Gerhard Klebe

List of Publications by Year
in descending order

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271 papers	22,636 citations	17440 63 h-index	9589 142 g-index
304 all docs	304 docs citations	304 times ranked	17897 citing authors

#	Article	IF	Citations
1	¹⁹F-NMR Unveils the Ligand-Induced Conformation of a Catalytically Inactive Twisted Homodimer of tRNAâ€“Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 1745-1755.	3.4	1
2	Structural and Biochemical Investigation of the Heterodimeric Murine tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 2229-2247.	3.4	7
3	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.	13.8	8
4	Two Methods, One Goal: Structural Differences between Cocrystallization and Crystal Soaking to Discover Ligand Binding Poses. ChemMedChem, 2021, 16, 292-300.	3.2	19
5	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.	2.0	0
6	Simultaneous determination of thermodynamic and kinetic data by isothermal titration calorimetry. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129772.	2.4	4
7	How a Fragment Draws Attention to Selectivity Discriminating Features between the Related Proteases Trypsin and Thrombin. Journal of Medicinal Chemistry, 2021, 64, 1611-1625.	6.4	2
8	The Basicity Makes the Difference: Improved Canavanine-Derived Inhibitors of the Proprotein Convertase Furin. ACS Medicinal Chemistry Letters, 2021, 12, 426-432.	2.8	11
9	Facilitated crystal handling using a simple device for evaporation reduction in microtiter plates. Journal of Applied Crystallography, 2021, 54, 376-382.	4.5	2
10	Workflow and Tools for Crystallographic Fragment Screening at the Helmholtz-Zentrum Berlin. Journal of Visualized Experiments, 2021, , .	0.3	7
11	Mapping Water Thermodynamics on Drug Candidates via Molecular Building Blocks: a Strategy to Improve Ligand Design and Rationalize SAR. Journal of Medicinal Chemistry, 2021, 64, 4662-4676.	6.4	5
12	Targeting a Cryptic Pocket in a Proteinâ€“Protein Contact by Disulfide-Induced Rupture of a Homodimeric Interface. ACS Chemical Biology, 2021, 16, 1090-1098.	3.4	2
13	OFF-State-Specific Inhibition of the Proprotein Convertase Furin. ACS Chemical Biology, 2021, 16, 1692-1700.	3.4	10
14	Frag4Lead: growing crystallographic fragment hits by catalog using fragment-guided template docking. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1168-1182.	2.3	11
15	Unraveling a Ligandâ€Induced Twist of a Homodimeric Enzyme by Pulsed Electronâ€“Electron Double Resonance. Angewandte Chemie - International Edition, 2021, 60, 23419-23426.	13.8	10
16	EntschlÃ¼sselung der ligandeninduzierten Verdrehung eines homodimeren Enzyms mit Hilfe der gepulsten Elektronâ€Elektronâ€Doppelresonanzâ€Spektroskopie. Angewandte Chemie, 2021, 133, 23607.	2.0	1
17	Which Properties Allow Ligands to Open and Bind to the Transient Binding Pocket of Human Aldose Reductase?. Biomolecules, 2021, 11, 1837.	4.0	5
18	Fragments as Novel Starting Points for tRNAâ€Guanine Transglycosylase Inhibitors Found by Alternative Screening Strategies. ChemMedChem, 2020, 15, 324-337.	3.2	7

