Roland G Huber

List of Publications by Year
in descending order

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75 papers	2,057 citations	257450 24 h-index	289244 40 g-index
82 all docs	82 docs citations	82 times ranked	3701 citing authors

#	Article	IF	Citations
1	Computational modelling of flavivirus dynamics: The ins and outs. Methods, 2021, 185, 28-38.	3.8	9
2	Antibody affinity versus dengue morphology influences neutralization. PLoS Pathogens, 2021, 17, e1009331.	4.7	8
3	The Pseudo-Circular Genomes of Flaviviruses: Structures, Mechanisms, and Functions of Circularization. Cells, 2021, 10, 642.	4.1	6
4	Allosteric Kinase Inhibitors Reshape MEK1 Kinase Activity Conformations in Cells and In Silico. Biomolecules, 2021, 11, 518.	4.0	4
5	Comprehensive mapping of SARS-CoV-2 interactions in vivo reveals functional virus-host interactions. Nature Communications, 2021, 12, 5113.	12.8	53
6	The nanotube express: Delivering a stapled peptide to the cell surface. Journal of Colloid and Interface Science, 2021, 604, 670-679.	9.4	3
7	Genome-wide RNA structure changes during human neurogenesis modulate gene regulatory networks. Molecular Cell, 2021, 81, 4942-4953.e8.	9.7	15
8	Alphaâ€Carbonic Acid Revisited: Carbonic Acid Monomethyl Ester as a Solid and its Conformational Isomerism in the Gas Phase. Chemistry - A European Journal, 2020, 26, 285-305.	3.3	9
9	On the ion coupling mechanism of the MATE transporter ClbM. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183137.	2.6	16
10	Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. Diagnostics, 2020, 10, 11.	2.6	16
11	Extending the Martini Coarse-Grained Force Field to N-Glycans. Journal of Chemical Information and Modeling, 2020, 60, 3864-3883.	5.4	30
12	Mutation-oriented profiling of autoinhibitory kinase conformations predicts RAF inhibitor efficacies. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 31105-31113.	7.1	9
13	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. Scientific Reports, 2020, 10, 17501.	3.3	52
14	3D reconstruction and flexibility of the hybrid engine Acetobacterium woodii F-ATP synthase. Biochemical and Biophysical Research Communications, 2020, 527, 518-524.	2.1	1
15	How Ligand Binding Affects the Dynamical Transition Temperature in Proteins. ChemPhysChem, 2020, 21, 916-926.	2.1	3
16	The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase Ïµ Subunit. ChemBioChem, 2020, 21, 3249-3254.	2.6	5
17	Thrombin-derived C-terminal fragments aggregate and scavenge bacteria and their proinflammatory products. Journal of Biological Chemistry, 2020, 295, 3417-3430.	3.4	24
18	Multiscale modelling and simulation of viruses. Current Opinion in Structural Biology, 2020, 61, 146-152.	5.7	26

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19	BRAF inhibitors promote intermediate BRAF(V600E) conformations and binary interactions with activated RAS. Science Advances, 2019, 5, eaav8463.	10.3	25
20	Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. Pharmacological Research, 2019, 147, 104372.	7.1	15
21	Linker length affects photostability of protein-targeted sensor of cellular microviscosity. Methods and Applications in Fluorescence, 2019, 7, 044004.	2.3	8
22	Directing GDNF-mediated neuronal signaling with proactively programmable cell-surface saccharide-free glycosaminoglycan mimetics. Chemical Communications, 2019, 55, 1259-1262.	4.1	0
23	Multiscale Modeling and Simulation Approaches to Lipidâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2003, 1-30.	0.9	7
24	Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit Î´. Journal of Structural Biology, 2019, 207, 199-208.	2.8	22
25	Structure mapping of dengue and Zika viruses reveals functional long-range interactions. Nature Communications, 2019, 10, 1408.	12.8	104
26	Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway. Journal of Chemical Information and Modeling, 2019, 59, 245-261.	5.4	4
27	Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices. Structure, 2019, 27, 302-314.e4.	3.3	11
28	An Optical Technique for Mapping Microviscosity Dynamics in Cellular Organelles. ACS Nano, 2018, 12, 4398-4407.	14.6	125
29	Molecular Simulations Detail the Thermal Expansion of the Pre-endosomal Dengue Virus. Biophysical Journal, 2018, 114, 458a-459a.	0.5	0
30	Virtual Dengue Virus: The INS and OUTS. Biophysical Journal, 2018, 114, 208a.	0.5	1
31	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. Structure, 2018, 26, 1151-1161.e4.	3.3	32
32	Partial Intrinsic Disorder Governs the Dengue Capsid Protein Conformational Ensemble. ACS Chemical Biology, 2018, 13, 1621-1630.	3.4	18
33	Facile saccharide-free mimetics that recapitulate key features of glycosaminoglycan sulfation patterns. Chemical Science, 2018, 9, 7940-7947.	7.4	10
34	A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. Journal of Chemical Theory and Computation, 2018, 14, 3920-3932.	5.3	9
35	Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling, 2017, 57, 345-354.	5.4	20
36	Aggregation of thrombin-derived C-terminal fragments as a previously undisclosed host defense mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4213-E4222.	7.1	49

