Nathan A Baker

List of Publications by Year
in descending order

119 papers	18,037 citations	61984 43 h-index	34986 98 g-index
124 all docs	124 docs citations	124 times ranked	22906 citing authors

#	Article	IF	Citations
1	Toward Quantum Computing for High-Energy Excited States in Molecular Systems: Quantum Phase Estimations of Core-Level States. Journal of Chemical Theory and Computation, 2021, 17, 201-210.	5.3	16
2	Visualizing biomolecular electrostatics in virtual reality with UnityMolâ€APBS. Protein Science, 2020, 29, 237-246.	7.6	31
3	Data-driven molecular modeling with the generalized Langevin equation. Journal of Computational Physics, 2020, 418, 109633.	3.8	21
4	A clustering-based biased Monte Carlo approach to protein titration curve prediction. , 2020, 2020, .		0
5	A data-driven framework for sparsity-enhanced surrogates with arbitrary mutually dependent randomness. Computer Methods in Applied Mechanics and Engineering, 2019, 350, 199-227.	6.6	6
6	Atomic Radius and Charge Parameter Uncertainty in Biomolecular Solvation Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 759-767.	5.3	13
7	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	7.6	1,399
8	How Much Chemistry Does a Deep Neural Network Need to Know to Make Accurate Predictions?. , 2018, , .		35
9	Spermine Condenses DNA, but Not RNA Duplexes. Biophysical Journal, 2017, 112, 22-30.	0.5	48
10	Bayesian Model Averaging for Ensemble-Based Estimates of Solvation-Free Energies. Journal of Physical Chemistry B, 2017, 121, 3458-3472.	2.6	8
11	PBâ€AM: An openâ€source, fully analytical linear poissonâ€boltzmann solver. Journal of Computational Chemistry, 2017, 38, 1275-1282.	3.3	9
12	Understanding nucleic acid structural changes by comparing wide-angle x-ray scattering (WAXS) experiments to molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 205102.	3.0	15
13	Data-driven parameterization of the generalized Langevin equation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 14183-14188.	7.1	103
14	Multi-shell model of ion-induced nucleic acid condensation. Journal of Chemical Physics, 2016, 144, 155101.	3.0	13
15	Condensation of Nucleic Acids by Multivalent Ions: Sequence Dependence and the Curious Case of RNA. Biophysical Journal, 2016, 110, 409a.	0.5	0
16	Energy Minimization of Discrete Protein Titration State Models Using Graph Theory. Journal of Physical Chemistry B, 2016, 120, 8354-8360.	2.6	2
17	Continuum Electrostatics Approaches to Calculating pKas and Ems in Proteins. Methods in Enzymology, 2016, 578, 1-20.	1.0	27
18	Smoothed dissipative particle dynamics model for mesoscopic multiphase flows in the presence of thermal fluctuations. Physical Review E, 2016, 94, 023304.	2.1	11

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19	Opposing Effects of Multivalent Ions on the Flexibility of DNA and RNA. Physical Review Letters, 2016, 117, 028101.	7.8	47
20	Adaptive visual sort and summary of micrographic images of nanoparticles for forensic analysis. , 2016, 2016, .		1
21	Enhancing sparsity of Hermite polynomial expansions by iterative rotations. Journal of Computational Physics, 2016, 307, 94-109.	3.8	39
22	The Role of Correlation and Solvation in Ion Interactions with B-DNA. Biophysical Journal, 2016, 110, 315-326.	0.5	33
23	Informatics Approaches to Data Preservation and Analysis in Protein Electrostatics. Biophysical Journal, 2015, 108, 369a.	0.5	0
24	Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity. Journal of Nanoparticle Research, 2015, 17, 250.	1.9	30
25	Constructing Surrogate Models of Complex Systems with Enhanced Sparsity: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation. Multiscale Modeling and Simulation, 2015, 13, 1327-1353.	1.6	27
26	Numerical calculation of protein-ligand binding rates through solution of the Smoluchowski equation using smoothed particle hydrodynamics. BMC Biophysics, 2015, 8, 7.	4.4	9
27	Why double-stranded RNA resists condensation. Nucleic Acids Research, 2014, 42, 10823-10831.	14.5	67
28	Physicochemical signatures of nanoparticle-dependent complement activation. Computational Science & Discovery, 2014, 7, 015003.	1.5	12
29	The Structural Basis of Cholesterol Accessibility in Membranes. Biophysical Journal, 2014, 106, 509a.	0.5	1
30	Bayesian model aggregation for ensembleâ€based estimates of protein pK_a values. Proteins: Structure, Function and Bioinformatics, 2014, 82, 354-363.	2.6	10
31	Side-Chain Oxysterols Modulate Cholesterol Accessibility through Membrane Remodeling. Biochemistry, 2014, 53, 3042-3051.	2.5	30
32	Improved Coarse-Grained Modeling of Cholesterol-Containing Lipid Bilayers. Journal of Chemical Theory and Computation, 2014, 10, 2137-2150.	5.3	48
33	Application of a hemolysis assay for analysis of complement activation by perfluorocarbon nanoparticles. Nanomedicine: Nanotechnology, Biology, and Medicine, 2014, 10, 651-660.	3.3	55
34	ISA-TAB-Nano: A Specification for Sharing Nanomaterial Research Data in Spreadsheet-based Format. BMC Biotechnology, 2013, 13, 2.	3.3	72
35	The Structural Basis of Cholesterol Accessibility in Membranes. Biophysical Journal, 2013, 105, 1838-1847.	0.5	46
36	Research towards a systematic signature discovery process. , 2013, , .		5