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19	Advancing GIST-Based Solvent Functionals through Multiobjective Optimization of Solvent Enthalpy and Entropy Scoring Terms. Journal of Chemical Information and Modeling, 2020, 60, 6654-6665.	5.4	5
20	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.	3.4	3
21	Fragmentâ€Based Discovery of Nonâ€bisphosphonate Binders of Trypanosoma brucei Farnesyl Pyrophosphate Synthase. ChemBioChem, 2020, 21, 3096-3111.	2.6	8
22	Fragment Screening Hit Draws Attention to a Novel Transient Pocket Adjacent to the Recognition Site of the tRNA-Modifying Enzyme TGT. Journal of Medicinal Chemistry, 2020, 63, 6802-6820.	6.4	4
23	Structureâ€Based Design of FXIIIaâ€Blockers: Addressing a Transient Hydrophobic Pocket in the Active Site of FXIIIa. ChemMedChem, 2020, 15, 900-905.	3.2	3
24	Rapid Discovery of Aspartyl Protease Inhibitors Using an Anchoring Approach. ChemMedChem, 2020, 15, 680-684.	3.2	4
25	Role of Water Molecules in Proteinâ€"Ligand Dissociation and Selectivity Discrimination: Analysis of the Mechanisms and Kinetics of Biomolecular Solvation Using Molecular Dynamics. Journal of Chemical Information and Modeling, 2020, 60, 1818-1832.	5.4	11
26	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.	6.4	8
27	Proteinâ€"Ligand Complex Solvation Thermodynamics: Development, Parameterization, and Testing of GIST-Based Solvent Functionals. Journal of Chemical Information and Modeling, 2020, 60, 1409-1423.	5.4	17
28	Conformational Changes in Alkyl Chains Determine the Thermodynamic and Kinetic Binding Profiles of Carbonic Anhydrase Inhibitors. ACS Chemical Biology, 2020, 15, 675-685.	3.4	16
29	The Influence of Varying Fluorination Patterns on the Thermodynamics and Kinetics of Benzenesulfonamide Binding to Human Carbonic Anhydrase II. Biomolecules, 2020, 10, 509.	4.0	7
30	A Proof-of-Concept Fragment Screening of a Hit-Validated 96-Compounds Library against Human Carbonic Anhydrase II. Biomolecules, 2020, 10, 518.	4.0	5
31	F2X-Universal and F2X-Entry: Structurally Diverse Compound Libraries for Crystallographic Fragment Screening. Structure, 2020, 28, 694-706.e5.	3.3	27
32	Der Flaschenhals â€" von der Forschung zur Entwicklung. , 2020, , 73-115.		2
33	Surprising Non-Additivity of Methyl Groups in Drugâ€"Kinase Interaction. ACS Chemical Biology, 2019, 14, 2585-2594.	3.4	14
34	Strategies for Late-Stage Optimization: Profiling Thermodynamics by Preorganization and Salt Bridge Shielding. Journal of Medicinal Chemistry, 2019, 62, 9753-9771.	6.4	15
35	Broad-scale analysis of thermodynamic signatures in medicinal chemistry: are enthalpy-favored binders the better development option?. Drug Discovery Today, 2019, 24, 943-948.	6.4	21
36	Diamondoid Amino Acidâ€Based Peptide Kinaseâ€...A Inhibitor Analogues. ChemMedChem, 2019, 14, 663-672.	3.2	7

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37	Conceptional Design of Self-Assembling Bisubstrate-like Inhibitors of Protein Kinase A Resulting in a Boronic Acid Glutamate Linkage. ACS Omega, 2019, 4, 775-784.	3.5	10
38	Intriguing role of water in protein-ligand binding studied by neutron crystallography on trypsin complexes. Nature Communications, 2018, 9, 3559.	12.8	140
39	Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin. ChemMedChem, 2018, 13, 2266-2270.	3.2	7
40	Sugar Acetonides are a Superior Motif for Addressing the Large, Solventâ€Exposed Riboseâ€33 Pocket of tRNAâ€Guanine Transglycosylase. Chemistry - A European Journal, 2018, 24, 9957-9967.	3.3	7
41	Austausch der ProteinkontaktflÃchen in der homodimeren tRNAâ€Guaninâ€Transglycosylase: ein Weg der funktionellen Regulation. Angewandte Chemie, 2018, 130, 10242-10247.	2.0	2
42	On the Implication of Water on Fragmentâ€toâ€Ligand Growth in Kinase Binding Thermodynamics. ChemMedChem, 2018, 13, 1988-1996.	3.2	8
43	Homodimer Architecture of QTRT2, the Noncatalytic Subunit of the Eukaryotic tRNA-Guanine Transglycosylase. Biochemistry, 2018, 57, 3953-3965.	2.5	8
44	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.	6.4	36
45	Swapping Interface Contacts in the Homodimeric tRNAâ€Guanine Transglycosylase: An Option for Functional Regulation. Angewandte Chemie - International Edition, 2018, 57, 10085-10090.	13.8	10
46	A Falseâ€Positive Screening Hit in Fragmentâ€Based Lead Discovery: Watch out for the Red Herring. Angewandte Chemie - International Edition, 2017, 56, 1908-1913.	13.8	12
47	Ladungen verschieben Protonierungen: Neutronenbeugung zeigt, dass Anilin und 2â€Aminopyridin protoniert an Trypsin binden. Angewandte Chemie, 2017, 129, 4965-4969.	2.0	4
48	Falschâ€positiver Treffer im Fragmentâ€basierten Wirkstoffdesign: Lass Dich nicht auf die falsche FÃhrte locken!. Angewandte Chemie, 2017, 129, 1934-1940.	2.0	0
49	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. ACS Chemical Biology, 2017, 12, 225-233.	3.4	14
50	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.	6.4	35
51	An Allyl Protection and Improved Purification Strategy Enables the Synthesis of Functionalized Phosphonamidate Peptides. Synthesis, 2017, 49, 1857-1866.	2.3	4
52	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.	13.8	18
53	Price for Opening the Transient Specificity Pocket in Human Aldose Reductase upon Ligand Binding: Structural, Thermodynamic, Kinetic, and Computational Analysis. ACS Chemical Biology, 2017, 12, 1397-1415.	3.4	23
54	Protoplast Swelling and Hypocotyl Growth Depend on Different Auxin Signaling Pathways. Plant Physiology, 2017, 175, 982-994.	4.8	19

