Sergio Decherchi

List of Publications by Year
in descending order

62 papers	1,791 citations	361413 20 h-index	276875 41 g-index
66 all docs	66 docs citations	66 times ranked	2151 citing authors

#	Article	IF	Citations
1	Probing Interplays between Human XBP1u Translational Arrest Peptide and 80S Ribosome. Journal of Chemical Theory and Computation, 2022, 18, 1905-1914.	5.3	5
2	Using Principal Paths to Walk Through Music and Visual Art Style Spaces Induced by Convolutional Neural Networks. Cognitive Computation, 2021, 13, 570-582.	5.2	15
3	Editorial: Molecular Dynamics and Machine Learning in Drug Discovery. Frontiers in Molecular Biosciences, 2021, 8, 673773.	3.5	8
4	Molecular Recognition by Gold Nanoparticle-Based Receptors as Defined through Surface Morphology and Pockets Fingerprint. Journal of Physical Chemistry Letters, 2021, 12, 5616-5622.	4.6	5
5	An Ab Initio Local Principal Path Algorithm. , 2021, , .		0
6	On the Stability of Feature Selection in Multiomics Data. , 2021, , .		1
7	Machine Learning and Enhanced Sampling Simulations for Computing the Potential of Mean Force and Standard Binding Free Energy. Journal of Chemical Theory and Computation, 2021, 17, 5287-5300.	5.3	23
8	Opportunities and Challenges for Machine Learning in Rare Diseases. Frontiers in Medicine, 2021, 8, 747612.	2.6	31
9	Multi-target dopamine D3 receptor modulators: Actionable knowledge for drug design from molecular dynamics and machine learning. European Journal of Medicinal Chemistry, 2020, 188, 111975.	5.5	19
10	Thermodynamics and Kinetics of Drug-Target Binding by Molecular Simulation. Chemical Reviews, 2020, 120, 12788-12833.	47.7	126
11	Fast and Memory-Efficient Import Vector Domain Description. Neural Processing Letters, 2020, 52, 511-524.	3.2	1
12	Spathial: an R package for the evolutionary analysis of biological data. Bioinformatics, 2020, 36, 4664-4667.	4.1	7
13	Solubility Advantage of Amorphous Ketoprofen. Thermodynamic and Kinetic Aspects by Molecular Dynamics and Free Energy Approaches. Journal of Chemical Theory and Computation, 2020, 16, 4126-4140.	5.3	3
14	Investigating Drugâ€“Target Residence Time in Kinases through Enhanced Sampling Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4646-4659.	5.3	32
15	Cognitive Insights into Sentic Spaces Using Principal Paths. Cognitive Computation, 2019, 11, 656-675.	5.2	8
16	Structure, Thermodynamics, and Kinetics of Plinabulin Binding to Two Tubulin Isotypes. CheM, 2019, 5, 2969-2986.	11.7	33
17	Simple Learning with a Teacher via Biased Regularized Least Squares. Lecture Notes in Computer Science, 2019, , 14-25.	1.3	1
18	NanoShaperâ€“VMD interface: computing and visualizing surfaces, pockets and channels in molecular systems. Bioinformatics, 2019, 35, 1241-1243.	4.1	23

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19	Finding Principal Paths in Data Space. IEEE Transactions on Neural Networks and Learning Systems, 2019, 30, 2449-2462.	11.3	15
20	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 219-224.	5.4	48
21	Fast Dynamic Docking Guided by Adaptive Electrostatic Bias: The MD-Binding Approach. Journal of Chemical Theory and Computation, 2018, 14, 1727-1736.	5.3	40
22	Import Vector Domain Description: A Kernel Logistic One-Class Learning Algorithm. IEEE Transactions on Neural Networks and Learning Systems, 2017, 28, 1722-1729.	11.3	11
23	Allosteric Communication Networks in Proteins Revealed through Pocket Crosstalk Analysis. ACS Central Science, 2017, 3, 949-960.	11.3	60
24	Distributed Kernel K-Means for Large Scale Clustering. , 2017, , .		3
25	Molecular Dynamics Simulations and Kinetic Measurements to Estimate and Predict Proteinâ€“Ligand Residence Times. Journal of Medicinal Chemistry, 2016, 59, 7167-7176.	6.4	81
26	Probing Hydration Patterns in Class-A GPCRs via Biased MD: The A_{2A} Receptor. Journal of Chemical Theory and Computation, 2016, 12, 6049-6061.	5.3	18
27	SIM-ELM: Connecting the ELM model with similarity-function learning. Neural Networks, 2016, 74, 22-34.	5.9	9
28	Inductive bias for semi-supervised extreme learning machine. Neurocomputing, 2016, 174, 154-167.	5.9	7
29	Kinetics of protein-ligand unbinding via smoothed potential molecular dynamics simulations. Scientific Reports, 2015, 5, 11539.	3.3	132
30	Implicit solvent methods for free energy estimation. European Journal of Medicinal Chemistry, 2015, 91, 27-42.	5.5	46
31	The ligand binding mechanism to purine nucleoside phosphorylase elucidated via molecular dynamics and machine learning. Nature Communications, 2015, 6, 6155.	12.8	98
32	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	5.4	65
33	Inductive Bias for Semi-supervised Extreme Learning Machine. Proceedings in Adaptation, Learning and Optimization, 2015, , 61-70.	1.6	4
34	Building and Analyzing Molecular Surfaces: A Tutorial on NanoShaper. , 2015, , 199-213.		1
35	Semi-supervised machine learning approach for unknown malicious software detection. , 2014, , .		4
36	CUDA accelerated molecular surface generation. Concurrency Computation Practice and Experience, 2014, 26, 1819-1831.	2.2	4

