naber, C. Wilson, R. Cooke, and D. D. Thomas

Names of Supercomputing Institute principal investigators appear in bold type.

Supercomputing Institute Research Bulletin
Fall 2008
2008/226, November 2008
and CB 2008-85
Activating Cleft Closure in Myosin II Probed by Site-directed Spin Labeling and Pulsed EPR
J. C. Klein, A. R. Burr, B. Svensson, D. J. Kennedy, J. Allingham, M. A. Titus, Ivan Rayment, and
D. D. Thomas
2008/227, November 2008
and CB 2008-86
Changes in Actin Structural Transitions Associated With Oxidative Inhibition of Muscle Contraction
E. Prochniewicz, D. Spakowicz, and D. D. Thomas
2008/228, November 2008
and CB 2008-87
Muscle and Nonmuscle Myosins Probed by a Spin Label at Equival-ent Sites in the Force-generating Domain
R. V. Agafonov, Y. E. Nesmelov, M. A. Titus, and D. D. Thomas

Center for Drug Design
2008/117, September 2008
and CB 2008-48
Design and Synthesis of Sulfoximine Based Inhibitors for HIV-1 Protease
A. Raza, Y. Sham, and R. Vince

Chemical Engineering and Materials Science
2008/101, September 2008
Low-pressure Clino- to High-pressure Clino-Enstatite Phase Transi-
tion: A Phonon Related Mechanism
Y. G. Yu and R. M. Wentzcovitch
2008/102, September 2008
Quasiharmonic Elastic Constants Corrected for Deviatoric Thermal Stresses
P. Carrier, R. M. Wentzcovitch, and J. F. Justo
2008/126, October 2008
First-principles Study for Low-spin LaCoO3 with Structurally Consis-
tent Hubbard U
H. Hsu, K. Umemoto, M. Cococioni, and R. Wentzcovitch
2008/192, October 2008
Buoyancy-driven Breakup of an Isolated Drop With Surfactant
M. A. Rother and R. H. Davis
2008/193, November 2008
Brownian Dynamics Simulations of Polyelectrolyte Adsorption in Shear Flow: Effects of Solvent Quality and Charge Patterning
N. Hoda and S. Kumar
2008/194, November 2008
Thermal Emission Control by Selective Heating of Periodic Struc-
tures
S. E. Han and D. J. Norris
2008/195, November 2008
Efficient Low-temperature Thermophotovoltaic Emitters From Metallic Photonic Crystals
P. Nagpal, S. E. Han, A. Stein, and D. J. Norris
2008/213, November 2008
On the Chain Length Dependence of Local Correlations in a Polymer Melt and a Perturbation Theory of Symmetric Polymer Blends
D. C. Morse and J. K. Chung
2008/220, November 2008
An Effective Semi-empirical Ansatz for Computing Anharmonic Free Energies
Z. Wu and R. M. Wentzcovitch
2008/221, November 2008
Anomalous Thermodynamics Properties in Ferroelectric Phase Through out Its Spin Crossover Transition
2008/222, November 2008
First-principles Study of Body-centered Tetragonal sp2-Carbon Al-
lotrope
K. Umemoto and R. M. Wentzcovitch
2008/223, November 2008
Order-Disorder Phase Transition Between Ice VII and VIII by First Principles
K. Umemoto and R. M. Wentzcovitch

Chemistry
2008/107, September 2008
Reactions of Copper(II)-H2O2 Adducts Supported by Tridentate Bist(2-pyrindylmethyl)amine Ligands: Sensitivity to Solvent and Variations in Ligand Substitution
Helical Extension as a Route to Molecular Wires
2008/109, September 2008
Performance of SM8 on a Test to Predict Small-molecule Solvation Free Energies
A. C. Chamberlain, C. J. Cramer, and D. G. Truhlar
2008/110, September 2008
The Restricted Active Space Fol-lowed by Second-order Perturbation Theory Method: Theory and Application to the Study of CuO2 and CuO2 Systems
2008/111, September 2008
Quantum Chemical Characteriza-
tion of the Structures, Thermo-
chemical Properties, and Dou-
blet–Quartet Splittings of Tridehy-
dropyrindinium Cations
J. J. Nash, H. I. Kenttäämaa, and C. J. Cramer
2008/112, September 2008
Perspective on Foundations of Sol-
vation Modeling: The Electrostatic Contribution to the Free Energy of Solvation
A. V. Marenich, C. J. Cramer, and D. G. Truhlar
2008/113, September 2008
A Universal Approach to Solvation Modeling
C. J. Cramer and D. G. Truhlar

