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<p><b>Education and Honors</b></p>	<p><b>Sandia National Laboratories Award for Excellence (2010)</b>  <b>Sandia National Laboratories Award for Excellence (2007)</b>  <b>Sandia National Laboratories Award for Excellence (2005)</b></p> <p><b>UNM SCHOOL OF MEDICINE (1999-2003)</b>  Ph.D. Biomedical Sciences</p> <ul style="list-style-type: none"> <li>• Distinction</li> <li>• DOD Breast Cancer Pre-doctoral Fellowship (3-year award)</li> <li>• Distinction on Comprehensive Exams</li> </ul> <p><b>UNIVERSITY OF NEW MEXICO (1999-2003)</b>  B.S. Computer Science</p> <ul style="list-style-type: none"> <li>• Magna Cum Laude</li> </ul> <p><b>UNIVERSITY OF NEW MEXICO (1995-1999)</b>  B.S. Biochemistry</p> <ul style="list-style-type: none"> <li>• Robert B. Lofffield Award for Research in Biochemistry and Molecular Biology</li> <li>• Biochemistry Departmental Honors: Summa Cum Laude</li> <li>• University Honors: Magna Cum Laude</li> <li>• UNM Presidential Scholarship</li> <li>• UNM New Mexico Scholarship</li> <li>• National Institute of Peace Essay Scholarship</li> </ul>
<p><b>Technical Proficiencies</b></p>	<p>Parallel Algorithms and High Performance Computing</p> <ul style="list-style-type: none"> <li>• MPI, OpenMP, CUDA, OpenCL, CUBLAS, CUFFT, Vectorization, etc.</li> </ul> <p>Scientific Computing and Software Development</p> <ul style="list-style-type: none"> <li>• C/C++/Fortran Programming, Object-Oriented Design, Standard Template Library, Template Meta-Programming, LAPACK, BLAS, GNU Scientific Library, Doxygen API, Subversion, GDB, TotalView, Dimensionality Reduction, Evolutionary Algorithms, Supervised Learning/Support Vector Machines, MATLAB/Octave, UNIX System Administration, Limited Windows Administration, Shell Scripting, Limited HTML, etc.</li> </ul> <p>Development and application of biophysics &amp; bio/chem – informatics:</p> <ul style="list-style-type: none"> <li>• LAMMPS, Dock, AutoDock, Tinker, Ghemical, Sybyl, InsightII, Affinity, FlexiDock, Discover, Modeler, Catalyst, Profit, Procheck, LUDI, VMD, Pymol, Molscript, ClustalW, Signature, SVMlight, PM-Dreamer, ESSEB, kMD, etc.</li> </ul>

**Research and Professional Experience****ADJUNCT ASSISTANT PROFESSOR (2009-Present)**

Department of Biochemistry and Molecular Biology  
University of New Mexico, Albuquerque, New Mexico

**SENIOR MEMBER OF THE TECHNICAL STAFF (2003-Present)**

Computational Biology (Dept 1412)

Sandia National Laboratories, Albuquerque, New Mexico

- Research and Development in Algorithms for High Performance Computing, Computational Biology, Structure-Based Design, and Neural Computation

**GRADUATE STUDIES (1999-2003)**

Mentor: David Vander Jagt, Ph.D.

- Topic: Type I 17- $\beta$ -Hydroxysteroid Dehydrogenase as a Target for Breast Cancer

**BIOCOMPUTING SYSTEM ADMINISTRATOR (2000-2003)**

Department of Biochemistry and Molecular Biology

University of New Mexico, Albuquerque, New Mexico

- Initial Installation of an IRIX Network and Software Packages for Biocomputing (now maintained by UNM Biocomputing Center)
- Departmental Irix/Linux Administrative Support Including Software Support for Biocomputing Applications

**COMPUTATIONAL BIOLOGY (Graduate Rotation, 1999)**

Aaron Halpern, PhD

- Programming Work in Multiple Sequence Alignment (ClustalW)

**RESEARCH ASSISTANT (1999)**

Department of Biochemistry and Molecular Biology

University of New Mexico, Albuquerque, New Mexico

- Computer Support for Molecular Modeling
- Lab Research in Enzyme Kinetics

**BIOCHEMISTRY UNDERGRADUATE RESEARCH (1998-1999)**

Dr. David Vander Jagt and Lucy Hunsaker

Department of Biochemistry and Molecular Biology

University of New Mexico, Albuquerque, New Mexico

- Kinetic and Computational Studies on Malarial LDH Inhibition

**CHEMISTRY UNDERGRADUATE RESEARCH (1997-1998)**

Dr. Lorraine Deck

Department of Chemistry

University of New Mexico, Albuquerque, New Mexico

- Performed Research in Organic Synthesis of Enzyme Inhibitors as Drug Targets

**DATABASE DESIGN CONSULTANT (1998)**

Capital Bank

Albuquerque, New Mexico

- Developed database for mailing lists and automated data entry from scanned documents containing addresses of the wealthy.

