

Roland G Huber

List of Publications by Year in descending order

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Version: 2024-02-01

75
papers

2,057
citations

257450

24
h-index

289244

40
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82
all docs

82
docs citations

82
times ranked

3701
citing authors

#	ARTICLE	IF	CITATIONS
1	Ice nucleation by water-soluble macromolecules. <i>Atmospheric Chemistry and Physics</i> , 2015, 15, 4077-4091.	4.9	198
2	Heteroaromatic π -Stacking Energy Landscapes. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1371-1379.	5.4	144
3	An Optical Technique for Mapping Microviscosity Dynamics in Cellular Organelles. <i>ACS Nano</i> , 2018, 12, 4398-4407.	14.6	125
4	Structure mapping of dengue and Zika viruses reveals functional long-range interactions. <i>Nature Communications</i> , 2019, 10, 1408.	12.8	104
5	Cross-reactive dengue human monoclonal antibody prevents severe pathologies and death from Zika virus infections. <i>JCI Insight</i> , 2017, 2, .	5.0	74
6	Hydrocarbons Are Essential for Optimal Cell Size, Division, and Growth of Cyanobacteria. <i>Plant Physiology</i> , 2016, 172, 1928-1940.	4.8	53
7	Comprehensive mapping of SARS-CoV-2 interactions in vivo reveals functional virus-host interactions. <i>Nature Communications</i> , 2021, 12, 5113.	12.8	53
8	Systematic analysis of protein identity between Zika virus and other arthropod-borne viruses. <i>Bulletin of the World Health Organization</i> , 2017, 95, 517-525I.	3.3	52
9	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. <i>Scientific Reports</i> , 2020, 10, 17501.	3.3	52
10	Cleavage Entropy as Quantitative Measure of Protease Specificity. <i>PLoS Computational Biology</i> , 2013, 9, e1003007.	3.2	49
11	Aggregation of thrombin-derived C-terminal fragments as a previously undisclosed host defense mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E4213-E4222.	7.1	49
12	Understanding Dengue Virus Capsid Protein Disordered N-Terminus and pep14-23-Based Inhibition. <i>ACS Chemical Biology</i> , 2015, 10, 517-526.	3.4	45
13	South-east Asian Zika virus strain linked to cluster of cases in Singapore, August 2016. <i>Eurosurveillance</i> , 2016, 21, .	7.0	44
14	Reciprocal regulation of PKA and Rac signaling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 8531-8536.	7.1	42
15	Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. <i>Structure</i> , 2016, 24, 1410-1420.	3.3	41
16	A Spring-Loaded Mechanism Governs the Clamp-like Dynamics of the Skp Chaperone. <i>Structure</i> , 2017, 25, 1079-1088.e3.	3.3	34
17	Matrix Isolation Studies of Carbonic Acidâ€™The Vapor Phase above the β -Polymorph. <i>Journal of the American Chemical Society</i> , 2013, 135, 7732-7737.	13.7	33
18	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. <i>Structure</i> , 2018, 26, 1151-1161.e4.	3.3	32

