Holger Gohlke

List of Publications by Year in descending order

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Version: 2024-02-01

241 papers	23,558 citations	44069 48 h-index	8630 146 g-index
263 all docs	263 docs citations	263 times ranked	24056 citing authors

#	Article	IF	Citations
1	Unsaturated fatty acids augment protein transport via the SecA:SecYEG translocon. FEBS Journal, 2022, 289, 140-162.	4.7	8
2	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.	6.6	0
3	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.	6.6	7
4	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.	4.1	7
5	Structure and Function of Redox-Sensitive Superfolder Green Fluorescent Protein Variant. Antioxidants and Redox Signaling, 2022, 37, 1-18.	5.4	5
6	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.	2.4	5
7	In vitro and in silico characterization of a novel NR1H4/FXR mutation causing Progressive Familial Intrahepatic Cholestasis Type 5. Zeitschrift Fur Gastroenterologie, 2022, 60, .	0.5	0
8	Time-resolved structural analysis of an RNA-cleaving DNA catalyst. Nature, 2022, 601, 144-149.	27.8	65
9	Mapping the helix arrangement of the reconstituted ETR1 ethylene receptor transmembrane domain by EPR spectroscopy. RSC Advances, 2022, 12, 7352-7356.	3.6	5
10	Molecular Modeling and Simulations of DNA and RNA: DNAzyme as a Model System. Methods in Molecular Biology, 2022, 2439, 153-170.	0.9	1
11	Single MHCâ€Ⅰ Expression Promotes Virusâ€Ⅰnduced Liver Immunopathology. Hepatology Communications, 2022, 6, 1620-1633.	4.3	2
12	Development of a First-in-Class Small-Molecule Inhibitor of the C-Terminal Hsp90 Dimerization. ACS Central Science, 2022, 8, 636-655.	11.3	12
13	Structural, mechanistic, and physiological insights into phospholipase A-mediated membrane phospholipid degradation in Pseudomonas aeruginosa. ELife, 2022, 11, .	6.0	13
14	Functional and structural characterization of interactions between opposite subunits in HCN pacemaker channels. Communications Biology, 2022, 5, 430.	4.4	1
15	Recurrent Germline Variant in RAD21 Predisposes Children to Lymphoblastic Leukemia or Lymphoma. International Journal of Molecular Sciences, 2022, 23, 5174.	4.1	2
16	Rational Design Yields Molecular Insights on Leaf-Binding of Anchor Peptides. ACS Applied Materials & Interfaces, 2022, 14, 28412-28426.	8.0	4
17	A MademoiseLLE domain binding platform links the key RNA transporter to endosomes. PLoS Genetics, 2022, 18, e1010269.	3.5	3
18	A promiscuous ancestral enzymeÂ´s structure unveils protein variable regions of the highly diverse metallo-Î²-lactamase family. Communications Biology, 2021, 4, 132.	4.4	16

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19	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.	5.4	14
20	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.	3.8	18
21	Foamy Viruses, Bet, and APOBEC3 Restriction. Viruses, 2021, 13, 504.	3.3	6
22	Allosteric signaling in C-linker and cyclic nucleotide-binding domain of HCN2 channels. Biophysical Journal, 2021, 120, 950-963.	0.5	8
23	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. Chemical Research in Toxicology, 2021, 34, 1503-1517.	3.3	13
24	Liver cell hydration and integrin signaling. Biological Chemistry, 2021, 402, 1033-1045.	2.5	1
25	The many facets of bile acids in the physiology and pathophysiology of the human liver. Biological Chemistry, 2021, 402, 1047-1062.	2.5	5
26	Glutamine synthetase as a central element in hepatic glutamine and ammonia metabolism: novel aspects. Biological Chemistry, 2021, 402, 1063-1072.	2.5	20
27	Promiscuous Esterases Counterintuitively Are Less Flexible than Specific Ones. Journal of Chemical Information and Modeling, 2021, 61, 2383-2395.	5.4	13
28	TopDomain: Exhaustive Protein Domain Boundary Metaprediction Combining Multisource Information and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 4599-4613.	5.3	5
29	Evidence for a credit-card-swipe mechanism in the human PC floppase ABCB4. Structure, 2021, 29, 1144-1155.e5.	3.3	11
30	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, .	7.1	8
31	Development of a Biosensor Platform for Phenolic Compounds Using a Transition Ligand Strategy. ACS Synthetic Biology, 2021, 10, 2002-2014.	3.8	10
32	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.	5.4	5
33	Structure and efflux mechanism of the yeast pleiotropic drug resistance transporter Pdr5. Nature Communications, 2021, 12, 5254.	12.8	51
34	Computational Analyses of the AtTPC1 (Arabidopsis Two-Pore Channel 1) Permeation Pathway. International Journal of Molecular Sciences, 2021, 22, 10345.	4.1	11
35	Interdependence of a mechanosensitive anion channel and glutamate receptors in distal wound signaling. Science Advances, 2021, 7, eabg4298.	10.3	45
36	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.	4.1	6