<b>Service</b>	<p><b>REFeree FOR</b></p> <ul style="list-style-type: none"> <li>• Journal of Chemical Information and Modeling</li> <li>• IEEE Engineering in Medicine and Biology</li> </ul> <p><b>AMERICAN CHEMICAL SOCIETY</b></p> <ul style="list-style-type: none"> <li>• Professional Member 2005-</li> <li>• Undergraduate Member 1997-1999</li> </ul>
<b>Teaching Experience</b>	<p><b>MENTOR FOR GRADUATE RESEARCH ROTATIONS (Sandia)</b></p> <ul style="list-style-type: none"> <li>• Ariella Sasson <ul style="list-style-type: none"> <li>○ DOE CSGF Graduate Fellow (Summer Practicum 2007)</li> <li>○ Modeling the activities of resveratrol analogs using Kernel Molecular Dynamics</li> </ul> </li> <li>• Babatunde Oguntade (Co-mentor with Steve Plimpton) <ul style="list-style-type: none"> <li>○ CSRI Graduate Student (Summer 2007)</li> <li>○ Anisotropic force-fields and rotational diffusivity for aspherical particles</li> </ul> </li> </ul> <p><b>BIOMEDICAL SCIENCES 548 (2009)</b></p> <ul style="list-style-type: none"> <li>• Guest speaker – “The domain and computation problems in molecular biophysics and informatics.”</li> </ul> <p><b>BIOMEDICAL SCIENCES 505-007 (Introduction to Biocomputing)</b></p> <ul style="list-style-type: none"> <li>• Wrote Introductory Handouts Including an Introduction to UNIX Computing</li> <li>• Wrote Handouts on the Theory of Docking for Independent Learning</li> <li>• Developed a Non-HTML-Based On-Screen Tutorial System for UNIX and Windows Systems (C++)</li> <li>• Developed Step-by-Step Tutorials for Independent Training in the Theory and use of UNIX, the Sybyl Computational Chemistry Package (Tripos), and Flexible Docking Software (AutoDock).</li> </ul> <p><b>UNDERGRADUATE, GRADUATE, AND MEDICAL STUDENT PROJECTS</b></p> <ul style="list-style-type: none"> <li>• Guided the Biocomputational Aspects of Student Projects</li> <li>• Trained Students in the Theory and Use of Various Biocomputing Packages Including Applications in Minimization, Dynamics, Flexible Ligand Docking, Molecule Superimposition, Protein Structure Analysis, Protein Structure Prediction, QSAR, De Novo Inhibitor Design, and Visualization (Sybyl, InsightII, AutoDock, Affinity, FlexiDock, Discover, Modeler, Catalyst, Profit, Procheck, LUDI, VMD, Pymol, Molscrip, and others).</li> <li>• Developed Software and Scripts to Aid in Student Work including Platform-Independent scripts for Distributing Docking jobs to run Embarrassingly Parallel Library Docking and a Suite of C++ software for PDB File Format Manipulations and Limited Docking Analysis.</li> </ul> <p><b>PRESENTATIONS REFLECTING STUDENT WORK</b></p> <p>Torres, V., <b>Brown, W.M.</b>, Deck, L.M. and Vander Jagt, D.L., Inhibition of Bacterial D-Specific Lactate Dehydrogenase by Gossypol Derivatives and Analogs. 2000: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p>

