Holger Gohlke

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1731220/publications.pdf

Version: 2024-02-01

241 papers	23,558 citations	43973 48 h-index	8599 146 g-index
263 all docs	263 docs citations	263 times ranked	24056 citing authors

#	Article	IF	Citations
1	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
2	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 3314-3321.	2.3	2,891
3	Insights into Proteinâ€“Protein Binding by Binding Free Energy Calculation and Free Energy Decomposition for the Rasâ€“Raf and Rasâ€“RalGDS Complexes. Journal of Molecular Biology, 2003, 330, 891-913.	2.0	1,079
4	Knowledge-based scoring function to predict protein-ligand interactions. Journal of Molecular Biology, 2000, 295, 337-356.	2.0	1,009
5	Free Energy Calculations by the Molecular Mechanics Poissonâ^'Boltzmann Surface Area Method. Molecular Informatics, 2012, 31, 114-122.	1.4	768
6	Converging free energy estimates: MM-PB(GB)SA studies on the protein-protein complex Ras-Raf. Journal of Computational Chemistry, 2004, 25, 238-250.	1.5	750
7	Approaches to the Description and Prediction of the Binding Affinity of Small-Molecule Ligands to Macromolecular Receptors. Angewandte Chemie - International Edition, 2002, 41, 2644-2676.	7.2	729
8	Assessing Scoring Functions for Proteinâ^'Ligand Interactions. Journal of Medicinal Chemistry, 2004, 47, 3032-3047.	2.9	464
9	A toolkit and benchmark study for FRET-restrained high-precision structural modeling. Nature Methods, 2012, 9, 1218-1225.	9.0	400
10	DrugScoreCSDKnowledge-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, 6296-6303.	2.9	314
11	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
12	Statistical potentials and scoring functions applied to proteinâ€“ligand binding. Current Opinion in Structural Biology, 2001, 11, 231-235.	2.6	186
13	Targeting Protein-Protein Interactions with Small Molecules: Challenges and Perspectives for omputational Binding Epitope Detection and Ligand Finding. Current Medicinal Chemistry, 2006, 13, 2607-2625.	1.2	174
14	A Novel Polyester Hydrolase From the Marine Bacterium Pseudomonas aestusnigri â€“ Structural and Functional Insights. Frontiers in Microbiology, 2020, 11, 114.	1.5	172
15	Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems. Current Opinion in Structural Biology, 2016, 40, 163-185.	2.6	156
16	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, 427-436.	2.9	152
17	DrugScorePPI webserver: fast and accurate in silico alanine scanning for scoring proteinâ€“protein interactions. Nucleic Acids Research, 2010, 38, W480-W486.	6.5	146
18	Protein rigidity and thermophilic adaptation. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1089-1108.	1.5	141

#	Article	IF	Citations
19	DrugScore Meets CoMFA:Â 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, 4153-4170.	2.9	139
20	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, 3331-3344.	2.3	139
21	A Natural Coarse Graining for Simulating Large Biomolecular Motion. Biophysical Journal, 2006, 91, 2115-2120.	0.2	129
22	Ligand-supported Homology Modelling of Protein Binding-sites using Knowledge-based Potentials. Journal of Molecular Biology, 2003, 334, 327-345.	2.0	126
23	PACKMOL-Memgen: A Simple-To-Use, Generalized Workflow for Membrane-Proteinâ€“Lipid-Bilayer System Building. Journal of Chemical Information and Modeling, 2019, 59, 2522-2528.	2.5	121
24	Hot Spots and Transient Pockets: Predicting the Determinants of Small-Molecule Binding to a Proteinâ€“Protein Interface. Journal of Chemical Information and Modeling, 2012, 52, 120-133.	2.5	120
25	CNA web server: rigidity theory-based thermal unfolding simulations of proteins for linking structure, (thermo-)stability, and function. Nucleic Acids Research, 2013, 41, W340-W348.	6.5	118
26	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, 322-337.	1.5	106
27	Structure-based computational analysis of protein binding sites for function and druggability prediction. Journal of Biotechnology, 2012, 159, 123-134.	1.9	100
28	DrugScore^{RNA}Knowledge-Based Scoring Function To Predict RNAâ^'Ligand Interactions. Journal of Chemical Information and Modeling, 2007, 47, 1868-1876.	2.5	98
29	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.	1.8	97
30	Docking into Knowledge-Based Potential Fields:â€‰ A Comparative Evaluation of DrugScore. Journal of Medicinal Chemistry, 2002, 45, 1967-1970.	2.9	96
31	Title is missing!. Journal of Computer - Aided Molecular Design, 2000, 20, 115-144.	1.0	92
32	Platelets contribute to amyloid-Î² aggregation in cerebral vessels through integrin Î± _{IIb} Î² ₃ â€“induced outside-in signaling and clusterin release. Science Signaling, 2016, 9, ra52.	1.6	89
33	Multiscale modeling of macromolecular conformational changes combining concepts from rigidity and elastic network theory. Proteins: Structure, Function and Bioinformatics, 2006, 63, 1038-1051.	1.5	88
34	FEW: A workflow tool for free energy calculations of ligand binding. Journal of Computational Chemistry, 2013, 34, 965-973.	1.5	86
35	Molecular recognition of RNA: challenges for modelling interactions and plasticity. Journal of Molecular Recognition, 2010, 23, 220-231.	1.1	85
36	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, 1007-1015.	2.5	81