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37	Improved Coarse-Grained Modeling of Cholesterol Activation in Lipid Bilayers. Biophysical Journal, 2013, 104, 590a-591a.	0.5	1
38	The Structural Basis of Cholesterol Activation in Membranes. Biophysical Journal, 2013, 104, 662a.	0.5	0
39	Parameterization of a geometric flow implicit solvation model. Journal of Computational Chemistry, 2013, 34, 687-695.	3.3	21
40	Structural phylogeny by profile extraction and multiple superimposition using electrostatic congruence as a discriminator. Intrinsically Disordered Proteins, 2013, 1, e25463.	1.9	7
41	Nanoinformatics workshop report: current resources, community needs and the proposal of a collaborative framework for data sharing and information integration. Computational Science & Discovery, 2013, 6, 014008.	1.5	9
42	Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. Journal of Chemical Physics, 2013, 139, 204108.	3.0	8
43	Standardizing data. Nature Nanotechnology, 2013, 8, 73-74.	31.5	19
44	Domain-specific languages for composing signature discovery workflows. , 2012, , .		2
45	iAPBS: a programming interface to the adaptive Poissonâ€“Boltzmann solver. Computational Science & Discovery, 2012, 5, 015005.	1.5	53
46	Annotating the structure and components of a nanoparticle formulation using computable string expressions. , 2012, 2012, 889-894.		1
47	Biomolecular electrostatics and solvation: a computational perspective. Quarterly Reviews of Biophysics, 2012, 45, 427-491.	5.7	152
48	APBSmem: A Tool for the Analysis of Membrane Protein Electrostatics. Biophysical Journal, 2012, 102, 682a.	0.5	0
49	Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers. Soft Matter, 2012, 8, 7024.	2.7	22
50	Variational approach for nonpolar solvation analysis. Journal of Chemical Physics, 2012, 137, 084101.	3.0	40
51	Side-chain oxysterols: From cells to membranes to molecules. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 330-336.	2.6	46
52	Improving Implicit Solvent Models with Differential Geometry. Biophysical Journal, 2012, 102, 169a.	0.5	0
53	Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq1 1 0.784314 rgBT /Ov	4.8	15
54	Interaction of Melittin Peptides with Perfluorocarbon Nanoemulsion Particles. Journal of Physical Chemistry B, 2011, 115, 15271-15279.	2.6	24

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55	25-Hydroxycholesterol Increases the Availability of Cholesterol in Phospholipid Membranes. Biophysical Journal, 2011, 100, 948-956.	0.5	50
56	NanoParticle Ontology for cancer nanotechnology research. Journal of Biomedical Informatics, 2011, 44, 59-74.	4.3	96
57	Differential geometry based solvation model II: Lagrangian formulation. Journal of Mathematical Biology, 2011, 63, 1139-1200.	1.9	58
58	On the development of protein pK_a calculation algorithms. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3287-3298.	2.6	19
59	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
60	Informatics and standards for nanomedicine technology. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2011, 3, 511-532.	6.1	36
61	Web servers and services for electrostatics calculations with APBS and PDB2PQR. Journal of Computational Chemistry, 2011, 32, 1488-1491.	3.3	254
62	Using physicochemical properties of amino acids to induce graphical models of residue couplings. , 2011, , .		0
63	Differential geometry based solvation model I: Eulerian formulation. Journal of Computational Physics, 2010, 229, 8231-8258.	3.8	110
64	APBSmem: A Graphical Interface for Electrostatic Calculations at the Membrane. PLoS ONE, 2010, 5, e12722.	2.5	83
65	Perturbation of Membrane Structure by Oxysterols. Biophysical Journal, 2010, 98, 491a.	0.5	1
66	Multi-Scale Modeling of the â€œContact-Facilitatedâ€•Delivery Mechanism ofÂPerfluorocarbon-Based Nanoemulsions. Biophysical Journal, 2010, 98, 672a.	0.5	0
67	Characterization of Perfluorooctylbromide-Based Nanoemulsion Particles Using Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 10086-10096.	2.6	15
68	A multiscale model linking ion-channel molecular dynamics and electrostatics to the cardiac action potential. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11102-11106.	7.1	124
69	Ontologies for cancer nanotechnology research. , 2009, 2009, 4158-61.		5
70	The physical basis of microtubule structure and stability. Protein Science, 2009, 12, 2257-2261.	7.6	123
71	Perturbations of Membrane Structure by Cholesterol and Cholesterol Derivatives Are Determined by Sterol Orientation. Journal of the American Chemical Society, 2009, 131, 4854-4865.	13.7	77
72	Simulations of RNA Interactions with Monovalent Ions. Methods in Enzymology, 2009, 469, 411-432.	1.0	48

