Rajarashi Guha

List of Publications by Year
in descending order

58 papers	4,391 citations	186209 28 h-index	161767 54 g-index
62 all docs	62 docs citations	62 times ranked	7497 citing authors

#	Article	IF	Citations
1	Diversifying cheminformatics. Journal of Cheminformatics, 2022, 14, 25.	2.8	6
2	A High-Throughput Screening Platform Identifies Novel Combination Treatments for Malignant Peripheral Nerve Sheath Tumors. Molecular Cancer Therapeutics, 2022, 21, 1246-1258.	1.9	2
3	What is the role of cheminformatics in a pandemic?. Journal of Cheminformatics, 2021, 13, 16.	2.8	3
4	Reply to â€œFAIR chemical structure in the Journal of Cheminformaticsâ€• Journal of Cheminformatics, 2021, 13, 49.	2.8	3
5	Brigatinib causes tumor shrinkage in both NF2-deficient meningioma and schwannoma through inhibition of multiple tyrosine kinases but not ALK. PLoS ONE, 2021, 16, e0252048.	1.1	19
6	Learning cheminformatics. Journal of Cheminformatics, 2020, 12, 4.	2.8	7
7	Drugs Targeting Tumor-Initiating Cells Prolong Survival in a Post-Surgery, Post-Chemotherapy Ovarian Cancer Relapse Model. Cancers, 2020, 12, 1645.	1.7	25
8	Journal of Cheminformatics, ORCID, and GitHub. Journal of Cheminformatics, 2019, 11, 44.	2.8	1
9	Scaffold-Based Analytics: Enabling Hit-to-Lead Decisions by Visualizing Chemical Series Linked across Large Datasets. Journal of Chemical Information and Modeling, 2019, 59, 4880-4892.	2.5	8
10	High-Throughput Screening for Drug Combinations. Methods in Molecular Biology, 2019, 1939, 11-35.	0.4	10
11	Implementing cheminformatics. Journal of Cheminformatics, 2019, 11, 12.	2.8	0
12	Therapeutic strategies for diffuse midline glioma from high-throughput combination drug screening. Science Translational Medicine, 2019, 11, .	5.8	129
13	The Rise and Fall of a Scaffold: A Trend Analysis of Scaffolds in the Medicinal Chemistry Literature. Journal of Medicinal Chemistry, 2018, 61, 4688-4703.	2.9	41
14	Canvass: A Crowd-Sourced, Natural-Product Screening Library for Exploring Biological Space. ACS Central Science, 2018, 4, 1727-1741.	5.3	32
15	Using Machine Learning to Predict Synergistic Antimalarial Compound Combinations With Novel Structures. Frontiers in Pharmacology, 2018, 9, 1096.	1.6	27
16	MEK inhibition induces MYOG and remodels super-enhancers in RAS-driven rhabdomyosarcoma. Science Translational Medicine, 2018, 10, .	5.8	104
17	Identification of Combinations of Approved Drugs With Synergistic Activity Against Ebola Virus in Cell Cultures. Journal of Infectious Diseases, 2018, 218, S672-S678.	1.9	49
18	A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria. Malaria Journal, 2018, 17, 160.	0.8	19

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19	Pharmacological and genomic profiling of neurofibromatosis type 1 plexiform neurofibroma-derived schwann cells. Scientific Data, 2018, 5, 180106.	2.4	20
20	Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002.	6.5	271
21	PAX3â€“FOXO1 Establishes Myogenic Super Enhancers and Confers BET Bromodomain Vulnerability. Cancer Discovery, 2017, 7, 884-899.	7.7	221
22	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	2.8	3
23	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	2.8	275
24	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives. Drug Discovery Today, 2016, 21, 225-238.	3.2	162
25	Augmented efficacy of brentuximab vedotin combined with ruxolitinib and/or Navitoclax in a murine model of human Hodgkinâ€™s lymphoma. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1624-1629.	3.3	38
26	High-throughput matrix screening identifies synergistic and antagonistic antimalarial drug combinations. Scientific Reports, 2015, 5, 13891.	1.6	92
27	BioAssay Research Database (BARD): chemical biology and probe-development enabled by structured metadata and result types. Nucleic Acids Research, 2015, 43, D1163-D1170.	6.5	20
28	Synergy Maps: exploring compound combinations using network-based visualization. Journal of Cheminformatics, 2015, 7, 36.	2.8	32
29	High-throughput combinatorial screening identifies drugs that cooperate with ibrutinib to kill activated B-cellâ€“like diffuse large B-cell lymphoma cells. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 2349-2354.	3.3	355
30	Blockade of oncogenic IÎºB kinase activity in diffuse large B-cell lymphoma by bromodomain and extraterminal domain protein inhibitors. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11365-11370.	3.3	166
31	On the validity versus utility of activity landscapes: are all activity cliffs statistically significant?. Journal of Cheminformatics, 2014, 6, 11.	2.8	9
32	What are we â€˜tweetingâ€™ about obesity? Mapping tweets with topic modeling and Geographic Information System. Cartography and Geographic Information Science, 2013, 40, 90-102.	1.4	171
33	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2012, 12, 1946-1956.	1.0	48
34	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	3.3	21
35	Exploring Uncharted Territories: Predicting Activity Cliï¬€s in Structureâ€“Activity Landscapes. Journal of Chemical Information and Modeling, 2012, 52, 2181-2191.	2.5	33
36	Exploring structureâ€“activity data using the landscape paradigm. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 829-841.	6.2	34

