BIOGRAPHICAL SKETCH

Nathan Andrew Baker

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| INSTITUTION AND LOCATION | DEGREE | Completion Date | FIELD OF STUDY |
| University of Iowa, Iowa City, IA | BS | 05/1997 | Chemistry |
| University of California San Diego, La Jolla, CA | PhD | 04/2001 | Physical Chemistry |
| University of California San Diego, La Jolla, CA | Postdoctoral Fellow | 07/2002 | Computational Biology |

### A. PERSONAL STATEMENT

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 research 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>). His research is currently funded by the National Institutes of Health and the Department of Energy.

Dr. Baker is Lead for the Signature Discovery Initiative at PNNL and serves as co-PI and program manager for the DOE ASCR Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4). He also manages the Applied Statistics and Computational Modeling Group at PNNL, which comprises approximately 50 staff with expertise in statistics, mathematics, and operations research.

Dr. Baker has served on numerous review panels for agencies including NIH and NSF and is currently a member of the NIH Macromolecular Structure and Function D study section. He is currently an Associate Editor for Biophysical Journal, serves on the editorial board for NPG Scientific Data, and has previously served as Editor-in-Chief for the Computational Science and Discovery journal and Section Editor for Annual Reports in Computational Chemistry.

Dr. Baker is the author of over 80 publications. He is a Fellow of the American Association for the Advancement of Science, has been awarded the Hewlett-Packard Junior Faculty Excellence Award by the American Chemical Society, the National Cancer Institute caBIG® Connecting Collaborators Award, and an Alfred P. Sloan Research Fellowship.

### B. POSITIONS AND HONORS

Positions and Employment

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| --- | --- |
| 1994 - 1997 | Undergraduate researcher, University of Iowa, Department of Chemistry, Iowa City, IA |
| 1997 - 2001 | Graduate research fellow, University of California San Diego, Department of Chemistry and Biochemistry, La Jolla, CA |
| 1999 - 2001 | Graduate research fellow, University of California San Diego, Department of Mathematics, La Jolla, CA |
| 2001 - 2002 | Postdoctoral fellow, University of California San Diego, Department of Chemistry and Biochemistry, La Jolla, CA |
| 2002 - 2006 | Assistant Professor, Washington University in St. Louis, Department of Biochemistry and Molecular Biophysics, St. Louis, MO |
| 2006 - 2010 | Associate Professor with tenure, Washington University in St. Louis, Department of Biochemistry and Molecular Biophysics, St. Louis, MO |
| 2010 - 2012 | Chief Scientist, Pacific Northwest National Laboratory, Computational and Statistical Analytics Division, Richland, WA |
| 2012 - | Laboratory Fellow, Pacific Northwest National Laboratory, Computational and Statistical Analytics, Richland, WA |
| 2013 - | Technical Group Manager, Pacific Northwest National Laboratory, Applied Statistics and Computational Modeling Group, Richland, WA |

