

# Gerhard Klebe

## List of Publications by Year in descending order

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271  
papers

22,636  
citations

20036

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10955

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docs citations

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citing authors

#	ARTICLE	IF	CITATIONS
1	<sup>19</sup> F-NMR Unveils the Ligand-Induced Conformation of a Catalytically Inactive Twisted Homodimer of tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 1745-1755.	1.6	1
2	Structural and Biochemical Investigation of the Heterodimeric Murine tRNA-Guanine Transglycosylase. ACS Chemical Biology, 2022, 17, 2229-2247.	1.6	7
3	Fragment Binding to Kinase Hinge: If Charge Distribution and Local p <i>K</i> <sub>a</sub> Shifts Mismatch Popular Bioisosterism Concepts. Angewandte Chemie - International Edition, 2021, 60, 252-258.	7.2	8
4	Two Methods, One Goal: Structural Differences between Cocrystallization and Crystal Soaking to Discover Ligand Binding Poses. ChemMedChem, 2021, 16, 292-300.	1.6	19
5	Fragment-Bindung an die Kinase-Scharnier-Region: Wenn Ladungsverteilung und lokale p <i>K</i> <sub>a</sub> -Verschiebungen etablierte Bioisosterie-Konzepte fehlleiten. Angewandte Chemie, 2021, 133, 256-262.	1.6	0
6	Simultaneous determination of thermodynamic and kinetic data by isothermal titration calorimetry. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129772.	1.1	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.	2.9	2
8	The Basicity Makes the Difference: Improved Canavanine-Derived Inhibitors of the Proprotein Convertase Furin. ACS Medicinal Chemistry Letters, 2021, 12, 426-432.	1.3	11
9	Facilitated crystal handling using a simple device for evaporation reduction in microtiter plates. Journal of Applied Crystallography, 2021, 54, 376-382.	1.9	2
10	Workflow and Tools for Crystallographic Fragment Screening at the Helmholtz-Zentrum Berlin. Journal of Visualized Experiments, 2021, , .	0.2	7
11	Mapping Water Thermodynamics on Drug Candidates <i>via</i> Molecular Building Blocks: a Strategy to Improve Ligand Design and Rationalize SAR. Journal of Medicinal Chemistry, 2021, 64, 4662-4676.	2.9	5
12	Targeting a Cryptic Pocket in a Protein-Protein Contact by Disulfide-Induced Rupture of a Homodimeric Interface. ACS Chemical Biology, 2021, 16, 1090-1098.	1.6	2
13	OFF-State-Specific Inhibition of the Proprotein Convertase Furin. ACS Chemical Biology, 2021, 16, 1692-1700.	1.6	10
14	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
15	Unraveling a Ligand-Induced Twist of a Homodimeric Enzyme by Pulsed Electron-Electron Double Resonance. Angewandte Chemie - International Edition, 2021, 60, 23419-23426.	7.2	10
16	Entschlüsselung der ligandeninduzierten Verdrehung eines homodimeren Enzyms mit Hilfe der gepulsten Elektron-Elektron-Doppelresonanzspektroskopie. Angewandte Chemie, 2021, 133, 23607.	1.6	1
17	Which Properties Allow Ligands to Open and Bind to the Transient Binding Pocket of Human Aldose Reductase?. Biomolecules, 2021, 11, 1837.	1.8	5
18	Fragments as Novel Starting Points for tRNA-Guanine Transglycosylase Inhibitors Found by Alternative Screening Strategies. ChemMedChem, 2020, 15, 324-337.	1.6	7

