CITATION REPORT List of articles citing

Random walk in orthogonal space to achieve efficient free-energy simulation of complex systems

DOI: 10.1073/pnas.0810631106 Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20227-32.

Source: https://exaly.com/paper-pdf/44379721/citation-report.pdf

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
267	Computing generalized Langevin equations and generalized Fokker-Planck equations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 10884-9	11.5	82
266	Enhanced sampling in generalized ensemble with large gap of sampling parameter: case study in temperature space random walk. <i>Journal of Chemical Physics</i> , 2009 , 130, 194112	3.9	18
265	Simultaneous escaping of explicit and hidden free energy barriers: application of the orthogonal space random walk strategy in generalized ensemble based conformational sampling. <i>Journal of Chemical Physics</i> , 2009 , 130, 234105	3.9	71
264	On-the-path random walk sampling for efficient optimization of minimum free-energy path. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1649-53	3.5	23
263	Artificial reaction coordinate "tunneling" in free-energy calculations: the catalytic reaction of RNase H. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1634-41	3.5	73
262	Calculation of free-energy differences by confinement simulations. Application to peptide conformers. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 9728-40	3.4	46
261	Theory of free energy and entropy in noncovalent binding. <i>Chemical Reviews</i> , 2009 , 109, 4092-107	68.1	291
260	Decomposition of energy and free energy changes by following the flow of work along reaction path. <i>Journal of Chemical Physics</i> , 2009 , 131, 144105	3.9	15
259	QM/MM Alchemical Free Energy Simulations: Challenges and Recent Developments. 2010 , 6, 51-62		18
258	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 35-47	6.4	310
257	(Un)Folding mechanisms of the FBP28 WW domain in explicit solvent revealed by multiple rare event simulation methods. 2010 , 98, 646-56		15
256	Chemical versus mechanical perturbations on the protonation state of arginine in complex lipid membranes: insights from microscopic pKa calculations. 2010 , 99, 1529-38		11
255	Practically Efficient QM/MM Alchemical Free Energy Simulations: The Orthogonal Space Random Walk Strategy. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2253-66	6.4	29
254	Elucidation of interactions of Alzheimer amyloid beta peptides (Abeta40 and Abeta42) with insulin degrading enzyme: a molecular dynamics study. 2010 , 49, 3947-56		13
253	Conformational consequences of ionization of Lys, Asp, and Glu buried at position 66 in staphylococcal nuclease. 2010 , 49, 4138-46		48
252	Electronic properties and desolvation penalties of metal ions plus protein electrostatics dictate the metal binding affinity and selectivity in the copper efflux regulator. <i>Journal of the American Chemical Society</i> , 2010 , 132, 18092-102	16.4	32
251	Conformational Free-Energy Difference of a Miniprotein from Nonequilibrium Simulations. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 1922-1926	6.4	17

(2011-2010)

250	Key residues that play a critical role in urea-induced lysozyme unfolding. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15687-93	3.4	17	
249	Sampling long time scale protein motions: OSRW simulation of active site loop conformational free energies in formyl-CoA:oxalate CoA transferase. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7252-3	16.4	9	
248	Constant pH replica exchange molecular dynamics in biomolecules using a discrete protonation model. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1401-1412	6.4	79	
247	Predicting the acid/base behavior of proteins: a constant-pH Monte Carlo approach with generalized born solvent. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 10634-48	3.4	28	
246	Balancing simulation accuracy and efficiency with the Amber united atom force field. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 2886-93	3.4	8	
245	Glycosidic bond conformation preference plays a pivotal role in catalysis of RNA pseudouridylation: a combined simulation and structural study. 2010 , 401, 690-5		9	
244	Free energy calculations: an efficient adaptive biasing potential method. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 5823-30	3.4	45	
243	Efficient Explicit-Solvent Molecular Dynamics Simulations of Molecular Association Kinetics: Methane/Methane, Na(+)/Cl(-), Methane/Benzene, and K(+)/18-Crown-6 Ether. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1189-97	6.4	37	
242	Enhancing QM/MM molecular dynamics sampling in explicit environments via an orthogonal-space-random-walk-based strategy. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 3924-35	3.4	20	
241	Allosteric activation via kinetic control: potassium accelerates a conformational change in IMP dehydrogenase. 2011 , 50, 8508-18		12	
240	Thermal Elimination of Precursors to Poly(phenylenevinylene) with a Macrocounterion versus a Small Counterion: A Coordinated Experimental and Simulation Study. 2011 , 44, 6663-6668		2	
239	A Combined Metadynamics and Umbrella Sampling Method for the Calculation of Ion Permeation Free Energy Profiles. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2277-2283	6.4	54	
238	Conformational relaxation and water penetration coupled to ionization of internal groups in proteins. 2011 , 115, 4042-53		32	
237	Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370		58	
236	Force-momentum-based self-guided Langevin dynamics: a rapid sampling method that approaches the canonical ensemble. <i>Journal of Chemical Physics</i> , 2011 , 135, 204101	3.9	18	
235	Computing Alchemical Free Energy Differences with Hamiltonian Replica Exchange Molecular Dynamics (H-REMD) Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2721-2727	6.4	59	
234	Multi-Site Edynamics for simulated Structure-Activity Relationship studies. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2728-2739	6.4	51	
233	Structural origins of high apparent dielectric constants experienced by ionizable groups in the hydrophobic core of a protein. 2011 , 405, 361-77		33	