Selected Other Experience and Professional Memberships

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| 2005 - 2014 | Ad hoc member, various study sections, National Institutes of Health |
| 2007 - 2010 | Director, Molecular Biophysics PhD Program, Washington University in St. Louis |
| 2007 - 2013 | Member, Committee for the Professional Opportunities for Women, Biophysical Society |
| 2008 - 2009 | Co-organizer, 23rd Annual Gibbs Conference on Biothermodynamics |
| 2008 - 2014 | Section Editor, Annual Reports in Computational Chemistry |
| 2008 - 2014 | Editorial Board Member, Biophysical Journal, Biophysical Society |
| 2008 - 2014 | Member, Faculty of 1000 Biology |
| 2009 - 2013 | Lead, Nanotechnology Working Group, National Cancer Institute National Cancer Informatics Program (formerly caBIG) |
| 2009 - 2014 | Chair, E56.01 Nanotechnology Subcommittee on Informatics and Terminology, ASTM |
| 2009 - 2014 | Editorial Board Member, Computational Science and Discovery |
| 2010 - 2010 | Member, Advisory Board, Integrated Graduate Education and Research Training (IGERT) in Health-Assistive Smart Environments, Washington State University |
| 2010 - 2011 | Member, College of Reviewers, National Institutes of Health College |
| 2010 - 2012 | Chief Scientist and Deputy Lead, Signature Discovery Initiative, Pacific Northwest National Laboratory |
| 2010 - 2013 | Ad hoc member, various review panels, National Science Foundation |
| 2010 - 2013 | Member, Advisory Board, Nano Registry, RTI, Inc. |
| 2011 - | Editor-in-Chief, Computational Science and Discovery |
| 2011 - 2011 | Reviewer, Defense Threat Reduction Agency |
| 2012 - | Lead, Signature Discovery Initiative, Pacific Northwest National Laboratory |
| 2012 - | Member, Council of Fellows Executive Committee, Pacific Northwest National Laboratory |
| 2012 - | Member, Macromolecular Structure & Function D Study Section, National Institutes of Health |
| 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 | Reviewer, A Research Strategy for Environmental, Health, and Safety Aspects of Engineered Nanomaterials, National Research Council |
| 2012 | Reviewer, US Air Force Office of Science and Research |
| 2012 - 2013 | Member, Mentor Center, Biophysical Society |
| 2012 - 2013 | Member, Working Group 1, Nomenclature and Terminology, U.S. Technical Advisory Group to the International Standards Organization TC-229 Committee on Nanotechnologies |
| 2012 - | Organizing committee member, Conference on Data Analysis (CoDA) 2014 |
| 2012 - 2015 | Co-chair, Nanomaterial Databases and Ontology, United States-European Union Communities of Research |
| 2013 - 2014 | Reviewer, INCITE Biological Sciences Panel, Department of Energy, Advanced Scientific Computing Research |
| 2013 | Reviewer, Progress in Research on Environmental, Health, and Safety Aspects of Engineered Nanomaterials, National Research Council |
| 2014 - | Editorial Board Member, Scientific Data, Nature Publishing Group |
| 2014 - | Associate Editor, Biophysical Journal, Biophysical Society |
| 2014 - | Chair, PNNL Institutional Computing Steering Committee, Pacific Northwest National Laboratory |
| 2015 | Member, Institutional Oversight Committee for Diversity and Inclusivity, Pacific Northwest National Laboratory |
| 2015 | R&D Data Management and Analysis Review, Novozymes |
| 2015 | Member, J9BA Life Sciences Red Team Review Panel, Defense Threat Reduction Agency |

Selected honors

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| --- | --- |
| 1995 | Undergraduate fellowship, Barry M. Goldwater fund |
| 1997 | Collegiate Scholar, University of Iowa |
| 1997 | Predoctoral fellowship, Howard Hughes Medical Institute |
| 1997 | Predoctoral fellowship, Burroughs-Wellcome La Jolla Interfaces in Science Program |
| 2004 | Research Fellow, Alfred P. Sloan Foundation |
| 2007 | Hewlett-Packard Junior Faculty Excellence Award, American Chemical Society |
| 2010 | Cancer Biomedical Informatics Grid (caBIG®) Connecting Collaborators Award, National Cancer Institute |
| 2012 | Fellow, American Association for the Advancement of Science |