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19	Advancing GIST-Based Solvent Functionals through Multiobjective Optimization of Solvent Enthalpy and Entropy Scoring Terms. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6654-6665.	2.5	5
20	The Importance of Charge in Perturbing the Aromatic Glue Stabilizing the Protein-Protein Interface of Homodimeric tRNA-Guanine Transglycosylase. <i>ACS Chemical Biology</i> , 2020, 15, 3021-3029.	1.6	3
21	Fragment-Based Discovery of Non-bisphosphonate Binders of <i>Trypanosoma brucei</i> Farnesyl Pyrophosphate Synthase. <i>ChemBioChem</i> , 2020, 21, 3096-3111.	1.3	8
22	Fragment Screening Hit Draws Attention to a Novel Transient Pocket Adjacent to the Recognition Site of the tRNA-Modifying Enzyme TGT. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 6802-6820.	2.9	4
23	Structure-Based Design of FXIIIa-Blockers: Addressing a Transient Hydrophobic Pocket in the Active Site of FXIIIa. <i>ChemMedChem</i> , 2020, 15, 900-905.	1.6	3
24	Rapid Discovery of Aspartyl Protease Inhibitors Using an Anchoring Approach. <i>ChemMedChem</i> , 2020, 15, 680-684.	1.6	4
25	Role of Water Molecules in Protein-Ligand Dissociation and Selectivity Discrimination: Analysis of the Mechanisms and Kinetics of Biomolecular Solvation Using Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1818-1832.	2.5	11
26	Protein-Induced Change in Ligand Protonation during Trypsin and Thrombin Binding: Hint on Differences in Selectivity Determinants of Both Proteins?. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 3274-3289.	2.9	8
27	Protein-Ligand Complex Solvation Thermodynamics: Development, Parameterization, and Testing of GIST-Based Solvent Functionals. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1409-1423.	2.5	17
28	Conformational Changes in Alkyl Chains Determine the Thermodynamic and Kinetic Binding Profiles of Carbonic Anhydrase Inhibitors. <i>ACS Chemical Biology</i> , 2020, 15, 675-685.	1.6	16
29	The Influence of Varying Fluorination Patterns on the Thermodynamics and Kinetics of Benzenesulfonamide Binding to Human Carbonic Anhydrase II. <i>Biomolecules</i> , 2020, 10, 509.	1.8	7
30	A Proof-of-Concept Fragment Screening of a Hit-Validated 96-Compounds Library against Human Carbonic Anhydrase II. <i>Biomolecules</i> , 2020, 10, 518.	1.8	5
31	F2X-Universal and F2X-Entry: Structurally Diverse Compound Libraries for Crystallographic Fragment Screening. <i>Structure</i> , 2020, 28, 694-706.e5.	1.6	27
32	Der Flaschenhals " von der Forschung zur Entwicklung. , 2020, , 73-115.		2
33	Surprising Non-Additivity of Methyl Groups in Drug-Kinase Interaction. <i>ACS Chemical Biology</i> , 2019, 14, 2585-2594.	1.6	14
34	Strategies for Late-Stage Optimization: Profiling Thermodynamics by Preorganization and Salt Bridge Shielding. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 9753-9771.	2.9	15
35	Broad-scale analysis of thermodynamic signatures in medicinal chemistry: are enthalpy-favored binders the better development option?. <i>Drug Discovery Today</i> , 2019, 24, 943-948.	3.2	21
36	Diamondoid Amino Acid-Based Peptide Kinase...A Inhibitor Analogues. <i>ChemMedChem</i> , 2019, 14, 663-672.	1.6	7

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37	Conceptual Design of Self-Assembling Bisubstrate-like Inhibitors of Protein Kinase A Resulting in a Boronic Acid Glutamate Linkage. <i>ACS Omega</i> , 2019, 4, 775-784.	1.6	10
38	Intriguing role of water in protein-ligand binding studied by neutron crystallography on trypsin complexes. <i>Nature Communications</i> , 2018, 9, 3559.	5.8	140
39	Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin. <i>ChemMedChem</i> , 2018, 13, 2266-2270.	1.6	7
40	Sugar Acetonides are a Superior Motif for Addressing the Large, Solvent-Exposed Ribose-33 Pocket of tRNA-Guanine Transglycosylase. <i>Chemistry - A European Journal</i> , 2018, 24, 9957-9967.	1.7	7
41	Austausch der Proteinkontaktflächen in der homodimeren tRNA-Guanin-Transglycosylase: ein Weg der funktionellen Regulation. <i>Angewandte Chemie</i> , 2018, 130, 10242-10247.	1.6	2
42	On the Implication of Water on Fragment-to-Ligand Growth in Kinase Binding Thermodynamics. <i>ChemMedChem</i> , 2018, 13, 1988-1996.	1.6	8
43	Homodimer Architecture of QTRT2, the Noncatalytic Subunit of the Eukaryotic tRNA-Guanine Transglycosylase. <i>Biochemistry</i> , 2018, 57, 3953-3965.	1.2	8
44	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drug-Kinase Binding. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 5922-5933.	2.9	36
45	Swapping Interface Contacts in the Homodimeric tRNA-Guanine Transglycosylase: An Option for Functional Regulation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10085-10090.	7.2	10
46	A False-Positive Screening Hit in Fragment-Based Lead Discovery: Watch out for the Red Herring. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 1908-1913.	7.2	12
47	Ladungen verschieben Protonierungen: Neutronenbeugung zeigt, dass Anilin und 2-Aminopyridin protoniert an Trypsin binden. <i>Angewandte Chemie</i> , 2017, 129, 4965-4969.	1.6	4
48	Falsch-positiver Treffer im Fragment-basierten Wirkstoffdesign: Lass Dich nicht auf die falsche Fährte locken!. <i>Angewandte Chemie</i> , 2017, 129, 1934-1940.	1.6	0
49	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. <i>ACS Chemical Biology</i> , 2017, 12, 225-233.	1.6	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. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5791-5799.	2.9	35
51	An Allyl Protection and Improved Purification Strategy Enables the Synthesis of Functionalized Phosphoramidate Peptides. <i>Synthesis</i> , 2017, 49, 1857-1866.	1.2	4
52	Charges Shift Protonation: Neutron Diffraction Reveals that Aniline and 2-Aminopyridine Become Protonated Upon Binding to Trypsin. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4887-4890.	7.2	18
53	Price for Opening the Transient Specificity Pocket in Human Aldose Reductase upon Ligand Binding: Structural, Thermodynamic, Kinetic, and Computational Analysis. <i>ACS Chemical Biology</i> , 2017, 12, 1397-1415.	1.6	23
54	Protoplast Swelling and Hypocotyl Growth Depend on Different Auxin Signaling Pathways. <i>Plant Physiology</i> , 2017, 175, 982-994.	2.3	19

