Rommie E Amaro

List of Publications by Year
in descending order

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176 papers	9,392 citations	46984 47 h-index	54882 84 g-index
201 all docs	201 docs citations	201 times ranked	11766 citing authors

#	Article	IF	Citations
1	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734.	5.3	727
2	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
3	An improved relaxed complex scheme for receptor flexibility in computer-aided drug design. Journal of Computer-Aided Molecular Design, 2008, 22, 693-705.	1.3	283
4	A glycan gate controls opening of the SARS-CoV-2 spike protein. Nature Chemistry, 2021, 13, 963-968.	6.6	254
5	SARS-CoV-2 escape from a highly neutralizing COVID-19 convalescent plasma. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	251
6	Structural basis for targeted DNA cytosine deamination and mutagenesis by APOBEC3A and APOBEC3B. Nature Structural and Molecular Biology, 2017, 24, 131-139.	3.6	214
7	POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics. Journal of Chemical Theory and Computation, 2014, 10, 5047-5056.	2.3	203
8	Ensemble-Based Virtual Screening Reveals Potential Novel Antiviral Compounds for Avian Influenza Neuraminidase. Journal of Medicinal Chemistry, 2008, 51, 3878-3894.	2.9	195
9	Computational identification of a transiently open L1/S3 pocket for reactivation of mutant p53. Nature Communications, 2013, 4, 1407.	5.8	184
10	D3R grand challenge 2015: Evaluation of proteinâ€“ligand pose and affinity predictions. Journal of Computer-Aided Molecular Design, 2016, 30, 651-668.	1.3	178
11	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. Chemical Reviews, 2016, 116, 6370-6390.	23.0	176
12	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	2.5	174
13	POVME 3.0: Software for Mapping Binding Pocket Flexibility. Journal of Chemical Theory and Computation, 2017, 13, 4584-4592.	2.3	169
14	Remarkable Loop Flexibility in Avian Influenza N1 and Its Implications for Antiviral Drug Design. Journal of the American Chemical Society, 2007, 129, 7764-7765.	6.6	157
15	D3R Grand Challenge 2: blind prediction of proteinâ€“ligand poses, affinity rankings, and relative binding free energies. Journal of Computer-Aided Molecular Design, 2018, 32, 1-20.	1.3	156
16	Exploring Residue Component Contributions to Dynamical Network Models of Allostery. Journal of Chemical Theory and Computation, 2012, 8, 2949-2961.	2.3	152
17	Weighted Implementation of Suboptimal Paths (WISP): An Optimized Algorithm and Tool for Dynamical Network Analysis. Journal of Chemical Theory and Computation, 2014, 10, 511-517.	2.3	147
18	A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 1097-1104.	0.2	139

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19	Characterizing Loop Dynamics and Ligand Recognition in Human- and Avian-Type Influenza Neuraminidases via Generalized Born Molecular Dynamics and End-Point Free Energy Calculations. Journal of the American Chemical Society, 2009, 131, 4702-4709.	6.6	129
20	Mechanism of 150-cavity formation in influenza neuraminidase. Nature Communications, 2011, 2, 388.	5.8	129
21	Discovery of drug-like inhibitors of an essential RNA-editing ligase in Trypanosoma brucei. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 17278-17283.	3.3	128
22	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
23	Computational approaches to mapping allosteric pathways. Current Opinion in Structural Biology, 2014, 25, 98-103.	2.6	122
24	Multiscale methods in drug design bridge chemical and biological complexity in the search for cures. Nature Reviews Chemistry, 2018, 2, .	13.8	112
