Stefan G Krimmer

List of Publications by Year
in descending order

21	614	686830 13	713013 21
papers	citations	h-index	g-index

23	23	23	1036
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Six Biophysical Screening Methods Miss a Large Proportion of Crystallographically Discovered Fragment Hits: A Case Study. ACS Chemical Biology, 2016, 11, 1693-1701.	1.6	87
2	Methyl, Ethyl, Propyl, Butyl: Futile But Not for Water, as the Correlation of Structure and Thermodynamic Signature Shows in a Congeneric Series of Thermolysin Inhibitors. ChemMedChem, 2014, 9, 833-846.	1.6	70
3	Rational Design of Thermodynamic and Kinetic Binding Profiles by Optimizing Surface Water Networks Coating Protein-Bound Ligands. Journal of Medicinal Chemistry, 2016, 59, 10530-10548.	2.9	64
4	High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits. Structure, 2016, 24, 1398-1409.	1.6	62
5	Thermodynamics of proteinâ€“ligand interactions as a reference for computational analysis: how to assess accuracy, reliability and relevance of experimental data. Journal of Computer-Aided Molecular Design, 2015, 29, 867-883.	1.3	54
6	Paying the Price of Desolvation in Solvent-Exposed Protein Pockets: Impact of Distal Solubilizing Groups on Affinity and Binding Thermodynamics in a Series of Thermolysin Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 5791-5799.	2.9	35
7	Synthesis and Characterization of Poly(ÎµÂ€caprolactone)Â€‹blockÂ€poly[NÂ€(2Â€hydroxypropyl)methacrylamide] Micelles for Drug Delivery. Macromolecular Bioscience, 2011, 11, 1041-1051.	2.1	33
8	Impact of Surface Water Layers on Proteinâ€“Ligand Binding: How Well Are Experimental Data Reproduced by Molecular Dynamics Simulations in a Thermolysin Test Case?. Journal of Chemical Information and Modeling, 2016, 56, 223-233.	2.5	29
9	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224.	1.1	24
10	How Nothing Boosts Affinity: Hydrophobic Ligand Binding to the Virtually Vacated S₁Â€² Pocket of Thermolysin. Journal of the American Chemical Society, 2017, 139, 10419-10431.	6.6	23
11	Structural basis for ligand reception by anaplastic lymphoma kinase. Nature, 2021, 600, 148-152.	13.7	21
12	Selective Janus Kinase 2 (JAK2) Pseudokinase Ligands with a Diaminotriazole Core. Journal of Medicinal Chemistry, 2020, 63, 5324-5340.	2.9	17
13	Experimental Active-Site Mapping by Fragments: Hot Spots Remote from the Catalytic Center of Endothiapepsin. Journal of Medicinal Chemistry, 2016, 59, 7561-7575.	2.9	14
14	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. ACS Chemical Biology, 2017, 12, 225-233.	1.6	14
15	Optimization of Pyrazoles as Phenol Surrogates to Yield Potent Inhibitors of Macrophage Migration Inhibitory Factor. ChemMedChem, 2018, 13, 1092-1097.	1.6	14
16	Active Site Mapping of an Aspartic Protease by Multiple Fragment Crystal Structures: Versatile Warheads To Address a Catalytic Dyad. Journal of Medicinal Chemistry, 2016, 59, 9743-9759.	2.9	12
17	Metadynamics as a Postprocessing Method for Virtual Screening with Application to the Pseudokinase Domain of JAK2. Journal of Chemical Information and Modeling, 2020, 60, 4403-4415.	2.5	12
18	Adding a Hydrogen Bond May Not Help: Naphthyridinone vs Quinoline Inhibitors of Macrophage Migration Inhibitory Factor. ACS Medicinal Chemistry Letters, 2017, 8, 1287-1291.	1.3	8

#	Article	IF	Citations
19	Indoloxytriazines as binding molecules for the JAK2 JH2 pseudokinase domain and its V617F variant. Tetrahedron Letters, 2021, 77, 153248.	0.7	7
20	Insights on JAK2 Modulation by Potent, Selective, and Cell-Permeable Pseudokinase-Domain Ligands. Journal of Medicinal Chemistry, 2022, 65, 8380-8400.	2.9	7
21	Conversion of a False Virtual Screen Hit into Selective JAK2 JH2 Domain Binders Using Convergent Design Strategies. ACS Medicinal Chemistry Letters, 2022, 13, 819-826.	1.3	6