#	Article	IF	Citations
37	On the Effects of Reactive Oxygen Species and Nitric Oxide on Red Blood Cell Deformability. Frontiers in Physiology, 2018, 9, 332.	1.3	80
38	NMSim Web Server: integrated approach for normal mode-based geometric simulations of biologically relevant conformational transitions in proteins. Nucleic Acids Research, 2012, 40, W310-W316.	6.5	79
39	Resolving dynamics and function of transient states in single enzyme molecules. Nature Communications, 2020, 11, 1231.	5.8	71
40	Î±₅ Î²₁ -integrins are sensors for tauroursodeoxycholic acid in hepatocytes. Hepatology, 2013, 57, 1117-1129.	3.6	67
41	Statics of the Ribosomal Exit Tunnel: Implications for Cotranslational Peptide Folding, Elongation Regulation, and Antibiotics Binding. Journal of Molecular Biology, 2009, 387, 502-517.	2.0	66
42	Targeting HSP90 dimerization via the C terminus is effective in imatinib-resistant CML and lacks the heat shock response. Blood, 2018, 132, 307-320.	0.6	66
43	Time-resolved structural analysis of an RNA-cleaving DNA catalyst. Nature, 2022, 601, 144-149.	13.7	65
44	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, 1064-1072.	2.9	64
45	Structural Rigidity and Protein Thermostability in Variants of Lipase A from Bacillus subtilis. PLoS ONE, 2015, 10, e0130289.	1.1	64
46	A Normal Mode-Based Geometric Simulation Approach for Exploring Biologically Relevant Conformational Transitions in Proteins. Journal of Chemical Information and Modeling, 2011, 51, 1604-1622.	2.5	62
47	Modulating Protein-Protein Interactions: From Structural Determinants of Binding to Druggability Prediction to Application. Current Pharmaceutical Design, 2012, 18, 4630-4647.	0.9	54
48	Effects of novel HDAC inhibitors on urothelial carcinoma cells. Clinical Epigenetics, 2018, 10, 100.	1.8	51
49	Structure and efflux mechanism of the yeast pleiotropic drug resistance transporter Pdr5. Nature Communications, 2021, 12, 5254.	5.8	51
50	Global and local indices for characterizing biomolecular flexibility and rigidity. Journal of Computational Chemistry, 2013, 34, 220-233.	1.5	50
51	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, 13824-13832.	1.6	48
52	Trading off stability against activity in extremophilic aldolases. Scientific Reports, 2016, 6, 17908.	1.6	48
53	Converging a Knowledge-Based Scoring Function: DrugScore²⁰¹⁸. Journal of Chemical Information and Modeling, 2019, 59, 509-521.	2.5	48
54	Application of Rigidity Theory to the Thermostabilization of Lipase A from Bacillus subtilis. PLoS Computational Biology, 2016, 12, e1004754.	1.5	48

