# J Andrew Mccammon

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | Coupling Monte Carlo, Variational Implicit Solvation, and Binary Level-Set for Simulations of Biomolecular Binding. *Journal of Chemical Theory and Computation*, **2021**, 17, 2465-2478 | 6.4 | 1 |
| 358 | The myosin II coiled-coil domain atomic structure in its native environment. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118, | 11.5 | 1 |
| 357 | Decoding allosteric regulation by the acyl carrier protein. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118, | 11.5 | 5 |
| 356 | Elucidation of Cryptic and Allosteric Pockets within the SARS-CoV-2 Main Protease. *Journal of Chemical Information and Modeling*, **2021**, 61, 3495-3501 | 6.1 | 16 |
| 355 | Characterizing protein kinase A (PKA) subunits as macromolecular regulators of PKA RI liquid-liquid phase separation. *Journal of Chemical Physics*, **2021**, 154, 221101 | 3.9 | 2 |
| 354 | A glycan gate controls opening of the SARS-CoV-2 spike protein **2021**, | | 22 |
| 353 | A glycan gate controls opening of the SARS-CoV-2 spike protein. *Nature Chemistry*, **2021**, 13, 963-968 | 17.6 | 63 |
| 352 | Data for molecular dynamics simulations of cytochrome oxidase with the Amber force field. *Data in Brief*, **2021**, 38, 107401 | 1.2 | 0 |
| 351 | An Open-Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries. *Biophysical Journal*, **2020**, 118, 1003-1008 | 2.9 | 7 |
| 350 | Gating mechanism of elongating ketoacyl-ACP synthases. *Nature Communications*, **2020**, 11, 1727 | 17.4 | 18 |
| 349 | Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. *Biophysical Journal*, **2020**, 119, 2275-2289 | 2.9 | 4 |
| 348 | Predicting the effects of dATP on cardiac contraction using multiscale modeling of the sarcomere. *Archives of Biochemistry and Biophysics*, **2020**, 695, 108582 | 4.1 | 1 |
| 347 | Interfacial plasticity facilitates high reaction rate of FAS malonyl-CoA:ACP transacylase, FabD. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 24224-24233 | 11.5 | 16 |
| 346 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries. *PLoS Computational Biology*, **2020**, 16, e1007756 | 5 | 19 |
| 345 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |
| 344 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |
| 343 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |

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| 342 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |
| 341 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |
| 340 | 3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries **2020**, 16, e1007756 | | |
| 339 | Brownian Dynamics Simulations of Biological Molecules. *Trends in Chemistry*, **2019**, 1, 727-738 | 14.8 | 16 |
| 338 | Modifying the Thioester Linkage Affects the Structure of the Acyl Carrier Protein. *Angewandte Chemie - International Edition*, **2019**, 58, 10888-10892 | 16.4 | 10 |
| 337 | Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. *ACS Central Science*, **2019**, 5, 651-662 | 16.8 | 57 |
| 336 | Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. *Journal of Structural Biology*, **2019**, 206, 267-279 | 3.4 | 22 |
| 335 | Structural and dynamical rationale for fatty acid unsaturation in. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 6775-6783 | 11.5 | 20 |
| 334 | The invisible dance of CRISPR-Cas9. Simulations unveil the molecular side of the gene-editing revolution. *Physics Today*, **2019**, 72, 30-36 | 0.9 | 7 |
| 333 | Computational Predictions of Drug-Protein Binding Kinetics with a Hybrid Molecular Dynamics, Brownian Dynamics, and Milestoning Approach. *Biophysical Journal*, **2019**, 116, 562a | 2.9 | 2 |
| 332 | Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578 | 5.2 | 158 |
