

Holger Gohlke

List of Publications by Year in descending order

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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	Unsaturated fatty acids augment protein transport via the SecA:SecYEG translocon. <i>FEBS Journal</i> , 2022, 289, 140-162.	2.2	8
2	Corrigendum to: Posttranslational Modification of the NADP-Malic Enzyme Involved in C4 Photosynthesis Modulates the Enzymatic Activity during the Day. <i>Plant Cell</i> , 2022, 34, 698-699.	3.1	0
3	Respiratory and C4-photosynthetic NAD-malic enzyme coexist in bundle sheath cell mitochondria and evolved via association of differentially adapted subunits. <i>Plant Cell</i> , 2022, 34, 597-615.	3.1	7
4	Critical assessment of structure-based approaches to improve protein resistance in aqueous ionic liquids by enzyme-wide saturation mutagenesis. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 399-409.	1.9	7
5	Structure and Function of Redox-Sensitive Superfolder Green Fluorescent Protein Variant. <i>Antioxidants and Redox Signaling</i> , 2022, 37, 1-18.	2.5	5
6	A phospholipase B from <i>Pseudomonas aeruginosa</i> with activity towards endogenous phospholipids affects biofilm assembly. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2022, 1867, 159101.	1.2	5
7	In vitro and in silico characterization of a novel NR1H4/FXR mutation causing Progressive Familial Intrahepatic Cholestasis Type 5. <i>Zeitschrift Fur Gastroenterologie</i> , 2022, 60, .	0.2	0
8	Time-resolved structural analysis of an RNA-cleaving DNA catalyst. <i>Nature</i> , 2022, 601, 144-149.	13.7	65
9	Mapping the helix arrangement of the reconstituted ETR1 ethylene receptor transmembrane domain by EPR spectroscopy. <i>RSC Advances</i> , 2022, 12, 7352-7356.	1.7	5
10	Molecular Modeling and Simulations of DNA and RNA: DNAzyme as a Model System. <i>Methods in Molecular Biology</i> , 2022, 2439, 153-170.	0.4	1
11	Single MHC ϵ Expression Promotes Virus-Induced Liver Immunopathology. <i>Hepatology Communications</i> , 2022, 6, 1620-1633.	2.0	2
12	Development of a First-in-Class Small-Molecule Inhibitor of the C-Terminal Hsp90 Dimerization. <i>ACS Central Science</i> , 2022, 8, 636-655.	5.3	12
13	Structural, mechanistic, and physiological insights into phospholipase A-mediated membrane phospholipid degradation in <i>Pseudomonas aeruginosa</i> . <i>ELife</i> , 2022, 11, .	2.8	13
14	Functional and structural characterization of interactions between opposite subunits in HCN pacemaker channels. <i>Communications Biology</i> , 2022, 5, 430.	2.0	1
15	Recurrent Germline Variant in RAD21 Predisposes Children to Lymphoblastic Leukemia or Lymphoma. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5174.	1.8	2
16	Rational Design Yields Molecular Insights on Leaf-Binding of Anchor Peptides. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 28412-28426.	4.0	4
17	A Mademoiselle domain binding platform links the key RNA transporter to endosomes. <i>PLoS Genetics</i> , 2022, 18, e1010269.	1.5	3
18	A promiscuous ancestral enzyme's structure unveils protein variable regions of the highly diverse metallo- β -lactamase family. <i>Communications Biology</i> , 2021, 4, 132.	2.0	16

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19	TopSuite Web Server: A Meta-Suite for Deep-Learning-Based Protein Structure and Quality Prediction. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 548-553.	2.5	14
20	40 Years of Research on Polybrominated Diphenyl Ethers (PBDEs) – A Historical Overview and Newest Data of a Promising Anticancer Drug. <i>Molecules</i> , 2021, 26, 995.	1.7	18
21	Foamy Viruses, Bet, and APOBEC3 Restriction. <i>Viruses</i> , 2021, 13, 504.	1.5	6
22	Allosteric signaling in C-linker and cyclic nucleotide-binding domain of HCN2 channels. <i>Biophysical Journal</i> , 2021, 120, 950-963.	0.2	8
23	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. <i>Chemical Research in Toxicology</i> , 2021, 34, 1503-1517.	1.7	13
24	Liver cell hydration and integrin signaling. <i>Biological Chemistry</i> , 2021, 402, 1033-1045.	1.2	1
