List of Publications by Year in descending order

33 papers	1,924 citations	516215 16 h-index	433756 31 g-index
47 all docs	47 docs citations	47 times ranked	3312 citing authors

#	Article	IF	Citations
1	CD28 Costimulation: From Mechanism to Therapy. Immunity, 2016, 44, 973-988.	6.6	607
2	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
3	Divergent Phenotypes of Human Regulatory T Cells Expressing the Receptors TIGIT and CD226. Journal of Immunology, 2015, 195, 145-155.	0.4	219
4	KoBaMIN: a knowledge-based minimization web server for protein structure refinement. Nucleic Acids Research, 2012, 40, W323-W328.	6.5	124
5	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
6	CANDO and the infinite drug discovery frontier. Drug Discovery Today, 2014, 19, 1353-1363.	3.2	67
7	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123.	0.9	50
8	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	1.5	48
9	Consistent refinement of submitted models at CASP using a knowledgeâ€based potential. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2668-2678.	1.5	46
10	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. Molecules, 2016, 21, 1537.	1.7	46
11	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
12	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
13	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
14	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
15	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	3.2	22
16	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
17	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
18	Accelerated Reactivity Mechanism and Interpretable Machine Learning Model of N-Sulfonylimines toward Fast Multicomponent Reactions. Organic Letters, 2020, 22, 8480-8486.	2.4	19

#	Article	IF	Citations
19	Monitoring phagocytic uptake of amyloid Î² into glial cell lysosomes in real time. Chemical Science, 2021, 12, 10901-10918.	3.7	19
20	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	1.6	18
21	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
22	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
23	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
24	A 2â€Tyrâ€1â€carboxylate Mononuclear Iron Center Forms the Active Site of a Paracoccus Dimethylformamidase. Angewandte Chemie - International Edition, 2020, 59, 16961-16966.	7.2	14
25	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
26	Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. Islets, 2020, 12, 99-107.	0.9	6
27	Lemon: a framework for rapidly mining structural information from the Protein Data Bank. Bioinformatics, 2019, 35, 4165-4167.	1.8	5
28	CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. Biophysical Journal, 2018, 114, 57a.	0.2	3
29	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	1.8	3
30	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
31	One Scaffold, Different Organelle Sensors: pHâ€Activable Fluorescent Probes for Targeting Live Microglial Cell Organelles**. ChemBioChem, 2022, 23, .	1.3	2
32	Abstract LB-076: Cancer cell specific lethality by degrading specific protein target network identified using a chemical screening based machine learning method. , 2018, , .		2
33	Abstract A35: Drug repurposing for castration resistant prostate cancer based on disease-disease relationships. , 2017, , .		1