Rommie E Amaro

List of Publications by Year
in descending order

176 papers	9,392 citations	47006 47 h-index	54911 84 g-index
201 all docs	201 docs citations	201 times ranked	11766 citing authors

#	Article	IF	Citations
1	Examining the Effect of Charged Lipids on Mitochondrial Outer Membrane Dynamics Using Atomistic Simulations. Biomolecules, 2022, 12, 183.	4.0	6
2	Developing inhibitors of the SARS-CoV-2 main protease. Biophysical Journal, 2022, 121, 192a.	0.5	0
3	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, .	7.1	83
4	Benchmarking ensemble docking methods in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2022, 36, 87-99.	2.9	0
5	Amino Acids Are Driven to the Interface by Salts and Acidic Environments. Journal of Physical Chemistry Letters, 2022, 13, 2824-2829.	4.6	14
6	GlycoGrip: Cell Surface-Inspired Universal Sensor for Betacoronaviruses. ACS Central Science, 2022, 8, 22-42.	11.3	31
7	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.	30.2	22
8	SEEKR2: Versatile Multiscale Milestoning Utilizing the OpenMM Molecular Dynamics Engine. Journal of Chemical Information and Modeling, 2022, 62, 3253-3262.	5.4	16
9	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.	2.6	4
10	The flexibility of ACE2 in the context of SARS-CoV-2 infection. Biophysical Journal, 2021, 120, 1072-1084.	0.5	102
11	A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 1097-1104.	0.5	139
12	RNA Metabolism Guided by RNA Modifications: The Role of SMUG1 in rRNA Quality Control. Biomolecules, 2021, 11, 76.	4.0	8
13	Calcium bridging drives polysaccharide co-adsorption to a proxy sea surface microlayer. Physical Chemistry Chemical Physics, 2021, 23, 16401-16416.	2.8	8
14	Markov state models and NMR uncover an overlooked allosteric loop in p53. Chemical Science, 2021, 12, 1891-1900.	7.4	22
15	Incorporation of sensing modalities into de novo designed fluorescence-activating proteins. Nature Communications, 2021, 12, 856.	12.8	31
16	Disease-related mutations in PI3KÎ³ disrupt regulatory C-terminal dynamics and reveal a path to selective inhibitors. ELife, 2021, 10, .	6.0	28
17	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. Biophysical Journal, 2021, 120, 983-993.	0.5	43
18	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	3.7	91

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19	Structural Characterization of a Minimal Antibody against Human APOBEC3B. Viruses, 2021, 13, 663.	3.3	2
20	Development of Dimethylisoxazole-Attached Imidazo[1,2-a]pyridines as Potent and Selective CBP/P300 Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 5787-5801.	6.4	15
21	An integrated view of p53 dynamics, function, and reactivation. Current Opinion in Structural Biology, 2021, 67, 187-194.	5.7	21
22	Elucidation of Cryptic and Allosteric Pockets within the SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2021, 61, 3495-3501.	5.4	51
23	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.	4.6	6
24	Independent Markov decomposition: Toward modeling kinetics of biomolecular complexes. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	11
25	A glycan gate controls opening of the SARS-CoV-2 spike protein. Nature Chemistry, 2021, 13, 963-968.	13.6	254
26	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, .	7.1	251
27	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
28	Derlin rhomboid pseudoproteases employ substrate engagement and lipid distortion to enable the retrotranslocation of ERAD membrane substrates. Cell Reports, 2021, 37, 109840.	6.4	22
29	Advancing Women in Chemistry. Journal of Chemical Information and Modeling, 2021, 61, 5305-5306.	5.4	5
30	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.	5.3	15
31	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. Frontiers in Molecular Biosciences, 2020, 7, 194.	3.5	8
32	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.	7.4	21
33	Biomolecular Simulations in the Time of COVID-19, and After. Computing in Science and Engineering, 2020, 22, 30-36.	1.2	25
34	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734.	11.3	727
35	An Analysis of Proteochemometric and Conformal Prediction Machine Learning Protein-Ligand Binding Affinity Models. Frontiers in Molecular Biosciences, 2020, 7, 93.	3.5	10
36	Predicting Ligand Binding Kinetics Using a Markovian Milestoning with Voronoi Tessellations Multiscale Approach. Journal of Chemical Theory and Computation, 2020, 16, 5348-5357.	5.3	37