25	D3R Grand Challenge 3: blind prediction of proteinâ€“ligand poses and affinity rankings. Journal of Computer-Aided Molecular Design, 2019, 33, 1-18.	1.3	104
26	The flexibility of ACE2 in the context of SARS-CoV-2 infection. Biophysical Journal, 2021, 120, 1072-1084.	0.2	102
27	MM-PBSA Captures Key Role of Intercalating Water Molecules at a Proteinâ^'Protein Interface. Journal of Chemical Theory and Computation, 2009, 5, 422-429.	2.3	101
28	Emerging Methods for Ensemble-Based Virtual Screening. Current Topics in Medicinal Chemistry, 2010, 10, 3-13.	1.0	99
29	Novel Druggable Hot Spots in Avian Influenza Neuraminidase H5N1 Revealed by Computational Solvent Mapping of a Reduced and Representative Receptor Ensemble. Chemical Biology and Drug Design, 2008, 71, 106-116.	1.5	97
30	AutoGrow: A Novel Algorithm for Protein Inhibitor Design. Chemical Biology and Drug Design, 2009, 73, 168-178.	1.5	91
31	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	2.4	91
32	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. ACS Central Science, 2020, 6, 189-196.	5.3	86
33	Application of Molecular-Dynamics Based Markov State Models to Functional Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2648-2657.	2.3	85
34	SEEKR: Simulation Enabled Estimation of Kinetic Rates, A Computational Tool to Estimate Molecular Kinetics and Its Application to Trypsinâ€“Benzamidine Binding. Journal of Physical Chemistry B, 2017, 121, 3597-3606.	1.2	84
35	Structure and dynamics of SARS-CoV-2 proofreading exoribonuclease ExoN. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	83
36	Allostery through the computational microscope: cAMP activation of a canonical signalling domain. Nature Communications, 2015, 6, 7588.	5.8	81

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37	D3R grand challenge 4: blind prediction of proteinâ€“ligand poses, affinity rankings, and relative binding free energies. Journal of Computer-Aided Molecular Design, 2020, 34, 99-119.	1.3	81
38	The Local Dinucleotide Preference of APOBEC3G Can Be Altered from 5â€²-CC to 5â€²-TC by a Single Amino Acid Substitution. Journal of Molecular Biology, 2013, 425, 4442-4454.	2.0	80
39	Back to the Future: Can Physical Models of Passive Membrane Permeability Help Reduce Drug Candidate Attrition and Move Us Beyond QSPR?. Chemical Biology and Drug Design, 2013, 81, 61-71.	1.5	77
40	Distinct Glycan Topology for Avian and Human Sialopentasaccharide Receptor Analogues upon Binding Different Hemagglutinins: A Molecular Dynamics Perspective. Journal of Molecular Biology, 2009, 387, 465-491.	2.0	75
41	Human Influenza A Virus Hemagglutinin Glycan Evolution Follows a Temporal Pattern to a Glycan Limit. MBio, 2019, 10, .	1.8	74
42	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	1.5	72
43	Novel Naphthalene-Based Inhibitors of Trypanosoma brucei RNA Editing Ligase 1. PLoS Neglected Tropical Diseases, 2010, 4, e803.	1.3	64
44	Multiscale Estimation of Binding Kinetics Using Brownian Dynamics, Molecular Dynamics and Milestoning. PLoS Computational Biology, 2015, 11, e1004381.	1.5	62
45	LipidWrapper: An Algorithm for Generating Large-Scale Membrane Models of Arbitrary Geometry. PLoS Computational Biology, 2014, 10, e1003720.	1.5	60
46	A Community Letter Regarding Sharing Biomolecular Simulation Data for COVID-19. Journal of Chemical Information and Modeling, 2020, 60, 2653-2656.	2.5	57
47	Role of Secondary Sialic Acid Binding Sites in Influenza N1 Neuraminidase. Journal of the American Chemical Society, 2010, 132, 2883-2885.	6.6	55
48	Elucidation of Cryptic and Allosteric Pockets within the SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2021, 61, 3495-3501.	2.5	51
49	Developing an energy landscape for the novel function of a (Â/Â)8 barrel: Ammonia conduction through HisF. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7599-7604.	3.3	50
50	Impact of calcium on N1 influenza neuraminidase dynamics and binding free energy. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2523-2532.	1.5	49
51	Machineâ€Learning Techniques Applied to Antibacterial Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 14-21.	1.5	49
52	Computational Studies of the Effect of the S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics. Biophysical Journal, 2014, 107, 1675-1685.	0.2	48
53	Conserved patterns hidden within group A Streptococcus M protein hypervariability recognize human C4b-binding protein. Nature Microbiology, 2016, 1, 16155.	5.9	47
54	3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries. PLoS Computational Biology, 2020, 16, e1007756.	1.5	46

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55	Molecular dynamics simulations of substrate channeling through an Î±â€“Î² barrel protein. Chemical Physics, 2004, 307, 147-155.	0.9	45
56	An Integrated Markov State Model and Path Metadynamics Approach To Characterize Drug Binding Processes. Journal of Chemical Theory and Computation, 2019, 15, 5689-5702.	2.3	45
57	A Virtual Screening Approach For Identifying Plants with Anti H5N1 Neuraminidase Activity. Journal of Chemical Information and Modeling, 2015, 55, 308-316.	2.5	43
58	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. Biophysical Journal, 2021, 120, 983-993.	0.2	43
59	Structural Elements in IGP Synthase Exclude Water to Optimize Ammonia Transfer. Biophysical Journal, 2005, 89, 475-487.	0.2	42
60	Mechanism of Glycan Receptor Recognition and Specificity Switch for Avian, Swine, and Human Adapted Influenza Virus Hemagglutinins: A Molecular Dynamics Perspective. Journal of the American Chemical Society, 2009, 131, 17430-17442.	6.6	42
61	APOBEC3B Nuclear Localization Requires Two Distinct N-Terminal Domain Surfaces. Journal of Molecular Biology, 2018, 430, 2695-2708.	2.0	42
62	Molecular Simulations of Aromatase Reveal New Insights Into the Mechanism of Ligand Binding. Journal of Chemical Information and Modeling, 2013, 53, 2047-2056.	2.5	40
63	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. Structure, 2019, 27, 1326-1335.e4.	1.6	39
64	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. Scientific Reports, 2016, 6, 27806.	1.6	38
65	Two Relations to Estimate Membrane Permeability Using Milestoning. Journal of Physical Chemistry B, 2016, 120, 8606-8616.	1.2	38
66	Adapting AlphaLISA high throughput screen to discover a novel small-molecule inhibitor targeting protein arginine methyltransferase 5 in pancreatic and colorectal cancers. Oncotarget, 2017, 8, 39963-39977.	0.8	38
67	Predicting Ligand Binding Kinetics Using a Markovian Milestoning with Voronoi Tessellations Multiscale Approach. Journal of Chemical Theory and Computation, 2020, 16, 5348-5357.	2.3	37
68	Microsecond Molecular Dynamics Simulations of Influenza Neuraminidase Suggest a Mechanism for the Increased Virulence of Stalk-Deletion Mutants. Journal of Physical Chemistry B, 2016, 120, 8590-8599.	1.2	36
69	Sea Spray Aerosol: Where Marine Biology Meets Atmospheric Chemistry. ACS Central Science, 2018, 4, 1617-1623.	5.3	36
70	Quantitative Ranking of Ligand Binding Kinetics with a Multiscale Milestoning Simulation Approach. Journal of Physical Chemistry Letters, 2018, 9, 4941-4948.	2.1	35
71	Ensemble-Based Computational Approach Discriminates Functional Activity of p53 Cancer and Rescue Mutants. PLoS Computational Biology, 2011, 7, e1002238.	1.5	34
72	The Binding Interface between Human APOBEC3F and HIV-1 Vif Elucidated by Genetic and Computational Approaches. Cell Reports, 2015, 13, 1781-1788.	2.9	34