| 331 | Shifting the Hydrolysis Equilibrium of Substrate Loaded Acyl Carrier Proteins. *Biochemistry*, **2019**, 58, 3557-3560 | 3.2 | 2 |
| 330 | Modifying the Thioester Linkage Affects the Structure of the Acyl Carrier Protein. *Angewandte Chemie*, **2019**, 131, 11004-11008 | 3.6 | 2 |
| 329 | Variational implicit-solvent predictions of the dry-wet transition pathways for ligand-receptor binding and unbinding kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 14989-14994 | 11.5 | 9 |
| 328 | A Stochastic Multiscale Model of Cardiac Thin Filament Activation Using Brownian-Langevin Dynamics. *Biophysical Journal*, **2019**, 117, 2255-2272 | 2.9 | 6 |
| 327 | The Implementation of the Colored Abstract Simplicial Complex and its Application to Mesh Generation. *ACM Transactions on Mathematical Software*, **2019**, 45, | 2.3 | 6 |
| 326 | Activation of atypical protein kinase C by sphingosine 1-phosphate revealed by an aPKC-specific activity reporter. *Science Signaling*, **2019**, 12, | 8.8 | 21 |
| 325 | Docking simulation and antibiotic discovery targeting the MlaC protein in Gram-negative bacteria. *Chemical Biology and Drug Design*, **2019**, 93, 647-652 | 2.9 | 2 |

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| 324 | Mechanisms for Benzene Dissociation through the Excited State of T4 Lysozyme L99A Mutant. *Biophysical Journal*, **2019**, 116, 205-214 | 2.9 | 11 |
| 323 | Mechanistic Probes for the Epimerization Domain of Nonribosomal Peptide Synthetases. *ChemBioChem*, **2019**, 20, 147-152 | 3.8 | 9 |
| 322 | pH-dependent conformational dynamics of beta-secretase 1: A molecular dynamics study. *Journal of Molecular Recognition*, **2019**, 32, e2765 | 2.6 | 7 |
| 321 | Mechanism of the G-protein mimetic nanobody binding to a muscarinic G-protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 3036-3041 | 11.5 | 64 |
| 320 | Replica Exchange Gaussian Accelerated Molecular Dynamics: Improved Enhanced Sampling and Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2018**, 14, 1853-1864 | 6.4 | 21 |
| 319 | Ligand Binding Pathways and Conformational Transitions of the HIV Protease. *Biochemistry*, **2018**, 57, 1533-1541 | 3.2 | 33 |
| 318 | Membrane Allostery and Unique Hydrophobic Sites Promote Enzyme Substrate Specificity. *Journal of the American Chemical Society*, **2018**, 140, 3285-3291 | 16.4 | 36 |
| 317 | Remarkable similarity in Plasmodium falciparum and Plasmodium vivax geranylgeranyl diphosphate synthase dynamics and its implication for antimalarial drug design. *Chemical Biology and Drug Design*, **2018**, 91, 1068-1077 | 2.9 | 4 |
| 316 | Ensemble Docking in Drug Discovery. *Biophysical Journal*, **2018**, 114, 2271-2278 | 2.9 | 203 |
| 315 | Improvements to the APBS biomolecular solvation software suite. *Protein Science*, **2018**, 27, 112-128 | 6.3 | 577 |
| 314 | HIERARCHICAL ORTHOGONAL MATRIX GENERATION AND MATRIX-VECTOR MULTIPLICATIONS IN RIGID BODY SIMULATIONS. *SIAM Journal of Scientific Computing*, **2018**, 40, A1345-A1361 | 2.6 | |
| 313 | Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. *Frontiers in Molecular Biosciences*, **2018**, 5, 13 | 5.6 | 5 |
| 312 | Membrane Allostery and Hydrophobic Binding Sites Control Substrate Specificity of Lipolytic Enzymes. *FASEB Journal*, **2018**, 32, 528.6 | 0.9 | |
| 311 | Atypical Protein Kinase C-specific Activity Reporter Reveals Novel Activation Mechanism of Atypical Protein Kinase C by Sphingosine 1-phosphate. *FASEB Journal*, **2018**, 32, 662.1 | 0.9 | |
| 310 | Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. *Protein Science*, **2018**, 27, 463-471 | 6.3 | 20 |
| 309 | Heterogeneous Solvation in Distinctive Protein-Protein Interfaces Revealed by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 11695-11701 | 3.4 | 4 |
