Nathan Andrew Baker

Computational and Statistical Analytics Division, Pacific Northwest National Laboratory, PO Box 999, MSID K7-20, Richland, WA 99352  
<http://signatures.pnnl.gov/>

# Professional preparation

University of Iowa Chemistry BS 1997

University of California San Diego Physical Chemistry PhD 2001

University of California San Diego Computational biology Postdoc 2002

# Appointments

2013-present Technical Group Manager, Applied Statistics and Computational Modeling, Pacific Northwest National Laboratory

2012-present Laboratory Fellow, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory

2010-2012 Chief Scientist, Computational and Statistical Analytics Division, Pacific Northwest National Laboratory

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

2006-2010 Director, Molecular Biophysics Graduate Program, Washington University in St. Louis

2004-2006 Alfred P. Sloan Research Fellow

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

# Publications

## Closely related to project

1. Gosink LJ, Hogan EA, Pulsipher TC, Baker NA. Bayesian model aggregation for ensemble-based estimates of protein pKa values. *Proteins*. **82** (3), 354-363, 2014.
2. Thomas DG, Chikkagoudar S, Heredia-Langner A, Tardiff MF, Xu Z, Hourcade DE, Pham CTN, Lanza GM, Weinberger KQ, Baker NA. Physicochemical signatures of nanoparticle-dependent complement activation. Computational Science and Discovery. **7**, 015003, 2014.
3. Baker NA, Klemm JD, Harper SL, Gaheen S, Heiskanen M, Rocca-Serra P, Sansone S-A. Standardizing Data. *Nature Nanotechnology*, **8**, 73-74, 2013.
4. Thomas DG, Gaheen S, Harper SL, Fritts M, Klaessig F, Hahn-Dantona E, Paik DS, Pan S, Stafford GA, Freund ET, Klemm JD, Baker NA. ISA-TAB-Nano: A Specification for Sharing Nanomaterial Research Data in Spreadsheet-based Format. *BMC Biotechnology*, **13**, 2, 2013.
5. Chen Z, Baker NA, Wei GW. Differential geometry based solvation model I: Eulerian formulation, *J Comput Phys*, **229**, 8231-58, 2010.

## Other significant

1. Daily M, Chun J, Heredia-Langner A, Baker NA. Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. J Chem Phys. **139**, 204108, 2013.
2. Lee S-J, Schlesinger PH, Wickline SA, Lanza GM, Baker NA. Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers. Soft Matter, **8**, 7024-35, 2012.
3. Ren P, Chun J, Thomas DG, Schnieders MJ, Marucho M, Zhang J, Baker NA. Biomolecular electrostatics and solvation: a computational perspective. Quart Rev Biophys, **45** (4), 427-491, 2012.
4. Dolinsky TJ, Czodrowski P, Li H, Nielsen JE, Jensen JH, Klebe G, Baker NA. PDB2PQR: Expanding and upgrading automated preparation of biomolecular structures for molecular simulations. *Nucleic Acids Res*, **35**, W522-5, 2007.
5. Wagoner JA, Baker NA. Assessing implicit models for nonpolar mean solvation forces: the importance of dispersion and volume terms. Proc Natl Acad Sci USA, **103**, 8331-6, 2006.

# Synergistic activities

* Developer of APBS & PDB2PQR biomolecular electrostatics software packages (<http://www.poissonboltzmann.org/>), in use by over 23,000 researchers.
* Lead for Signature Discovery Initiative (<http://signatures.pnnl.gov/>).
* Associate Editor for *Biophysical Journal* and Editor-in-Chief for *Computational Science & Discovery*.
* Member of NIH *Macromolecular Structure & Function D* review panel.
* US chair of US-EU US-EU Nanotechnology Databases & Ontology Community of Research, Databases & Ontologies.

# Collaborators and other affiliations

**Collaborators and co-editors**. Emil Alexov (Clemson Univ), Paul Atzberger (UC Santa Barbara), Antonio Baptista (Univ Nova de Lisboa), Steve Bond (Sandia), Zhan Chen (Univ of Minnesota), Peter Chivers (Univ of Durham), Doug Covey (Washington Univ St Louis), Eric Darve (Stanford Univ), David Gohara (St Louis Univ), Jeff Gray (Univ Alabama), Liz Hahn-Dantona (National Institutes of Health), Robert Hanson (St Olaf College), Stacey Harper (Oregon State Univ), Mervi Heiskanen (National Institutes of Health), Mark Hoover (Centers for Disease Control), Dennis Hourcade (Washington Univ St Louis), Jonathan Hu (Sandia), George Karniadakis (Brown Univ), Fred Klaessig (Pennsylvania Nano-Bio), Juli Klemm (National Institutes of Health), Robert Konecny (UC San Diego), Sriram Krishnan (Google), Greg Lanza (Washington Univ St Louis), Wilfred Li (UC San Diego), Victor Maojo (Univ. Politécnica de Madrid), Martin Maxey (Brown Univ), Ernie Mehler (Cornell Medical College), Julie Mitchell (Univ Wisconsin), Anthony Nicholls (Open Eye Software), Jens Nielsen (Novozymes), Alexey Onufriev (Virginia Tech), Dan Ory (Washington Univ St Louis), Mark Oxley (Air Force Institute of Technology), Suzette Pabit (Cornell), David Paik (Stanford Univ), Rohit Pappu (Washington Univ St Louis), Mike Parks (Sandia), Christine Pham (Washington Univ St Louis), Lois Pollack (Cornell), Naren Ramakrishnan (Virginia Tech), Pengyu Ren (UT Austin), Philippe Rocca-Serra (Oxford Univ), Yoram Rudy (Washington Univ St Louis), Susanna Sansone (Oxford Univ), Paul Schlesinger (Washington Univ St Louis), Mike Schnieders (Univ Iowa), David Sept (Univ Michigan), Jana Shen (Univ Maryland Baltimore County), Chris Siefert (Sandia), Jonathan Silva (Washington Univ St Louis), Grace Stafford (Jackson Labs), Panos Stinis (Univ Minnesota), Igor Tolokh (VA Tech), Jim Warwicker (Univ Manchester), Guowei Wei (Michigan State Univ), Sam Wickline (Washington Univ St Louis), Mike Word (OpenEye Software), Jinchao Xu (Penn State Univ), Xiu Yan (PNNL), Bin Zheng (PNNL).

**Graduate advisors and postdoc sponsors**. Michael Holst (UC San Diego) and J. Andrew McCammon (UC San Diego).

**Thesis advisor & postdoc sponsor**. Mike Bradley (Yale Univ), Mike Daily (PNNL) Feng Dong (Merck), Sun Joo Lee (Washington Univ St. Louis), Huan Lei (PNNL), Marcelo Marucho (UT San Antonio), Brett Olsen (Washington Univ St Louis), Rachel Rice (Duke Univ), Yuhua Song (Univ Alabama), Jason Wagoner (SUNY Stony Brook)