Krzysztof Kuczera

List of Publications by Year
in descending order

45	920	567281 15	454955 30
papers	citations	h-index	g-index

50	50	50	1094
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Observing reorientation dynamics with Time-Resolved fluorescence and molecular dynamics in varying periodic boundary conditions. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10614-10628.	3.5	2
2	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
3	Enhancing the Inhomogeneous Photodynamics of Canonical Bacteriophytochrome. Journal of Physical Chemistry B, 2022, 126, 2647-2657.	2.6	3
4	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
5	Probing coupled motions of peptides in solution with fluorescence anisotropy and molecular dynamics simulation. Chemical Physics, 2021, 541, 111018.	1.9	3
6	Length Dependent Folding Kinetics of Alanine-Based Helical Peptides from Optimal Dimensionality Reduction. Life, 2021, 11, 385.	2.4	3
7	Free energy simulations to understand the effect of Met â†' Ala mutations at positions 205, 206 and 213 on stability of human prion protein. Biophysical Chemistry, 2021, 275, 106620.	2.8	6
8	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
9	Dissecting Multiple Pathways in the Relaxation Dynamics of Helix <==> Coil Transitions with Optimum Dimensionality Reduction. Biomolecules, 2021, 11, 1351.	4.0	2
10	Oligomeric States and Hydrodynamic Properties of Lysyl Oxidase-Like 2. Biomolecules, 2021, 11, 1846.	4.0	7
11	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
12	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
13	Kinetic pathway analysis of an Î±-helix in two protonation states: Direct observation and optimal dimensionality reduction. Journal of Chemical Physics, 2019, 150, 074902.	3.0	2
14	Dynamic elements and kinetics: Most favorable conformations of peptides in solution with measurements and simulations. Journal of Chemical Physics, 2019, 151, 225102.	3.0	6
15	Simulating the free energy of passive membrane permeation for small molecules. Molecular Simulation, 2018, 44, 1147-1157.	2.0	9
16	Helixâ€"Coil Transition Courses Through Multiple Pathways and Intermediates: Fast Kinetic Measurements and Dimensionality Reduction. Journal of Physical Chemistry B, 2018, 122, 10806-10816.	2.6	12
17	Deprotonation of a Single Amino Acid Residue Induces Significant Stability in an Î±-Helical Heteropeptide. Journal of Physical Chemistry B, 2018, 122, 11508-11518.	2.6	9
18	Probing the interaction between cHAVc3 peptide and the EC1 domain of E-cadherin using NMR and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 92-104.	3.5	17

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19	Finding optimal paths through biomolecular mazes. Physics of Life Reviews, 2017, 22-23, 77-78.	2.8	1
20	Permeation of the three aromatic dipeptides through lipid bilayers: Experimental and computational study. Journal of Chemical Physics, 2016, 144, 245103.	3.0	20
21	Publisherâ€™s Note: â€œPermeation of the three aromatic dipeptides through lipid bilayers: Experimental and computational studyâ€•[J. Chem. Phys. 144, 245103 (2016)]. Journal of Chemical Physics, 2016, 145, 059902.	3.0	1
22	Probing Selection Mechanism of the Most Favorable Conformation of a Dipeptide in Chaotropic and Kosmotropic Solution. Journal of Physical Chemistry B, 2016, 120, 6939-6950.	2.6	5
23	Reorientation Motion and Preferential Interactions of a Peptide in Denaturants and Osmolyte. Journal of Physical Chemistry B, 2016, 120, 3089-3099.	2.6	22
24	Molecular Modeling of Peptides. Methods in Molecular Biology, 2015, 1268, 15-41.	0.9	6
25	Non-Exponential Kinetics and a Complete Folding Pathway of an Î±-Helical Heteropeptide: Direct Observation and Comprehensive Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 639-647.	2.6	10
26	Detailed Microscopic Unfolding Pathways of an Î±-Helix and a Î²-Hairpin: Direct Observation and Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 7233-7246.	2.6	11
27	Milestoning Simulation Reveals Mechanism of Helix-Breaking. Biophysical Journal, 2013, 105, 832.	0.5	0
28	Computer simulations of helix folding in homo- and heteropeptides. Molecular Simulation, 2012, 38, 682-694.	2.0	13
29	Experiments and Comprehensive Simulations of the Formation of a Helical Turn. Journal of Physical Chemistry B, 2012, 116, 6598-6610.	2.6	22
30	Unassisted Transport of N-Acetyl-<scp>l</scp>-tryptophanamide through Membrane: Experiment and Simulation of Kinetics. Journal of Physical Chemistry B, 2012, 116, 2739-2750.	2.6	59
31	Reorientations of Aromatic Amino Acids and Their Side Chain Models: Anisotropy Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2010, 114, 133-142.	2.5	15
32	Helix Formation in a Pentapeptide: Experiment and Force-field Dependent Dynamics. Journal of Physical Chemistry A, 2010, 114, 12391-12402.	2.5	39
33	Divergence in proteinsâ€•Study of Cytochrome b5 isoforms using coreâ€swap mutants. FASEB Journal, 2010, 24, 521.6.	0.5	0
34	Kinetics of Helix Unfolding: Molecular Dynamics Simulations with Milestoning. Journal of Physical Chemistry A, 2009, 113, 7461-7473.	2.5	63
35	Effects of CMAP and Electrostatic Cutoffs on the Dynamics of an Integral Membrane Protein: The Phospholamban Study. Journal of Biomolecular Structure and Dynamics, 2008, 26, 17-34.	3.5	5
36	Equilibrium Structure and Folding of a Helix-Forming Peptide: Circular Dichroism Measurements and Replica-Exchange Molecular Dynamics Simulations. Biophysical Journal, 2004, 87, 3786-3798.	0.5	46

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37	Molecular Dynamics Simulations of Conformational Behavior of Linear RGD Peptidomimetics and Cyclic Prodrugs in Aqueous and Octane Solutions. Journal of Biomolecular Structure and Dynamics, 2002, 19, 775-788.	3.5	12
38	Computational Characterization of Substrate Binding and Catalysis in S-Adenosylhomocysteine Hydrolase. Biochemistry, 2001, 40, 15143-15152.	2.5	17
39	Structure and Dynamics of Calcium-activated Calmodulin in Solution. Journal of Biomolecular Structure and Dynamics, 2001, 19, 247-271.	3.5	40
40	Structure and Function of S-Adenosylhomocysteine Hydrolase. Cell Biochemistry and Biophysics, 2000, 33, 101-125.	1.8	148
41	Transitions from Î± to Ï€ Helix Observed in Molecular Dynamics Simulations of Synthetic Peptidesâ€. Biochemistry, 2000, 39, 13737-13747.	2.5	51
42	Conformational free energy surface of the linear DPDPE peptide: cost of pre-organization for disulfide bond formation. Theoretical Chemistry Accounts, 1999, 101, 274-281.	1.4	6
43	One-Electron Photooxidation ofN-Methionyl Peptides. Mechanism of Sulfoxide and Azasulfonium Diastereomer Formation through Reaction of Sulfide Radical Cation Complexes with Oxygen or Superoxide. Journal of the American Chemical Society, 1998, 120, 3345-3356.	13.7	68
44	Unusual Encapsulation of Two Nitrates in a Single Bicyclic Cage. Journal of the American Chemical Society, 1998, 120, 8899-8900.	13.7	140
45	Picosecond Time-Resolved Fourier-Transform Raman Spectroscopy and Normal-Mode Analysis of the Ground State and Singlet Excited State of Anthraceneâ€. The Journal of Physical Chemistry, 1996, 100, 11857-11862.	2.9	15