List of Publications by Year in descending order

100 papers	7,354 citations	61945 43 h-index	66879 78 g-index
107 all docs	107 docs citations	107 times ranked	8105 citing authors

#	Article	IF	Citations
1	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	3.1	1,399
2	Omicron Variant (B.1.1.529): Infectivity, Vaccine Breakthrough, and Antibody Resistance. Journal of Chemical Information and Modeling, 2022, 62, 412-422.	2.5	507
3	Mutations Strengthened SARS-CoV-2 Infectivity. Journal of Molecular Biology, 2020, 432, 5212-5226.	2.0	386
4	TopologyNet: Topology based deep convolutional and multi-task neural networks for biomolecular property predictions. PLoS Computational Biology, 2017, 13, e1005690.	1.5	194
5	Persistent homology analysis of protein structure, flexibility, and folding. International Journal for Numerical Methods in Biomedical Engineering, 2014, 30, 814-844.	1.0	174
6	Representability of algebraic topology for biomolecules in machine learning based scoring and virtual screening. PLoS Computational Biology, 2018, 14, e1005929.	1.5	168
7	Mutations on COVID-19 diagnostic targets. Genomics, 2020, 112, 5204-5213.	1.3	164
8	Vaccine-escape and fast-growing mutations in the United Kingdom, the United States, Singapore, Spain, India, and other COVID-19-devastated countries. Genomics, 2021, 113, 2158-2170.	1.3	164
9	AGL-Score: Algebraic Graph Learning Score for Proteinâ€“Ligand Binding Scoring, Ranking, Docking, and Screening. Journal of Chemical Information and Modeling, 2019, 59, 3291-3304.	2.5	145
10	Treatment of charge singularities in implicit solvent models. Journal of Chemical Physics, 2007, 127, 114106.	1.2	128
11	MIBPB: A software package for electrostatic analysis. Journal of Computational Chemistry, 2011, 32, 756-770.	1.5	127
12	Analysis of SARS-CoV-2 mutations in the United States suggests presence of four substrains and novel variants. Communications Biology, 2021, 4, 228.	2.0	126
13	Poissonâ€“Boltzmannâ€“Nernstâ€“Planck model. Journal of Chemical Physics, 2011, 134, 194101.	1.2	124
14	Quantitative Toxicity Prediction Using Topology Based Multitask Deep Neural Networks. Journal of Chemical Information and Modeling, 2018, 58, 520-531.	2.5	116
15	Integration of element specific persistent homology and machine learning for proteinâ€ligand binding affinity prediction. International Journal for Numerical Methods in Biomedical Engineering, 2018, 34, e2914.	1.0	115
16	A topology-based network tree for the prediction of proteinâ€“protein binding affinity changes following mutation. Nature Machine Intelligence, 2020, 2, 116-123.	8.3	112
17	Mathematical deep learning for pose and binding affinity prediction and ranking in D3R Grand Challenges. Journal of Computer-Aided Molecular Design, 2019, 33, 71-82.	1.3	106
18	Variational Multiscale Models for Charge Transport. SIAM Review, 2012, 54, 699-754.	4.2	99

#	Article	IF	Citations
19	Differential Geometry Based Multiscale Models. Bulletin of Mathematical Biology, 2010, 72, 1562-1622.	0.9	95
20	Decoding SARS-CoV-2 Transmission and Evolution and Ramifications for COVID-19 Diagnosis, Vaccine, and Medicine. Journal of Chemical Information and Modeling, 2020, 60, 5853-5865.	2.5	91
21	Prediction and mitigation of mutation threats to COVID-19 vaccines and antibody therapies. Chemical Science, 2021, 12, 6929-6948.	3.7	85
22	Generative Network Complex for the Automated Generation of Drug-like Molecules. Journal of Chemical Information and Modeling, 2020, 60, 5682-5698.	2.5	79
23	Omicron BA.2 (B.1.1.529.2): High Potential for Becoming the Next Dominant Variant. Journal of Physical Chemistry Letters, 2022, 13, 3840-3849.	2.1	79
24	Rigidity Strengthening: A Mechanism for Proteinâ€“Ligand Binding. Journal of Chemical Information and Modeling, 2017, 57, 1715-1721.	2.5	78
25	Repositioning of 8565 Existing Drugs for COVID-19. Journal of Physical Chemistry Letters, 2020, 11, 5373-5382.	2.1	78
26	Are 2D fingerprints still valuable for drug discovery?. Physical Chemistry Chemical Physics, 2020, 22, 8373-8390.	1.3	77
27	Algebraic graph-assisted bidirectional transformers for molecular property prediction. Nature Communications, 2021, 12, 3521.	5.8	76
28	Mechanisms of SARS-CoV-2 Evolution Revealing Vaccine-Resistant Mutations in Europe and America. Journal of Physical Chemistry Letters, 2021, 12, 11850-11857.	2.1	73
29	TopPâ€“S: Persistent homologyâ€based multiâ€task deep neural networks for simultaneous predictions of partition coefficient and aqueous solubility. Journal of Computational Chemistry, 2018, 39, 1444-1454.	1.5	71
30	Multiscale multiphysics and multidomain modelsâ€”Flexibility and rigidity. Journal of Chemical Physics, 2013, 139, 194109.	1.2	68
31	Host Immune Response Driving SARS-CoV-2 Evolution. Viruses, 2020, 12, 1095.	1.5	68
32	Boosting Tree-Assisted Multitask Deep Learning for Small Scientific Datasets. Journal of Chemical Information and Modeling, 2020, 60, 1235-1244.	2.5	66
33	Perspectives on SARS-CoV-2 Main Protease Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 16922-16955.	2.9	63
34	Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 137 crystal structures using algebraic topology and deep learning. Chemical Science, 2020, 11, 12036-12046.	3.7	62
35	Decoding Asymptomatic COVID-19 Infection and Transmission. Journal of Physical Chemistry Letters, 2020, 11, 10007-10015.	2.1	61
36	Emerging Vaccine-Breakthrough SARS-CoV-2 Variants. ACS Infectious Diseases, 2022, 8, 546-556.	1.8	59