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37	Aqueous ionic liquids redistribute local enzyme stability via long-range perturbation pathways. Computational and Structural Biotechnology Journal, 2021, 19, 4248-4264.	4.1	14
38	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.	5.2	21
39	Targeting spectrin redox switches to regulate the mechanoproperties of red blood cells. Biological Chemistry, 2021, 402, 317-331.	2.5	9
40	TopProperty: Robust Metaprediction of Transmembrane and Globular Protein Features Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2021, 17, 7281-7289.	5.3	5
41	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.	5.4	7
42	The Membraneâ€Integrated Steric Chaperone Lif Facilitates Active Site Opening ofPseudomonas aeruginosaLipase A. Journal of Computational Chemistry, 2020, 41, 500-512.	3.3	9
43	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.	5.4	21
44	Dimerization energetics of the Gâ€protein coupled bile acid receptor TGR5 from allâ€atom simulations. Journal of Computational Chemistry, 2020, 41, 874-884.	3.3	6
45	Loop 1 of APOBEC3C Regulates its Antiviral Activity against HIV-1. Journal of Molecular Biology, 2020, 432, 6200-6227.	4.2	11
46	Semisynthetic Analogs of the Antibiotic Fidaxomicinâ€”Design, Synthesis, and Biological Evaluation. ACS Medicinal Chemistry Letters, 2020, 11, 2414-2420.	2.8	12
47	Automated and optimally FRET-assisted structural modeling. Nature Communications, 2020, 11, 5394.	12.8	39
48	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.	3.3	6
49	Cell Type-Dependent Escape of Capsid Inhibitors by Simian Immunodeficiency Virus SIVcpz. Journal of Virology, 2020, 94, .	3.4	5
50	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.	3.5	13
51	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.	4.8	4
52	Fluorophoreâ€Labeled Cyclic Nucleotides as Potent Agonists of Cyclic Nucleotideâ€Regulated Ion Channels. ChemBioChem, 2020, 21, 2311-2320.	2.6	2
53	Binding modes of thioflavin T and Congo red to the fibril structure of amyloid-Î²(1â€“42). Chemical Communications, 2020, 56, 7589-7592.	4.1	38
54	Mechanism of Fully Reversible, pH-Sensitive Inhibition of Human Glutamine Synthetase by Tyrosine Nitration. Journal of Chemical Theory and Computation, 2020, 16, 4694-4705.	5.3	5