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55	How Nothing Boosts Affinity: Hydrophobic Ligand Binding to the Virtually Vacated S <sub>1</sub> Pocket of Thermolysin. <i>Journal of the American Chemical Society</i> , 2017, 139, 10419-10431.	6.6	23
56	Soaking suggests "alternative facts": Only co-crystallization discloses major ligand-induced interface rearrangements of a homodimeric tRNA-binding protein indicating a novel mode-of-inhibition. <i>PLoS ONE</i> , 2017, 12, e0175723.	1.1	30
57	Six Biophysical Screening Methods Miss a Large Proportion of Crystallographically Discovered Fragment Hits: A Case Study. <i>ACS Chemical Biology</i> , 2016, 11, 1693-1701.	1.6	87
58	Structures of endothiapepsin "fragment complexes from crystallographic fragment screening using a novel, diverse and affordable 96-compound fragment library. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2016, 72, 346-355.	0.4	29
59	Changing the selectivity profile " from substrate analog inhibitors of thrombin and factor Xa to potent matriptase inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 89-97.	2.5	6
60	Active Site Mapping of an Aspartic Protease by Multiple Fragment Crystal Structures: Versatile Warheads To Address a Catalytic Dyad. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 9743-9759.	2.9	12
61	Experimental Active-Site Mapping by Fragments: Hot Spots Remote from the Catalytic Center of Endothiapepsin. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 7561-7575.	2.9	14
62	Occupying a flat subpocket in a tRNA-modifying enzyme with ordered or disordered side chains: Favorable or unfavorable for binding?. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4900-4910.	1.4	11
63	Fragment Linking and Optimization of Inhibitors of the Aspartic Protease Endothiapepsin: Fragment-Based Drug Design Facilitated by Dynamic Combinatorial Chemistry. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9422-9426.	7.2	55
64	High-Throughput Crystallography: Reliable and Efficient Identification of Fragment Hits. <i>Structure</i> , 2016, 24, 1398-1409.	1.6	62
65	Rational Design of Thermodynamic and Kinetic Binding Profiles by Optimizing Surface Water Networks Coating Protein-Bound Ligands. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 10530-10548.	2.9	64
66	Boosting Affinity by Correct Ligand Preorganization for the S2 Pocket of Thrombin: A Study by Isothermal Titration Calorimetry, Molecular Dynamics, and High-Resolution Crystal Structures. <i>ChemMedChem</i> , 2016, 11, 309-319.	1.6	17
67	An Immucillin-Based Transition-State Analogous Inhibitor of tRNA "Guanine Transglycosylase (TGT). <i>Chemistry - A European Journal</i> , 2016, 22, 6750-6754.	1.7	4
68	Impact of Surface Water Layers on Protein "Ligand Binding: How Well Are Experimental Data Reproduced by Molecular Dynamics Simulations in a Thermolysin Test Case?. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 223-233.	2.5	29
69	Kinetic and Structural Insights into the Mechanism of Binding of Sulfonamides to Human Carbonic Anhydrase by Computational and Experimental Studies. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4245-4256.	2.9	60
70	Fragmentverknüpfung und "optimierung von Hemmstoffen der Aspartylprotease Endothiapepsin: Fragmentbasiertes Wirkstoffdesign beschleunigt durch dynamische kombinatorische Chemie. <i>Angewandte Chemie</i> , 2016, 128, 9569-9574.	1.6	21
71	Charakteristische Bindungsmodi in der Leitstrukturoptimierung: wechselnde Bindungsgeometrien bei Aspartylprotease-Inhibitoren. <i>Angewandte Chemie</i> , 2015, 127, 2891-2896.	1.6	1
72	Structural Determinants of the Selectivity of 3-Benzyluracil "acetic Acids toward Human Enzymes Aldose Reductase and AKR1B10. <i>ChemMedChem</i> , 2015, 10, 1989-2003.	1.6	13

