Holger Gohlke

List of Publications by Year in Descending Order

228 papers	17,969 citations	45 h-index	132 g-index
263 ext. papers	20,978 ext. citations	5.9 avg, IF	6.8 L-index

#	Paper	IF	Citations
228	A phospholipase B from Pseudomonas aeruginosa with activity towards endogenous phospholipids affects biofilm assembly.. *Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids*, **2022**, 1867, 159101	5	1
227	Critical assessment of structure-based approaches to improve protein resistance in aqueous ionic liquids by enzyme-wide saturation mutagenesis.. *Computational and Structural Biotechnology Journal*, **2022**, 20, 399-409	6.8	2
226	Mapping the helix arrangement of the reconstituted ETR1 ethylene receptor transmembrane domain by EPR spectroscopy.. *RSC Advances*, **2022**, 12, 7352-7356	3.7	0
225	Molecular Modeling and Simulations of DNA and RNA: DNAzyme as a Model System.. *Methods in Molecular Biology*, **2022**, 2439, 153-170	1.4	0
224	Structural, mechanistic and physiological insights into phospholipase A-mediated membrane phospholipid degradation in .. *ELife*, **2022**, 11,	8.9	1
223	Functional and structural characterization of interactions between opposite subunits in HCN pacemaker channels.. *Communications Biology*, **2022**, 5, 430	6.7	
222	Time-resolved structural analysis of an RNA-cleaving DNA catalyst.. *Nature*, **2021**,	50.4	7
221	Targeting spectrin redox switches to regulate the mechanoproperties of red blood cells. *Biological Chemistry*, **2021**, 402, 317-331	4.5	2
220	Substrate Access Mechanism in a Novel Membrane-Bound Phospholipase A of Concordant with Specificity and Regioselectivity. *Journal of Chemical Information and Modeling*, **2021**, 61, 5626-5643	6.1	0
219	TopProperty: Robust Metaprediction of Transmembrane and Globular Protein Features Using Deep Neural Networks. *Journal of Chemical Theory and Computation*, **2021**, 17, 7281-7289	6.4	0
218	Foamy Viruses, Bet, and APOBEC3 Restriction. *Viruses*, **2021**, 13,	6.2	1
217	Allosteric signaling in C-linker and cyclic nucleotide-binding domain of HCN2 channels. *Biophysical Journal*, **2021**, 120, 950-963	2.9	1
216	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. *Chemical Research in Toxicology*, **2021**, 34, 1503-1517	4	2
215	Liver cell hydration and integrin signaling. *Biological Chemistry*, **2021**, 402, 1033-1045	4.5	0
214	The many facets of bile acids in the physiology and pathophysiology of the human liver. *Biological Chemistry*, **2021**, 402, 1047-1062	4.5	2
213	Glutamine synthetase as a central element in hepatic glutamine and ammonia metabolism: novel aspects. *Biological Chemistry*, **2021**, 402, 1063-1072	4.5	5
212	Promiscuous Esterases Counterintuitively Are Less Flexible than Specific Ones. *Journal of Chemical Information and Modeling*, **2021**, 61, 2383-2395	6.1	2

211	TopDomain: Exhaustive Protein Domain Boundary Metaprediction Combining Multisource Information and Deep Learning. *Journal of Chemical Theory and Computation*, **2021**, 17, 4599-4613	6.4	1
210	Evidence for a credit-card-swipe mechanism in the human PC floppase ABCB4. *Structure*, **2021**, 29, 1144-1155.e5	5.7	5
209	A promiscuous ancestral enzyme's structure unveils protein variable regions of the highly diverse metallo-β-lactamase family. *Communications Biology*, **2021**, 4, 132	6.7	4
208	TopSuite Web Server: A Meta-Suite for Deep-Learning-Based Protein Structure and Quality Prediction. *Journal of Chemical Information and Modeling*, **2021**, 61, 548-553	6.1	5
207	40 Years of Research on Polybrominated Diphenyl Ethers (PBDEs)-A Historical Overview and Newest Data of a Promising Anticancer Drug. *Molecules*, **2021**, 26,	4.8	6
206	Thermodynamic profile of mutual subunit control in a heteromeric receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	1
205	Development of a Biosensor Platform for Phenolic Compounds Using a Transition Ligand Strategy. *ACS Synthetic Biology*, **2021**, 10, 2002-2014	5.7	2
204	F/G Region Rigidity is Inversely Correlated to Substrate Promiscuity of Human CYP Isoforms Involved in Metabolism. *Journal of Chemical Information and Modeling*, **2021**, 61, 4023-4030	6.1	0
203	Structure and efflux mechanism of the yeast pleiotropic drug resistance transporter Pdr5. *Nature Communications*, **2021**, 12, 5254	17.4	8
202	Interdependence of a mechanosensitive anion channel and glutamate receptors in distal wound signaling. *Science Advances*, **2021**, 7, eabg4298	14.3	11
201	Can constraint network analysis guide the identification phase of KnowVolution? A case study on improved thermostability of an endo-β-glucanase. *Computational and Structural Biotechnology Journal*, **2021**, 19, 743-751	6.8	3
200	Aqueous ionic liquids redistribute local enzyme stability via long-range perturbation pathways. *Computational and Structural Biotechnology Journal*, **2021**, 19, 4248-4264	6.8	6
199	Discovery of new acetylcholinesterase inhibitors for Alzheimer's disease: virtual screening and characterisation. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 491-496	5.6	5
198	Cumulative Submillisecond All-Atom Simulations of the Temperature-Induced Coil-to-Globule Transition of Poly(N-vinylcaprolactam) in Aqueous Solution. *Macromolecules*, **2020**, 53, 9793-9810	5.5	2
197	Fluorophore-Labeled Cyclic Nucleotides as Potent Agonists of Cyclic Nucleotide-Regulated Ion Channels. *ChemBioChem*, **2020**, 21, 2311-2320	3.8	2
196	Binding modes of thioflavin T and Congo red to the fibril structure of amyloid-β(1-42). *Chemical Communications*, **2020**, 56, 7589-7592	5.8	10
195	Mechanism of Fully Reversible, pH-Sensitive Inhibition of Human Glutamine Synthetase by Tyrosine Nitration. *Journal of Chemical Theory and Computation*, **2020**, 16, 4694-4705	6.4	4
194	Resolving dynamics and function of transient states in single enzyme molecules. *Nature Communications*, **2020**, 11, 1231	17.4	31