Fall 2008
Supercomputing Institute Research Bulletin
2008/114, September 2008
Stereoelectronic Effects on Mole- 
lar Geometries and State-Energy 
Splittings of Ligated Monocopper
Dioxygen Complexes
C. J. Cramer, J. R. Gour, 
A. Kinal, M. Woch, P. Piekuch, 
A. R. M. Shahi, and L. Gagliardi

2008/115, September 2008
A Thermal Decarbonylation of 
Penam β-Lactams 
K. W. Wiitala, Z. Tian, C. J. 
Cramer, and T. R. Hoye

2008/116, September 2008 
and CB 2008-47
Direct Examination of H₂O₂ Acti- 
vation by a Heme Peroxidase 
J. P. Roth and C. J. Cramer

2008/120, September 2008
Electric Dipole Moment of Sulfuric 
Acid From Fourier Transform Mi-
crowave Spectroscopy 
G. Sedo, J. Schultz, and K. R. 
Leopold

2008/121, September 2008
Effects of ¹⁸O Isotopic Substitution 
on the Rotational Spectra and Po- 
tential Splitting in the OH-OH₂ 
Complex: Improved Measurements for 
¹⁶OH-¹⁶OH₂ and ¹⁸OH-¹⁸OH₂. 
New Measurements for the Mixed 
Isotopic Forms, and Ab Initio Cal-
culations of the ²A¹'-²A¹⁺ Energy 
Separation 
C. S. Brauer, G. Sedo, E. Dahlke, 
S. Wu, E. M. Grunstrup, K. R. 
Leopold, M. D. Marshall, H. O. 
Leung, and D. G. Truhlar

2008/127, October 2008
Spherical Tensor Gradient Opera-
tor Method for Integral Rotation: A 
Simple, Efficient, and Extendable 
Alternative to Slater-Koster Tables 
T. J. Giese and D. M. York

2008/128, October 2008 
and CB 2008-50
Density Functional Study of C-5 
Cytosine Substitution 
A. Moser, B. Guza, N. Tretyakova, 
and D. M. York

2008/129, October 2008 
and CB 2008-51
Threshold Occupancy and Specific 
Cation Binding Modes in the Ham-
merhead Ribozyme Active Site Are 
Required for Active Conformation 
T.-S. Lee, G. M. Giambasu, C. P. 
Sosa, M. Martick, W. G. Scott, and 
D. M. York

2008/135, October 2008
Assessment of Multicoefficient Cor-
relation Methods, Second-order
Moller-Plesset Perturbation Theo-
ry, and Density Functional Theory 
for H₂O¹⁺(H₂O)ₙ (n = 1–5) and 
OH⁻(H₂O)ₙ (n = 1–4) 
E. W. Dahlke, M. A. Ortmeyer, and 
D. G. Truhlar

2008/136, October 2008
Conservative Algorithm for an 
Adaptive Change of Resolution in 
Mixed Atomicistic/Coarse-grained 
Multiscale Simulations 
A. Heyden and D. G. Truhlar

2008/137, October 2008
Assessment of the Accuracy of 
Density Functionals for Prediction of 
Relative Energies and Geome-
tries of Low-lying Isomers of Water 
Hexamers 
E. W. Dahlke, R. M. Olson, H. R. 
Leverentz, and D. G. Truhlar

