Andreas Heine

List of Publications by Year
in descending order

53 papers	1,285 citations	361045 20 h-index	377514 34 g-index
54 all docs	54 docs citations	54 times ranked	2015 citing authors

#	Article	IF	Citations
1	Expect the Unexpected or Caveat for Drug Designers: Multiple Structure Determinations Using Aldose Reductase Crystals Treated under Varying Soaking and Co-crystallisation Conditions. Journal of Molecular Biology, 2006, 363, 174-187.	2.0	101
2	A Small Nonrule of 3 Compatible Fragment Library Provides High Hit Rate of Endothiapepsin Crystal Structures with Various Fragment Chemotypes. Journal of Medicinal Chemistry, 2011, 54, 7784-7796.	2.9	97
3	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
4	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
5	Structure of Active Coagulation Factorâ€…XIII Triggered by Calcium Binding: Basis for the Design of Nextâ€Generation Anticoagulants. Angewandte Chemie - International Edition, 2013, 52, 11930-11934.	7.2	62
6	High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits. Structure, 2016, 24, 1398-1409.	1.6	62
7	Kinetic and Structural Insights into the Mechanism of Binding of Sulfonamides to Human Carbonic Anhydrase by Computational and Experimental Studies. Journal of Medicinal Chemistry, 2016, 59, 4245-4256.	2.9	60
8	Crystal Structures of tRNA-guanine Transglycosylase (TGT) in Complex with Novel and Potent Inhibitors Unravel Pronounced Induced-fit Adaptations and Suggest Dimer Formation Upon Substrate Binding. Journal of Molecular Biology, 2007, 370, 492-511.	2.0	57
9	One Question, Multiple Answers: Biochemical and Biophysical Screening Methods Retrieve Deviating Fragment Hit Lists. ChemMedChem, 2015, 10, 1511-1521.	1.6	54
10	Identification of Novel Aldose Reductase Inhibitors Based on Carboxymethylated Mercaptotriazinoindole Scaffold. Journal of Medicinal Chemistry, 2015, 58, 2649-2657.	2.9	42
11	Fragment Binding Can Be Either More Enthalpy-Driven or Entropy-Driven: Crystal Structures and Residual Hydration Patterns Suggest Why. Journal of Medicinal Chemistry, 2015, 58, 6960-6971.	2.9	37
12	Thermodynamic signatures of fragment binding: Validation of direct versus displacement ITC titrations. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 647-656.	1.1	36
13	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drugâ€“Kinase Binding. Journal of Medicinal Chemistry, 2018, 61, 5922-5933.	2.9	36
14	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
15	Soaking suggests â€œalternative factsâ€: Only co-crystallization discloses major ligand-induced interface rearrangements of a homodimeric tRNA-binding protein indicating a novel mode-of-inhibition. PLoS ONE, 2017, 12, e0175723.	1.1	30
16	Structures of endothiapepsinâ€“fragment complexes from crystallographic fragment screening using a novel, diverse and affordable 96-compound fragment library. Acta Crystallographica Section F, Structural Biology Communications, 2016, 72, 346-355.	0.4	29
17	Structureâ€Based Macrocyclization of Substrate Analogue NS2Bâ€NS3 Protease Inhibitors of Zika, West Nile and Dengue viruses. ChemMedChem, 2020, 15, 1439-1452.	1.6	29
18	Tracing Binding Modes in Hitâ€toâ€Lead Optimization: Chameleonâ€Like Poses of Aspartic Protease Inhibitors. Angewandte Chemie - International Edition, 2015, 54, 2849-2853.	7.2	27