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73	Development of an AlphaLISA high throughput technique to screen for small molecule inhibitors targeting protein arginine methyltransferases. Molecular BioSystems, 2017, 13, 2509-2520.	2.9	32
74	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. Journal of Chemical Information and Modeling, 2015, 55, 1953-1961.	2.5	31
75	Incorporation of sensing modalities into de novo designed fluorescence-activating proteins. Nature Communications, 2021, 12, 856.	5.8	31
76	GlycoGrip: Cell Surface-Inspired Universal Sensor for Betacoronaviruses. ACS Central Science, 2022, 8, 22-42.	5.3	31
77	A 3-Dimensional Trimeric Î²-Barrel Model for Chlamydia MOMP Contains Conserved and Novel Elements of Gram-Negative Bacterial Porins. PLoS ONE, 2013, 8, e68934.	1.1	30
78	Multiscale simulation approaches to modeling drugâ€“protein binding. Current Opinion in Structural Biology, 2020, 61, 213-221.	2.6	29
79	Conformational Switch Regulates the DNA Cytosine Deaminase Activity of Human APOBEC3B. Scientific Reports, 2017, 7, 17415.	1.6	28
80	Disease-related mutations in PI3KÎ³ disrupt regulatory C-terminal dynamics and reveal a path to selective inhibitors. ELife, 2021, 10, .	2.8	28
81	A Kepler Workflow Tool for Reproducible AMBER GPU Molecular Dynamics. Biophysical Journal, 2017, 112, 2469-2474.	0.2	27
82	Computation-Guided Discovery of Influenza Endonuclease Inhibitors. ACS Medicinal Chemistry Letters, 2014, 5, 61-64.	1.3	26
83	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. ACS Chemical Biology, 2017, 12, 422-434.	1.6	26
84	Structural basis for ligand modulation of the CCR2 conformational landscape. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 8131-8136.	3.3	26
85	A Computational Assay that Explores the Hemagglutinin/Neuraminidase Functional Balance Reveals the Neuraminidase Secondary Site as a Novel Anti-Influenza Target. ACS Central Science, 2018, 4, 1570-1577.	5.3	25
86	Biomolecular Simulations in the Time of COVID-19, and After. Computing in Science and Engineering, 2020, 22, 30-36.	1.2	25
87	An Open-Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries. Biophysical Journal, 2020, 118, 1003-1008.	0.2	24
88	Rational Prediction with Molecular Dynamics for Hit Identification. Current Topics in Medicinal Chemistry, 2012, 12, 2002-2012.	1.0	23
89	Exascale Computing: A New Dawn for Computational Biology. Computing in Science and Engineering, 2018, 20, 18-25.	1.2	23
90	Markov state models and NMR uncover an overlooked allosteric loop in p53. Chemical Science, 2021, 12, 1891-1900.	3.7	22

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91	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	2.5	22
92	Derlin rhomboid pseudoproteases employ substrate engagement and lipid distortion to enable the retrotranslocation of ERAD membrane substrates. Cell Reports, 2021, 37, 109840.	2.9	22
93	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	13.8	22
94	Knowledge-Based Methods To Train and Optimize Virtual Screening Ensembles. Journal of Chemical Information and Modeling, 2016, 56, 830-842.	2.5	21
95	Insights into the behavior of nonanoic acid and its conjugate base at the air/water interface through a combined experimental and theoretical approach. Chemical Science, 2020, 11, 10647-10656.	3.7	21
96	Ranking of Ligand Binding Kinetics Using a Weighted Ensemble Approach and Comparison with a Multiscale Milestoning Approach. Journal of Chemical Information and Modeling, 2020, 60, 5340-5352.	2.5	21
97	An integrated view of p53 dynamics, function, and reactivation. Current Opinion in Structural Biology, 2021, 67, 187-194.	2.6	21
