David E Shaw

List of Publications by Year
in descending order

129 papers	41,540 citations	8755 75 h-index	19749 117 g-index
138 all docs	138 docs citations	138 times ranked	39198 citing authors

#	Article	IF	Citations
1	Glide:Â A New Approach for Rapid, Accurate Docking and Scoring. 1. Method and Assessment of Docking Accuracy. Journal of Medicinal Chemistry, 2004, 47, 1739-1749.	6.4	7,428
2	Improved sideâ€chain torsion potentials for the Amber ff99SB protein force field. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1950-1958.	2.6	4,694
3	A hierarchical approach to all-atom protein loop prediction. Proteins: Structure, Function and Bioinformatics, 2004, 55, 351-367.	2.6	1,874
4	How Fast-Folding Proteins Fold. Science, 2011, 334, 517-520.	12.6	1,609
5	Atomic-Level Characterization of the Structural Dynamics of Proteins. Science, 2010, 330, 341-346.	12.6	1,583
6	Molecular dynamics---Scalable algorithms for molecular dynamics simulations on commodity clusters. , 2006, , .		1,113
7	Biomolecular Simulation: A Computational Microscope for Molecular Biology. Annual Review of Biophysics, 2012, 41, 429-452.	10.0	936
8	Structure and function of an irreversible agonist-Î²2 adrenoceptor complex. Nature, 2011, 469, 236-240.	27.8	741
9	Developing a molecular dynamics force field for both folded and disordered protein states. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4758-E4766.	7.1	738
10	Scalable Algorithms for Molecular Dynamics Simulations on Commodity Clusters. , 2006, , .		726
11	How Robust Are Protein Folding Simulations with Respect to Force Field Parameterization?. Biophysical Journal, 2011, 100, L47-L49.	0.5	725
12	The Dynamic Process of Î²2-Adrenergic Receptor Activation. Cell, 2013, 152, 532-542.	28.9	723
13	Structure and dynamics of the M3 muscarinic acetylcholine receptor. Nature, 2012, 482, 552-556.	27.8	714
14	Pathway and mechanism of drug binding to G-protein-coupled receptors. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13118-13123.	7.1	673
15	Long-timescale molecular dynamics simulations of protein structure and function. Current Opinion in Structural Biology, 2009, 19, 120-127.	5.7	671
16	Water Dispersion Interactions Strongly Influence Simulated Structural Properties of Disordered Protein States. Journal of Physical Chemistry B, 2015, 119, 5113-5123.	2.6	671
17	Systematic Validation of Protein Force Fields against Experimental Data. PLoS ONE, 2012, 7, e32131.	2.5	570
18	How Does a Drug Molecule Find Its Target Binding Site?. Journal of the American Chemical Society, 2011, 133, 9181-9183.	13.7	564

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19	Activation mechanism of theÎ²₂-adrenergic receptor. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18684-18689.	7.1	539
20	Mechanism of Voltage Gating in Potassium Channels. Science, 2012, 336, 229-233.	12.6	516
21	Assessing the accuracy of physical models used in protein-folding simulations: quantitative evidence from long molecular dynamics simulations. Current Opinion in Structural Biology, 2014, 24, 98-105.	5.7	424
22	Conformational Coupling across the Plasma Membrane in Activation of the EGF Receptor. Cell, 2013, 152, 543-556.	28.9	423
23	Architecture and Membrane Interactions of the EGF Receptor. Cell, 2013, 152, 557-569.	28.9	417
24	High-resolution crystal structure of human protease-activated receptor 1. Nature, 2012, 492, 387-392.	27.8	416
25	Anton 2: Raising the Bar for Performance and Programmability in a Special-Purpose Molecular Dynamics Supercomputer. , 2014, , .		369
26	Structural basis for modulation of a G-protein-coupled receptor by allosteric drugs. Nature, 2013, 503, 295-299.	27.8	365
27	Gaussian split Ewald: A fast Ewald mesh method for molecular simulation. Journal of Chemical Physics, 2005, 122, 054101.	3.0	351
28	Molecular determinants of drugâ€“receptor binding kinetics. Drug Discovery Today, 2013, 18, 667-673.	6.4	307
29	Oncogenic Mutations Counteract Intrinsic Disorder in the EGFR Kinase and Promote Receptor Dimerization. Cell, 2012, 149, 860-870.	28.9	304
30	Identification of two distinct inactive conformations of the Î² ₂ -adrenergic receptor reconciles structural and biochemical observations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4689-4694.	7.1	298
31	Principles of conduction and hydrophobic gating in K ⁺ channels. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5833-5838.	7.1	298
32	Atomic-level description of ubiquitin folding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5915-5920.	7.1	281
33	Structural analysis of the catalytically inactive kinase domain of the human EGF receptor 3. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 21608-21613.	7.1	278
34	Structure of Human Urokinase Plasminogen Activator in Complex with Its Receptor. Science, 2006, 311, 656-659.	12.6	273
35	Protein folding kinetics and thermodynamics from atomistic simulation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17845-17850.	7.1	262
36	Structural basis for nucleotide exchange in heterotrimeric G proteins. Science, 2015, 348, 1361-1365.	12.6	250

