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	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
2	Emerging Vaccine-Breakthrough SARS-CoV-2 Variants. ACS Infectious Diseases, 2022, 8, 546-556.	1.8	59
3	Aspects of topological approaches for data science. , 2022, 4, 165.		10
4	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
5	Geometric algebra generation of molecular surfaces. Journal of the Royal Society Interface, 2022, 19, 20220117.	1.5	1
6	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
7	Methodology-Centered Review of Molecular Modeling, Simulation, and Prediction of SARS-CoV-2. Chemical Reviews, 2022, 122, 11287-11368.	23.0	38
8	Review of COVID-19 Antibody Therapies. Annual Review of Biophysics, 2021, 50, 1-30.	4.5	34
9	Evolutionary de Rham-Hodge method. Discrete and Continuous Dynamical Systems - Series B, 2021, 26, 3785.	0.5	20
10	Prediction and mitigation of mutation threats to COVID-19 vaccines and antibody therapies. Chemical Science, 2021, 12, 6929-6948.	3.7	85
11	HERMES: Persistent spectral graph software. , 2021, 3, 67.		16
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	Topological representations of crystalline compounds for the machine-learning prediction of materials properties. Npj Computational Materials, 2021, 7, .	3.5	36
14	GGL-Tox: Geometric Graph Learning for Toxicity Prediction. Journal of Chemical Information and Modeling, 2021, 61, 1691-1700.	2.5	43
15	UMAP-assisted K-means clustering of large-scale SARS-CoV-2 mutation datasets. Computers in Biology and Medicine, 2021, 131, 104264.	3.9	57
16	Algebraic graph-assisted bidirectional transformers for molecular property prediction. Nature Communications, 2021, 12, 3521.	5.8	76
17	AweGNN: Auto-parametrized weighted element-specific graph neural networks for molecules. Computers in Biology and Medicine, 2021, 134, 104460.	3.9	2
18	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

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19	Revealing the Threat of Emerging SARS-CoV-2 Mutations to Antibody Therapies. Journal of Molecular Biology, 2021, 433, 167155.	2.0	53
20	Extracting Predictive Representations from Hundreds of Millions of Molecules. Journal of Physical Chemistry Letters, 2021, 12, 10793-10801.	2.1	28
21	Proteome-Informed Machine Learning Studies of Cocaine Addiction. Journal of Physical Chemistry Letters, 2021, 12, 11122-11134.	2.1	8
22	Perspectives on SARS-CoV-2 Main Protease Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 16922-16955.	2.9	63
23	MLIMC: Machine learning-based implicit-solvent Monte Carlo. Chinese Journal of Chemical Physics, 2021, 34, 683-694.	0.6	8
24	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
25	Cluster learning-assisted directed evolution. Nature Computational Science, 2021, 1, 809-818.	3.8	30
26	MathDL: mathematical deep learning for D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 131-147.	1.3	56
27	Host Immune Response Driving SARS-CoV-2 Evolution. Viruses, 2020, 12, 1095.	1.5	68
28	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
29	Generative Network Complex for the Automated Generation of Drug-like Molecules. Journal of Chemical Information and Modeling, 2020, 60, 5682-5698.	2.5	79
30	Persistent spectral graph. International Journal for Numerical Methods in Biomedical Engineering, 2020, 36, e3376.	1.0	47
31	Decoding Asymptomatic COVID-19 Infection and Transmission. Journal of Physical Chemistry Letters, 2020, 11, 10007-10015.	2.1	61
32	The de Rhamâ€“Hodge Analysis and Modeling of Biomolecules. Bulletin of Mathematical Biology, 2020, 82, 108.	0.9	11
33	Mutations Strengthened SARS-CoV-2 Infectivity. Journal of Molecular Biology, 2020, 432, 5212-5226.	2.0	386
34	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
35	Mutations on COVID-19 diagnostic targets. Genomics, 2020, 112, 5204-5213.	1.3	164
36	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