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73	Communication Via Structural Water: Changes In The Thrombin Water Channel And Active Site Due To Sodium Binding. Biophysical Journal, 2009, 96, 595a-596a.	0.5	0
74	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, 2008, 94, 3565-3576.	0.5	106
75	Computational Methods for Biomolecular Electrostatics. Methods in Cell Biology, 2008, 84, 843-870.	1.1	65
76	Molecular Dynamics Simulation of the Escherichia coli NikR Protein: Equilibrium Conformational Fluctuations Reveal Interdomain Allosteric Communication Pathways. Journal of Molecular Biology, 2008, 378, 1155-1173.	4.2	63
77	Assessing the performance of implicit solvation models at a nucleic acid surface. Physical Chemistry Chemical Physics, 2008, 10, 4889.	2.8	18
78	Molecular dynamics simulation of the NikR protein: Equilibrium conformational fluctuations reveal interâ€domain allosteric communication pathways. FASEB Journal, 2008, 22, 612.2.	0.5	0
79	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	3.0	79
80	Solvent reaction field potential inside an uncharged globular protein: A bridge between implicit and explicit solvent models?. Journal of Chemical Physics, 2007, 127, 155101.	3.0	36
81	Erratum to â€œProbing 3â€²-ssDNA Loop Formation in E. coli RecBCD/RecBCâ€“DNA Complexes Using Non-natural DNA: A Model for â€œChiâ€•Recognition Complexesâ€•[J. Mol. Biol. 359 (2006) 1137â€“1149]. Journal of Molecular Biology, 2007, 365, 900.	4.2	0
82	PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. Nucleic Acids Research, 2007, 35, W522-W525.	14.5	1,659
83	Optimizing the Poisson Dielectric Boundary with Explicit Solvent Forces and Energies:â€‰ Lessons Learned with Atom-Centered Dielectric Functions. Journal of Chemical Theory and Computation, 2007, 3, 170-183.	5.3	42
84	Finite Element Analysis of the Time-Dependent Smoluchowski Equation for Acetylcholinesterase Reaction Rate Calculations. Biophysical Journal, 2007, 92, 3397-3406.	0.5	33
85	Application of New Multiresolution Methods for the Comparison of Biomolecular Electrostatic Properties in the Absence of Global Structural Similarity. Multiscale Modeling and Simulation, 2006, 5, 1196-1213.	1.6	32
86	Probing 3â€²-ssDNA Loop Formation in E. coli RecBCD/RecBCâ€“DNA Complexes Using Non-natural DNA: A Model for â€œChiâ€•Recognition Complexes. Journal of Molecular Biology, 2006, 362, 26-43.	4.2	22
87	Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. Biopolymers, 2006, 82, 106-120.	2.4	59
88	Assessing implicit models for nonpolar mean solvation forces: The importance of dispersion and volume terms. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8331-8336.	7.1	270
89	Implicit Solvent Electrostatics in Biomolecular Simulation. , 2006, , 263-295.		29
90	Determining the mechanism of allosteric regulation of NikR binding to DNA activated by Ni ²⁺. FASEB Journal, 2006, 20, A489.	0.5	0

