Nathan Andrew Baker

Curriculum Vitae

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Nathan A. Baker, Ph.D. is a Laboratory Fellow in the Applied Statistics and Computational Modeling Group at Pacific Northwest National Laboratory (PNNL). His research focuses on the development of new algorithms and mathematical methods in biophysics, nanotechnology, and informatics. Current projects include new computational methods for modeling solvation in biomolecular systems (`http://www.poissonboltzmann.org/`), mathematical methods for mesoscale materials modeling (`http://www.pnnl.gov/computing/cm4/`), and development of new methods for signature discovery (`http://signatures.pnnl.gov`).

Experience

2015–present **Visiting Professor**, *Division of Applied Mathematics, Brown University*, Providence, RI.

2012–present **Laboratory Fellow**, *Computational and Statistical Analytics Division, Pacific Northwest National Laboratory*, Richland, WA.

2013–2015 **Technical Group Manager**, *Applied Statistics and Computational Modeling Group, Pacific Northwest National Laboratory*, Richland, WA.

2010–2012 **Chief Scientist**, *Computational and Statistical Analytics Division, Pacific Northwest National Laboratory*, Richland, WA.

2006–2010 **Associate Professor (tenured)**, *Department of Biochemistry and Molecular Biophysics, Washington University in St Louis*, St Louis, MO.

2002–2006 **Assistant Professor**, *Department of Biochemistry and Molecular Biophysics, Washington University in St Louis*, St Louis, MO.

Education

2001–2002 **Postdoctoral Researcher**, *Department of Chemistry and Biochemistry, University of California San Diego*, La Jolla, CA.

1997–2001 **PhD, Physical Chemistry**, *University of California San Diego*, La Jolla, CA.

1993–1997 **BS, Chemistry**, *University of Iowa*, Iowa City, IA, Honors and highest distinction.

Selected honors and awards

2012 **Fellow**, *American Association for the Advancement of Science*.

2010 **Cancer Biomedical Informatics Grid (caBIG) Connecting Collaborators Award**, *National Cancer Institute*.

2007 **Hewlett-Packard Junior Faculty Excellence Award**, *American Chemical Society*.

2004 **Research Fellowship**, *Alfred P Sloan Foundation*.

2001 **All-hands Meeting Student Poster Award**, *National Partnership Advanced Computational Infrastructure*.

2001 **Kamen Award for Outstanding Thesis in the Biological Sciences**, *University of California San Diego*.

2000 **IBM Student Award in Computational Chemistry, First Place**, *American Chemical Society*.

1999 **Predoctoral Fellowship**, *Burroughs-Wellcome La Jolla Interfaces in Science Program*.

1998–1999 **Letters of Commendation for Teaching**, *University of California San Diego*.

1997 **Predoctoral Fellowship**, *Howard Hughes Medical Institute*.

1997 **Collegiate Scholar**, *University of Iowa*.

1997 **Member**, *Phi Beta Kappa*, University of Iowa.

1997 **Undergraduate Liberal Arts Commencement Speaker**, *University of Iowa*.

1995 **Undergraduate Fellowship**, *Barry M Goldwater Foundation*.

Service

Selected extramural service

2014–2017 **Associate Editor**, *Biophysical Journal*, Biophysical Society.

2015–2016 **External Advisory Board Member**, *Visual Analytics for sense-making in Criminal Intelligence analysis (VALCRI) Project*, European Commission.

2014–present **Editorial Board member**, *Scientific Data*, Nature Publishing Group.

2012–2016 **Member**, *Macromolecular Structure and Function D Study Section*, National Institutes of Health.

2014–2016 **Organizing committee member**, *Conference on Data Analysis (CoDA)*.

2014–2015 **Reviewer**, *INCITE Biological Sciences Review Panel*, Advanced Scientific Computing Research, Department of Energy.

2015 **Panelist**, *National Strategic Computing Initiative Panel*, HPC User Forum meeting.

2015 **Reviewer**, *J9BA Life Sciences Red Team Review*, Defense Threat Reduction Agency.

2015 **Advisory board member**, *Data Management and Analysis Advisory Board*, Novozymes.

2014 **Scientific Advisory Board member**, *eNanoMapper Project*, European Commission.

2012–2014 **Co-Chair**, *Nanotechnology Databases and Ontologies, US-EU Communities of Research*, OSTP National Nanotechnology Coordinating Office.

2011–2014 **Editor-in-Chief**, *Computational Science and Discovery*, Institute of Physics.

2009–2014 **Editorial Board member**, *Computational Science and Discovery*, Institute of Physics.

2009–2014 **Chair**, *E56.01 Nanotechnology Subcommittee on Informatics and Terminology*, ASTM.

2008–2014 **Section Editor**, *Annual Reports in Computational Chemistry*, American Chemical Society.

2008–2014 **Editorial Board member**, *Biophysical Journal*, Biophysical Society.

2008–2014 **Member**, *Faculty of 1000 Biology*.

2005–2014 **Ad hoc member**, *Various study sections*, National Institutes of Health.

2013 **Reviewer**, *Progress in Research on Environmental, Health, and Safety Aspects of Engineered Nanomaterials*, National Academy of Sciences.

2012–2013 **Member**, *Working Group 1, Nomenclature and Terminology, U.S. Technical Advisory Group*, ANSI, ISO International Organization for Standardization.

2011–2013 **Organizing committee member**, *Nanoinformatics Workshop*.

2011–2013 **Organizing committee member**, *Protein Electrostatics Workshop*, Telluride Science Research Center.

2010–2013 **Advisory committee member**, *Nanomaterial Registry*, RTI International & National Institutes of Health.

2009–2013 **Working group lead**, *Nanotechnology Working Group, caBIG Integrated Cancer Research Workspace*, National Cancer Institute.

2008–2013 **Member**, *Nanotechnology Working Group, caBIG Integrated Cancer Research Workspace*, National Cancer Institute.

2007–2013 **Member**, *Committee for Professional Opportunities for Women*, Biophysical Society.

2006–2013 **Reviewer**, National Science Foundation.

2012 **Panelist**, *National Academies Board on Environmental Studies and Toxicology Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology Workshop*, National Academies of Science.

2012 **Member**, *Program Committee, caBIG Annual Meeting*, National Cancer Institute.

2010–2012 **Member**, *Public Affairs Committee*, Biophysical Society.

2010 **Advisory board member**, *Integrated Graduate Education and Research Training (IGERT) in Health-Assistive Smart Environments*, Washington State University.