| 308 | A Computational Modeling Approach Predicts Interaction of the Antifungal Protein AFP from with Fungal Membranes via Its Core Motif. *MSphere*, **2018**, 3, | 5 | 12 |
| 307 | Identification of SLAC1 anion channel residues required for CO/bicarbonate sensing and regulation of stomatal movements. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 11129-11137 | 11.5 | 32 |

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| 306 | Key role of the REC lobe during CRISPR-Cas9 activation by ‘sensing’, ‘regulating’, and ‘locking’ the catalytic HNH domain. *Quarterly Reviews of Biophysics*, **2018**, 51, | 7 | 42 |
| 305 | Spectroscopic and Computational Investigations of Ligand Binding to IspH: Discovery of Non-diphosphate Inhibitors. *ChemBioChem*, **2017**, 18, 914-920 | 3.8 | 5 |
| 304 | Effect of donor atom identity on metal-binding pharmacophore coordination. *Journal of Biological Inorganic Chemistry*, **2017**, 22, 605-613 | 3.7 | 7 |
| 303 | Activation mechanisms of the first sphingosine-1-phosphate receptor. *Protein Science*, **2017**, 26, 1150-1160 | 6.9 | 11 |
| 302 | Gaussian Accelerated Molecular Dynamics in NAMD. *Journal of Chemical Theory and Computation*, **2017**, 13, 9-19 | 6.4 | 64 |
| 301 | Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. *Annual Reports in Computational Chemistry*, **2017**, 13, 231-278 | 1.8 | 47 |
| 300 | Manipulating Protein-Protein Interactions in Nonribosomal Peptide Synthetase Type II Peptidyl Carrier Proteins. *Biochemistry*, **2017**, 56, 5269-5273 | 3.2 | 12 |
| 299 | Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. *Journal of the American Chemical Society*, **2017**, 139, 16028-16031 | 16.4 | 66 |
| 298 | "Martinizing" the Variational Implicit Solvent Method (VISM): Solvation Free Energy for Coarse-Grained Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 6538-6548 | 3.4 | 8 |
| 297 | 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 |
| 296 | Dynamic Structure and Inhibition of a Malaria Drug Target: Geranylgeranyl Diphosphate Synthase. *Biochemistry*, **2016**, 55, 5180-90 | 3.2 | 7 |
| 295 | Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations. *ACS Central Science*, **2016**, 2, 756-763 | 16.8 | 67 |
| 294 | Molecular dynamic study of MlaC protein in Gram-negative bacteria: conformational flexibility, solvent effect and protein-phospholipid binding. *Protein Science*, **2016**, 25, 1430-7 | 6.3 | 15 |
| 293 | G-protein coupled receptors: advances in simulation and drug discovery. *Current Opinion in Structural Biology*, **2016**, 41, 83-89 | 8.1 | 60 |
| 292 | General trends of dihedral conformational transitions in a globular protein. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 501-14 | 4.2 | 6 |
| 291 | Unconstrained Enhanced Sampling for Free Energy Calculations of Biomolecules: A Review. *Molecular Simulation*, **2016**, 42, 1046-1055 | 2 | 93 |
| 290 | Stochastic level-set variational implicit-solvent approach to solute-solvent interfacial fluctuations. *Journal of Chemical Physics*, **2016**, 145, 054114 | 3.9 | 8 |
| 289 | Hybrid finite element and Brownian dynamics method for charged particles. *Journal of Chemical Physics*, **2016**, 144, 164107 | 3.9 | 1 |

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| 288 | Substrate channeling between the human dihydrofolate reductase and thymidylate synthase. *Protein Science*, **2016**, 25, 79-86 | 6.3 | 20 |
| 287 | Development of Potent and Selective Inhibitors for Group VIA Calcium-Independent Phospholipase A2 Guided by Molecular Dynamics and Structure-Activity Relationships. *Journal of Medicinal Chemistry*, **2016**, 59, 4403-14 | 8.3 | 27 |
