J Andrew Mccammon

List of Publications by Citations

359 papers	29,194 citations	79 h-index	162 g-index
374 ext. papers	33,200 ext. citations	6.7 avg, IF	7.37 L-index

#	Paper	IF	Citations
359	PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. *Nucleic Acids Research*, **2004**, 32, W665-7	20.1	2395
358	Molecular dynamics simulations of biomolecules. *Nature Structural Biology*, **2002**, 9, 646-52		1990
357	Dynamics of folded proteins. *Nature*, **1977**, 267, 585-90	50.4	1471
356	Accelerated molecular dynamics: a promising and efficient simulation method for biomolecules. *Journal of Chemical Physics*, **2004**, 120, 11919-29	3.9	1089
355	Bio3d: an R package for the comparative analysis of protein structures. *Bioinformatics*, **2006**, 22, 2695-6	7.2	947
354	Molecular dynamics: survey of methods for simulating the activity of proteins. *Chemical Reviews*, **2006**, 106, 1589-615	68.1	818
353	Molecular dynamics simulations and drug discovery. *BMC Biology*, **2011**, 9, 71	7.3	615
352	Electrostatics in biomolecular structure and dynamics. *Chemical Reviews*, **1990**, 90, 509-521	68.1	586
351	Improvements to the APBS biomolecular solvation software suite. *Protein Science*, **2018**, 27, 112-128	6.3	577
350	The determinants of pKas in proteins. *Biochemistry*, **1996**, 35, 7819-33	3.2	424
349	The internal dynamics of globular proteins. *Critical Reviews in Biochemistry*, **1981**, 9, 293-349		418
348	Computational drug design accommodating receptor flexibility: the relaxed complex scheme. *Journal of the American Chemical Society*, **2002**, 124, 5632-3	16.4	353
347	Routine Access to Millisecond Time Scale Events with Accelerated Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 2997-3002	6.4	344
346	Brownian dynamics simulation of diffusion-influenced bimolecular reactions. *Journal of Chemical Physics*, **1984**, 80, 1517-1524	3.9	326
345	The hinge-bending mode in lysozyme. *Nature*, **1976**, 262, 325-6	50.4	324
344	Computation of electrostatic forces on solvated molecules using the Poisson-Boltzmann equation. *The Journal of Physical Chemistry*, **1993**, 97, 3591-3600		304
343	Ewald artifacts in computer simulations of ionic solvation and ion□on interaction: A continuum electrostatics study. *Journal of Chemical Physics*, **1999**, 110, 1856-1872	3.9	303

342	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2015**, 11, 3584-3595	6.4	302
341	Discovery of a novel binding trench in HIV integrase. *Journal of Medicinal Chemistry*, **2004**, 47, 1879-81	8.3	286
340	Developing a dynamic pharmacophore model for HIV-1 integrase. *Journal of Medicinal Chemistry*, **2000**, 43, 2100-14	8.3	248
339	An improved relaxed complex scheme for receptor flexibility in computer-aided drug design. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 693-705	4.2	243
338	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2014**, 10, 2677-2689	6.4	225
337	Water in cavity-ligand recognition. *Journal of the American Chemical Society*, **2010**, 132, 12091-7	16.4	215
336	Ensemble Docking in Drug Discovery. *Biophysical Journal*, **2018**, 114, 2271-2278	2.9	203
335	Conformation gating as a mechanism for enzyme specificity. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 9280-3	11.5	201
334	HIV-1 protease molecular dynamics of a wild-type and of the V82F/I84V mutant: possible contributions to drug resistance and a potential new target site for drugs. *Protein Science*, **2004**, 13, 1108-23	6.3	197
333	Ensemble-based virtual screening reveals potential novel antiviral compounds for avian influenza neuraminidase. *Journal of Medicinal Chemistry*, **2008**, 51, 3878-94	8.3	190
332	Stochastically gated diffusion-influenced reactions. *Journal of Chemical Physics*, **1982**, 77, 4484-4493	3.9	188
331	Trapping the dynamic acyl carrier protein in fatty acid biosynthesis. *Nature*, **2014**, 505, 427-31	50.4	174
330	Activation and dynamic network of the M2 muscarinic receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 10982-7	11.5	174
329	How Can Hydrophobic Association Be Enthalpy Driven?. *Journal of Chemical Theory and Computation*, **2010**, 6, 2866-2871	6.4	169
328	Large conformational changes in proteins: signaling and other functions. *Current Opinion in Structural Biology*, **2010**, 20, 142-7	8.1	167
327	POVME: an algorithm for measuring binding-pocket volumes. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 773-6	2.8	164
326	The relaxed complex method: Accommodating receptor flexibility for drug design with an improved scoring scheme. *Biopolymers*, **2003**, 68, 47-62	2.2	160
325	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158