### C. SELECTED PUBLICATIONS (of 88 total)

1. Holst M, Baker N, Wang F. Adaptive multilevel finite element solution of the Poisson–Boltzmann equation I. Algorithms and examples. Journal of computational chemistry. 2000 October; 21(15):1319-1342.
2. Baker N, Holst M, Wang F. Adaptive multilevel finite element solution of the Poisson–Boltzmann equation II. Refinement at solvent-accessible surfaces in biomolecular systems. Journal of Computational Chemistry. 2000 November; 21(15):1343-1352.
3. Baker NA, Sept DS, Holst MJ, McCammon JA. The adaptive multilevel finite element solution of the Poisson-Boltzmann equation on massively parallel computers. IBM Journal of Research and Development. 2001 May; 45(3-4):427-438.
4. Baker NA, Sept D, Joseph S, Holst MJ, McCammon JA. Electrostatics of nanosystems: application to microtubules and the ribosome. Proc Natl Acad Sci U S A. 2001 Aug 28;98(18):10037-41. PubMed PMID: [11517324](http://www.ncbi.nlm.nih.gov/pubmed/11517324/); PubMed Central PMCID: [PMC56910](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC56910/).
5. Tai K, Bond SD, MacMillan HR, Baker NA, Holst MJ, et al. Finite element simulations of acetylcholine diffusion in neuromuscular junctions. Biophys J. 2003 Apr;84(4):2234-41. PubMed PMID: [12668432](http://www.ncbi.nlm.nih.gov/pubmed/12668432/); PubMed Central PMCID: [PMC1302790](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1302790/).
6. Baker NA. Poisson-Boltzmann methods for biomolecular electrostatics. Methods Enzymol. 2004;383:94-118. PubMed PMID: [15063648](http://www.ncbi.nlm.nih.gov/pubmed/15063648/).
7. Song Y, Zhang Y, Shen T, Bajaj CL, McCammon JA, et al. Finite element solution of the steady-state Smoluchowski equation for rate constant calculations. Biophys J. 2004 Apr;86(4):2017-29. PubMed PMID: [15041644](http://www.ncbi.nlm.nih.gov/pubmed/15041644/); PubMed Central PMCID: [PMC1304055](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1304055/).
8. Dolinsky TJ, Nielsen JE, McCammon JA, Baker NA. PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. Nucleic Acids Res. 2004 Jul 1;32(Web Server issue):W665-7. PubMed PMID: [15215472](http://www.ncbi.nlm.nih.gov/pubmed/15215472/); PubMed Central PMCID: [PMC441519](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC441519/).
9. Song Y, Zhang Y, Bajaj CL, Baker NA. Continuum diffusion reaction rate calculations of wild-type and mutant mouse acetylcholinesterase: adaptive finite element analysis. Biophys J. 2004 Sep;87(3):1558-66. PubMed PMID: [15345536](http://www.ncbi.nlm.nih.gov/pubmed/15345536/); PubMed Central PMCID: [PMC1304562](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1304562/).
10. Dolinsky TJ, Burgers PM, Karplus K, Baker NA. SPrCY: comparison of structural predictions in the Saccharomyces cerevisiae genome. Bioinformatics. 2004 Sep 22;20(14):2312-4. PubMed PMID: [15059824](http://www.ncbi.nlm.nih.gov/pubmed/15059824/).
11. Wagoner J, Baker NA. Solvation forces on biomolecular structures: a comparison of explicit solvent and Poisson-Boltzmann models. J Comput Chem. 2004 Oct;25(13):1623-9. PubMed PMID: [15264256](http://www.ncbi.nlm.nih.gov/pubmed/15264256/).
12. Zhang D, Konecny R, Baker NA, McCammon JA. 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. 2004 Nov;75(4):325-37. PubMed PMID: [15386271](http://www.ncbi.nlm.nih.gov/pubmed/15386271/); PubMed Central PMCID: [PMC2426774](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2426774/).
13. Baker NA, McCammon JA. Electrostatic Interactions. Structural Bioinformatics. 2005 January; 44.
14. Zhang D, Suen J, Zhang Y, Song Y, Radic Z, et al. Tetrameric mouse acetylcholinesterase: continuum diffusion rate calculations by solving the steady-state Smoluchowski equation using finite element methods. Biophys J. 2005 Mar;88(3):1659-65. PubMed PMID: [15626705](http://www.ncbi.nlm.nih.gov/pubmed/15626705/); PubMed Central PMCID: [PMC1305222](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1305222/).
15. Baker NA. Improving implicit solvent simulations: a Poisson-centric view. Curr Opin Struct Biol. 2005 Apr;15(2):137-43. PubMed PMID: [15837170](http://www.ncbi.nlm.nih.gov/pubmed/15837170/).
16. Baker NA. Biomolecular Applications of Poisson–Boltzmann Methods. Reviews in Computational Chemistry. 2005 April; 21:349-379.