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37	Repositioning of 8565 Existing Drugs for COVID-19. Journal of Physical Chemistry Letters, 2020, 11, 5373-5382.	2.1	78
38	A review of mathematical representations of biomolecular data. Physical Chemistry Chemical Physics, 2020, 22, 4343-4367.	1.3	56
39	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
40	Boosting Tree-Assisted Multitask Deep Learning for Small Scientific Datasets. Journal of Chemical Information and Modeling, 2020, 60, 1235-1244.	2.5	66
41	Are 2D fingerprints still valuable for drug discovery?. Physical Chemistry Chemical Physics, 2020, 22, 8373-8390.	1.3	77
42	Generative Models for Molecular Design. Journal of Chemical Information and Modeling, 2020, 60, 5635-5636.	2.5	9
43	Persistent Cohomology for Data With Multicomponent Heterogeneous Information. SIAM Journal on Mathematics of Data Science, 2020, 2, 396-418.	1.0	10
44	Atom-specific persistent homology and its application to protein flexibility analysis. Computational and Mathematical Biophysics, 2020, 8, 1-35.	0.6	6
45	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
46	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
47	DGâ€GL: Differential geometryâ€based geometric learning of molecular datasets. International Journal for Numerical Methods in Biomedical Engineering, 2019, 35, e3179.	1.0	52
48	Generative network complex (GNC) for drug discovery. Communications in Information and Systems, 2019, 19, 241-277.	0.3	14
49	Review of quantitative systems pharmacological modeling in thrombosis. Communications in Information and Systems, 2019, 19, 219-240.	0.3	3
50	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
51	Multiscale weighted colored graphs for protein flexibility and rigidity analysis. Journal of Chemical Physics, 2018, 148, 054103.	1.2	29
52	Quantitative Toxicity Prediction Using Topology Based Multitask Deep Neural Networks. Journal of Chemical Information and Modeling, 2018, 58, 520-531.	2.5	116
53	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
54	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	3.1	1,399

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55	Breaking the polarâ€nonpolar division in solvation free energy prediction. Journal of Computational Chemistry, 2018, 39, 217-233.	1.5	24
56	Blind prediction of protein B-factor and flexibility. Journal of Chemical Physics, 2018, 149, 134107.	1.2	17
57	Protein pocket detection via convex hull surface evolution and associated Reeb graph. Bioinformatics, 2018, 34, i830-i837.	1.8	23
58	Representability of algebraic topology for biomolecules in machine learning based scoring and virtual screening. PLoS Computational Biology, 2018, 14, e1005929.	1.5	168
59	Divide-and-conquer strategy for large-scale Eulerian solvent excluded surface. Communications in Information and Systems, 2018, 18, 299-329.	0.3	2
60	ESES: Software for <scp>E</scp>ulerian solvent excluded surface. Journal of Computational Chemistry, 2017, 38, 446-466.	1.5	29
61	Accurate, robust, and reliable calculations of Poissonâ€“Boltzmann binding energies. Journal of Computational Chemistry, 2017, 38, 941-948.	1.5	29
62	Feature functional theoryâ€“binding predictor (FFTâ€“BP) for the blind prediction of binding free energies. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	27
63	Analysis and prediction of protein folding energy changes upon mutation by element specific persistent homology. Bioinformatics, 2017, 33, 3549-3557.	1.8	48
64	Rigidity Strengthening: A Mechanism for Proteinâ€“Ligand Binding. Journal of Chemical Information and Modeling, 2017, 57, 1715-1721.	2.5	78
65	Geometric and electrostatic modeling using molecular rigidity functions. Journal of Computational and Applied Mathematics, 2017, 313, 18-37.	1.1	6
66	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
67	A Review of Mathematical Modeling, Simulation and Analysis of Membrane Channel Charge Transport â˜†. , 2017, , .		3
68	TopologyNet: Topology based deep convolutional and multi-task neural networks for biomolecular property predictions. PLoS Computational Biology, 2017, 13, e1005690.	1.5	194
69	Mathematics at the eve of a historic transition in biology. Computational and Mathematical Biophysics, 2017, 5, 138-141.	0.6	3
70	Flexibilityâ€“rigidity index for proteinâ€“nucleic acid flexibility and fluctuation analysis. Journal of Computational Chemistry, 2016, 37, 1283-1295.	1.5	15
71	Generalized flexibility-rigidity index. Journal of Chemical Physics, 2016, 144, 234106.	1.2	27
72	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