2008–2010 **Topic Page contributor**, Scirus.

2008 **Panelist**, *"Transition from Postdoc to Faculty" Workshop*, Biophysical Society.

2008–2009 **Co-organizer**, *23rd Annual Meeting*, Gibbs Society for Biothermodynamics.

2006–2008 **Member**, *Nanotechnology Alliance Informatics Working Group*, National Cancer Institute.

2005–2008 **Member**, *Program Committee*, Biophysical Society.

2007 **Organizer and chair**, *Early Careers Panel Discussion: Negotiating the Transition to Non-Traditional Careers*, Biophysical Society.

2004–2007 **Member**, *Early Careers Committee*, Biophysical Society.

Selected intramural service

2015–present **Member**, *Interdisciplinary Applied Sciences Planning Committee*, Washington State University Tri-Cities and Pacific Northwest National Laboratory.

2015–present **Advisory committee member**, *Microbes in Transition Initiative Advisory Committee*, Pacific Northwest National Laboratory.

2014–present **Chair**, *PNNL Institutional Computing Steering Committee*, Pacific Northwest National Laboratory.

2015 **Co-chair**, *National Strategic Computing Initiative Planning Committee, co-chair*, Pacific Northwest National Laboratory.

2014–present **Advisory committee member**, *Analysis in Motion Initiative Advisory Committee*, Pacific Northwest National Laboratory.

2013–present **Reviewer**, *ASCR Early Career pre-proposals*, Pacific Northwest National Laboratory.

2013–present **Member**, *Council of Fellows Executive Committee*, Pacific Northwest National Laboratory.

2012–2015 **Lead**, *Signature Discovery Initiative*, Pacific Northwest National Laboratory.

2011–present **Reviewer**, *HHS LDRD proposals*, Pacific Northwest National Laboratory.

2010–present **Chief Scientist**, *Signature Discovery Initiative*, Pacific Northwest National Laboratory.

2014–2015 **Judge**, *Postdoc Symposium*, Pacific Northwest National Laboratory.

2015 **Presenter**, *Computing Assessment Committee*, Pacific Northwest National Laboratory.

2015 **Member**, *Physical and Computational Sciences Directorate Strategy Committee*, Pacific Northwest National Laboratory.

2015 **Advocate**, *Proposal-Writing Workshop development*, Pacific Northwest National Laboratory.

2013–2015 **Presenter**, *Publishing Workshop*, National Security Directorate, Pacific Northwest National Laboratory.

2011–2015 **Lead**, *Signatures Community of Interest Network*, Pacific Northwest National Laboratory.

2015 **Member**, *Diversity Internal Oversight Committee*, Pacific Northwest National Laboratory.

2015 **Member**, *Employee Time Reporting Reform Committee*, Pacific Northwest National Laboratory.

2015 **Member**, *Computational Materials Science Red Team*, Pacific Northwest National Laboratory.

2015 **Biomarkers briefer to Rep. McMorris-Rodgers staffers**, Pacific Northwest National Laboratory.

2011–2014 **Reviewer**, *DHHS Sector LDRD Proposals*, Pacific Northwest National Laboratory.

2012–2014 **Reviewer**, *BES pre-proposals*, Pacific Northwest National Laboratory.

2005–2010 **Director**, *Siteman Center for Cancer Nanotechnology Excellence Biocomputing Core*, Washington University in St Louis.

2007–2010 **Member**, *Program and Student Affairs Committee, Division of Biology and Biomedical Sciences*, Washington University in St Louis.

2009–2010 **Member**, *Nominating Committee*, Biophysical Society.

2007–2010 **Director**, *Computational and Molecular Biophysics graduate program*, Washington University in St Louis.

2004–2010 **Steering committee member**, *Computational and Molecular Biophysics graduate program*, Washington University in St Louis.

2008 **Chair**, *Scientific Collaboration Panel Discussion, Annual Conference on Effective Research Management*, Washington University in St Louis.

2008 **Co-organizer**, *Bridging Research and Teaching Workshop: Innovation at the Crossroads of Chemistry, Physics, and Biology*, Washington University in St Louis.

2003–2008 **Seminar co-organizer**, *Center for Computational Biology*, Washington University in St Louis.

2007 **Member**, *Education Planning Committee, Division of Biology and Biomedical Sciences*, Washington University in St Louis.

2004–2007 **Member**, *Admissions Committee, Division of Biology and Biomedical Sciences*, Washington University in St Louis.

2004–2007 **Mentor**, *Students and Teachers as Researchers (STARS) program*, University of Missouri St Louis.

2006–2007 **Member**, *Faculty Search Committee, Department of Mechanical and Aerospace Engineering*, Washington University in St Louis.

2006 **Member**, *Liaison Committee on Medical Education and IT, School of Medicine*, Washington University in St Louis.

2006 **Co-organizer**, *ICAM/Center for Computational Biology Multiscale Interactions and Dynamics in Biological Systems Workshop*, Washington University in St Louis.

2004 **Member**, *Oversight Committee, Center for Scientific Parallel Computing*, Washington University in St Louis.

Selected community service

2014–present **Communications representative**, *Hansen Park Homeowners Association*, Kennewick, WA.

2012–2014 **Webmaster**, *Hansen Park Homeowners Association*, Kennewick, WA.

2010–2011 **Den leader**, *Cub Scouts*, Kennewick, WA.

2006–2010 **Member, Technology Committee**, *Our Lady of Lourdes School*, St Louis, MO.

2005–2010 **Webmaster**, *Ethical Society Nursery School*, St Louis, MO.