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91	Improving implicit solvent simulations: a Poisson-centric view. Current Opinion in Structural Biology, 2005, 15, 137-143.	5.7	322
92	Iron Responsive Element RNA Flexibility Described by NMR and Isotropic Reorientational Eigenmode Dynamics. Journal of Biomolecular NMR, 2005, 32, 179-193.	2.8	29
93	Electrostatic Interactions. Methods of Biochemical Analysis, 2005, , 427-440.	0.2	10
94	Biomolecular Applications of Poisson-Boltzmann Methods. Reviews in Computational Chemistry, 2005, , 349-379.	1.5	36
95	Molecular Dynamics Simulations of Salicylate Effects on the Micro- and Mesoscopic Properties of a Dipalmitoylphosphatidylcholine Bilayer. Biochemistry, 2005, 44, 13425-13438.	2.5	44
96	Tetrameric Mouse Acetylcholinesterase: Continuum Diffusion Rate Calculations by Solving the Steady-State Smoluchowski Equation Using Finite Element Methods. Biophysical Journal, 2005, 88, 1659-1665.	0.5	31
97	SPrCY: comparison of structural predictions in the Saccharomyces cerevisiae genome. Bioinformatics, 2004, 20, 2312-2314.	4.1	14
98	ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. Molecular Simulation, 2004, 30, 45-61.	2.0	21
99	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, 75, 325-337.	2.4	54
100	Solvation forces on biomolecular structures: A comparison of explicit solvent and Poisson-Boltzmann models. Journal of Computational Chemistry, 2004, 25, 1623-1629.	3.3	92
101	Poissonâ€“Boltzmann Methods for Biomolecular Electrostatics. Methods in Enzymology, 2004, 383, 94-118.	1.0	182
102	Continuum Diffusion Reaction Rate Calculations of Wild-Type and Mutant Mouse Acetylcholinesterase: Adaptive Finite Element Analysis. Biophysical Journal, 2004, 87, 1558-1566.	0.5	37
103	PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. Nucleic Acids Research, 2004, 32, W665-W667.	14.5	3,014
104	Finite Element Solution of the Steady-State Smoluchowski Equation for Rate Constant Calculations. Biophysical Journal, 2004, 86, 2017-2029.	0.5	81
105	Finite Element Simulations of Acetylcholine Diffusion in Neuromuscular Junctions. Biophysical Journal, 2003, 84, 2234-2241.	0.5	54
106	Binding of Aminoglycoside Antibiotics to the Small Ribosomal Subunit:Â A Continuum Electrostatics Investigation. Journal of the American Chemical Society, 2002, 124, 1438-1442.	13.7	52
107	Bridging Implicit and Explicit Solvent Approaches for Membrane Electrostatics. Biophysical Journal, 2002, 83, 1374-1379.	0.5	66
108	Mathematics and Molecular Neurobiology. Lecture Notes in Computational Science and Engineering, 2002, , 31-60.	0.3	0

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109	Electrostatics of nanosystems: Application to microtubules and the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 10037-10041.	7.1	6,623
110	Adaptive multilevel finite element solution of the Poisson-Boltzmann equation I. Algorithms and examples. Journal of Computational Chemistry, 2000, 21, 1319-1342.	3.3	255
111	Adaptive multilevel finite element solution of the Poisson-Boltzmann equation II. Refinement at solvent-accessible surfaces in biomolecular systems. Journal of Computational Chemistry, 2000, 21, 1343-1352.	3.3	169
112	Delineation and Decomposition of Energies Involved in Quaternary Ammonium Binding in the Active Site of Acetylcholinesterase. Journal of the American Chemical Society, 2000, 122, 2975-2980.	13.7	37
113	Theoretical and experimental investigations of electrostatic effects on acetylcholinesterase catalysis and inhibition. Chemico-Biological Interactions, 1999, 119-120, 99-110.	4.0	16
114	Dynamical properties of fasciculin-2. , 1999, 36, 447-453.		12
115	Polarization around an ion in a dielectric continuum with truncated electrostatic interactions. Journal of Chemical Physics, 1999, 110, 10679-10692.	3.0	34
116	Non-Boltzmann Rate Distributions in Stochastically Gated Reactions. Journal of Physical Chemistry B, 1999, 103, 615-617.	2.6	10
117	Weighted-Ensemble Brownian Dynamics for Charged Ligand Diffusion onto Acetylcholinesterase. , 1998, , 367-367.		1
118	Low-Barrier Hydrogen Bond in the Catalytic Triad of Serine Enzymes. , 1998, , 233-233.		0
119	Molecular Recognition by Cholesterol Esterase of Active Site Ligands:Â Structureâ^'Reactivity Effects for Inhibition by Aryl Carbamates and Subsequent Carbamylenzyme Turnoverâ€. Biochemistry, 1996, 35, 16723-16734.	2.5	78