Peter Kasson

List of Publications by Year
in descending order

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75 papers	8,295 citations	201575 27 h-index	110317 64 g-index
89 all docs	89 docs citations	89 times ranked	13463 citing authors

#	Article	IF	Citations
1	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	1.8	6,072
2	Heterogeneity Even at the Speed Limit of Folding: Large-scale Molecular Dynamics Study of a Fast-folding Variant of the Villin Headpiece. Journal of Molecular Biology, 2007, 374, 806-816.	2.0	182
3	Ensemble molecular dynamics yields submillisecond kinetics and intermediates of membrane fusion. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11916-11921.	3.3	139
4	Formation of a Highly Peptide-Receptive State of Class II MHC. Immunity, 1998, 9, 699-709.	6.6	126
5	Control of Membrane Fusion Mechanism by Lipid Composition: Predictions from Ensemble Molecular Dynamics. PLoS Computational Biology, 2007, 3, e220.	1.5	118
6	Atomic-Resolution Simulations Predict a Transition State for Vesicle Fusion Defined by Contact of a Few Lipid Tails. PLoS Computational Biology, 2010, 6, e1000829.	1.5	108
7	Viral factors in influenza pandemic risk assessment. ELife, 2016, 5, .	2.8	82
8	Lipid Tail Protrusion in Simulations Predicts Fusogenic Activity of Influenza Fusion Peptide Mutants and Conformational Models. PLoS Computational Biology, 2013, 9, e1002950.	1.5	76
9	Managing Coronavirus Disease 2019 Spread With Voluntary Public Health Measures: Sweden as a Case Study for Pandemic Control. Clinical Infectious Diseases, 2020, 71, 3174-3181.	2.9	73
10	SARS-CoV-2 receptor networks in diabetic and COVID-19â€“associated kidney disease. Kidney International, 2020, 98, 1502-1518.	2.6	64
11	Dynamic heterogeneity controls diffusion and viscosity near biological interfaces. Nature Communications, 2014, 5, 3034.	5.8	58
12	Improving pandemic influenza risk assessment. ELife, 2014, 3, e03883.	2.8	53
13	Structure of the Neisserial Outer Membrane Protein Opa₆₀:ÂLoop Flexibility Essential to Receptor Recognition and Bacterial Engulfment. Journal of the American Chemical Society, 2014, 136, 9938-9946.	6.6	52
14	Cholesterol enhances influenza binding avidity by controlling nanoscale receptor clustering. Chemical Science, 2018, 9, 2340-2347.	3.7	50
15	Kinetics of Peptide Binding to the Class II MHC Protein Iâ^'Ekâ€. Biochemistry, 2000, 39, 1048-1058.	1.2	48
16	Water Ordering at Membrane Interfaces Controls Fusion Dynamics. Journal of the American Chemical Society, 2011, 133, 3812-3815.	6.6	47
17	Persistent voids: a new structural metric for membrane fusion. Bioinformatics, 2007, 23, 1753-1759.	1.8	46
18	Influenza hemagglutinin drives viral entry via two sequential intramembrane mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 7200-7207.	3.3	46