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37	UMAP-assisted K-means clustering of large-scale SARS-CoV-2 mutation datasets. Computers in Biology and Medicine, 2021, 131, 104264.	3.9	57
38	MathDL: mathematical deep learning for D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 131-147.	1.3	56
39	A review of mathematical representations of biomolecular data. Physical Chemistry Chemical Physics, 2020, 22, 4343-4367.	1.3	56
40	Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis. Journal of Chemical Physics, 2014, 140, 234105.	1.2	53
41	Revealing the Threat of Emerging SARS-CoV-2 Mutations to Antibody Therapies. Journal of Molecular Biology, 2021, 433, 167155.	2.0	53
42	DGâ€GL: Differential geometryâ€based geometric learning of molecular datasets. International Journal for Numerical Methods in Biomedical Engineering, 2019, 35, e3179.	1.0	52
43	Analysis and prediction of protein folding energy changes upon mutation by element specific persistent homology. Bioinformatics, 2017, 33, 3549-3557.	1.8	48
44	Persistent spectral graph. International Journal for Numerical Methods in Biomedical Engineering, 2020, 36, e3376.	1.0	47
45	GGL-Tox: Geometric Graph Learning for Toxicity Prediction. Journal of Chemical Information and Modeling, 2021, 61, 1691-1700.	2.5	43
46	A topological approach for protein classification. Computational and Mathematical Biophysics, 2015, 3, .	0.6	42
47	Methodology-Centered Review of Molecular Modeling, Simulation, and Prediction of SARS-CoV-2. Chemical Reviews, 2022, 122, 11287-11368.	23.0	38
48	Topological representations of crystalline compounds for the machine-learning prediction of materials properties. Npj Computational Materials, 2021, 7, .	3.5	36
49	MULTISCALE, MULTIPHYSICS AND MULTIDOMAIN MODELS I: BASIC THEORY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341006.	1.8	35
50	Object-oriented persistent homology. Journal of Computational Physics, 2016, 305, 276-299.	1.9	34
51	Review of COVID-19 Antibody Therapies. Annual Review of Biophysics, 2021, 50, 1-30.	4.5	34
52	Biomolecular surface construction by PDE transform. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 291-316.	1.0	32
53	Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM). Journal of Chemical Physics, 2015, 143, 204106.	1.2	32
54	Communication: Capturing protein multiscale thermal fluctuations. Journal of Chemical Physics, 2015, 142, 211101.	1.2	31

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55	MIB Galerkin method for elliptic interface problems. Journal of Computational and Applied Mathematics, 2014, 272, 195-220.	1.1	30
56	Cluster learning-assisted directed evolution. Nature Computational Science, 2021, 1, 809-818.	3.8	30
57	ESES: Software for <scp>E</scp>ulerian solvent excluded surface. Journal of Computational Chemistry, 2017, 38, 446-466.	1.5	29
58	Accurate, robust, and reliable calculations of Poissonâ€“Boltzmann binding energies. Journal of Computational Chemistry, 2017, 38, 941-948.	1.5	29
59	Multiscale weighted colored graphs for protein flexibility and rigidity analysis. Journal of Chemical Physics, 2018, 148, 054103.	1.2	29
60	Extracting Predictive Representations from Hundreds of Millions of Molecules. Journal of Physical Chemistry Letters, 2021, 12, 10793-10801.	2.1	28
61	Multiresolution persistent homology for excessively large biomolecular datasets. Journal of Chemical Physics, 2015, 143, 134103.	1.2	27
62	Generalized flexibility-rigidity index. Journal of Chemical Physics, 2016, 144, 234106.	1.2	27
63	Feature functional theoryâ€“binding predictor (FFTâ€“BP) for the blind prediction of binding free energies. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	27
64	Persistent topology for cryoâ€EM data analysis. International Journal for Numerical Methods in Biomedical Engineering, 2015, 31, .	1.0	26
65	Differential geometry based solvation model. III. Quantum formulation. Journal of Chemical Physics, 2011, 135, 194108.	1.2	25
66	Geometric modeling of subcellular structures, organelles, andâ€‰multiprotein complexes. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 1198-1223.	1.0	24
67	Multiscale geometric modeling of macromolecules I: Cartesian representation. Journal of Computational Physics, 2014, 257, 912-936.	1.9	24
68	Multiresolution Topological Simplification. Journal of Computational Biology, 2015, 22, 887-891.	0.8	24
69	Breaking the polarâ€nonpolar division in solvation free energy prediction. Journal of Computational Chemistry, 2018, 39, 217-233.	1.5	24
70	Protein pocket detection via convex hull surface evolution and associated Reeb graph. Bioinformatics, 2018, 34, i830-i837.	1.8	23
71	Multiscale geometric modeling of macromolecules II: Lagrangian representation. Journal of Computational Chemistry, 2013, 34, 2100-2120.	1.5	22
72	Quantum dynamics in continuum for proton transport II: Variational solventâ€“solute interface. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 25-51.	1.0	21