98	Bridging scales through multiscale modeling: a case study on protein kinase A. Frontiers in Physiology, 2015, 6, 250.	1.3	20
99	Enhancing Virtual Screening Performance of Protein Kinases with Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1923-1935.	2.5	20
100	Improving the Efficiency of Ligand-Binding Protein Design with Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 5703-5715.	2.3	20
101	Mechanisms for Benzene Dissociation through the Excited State of T4 Lysozyme L99A Mutant. Biophysical Journal, 2019, 116, 205-214.	0.2	20
102	Functional and Structural Insights Revealed by Molecular Dynamics Simulations of an Essential RNA Editing Ligase in Trypanosoma brucei. PLoS Neglected Tropical Diseases, 2007, 1, e68.	1.3	18
103	Capturing Invisible Motions in the Transition from Ground to Rare Excited States of T4 Lysozyme L99A. Biophysical Journal, 2016, 111, 1631-1640.	0.2	18
104	Molecular Docking to Flexible Targets. Methods in Molecular Biology, 2015, 1215, 445-469.	0.4	18
105	Structural Characterisation of Tpx from Yersinia pseudotuberculosis Reveals Insights into the Binding of Salicylidene Acylhydrazide Compounds. PLoS ONE, 2012, 7, e32217.	1.1	17
106	Molecular Dynamics Analysis of Antibody Recognition and Escape by Human H1N1 Influenza Hemagglutinin. Biophysical Journal, 2015, 108, 2704-2712.	0.2	17
107	Biochemical, Structural and Molecular Dynamics Analyses of the Potential Virulence Factor RipA from Yersinia pestis. PLoS ONE, 2011, 6, e25084.	1.1	16
108	Electrostatic Interactions as Mediators in the Allosteric Activation of Protein Kinase A RÎ±. Biochemistry, 2017, 56, 1536-1545.	1.2	16

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109	Protein Cofactors Are Essential for High-Affinity DNA Binding by the Nuclear Factor ÎºB RelA Subunit. Biochemistry, 2018, 57, 2943-2957.	1.2	16
110	SEEKR2: Versatile Multiscale Milestoning Utilizing the OpenMM Molecular Dynamics Engine. Journal of Chemical Information and Modeling, 2022, 62, 3253-3262.	2.5	16
111	Teachâ€“Discoverâ€“Treat (TDT): Collaborative computational drug discovery for neglected diseases. Journal of Molecular Graphics and Modelling, 2012, 38, 360-362.	1.3	15
112	RNA Editing TUTase 1: structural foundation of substrate recognition, complex interactions and drug targeting. Nucleic Acids Research, 2016, 44, 10862-10878.	6.5	15
113	ENRI: A tool for selecting structureâ€based virtual screening target conformations. Chemical Biology and Drug Design, 2017, 89, 762-771.	1.5	15
114	Development of Dimethylisoxazole-Attached Imidazo[1,2-a]pyridines as Potent and Selective CBP/P300 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 5787-5801.	2.9	15
115	Gaussian-Accelerated Molecular Dynamics with the Weighted Ensemble Method: A Hybrid Method Improves Thermodynamic and Kinetic Sampling. Journal of Chemical Theory and Computation, 2021, 17, 7938-7951.	2.3	15
116	The substrate-binding cap of the UDP-diacylglucosamine pyrophosphatase LpxH is highly flexible, enabling facile substrate binding and product release. Journal of Biological Chemistry, 2018, 293, 7969-7981.	1.6	14
117	Amino Acids Are Driven to the Interface by Salts and Acidic Environments. Journal of Physical Chemistry Letters, 2022, 13, 2824-2829.	2.1	14
118	Neolymphostin A Is a Covalent Phosphoinositide 3-Kinase (PI3K)/Mammalian Target of Rapamycin (mTOR) Dual Inhibitor That Employs an Unusual Electrophilic Vinylogous Ester. Journal of Medicinal Chemistry, 2018, 61, 10463-10472.	2.9	13
119	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. Biophysical Journal, 2020, 119, 2275-2289.	0.2	13
120	COVID19 - Computational Chemists Meet the Moment. Journal of Chemical Information and Modeling, 2020, 60, 5724-5726.	2.5	13