2008/138, October 2008
A Unified Perspective on the Hy-
drogen Atom Transfer and Proton-
coupled Electron Transfer Mecha-
isms in Terms of Topographic 
Features of the Ground and Excit-
ed Potential Energy Surfaces as 
Exemplified by the Reaction Be-
tween Phenol and Radicals 
O. Tishchenko, D. G. Truhlar, 
A. Culemants, and M. T. Nguyen

2008/139, October 2008
A Prototype for Graphene Material 
Simulation: Structures and Interac-
tion Potentials of Coronene Dimers 
Y. Zhao and D. G. Truhlar

2008/140, October 2008
How Well Can New-generation
Density Functionals Describe the 
Energetics of Bond-dissociation 
Reactions Producing Radicals? 
Y. Zhao and D. G. Truhlar

2008/141, October 2008
Benchmark Data for Interactions 
in Zeolite Model Complexes and 
Their Use for Assessment and Vali-
dation of Electronic Structure 
Methods 
Y. Zhao and D. G. Truhlar

2008/142, October 2008
Computational Characterization 
and Modeling of Buckyball Twee-
ers: Density Functional Study of 
Concave-Convex π-π Interactions 
Y. Zhao and D. G. Truhlar

2008/143, October 2008
Cluster and Nanoparticle Conden-
sation and Evaporation Reactions. 
Thermal Rate Constants and Equi-
librium Constants of A⁻m + A¹⁺⁻m 
↔ A¹⁻n With n = 2–60 and m = 
1–8 
Z. Hua Li and D. G. Truhlar

2008/144, October 2008
VBSM: A Solution Model Based 
on Valence Bond Theory 
P. Su, W. Wu, C. P. Kelly, C. J. 
Cramer, and D. G. Truhlar

2008/145, October 2008
Application of the Electrostatically 
Embedded Many-body Expansion 
to Microsolvation of Ammonia in 
Water Clusters 
A. Sorkin, E. E. Dahlke, and D. G. 
Truhlar

2008/146, October 2008
Performance of the M06 Family of 
Exchange-correlation Functionals 
for Predicting Magnetic Coupling 
in Organic and Inorganic Mole-
cules 
R. Valero, R. Costa, I. de P. R. 
Moreira, D. G. Truhlar, and 
F. Illas

2008/147, October 2008
Tight Binding Configuration Inter-
action (TBCI): A Non-iterative Ap-
proach to Incorporating Electro-
statics Into Tight Binding 
M. A. Iron, A. Heyden, 
G. Staszewska, and D. G. Truhlar
2008/148, October 2008
Electrostatically Embedded Multi-configuration Molecular Mechanics Based on the Combined Density Functional and Molecular Mechanical Method
M. Higashi and D. G. Truhlar

2008/149, October 2008
Stereochemistry of Eudesmane Cation Formation During Catalysis by Aristolochene Synthase From Penicillum Roqueforti
D. J. Miller, J. Gao, D. G. Truhlar, N. J. Young, V. Gonzalez, and R. K. Allemann

2008/150, October 2008
Adiabatic States Derived From a Spin-coupled Diabatic Transformation: Semiclassical Trajectory Study of Photodissociation of HBr and the Construction of Potential Curves for LiBr+
R. Valero, D. G. Truhlar, and A. W. Jasper

2008/151, October 2008
Construction of a Generalized Gradient Approximation by Restoring the Density-gradient Expansion and Enforcing a Tight Lieb-Oxford Bound
Y. Zhao and D. G. Truhlar

2008/152, October 2008
Assessment of New Meta and Hybrid Density Functional for Predicting the Geometry and Binding Energy of a Challenging System: The Dimer of H$_2$S and Benzen
H. R. Leverentz and D. G. Truhlar

2008/153, October 2008
The Variational Explicit Polarization Potential and Analytical First Derivative of Energy: Towards a Next Generation Force Field
W. Xie, L. Song, D. G. Truhlar, and J. Gao

2008/154, October 2008
Multireference Model Chemistries for thermochemical Kinetics
O. Tishchenko, J. Zheng, and D. G. Truhlar

