NATHAN ANDREW BAKER

CURRICULUM VITAE
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Nathan Baker, Ph.D. is the Director of the Advanced Computing, Mathematics, and Data Division at Pacific Northwest National Laboratory (PNNL) and a Visiting Faculty member at Brown University. His research interests include the development of new algorithms and mathematical methods in biophysics, nanotechnology, and informatics. Current research projects include computational methods for modeling solvation in biomolecular systems, mathematical methods for mesoscale materials modeling, and development of new methods for signature discovery. His research is primarily funded by the National Institutes of Health and the Department of Energy.

EXPERIENCE

2016–present	**Director**, Advanced Computing, Mathematics, and Data Division, Pacific Northwest National Laboratory, Richland, WA.
2015–present	**Visiting Professor**, Division of Applied Mathematics, Brown University, Providence, RI.
2012–2016	**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), Dept of Biochemistry and Molecular Biophysics, Washington University, St Louis, MO.
2002–2006	**Assistant Professor**, Dept of Biochemistry and Molecular Biophysics, Washington University, St Louis, MO.

EDUCATION

2001–2002	**Postdoctoral Researcher**, Dept 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, Univ 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**, Univ California San Diego.
1997	**Predoctoral Fellowship**, Howard Hughes Medical Institute.
1997	**Collegiate Scholar**, Univ Iowa.
1997	**Member**, Phi Beta Kappa, Univ Iowa.
1997	Undergraduate Liberal Arts Commencement Speaker, Univ Iowa.
1995	**Undergraduate Fellowship**, Barry M Goldwater Foundation.

SERVICE

SELECTED EXTRAMURAL SERVICE

2014-2017	**Associate Editor**, Biophysical Journal, Biophysical Society.
2016-present	**Executive Committee Member**, Carbon Capture Simulation Initiative, Department of Energy.
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.

2016	**Reviewer**, MIT Sea Grants, Massachusetts Institute of Technology.
2014-2016	**Organizing committee member**, Conference on Data Analysis (CoDA).
2014-2015	**Reviewer**, INCITE Biological Sciences Review Panel, Advanced Scientific Computing Research, Dept 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 Univ.
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

2016-present	**Member**, Compensation Manager search committee, Pacific Northwest Natl Lab.
2016-present	**Member**, Scientist & Engineer Job Family review panel, Pacific Northwest Natl Lab.
2016-present	**Executive secretary**, Integrated Plant, Atmosphere, & Soil System Initiative, Pacific Northwest Natl Lab.
2014-present	**Lecturer and panelist**, Scientist & Engineer Development Program, Pacific Northwest Natl Lab
2015	**Panelist**, Council of Fellows "Increasing Scientific Impact" session, Pacific Northwest Natl Lab.
2015	**Member**, Interdisciplinary Applied Sciences Planning Committee, Washington State Univ Tri-Cities and Pacific Northwest Natl Lab.
2015-present	**Advisory committee member**, Microbes in Transition Initiative Advisory Committee, Pacific Northwest Natl Lab.
2014-present	**Executive secretary**, Analysis in Motion Initiative, Pacific Northwest Natl Lab.

2014-2016	**Chair**, PNNL Institutional Computing Steering Committee, Pacific Northwest Natl Lab.
2015	**Co-chair**, National Strategic Computing Initiative Planning Committee, co-chair, Pacific Northwest Natl Lab.
2014-present	**Advisory committee member**, Analysis in Motion Initiative Advisory Committee, Pacific Northwest Natl Lab.
2013-present	**Reviewer**, ASCR Early Career pre-proposals, Pacific Northwest Natl Lab.
2013-2016	**Member**, Council of Fellows Executive Committee, Pacific Northwest Natl Lab.
2012-2015	**Lead**, Signature Discovery Initiative, Pacific Northwest Natl Lab.
2011-present	**Reviewer**, HHS LDRD proposals, Pacific Northwest Natl Lab.
2010-present	**Chief Scientist**, Signature Discovery Initiative, Pacific Northwest Natl Lab.
2014-2015	**Judge**, Postdoc Symposium, Pacific Northwest Natl Lab.
2015	**Presenter**, Computing Assessment Committee, Pacific Northwest Natl Lab.
2015	**Member**, Physical and Computational Sciences Directorate Strategy Committee, Pacific Northwest Natl Lab.
2015	**Advocate**, Proposal-Writing Workshop development, Pacific Northwest Natl Lab.
2013-2015	**Presenter**, Publishing Workshop, National Security Directorate, Pacific Northwest Natl Lab.
2011-2015	**Lead**, Signatures Community of Interest Network, Pacific Northwest Natl Lab.
2015	**Member**, Diversity Internal Oversight Committee, Pacific Northwest Natl Lab.
2015	**Member**, Employee Time Reporting Reform Committee, Pacific Northwest Natl Lab.
2015	**Member**, Computational Materials Science Red Team, Pacific Northwest Natl Lab.
2011-2014	**Reviewer**, DHHS Sector LDRD Proposals, Pacific Northwest Natl Lab.
2012-2014	**Reviewer**, BES pre-proposals, Pacific Northwest Natl Lab.
2005-2010	**Director**, Siteman Center for Cancer Nanotechnology Excellence Biocomputing Core, Washington Univ St Louis
2007-2010	**Member**, Program and Student Affairs Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.
2009-2010	**Member**, Nominating Committee, Biophysical Society.
2007-2010	**Director**, Computational and Molecular Biophysics graduate program, Washington Univ St Louis
2004-2010	**Steering committee member**, Computational and Molecular Biophysics graduate program, Washington Univ St Louis.
2008	**Chair**, Scientific Collaboration Panel Discussion, Annual Conference on Effective Research Management, Washington Univ St Louis.
2008	**Co-organizer**, Bridging Research and Teaching Workshop: Innovation at the Crossroads of Chemistry, Physics, and Biology, Washington Univ St Louis.
2003-2008	**Seminar co-organizer**, Center for Computational Biology, Washington Univ St Louis.
2007	**Member**, Education Planning Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.
2004-2007	**Member**, Admissions Committee, Division of Biology and Biomedical Sciences, Washington Univ St Louis.
2004-2007	**Mentor**, Students and Teachers as Researchers (STARS) program, Univ Missouri St Louis.
2006-2007	**Member**, Faculty Search Committee, Dept of Mechanical and Aerospace Engineering, Washington Univ St Louis.
2006	**Member**, Liaison Committee on Medical Education and IT, School of Medicine, Washington Univ St Louis.
2006	**Co-organizer**, ICAM/Center for Computational Biology Multiscale Interactions and Dynamics in Biological Systems Workshop, Washington Univ St Louis.
2004	**Member**, Oversight Committee, Center for Scientific Parallel Computing, Washington Univ St Louis.