#	Article	IF	Citations
55	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.	2.5	46
56	Interdependence of a mechanosensitive anion channel and glutamate receptors in distal wound signaling. Science Advances, 2021, 7, eabg4298.	4.7	45
57	Largeâ€scale comparison of protein essential dynamics from molecular dynamics simulations and coarseâ€grained normal mode analyses. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3341-3352.	1.5	44
58	Thermostabilizing mutations preferentially occur at structural weak spots with a high mutation ratio. Journal of Biotechnology, 2012, 159, 135-144.	1.9	44
59	C-terminal modulators of heat shock protein of 90â€¯kDa (HSP90): State of development and modes of action. Bioorganic and Medicinal Chemistry, 2019, 27, 115080.	1.4	44
60	Analyzing the Flexibility of RNA Structures by Constraint Counting. Biophysical Journal, 2008, 94, 4202-4219.	0.2	43
61	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.	2.0	43
62	Structural basis of lantibiotic recognition by the nisin resistance protein from Streptococcus agalactiae. Scientific Reports, 2016, 6, 18679.	1.6	42
63	Double-strand DNA end-binding and sliding of the toroidal CRISPR-associated protein Csn2. Nucleic Acids Research, 2013, 41, 6347-6359.	6.5	41
64	3D QSAR Analyses-Guided Rational Design of Novel Ligands for the (Î±4)2(Î²2)3Nicotinic Acetylcholine Receptor. Journal of Medicinal Chemistry, 2003, 46, 2031-2048.	2.9	40
65	Determinants of the Unexpected Stability of RNA Fluorobenzene Self Pairs. ChemBioChem, 2008, 9, 2619-2622.	1.3	40
66	Dimer-tetramer transition controls RUNX1/ETO leukemogenic activity. Blood, 2010, 116, 603-613.	0.6	40
67	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.	2.3	40
68	Pocket-Space Maps To Identify Novel Binding-Site Conformations in Proteins. Journal of Chemical Information and Modeling, 2011, 51, 2666-2679.	2.5	39
69	Partially inserted nascent chain unzips the lateral gate of the Sec translocon. EMBO Reports, 2019, 20, e48191.	2.0	39
70	Automated and optimally FRET-assisted structural modeling. Nature Communications, 2020, 11, 5394.	5.8	39
71	Systematic analysis of ATG13 domain requirements for autophagy induction. Autophagy, 2018, 14, 743-763.	4.3	38
72	Binding modes of thioflavin T and Congo red to the fibril structure of amyloid-Î²(1â€“42). Chemical Communications, 2020, 56, 7589-7592.	2.2	38

#	Article	IF	Citations
73	Steering Proteinâ"Ligand Docking with Quantitative NMR Chemical Shift Perturbations. Journal of Chemical Information and Modeling, 2009, 49, 2260-2271.	2.5	37
74	Alkoxyurea-Based Histone Deacetylase Inhibitors Increase Cisplatin Potency in Chemoresistant Cancer Cell Lines. Journal of Medicinal Chemistry, 2017, 60, 5334-5348.	2.9	37
75	Co-culture of the fungusFusarium tricinctumwithStreptomyces lividansinduces production of cryptic naphthoquinone dimers. RSC Advances, 2019, 9, 1491-1500.	1.7	37
76	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, 3133-3146.	6.5	36
77	Biallelic mutation of human SLC6A6 encoding the taurine transporter TAUT is linked to early retinal degeneration. FASEB Journal, 2019, 33, 11507-11527.	0.2	36
78	Quantitative assessment of the determinant structural differences between redox-active and inactive glutaredoxins. Nature Communications, 2020, 11, 1725.	5.8	34
79	Starting Structure Dependence of NMR Order Parameters Derived from MD Simulations: Implications for Judging Force-Field Quality. Biophysical Journal, 2008, 95, L04-L06.	0.2	33
80	Structural Model of the ETR1 Ethylene Receptor Transmembrane Sensor Domain. Scientific Reports, 2019, 9, 8869.	1.6	33
81	Calcium-Promoted Interaction between the C2-Domain Protein EHB1 and Metal Transporter IRT1 Inhibits Arabidopsis Iron Acquisition. Plant Physiology, 2019, 180, 1564-1581.	2.3	33
82	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.	2.9	32
83	Elastic Potential Grids: Accurate and Efficient Representation of Intermolecular Interactions for Fully Flexible Docking. ChemMedChem, 2009, 4, 1264-1268.	1.6	31
84	Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery. Journal of Chemical Theory and Computation, 2017, 13, 6343-6357.	2.3	31
85	Improving Binding Mode Predictions by Docking into Protein-Specifically Adapted Potential Fields. Journal of Medicinal Chemistry, 2005, 48, 5466-5479.	2.9	30
86	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.	2.3	30
87	How Good Are State-of-the-Art Docking Tools in Predicting Ligand Binding Modes in Proteinâ€"Protein Interfaces?. Journal of Chemical Information and Modeling, 2012, 52, 2807-2811.	2.5	29
88	Binding Region of Alanopine Dehydrogenase Predicted by Unbiased Molecular Dynamics Simulations of Ligand Diffusion. Journal of Chemical Information and Modeling, 2013, 53, 2493-2498.	2.5	29
89	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.	1.7	29
90	Rigidity theory for biomolecules: concepts, software, and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1311.	6.2	29

