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	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
2	The Effect of Core Replacement on S64315, a Selective MCL-1 Inhibitor, and Its Analogues. ACS Omega, 2021, 6, 22073-22102.	3.5	0
3	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
4	Modelling the binding mode of macrocycles: Docking and conformational sampling. Bioorganic and Medicinal Chemistry, 2020, 28, 115143.	3.0	12
5	Exploring IDPâ€“Ligand Interactions: Tau K18 as a Test Case. International Journal of Molecular Sciences, 2020, 21, 5257.	4.1	9
6	Discovery of S64315, a Potent and Selective Mcl-1 Inhibitor. Journal of Medicinal Chemistry, 2020, 63, 13762-13795.	6.4	43
7	Energy windows for computed compound conformers: covering artefacts or truly large reorganization energies?. Future Medicinal Chemistry, 2019, 11, 97-118.	2.3	10
8	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
9	Structure-Guided Discovery of a Selective Mcl-1 Inhibitor with Cellular Activity. Journal of Medicinal Chemistry, 2019, 62, 6913-6924.	6.4	45
10	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
11	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
12	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
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	The MCL1 inhibitor S63845 is tolerable and effective in diverse cancer models. Nature, 2016, 538, 477-482.	27.8	830
15	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
16	Is conformational sampling of drugâ€like molecules a solved problem?. Drug Development Research, 2011, 72, 85-94.	2.9	25
17	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
18	Conformational Sampling and Energetics of Drug-Like Molecules. Current Medicinal Chemistry, 2009, 16, 3381-3413.	2.4	67

#	Article	IF	Citations
19	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
20	Chemical Substituent Effect on Pyridine Permeability and Mechanistic Insight from Computational Molecular Descriptors. Molecular Pharmaceutics, 2006, 3, 745-755.	4.6	10
21	Structure-Based Inhibitor Design Targeting HIV-1 Integrase. Current Drug Targets Infectious Disorders, 2002, 2, 217-234.	2.1	32
22	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