Rajarshi Guha

List of Publications by Year
in descending order

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102	7,077	66343	60623
papers	citations	42 h-index	81 g-index

112	112	112	11658
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploiting Synthetic Lethality for the Therapy of ABC Diffuse Large B Cell Lymphoma. Cancer Cell, 2012, 21, 723-737.	16.8	460
2	Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. Current Pharmaceutical Design, 2006, 12, 2111-2120.	1.9	418
3	The Blue Obeliskâ€"Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	5.4	366
4	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.	7.1	355
5	High-content genome-wide RNAi screens identify regulators of parkin upstream of mitophagy. Nature, 2013, 504, 291-295.	27.8	301
6	Structureâ^'Activity Landscape Index:â€‰ Identifying and Quantifying Activity Cliffs. Journal of Chemical Information and Modeling, 2008, 48, 646-658.	5.4	281
7	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	6.1	275
8	Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002.	14.5	271
9	Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332.	46.4	263
10	Blockade of oncogenic Ií¤B 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.	7.1	166
11	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.	6.4	162
12	Navigating structureâ€"activity landscapes. Drug Discovery Today, 2009, 14, 698-705.	6.4	161
13	Chemoinformatic Analysis of Combinatorial Libraries, Drugs, Natural Products, and Molecular Libraries Small Molecule Repository. Journal of Chemical Information and Modeling, 2009, 49, 1010-1024.	5.4	138
14	Chemical Genomic Profiling for Antimalarial Therapies, Response Signatures, and Molecular Targets. Science, 2011, 333, 724-729.	12.6	130
15	Therapeutic strategies for diffuse midline glioma from high-throughput combination drug screening. Science Translational Medicine, 2019, 11, .	12.4	129
16	KNIME Workflow to Assess PAINS Filters in SMARTS Format. Comparison of RDKit and Indigo Cheminformatics Libraries. Molecular Informatics, 2011, 30, 847-850.	2.5	118
17	A Druggable TCF4- and BRD4-Dependent Transcriptional Network Sustains Malignancy in Blastic Plasmacytoid Dendritic Cell Neoplasm. Cancer Cell, 2016, 30, 764-778.	16.8	116
18	On Exploring Structureâ€"Activity Relationships. Methods in Molecular Biology, 2013, 993, 81-94.	0.9	102

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19	The phosphatidylinositol-3-phosphate 5-kinase inhibitor apilimod blocks filoviral entry and infection. PLoS Neglected Tropical Diseases, 2017, 11, e0005540.	3.0	97
20	Interpreting Computational Neural Network QSAR Models:Â A Measure of Descriptor Importance. Journal of Chemical Information and Modeling, 2005, 45, 800-806.	5.4	94
21	High-throughput matrix screening identifies synergistic and antagonistic antimalarial drug combinations. Scientific Reports, 2015, 5, 13891.	3.3	92
22	Determining the Validity of a QSAR Model â^' A Classification Approach. Journal of Chemical Information and Modeling, 2005, 45, 65-73.	5.4	88
23	Assessing How Well a Modeling Protocol Captures a Structureâ^'Activity Landscape. Journal of Chemical Information and Modeling, 2008, 48, 1716-1728.	5.4	84
24	Selective targeting of JAK/STAT signaling is potentiated by Bcl-xL blockade in IL-2â€“dependent adult T-cell leukemia. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12480-12485.	7.1	81
25	Development of Linear, Ensemble, and Nonlinear Models for the Prediction and Interpretation of the Biological Activity of a Set of PDGFR Inhibitors. Journal of Chemical Information and Computer Sciences, 2004, 44, 2179-2189.	2.8	78
26	On the interpretation and interpretability of quantitative structureâ€“activity relationship models. Journal of Computer-Aided Molecular Design, 2008, 22, 857-871.	2.9	70
27	A Combination CDK4/6 and IGF1R Inhibitor Strategy for Ewing Sarcoma. Clinical Cancer Research, 2019, 25, 1343-1357.	7.0	69
28	Local Lazy Regression:Â Making Use of the Neighborhood to Improve QSAR Predictions. Journal of Chemical Information and Modeling, 2006, 46, 1836-1847.	5.4	65
29	Profile of the GSK Published Protein Kinase Inhibitor Set Across ATP-Dependent and-Independent Luciferases: Implications for Reporter-Gene Assays. PLoS ONE, 2013, 8, e57888.	2.5	65
30	Glypicanâ€3â€Specific Antibody Drug Conjugates Targeting Hepatocellular Carcinoma. Hepatology, 2019, 70, 563-576.	7.3	65
31	Interpreting Computational Neural Network Quantitative Structureâ^'Activity Relationship Models:Â A Detailed Interpretation of the Weights and Biases. Journal of Chemical Information and Modeling, 2005, 45, 1109-1121.	5.4	63
32	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	6.1	63
33	Drug target ontology to classify and integrate drug discovery data. Journal of Biomedical Semantics, 2017, 8, 50.	1.6	63
34	Resistance to Epigenetic-Targeted Therapy Engenders Tumor Cell Vulnerabilities Associated with Enhancer Remodeling. Cancer Cell, 2018, 34, 922-938.e7.	16.8	63
35	Development of QSAR Models To Predict and Interpret the Biological Activity of Artemisinin Analogues. Journal of Chemical Information and Computer Sciences, 2004, 44, 1440-1449.	2.8	60
36	Generation of QSAR sets with a self-organizing map. Journal of Molecular Graphics and Modelling, 2004, 23, 1-14.	2.4	52