#	Article	IF	Citations
91	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, 1489-1501.	2.5	28
92	Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. PLoS Computational Biology, 2016, 12, e1004693.	1.5	28
93	Constraint counting on RNA structures: Linking flexibility and function. Methods, 2009, 49, 181-188.	1.9	27
94	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.	2.6	27
95	Recognition motif and mechanism of ripening inhibitory peptides in plant hormone receptor ETR1. Scientific Reports, 2018, 8, 3890.	1.6	27
96	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.	2.3	27
97	Synthesis of Peptoid-Based Class I-Selective Histone Deacetylase Inhibitors with Chemosensitizing Properties. Journal of Medicinal Chemistry, 2019, 62, 11260-11279.	2.9	27
98	Resolving Hot Spots in the C-Terminal Dimerization Domain that Determine the Stability of the Molecular Chaperone Hsp90. PLoS ONE, 2014, 9, e96031.	1.1	27
99	EDTA aggregates induce SYPRO orange-based fluorescence in thermal shift assay. PLoS ONE, 2017, 12, e0177024.	1.1	27
100	Chlorflavonin Targets Acetohydroxyacid Synthase Catalytic Subunit IlvB1 for Synergistic Killing of Mycobacterium tuberculosis. ACS Infectious Diseases, 2018, 4, 123-134.	1.8	26
101	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.	2.0	25
102	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, 862-876.	2.5	25
103	Target Flexibility in RNAâ^'Ligand Docking Modeled by Elastic Potential Grids. ACS Medicinal Chemistry Letters, 2011, 2, 489-493.	1.3	24
104	The crystal structure of the CRISPR-associated protein Csn2 from Streptococcus agalactiae. Journal of Structural Biology, 2012, 178, 350-362.	1.3	24
105	Interaction of Ochratoxin A and Its Thermal Degradation Product 2â€²R-Ochratoxin A with Human Serum Albumin. Toxins, 2018, 10, 256.	1.5	24
106	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.	1.6	23
107	From Determinants of RUNX1/ETO Tetramerization to Small-Molecule Proteinâ€“Protein Interaction Inhibitors Targeting Acute Myeloid Leukemia. Journal of Chemical Information and Modeling, 2013, 53, 2197-2202.	2.5	22
108	Structure of the Response Regulator NsrR from Streptococcus agalactiae, Which Is Involved in Lantibiotic Resistance. PLoS ONE, 2016, 11, e0149903.	1.1	22

#	Article	IF	Citations
109	Efficient and Robust Analysis of Biomacromolecular Flexibility Using Ensembles of Network Topologies Based on Fuzzy Noncovalent Constraints. Structure, 2013, 21, 1725-1734.	1.6	21
110	Determinants of FIV and HIV Vif sensitivity of feline APOBEC3 restriction factors. Retrovirology, 2016, 13, 46.	0.9	21
111	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, 110-126.	2.5	21
112	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPARÎ³ activators. European Journal of Medicinal Chemistry, 2016, 108, 423-435.	2.6	21
113	Systematically Scrutinizing the Impact of Substitution Sites on Thermostability and Detergent Tolerance for Bacillus subtilis Lipase A. Journal of Chemical Information and Modeling, 2020, 60, 1568-1584.	2.5	21
114	Discovery of new acetylcholinesterase inhibitors for Alzheimerâ€™s disease: virtual screening and inÂvitro characterisation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 491-496.	2.5	21
115	Extension of the free energy workflow FEW towards implicit solvent/implicit membrane MMâ€“PBSA calculations. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 972-982.	1.1	20
116	Posttranslational Modification of the NADP-Malic Enzyme Involved in C₄ Photosynthesis Modulates the Enzymatic Activity during the Day. Plant Cell, 2019, 31, 2525-2539.	3.1	20
117	FK506 Resistance of Saccharomyces cerevisiae Pdr5 and Candida albicans Cdr1 Involves Mutations in the Transmembrane Domains and Extracellular Loops. Antimicrobial Agents and Chemotherapy, 2019, 63, .	1.4	20
118	Glutamine synthetase as a central element in hepatic glutamine and ammonia metabolism: novel aspects. Biological Chemistry, 2021, 402, 1063-1072.	1.2	20
119	Nutrient exchange in arbuscular mycorrhizal symbiosis from a thermodynamic point of view. New Phytologist, 2019, 222, 1043-1053.	3.5	19
120	DrugScorePPI Knowledge-Based Potentials Used as Scoring and Objective Function in Protein-Protein Docking. PLoS ONE, 2014, 9, e89466.	1.1	19
121	Understanding the Inhibitory Effect of Highly Potent and Selective Archazolides Binding to the Vacuolar ATPase. Journal of Chemical Information and Modeling, 2012, 52, 2265-2272.	2.5	18
122	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, 1043-1055.	1.1	18
123	On the contributing role of the transmembrane domain for subunit-specific sensitivity of integrin activation. Scientific Reports, 2018, 8, 5733.	1.6	18
124	Fluorescent analogs of peptoid-based HDAC inhibitors: Synthesis, biological activity and cellular uptake kinetics. Bioorganic and Medicinal Chemistry, 2019, 27, 115039.	1.4	18
125	40 Years of Research on Polybrominated Diphenyl Ethers (PBDEs)â€”A Historical Overview and Newest Data of a Promising Anticancer Drug. Molecules, 2021, 26, 995.	1.7	18
126	Influence of the solvent representation on vibrational entropy calculations: Generalized born versus distanceâ€dependent dielectric model. Journal of Computational Chemistry, 2012, 33, 1004-1013.	1.5	17