17. Showalter SA, Baker NA, Tang C, Hall KB. Iron responsive element RNA flexibility described by NMR and isotropic reorientational eigenmode dynamics. J Biomol NMR. 2005 Jul;32(3):179-93. PubMed PMID: [16132819](http://www.ncbi.nlm.nih.gov/pubmed/16132819/).
18. Zhang X, Bajaj CL, Kwon B, Dolinsky TJ, Nielsen JE, et al. Application of new multi-resolution methods for the comparison of biomolecular electrostatic properties in the absence of global structural similarity. Multiscale Model Simul. 2006;5(4):1196-1213. PubMed PMID: [18841247](http://www.ncbi.nlm.nih.gov/pubmed/18841247/); PubMed Central PMCID: [PMC2561295](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2561295/).
19. Baker NA, Bashford D, Case DA. Implicit Solvent Electrostatics in Biomolecular Simulation. Lecture Notes in Computational Science and Engineering. 2006; 49:263-295.
20. Wagoner JA, Baker NA. Assessing implicit models for nonpolar mean solvation forces: the importance of dispersion and volume terms. Proc Natl Acad Sci U S A. 2006 May 30;103(22):8331-6. PubMed PMID: [16709675](http://www.ncbi.nlm.nih.gov/pubmed/16709675/); PubMed Central PMCID: [PMC1482494](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1482494/).
21. Konecny R, Trylska J, Tama F, Zhang D, Baker NA, et al. Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. Biopolymers. 2006 Jun 5;82(2):106-20. PubMed PMID: [16278831](http://www.ncbi.nlm.nih.gov/pubmed/16278831/); PubMed Central PMCID: [PMC2440512](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2440512/).
22. Vitalis A, Baker NA, McCammon JA. ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. Molecular simulation. 2006 August; 30(1):45-61.
23. Schnieders MJ, Baker NA, Ren P, Ponder JW. Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. J Chem Phys. 2007 Mar 28;126(12):124114. PubMed PMID: [17411115](http://www.ncbi.nlm.nih.gov/pubmed/17411115/); PubMed Central PMCID: [PMC2430168](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2430168/).
24. Cheng Y, Suen JK, Zhang D, Bond SD, Zhang Y, et al. Finite element analysis of the time-dependent Smoluchowski equation for acetylcholinesterase reaction rate calculations. Biophys J. 2007 May 15;92(10):3397-406. PubMed PMID: [17307827](http://www.ncbi.nlm.nih.gov/pubmed/17307827/); PubMed Central PMCID: [PMC1853150](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1853150/).
25. Dolinsky TJ, Czodrowski P, Li H, Nielsen JE, Jensen JH, et al. PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. Nucleic Acids Res. 2007 Jul;35(Web Server issue):W522-5. PubMed PMID: [17488841](http://www.ncbi.nlm.nih.gov/pubmed/17488841/); PubMed Central PMCID: [PMC1933214](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1933214/).
26. Cerutti DS, Baker NA, McCammon JA. Solvent reaction field potential inside an uncharged globular protein: a bridge between implicit and explicit solvent models?. J Chem Phys. 2007 Oct 21;127(15):155101. PubMed PMID: [17949217](http://www.ncbi.nlm.nih.gov/pubmed/17949217/); PubMed Central PMCID: [PMC2556216](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2556216/).
27. Swanson JJ, Wagoner JA, McCammon JA. Optimizing the Poisson Dielectric Boundary with Explicit Solvent Forces and Energies:  Lessons Learned with Atom-Centered Dielectric Functions. Journal of chemical theory and computation. 2007 November; 3(1):170-183.
28. Dong F, Olsen B, Baker NA. Computational methods for biomolecular electrostatics. Methods Cell Biol. 2008;84:843-70. PubMed PMID: [17964951](http://www.ncbi.nlm.nih.gov/pubmed/17964951/); PubMed Central PMCID: [PMC2423940](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2423940/).
29. Bradley MJ, Chivers PT, Baker NA. Molecular dynamics simulation of the Escherichia coli NikR protein: equilibrium conformational fluctuations reveal interdomain allosteric communication pathways. J Mol Biol. 2008 May 16;378(5):1155-73. PubMed PMID: [18433769](http://www.ncbi.nlm.nih.gov/pubmed/18433769/); PubMed Central PMCID: [PMC2478562](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2478562/).
30. Dong F, Wagoner JA, Baker NA. Assessing the performance of implicit solvation models at a nucleic acid surface. Phys Chem Chem Phys. 2008 Aug 28;10(32):4889-902. PubMed PMID: [18688533](http://www.ncbi.nlm.nih.gov/pubmed/18688533/); PubMed Central PMCID: [PMC2538626](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2538626/).