2008/155, October 2008
Combined Electrostatically Embedded Multiconfiguration Molecular Mechanics and Molecular Mechanical Method: Application to Molecular Dynamics Simulation of a Chemical Reaction in Aqueous Solution With Hybrid Density Functional Theory
M. Higashi and D. G. Truhlar

2008/156, October 2008
Mixed Quantum/Classical Investigation of the Photodissociation of NH$_3$(Å) and a Practical Method for Maintaining Zero-Point Energy in Classical Trajectories
D. Bonhommeau and D. G. Truhlar

2008/157, October 2008
Nan_solids, Slu_shes, and Nanoliquids: Characterization of Nanophases in Metal Clusters and Nanoparticles
Z. Hua Li and D. G. Truhlar

2008/158, October 2008
Algorithmic Decoherence Time for Decay-of-Mixing Non-Born-Oppenheimer Dynamics
S. C. Cheng, C. Zhu, K. K. Liang, S. H. Lin, and D. G. Truhlar

2008/159, October 2008
Improved Description of Nuclear Magnetic Resonance Chemical Shielding Constants Using the M06-L Meta-generalized Gradient-approximation Density Functional
Y. Zhao and D. G. Truhlar

2008/169, October 2008
Lithium Monoxide Anion: A Ground-state Triplet With the Strongest Base to Date

2008/170, October 2008
Does Electrospray Ionization Produce Gas-Phase or Liquid-Phase Structures?
Z. Tian and S. R. Kass

2008/173, October 2008
On the Accuracy of Computed Excited-state Dipole Moments
R. A. King

2008/175, October 2008
Combined QM/MM and Path Integral Simulations of Kinetic Isotope Effects in the Proton Transfer Reaction Between Nitroethane and Acetate Ion in Water
J. Gao, K.-Y. Wong, and D. T. Major

2008/176, October 2008
and CB 2008-61
Molecular Dynamics Simulations of Biotin Carboxylase
S. O. Nilsson Lilj, J. Gao, and G. L. Waldrop

2008/177, October 2008
and CB 2008-62
Kinetic Isotope Effects From Hybrid Classical and Quantum Path Integral Computations
J. Gao, K.-Y. Wong, D. T. Major, A. Cembran, L. Song, Y.-L. Lin, Y. Fan, and S. Ma

2008/178, October 2008
and CB 2008-63
Systematic Approach for Computing Zero-point Energy, Quantum Partition Function, and Tunneling Effect Based on Kleinert’s Variational Perturbation Theory
K.-Y. Wong and J. Gao

2008/179, October 2008
On the Construction of Diabatic and Adiabatic Potential Energy Surfaces Based on Ab Initio Valentine Bond Theory
L. Song and J. Gao

2008/180, October 2008
Incorporation of a QM/MM Buffer Zone in the Variational Double Self-consistent Field Method
W. Xie, L. Song, D. G. Truhlar, and J. Gao

2008/181, October 2008
A Coupled Polarization-matrix Inversion and Iteration Approach for Accelerating the Dipole Convergence in a Polarizable Potential Function
W. Xie, J. Pu, and J. Gao
Computer Science and Engineering

2008/104, September 2008
Whole Genome Alignments Using MPI-LAGAN
R. Zhang, H. Rangwala, and G. Karypis

2008/124, October 2008
Fast Approximate kNN Graph Construction for High Dimensional Data via Recursive Lanczos Bisection
J. Chen, H. Fang, and Y. Saad

Electrical and Computer Engineering

2008/203, November 2008
Spin Injection Effects on Exciton Formation in Organic Semiconductors
M. Yunus, P. P. Ruden, and D. L. Smith

2008/204, November 2008
Ambipolar Electrical Spin Injection and Spin Transport in Organic Semiconductors
M. Yunus, P. P. Ruden, and D. L. Smith

2008/233, November 2008
and CB 2008-89
Imaging With Concave Large-aperture Therapeutic Ultrasound Arrays Using Conventional Synthetic-aperture Beamforming
Y. Wan and E. S. Ebbini

