Kelin Xia

List of Publications by Year
in descending order

71 papers	1,553 citations	304743 22 h-index	345221 36 g-index
74 all docs	74 docs citations	74 times ranked	780 citing authors

#	Article	IF	Citations
1	Molecular persistent spectral image (Mol-PSI) representation for machine learning models in drug design. Briefings in Bioinformatics, 2022, 23, .	6.5	12
2	Flexibility and rigidity index for chromosome packing, flexibility and dynamics analysis. Frontiers of Computer Science, 2022, 16, 1.	2.4	1
3	Persistent spectral based ensemble learning (PerSpect-EL) for proteinâ€“protein binding affinity prediction. Briefings in Bioinformatics, 2022, 23, .	6.5	21
4	Aspects of topological approaches for data science. , 2022, 4, 165.		10
5	Persistent-homology-based machine learning: a survey and a comparative study. Artificial Intelligence Review, 2022, 55, 5169-5213.	15.7	23
6	Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction. PLoS Computational Biology, 2022, 18, e1009943.	3.2	14
7	Persistent spectral simplicial complex-based machine learning for chromosomal structural analysis in cellular differentiation. Briefings in Bioinformatics, 2022, 23, .	6.5	4
8	Hodge theory-based biomolecular data analysis. Scientific Reports, 2022, 12, .	3.3	2
9	Hypergraph-based persistent cohomology (HPC) for molecular representations in drug design. Briefings in Bioinformatics, 2021, 22, .	6.5	22
10	Fast random algorithms for manifold based optimization in reconstructing 3D chromosomal structures. Communications in Information and Systems, 2021, 21, 1-29.	0.5	1
11	Ollivier Persistent Ricci Curvature-Based Machine Learning for the Proteinâ€“Ligand Binding Affinity Prediction. Journal of Chemical Information and Modeling, 2021, 61, 1617-1626.	5.4	29
12	Persistent spectral hypergraph based machine learning (PSH-ML) for protein-ligand binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	26
13	Forman persistent Ricci curvature (FPRC)-based machine learning models for proteinâ€“ligand binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	32
14	Persistent spectralâ€“based machine learning (PerSpect ML) for protein-ligand binding affinity prediction. Science Advances, 2021, 7, .	10.3	89
15	Predicting Chromosome Flexibility from the Genomic Sequence Based on Deep Learning Neural Networks. Current Bioinformatics, 2021, 16, 1311-1319.	1.5	5
16	Understanding Changes in the Topology and Geometry of Financial Market Correlations during a Market Crash. Entropy, 2021, 23, 1211.	2.2	8
17	Mathematical-based microbiome analytics for clinical translation. Computational and Structural Biotechnology Journal, 2021, 19, 6272-6281.	4.1	13
18	Determining Optimal Coarseâ€Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. Journal of Computational Chemistry, 2020, 41, 14-20.	3.3	9

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19	Discrete Morse theory for weighted simplicial complexes. Topology and Its Applications, 2020, 270, 107038.	0.4	6
20	Weighted-persistent-homology-based machine learning for RNA flexibility analysis. PLoS ONE, 2020, 15, e0237747.	2.5	4
21	Weighted persistent homology for osmolyte molecular aggregation and hydrogen-bonding network analysis. Scientific Reports, 2020, 10, 9685.	3.3	20
22	Weighted Fundamental Group. Bulletin of the Malaysian Mathematical Sciences Society, 2020, 43, 4065-4088.	0.9	2
23	Weighted persistent homology for biomolecular data analysis. Scientific Reports, 2020, 10, 2079.	3.3	33
24	Coarse-Grained Simulation of Mechanical Properties of Single Microtubules With Micrometer Length. Frontiers in Molecular Biosciences, 2020, 7, 632122.	3.5	6
25	Magnus representation of genome sequences. Journal of Theoretical Biology, 2019, 480, 104-111.	1.7	2
26	A Malicious Web Site Identification Technique Using Web Structure Clustering. IEICE Transactions on Information and Systems, 2019, E102.D, 1665-1672.	0.7	4
27	Ligand Binding Induces Agonistic-Like Conformational Adaptations in Helix 12 of Progesterone Receptor Ligand Binding Domain. Frontiers in Chemistry, 2019, 7, 315.	3.6	7
28	Persistent homology analysis of osmolyte molecular aggregation and their hydrogen-bonding networks. Physical Chemistry Chemical Physics, 2019, 21, 21038-21048.	2.8	7
29	A complex multiscale virtual particle model based elastic network model (CMVP-ENM) for the normal mode analysis of biomolecular complexes. Physical Chemistry Chemical Physics, 2019, 21, 4359-4366.	2.8	5
30	A new method for the construction of coarse-grained models of large biomolecules from low-resolution cryo-electron microscopy data. Physical Chemistry Chemical Physics, 2019, 21, 9720-9727.	2.8	6
31	Sequence- And Structure-Specific Probing of RNAs by Short Nucleobase-Modified dsRNA-Binding PNAs Incorporating a Fluorescent Light-up Uracil Analog. Analytical Chemistry, 2019, 91, 5331-5338.	6.5	20
32	General Recognition of U-G, U-A, and C-G Pairs by Double-Stranded RNA-Binding PNAs Incorporated with an Artificial Nucleobase. Biochemistry, 2019, 58, 1319-1331.	2.5	19
33	Understanding Attack Trends from Security Blog Posts Using Guided-topic Model. Journal of Information Processing, 2019, 27, 802-809.	0.4	2
34	Persistent homology analysis of ion aggregations and hydrogen-bonding networks. Physical Chemistry Chemical Physics, 2018, 20, 13448-13460.	2.8	20
35	Multiscale virtual particle based elastic network model (MVP-ENM) for normal mode analysis of large-sized biomolecules. Physical Chemistry Chemical Physics, 2018, 20, 658-669.	2.8	12
36	Multiscale Persistent Functions for Biomolecular Structure Characterization. Bulletin of Mathematical Biology, 2018, 80, 1-31.	1.9	24