31. Thomas DG, Pappu RV, Baker NA. Ontologies for cancer nanotechnology research. Conf Proc IEEE Eng Med Biol Soc. 2009;2009:4158-61. PubMed PMID: [19964619](http://www.ncbi.nlm.nih.gov/pubmed/19964619/).
32. Chen AA, Marucho M, Baker NA, Pappu RV. Simulations of RNA interactions with monovalent ions. Methods Enzymol. 2009;469:411-32. PubMed PMID: [20946801](http://www.ncbi.nlm.nih.gov/pubmed/20946801/).
33. Silva JR, Pan H, Wu D, Nekouzadeh A, Decker KF, et al. A multiscale model linking ion-channel molecular dynamics and electrostatics to the cardiac action potential. Proc Natl Acad Sci U S A. 2009 Jul 7;106(27):11102-6. PubMed PMID: [19549851](http://www.ncbi.nlm.nih.gov/pubmed/19549851/); PubMed Central PMCID: [PMC2700153](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2700153/).
34. Callenberg KM, Choudhary OP, de Forest GL, Gohara DW, Baker NA, et al. APBSmem: a graphical interface for electrostatic calculations at the membrane. PLoS One. 2010 Sep 29;5(9)PubMed PMID: [20949122](http://www.ncbi.nlm.nih.gov/pubmed/20949122/); PubMed Central PMCID: [PMC2947494](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2947494/).
35. Chen Z, Baker NA, Wei GW. Differential geometry based solvation model I: Eulerian formulation. J Comput Phys. 2010 Nov 1;229(22):8231-8258. PubMed PMID: [20938489](http://www.ncbi.nlm.nih.gov/pubmed/20938489/); PubMed Central PMCID: [PMC2951687](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2951687/).
36. Hossain K, Bailey-Kellogg C, Friedman AM, Bradley MJ, Baker NA, et al. Using physicochemical properties of amino acids to induce graphical models of residue couplings. BIOKDD 11. 2011;
37. Thomas DG, Pappu RV, Baker NA. NanoParticle Ontology for cancer nanotechnology research. J Biomed Inform. 2011 Feb;44(1):59-74. PubMed PMID: [20211274](http://www.ncbi.nlm.nih.gov/pubmed/20211274/); PubMed Central PMCID: [PMC3042056](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3042056/).
38. Unni S, Huang Y, Hanson RM, Tobias M, Krishnan S, et al. Web servers and services for electrostatics calculations with APBS and PDB2PQR. J Comput Chem. 2011 May;32(7):1488-91. PubMed PMID: [21425296](http://www.ncbi.nlm.nih.gov/pubmed/21425296/); PubMed Central PMCID: [PMC3062090](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3062090/).
39. Thomas DG, Klaessig F, Harper SL, Fritts M, Hoover MD, et al. Informatics and standards for nanomedicine technology. Wiley Interdiscip Rev Nanomed Nanobiotechnol. 2011 Sep-Oct;3(5):511-32. PubMed PMID: [21721140](http://www.ncbi.nlm.nih.gov/pubmed/21721140/); PubMed Central PMCID: [PMC3189420](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3189420/).
40. Carstensen T, Farrell D, Huang Y, Baker NA, Nielsen JE. On the development of protein pKa calculation algorithms. Proteins. 2011 Dec;79(12):3287-98. PubMed PMID: [21744393](http://www.ncbi.nlm.nih.gov/pubmed/21744393/); PubMed Central PMCID: [PMC3193850](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3193850/).
41. Alexov E, Mehler EL, Baker N, Baptista AM, Huang Y, et al. Progress in the prediction of pKa values in proteins. Proteins. 2011 Dec;79(12):3260-75. PubMed PMID: [22002859](http://www.ncbi.nlm.nih.gov/pubmed/22002859/); PubMed Central PMCID: [PMC3243943](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3243943/).
42. Chen Z, Baker NA, Wei GW. Differential geometry based solvation model II: Lagrangian formulation. J Math Biol. 2011 Dec;63(6):1139-200. PubMed PMID: [21279359](http://www.ncbi.nlm.nih.gov/pubmed/21279359/); PubMed Central PMCID: [PMC3113640](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3113640/).
43. Lee SJ, Schlesinger PH, Wickline SA, Lanza GM, Baker NA. Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers. Soft Matter. 2012 Jan 1;8(26):3024-3035. PubMed PMID: [22712024](http://www.ncbi.nlm.nih.gov/pubmed/22712024/); PubMed Central PMCID: [PMC3375911](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3375911/).
44. Jacob F, Wynne AS, Liu YJ, Baker NA, Gray J. Domain Specific Languages for Composing Signature Discovery Workflows. Domain Specific Languages for Composing Signature Discovery Workflows. 2012; :61-64.