Manuscript review service

Acta Crystallographica, Annals of Biomedical Engineering, Biochemistry, Biochimica et Biophysica Acta - Biomembranes, Bioinformatics, Biomechanics and Modeling in Mechanobiology, Bioorganic and Medicinal Chemistry Letters, Biophysical Chemistry, Biophysical Journal, Biopolymers, BMC Biophysics, Cancer Biomarkers, Communications in Computational Physics, Computational Science and Discovery, Integrative Biology, Journal of Chemical Information and Modeling, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Computational Physics, Journal of Computer-Aided Molecular Design, Journal of Electrostatics, Journal of General Physiology, Journal of Lipid Research, Journal of Mathematical Analysis and Applications, Journal of Mathematical Biology, Journal of Molecular Biology, Journal of Molecular Graphics and Modeling, Journal of Neurophysiology, Journal of Physical Chemistry, Journal of Physical Chemistry B, Journal of Physical Chemistry C, Journal of Physical Chemistry Letters, Journal of Physics Condensed Matter, Journal of the American Chemical Society, Journal of Theoretical Biology, Molecular Informatics, Nature Nanotechnology, Nucleic Acids Research, Physical Biology, Physical Chemistry Chemical Physics, PLoS Computational Biology, PLoS ONE, PMC Biophysics, Proceedings of the National Academy of Sciences, Protein Engineering, Protein Science, Proteins, SIAM Journal on Applied Mathematics, SIAM Review, Soft Matter, Structure, Theoretical Chemistry Accounts,

Grant proposal reviews

American Chemical Society Petroleum Research Fund, National Institutes of Health, National Science Foundation, United States Civilian Research and Development Foundation, United States-Israel Binational Science Foundation, Defense Threat Reduction Agency, United States Air Force Office of Science and Research, DOE ASCR INCITE

Selected funding

2012–2017 **PNNL lead**, *Collaboratory on Mathematics for Mesoscopic Modeling of Materials (FWP 63024)*, DOE ASCR.

2004–2017 **PI**, *APBS: Nanoscale biomolecular electrostatics software (R01 GM069702)*, NIH NIGMS.

2012–2016 **co-PI**, *DNA-DNA interactions with atomic detail (R01 GM099450)*, NIH NIGMS.

2011–2014 **co-I**, *Mechanism of oxysterol activation of membrane cholesterol (R01 HL067773)*, NIH NHLBI.

2012–2013 **PI**, *ISA-TAB curation of electrostatic data*, OpenEye Software.

2010–2013 **co-I**, *Characterization/bioinformatics-modeling of nanoparticle-complement interactions (U01 NS073457)*, NIH NINDS.

2009–2013 **co-PI**, *Collaborative research: Geometric flow approach to implicit solvation modeling (R01 GM090208-01)*, NIH NIGMS.

2004–2013 **co-I**, *National Biomedical Computation Resource (P41 RR0860516)*, NIH NCRR.

2008–2011 **DBP PI**, *Cancer Nanotechnology Knowledgebase for Nanoparticle Analysis and Design (U54 HG004028)*, NIH NHGRI.

2008–2011 **PI**, *caBIG Integrative Cancer Research Workspace (GS-35F-0306J)*, NIH NCI subcontract.

2007–2010 **PI**, *caNanoLab Data Submission Support (N01-CN-12400)*, NIH NCI subcontract.

2005–2010 **Core PI**, *The Siteman Cancer Center Nanotechnology Excellence at Washington University Biocomputing Core (U54 CA11934205)*.

2008–2010 **co-I**, *New Inhibitors of Acetylcholinesterase that Block Inactivation by Organophosphates (HDTRA1-08-C-0015)*, DoD DTRA.

2007–2009 **co-I**, *Loss of Vascular Control in Pediatric Lung Injury: Disruption of NO Biotransport by Oxidative Stress*, Children's Discovery Institute.

2006–2009 **co-PI**, *Allosteric Regulation of the Nickel-dependent NikR Repressor (MCB-0520877)*, NSF MCB.

2005–2007 **PI**, *Molecular Engineering of Thrombin-Based Nanocatalysts*, National Academies Keck Futures Initiative.

Selected mentoring

2015–present **Huan Lei**, *Staff*, Pacific Northwest National Laboratory.

2015–present **Ilke Arslan**, *Staff*, Pacific Northwest National Laboratory.

2015–present **Nathan Hodas**, *Staff*, Pacific Northwest National Laboratory.

2015–present **Juan Brandi**, *Postbac*, Pacific Northwest National Laboratory.

2015–present **Xiu Yang**, *Postdoc*, Pacific Northwest National Laboratory.

2014–2015 **Peter Li**, *High school researcher*, Pacific Northwest National Laboratory.

2014–present **Luke Gosink**, *Staff*, Pacific Northwest National Laboratory.

2013–present **Landon Sego**, *Staff*, Pacific Northwest National Laboratory.

2013–2015 **Huan Lei**, *Postdoc*, Pacific Northwest National Laboratory.

2013–present **Paul Bruillard**, *Staff*, Pacific Northwest National Laboratory.

2013–present **Courtney Corley**, *Staff*, Pacific Northwest National Laboratory.

2015 **Shadya Maldonado**, *Postbac*, Pacific Northwest National Laboratory.

2014–2015 **Minju Chun**, *High school researcher*, Pacific Northwest National Laboratory.

2012–2013 **Max Li**, *High school researcher*, Pacific Northwest National Laboratory.

2011–2013 **Mike Daily**, *Postdoc*, Pacific Northwest National Laboratory.

2011–2013 **Emilie Hogan**, *Postdoc*, Pacific Northwest National Laboratory.

2010–2011 **Shy Brown**, *Postbac*, Pacific Northwest National Laboratory.

2010–2011 **Tyler Harmon**, *Postbac*, Pacific Northwest National Laboratory.

2010 **Marc Sherman**, *MD/PhD student*, Washington University in St Louis.

2009–2010 **Arjun Bahl**, *Undergraduate researcher*, Washington University in St Louis.

2008–2010 **Marcelo Marucho**, *Postdoc*, Washington University in St Louis.

2008–2010 **Michal Lijowksi**, *Bioinformatics curator*, Washington University in St Louis.

2007–2010 **Yong Huang**, *Programmer*, Washington University in St Louis.

2007–2010 **Samir Unni**, *High school and undergraduate researcher*, Washington University in St Louis.

2006–2010 **Dennis Thomas**, *Postdoc*, Washington University in St Louis.

2006–2010 **Brett Olsen**, *PhD student*, Washington University in St Louis.

2006–2010 **Dave Gohara**, *Programmer*, Washington University in St Louis.

2005–2010 **Sunjoo Lee**, *PhD student*, Washington University in St Louis.

2009 **Aditya Nath**, *Undergraduate researcher*, Washington University in St Louis.

2009 **Mark Rosenberg**, *Undergraduate researcher*, Washington University in St Louis.

2007–2009 **Stephen Gradwohl**, *Undergraduate researcher*, Washington University in St Louis.

2008 **Sechin Jain**, *Undergraduate researcher*, Washington University in St Louis.

2003–2009 **Rachel Rice**, *PhD student*, Washington University in St Louis.

2003–2009 **Michael Bradley**, *PhD student*, Washington University in St Louis.