SELECTED COMMUNITY SERVICE

2016	**Judge**, Mathematics, Engineering, Science Achievement (MESA) USA Engineering Design Competition, Pasco, WA.
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.

SELECTED 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.

SELECTED 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, Dept of Energy Advanced Scientific Computing Research.

SELECTED FUNDING

2012-2016	**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 Univ 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.

MENTORING

POSTDOCTORAL RESEARCHERS

2013-2015	Huan Lei, Pacific Northwest Natl Lab.
2015	Xiu Yang, Pacific Northwest Natl Lab.
2011-2013	Mike Daily, Pacific Northwest Natl Lab.
2011-2013	Emilie Hogan, Pacific Northwest Natl Lab.
2008-2010	Marcelo Marucho, Washington Univ St Louis.
2006-2010	Dennis Thomas, Washington Univ St Louis.
2005-2007	Feng Dong, Washington Univ St Louis.
2002-2006	Yuhua Song, Washington Univ St Louis.
2002-2003	Seongeun Yang, Postdoc, Washington Univ St Louis.

GRADUATE STUDENTS

2015-2016	Mingge Deng, Brown Univ.
2010	Marc Sherman, Washington Univ St Louis.
2006-2010	Brett Olsen, Washington Univ St Louis.
2005-2010	Sunjoo Lee, Washington Univ St Louis.
2003-2009	Rachel Rice, Washington Univ St Louis.
2003-2009	Michael Bradley, Washington Univ St Louis.

UNDERGRADUATE RESEARCHERS

2009-2010	Arjun Bahl, Washington Univ St Louis.
2009	Aditya Nath, Washington Univ St Louis.
2009	Mark Rosenberg, Washington Univ St Louis.
2007-2009	Stephen Gradwohl, Washington Univ St Louis.

2008	Sechin Jain, Washington Univ St Louis.
2007-2008	Tom Richner, Washington Univ St Louis.
2005	Jeff Poskin, Washington Univ St Louis.
2002-2006	Jason Wagoner, Washington Univ St Louis.

OTHER RESEARCHERS

2015-present	Juan Brandi, Postbac researcher, Pacific Northwest Natl Lab.
2015-2016	Maria Tartakovsky, High school researcher, Pacific Northwest Natl Lab.
2014-2015	Peter Li, High school researcher, Pacific Northwest Natl Lab.
2015	Shadya Maldonado, Postbac researcher, Pacific Northwest Natl Lab.
2014-2015	Minju Chun, High school researcher, Pacific Northwest Natl Lab.
2012-2013	Max Li, High school researcher, Pacific Northwest Natl Lab.
2010-2011	Shy Brown, Postbac, Pacific Northwest Natl Lab.
2010-2011	Tyler Harmon, Postbac, Pacific Northwest Natl Lab.
2008-2010	Michal Lijowksi, Bioinformatics curator, Washington Univ St Louis.
2007-2010	Yong Huang, Programmer, Washington Univ St Louis.
2007-2010	Samir Unni, High school and undergraduate researcher, Washington Univ St Louis.
2006-2010	Dave Gohara, Programmer, Washington Univ St Louis.
2006-2008	Peter Jones, Programmer, Washington Univ St Louis.
2005	Eric Mintun, High school researcher, Washington Univ St Louis.
2004	Prachi Mayenkar, High school researcher, Washington Univ St Louis.
2002-2006	Todd Dolinsky, Programmer, Washington Univ St Louis.

CURRENT PROFESSIONAL MEMBERSHIPS

American Chemical Society, Association for Computing Machinery, Biophysical Society, IEEE, Society for Industrial and Applied Mathematics.