| 286 | Computer-aided drug design guided by hydrogen/deuterium exchange mass spectrometry: A powerful combination for the development of potent and selective inhibitors of Group VIA calcium-independent phospholipase A. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4801-4811 | 3.4 | 15 |
| 285 | Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E5675-84 | 11.5 | 69 |
| 284 | Graded activation and free energy landscapes of a muscarinic G-protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12162-12167 | 11.5 | 79 |
| 283 | Computation of pH-dependent binding free energies. *Biopolymers*, **2016**, 105, 43-9 | 2.2 | 16 |
| 282 | Effects of HCM cTnI mutation R145G on troponin structure and modulation by PKA phosphorylation elucidated by molecular dynamics simulations. *Biophysical Journal*, **2015**, 108, 395-407 | 2.9 | 30 |
| 281 | Enhanced ligand sampling for relative protein-ligand binding free energy calculations. *Journal of Physical Chemistry B*, **2015**, 119, 6190-7 | 3.4 | 13 |
| 280 | Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2015**, 11, 3584-3595 | 6.4 | 302 |
| 279 | LS-VISM: A software package for analysis of biomolecular solvation. *Journal of Computational Chemistry*, **2015**, 36, 1047-59 | 3.5 | 16 |
| 278 | Allosteric effects of sodium ion binding on activation of the m3 muscarinic g-protein-coupled receptor. *Biophysical Journal*, **2015**, 108, 1796-1806 | 2.9 | 53 |
| 277 | Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor. *Quarterly Reviews of Biophysics*, **2015**, 48, 479-87 | 7 | 100 |
| 276 | Troponin I Mutations R146G and R21C Alter Cardiac Troponin Function, Contractile Properties, and Modulation by Protein Kinase A (PKA)-mediated Phosphorylation. *Journal of Biological Chemistry*, **2015**, 290, 27749-66 | 5.4 | 25 |
| 275 | A self-consistent phase-field approach to implicit solvation of charged molecules with Poisson-Boltzmann electrostatics. *Journal of Chemical Physics*, **2015**, 143, 243110 | 3.9 | 6 |
| 274 | Accelerated molecular dynamics simulations of protein folding. *Journal of Computational Chemistry*, **2015**, 36, 1536-49 | 3.5 | 106 |
| 273 | Electrostatic steering enhances the rate of cAMP binding to phosphodiesterase: Brownian dynamics modeling. *Protein Science*, **2015**, 24, 1884-9 | 6.3 | 13 |
| 272 | Investigation of the conformational dynamics of the apo A2A adenosine receptor. *Protein Science*, **2015**, 24, 1004-12 | 6.3 | 10 |
| 271 | Conformational Dynamics and Binding Free Energies of Inhibitors of BACE-1: From the Perspective of Protonation Equilibria. *PLoS Computational Biology*, **2015**, 11, e1004341 | 5 | 25 |

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| 270 | How to deal with multiple binding poses in alchemical relative protein-ligand binding free energy calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2670-9 | 6.4 | 42 |
| 269 | 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 |
| 268 | Membranes serve as allosteric activators of phospholipase A2, enabling it to extract, bind, and hydrolyze phospholipid substrates. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E516-25 | 11.5 | 64 |
| 267 | Exploring the role of receptor flexibility in structure-based drug discovery. *Biophysical Chemistry*, **2014**, 186, 31-45 | 3.5 | 105 |
| 266 | Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 6398-406 | 3.6 | 62 |
| 265 | A model study of sequential enzyme reactions and electrostatic channeling. *Journal of Chemical Physics*, **2014**, 140, 105101 | 3.9 | 39 |
| 264 | Trapping the dynamic acyl carrier protein in fatty acid biosynthesis. *Nature*, **2014**, 505, 427-31 | 50.4 | 174 |
| 263 | Electrostatic channeling in P. falciparum DHFR-TS: Brownian dynamics and Smoluchowski modeling. *Biophysical Journal*, **2014**, 107, 2394-402 | 2.9 | 18 |