2007–2008 **Tom Richner**, *Undergraduate researcher*, Washington University in St Louis.

2006–2008 **Peter Jones**, *Programmer*, Washington University in St Louis.

2005–2007 **Feng Dong**, *Postdoc*, Washington University in St Louis.

2005 **Jeff Poskin**, *Undergraduate researcher*, Washington University in St Louis.

2005 **Eric Mintun**, *High school researcher*, Washington University in St Louis.

2004 **Prachi Mayenkar**, *High school researcher*, Washington University in St Louis.

2002–2006 **Yuhua Song**, *Postdoc*, Washington University in St Louis.

2002–2006 **Jason Wagoner**, *Undergraduate researcher*, Washington University in St Louis.

2002–2006 **Todd Dolinsky**, *Programmer*, Washington University in St Louis.

2002–2003 **Seongeun Yang**, *Postdoc*, Washington University in St Louis.

Selected publications

Lei, Huan, Xiu Yang, Bin Zheng, Guang Lin, and Nathan A Baker (in press). "Quantifying the influence of conformational uncertainty in biomolecular solvation". In: *Multiscale Modeling & Simulation*.

Harper, Bryan, Dennis Thomas, Satish Chikkagoudar, Nathan Baker, Kaizhi Tang, Alejandro Heredia-Langner, Roberto Lins, and Stacey Harper (2015). "Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity". In: *Journal of Nanoparticle Research* 17.6, pp. 1–12.

Hogan, Emilie, Kyle Monson, and Nathan A Baker (2015). "Energy Minimization of Discrete Protein Titration State Models Using Graph Theory". In: *arXiv preprint arXiv:1507.07021*.

Pan, Wenxiao, Michael Daily, and Nathan A Baker (2015). "Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smoothed particle hydrodynamics". In: *BMC Biophysics* 8.1, p. 7.

Sushko, Maria L, Dennis G Thomas, Suzette A Pabit, Lois Pollack, Alexey V Onufriev, and Nathan A Baker (2015). "The role of correlation and solvation in ion interactions with B-DNA". In: *arXiv preprint arXiv:1506.07951*.

Bielska, Agata A, Brett N Olsen, Sarah E Gale, Laurel Mydock-McGrane, Kathiresan Krishnan, Nathan Andrew Baker, Paul H Schlesinger, Douglas F Covey, and Daniel S Ory (2014). "Side-Chain Oxysterols Modulate Cholesterol Accessibility through Membrane Remodeling". In: *Biochemistry* 53.18, pp. 3042–3051.

Daily, Michael D, Brett N Olsen, Paul H Schlesinger, Daniel S Ory, and Nathan A Baker (2014). "Improved coarse-grained modeling of cholesterol-containing lipid bilayers". In: *Journal of Chemical Theory and Computation* 10.5, pp. 2137–2150.

Gosink, Luke J, Emilie A Hogan, Trenton C Pulsipher, and Nathan A Baker (2014). "Bayesian model aggregation for ensemble-based estimates of protein pK_a values". In: *Proteins: Structure, Function, and Bioinformatics* 82.3, pp. 354–363.

Pham, Christine TN et al. (2014). "Application of a hemolysis assay for analysis of complement activation by perfluorocarbon nanoparticles". In: *Nanomedicine: Nanotechnology, Biology and Medicine* 10.3, pp. 651–660.

Richardson, C et al. (2014). *Materials Frontiers to Empower Quantum Computing*. Technical report. Los Alamos National Laboratory.

Thomas, Dennis G, Satish Chikkagoudar, Alejandro Heredia-Langner, et al. (2014). "Physicochemical signatures of nanoparticle-dependent complement activation". In: *Computational Science & Discovery* 7.1, p. 015003.

Tolokh, Igor S, Suzette A Pabit, Andrea M Katz, Yujie Chen, Aleksander Drozdetski, Nathan Baker, Lois Pollack, and Alexey V Onufriev (2014). "Why double-stranded RNA resists condensation". In: *Nucleic Acids Research* 42.16, pp. 10823–31.

Wei, Guo Wei and Nathan A Baker (2014). "Differential geometry-based solvation and electrolyte transport models for biomolecular modeling: a review". In: *arXiv preprint arXiv:1412.0176*.

Baker, Nathan A, Juli D Klemm, Stacey L Harper, Sharon Gaheen, Mervi Heiskanen, Philippe Rocca-Serra, and Susanna-Assunta Sansone (2013). "Standardizing data". In: *Nature Nanotechnology* 8.2, pp. 73–74.

Baker, Nathan et al. (2013). "Research towards a systematic signature discovery process". In: *Intelligence and Security Informatics (ISI), 2013 IEEE International Conference on*. IEEE, pp. 301–308.

Chakraborty, Sandeep, Basuthkar J Rao, Nathan Baker, and Bjarni Ásgeirsson (2013). "Structural phylogeny by profile extraction and multiple superimposition using electrostatic congruence as a discriminator". In: *Intrinsically Disordered Proteins* 1.1, e25463.

Daily, Michael D, Jaehun Chun, Alejandro Heredia-Langner, Guowei Wei, and Nathan A Baker (2013). "Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies". In: *The Journal of Chemical Physics* 139.20, p. 204108.

Harper, Stacey L et al. (2013). "Nanoinformatics workshop report: current resources, community needs and the proposal of a collaborative framework for data sharing and information integration". In: *Computational Science & Discovery* 6.1, p. 014008.

Olsen, Brett N, Agata A Bielska, Tiffany Lee, Michael D Daily, Douglas F Covey, Paul H Schlesinger, Nathan A Baker, and Daniel S Ory (2013). "The structural basis of cholesterol accessibility in membranes". In: *Biophysical Journal* 105.8, pp. 1838–1847.

Thomas, Dennis G, Jaehun Chun, Zhan Chen, Guowei Wei, and Nathan A Baker (2013). "Parameterization of a geometric flow implicit solvation model". In: *Journal of Computational Chemistry* 34.8, pp. 687–695.

Thomas, Dennis G, Sharon Gaheen, et al. (2013). "ISA-TAB-Nano: a specification for sharing nanomaterial research data in spreadsheet-based format". In: *BMC Biotechnology* 13.1, p. 2.

Chen, Zhan, Shan Zhao, Jaehun Chun, Dennis G Thomas, Nathan A Baker, Peter W Bates, and GW Wei (2012). "Variational approach for nonpolar solvation analysis". In: *The Journal of Chemical Physics* 137.8, p. 084101.