<p><b>Teaching Experience (Continued)</b></p>	<p>Woodcock, K.A., Deck, J., <b>Brown, W.M.</b> and Vander Jagt, D.L., Pancreatic Cholesterol Esterase: A Potential Drug Target in the Treatment of Heart Disease and the Development of Selective Inhibitors. 2000: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p>Hatch, M.S., <b>Brown, W.M.</b>, Deck, L.M. and Vander Jagt, D.L., Inhibition of Cholesterol Esterase from <i>Candida cylindracea</i> by Substituted Pyrones. 2001: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p>Metzger IV, L.E., <b>Brown, W.M.</b>, Hunsaker, L.A. and Vander Jagt, D.L., Comparative Computational Modelling and Experimental Assessment of Bifunctional Upa Inhibitors. 2001: <i>N.S.F. Research Experience for Undergraduates Program, Dept. of Chemistry, UNM.</i></p> <p>Metzger IV, L.E., <b>Brown, W.M.</b>, Montes, V. and Vander Jagt, D.L., Urokinase Plasminogen Activator (Upa) and Metastasis: Developing New Inhibitors of Human Upa. 2001: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p>Montes, V. and Vander Jagt, D.L., Urokinase Plasminogen Activator (Upa) and Metastasis: Developing New Inhibitors of Human Urokinase (Upa). 2001: <i>Medical Student Research Day (First Place Winner).</i></p> <p>Hoard, A., <b>Brown, W.M.</b> and Vander Jagt, D.L., Homology Modeling of Lactate Dehydrogenases from Four Species of Human Malarial Parasites. 2002: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p>Hoard, A., <b>Brown, W.M.</b> and Vander Jagt, D.L., Lactate Dehydrogenase a as a Target for Anti-Cancer Drug Sensitization. 2002: <i>Pathways to Research Careers.</i></p> <p>Metzger IV, L.E., <b>Brown, W.M.</b> and Vander Jagt, D.L., Qsar Analysis and Structure-Based Drug Design of Novel Inhibitors of Human Urokinase. 2002: <i>Pathways to Research Careers.</i></p> <p>Metzger IV, L.E., Heynekamp, J., <b>Brown, W.M.</b>, Montes, V., Hunsaker, L.A., Deck, L.M. and Vander Jagt, D.L., Structure-Based Design of Bifunctional S1-Site Inhibitors of Human Urokinase-Type Plasminogen Activator. 2002: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p>Mickelsen, S.R., <b>Brown, W.M.</b>, Hunsaker, L.A., Royer, R.E., Deck, L.M. and Vander Jagt, D.L., Modeling Selective Inhibitors of Lactate Dehydrogenase a Suggests Key Interactions for Rational Drug Design. 2002: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p>
<p><b>Invited Talks</b></p>	<p>UNM Biocomputing Software and Applications to Structure-Based Drug Design. 2001: <i>University of New Mexico School of Medicine, Albuquerque, NM.</i></p> <p>Creating Active Site Boundaries: A Comparison of Two Algorithms and Application to Flexible Docking. 2002: <i>Rocky Mountain Regional American Chemical Society Symposium on Drug Discovery. Albuquerque, NM.</i></p>

<b>Invited Talks (Continued)</b>	<p>New Approach for Characterization of Binding-Site Search Space. 2003: <i>UNM Biocomputing Symposium. Albuquerque, NM.</i></p> <p>Calculating Molecular Properties from Simulation Using Kernel Molecular Dynamics. 2007: <i>UNM Biocomputing Symposium. Albuquerque, NM.</i></p> <p>Kernel Molecular Dynamics. 2007: <i>Army Research Laboratory. Baltimore, MD.</i></p> <p>Advanced Mathematical Methods for Molecular Property Prediction. 2009: <i>Innovation in Cancer Management Workshop, MD Anderson Cancer Center, Houston, TX.</i></p> <p>Porting LAMMPS to GPUs. 2010: <i>SOS 14 Conference, Savannah, GA.</i></p>
<b>Presentations</b>	<p><b>Brown, W.M.</b> and Deck, L.M., Organic Synthesis of Substituted Hydroxynaphthoic Acids. 1998: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p><b>Brown, W.M.</b>, Selective Inhibitors of <i>Plasmodium Falciparum</i> Lactate Dehydrogenase: A Target for Anti-Malarial Drug Design. 1999: <i>Biochemistry and Molecular Biology Annual Retreat.</i></p> <p><b>Brown, W.M.</b>, Hunsaker, L.A., Deck, L.M. and Vander Jagt, D.L., Pan-Active Site Inhibition: Inhibitor Specificity through Competitive Binding at Both Substrate and Cofactor Sites. 2000: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p><b>Brown, W.M.</b>, Computational Methods in Drug Design: Targets for Cancer, Malaria, Diabetes, and Heart Disease. 2001: <i>Biomedical Sciences Graduate Recruitment Day, University of New Mexico.</i></p> <p><b>Brown, W.M.</b>, Royer, R.E., Deck, L.M., Hunsaker, L.A. and Vander Jagt, D.L., The Cofactor Binding Site of Human 17-Beta-Hydroxysteroid Dehydrogenase Type I as a Drug Target. 2001: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p> <p><b>Brown, W.M.</b>, Royer, R.E., Deck, L.M., Hunsaker, L.A. and Vander Jagt, D.L., The Cofactor Binding Site of Human 17-Beta-Hydroxysteroid Dehydrogenase Type 1 as a Drug Target. 2001: <i>Experimental Biology 2001, Orlando Florida.</i></p> <p><b>Brown, W.M.</b>, Barlow, J., Hunsaker, L.A., Royer, R.E., Deck, L.M. and Vander Jagt, D.L., Active Site Analysis and Rational Design of Hydroxysteroid Dehydrogenase Inhibitors. 2002: <i>Department of Defense Breast Cancer Research Meeting, Orlando Florida.</i></p> <p><b>Brown, W.M.</b>, Barlow, J., Royer, R.E., Deck, L.M., Hunsaker, L.A. and Vander Jagt, D.L., Rational Design of 17-Beta-Hydroxysteroid Dehydrogenase Inhibitors: Computational Methods for Lead Optimization. 2002: <i>Biochemistry and Molecular Biology Sevilleta Research Retreat.</i></p>

