Peter Kasson

List of Publications by Year
in descending order

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75 papers	8,295 citations	201674 27 h-index	110387 64 g-index
89 all docs	89 docs citations	89 times ranked	13463 citing authors

#	Article	IF	Citations
1	Modeling biomolecular kinetics with large-scale simulation. Current Opinion in Structural Biology, 2022, 72, 95-102.	5.7	0
2	gmxapi: A GROMACS-native Python interface for molecular dynamics with ensemble and plugin support. PLoS Computational Biology, 2022, 18, e1009835.	3.2	1
3	Inference of Joint Conformational Distributions from Separately Acquired Experimental Measurements. Journal of Physical Chemistry Letters, 2021, 12, 1606-1611.	4.6	3
4	Understanding Activation and Inhibition of SARS-CoV-2 Viral Entry with Single-Virus Microscopy. Biophysical Journal, 2021, 120, 321a.	0.5	0
5	Bilayer-Coated Nanoparticles to Probe the Effect of Membrane Deformability on Fusion intermediates. Biophysical Journal, 2021, 120, 41a.	0.5	0
6	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.	2.6	6
7	Development of COVID-19 vaccine using a dual Toll-like receptor ligand liposome adjuvant. Npj Vaccines, 2021, 6, 137.	6.0	15
8	Computational methods to study enveloped viral entry. Biochemical Society Transactions, 2021, 49, 2527-2537.	3.4	1
9	SARS-CoV-2 receptor networks in diabetic and COVID-19â€“associated kidney disease. Kidney International, 2020, 98, 1502-1518.	5.2	64
10	Bilayer-Coated Nanoparticles Reveal How Influenza Viral Entry Depends on Membrane Deformability but Not Curvature. Journal of Physical Chemistry Letters, 2020, 11, 7190-7196.	4.6	14
11	Precise Triggering and Chemical Control of Single-Virus Fusion within Endosomes. Journal of Virology, 2020, 95, .	3.4	9
12	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.	7.1	46
13	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.	5.8	73
14	Acquired Functional Capsid Structures in Metazoan Totivirus-like dsRNA Virus. Structure, 2020, 28, 888-896.e3.	3.3	12
15	Adaptive Ensemble Biomolecular Applications at Scale. SN Computer Science, 2020, 1, 1.	3.6	14
16	Infectious Disease Research in the Era of Big Data. Annual Review of Biomedical Data Science, 2020, 3, 43-59.	6.5	10
17	Detecting and Controlling Dye Effects in Single-Virus Fusion Experiments. Biophysical Journal, 2019, 117, 445-452.	0.5	26
18	Antibiotic Uptake Across Gram-Negative Outer Membranes: Better Predictions Towards Better Antibiotics. ACS Infectious Diseases, 2019, 5, 2096-2104.	3.8	37

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19	Hybrid Refinement of Heterogeneous Conformational Ensembles Using Spectroscopic Data. Journal of Physical Chemistry Letters, 2019, 10, 3410-3414.	4.6	8
20	Atomic-Resolution Simulations Show Two Sequential Fusion Peptide Mechanisms in Influenza Membrane Fusion. Biophysical Journal, 2019, 116, 368a.	0.5	0
21	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. Journal of Physical Chemistry B, 2019, 123, 3576-3590.	2.6	21
22	Conformational Intermediate That Controls KPC-2 Catalysis and Beta-Lactam Drug Resistance. ACS Catalysis, 2018, 8, 2741-2747.	11.2	22
23	Influenza Hemifusion Phenotype Depends on Membrane Context: Differences in Cellâ€“Cell and Virusâ€“Cell Fusion. Journal of Molecular Biology, 2018, 430, 594-601.	4.2	21
24	Cholesterol enhances influenza binding avidity by controlling nanoscale receptor clustering. Chemical Science, 2018, 9, 2340-2347.	7.4	50
25	Refinement of Highly Flexible Protein Structures using Simulationâ€Guided Spectroscopy. Angewandte Chemie, 2018, 130, 17356-17360.	2.0	1
26	Refinement of Highly Flexible Protein Structures using Simulationâ€Guided Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 17110-17114.	13.8	10
27	Predicting allostery and microbial drug resistance with molecular simulations. Current Opinion in Structural Biology, 2018, 52, 80-86.	5.7	10
28	Adaptive ensemble simulations of biomolecules. Current Opinion in Structural Biology, 2018, 52, 87-94.	5.7	24
29	pH Dependence of Zika Membrane Fusion Kinetics Reveals an Off-Pathway State. ACS Central Science, 2018, 4, 1503-1510.	11.3	43
30	Kinetic Models of Zika Virus Membrane Fusion. Biophysical Journal, 2018, 114, 604a.	0.5	0
31	gmxapi: a high-level interface for advanced control and extension of molecular dynamics simulations. Bioinformatics, 2018, 34, 3945-3947.	4.1	9
32	Cholesterol-Induced Membrane Organization Promotes Influenza Virus Binding. Biophysical Journal, 2018, 114, 379a.	0.5	1
33	Structural conservation in a membrane-enveloped filamentous virus infecting a hyperthermophilic acidophile. Nature Communications, 2018, 9, 3360.	12.8	24
34	Predicting allosteric mutants that increase activity of a major antibiotic resistance enzyme. Chemical Science, 2017, 8, 6484-6492.	7.4	25
35	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. ELife, 2017, 6, .	6.0	37
36	Excess positional mutual information predicts both local and allosteric mutations affecting beta lactamase drug resistance. Bioinformatics, 2016, 32, 3420-3427.	4.1	19