#	Article	IF	Citations
127	Rigidity Theory-Based Approximation of Vibrational Entropy Changes upon Binding to Biomolecules. Journal of Chemical Theory and Computation, 2017, 13, 1495-1502.	2.3	17
128	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.	1.9	17
129	Relevance of N-terminal residues for amyloid-Î² binding to platelet integrin Î± IIb Î² 3 , integrin outside-in signaling and amyloid-Î² fibril formation. Cellular Signalling, 2018, 50, 121-130.	1.7	17
130	AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools. Journal of Chemical Physics, 2020, 152, 221103.	1.2	17
131	Î±â€Aminoxy Oligopeptides: Synthesis, Secondary Structure, and Cytotoxicity of a New Class of Anticancer Foldamers. Chemistry - A European Journal, 2016, 22, 17600-17611.	1.7	16
132	Structural intermediates and directionality of the swiveling motion of Pyruvate Phosphate Dikinase. Scientific Reports, 2017, 7, 45389.	1.6	16
133	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.	1.6	16
134	A promiscuous ancestral enzymeÂ´s structure unveils protein variable regions of the highly diverse metallo-Î²-lactamase family. Communications Biology, 2021, 4, 132.	2.0	16
135	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, 2383-2400.	2.5	15
136	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, 36536-36543.	1.6	15
137	A Membrane-proximal, C-terminal Î±-Helix Is Required for Plasma Membrane Localization and Function of the G Protein-coupled Receptor (GPCR) TGR5. Journal of Biological Chemistry, 2014, 289, 3689-3702.	1.6	15
138	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low Î²² Values. Journal of Physical Chemistry B, 2016, 120, 8845-8862.	1.2	15
139	Determinants of the species selectivity of oxazolidinone antibiotics targeting the large ribosomal subunit. Biological Chemistry, 2013, 394, 1529-1541.	1.2	14
140	Surprising Non-Additivity of Methyl Groups in Drugâ€“Kinase Interaction. ACS Chemical Biology, 2019, 14, 2585-2594.	1.6	14
141	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.	2.5	14
142	Aqueous ionic liquids redistribute local enzyme stability via long-range perturbation pathways. Computational and Structural Biotechnology Journal, 2021, 19, 4248-4264.	1.9	14
143	Activation of Integrins by Urea in Perfused Rat Liver. Journal of Biological Chemistry, 2010, 285, 29348-29356.	1.6	13
144	VisualCNA: a GUI for interactive constraint network analysis and protein engineering for improving thermostability. Bioinformatics, 2015, 31, 2394-2396.	1.8	13

#	Article	IF	Citations
145	Suppression of RUNX1/ETO oncogenic activity by a small molecule inhibitor of tetramerization. Haematologica, 2017, 102, e170-e174.	1.7	13
146	The tetrahydroxanthone-dimer phomoxanthone A is a strong inducer of apoptosis in cisplatin-resistant solid cancer cells. Bioorganic and Medicinal Chemistry, 2019, 27, 115044.	1.4	13
147	Novel Fluorescent Cyclic Nucleotide Derivatives to Study CNG and HCN Channel Function. Biophysical Journal, 2019, 116, 2411-2422.	0.2	13
148	The Puzzle of Metabolite Exchange and Identification of Putative Octotrico Peptide Repeat Expression Regulators in the Nascent Photosynthetic Organelles of Paulinella chromatophora. Frontiers in Microbiology, 2020, 11, 607182.	1.5	13
149	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. Chemical Research in Toxicology, 2021, 34, 1503-1517.	1.7	13
150	Promiscuous Esterases Counterintuitively Are Less Flexible than Specific Ones. Journal of Chemical Information and Modeling, 2021, 61, 2383-2395.	2.5	13
151	Structural, mechanistic, and physiological insights into phospholipase A-mediated membrane phospholipid degradation in Pseudomonas aeruginosa. ELife, 2022, 11, .	2.8	13
152	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, 1110-1118.	1.7	12
153	Semisynthetic Analogs of the Antibiotic Fidaxomicinâ€"Design, Synthesis, and Biological Evaluation. ACS Medicinal Chemistry Letters, 2020, 11, 2414-2420.	1.3	12
154	Structural and dynamic insights revealing how lipase binding domain MD1 of Pseudomonas aeruginosa foldase affects lipase activation. Scientific Reports, 2020, 10, 3578.	1.6	12
155	Pseudomonas aeruginosaesterase 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.	0.4	12
156	Development of a First-in-Class Small-Molecule Inhibitor of the C-Terminal Hsp90 Dimerization. ACS Central Science, 2022, 8, 636-655.	5.3	12
157	Conformations and lipophilicity profiles of some cyclic Î²-(1â†'3)- and Î²-(1â†'6)-linked oligogalactofuranosides. Carbohydrate Research, 1999, 321, 96-104.	1.1	11
158	Modular Solidâ€Phase Synthesis of Teroxazoles as a Class of Îµâ€Helix Mimetics. European Journal of Organic Chemistry, 2012, 2012, 3270-3277.	1.2	11
159	Quality Matters: Extension of Clusters of Residues with Good Hydrophobic Contacts Stabilize (Hyper)Thermophilic Proteins. Journal of Chemical Information and Modeling, 2014, 54, 355-361.	2.5	11
160	Design, Synthesis, and Biological Evaluation of Simplified Side Chain Hybrids of the Potent Actin Binding Polyketides Rhizopodin and Bistramide. ChemMedChem, 2015, 10, 470-489.	1.6	11
161	Basal Histamine H₄ Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. Chemistry - A European Journal, 2019, 25, 14613-14624.	1.7	11
162	Design, synthesis and biological evaluation of Î²-peptoid-capped HDAC inhibitors with anti-neuroblastoma and anti-glioblastoma activity. MedChemComm, 2019, 10, 1109-1115.	3.5	11