**Presentations  
(Continued)**

**Brown, W.M.**, Hunsaker, L.A., Deck, L.M., Royer, R.E. and Vander Jagt, D.L., 17-Beta-Hydroxysteroid Dehydrogenase Type 1: Computational Design of Active Site Inhibitors Targeted to the Rossmann Fold. 2002: *Enzymology and Molecular Biology of Carbonyl Metabolism 11th International Meeting, Ystad Sweden.*

Vander Jagt, T., **Brown, W.M.**, Hoard, A., Hunsaker, L.A., Deck, L.M., Royer, R.E. Piper, R., Dame, J., Makler, M., Vander Jagt, D.L. Structure and Kinetic Properties of Lactate Dehydrogenases from Four Species of Human Malarial Parasites. 2003: *Experimental Biology, San Diego, California.*

Martin, S., **Brown, W.M.**, Strauss, C., Rintoul, M., Faulon, J.L. Predicting Protein-Protein Interactions with Applications to  $\beta$ -strand Ordering. 2005: *Genomes-to-Life Program Project Meeting, Washington D.C.*

Faulon, J.L., **Brown, W.M.**, Martin, S. Structure Inference and Design in Cheminformatics and Bioinformatics. 2005: *SIAM Conference on Computational Science and Engineering, Orlando, Florida.*

Faulon, J.L., **Brown, W.M.**, Martin, S. Reverse Engineering Chemical Structure from Molecular Descriptors: How Many Solutions? 2005: *American Chemical Society National Meeting, San Diego, California.*

Martin, S., Kenneke, J., **Brown, W.M.**, Faulon, J.L. Inverse QSAR Analysis for Improving Predictions of Chemical Toxicity. 2005: *EPA Science Forum, Washington, D.C.*

**Brown, W.M.**, Martin, S., Kenneke, J. Predicting Protein-Protein Interactions Using Signature Products with an Application to  $\beta$ -strand Ordering, 2005: *NM Bioinformatics Symposium, Santa Fe, NM.*

**Brown, W.M.**, Martin, S., Faulon, J.L. Protein Informatics. 2005: *GTL Project Meeting, Seattle, WA.*

Faulon, J.L., **Brown, W.M.**, Martin, S. Structure Inference and Design in Cheminformatics and Bioinformatics. 2005: *SIAM Conference on Computational Science and Engineering, Orlando, FL.*

Martin, S., **Brown, W.M.**, Faulon, J.L.. Predicting Activated Metabolites using QSAR. 2005: *Sandia Biotech Council Meeting, Santa Fe, NM.*

**Brown, W.M.**, Faulon, J.L., Martin, S. Inverse Problems in Cheminformatics and Bioinformatics. 2005: *UNM Biocomputing Symposium, Albuquerque, NM.*