45. Maojo V, Fritts M, Martin-Sanchez F, De la Iglesia D, Cachau RE, et al. Nanoinformatics: developing new computing applications for nanomedicine. Comput Sci Eng. 2012 Jun 1;94(6):521-539. PubMed PMID: [22942787](http://www.ncbi.nlm.nih.gov/pubmed/22942787/); PubMed Central PMCID: [PMC3430140](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3430140/).
46. Konecny R, Baker NA, McCammon JA. iAPBS: a programming interface to Adaptive Poisson-Boltzmann Solver (APBS). Comput Sci Discov. 2012 Jul 26;5(1)PubMed PMID: [22905037](http://www.ncbi.nlm.nih.gov/pubmed/22905037/); PubMed Central PMCID: [PMC3419494](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3419494/).
47. Chen Z, Zhao S, Chun J, Thomas DG, Baker NA, et al. Variational approach for nonpolar solvation analysis. J Chem Phys. 2012 Aug 28;137(8):084101. PubMed PMID: [22938212](http://www.ncbi.nlm.nih.gov/pubmed/22938212/); PubMed Central PMCID: [PMC3436914](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3436914/).
48. Thomas DG, Chikkagoudar S, Chappell AR, Baker NA. Annotating the structure and components of a nanoparticle formulation using computable string expressions. Bioinformatics and Biomedicine Workshops (BIBMW), 2012 IEEE International Conference on . 2012 October; :889-894.
49. Ren P, Chun J, Thomas DG, Schnieders MJ, Marucho M, et al. Biomolecular electrostatics and solvation: a computational perspective. Q Rev Biophys. 2012 Nov;45(4):427-91. PubMed PMID: [23217364](http://www.ncbi.nlm.nih.gov/pubmed/23217364/); PubMed Central PMCID: [PMC3533255](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3533255/).
50. Harper SL, Hutchison JE, Baker N, Ostraat M, Tinkle S, et al. Nanoinformatics workshop report: Current resources, community needs, and the proposal of a collaborative framework for data sharing and information integration. Comput Sci Discov. 2013;6(1):14008. PubMed PMID: [24454543](http://www.ncbi.nlm.nih.gov/pubmed/24454543/); PubMed Central PMCID: [PMC3895330](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3895330/).
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52. Baker NA, Klemm JD, Harper SL, Gaheen S, Heiskanen M, et al. Standardizing data. Nat Nanotechnol. 2013 Feb;8(2):73-4. PubMed PMID: [23380926](http://www.ncbi.nlm.nih.gov/pubmed/23380926/); PubMed Central PMCID: [PMC4054689](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4054689/).
53. Thomas DG, Chun J, Chen Z, Wei G, Baker NA. Parameterization of a geometric flow implicit solvation model. J Comput Chem. 2013 Mar 30;34(8):687-95. PubMed PMID: [23212974](http://www.ncbi.nlm.nih.gov/pubmed/23212974/); PubMed Central PMCID: [PMC3578971](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3578971/).
54. Chakraborty S, Rao BJ, Baker N, Ásgeirsson B. Structural phylogeny by profile extraction and multiple superimposition using electrostatic congruence as a discriminator. Intrinsically Disordered Proteins. 2013 April; 1:69-81.
55. Baker NA, Barr JL, Bonheyo GT, Joslyn CA, Krishnaswami K, et al. Research towards a systematic signature discovery process. Intelligence and Security Informatics (ISI), 2013 IEEE International Conference on . 2013 June; :301-308.
56. Olsen BN, Bielska AA, Lee T, Daily MD, Covey DF, et al. The structural basis of cholesterol accessibility in membranes. Biophys J. 2013 Oct 15;105(8):1838-47. PubMed PMID: [24138860](http://www.ncbi.nlm.nih.gov/pubmed/24138860/); PubMed Central PMCID: [PMC3797575](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3797575/).
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60. Thomas DG, Chikkagoudar S, Heredia-Langer A, Tardiff MF, Xu Z, et al. Physicochemical signatures of nanoparticle-dependent complement activation. Comput Sci Discov. 2014 Mar 21;7(1):015003. PubMed PMID: [25254068](http://www.ncbi.nlm.nih.gov/pubmed/25254068/); PubMed Central PMCID: [PMC4169987](http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4169987/).
61. Lei H, Yang X, Lin G, Baker NA. Quantifying the influence of conformational uncertainty in biomolecular solvation. 2014 August. <http://arxiv.org/abs/1408.5629>
62. Wei G, Baker NA. Differential geometry-based solvation and electrolyte transport models for biomolecular modeling: a review. 2014 November. <http://arxiv.org/abs/1412.0176>
63. Pan W, Daily M, Baker NA. Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smooth particle hydrodynamics. BMC biophysics. In press. <http://arxiv.org/abs/1501.04240>