Jacob, Ferosh, Jeff Gray, Adam Wynne, Yan Liu, and Nathan Baker (2012). "Domain-specific languages for composing signature discovery workflows". In: *Proceedings of the 2012 workshop on Domain-specific modeling*. ACM, pp. 61–64.

Konecny, Robert, Nathan A Baker, and J Andrew McCammon (2012). "iAPBS: a programming interface to the adaptive Poisson–Boltzmann solver". In: *Computational Science & Discovery* 5.1, p. 015005.

Lee, Sun-Joo, Paul H Schlesinger, Samuel A Wickline, Gregory M Lanza, and Nathan A Baker (2012). "Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers". In: *Soft Matter* 8.26, pp. 7024–7035.

Maojo, Victor et al. (2012). "Nanoinformatics: developing new computing applications for nanomedicine". In: *Computing* 94.6, pp. 521–539.

Olsen, Brett N, Paul H Schlesinger, Daniel S Ory, and Nathan A Baker (2012). "Side-chain oxysterols: from cells to membranes to molecules". In: *Biochimica et Biophysica Acta (BBA)-Biomembranes* 1818.2, pp. 330–336.

Ren, Pengyu, Jaehun Chun, Dennis G Thomas, Michael J Schnieders, Marcelo Marucho, Jiajing Zhang, and Nathan A Baker (2012). "Biomolecular electrostatics and solvation: a computational perspective". In: *Quarterly Reviews of Biophysics* 45.04, pp. 427–491.

Thomas, Dennis G, Satish Chikkagoudar, Alan R Chappell, Nathan Baker, et al. (2012). "Annotating the structure and components of a nanoparticle formulation using computable string expressions". In: *Bioinformatics and Biomedicine Workshops (BIBMW), 2012 IEEE International Conference on*. IEEE, pp. 889–894.

Alexov, Emil et al. (2011). "Progress in the prediction of pK_a values in proteins". In: *Proteins: structure, function, and bioinformatics* 79.12, pp. 3260–3275.

Carstensen, Tommy, Damien Farrell, Yong Huang, Nathan A Baker, and Jens Erik Nielsen (2011). "On the development of protein pK_a calculation algorithms". In: *Proteins: Structure, Function, and Bioinformatics* 79.12, pp. 3287–3298.

Chen, Zhan, Nathan A Baker, and GW Wei (2011). "Differential geometry based solvation model II: Lagrangian formulation". In: *Journal of Mathematical Biology* 63.6, pp. 1139–1200.

Hossain, KSM Tozammel, Chris Bailey-Kellogg, Alan M Friedman, Michael J Bradley, Nathan Baker, and Naren Ramakrishnan (2011). "Using Physicochemical Properties of Amino Acids to induce Graphical Models of Residue Couplings". In: *BIOKDD '11*.

Lee, Sun-Joo, Paul H Schlesinger, Samuel A Wickline, Gregory M Lanza, and Nathan A Baker (2011). "Interaction of melittin peptides with perfluorocarbon nanoemulsion particles". In: *The Journal of Physical Chemistry B* 115.51, pp. 15271–15279.

Olsen, Brett N, Paul H Schlesinger, Daniel S Ory, and Nathan A Baker (2011). "25-Hydroxycholesterol increases the availability of cholesterol in phospholipid membranes". In: *Biophysical Journal* 100.4, pp. 948–956.

Thomas, Dennis G, Fred Klaessig, et al. (2011). "Informatics and standards for nanomedicine technology". In: *Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology* 3, pp. 511–532.

Unni, Samir, Yong Huang, Robert M Hanson, Malcolm Tobias, Sriram Krishnan, Wilfred W Li, Jens E Nielsen, and Nathan A Baker (2011). "Web servers and services for electrostatics calculations with APBS and PDB2PQR". In: *Journal of Computational Chemistry* 32.7, pp. 1488–1491.

Callenberg, Keith M, Om P Choudhary, Gabriel L de Forest, David W Gohara, Nathan A Baker, and Michael Grabe (2010). "APBSmem: a graphical interface for electrostatic calculations at the membrane". In: *PloS ONE* 5.9, e12722.

Chen, Zhan, Nathan A Baker, and Guo-Wei Wei (2010). "Differential geometry based solvation model I: Eulerian formulation". In: *Journal of Computational Physics* 229.22, pp. 8231–8258.

Lee, Sun-Joo, Brett Olsen, Paul H Schlesinger, and Nathan A Baker (2010). "Characterization of Perfluorooctylbromide-Based Nanoemulsion Particles Using Atomistic Molecular Dynamics Simulations". In: *The Journal of Physical Chemistry B* 114.31, pp. 10086–10096.

Thomas, Dennis G, Rohit V Pappu, and Nathan A Baker (2010). "NanoParticle Ontology for cancer nanotechnology research". In: *Journal of Biomedical Informatics* 44.1, pp. 59–74.

Chen, Alan A, Marcelo Marucho, Nathan A Baker, and Rohit V Pappu (2009). "Simulations of RNA interactions with monovalent ions". In: *Methods in Enzymology* 469, pp. 411–432.

Olsen, Brett N, Paul H Schlesinger, and Nathan A Baker (2009). "Perturbations of membrane structure by cholesterol and cholesterol derivatives are determined by sterol orientation". In: *Journal of the American Chemical Society* 131.13, pp. 4854–4865.

Silva, Jonathan R, Hua Pan, Dick Wu, Ali Nekouzadeh, Keith F Decker, Jianmin Cui, Nathan A Baker, David Sept, and Yoram Rudy (2009). "A multiscale model linking ion-channel molecular dynamics

and electrostatics to the cardiac action potential". In: *Proceedings of the National Academy of Sciences* 106.27, pp. 11102–11106.

Thomas, Dennis G, Rohit V Pappu, Nathan Baker, et al. (2009). "Ontologies for cancer nanotechnology research". In: *Engineering in Medicine and Biology Society, 2009. EMBC 2009. Annual International Conference of the IEEE*. IEEE, pp. 4158–4161.

Bradley, Michael J, Peter T Chivers, and Nathan A Baker (2008). "Molecular dynamics simulation of the Escherichia coli NikR protein: equilibrium conformational fluctuations reveal interdomain allosteric communication pathways". In: *Journal of Molecular Biology* 378.5, pp. 1155–1173.

