Holger Gohlke

List of Publications by Citations

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	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
227	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3314-21	6.4	1807
226	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
225	Knowledge-based scoring function to predict protein-ligand interactions. *Journal of Molecular Biology*, **2000**, 295, 337-56	6.5	871
224	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
223	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
222	Free Energy Calculations by the Molecular Mechanics Poisson-Boltzmann Surface Area Method. *Molecular Informatics*, **2012**, 31, 114-22	3.8	563
221	Assessing scoring functions for protein-ligand interactions. *Journal of Medicinal Chemistry*, **2004**, 47, 3032-47	8.3	433
220	A toolkit and benchmark study for FRET-restrained high-precision structural modeling. *Nature Methods*, **2012**, 9, 1218-25	21.6	296
219	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
218	Target flexibility: an emerging consideration in drug discovery and design. *Journal of Medicinal Chemistry*, **2008**, 51, 6237-55	8.3	244
217	Statistical potentials and scoring functions applied to protein-ligand binding. *Current Opinion in Structural Biology*, **2001**, 11, 231-5	8.1	174
216	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
215	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
214	A natural coarse graining for simulating large biomolecular motion. *Biophysical Journal*, **2006**, 91, 2115-20	4.9	123
213	DrugScorePPI webserver: fast and accurate in silico alanine scanning for scoring protein-protein interactions. *Nucleic Acids Research*, **2010**, 38, W480-6	20.1	118
212	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

211	Ligand-supported homology modelling of protein binding-sites using knowledge-based potentials. *Journal of Molecular Biology*, **2003**, 334, 327-45	6.5	116
210	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
209	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
208	Protein rigidity and thermophilic adaptation. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1089-108	4.2	104
207	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
206	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
205	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
204	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
203	Docking into knowledge-based potential fields: a comparative evaluation of DrugScore. *Journal of Medicinal Chemistry*, **2002**, 45, 1967-70	8.3	83
202	Structure-based computational analysis of protein binding sites for function and druggability prediction. *Journal of Biotechnology*, **2012**, 159, 123-34	3.7	82
201	Towards targeting protein-protein interfaces with small molecules. *Journal of Cheminformatics*, **2011**, 3,	8.6	78
200	DrugScoreRNA--knowledge-based scoring function to predict RNA-ligand interactions. *Journal of Chemical Information and Modeling*, **2007**, 47, 1868-76	6.1	78
199	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
198	FEW: a workflow tool for free energy calculations of ligand binding. *Journal of Computational Chemistry*, **2013**, 34, 965-73	3.5	73
197	Molecular recognition of RNA: challenges for modelling interactions and plasticity. *Journal of Molecular Recognition*, **2010**, 23, 220-31	2.6	69
196	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
195	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
194	A Novel Polyester Hydrolase From the Marine Bacterium Structural and Functional Insights. *Frontiers in Microbiology*, **2020**, 11, 114	5.7	62

193	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
192	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
191	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
190	α5β1-integrins are sensors for tauroursodeoxycholic acid in hepatocytes. *Hepatology*, **2013**, 57, 1117-29	11.2	56
189	On the Effects of Reactive Oxygen Species and Nitric Oxide on Red Blood Cell Deformability. *Frontiers in Physiology*, **2018**, 9, 332	4.6	54
188	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
187	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
186	Modulating protein-protein interactions: from structural determinants of binding to druggability prediction to application. *Current Pharmaceutical Design*, **2012**, 18, 4630-47	3.3	47
185	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
184	Structural Rigidity and Protein Thermostability in Variants of Lipase A from Bacillus subtilis. *PLoS ONE*, **2015**, 10, e0130289	3.7	46
183	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
182	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
181	Analyzing the flexibility of RNA structures by constraint counting. *Biophysical Journal*, **2008**, 94, 4202-19	2.9	40
180	Trading off stability against activity in extremophilic aldolases. *Scientific Reports*, **2016**, 6, 17908	4.9	39
179	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
178	Effects of novel HDAC inhibitors on urothelial carcinoma cells. *Clinical Epigenetics*, **2018**, 10, 100	7.7	38
177	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
176	Double-strand DNA end-binding and sliding of the toroidal CRISPR-associated protein Csn2. *Nucleic Acids Research*, **2013**, 41, 6347-59	20.1	37

175	Pocket-space maps to identify novel binding-site conformations in proteins. *Journal of Chemical Information and Modeling*, **2011**, 51, 2666-79	6.1	37
174	Thermostabilizing mutations preferentially occur at structural weak spots with a high mutation ratio. *Journal of Biotechnology*, **2012**, 159, 135-44	3.7	36
173	Determinants of the unexpected stability of RNA fluorobenzene self pairs. *ChemBioChem*, **2008**, 9, 2619-28	3.2	36
172	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
171	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
170	Dimer-tetramer transition controls RUNX1/ETO leukemogenic activity. *Blood*, **2010**, 116, 603-13	2.2	35
169	Application of Rigidity Theory to the Thermostabilization of Lipase A from Bacillus subtilis. *PLoS Computational Biology*, **2016**, 12, e1004754	5	35
168	Global and local indices for characterizing biomolecular flexibility and rigidity. *Journal of Computational Chemistry*, **2013**, 34, 220-33	3.5	33
167	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
166	Steering protein-ligand docking with quantitative NMR chemical shift perturbations. *Journal of Chemical Information and Modeling*, **2009**, 49, 2260-71	6.1	32
165	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
164	Resolving dynamics and function of transient states in single enzyme molecules. *Nature Communications*, **2020**, 11, 1231	17.4	31
163	Structural basis of lantibiotic recognition by the nisin resistance protein from Streptococcus agalactiae. *Scientific Reports*, **2016**, 6, 18679	4.9	31
162	Alkoxyurea-Based Histone Deacetylase Inhibitors Increase Cisplatin Potency in Chemoresistant Cancer Cell Lines. *Journal of Medicinal Chemistry*, **2017**, 60, 5334-5348	8.3	31
161	Improving binding mode predictions by docking into protein-specifically adapted potential fields. *Journal of Medicinal Chemistry*, **2005**, 48, 5466-79	8.3	29
160	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
159	Converging a Knowledge-Based Scoring Function: DrugScore. *Journal of Chemical Information and Modeling*, **2019**, 59, 509-521	6.1	28
158	Systematic analysis of ATG13 domain requirements for autophagy induction. *Autophagy*, **2018**, 14, 743-763	13.2	28

