

# Krzysztof Kuczera

## List of Publications by Year in descending order

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45  
papers

920  
citations

567281

15  
h-index

454955

30  
g-index

50  
all docs

50  
docs citations

50  
times ranked

1094  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure and Function of S-Adenosylhomocysteine Hydrolase. <i>Cell Biochemistry and Biophysics</i> , 2000, 33, 101-125.	1.8	148
2	Unusual Encapsulation of Two Nitrates in a Single Bicyclic Cage. <i>Journal of the American Chemical Society</i> , 1998, 120, 8899-8900.	13.7	140
3	One-Electron Photooxidation of N-Methionyl Peptides. Mechanism of Sulfoxide and Azasulfonium Diastereomer Formation through Reaction of Sulfide Radical Cation Complexes with Oxygen or Superoxide. <i>Journal of the American Chemical Society</i> , 1998, 120, 3345-3356.	13.7	68
4	Kinetics of Helix Unfolding: Molecular Dynamics Simulations with Milestoning. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7461-7473.	2.5	63
5	Unassisted Transport of N-Acetyl-L-tryptophanamide through Membrane: Experiment and Simulation of Kinetics. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2739-2750.	2.6	59
6	Transitions from $\hat{I}_{\pm}$ to $\hat{I}_{\infty}$ Helix Observed in Molecular Dynamics Simulations of Synthetic Peptides. <i>Biochemistry</i> , 2000, 39, 13737-13747.	2.5	51
7	Equilibrium Structure and Folding of a Helix-Forming Peptide: Circular Dichroism Measurements and Replica-Exchange Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2004, 87, 3786-3798.	0.5	46
8	Structure and Dynamics of Calcium-activated Calmodulin in Solution. <i>Journal of Biomolecular Structure and Dynamics</i> , 2001, 19, 247-271.	3.5	40
9	Helix Formation in a Pentapeptide: Experiment and Force-field Dependent Dynamics. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12391-12402.	2.5	39
10	Experiments and Comprehensive Simulations of the Formation of a Helical Turn. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6598-6610.	2.6	22
11	Reorientation Motion and Preferential Interactions of a Peptide in Denaturants and Osmolyte. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3089-3099.	2.6	22
12	Permeation of the three aromatic dipeptides through lipid bilayers: Experimental and computational study. <i>Journal of Chemical Physics</i> , 2016, 144, 245103.	3.0	20
13	Computational Characterization of Substrate Binding and Catalysis in S-Adenosylhomocysteine Hydrolase. <i>Biochemistry</i> , 2001, 40, 15143-15152.	2.5	17
14	Probing the interaction between cHAVc3 peptide and the EC1 domain of E-cadherin using NMR and molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 92-104.	3.5	17
15	Picosecond Time-Resolved Fourier-Transform Raman Spectroscopy and Normal-Mode Analysis of the Ground State and Singlet Excited State of Anthracene. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11857-11862.	2.9	15
16	Reorientations of Aromatic Amino Acids and Their Side Chain Models: Anisotropy Measurements and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 133-142.	2.5	15
17	Computer simulations of helix folding in homo- and heteropeptides. <i>Molecular Simulation</i> , 2012, 38, 682-694.	2.0	13
18	Molecular Dynamics Simulations of Conformational Behavior of Linear RGD Peptidomimetics and Cyclic Prodrugs in Aqueous and Octane Solutions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2002, 19, 775-788.	3.5	12

