Rajiv Kumar Kar

List of Publications by Year
in descending order

59 papers	1,322 citations	361045 20 h-index	395343 33 g-index
62 all docs	62 docs citations	62 times ranked	2313 citing authors

#	Article	IF	Citations
1	Understanding flavin electronic structure and spectra. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1541.	6.2	19
2	Insight into the isomerization mechanism of retinal proteins from hybrid quantum mechanics/molecular mechanics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1562.	6.2	7
3	Cover Image, Volume 12, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	0
4	Doubling FÃ¶rster Resonance Energy Transfer Efficiency in Proteins with Extrinsic Thioamide Probes: Implications for Thiomodified Nucleobases. Chemistry - A European Journal, 2021, 27, 4373-4383.	1.7	6
5	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	1.3	26
6	Two-photon conversion of a bacterial phytochrome. Biophysical Journal, 2021, 120, 964-974.	0.2	8
7	LC-MS characterized methanolic extract of zanthoxylum armatum possess anti-breast cancer activity through Nrf2-Keap1 pathway: An in-silico, in-vitro and in-vivo evaluation. Journal of Ethnopharmacology, 2021, 269, 113758.	2.0	16
8	Computational Resources for Bioscience Education. Applied Biochemistry and Biotechnology, 2021, 193, 3418-3424.	1.4	0
9	Solvent Relaxation NMR: A Tool for Real-Time Monitoring Water Dynamics in Protein Aggregation Landscape. ACS Chemical Neuroscience, 2021, 12, 2903-2916.	1.7	8
10	Gram-Scale Synthesis of 1,8-Naphthyridines in Water: The Friedlander Reaction Revisited. ACS Omega, 2021, 6, 19304-19313.	1.6	11
11	Transient Near-UV Absorption of the Light-Driven Sodium Pump Krokinobacter eikastus Rhodopsin 2: A Spectroscopic Marker for Retinal Configuration. Journal of Physical Chemistry Letters, 2021, 12, 6284-6291.	2.1	9
12	Structural Dynamics of RNA in the Presence of Choline Amino Acid Based Ionic Liquid: A Spectroscopic and Computational Outlook. ACS Central Science, 2021, 7, 1688-1697.	5.3	8
13	Tuning the Quantum Chemical Properties of Flavins via Modification at C8. Journal of Physical Chemistry B, 2021, 125, 12654-12669.	1.2	7
14	Highâ€resolution structure of a partially folded insulin aggregation intermediate. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1648-1659.	1.5	13
15	Quercetin loaded folate targeted plasmonic silver nanoparticles for light activated chemo-photothermal therapy of DMBA induced breast cancer in Sprague Dawley rats. RSC Advances, 2020, 10, 31961-31978.	1.7	30
16	Femtosecond-to-millisecond structural changes in a light-driven sodium pump. Nature, 2020, 583, 314-318.	13.7	115
17	Structural and biochemical investigation of MARK4 inhibitory potential of cholic acid: Towards therapeutic implications in neurodegenerative diseases. International Journal of Biological Macromolecules, 2020, 161, 596-604.	3.6	37
18	Effect of pH on the structure and function of pyruvate dehydrogenase kinase 3: Combined spectroscopic and MD simulation studies. International Journal of Biological Macromolecules, 2020, 147, 768-777.	3.6	16

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19	Molecular Details of a Salt Bridge and Its Role in Insulin Fibrillation by NMR and Raman Spectroscopic Analysis. Journal of Physical Chemistry B, 2020, 124, 1125-1136.	1.2	10
20	Characterization of Antimicrobial Peptideâ€“Membrane Interaction Using All-Atom Molecular Dynamic Simulation. Springer Protocols, 2020, , 163-176.	0.1	2
21	A Peptide-Nanoparticle System with Improved Efficacy against Multidrug Resistant Bacteria. Scientific Reports, 2019, 9, 4485.	1.6	80
22	Atomistic Insight into the Role of Threonine 127 in the Functional Mechanism of Channelrhodopsin-2. Applied Sciences (Switzerland), 2019, 9, 4905.	1.3	4
23	Nuclear spin-hyperpolarization generated in a flavoprotein under illumination: experimental field-dependence and theoretical level crossing analysis. Scientific Reports, 2019, 9, 18436.	1.6	14
24	Sequence specificity of amylin-insulin interaction: a fragment-based insulin fibrillation inhibition study. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2019, 1867, 405-415.	1.1	13
25	Spectroscopic Properties of Lumiflavin: A Quantum Chemical Study. Photochemistry and Photobiology, 2019, 95, 662-674.	1.3	15
26	Nonproductive Binding Modes as a Prominent Feature of AÎ²₄₀ Fiber Elongation: Insights from Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2018, 58, 1576-1586.	2.5	11
27	Evidences for zinc (II) and copper (II) ion interactions with Mycobacterium leprae HSP18: Effect on its structure and chaperone function. Journal of Inorganic Biochemistry, 2018, 188, 62-75.	1.5	6
28	Synthesis of novel muramic acid derivatives and their interaction with lysozyme: Action of lysozyme revisited. Journal of Colloid and Interface Science, 2017, 498, 395-404.	5.0	12
29	Accelerated molecular dynamics simulation analysis of MSI-594 in a lipid bilayer. Physical Chemistry Chemical Physics, 2017, 19, 19289-19299.	1.3	46
30	Activity of a novel sulfonamide compound 2-nitro-N-(pyridin-2-ylmethyl)benzenesulfonamide against Leishmania donovani. Drug Design, Development and Therapy, 2016, 10, 1753.	2.0	3
31	Evidence for Inhibition of Lysozyme Amyloid Fibrillization by Peptide Fragments from Human Lysozyme: A Combined Spectroscopy, Microscopy, and Docking Study. Biomacromolecules, 2016, 17, 1998-2009.	2.6	35
32	Deciphering the role of the AT-rich interaction domain and the HMG-box domain of ARID-HMG proteins of Arabidopsis thaliana. Plant Molecular Biology, 2016, 92, 371-388.	2.0	16
33	Structural Elucidation of the Cell-Penetrating Penetratin Peptide in Model Membranes at the Atomic Level: Probing Hydrophobic Interactions in the Bloodâ€“Brain Barrier. Biochemistry, 2016, 55, 4982-4996.	1.2	24
34	Mode of Action of a Designed Antimicrobial Peptide: High Potency against Cryptococcus neoformans. Biophysical Journal, 2016, 111, 1724-1737.	0.2	37
35	Expedient synthesis of the pentasaccharide repeating unit of the O-antigen of Escherichia coli O86 and its conformational analysis. Glycoconjugate Journal, 2016, 33, 887-896.	1.4	5
36	Biophysical insights into the membrane interaction of the core amyloid-forming AÎ²₄₀fragment K16â€“K28 and its role in the pathogenesis of Alzheimer's disease. Physical Chemistry Chemical Physics, 2016, 18, 16890-16901.	1.3	16