SELECTED PRESENTATIONS

2016	N Baker. Univ Illinois Computational Science and Engineering Annual Symposium, Keynote talk.
2015	NA Baker*, H Lei, X Yang, B Zheng, G Lin. Brown Univ, Division of Applied Mathematics Seminar, Invited talk.
2015	NA Baker*, H Lei, X Yang, B Zheng, G Lin. Multiple faces of biomolecular electrostatics workshop, Mathematical Biosciences Institute, Invited talk.
2015	NA Baker. IDC HPC User Forum NSCI Panel Discussion, Panelist.
2015	C Dowling, T Pulsipher, L Gosink, S-A Sansone, NA Baker*. Biophysical Society Annual Meeting, Invited talk.
2014	NA Baker. VALCRI seminar, Linköping Univ, Invited talk.
2014	NA Baker. Materials Frontiers to Empower Quantum Computing, LANL workshop, Invited talk.
2014	NA Baker. SCIX Conference, Reno, NV, Keynote.
2014	NA Baker. Univ Pittsburgh, Computational & Systems Biology Seminar, Invited talk.
2014	NA Baker. Univ Maryland Baltimore County Seminar, Invited talk.
2014	NA Baker. Conference on Data Analysis (CoDA 2014), Invited talk.
2014	NA Baker. Lawrence Livermore Natl Lab Lab Days, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. Univ Washington Nanotechnology Seminar, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. Third Biological Diffusion and Brownian Dynamics Brainstorm: BDBDB3, Invited talk.
2013	C Dowling, S-A Sansone, NA Baker*. Gordon Research Conference Computer-Aided Drug Design, Invited talk.
2013	L Gosink, E Hogan, T Pulsipher, NA Baker*. Telluride Science Research Center Protein Electrostatics Workshop, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. Tsinghua Univ Chemistry Seminar, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. Wuhan Univ Physics Seminar, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. International Conference on Mathematical Modeling and Computation, Invited talk.
2013	J Chun, DG Thomas, M Daily, L Gosink, E Hogan, GW Wei, NA Baker*. Chinese Academy of Sciences Applied Mathematics Seminar, Invited talk.
2013	NA Baker. Arizona State Univ Biophysics Seminar, Invited talk.

2013 NA Baker, H Rauscher. Society of Toxicology Annual Meeting presentation, Invited talk.
2013 NA Baker. Acoustics Dept, Univ Washington Applied Physics Laboratory, Invited talk.
2013 NA Baker. Microproducts Breakthrough Institute Seminar, Oregon State Univ, Invited talk.
2012 NA Baker. EU-US: Bridging NanoEHS Research Efforts, Invited talk.
2012 NA Baker. National Academies Research Progress on Environmental, Health, and Safety Aspects of Nanotechnology, Invited talk.
2012 NA Baker. Science of Multi-INT Workshop, Contributed talk.
2012 J Chun, DG Thomas, GW Wei, NA Baker*. American Chemical Society National Meeting, Invited talk.
2012 DG Thomas, J Chun, GW Wei, NA Baker*. Georgia Tech Mathematics Seminar, Invited talk.
2012 NA Baker. EU-US Communities of Research in Nanotechnology Databases and Ontology, Invited talk.
2012 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker*. ICSU-CODATA Paris Meeting on Nanotechnology Informatics, Invited talk.
2012 NA Baker. National Geospatial-Intelligence Agency Technical Exchange, Invited talk.
2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker*. Nanoinformatics 2011, Invited talk.
2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker*. American Society for Nanomedicine Annual Meeting, Invited talk.
2011 DG Thomas, A Chappell, E Freund, S Gaheen, S Harper, JD Klemm, DS Paik, NA Baker*. SRC-SEMATECH Environmental Research Center, Invited talk.
2011 DS Thomas, J Chun, Z Chen, G Wei, NA Baker*. MBI Modeling and Computation of Biomolecular Structure and Dynamics, Invited talk.
2011 DS Thomas, J Chun, Z Chen, G Wei, NA Baker*. Univ Washington Applied Mathematics Seminar, Invited talk.
2011 BN Olsen, Schlesinger PH, DS Ory, NA Baker*. American Chemical Society National Meeting, Invited talk.
2011 DS Paik, NA Baker*. National Center for Biomedical Ontology Annual Meeting, Invited talk.
2010 NA Baker. Nanoinformatics 2010, Invited talk.
2010 NA Baker. Univ North Carolina Chapel Hill Physical Chemistry Seminar, Invited talk.
2006 NA Baker. Bioinformatics Institute, Agency for Science, Technology, and Research (A*STAR Biopolis), Singapore, Visiting scientist lecture series.
2005 NA Baker. Japan Society for the Promotion of Science, U.S. National Academy of Sciences: Eighth Annual Japanese-American Frontiers of Science Symposium, Invited poster.
2004 NA Baker. 2nd Annual National Academies Keck Futures Initiative, Invited poster.

SELECTED PUBLICATIONS

A full publication list with bibliometrics is available from Google Scholar.

Drozdetski, A. V., Tolokh, I. S., Pollack, L., Baker, N., & Onufriev, A. V. (2016). Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. *Physical Review Letters*, *117*(2), 028101. http://doi.org/10.1103/PhysRevLett.117.028101

Gunner, M. R., & Baker, N. A. (2016). Continuum Electrostatics Approaches to Calculating pKas and Ems in Proteins. In *Methods in Enzymology*. http://doi.org/10.1016/bs.mie.2016.05.052

Tolokh, I. S., Drozdetski, A. V., Pollack, L., Baker, N. A., & Onufriev, A. V. (2016). Multi-shell model of ion-induced nucleic acid condensation. *The Journal of Chemical Physics*, *144*(15), 155101. http://doi.org/10.1063/1.4945382

Yang, X., Lei, H., Baker, N. A., & Lin, G. (2016). Enhancing sparsity of Hermite polynomial expansions by iterative rotations. *Journal of Computational Physics*, *307*, 94–109. http://doi.org/10.1016/j.jcp.2015.11.038

Purvine, E., Monson, K., Jurrus, E., Star, K., & Baker, N. A. (2016). Energy Minimization of Discrete Protein Titration State Models Using Graph Theory. *The Journal of Physical Chemistry. B*, acs.jpcb.6b02059. http://doi.org/10.1021/acs.jpcb.6b02059

Pabit, S. A., Katz, A. M., Tolokh, I. S., Drozdetski, A., Baker, N., Onufriev, A. V., & Pollack, L. (2016, May 24). Understanding nucleic acid structural changes by comparing wide-angle x-ray scattering (WAXS) experiments to molecular dynamics simulations. *The Journal of Chemical Physics*. AIP Publishing. http://doi.org/10.1063/1.4950814