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73	One Question, Multiple Answers: Biochemical and Biophysical Screening Methods Retrieve Deviating Fragment Hit Lists. <i>ChemMedChem</i> , 2015, 10, 1511-1521.	1.6	54
74	Acceleration of Binding Site Comparisons by Graph Partitioning. <i>Molecular Informatics</i> , 2015, 34, 550-558.	1.4	2
75	Structure-Based Optimization of Inhibitors of the Aspartic Protease Endothiapepsin. <i>International Journal of Molecular Sciences</i> , 2015, 16, 19184-19194.	1.8	13
76	Thermodynamic signatures of fragment binding: Validation of direct versus displacement ITC titrations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 647-656.	1.1	36
77	The Use of Thermodynamic and Kinetic Data in Drug Discovery: Decisive Insight or Increasing the Puzzlement?. <i>ChemMedChem</i> , 2015, 10, 229-231.	1.6	36
78	Replacement of Water Molecules in a Phosphate Binding Site by Furanoside-Appended Benzoguanine Ligands of tRNA-Guanine Transglycosylase (TGT). <i>Chemistry - A European Journal</i> , 2015, 21, 126-135.	1.7	8
79	Frontispiece: Replacement of Water Molecules in a Phosphate Binding Site by Furanoside-Appended Benzoguanine Ligands of tRNA-Guanine Transglycosylase (TGT). <i>Chemistry - A European Journal</i> , 2015, 21, n/a-n/a.	1.7	0
80	Tracing Binding Modes in Hit-to-Lead Optimization: Chameleon-Like Poses of Aspartic Protease Inhibitors. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2849-2853.	7.2	27
81	Applying thermodynamic profiling in lead finding and optimization. <i>Nature Reviews Drug Discovery</i> , 2015, 14, 95-110.	21.5	240
82	Identification of Novel Aldose Reductase Inhibitors Based on Carboxymethylated Mercaptotriazinoindole Scaffold. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2649-2657.	2.9	42
83	What Glues a Homodimer Together: Systematic Analysis of the Stabilizing Effect of an Aromatic Hot Spot in the Protein-Protein Interface of the tRNA-Modifying Enzyme Tgt. <i>ACS Chemical Biology</i> , 2015, 10, 1897-1907.	1.6	19
84	Thermodynamics of protein-ligand interactions as a reference for computational analysis: how to assess accuracy, reliability and relevance of experimental data. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 867-883.	1.3	54
85	Fragment Binding Can Be Either More Enthalpy-Driven or Entropy-Driven: Crystal Structures and Residual Hydration Patterns Suggest Why. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6960-6971.	2.9	37
86	Large-Scale Mining for Similar Protein Binding Pockets: With RAPMAD Retrieval on the Fly Becomes Real. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 165-179.	2.5	18
87	Protein-Ligand Interactions as the Basis for Drug Action. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 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. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2015, , 209-221.	0.5	0
89	Extended Graph-Based Models for Enhanced Similarity Search in Cavbase. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2014, 11, 878-890.	1.9	11
90	Hot-spot analysis to dissect the functional protein-protein interface of a tRNA-modifying enzyme. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2713-2732.	1.5	17