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37	Faces of Contemporary CryoEM Information and Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2407-2409.	5.4	1
38	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.	5.4	5
39	An Open-Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries. Biophysical Journal, 2020, 118, 1003-1008.	0.5	24
40	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. ACS Central Science, 2020, 6, 189-196.	11.3	86
41	Active site plasticity and possible modes of chemical inhibition of the human DNA deaminase APOBEC3B. FASEB BioAdvances, 2020, 2, 49-58.	2.4	9
42	Multiscale simulation approaches to modeling drugâ€“protein binding. Current Opinion in Structural Biology, 2020, 61, 213-221.	5.7	29
43	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.	2.9	81
44	Drug Design Data Resource, Grand Challenge 4, second of two issues. Journal of Computer-Aided Molecular Design, 2020, 34, 97-97.	2.9	0
45	A Community Letter Regarding Sharing Biomolecular Simulation Data for COVID-19. Journal of Chemical Information and Modeling, 2020, 60, 2653-2656.	5.4	57
46	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.	5.4	21
47	3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries. PLoS Computational Biology, 2020, 16, e1007756.	3.2	46
48	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. Biophysical Journal, 2020, 119, 2275-2289.	0.5	13
49	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	5.4	22
50	COVID19 - Computational Chemists Meet the Moment. Journal of Chemical Information and Modeling, 2020, 60, 5724-5726.	5.4	13
51	Title is missing!. , 2020, 16, e1007756.		0
52	Title is missing!. , 2020, 16, e1007756.		0
53	Title is missing!. , 2020, 16, e1007756.		0
54	Title is missing!. , 2020, 16, e1007756.		0

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55	Title is missing!. , 2020, 16, e1007756.		0
56	Title is missing!. , 2020, 16, e1007756.		0
57	Determinants of Oligonucleotide Selectivity of APOBEC3B. Journal of Chemical Information and Modeling, 2019, 59, 2264-2273.	5.4	10
58	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. Structure, 2019, 27, 1326-1335.e4.	3.3	39
59	Improving the Efficiency of Ligand-Binding Protein Design with Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 5703-5715.	5.3	20
60	An Integrated Markov State Model and Path Metadynamics Approach To Characterize Drug Binding Processes. Journal of Chemical Theory and Computation, 2019, 15, 5689-5702.	5.3	45
61	Molecular Docking of Broad-Spectrum Antibodies on Hemagglutinins of Influenza A Virus. Evolutionary Bioinformatics, 2019, 15, 117693431987693.	1.2	4
62	Surfactant Charge Modulates Structure and Stability of Lipase-Embedded Monolayers at Marine-Relevant Aerosol Surfaces. Langmuir, 2019, 35, 9050-9060.	3.5	8
63	A Celebration of Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 1683-1692.	5.4	5
64	Frontiers in CryoEM Modeling. Journal of Chemical Information and Modeling, 2019, 59, 3091-3093.	5.4	2
65	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.	3.2	4
66	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.	7.1	26
67	Human Influenza A Virus Hemagglutinin Glycan Evolution Follows a Temporal Pattern to a Glycan Limit. MBio, 2019, 10, .	4.1	74
68	Will the Real Cryptic Pocket Please Stand Out?. Biophysical Journal, 2019, 116, 753-754.	0.5	6
69	D3R Grand Challenge 3: blind prediction of proteinâ€“ligand poses and affinity rankings. Journal of Computer-Aided Molecular Design, 2019, 33, 1-18.	2.9	104
70	Mechanisms for Benzene Dissociation through the Excited State of T4 Lysozyme L99A Mutant. Biophysical Journal, 2019, 116, 205-214.	0.5	20
71	The Implementation of the Colored Abstract Simplicial Complex and Its Application to Mesh Generation. ACM Transactions on Mathematical Software, 2019, 45, 1-20.	2.9	6
72	Multiscale methods in drug design bridge chemical and biological complexity in the search for cures. Nature Reviews Chemistry, 2018, 2, .	30.2	112