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55	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.	13.7	23
56	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.	2.5	30
57	Six Biophysical Screening Methods Miss a Large Proportion of Crystallographically Discovered Fragment Hits: A Case Study. ACS Chemical Biology, 2016, 11, 1693-1701.	3.4	87
58	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.	0.8	29
59	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.	5.2	6
60	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.	6.4	12
61	Experimental Active-Site Mapping by Fragments: Hot Spots Remote from the Catalytic Center of Endothiapepsin. Journal of Medicinal Chemistry, 2016, 59, 7561-7575.	6.4	14
62	Occupying a flat subpocket in a tRNA-modifying enzyme with ordered or disordered side chains: Favorable or unfavorable for binding?. Bioorganic and Medicinal Chemistry, 2016, 24, 4900-4910.	3.0	11
63	Fragment Linking and Optimization of Inhibitors of the Aspartic Protease Endothiapepsin: Fragmentâ€Based Drug Design Facilitated by Dynamic Combinatorial Chemistry. Angewandte Chemie - International Edition, 2016, 55, 9422-9426.	13.8	55
64	High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits. Structure, 2016, 24, 1398-1409.	3.3	62
65	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.	6.4	64
66	Boosting Affinity by Correct Ligand Preorganization for the S2 Pocket of Thrombin: A Study by Isothermal Titration Calorimetry, Molecular Dynamics, and Highâ€Resolution Crystal Structures. ChemMedChem, 2016, 11, 309-319.	3.2	17
67	An Immucillinâ€Based Transitionâ€Stateâ€Analogous Inhibitor of tRNAâ€“Guanine Transglycosylase (TGT). Chemistry - A European Journal, 2016, 22, 6750-6754.	3.3	4
68	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.	5.4	29
69	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.	6.4	60
70	FragmentverknÃ¼pfung und â€optimierung von Hemmstoffen der Aspartylprotease Endothiapepsin: Fragmentbasiertes Wirkstoffdesign beschleunigt durch dynamische kombinatorische Chemie. Angewandte Chemie, 2016, 128, 9569-9574.	2.0	21
71	ChamÃleonâ€artige Bindungsmodi in der Leitstrukturoptimierung: wechselnde Bindungsgeometrien bei Aspartylproteaseâ€Inhibitoren. Angewandte Chemie, 2015, 127, 2891-2896.	2.0	1
72	Structural Determinants of the Selectivity of 3â€Benzyluracilâ€1â€acetic Acids toward Human Enzymes Aldose Reductase and AKR1B10. ChemMedChem, 2015, 10, 1989-2003.	3.2	13