Engineering

2008/99, September 2008
Breakdown of Laminar Pipe Flow Into Transitional Intermittency and Subsequent Attainment of Fully Developed Intermittent or Turbulent Flow
J. Abraham, E. M. Sparrow, and J. C. Tong

Genetics, Cell Biology, and Development

2008/134, October 2008
and CB 2008-55
A Facile Method for Somatic, Life-long Manipulation of Multiple Genes in the Mouse Liver

Geology and Geophysics

2008/119, September 2008
Ubiquitous Interactive Visualization of 3-D Mantle Convection Through Web Applications Using Java

2008/123, October 2008
Landslides, Ice Quakes, Earthquakes: A Thermodynamic Approach to Surface Instabilities
K. Regenauer-Lieb, D. A. Yuen, and F. Fusseis

2008/188, October 2008
Is the Long-wavelength Geoid Sensitive to the Presence of Postperovskite Above the Core-Mantle Boundary?
N. Tosi, O. Cadek, Z. Martinec, D. A. Yuen, and G. Kaufmann
2008/229, November 2008  
Numerical Evaluation of Tsunami Wave Hazards in Harbors Along the South China Sea  
H. H. Jing, H. Zhang, D. A. Yuen, and Y. Shi

2008/230, November 2008  
Simulating Tsunami Shallow-water Equations With Graphics Accelerated Hardware (GPU) and Radial Basis Functions (RBF)  

2008/132, October 2008  
and CB 2008-53  
Data-driven Extraction of Relative Reasoning Rules to Limit Combinatorial Explosion in Biodegradation Pathway Prediction  
K. Fenner, J. Gao, S. Kramer, L. B. M. Ellis, and L. P. Wackett

2008/133, October 2008  
and CB 2008-54  
The University of Minnesota Pathway Prediction System: Predicting Metabolic Logic  
L. B. M. Ellis, J. Gao, K. Fenner, and L. P. Wackett

2008/164, October 2008  
and CB 2008-56  
Reasons for a Protocol for Radiation Treatment Aimed at Exploiting Weekly Rhythms  
F. Halberg, G. Cornélissen, F. Halberg, W. Ulmer, S. Sanchez de la Penia, J. Siegelova, O. Schwartzkopff, and BIOCOS project

2008/165, October 2008  
and CB 2008-57  
Breuker-Egeson-Lockyer (BEL) Cycle in Heliogeomagnetics  

2008/166, October 2008  
and CB 2008-58  
On Gaps and Interpolation Methods to Avoid Errors in Period Estimation With Conventional Time Series Analysis  
J. Czaplicki, J. Siegelova, B. Fiser, G. Cornélissen, and F. Halberg

2008/167, October 2008  
and CB 2008-59  
Prediabetes is Associated With Abnormal Circadian Blood Pressure Variability  
A. K. Gupta, F. L. Greenway, G. Cornélissen, W. Pan, and F. Halberg

2008/168, October 2008  
and CB 2008-60  
Stress, Geomagnetic Disturbance, Infradian and Circadian Sampling for Circulating Corticosterone and Models of Human Depression?  
A. Olah, R. Jozsa, V. Csernus, J. Sandor, A. Muller, M. Zeman, W. Hoogerwerf, G. Cornélissen, and F. Halberg

2008/189, October 2008  
and CB 2008-66  
Chronobiology, Chronomics and N-of-1 Tests of Timing Coenzyme Q10  

2008/118, September 2008  
Efficient Sticking of Surface-passivated Si Nanospheres via Phasetransition Plasticity  
M. Suri and T. Dumitrica

2008/131, October 2008  
Anisotropy of a Turbulent Boundary Layer  
K. Liu and R. H. Pletcher

2008/160, October 2008  
A Robust Consistent Configuration Framework and Formulation for 3D Finite Strain Dynamic Impact Problems  
X. Zhou, D. Sha, and K. K. Tamma

2008/161, October 2008  
Total Energy Framework, Finite Elements, and Discretization via Hamilton’s Law of Varying Action  
J. Har and K. K. Tamma