157	Co-culture of the fungus with induces production of cryptic naphthoquinone dimers.. *RSC Advances*, **2019**, 9, 1491-1500	3.7	27
156	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
155	Elastic potential grids: accurate and efficient representation of intermolecular interactions for fully flexible docking. *ChemMedChem*, **2009**, 4, 1264-8	3.7	26
154	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
153	Constraint counting on RNA structures: linking flexibility and function. *Methods*, **2009**, 49, 181-8	4.6	25
152	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
151	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
150	Partially inserted nascent chain unzips the lateral gate of the Sec translocon. *EMBO Reports*, **2019**, 20, e48191	6.5	22
149	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
148	Rigidity theory for biomolecules: concepts, software, and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1311	7.9	21
147	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
146	The crystal structure of the CRISPR-associated protein Csn2 from Streptococcus agalactiae. *Journal of Structural Biology*, **2012**, 178, 350-62	3.4	21
145	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
144	Quantitative assessment of the determinant structural differences between redox-active and inactive glutaredoxins. *Nature Communications*, **2020**, 11, 1725	17.4	20
143	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
142	Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery. *Journal of Chemical Theory and Computation*, **2017**, 13, 6343-6357	6.4	20
141	Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. *PLoS Computational Biology*, **2016**, 12, e1004693	5	20
140	Target Flexibility in RNA-Ligand Docking Modeled by Elastic Potential Grids. *ACS Medicinal Chemistry Letters*, **2011**, 2, 489-93	4.3	19

139	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
138	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
137	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
136	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
135	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
134	Recognition motif and mechanism of ripening inhibitory peptides in plant hormone receptor ETR1. *Scientific Reports*, **2018**, 8, 3890	4.9	17
133	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
132	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPAR□activators. *European Journal of Medicinal Chemistry*, **2016**, 108, 423-435	6.8	17
131	Biallelic mutation of human encoding the taurine transporter TAUT is linked to early retinal degeneration. *FASEB Journal*, **2019**, 33, 11507-11527	0.9	17
130	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
129	DrugScorePPI knowledge-based potentials used as scoring and objective function in protein-protein docking. *PLoS ONE*, **2014**, 9, e89466	3.7	17
128	Determinants of FIV and HIV Vif sensitivity of feline APOBEC3 restriction factors. *Retrovirology*, **2016**, 13, 46	3.6	17
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126	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
125	Synthesis of Peptoid-Based Class I-Selective Histone Deacetylase Inhibitors with Chemosensitizing Properties. *Journal of Medicinal Chemistry*, **2019**, 62, 11260-11279	8.3	16
124	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
123	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
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115	Determinants of the species selectivity of oxazolidinone antibiotics targeting the large ribosomal subunit. *Biological Chemistry*, **2013**, 394, 1529-41	4.5	13
114	Activation of integrins by urea in perfused rat liver. *Journal of Biological Chemistry*, **2010**, 285, 29348-56	5.4	13
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110	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
109	On the contributing role of the transmembrane domain for subunit-specific sensitivity of integrin activation. *Scientific Reports*, **2018**, 8, 5733	4.9	12
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105	β-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
104	Nutrient exchange in arbuscular mycorrhizal symbiosis from a thermodynamic point of view. *New Phytologist*, **2019**, 222, 1043-1053	9.8	12

103	Structural intermediates and directionality of the swiveling motion of Pyruvate Phosphate Dikinase. *Scientific Reports*, **2017**, 7, 45389	4.9	11
102	Conformations and lipophilicity profiles of some cyclic α(1-3)- and α(1-6)-linked oligogalactofuranosides. *Carbohydrate Research*, **1999**, 321, 96-104	2.9	11
101	Interdependence of a mechanosensitive anion channel and glutamate receptors in distal wound signaling. *Science Advances*, **2021**, 7, eabg4298	14.3	11
100	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
99	VisualCNA: a GUI for interactive constraint network analysis and protein engineering for improving thermostability. *Bioinformatics*, **2015**, 31, 2394-6	7.2	10
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87	Surprising Non-Additivity of Methyl Groups in Drug-Kinase Interaction. *ACS Chemical Biology*, **2019**, 14, 2585-2594	4.9	8
86	Structure and efflux mechanism of the yeast pleiotropic drug resistance transporter Pdr5. *Nature Communications*, **2021**, 12, 5254	17.4	8

85	AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools. *Journal of Chemical Physics*, **2020**, 152, 221103	3.9	7
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70	Novel Fluorescent Cyclic Nucleotide Derivatives to Study CNG and HCN Channel Function. *Biophysical Journal*, **2019**, 116, 2411-2422	2.9	5
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