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73	One Question, Multiple Answers: Biochemical and Biophysical Screening Methods Retrieve Deviating Fragment Hit Lists. ChemMedChem, 2015, 10, 1511-1521.	3.2	54
74	Acceleration of Binding Site Comparisons by Graph Partitioning. Molecular Informatics, 2015, 34, 550-558.	2.5	2
75	Structure-Based Optimization of Inhibitors of the Aspartic Protease Endothiapepsin. International Journal of Molecular Sciences, 2015, 16, 19184-19194.	4.1	13
76	Thermodynamic signatures of fragment binding: Validation of direct versus displacement ITC titrations. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 647-656.	2.4	36
77	The Use of Thermodynamic and Kinetic Data in Drug Discovery: Decisive Insight or Increasing the Puzzlement?. ChemMedChem, 2015, 10, 229-231.	3.2	36
78	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.	3.3	8
79	Frontispiece: Replacement of Water Molecules in a Phosphate Binding Site by Furanoside-Appendedlin-Benzoguanine Ligands of tRNA-Guanine Transglycosylase (TGT). Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
80	Tracing Binding Modes in Hitâ€toâ€Lead Optimization: Chameleonâ€Like Poses of Aspartic Protease Inhibitors. Angewandte Chemie - International Edition, 2015, 54, 2849-2853.	13.8	27
81	Applying thermodynamic profiling in lead finding and optimization. Nature Reviews Drug Discovery, 2015, 14, 95-110.	46.4	240
82	Identification of Novel Aldose Reductase Inhibitors Based on Carboxymethylated Mercaptotriazinoindole Scaffold. Journal of Medicinal Chemistry, 2015, 58, 2649-2657.	6.4	42
83	What Glues a Homodimer Together: Systematic Analysis of the Stabilizing Effect of an Aromatic Hot Spot in the Proteinâ€"Protein Interface of the tRNA-Modifying Enzyme Tgt. ACS Chemical Biology, 2015, 10, 1897-1907.	3.4	19
84	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.	2.9	54
85	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.	6.4	37
86	Large-Scale Mining for Similar Protein Binding Pockets: With RAPMAD Retrieval on the Fly Becomes Real. Journal of Chemical Information and Modeling, 2015, 55, 165-179.	5.4	18
87	Protein-Ligand Interactions as the Basis for Drug Action. NATO Science for Peace and Security Series A: Chemistry and Biology, 2015, , 83-92.	0.5	7
88	Structure-Based Drug Design to Perturb Function of a tRNA-Modifying Enzyme by Active Site and Protein-Protein Interface Inhibition. NATO Science for Peace and Security Series A: Chemistry and Biology, 2015, , 209-221.	0.5	0
89	Extended Graph-Based Models for Enhanced Similarity Search in Cavbase. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2014, 11, 878-890.	3.0	11
90	Hot-spot analysis to dissect the functional protein-protein interface of a tRNA-modifying enzyme. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2713-2732.	2.6	17

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91	Impact of protein and ligand impurities on ITC-derived proteinâ€“ligand thermodynamics. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 2843-2850.	2.4	21
92	Structureâ€Based Design of Inhibitors of the Aspartic Protease Endothiapepsin by Exploiting Dynamic Combinatorial Chemistry. Angewandte Chemie - International Edition, 2014, 53, 3259-3263.	13.8	71
93	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.	3.2	70
94	Beyond Affinity: Enthalpyâ€“Entropy Factorization Unravels Complexity of a Flat Structureâ€“Activity Relationship for Inhibition of a tRNA-Modifying Enzyme. Journal of Medicinal Chemistry, 2014, 57, 5566-5578.	6.4	15
95	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.	6.4	26
96	Identification of a novel polyfluorinated compound as a lead to inhibit the human enzymes aldose reductase and AKR1B10: structure determination of both ternary complexes and implications for drug design. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 889-903.	2.5	28
97	Cavities Tell More than Sequences: Exploring Functional Relationships of Proteases via Binding Pockets. Journal of Chemical Information and Modeling, 2013, 53, 2082-2092.	5.4	18
98	Proteinâ€“Ligand Interactions as the Basis for Drug Action. , 2013, , 61-88.		9
99	Screening Technologies for Lead Structure Discovery. , 2013, , 129-152.		0
100	Optimization of Lead Structures. , 2013, , 153-172.		1
101	Three-Dimensional Structure of Biomolecules. , 2013, , 291-314.		0
102	Quantitative Structureâ€“Activity Relationships. , 2013, , 371-396.		0
103	A Case Study: Structure-Based Inhibitor Design for tRNA-Guanine Transglycosylase. , 2013, , 449-468.		0
104	Launching Spiking Ligands into a Proteinâ€“Protein Interface: A Promising Strategy To Destabilize and Break Interface Formation in a tRNA Modifying Enzyme. ACS Chemical Biology, 2013, 8, 1163-1178.	3.4	24
105	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.	13.8	62
106	Graphâ€based methods for protein structure comparison. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery, 2013, 3, 307-320.	6.8	5
107	Das NadelÃ¶hr â€“ von der Forschung zur Entwicklung. , 2013, , 53-115.		1
108	Dissecting the Hydrophobic Effect on the Molecular Level: The Role of Water, Enthalpy, and Entropy in Ligand Binding to Thermolysin. Angewandte Chemie - International Edition, 2013, 52, 1822-1828.	13.8	134