232	A Benchmark Test Set for Alchemical Free Energy Transformations and Its Use to Quantify Error in Common Free Energy Methods. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 4115-34	6.4	99
231	Free Energy Calculations for Cyclodextrin Inclusion Complexes. 2011 , 15, 839-847		12
230	Alchemical free energy methods for drug discovery: progress and challenges. 2011 , 21, 150-60		382
229	Equilibrium sampling in biomolecular simulations. 2011 , 40, 41-62		171
228	Structural plasticity of staphylococcal nuclease probed by perturbation with pressure and pH. 2011 , 79, 1293-305		26
227	Developing hybrid approaches to predict pKa values of ionizable groups. 2011 , 79, 3389-99		27
226	pH replica-exchange method based on discrete protonation states. 2011 , 79, 3420-36		89
225	Extending fragment-based free energy calculations with library Monte Carlo simulation: annealing in interaction space. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1135-43	3.5	8
224	Avoiding the van der Waals endpoint problem using serial atomic insertion. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2449-58	3.5	14
223	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3423-32	3.5	32
222	Approaching post-Hartreeflock quality potential energy surfaces with simple pair-wise expressions: parameterising point-charge-based force fields for liquid water using the adaptive force matching method. 2011 , 37, 591-605		39
221	Large shifts in pKa values of lysine residues buried inside a protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 5260-5	11.5	301
220	Generalized essential energy space random walks to more effectively accelerate solute sampling in aqueous environment. <i>Journal of Chemical Physics</i> , 2012 , 136, 044103	3.9	13
219	Transmembrane helix assembly by window exchange umbrella sampling. <i>Physical Review Letters</i> , 2012 , 108, 108102	7.4	51
218	Computational insights for the discovery of non-ATP competitive inhibitors of MAP kinases. 2012 , 18, 1173-85		18
217	Biomolecular electrostatics and solvation: a computational perspective. 2012 , 45, 427-91		132
216	Sampling protein motion and solvent effect during ligand binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 1467-72	11.5	86
215	Exact Relation between Potential of Mean Force and Free-Energy Profile. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3998-4003	6.4	21

(2013-2012)