193	AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools. *Journal of Chemical Physics*, **2020**, 152, 221103	3.9	7
192	Structural and dynamic insights revealing how lipase binding domain MD1 of Pseudomonas aeruginosa foldase affects lipase activation. *Scientific Reports*, **2020**, 10, 3578	4.9	6
191	A Novel Polyester Hydrolase From the Marine Bacterium Structural and Functional Insights. *Frontiers in Microbiology*, **2020**, 11, 114	5.7	62
190	TopModel: Template-Based Protein Structure Prediction at Low Sequence Identity Using Top-Down Consensus and Deep Neural Networks. *Journal of Chemical Theory and Computation*, **2020**, 16, 1953-1967	6.4	14
189	TGR5 (GPBAR1) in the Liver **2020**, 286-298		
188	Quantitative assessment of the determinant structural differences between redox-active and inactive glutaredoxins. *Nature Communications*, **2020**, 11, 1725	17.4	20
187	Bile Acids and TGR5 (Gpbar1) Signaling **2020**, 81-100		2
186	The Membrane-Integrated Steric Chaperone Lif Facilitates Active Site Opening of Pseudomonas aeruginosa Lipase A. *Journal of Computational Chemistry*, **2020**, 41, 500-512	3.5	3
185	Systematically Scrutinizing the Impact of Substitution Sites on Thermostability and Detergent Tolerance for Lipase A. *Journal of Chemical Information and Modeling*, **2020**, 60, 1568-1584	6.1	9
184	Dimerization energetics of the G-protein coupled bile acid receptor TGR5 from all-atom simulations. *Journal of Computational Chemistry*, **2020**, 41, 874-884	3.5	3
183	Loop 1 of APOBEC3C Regulates its Antiviral Activity against HIV-1. *Journal of Molecular Biology*, **2020**, 432, 6200-6227	6.5	7
182	Semisynthetic Analogs of the Antibiotic Fidaxomicin-Design, Synthesis, and Biological Evaluation. *ACS Medicinal Chemistry Letters*, **2020**, 11, 2414-2420	4.3	5
181	Automated and optimally FRET-assisted structural modeling. *Nature Communications*, **2020**, 11, 5394	17.4	12
180	Characterization of the nucleotide-binding domain NsrF from the BceAB-type ABC-transporter NsrFP from the human pathogen Streptococcus agalactiae. *Scientific Reports*, **2020**, 10, 15208	4.9	4
179	Cell Type-Dependent Escape of Capsid Inhibitors by Simian Immunodeficiency Virus SIVcpz. *Journal of Virology*, **2020**, 94,	6.6	2
178	The Puzzle of Metabolite Exchange and Identification of Putative Octotrico Peptide Repeat Expression Regulators in the Nascent Photosynthetic Organelles of. *Frontiers in Microbiology*, **2020**, 11, 607182	5.7	7
177	Evidence for functional selectivity in TUDC- and norUDCA-induced signal transduction via β integrin towards choleresis. *Scientific Reports*, **2020**, 10, 5795	4.9	4
176	C-terminal modulators of heat shock protein of 90 kDa (HSP90): State of development and modes of action. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 115080	3.4	21