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37	Carbonic acid monoethyl ester as a pure solid and its conformational isomerism in the gas-phase. RSC Advances, 2017, 7, 22222-22233.	3.6	11
38	A Spring-Loaded Mechanism Governs the Clamp-like Dynamics of the Skp Chaperone. Structure, 2017, 25, 1079-1088.e3.	3.3	34
39	Simulations Help Unravel Flavivirus Envelope Structure and Function. Biophysical Journal, 2017, 112, 309a.	0.5	1
40	Multiscale Dynamics of Flavivirus Fusion Peptides - Membrane Interactions via Simulation and Experiments. Biophysical Journal, 2017, 112, 328a.	0.5	0
41	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
42	Systematic analysis of protein identity between Zika virus and other arthropod-borne viruses. Bulletin of the World Health Organization, 2017, 95, 517-525I.	3.3	52
43	Protein-protein interactions in paralogues: Electrostatics modulates specificity on a conserved steric scaffold. PLoS ONE, 2017, 12, e0185928.	2.5	7
44	Cross-reactive dengue human monoclonal antibody prevents severe pathologies and death from Zika virus infections. JCI Insight, 2017, 2, .	5.0	74
45	South-east Asian Zika virus strain linked to cluster of cases in Singapore, August 2016. Eurosurveillance, 2016, 21, .	7.0	44
46	Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. PLoS ONE, 2016, 11, e0156963.	2.5	28
47	Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. Structure, 2016, 24, 1410-1420.	3.3	41
48	Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. Scientific Reports, 2016, 6, 19160.	3.3	17
49	praja2 regulates KSR1 stability and mitogenic signaling. Cell Death and Disease, 2016, 7, e2230-e2230.	6.3	22
50	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
51	Impairing Cohesin Smc1/3 Head Engagement Compensates for the Lack of Eco1 Function. Structure, 2016, 24, 1991-1999.	3.3	23
52	Hydrocarbons Are Essential for Optimal Cell Size, Division, and Growth of Cyanobacteria. Plant Physiology, 2016, 172, 1928-1940.	4.8	53
53	Energetics and Dynamics Across the Bcl-2-Regulated Apoptotic Pathway Reveal Distinct Evolutionary Determinants of Specificity and Affinity. Structure, 2016, 24, 2024-2033.	3.3	16
54	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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55	Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases. Journal of Physical Chemistry B, 2016, 120, 299-308.	2.6	5
56	Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091.	4.9	198
57	Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics, 2015, 33, 104-120.	3.5	24
58	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
59	Intrinsic flexibility of <scp>NLRP</scp> pyrin domains is a key factor in their conformational dynamics, fold stability, and dimerization. Protein Science, 2015, 24, 174-181.	7.6	24
60	Understanding Dengue Virus Capsid Protein Disordered N-Terminus and pep14-23-Based Inhibition. ACS Chemical Biology, 2015, 10, 517-526.	3.4	45
61	The Structural Basis for Activation and Inhibition of ZAP-70 Kinase Domain. PLoS Computational Biology, 2015, 11, e1004560.	3.2	12
62	Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. PLoS ONE, 2015, 10, e0140713.	2.5	24
63	Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658.	2.5	25
64	Specificity of a proteinâ€“protein interface: Local dynamics direct substrate recognition of effector caspases. Proteins: Structure, Function and Bioinformatics, 2014, 82, 546-555.	2.6	20
65	Heteroaromatic Ï€-Stacking Energy Landscapes. Journal of Chemical Information and Modeling, 2014, 54, 1371-1379.	5.4	144
66	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
67	Matrix Isolation Studies of Carbonic Acidâ€”The Vapor Phase above the Î²-Polymorph. Journal of the American Chemical Society, 2013, 135, 7732-7737.	13.7	33
68	Entropy from State Probabilities: Hydration Entropy of Cations. Journal of Physical Chemistry B, 2013, 117, 6466-6472.	2.6	23
69	Substrate-Driven Mapping of the Degradome by Comparison of Sequence Logos. PLoS Computational Biology, 2013, 9, e1003353.	3.2	23
70	Cleavage Entropy as Quantitative Measure of Protease Specificity. PLoS Computational Biology, 2013, 9, e1003007.	3.2	49
71	Reciprocal regulation of PKA and Rac signaling. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8531-8536.	7.1	42
72	Porphyrin-LEGOÂ®: synthesis of a hexafullereno-diporphyrin using porphyrins programmed for [4+2]-cycloaddition. Chemical Communications, 2012, 48, 4359.	4.1	17

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73	Dynamic Regulation of Phenylalanine Hydroxylase by Simulated Redox Manipulation. PLoS ONE, 2012, 7, e53005.	2.5	27
74	Dengue and Zika RNA-RNA Interactomes Reveal Virus Permissive and Restrictive Factors in Human Cells. SSRN Electronic Journal, 0, , .	0.4	0
75	RNAvigator: A Pipeline to Identify Candidates for Functional RNA Structure Elements. Frontiers in Virology, 0, 2, .	1.4	1