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19	F2X-Universal and F2X-Entry: Structurally Diverse Compound Libraries for Crystallographic Fragment Screening. Structure, 2020, 28, 694-706.e5.	1.6	27
20	Chasing Protons: How Isothermal Titration Calorimetry, Mutagenesis, and pK_a Calculations Trace the Locus of Charge in Ligand Binding to a tRNA-Binding Enzyme. Journal of Medicinal Chemistry, 2014, 57, 5554-5565.	2.9	26
21	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
22	Two Methods, One Goal: Structural Differences between Cocrystallization and Crystal Soaking to Discover Ligand Binding Poses. ChemMedChem, 2021, 16, 292-300.	1.6	19
23	Charges Shift Protonation: Neutron Diffraction Reveals that Aniline and 2â€Aminopyridine Become Protonated Upon Binding to Trypsin. Angewandte Chemie - International Edition, 2017, 56, 4887-4890.	7.2	18
24	Investigation of Specificity Determinants in Bacterial tRNA-Guanine Transglycosylase Reveals Queuine, the Substrate of Its Eucaryotic Counterpart, as Inhibitor. PLoS ONE, 2013, 8, e64240.	1.1	16
25	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
26	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. ACS Chemical Biology, 2017, 12, 225-233.	1.6	14
27	Surprising Non-Additivity of Methyl Groups in Drugâ€“Kinase Interaction. ACS Chemical Biology, 2019, 14, 2585-2594.	1.6	14
28	Glutamate versus Glutamine Exchange Swaps Substrate Selectivity in tRNA-Guanine Transglycosylase: Insight into the Regulation of Substrate Selectivity by Kinetic and Crystallographic Studies. Journal of Molecular Biology, 2007, 374, 764-776.	2.0	12
29	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
30	Frag4Lead: growing crystallographic fragment hits by catalog using fragment-guided template docking. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1168-1182.	1.1	11
31	High-affinity inhibitors ofZymomonas mobilistRNAâ€“guanine transglycosylase through convergent optimization. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1798-1807.	2.5	10
32	Structural basis for catalysis and substrate specificity of a 3C-like cysteine protease from a mosquito mesonivirus. Virology, 2019, 533, 21-33.	1.1	10
33	Unraveling a Ligandâ€Induced Twist of a Homodimeric Enzyme by Pulsed Electronâ€“Electron Double Resonance. Angewandte Chemie - International Edition, 2021, 60, 23419-23426.	7.2	10
34	Swapping Interface Contacts in the Homodimeric tRNAâ€Guanine Transglycosylase: An Option for Functional Regulation. Angewandte Chemie - International Edition, 2018, 57, 10085-10090.	7.2	10
35	Replacement of Water Molecules in a Phosphate Binding Site by Furanosideâ€Appended linâ€Benzoguanine Ligands of tRNAâ€Guanine Transglycosylase (TGT). Chemistry - A European Journal, 2015, 21, 126-135.	1.7	8
36	On the Implication of Water on Fragmentâ€toâ€Ligand Growth in Kinase Binding Thermodynamics. ChemMedChem, 2018, 13, 1988-1996.	1.6	8

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37	Protein-Induced Change in Ligand Protonation during Trypsin and Thrombin Binding: Hint on Differences in Selectivity Determinants of Both Proteins?. Journal of Medicinal Chemistry, 2020, 63, 3274-3289.	2.9	8
38	Fragment Binding to Kinase Hinge: If Charge Distribution and Local pK_a Shifts Mislead Popular Bioisosterism Concepts. Angewandte Chemie - International Edition, 2021, 60, 252-258.	7.2	8
39	Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin. ChemMedChem, 2018, 13, 2266-2270.	1.6	7
40	Fragments as Novel Starting Points for tRNAâ€Guanine Transglycosylase Inhibitors Found by Alternative Screening Strategies. ChemMedChem, 2020, 15, 324-337.	1.6	7
41	Workflow and Tools for Crystallographic Fragment Screening at the Helmholtz-Zentrum Berlin. Journal of Visualized Experiments, 2021, , .	0.2	7
42	Structure-Based Optimization and Characterization of Macrocyclic Zika Virus NS2B-NS3 Protease Inhibitors. Journal of Medicinal Chemistry, 2022, 65, 6555-6572.	2.9	7
43	Structural and Biochemical Investigation of the Heterodimeric Murine tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 2229-2247.	1.6	7
44	Changing the selectivity profile â€“ from substrate analog inhibitors of thrombin and factor Xa to potent matriptase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 89-97.	2.5	6
45	A Proof-of-Concept Fragment Screening of a Hit-Validated 96-Compounds Library against Human Carbonic Anhydrase II. Biomolecules, 2020, 10, 518.	1.8	5
46	Ladungen verschieben Protonierungen: Neutronenbeugung zeigt, dass Anilin und 2â€Aminopyridin protoniert an Trypsin binden. Angewandte Chemie, 2017, 129, 4965-4969.	1.6	4
47	The Importance of Charge in Perturbing the Aromatic Glue Stabilizing the Proteinâ€“Protein Interface of Homodimeric tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2020, 15, 3021-3029.	1.6	3
48	Structureâ€Based Design of FXIIIaâ€Blockers: Addressing a Transient Hydrophobic Pocket in the Active Site of FXIIIa. ChemMedChem, 2020, 15, 900-905.	1.6	3
49	Austausch der ProteinkontaktflÃchen in der homodimeren tRNAâ€Guaninâ€Transglycosylase: ein Weg der funktionellen Regulation. Angewandte Chemie, 2018, 130, 10242-10247.	1.6	2
50	Targeting a Cryptic Pocket in a Proteinâ€“Protein Contact by Disulfide-Induced Rupture of a Homodimeric Interface. ACS Chemical Biology, 2021, 16, 1090-1098.	1.6	2
51	EntschlÃ¼sselung der ligandeninduzierten Verdrehung eines homodimeren Enzyms mit Hilfe der gepulsten Elektronâ€Elektronâ€Doppelresonanzâ€Spektroskopie. Angewandte Chemie, 2021, 133, 23607.	1.6	1
52	¹⁹F-NMR Unveils the Ligand-Induced Conformation of a Catalytically Inactive Twisted Homodimer of tRNAâ€“Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 1745-1755.	1.6	1
53	Fragmentâ€Bindung an die Kinaseâ€Scharnierâ€Region: Wenn Ladungsverteilung und lokale p K a â€Verschiebungen etablierte Bioisosterieâ€Konzepte fehlleiten. Angewandte Chemie, 2021, 133, 256-262.	1.6	0