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73	Protein Cofactors Are Essential for High-Affinity DNA Binding by the Nuclear Factor ÎºB RelA Subunit. Biochemistry, 2018, 57, 2943-2957.	2.5	16
74	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.	3.4	14
75	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.5	318
76	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.	2.9	156
77	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.	11.3	25
78	Sea Spray Aerosol: Where Marine Biology Meets Atmospheric Chemistry. ACS Central Science, 2018, 4, 1617-1623.	11.3	36
79	Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2018, 58, 2175-2177.	5.4	6
80	Dynamics and Molecular Mechanisms of p53 Transcriptional Activation. Biochemistry, 2018, 57, 6528-6537.	2.5	6
81	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.	6.4	13
82	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.	0.5	2
83	Exascale Computing: A New Dawn for Computational Biology. Computing in Science and Engineering, 2018, 20, 18-25.	1.2	23
84	APOBEC3B Nuclear Localization Requires Two Distinct N-Terminal Domain Surfaces. Journal of Molecular Biology, 2018, 430, 2695-2708.	4.2	42
85	Influenza Viral Envelope Simulation Reveals Novel Druggable Pockets on Surface Glycoproteins. Biophysical Journal, 2018, 114, 341a.	0.5	1
86	Quantitative Ranking of Ligand Binding Kinetics with a Multiscale Milestoning Simulation Approach. Journal of Physical Chemistry Letters, 2018, 9, 4941-4948.	4.6	35
87	Investigating the Dynamics of Designed Ligand-Binding Proteins. Biophysical Journal, 2018, 114, 527a.	0.5	0
88	Electrostatic Interactions as Mediators in the Allosteric Activation of Protein Kinase A RIÎ±. Biochemistry, 2017, 56, 1536-1545.	2.5	16
89	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.	2.6	84
90	Biography of Klaus Schulten. Journal of Physical Chemistry B, 2017, 121, 3206-3206.	2.6	0

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91	A Kepler Workflow Tool for Reproducible AMBER GPU Molecular Dynamics. Biophysical Journal, 2017, 112, 2469-2474.	0.5	27
92	Construing the Dynamic Complexity at a Plausible IKK2-Nemo Interface. Biophysical Journal, 2017, 112, 352a.	0.5	0
93	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.	2.9	7
94	A Reflection on Klaus Schulten. Journal of Chemical Theory and Computation, 2017, 13, 1-2.	5.3	6
95	ENRI: A tool for selecting structureâ€based virtual screening target conformations. Chemical Biology and Drug Design, 2017, 89, 762-771.	3.2	15
96	Structural basis for targeted DNA cytosine deamination and mutagenesis by APOBEC3A and APOBEC3B. Nature Structural and Molecular Biology, 2017, 24, 131-139.	8.2	214
97	Rapid Chagas Disease Drug Target Discovery Using Directed Evolution in Drug-Sensitive Yeast. ACS Chemical Biology, 2017, 12, 422-434.	3.4	26
98	Toward Understanding â€œthe Waysâ€•of Allosteric Drugs. ACS Central Science, 2017, 3, 925-926.	11.3	7
99	POVME 3.0: Software for Mapping Binding Pocket Flexibility. Journal of Chemical Theory and Computation, 2017, 13, 4584-4592.	5.3	169
100	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
101	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.	2.5	9
102	Conformational Switch Regulates the DNA Cytosine Deaminase Activity of Human APOBEC3B. Scientific Reports, 2017, 7, 17415.	3.3	28
103	Reliability assessment for large-scale molecular dynamics approximations. Journal of Chemical Physics, 2017, 147, 234106.	3.0	4
104	A Comparative Study of the Structural Dynamics of Four Terminal Uridylyl Transferases. Genes, 2017, 8, 166.	2.4	1
105	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.	1.8	38
106	Model of the Ankyrin and SOCS Box Protein, ASB9, E3 Ligase Reveals a Mechanism for Dynamic Ubiquitin Transfer. Structure, 2016, 24, 1248-1256.	3.3	10
107	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
108	Emerging Computational Methods for the Rational Discovery of Allosteric Drugs. Chemical Reviews, 2016, 116, 6370-6390.	47.7	176