**Brown, W.M.**, Aspherical Particles in Molecular Dynamics. 2007: *Nanoparticle Flow Consortium, Albuquerque, NM.*

**Brown, W.M.**, Martin, S. Molecular Property Prediction Using Kernel Molecular Dynamics. 2007: *SIAM Conference on Computational Science and Engineering, Costa Mesa, CA.*

<p><b>Presentations (Continued)</b></p>	<p>Coutsias, E.A., <b>Brown, W.M.</b>, Watson, J.-P. Geometrical methods for the efficient exploration of protein conformation space. 2008: <i>IMA Conference on Protein Folding, Minneapolis, MN.</i></p> <p><b>Brown, W.M.</b> Molecular Modeling of Ellipsoidal Nanoparticles. 2008: <i>Nanoparticle Flow Consortium, Sante Fe, NM.</i></p> <p>Crozier, P.S., <b>Brown, W.M.</b>, Wang, P. Harnessing GPU speed to accelerate LAMMPS particle simulations. 2009: <i>SC - Supercomputing, Portland, OR.</i></p> <p><b>Brown, W.M.</b>, Wang, P., Crozier, P.S., Plimpton, S. LAMMPS on GPUs – A Tutorial. 2010: <i>LAMMPS Users Workshop, Albuquerque, NM.</i></p> <p><b>Brown, W.M.</b>, Crozier, P.S. GPU Acceleration of Aspherical Particle Simulations. 2010: <i>LAMMPS Users Workshop, Albuquerque, NM.</i></p>
<p><b>Published Abstracts and Conference Proceedings</b></p>	<p><b>Brown, W.M.</b> and Vander Jagt, D.L., Pan-Active Site Inhibition: Inhibitor Specificity through Competitive Binding at Both Substrate and Cofactor Sites. <i>FASEB Journal</i>, 2000. <b>14</b>(8): p. 486.</p> <p><b>Brown, W.M.</b>, Royer, R.E., Deck, L.M., Hunsaker, L.A. and Vander Jagt, D.L., The Cofactor Binding Site of Human 17-Beta-Hydroxysteroid Dehydrogenase Type 1 as a Drug Target. <i>FASEB Journal</i>, 2001. <b>15</b>(5): p. A1159.</p> <p>Deck, L.M., Stoddard, M., Hunsaker, L.A., <b>Brown, W.M.</b> and Vander Jagt, D.L., Selective Inhibition of Cholesterol Esterase from <i>Candida cylindracea</i> by 3-Alkyl-6-Chloro-2-Pyrones. <i>FASEB Journal</i>, 2001. <b>15</b>(5): p. A1161.</p> <p><b>Brown, W.M.</b>, Barlow, J., Royer, R.E., Deck, L.M., Hunsaker, L.A. and Vander Jagt, D.L., Rational Design of 17-Beta-Hydroxysteroid Dehydrogenase Inhibitors: Computational Methods for Lead Optimization. <i>Cancer Research</i>, 2002. <b>43</b>: p. A738.</p> <p>Deck, L.M., Heynekamp, J., Metzger IV, L.E., <b>Brown, W.M.</b>, Montes, V.N. and Vander Jagt, D.L., Structure-Based Design of Bifunctional S1-Site Inhibitors of Human Urokinase-Type Plasminogen Activator. <i>Cancer Research</i>, 2002. <b>43</b>: p. A739.</p> <p>Vander Jagt, T., <b>Brown, W.M.</b>, Hoard, A., Hunsaker, L.A., Deck, L.M., Royer, R.E., Piper, R., Dame, J., Makler, M., Vander Jagt, D.L. Structure and Kinetic Properties of Lactate Dehydrogenases from Four Species of Human Malarial Parasites. <i>FASEB Journal</i>, 2003. <b>17</b>: p. A981.</p> <p>Faulon, J.L., <b>Brown, W.M.</b>, Martin, S. Reverse engineering chemical structures from molecular descriptors: How many solutions? <i>Abstracts of Papers of the American Chemical Society</i>, 2005. <b>229</b>: p. U600-U600.</p> <p>Martin, S., <b>Brown, W.M.</b>, Faulon, J.L., Weis, D., Visco, D., Kenneke, S. Inverse Design of Large Molecules using Linear Diophantine Equations. <i>Proceedings of the IEEE Computational Systems Biology Conference</i>, 2005. p. 11-16.</p>

Peer-  
Reviewed  
Publications

Vander Jagt, D.L., Hassebrook, R.K., Hunsaker, L.A., **Brown, W.M.** and Royer, R.E. Metabolism of the 2-Oxoaldehyde Methylglyoxal by Aldose Reductase and by Glyoxalase-I: Roles for Glutathione in Both Enzymes and Implications for Diabetic Complications. *Chemico-Biological Interactions*, 2001. **130**(1-3): p. 549-562.