175	Small-molecule inhibitors of nisin resistance protein NSR from the human pathogen Streptococcus agalactiae. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 115079	3.4	4
174	Design, synthesis and biological evaluation of peptoid-capped HDAC inhibitors with anti-neuroblastoma and anti-glioblastoma activity. *MedChemComm*, **2019**, 10, 1109-1115	5	5
173	Co-culture of the fungus with induces production of cryptic naphthoquinone dimers.. *RSC Advances*, **2019**, 9, 1491-1500	3.7	27
172	Novel Fluorescent Cyclic Nucleotide Derivatives to Study CNG and HCN Channel Function. *Biophysical Journal*, **2019**, 116, 2411-2422	2.9	5
171	PACKMOL-Memgen: A Simple-To-Use, Generalized Workflow for Membrane-Protein-Lipid-Bilayer System Building. *Journal of Chemical Information and Modeling*, **2019**, 59, 2522-2528	6.1	46
170	Novel 3,4-Dihydroisocoumarins Inhibit Human P-gp and BCRP in Multidrug Resistant Tumors and Demonstrate Substrate Inhibition of Yeast Pdr5. *Frontiers in Pharmacology*, **2019**, 10, 400	5.6	10
169	Cosolvent-Enhanced Sampling and Unbiased Identification of Cryptic Pockets Suitable for Structure-Based Drug Design. *Journal of Chemical Theory and Computation*, **2019**, 15, 3331-3343	6.4	14
168	Calcium-Promoted Interaction between the C2-Domain Protein EHB1 and Metal Transporter IRT1 Inhibits Arabidopsis Iron Acquisition. *Plant Physiology*, **2019**, 180, 1564-1581	6.6	18
167	Phosphorylated tyrosine 93 of hepatitis C virus nonstructural protein 5A is essential for interaction with host c-Src and efficient viral replication. *Journal of Biological Chemistry*, **2019**, 294, 7388-7402	5.4	4
166	JAK2 p.G571S in B-cell precursor acute lymphoblastic leukemia: a synergizing germline susceptibility. *Leukemia*, **2019**, 33, 2331-2335	10.7	6
165	The tetrahydroxanthone-dimer phomoxanthone A is a strong inducer of apoptosis in cisplatin-resistant solid cancer cells. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 115044	3.4	7
164	Fluorescent analogs of peptoid-based HDAC inhibitors: Synthesis, biological activity and cellular uptake kinetics. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 115039	3.4	9
163	Biallelic mutation of human encoding the taurine transporter TAUT is linked to early retinal degeneration. *FASEB Journal*, **2019**, 33, 11507-11527	0.9	17
162	Isoform-specific Inhibition of N-methyl-D-aspartate Receptors by Bile Salts. *Scientific Reports*, **2019**, 9, 10068	4.9	5
161	Xanthone, benzophenone and bianthrone derivatives from the hypersaline lake-derived fungus Aspergillus wentii. *Bioorganic and Medicinal Chemistry*, **2019**, 27, 115005	3.4	3
160	Posttranslational Modification of the NADP-Malic Enzyme Involved in C Photosynthesis Modulates the Enzymatic Activity during the Day. *Plant Cell*, **2019**, 31, 2525-2539	11.6	7
159	Structural Model of the ETR1 Ethylene Receptor Transmembrane Sensor Domain. *Scientific Reports*, **2019**, 9, 8869	4.9	12
158	Surprising Non-Additivity of Methyl Groups in Drug-Kinase Interaction. *ACS Chemical Biology*, **2019**, 14, 2585-2594	4.9	8

157	Basal Histamine H Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. *Chemistry - A European Journal*, **2019**, 25, 14613-14624	4.8	7
156	Partially inserted nascent chain unzips the lateral gate of the Sec translocon. *EMBO Reports*, **2019**, 20, e48191	6.5	22
155	Pseudomonas aeruginosa esterase PA2949, a bacterial homolog of the human membrane esterase ABHD6: expression, purification and crystallization. *Acta Crystallographica Section F, Structural Biology Communications*, **2019**, 75, 270-277	1.1	5
154	-modified cAMP derivatives that activate protein kinase A also act as full agonists of murine HCN2 channels. *Journal of Biological Chemistry*, **2019**, 294, 17978-17987	5.4	
153	Synthesis of Peptoid-Based Class I-Selective Histone Deacetylase Inhibitors with Chemosensitizing Properties. *Journal of Medicinal Chemistry*, **2019**, 62, 11260-11279	8.3	16
152	Nutrient exchange in arbuscular mycorrhizal symbiosis from a thermodynamic point of view. *New Phytologist*, **2019**, 222, 1043-1053	9.8	12
151	FK506 Resistance of Pdr5 and Cdr1 Involves Mutations in the Transmembrane Domains and Extracellular Loops. *Antimicrobial Agents and Chemotherapy*, **2019**, 63,	5.9	13
150	Converging a Knowledge-Based Scoring Function: DrugScore. *Journal of Chemical Information and Modeling*, **2019**, 59, 509-521	6.1	28
149	The human platelet antigen-1b (Pro) variant of allosterically shifts the dynamic conformational equilibrium of this integrin toward the active state. *Journal of Biological Chemistry*, **2018**, 293, 4830-4844	5.4	3
148	Recognition motif and mechanism of ripening inhibitory peptides in plant hormone receptor ETR1. *Scientific Reports*, **2018**, 8, 3890	4.9	17
147	Identification of a Conserved Interface of Human Immunodeficiency Virus Type 1 and Feline Immunodeficiency Virus Vifs with Cullin 5. *Journal of Virology*, **2018**, 92,	6.6	7
146	Effects of novel HDAC inhibitors on urothelial carcinoma cells. *Clinical Epigenetics*, **2018**, 10, 100	7.7	38
145	On the Effects of Reactive Oxygen Species and Nitric Oxide on Red Blood Cell Deformability. *Frontiers in Physiology*, **2018**, 9, 332	4.6	54
144	Targeting HSP90 dimerization via the C terminus is effective in imatinib-resistant CML and lacks the heat shock response. *Blood*, **2018**, 132, 307-320	2.2	37
143	On the contributing role of the transmembrane domain for subunit-specific sensitivity of integrin activation. *Scientific Reports*, **2018**, 8, 5733	4.9	12
142	Novel Recurrent Germline JAK2 G571S Variant in Childhood Acute B-Lymphoblastic Leukemia: A Double Hit One Pathway Scenario. *Blood*, **2018**, 132, 387-387	2.2	3
141	Therapeutic Targeting of HSP90 in AML and ALL. *Blood*, **2018**, 132, 4680-4680	2.2	
140	Systematic analysis of ATG13 domain requirements for autophagy induction. *Autophagy*, **2018**, 14, 743-763	13.2	28