### D. RESEARCH SUPPORT

Ongoing Research Support

2014/08/01-2019/07/30

FWP 60650, DOE NNSA: DNN R&D

Baker, Nathan (PI)

Consortium for Nonproliferation Enabling Capabilities (CNEC)

CNEC is a consortium of universities and DOE National Laboratories designed enhance US nonproliferation capabilities through a combination of education R&D.

Role: Co-Investigator

2012/08/01-2017/07/31

FWP 63024, DOE Office of Science: Advanced Scientific Computing Research

Karniadakis, George (PI)

Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4)

Develop a systematic mathematical foundation for the understanding and control of the fundamental mechanisms in the mesoscale processes that permit the scalable synthesis of complex materials, through the design of effective and rigorous modeling and simulation methods and the corresponding scalable algorithms.

Role: CPI

2004/01/01-2017/02/28

R01 GM069702, National Institutes of Health

Baker, Nathan (PI)

APBS: Nanoscale biomolecular electrostatics software

The goal of this project is to enable the investigation of the solvation and electrostatic properties of macromolecules in biomedical research by supporting the maintenance and continued development of the open-source Adaptive Poisson-Boltzmann Solver (APBS) and PDB2PQR software packages.

Role: PI

2012/09/01-2016/07/30

R01 GM099450, National Institutes of Health

Onufriev, Alexey (PI)

DNA-DNA interactions with atomic detail

Provide Monte Carlo simulations and classical density functional analysis of ion atomspheres around DNA complexes

Role: PI

Completed Research Support

2011/01/01-2014/11/30

R01 HL067773, National Institutes of Health

Ory, Daniel (PI)

Mechanism of oxysterol activation of membrane cholesterol

Provide molecular simulation support to oxysterol-membrane interaction analysis.

Role: KP

2010/09/01-2013/08/30

U01 NS073457, National Institutes of Health

Hourcade, Dennis (PI)

Characterization/bioinformatics-modeling of nanoparticle-complement interactions

Predict the propensity of nanomaterials to activate the complement pathway.