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37	A conserved protonation-dependent switch controls drug binding in the Abl kinase. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 139-144.	7.1	240
38	Millisecond-scale molecular dynamics simulations on Anton. , 2009, , .		238
39	The future of molecular dynamics simulations in drug discovery. Journal of Computer-Aided Molecular Design, 2012, 26, 15-26.	2.9	233
40	Preconfiguration of the antigen-binding site during affinity maturation of a broadly neutralizing influenza virus antibody. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 264-269.	7.1	227
41	Refinement of protein structure homology models via long, allâ€atom molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2071-2079.	2.6	226
42	Structure and Dynamics of an Unfolded Protein Examined by Molecular Dynamics Simulation. Journal of the American Chemical Society, 2012, 134, 3787-3791.	13.7	222
43	Superoxide dismutase 1 (SOD1) is essential for H ₂ O ₂ -mediated oxidation and inactivation of phosphatases in growth factor signaling. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7147-7152.	7.1	221
44	RNA force field with accuracy comparable to state-of-the-art protein force fields. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E1346-E1355.	7.1	214
45	Crystal structures of the JAK2 pseudokinase domain and the pathogenic mutant V617F. Nature Structural and Molecular Biology, 2012, 19, 754-759.	8.2	196
46	A fast, scalable method for the parallel evaluation of distance-limited pairwise particle interactions. Journal of Computational Chemistry, 2005, 26, 1318-1328.	3.3	189
47	Microsecond Molecular Dynamics Simulation Shows Effect of Slow Loop Dynamics on Backbone Amide Order Parameters of Proteinsâ€. Journal of Physical Chemistry B, 2008, 112, 6155-6158.	2.6	188
48	Transitions to catalytically inactive conformations in EGFR kinase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7270-7275.	7.1	186
49	Mechanism of NMDA receptor channel block by MK-801 and memantine. Nature, 2018, 556, 515-519.	27.8	177
50	A nonâ€“RGD-based integrin binding peptide (ATN-161) blocks breast cancer growth and metastasis in vivo. Molecular Cancer Therapeutics, 2006, 5, 2271-2280.	4.1	176
51	Structural origin of slow diffusion in protein folding. Science, 2015, 349, 1504-1510.	12.6	175
52	Exploring atomic resolution physiology on a femtosecond to millisecond timescale using molecular dynamics simulations. Journal of General Physiology, 2010, 135, 555-562.	1.9	168
53	Atomic-level characterization of proteinâ€“protein association. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4244-4249.	7.1	163
54	Accurate and efficient integration for molecular dynamics simulations at constant temperature and pressure. Journal of Chemical Physics, 2013, 139, 164106.	3.0	159