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19	Ebolavirus Entry Requires a Compact Hydrophobic Fist at the Tip of the Fusion Loop. Journal of Virology, 2014, 88, 6636-6649.	1.5	44
20	pH Dependence of Zika Membrane Fusion Kinetics Reveals an Off-Pathway State. ACS Central Science, 2018, 4, 1503-1510.	5.3	43
21	Disentangling Viral Membrane Fusion from Receptor Binding Using Synthetic DNA-Lipid Conjugates. Biophysical Journal, 2016, 111, 123-131.	0.2	42
22	Molecular Simulation Workflows as Parallel Algorithms: The Execution Engine of Copernicus, a Distributed High-Performance Computing Platform. Journal of Chemical Theory and Computation, 2015, 11, 2600-2608.	2.3	40
23	Antibiotic Uptake Across Gram-Negative Outer Membranes: Better Predictions Towards Better Antibiotics. ACS Infectious Diseases, 2019, 5, 2096-2104.	1.8	37
24	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. ELife, 2017, 6, .	2.8	37
25	Multiphasic Effects of Cholesterol on Influenza Fusion Kinetics Reflect Multiple Mechanistic Roles. Biophysical Journal, 2013, 105, 1383-1387.	0.2	36
26	Combining Molecular Dynamics with Bayesian Analysis To Predict and Evaluate Ligand-Binding Mutations in Influenza Hemagglutinin. Journal of the American Chemical Society, 2009, 131, 11338-11340.	6.6	30
27	Molecular Dynamics Simulation of Lipid Reorientation at Bilayer Edges. Biophysical Journal, 2004, 86, 3744-3749.	0.2	27
28	Copernicus. , 2011, , .		27
29	Influenza viral membrane fusion is sensitive to sterol concentration but surprisingly robust to sterol chemical identity. Scientific Reports, 2016, 6, 29842.	1.6	26
30	Detecting and Controlling Dye Effects in Single-Virus Fusion Experiments. Biophysical Journal, 2019, 117, 445-452.	0.2	26
31	Predicting allosteric mutants that increase activity of a major antibiotic resistance enzyme. Chemical Science, 2017, 8, 6484-6492.	3.7	25
32	Structural Basis for Influence of Viral Glycans on Ligand Binding by Influenza Hemagglutinin. Biophysical Journal, 2008, 95, L48-L50.	0.2	24
33	Adaptive ensemble simulations of biomolecules. Current Opinion in Structural Biology, 2018, 52, 87-94.	2.6	24
34	Structural conservation in a membrane-enveloped filamentous virus infecting a hyperthermophilic acidophile. Nature Communications, 2018, 9, 3360.	5.8	24
35	Hemagglutinin Spatial Distribution Shifts in Response to Cholesterol in the Influenza Viral Envelope. Biophysical Journal, 2015, 109, 1917-1924.	0.2	23
36	Conformational Intermediate That Controls KPC-2 Catalysis and Beta-Lactam Drug Resistance. ACS Catalysis, 2018, 8, 2741-2747.	5.5	22

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37	Influenza Hemifusion Phenotype Depends on Membrane Context: Differences in Cellâ€“Cell and Virusâ€“Cell Fusion. Journal of Molecular Biology, 2018, 430, 594-601.	2.0	21
38	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. Journal of Physical Chemistry B, 2019, 123, 3576-3590.	1.2	21
39	Excess positional mutual information predicts both local and allosteric mutations affecting beta lactamase drug resistance. Bioinformatics, 2016, 32, 3420-3427.	1.8	19
40	Development of COVID-19 vaccine using a dual Toll-like receptor ligand liposome adjuvant. Npj Vaccines, 2021, 6, 137.	2.9	15
41	Coupled Diffusion in Lipid Bilayers upon Close Approach. Journal of the American Chemical Society, 2015, 137, 708-714.	6.6	14
42	Bilayer-Coated Nanoparticles Reveal How Influenza Viral Entry Depends on Membrane Deformability but Not Curvature. Journal of Physical Chemistry Letters, 2020, 11, 7190-7196.	2.1	14
43	Adaptive Ensemble Biomolecular Applications at Scale. SN Computer Science, 2020, 1, 1.	2.3	14
44	Acquired Functional Capsid Structures in Metazoan Totivirus-like dsRNA Virus. Structure, 2020, 28, 888-896.e3.	1.6	12
45	A hybrid machine-learning approach for segmentation of protein localization data. Bioinformatics, 2005, 21, 3778-3786.	1.8	11
46	Probing microscopic material properties inside simulated membranes through spatially resolved three-dimensional local pressure fields and surface tensions. Chemistry and Physics of Lipids, 2013, 169, 106-112.	1.5	11
47	Refinement of Highly Flexible Protein Structures using Simulationâ€Guided Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 17110-17114.	7.2	10
48	Predicting allostery and microbial drug resistance with molecular simulations. Current Opinion in Structural Biology, 2018, 52, 80-86.	2.6	10
49	Infectious Disease Research in the Era of Big Data. Annual Review of Biomedical Data Science, 2020, 3, 43-59.	2.8	10
50	gmxapi: a high-level interface for advanced control and extension of molecular dynamics simulations. Bioinformatics, 2018, 34, 3945-3947.	1.8	9
51	Precise Triggering and Chemical Control of Single-Virus Fusion within Endosomes. Journal of Virology, 2020, 95, .	1.5	9
52	Hybrid Refinement of Heterogeneous Conformational Ensembles Using Spectroscopic Data. Journal of Physical Chemistry Letters, 2019, 10, 3410-3414.	2.1	8
53	Receptor Binding by Influenza Virus: Using Computational Techniques To Extend Structural Data. Biochemistry, 2012, 51, 2359-2365.	1.2	7
54	Lipid Converter, A Framework for Lipid Manipulations in Molecular Dynamics Simulations. Journal of Membrane Biology, 2014, 247, 1137-1140.	1.0	7

