Tiejun Cheng

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4543481/publications.pdf

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35	7,933	304368	360668
papers	citations	22 h-index	35 g-index

37	37	37	10746
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	PubChem 2019 update: improved access to chemical data. Nucleic Acids Research, 2019, 47, D1102-D1109.	6.5	2,217
2	PubChem in 2021: new data content and improved web interfaces. Nucleic Acids Research, 2021, 49, D1388-D1395.	6.5	2,146
3	Computation of Octanolâ^'Water Partition Coefficients by Guiding an Additive Model with Knowledge. Journal of Chemical Information and Modeling, 2007, 47, 2140-2148.	2.5	601
4	Structure-Based Virtual Screening for Drug Discovery: a Problem-Centric Review. AAPS Journal, 2012, 14, 133-141.	2.2	461
5	Comparative Assessment of Scoring Functions on a Diverse Test Set. Journal of Chemical Information and Modeling, 2009, 49, 1079-1093.	2.5	444
6	PubChem BioAssay: 2017 update. Nucleic Acids Research, 2017, 45, D955-D963.	6.5	398
7	PubChem as a public resource for drug discovery. Drug Discovery Today, 2010, 15, 1052-1057.	3.2	308
8	Evaluation of the performance of four molecular docking programs on a diverse set of proteinâ€ligand complexes. Journal of Computational Chemistry, 2010, 31, 2109-2125.	1.5	277
9	PubChem BioAssay: 2014 update. Nucleic Acids Research, 2014, 42, D1075-D1082.	6.5	250
10	Predicting drugâ€“drug interactions through drug structural similarities and interaction networks incorporating pharmacokinetics and pharmacodynamics knowledge. Journal of Cheminformatics, 2017, 9, 16.	2.8	82
11	Identifying Compound-Target Associations by Combining Bioactivity Profile Similarity Search and Public Databases Mining. Journal of Chemical Information and Modeling, 2011, 51, 2440-2448.	2.5	71
12	An update on PUG-REST: RESTful interface for programmatic access to PubChem. Nucleic Acids Research, 2018, 46, W563-W570.	6.5	69
13	Literature information in PubChem: associations between PubChem records and scientific articles. Journal of Cheminformatics, 2016, 8, 32.	2.8	58
14	PubChem applications in drug discovery: a bibliometric analysis. Drug Discovery Today, 2014, 19, 1751-1756.	3.2	53
15	FSelector: a Ruby gem for feature selection. Bioinformatics, 2012, 28, 2851-2852.	1.8	48
16	Binary Classification of Aqueous Solubility Using Support Vector Machines with Reduction and Recombination Feature Selection. Journal of Chemical Information and Modeling, 2011, 51, 229-236.	2.5	47
17	Plant Reactome: a knowledgebase and resource for comparative pathway analysis. Nucleic Acids Research, 2020, 48, D1093-D1103.	6.5	44
18	Pathway Analysis for Drug Repositioning Based on Public Database Mining. Journal of Chemical Information and Modeling, 2014, 54, 407-418.	2.5	40

#	Article	IF	Citations
19	Large-Scale Prediction of Drug-Target Interaction: a Data-Centric Review. AAPS Journal, 2017, 19, 1264-1275.	2.2	39
20	PubChem BioAssay: A Decadeâ€™s Development toward Open High-Throughput Screening Data Sharing. SLAS Discovery, 2017, 22, 655-666.	1.4	38
21	Automatic Perception of Organic Molecules Based on Essential Structural Information. Journal of Chemical Information and Modeling, 2007, 47, 1379-1385.	2.5	37
22	Investigating the correlations among the chemical structures, bioactivity profiles and molecular targets of small molecules. Bioinformatics, 2010, 26, 2881-2888.	1.8	26
23	PubChem Protein, Gene, Pathway, and Taxonomy Data Collections: Bridging Biology and Chemistry through Target-Centric Views of PubChem Data. Journal of Molecular Biology, 2022, 434, 167514.	2.0	26
24	iCn3D: From Web-Based 3D Viewer to Structural Analysis Tool in Batch Mode. Frontiers in Molecular Biosciences, 2022, 9, 831740.	1.6	26
25	PUG-View: programmatic access to chemical annotations integrated in PubChem. Journal of Cheminformatics, 2019, 11, 56.	2.8	23
26	A knowledge-guided strategy for improving the accuracy of scoring functions in binding affinity prediction. BMC Bioinformatics, 2010, 11, 193.	1.2	18
27	Total Synthesis of Clavepictines A and B and Pictamine. Organic Letters, 2006, 8, 3179-3182.	2.4	17
28	Web search and data mining of natural products and their bioactivities in PubChem. Science China Chemistry, 2013, 56, 1424-1435.	4.2	15
29	Discovering and Summarizing Relationships Between Chemicals, Genes, Proteins, and Diseases in PubChem. Frontiers in Research Metrics and Analytics, 2021, 6, 689059.	0.9	14
30	Studying the Parkinsonâ€™s disease metabolome and exposome in biological samples through different analytical and cheminformatics approaches: a pilot study. Analytical and Bioanalytical Chemistry, 2022, 414, 7399-7419.	1.9	12
31	Supporting precision medicine by data mining across multi-disciplines: an integrative approach for generating comprehensive linkages between single nucleotide variants (SNVs) and drug-binding sites. Bioinformatics, 2017, 33, 1621-1629.	1.8	11
32	Plant Reactome and PubChem: The Plant Pathway and (Bio)Chemical Entity Knowledgebases. Methods in Molecular Biology, 2022, 2443, 511-525.	0.4	7
33	An Empirical Additive Model for Aqueous Solubility Computation: Success and Limitations. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2012, 28, 2249-2257.	2.2	5
34	I-SOLV: A new surface-based empirical model for computing solvation free energies. Journal of Molecular Graphics and Modelling, 2007, 26, 368-377.	1.3	3
35	Enhancing the interoperability of glycan data flow between ChEBI, PubChem, and GlyGen. Glycobiology, 2021, , .	1.3	2