214	Practically Efficient and Robust Free Energy Calculations: Double-Integration Orthogonal Space Tempering. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 810-23	6.4	70	
213	Structural and electrostatic asymmetry at the active site in typical and atypical peroxiredoxin dimers. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6832-43	3.4	14	
212	Force and Stress along Simulated Dissociation Pathways of Cucurbituril-Guest Systems. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 966-976	6.4	13	
211	Computational Insights into Dynamics of Protein Aggregation and Enzyme-Substrate Interactions. Journal of Physical Chemistry Letters, 2012 , 3, 3460-9	6.4	4	
210	Constant pH Molecular Dynamics Simulations of Nucleic Acids in Explicit Solvent. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 36-46	6.4	73	
209	Free-energy simulations reveal that both hydrophobic and polar interactions are important for influenza hemagglutinin antibody binding. 2012 , 102, 1453-61		22	
208	Novel Design of a Nanoflowmeter Based on Carbon Nanotubes. 2012 , 116, 13429-13434		6	
207	Analysis and elimination of a bias in targeted molecular dynamics simulations of conformational transitions: application to calmodulin. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8584-603	3.4	42	
206	Development and application of enhanced sampling techniques to simulate the long-time scale dynamics of biomolecular systems. 2012 , 112, 33-43		23	
205	The Structure, Thermodynamics and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1721-1736	6.4	65	
204	Protonation states of the catalytic dyad of Becretase (BACE1) in the presence of chemically diverse inhibitors: a molecular docking study. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 1275-87	6.1	28	
203	Amino acid analogues bind to carbon nanotube via Einteractions: comparison of molecular mechanical and quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 2012 , 136, 025103	3.9	82	
202	Blind prediction of host-guest binding affinities: a new SAMPL3 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2012 , 26, 475-87	4.2	101	
201	Structural reorganization triggered by charging of Lys residues in the hydrophobic interior of a protein. 2012 , 20, 1071-85		37	
200	Toward molecular models of proton pumping: Challenges, methods and relevant applications. 2012 , 55, 3-18		6	
199	Enhanced and effective conformational sampling of protein molecular systems for their free energy landscapes. 2012 , 4, 27-44		48	
198	Elucidating the catalytic mechanism of Becretase (BACE1): a quantum mechanics/molecular mechanics (QM/MM) approach. 2013 , 40, 1-9		24	
197	Binding preference of carbon nanotube over proline-rich motif ligand on SH3-domain: a comparison with different force fields. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 3541-7	3.4	12	

196	Using collective variables to drive molecular dynamics simulations. <i>Molecular Physics</i> , 2013 , 111, 3345-	33 <u>6</u> 7	463
195	Hidden Conformation Events in DNA Base Extrusions: A Generalized Ensemble Path Optimization and Equilibrium Simulation Study. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9,	6.4	15
194	Optimization of Umbrella Sampling Replica Exchange Molecular Dynamics by Replica Positioning. Journal of Chemical Theory and Computation, 2013 , 9, 4692-9	6.4	28
193	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 13-17	6.4	33
192	Hemoglobin Bohr effects: atomic origin of the histidine residue contributions. 2013 , 52, 8539-55		21
191	Towards Accurate Prediction of Protonation Equilibrium of Nucleic Acids. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 760-766	6.4	26
190	Free-energy differences between states with different conformational ensembles. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1398-408	3.5	15
189	Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1885-1895	6.4	63
188	Standard binding free energies from computer simulations: What is the best strategy?. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 794-802	6.4	224
187	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 153-164	6.4	59
186	pH-dependent dynamics of complex RNA macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 935-943	6.4	47
185	Efficient Computation of Small-Molecule Configurational Binding Entropy and Free Energy Changes by Ensemble Enumeration. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5098-5115	6.4	24
184	Unusual sequence effects on nucleotide excision repair of arylamine lesions: DNA bending/distortion as a primary recognition factor. 2013 , 41, 869-80		38
183	A virtual-system coupled multicanonical molecular dynamics simulation: principles and applications to free-energy landscape of protein-protein interaction with an all-atom model in explicit solvent. <i>Journal of Chemical Physics</i> , 2013 , 138, 184106	3.9	29
182	Adaptive single replica multiple state transition interface sampling. <i>Journal of Chemical Physics</i> , 2013 , 139, 044105	3.9	24
181	Enhanced sampling of molecular dynamics simulation of peptides and proteins by double coupling to thermal bath. 2013 , 31, 206-14		5
180	UV-radiation induced disruption of dry-cavities in human D -crystallin results in decreased stability and faster unfolding. 2013 , 3, 1560		33
179	Achieving ergodic sampling using replica-exchange free-energy calculations. 2014 , 40, 218-228		19