139	Chlorflavonin Targets Acetohydroxyacid Synthase Catalytic Subunit IlvB1 for Synergistic Killing of Mycobacterium tuberculosis. *ACS Infectious Diseases*, **2018**, 4, 123-134	5.5	13
138	Hydrophobic alkyl chains substituted to the 8-position of cyclic nucleotides enhance activation of CNG and HCN channels by an intricate enthalpy - entropy compensation. *Scientific Reports*, **2018**, 8, 14960	4.9	6
137	TopScore: Using Deep Neural Networks and Large Diverse Data Sets for Accurate Protein Model Quality Assessment. *Journal of Chemical Theory and Computation*, **2018**, 14, 6117-6126	6.4	18
136	Interaction of Ochratoxin A and Its Thermal Degradation Product 2SOchratoxin A with Human Serum Albumin. *Toxins*, **2018**, 10,	4.9	17
135	Relevance of N-terminal residues for amyloid-□binding to platelet integrin □integrin outside-in signaling and amyloid-□fibril formation. *Cellular Signalling*, **2018**, 50, 121-130	4.9	10
134	Efficient Approximation of Ligand Rotational and Translational Entropy Changes upon Binding for Use in MM-PBSA Calculations. *Journal of Chemical Information and Modeling*, **2017**, 57, 170-189	6.1	31
133	□Aminoxy Peptoids: A Unique Peptoid Backbone with a Preference for cis-Amide Bonds. *Chemistry - A European Journal*, **2017**, 23, 3699-3707	4.8	4
132	Suppression of RUNX1/ETO oncogenic activity by a small molecule inhibitor of tetramerization. *Haematologica*, **2017**, 102, e170-e174	6.6	8
131	Rigidity theory for biomolecules: concepts, software, and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1311	7.9	21
130	Design, Multicomponent Synthesis, and Anticancer Activity of a Focused Histone Deacetylase (HDAC) Inhibitor Library with Peptoid-Based Cap Groups. *Journal of Medicinal Chemistry*, **2017**, 60, 5493-5506	8.3	22
129	Structural intermediates and directionality of the swiveling motion of Pyruvate Phosphate Dikinase. *Scientific Reports*, **2017**, 7, 45389	4.9	11
128	Rigidity Theory-Based Approximation of Vibrational Entropy Changes upon Binding to Biomolecules. *Journal of Chemical Theory and Computation*, **2017**, 13, 1495-1502	6.4	14
127	Human RAD52 - a novel player in DNA repair in cancer and immunodeficiency. *Haematologica*, **2017**, 102, e69-e72	6.6	4
126	Tertiary Interactions in the Unbound Guanine-Sensing Riboswitch Focus Functional Conformational Variability on the Binding Site. *Journal of Chemical Information and Modeling*, **2017**, 57, 2822-2832	6.1	1
125	Pyrazolidine-3,5-dione-based inhibitors of phosphoenolpyruvate carboxylase as a new class of potential C plant herbicides. *FEBS Letters*, **2017**, 591, 3369-3377	3.8	1
124	On the potential alternate binding change mechanism in a dimeric structure of Pyruvate Phosphate Dikinase. *Scientific Reports*, **2017**, 7, 8020	4.9	5
123	Sequencing of FIC1, BSEP and MDR3 in a large cohort of patients with cholestasis revealed a high number of different genetic variants. *Journal of Hepatology*, **2017**, 67, 1253-1264	13.4	68
122	Cover Image, Volume 7, Issue 4. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1324	7.9	

