Paul N Mortenson

List of Publications by Year
in descending order

30 papers	2,106 citations	331670 21 h-index	434195 31 g-index
32 all docs	32 docs citations	32 times ranked	2879 citing authors

#	Article	IF	Citations
1	ParaMol: A Package for Automatic Parameterization of Molecular Mechanics Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 2026-2047.	5.4	22
2	A knowledge-based, structural-aided discovery of a novel class of 2-phenylimidazo[1,2-a]pyridine-6-carboxamide H-PGDS inhibitors. Bioorganic and Medicinal Chemistry Letters, 2021, 47, 128113.	2.2	3
3	Câ€“H functionalisation tolerant to polar groups could transform fragment-based drug discovery (FBDD). Chemical Science, 2021, 12, 11976-11985.	7.4	30
4	Generation of Quantum Configurational Ensembles Using Approximate Potentials. Journal of Chemical Theory and Computation, 2021, 17, 7021-7042.	5.3	2
5	Fragment-to-Lead Medicinal Chemistry Publications in 2018. Journal of Medicinal Chemistry, 2020, 63, 4430-4444.	6.4	61
6	The exploration of aza-quinolines as hematopoietic prostaglandin D synthase (H-PGDS) inhibitors with low brain exposure. Bioorganic and Medicinal Chemistry, 2020, 28, 115791.	3.0	4
7	Fragment-to-Lead Medicinal Chemistry Publications in 2019. Journal of Medicinal Chemistry, 2020, 63, 15494-15507.	6.4	41
8	Structureâ€“Activity and Structureâ€“Conformation Relationships of Aryl Propionic Acid Inhibitors of the Kelch-like ECH-Associated Protein 1/Nuclear Factor Erythroid 2-Related Factor 2 (KEAP1/NRF2) Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2019, 62, 4683-4702.	6.4	59
9	The discovery of quinoline-3-carboxamides as hematopoietic prostaglandin D synthase (H-PGDS) inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 1456-1478.	3.0	17
10	Fragment-to-Lead Medicinal Chemistry Publications in 2017. Journal of Medicinal Chemistry, 2019, 62, 3857-3872.	6.4	47
11	Fragment-to-Lead Medicinal Chemistry Publications in 2016. Journal of Medicinal Chemistry, 2018, 61, 1774-1784.	6.4	41
12	Predicting â€œHotâ€•and â€œWarmâ€•Spots for Fragment Binding. Journal of Medicinal Chemistry, 2017, 60, 4036-4046.	6.4	32
13	Fragment-Based Discovery of Potent and Selective DDR1/2 Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 798-803.	2.8	49
14	Allosteric Inhibition of the Neuropeptidase Neurolysin. Journal of Biological Chemistry, 2014, 289, 35605-35619.	3.4	18
15	Efficient exploration of chemical space by fragment-based screening. Progress in Biophysics and Molecular Biology, 2014, 116, 82-91.	2.9	127
16	Fragment-Based Approaches to the Discovery of Kinase Inhibitors. Methods in Enzymology, 2014, 548, 69-92.	1.0	13
17	Identification of orally bioavailable small-molecule inhibitors of hematopoietic prostaglandin D2 synthase using X-ray fragment based drug discovery. MedChemComm, 2014, 5, 134-141.	3.4	8
18	Fragment-Based Discovery of 6-Azaindazoles As Inhibitors of Bacterial DNA Ligase. ACS Medicinal Chemistry Letters, 2013, 4, 1208-1212.	2.8	21

#	Article	IF	Citations
19	Fragment-Based Discovery of 7-Azabenzimidazoles as Potent, Highly Selective, and Orally Active CDK4/6 Inhibitors. ACS Medicinal Chemistry Letters, 2012, 3, 445-449.	2.8	34
20	Docking Performance of Fragments and Druglike Compounds. Journal of Medicinal Chemistry, 2011, 54, 5422-5431.	6.4	109
21	Assessing the lipophilicity of fragments and early hits. Journal of Computer-Aided Molecular Design, 2011, 25, 663-667.	2.9	95
22	Discovery of 2-(6-{[(6-Fluoroquinolin-2-yl)methyl]amino}bicyclo[3.1.0]hex-3-yl)-N-hydroxypyrimidine-5-carboxamide (CHR-3996), a Class I Selective Orally Active Histone Deacetylase Inhibitor. Journal of Medicinal Chemistry, 2010, 53, 8663-8678.	6.4	74
23	DNA gyrase (GyrB)/topoisomerase IV (ParE) inhibitors: Synthesis and antibacterial activity. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 894-899.	2.2	70
24	Discovery of novel inhibitors of Trypanosoma cruzi trans-sialidase from in silico screening. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 589-596.	2.2	68
25	Proteinâ~Ligand Docking against Non-Native Protein Conformers. Journal of Chemical Information and Modeling, 2008, 48, 2214-2225.	5.4	129
26	Energy Landscapes: From Clusters to Biomolecules. Advances in Chemical Physics, 2007, , 1-111.	0.3	153
27	Diverse, High-Quality Test Set for the Validation of Proteinâ~Ligand Docking Performance. Journal of Medicinal Chemistry, 2007, 50, 726-741.	6.4	546
28	Energy landscapes of model polyalanines. Journal of Chemical Physics, 2002, 117, 1363-1376.	3.0	78
29	Energy landscapes, global optimization and dynamics of the polyalanine Ac(ala)8NHMe. Journal of Chemical Physics, 2001, 114, 6443-6454.	3.0	77
30	Crystals of binary Lennard-Jones solids. Physical Review B, 2001, 64, .	3.2	77