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91	Impact of protein and ligand impurities on ITC-derived proteinâ€“ligand thermodynamics. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2014, 1840, 2843-2850.	1.1	21
92	Structureâ€“Based Design of Inhibitors of the Aspartic Protease Endothiapepsin by Exploiting Dynamic Combinatorial Chemistry. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 3259-3263.	7.2	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. <i>ChemMedChem</i> , 2014, 9, 833-846.	1.6	70
94	Beyond Affinity: Enthalpyâ€“Entropy Factorization Unravels Complexity of a Flat Structureâ€“Activity Relationship for Inhibition of a tRNA-Modifying Enzyme. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 5566-5578.	2.9	15
95	Chasing Protons: How Isothermal Titration Calorimetry, Mutagenesis, and p <i>K<sub>a</sub></i> Calculations Trace the Locus of Charge in Ligand Binding to a tRNA-Binding Enzyme. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 5554-5565.	2.9	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. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 889-903.	2.5	28
97	Cavities Tell More than Sequences: Exploring Functional Relationships of Proteases via Binding Pockets. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2082-2092.	2.5	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. <i>ACS Chemical Biology</i> , 2013, 8, 1163-1178.	1.6	24
105	Structure of Active Coagulation Factorâ€“XIII Triggered by Calcium Binding: Basis for the Design of Nextâ€“Generation Anticoagulants. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 11930-11934.	7.2	62
106	Graphâ€“based methods for protein structure comparison. <i>Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery</i> , 2013, 3, 307-320.	4.6	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. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 1822-1828.	7.2	134

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109	High-affinity inhibitors of <i>Zymomonas mobilis</i> tRNA <sup>G</sup> 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.	1.1	16
112	Das Nadelnhr " 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.	2.9	86
114	Concise and efficient syntheses of preQ1 base, Q base, and (ent)-Q base. Organic and Biomolecular Chemistry, 2012, 10, 8660.	1.5	12
115	Beyond Heparinization: Design of Highly Potent Thrombin Inhibitors Suitable for Surface Coupling. ChemMedChem, 2012, 7, 1965-1973.	1.6	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.	7.3	83
118	Cofactor 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.	1.5	19
119	Fingerprint Kernels for Protein Structure Comparison. Molecular Informatics, 2012, 31, 443-452.	1.4	5
120	From <i>lin</i> Benzoguanines to <i>lin</i> Benzohypoxanthines as Ligands for <i>Zymomonas mobilis</i> tRNA <sup>G</sup> Guanine Transglycosylase: Replacement of Protein Ligand Hydrogen Bonding by Importing Water Clusters. Chemistry - A European Journal, 2012, 18, 9246-9257.	1.7	19
121	Experimental and Computational Active Site Mapping as a Starting Point to Fragment-Based Lead Discovery. ChemMedChem, 2012, 7, 248-261.	1.6	31
122	Water Makes the Difference: Rearrangement of Water Solvation Layer Triggers Non-additivity of Functional Group Contributions in Protein Ligand Binding. ChemMedChem, 2012, 7, 1423-1434.	1.6	64
123	Superposition and Alignment of Labeled Point Clouds. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 1653-1666.	1.9	14
124	SEGA: Semiglobal Graph Alignment for Structure-Based Protein Comparison. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2011, 8, 1330-1343.	1.9	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.	2.9	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.	1.1	15



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127	Congeneric but Still Distinct: How Closely Related Trypsin Ligands Exhibit Different Thermodynamic and Structural Properties. <i>Journal of Molecular Biology</i> , 2011, 405, 1170-1187.	2.0	49
128	Tracing the Detail: How Mutations Affect Binding Modes and Thermodynamic Signatures of Closely Related Aldose Reductase Inhibitors. <i>Journal of Molecular Biology</i> , 2011, 406, 700-712.	2.0	23
129	Two Solutions for the Same Problem: Multiple Binding Modes of Pyrrolidine-Based HIV-1 Protease Inhibitors. <i>Journal of Molecular Biology</i> , 2011, 410, 745-755.	2.0	8
130	DSX: A Knowledge-Based Scoring Function for the Assessment of Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2731-2745.	2.5	249
131	Radiation damage reveals promising interaction position. <i>Journal of Synchrotron Radiation</i> , 2011, 18, 782-789.	1.0	5
132	The Golden Age of GPCR Structural Biology: Any Impact on Drug Design?. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11573-11575.	7.2	16
133	Stereo- and Regioselective Azide/Alkyne Cycloadditions in Carbonic Anhydrase II via Tethering, Monitored by Crystallography and Mass Spectrometry. <i>Chemistry - A European Journal</i> , 2011, 17, 5842-5851.	1.7	16
134	fconv: format conversion, manipulation and feature computation of molecular data. <i>Bioinformatics</i> , 2011, 27, 1021-1022.	1.8	64
135	Pyrrolidine Derivatives as Plasmepsin Inhibitors: Binding Mode Analysis Assisted by Molecular Dynamics Simulations of a Highly Flexible Protein. <i>ChemMedChem</i> , 2010, 5, 443-454.	1.6	14
136	Fragment-Based Lead Discovery: Screening and Optimizing Fragments for Thermolysin Inhibition. <i>ChemMedChem</i> , 2010, 5, 930-940.	1.6	22
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