121	Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery. *Journal of Chemical Theory and Computation*, **2017**, 13, 6343-6357	6.4	20
120	Structural features of FAP174, a MYCBP-1 orthologue from Chlamydomonas reinhardtii, revealed by computational and experimental analyses. *RSC Advances*, **2017**, 7, 51391-51402	3.7	1
119	Alkoxyurea-Based Histone Deacetylase Inhibitors Increase Cisplatin Potency in Chemoresistant Cancer Cell Lines. *Journal of Medicinal Chemistry*, **2017**, 60, 5334-5348	8.3	31
118	Contribution of single amino acid and codon substitutions to the production and secretion of a lipase by Bacillus subtilis. *Microbial Cell Factories*, **2017**, 16, 160	6.4	13
117	EDTA aggregates induce SYPRO orange-based fluorescence in thermal shift assay. *PLoS ONE*, **2017**, 12, e0177024	3.7	12
116	Ligand-mediated and tertiary interactions cooperatively stabilize the P1 region in the guanine-sensing riboswitch. *PLoS ONE*, **2017**, 12, e0179271	3.7	4
115	Trading off stability against activity in extremophilic aldolases. *Scientific Reports*, **2016**, 6, 17908	4.9	39
114	Structural assemblies of the di- and oligomeric G-protein coupled receptor TGR5 in live cells: an MFIS-FRET and integrative modelling study. *Scientific Reports*, **2016**, 6, 36792	4.9	17
113	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low (κ^2) Values. *Journal of Physical Chemistry B*, **2016**, 120, 8845-62	3.4	12
112	Platelets contribute to amyloid-β aggregation in cerebral vessels through integrin αIIbβ3-induced outside-in signaling and clusterin release. *Science Signaling*, **2016**, 9, ra52	8.8	56
111	Structural basis of lantibiotic recognition by the nisin resistance protein from Streptococcus agalactiae. *Scientific Reports*, **2016**, 6, 18679	4.9	31
110	Design and biological testing of peptidic dimerization inhibitors of human Hsp90 that target the C-terminal domain. *Biochimica Et Biophysica Acta - General Subjects*, **2016**, 1860, 1043-55	4	13
109	Interpreting Thermodynamic Profiles of Aminoadamantane Compounds Inhibiting the M2 Proton Channel of Influenza A by Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2016**, 56, 110-26	6.1	18
108	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPARγ activators. *European Journal of Medicinal Chemistry*, **2016**, 108, 423-435	6.8	17
107	Application of Rigidity Theory to the Thermostabilization of Lipase A from Bacillus subtilis. *PLoS Computational Biology*, **2016**, 12, e1004754	5	35
106	Redesigning Aldolase Stereoselectivity by Homologous Grafting. *PLoS ONE*, **2016**, 11, e0156525	3.7	5
105	Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. *PLoS Computational Biology*, **2016**, 12, e1004693	5	20
104	Structure of the Response Regulator NsrR from Streptococcus agalactiae, Which Is Involved in Lantibiotic Resistance. *PLoS ONE*, **2016**, 11, e0149903	3.7	10

103	Determinants of FIV and HIV Vif sensitivity of feline APOBEC3 restriction factors. *Retrovirology*, **2016**, 13, 46	3.6	17
102	Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems. *Current Opinion in Structural Biology*, **2016**, 40, 163-185	8.1	102
101	Alchemical Free Energy Calculations and Isothermal Titration Calorimetry Measurements of Aminoadamantanes Bound to the Closed State of Influenza A/M2TM. *Journal of Chemical Information and Modeling*, **2016**, 56, 862-76	6.1	18
100	-Aminoxy Oligopeptides: Synthesis, Secondary Structure, and Cytotoxicity of a New Class of Anticancer Foldamers. *Chemistry - A European Journal*, **2016**, 22, 17600-17611	4.8	12
99	Synthesis, Biological Evaluation and Molecular Modeling of Substituted Indeno[1,2-b]indoles as Inhibitors of Human Protein Kinase CK2. *Pharmaceuticals*, **2015**, 8, 279-302	5.2	25
98	VisualCNA: a GUI for interactive constraint network analysis and protein engineering for improving thermostability. *Bioinformatics*, **2015**, 31, 2394-6	7.2	10
97	Mutational mapping of the transmembrane binding site of the G-protein coupled receptor TGR5 and binding mode prediction of TGR5 agonists. *European Journal of Medicinal Chemistry*, **2015**, 104, 57-72	6.8	22
96	Toolkit for Multi-Conformation Biomolecular Structure Determination by High-Precision FRET and Molecular Simulations. *Biophysical Journal*, **2015**, 108, 163a-164a	2.9	
95	Complex long-distance effects of mutations that confer linezolid resistance in the large ribosomal subunit. *Nucleic Acids Research*, **2015**, 43, 7731-43	20.1	5
94	Extension of the free energy workflow FEW towards implicit solvent/implicit membrane MM-PBSA calculations. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 972-982	4	15
93	Force field dependence of riboswitch dynamics. *Methods in Enzymology*, **2015**, 553, 163-91	1.7	5
92	Design, synthesis, and biological evaluation of simplified side chain hybrids of the potent actin binding polyketides rhizopodin and bistramide. *ChemMedChem*, **2015**, 10, 470-89	3.7	10
91	Structural Rigidity and Protein Thermostability in Variants of Lipase A from Bacillus subtilis. *PLoS ONE*, **2015**, 10, e0130289	3.7	46
90	Molecular dynamics simulations and structure-guided mutagenesis provide insight into the architecture of the catalytic core of the ectoine hydroxylase. *Journal of Molecular Biology*, **2014**, 426, 586-600	6.5	39
89	Quality matters: extension of clusters of residues with good hydrophobic contacts stabilize (hyper)thermophilic proteins. *Journal of Chemical Information and Modeling*, **2014**, 54, 355-61	6.1	10
88	A membrane-proximal, C-terminal -helix is required for plasma membrane localization and function of the G Protein-coupled receptor (GPCR) TGR5. *Journal of Biological Chemistry*, **2014**, 289, 3689-702	5.4	13
87	Binding Free Energy Calculations for Lead Optimization: Assessment of Their Accuracy in an Industrial Drug Design Context. *Journal of Chemical Theory and Computation*, **2014**, 10, 3331-44	6.4	104
86	Design, synthesis, and conformational analysis of trispyrimidonamides as -helix mimetics. *Journal of Organic Chemistry*, **2014**, 79, 1582-93	4.2	3