121	Computerâ€Aided Discovery of Trypanosoma brucei <scp>RNA</scp>â€Editing Terminal Uridylyl Transferase 2 Inhibitors. Chemical Biology and Drug Design, 2014, 84, 131-139.	1.5	11
122	A novel high-throughput activity assay for theTrypanosoma bruceieditosome enzyme REL1 and other RNA ligases. Nucleic Acids Research, 2016, 44, e24-e24.	6.5	11
123	Independent Markov decomposition: Toward modeling kinetics of biomolecular complexes. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
124	Discovery and design of DNA and RNA ligase inhibitors in infectious microorganisms. Expert Opinion on Drug Discovery, 2009, 4, 1281-1294.	2.5	10
125	Model of the Ankyrin and SOCS Box Protein, ASB9, E3 Ligase Reveals a Mechanism for Dynamic Ubiquitin Transfer. Structure, 2016, 24, 1248-1256.	1.6	10
126	Determinants of Oligonucleotide Selectivity of APOBEC3B. Journal of Chemical Information and Modeling, 2019, 59, 2264-2273.	2.5	10

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127	An Analysis of Proteochemometric and Conformal Prediction Machine Learning Protein-Ligand Binding Affinity Models. Frontiers in Molecular Biosciences, 2020, 7, 93.	1.6	10
128	Molecular Simulations Reveal an Unresolved Conformation of the Type IA Protein Kinase A Regulatory Subunit and Suggest Its Role in the cAMP Regulatory Mechanism. Biochemistry, 2017, 56, 3885-3888.	1.2	9
129	Active site plasticity and possible modes of chemical inhibition of the human DNA deaminase APOBEC3B. FASEB BioAdvances, 2020, 2, 49-58.	1.3	9
130	Elements of Nucleotide Specificity in the Trypanosoma brucei Mitochondrial RNA Editing Enzyme RET2. Journal of Chemical Information and Modeling, 2012, 52, 1308-1318.	2.5	8
131	Surfactant Charge Modulates Structure and Stability of Lipase-Embedded Monolayers at Marine-Relevant Aerosol Surfaces. Langmuir, 2019, 35, 9050-9060.	1.6	8
132	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. Frontiers in Molecular Biosciences, 2020, 7, 194.	1.6	8
133	RNA Metabolism Guided by RNA Modifications: The Role of SMUG1 in rRNA Quality Control. Biomolecules, 2021, 11, 76.	1.8	8
134	Calcium bridging drives polysaccharide co-adsorption to a proxy sea surface microlayer. Physical Chemistry Chemical Physics, 2021, 23, 16401-16416.	1.3	8
135	Biomedical Big Data Training Collaborative (BBDTC): An effort to bridge the talent gap in biomedical science and research. Journal of Computational Science, 2017, 20, 205-214.	1.5	7
136	Toward Understanding â€œthe Waysâ€•of Allosteric Drugs. ACS Central Science, 2017, 3, 925-926.	5.3	7
137	Progress towards Automated Kepler Scientific Workflows for Computer-aided Drug Discovery and Molecular Simulations. Procedia Computer Science, 2014, 29, 1745-1755.	1.2	6
138	A Reflection on Klaus Schulten. Journal of Chemical Theory and Computation, 2017, 13, 1-2.	2.3	6
139	Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2018, 58, 2175-2177.	2.5	6
140	Dynamics and Molecular Mechanisms of p53 Transcriptional Activation. Biochemistry, 2018, 57, 6528-6537.	1.2	6
141	Will the Real Cryptic Pocket Please Stand Out?. Biophysical Journal, 2019, 116, 753-754.	0.2	6
142	Cation-Driven Lipopolysaccharide Morphological Changes Impact Heterogeneous Reactions of Nitric Acid with Sea Spray Aerosol Particles. Journal of Physical Chemistry Letters, 2021, 12, 5023-5029.	2.1	6
143	The Implementation of the Colored Abstract Simplicial Complex and Its Application to Mesh Generation. ACM Transactions on Mathematical Software, 2019, 45, 1-20.	1.6	6
144	Examining the Effect of Charged Lipids on Mitochondrial Outer Membrane Dynamics Using Atomistic Simulations. Biomolecules, 2022, 12, 183.	1.8	6

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145	A Celebration of Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 1683-1692.	2.5	5