25	The many facets of bile acids in the physiology and pathophysiology of the human liver. <i>Biological Chemistry</i> , 2021, 402, 1047-1062.	1.2	5
26	Glutamine synthetase as a central element in hepatic glutamine and ammonia metabolism: novel aspects. <i>Biological Chemistry</i> , 2021, 402, 1063-1072.	1.2	20
27	Promiscuous Esterases Counterintuitively Are Less Flexible than Specific Ones. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2383-2395.	2.5	13
28	TopDomain: Exhaustive Protein Domain Boundary Metaprediction Combining Multisource Information and Deep Learning. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4599-4613.	2.3	5
29	Evidence for a credit-card-swipe mechanism in the human PC floppase ABCB4. <i>Structure</i> , 2021, 29, 1144-1155.e5.	1.6	11
30	Thermodynamic profile of mutual subunit control in a heteromeric receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	8
31	Development of a Biosensor Platform for Phenolic Compounds Using a Transition Ligand Strategy. <i>ACS Synthetic Biology</i> , 2021, 10, 2002-2014.	1.9	10
32	F/G Region Rigidity is Inversely Correlated to Substrate Promiscuity of Human CYP Isoforms Involved in Metabolism. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4023-4030.	2.5	5
33	Structure and efflux mechanism of the yeast pleiotropic drug resistance transporter Pdr5. <i>Nature Communications</i> , 2021, 12, 5254.	5.8	51
34	Computational Analyses of the AtTPC1 (Arabidopsis Two-Pore Channel 1) Permeation Pathway. <i>International Journal of Molecular Sciences</i> , 2021, 22, 10345.	1.8	11
35	Interdependence of a mechanosensitive anion channel and glutamate receptors in distal wound signaling. <i>Science Advances</i> , 2021, 7, eabg4298.	4.7	45
36	Can constraint network analysis guide the identification phase of KnowVolution? A case study on improved thermostability of an endo- β -glucanase. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 743-751.	1.9	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.	1.9	14
38	Discovery of new acetylcholinesterase inhibitors for Alzheimer's disease: virtual screening and <i>in vitro</i> characterisation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 491-496.	2.5	21
39	Targeting spectrin redox switches to regulate the mechanoproperties of red blood cells. Biological Chemistry, 2021, 402, 317-331.	1.2	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.	2.3	5
41	Substrate Access Mechanism in a Novel Membrane-Bound Phospholipase A of <i>Pseudomonas aeruginosa</i> Concordant with Specificity and Regioselectivity. Journal of Chemical Information and Modeling, 2021, 61, 5626-5643.	2.5	7
42	The Membrane-Integrated Steric Chaperone LipA Facilitates Active Site Opening of <i>Pseudomonas aeruginosa</i> Lipase A. Journal of Computational Chemistry, 2020, 41, 500-512.	1.5	9
43	Systematically Scrutinizing the Impact of Substitution Sites on Thermostability and Detergent Tolerance for <i>Bacillus subtilis</i> Lipase A. Journal of Chemical Information and Modeling, 2020, 60, 1568-1584.	2.5	21
44	Dimerization energetics of the G-protein coupled bile acid receptor TGR5 from all-atom simulations. Journal of Computational Chemistry, 2020, 41, 874-884.	1.5	6
45	Loop 1 of APOBEC3C Regulates its Antiviral Activity against HIV-1. Journal of Molecular Biology, 2020, 432, 6200-6227.	2.0	11
46	Semisynthetic Analogs of the Antibiotic Fidaxomicin: Design, Synthesis, and Biological Evaluation. ACS Medicinal Chemistry Letters, 2020, 11, 2414-2420.	1.3	12
47	Automated and optimally FRET-assisted structural modeling. Nature Communications, 2020, 11, 5394.	5.8	39
48	Characterization of the nucleotide-binding domain NsrF from the BceAB-type ABC-transporter NsrFP from the human pathogen <i>Streptococcus agalactiae</i> . Scientific Reports, 2020, 10, 15208.	1.6	6
49	Cell Type-Dependent Escape of Capsid Inhibitors by Simian Immunodeficiency Virus SIVcpz. Journal of Virology, 2020, 94, .	1.5	5
