# Gaurav Chopra

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 36 papers | 1,800 citations | 516215 16 h-index | 395343 33 g-index |
| 70 all docs | 70 docs citations | 70 times ranked | 2861 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 | Neurotoxic reactive astrocytes induce cell death via saturated lipids. Nature, 2021, 599, 102-107. | 13.7 | 277 |
| 4 | Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513. | 1.8 | 3 |
| 5 | Graph-based machine learning interprets and predicts diagnostic isomer-selective ionâ€“molecule reactions in tandem mass spectrometry. Chemical Science, 2020, 11, 11849-11858. | 3.7 | 12 |
| 6 | Accelerated Reactivity Mechanism and Interpretable Machine Learning Model of N-Sulfonylimines toward Fast Multicomponent Reactions. Organic Letters, 2020, 22, 8480-8486. | 2.4 | 19 |
| 7 | 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 |
| 8 | Targeting polyamine biosynthesis to stimulate beta cell regeneration in zebrafish. Islets, 2020, 12, 99-107. | 0.9 | 6 |
| 9 | Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128. | 3.2 | 22 |
| 10 | 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 |
| 11 | Spectral deep learning for prediction and prospective validation of functional groups. Chemical Science, 2020, 11, 4618-4630. | 3.7 | 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. | 2.5 | 36 |
| 13 | 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 |
| 14 | A 2â€Tyrâ€1â€carboxylate Mononuclear Iron Center Forms the Active Site of a Paracoccus Dimethylformamidase. Angewandte Chemie, 2020, 132, 17109-17114. | 1.6 | 0 |
| 15 | Lemon: a framework for rapidly mining structural information from the Protein Data Bank. Bioinformatics, 2019, 35, 4165-4167. | 1.8 | 5 |
| 16 | Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155. | 1.6 | 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. | 0.9 | 13 |
| 18 | Integrated Pan-Cancer Map of EBV-Associated Neoplasms Reveals Functional Hostâ€“Virus Interactions. Cancer Research, 2019, 79, 6010-6023. | 0.4 | 43 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Virtual Reality Environment to Visualize and Manipulate Molecular Structures. Biophysical Journal, 2018, 114, 184a. | 0.2 | 1 |
| 20 | CANDOCK: Conformational Entropy Driven Analytics for Class-Specific Proteome-Wide Docking. Biophysical Journal, 2018, 114, 57a. | 0.2 | 3 |
| 21 | Targeting Proteome-Scale Networks to Design and Synthesize Potent Anticancer and Cell-Specific Immunomodulatory Compounds. Biophysical Journal, 2018, 114, 663a. | 0.2 | 0 |
| 22 | Live Cell Surface Conjugation Methods for Imaging, Sensing and Therapy. Biophysical Journal, 2018, 114, 20a. | 0.2 | 1 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 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. Molecules, 2016, 21, 1537. | 1.7 | 46 |
| 28 | CD28 Costimulation: From Mechanism to Therapy. Immunity, 2016, 44, 973-988. | 6.6 | 607 |
| 29 | Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123. | 0.9 | 50 |
| 30 | 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 |
| 31 | Oxido-reductive regulation of vascular remodeling by receptor tyrosine kinase ROS1. Journal of Clinical Investigation, 2014, 124, 5159-5174. | 3.9 | 38 |
| 32 | CANDO and the infinite drug discovery frontier. Drug Discovery Today, 2014, 19, 1353-1363. | 3.2 | 67 |
| 33 | 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 |
| 34 | KoBaMIN: a knowledge-based minimization web server for protein structure refinement. Nucleic Acids Research, 2012, 40, W323-W328. | 6.5 | 124 |
| 35 | Consistent refinement of submitted models at CASP using a knowledgeâ€based potential. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2668-2678. | 1.5 | 46 |
| 36 | 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 |