Dong, Feng, Brett Olsen, and Nathan A Baker (2008). "Computational methods for biomolecular electrostatics". In: *Methods in Cell Biology* 84, pp. 843–870.

Dong, Feng, Jason A Wagoner, and Nathan A Baker (2008). "Assessing the performance of implicit solvation models at a nucleic acid surface". In: *Physical Chemistry Chemical Physics* 10.32, pp. 4889–4902.

Lee, Sun-Joo, Yuhua Song, and Nathan A Baker (2008). "Molecular dynamics simulations of asymmetric NaCl and KCl solutions separated by phosphatidylcholine bilayers: potential drops and structural changes induced by strong Na+-lipid interactions and finite size effects". In: *Biophysical Journal* 94.9, pp. 3565–3576.

Cerutti, David S, Nathan A Baker, and J Andrew McCammon (2007). "Solvent reaction field potential inside an uncharged globular protein: A bridge between implicit and explicit solvent models?" In: *The Journal of Chemical Physics* 127, p. 155101.

Cheng, Yuhui et al. (2007). "Finite element analysis of the time-dependent Smoluchowski equation for acetylcholinesterase reaction rate calculations". In: *Biophysical Journal* 92.10, pp. 3397–3406.

Dolinsky, Todd J, Paul Czodrowski, Hui Li, Jens E Nielsen, Jan H Jensen, Gerhard Klebe, and Nathan A Baker (2007). "PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations". In: *Nucleic Acids Research* 35.suppl 2, W522–W525.

Schnieders, Michael J, Nathan A Baker, Pengyu Ren, and Jay W Ponder (2007). "Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum". In: *The Journal of Chemical Physics* 126, p. 124114.

Swanson, Jessica MJ, Jason A Wagoner, Nathan A Baker, and J Andrew McCammon (2007). "Optimizing the Poisson dielectric boundary with explicit solvent forces and energies: lessons learned with atom-centered dielectric functions". In: *Journal of Chemical Theory and Computation* 3.1, pp. 170–183.

Baker, Nathan A, Donald Bashford, and David A Case (2006). "Implicit solvent electrostatics in biomolecular simulation". In: *New Algorithms for Macromolecular Simulation*. Springer Berlin Heidelberg, pp. 263–295.

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Selected presentations

Baker, NA (2015). *IDC HPC User Forum NSCI Panel Discussion*. Panelist.

Baker*, NA, H Lei, X Yang, B Zheng, and G Lin (2015a). *Brown University, Division of Applied Mathematics Seminar*. Invited talk.

– (2015b). *Multiple faces of biomolecular electrostatics workshop, Mathematical Biosciences Institute*. Invited talk.

Dowling, C, T Pulsipher, L Gosink, S-A Sansone, and NA Baker* (2015). *Biophysical Society Annual Meeting*. Invited talk.

Baker, NA (2014a). *Conference on Data Analysis (CoDA 2014)*. Invited talk.

Baker, NA (2014b). *Lawrence Livermore National Laboratory Lab Days*. Invited talk.

– (2014c). *Materials Frontiers to Empower Quantum Computing, LANL workshop*. Invited talk.

– (2014d). *SCIX Conference, Reno, NV*. Keynote.

– (2014e). *University of Maryland Baltimore County Seminar*. Invited talk.

– (2014f). *University of Pittsburgh, Computational & Systems Biology Seminar*. Invited talk.

– (2014g). *VALCRI seminar, Linköping University*. Invited talk.

– (2013a). *Acoustics Department, University of Washington Applied Physics Laboratory*. Invited talk.

– (2013b). *Arizona State University Biophysics Seminar*. Invited talk.

– (2013c). *Microproducts Breakthrough Institute Seminar, Oregon State University*. Invited talk.

Baker, NA and H Rauscher (2013). *Society of Toxicology Annual Meeting presentation*. Invited talk.

Chun, J, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, and NA Baker* (2013a). *Chinese Academy of Sciences Applied Mathematics Seminar*. Invited talk.

– (2013b). *International Conference on Mathematical Modeling and Computation*. Invited talk.

– (2013c). *Third Biological Diffusion and Brownian Dynamics Brainstorm: BDBDB3*. Invited talk.

– (2013d). *Tsinghua University Chemistry Seminar*. Invited talk.

– (2013e). *University of Washington Nanotechnology Seminar*. Invited talk.

– (2013f). *Wuhan University Physics Seminar*.

Dowling, C, S-A Sansone, and NA Baker* (2013). *Gordon Research Conference Computer-Aided Drug Design*. Invited talk.

Gosink, L, E Hogan, T Pulsipher, and NA Baker* (2013). *Telluride Science Research Center Protein Electrostatics Workshop*. Invited talk.

Baker, NA (2012a). *EU-US: Bridging NanoEHS Research Efforts*. Invited talk.

– (2012b). *EU-US Communities of Research in Nanotechnology Databases and Ontology*. Invited talk.

– (2012c). *National Academies Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology*. Invited talk.

– (2012d). *National Geospatial-Intelligence Agency Technical Exchange*. Invited talk.

– (2012e). *Science of Multi-INT Workshop*. Contributed talk.

Chun, J, DG Thomas, GW Wei, and NA Baker* (2012). *American Chemical Society National Meeting*. Invited talk.

Thomas, DG, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, and NA Baker* (2012). *ICSU-CODATA Paris Meeting on Nanotechnology Informatics*. Invited talk.

Thomas, DG, J Chun, GW Wei, and NA Baker* (2012). *Georgia Tech Mathematics Seminar*. Invited talk.

Olsen, BN, Schlesinger PH, DS Ory, and NA Baker* (2011). *American Chemical Society National Meeting*. Invited talk.

Paik, DS and NA Baker* (2011). *National Center for Biomedical Ontology Annual Meeting*. Invited talk.

Thomas, DG, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, and NA Baker* (2011a). *American Society for Nanomedicine Annual Meeting*. Invited talk.

– (2011b). *Nanoinformatics 2011*. Invited talk.

– (2011c). *SRC-SEMATECH Environmental Research Center*. Invited talk.

Thomas, DS, J Chun, Z Chen, G Wei, and NA Baker* (2011a). *MBI Modeling and Computation of Biomolecular Structure and Dynamics*. Invited talk.

– (2011b). *University of Washington Applied Mathematics Seminar*. Invited talk.

Baker*, N et al. (2010). *caBIG Annual Meeting*. Contributed poster.