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37	Sequence-based multiscale modeling for high-throughput chromosome conformation capture (Hi-C) data analysis. PLoS ONE, 2018, 13, e0191899.	2.5	3
38	Persistent similarity for biomolecular structure comparison. Communications in Information and Systems, 2018, 18, 269-298.	0.5	1
39	Finite volume formulation of the MIB method for elliptic interface problems. Journal of Computational and Applied Mathematics, 2017, 321, 60-77.	2.0	6
40	Geometric and electrostatic modeling using molecular rigidity functions. Journal of Computational and Applied Mathematics, 2017, 313, 18-37.	2.0	6
41	Flexibilityâ€“rigidity index for proteinâ€“nucleic acid flexibility and fluctuation analysis. Journal of Computational Chemistry, 2016, 37, 1283-1295.	3.3	15
42	Generalized flexibility-rigidity index. Journal of Chemical Physics, 2016, 144, 234106.	3.0	27
43	Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM). Journal of Chemical Physics, 2015, 143, 204106.	3.0	32
44	Multiresolution persistent homology for excessively large biomolecular datasets. Journal of Chemical Physics, 2015, 143, 134103.	3.0	27
45	Persistent topology for cryoâ€EM data analysis. International Journal for Numerical Methods in Biomedical Engineering, 2015, 31, .	2.1	26
46	Multidimensional persistence in biomolecular data. Journal of Computational Chemistry, 2015, 36, 1502-1520.	3.3	53
47	A topological approach for protein classification. Computational and Mathematical Biophysics, 2015, 3, .	1.1	42
48	Multiresolution Topological Simplification. Journal of Computational Biology, 2015, 22, 887-891.	1.6	24
49	Matched interface and boundary method for elasticity interface problems. Journal of Computational and Applied Mathematics, 2015, 285, 203-225.	2.0	15
50	Second order method for solving 3D elasticity equations with complex interfaces. Journal of Computational Physics, 2015, 294, 405-438.	3.8	23
51	Atomic scale design and three-dimensional simulation of ionic diffusive nanofluidic channels. Microfluidics and Nanofluidics, 2015, 19, 665-692.	2.2	7
52	Communication: Capturing protein multiscale thermal fluctuations. Journal of Chemical Physics, 2015, 142, 211101.	3.0	31
53	Persistent homology for the quantitative prediction of fullerene stability. Journal of Computational Chemistry, 2015, 36, 408-422.	3.3	63
54	Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis. Journal of Chemical Physics, 2014, 140, 234105.	3.0	53

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55	Persistent homology analysis of protein structure, flexibility, and folding. International Journal for Numerical Methods in Biomedical Engineering, 2014, 30, 814-844.	2.1	174
56	Molecular nonlinear dynamics and protein thermal uncertainty quantification. Chaos, 2014, 24, 013103.	2.5	16
57	A Galerkin formulation of the MIB method for three dimensional elliptic interface problems. Computers and Mathematics With Applications, 2014, 68, 719-745.	2.7	15
58	MIB Galerkin method for elliptic interface problems. Journal of Computational and Applied Mathematics, 2014, 272, 195-220.	2.0	30
59	Multiscale geometric modeling of macromolecules I: Cartesian representation. Journal of Computational Physics, 2014, 257, 912-936.	3.8	24
60	Multiscale geometric modeling of macromolecules II: Lagrangian representation. Journal of Computational Chemistry, 2013, 34, 2100-2120.	3.3	22
61	Multiscale multiphysics and multidomain modelsâ€”Flexibility and rigidity. Journal of Chemical Physics, 2013, 139, 194109.	3.0	68
62	Stochastic model for protein flexibility analysis. Physical Review E, 2013, 88, 062709.	2.1	16
63	MATHEMATICAL MODELS AND TECHNIQUES FOR BIOMOLECULAR GEOMETRIC ANALYSIS. , 2013, , .		0
64	Variational Multiscale Models for Charge Transport. SIAM Review, 2012, 54, 699-754.	9.5	99
65	Geometric modeling of subcellular structures, organelles, andâ€‰multiprotein complexes. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 1198-1223.	2.1	24
66	Adaptively deformed mesh based interface method for elliptic equations with discontinuous coefficients. Journal of Computational Physics, 2012, 231, 1440-1461.	3.8	14
67	MIB method for elliptic equations with multi-material interfaces. Journal of Computational Physics, 2011, 230, 4588-4615.	3.8	18
68	Theoretical study for regulatory property of scaffold protein on MAPK cascade: A qualitative modeling. Biophysical Chemistry, 2010, 147, 130-139.	2.8	6
69	Information propagation from IP3 to target protein: A combined model for encoding and decoding of Ca2+ signal. Physica A: Statistical Mechanics and Its Applications, 2009, 388, 4105-4114.	2.6	12
70	Persistent-Homology-Based Machine Learning and Its Applications -- A Survey. SSRN Electronic Journal, 0, , .	0.4	37
71	Weighted-Persistent-Homology-based Machine Learning for RNA Flexibility Analysis. SSRN Electronic Journal, 0, , .	0.4	0