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37	Structure and Dynamics of Antifreeze Proteinâ€“Model Membrane Interactions: A Combined Spectroscopic and Molecular Dynamics Study. Journal of Physical Chemistry B, 2016, 120, 902-914.	1.2	20
38	C -cinnamoyl glycosides as a new class of anti-filarial agents. European Journal of Medicinal Chemistry, 2016, 114, 308-317.	2.6	14
39	Biophysical Characterization of Essential Phosphorylation at the Flexible C-Terminal Region of C-Raf with 14-3-3Î¶ Protein. PLoS ONE, 2015, 10, e0135976.	1.1	9
40	Structural and sequential context of p53: A review of experimental and theoretical evidence. Progress in Biophysics and Molecular Biology, 2015, 117, 250-263.	1.4	48
41	Interaction of ATP with a Small Heat Shock Protein from Mycobacterium leprae: Effect on Its Structure and Function. PLoS Neglected Tropical Diseases, 2015, 9, e0003661.	1.3	13
42	Will It Be Beneficial To Simulate the Antifreeze Proteins at Ice Freezing Condition or at Lower Temperature?. Journal of Physical Chemistry B, 2015, 119, 11485-11495.	1.2	12
43	Biophysical and biochemical aspects of antifreeze proteins: Using computational tools to extract atomistic information. Progress in Biophysics and Molecular Biology, 2015, 119, 194-204.	1.4	15
44	Membrane disruptive antimicrobial activities of human Î²-defensin-3 analogs. European Journal of Medicinal Chemistry, 2015, 91, 91-99.	2.6	44
45	Double GC:GC Mismatch in dsDNA Enhances Local Dynamics Retaining the DNA Footprint: A Highâ€Resolution NMR Study. ChemMedChem, 2014, 9, 2059-2064.	1.6	14
46	Linear synthesis and conformational analysis of the pentasaccharide repeating unit of the cell wall O-antigen of Escherichia coli O13. Carbohydrate Research, 2014, 391, 9-15.	1.1	3
47	Acetylation of Gly1 and Lys2 Promotes Aggregation of Human Î³D-Crystallin. Biochemistry, 2014, 53, 7269-7282.	1.2	26
48	Synthesis of the pentasaccharide repeating unit of the O-antigen of Escherichia coli O175 using one-pot glycosylations and its conformational analysis. Tetrahedron, 2014, 70, 9262-9267.	1.0	2
49	Sequence context induced antimicrobial activity: insight into lipopolysaccharide permeabilization. Molecular BioSystems, 2014, 10, 1596-1612.	2.9	30
50	Synthesis of the tetrasaccharide repeating unit of the O-antigen of the Escherichia coli O69 strain and its conformational analysis. RSC Advances, 2014, 4, 37079-37084.	1.7	3
51	Indolicidin Targets Duplex DNA: Structural and Mechanistic Insight through a Combination of Spectroscopy and Microscopy. ChemMedChem, 2014, 9, 2052-2058.	1.6	75
52	Convergent Synthesis and Conformational Analysis of the Hexasaccharide Repeating Unit of the Oâ€Antigen of Shigella flexneri Serotype 1d. European Journal of Organic Chemistry, 2014, 2014, 4577-4584.	1.2	20
53	Interaction between Nbp35 and Cfd1 Proteins of Cytosolic Fe-S Cluster Assembly Reveals a Stable Complex Formation in Entamoeba histolytica. PLoS ONE, 2014, 9, e108971.	1.1	19
54	Human cathelicidin peptide LL37 binds telomeric G-quadruplex. Molecular BioSystems, 2013, 9, 1833.	2.9	25

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55	Novel G-quadruplex stabilizing agents: in-silico approach and dynamics. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1497-1518.	2.0	15
56	Computational Elucidation of Structural Basis for Ligand Binding withLeishmania donovaniAdenosine Kinase. BioMed Research International, 2013, 2013, 1-14.	0.9	32
57	Use of a Small Peptide Fragment as an Inhibitor of Insulin Fibrillation Process: A Study by High and Low Resolution Spectroscopy. PLoS ONE, 2013, 8, e72318.	1.1	64
58	Quantifying the Structural Requirements for Designing Newer FLT3 Inhibitors. Medicinal Chemistry, 2012, 8, 913-927.	0.7	5
59	Solution Structures, Dynamics, and Ice Growth Inhibitory Activity of Peptide Fragments Derived from an Antarctic Yeast Protein. PLoS ONE, 2012, 7, e49788.	1.1	21