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55	The Role of Ligands on the Equilibria Between Functional States of a G Protein-Coupled Receptor. Journal of the American Chemical Society, 2013, 135, 9465-9474.	13.7	156
56	Structural insights into binding specificity, efficacy and bias of a Î²2AR partial agonist. Nature Chemical Biology, 2018, 14, 1059-1066.	8.0	155
57	EGFR oligomerization organizes kinase-active dimers into competent signalling platforms. Nature Communications, 2016, 7, 13307.	12.8	146
58	Mechanism of Na ⁺ /H ⁺ Antiporting. Science, 2007, 317, 799-803.	12.6	141
59	Equally Potent Inhibition of c-Src and Abl by Compounds that Recognize Inactive Kinase Conformations. Cancer Research, 2009, 69, 2384-2392.	0.9	134
60	Molecular basis for pseudokinase-dependent autoinhibition of JAK2 tyrosine kinase. Nature Structural and Molecular Biology, 2014, 21, 579-584.	8.2	132
61	Copper Binding by Tetrathiomolybdate Attenuates Angiogenesis and Tumor Cell Proliferation through the Inhibition of Superoxide Dismutase 1. Clinical Cancer Research, 2006, 12, 4974-4982.	7.0	131
62	Angiogenesis blockade as a new therapeutic approach to experimental colitis. Gut, 2007, 56, 855-862.	12.1	118
63	Quantitative Characterization of the Binding and Unbinding of Millimolar Drug Fragments with Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3372-3377.	5.3	115
64	Parallel random numbers. , 2011, , .		112
65	IRAK4 Dimerization and trans -Autophosphorylation Are Induced by Myddosome Assembly. Molecular Cell, 2014, 55, 891-903.	9.7	108
66	Computational Design and Experimental Testing of the Fastest-Folding Î²-Sheet Protein. Journal of Molecular Biology, 2011, 405, 43-48.	4.2	106
67	The midpoint method for parallelization of particle simulations. Journal of Chemical Physics, 2006, 124, 184109.	3.0	104
68	Regulation of RAS oncogenicity by acetylation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10843-10848.	7.1	104
69	Atomic structure of a toxic, oligomeric segment of SOD1 linked to amyotrophic lateral sclerosis (ALS). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8770-8775.	7.1	104
70	Development of a Force Field for the Simulation of Single-Chain Proteins and Proteinâ€“Protein Complexes. Journal of Chemical Theory and Computation, 2020, 16, 2494-2507.	5.3	104
71	Structural Basis of Interaction between Urokinase-type Plasminogen Activator and its Receptor. Journal of Molecular Biology, 2006, 363, 482-495.	4.2	103
72	Crystal structures of two human vitronectin, urokinase and urokinase receptor complexes. Nature Structural and Molecular Biology, 2008, 15, 422-423.	8.2	103

