Gaurav Chopra

List of Publications by Year
in descending order

36	1,800	516710 16	395702 33
papers	citations	h-index	g-index

70	70	70	2861
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CD28 Costimulation: From Mechanism to Therapy. Immunity, 2016, 44, 973-988.	14.3	607
2	Neurotoxic reactive astrocytes induce cell death via saturated lipids. Nature, 2021, 599, 102-107.	27.8	277
3	KoBaMIN: a knowledge-based minimization web server for protein structure refinement. Nucleic Acids Research, 2012, 40, W323-W328.	14.5	124
4	Solvent dramatically affects protein structure refinement. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20239-20244.	7.1	99
5	CANDO and the infinite drug discovery frontier. Drug Discovery Today, 2014, 19, 1353-1363.	6.4	67
6	Spectral deep learning for prediction and prospective validation of functional groups. Chemical Science, 2020, 11, 4618-4630.	7.4	61
7	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123.	1.9	50
8	Consistent refinement of submitted models at CASP using a knowledgeâ€based potential. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2668-2678.	2.6	46
9	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. Molecules, 2016, 21, 1537.	3.8	46
10	Integrated Pan-Cancer Map of EBV-Associated Neoplasms Reveals Functional Hostâ€“Virus Interactions. Cancer Research, 2019, 79, 6010-6023.	0.9	43
11	Oxido-reductive regulation of vascular remodeling by receptor tyrosine kinase ROS1. Journal of Clinical Investigation, 2014, 124, 5159-5174.	8.2	38
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	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.	0.6	34
14	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.	2.4	34
15	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	6.4	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.	5.4	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.	3.3	19
18	Accelerated Reactivity Mechanism and Interpretable Machine Learning Model of N-Sulfonylimines toward Fast Multicomponent Reactions. Organic Letters, 2020, 22, 8480-8486.	4.6	19

#	Article	IF	Citations
19	Monitoring phagocytic uptake of amyloid Î² into glial cell lysosomes in real time. Chemical Science, 2021, 12, 10901-10918.	7.4	19
20	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	3.3	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.	2.8	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.	2.5	16
23	A 2â€Tyrâ€1â€carboxylate Mononuclear Iron Center Forms the Active Site of a Paracoccus Dimethylformamidase. Angewandte Chemie - International Edition, 2020, 59, 16961-16966.	13.8	14
24	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
25	Graph-based machine learning interprets and predicts diagnostic isomer-selective ionâ€“molecule reactions in tandem mass spectrometry. Chemical Science, 2020, 11, 11849-11858.	7.4	12
26	Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. Islets, 2020, 12, 99-107.	1.8	6
27	Lemon: a framework for rapidly mining structural information from the Protein Data Bank. Bioinformatics, 2019, 35, 4165-4167.	4.1	5
28	CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. Biophysical Journal, 2018, 114, 57a.	0.5	3
29	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	3.6	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.	5.4	2
31	One Scaffold, Different Organelle Sensors: pHâ€Activable Fluorescent Probes for Targeting Live Microglial Cell Organelles**. ChemBioChem, 2022, 23, .	2.6	2
32	Virtual Reality Environment to Visualize and Manipulate Molecular Structures. Biophysical Journal, 2018, 114, 184a.	0.5	1
33	Live Cell Surface Conjugation Methods for Imaging, Sensing and Therapy. Biophysical Journal, 2018, 114, 20a.	0.5	1
34	Abstract A35: Drug repurposing for castration resistant prostate cancer based on disease-disease relationships. , 2017, , .		1
35	Targeting Proteome-Scale Networks to Design and Synthesize Potent Anticancer and Cell-Specific Immunomodulatory Compounds. Biophysical Journal, 2018, 114, 663a.	0.5	0
36	A 2â€Tyrâ€1â€carboxylate Mononuclear Iron Center Forms the Active Site of a Paracoccus Dimethylformamidase. Angewandte Chemie, 2020, 132, 17109-17114.	2.0	0