178	Payoffs, not tradeoffs, in the adaptation of a virus to ostensibly conflicting selective pressures. 2014 , 10, e1004611		19
177	Combine umbrella sampling with integrated tempering method for efficient and accurate calculation of free energy changes of complex energy surface. <i>Journal of Chemical Physics</i> , 2014 , 141, 044108	3.9	21
176	Multiple-Replica Strategies for Free-Energy Calculations in NAMD: Multiple-Walker Adaptive Biasing Force and Walker Selection Rules. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5276-8.	6 .4	52
175	A replica exchange transition interface sampling method with multiple interface sets for investigating networks of rare events. <i>Journal of Chemical Physics</i> , 2014 , 141, 044101	3.9	23
174	Thermodynamics of Deca-alanine Folding in Water. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2836-2844	6.4	37
173	Absolute Organic Crystal Thermodynamics: Growth of the Asymmetric Unit into a Crystal via Alchemy. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2781-91	6.4	19
172	Computing the relative stabilities and the per-residue components in protein conformational changes. 2014 , 22, 168-75		21
171	Bayesian model aggregation for ensemble-based estimates of protein pKa values. 2014 , 82, 354-63		9
170	Quantum mechanical/molecular mechanical studies of zinc hydrolases. 2014 , 33, 1-41		19
169	Hydration Free Energy from Orthogonal Space Random Walk and Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2792-2801	6.4	12
168	A large-scale test of free-energy simulation estimates of protein-ligand binding affinities. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2794-806	6.1	49
167	Well-tempered metadynamics converges asymptotically. <i>Physical Review Letters</i> , 2014 , 112, 240602	7.4	182
166	Recent developments in methods for identifying reaction coordinates. 2014 , 40, 784-793		50
165	Theory of Adaptive Optimization for Umbrella Sampling. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2719-2728	6.4	16
164	Roadmaps through free energy landscapes calculated using the multi-dimensional vFEP approach. Journal of Chemical Theory and Computation, 2014 , 10, 24-34	6.4	45
163	Simultaneous Computation of Dynamical and Equilibrium Information Using a Weighted Ensemble of Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2658-2667	6.4	60
162	Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3626-33	6.4	47
161	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. 2014 , 82, 1319	-31	73

160	Integrated Hamiltonian sampling: a simple and versatile method for free energy simulations and conformational sampling. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 8210-20	3.4	13
159	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. Journal of Chemical Theory and Computation, 2014 , 10, 2677-2689	6.4	225
158	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2738-2750	6.4	54
157	Local Elevation Umbrella Sampling Applied to the Calculation of Alchemical Free-Energy Changes via EDynamics: The ELEUS Scheme. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3006-22	6.4	16
156	Computational Recipe for Efficient Description of Large-Scale Conformational Changes in Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2866-2880	6.4	52
155	Frontiers in free-energy calculations of biological systems. 2014 , 4, 71-89		104
154	Free-Energy Calculations with Metadynamics: Theory and Practice. 2015 , 1-49		29
153	Polarizable Force Fields for Biomolecular Modeling. 2015 , 51-86		29
152	Reducing the cost of evaluating the committor by a fitting procedure. <i>Journal of Chemical Physics</i> , 2015 , 143, 174103	3.9	10
151	In silico ADME/T modelling for rational drug design. 2015 , 48, 488-515		137
150	The complex and specific pMHC interactions with diverse HIV-1 TCR clonotypes reveal a structural basis for alterations in CTL function. 2014 , 4, 4087		16
149	Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI versus ELEUS. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1686-97	3.5	10
148	. 2015,		2
147	FAST Conformational Searches by Balancing Exploration/Exploitation Trade-Offs. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5747-57	6.4	90
146	Theoretical insights into the functioning of metallopeptidases and their synthetic analogues. <i>Accounts of Chemical Research</i> , 2015 , 48, 192-200	24.3	26
145	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 9423-9437	3.4	149
144	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. Journal of Chemical Theory and Computation, 2015, 11, 1255-66	6.4	8
143	Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. <i>Journal of the American Chemical Society</i> 2015 , 137, 2695-703	16.4	633

(2016-2015)