#	Article	IF	Citations
163	Loop 1 of APOBEC3C Regulates its Antiviral Activity against HIV-1. Journal of Molecular Biology, 2020, 432, 6200-6227.	2.0	11
164	Evidence for a credit-card-swipe mechanism in the human PC floppase ABCB4. Structure, 2021, 29, 1144-1155.e5.	1.6	11
165	Computational Analyses of the AtTPC1 (Arabidopsis Two-Pore Channel 1) Permeation Pathway. International Journal of Molecular Sciences, 2021, 22, 10345.	1.8	11
166	JAK2 p.G571S in B-cell precursor acute lymphoblastic leukemia: a synergizing germline susceptibility. Leukemia, 2019, 33, 2331-2335.	3.3	10
167	Development of a Biosensor Platform for Phenolic Compounds Using a Transition Ligand Strategy. ACS Synthetic Biology, 2021, 10, 2002-2014.	1.9	10
168	Î±-Aminoxy Peptoids: A Unique Peptoid Backbone with a Preference forcis-Amide Bonds. Chemistry - A European Journal, 2017, 23, 3699-3707.	1.7	9
169	Isoform-specific Inhibition of N-methyl-D-aspartate Receptors by Bile Salts. Scientific Reports, 2019, 9, 10068.	1.6	9
170	The Membraneâ€Integrated Steric Chaperone Lif Facilitates Active Site Opening ofPseudomonas aeruginosaLipase A. Journal of Computational Chemistry, 2020, 41, 500-512.	1.5	9
171	Targeting spectrin redox switches to regulate the mechanoproperties of red blood cells. Biological Chemistry, 2021, 402, 317-331.	1.2	9
172	Complex long-distance effects of mutations that confer linezolid resistance in the large ribosomal subunit. Nucleic Acids Research, 2015, 43, 7731-7743.	6.5	8
173	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.	1.6	8
174	Allosteric signaling in C-linker and cyclic nucleotide-binding domain of HCN2 channels. Biophysical Journal, 2021, 120, 950-963.	0.2	8
175	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, .	3.3	8
176	Unsaturated fatty acids augment protein transport via the SecA:SecYEG translocon. FEBS Journal, 2022, 289, 140-162.	2.2	8
177	Ligand-mediated and tertiary interactions cooperatively stabilize the P1 region in the guanine-sensing riboswitch. PLoS ONE, 2017, 12, e0179271.	1.1	8
178	Predicting transmembrane helix pair configurations with knowledgeâ€based distanceâ€dependent pair potentials. Proteins: Structure, Function and Bioinformatics, 2008, 70, 984-999.	1.5	7
179	Human RAD52 â€“ a novel player in DNA repair in cancer and immunodeficiency. Haematologica, 2017, 102, e69-e72.	1.7	7
180	The human platelet antigen-1b (Pro33) variant of Î±IIbÎ²3 allosterically shifts the dynamic conformational equilibrium of this integrin toward the active state. Journal of Biological Chemistry, 2018, 293, 4830-4844.	1.6	7

