I-Jen Chen

List of Publications by Year
in descending order

22 papers	1,693 citations	623734 14 h-index	713466 21 g-index
22 all docs	22 docs citations	22 times ranked	3407 citing authors

#	Article	IF	Citations
1	The MCL1 inhibitor S63845 is tolerable and effective in diverse cancer models. Nature, 2016, 538, 477-482.	27.8	830
2	Drug-like Bioactive Structures and Conformational Coverage with the LigPrep/ConfGen Suite: Comparison to Programs MOE and Catalyst. Journal of Chemical Information and Modeling, 2010, 50, 822-839.	5.4	142
3	Conformational Sampling of Druglike Molecules with MOE and Catalyst: Implications for Pharmacophore Modeling and Virtual Screening. Journal of Chemical Information and Modeling, 2008, 48, 1773-1791.	5.4	122
4	S55746 is a novel orally active BCL-2 selective and potent inhibitor that impairs hematological tumor growth. Oncotarget, 2018, 9, 20075-20088.	1.8	82
5	Tackling the conformational sampling of larger flexible compounds and macrocycles in pharmacology and drug discovery. Bioorganic and Medicinal Chemistry, 2013, 21, 7898-7920.	3.0	79
6	Conformational Sampling and Energetics of Drug-Like Molecules. Current Medicinal Chemistry, 2009, 16, 3381-3413.	2.4	67
7	Structure-Guided Discovery of a Selective Mcl-1 Inhibitor with Cellular Activity. Journal of Medicinal Chemistry, 2019, 62, 6913-6924.	6.4	45
8	Discovery of S64315, a Potent and Selective Mcl-1 Inhibitor. Journal of Medicinal Chemistry, 2020, 63, 13762-13795.	6.4	43
9	Computation of the influence of chemical substitution on the p K a of pyridine using semiempirical and ab initio methods. Theoretical Chemistry Accounts, 2000, 103, 483-494.	1.4	42
10	Design of Leucine-Rich Repeat Kinase 2 (LRRK2) Inhibitors Using a Crystallographic Surrogate Derived from Checkpoint Kinase 1 (CHK1). Journal of Medicinal Chemistry, 2017, 60, 8945-8962.	6.4	41
11	Establishing Drug Discovery and Identification of Hit Series for the Anti-apoptotic Proteins, Bcl-2 and Mcl-1. ACS Omega, 2019, 4, 8892-8906.	3.5	35
12	Structure-Based Inhibitor Design Targeting HIV-1 Integrase. Current Drug Targets Infectious Disorders, 2002, 2, 217-234.	2.1	32
13	Towards understanding the unbound state of drug compounds: Implications for the intramolecular reorganization energy upon binding. Bioorganic and Medicinal Chemistry, 2016, 24, 2159-2189.	3.0	29
14	Is conformational sampling of drugâ€like molecules a solved problem?. Drug Development Research, 2011, 72, 85-94.	2.9	25
15	Design and Synthesis of Pyrrolo[2,3-d]pyrimidine-Derived Leucine-Rich Repeat Kinase 2 (LRRK2) Inhibitors Using a Checkpoint Kinase 1 (CHK1)-Derived Crystallographic Surrogate. Journal of Medicinal Chemistry, 2021, 64, 10312-10332.	6.4	21
16	The design and SAR of a novel series of 2-aminopyridine based LRRK2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4500-4505.	2.2	15
17	Modelling the binding mode of macrocycles: Docking and conformational sampling. Bioorganic and Medicinal Chemistry, 2020, 28, 115143.	3.0	12
18	Chemical Substituent Effect on Pyridine Permeability and Mechanistic Insight from Computational Molecular Descriptors. Molecular Pharmaceutics, 2006, 3, 745-755.	4.6	10

#	Article	IF	Citations
19	Energy windows for computed compound conformers: covering artefacts or truly large reorganization energies?. Future Medicinal Chemistry, 2019, 11, 97-118.	2.3	10
20	Exploring IDPâ€“Ligand Interactions: Tau K18 as a Test Case. International Journal of Molecular Sciences, 2020, 21, 5257.	4.1	9
21	The reorganization energy of compounds upon binding to proteins, from dynamic and solvated bound and unbound states. Bioorganic and Medicinal Chemistry, 2021, 51, 116464.	3.0	2
22	The Effect of Core Replacement on S64315, a Selective MCL-1 Inhibitor, and Its Analogues. ACS Omega, 2021, 6, 22073-22102.	3.5	0