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37	Chemogenomic Profiling of Endogenous PARK2 Expression Using a Genome-Edited Coincidence Reporter. ACS Chemical Biology, 2015, 10, 1188-1197.	3.4	52
38	Aurora B kinase is a potent and selective target in MYCN-driven neuroblastoma. Oncotarget, 2015, 6, 35247-35262.	1.8	52
39	Ensemble Feature Selection:â€‰ Consistent Descriptor Subsets for Multiple QSAR Models. Journal of Chemical Information and Modeling, 2007, 47, 989-997.	5.4	51
40	Identification of Combinations of Approved Drugs With Synergistic Activity Against Ebola Virus in Cell Cultures. Journal of Infectious Diseases, 2018, 218, S672-S678.	4.0	49
41	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2012, 12, 1946-1956.	2.1	48
42	Matrix Screen Identifies Synergistic Combination of PARP Inhibitors and Nicotinamide Phosphoribosyltransferase (NAMPT) Inhibitors in Ewing Sarcoma. Clinical Cancer Research, 2017, 23, 7301-7311.	7.0	44
43	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.	2.9	43
44	Discovery of new antimalarial chemotypes through chemical methodology and library development. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6775-6780.	7.1	42
45	Web Service Infrastructure for Chemoinformatics. Journal of Chemical Information and Modeling, 2007, 47, 1303-1307.	5.4	41
46	Large-scale screening identifies a novel microRNA, miR-15a-3p, which induces apoptosis in human cancer cell lines. RNA Biology, 2013, 10, 287-300.	3.1	41
47	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. Journal of Cheminformatics, 2010, 2, 5.	6.1	39
48	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.	7.1	38
49	A 1536-Well Quantitative High-Throughput Screen to Identify Compounds Targeting Cancer Stem Cells. Journal of Biomolecular Screening, 2012, 17, 1231-1242.	2.6	35
50	Exploring structureâ€“activity data using the landscape paradigm. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 829-841.	14.6	34
51	Exploring Uncharted Territories: Predicting Activity Cliï¬€s in Structureâ€“Activity Landscapes. Journal of Chemical Information and Modeling, 2012, 52, 2181-2191.	5.4	33
52	Synergy Maps: exploring compound combinations using network-based visualization. Journal of Cheminformatics, 2015, 7, 36.	6.1	32
53	Canvass: A Crowd-Sourced, Natural-Product Screening Library for Exploring Biological Space. ACS Central Science, 2018, 4, 1727-1741.	11.3	32
54	Genome Editing-Enabled HTS Assays Expand Drug Target Pathways for Charcotâ€“Marieâ€“Tooth Disease. ACS Chemical Biology, 2014, 9, 2594-2602.	3.4	31