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109	High-affinity inhibitors ofZymomonas mobilistRNAâ€“guanine transglycosylase through convergent optimization. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1798-1807.	2.5	10
110	Conformational Analysis. , 2013, , 335-346.		0
111	Investigation of Specificity Determinants in Bacterial tRNA-Guanine Transglycosylase Reveals Queuine, the Substrate of Its Eucaryotic Counterpart, as Inhibitor. PLoS ONE, 2013, 8, e64240.	2.5	16
112	Das NadelÃ¶hr â€“ von der Forschung zur Entwicklung. , 2013, , 53-115.		0
113	Ligand Binding Stepwise Disrupts Water Network in Thrombin: Enthalpic and Entropic Changes Reveal Classical Hydrophobic Effect. Journal of Medicinal Chemistry, 2012, 55, 6094-6110.	6.4	86
114	Concise and efficient syntheses of preQ1 base, Q base, and (ent)-Q base. Organic and Biomolecular Chemistry, 2012, 10, 8660.	2.8	12
115	Beyond Heparinization: Design of Highly Potent Thrombin Inhibitors Suitable for Surface Coupling. ChemMedChem, 2012, 7, 1965-1973.	3.2	9
116	GPU-based Cloud computing for comparing the structure of protein binding sites. , 2012, , .		7
117	Targeting the Blind Spot of Polycationic Nanocarrier-Based siRNA Delivery. ACS Nano, 2012, 6, 9447-9454.	14.6	83
118	Cofactorâ€binding sites in proteins of deviating sequence: Comparative analysis and clustering in torsion angle, cavity, and fold space. Proteins: Structure, Function and Bioinformatics, 2012, 80, 626-648.	2.6	19
119	Fingerprint Kernels for Protein Structure Comparison. Molecular Informatics, 2012, 31, 443-452.	2.5	5
120	From linâ€Benzoguanines to linâ€Benzohypoxanthines as Ligands for Zymomonas mobilis tRNAâ€“Guanine Transglycosylase: Replacement of Proteinâ€“Ligand Hydrogen Bonding by Importing Water Clusters. Chemistry - A European Journal, 2012, 18, 9246-9257.	3.3	19
121	Experimental and Computational Active Site Mapping as a Starting Point to Fragmentâ€Based Lead Discovery. ChemMedChem, 2012, 7, 248-261.	3.2	31
122	Water Makes the Difference: Rearrangement of Water Solvation Layer Triggers Nonâ€additivity of Functional Group Contributions in Proteinâ€“Ligand Binding. ChemMedChem, 2012, 7, 1423-1434.	3.2	64
123	Superposition and Alignment of Labeled Point Clouds. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 1653-1666.	3.0	14
124	SEGA: Semiglobal Graph Alignment for Structure-Based Protein Comparison. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 1330-1343.	3.0	11
125	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.	6.4	97
126	Ligand-induced fit affects binding modes and provokes changes in crystal packing of aldose reductase. Biochimica Et Biophysica Acta - General Subjects, 2011, 1810, 879-887.	2.4	15