142	Kinetics of protein-ligand unbinding: Predicting pathways, rates, and rate-limiting steps. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E386-91	11.5	234
141	Efficient Calculation of Enzyme Reaction Free Energy Profiles Using a Hybrid Differential Relaxation Algorithm: Application to Mycobacterial Zinc Hydrolases. 2015 , 100, 33-65		4
140	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3584-3595	6.4	302
139	Enhanced conformational sampling using replica exchange with concurrent solute scaling and hamiltonian biasing realized in one dimension. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2855-67	6.4	25
138	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2234-44	6.4	10
137	From thermodynamics to kinetics: enhanced sampling of rare events. <i>Accounts of Chemical Research</i> , 2015 , 48, 947-55	24.3	47
136	Theoretical and simulation studies on voltage-gated sodium channels. 2015 , 6, 413-22		9
135	Mixed Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations of Biological Systems in Ground and Electronically Excited States. <i>Chemical Reviews</i> , 2015 , 115, 6217-63	68.1	277
134	Multistate Elocal-elevation umbrella-sampling (MS-ELEUS): method and application to the complexation of cations by crown ethers. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2575-8	86.4	13
133	Modeling of Nanotoxicity. 2015,		10
132	Exploring Valleys without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5638-50	6.4	23
131	Free energy and hidden barriers of the Esheet structure of prion protein. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5024-34	6.4	14
130	Molecular density functional theory for multiscale modeling of hydration free energy. 2015 , 126, 370-38	82	19
129	Toward structure prediction of cyclic peptides. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 4210-9	3.6	39
128	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. 2015 , 1850, 944-953		25
127	The adaptive biasing force method: everything you always wanted to know but were afraid to ask. Journal of Physical Chemistry B, 2015 , 119, 1129-51	3.4	240
126	Electrostatic free energies in translational GTPases: Classic allostery and the rest. 2015 , 1850, 1006-101	6	4
125	Methods for Efficiently and Accurately Computing Quantum Mechanical Free Energies for Enzyme Catalysis. 2016 , 577, 75-104		4

124	Advanced Sampling for Molecular Simulation is Coming of Age. <i>Journal of Computational Chemistry</i> , 2016 , 37, 549	3.5	5
123	Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. <i>Journal of Computational Chemistry</i> , 2016 , 37, 558-66	3.5	37
122	Free energy simulations with the AMOEBA polarizable force field and metadynamics on GPU platform. <i>Journal of Computational Chemistry</i> , 2016 , 37, 614-22	3.5	9
121	Unconstrained Enhanced Sampling for Free Energy Calculations of Biomolecules: A Review. 2016 , 42, 1046-1055		93
120	Concepts and protocols for electrostatic free energies. 2016 , 42, 1090-1101		25
119	A benchmark for reaction coordinates in the transition path ensemble. <i>Journal of Chemical Physics</i> , 2016 , 144, 134104	3.9	14
118	Free energy landscape of a minimalist salt bridge model. <i>Protein Science</i> , 2016 , 25, 270-6	6.3	
117	Insights into How Cyclic Peptides Switch Conformations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2480-8	6.4	34
116	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 30261-30269	3.6	36
115	Understanding enzyme reactions using enhanced sampling techniques. 2016 , 42, 846-854		
114	Decrypting protein insertion through the translocon with free-energy calculations. 2016 , 1858, 1663-71		12
114	Decrypting protein insertion through the translocon with free-energy calculations. 2016 , 1858, 1663-71 Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301	3.4	12 25
·	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping		
113	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301 A Simple and Accurate Method To Calculate Free Energy Profiles and Reaction Rates from		25
113	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301 A Simple and Accurate Method To Calculate Free Energy Profiles and Reaction Rates from Restrained Molecular Simulations of Diffusive Processes. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 845	7 -42	25
113	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301 A Simple and Accurate Method To Calculate Free Energy Profiles and Reaction Rates from Restrained Molecular Simulations of Diffusive Processes. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 845 Generalized Ensemble Sampling of Enzyme Reaction Free Energy Pathways. 2016 , 577, 57-74	7 -42	25 11 3
113 112 111 110	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301 A Simple and Accurate Method To Calculate Free Energy Profiles and Reaction Rates from Restrained Molecular Simulations of Diffusive Processes. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 845 Generalized Ensemble Sampling of Enzyme Reaction Free Energy Pathways. 2016 , 577, 57-74 Steered Molecular Dynamics Methods Applied to Enzyme Mechanism and Energetics. 2016 , 578, 123-43	7 -42	25 11 3