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37	Disentangling Viral Membrane Fusion from Receptor Binding Using Synthetic DNA-Lipid Conjugates. Biophysical Journal, 2016, 111, 123-131.	0.5	42
38	Influenza viral membrane fusion is sensitive to sterol concentration but surprisingly robust to sterol chemical identity. Scientific Reports, 2016, 6, 29842.	3.3	26
39	Viral factors in influenza pandemic risk assessment. ELife, 2016, 5, .	6.0	82
40	Effect of Cholesterol Depletion on HA Distribution in the Viral Membrane of Influenza. Biophysical Journal, 2015, 108, 406a-407a.	0.5	1
41	Coupled Diffusion in Lipid Bilayers upon Close Approach. Journal of the American Chemical Society, 2015, 137, 708-714.	13.7	14
42	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.	5.3	40
43	Hemagglutinin Spatial Distribution Shifts in Response to Cholesterol in the Influenza Viral Envelope. Biophysical Journal, 2015, 109, 1917-1924.	0.5	23
44	Improving pandemic influenza risk assessment. ELife, 2014, 3, e03883.	6.0	53
45	Lipid Converter, A Framework for Lipid Manipulations in Molecular Dynamics Simulations. Journal of Membrane Biology, 2014, 247, 1137-1140.	2.1	7
46	Dynamic heterogeneity controls diffusion and viscosity near biological interfaces. Nature Communications, 2014, 5, 3034.	12.8	58
47	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.	13.7	52
48	Ebolavirus Entry Requires a Compact Hydrophobic Fist at the Tip of the Fusion Loop. Journal of Virology, 2014, 88, 6636-6649.	3.4	44
49	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.	3.2	11
50	Multiphasic Effects of Cholesterol on Influenza Fusion Kinetics Reflect Multiple Mechanistic Roles. Biophysical Journal, 2013, 105, 1383-1387.	0.5	36
51	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	4.1	6,072
52	Lipid Tail Protrusion in Simulations Predicts Fusogenic Activity of Influenza Fusion Peptide Mutants and Conformational Models. PLoS Computational Biology, 2013, 9, e1002950.	3.2	76
53	COMPUTATIONAL BIOLOGY IN THE CLOUD: METHODS AND NEW INSIGHTS FROM COMPUTING AT SCALE. , 2012, , .		5
54	Receptor Binding by Influenza Virus: Using Computational Techniques To Extend Structural Data. Biochemistry, 2012, 51, 2359-2365.	2.5	7

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55	Water Ordering at Membrane Interfaces Controls Fusion Dynamics. Journal of the American Chemical Society, 2011, 133, 3812-3815.	13.7	47
56	A bundling of viral fusion mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3827-3828.	7.1	5
57	Copernicus. , 2011, , .		27
58	Atomic-Resolution Simulations Predict a Transition State for Vesicle Fusion Defined by Contact of a Few Lipid Tails. PLoS Computational Biology, 2010, 6, e1000829.	3.2	108
59	"Cross-graining": efficient multi-scale simulation via Markov state models. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2010, , 260-8.	0.7	1
60	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.	13.7	30
61	Structural Basis for Influence of Viral Glycans on Ligand Binding by Influenza Hemagglutinin. Biophysical Journal, 2008, 95, L48-L50.	0.5	24
62	COMBINING MUTUAL INFORMATION WITH STRUCTURAL ANALYSIS TO SCREEN FOR FUNCTIONALLY IMPORTANT RESIDUES IN INFLUENZA HEMAGGLUTININ. , 2008, , 492-503.		5
63	Control of Membrane Fusion Mechanism by Lipid Composition: Predictions from Ensemble Molecular Dynamics. PLoS Computational Biology, 2007, 3, e220.	3.2	118
64	Persistent voids: a new structural metric for membrane fusion. Bioinformatics, 2007, 23, 1753-1759.	4.1	46
65	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.	4.2	182
66	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
67	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.	7.1	139
68	PREDICTING STRUCTURE AND DYNAMICS OF LOOSELY-ORDERED PROTEIN COMPLEXES: INFLUENZA HEMAGGLUTININ FUSION PEPTIDE. , 2006, , .		3
69	A hybrid machine-learning approach for segmentation of protein localization data. Bioinformatics, 2005, 21, 3778-3786.	4.1	11
70	Quantitative Imaging of Lymphocyte Membrane Protein Reorganization and Signaling. Biophysical Journal, 2005, 88, 579-589.	0.5	6
71	Deformable modeling for improved calculation of molecular velocities from single-particle tracking. , 2005, , 208-11.		0
72	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. PLoS Computational Biology, 2005, preprint, e220.	3.2	2

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73	Molecular Dynamics Simulation of Lipid Reorientation at Bilayer Edges. Biophysical Journal, 2004, 86, 3744-3749.	0.5	27
74	Kinetics of Peptide Binding to the Class II MHC Protein Iâ^'Ekâ€. Biochemistry, 2000, 39, 1048-1058.	2.5	48
75	Formation of a Highly Peptide-Receptive State of Class II MHC. Immunity, 1998, 9, 699-709.	14.3	126