Baker, NA (2010a). *Nanoinformatics 2010*. Invited talk.

– (2010b). *Pacific Northwest National Laboratory seminar*. Invited talk.

– (2010c). *University of North Carolina Chapel Hill Physical Chemistry Seminar*. Invited talk.

– (2010d). *Washington University School of Medicine Dept. of Genetics Seminar*. Invited talk.

Gaheen*, S et al. (2010). *caBIG Annual Meeting*. Contributed poster.

Baker, NA (2009a). *Bioinformatics Institute, Agency for Science, Technology, and Research (A*STAR Biopolis), Singapore*. Visiting scientist lecture series and workshop.

– (2009b). *caBIG Integrative Cancer Research Workspace Meeting*. Invited talk.

– (2009c). *National Cancer Institute Nanotechnology Alliance Meeting*. Co-chair and invited talk.

– (2009d). *National Center for Biomedical Ontology Seminar, Stanford University*. Invited talk.

– (2009e). *University of California Davis, Department of Chemistry Seminar*. Invited talk.

– (2009f). *University of Texas at Austin ICES Seminar*. Invited talk.

Baker*, NA and K Tai (2009). *Specialised Training Workshop on Electrostatics Calculations, Collaborative Computational Project for Biomolecular Simulation*. Invited workshop.

Bradley, MJ, RL Rice, and NA Baker* (2009). *Biomolecular Modeling and Simulations, Israel Science Foundation Workshop*. Invited talk.

Carstensen, T, JE Nielsen, Y Huang, and NA Baker (2009). *TSRC Protein Electrostatics Workshop*. Invited talk.

Lee*, SJ and NA Baker (2009). *National Biomedical Computation Resource Summer Institute*. Invited talk.

Lee*, SJ, BN Olsen, Schlesinger PH, and NA Baker (2009). *Gibbs Conference on Biothermodynamics*. Invited talk.

NA*, Baker* et al. (2009). *caBIG Annual Meeting*. Contributed poster.

Olsen*, B, P Schlesinger, and N Baker (2009). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Olsen, BN and NA Baker* (2009). *Anesthesiology Research Unit Seminar, Washington University in St Louis*. Invited talk.

Thomas, DG, RV Pappu, and NA Baker* (2009a). *caBIG Annual Meeting*. Contributed poster.

– (2009b). *International Conference on Biomedical Ontology*. Contributed poster.

Wagoner, JA, F Dong, and NA Baker* (2009). *Biomolecular simulation 2009, Collaborative Computational Project for Biomolecular Simulation*. Plenary talk.

Baker, NA (2008a). *Mechanical Engineering Seminar, Washington University*. Invited talk.

– (2008b). *Protein Folding Workshop, Institute for Mathematics and its Applications*. Invited talk.

– (2008c). *Rensselaer Polytechnic Institute Seminar*. Invited talk.

– (2008d). *Seminar, Conway Institute, University College Dublin*. Invited talk.

– (2008e). *Seminar, Department of Biological Science, Florida State University*. Invited talk.

– (2008f). *University of Illinois Materials Science and Engineering Seminar*. Invited talk.

– (2008g). *University of Iowa Physical Chemistry Seminar*. Invited talk.

Baker, NA and D Sept* (2008). *Center for Theoretical Biological Physics Summer Workshop, University of California San Diego*. Invited talk.

Bradley, M, R Rice, E Di Cera, and N Baker* (2008). *American Chemical Society National Meeting*. Invited talk.

Hahn-Dantona*, EA, MJ Fritts, AK Patri, NA Baker, DG Thomas, and FW Hartel (2008). *Nanobiology Think Tank Meeting*. Contributed poster.

Paik*, D et al. (2008). *Radiological Society of North America 94th Scientific Sessions*. Contributed poster.

Rice, RL and NA Baker* (2008). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Thomas, DG, PL Jones, RV Pappu, and NA Baker (2008). *caBIG Annual Meeting*. Invited talk.

Wagoner, J, F Dong, and NA Baker* (2008a). *Biopolymers Gordon Research Conference*. Invited talk.

– (2008b). *Computational Chemistry Gordon Research Conference*. Invited talk.

Wagoner, J, F Dong, and NA Baker* (2008c). *Protein Electrostatics Workshop, Telluride Science Research Center*. Invited talk.

Wagoner, J, F Dong, D Cerutti, JA McCammon, and NA Baker (2008). *American Chemical Society National Meeting*. Invited talk.

Wagoner, JA, F Dong, and NA Baker* (2008). *Solvation Workshop, Institute for Mathematics and its Applications*. Invited talk.

Baker, NA (2007a). *Biophysical Evenings, Washington University in St Louis*. Invited talk.

– (2007b). *Mathematics of DNA Structure, Function, and Interactions, Institute for Mathematics and its Applications*. Invited talk.

– (2007c). *National Biomedical Computation Resource Summer Institute Mini-Symposium*. Invited talk.

Baker*, NA et al. (2007). *National Cancer Institute Nanotechnology Alliance Meeting*. Invited talk.

Baker, NA (2007d). *Quantitative Biology and Modeling/Dept. of Mathematics Seminar, Michigan State University*. Invited talk.

– (2007e). *Seminar, Integrated DNA Technologies*. Invited talk.

– (2007f). *Seminar, University of Kansas*. Invited talk.

Bradley*, M, P Chivers, and Baker N (2007). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Dong, F, JA Wagoner, and NA Baker* (2007). *American Chemical Society National Meeting*. Invited talk.

Lee, SJ, Y Song, and NA Baker (2007). *Biophysical Society Meeting*. Contributed poster.

Li*, P-C, MJ Bradley, NA Baker, and D Sept (2007). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Olsen, B, Y Song, SJ Lee, Tieleman DP, and NA Baker* (2007). *American Chemical Society National Meeting*. Invited talk.

Olsen*, B, Y Song, DP Tieleman, and Baker N (2007). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Rice*, RL and NA Baker (2007). *Biophysical Society Meeting*. Contributed poster.

Thomas, D, P Jones, R Pappu, D Sept, and N Baker* (2007). *Trans-NIH Nano Task Force Meeting*. Invited talk.

Thomas, D, H Sim, P Jones, R Pappu, D Sept, and N Baker* (2007). *Nanotechnology and the Life Sciences Symposium*. Talk and poster.

Thomas, DG, H Sim, P Jones, D Sept, R Pappu, and NA Baker (2007). *National Cancer Institute Nanotechnology Alliance Meeting*. Invited talk.