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19	A Novel Paramagnetic Relaxation Enhancement Tag for Nucleic Acids: A Tool to Study Structure and Dynamics of RNA. ACS Chemical Biology, 2013, 8, 2697-2706.	3.4	31
20	Multiscale molecular dynamics simulation approaches to the structure and dynamics of viruses. Progress in Biophysics and Molecular Biology, 2017, 128, 121-132.	2.9	31
21	Extending the Martini Coarse-Grained Force Field to <i>N</i> -Glycans. Journal of Chemical Information and Modeling, 2020, 60, 3864-3883.	5.4	30
22	Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. PLoS ONE, 2016, 11, e0156963.	2.5	28
23	Dynamic Regulation of Phenylalanine Hydroxylase by Simulated Redox Manipulation. PLoS ONE, 2012, 7, e53005.	2.5	27
24	A Reversible Association between Smc Coiled Coils Is Regulated by Lysine Acetylation and Is Required for Cohesin Association with the DNA. Molecular Cell, 2016, 63, 1044-1054.	9.7	27
25	Multiscale modelling and simulation of viruses. Current Opinion in Structural Biology, 2020, 61, 146-152.	5.7	26
26	BRAF inhibitors promote intermediate BRAF(V600E) conformations and binary interactions with activated RAS. Science Advances, 2019, 5, eaav8463.	10.3	25
27	Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658.	2.5	25
28	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 104-120.	3.5	24
29	Independent Metrics for Protein Backbone and Side-Chain Flexibility: Time Scales and Effects of Ligand Binding. Journal of Chemical Theory and Computation, 2015, 11, 851-860.	5.3	24
30	Intrinsic flexibility of <i>NLRP</i> pyrin domains is a key factor in their conformational dynamics, fold stability, and dimerization. Protein Science, 2015, 24, 174-181.	7.6	24
31	Thrombin-derived C-terminal fragments aggregate and scavenge bacteria and their proinflammatory products. Journal of Biological Chemistry, 2020, 295, 3417-3430.	3.4	24
32	Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. PLoS ONE, 2015, 10, e0140713.	2.5	24
33	Entropy from State Probabilities: Hydration Entropy of Cations. Journal of Physical Chemistry B, 2013, 117, 6466-6472.	2.6	23
34	Substrate-Driven Mapping of the Degradome by Comparison of Sequence Logos. PLoS Computational Biology, 2013, 9, e1003353.	3.2	23
35	Impairing Cohesin Smc1/3 Head Engagement Compensates for the Lack of Eco1 Function. Structure, 2016, 24, 1991-1999.	3.3	23
36	Chlorophyll Catabolites in Fall Leaves of the Wych Elm Tree Present a Novel Glycosylation Motif. Chemistry - A European Journal, 2016, 22, 9498-9503.	3.3	23

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37	praja2 regulates KSR1 stability and mitogenic signaling. <i>Cell Death and Disease</i> , 2016, 7, e2230-e2230.	6.3	22
38	Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit F ₁ . <i>Journal of Structural Biology</i> , 2019, 207, 199-208.	2.8	22
39	Specificity of a protein-protein interface: Local dynamics direct substrate recognition of effector caspases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 546-555.	2.6	20
40	Binding Pose Flip Explained via Enthalpic and Entropic Contributions. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 345-354.	5.4	20
41	Partial Intrinsic Disorder Governs the Dengue Capsid Protein Conformational Ensemble. <i>ACS Chemical Biology</i> , 2018, 13, 1621-1630.	3.4	18
42	Porphyrin-LEGO [®] : synthesis of a hexafullereno-diporphyrin using porphyrins programmed for [4+2]-cycloaddition. <i>Chemical Communications</i> , 2012, 48, 4359.	4.1	17
43	Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. <i>Scientific Reports</i> , 2016, 6, 19160.	3.3	17
44	Energetics and Dynamics Across the Bcl-2-Regulated Apoptotic Pathway Reveal Distinct Evolutionary Determinants of Specificity and Affinity. <i>Structure</i> , 2016, 24, 2024-2033.	3.3	16
45	On the ion coupling mechanism of the MATE transporter ClbM. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183137.	2.6	16
46	Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. <i>Diagnostics</i> , 2020, 10, 11.	2.6	16
47	Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. <i>Pharmacological Research</i> , 2019, 147, 104372.	7.1	15
48	Genome-wide RNA structure changes during human neurogenesis modulate gene regulatory networks. <i>Molecular Cell</i> , 2021, 81, 4942-4953.e8.	9.7	15
49	The Structural Basis for Activation and Inhibition of ZAP-70 Kinase Domain. <i>PLoS Computational Biology</i> , 2015, 11, e1004560.	3.2	12
50	Carbonic acid monoethyl ester as a pure solid and its conformational isomerism in the gas-phase. <i>RSC Advances</i> , 2017, 7, 22222-22233.	3.6	11
51	Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices. <i>Structure</i> , 2019, 27, 302-314.e4.	3.3	11
52	Facile saccharide-free mimetics that recapitulate key features of glycosaminoglycan sulfation patterns. <i>Chemical Science</i> , 2018, 9, 7940-7947.	7.4	10
53	A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3920-3932.	5.3	9
54	Alpha-Carbonic Acid Revisited: Carbonic Acid Monomethyl Ester as a Solid and its Conformational Isomerism in the Gas Phase. <i>Chemistry - A European Journal</i> , 2020, 26, 285-305.	3.3	9