85	DrugScorePPI knowledge-based potentials used as scoring and objective function in protein-protein docking. *PLoS ONE*, **2014**, 9, e89466	3.7	17
84	Resolving hot spots in the C-terminal dimerization domain that determine the stability of the molecular chaperone Hsp90. *PLoS ONE*, **2014**, 9, e96031	3.7	21
83	Efficient and robust analysis of biomacromolecular flexibility using ensembles of network topologies based on fuzzy noncovalent constraints. *Structure*, **2013**, 21, 1725-34	5.2	17
82	From determinants of RUNX1/ETO tetramerization to small-molecule protein-protein interaction inhibitors targeting acute myeloid leukemia. *Journal of Chemical Information and Modeling*, **2013**, 53, 2197-202	6.1	16
81	Proteinstabilität webbasiert analysieren. *Nachrichten Aus Der Chemie*, **2013**, 61, 909-911	0.1	
80	Binding region of alanopine dehydrogenase predicted by unbiased molecular dynamics simulations of ligand diffusion. *Journal of Chemical Information and Modeling*, **2013**, 53, 2493-8	6.1	20
79	CNA web server: rigidity theory-based thermal unfolding simulations of proteins for linking structure, (thermo-)stability, and function. *Nucleic Acids Research*, **2013**, 41, W340-8	20.1	97
78	FEW: a workflow tool for free energy calculations of ligand binding. *Journal of Computational Chemistry*, **2013**, 34, 965-73	3.5	73
77	Histone deacetylase (HDAC) inhibitors with a novel connecting unit linker region reveal a selectivity profile for HDAC4 and HDAC5 with improved activity against chemoresistant cancer cells. *Journal of Medicinal Chemistry*, **2013**, 56, 427-36	8.3	116
76	Constraint Network Analysis (CNA): a Python software package for efficiently linking biomacromolecular structure, flexibility, (thermo-)stability, and function. *Journal of Chemical Information and Modeling*, **2013**, 53, 1007-15	6.1	56
75	Global and local indices for characterizing biomolecular flexibility and rigidity. *Journal of Computational Chemistry*, **2013**, 34, 220-33	3.5	33
74	5 1-integrins are sensors for tauroursodeoxycholic acid in hepatocytes. *Hepatology*, **2013**, 57, 1117-29	11.2	56
73	Determinants of the species selectivity of oxazolidinone antibiotics targeting the large ribosomal subunit. *Biological Chemistry*, **2013**, 394, 1529-41	4.5	13
72	Advances in molecular dynamics simulations and free-energy calculations relevant for drug design **2013**, 50-63		4
71	Double-strand DNA end-binding and sliding of the toroidal CRISPR-associated protein Csn2. *Nucleic Acids Research*, **2013**, 41, 6347-59	20.1	37
70	Influence of the solvent representation on vibrational entropy calculations: generalized born versus distance-dependent dielectric model. *Journal of Computational Chemistry*, **2012**, 33, 1004-13	3.5	15
69	A toolkit and benchmark study for FRET-restrained high-precision structural modeling. *Nature Methods*, **2012**, 9, 1218-25	21.6	296
68	Structure-based computational analysis of protein binding sites for function and druggability prediction. *Journal of Biotechnology*, **2012**, 159, 123-34	3.7	82