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73	A dynamically coupled allosteric network underlies binding cooperativity in Src kinase. Nature Communications, 2015, 6, 5939.	12.8	101
74	Atomic-level simulation of currentâ€“voltage relationships in single-file ion channels. Journal of General Physiology, 2013, 141, 619-632.	1.9	98
75	Structural analysis of the EGFR/HER3 heterodimer reveals the molecular basis for activating HER3 mutations. Science Signaling, 2014, 7, ra114.	3.6	98
76	A common, avoidable source of error in molecular dynamics integrators. Journal of Chemical Physics, 2007, 126, 046101.	3.0	95
77	Picosecond to Millisecond Structural Dynamics in Human Ubiquitin. Journal of Physical Chemistry B, 2016, 120, 8313-8320.	2.6	93
78	Evaluating the Effects of Cutoffs and Treatment of Long-range Electrostatics in Protein Folding Simulations. PLoS ONE, 2012, 7, e39918.	2.5	83
79	Pharmacology of the Novel Antiangiogenic Peptide ATN-161 (Ac-PHSCN-NH2): Observation of a U-Shaped Dose-Response Curve in Several Preclinical Models of Angiogenesis and Tumor Growth. Clinical Cancer Research, 2008, 14, 2137-2144.	7.0	82
80	Mechanism of Coupled Folding-upon-Binding of an Intrinsically Disordered Protein. Journal of the American Chemical Society, 2020, 142, 11092-11101.	13.7	81
81	Zonal methods for the parallel execution of range-limited N-body simulations. Journal of Computational Physics, 2007, 221, 303-329.	3.8	80
82	Demonstrating an Order-of-Magnitude Sampling Enhancement in Molecular Dynamics Simulations of Complex Protein Systems. Journal of Chemical Theory and Computation, 2016, 12, 1360-1367.	5.3	79
83	An Anti-Urokinase Plasminogen Activator Receptor Antibody (ATN-658) Blocks Prostate Cancer Invasion, Migration, Growth, and Experimental Skeletal Metastasis In Vitro and In Vivo. Neoplasia, 2010, 12, 778-788.	5.3	78
84	Interaction Networks in Protein Folding via Atomic-Resolution Experiments and Long-Time-Scale Molecular Dynamics Simulations. Journal of the American Chemical Society, 2015, 137, 6506-6516.	13.7	76
85	Structural basis for backtracking by the SARS-CoV-2 replicationâ€“transcription complex. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	76
86	Dynamic control of slow water transport by aquaporin 0: Implications for hydration and junction stability in the eye lens. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14430-14435.	7.1	74
87	Improving the accuracy of MÃ¸ller-Plesset perturbation theory with neural networks. Journal of Chemical Physics, 2017, 147, 161725.	3.0	74
88	Molecular Basis of Ligand Dissociation from the Adenosine A_{2A} Receptor. Molecular Pharmacology, 2016, 89, 485-491.	2.3	72
89	Structural Basis of AZD9291 Selectivity for EGFR T790M. Journal of Medicinal Chemistry, 2020, 63, 8502-8511.	6.4	71
90	Targeting the Urokinase Plasminogen Activator Receptor Inhibits Ovarian Cancer Metastasis. Clinical Cancer Research, 2011, 17, 459-471.	7.0	69

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91	Minimizing thermodynamic length to select intermediate states for free-energy calculations and replica-exchange simulations. Physical Review E, 2009, 80, 046705.	2.1	64
92	Her2 activation mechanism reflects evolutionary preservation of asymmetric ectodomain dimers in the human EGFR family. ELife, 2013, 2, e00708.	6.0	62
93	Anton 3. , 2021, , .		56
94	Fragment Hits: What do They Look Like and How do They Bind?. Journal of Medicinal Chemistry, 2019, 62, 3381-3394.	6.4	53
95	Peptides Derived from the Histidine-Proline Domain of the Histidine-Proline-Rich Glycoprotein Bind to Tropomyosin and Have Antiangiogenic and Antitumor Activities. Cancer Research, 2004, 64, 5812-5817.	0.9	51
96	Allosteric activation of apicomplexan calcium-dependent protein kinases. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E4975-84.	7.1	51
97	Structural mechanism for Brutonâ€™s tyrosine kinase activation at the cell membrane. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9390-9399.	7.1	49
98	Molecular Basis of Small-Molecule Binding to Î±-Synuclein. Journal of the American Chemical Society, 2022, 144, 2501-2510.	13.7	48
99	Atomistic Description of the Folding of a Dimeric Protein. Journal of Physical Chemistry B, 2013, 117, 12935-12942.	2.6	45
100	A Simple Model of Multivalent Adhesion and Its Application to Influenza Infection. Biophysical Journal, 2016, 110, 218-233.	0.5	45
101	The u-series: A separable decomposition for electrostatics computation with improved accuracy. Journal of Chemical Physics, 2020, 152, 084113.	3.0	45
102	A structural model of a Rasâ€“Raf signalosome. Nature Structural and Molecular Biology, 2021, 28, 847-857.	8.2	44
103	Equipartition and the Calculation of Temperature in Biomolecular Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2045-2058.	5.3	42
104	Membrane Interaction of Bound Ligands Contributes to the Negative Binding Cooperativity of the EGF Receptor. PLoS Computational Biology, 2014, 10, e1003742.	3.2	39
105	Ensemble cryo-EM reveals conformational states of the nsp13 helicase in the SARS-CoV-2 helicase replicationâ€“transcription complex. Nature Structural and Molecular Biology, 2022, 29, 250-260.	8.2	35
106	Key mutations stabilize antigenâ€binding conformation during affinity maturation of a broadly neutralizing influenza antibody lineage. Proteins: Structure, Function and Bioinformatics, 2015, 83, 771-780.	2.6	34
107	Quantum chemical benchmark databases of gold-standard dimer interaction energies. Scientific Data, 2021, 8, 55.	5.3	34
108	Exploiting Allosteric Properties of RAF and MEK Inhibitors to Target Therapy-Resistant Tumors Driven by Oncogenic BRAF Signaling. Cancer Discovery, 2021, 11, 1716-1735.	9.4	30

