Ray Unwalla

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5167054/publications.pdf

Version: 2024-02-01

9 papers	528 citations	1040056 9 h-index	1474206 9 g-index
9 all docs	9 docs citations	9 times ranked	815 citing authors

#	Article	IF	Citations
1	TorsionNet: A Deep Neural Network to Rapidly Predict Small-Molecule Torsional Energy Profiles with the Accuracy of Quantum Mechanics. Journal of Chemical Information and Modeling, 2022, 62, 785-800.	5.4	16
2	Comprehensive Assessment of Torsional Strain in Crystal Structures of Small Molecules and Proteinâ€“Ligand Complexes using ab Initio Calculations. Journal of Chemical Information and Modeling, 2019, 59, 4195-4208.	5.4	23
3	Identification of N-{cis-3-[Methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclobutyl}propane-1-sulfonamide (PF-04965842): A Selective JAK1 Clinical Candidate for the Treatment of Autoimmune Diseases. Journal of Medicinal Chemistry, 2018, 61, 1130-1152.	6.4	115
4	Identification of Cyanamide-Based Janus Kinase 3 (JAK3) Covalent Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 10665-10699.	6.4	55
5	Discovery of 3-Cyano-N-(3-(1-isobutyrylpiperidin-4-yl)-1-methyl-4-(trifluoromethyl)-1H-pyrrolo[2,3-b]pyridin-5-yl)benzamide: A Potent, Selective, and Orally Bioavailable Retinoic Acid Receptor-Related Orphan Receptor C2 Inverse Agonist. Journal of Medicinal Chemistry, 2018, 61, 10415-10439.	6.4	26
6	Design of a Janus Kinase 3 (JAK3) Specific Inhibitor 1-((2S,5R)-5-((7H-Pyrrolo[2,3-d]pyrimidin-4-yl)amino)-2-methylpiperidin-1-yl)prop-2-en-1-one (PF-06651600) Allowing for the Interrogation of JAK3 Signaling in Humans. Journal of Medicinal Chemistry, 2017, 60, 1971-1993.	6.4	111
7	Millisecond dynamics of BTK reveal kinome-wide conformational plasticity within the apo kinase domain. Scientific Reports, 2017, 7, 15604.	3.3	43
8	Structure-Based Approach To Identify 5-[4-Hydroxyphenyl]pyrrole-2-carbonitrile Derivatives as Potent and Tissue Selective Androgen Receptor Modulators. Journal of Medicinal Chemistry, 2017, 60, 6451-6457.	6.4	12
9	Discovery of a JAK3-Selective Inhibitor: Functional Differentiation of JAK3-Selective Inhibition over pan-JAK or JAK1-Selective Inhibition. ACS Chemical Biology, 2016, 11, 3442-3451.	3.4	127