Baker, NA (2006a). *Biocomplexity Institute Seminar, University of Indiana*. Invited talk.

– (2006b). *Bioinformatics Institute, Agency for Science, Technology, and Research (A*STAR Biopolis), Singapore*. Visiting scientist lecture series.

– (2006c). *Computer Science and Engineering Seminar Series, University of Notre Dame*. Invited talk.

– (2006d). *Future of Biomolecular Simulations: From Ab Initio to Nano-molecular Machines, National Center for Computational Sciences, Oak Ridge National Lab*. Invited talk.

– (2006e). *National Biomedical Computation Resource Summer Institute*. Invited workshop.

– (2006f). *Theoretical and Computational Biophysics Seminar, University of Illinois Urbana-Champaign*. Invited talk.

Bradley*, M and Baker N Chivers P (2006). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Dong*, F, J Wagoner, and NA Baker (2006). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Olsen*, B, SJ Lee, Y Song, and NA Baker (2006). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Song*, Y and NA Baker (2006). *Biophysical Society Meeting*. Contributed poster.

Wagoner*, JA and NA Baker (2006). *Biophysical Society Meeting*. Contributed poster.

Wagoner, JA, F Dong, and NA Baker* (2006). *Gibbs Conference on Biothermodynamics*. Invited talk.

Baker, NA (2005a). *Contemporary Biochemistry Seminar Series, University of Wisconsin at Madison*. Invited talk.

– (2005b). *Institute for Computational Engineering and Sciences, University of Texas at Austin*. Invited talk.

– (2005c). *IPAM Workshop: Bridging Time and Length Scales in Materials Science and Bio-Physics*. Invited talk.

– (2005d). *Japan Society for the Promotion of Science, U.S. National Academy of Sciences: Eighth Annual Japanese-American Frontiers of Science Symposium*. Invited poster.

– (2005e). *St Louis RCGA Bioinformatics Network Seminar*. Invited talk.

– (2005f). *University of Iowa Department of Chemistry Seminar*. Invited talk.

Baker*, NA, T Dolinsky, J Wagoner, and Y Song (2005). *QBMI Computational Structural Biology Workshop*. Invited talk.

Bradley*, M, P Chivers, and N Baker (2005). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Song*, Y and NA Baker (2005). *Biophysical Society Meeting*. Contributed poster.

Song*, Y, V Guallar, and NA Baker (2005). *Gibbs Conference on Biothermodynamics*. Invited talk.

Wagoner*, JA and NA Baker (2005). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Baker, NA (2004a). *2nd Annual National Academies Keck Futures Initiative*. Invited poster.

– (2004b). *Algorithms for Multiscale Modeling IV*. Invited talk.

– (2004c). *JASON Summer Study 2004 Computation for Biology and Medicine, JASON group (Mitre Corporation)*. Invited briefing.

– (2004d). *Multiscale Computational Models for Biomolecular Research, National Biomedical Computation Resource*. Invited talk.

Song*, Y, Y Zhang, T Shen, CL Bajaj, JA McCammon, and NA Baker (2004). *Biophysical Society Meeting*. Contributed poster.

Wagoner*, J, A Melnykov, and NA Baker (2004). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Baker, NA (2003a). *Rush Medical College, Department of Molecular Biophysics and Physiology Seminar*. Invited talk.

– (2003b). *The Third Virtual Conference on Genomics and Bioinformatics*. Invited talk.

– (2003c). *University of Texas at Austin, Center for Computational Visualization Seminar*. Invited talk.

Baker, NA, C Bajaj*, JA McCammon, Sanner M, and Olson A (2003). *NPACI All-Hands Meeting*. Invited talk.

Baker*, NA, D Sept, S Joseph, MJ Holst, and JA McCammon (2003). *SIAM Computation Science and Engineering meeting*. Contributed talk.

Baker*, NA, X Zhang, Z Xu, and CL Bajaj (2003). *Digital Biology: The Emerging Paradigm (NIH BISTIC)*. Contributed poster.

Bradley*, M, E Schreiter, C Drennan, P Chivers, and Baker N (2003). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Song*, Y, Y Zhang, T Shen, C Bajaj, JA McCammon, and NA Baker (2003). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Baker, NA (2002a). *NPACI All-Hands Meeting*. Invited talk.

– (2002b). *The Salk Institute, Young Investigator Symposium*. Invited talk.

– (2002c). *University of Illinois Urbana-Champaign, Theoretical Biophysics Seminar*. Invited talk.

Baker*, NA, D Sept, MJ Holst, and JA McCammon (2002). *NPACI All-Hands Meeting*. Contributed poster, first place student award.

Baker*, NA, D Sept, S Joseph, MJ Holst, and JA McCammon (2002). *Biophysical Society Annual Meeting*. Contributed poster.

Baker, NA*, D Sept, S Joseph, MJ Holst, and JA McCammon (2002). *Gibbs Conference on Biothermodynamics*. Contributed poster.

Sept*, D, NA Baker, and JA McCammon (2002). *Biophysical Society Annual Meeting*. Contributed poster.

Baker, NA (2001a). *Seminar, The Burnham Institute*. Invited talk.

– (2001b). *University of California at San Diego, Biochemistry Seminar*. Invited talk.

– (2001c). *University of Chicago, Computations in Science Seminar*. Invited talk.

– (2001d). *University of Michigan, Bioinformatics Program Seminar*. Invited talk.

– (2001e). *Washington University School of Medicine, Department of Biochemistry and Molecular Biophysics Special Seminar*. Invited talk.

Baker*, NA, D Sept, M Holst, and JA McCammon (2001). *American Chemical Society National Meeting*. Invited talk.

Baker*, NA (2000). *The First SIAM Conference on Computational Science and Engineering*. Contributed talk.

Baker*, NA, MJ Holst, and JA McCammon (2000). *La Jolla Interfaces in Science 2000 Symposium: Quantitative Challenges in the Post-genomic Sequence*. Contributed poster.

Baker*, NA, G Huber, and JA McCammon (1998). *The Sixth International Meeting on Cholinesterases*. Contributed poster.

Baker, N, W Kearney, and D Quinn* (1997). *Experimental Nuclear Magnetic Resonance Conference*. Contributed poster.

Baker, N, S Feaster, and D Quinn* (1996). *Gordon Conference: Enzymes, Coenzymes, Metabolic Pathways*. Contributed poster.