2008/162, October 2008  
Algorithms by Design: Part I—On the Hidden Point Collocation With in LMS Methods and Implications for Nonlinear Dynamics Applications  
A. Hoitink, S. Masuri, X. Zhou, and K. K. Tamma

2008/163, October 2008  
Modeling the Spatiotemporal Evolution of a Nanodusty Plasma  
L. Ravi and S. L. Girshick

2008/209, November 2008  
Filtration of Aerosol Particles by Elliptical Fibers: A Numerical Study  
J. Wang and D. Y. H. Pui

2008/216, November 2008  
Elasticity of Ideal Single-wall Carbon Nanotubes Via Symmetry-adapted Tight-binding Objective Modeling  
D.-B. Zhang and T. Dumitrica

2008/210, November 2008  
and CB 2008-77  
Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Drug-like Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and in Aqueous Solution  
B. R. White, C. R. Wagner, D. G. Truhlar, and E. A. Amin

2008/211, November 2008  
and CB 2008-78  
Assessment of Density Functionals, Semiempirical Methods, and SCC-DFTB for Protonated Creatinine Geometries  
N. M. Settgren, P. Buhmann, and E. A. Amin
2008/212, November 2008 and CB 2008-79

Total Synthesis and Evaluation of C25-benzylxoyepothilone C for Tubulin Assembly and Cytotoxicity Against MCF-7 Breast Cancer Cells

**Medicine**

2008/134, October 2008 and CB 2008-55

A Facile Method for Somatic, Life-long Manipulation of Multiple Genes in the Mouse Liver

2008/191, October 2008 and CB 2008-68

Identification of Heterogeneity Among Soft Tissue Sarcomas by Gene Expression Profiles From Different Tumors
K. M. Skubitz, S. Pambuccian, J. C. Manivel, and A. P. N. Skubitz

**Microbiology**

2008/197, November 2008 and CB 2008-69

Development and Use of an Efficient System for Random Mariner Transposon Mutagenesis To Identify Novel Genetic Determinants of Biofilm Formation in the Core Enterococcus faecalis Genome
C. J. Kristich, V. T. Nguyen, T. Le, A. M. T. Barnes, S. Grindle, and G. M. Dunny

2008/207, November 2008 and CB 2008-76

Transcriptional Analysis of Diverse Strains Mycobacterium avium Sub-species Paratuberculosis in Primates Bovine Monocyte Derived Macrophages
X. Zhu, Z. J. Tu, P. M. Coussens, V. Kapur, H. Janagama, S. Naser, and S. Sreevatsan

**Pharmaceutics**

2008/231, November 2008 and CB 2008-88

Optimal Periodic Control of a Drug Delivery System
S. Varigonda, T. T. Georgiou, R. A. Siegel, and P. Daoutidis

2008/171, October 2008

Supersymmetric Theories at Finite Temperature
J. Hiller

2008/172, October 2008

Exploring a Nonperturbative Method for Calculation of the Anomalous Magnetic Moment of the Electron
S. Chabysheva

2008/196, November 2008

The Effect of Anisotropy on the Ground-state Magnetic Ordering of the Spin-1 Quantum \( J_{1}^{XXZ} J_{2}^{XXZ} \) Model on the Square Lattice
R. F. Bishop, P. H. Y. Li, R. Darra-di, J. Richter, and C. E. Campbell

2008/198, November 2008

Effect of Anisotropy on the Ground-state Magnetic Ordering of the Spin-half Quantum \( J_{1}^{XXZ} J_{2}^{XXZ} \) Model on the Square Lattice

2008/217, November 2008

The Chiral Critical Point of \( N_f = 3 \) QCD at Finite Density to the Order \((\mu/T)^4\)

P. de Forcrand and O. Philipson

**Physiology**

2008/105, September 2008 and CB 2008-46

Reconstructing the Phylogeny of Figs (Ficus, Moraceae) to Reveal the History of the Fig Pollination Mutualism
N. Ronsted, G. Weiblen, W. L. Clement, N. J. C. Zerega, and V Savolainen