Wei, G. W., & Baker, N. A. (2016). Differential geometry-based solvation and electrolyte transport models for biomolecular modeling: a review. In *Many-Body Effects and Electrostatics in Biomolecules* (pp. 417–461). Pan Stanford. http://doi.org/10.1201/b21343-15

Sushko, M. L., Thomas, D. G., Pabit, S. A., Pollack, L., Onufriev, A. V., & Baker, N. A. (2016). The Role of Correlation and Solvation in Ion Interactions with B-DNA. *Biophysical Journal*, *110*(2), 315–26. http://doi.org/10.1016/j.bpj.2015.12.011

Dowling, C. P., Johnson, S., Jurrus, E., & Baker, N. A. (2015). An ISA-Tab specification for protein titration data exchange. Retrieved from http://arxiv.org/abs/1511.06431

Pan, W., Daily, M., & Baker, N. A. (2015). Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smoothed particle hydrodynamics. *BMC Biophysics*, *8*(1), 7. http://doi.org/10.1186/s13628-015-0021-y

Harper, B., Thomas, D., Chikkagoudar, S., Baker, N., Tang, K., Heredia-Langner, A., … Harper, S. (2015). Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity. *Journal of Nanoparticle Research : An Interdisciplinary Forum for Nanoscale Science and Technology*, *17*(6), 250. http://doi.org/10.1007/s11051-015-3051-0

Lei, H., Yang, X., Zheng, B., Lin, G., & Baker, N. A. (2015). Constructing Surrogate Models of Complex Systems with Enhanced Sparsity: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation. *Multiscale Modeling and Simulation*, *13*(4), 1327–1353. http://doi.org/10.1137/140981587

Daily, M. D., Olsen, B. N., Schlesinger, P. H., Ory, D. S., & Baker, N. A. (2014). Improved Coarse-Grained Modeling of Cholesterol-Containing Lipid Bilayers. *Journal of Chemical Theory and Computation*, *10*(5), 2137–2150. http://doi.org/10.1021/ct401028g

Gosink, L. J., Hogan, E. A., Pulsipher, T. C., & Baker, N. A. (2014). Bayesian model aggregation for ensemble-based estimates of protein pKa values. *Proteins: Structure, Function and Bioinformatics*, *82*(3), 354–363. http://doi.org/10.1002/prot.24390

Pham, C. T. N., Thomas, D. G., Beiser, J., Mitchell, L. M., Huang, J. L., Senpan, A., … Hourcade, D. E. (2014). Application of a hemolysis assay for analysis of complement activation by perfluorocarbon nanoparticles. *Nanomedicine: Nanotechnology, Biology, and Medicine*, *10*(3), 651–660. http://doi.org/10.1016/j.nano.2013.10.012

Thomas, D. G., Chikkagoudar, S., Heredia-Langer, A., Tardiff, M. F., Xu, Z., Hourcade, D. E., … Baker, N. A. (2014). Physicochemical signatures of nanoparticle-dependent complement activation. *Computational Science & Discovery*, *7*(1), 015003. http://doi.org/10.1088/1749-4699/7/1/015003

Bielska, A. A., Olsen, B. N., Gale, S. E., Mydock-McGrane, L., Krishnan, K., Baker, N. A., … Ory, D. S. (2014). Side-chain oxysterols modulate cholesterol accessibility through membrane remodeling. *Biochemistry*, *53*(18), 3042–51. http://doi.org/10.1021/bi5000096

Tolokh, I. S., Pabit, S. A., Katz, A. M., Chen, Y., Drozdetski, A., Baker, N. A., … Onufriev, A. V. (2014). Why double-stranded RNA resists condensation. *Nucleic Acids Research*, *42*(16), 10823–31. http://doi.org/10.1093/nar/gku756

Richardson, C., Sarrao, J., Taylor, A., Baker, N. A., Ballarotto, V., Blain, M., … Warner, M. G. (2014). *Materials Frontiers to Empower Quantum Computing*. Los Alamos, NM.

Baker, N. A., Barr, J. L., Bonheyo, G. T., Joslyn, C. A., Krishnaswami, K., Oxley, M. E., … Wynne, A. S. (2013). Research towards a systematic signature discovery process. In *Intelligence and Security Informatics (ISI), 2013 IEEE International Conference on* (pp. 301–308). IEEE. http://doi.org/10.1109/isi.2013.6578848

Thomas, D. G., Chun, J., Chen, Z., Wei, G., & Baker, N. A. (2013). Parameterization of a geometric flow implicit solvation model. *Journal of Computational Chemistry*, *34*(8), 687–95. http://doi.org/10.1002/jcc.23181

Thomas, D. G., Gaheen, S., Harper, S. L., Fritts, M., Klaessig, F., Hahn-Dantona, E., … Baker, N. A. (2013). ISA-TAB-Nano: a specification for sharing nanomaterial research data in spreadsheet-based format. *BMC Biotechnology*, *13*(1), 2. http://doi.org/10.1186/1472-6750-13-2

Baker, N. A., Klemm, J. D., Harper, S. L., Gaheen, S., Heiskanen, M., Rocca-Serra, P., & Sansone, S.-A. (2013). Standardizing data. *Nature Nanotechnology*, *8*(2), 73–74. http://doi.org/10.1038/nnano.2013.12

Chakraborty, S., Rao, B. J., Baker, N. A., Asgeirsson, B., & Ásgeirsson, B. (2013). Structural phylogeny by profile extraction and multiple superimposition using electrostatic congruence as a discriminator. *Intrinsically Disordered Proteins*, *1*(1), e25463. http://doi.org/10.4161/idp.25463