146	Impact of the Journal of Chemical Information and Modeling Special Issue on Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2020, 60, 3328-3330.	2.5	5
147	DelEnsembleElec: Computing Ensemble-Averaged Electrostatics Using DelPhi. Communications in Computational Physics, 2013, 13, 256-268.	0.7	5
148	Advancing Women in Chemistry. Journal of Chemical Information and Modeling, 2021, 61, 5305-5306.	2.5	5
149	Computational chemistry and drug discovery: a call to action. Future Medicinal Chemistry, 2012, 4, 1893-1896.	1.1	4
150	Drug Discovery Gets a Boost from Data Science. Structure, 2016, 24, 1225-1226.	1.6	4
151	Biomedical Big Data Training Collaborative (BBDTC): An Effort to Bridge the Talent Gap in Biomedical Science and Research. Procedia Computer Science, 2016, 80, 1791-1800.	1.2	4
152	Reliability assessment for large-scale molecular dynamics approximations. Journal of Chemical Physics, 2017, 147, 234106.	1.2	4
153	Molecular Docking of Broad-Spectrum Antibodies on Hemagglutinins of Influenza A Virus. Evolutionary Bioinformatics, 2019, 15, 117693431987693.	0.6	4
154	A demonstration of modularity, reuse, reproducibility, portability and scalability for modeling and simulation of cardiac electrophysiology using Kepler Workflows. PLoS Computational Biology, 2019, 15, e1006856.	1.5	4
155	OCRE Domains of Splicing Factors RBM5 and RBM10: Tyrosine Ringâ€Flip Frequencies Determined by Integrated Use of 1 H NMR Spectroscopy and Molecular Dynamics Simulations. ChemBioChem, 2021, 22, 565-570.	1.3	4
156	SEEKR: Simulation Enabled Estimation of Kinetic Rates, A Multiscale Approach for the Calculation of Protein-Ligand Association and Dissociation Kinetics. Biophysical Journal, 2018, 114, 42a.	0.2	2
157	Frontiers in CryoEM Modeling. Journal of Chemical Information and Modeling, 2019, 59, 3091-3093.	2.5	2
158	Structural Characterization of a Minimal Antibody against Human APOBEC3B. Viruses, 2021, 13, 663.	1.5	2
159	A Comparative Study of the Structural Dynamics of Four Terminal Uridylyl Transferases. Genes, 2017, 8, 166.	1.0	1
160	Influenza Viral Envelope Simulation Reveals Novel Druggable Pockets on Surface Glycoproteins. Biophysical Journal, 2018, 114, 341a.	0.2	1
161	Faces of Contemporary CryoEM Information and Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2407-2409.	2.5	1
162	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. BMC Bioinformatics, 2014, 15, 159.	1.2	0

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163	Tribute to J. Andrew McCammon. Journal of Physical Chemistry B, 2016, 120, 8055-8056.	1.2	0
164	Biography of Klaus Schulten. Journal of Physical Chemistry B, 2017, 121, 3206-3206.	1.2	0
165	Construing the Dynamic Complexity at a Plausible IKK2-Nemo Interface. Biophysical Journal, 2017, 112, 352a.	0.2	0
166	Investigating the Dynamics of Designed Ligand-Binding Proteins. Biophysical Journal, 2018, 114, 527a.	0.2	0
167	Drug Design Data Resource, Grand Challenge 4, second of two issues. Journal of Computer-Aided Molecular Design, 2020, 34, 97-97.	1.3	0
168	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. SSRN Electronic Journal, 0, , .	0.4	0
169	Developing inhibitors of the SARS-CoV-2 main protease. Biophysical Journal, 2022, 121, 192a.	0.2	0
170	Benchmarking ensemble docking methods in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2022, 36, 87-99.	1.3	0
171	Title is missing!. , 2020, 16, e1007756.		0
172	Title is missing!. , 2020, 16, e1007756.		0
173	Title is missing!. , 2020, 16, e1007756.		0
174	Title is missing!. , 2020, 16, e1007756.		0
175	Title is missing!. , 2020, 16, e1007756.		0
176	Title is missing!. , 2020, 16, e1007756.		0