2008/125, October 2008

Physiological and Molecular Characterization of Aluminum Resistance in Medicago truncatula
D. Chandran, N. Sharopova, K. A. VandenBosch, D. F. Garvin, and D. A. Samac

2008/190, October 2008

Transcriptome Profiling Identified Novel Genes Associated With Aluminum Toxicity, Resistance and Tolerance in Medicago truncatul
A. D. Samac

2008/218, November 2008 and CB 2008-81

Phylogeny, Biogeography, and Ecology of Ficus Section Malvinae (Moraceae)
N. Ronsted, G. D. Weiblen, V. Savolainen, and J. M. Cook

2008/219, November 2008 and CB 2008-82

The Genetic Network Controlling the Arabidopsis Transcriptional Response to Pseudomonas syringae pv. maculicola: Roles of Major Regulators and the Phytotoxin Coronatine

**Plant Biology**
Physiological and Molecular Characterization of Aluminum Resistance in Medicago Truncatula
D. Chandran, N. Sharopova, K. A. VandenBosch, D. F. Garvin, and D. A. Samac

Transcriptome Profiling Identified Novel Genes Associated With Aluminum Toxicity, Resistance and Tolerance in Medicago truncatula
D. Chandran, N. Sharopova, S. Ivashuta, J. S. Gantt, K. A. VandenBosch, and D. A. Samac

Prion Disease Induced Alterations in Gene Expression in Spleen and Brain Prior to Clinical Symptoms
H. O. Kim, G. P. Snyder, T. M. Blazey, R. E. Race, B. Chesebro, and P. Skinner

Transcriptional Analysis of Diverse Strains Mycobacterium avium Subspecies Paratuberculosis in Primary Bovine Monocyte Derived Macrophages
X. Zhu, Z. J. Tu, P. M. Coussens, V. Kapur, H. Janagama, S. Naser, and S. Sreevatsan

Past editions of the Research Bulletin are available in PDF on our Web site:
www.msi.umn.edu/about/publications/researchbulletin/index.html

UMSI Research Reports can be accessed on our Web site:
www.msi.umn.edu/cgi-bin/reports/searchv2.html

MSI’s Annual Report is now available as a printed publication. The Annual Report contains highlights of research at MSI during 2007 and 2008. To obtain a copy, please send email with your complete address to: requests@msi.umn.edu

or mail to:

University of Minnesota
Supercomputing Institute
599 Walter
117 Pleasant St. SE
Minneapolis, MN 55455

MSI 2007–Annual Report of Research, which contains abstracts of all research projects at MSI during the period January 1, 2007–March 15, 2008, is available in PDF on our Web site:
www.msi.umn.edu/about/publications/annualreport/index.html
Please help us keep our mailing list up to date

Check one:
☐ Add name to mailing list
☐ Make corrections/changes as shown
☐ Remove name from mailing list

Name __________________________
Institution _____________________
Address __________________________
______________________________
______________________________
Phone __________________________
Email __________________________

This information can be mailed to the
Supercomputing Institute, 599 Walter,
117 Pleasant Street SE, Minneapolis, MN 55455,
faxed to (612) 624-8861, or emailed to requests@msi.umn.edu

For more information on the University of Minnesota Supercomputing Institute, please contact us at the address given below. You may also consult the Supercomputing Institute’s Internet pages:

www.msi.umn.edu

This information is available in alternative formats upon request by individuals with disabilities. Please send email to alt-format@msi.umn.edu or call 612-624-0528.

Editor/photographer: Tracey A. Bartlett

The University of Minnesota is committed to the policy that all persons shall have equal access to its programs, facilities, and employment without regard to race, color, creed, religion, national origin, sex, age, marital status, disability, public assistance status, veteran status, or sexual orientation.

© 2008 University of Minnesota

Contains a minimum of 10% postconsumer waste

UNIVERSITY OF MINNESOTA
Supercomputing Institute
599 Walter
117 Pleasant Street SE
Minneapolis, MN 55455

Change Service Requested