Olsen, B. N., Bielska, A. A., Lee, T., Daily, M. D., Covey, D. F., Schlesinger, P. H., … Ory, D. S. (2013). The structural basis of cholesterol accessibility in membranes. *Biophysical Journal*, *105*(8), 1838–1847. http://doi.org/10.1016/j.bpj.2013.08.042

Harper, S. L., Hutchison, J. E., Baker, N. A., Ostraat, M., Tinkle, S., Steevens, J., … Tuominen, M. (2013). Nanoinformatics workshop report: Current resources, community needs, and the proposal of a collaborative framework for data sharing and information integration. *Computational Science & Discovery*, *6*(1), 14008. http://doi.org/10.1088/1749-4699/6/1/014008

Daily, M. D., Chun, J., Heredia-Langner, A., Wei, G. W., & Baker, N. A. (2013). Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. *The Journal of Chemical Physics*, *139*(20), 204108. http://doi.org/10.1063/1.4832900

Olsen, B. N., Schlesinger, P. H., Ory, D. S., & Baker, N. A. (2012). Side-chain oxysterols: From cells to membranes to molecules. *Biochimica et Biophysica Acta (BBA) - Biomembranes*, *1818*(2), 330–336. http://doi.org/10.1016/j.bbamem.2011.06.014

Konecny, R., Baker, N. A., & McCammon, J. A. (2012). iAPBS: a programming interface to Adaptive Poisson-Boltzmann Solver (APBS). *Computational Science & Discovery*, *5*(1), 015005. http://doi.org/10.1088/1749-4699/5/1/015005

Maojo, V., Fritts, M., Martin-Sanchez, F., De la Iglesia, D., Cachau, R. E., Garcia-Remesal, M., … Kulikowski, C. (2012). Nanoinformatics: developing new computing applications for nanomedicine. *Computing*, *94*(6), 521–539. http://doi.org/10.1007/s00607-012-0191-2

Lee, S.-J., Schlesinger, P. H., Wickline, S. A., Lanza, G. M., & Baker, N. A. (2012). Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers. *Soft Matter*, *8*(26), 7024. http://doi.org/10.1039/c2sm25847a

Chen, Z., Zhao, S., Chun, J., Thomas, D. G., Baker, N. A., Bates, P. W., & Wei, G. W. (2012). Variational approach for nonpolar solvation analysis. *The Journal of Chemical Physics*, *137*(8), 084101. http://doi.org/10.1063/1.4745084

Ren, P., Chun, J., Thomas, D. G., Schnieders, M. J., Marucho, M., Zhang, J., & Baker, N. A. (2012). Biomolecular electrostatics and solvation: a computational perspective. *Quarterly Reviews of Biophysics*, *45*(4), 427–91. http://doi.org/10.1017/S003358351200011X

Thomas, D. G., Chikkagoudar, S., Chappell, A. R., & Baker, N. A. (2012). Annotating the structure and components of a nanoparticle formulation using computable string expressions. *Proceedings. IEEE International Conference on Bioinformatics and Biomedicine*, *2012*, 889–894. http://doi.org/10.1109/BIBMW.2012.6470259

Jacob, F., Gray, J., Wynne, A. S., Liu, Y., & Baker, N. A. (2012). Domain-specific Languages for Composing Signature Discovery Workflows. In *Proceedings of the 2012 Workshop on Domain-specific Modeling* (pp. 61–64). New York, NY, USA: ACM. http://doi.org/10.1145/2420918.2420934

Hossain, K. S. M. T., Bailey-Kellogg, C., Friedman, A. M., Bradley, M. J., Baker, N., & Ramakrishnan, N. (2011). Using physicochemical properties of amino acids to induce graphical models of residue couplings. In *Proceedings of the Tenth International Workshop on Data Mining in Bioinformatics - BIOKDD '11* (pp. 1–10). New York, New York, USA: ACM Press. http://doi.org/10.1145/2003351.2003354

Chen, Z., Baker, N. A., & Wei, G. W. (2011). Differential geometry based solvation model II: Lagrangian formulation. *Journal of Mathematical Biology*, *63*(6), 1139–1200. http://doi.org/10.1007/s00285-011-0402-z

Thomas, D. G., Pappu, R. V, & Baker, N. A. (2011). NanoParticle Ontology for cancer nanotechnology research. *Journal of Biomedical Informatics*, *44*(1), 59–74. http://doi.org/10.1016/j.jbi.2010.03.001

Thomas, D. G., Klaessig, F., Harper, S. L., Fritts, M., Hoover, M. D., Gaheen, S., … Baker, N. A. (2011). Informatics and standards for nanomedicine technology. *Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology*, *3*(5), n/a–n/a. http://doi.org/10.1002/wnan.152

Unni, S., Huang, Y., Hanson, R. M., Tobias, M., Krishnan, S., Li, W. W., … Baker, N. A. (2011). Web servers and services for electrostatics calculations with APBS and PDB2PQR. *Journal of Computational Chemistry*, *32*(7), 1488–1491. http://doi.org/10.1002/jcc.21720

Carstensen, T., Farrell, D., Huang, Y., Baker, N. A., & Nielsen, J. E. (2011). On the development of protein pKa calculation algorithms. *Proteins: Structure, Function, and Bioinformatics*, *79*(12), 3287–3298. http://doi.org/10.1002/prot.23091

Lee, S.-J., Schlesinger, P. H., Wickline, S. A., Lanza, G. M., & Baker, N. A. (2011). Interaction of melittin peptides with perfluorocarbon nanoemulsion particles. *The Journal of Physical Chemistry. B*, *115*(51), 15271–9. http://doi.org/10.1021/jp209543c