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55	Quantitative Imaging of Lymphocyte Membrane Protein Reorganization and Signaling. Biophysical Journal, 2005, 88, 579-589.	0.2	6
56	The N-terminal Helix-Turn-Helix Motif of Transcription Factors MarA and Rob Drives DNA Recognition. Journal of Physical Chemistry B, 2021, 125, 6791-6806.	1.2	6
57	COMBINING MUTUAL INFORMATION WITH STRUCTURAL ANALYSIS TO SCREEN FOR FUNCTIONALLY IMPORTANT RESIDUES IN INFLUENZA HEMAGGLUTININ. , 2008, , 492-503.		5
58	A bundling of viral fusion mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3827-3828.	3.3	5
59	COMPUTATIONAL BIOLOGY IN THE CLOUD: METHODS AND NEW INSIGHTS FROM COMPUTING AT SCALE. , 2012, , .		5
60	Predicting structure and dynamics of loosely-ordered protein complexes: influenza hemagglutinin fusion peptide. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2007, , 40-50.	0.7	5
61	Inference of Joint Conformational Distributions from Separately Acquired Experimental Measurements. Journal of Physical Chemistry Letters, 2021, 12, 1606-1611.	2.1	3
62	PREDICTING STRUCTURE AND DYNAMICS OF LOOSELY-ORDERED PROTEIN COMPLEXES: INFLUENZA HEMAGGLUTININ FUSION PEPTIDE. , 2006, , .		3
63	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. PLoS Computational Biology, 2005, preprint, e220.	1.5	2
64	Effect of Cholesterol Depletion on HA Distribution in the Viral Membrane of Influenza. Biophysical Journal, 2015, 108, 406a-407a.	0.2	1
65	Refinement of Highly Flexible Protein Structures using Simulationâ€Guided Spectroscopy. Angewandte Chemie, 2018, 130, 17356-17360.	1.6	1
66	Cholesterol-Induced Membrane Organization Promotes Influenza Virus Binding. Biophysical Journal, 2018, 114, 379a.	0.2	1
67	Computational methods to study enveloped viral entry. Biochemical Society Transactions, 2021, 49, 2527-2537.	1.6	1
68	"Cross-graining": efficient multi-scale simulation via Markov state models. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2010, , 260-8.	0.7	1
69	gmxapi: A GROMACS-native Python interface for molecular dynamics with ensemble and plugin support. PLoS Computational Biology, 2022, 18, e1009835.	1.5	1
70	Deformable modeling for improved calculation of molecular velocities from single-particle tracking. , 2005, , 208-11.		0
71	Kinetic Models of Zika Virus Membrane Fusion. Biophysical Journal, 2018, 114, 604a.	0.2	0
72	Atomic-Resolution Simulations Show Two Sequential Fusion Peptide Mechanisms in Influenza Membrane Fusion. Biophysical Journal, 2019, 116, 368a.	0.2	0

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73	Understanding Activation and Inhibition of SARS-CoV-2 Viral Entry with Single-Virus Microscopy. Biophysical Journal, 2021, 120, 321a.	0.2	0
74	Bilayer-Coated Nanoparticles to Probe the Effect of Membrane Deformability on Fusion intermediates. Biophysical Journal, 2021, 120, 41a.	0.2	0
75	Modeling biomolecular kinetics with large-scale simulation. Current Opinion in Structural Biology, 2022, 72, 95-102.	2.6	0