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55	Chemical Data Mining of the NCI Human Tumor Cell Line Database. Journal of Chemical Information and Modeling, 2007, 47, 2063-2076.	5.4	30
56	Actinoramide A Identified as a Potent Antimalarial from Titration-Based Screening of Marine Natural Product Extracts. Journal of Natural Products, 2015, 78, 2411-2422.	3.0	30
57	A single nucleotide polymorphism in the Plasmodium falciparum atg18 gene associates with artemisinin resistance and confers enhanced parasite survival under nutrient deprivation. Malaria Journal, 2018, 17, 391.	2.3	30
58	High-throughput Chemical Screening Identifies Focal Adhesion Kinase and Aurora Kinase B Inhibition as a Synergistic Treatment Combination in Ewing Sarcoma. Clinical Cancer Research, 2019, 25, 4552-4566.	7.0	30
59	High-throughput screens identify HSP90 inhibitors as potent therapeutics that target inter-related growth and survival pathways in advanced prostate cancer. Scientific Reports, 2018, 8, 17239.	3.3	29
60	The Ups and Downs of Structureâ€“Activity Landscapes. Methods in Molecular Biology, 2010, 672, 101-117.	0.9	28
61	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.	1.2	28
62	Evaluation of the Activity of Lamivudine and Zidovudine against Ebola Virus. PLoS ONE, 2016, 11, e0166318.	2.5	28
63	Chemotaxis of Molecular Dyes in Polymer Gradients in Solution. Journal of the American Chemical Society, 2017, 139, 15588-15591.	13.7	28
64	Exploratory analysis of kinetic solubility measurements of a small molecule library. Bioorganic and Medicinal Chemistry, 2011, 19, 4127-4134.	3.0	27
65	Characterization of clinically used oral antiseptics as quadruplex-binding ligands. Nucleic Acids Research, 2018, 46, 2722-2732.	14.5	27
66	Using Machine Learning to Predict Synergistic Antimalarial Compound Combinations With Novel Structures. Frontiers in Pharmacology, 2018, 9, 1096.	3.5	27
67	Large-scale pharmacological profiling of 3D tumor models of cancer cells. Cell Death and Disease, 2016, 7, e2492-e2492.	6.3	26
68	A High-Throughput Screening Model of the Tumor Microenvironment for Ovarian Cancer Cell Growth. SLAS Discovery, 2017, 22, 494-506.	2.7	26
69	Drugs Targeting Tumor-Initiating Cells Prolong Survival in a Post-Surgery, Post-Chemotherapy Ovarian Cancer Relapse Model. Cancers, 2020, 12, 1645.	3.7	25
70	Moving targets in drug discovery. Scientific Reports, 2020, 10, 20213.	3.3	23
71	Scalable Partitioning and Exploration of Chemical Spaces Using Geometric Hashing. Journal of Chemical Information and Modeling, 2006, 46, 321-333.	5.4	22
72	Flexible Web Service Infrastructure for the Development and Deployment of Predictive Models. Journal of Chemical Information and Modeling, 2008, 48, 456-464.	5.4	22