#	ARTICLE	IF	CITATIONS
19	Helix-Coil Transition Courses Through Multiple Pathways and Intermediates: Fast Kinetic Measurements and Dimensionality Reduction. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10806-10816.	2.6	12
20	Detailed Microscopic Unfolding Pathways of an $\alpha$ -Helix and a $\beta$ -Hairpin: Direct Observation and Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7233-7246.	2.6	11
21	Non-Exponential Kinetics and a Complete Folding Pathway of an $\alpha$ -Helical Heteropeptide: Direct Observation and Comprehensive Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 639-647.	2.6	10
22	Simulating the free energy of passive membrane permeation for small molecules. <i>Molecular Simulation</i> , 2018, 44, 1147-1157.	2.0	9
23	Deprotonation of a Single Amino Acid Residue Induces Significant Stability in an $\alpha$ -Helical Heteropeptide. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11508-11518.	2.6	9
24	Oligomeric States and Hydrodynamic Properties of Lysyl Oxidase-Like 2. <i>Biomolecules</i> , 2021, 11, 1846.	4.0	7
25	Conformational free energy surface of the linear DPDPE peptide: cost of pre-organization for disulfide bond formation. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 274-281.	1.4	6
26	Dynamic elements and kinetics: Most favorable conformations of peptides in solution with measurements and simulations. <i>Journal of Chemical Physics</i> , 2019, 151, 225102.	3.0	6
27	Free energy simulations to understand the effect of Met $\rightarrow$ Ala mutations at positions 205, 206 and 213 on stability of human prion protein. <i>Biophysical Chemistry</i> , 2021, 275, 106620.	2.8	6
28	Molecular Modeling of Peptides. <i>Methods in Molecular Biology</i> , 2015, 1268, 15-41.	0.9	6
29	Effects of CMAP and Electrostatic Cutoffs on the Dynamics of an Integral Membrane Protein: The Phospholamban Study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2008, 26, 17-34.	3.5	5
30	Probing Selection Mechanism of the Most Favorable Conformation of a Dipeptide in Chaotropic and Kosmotropic Solution. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6939-6950.	2.6	5
31	Probing coupled motions of peptides in solution with fluorescence anisotropy and molecular dynamics simulation. <i>Chemical Physics</i> , 2021, 541, 111018.	1.9	3
32	Length Dependent Folding Kinetics of Alanine-Based Helical Peptides from Optimal Dimensionality Reduction. <i>Life</i> , 2021, 11, 385.	2.4	3
33	Enhancing the Inhomogeneous Photodynamics of Canonical Bacteriophytochrome. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2647-2657.	2.6	3
34	Kinetic pathway analysis of an $\alpha$ -helix in two protonation states: Direct observation and optimal dimensionality reduction. <i>Journal of Chemical Physics</i> , 2019, 150, 074902.	3.0	2
35	Observing reorientation dynamics with Time-Resolved fluorescence and molecular dynamics in varying periodic boundary conditions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10614-10628.	3.5	2
36	Dissecting Multiple Pathways in the Relaxation Dynamics of Helix $\rightleftharpoons$ Coil Transitions with Optimum Dimensionality Reduction. <i>Biomolecules</i> , 2021, 11, 1351.	4.0	2

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37	Publisher's Note: "Permeation of the three aromatic dipeptides through lipid bilayers: Experimental and computational study". J. Chem. Phys. 144, 245103 (2016). Journal of Chemical Physics, 2016, 145, 059902.	3.0	1
38	Finding optimal paths through biomolecular mazes. Physics of Life Reviews, 2017, 22-23, 77-78.	2.8	1
39	Unassisted N-acetyl-phenylalanine-amide transport across membrane with varying lipid size and composition: kinetic measurements and atomistic molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, , 1-16.	3.5	1
40	Probing the Internal Dynamics and Shape of Simple Peptides in Urea, Guanidinium Hydrochloride, and Proline Solutions with Time-Resolved Fluorescence Anisotropy and Atomistic Cosolvent Simulations. Journal of Physical Chemistry B, 2021, 125, 10972-10984.	2.6	1
41	Reorientation motions of N-acetyl-tryptophan-amide (NATA dipeptide) in aqueous solution and with co-solvents: Molecular dynamics vs hydrodynamic model. Physics of Fluids, 2020, 32, .	4.0	1
42	Modulation of human transthyretin stability by the mutations at histidine 88 studied by free energy simulation. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1825-1836.	2.6	1
43	Milestoning Simulation Reveals Mechanism of Helix-Breaking. Biophysical Journal, 2013, 105, 832.	0.5	0
44	Divergence in proteins' Study of Cytochrome b5 isoforms using core swap mutants. FASEB Journal, 2010, 24, 521.6.	0.5	0
45	Simulation analysis of selective alanine mutation effect on stability of human prion protein. Journal of Biomolecular Structure and Dynamics, 2022, , 1-11.	3.5	0