106	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8733-42	3.4	11
105	Extended Adaptive Biasing Force Algorithm. An On-the-Fly Implementation for Accurate Free-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3506-13	6.4	71
104	Ligand Release Pathways Obtained with WExplore: Residence Times and Mechanisms. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 5377-85	3.4	40
103	Comparative exploration of hydrogen sulfide and water transmembrane free energy surfaces via orthogonal space tempering free energy sampling. <i>Journal of Computational Chemistry</i> , 2016 , 37, 567-	74 ^{3.5}	11
102	Toward high-throughput predictions of the hydration free energies of small organic molecules from first principles. 2016 , 407, 304-313		11
101	Predictive Sampling of Rare Conformational Events in Aqueous Solution: Designing a Generalized Orthogonal Space Tempering Method. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 41-52	6.4	9
100	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 126-30	6.4	9
99	Sampling errors in free energy simulations of small molecules in lipid bilayers. 2016 , 1858, 2539-2548		70
98	Spectral gap optimization of order parameters for sampling complex molecular systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 2839-44	11.5	135
97	Efficient free energy calculations by combining two complementary tempering sampling methods. <i>Journal of Chemical Physics</i> , 2017 , 146, 024103	3.9	9
96	Microscopic mechanisms that govern the titration response and pK values of buried residues in staphylococcal nuclease mutants. 2017 , 85, 268-281		22
95	Computing converged free energy differences between levels of theory via nonequilibrium work methods: Challenges and opportunities. <i>Journal of Computational Chemistry</i> , 2017 , 38, 1376-1388	3.5	22
94	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1566-1576	6.4	24
93	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite Dynamics. Journal of Physical Chemistry B, 2017 , 121, 3626-3635	3.4	34
92	Identifying the structural and kinetic elements in protein large-amplitude conformational motions. 2017 , 36, 185-227		3
91	Pitfall in Free-Energy Simulations on Simplest Systems. 2017 , 2, 4398-4418		
90	Gibbs Sampler-Based Dynamics and Rao-Blackwell Estimator for Alchemical Free Energy Calculation. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2501-2510	6.4	23
89	Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. <i>Journal of Computational Chemistry</i> , 2017 , 38, 2047-2055	3.5	70

88	Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4660-4674	6.4	5
87	Molecular dynamics investigations of an indicator displacement assay mechanism in a liquid crystal sensor. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 23924-23933	3.6	10
86	Mapping the Drude polarizable force field onto a multipole and induced dipole model. <i>Journal of Chemical Physics</i> , 2017 , 147, 161702	3.9	32
85	Molecular Theory of Hydration at Different Temperatures. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 6898-6908	3.4	7
84	Coalescence of Nanoclusters Analyzed by Well-Tempered Metadynamics. Comparison with Straightforward Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3874-3880	6.4	7
83	Estimation of relative free energies of binding using pre-computed ensembles based on the single-step free energy perturbation and the site-identification by Ligand competitive saturation approaches. <i>Journal of Computational Chemistry</i> , 2017 , 38, 1238-1251	3.5	22
82	Origin of pK Shifts of Internal Lysine Residues in SNase Studied Via Equal-Molar VMMS Simulations in Explicit Water. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 3318-3330	3.4	16
81	Polymorphism at 129 dictates metastable conformations of the human prion protein N-terminal Esheet. <i>Chemical Science</i> , 2017 , 8, 1225-1232	9.4	9
80	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 42-54	6.4	68
79	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017 , 13, 231-278	3	47
79 78		6.4	47 24
	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy		24
78	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1216-1227 Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. <i>Chemical</i>	6.4	24
78 77	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1216-1227 Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. <i>Chemical Reviews</i> , 2018, 118, 1691-1741 Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations.	6.4	24
78 77 76	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 1216-1227 Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. Chemical Reviews, 2018, 118, 1691-1741 Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. 2018, 114, 1091-1102 Constructing Markov State Models to elucidate the functional conformational changes of complex	6.4	24 290 16
78 77 76 75	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 1216-1227 Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. Chemical Reviews, 2018, 118, 1691-1741 Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. 2018, 114, 1091-1102 Constructing Markov State Models to elucidate the functional conformational changes of complex biomolecules. 2018, 8, e1343 Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. 2018, 498, 282-287	6.4	242901649
78 77 76 75 74	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. 2017, 13, 231-278 Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 1216-1227 Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. Chemical Reviews, 2018, 118, 1691-1741 Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. 2018, 114, 1091-1102 Constructing Markov State Models to elucidate the functional conformational changes of complex biomolecules. 2018, 8, e1343 Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. 2018, 498, 282-287 Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional	6.4	24290164914