324	A molecular mechanics/grid method for evaluation of ligand receptor interactions. *Journal of Computational Chemistry*, **1995**, 16, 454-464	3.5	158
323	Free energy difference calculations by thermodynamic integration: Difficulties in obtaining a precise value. *Journal of Computational Chemistry*, **1991**, 12, 271-275	3.5	149
322	Molecular recognition and ligand association. *Annual Review of Physical Chemistry*, **2013**, 64, 151-75	15.7	145
321	Acetylcholinesterase: electrostatic steering increases the rate of ligand binding. *Biochemistry*, **1993**, 32, 401-3	3.2	138
320	Gated binding of ligands to proteins. *Nature*, **1981**, 293, 316-7	50.4	136
319	A gating mechanism proposed from a simulation of a human alpha7 nicotinic acetylcholine receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6813-8	11.5	127
318	Computing ionization states of proteins with a detailed charge model. *Journal of Computational Chemistry*, **1996**, 17, 1633-1644	3.5	127
317	Allosteric networks in thrombin distinguish procoagulant vs. anticoagulant activities. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 21216-22	11.5	117
316	Structure-based drug design: computational advances. *Annual Review of Pharmacology and Toxicology*, **1997**, 37, 71-90	17.9	117
315	Order N algorithm for computation of electrostatic interactions in biomolecular systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 19314-9	11.5	115
314	Exploring global motions and correlations in the ribosome. *Biophysical Journal*, **2005**, 89, 1455-63	2.9	115
313	Agonist-mediated conformational changes in acetylcholine-binding protein revealed by simulation and intrinsic tryptophan fluorescence. *Journal of Biological Chemistry*, **2005**, 280, 8443-51	5.4	115
312	Dielectric boundary smoothing in finite difference solutions of the poisson equation: An approach to improve accuracy and convergence. *Journal of Computational Chemistry*, **1991**, 12, 909-912	3.5	115
311	Discovery of drug-like inhibitors of an essential RNA-editing ligase in Trypanosoma brucei. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 17278-83	11.5	114
310	Diffusive langevin dynamics of model alkanes. *Chemical Physics Letters*, **1979**, 65, 4-11	2.5	111
309	Antiinfectives targeting enzymes and the proton motive force. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E7073-82	11.5	107
308	A coarse grained model for the dynamics of flap opening in HIV-1 protease. *Chemical Physics Letters* , **2005**, 413, 123-128	2.5	107
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306	Accelerated molecular dynamics simulations of protein folding. *Journal of Computational Chemistry*, **2015**, 36, 1536-49	3.5	106
305	Exploring the role of receptor flexibility in structure-based drug discovery. *Biophysical Chemistry*, **2014**, 186, 31-45	3.5	105
304	Targeted molecular dynamics study of C-loop closure and channel gating in nicotinic receptors. *PLoS Computational Biology*, **2006**, 2, e134	5	104
303	Channel opening motion of alpha7 nicotinic acetylcholine receptor as suggested by normal mode analysis. *Journal of Molecular Biology*, **2006**, 355, 310-24	6.5	102
302	Poisson-Nernst-Planck Equations for Simulating Biomolecular Diffusion-Reaction Processes I: Finite Element Solutions. *Journal of Computational Physics*, **2010**, 229, 6979-6994	4.1	101
301	Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor. *Quarterly Reviews of Biophysics*, **2015**, 48, 479-87	7	100
300	Toward a unified representation of protein structural dynamics in solution. *Journal of the American Chemical Society*, **2009**, 131, 16968-75	16.4	98
299	Unconstrained Enhanced Sampling for Free Energy Calculations of Biomolecules: A Review. *Molecular Simulation*, **2016**, 42, 1046-1055	2	93
298	Accessing a hidden conformation of the maltose binding protein using accelerated molecular dynamics. *PLoS Computational Biology*, **2011**, 7, e1002034	5	92
297	Studying enzyme binding specificity in acetylcholinesterase using a combined molecular dynamics and multiple docking approach. *Journal of the American Chemical Society*, **2002**, 124, 8260-7	16.4	92
296	Active site binding modes of HIV-1 integrase inhibitors. *Journal of Medicinal Chemistry*, **2000**, 43, 4109-17	8.3	92
295	CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7260-7265	11.5	91
294	Mapping the druggable allosteric space of G-protein coupled receptors: a fragment-based molecular dynamics approach. *Chemical Biology and Drug Design*, **2010**, 76, 201-17	2.9	91
293	Method for Including the Dynamic Fluctuations of a Protein in Computer-Aided Drug Design. *Journal of Physical Chemistry A*, **1999**, 103, 10213-10219	2.8	91
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290	Accounting for receptor flexibility and enhanced sampling methods in computer-aided drug design. *Chemical Biology and Drug Design*, **2013**, 81, 41-9	2.9	90
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282	Phosphorylation effects on cis/trans isomerization and the backbone conformation of serine-proline motifs: accelerated molecular dynamics analysis. *Journal of the American Chemical Society*, **2005**, 127, 1969-74	16.4	80
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280	Electrostatic free energy and its variations in implicit solvent models. *Journal of Physical Chemistry B*, **2008**, 112, 3058-69	3.4	78
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268	Finite element solution of the steady-state Smoluchowski equation for rate constant calculations. *Biophysical Journal*, **2004**, 86, 2017-29	2.9	70
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