50	The Puzzle of Metabolite Exchange and Identification of Putative Octotrico Peptide Repeat Expression Regulators in the Nascent Photosynthetic Organelles of <i>Paulinella chromatophora</i> . Frontiers in Microbiology, 2020, 11, 607182.	1.5	13
51	Cumulative Submillisecond All-Atom Simulations of the Temperature-Induced Coil-to-Globule Transition of Poly(<i>N</i> -vinylcaprolactam) in Aqueous Solution. Macromolecules, 2020, 53, 9793-9810.	2.2	4
52	Fluorophore-Labeled Cyclic Nucleotides as Potent Agonists of Cyclic Nucleotide-Regulated Ion Channels. ChemBioChem, 2020, 21, 2311-2320.	1.3	2
53	Binding modes of thioflavin T and Congo red to the fibril structure of amyloid- β (1-42). Chemical Communications, 2020, 56, 7589-7592.	2.2	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.	2.3	5

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55	Resolving dynamics and function of transient states in single enzyme molecules. <i>Nature Communications</i> , 2020, 11, 1231.	5.8	71
56	AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools. <i>Journal of Chemical Physics</i> , 2020, 152, 221103.	1.2	17
57	Structural and dynamic insights revealing how lipase binding domain MD1 of <i>Pseudomonas aeruginosa</i> foldase affects lipase activation. <i>Scientific Reports</i> , 2020, 10, 3578.	1.6	12
58	A Novel Polyester Hydrolase From the Marine Bacterium <i>Pseudomonas aestusnigri</i> – Structural and Functional Insights. <i>Frontiers in Microbiology</i> , 2020, 11, 114.	1.5	172
59	TopModel: Template-Based Protein Structure Prediction at Low Sequence Identity Using Top-Down Consensus and Deep Neural Networks. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1953-1967.	2.3	40
60	Quantitative assessment of the determinant structural differences between redox-active and inactive glutaredoxins. <i>Nature Communications</i> , 2020, 11, 1725.	5.8	34
61	Foreword. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115460.	1.4	0
62	FRET-Assisted Protein Structure Prediction of CASP13 Targets. <i>Biophysical Journal</i> , 2020, 118, 481a-482a.	0.2	1
63	Evidence for functional selectivity in TUDC- and norUDCA-induced signal transduction via $\beta 1$ integrin towards choleresis. <i>Scientific Reports</i> , 2020, 10, 5795.	1.6	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. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115044.	1.4	13
66	Fluorescent analogs of peptoid-based HDAC inhibitors: Synthesis, biological activity and cellular uptake kinetics. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115039.	1.4	18
67	Biallelic mutation of human <i>SLC6A6</i> encoding the taurine transporter TAUT is linked to early retinal degeneration. <i>FASEB Journal</i> , 2019, 33, 11507-11527.	0.2	36
68	Isoform-specific Inhibition of N-methyl-D-aspartate Receptors by Bile Salts. <i>Scientific Reports</i> , 2019, 9, 10068.	1.6	9
69	Xanthone, benzophenone and bianthrone derivatives from the hypersaline lake-derived fungus <i>Aspergillus wentii</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115005.	1.4	7
70	Posttranslational Modification of the NADP-Malic Enzyme Involved in C_4 Photosynthesis Modulates the Enzymatic Activity during the Day. <i>Plant Cell</i> , 2019, 31, 2525-2539.	3.1	20
71	Structural Model of the ETR1 Ethylene Receptor Transmembrane Sensor Domain. <i>Scientific Reports</i> , 2019, 9, 8869.	1.6	33
72	Surprising Non-Additivity of Methyl Groups in Drug-Kinase Interaction. <i>ACS Chemical Biology</i> , 2019, 14, 2585-2594.	1.6	14

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73	Basal Histamine H ₄ Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. <i>Chemistry - A European Journal</i> , 2019, 25, 14613-14624.	1.7	11
74	Partially inserted nascent chain unzips the lateral gate of the Sec translocon. <i>EMBO Reports</i> , 2019, 20, e48191.	2.0	39
75	C-terminal modulators of heat shock protein of 90 kDa (HSP90): State of development and modes of action. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115080.	1.4	44