Olsen, B. N., Schlesinger, P. H., Ory, D. S., & Baker, N. A. (2011). 25-Hydroxycholesterol increases the availability of cholesterol in phospholipid membranes. *Biophysical Journal*, *100*(4), 948–956. http://doi.org/10.1016/j.bpj.2010.12.3728

Alexov, E., Mehler, E. L., Baker, N., M. Baptista, A., Huang, Y., Milletti, F., … Word, J. M. (2011). Progress in the prediction of pKa values in proteins. *Proteins: Structure, Function, and Bioinformatics*, *79*(12), 3260–3275. http://doi.org/10.1002/prot.23189

Callenberg, K. M., Choudhary, O. P., de Forest, G. L., Gohara, D. W., Baker, N. A., & Grabe, M. (2010). APBSmem: A Graphical Interface for Electrostatic Calculations at the Membrane. *PLoS ONE*, *5*(9), e12722. http://doi.org/10.1371/journal.pone.0012722

Chen, Z., Baker, N. a, & Wei, G. W. (2010). Differential geometry based solvation model I: Eulerian formulation. *Journal of Computational Physics*, *229*(22), 8231–8258. http://doi.org/10.1016/j.jcp.2010.06.036

Lee, S.-J., Olsen, B., Schlesinger, P. H., & Baker, N. A. (2010). Characterization of perfluorooctylbromide-based nanoemulsion particles using atomistic molecular dynamics simulations. *The Journal of Physical Chemistry. B*, *114*(31), 10086–96. http://doi.org/10.1021/jp103228c

Sept, D., Baker, N. A., & McCammon, J. A. (2009). The physical basis of microtubule structure and stability. *Protein Science*, *12*(10), 2257–2261. http://doi.org/10.1110/ps.03187503

Chen, A. A., Marucho, M., Baker, N. A., & Pappu, R. V. (2009). *Simulations of RNA interactions with monovalent ions. Methods in Enzymology* (Vol. 469). Elsevier. http://doi.org/10.1016/S0076-6879(09)69020-0

Silva, J. R., Pan, H., Wu, D., Nekouzadeh, A., Decker, K. F., Cui, J., … Rudy, Y. (2009). A multiscale model linking ion-channel molecular dynamics and electrostatics to the cardiac action potential. *Proceedings of the National Academy of Sciences*, *106*(27), 11102–11106. http://doi.org/10.1073/pnas.0904505106

Olsen, B. N., Schlesinger, P. H., & Baker, N. A. (2009). Perturbations of membrane structure by cholesterol and cholesterol derivatives are determined by sterol orientation. *Journal of the American Chemical Society*, *131*(13), 4854–65. http://doi.org/10.1021/ja8095224

Thomas, D. G., Pappu, R. V., & Baker, N. A. (2009). Ontologies for cancer nanotechnology research. In *2009 Annual International Conference of the IEEE Engineering in Medicine and Biology Society* (Vol. 2009, pp. 4158–4161). IEEE. http://doi.org/10.1109/IEMBS.2009.5333941

Bradley, M. J., Chivers, P. T., & Baker, N. A. (2008). Molecular Dynamics Simulation of the Escherichia coli NikR Protein: Equilibrium Conformational Fluctuations Reveal Interdomain Allosteric Communication Pathways. *Journal of Molecular Biology*, *378*(5), 1155–1173. http://doi.org/10.1016/j.jmb.2008.03.010

Dong, F., Wagoner, J. A., & Baker, N. A. (2008). Assessing the performance of implicit solvation models at a nucleic acid surface. *Physical Chemistry Chemical Physics : PCCP*, *10*(32), 4889–902. http://doi.org/10.1039/b807384h

Lee, S.-J., Song, Y., & Baker, N. a. (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. *Biophysical Journal*, *94*(9), 3565–3576. http://doi.org/10.1529/biophysj.107.116335

Dong, F., Olsen, B., & Baker, N. A. (2008). Computational Methods for Biomolecular Electrostatics. In *Methods in Cell Biology* (Vol. 84, pp. 843–870). http://doi.org/10.1016/S0091-679X(07)84026-X

Cerutti, D. S., Baker, N. a, & McCammon, J. A. (2007). Solvent reaction field potential inside an uncharged globular protein: A bridge between implicit and explicit solvent models? *The Journal of Chemical Physics*, *127*(15), 155101. http://doi.org/10.1063/1.2771171

Schnieders, M. J., Baker, N. A., Ren, P., & Ponder, J. W. (2007). Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. *The Journal of Chemical Physics*, *126*(12), 124114. http://doi.org/10.1063/1.2714528

Swanson, J. M. J., Wagoner, J. A., Baker, N. A., & McCammon, J. A. (2007). Optimizing the Poisson Dielectric Boundary with Explicit Solvent Forces and Energies: Lessons Learned with Atom-Centered Dielectric Functions. *Journal of Chemical Theory and Computation*, *3*(1), 170–183. http://doi.org/10.1021/ct600216k

Dolinsky, T. J., Czodrowski, P., Li, H., Nielsen, J. E., Jensen, J. H., Klebe, G., & Baker, N. A. (2007). PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. *Nucleic Acids Research*, *35*(Web Server), W522–W525. http://doi.org/10.1093/nar/gkm276

Cheng, Y., Suen, J. K., Zhang, D., Bond, S. D., Zhang, Y., Song, Y., … McCammon, J. A. (2007). Finite Element Analysis of the Time-Dependent Smoluchowski Equation for Acetylcholinesterase Reaction Rate Calculations. *Biophysical Journal*, *92*(10), 3397–3406. http://doi.org/10.1529/biophysj.106.102533