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109	Knowledge-Based Methods To Train and Optimize Virtual Screening Ensembles. Journal of Chemical Information and Modeling, 2016, 56, 830-842.	5.4	21
110	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.	2.6	36
111	D3R grand challenge 2015: Evaluation of proteinâ€“ligand pose and affinity predictions. Journal of Computer-Aided Molecular Design, 2016, 30, 651-668.	2.9	178
112	Enhancing Virtual Screening Performance of Protein Kinases with Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1923-1935.	5.4	20
113	Drug Discovery Gets a Boost from Data Science. Structure, 2016, 24, 1225-1226.	3.3	4
114	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.	2.0	4
115	Tribute to J. Andrew McCammon. Journal of Physical Chemistry B, 2016, 120, 8055-8056.	2.6	0
116	Comparative chemical genomics reveal that the spiroindolone antimalarial KAE609 (Cipargamin) is a P-type ATPase inhibitor. Scientific Reports, 2016, 6, 27806.	3.3	38
117	Conserved patterns hidden within group A Streptococcus M protein hypervariability recognize human C4b-binding protein. Nature Microbiology, 2016, 1, 16155.	13.3	47
118	RNA Editing TUTase 1: structural foundation of substrate recognition, complex interactions and drug targeting. Nucleic Acids Research, 2016, 44, 10862-10878.	14.5	15
119	Capturing Invisible Motions in the Transition from Ground to Rare Excited States of T4 Lysozyme L99A. Biophysical Journal, 2016, 111, 1631-1640.	0.5	18
120	Two Relations to Estimate Membrane Permeability Using Milestoning. Journal of Physical Chemistry B, 2016, 120, 8606-8616.	2.6	38
121	A novel high-throughput activity assay for theTrypanosoma bruceieditosome enzyme REL1 and other RNA ligases. Nucleic Acids Research, 2016, 44, e24-e24.	14.5	11
122	The Binding Interface between Human APOBEC3F and HIV-1 Vif Elucidated by Genetic and Computational Approaches. Cell Reports, 2015, 13, 1781-1788.	6.4	34
123	Machineâ€Learning Techniques Applied to Antibacterial Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 14-21.	3.2	49
124	Multiscale Estimation of Binding Kinetics Using Brownian Dynamics, Molecular Dynamics and Milestoning. PLoS Computational Biology, 2015, 11, e1004381.	3.2	62
125	Bridging scales through multiscale modeling: a case study on protein kinase A. Frontiers in Physiology, 2015, 6, 250.	2.8	20
126	Molecular Dynamics Analysis of Antibody Recognition and Escape by Human H1N1 Influenza Hemagglutinin. Biophysical Journal, 2015, 108, 2704-2712.	0.5	17

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127	A Virtual Screening Approach For Identifying Plants with Anti H5N1 Neuraminidase Activity. Journal of Chemical Information and Modeling, 2015, 55, 308-316.	5.4	43
128	Allostery through the computational microscope: cAMP activation of a canonical signalling domain. Nature Communications, 2015, 6, 7588.	12.8	81
129	Neural-Network Scoring Functions Identify Structurally Novel Estrogen-Receptor Ligands. Journal of Chemical Information and Modeling, 2015, 55, 1953-1961.	5.4	31
130	Molecular Docking to Flexible Targets. Methods in Molecular Biology, 2015, 1215, 445-469.	0.9	18
131	LipidWrapper: An Algorithm for Generating Large-Scale Membrane Models of Arbitrary Geometry. PLoS Computational Biology, 2014, 10, e1003720.	3.2	60
132	Computational approaches to mapping allosteric pathways. Current Opinion in Structural Biology, 2014, 25, 98-103.	5.7	122
133	Computation-Guided Discovery of Influenza Endonuclease Inhibitors. ACS Medicinal Chemistry Letters, 2014, 5, 61-64.	2.8	26
134	POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics. Journal of Chemical Theory and Computation, 2014, 10, 5047-5056.	5.3	203
135	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.	3.2	11
136	Computational Studies of the Effect of the S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics. Biophysical Journal, 2014, 107, 1675-1685.	0.5	48
137	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. BMC Bioinformatics, 2014, 15, 159.	2.6	0
138	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.	5.3	147
139	Progress towards Automated Kepler Scientific Workflows for Computer-aided Drug Discovery and Molecular Simulations. Procedia Computer Science, 2014, 29, 1745-1755.	2.0	6
140	Application of Molecular-Dynamics Based Markov State Models to Functional Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2648-2657.	5.3	85
141	Molecular Simulations of Aromatase Reveal New Insights Into the Mechanism of Ligand Binding. Journal of Chemical Information and Modeling, 2013, 53, 2047-2056.	5.4	40
142	Computational identification of a transiently open L1/S3 pocket for reactivation of mutant p53. Nature Communications, 2013, 4, 1407.	12.8	184
143	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.	4.2	80
144	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.	3.2	77