76	Small-molecule inhibitors of nisin resistance protein NSR from the human pathogen <i>Streptococcus agalactiae</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115079.	1.4	4
77	Design, synthesis and biological evaluation of Î ² -peptoid-capped HDAC inhibitors with anti-neuroblastoma and anti-glioblastoma activity. <i>MedChemComm</i> , 2019, 10, 1109-1115.	3.5	11
78	Co-culture of the fungus <i>Fusarium tricinctum</i> with <i>Streptomyces lividans</i> induces production of cryptic naphthoquinone dimers. <i>RSC Advances</i> , 2019, 9, 1491-1500.	1.7	37
79	Novel Fluorescent Cyclic Nucleotide Derivatives to Study CNG and HCN Channel Function. <i>Biophysical Journal</i> , 2019, 116, 2411-2422.	0.2	13
80	PACKMOL-Memgen: A Simple-To-Use, Generalized Workflow for Membrane-Protein-Lipid-Bilayer System Building. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2522-2528.	2.5	121
81	Novel 3,4-Dihydroisocoumarins Inhibit Human P-gp and BCRP in Multidrug Resistant Tumors and Demonstrate Substrate Inhibition of Yeast Pdr5. <i>Frontiers in Pharmacology</i> , 2019, 10, 400.	1.6	16
82	Cosolvent-Enhanced Sampling and Unbiased Identification of Cryptic Pockets Suitable for Structure-Based Drug Design. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3331-3343.	2.3	30
83	Calcium-Promoted Interaction between the C2-Domain Protein EHB1 and Metal Transporter IRT1 Inhibits Arabidopsis Iron Acquisition. <i>Plant Physiology</i> , 2019, 180, 1564-1581.	2.3	33
84	High-Precision FRET Reveals Sequence Dependent Structures of RNA Three-Way Junctions. <i>Biophysical Journal</i> , 2019, 116, 139a-140a.	0.2	0
85	Phosphorylated tyrosine 93 of hepatitis C virus nonstructural protein 5A is essential for interaction with host c-Src and efficient viral replication. <i>Journal of Biological Chemistry</i> , 2019, 294, 7388-7402.	1.6	5
86	Integrative Dynamic Structural Biology with Fluorescence Spectroscopy. <i>Biophysical Journal</i> , 2019, 116, 469a-470a.	0.2	0
87	JAK2 p.G571S in B-cell precursor acute lymphoblastic leukemia: a synergizing germline susceptibility. <i>Leukemia</i> , 2019, 33, 2331-2335.	3.3	10
88	Opposing Subunits Interact to Stabilize the Closed State in HCN2 Channels. <i>Biophysical Journal</i> , 2019, 116, 108a.	0.2	0
89	N6-modified cAMP derivatives that activate protein kinase A also act as full agonists of murine HCN2 channels. <i>Journal of Biological Chemistry</i> , 2019, 294, 17978-17987.	1.6	1
90	Synthesis of Peptoid-Based Class I-Selective Histone Deacetylase Inhibitors with Chemosensitizing Properties. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 11260-11279.	2.9	27

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91	Nutrient exchange in arbuscular mycorrhizal symbiosis from a thermodynamic point of view. <i>New Phytologist</i> , 2019, 222, 1043-1053.	3.5	19
92	FK506 Resistance of <i>Saccharomyces cerevisiae</i> Pdr5 and <i>Candida albicans</i> Cdr1 Involves Mutations in the Transmembrane Domains and Extracellular Loops. <i>Antimicrobial Agents and Chemotherapy</i> , 2019, 63, .	1.4	20
93	Converging a Knowledge-Based Scoring Function: DrugScore ²⁰¹⁸ . <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 509-521.	2.5	48
94	<i>Pseudomonas aeruginosa</i> esterase PA2949, a bacterial homolog of the human membrane esterase ABHD6: expression, purification and crystallization. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019, 75, 270-277.	0.4	12
95	The human platelet antigen-1b (Pro33) variant of $\alpha\text{IIb}\beta\text{3}$ allosterically shifts the dynamic conformational equilibrium of this integrin toward the active state. <i>Journal of Biological Chemistry</i> , 2018, 293, 4830-4844.	1.6	7
96	Recognition motif and mechanism of ripening inhibitory peptides in plant hormone receptor ETR1. <i>Scientific Reports</i> , 2018, 8, 3890.	1.6	27
97	Identification of a Conserved Interface of Human Immunodeficiency Virus Type 1 and Feline Immunodeficiency Virus Vifs with Cullin 5. <i>Journal of Virology</i> , 2018, 92, .	1.5	7