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127	Congeneric but Still Distinct: How Closely Related Trypsin Ligands Exhibit Different Thermodynamic and Structural Properties. Journal of Molecular Biology, 2011, 405, 1170-1187.	4.2	49
128	Tracing the Detail: How Mutations Affect Binding Modes and Thermodynamic Signatures of Closely Related Aldose Reductase Inhibitors. Journal of Molecular Biology, 2011, 406, 700-712.	4.2	23
129	Two Solutions for the Same Problem: Multiple Binding Modes of Pyrrolidine-Based HIV-1 Protease Inhibitors. Journal of Molecular Biology, 2011, 410, 745-755.	4.2	8
130	DSX: A Knowledge-Based Scoring Function for the Assessment of Proteinâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2011, 51, 2731-2745.	5.4	249
131	Radiation damage reveals promising interaction position. Journal of Synchrotron Radiation, 2011, 18, 782-789.	2.4	5
132	The Golden Age of GPCR Structural Biology: Any Impact on Drug Design?. Angewandte Chemie - International Edition, 2011, 50, 11573-11575.	13.8	16
133	Stereoâ€•and Regioselective Azide/Alkyne Cycloadditions in Carbonic Anhydrase II via Tethering, Monitored by Crystallography and Mass Spectrometry. Chemistry - A European Journal, 2011, 17, 5842-5851.	3.3	16
134	fconv: format conversion, manipulation and feature computation of molecular data. Bioinformatics, 2011, 27, 1021-1022.	4.1	64
135	Pyrrolidine Derivatives as Plasmepsin Inhibitors: Binding Mode Analysis Assisted by Molecular Dynamics Simulations of a Highly Flexible Protein. ChemMedChem, 2010, 5, 443-454.	3.2	14
136	Fragmentâ€Based Lead Discovery: Screening and Optimizing Fragments for Thermolysin Inhibition. ChemMedChem, 2010, 5, 930-940.	3.2	22
137	Bidentate Zinc Chelators for Î±â€Carbonic Anhydrases that Produce a Trigonal Bipyramidal Coordination Geometry. ChemMedChem, 2010, 5, 1609-1615.	3.2	27
138	Adding calorimetric data to decision making in lead discovery: a hot tip. Nature Reviews Drug Discovery, 2010, 9, 23-27.	46.4	354
139	Enhancement of Hydrophobic Interactions and Hydrogen Bond Strength by Cooperativity: Synthesis, Modeling, and Molecular Dynamics Simulations of a Congeneric Series of Thrombin Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 2126-2135.	6.4	79
140	GARLig: A Fully Automated Tool for Subset Selection of Large Fragment Spaces via a Self-Adaptive Genetic Algorithm. Journal of Chemical Information and Modeling, 2010, 50, 1644-1659.	5.4	14
141	Non-additivity of Functional Group Contributions in Proteinâ€“Ligand Binding: A Comprehensive Study by Crystallography and Isothermal Titration Calorimetry. Journal of Molecular Biology, 2010, 397, 1042-1054.	4.2	137
142	Evolutionary construction of multiple graph alignments for the structural analysis of biomolecules. Bioinformatics, 2009, 25, 2110-2117.	4.1	23
143	Highâ€Affinity Inhibitors of tRNAâ€Guanine Transglycosylase Replacing the Function of a Structural Water Cluster. Chemistry - A European Journal, 2009, 15, 10809-10817.	3.3	30
144	Crystal Structure Analysis and in Silico pK_a Calculations Suggest Strong pK_a Shifts of Ligands as Driving Force for Highâ€Affinity Binding to TGT. ChemBioChem, 2009, 10, 716-727.	2.6	23

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145	Structureâ€Based Optimization of Aldose Reductase Inhibitors Originating from Virtual Screening. ChemMedChem, 2009, 4, 809-819.	3.2	15
146	How to Replace the Residual Solvation Shell of Polar Active Site Residues to Achieve Nanomolar Inhibition of tRNAâ€Guanine Transglycosylase. ChemMedChem, 2009, 4, 2012-2023.	3.2	26
147	Prediction of turn types in protein structure by machineâ€learning classifiers. Proteins: Structure, Function and Bioinformatics, 2009, 74, 344-352.	2.6	23
148	Turns revisited: A uniform and comprehensive classification of normal, open, and reverse turn families minimizing unassigned random chain portions. Proteins: Structure, Function and Bioinformatics, 2009, 74, 353-367.	2.6	46
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