70	Exploring Configuration Space and Path Space of Biomolecules Using Enhanced Sampling Techniques-Searching for Mechanism and Kinetics of Biomolecular Functions. 2018 , 19,		2
69	Molecular mechanism of phosphoinositides & pecificity for the inwardly rectifying potassium channel Kir2.2. <i>Chemical Science</i> , 2018 , 9, 8352-8362	9.4	O
68	Tinker 8: Software Tools for Molecular Design. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5273-5289	6.4	188
67	Approaching protein design with multisite dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. <i>Protein Science</i> , 2018 , 27, 1910-1922	6.3	11
66	Hydronium Ions Accompanying Buried Acidic Residues Lead to High Apparent Dielectric Constants in the Interior of Proteins. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 6215-6223	3.4	5
65	Unfolding Hidden Barriers by Active Enhanced Sampling. <i>Physical Review Letters</i> , 2018 , 121, 010601	7.4	21
64	Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1356-1371	6.1	6
63	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4738-4745	6.4	47
62	Assessment of a Single Decoupling Alchemical Approach for the Calculation of the Absolute Binding Free Energies of Protein-Peptide Complexes. <i>Frontiers in Molecular Biosciences</i> , 2018 , 5, 22	5.6	10
61	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018 , 9, 956-97	2 ^{9.4}	122
60	Lanosterol Disrupts Aggregation of Human D -Crystallin by Binding to the Hydrophobic Dimerization Interface. <i>Journal of the American Chemical Society</i> , 2018 , 140, 8479-8486	16.4	23
59	Exploration of HIV-1 fusion peptide-antibody VRC34.01 binding reveals fundamental neutralization sites. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18569-18576	3.6	3
58	Molecular Simulations of Supramolecular Architectures. 2019 , 1-27		
57	Scalable Indirect Free Energy Method Applied to Divalent Cation-Metalloprotein Binding. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4602-4614	6.4	2
56	Accurate Determination of Cavitand Binding Free Energies via Unrestrained Advanced Sampling. Journal of Chemical Theory and Computation, 2019 , 15, 5761-5768	6.4	4
55	Taming Rugged Free Energy Landscapes Using an Average Force. <i>Accounts of Chemical Research</i> , 2019 , 52, 3254-3264	24.3	36
54	Applications of Laplacian spectrum for the vertexWertex graph. <i>Modern Physics Letters B</i> , 2019 , 33, 1950	O 118 / 4	1
53	Delineating Protein-Protein Curvilinear Dissociation Pathways and Energetics with NaWe Multiple-Walker Umbrella Sampling Simulations. <i>Journal of Computational Chemistry</i> , 2019 , 40, 1652-16	563 ⁵	6

52	Force Field Development and Nanoreactor Chemistry. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019 , 127-159	0.7	
51	Biological Membrane Organization and Cellular Signaling. <i>Chemical Reviews</i> , 2019 , 119, 5849-5880	68.1	59
50	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 1382-1397	6.1	3
49	Multiscale (re)modeling of lipid bilayer membranes. <i>Advances in Biomembranes and Lipid Self-Assembly</i> , 2019 , 30, 39-104	1	1
48	Approximating free energy and committor landscapes in standard transition path sampling using virtual interface exchange. <i>Journal of Chemical Physics</i> , 2019 , 151, 174111	3.9	8
47	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 837-856	6.4	20
46	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 813-836	6.4	27
45	Toward Achieving Efficient and Accurate Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 708-719	6.4	33
44	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1115-1127	6.4	8
43	Prediction of pKa in a system with high orthogonal barriers: Alchemical flying Gaussian method. <i>Chemical Physics Letters</i> , 2020 , 760, 138012	2.5	2
42	Accelerated Computation of Free Energy Profile at Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 3. Gaussian Smoothing on Density-of-States. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6814-6822	6.4	5
41	Scalable molecular dynamics on CPU and GPU architectures with NAMD. <i>Journal of Chemical Physics</i> , 2020 , 153, 044130	3.9	483
40	A fast and high-quality charge model for the next generation general AMBER force field. <i>Journal of Chemical Physics</i> , 2020 , 153, 114502	3.9	36
39	Entropy deepens loading chemical potentials of small alcohols by narrow carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 22369-22379	3.6	
38	Kinetic energy flows in activated dynamics of biomolecules. <i>Journal of Chemical Physics</i> , 2020 , 153, 094	11999	4
37	Structural Basis of the Potential Binding Mechanism of Remdesivir to SARS-CoV-2 RNA-Dependent RNA Polymerase. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 6955-6962	3.4	65
36	Conformational Free-Energy Differences of Large Solvated Systems with the Focused Confinement Method. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5163-5173	6.4	1
35	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. <i>ACS Omega</i> , 2020 , 5, 4611-4619	3.9	31