Stoddard Hatch, M., **Brown, W.M.**, Deck, J.A., Hunsaker, L.A., Deck, L.M. and Vander Jagt, D.L. Inhibition of Yeast Lipase (Crl1) and Cholesterol Esterase (Crl3) by 6-Chloro-2-Pyrones: Comparison with Porcine Cholesterol Esterase. *Biochim Biophys Acta*, 2002. **1596**(2): p. 381-91.

**Brown, W.M.**, Hunsaker, L.A., Deck, J.A., Royer, R.E. and Vander Jagt, D.L. 17-Beta-Hydroxysteroid Dehydrogenase Type 1: Computational Design of Active Site Inhibitors Targeted to the Rossmann Fold. *Chemico-Biological Interactions*, 2003. **143**: p. 481-491.

Vander Jagt, D.L., Hunsaker, L.A., Young, B.S. and **Brown, W.M.** Aldo-Keto Reductase-Catalyzed Detoxication of Endogenous Aldehydes Associated with Diabetic Complications. *American Chemical Society Series*, 2004. **865**: p. 23-35.

**Brown, W.M.**, Hoard, A., Vanderjagt, T.A., Hunsaker, L.A., Deck, L.M., Royer, R.E., Piper, R.C., Dame, J., Makler, D.L., and Vander Jagt, D.L. Comparative structural analysis and kinetic properties of lactate dehydrogenases from four species of human malarial parasites. *Biochemistry*, 2004. **43**: p. 6219-6229.

**Brown, W.M.** and Vander Jagt, D.L. Creating Artificial Binding Pocket Boundaries to Improve the Efficiency of Flexible Ligand Docking. *Journal of Chemical Information and Computer Science*, 2004. **44**: p. 1412-1422.

Sillerud, L.O., Burks, E.J., **Brown, W.M.**, Brown, D.C., and Larson, R.S. NMR solution structure of a potent cyclic nonapeptide inhibitor of ICAM-1-mediated leukocyte adhesion produced by homologous amino acid substitution. *Journal of Peptide Research*, 2004. **44**: p. 1412-1422.

**Brown, W. M.**, Faulon, J.L., Sale, K. A Deterministic Algorithm for Constrained Enumeration of Transmembrane Protein Folds. *Computational Biology and Chemistry*, 2005. **29**: p. 143-150.

Faulon, J.L., **Brown, W.M.**, Martin, S. Reverse Engineering Chemical Structures from Molecular Descriptors: How Many Solutions? *Journal of Computer-Aided Molecular Design*, 2005. **19**: p. 637-650.

**Brown, W.M.**, Martin, S., Strauss, C., Faulon, J.L. Predicting  $\beta$ -strand Packing Interactions using the Signature Product. *Journal of Molecular Modeling*, 2006. **12**: p. 355-361.

**Brown, W. M.** and Bäckér, A. Optimal Neuronal Tuning for Finite Stimulus Spaces. *Neural Computation*, 2006. **18**: p. 1511-1526.

**Brown, W.M.**, Martin, S., Rintoul, M.D., Faulon, J.L. Designing Novel Polymers with Targeted Properties using the Signature Molecular Descriptor. *Journal of Chemical Information and Modeling*, 2006. **46**: p. 826-835.

