List of Publications by Year in descending order

33 papers	1,924 citations	516561 16 h-index	434063 31 g-index
47 all docs	47 docs citations	47 times ranked	3312 citing authors

#	Article	IF	Citations
1	One Scaffold, Different Organelle Sensors: pHâ€Activable Fluorescent Probes for Targeting Live Microglial Cell Organelles**. ChemBioChem, 2022, 23, .	1.3	2
2	Monitoring phagocytic uptake of amyloid Î² into glial cell lysosomes in real time. Chemical Science, 2021, 12, 10901-10918.	3.7	19
3	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	1.8	3
4	Accelerated Reactivity Mechanism and Interpretable Machine Learning Model of N-Sulfonylimines toward Fast Multicomponent Reactions. Organic Letters, 2020, 22, 8480-8486.	2.4	19
5	DUBS: A Framework for Developing <u>D</u>irectory of <u>U</u>seful <u>B</u>enchmarking <u>S</u>ets for Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4137-4143.	2.5	2
6	Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. Islets, 2020, 12, 99-107.	0.9	6
7	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	3.2	22
8	cando.py: Open Source Software for Predictive Bioanalytics of Large Scale Drugâ€“Proteinâ€“Disease Data. Journal of Chemical Information and Modeling, 2020, 60, 4131-4136.	2.5	21
9	CANDOCK: Chemical Atomic Network-Based Hierarchical Flexible Docking Algorithm Using Generalized Statistical Potentials. Journal of Chemical Information and Modeling, 2020, 60, 1509-1527.	2.5	36
10	A 2â€Tyrâ€Hâ€carboxylate Mononuclear Iron Center Forms the Active Site of a Paracoccus Dimethylformamidase. Angewandte Chemie - International Edition, 2020, 59, 16961-16966.	7.2	14
11	Lemon: a framework for rapidly mining structural information from the Protein Data Bank. Bioinformatics, 2019, 35, 4165-4167.	1.8	5
12	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	1.6	18
13	Rapid, Refined, and Robust Method for Expression, Purification, and Characterization of Recombinant Human Amyloid beta 1-42. Methods and Protocols, 2019, 2, 48.	0.9	13
14	CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. Biophysical Journal, 2018, 114, 57a.	0.2	3
15	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	1.6	19
16	Abstract LB-076: Cancer cell specific lethality by degrading specific protein target network identified using a chemical screening based machine learning method. , 2018, , .		2
17	Identification of New FLT3 Inhibitors That Potently Inhibit AML Cell Lines via an Azo Click-It/Staple-It Approach. ACS Medicinal Chemistry Letters, 2017, 8, 492-497.	1.3	16
18	Aminoisoquinoline benzamides, FLT3 and Src-family kinase inhibitors, potently inhibit proliferation of acute myeloid leukemia cell lines. Future Medicinal Chemistry, 2017, 9, 1213-1225.	1.1	15

#	Article	IF	Citations
19	Inhibition of 12/15-Lipoxygenase Protects Against Î²-Cell Oxidative Stress and Glycemic Deterioration in Mouse Models of Type 1 Diabetes. Diabetes, 2017, 66, 2875-2887.	0.3	34
20	Abstract A35: Drug repurposing for castration resistant prostate cancer based on disease-disease relationships. , 2017, , .		1
21	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. Molecules, 2016, 21, 1537.	1.7	46
22	CD28 Costimulation: From Mechanism to Therapy. Immunity, 2016, 44, 973-988.	6.6	607
23	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123.	0.9	50
24	Divergent Phenotypes of Human Regulatory T Cells Expressing the Receptors TIGIT and CD226. Journal of Immunology, 2015, 195, 145-155.	0.4	219
25	The Chromatin-Modifying Enzyme Ezh2 Is Critical for the Maintenance of Regulatory T Cell Identity after Activation. Immunity, 2015, 42, 227-238.	6.6	253
26	Multiscale Modelling of Relationships between Protein Classes and Drug Behavior Across all Diseases Using the CANDO Platform. Mini-Reviews in Medicinal Chemistry, 2015, 15, 705-717.	1.1	34
27	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	1.5	48
28	CANDO and the infinite drug discovery frontier. Drug Discovery Today, 2014, 19, 1353-1363.	3.2	67
29	Distal Effect of Amino Acid Substitutions in CYP2C9 Polymorphic Variants Causes Differences in Interatomic Interactions against (S)-Warfarin. PLoS ONE, 2013, 8, e74053.	1.1	16
30	KoBaMIN: a knowledge-based minimization web server for protein structure refinement. Nucleic Acids Research, 2012, 40, W323-W328.	6.5	124
31	Remarkable patterns of surface water ordering around polarized buckminsterfullerene. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 14455-14460.	3.3	25
32	Consistent refinement of submitted models at CASP using a knowledgeâ€based potential. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2668-2678.	1.5	46
33	Solvent dramatically affects protein structure refinement. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20239-20244.	3.3	99