Wagoner, J. A., & Baker, N. A. (2006). Assessing implicit models for nonpolar mean solvation forces: The importance of dispersion and volume terms. *Proceedings of the National Academy of Sciences*, *103*(22), 8331–8336. http://doi.org/10.1073/pnas.0600118103

Konecny, R., Trylska, J., Tama, F., Zhang, D., Baker, N. A., Brooks, C. L., & McCammon, J. A. (2006). Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. *Biopolymers*, *82*(2), 106–120. http://doi.org/10.1002/bip.20409

Zhang, X., Bajaj, C. L., Kwon, B., Dolinsky, T. J., Nielsen, J. E., & Baker, N. A. (2006). Application of New Multiresolution Methods for the Comparison of Biomolecular Electrostatic Properties in the Absence of Global Structural Similarity. *Multiscale Modeling & Simulation*, *5*(4), 1196–1213. http://doi.org/10.1137/050647670

Baker, N. A., Bashford, D., & Case, D. A. (2006). *Implicit solvent electrostatics in biomolecular simulation.* (B. Leimkuhler, C. Chipot, R. Elber, A. Laaksonen, A. Mark, T. Schlick, … R. Skeel, Eds.), *New Algorithms for Macromolecular Simulation* (Vol. 49). Berlin/Heidelberg: Springer-Verlag. http://doi.org/10.1007/3-540-31618-3

Wong, C. J., Rice, R. L., Baker, N. A., Ju, T., & Lohman, T. M. (2006). Probing 3'-ssDNA loop formation in E. coli RecBCD/RecBC-DNA complexes using non-natural DNA: a model for "Chi" recognition complexes. *Journal of Molecular Biology*, *362*(1), 26–43. http://doi.org/10.1016/j.jmb.2006.07.016

Baker, N. A. (2005). Improving implicit solvent simulations: a Poisson-centric view. *Current Opinion in Structural Biology*, *15*(2), 137–143. http://doi.org/10.1016/j.sbi.2005.02.001

Song, Y., Guallar, V., & Baker, N. A. (2005). Molecular Dynamics Simulations of Salicylate Effects on the Micro- and Mesoscopic Properties of a Dipalmitoylphosphatidylcholine Bilayer. *Biochemistry*, *44*(41), 13425–13438. http://doi.org/10.1021/bi0506829

Baker, N. A. (2005). Biomolecular Applications of Poisson-Boltzmann Methods. In K. B. Lipkowitz, R. Larter, & T. R. Cundari (Eds.), *Reviews in Computational Chemistry* (21st ed., Vol. 21, pp. 349–379). Hoboken, NJ, USA: John Wiley & Sons, Inc. http://doi.org/10.1002/0471720895

Showalter, S. A., Baker, N. A., Tang, C., & Hall, K. B. (2005). Iron Responsive Element RNA Flexibility Described by NMR and Isotropic Reorientational Eigenmode Dynamics. *Journal of Biomolecular NMR*, *32*(3), 179–193. http://doi.org/10.1007/s10858-005-7948-2

Zhang, D., Suen, J., Zhang, Y., Song, Y., Radic, Z., Taylor, P., … McCammon, J. A. (2005). Tetrameric Mouse Acetylcholinesterase: Continuum Diffusion Rate Calculations by Solving the Steady-State Smoluchowski Equation Using Finite Element Methods. *Biophysical Journal*, *88*(3), 1659–1665. http://doi.org/10.1529/biophysj.104.053850

Wagoner, J., & Baker, N. A. (2004). Solvation forces on biomolecular structures: A comparison of explicit solvent and Poisson-Boltzmann models. *Journal of Computational Chemistry*, *25*(13), 1623–1629. http://doi.org/10.1002/jcc.20089

Zhang, D., Konecny, R., Baker, N. A., & McCammon, J. A. (2004). Electrostatic interaction between RNA and protein capsid in cowpea chlorotic mottle virus simulated by a coarse-grain RNA model and a Monte Carlo approach. *Biopolymers*, *75*(4), 325–337. http://doi.org/10.1002/bip.20120

Song, Y., Zhang, Y., Bajaj, C. L., & Baker, N. A. (2004). Continuum diffusion reaction rate calculations of wild-type and mutant mouse acetylcholinesterase: adaptive finite element analysis. *Biophysical Journal*, *87*(3), 1558–66. http://doi.org/10.1529/biophysj.104.041517

Vitalis, A., Baker, N. A., & McCammon, J. A. (2004). ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. *Molecular Simulation*, *30*(1), 45–61. http://doi.org/10.1080/08927020310001597862

Dolinsky, T. J., Burgers, P. M. J., Karplus, K., & Baker, N. A. (2004). SPrCY: comparison of structural predictions in the Saccharomyces cerevisiae genome. *Bioinformatics (Oxford, England)*, *20*(14), 2312–4. http://doi.org/10.1093/bioinformatics/bth223

Baker, N. A. (2004). Poisson–Boltzmann Methods for Biomolecular Electrostatics. In *Methods in enzymology* (Vol. 383, pp. 94–118). American Chemical Society. http://doi.org/10.1016/S0076-6879(04)83005-2

Dolinsky, T. J., Nielsen, J. E., McCammon, J. A., & Baker, N. A. (2004). PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. *Nucleic Acids Research*, *32*(Web Server), W665–W667. http://doi.org/10.1093/nar/gkh381

Song, Y., Zhang, Y., Shen, T., Bajaj, C. L., McCammon, J. A., & Baker, N. A. (2004). Finite Element Solution of the Steady-State Smoluchowski Equation for Rate Constant Calculations. *Biophysical Journal*, *86*(4), 2017–2029. http://doi.org/10.1016/S0006-3495(04)74263-0