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55	Resolving dynamics and function of transient states in single enzyme molecules. Nature Communications, 2020, 11, 1231.	12.8	71
56	AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools. Journal of Chemical Physics, 2020, 152, 221103.	3.0	17
57	Structural and dynamic insights revealing how lipase binding domain MD1 of Pseudomonas aeruginosa foldase affects lipase activation. Scientific Reports, 2020, 10, 3578.	3.3	12
58	A Novel Polyester Hydrolase From the Marine Bacterium Pseudomonas aestusnigri â€“ Structural and Functional Insights. Frontiers in Microbiology, 2020, 11, 114.	3.5	172
59	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.	5.3	40
60	Quantitative assessment of the determinant structural differences between redox-active and inactive glutaredoxins. Nature Communications, 2020, 11, 1725.	12.8	34
61	Foreword. Bioorganic and Medicinal Chemistry, 2020, 28, 115460.	3.0	0
62	FRET-Assisted Protein Structure Postdiction of CASP13 Targets. Biophysical Journal, 2020, 118, 481a-482a.	0.5	1
63	Evidence for functional selectivity in TUDC- and norUDCA-induced signal transduction via Î±5Î²1 integrin towards choleresis. Scientific Reports, 2020, 10, 5795.	3.3	5
64	Bile Acids and TGR5 (Gpbar1) Signaling. , 2020, , 81-100.		3
65	The tetrahydroxanthone-dimer phomoxanthone A is a strong inducer of apoptosis in cisplatin-resistant solid cancer cells. Bioorganic and Medicinal Chemistry, 2019, 27, 115044.	3.0	13
66	Fluorescent analogs of peptoid-based HDAC inhibitors: Synthesis, biological activity and cellular uptake kinetics. Bioorganic and Medicinal Chemistry, 2019, 27, 115039.	3.0	18
67	Biallelic mutation of human SLC6A6 encoding the taurine transporter TAUT is linked to early retinal degeneration. FASEB Journal, 2019, 33, 11507-11527.	0.5	36
68	Isoform-specific Inhibition of N-methyl-D-aspartate Receptors by Bile Salts. Scientific Reports, 2019, 9, 10068.	3.3	9
69	Xanthone, benzophenone and bianthrone derivatives from the hypersaline lake-derived fungus Aspergillus wentii. Bioorganic and Medicinal Chemistry, 2019, 27, 115005.	3.0	7
70	Posttranslational Modification of the NADP-Malic Enzyme Involved in C₄ Photosynthesis Modulates the Enzymatic Activity during the Day. Plant Cell, 2019, 31, 2525-2539.	6.6	20
71	Structural Model of the ETR1 Ethylene Receptor Transmembrane Sensor Domain. Scientific Reports, 2019, 9, 8869.	3.3	33
72	Surprising Non-Additivity of Methyl Groups in Drugâ€“Kinase Interaction. ACS Chemical Biology, 2019, 14, 2585-2594.	3.4	14

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73	Basal Histamine H₄ Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. Chemistry - A European Journal, 2019, 25, 14613-14624.	3.3	11
74	Partially inserted nascent chain unzips the lateral gate of the Sec translocon. EMBO Reports, 2019, 20, e48191.	4.5	39
75	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.	3.0	44
76	Small-molecule inhibitors of nisin resistance protein NSR from the human pathogen Streptococcus agalactiae. Bioorganic and Medicinal Chemistry, 2019, 27, 115079.	3.0	4
77	Design, synthesis and biological evaluation of Î²-peptoid-capped HDAC inhibitors with anti-neuroblastoma and anti-glioblastoma activity. MedChemComm, 2019, 10, 1109-1115.	3.4	11
78	Co-culture of the fungusFusarium tricinctumwithStreptomyces lividansinduces production of cryptic naphthoquinone dimers. RSC Advances, 2019, 9, 1491-1500.	3.6	37
79	Novel Fluorescent Cyclic Nucleotide Derivatives to Study CNG and HCN Channel Function. Biophysical Journal, 2019, 116, 2411-2422.	0.5	13
80	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.	5.4	121
81	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.	3.5	16
82	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.	5.3	30
83	Calcium-Promoted Interaction between the C2-Domain Protein EHB1 and Metal Transporter IRT1 Inhibits Arabidopsis Iron Acquisition. Plant Physiology, 2019, 180, 1564-1581.	4.8	33
84	High-Precision FRET Reveals Sequence Dependent Structures of RNA Three-Way Junctions. Biophysical Journal, 2019, 116, 139a-140a.	0.5	0
85	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.	3.4	5
86	Integrative Dynamic Structural Biology with Fluorescence Spectroscopy. Biophysical Journal, 2019, 116, 469a-470a.	0.5	0
87	JAK2 p.G571S in B-cell precursor acute lymphoblastic leukemia: a synergizing germline susceptibility. Leukemia, 2019, 33, 2331-2335.	7.2	10
88	Opposing Subunits Interact to Stabilize the Closed State in HCN2 Channels. Biophysical Journal, 2019, 116, 108a.	0.5	0
89	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.	3.4	1
90	Synthesis of Peptoid-Based Class I-Selective Histone Deacetylase Inhibitors with Chemosensitizing Properties. Journal of Medicinal Chemistry, 2019, 62, 11260-11279.	6.4	27