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145	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.	2.5	30
146	DelEnsembleElec: Computing Ensemble-Averaged Electrostatics Using DelPhi. Communications in Computational Physics, 2013, 13, 256-268.	1.7	5
147	Rational Prediction with Molecular Dynamics for Hit Identification. Current Topics in Medicinal Chemistry, 2012, 12, 2002-2012.	2.1	23
148	Exploring Residue Component Contributions to Dynamical Network Models of Allostery. Journal of Chemical Theory and Computation, 2012, 8, 2949-2961.	5.3	152
149	Elements of Nucleotide Specificity in the Trypanosoma brucei Mitochondrial RNA Editing Enzyme RET2. Journal of Chemical Information and Modeling, 2012, 52, 1308-1318.	5.4	8
150	Teachâ€“Discoverâ€“Treat (TDT): Collaborative computational drug discovery for neglected diseases. Journal of Molecular Graphics and Modelling, 2012, 38, 360-362.	2.4	15
151	Computational chemistry and drug discovery: a call to action. Future Medicinal Chemistry, 2012, 4, 1893-1896.	2.3	4
152	Structural Characterisation of Tpx from Yersinia pseudotuberculosis Reveals Insights into the Binding of Salicylidene Acylhydrazide Compounds. PLoS ONE, 2012, 7, e32217.	2.5	17
153	Mechanism of 150-cavity formation in influenza neuraminidase. Nature Communications, 2011, 2, 388.	12.8	129
154	Biochemical, Structural and Molecular Dynamics Analyses of the Potential Virulence Factor RipA from Yersinia pestis. PLoS ONE, 2011, 6, e25084.	2.5	16
155	Ensemble-Based Computational Approach Discriminates Functional Activity of p53 Cancer and Rescue Mutants. PLoS Computational Biology, 2011, 7, e1002238.	3.2	34
156	Emerging Methods for Ensemble-Based Virtual Screening. Current Topics in Medicinal Chemistry, 2010, 10, 3-13.	2.1	99
157	Impact of calcium on N1 influenza neuraminidase dynamics and binding free energy. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2523-2532.	2.6	49
158	A Multidimensional Strategy to Detect Polypharmacological Targets in the Absence of Structural and Sequence Homology. PLoS Computational Biology, 2010, 6, e1000648.	3.2	72
159	Novel Naphthalene-Based Inhibitors of Trypanosoma brucei RNA Editing Ligase 1. PLoS Neglected Tropical Diseases, 2010, 4, e803.	3.0	64
160	Role of Secondary Sialic Acid Binding Sites in Influenza N1 Neuraminidase. Journal of the American Chemical Society, 2010, 132, 2883-2885.	13.7	55
161	AutoGrow: A Novel Algorithm for Protein Inhibitor Design. Chemical Biology and Drug Design, 2009, 73, 168-178.	3.2	91
162	MM-PBSA Captures Key Role of Intercalating Water Molecules at a Proteinâ^'Protein Interface. Journal of Chemical Theory and Computation, 2009, 5, 422-429.	5.3	101

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163	Discovery and design of DNA and RNA ligase inhibitors in infectious microorganisms. Expert Opinion on Drug Discovery, 2009, 4, 1281-1294.	5.0	10
164	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.	13.7	42
165	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.	4.2	75
166	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.	13.7	129
167	An improved relaxed complex scheme for receptor flexibility in computer-aided drug design. Journal of Computer-Aided Molecular Design, 2008, 22, 693-705.	2.9	283
168	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.	3.2	97
169	Ensemble-Based Virtual Screening Reveals Potential Novel Antiviral Compounds for Avian Influenza Neuraminidase. Journal of Medicinal Chemistry, 2008, 51, 3878-3894.	6.4	195
170	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.	7.1	128
171	Remarkable Loop Flexibility in Avian Influenza N1 and Its Implications for Antiviral Drug Design. Journal of the American Chemical Society, 2007, 129, 7764-7765.	13.7	157
172	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.	3.0	18
173	Structural Elements in IGP Synthase Exclude Water to Optimize Ammonia Transfer. Biophysical Journal, 2005, 89, 475-487.	0.5	42
174	Molecular dynamics simulations of substrate channeling through an Î±â€“Î² barrel protein. Chemical Physics, 2004, 307, 147-155.	1.9	45
175	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.	7.1	50
176	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. SSRN Electronic Journal, 0, , .	0.4	0