#	Article	IF	Citations
181	Identification of a Conserved Interface of Human Immunodeficiency Virus Type 1 and Feline Immunodeficiency Virus Vifs with Cullin 5. Journal of Virology, 2018, 92, .	1.5	7
182	Xanthone, benzophenone and bianthrone derivatives from the hypersaline lake-derived fungus Aspergillus wentii. Bioorganic and Medicinal Chemistry, 2019, 27, 115005.	1.4	7
183	Redesigning Aldolase Stereoselectivity by Homologous Grafting. PLoS ONE, 2016, 11, e0156525.	1.1	7
184	Substrate Access Mechanism in a Novel Membrane-Bound Phospholipase A of Pseudomonas aeruginosa Concordant with Specificity and Regioselectivity. Journal of Chemical Information and Modeling, 2021, 61, 5626-5643.	2.5	7
185	Respiratory and C4-photosynthetic NAD-malic enzyme coexist in bundle sheath cell mitochondria and evolved via association of differentially adapted subunits. Plant Cell, 2022, 34, 597-615.	3.1	7
186	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.	1.9	7
187	Force Field Dependence of Riboswitch Dynamics. Methods in Enzymology, 2015, 553, 163-191.	0.4	6
188	On the potential alternate binding change mechanism in a dimeric structure of Pyruvate Phosphate Dikinase. Scientific Reports, 2017, 7, 8020.	1.6	6
189	Dimerization energetics of the Gâ€protein coupled bile acid receptor TGR5 from allâ€atom simulations. Journal of Computational Chemistry, 2020, 41, 874-884.	1.5	6
190	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.	1.6	6
191	Foamy Viruses, Bet, and APOBEC3 Restriction. Viruses, 2021, 13, 504.	1.5	6
192	Can constraint network analysis guide the identification phase of KnowVolution? A case study on improved thermostability of an endo-Î²-glucanase. Computational and Structural Biotechnology Journal, 2021, 19, 743-751.	1.9	6
193	Design, Synthesis, and Conformational Analysis of Trispyrimidonamides as Î±-Helix Mimetics. Journal of Organic Chemistry, 2014, 79, 1582-1593.	1.7	5
194	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.	1.6	5
195	Cell Type-Dependent Escape of Capsid Inhibitors by Simian Immunodeficiency Virus SIVcpz. Journal of Virology, 2020, 94, .	1.5	5
196	Mechanism of Fully Reversible, pH-Sensitive Inhibition of Human Glutamine Synthetase by Tyrosine Nitration. Journal of Chemical Theory and Computation, 2020, 16, 4694-4705.	2.3	5
197	Evidence for functional selectivity in TUDC- and norUDCA-induced signal transduction via Î±5Î²1 integrin towards choleresis. Scientific Reports, 2020, 10, 5795.	1.6	5
198	The many facets of bile acids in the physiology and pathophysiology of the human liver. Biological Chemistry, 2021, 402, 1047-1062.	1.2	5

#	Article	IF	Citations
199	TopDomain: Exhaustive Protein Domain Boundary Metaprediction Combining Multisource Information and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 4599-4613.	2.3	5
200	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.	2.5	5
201	TopProperty: Robust Metaprediction of Transmembrane and Globular Protein Features Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2021, 17, 7281-7289.	2.3	5
202	Structure and Function of Redox-Sensitive Superfolder Green Fluorescent Protein Variant. Antioxidants and Redox Signaling, 2022, 37, 1-18.	2.5	5
203	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.	1.2	5
204	Mapping the helix arrangement of the reconstituted ETR1 ethylene receptor transmembrane domain by EPR spectroscopy. RSC Advances, 2022, 12, 7352-7356.	1.7	5
205	Alignment-Independent Comparison of Binding Sites Based on DrugScore Potential Fields Encoded by 3D Zernike Descriptors. Journal of Chemical Information and Modeling, 2012, 52, 2339-2347.	2.5	4
206	Pyrazolidineâ€3,5â€dioneâ€based inhibitors of phosphoenolpyruvate carboxylase as a new class of potential C₄ plant herbicides. FEBS Letters, 2017, 591, 3369-3377.	1.3	4
207	Small-molecule inhibitors of nisin resistance protein NSR from the human pathogen Streptococcus agalactiae. Bioorganic and Medicinal Chemistry, 2019, 27, 115079.	1.4	4
208	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.	2.2	4
209	Flexibility Analysis of Biomacromolecules with Application to Computer-Aided Drug Design. Methods in Molecular Biology, 2012, 819, 75-91.	0.4	4
210	Rational Design Yields Molecular Insights on Leaf-Binding of Anchor Peptides. ACS Applied Materials & Interfaces, 2022, 14, 28412-28426.	4.0	4
211	Bile Acids and TGR5 (Gpbar1) Signaling. , 2020, , 81-100.		3
212	Novel Recurrent Germline JAK2 G571S Variant in Childhood Acute B-Lymphoblastic Leukemia: A Double Hit One Pathway Scenario. Blood, 2018, 132, 387-387.	0.6	3
213	Protein Flexibility and Mobility in Structure-Based Drug Design. , 2012, , 455-476.		3
214	A MademoiseLLE domain binding platform links the key RNA transporter to endosomes. PLoS Genetics, 2022, 18, e1010269.	1.5	3
215	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.	2.5	2
216	Structural features of FAP174, a MYCBP-1 orthologue from Chlamydomonas reinhardtii, revealed by computational and experimental analyses. RSC Advances, 2017, 7, 51391-51402.	1.7	2