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109	Unifying on-chip and inter-node switching within the Anton 2 network. , 2014, , .		26
110	Assessment of the utility of contactâ€based restraints in accelerating the prediction of protein structure using molecular dynamics simulations. Protein Science, 2016, 25, 19-29.	7.6	26
111	Development of Force Field Parameters for the Simulation of Single- and Double-Stranded DNA Molecules and DNAâ€“Protein Complexes. Journal of Physical Chemistry B, 2022, 126, 4442-4457.	2.6	25
112	Identifying localized changes in large systems: Change-point detection for biomolecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7454-7459.	7.1	24
113	A Deep-Learning View of Chemical Space Designed to Facilitate Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 4487-4496.	5.4	24
114	Entry from the Lipid Bilayer: A Possible Pathway for Inhibition of a Peptide G Protein-Coupled Receptor by a Lipophilic Small Molecule. Biochemistry, 2018, 57, 5748-5758.	2.5	23
115	How does a small molecule bind at a cryptic binding site?. PLoS Computational Biology, 2022, 18, e1009817.	3.2	21
116	Computationally efficient molecular dynamics integrators with improved sampling accuracy. Molecular Physics, 2012, 110, 967-983.	1.7	20
117	Filtering, Reductions and Synchronization in the Anton 2 Network. , 2015, , .		20
118	AutoPH4: An Automated Method for Generating Pharmacophore Models from Protein Binding Pockets. Journal of Chemical Information and Modeling, 2020, 60, 4326-4338.	5.4	19
119	Structural basis for ALK2/BMPR2 receptor complex signaling through kinase domain oligomerization. Nature Communications, 2021, 12, 4950.	12.8	15
120	Anton: A Specialized Machine for Millisecond-Scale Molecular Dynamics Simulations of Proteins. , 2009, , .		13
121	Extending the Generality of Molecular Dynamics Simulations on a Special-Purpose Machine. , 2013, , .		13
122	Atomic-Level Description of Protein Folding inside the GroEL Cavity. Journal of Physical Chemistry B, 2018, 122, 11440-11449.	2.6	10
123	Targetable HER3 functions driving tumorigenic signaling in HER2-amplified cancers. Cell Reports, 2022, 38, 110291.	6.4	7
124	Overcoming Communication Latency Barriers in Massively Parallel Scientific Computation. IEEE Micro, 2011, 31, 8-19.	1.8	5
125	Tight Certification Techniques for Digit-by-Rounding Algorithms with Application to a New 1/sqrt(x) Design. , 2011, , .		3
126	Characterizing Receptor Flexibility to Predict Mutations That Lead to Human Adaptation of Influenza Hemagglutinin. Journal of Chemical Theory and Computation, 2022, 18, 4995-5005.	5.3	3

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127	Anton. , 2013, , .		2
128	Midtown splines: An optimal charge assignment for electrostatics calculations. Journal of Chemical Physics, 2020, 153, 224117.	3.0	1
129	Hardware support for fine-grained event-driven computation in Anton 2. Computer Architecture News, 2013, 41, 549-560.	2.5	0