(2020-2020)

34	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of Evariations, Extrapolations, and Biasing. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1630-16	6 ⁶ 5 ⁴	12
33	Orientational dependence of the potential of mean force for a discotic liquid crystal near a substrate. <i>Molecular Physics</i> , 2020 , 118, e1748241	1.7	
32	AMOEBA binding free energies for the SAMPL7 TrimerTrip host-guest challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 79-93	4.2	8
31	Molecular dynamics: a powerful tool for studying the medicinal chemistry of ion channel modulators. <i>RSC Medicinal Chemistry</i> , 2021 , 12, 1503-1518	3.5	1
30	Binding of SARS-CoV-2/SARS-CoV spike protein with human ACE2 receptor. <i>Journal of Physics Communications</i> , 2021 , 5, 035010	1.2	4
29	Transition Path Sampling as Markov Chain Monte Carlo of Trajectories: Recent Algorithms, Software, Applications, and Future Outlook. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2000237	3.5	8
28	Overcoming Free-Energy Barriers with a Seamless Combination of a Biasing Force and a Collective Variable-Independent Boost Potential. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3886-389	94 ^{6.4}	1
27	Optimizing String Method@Reproducibility Using Generalized Solute Tempering Replica Exchange. Journal of Physical Chemistry B, 2021 , 125, 6609-6616	3.4	
26	Cyclosporin Structure and Permeability: From A to Z and Beyond. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 13131-13151	8.3	7
25	Strategies for the exploration of free energy landscapes: Unity in diversity and challenges ahead. <i>Reviews in Physics</i> , 2017 , 2, 32-45	11.3	73
24	Free Energy Calculation Methods of Biomolecules. Sheng Wu Wu Li Hsueh Bao, 2011, 27, 395-402		1
23	Sensitivity in binding free energies due to protein reorganization.		
22	OpenPathSampling: A Python framework for path sampling simulations. II. Building and customizing path ensembles and sample schemes.		
21	OpenPathSampling: A Python framework for path sampling simulations. I. Basics.		
20	Achieving Reversible Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE.		
20			
	through RAVE. Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional	6.4	1

16	Uncovering One-Dimensional Reaction Coordinate that Underlies Structure-Function Relationship of Proteins.		
15	A Rigorous Method for Identifying a One-Dimensional Reaction Coordinate in Complex Molecules <i>Journal of Chemical Theory and Computation</i> , 2022 ,	6.4	2
14	DataSheet1.PDF. 2018 ,		
13	A Computational Model for the PLP-Dependent Enzyme Methionine -Lyase <i>Frontiers in Molecular Biosciences</i> , 2022 , 9, 886358	5.6	
12	Drug Discovery by Automated Adaptation of Chemical Structure and Identity. <i>Journal of Chemical Theory and Computation</i> ,	6.4	
11	Engineering EmbdenMeyerhofParnas Glycolysis to Generate Noncanonical Reducing Power. <i>ACS Catalysis</i> , 2022 , 12, 8582-8592	13.1	1
10	Capabilities and limits of autoencoders for extracting collective variables in atomistic materials science. 2022 , 24, 23152-23163		0
9	Accurate pKa Calculations in Proteins with Reactive Molecular Dynamics Provide Physical Insight Into the Electrostatic Origins of Their Values. 2022 , 126, 7321-7330		1
8	Electrostatic Contributions to the Binding Free Energy of Nicotine to the Acetylcholine Binding Protein. 2022 , 126, 8669-8679		1
7	Enhancing sampling with free-energy calculations. 2022 , 77, 102497		O
6	A Comparison of Methods for Computing Relative Anhydrous Hydrate Stability with Molecular Simulation.		O
5	Free Energy Methods for the Description of Molecular Processes. 2023 , 52,		O
4	ACES: Optimized Alchemically Enhanced Sampling.		0
3	Anharmonic thermo-elasticity of tungsten from accelerated Bayesian adaptive biasing force calculations with data-driven force fields. 2023 , 7,		Ο
2	Alchemical Metadynamics: Adding Alchemical Variables to Metadynamics to Enhance Sampling in Free Energy Calculations. 2023 , 19, 1805-1817		0
1	Identifying and overcoming the sampling challenges in relative binding free energy calculations of a model protein:protein complex.		O