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91	Nutrient exchange in arbuscular mycorrhizal symbiosis from a thermodynamic point of view. New Phytologist, 2019, 222, 1043-1053.	7.3	19
92	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, .	3.2	20
93	Converging a Knowledge-Based Scoring Function: DrugScore²⁰¹⁸. Journal of Chemical Information and Modeling, 2019, 59, 509-521.	5.4	48
94	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.	0.8	12
95	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.	3.4	7
96	Recognition motif and mechanism of ripening inhibitory peptides in plant hormone receptor ETR1. Scientific Reports, 2018, 8, 3890.	3.3	27
97	Identification of a Conserved Interface of Human Immunodeficiency Virus Type 1 and Feline Immunodeficiency Virus Vifs with Cullin 5. Journal of Virology, 2018, 92, .	3.4	7
98	Systematic analysis of ATG13 domain requirements for autophagy induction. Autophagy, 2018, 14, 743-763.	9.1	38
99	Chlorflavonin Targets Acetohydroxyacid Synthase Catalytic Subunit IlvB1 for Synergistic Killing of Mycobacterium tuberculosis. ACS Infectious Diseases, 2018, 4, 123-134.	3.8	26
100	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.	3.3	8
101	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.	5.3	27
102	Interaction of Ochratoxin A and Its Thermal Degradation Product 2â€²R-Ochratoxin A with Human Serum Albumin. Toxins, 2018, 10, 256.	3.4	24
103	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.	3.6	17
104	Effects of novel HDAC inhibitors on urothelial carcinoma cells. Clinical Epigenetics, 2018, 10, 100.	4.1	51
105	On the Effects of Reactive Oxygen Species and Nitric Oxide on Red Blood Cell Deformability. Frontiers in Physiology, 2018, 9, 332.	2.8	80
106	Targeting HSP90 dimerization via the C terminus is effective in imatinib-resistant CML and lacks the heat shock response. Blood, 2018, 132, 307-320.	1.4	66
107	On the contributing role of the transmembrane domain for subunit-specific sensitivity of integrin activation. Scientific Reports, 2018, 8, 5733.	3.3	18
108	Novel Recurrent Germline JAK2 G571S Variant in Childhood Acute B-Lymphoblastic Leukemia: A Double Hit One Pathway Scenario. Blood, 2018, 132, 387-387.	1.4	3

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109	Therapeutic Targeting of HSP90 in AML and ALL. Blood, 2018, 132, 4680-4680.	1.4	0
110	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.	5.4	46
111	Î±-Aminoxy Peptoids: A Unique Peptoid Backbone with a Preference forcis-Amide Bonds. Chemistry - A European Journal, 2017, 23, 3699-3707.	3.3	9
112	Suppression of RUNX1/ETO oncogenic activity by a small molecule inhibitor of tetramerization. Haematologica, 2017, 102, e170-e174.	3.5	13
113	Rigidity theory for biomolecules: concepts, software, and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1311.	14.6	29
114	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.	6.4	32
115	Structural intermediates and directionality of the swiveling motion of Pyruvate Phosphate Dikinase. Scientific Reports, 2017, 7, 45389.	3.3	16
116	Rigidity Theory-Based Approximation of Vibrational Entropy Changes upon Binding to Biomolecules. Journal of Chemical Theory and Computation, 2017, 13, 1495-1502.	5.3	17
117	Protein Structure Determination by High-Precision FRET and Molecular Modeling. Biophysical Journal, 2017, 112, 48a.	0.5	0
118	Human RAD52 â€“ a novel player in DNA repair in cancer and immunodeficiency. Haematologica, 2017, 102, e69-e72.	3.5	7
119	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.	5.4	2
120	Pyrazolidineâ€3,5â€dioneâ€based inhibitors of phosphoenolpyruvate carboxylase as a new class of potential C₄ plant herbicides. FEBS Letters, 2017, 591, 3369-3377.	2.8	4
121	On the potential alternate binding change mechanism in a dimeric structure of Pyruvate Phosphate Dikinase. Scientific Reports, 2017, 7, 8020.	3.3	6
122	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.	3.7	97
123	Cover Image, Volume 7, Issue 4. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1324.	14.6	0
124	Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery. Journal of Chemical Theory and Computation, 2017, 13, 6343-6357.	5.3	31
125	Structural features of FAP174, a MYCBP-1 orthologue from Chlamydomonas reinhardtii, revealed by computational and experimental analyses. RSC Advances, 2017, 7, 51391-51402.	3.6	2
126	Alkoxyurea-Based Histone Deacetylase Inhibitors Increase Cisplatin Potency in Chemoresistant Cancer Cell Lines. Journal of Medicinal Chemistry, 2017, 60, 5334-5348.	6.4	37