<p><b>Peer-Reviewed Publications (Continued)</b></p>	<p><b>Brown, W.M.</b>, Sasson, A., Bellew, D.R., Hunsaker, L.A., Martin, S., Leitao, A., Deck, L.M., Vander Jagt, D.L., Oprea, T.I. Efficient Calculation of Molecular Properties from Simulation using Kernel Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i>, 2008. <b>48</b>: 1626-1637.</p> <p><b>Brown, W.M.</b>, Martin, S., Pollock, S.N., Coutsiyas, E.A., Watson, J.-P., Algorithmic Dimensionality Reduction for Molecular Structure Analysis. <i>Journal of Chemical Physics</i>, 2008. <b>129</b>: 064118 p. 1-13.</p> <p><b>Brown, W.M.</b>, Petersen, M.K., Plimpton, S.J., Grest, G.S., Liquid Crystal Nanodroplets in Solution. <i>Journal of Chemical Physics</i>, 2009. <b>130</b>: 044901 p. 1-7.</p> <p>Gray, G.A., Williams, P.J., Sale, K.L., <b>Brown, W.M.</b>, Faulon, J.-L. Disparate Data Fusion for Protein Phosphorylation Prediction. <i>Annals of Operations Research</i>, 2010. <b>174</b>: p. 219-235.</p> <p><b>Brown, W.M.</b>, Thompson, A.P., Schultz, P.A., Efficient Hybrid Evolutionary Optimization of Interatomic Potential Models. <i>Journal of Chemical Physics</i>, 2010. 024312 p. 1-10.</p>
<p><b>Book Chapters</b></p>	<p>Martin, S., <b>Brown, W.M.</b>, Faulon, J.-L., "Using Product Kernels to Predict Protein Interactions," in <i>Advances in Biochemical Engineering/Biotechnology: Protein-Protein Interactions</i>, H. Seitz and M. Werther, Eds., Springer-Verlag.</p>
<p><b>Technical Reports</b></p>	<p><b>Brown, W.M.</b>, Faulon, J.L., Gray, G.A., Hunt, T.W., Schoeniger, J.S., Shirley, D., Slepoy, A., Young, M.M., Sale, K.L. Model-Building Codes for Membrane Proteins. <i>SAND Reports</i>, 2004. 6383: p. 1-75.</p> <p>May, E.E., Johnston, A.M., Watson, J.P., Hart, W.E., <b>Brown, W.M.</b> Deciphering the Genetic Regulatory Code Using an Inverse Error Control Coding Framework. <i>SAND Reports</i>, 2005. 1029: p. 1-41.</p> <p><b>Brown, W.M.</b>, Davidson, G.S. Interactomes to Biological Phase Space: A call to begin thinking at a new level in computational biology. <i>SAND Reports</i>, 2007. 6278: p.1-30.</p> <p>Martin, S., <b>Brown, W.M.</b>, Klavans, R., Boyack, K.W., DrL: Distributed Recursive (Graph) Layout. <i>SAND Reports</i>, 2008. 2936: p. 1-10.</p> <p><b>Brown, W.M.</b>, Thompson, A.P., Watson, J.-P., Schultz, P.A. Bridging Scales from Ab Initio Models to Predictive Empirical Models for Complex Materials. <i>SAND Reports</i>, 2008. 6454: p. 1-57.</p> <p>Grest, G. S., <b>Brown, W. M.</b>, Lechman, J. B., Petersen, M. K., Plimpton, S. J., Schunk, P. R. Nanoparticle Flow, Ordering, and Self-Assembly. <i>SAND Reports</i>, 2008. 6516: p. 1-29.</p>

<b>Research Highlights</b>	<p>Scalable GPGPU Accelerated MD Simulations Achieve &gt;150x Speedup on a Single Node. <i>NNSA ASC Quarterly Newsletter</i>. December 2009.</p> <p>Klein Bottle Discovered in Molecular Conformation Data. <i>CCIM News Notes</i>. 2009.</p> <p>New Computational Methods Enable Novel Nanoparticle Simulations. <i>Computational Science Research Highlights</i>. 2009. 1-42 - 1-43.</p> <p>German, J. Beauty, molecules deep. <i>Sandia Technology - A Quarterly Research and Development Magazine</i>. 2008. 9: p. 5-7.</p> <p>German, J. Sandia leads three-year alliance with companies interested in nanoparticle coatings, films. <i>Sandia Lab News</i>. March 14 , 2008.</p>
<b>Software</b>	<p><b>Binding Pocket Surveryor (1999)</b>. <i>W. Michael Brown</i>. Calculation of the macromolecule encapsulating surface, identification of binding pockets and calculation of binding pocket statistics, incorporation into energetic calculations for flexible docking.</p> <p><b>SigProd Ver. 1.0 (2004)</b>. <i>Shawn Martin, Carla Churchwell, and W. Michael Brown</i>. Support vector machines for prediction of protein/peptide/secondary structure element interactions using the signature product. <i>Sandia Copyright Number 764</i>.</p> <p><b>Signature Translator (2004)</b>. <i>Jean-Loup Faulon, Carla Churchwell, and W. Michael Brown</i>. Calculation of the signature molecular descriptor from molecular structure.</p> <p><b>ESSEB (2004)</b>. <i>W. Michael Brown and Jean-Loup Faulon</i>. Constrained enumeration of secondary structure element bundles for prediction of integral membrane protein structures. <i>Sandia Copyright Number 789</i>.</p> <p><b>PVxOrd (2006)</b>. <i>W. Michael Brown, Shawn Martin, and Brian Wylie</i>. Parallel graph drawing and high dimensional embedding.</p> <p><b>LAMMPS</b>. <i>Steve Plimpton, Many Others, W. Michael Brown</i>. Developed a framework for simulation of aspherical particles, an implementation of parallel replica dynamics, and GPGPU acceleration package (Released under GPL).</p> <p><b>Dr. L (2007)</b>. <i>W. Michael Brown, Shawn Martin, Haixia Jia, Jean-Paul Watson</i>. Linear and non-linear dimensionality reduction. (Released under GPL). <i>Sandia Copyright Number 1214</i>.</p> <p><b>PM-Dreamer (2008)</b>. <i>W. Michael Brown</i>. Hybrid evolutionary optimization of empirical models for particle mechanics. (Pending release under GPL). <i>Sandia Copyright Number 1283</i>.</p> <p><b>Geryon (2010)</b>. <i>W. Michael Brown</i>. A unified coprocessor library for OpenCL, CUDA runtime, and CUDA driver. (Pending release under FreeBSD). <i>Sandia Copyright Number 1293</i>.</p>