| 262 | Use of Broken-Symmetry Density Functional Theory To Characterize the IspH Oxidized State: Implications for IspH Mechanism and Inhibition. *Journal of Chemical Theory and Computation*, **2014**, 10, 3871-3884 | 6.4 | 13 |
| 261 | Accelerated adaptive integration method. *Journal of Physical Chemistry B*, **2014**, 118, 5109-18 | 3.4 | 11 |
| 260 | Mapping of allosteric druggable sites in activation-associated conformers of the M2 muscarinic receptor. *Chemical Biology and Drug Design*, **2014**, 83, 237-46 | 2.9 | 36 |
| 259 | Variational Implicit Solvation with Poisson-Boltzmann Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 1454-1467 | 6.4 | 35 |
| 258 | Trypsinogen activation as observed in accelerated molecular dynamics simulations. *Protein Science*, **2014**, 23, 1550-8 | 6.3 | 3 |
| 257 | Heterogeneous Hydration of p53/MDM2 Complex. *Journal of Chemical Theory and Computation*, **2014**, 10, 1302-1313 | 6.4 | 17 |
| 256 | Computational studies of the effect of the S23D/S24D troponin I mutation on cardiac troponin structural dynamics. *Biophysical Journal*, **2014**, 107, 1675-85 | 2.9 | 35 |
| 255 | Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2014**, 10, 2677-2689 | 6.4 | 225 |
| 254 | Structure, mechanism, and dynamics of UDP-galactopyranose mutase. *Archives of Biochemistry and Biophysics*, **2014**, 544, 128-41 | 4.1 | 39 |
| 253 | Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. *Journal of Chemical Theory and Computation*, **2014**, 10, 1631-1637 | 6.4 | 8 |

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| 252 | PKA phosphorylation of cardiac troponin I modulates activation and relaxation kinetics of ventricular myofibrils. *Biophysical Journal*, **2014**, 107, 1196-1204 | 2.9 | 35 |
| 251 | Drug screening strategy for human membrane proteins: from NMR protein backbone structure to in silica- and NMR-screened hits. *Biochemical and Biophysical Research Communications*, **2014**, 445, 724-33 | 2.4 | 9 |
| 250 | Taxodione and arenarone inhibit farnesyl diphosphate synthase by binding to the isopentenyl diphosphate site. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E2530-9 | 11.5 | 27 |
| 249 | Poisson-Boltzmann versus Size-Modified Poisson-Boltzmann Electrostatics Applied to Lipid Bilayers. *Journal of Physical Chemistry B*, **2014**, 118, 14827-32 | 3.4 | 10 |
| 248 | Allosteric inhibition of Epac: computational modeling and experimental validation to identify allosteric sites and inhibitors. *Journal of Biological Chemistry*, **2014**, 289, 29148-57 | 5.4 | 24 |
| 247 | Molecular dynamics simulation study of conformational changes of transcription factor TFIIS during RNA polymerase II transcriptional arrest and reactivation. *PLoS ONE*, **2014**, 9, e97975 | 3.7 | 5 |
| 246 | Substrate-dependent dynamics of UDP-galactopyranose mutase: Implications for drug design. *Protein Science*, **2013**, 22, 1490-501 | 6.3 | 11 |
| 245 | Improving the Efficiency of Free Energy Calculations in the Amber Molecular Dynamics Package. *Journal of Chemical Theory and Computation*, **2013**, 9, | 6.4 | 72 |
| 244 | Population based reweighting of scaled molecular dynamics. *Journal of Physical Chemistry B*, **2013**, 117, 12759-68 | 3.4 | 75 |
| 243 | AFMPB: An adaptive fast multipole PoissonBoltzmann solver for calculating electrostatics in biomolecular systems. *Computer Physics Communications*, **2013**, 184, 2618-2619 | 4.2 | 2 |
| 242 | Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2013**, 9, 4684-4691 | 6.4 | 32 |
| 241 | Variational Implicit-Solvent Modeling of Host-Guest Binding: A Case Study on Cucurbit[7]uril. *Journal of Chemical Theory and Computation*, **2013**, 9, 4195-4204 | 6.4 | 11 |
| 240 | Simulations of biased agonists in the 2 adrenergic receptor with accelerated molecular dynamics. *Biochemistry*, **2013**, 52, 5593-603 | 3.2 | 31 |