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37	Describing the Conformational Landscape of Small Organic Molecules through Gaussian Mixtures in Dihedral Space. Journal of Chemical Theory and Computation, 2014, 10, 2557-2568.	5.3	10
38	Solving the Linearized Poisson-Boltzmann Equation on GPUs Using CUDA. , 2013, , .		2
39	Circular-ELM for the reduced-reference assessment of perceived image quality. Neurocomputing, 2013, 102, 78-89.	5.9	66
40	Extreme Learning Machines [Trends & Controversies]. IEEE Intelligent Systems, 2013, 28, 30-59.	4.0	329
41	Between Algorithm and Model: Different Molecular Surface Definitions for the Poisson-Boltzmann Based Electrostatic Characterization of Biomolecules in Solution. Communications in Computational Physics, 2013, 13, 61-89.	1.7	46
42	A general and Robust Ray-Casting-Based Algorithm for Triangulating Surfaces at the Nanoscale. PLoS ONE, 2013, 8, e59744.	2.5	98
43	Efficient Digital Implementation of Extreme Learning Machines for Classification. IEEE Transactions on Circuits and Systems II: Express Briefs, 2012, 59, 496-500.	3.0	73
44	Learning the mean: A neural network approach. Neurocomputing, 2012, 77, 129-143.	5.9	4
45	CUDA Accelerated Blobby Molecular Surface Generation. Lecture Notes in Computer Science, 2012, , 347-356.	1.3	5
46	Computational intelligence methods for underwater magnetic-based protection systems. , 2011, , .		2
47	Tactile-Data Classification of Contact Materials Using Computational Intelligence. IEEE Transactions on Robotics, 2011, 27, 635-639.	10.3	91
48	Efficient approximate Regularized Least Squares by Toeplitz matrix. Pattern Recognition Letters, 2011, 32, 468-475.	4.2	1
49	Operative assessment of predicted generalization errors on non-stationary distributions in data-intensive applications. Intelligent Data Analysis, 2011, 15, 193-214.	0.9	0
50	SeaLab Advanced Information Retrieval. , 2010, , .		7
51	Using Unsupervised Analysis to Constrain Generalization Bounds for Support Vector Classifiers. IEEE Transactions on Neural Networks, 2010, 21, 424-438.	4.2	20
52	A neural model approach for regularization in the mean estimation case. , 2010, , .		1
53	Circuit implementation of SVM training. , 2009, , .		0
54	Maximal-discrepancy bounds for regularized classifiers. , 2009, , .		1

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55	Text Clustering for Digital Forensics Analysis. Advances in Intelligent and Soft Computing, 2009, , 29-36.	0.2	26
56	K-Means Clustering for Content-Based Document Management in Intelligence. Intelligent Information Systems, 2009, , 287-323.	0.1	7
57	A Preliminary Study on SVM Based Analysis of Underwater Magnetic Signals for Port Protection. Advances in Intelligent and Soft Computing, 2009, , 37-44.	0.2	3
58	Hypermetric k-Means Clustering for Content-Based Document Management. Advances in Soft Computing, 2009, , 61-68.	0.4	0
59	Low-complexity, linear circuit implementation of support vector machines training. Electronics Letters, 2008, 44, 1478.	1.0	2
60	Non-stationary Data Mining: The Network Security Issue. Lecture Notes in Computer Science, 2008, , 32-41.	1.3	1
61	Embedded Electronics Systems for Training Support Vector Machines. , 2006, , .		1
62	Probabilistic Pocket Druggability Prediction via One-Class Learning. Frontiers in Pharmacology, 0, 13, .	3.5	4