#	Article	IF	Citations
217	Fluorophoreâ€Labeled Cyclic Nucleotides as Potent Agonists of Cyclic Nucleotideâ€Regulated Ion Channels. ChemBioChem, 2020, 21, 2311-2320.	1.3	2
218	Single MHCâ€I Expression Promotes Virusâ€Induced Liver Immunopathology. Hepatology Communications, 2022, 6, 1620-1633.	2.0	2
219	Recurrent Germline Variant in RAD21 Predisposes Children to Lymphoblastic Leukemia or Lymphoma. International Journal of Molecular Sciences, 2022, 23, 5174.	1.8	2
220	Proteinâ€Proteinâ€Interaktionen webbasiert analysieren. Nachrichten Aus Der Chemie, 2011, 59, 44-45.	0.0	1
221	From Hanschâ€Fujita Analysis to AFMoC: A Road to Structureâ€Based QSAR. Molecular Informatics, 2012, 31, 698-704.	1.4	1
222	N6-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.	1.6	1
223	FRET-Assisted Protein Structure Postdiction of CASP13 Targets. Biophysical Journal, 2020, 118, 481a-482a.	0.2	1
224	Liver cell hydration and integrin signaling. Biological Chemistry, 2021, 402, 1033-1045.	1.2	1
225	Molecular Modeling and Simulations of DNA and RNA: DNAzyme as a Model System. Methods in Molecular Biology, 2022, 2439, 153-170.	0.4	1
226	Functional and structural characterization of interactions between opposite subunits in HCN pacemaker channels. Communications Biology, 2022, 5, 430.	2.0	1
227	Towards targeting protein-protein interfaces with small molecules. Journal of Cheminformatics, 2011, 3, .	2.8	0
228	ProteinstabilitÃt webbasiert analysieren. Nachrichten Aus Der Chemie, 2013, 61, 909-911.	0.0	0
229	RNA Junctions Structure and Distance Determination via Accurate Single-Molecule High-Precision FRET Measurements. Biophysical Journal, 2015, 108, 236a.	0.2	0
230	Toolkit for Multi-Conformation Biomolecular Structure Determination by High-Precision FRET and Molecular Simulations. Biophysical Journal, 2015, 108, 163a-164a.	0.2	0
231	The Role of Cytoskeletal S-Nitrosation in Red Blood Cell Deformability. Free Radical Biology and Medicine, 2016, 100, S140.	1.3	0
232	Mapping Motions and Structure to a State Necessary for Oligomerization of a Large GTPase: A Joint SAXS, NSE, EPR and FRET Study. Biophysical Journal, 2016, 110, 514a.	0.2	0
233	Protein Structure Determination by High-Precision FRET and Molecular Modeling. Biophysical Journal, 2017, 112, 48a.	0.2	0
234	Cover Image, Volume 7, Issue 4. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1324.	6.2	0

#	Article	IF	Citations
235	High-Precision FRET Reveals Sequence Dependent Structures of RNA Three-Way Junctions. Biophysical Journal, 2019, 116, 139a-140a.	0.2	0
236	Integrative Dynamic Structural Biology with Fluorescence Spectroscopy. Biophysical Journal, 2019, 116, 469a-470a.	0.2	0
237	Opposing Subunits Interact to Stabilize the Closed State in HCN2 Channels. Biophysical Journal, 2019, 116, 108a.	0.2	0
238	Foreword. Bioorganic and Medicinal Chemistry, 2020, 28, 115460.	1.4	0
239	Corrigendum to: Posttranslational Modification of the NADP-Malic Enzyme Involved in C4 Photosynthesis Modulates the Enzymatic Activity during the Day. Plant Cell, 2022, 34, 698-699.	3.1	0
240	Therapeutic Targeting of HSP90 in AML and ALL. Blood, 2018, 132, 4680-4680.	0.6	0
241	In vitro and in silico characterization of a novel NR1H4/FXR mutation causing Progressive Familial Intrahepatic Cholestasis Type 5. Zeitschrift Fur Gastroenterologie, 2022, 60, .	0.2	0