| 239 | Solvent fluctuations in hydrophobic cavity-ligand binding kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 1197-202 | 11.5 | 77 |
| 238 | Structural insight into the separate roles of inositol tetraphosphate and deacetylase-activating domain in activation of histone deacetylase 3. *Protein Science*, **2013**, 22, 83-92 | 6.3 | 24 |
| 237 | 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 |
| 236 | Molecular recognition and ligand association. *Annual Review of Physical Chemistry*, **2013**, 64, 151-75 | 15.7 | 145 |
| 235 | w-REXAMD: A Hamiltonian Replica Exchange Approach to Improve Free Energy Calculations for Systems with Kinetically Trapped Conformations. *Journal of Chemical Theory and Computation*, **2013**, 9, 18-23 | 6.4 | 36 |

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| 234 | Evaluation of Hydration Free Energy by Level-Set Variational Implicit-Solvent Model with Coulomb-Field Approximation. *Journal of Chemical Theory and Computation*, **2013**, 9, 1778-1787 | 6.4 | 24 |
| 233 | Utilizing a dynamical description of IspH to aid in the development of novel antimicrobial drugs. *PLoS Computational Biology*, **2013**, 9, e1003395 | 5 | 7 |
| 232 | Insertion of the Ca□+-independent phospholipase A□into a phospholipid bilayer via coarse-grained and atomistic molecular dynamics simulations. *PLoS Computational Biology*, **2013**, 9, e1003156 | 5 | 27 |
| 231 | Inactivating mutation in histone deacetylase 3 stabilizes its active conformation. *Protein Science*, **2013**, 22, 1306-12 | 6.3 | 6 |
| 230 | 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 |
| 229 | Multi-core CPU or GPU-accelerated Multiscale Modeling for Biomolecular Complexes. *Computational and Mathematical Biophysics*, **2013**, 1, | 1.7 | 14 |
| 228 | Mapping the Population of Protein Conformational Energy Sub-States from NMR Dipolar Couplings. *Angewandte Chemie*, **2013**, 125, 3263-3267 | 3.6 | 1 |
| 227 | Phase-field approach to implicit solvation of biomolecules with Coulomb-field approximation. *Journal of Chemical Physics*, **2013**, 139, 024111 | 3.9 | 12 |
| 226 | Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver. *Communications in Computational Physics*, **2013**, 13, 107-128 | 2.4 | 9 |
| 225 | Modelling cardiac calcium sparks in a three-dimensional reconstruction of a calcium release unit. *Journal of Physiology*, **2012**, 590, 4403-22 | 3.9 | 67 |
| 224 | 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 |
| 223 | The binding mechanism, multiple binding modes, and allosteric regulation of Staphylococcus aureus Sortase A probed by molecular dynamics simulations. *Protein Science*, **2012**, 21, 1858-71 | 6.3 | 28 |
| 222 | Dynamics and calcium association to the N-terminal regulatory domain of human cardiac troponin C: a multiscale computational study. *Journal of Physical Chemistry B*, **2012**, 116, 8449-59 | 3.4 | 39 |
| 221 | Level-Set Variational Implicit-Solvent Modeling of Biomolecules with the Coulomb-Field Approximation. *Journal of Chemical Theory and Computation*, **2012**, 8, 386-397 | 6.4 | 28 |
| 220 | Routine Access to Millisecond Time Scale Events with Accelerated Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 2997-3002 | 6.4 | 344 |
| 219 | Calcium binding and allosteric signaling mechanisms for the sarcoplasmic reticulum Ca□+ ATPase. *Protein Science*, **2012**, 21, 1429-43 | 6.3 | 21 |
| 218 | Hydrophobic Association and Volume-Confined Water Molecules **2012**, 145-170 | | 9 |
| 217 | The dynamic structure of thrombin in solution. *Biophysical Journal*, **2012**, 103, 79-88 | 2.9 | 43 |

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| 216 | Multi-Timescale Conformational Dynamics of the SH3 Domain of CD2-Associated Protein using NMR Spectroscopy and Accelerated Molecular Dynamics. *Angewandte Chemie*, **2012**, 124, 6207-6210 | 3.6 | 3 |