98	Systematic analysis of ATG13 domain requirements for autophagy induction. <i>Autophagy</i> , 2018, 14, 743-763.	4.3	38
99	Chlorflavonin Targets Acetohydroxyacid Synthase Catalytic Subunit IlvB1 for Synergistic Killing of <i>Mycobacterium tuberculosis</i> . <i>ACS Infectious Diseases</i> , 2018, 4, 123-134.	1.8	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. <i>Scientific Reports</i> , 2018, 8, 14960.	1.6	8
101	TopScore: Using Deep Neural Networks and Large Diverse Data Sets for Accurate Protein Model Quality Assessment. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6117-6126.	2.3	27
102	Interaction of Ochratoxin A and Its Thermal Degradation Product 2 α -Ochratoxin A with Human Serum Albumin. <i>Toxins</i> , 2018, 10, 256.	1.5	24
103	Relevance of N-terminal residues for amyloid- β binding to platelet integrin $\alpha\text{IIb}\beta\text{3}$, integrin outside-in signaling and amyloid- β fibril formation. <i>Cellular Signalling</i> , 2018, 50, 121-130.	1.7	17
104	Effects of novel HDAC inhibitors on urothelial carcinoma cells. <i>Clinical Epigenetics</i> , 2018, 10, 100.	1.8	51
105	On the Effects of Reactive Oxygen Species and Nitric Oxide on Red Blood Cell Deformability. <i>Frontiers in Physiology</i> , 2018, 9, 332.	1.3	80
106	Targeting HSP90 dimerization via the C terminus is effective in imatinib-resistant CML and lacks the heat shock response. <i>Blood</i> , 2018, 132, 307-320.	0.6	66
107	On the contributing role of the transmembrane domain for subunit-specific sensitivity of integrin activation. <i>Scientific Reports</i> , 2018, 8, 5733.	1.6	18
108	Novel Recurrent Germline JAK2 G571S Variant in Childhood Acute B-Lymphoblastic Leukemia: A Double Hit One Pathway Scenario. <i>Blood</i> , 2018, 132, 387-387.	0.6	3

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109	Therapeutic Targeting of HSP90 in AML and ALL. <i>Blood</i> , 2018, 132, 4680-4680.	0.6	0
110	Efficient Approximation of Ligand Rotational and Translational Entropy Changes upon Binding for Use in MM-PBSA Calculations. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 170-189.	2.5	46
111	Î±-Aminoxy Peptoids: A Unique Peptoid Backbone with a Preference for cis-Amide Bonds. <i>Chemistry - A European Journal</i> , 2017, 23, 3699-3707.	1.7	9
112	Suppression of RUNX1/ETO oncogenic activity by a small molecule inhibitor of tetramerization. <i>Haematologica</i> , 2017, 102, e170-e174.	1.7	13
113	Rigidity theory for biomolecules: concepts, software, and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1311.	6.2	29
114	Design, Multicomponent Synthesis, and Anticancer Activity of a Focused Histone Deacetylase (HDAC) Inhibitor Library with Peptoid-Based Cap Groups. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5493-5506.	2.9	32
115	Structural intermediates and directionality of the swiveling motion of Pyruvate Phosphate Dikinase. <i>Scientific Reports</i> , 2017, 7, 45389.	1.6	16
116	Rigidity Theory-Based Approximation of Vibrational Entropy Changes upon Binding to Biomolecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1495-1502.	2.3	17
117	Protein Structure Determination by High-Precision FRET and Molecular Modeling. <i>Biophysical Journal</i> , 2017, 112, 48a.	0.2	0
118	Human RAD52 â€“ a novel player in DNA repair in cancer and immunodeficiency. <i>Haematologica</i> , 2017, 102, e69-e72.	1.7	7
119	Tertiary Interactions in the Unbound Guanine-Sensing Riboswitch Focus Functional Conformational Variability on the Binding Site. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2822-2832.	2.5	2
120	Pyrazolidine- and Oxadiazole-Based inhibitors of phosphoenolpyruvate carboxylase as a new class of potential C ₄ plant herbicides. <i>FEBS Letters</i> , 2017, 591, 3369-3377.	1.3	4
121	On the potential alternate binding change mechanism in a dimeric structure of Pyruvate Phosphate Dikinase. <i>Scientific Reports</i> , 2017, 7, 8020.	1.6	6
122	Sequencing of FIC1, BSEP and MDR3 in a large cohort of patients with cholestasis revealed a high number of different genetic variants. <i>Journal of Hepatology</i> , 2017, 67, 1253-1264.	1.8	97