67	Thermostabilizing mutations preferentially occur at structural weak spots with a high mutation ratio. *Journal of Biotechnology*, **2012**, 159, 135-44	3.7	36
66	Understanding the inhibitory effect of highly potent and selective archazolides binding to the vacuolar ATPase. *Journal of Chemical Information and Modeling*, **2012**, 52, 2265-72	6.1	18
65	Alignment-independent comparison of binding sites based on DrugScore potential fields encoded by 3D Zernike descriptors. *Journal of Chemical Information and Modeling*, **2012**, 52, 2339-47	6.1	3
64	The crystal structure of the CRISPR-associated protein Csn2 from Streptococcus agalactiae. *Journal of Structural Biology*, **2012**, 178, 350-62	3.4	21
63	How good are state-of-the-art docking tools in predicting ligand binding modes in protein-protein interfaces?. *Journal of Chemical Information and Modeling*, **2012**, 52, 2807-11	6.1	27
62	From Hansch-Fujita Analysis to AFMoC: A Road to Structure-Based QSAR. *Molecular Informatics*, **2012**, 31, 698-704	3.8	1
61	Hot spots and transient pockets: predicting the determinants of small-molecule binding to a protein-protein interface. *Journal of Chemical Information and Modeling*, **2012**, 52, 120-33	6.1	106
60	Scoring Functions for Protein□ligand Interactions **2012**, 237-263		9
59	Free Energy Calculations by the Molecular Mechanics Poisson-Boltzmann Surface Area Method. *Molecular Informatics*, **2012**, 31, 114-22	3.8	563
58	Modular Solid-Phase Synthesis of Teroxazoles as a Class of □-Helix Mimetics. *European Journal of Organic Chemistry*, **2012**, 2012, 3270-3277	3.2	9
57	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3314-21	6.4	1807
56	Resolving the negative potential side (n-side) water-accessible proton pathway of F-type ATP synthase by molecular dynamics simulations. *Journal of Biological Chemistry*, **2012**, 287, 36536-43	5.4	13
55	NMSim web server: integrated approach for normal mode-based geometric simulations of biologically relevant conformational transitions in proteins. *Nucleic Acids Research*, **2012**, 40, W310-6	20.1	64
54	Modulating protein-protein interactions: from structural determinants of binding to druggability prediction to application. *Current Pharmaceutical Design*, **2012**, 18, 4630-47	3.3	47
53	Flexibility analysis of biomacromolecules with application to computer-aided drug design. *Methods in Molecular Biology*, **2012**, 819, 75-91	1.4	4
52	Statics of Biomacromolecules **2011**, 281-299		2
51	Protein-Protein-Interaktionen webbasiert analysieren. *Nachrichten Aus Der Chemie*, **2011**, 59, 44-45	0.1	1
50	A normal mode-based geometric simulation approach for exploring biologically relevant conformational transitions in proteins. *Journal of Chemical Information and Modeling*, **2011**, 51, 1604-22	6.1	53

49	Pocket-space maps to identify novel binding-site conformations in proteins. *Journal of Chemical Information and Modeling*, **2011**, 51, 2666-79	6.1	37
48	Arg149 is involved in switching the low affinity, open state of the binding protein AfProX into its high affinity, closed state. *Journal of Molecular Biology*, **2011**, 411, 36-52	6.5	22
47	Towards targeting protein-protein interfaces with small molecules. *Journal of Cheminformatics*, **2011**, 3,	8.6	78
46	Protein rigidity and thermophilic adaptation. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1089-108	4.2	104
45	Target Flexibility in RNA-Ligand Docking Modeled by Elastic Potential Grids. *ACS Medicinal Chemistry Letters*, **2011**, 2, 489-93	4.3	19
44	DrugScorePPI webserver: fast and accurate in silico alanine scanning for scoring protein-protein interactions. *Nucleic Acids Research*, **2010**, 38, W480-6	20.1	118
43	Activation of integrins by urea in perfused rat liver. *Journal of Biological Chemistry*, **2010**, 285, 29348-56	5.4	13
42	Aromatic N versus aromatic F: bioisosterism discovered in RNA base pairing interactions leads to a novel class of universal base analogs. *Nucleic Acids Research*, **2010**, 38, 3133-46	20.1	35
41	HIV-1 TAR RNA spontaneously undergoes relevant apo-to-holo conformational transitions in molecular dynamics and constrained geometrical simulations. *Journal of Chemical Information and Modeling*, **2010**, 50, 1489-501	6.1	28
40	Molecular recognition of RNA: challenges for modelling interactions and plasticity. *Journal of Molecular Recognition*, **2010**, 23, 220-31	2.6	69
39	Protein Flexibility in In Silico Screening **2010**, 867-887		
38	Dimer-tetramer transition controls RUNX1/ETO leukemogenic activity. *Blood*, **2010**, 116, 603-13	2.2	35
37	Large-scale comparison of protein essential dynamics from molecular dynamics simulations and coarse-grained normal mode analyses. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3341-52	4.2	42
36	Elastic potential grids: accurate and efficient representation of intermolecular interactions for fully flexible docking. *ChemMedChem*, **2009**, 4, 1264-8	3.7	26
35	Steering protein-ligand docking with quantitative NMR chemical shift perturbations. *Journal of Chemical Information and Modeling*, **2009**, 49, 2260-71	6.1	32
34	Constraint counting on RNA structures: linking flexibility and function. *Methods*, **2009**, 49, 181-8	4.6	25
33	Statics of the ribosomal exit tunnel: implications for cotranslational peptide folding, elongation regulation, and antibiotics binding. *Journal of Molecular Biology*, **2009**, 387, 502-17	6.5	60
32	Analyzing the flexibility of RNA structures by constraint counting. *Biophysical Journal*, **2008**, 94, 4202-19	2.9	40