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73	Whole-genome RNAi screen highlights components of the endoplasmic reticulum/Golgi as a source of resistance to immunotoxin-mediated cytotoxicity. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E1135-42.	7.1	22
74	A High-Throughput Screen of a Library of Therapeutics Identifies Cytotoxic Substrates of P-glycoprotein. Molecular Pharmacology, 2019, 96, 629-640.	2.3	22
75	A furoxanâ€“amodiaquine hybrid as a potential therapeutic for three parasitic diseases. MedChemComm, 2012, 3, 1505.	3.4	21
76	R-NN Curves:Â An Intuitive Approach to Outlier Detection Using a Distance Based Method. Journal of Chemical Information and Modeling, 2006, 46, 1713-1722.	5.4	20
77	Pharmacological and genomic profiling of neurofibromatosis type 1 plexiform neurofibroma-derived schwann cells. Scientific Data, 2018, 5, 180106.	5.3	20
78	A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria. Malaria Journal, 2018, 17, 160.	2.3	19
79	Novel Phenotypic Outcomes Identified for a Public Collection of Approved Drugs from a Publicly Accessible Panel of Assays. PLoS ONE, 2015, 10, e0130796.	2.5	18
80	High-throughput screening identifies candidate drugs for the treatment of recurrent respiratory papillomatosis. Papillomavirus Research (Amsterdam, Netherlands), 2019, 8, 100181.	4.5	18
81	A High-Throughput Assay for Small Molecule Destabilizers of the KRAS Oncoprotein. PLoS ONE, 2014, 9, e103836.	2.5	18
82	Target Deconvolution of a Multikinase Inhibitor with Antimetastatic Properties Identifies TAOK3 as a Key Contributor to a Cancer Stem Cellâ€“Like Phenotype. Molecular Cancer Therapeutics, 2019, 18, 2097-2110.	4.1	16
83	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	2.6	14
84	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.	7.1	14
85	Mutation Profiles in Glioblastoma 3D Oncospheres Modulate Drug Efficacy. SLAS Technology, 2019, 24, 28-40.	1.9	14
86	Using a neural network for mining interpretable relationships of West Nile risk factors. Social Science and Medicine, 2011, 72, 418-429.	3.8	13
87	High-throughput screening for genes that prevent excess DNA replication in human cells and for molecules that inhibit them. Methods, 2012, 57, 234-248.	3.8	11
88	High-Throughput Screening for Drug Combinations. Methods in Molecular Biology, 2019, 1939, 11-35.	0.9	10
89	On the validity versus utility of activity landscapes: are all activity cliffs statistically significant?. Journal of Cheminformatics, 2014, 6, 11.	6.1	9
90	mQC: A Heuristic Quality-Control Metric for High-Throughput Drug Combination Screening. Scientific Reports, 2016, 6, 37741.	3.3	8

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91	The synergy of BET inhibitors with aurora A kinase inhibitors in MYCN-amplified neuroblastoma is heightened with functional TP53. Neoplasia, 2021, 23, 624-633.	5.3	8
92	Chemical Screens Identify Drugs that Enhance or Mitigate Cellular Responses to Antibody-Toxin Fusion Proteins. PLoS ONE, 2016, 11, e0161415.	2.5	8
93	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2013, 12, 1946-1956.	2.1	6
94	Ranking Differential Drug Activities from Dose-Response Synthetic Lethality Screens. Journal of Biomolecular Screening, 2016, 21, 942-955.	2.6	4
95	Counting Clusters Using R-NN Curves. Journal of Chemical Information and Modeling, 2007, 47, 1308-1318.	5.4	3
96	Selective targeting of JAK/STAT signaling is potentiated by Bcl-xL blockade in IL-2-dependent adult T-cell leukemia. Retrovirology, 2015, 12, .	2.0	3
97	Matrix Drug Screen Identifies Synergistic Drug Combinations to Augment SMAC Mimetic Activity in Ovarian Cancer. Cancers, 2020, 12, 3784.	3.7	3
98	A Risk Factor Analysis of West Nile Virus: Extraction of Relationships from a Neural-Network Model. Lecture Notes in Computer Science, 2010, , 208-217.	1.3	1
99	Development of QSAR Models to Predict and Interpret the Biological Activity of Artemisinin Analogues.. ChemInform, 2004, 35, no.	0.0	0
100	Development of Linear, Ensemble, and Nonlinear Models for the Prediction and Interpretation of the Biological Activity of a Set of PDGFR Inhibitors.. ChemInform, 2005, 36, no.	0.0	0
101	Determining the Validity of a QSAR Model ? A Classification Approach.. ChemInform, 2005, 36, no.	0.0	0
102	Interpreting Computational Neural Network Quantitative Structureâ€"Activity Relationship Models: A Detailed Interpretation of the Weights and Biases.. ChemInform, 2005, 36, no.	0.0	0