<b>Completed and Ongoing Research Funding</b>	DAMD17-00-0368 (Brown PI) 2000 – 2003 US Army/DOD Breast Cancer Program Type I 17- $\beta$ -Hydroxysteroid Dehydrogenase as a Target for Breast Cancer Role: PI
	DE-AC04-94AL85000 69193/3.1 (Joe Schoeniger PI) 2003 – 2004 DOE Laboratory Directed Research and Development (LDRD) Interfacial Bioscience Grand Challenge (IBIG) Role: Co-Investigator
	DE-AC04-94AL85000 7101/13.10 (Mark Rintoul PI) 2004 – 2005 DOE Computer Science Research Foundation (CSRF) Inverse Molecular Design Role: Co-Investigator
	DE-AC04-94AL85000 547/02.09 (Alex Backer PI) 2004 – 2005 DOE Mathematical, Information, and Computational Sciences Meaning: Dimensionality, Representation, Networks and Learning Role: Co-Investigator
	DE-AC04-94AL85000 54542/04 (Grant Heffelfinger PI) 2004 – 2005 DOE Genomes-to-Life Carbon Sequestration in Synechococcus Sp.: From Molecular Machines to Hierarchical Modeling Role: Co-Investigator
	IAG DW89921601 Task 3 (Shawn Martin PI) 2004-2006 Environmental Protection Agency Inverse-QSAR for Prediction of Activated Metabolites Role: Co-Investigator
	U54 MH074411-01 (John Lazo PI) 2005 NIH Molecular Libraries Screening Network (Informatics Core) Role: Co-Investigator
	DE-AC04-94AL85000 7101/23.5 (Jean-Paul Watson PI) 2006-2008 DOE Computer Science Research Foundation (CSRF) A Visualization Framework for Optimization and Uncertainty Calculations Role: Co-Investigator
	Nanoparticle Consortium CRADA (Randall Schunk PI) 2006-2008 DOE, 3M, BASF, Corning, Proctor & Gamble, National Starch and Chemical Coupled Molecular Dynamics Flow Solver Role: Co-Investigator
	DE-AC04-94AL85000 127740/1 (W. Michael Brown PI) 2008-2009 DOE (LDRD) Bridging Scales from Ab Initio Models to Predictive Empirical Models for Complex Materials Role: PI

<b>Completed and Ongoing Research Funding (Continued)</b>	DE-AC04-94AL85000 7101/24.1 (Mark Rintoul PI) DOE (CSRF) Exascale Computing Role: Co-Investigator	2009-2011
	DE-AC04-94AL85000 130732/03 (Greg Wagner PI) DOE (LDRD) Equation Free Simulation Methods Role: Co-Investigator	2009-2011
	DE-AC04-94AL85000 131762/3 (W. Michael Brown PI) DOE (CSRF) Developing Interatomic Potentials from Ab Initio Simulation Role: PI	2009-2011