

Gaurav Chopra

List of Publications by Year in descending order

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Version: 2024-02-01

36
papers

1,800
citations

516710

16
h-index

395702

33
g-index

70
all docs

70
docs citations

70
times ranked

2861
citing authors

#	ARTICLE	IF	CITATIONS
1	One Scaffold, Different Organelle Sensors: pH-Activable Fluorescent Probes for Targeting Live Microglial Cell Organelles**. ChemBioChem, 2022, 23, .	2.6	2
2	Monitoring phagocytic uptake of amyloid I ² into glial cell lysosomes in real time. Chemical Science, 2021, 12, 10901-10918.	7.4	19
3	Neurotoxic reactive astrocytes induce cell death via saturated lipids. Nature, 2021, 599, 102-107.	27.8	277
4	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	3.6	3
5	Graph-based machine learning interprets and predicts diagnostic isomer-selective ion-molecule reactions in tandem mass spectrometry. Chemical Science, 2020, 11, 11849-11858.	7.4	12
6	Accelerated Reactivity Mechanism and Interpretable Machine Learning Model of <i>N</i> -Sulfonylimines toward Fast Multicomponent Reactions. Organic Letters, 2020, 22, 8480-8486.	4.6	19
7	DUBS: A Framework for Developing Directory of Useful Benchmarks Sets for Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4137-4143.	5.4	2
8	Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. Islets, 2020, 12, 99-107.	1.8	6
9	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	6.4	22
10	cando.py: Open Source Software for Predictive Bioanalytics of Large Scale Drug-Protein-Disease Data. Journal of Chemical Information and Modeling, 2020, 60, 4131-4136.	5.4	21
11	Spectral deep learning for prediction and prospective validation of functional groups. Chemical Science, 2020, 11, 4618-4630.	7.4	61
12	CANDOCK: Chemical Atomic Network-Based Hierarchical Flexible Docking Algorithm Using Generalized Statistical Potentials. Journal of Chemical Information and Modeling, 2020, 60, 1509-1527.	5.4	36
13	A 2-Tyrosyl-carboxylate Mononuclear Iron Center Forms the Active Site of a <i>Paracoccus</i> Dimethylformamidase. Angewandte Chemie - International Edition, 2020, 59, 16961-16966.	13.8	14
14	A 2-Tyrosyl-carboxylate Mononuclear Iron Center Forms the Active Site of a <i>Paracoccus</i> Dimethylformamidase. Angewandte Chemie, 2020, 132, 17109-17114.	2.0	0
15	Lemon: a framework for rapidly mining structural information from the Protein Data Bank. Bioinformatics, 2019, 35, 4165-4167.	4.1	5
16	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	3.3	18
17	Rapid, Refined, and Robust Method for Expression, Purification, and Characterization of Recombinant Human Amyloid beta 1-42. Methods and Protocols, 2019, 2, 48.	2.0	13
18	Integrated Pan-Cancer Map of EBV-Associated Neoplasms Reveals Functional Host-Virus Interactions. Cancer Research, 2019, 79, 6010-6023.	0.9	43

#	ARTICLE	IF	CITATIONS
19	Virtual Reality Environment to Visualize and Manipulate Molecular Structures. <i>Biophysical Journal</i> , 2018, 114, 184a.	0.5	1
20	CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. <i>Biophysical Journal</i> , 2018, 114, 57a.	0.5	3
21	Targeting Proteome-Scale Networks to Design and Synthesize Potent Anticancer and Cell-Specific Immunomodulatory Compounds. <i>Biophysical Journal</i> , 2018, 114, 663a.	0.5	0
22	Live Cell Surface Conjugation Methods for Imaging, Sensing and Therapy. <i>Biophysical Journal</i> , 2018, 114, 20a.	0.5	1
23	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. <i>Scientific Reports</i> , 2018, 8, 9939.	3.3	19
24	Identification of New FLT3 Inhibitors That Potently Inhibit AML Cell Lines via an Azo Click-It/Staple-It Approach. <i>ACS Medicinal Chemistry Letters</i> , 2017, 8, 492-497.	2.8	16
25	Inhibition of 12/15-Lipoxygenase Protects Against β -Cell Oxidative Stress and Glycemic Deterioration in Mouse Models of Type 1 Diabetes. <i>Diabetes</i> , 2017, 66, 2875-2887.	0.6	34
26	Abstract A35: Drug repurposing for castration resistant prostate cancer based on disease-disease relationships. , 2017, . .		1
27	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. <i>Molecules</i> , 2016, 21, 1537.	3.8	46
28	CD28 Costimulation: From Mechanism to Therapy. <i>Immunity</i> , 2016, 44, 973-988.	14.3	607
29	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. <i>Current Pharmaceutical Design</i> , 2016, 22, 3109-3123.	1.9	50
30	Multiscale Modelling of Relationships between Protein Classes and Drug Behavior Across all Diseases Using the CANDO Platform. <i>Mini-Reviews in Medicinal Chemistry</i> , 2015, 15, 705-717.	2.4	34
31	Oxido-reductive regulation of vascular remodeling by receptor tyrosine kinase ROS1. <i>Journal of Clinical Investigation</i> , 2014, 124, 5159-5174.	8.2	38
32	CANDO and the infinite drug discovery frontier. <i>Drug Discovery Today</i> , 2014, 19, 1353-1363.	6.4	67
33	Distal Effect of Amino Acid Substitutions in CYP2C9 Polymorphic Variants Causes Differences in Interatomic Interactions against (S)-Warfarin. <i>PLoS ONE</i> , 2013, 8, e74053.	2.5	16
34	KoBaMIN: a knowledge-based minimization web server for protein structure refinement. <i>Nucleic Acids Research</i> , 2012, 40, W323-W328.	14.5	124
35	Consistent refinement of submitted models at CASP using a knowledge-based potential. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2668-2678.	2.6	46
36	Solvent dramatically affects protein structure refinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 20239-20244.	7.1	99