123	Cover Image, Volume 7, Issue 4. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1324.	6.2	0
124	Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6343-6357.	2.3	31
125	Structural features of FAP174, a MYCBP-1 orthologue from <i>Chlamydomonas reinhardtii</i> , revealed by computational and experimental analyses. <i>RSC Advances</i> , 2017, 7, 51391-51402.	1.7	2
126	Alkoxyurea-Based Histone Deacetylase Inhibitors Increase Cisplatin Potency in Chemoresistant Cancer Cell Lines. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5334-5348.	2.9	37

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127	Contribution of single amino acid and codon substitutions to the production and secretion of a lipase by <i>Bacillus subtilis</i> . <i>Microbial Cell Factories</i> , 2017, 16, 160.	1.9	17
128	EDTA aggregates induce SYPRO orange-based fluorescence in thermal shift assay. <i>PLoS ONE</i> , 2017, 12, e0177024.	1.1	27
129	Ligand-mediated and tertiary interactions cooperatively stabilize the P1 region in the guanine-sensing riboswitch. <i>PLoS ONE</i> , 2017, 12, e0179271.	1.1	8
130	Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. <i>PLoS Computational Biology</i> , 2016, 12, e1004693.	1.5	28
131	Structure of the Response Regulator NsrR from <i>Streptococcus agalactiae</i> , Which Is Involved in Lantibiotic Resistance. <i>PLoS ONE</i> , 2016, 11, e0149903.	1.1	22
132	The Role of Cytoskeletal S-Nitrosation in Red Blood Cell Deformability. <i>Free Radical Biology and Medicine</i> , 2016, 100, S140.	1.3	0
133	Determinants of FIV and HIV Vif sensitivity of feline APOBEC3 restriction factors. <i>Retrovirology</i> , 2016, 13, 46.	0.9	21
134	Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems. <i>Current Opinion in Structural Biology</i> , 2016, 40, 163-185.	2.6	156
135	Alchemical Free Energy Calculations and Isothermal Titration Calorimetry Measurements of Aminoadamantanes Bound to the Closed State of Influenza A/M2TM. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 862-876.	2.5	25
136	Î±-Aminoxy Oligopeptides: Synthesis, Secondary Structure, and Cytotoxicity of a New Class of Anticancer Foldamers. <i>Chemistry - A European Journal</i> , 2016, 22, 17600-17611.	1.7	16
137	Trading off stability against activity in extremophilic aldolases. <i>Scientific Reports</i> , 2016, 6, 17908.	1.6	48
138	Structural assemblies of the di- and oligomeric G-protein coupled receptor TGR5 in live cells: an MFIS-FRET and integrative modelling study. <i>Scientific Reports</i> , 2016, 6, 36792.	1.6	23
139	Failure of the IDA in FRET Systems at Close Inter-Dye Distances Is Moderated by Frequent Low $\langle r^2 \rangle$ Values. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8845-8862.	1.2	15
140	Platelets contribute to amyloid-Î² aggregation in cerebral vessels through integrin Î± _{IIb} Î² ₃ induced outside-in signaling and clusterin release. <i>Science Signaling</i> , 2016, 9, ra52.	1.6	89
141	Structural basis of lantibiotic recognition by the nisin resistance protein from <i>Streptococcus agalactiae</i> . <i>Scientific Reports</i> , 2016, 6, 18679.	1.6	42
142	Mapping Motions and Structure to a State Necessary for Oligomerization of a Large GTPase: A Joint SAXS, NSE, EPR and FRET Study. <i>Biophysical Journal</i> , 2016, 110, 514a.	0.2	0
143	Design and biological testing of peptidic dimerization inhibitors of human Hsp90 that target the C-terminal domain. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016, 1860, 1043-1055.	1.1	18
144	Interpreting Thermodynamic Profiles of Aminoadamantane Compounds Inhibiting the M2 Proton Channel of Influenza A by Free Energy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 110-126.	2.5	21

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145	Design and synthesis of novel Y-shaped barbituric acid derivatives as PPAR β activators. <i>European Journal of Medicinal Chemistry</i> , 2016, 108, 423-435.	2.6	21
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