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127	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.	4.0	17
128	EDTA aggregates induce SYPRO orange-based fluorescence in thermal shift assay. PLoS ONE, 2017, 12, e0177024.	2.5	27
129	Ligand-mediated and tertiary interactions cooperatively stabilize the P1 region in the guanine-sensing riboswitch. PLoS ONE, 2017, 12, e0179271.	2.5	8
130	Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. PLoS Computational Biology, 2016, 12, e1004693.	3.2	28
131	Structure of the Response Regulator NsrR from Streptococcus agalactiae, Which Is Involved in Lantibiotic Resistance. PLoS ONE, 2016, 11, e0149903.	2.5	22
132	The Role of Cytoskeletal S-Nitrosation in Red Blood Cell Deformability. Free Radical Biology and Medicine, 2016, 100, S140.	2.9	0
133	Determinants of FIV and HIV Vif sensitivity of feline APOBEC3 restriction factors. Retrovirology, 2016, 13, 46.	2.0	21
134	Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems. Current Opinion in Structural Biology, 2016, 40, 163-185.	5.7	156
135	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.	5.4	25
136	Î±â€Aminoxy Oligopeptides: Synthesis, Secondary Structure, and Cytotoxicity of a New Class of Anticancer Foldamers. Chemistry - A European Journal, 2016, 22, 17600-17611.	3.3	16
137	Trading off stability against activity in extremophilic aldolases. Scientific Reports, 2016, 6, 17908.	3.3	48
138	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.	3.3	23
139	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.	2.6	15
140	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.	3.6	89
141	Structural basis of lantibiotic recognition by the nisin resistance protein from Streptococcus agalactiae. Scientific Reports, 2016, 6, 18679.	3.3	42
142	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.	0.5	0
143	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.	2.4	18
144	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.	5.4	21

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145	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPARÎ³ activators. European Journal of Medicinal Chemistry, 2016, 108, 423-435.	5.5	21
146	Application of Rigidity Theory to the Thermostabilization of Lipase A from Bacillus subtilis. PLoS Computational Biology, 2016, 12, e1004754.	3.2	48
147	Redesigning Aldolase Stereoselectivity by Homologous Grafting. PLoS ONE, 2016, 11, e0156525.	2.5	7
148	Complex long-distance effects of mutations that confer linezolid resistance in the large ribosomal subunit. Nucleic Acids Research, 2015, 43, 7731-7743.	14.5	8
149	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.	2.4	20
150	Force Field Dependence of Riboswitch Dynamics. Methods in Enzymology, 2015, 553, 163-191.	1.0	6
151	Design, Synthesis, and Biological Evaluation of Simplified Side Chain Hybrids of the Potent Actin Binding Polyketides Rhizopodin and Bistramide. ChemMedChem, 2015, 10, 470-489.	3.2	11
152	RNA Junctions Structure and Distance Determination via Accurate Single-Molecule High-Precision FRET Measurements. Biophysical Journal, 2015, 108, 236a.	0.5	0
153	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.	3.8	29
154	VisualCNA: a GUI for interactive constraint network analysis and protein engineering for improving thermostability. Bioinformatics, 2015, 31, 2394-2396.	4.1	13
155	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.	5.5	27
156	Toolkit for Multi-Conformation Biomolecular Structure Determination by High-Precision FRET and Molecular Simulations. Biophysical Journal, 2015, 108, 163a-164a.	0.5	0
157	Structural Rigidity and Protein Thermostability in Variants of Lipase A from Bacillus subtilis. PLoS ONE, 2015, 10, e0130289.	2.5	64
158	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.	4.2	43
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.	5.4	11
160	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.	3.4	15
161	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.	5.3	139
162	Design, Synthesis, and Conformational Analysis of Trispyrimidonamides as Î±-Helix Mimetics. Journal of Organic Chemistry, 2014, 79, 1582-1593.	3.2	5

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