Role: CPI

2009/08/01-2013/07/31

R01 GM090208, National Institutes of Health

Wei, Guowei (PI)

Collaborative research: Geometric flow approach to implicit solvation modeling

Develop new geometric flow methods for the electrostatic and solvation analysis of large biomolecules.

Role: PI

2004/06/01-2013/04/01

P41 RR0860516, National Institutes of Health

Arzberger, Peter (PI)

National Biomedical Computation Resource

This grant supports the integration of Baker group software (APBS, PDB2PQR, and SMOL) with NBCR infrastructure developed through the sub-cellular modeling core.

Role: CPI

2008/11/01-2012/08/01

U54 HG004028, National Institutes of Health

Musen, Mark (PI)

Cancer Nanotechnology Knowledgebase for Nanoparticle Analysis and Design

Provide semantic annotation to caNanoLab data and provide Bioportal users of the NanoParticle Ontology easy-to-use access to this valuable nanomedicine database.

Role: CPI

2009/08/01-2011/12/01

R01 GM076121-04S1-VT, National Institutes of Health

Onufriev, Alexey (PI)

Analytical Electrostatics: Methods and Biological Applications

Pioneer a new approach, bridging theory and experiment to simulate ions around DNA and understand their interactions with the polymer.

Role: CPI

2010/10/01-2011/09/30

HHS LDRD, Pacific Northwest National Laboratory

Baker, Nathan (PI)

Modeling and predicting nanoparticle interactions with biological materials

Predict the interaction of proteins and related biomolecules with nanoparticle surfaces.

Role: PI

2010/02/01-2011/01/31

R01 GM069702-06S1, National Institutes of Health (ARRA Admin Supp)

Baker, Nathan (PI)

APBS: Nanoscale biomolecular electrostatics software

Improve the APBS and PDB2PQR packages through the introduction of new technology and algorithms.

Role: PI

2008/03/01-2011/01/01

GS-35F-0306J, National Institutes of Health

Baker, Nathan (PI)

caBIG Integrative Cancer Research Workspace

Expedite the cancer research community’s access to increasing amounts of relevant date, creating a common, extensible informatics platform that integrates diverse data types and supports interoperable analytic tools.

Role: PI

2007/10/01-2010/12/01

N01-CN-12400, National Institutes of Health

Baker, Nathan (PI)

caNanoLab Data Submission Support

Assist other CCNEs in the NCI Nanotechnology Alliance community in submitting nanoparticle data into the caNanoLab Data Portal to promote and expedite data sharing in the nanotechnology biomedical community.

Role: PI

2005/09/01-2010/08/30

U54 CA11934205-CCNE, National Institutes of Health

Wickline, Samuel (PI)

The Siteman Cancer Center Nanotechnology Excellence at Washington Univ.

Supports the development of informatics resources to describe the biological function of nanoparticle therapeutics and imaging platforms. Our specific focus is the development of ontologies and databases for characterizing nanoparticle properties and functions with a long term goal of inference.

Role: CPI

2008/04/01-2010/04/01

HDTRA1-08-C-0015, Defense Threat Reduction Agency

Rosenberry, Terrone (PI)

New Inhibitors of Acetylcholinesterase that Block Inactivation by Organophosphates

Design drugs that prevent AChE inactivation by OPs while providing for the normal hydrolysis of ACh by AChE

Role: KP

2006/02/01-2009/01/31

MCB-0520877, National Science Foundation

Chivers, Peter (PI)

Allosteric Regulation on the Nickel-dependent NikR Repressor

Role: CPI

2007/02/01-2009/01/31

Research grant, Children's Discovery Institute

Doctor, Allan (PI)

Loss of Vascular Control in Pediatric Lung Injury: Disruption of NO Biotransport by Oxidative Stress

Role: CPI

2005/05/01-2007/06/01

NAKFI Nano02, National Academies Keck Futures Initiative

Baker, Nathan (PI)

Molecular Engineering of Thrombin-Based Nanocatalysts

Role: PI