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37	Chemical Genomic Profiling for Antimalarial Therapies, Response Signatures, and Molecular Targets. Science, 2011, 333, 724-729.	6.0	130
38	Using a neural network for mining interpretable relationships of West Nile risk factors. Social Science and Medicine, 2011, 72, 418-429.	1.8	13
39	Exploratory analysis of kinetic solubility measurements of a small molecule library. Bioorganic and Medicinal Chemistry, 2011, 19, 4127-4134.	1.4	27
40	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
41	The Ups and Downs of Structureâ€“Activity Landscapes. Methods in Molecular Biology, 2010, 672, 101-117.	0.4	28
42	Use of genetic algorithm and neural network approaches for risk factor selection: A case study of West Nile virus dynamics in an urban environment. Computers, Environment and Urban Systems, 2010, 34, 189-203.	3.3	14
43	Advances in Cheminformatics Methodologies and Infrastructure to Support the Data Mining of Large, Heterogeneous Chemical Datasets. Current Computer-Aided Drug Design, 2010, 6, 50-67.	0.8	28
44	GOAssay: from Gene Ontology to Assays IDentifiers - Towards Automatic Functional Annotation of PubChem BioAssays. Nature Precedings, 2009, , .	0.1	1
45	PubChem as a Source of Polypharmacology. Journal of Chemical Information and Modeling, 2009, 49, 2044-2055.	2.5	130
46	Utilizing high throughput screening data for predictive toxicology models: protocols and application to MLSCN assays. Journal of Computer-Aided Molecular Design, 2008, 22, 367-384.	1.3	43
47	On the interpretation and interpretability of quantitative structureâ€“activity relationship models. Journal of Computer-Aided Molecular Design, 2008, 22, 857-871.	1.3	70
48	Structureâ^'Activity Landscape Index:â€‰ Identifying and Quantifying Activity Cliffs. Journal of Chemical Information and Modeling, 2008, 48, 646-658.	2.5	281
49	Assessing How Well a Modeling Protocol Captures a Structureâ^'Activity Landscape. Journal of Chemical Information and Modeling, 2008, 48, 1716-1728.	2.5	84
50	SQMD: Architecture for Scalable, Distributed Database System Built on Virtual Private Servers. , 2008, , .		2
51	Open Notebook Science - Falcipain-2 Preliminary Results. Nature Precedings, 2008, , .	0.1	1
52	The CombiUgi Project and Closing the Open Science Loop. Nature Precedings, 2007, , .	0.1	0
53	Chemical Informatics Functionality inR. Journal of Statistical Software, 2007, 18, .	1.8	189
54	The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	2.5	366

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55	Scalable Partitioning and Exploration of Chemical Spaces Using Geometric Hashing. Journal of Chemical Information and Modeling, 2006, 46, 321-333.	2.5	22
56	Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. Current Pharmaceutical Design, 2006, 12, 2111-2120.	0.9	418
57	Determining the Validity of a QSAR Model ? A Classification Approach.. ChemInform, 2005, 36, no.	0.1	0
58	Development of QSAR Models to Predict and Interpret the Biological Activity of Artemisinin Analogues.. ChemInform, 2004, 35, no.	0.1	0