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55	Mutation-oriented profiling of autoinhibitory kinase conformations predicts RAF inhibitor efficacies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 31105-31113.	7.1	9
56	Computational modelling of flavivirus dynamics: The ins and outs. <i>Methods</i> , 2021, 185, 28-38.	3.8	9
57	Linker length affects photostability of protein-targeted sensor of cellular microviscosity. <i>Methods and Applications in Fluorescence</i> , 2019, 7, 044004.	2.3	8
58	Antibody affinity versus dengue morphology influences neutralization. <i>PLoS Pathogens</i> , 2021, 17, e1009331.	4.7	8
59	Protein-protein interactions in paralogues: Electrostatics modulates specificity on a conserved steric scaffold. <i>PLoS ONE</i> , 2017, 12, e0185928.	2.5	7
60	Multiscale Modeling and Simulation Approaches to Lipid-Protein Interactions. <i>Methods in Molecular Biology</i> , 2019, 2003, 1-30.	0.9	7
61	The Pseudo-Circular Genomes of Flaviviruses: Structures, Mechanisms, and Functions of Circularization. <i>Cells</i> , 2021, 10, 642.	4.1	6
62	Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases. <i>Journal of Physical Chemistry B</i> , 2016, 120, 299-308.	2.6	5
63	The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase μ Subunit. <i>ChemBioChem</i> , 2020, 21, 3249-3254.	2.6	5
64	Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 245-261.	5.4	4
65	Allosteric Kinase Inhibitors Reshape MEK1 Kinase Activity Conformations in Cells and In Silico. <i>Biomolecules</i> , 2021, 11, 518.	4.0	4
66	How Ligand Binding Affects the Dynamical Transition Temperature in Proteins. <i>ChemPhysChem</i> , 2020, 21, 916-926.	2.1	3
67	The nanotube express: Delivering a stapled peptide to the cell surface. <i>Journal of Colloid and Interface Science</i> , 2021, 604, 670-679.	9.4	3
68	Simulations Help Unravel Flavivirus Envelope Structure and Function. <i>Biophysical Journal</i> , 2017, 112, 309a.	0.5	1
69	Virtual Dengue Virus: The INS and OUTS. <i>Biophysical Journal</i> , 2018, 114, 208a.	0.5	1
70	3D reconstruction and flexibility of the hybrid engine <i>Acetobacterium woodii</i> F-ATP synthase. <i>Biochemical and Biophysical Research Communications</i> , 2020, 527, 518-524.	2.1	1
71	RNAvigator: A Pipeline to Identify Candidates for Functional RNA Structure Elements. <i>Frontiers in Virology</i> , 0, 2, .	1.4	1
72	Multiscale Dynamics of Flavivirus Fusion Peptides - Membrane Interactions via Simulation and Experiments. <i>Biophysical Journal</i> , 2017, 112, 328a.	0.5	0

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73	Molecular Simulations Detail the Thermal Expansion of the Pre-endosomal Dengue Virus. Biophysical Journal, 2018, 114, 458a-459a.	0.5	0
74	Directing GDNF-mediated neuronal signaling with proactively programmable cell-surface saccharide-free glycosaminoglycan mimetics. Chemical Communications, 2019, 55, 1259-1262.	4.1	0
75	Dengue and Zika RNA-RNA Interactomes Reveal Virus Permissive and Restrictive Factors in Human Cells. SSRN Electronic Journal, 0, , .	0.4	0