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73	Object-oriented persistent homology. Journal of Computational Physics, 2016, 305, 276-299.	1.9	34
74	Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM). Journal of Chemical Physics, 2015, 143, 204106.	1.2	32
75	Multiresolution persistent homology for excessively large biomolecular datasets. Journal of Chemical Physics, 2015, 143, 134103.	1.2	27
76	Persistent topology for cryoâ€EM data analysis. International Journal for Numerical Methods in Biomedical Engineering, 2015, 31, .	1.0	26
77	A topological approach for protein classification. Computational and Mathematical Biophysics, 2015, 3, .	0.6	42
78	Multiresolution Topological Simplification. Journal of Computational Biology, 2015, 22, 887-891.	0.8	24
79	Communication: Capturing protein multiscale thermal fluctuations. Journal of Chemical Physics, 2015, 142, 211101.	1.2	31
80	Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis. Journal of Chemical Physics, 2014, 140, 234105.	1.2	53
81	Persistent homology analysis of protein structure, flexibility, and folding. International Journal for Numerical Methods in Biomedical Engineering, 2014, 30, 814-844.	1.0	174
82	MIB Galerkin method for elliptic interface problems. Journal of Computational and Applied Mathematics, 2014, 272, 195-220.	1.1	30
83	Multiscale geometric modeling of macromolecules I: Cartesian representation. Journal of Computational Physics, 2014, 257, 912-936.	1.9	24
84	Multiscale geometric modeling of macromolecules II: Lagrangian representation. Journal of Computational Chemistry, 2013, 34, 2100-2120.	1.5	22
85	Parameterization of a geometric flow implicit solvation model. Journal of Computational Chemistry, 2013, 34, 687-695.	1.5	21
86	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
87	Multiscale multiphysics and multidomain modelsâ€”Flexibility and rigidity. Journal of Chemical Physics, 2013, 139, 194109.	1.2	68
88	MULTISCALE, MULTIPHYSICS AND MULTIDOMAIN MODELS I: BASIC THEORY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341006.	1.8	35
89	Quantum Dynamics in Continuum for Proton Transport I: Basic Formulation. Communications in Computational Physics, 2013, 13, 285-324.	0.7	13
90	Variational Multiscale Models for Charge Transport. SIAM Review, 2012, 54, 699-754.	4.2	99

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91	Geometric modeling of subcellular structures, organelles, andâ€‰multiprotein complexes. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 1198-1223.	1.0	24
92	Quantum dynamics in continuum for proton transportâ€”Generalized correlation. Journal of Chemical Physics, 2012, 136, 134109.	1.2	20
93	Biomolecular surface construction by PDE transform. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 291-316.	1.0	32
94	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
95	Poissonâ€“Boltzmannâ€“Nernstâ€“Planck model. Journal of Chemical Physics, 2011, 134, 194101.	1.2	124
96	Partial differential equation transformâ€”Variational formulation and Fourier analysis. International Journal for Numerical Methods in Biomedical Engineering, 2011, 27, 1996-2020.	1.0	19
97	MIBPB: A software package for electrostatic analysis. Journal of Computational Chemistry, 2011, 32, 756-770.	1.5	127
98	Differential geometry based solvation model. III. Quantum formulation. Journal of Chemical Physics, 2011, 135, 194108.	1.2	25
99	Differential Geometry Based Multiscale Models. Bulletin of Mathematical Biology, 2010, 72, 1562-1622.	0.9	95
100	Treatment of charge singularities in implicit solvent models. Journal of Chemical Physics, 2007, 127, 114106.	1.2	128