| 215 | Innenr□ktitelbild: Multi-Timescale Conformational Dynamics of the SH3 Domain of CD2-Associated Protein using NMR Spectroscopy and Accelerated Molecular Dynamics (Angew. Chem. 25/2012). *Angewandte Chemie*, **2012**, 124, 6383-6383 | 3.6 | |
| 214 | Inside Back Cover: Multi-Timescale Conformational Dynamics of the SH3 Domain of CD2-Associated Protein using NMR Spectroscopy and Accelerated Molecular Dynamics (Angew. Chem. Int. Ed. 25/2012). *Angewandte Chemie - International Edition*, **2012**, 51, 6279-6279 | 16.4 | |
| 213 | Modeling effects of L-type ca(2+) current and na(+)-ca(2+) exchanger on ca(2+) trigger flux in rabbit myocytes with realistic T-tubule geometries. *Frontiers in Physiology*, **2012**, 3, 351 | 4.6 | 23 |
| 212 | Accelerated molecular dynamics: Theory, implementation and applications **2012**, | | 3 |
| 211 | A molecular dynamics ensemble-based approach for the mapping of druggable binding sites. *Methods in Molecular Biology*, **2012**, 819, 3-12 | 1.4 | 21 |
| 210 | Molecular recognition in the case of flexible targets. *Current Pharmaceutical Design*, **2011**, 17, 1663-71 | 3.3 | 39 |
| 209 | Novel inhibitors of Mycobacterium tuberculosis dTDP-6-deoxy-L-lyxo-4-hexulose reductase (RmlD) identified by virtual screening. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 7064-7 | 2.9 | 14 |
| 208 | Molecular dynamics simulations and drug discovery. *BMC Biology*, **2011**, 9, 71 | 7.3 | 615 |
| 207 | Gated Diffusion-controlled Reactions. *BMC Biophysics*, **2011**, 4, 4 | 0 | 18 |
| 206 | Predictive power of molecular dynamics receptor structures in virtual screening. *Journal of Chemical Information and Modeling*, **2011**, 51, 1439-46 | 6.1 | 75 |
| 205 | Induced fit or conformational selection? The role of the semi-closed state in the maltose binding protein. *Biochemistry*, **2011**, 50, 10530-9 | 3.2 | 76 |
| 204 | POVME: an algorithm for measuring binding-pocket volumes. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 773-6 | 2.8 | 164 |
| 203 | Accessing a hidden conformation of the maltose binding protein using accelerated molecular dynamics. *PLoS Computational Biology*, **2011**, 7, e1002034 | 5 | 92 |
| 202 | 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 |
| 201 | Numerical analysis of Ca2+ signaling in rat ventricular myocytes with realistic transverse-axial tubular geometry and inhibited sarcoplasmic reticulum. *PLoS Computational Biology*, **2010**, 6, e1000972 | 5 | 34 |
| 200 | How Can Hydrophobic Association Be Enthalpy Driven?. *Journal of Chemical Theory and Computation*, **2010**, 6, 2866-2871 | 6.4 | 169 |
| 199 | Enhanced conformational space sampling improves the prediction of chemical shifts in proteins. *Journal of the American Chemical Society*, **2010**, 132, 1220-1 | 16.4 | 82 |

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| 198 | Water in cavity-ligand recognition. *Journal of the American Chemical Society*, **2010**, 132, 12091-7 | 16.4 | 215 |
| 197 | A dynamic model of HIV integrase inhibition and drug resistance. *Journal of Molecular Biology*, **2010**, 397, 600-15 | 6.5 | 52 |
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| 5 | Multiscale simulations examining glycan shield effects on drug binding to influenza neuraminidase | | 2 |
| 4 | Structure and Dynamic Basis of Molecular Recognition Between Acyltransferase and Carrier Protein in E. coli Fatty Acid Synthesis | | 2 |
| 3 | Molecular mechanism of off-target effects in CRISPR-Cas9 | | 4 |
| 2 | GAMer 2: A System for 3D Mesh Processing of Cellular Electron Micrographs | | 4 |
| 1 | An Open Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries | | 1 |