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73	Parameterization of a geometric flow implicit solvation model. Journal of Computational Chemistry, 2013, 34, 687-695.	1.5	21
74	Quantum dynamics in continuum for proton transportâ€"Generalized correlation. Journal of Chemical Physics, 2012, 136, 134109.	1.2	20
75	Evolutionary de Rham-Hodge method. Discrete and Continuous Dynamical Systems - Series B, 2021, 26, 3785.	0.5	20
76	Partial differential equation transformâ€"Variational formulation and Fourier analysis. International Journal for Numerical Methods in Biomedical Engineering, 2011, 27, 1996-2020.	1.0	19
77	Automatic parametrization of non-polar implicit solvent models for the blind prediction of solvation free energies. Journal of Chemical Physics, 2016, 145, 124110.	1.2	18
78	Blind prediction of protein B-factor and flexibility. Journal of Chemical Physics, 2018, 149, 134107.	1.2	17
79	HERMES: Persistent spectral graph software. , 2021, 3, 67.		16
80	Flexibilityâ€"rigidity index for proteinâ€"nucleic acid flexibility and fluctuation analysis. Journal of Computational Chemistry, 2016, 37, 1283-1295.	1.5	15
81	Generative network complex (GNC) for drug discovery. Communications in Information and Systems, 2019, 19, 241-277.	0.3	14
82	Quantum Dynamics in Continuum for Proton Transport I: Basic Formulation. Communications in Computational Physics, 2013, 13, 285-324.	0.7	13
83	The de Rhamâ€"Hodge Analysis and Modeling of Biomolecules. Bulletin of Mathematical Biology, 2020, 82, 108.	0.9	11
84	Persistent Cohomology for Data With Multicomponent Heterogeneous Information. SIAM Journal on Mathematics of Data Science, 2020, 2, 396-418.	1.0	10
85	Aspects of topological approaches for data science. , 2022, 4, 165.		10
86	The impact of surface area, volume, curvature, and Lennardâ€"Jones potential to solvation modeling. Journal of Computational Chemistry, 2017, 38, 24-36.	1.5	9
87	Generative Models for Molecular Design. Journal of Chemical Information and Modeling, 2020, 60, 5635-5636.	2.5	9
88	Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. Journal of Chemical Physics, 2013, 139, 204108.	1.2	8
89	Proteome-Informed Machine Learning Studies of Cocaine Addiction. Journal of Physical Chemistry Letters, 2021, 12, 11122-11134.	2.1	8
90	MLIMC: Machine learning-based implicit-solvent Monte Carlo. Chinese Journal of Chemical Physics, 2021, 34, 683-694.	0.6	8

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91	Machine Learning Analysis of Cocaine Addiction Informed by DAT, SERT, and NET-Based Interactome Networks. Journal of Chemical Theory and Computation, 2022, 18, 2703-2719.	2.3	8
92	Geometric and electrostatic modeling using molecular rigidity functions. Journal of Computational and Applied Mathematics, 2017, 313, 18-37.	1.1	6
93	Evolutionary homology on coupled dynamical systems with applications to protein flexibility analysis. Journal of Applied and Computational Topology, 2020, 4, 481-507.	1.0	6
94	Atom-specific persistent homology and its application to protein flexibility analysis. Computational and Mathematical Biophysics, 2020, 8, 1-35.	0.6	6
95	A Review of Mathematical Modeling, Simulation and Analysis of Membrane Channel Charge Transport â˜†. , 2017, , .		3
96	Mathematics at the eve of a historic transition in biology. Computational and Mathematical Biophysics, 2017, 5, 138-141.	0.6	3
97	Review of quantitative systems pharmacological modeling in thrombosis. Communications in Information and Systems, 2019, 19, 219-240.	0.3	3
98	AweGNN: Auto-parametrized weighted element-specific graph neural networks for molecules. Computers in Biology and Medicine, 2021, 134, 104460.	3.9	2
99	Divide-and-conquer strategy for large-scale Eulerian solvent excluded surface. Communications in Information and Systems, 2018, 18, 299-329.	0.3	2
100	Geometric algebra generation of molecular surfaces. Journal of the Royal Society Interface, 2022, 19, 20220117.	1.5	1