Tai, K., Bond, S. D., MacMillan, H. R., Baker, N. A., Holst, M. J., & McCammon, J. A. (2003). Finite element simulations of acetylcholine diffusion in neuromuscular junctions. *Biophysical Journal*, *84*(4), 2234–41. http://doi.org/10.1016/S0006-3495(03)75029-2

Lin, J.-H., Baker, N. A., & McCammon, J. A. (2002). Bridging Implicit and Explicit Solvent Approaches for Membrane Electrostatics. *Biophysical Journal*, *83*(3), 1374–1379. http://doi.org/10.1016/S0006-3495(02)73908-8

Ma, C., Baker, N. A., Joseph, S., & McCammon, J. A. (2002). Binding of Aminoglycoside Antibiotics to the Small Ribosomal Subunit: A Continuum Electrostatics Investigation. *Journal of the American Chemical Society*, *124*(7), 1438–1442. http://doi.org/10.1021/ja016830+

Baker, N. A., Tai, K., Henchman, R., Sept, D., Elcock, A., Holst, M. J., & McCammon, J. A. (2002). Mathematics and Molecular Neurobiology. In T. Schlick & H. H. Gan (Eds.), *Computational Methods for Macromolecules: Challenges and Applications* (Vol. 24, pp. 31–60). Berlin, Heidelberg: Springer Berlin Heidelberg. http://doi.org/10.1007/978-3-642-56080-4

Baker, N. A., Sept, D., Holst, M. J., & McCammon, J. A. (2001). The adaptive multilevel finite element solution of the Poisson-Boltzmann equation on massively parallel computers. *IBM Journal of Research and Development*, *45*(3.4), 427–438. http://doi.org/10.1147/rd.453.0427

Baker, N. A., Sept, D., Joseph, S., Holst, M. J., & McCammon, J. A. (2001). Electrostatics of nanosystems: Application to microtubules and the ribosome. *Proceedings of the National Academy of Sciences*, *98*(18), 10037–10041. http://doi.org/10.1073/pnas.181342398

Holst, M. J., Baker, N. A., Wang, F., & McCammon, J. A. (2000). Adaptive multilevel finite element solution of the Poisson-Boltzmann equation I. Algorithms and examples. *Journal of Computational Chemistry*, *21*(15), 1319–1342. http://doi.org/10.1002/1096-987X(20001130)21:15<1319::AID-JCC1>3.0.CO;2-8

Baker, N., Holst, M., & Wang, F. (2000). Adaptive multilevel finite element solution of the Poisson-Boltzmann equation II. Refinement at solvent-accessible surfaces in biomolecular systems. *Journal of Computational Chemistry*, *21*(15), 1343–1352. http://doi.org/10.1002/1096-987X(20001130)21:15<1343::AID-JCC2>3.0.CO;2-K

Quinn, D. M., Feaster, S. R., Nair, H. K., Baker, N. A., Radić, Z., & Taylor, P. (2000). Delineation and Decomposition of Energies Involved in Quaternary Ammonium Binding in the Active Site of Acetylcholinesterase. *Journal of the American Chemical Society*, *122*(13), 2975–2980. http://doi.org/10.1021/ja9933588

Baker, N. A., Hünenberger, P. H., & McCammon, J. A. (1999). Polarization around an ion in a dielectric continuum with truncated electrostatic interactions. *The Journal of Chemical Physics*, *110*(22), 10679. http://doi.org/10.1063/1.479013

Quinn, D. M., Medhekar, R., & Baker, N. A. (1999). Ester hydrolysis. In *Comprehensive Natural Products Chemistry: Enzymes, Enzyme Mechanisms, Proteins, and Aspects of NO Chemistry* (pp. 101–137). Oxford, UK: Elsevier Science Inc.

Baker, N. A., & McCammon, J. A. (1999). Non-Boltzmann Rate Distributions in Stochastically Gated Reactions. *The Journal of Physical Chemistry B*, *103*(4), 615–617. http://doi.org/10.1021/jp984151o

Baker, N. A., Helms, V., & McCammon, J. A. (1999). Dynamical properties of fasciculin-2. *Proteins*, *36*(4), 447–53. http://doi.org/10.1002/(SICI)1097-0134(19990901)36:4<447::AID-PROT8>3.0.CO;2-E

Malany, S., Baker, N., Verweyst, M., Medhekar, R., Quinn, D. M., Velan, B., … Shafferman, A. (1999). Theoretical and experimental investigations of electrostatic effects on acetylcholinesterase catalysis and inhibition. *Chemico-Biological Interactions*, *119-120*, 99–110. http://doi.org/10.1016/S0009-2797(99)00018-6

Medhekar, R., Baker, N., Kearney, W., Sando, K., & Quinn, D. M. (1998). Low-barrier hydrogen bond in the catalytic triad of serine esterases. In B. P. Doctor, P. Taylor, D. M. Quinn, R. L. Rotundo, & M. K. Gentry (Eds.), *Structure and Function of Cholinesterases and Related Proteins* (p. 233). Boston, MA: Springer US. http://doi.org/10.1007/978-1-4899-1540-5

Feaster, S. R., Lee, K., Baker, N., Hui, D. Y., & Quinn, D. M. (1996). Molecular Recognition by Cholesterol Esterase of Active Site Ligands: Structure−Reactivity Effects for Inhibition by Aryl Carbamates and Subsequent Carbamylenzyme Turnover. *Biochemistry*, *35*(51), 16723–16734. http://doi.org/10.1021/bi961677v