31	Starting structure dependence of NMR order parameters derived from MD simulations: implications for judging force-field quality. *Biophysical Journal*, **2008**, 95, L04-6	2.9	33
30	Target flexibility: an emerging consideration in drug discovery and design. *Journal of Medicinal Chemistry*, **2008**, 51, 6237-55	8.3	244
29	Predicting transmembrane helix pair configurations with knowledge-based distance-dependent pair potentials. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 984-99	4.2	7
28	Determinants of the unexpected stability of RNA fluorobenzene self pairs. *ChemBioChem*, **2008**, 9, 2619-28	3.2	36
27	DrugScoreRNA--knowledge-based scoring function to predict RNA-ligand interactions. *Journal of Chemical Information and Modeling*, **2007**, 47, 1868-76	6.1	78
26	Consensus adaptation of fields for molecular comparison (AFMoC) models incorporate ligand and receptor conformational variability into tailor-made scoring functions. *Journal of Chemical Information and Modeling*, **2007**, 47, 2383-400	6.1	15
25	Structure of Aquifex aeolicus argonaute highlights conformational flexibility of the PAZ domain as a potential regulator of RNA-induced silencing complex function. *Journal of Biological Chemistry*, **2007**, 282, 13824-32	5.4	41
24	Targeting protein-protein interactions with small molecules: challenges and perspectives for computational binding epitope detection and ligand finding. *Current Medicinal Chemistry*, **2006**, 13, 2607-25	4.3	144
23	A natural coarse graining for simulating large biomolecular motion. *Biophysical Journal*, **2006**, 91, 2115-20	2.9	123
22	Multiscale modeling of macromolecular conformational changes combining concepts from rigidity and elastic network theory. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 1038-51	4.2	78
21	Improving binding mode predictions by docking into protein-specifically adapted potential fields. *Journal of Medicinal Chemistry*, **2005**, 48, 5466-79	8.3	29
20	DrugScore(CSD)-knowledge-based scoring function derived from small molecule crystal data with superior recognition rate of near-native ligand poses and better affinity prediction. *Journal of Medicinal Chemistry*, **2005**, 48, 6296-303	8.3	284
19	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
18	Change in protein flexibility upon complex formation: analysis of Ras-Raf using molecular dynamics and a molecular framework approach. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 322-37	4.2	94
17	Converging free energy estimates: MM-PB(GB)SA studies on the protein-protein complex Ras-Raf. *Journal of Computational Chemistry*, **2004**, 25, 238-50	3.5	652
16	Assessing scoring functions for protein-ligand interactions. *Journal of Medicinal Chemistry*, **2004**, 47, 3032-47	8.3	433
15	3D QSAR analyses-guided rational design of novel ligands for the (alpha4)2(beta2)3 nicotinic acetylcholine receptor. *Journal of Medicinal Chemistry*, **2003**, 46, 2031-48	8.3	36
14	Ligand-supported homology modelling of protein binding-sites using knowledge-based potentials. *Journal of Molecular Biology*, **2003**, 334, 327-45	6.5	116

13	Insights into protein-protein binding by binding free energy calculation and free energy decomposition for the Ras-Raf and Ras-RalGDS complexes. *Journal of Molecular Biology*, **2003**, 330, 891-913	6.5	924
12	Approaches to the description and prediction of the binding affinity of small-molecule ligands to macromolecular receptors. *Angewandte Chemie - International Edition*, **2002**, 41, 2644-76	16.4	595
11	DrugScore meets CoMFA: adaptation of fields for molecular comparison (AFMoC) or how to tailor knowledge-based pair-potentials to a particular protein. *Journal of Medicinal Chemistry*, **2002**, 45, 4153-70	8.3	134
10	Synthesis and nicotinic binding studies on enantiopure diazine analogues of the novel (2-chloro-5-pyridyl)-9-azabicyclo[4.2.1]non-2-ene UB-165. *Journal of Medicinal Chemistry*, **2002**, 45, 1064-72	8.3	53
9	Docking into knowledge-based potential fields: a comparative evaluation of DrugScore. *Journal of Medicinal Chemistry*, **2002**, 45, 1967-70	8.3	83
8	Transport of peptidomimetic thrombin inhibitors with a 3-amidino-phenylalanine structure: permeability and efflux mechanism in monolayers of a human intestinal cell line (Caco-2). *Pharmaceutical Research*, **2001**, 18, 1110-8	4.5	10
7	Statistical potentials and scoring functions applied to protein-ligand binding. *Current Opinion in Structural Biology*, **2001**, 11, 231-5	8.1	174
6	Predicting binding modes, binding affinities and □hot spotsSfor protein-ligand complexes using a knowledge-based scoring function. *Journal of Computer - Aided Molecular Design*, **2000**, 20, 115-144		86
5	Knowledge-based scoring function to predict protein-ligand interactions. *Journal of Molecular Biology*, **2000**, 295, 337-56	6.5	871
4	Conformations and lipophilicity profiles of some cyclic Ð(1-3)- and Ð(1-6)-linked oligogalactofuranosides. *Carbohydrate Research*, **1999**, 321, 96-104	2.9	11
3	Respiratory and C4-photosynthetic NAD-malic enzyme coexist in bundle sheath cells mitochondria and evolved via association of differentially adapted subunits		1
2	Novel intracellular phospholipase B from Pseudomonas aeruginosa with activity towards endogenous phospholipids affects biofilm assembly		1
1	Evidence for a bacterial Lands cycle phospholipase A: Structural and mechanistic insights into membrane phospholipid remodeling		1