# 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 | 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 |
| 2 | Insights on JAK2 Modulation by Potent, Selective, and Cell-Permeable Pseudokinase-Domain Ligands. Journal of Medicinal Chemistry, 2022, 65, 8380-8400. | 2.9 | 7 |
| 3 | Indoloxytriazines as binding molecules for the JAK2 JH2 pseudokinase domain and its V617F variant. Tetrahedron Letters, 2021, 77, 153248. | 0.7 | 7 |
| 4 | Structural basis for ligand reception by anaplastic lymphoma kinase. Nature, 2021, 600, 148-152. | 13.7 | 21 |
| 5 | 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 |
| 6 | Selective Janus Kinase 2 (JAK2) Pseudokinase Ligands with a Diaminotriazole Core. Journal of Medicinal Chemistry, 2020, 63, 5324-5340. | 2.9 | 17 |
| 7 | Optimization of Pyrazoles as Phenol Surrogates to Yield Potent Inhibitors of Macrophage Migration Inhibitory Factor. ChemMedChem, 2018, 13, 1092-1097. | 1.6 | 14 |
| 8 | Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224. | 1.1 | 24 |
| 9 | Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. ACS Chemical Biology, 2017, 12, 225-233. | 1.6 | 14 |
| 10 | 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 |
| 11 | How Nothing Boosts Affinity: Hydrophobic Ligand Binding to the Virtually Vacated S<sub>1</sub>â€² Pocket of Thermolysin. Journal of the American Chemical Society, 2017, 139, 10419-10431. | 6.6 | 23 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits. Structure, 2016, 24, 1398-1409. | 1.6 | 62 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |