

Prem P Chapagain

List of Publications by Year in descending order

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Version: 2024-02-01

90
papers

1,780
citations

257101

24
h-index

344852

36
g-index

106
all docs

106
docs citations

106
times ranked

2563
citing authors

#	ARTICLE	IF	CITATIONS
1	Intricate Functions of Matrix Metalloproteinases in Physiological and Pathological Conditions. <i>Journal of Cellular Physiology</i> , 2016, 231, 2599-2621.	2.0	133
2	The importance of culling in Johne's disease control. <i>Journal of Theoretical Biology</i> , 2008, 254, 135-146.	0.8	73
3	The Integrin Binding Peptide, ATN-161, as a Novel Therapy for SARS-CoV-2 Infection. <i>JACC Basic To Translational Science</i> , 2021, 6, 1-8.	1.9	73
4	Mutation-induced changes in the receptor-binding interface of the SARS-CoV-2 Delta variant B.1.617.2 and implications for immune evasion. <i>Biochemical and Biophysical Research Communications</i> , 2021, 574, 14-19.	1.0	70
5	Simulation modeling to evaluate the persistence of <i>Mycobacterium avium</i> subsp. <i>paratuberculosis</i> (MAP) on commercial dairy farms in the United States. <i>Preventive Veterinary Medicine</i> , 2008, 83, 360-380.	0.7	58
6	Indispensable Role of Ion Channels and Transporters in the Auditory System. <i>Journal of Cellular Physiology</i> , 2017, 232, 743-758.	2.0	55
7	Potential RNA-dependent RNA polymerase inhibitors as prospective therapeutics against SARS-CoV-2. <i>Journal of Medical Microbiology</i> , 2020, 69, 864-873.	0.7	49
8	Zika Virus: An Emerging Global Health Threat. <i>Frontiers in Cellular and Infection Microbiology</i> , 2017, 7, 486.	1.8	47
9	The Ebola virus protein VP40 hexamer enhances the clustering of PI(4,5)P ₂ lipids in the plasma membrane. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28409-28417.	1.3	44
10	Structures of the kinetically trapped i-motif DNA intermediates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26691-26702.	1.3	43
11	Molecular Dynamics Investigations of the $\hat{1}\pm$ -Helix to $\hat{1}^2$ -Barrel Conformational Transformation in the RfaH Transcription Factor. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5101-5108.	1.2	40
12	Potential Autoimmunity Resulting from Molecular Mimicry between SARS-CoV-2 Spike and Human Proteins. <i>Viruses</i> , 2022, 14, 1415.	1.5	39
13	A cationic, C-terminal patch and structural rearrangements in Ebola virus matrix VP40 protein control its interactions with phosphatidylserine. <i>Journal of Biological Chemistry</i> , 2018, 293, 3335-3349.	1.6	38
14	A dominant variant in the PDE1C gene is associated with nonsyndromic hearing loss. <i>Human Genetics</i> , 2018, 137, 437-446.	1.8	36
15	Self-organization in protein folding and the hydrophobic interaction. <i>Journal of Chemical Physics</i> , 2005, 123, 054901.	1.2	35
16	Fluorescent protein barrel fluctuations and oxygen diffusion pathways in mCherry. <i>Journal of Chemical Physics</i> , 2011, 135, 235101.	1.2	35
17	DNA supercoiling, a critical signal regulating the basal expression of the lac operon in <i>Escherichia coli</i> . <i>Scientific Reports</i> , 2016, 6, 19243.	1.6	35
18	Membrane association and localization dynamics of the Ebola virus matrix protein VP40. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2012-2020.	1.4	33

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19	Exploring Structural and Optical Properties of Fluorescent Proteins by Squeezing: Modeling High-Pressure Effects on the mStrawberry and mCherry Red Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12426-12440.	1.2	32
20	The effect of heterogeneous infectious period and contagiousness on the dynamics of <i>Salmonella</i> transmission in dairy cattle. <i>Epidemiology and Infection</i> , 2008, 136, 1496-1510.	1.0	31
21	A mathematical model of the dynamics of <i>Salmonella</i> Cerro infection in a US dairy herd. <i>Epidemiology and Infection</i> , 2008, 136, 263-272.	1.0	31
22	Exploring the Diffusion of Molecular Oxygen in the Red Fluorescent Protein mCherry Using Explicit Oxygen Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2247-2253.	1.2	31
23	Detection of lipid-induced structural changes of the Marburg virus matrix protein VP40 using hydrogen/deuterium exchange-mass spectrometry. <i>Journal of Biological Chemistry</i> , 2017, 292, 6108-6122.	1.6	30
24	Structural and Dynamical Differences in the Spike Protein RBD in the SARS-CoV-2 Variants B.1.1.7 and B.1.351. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7101-7107.	1.2	30
25	The Role of the Interdomain Interactions on RfaH Dynamics and Conformational Transformation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12750-12759.	1.2	28
26	Molecular mechanisms of pore formation and membrane disruption by the antimicrobial lantibiotic peptide Mutacin 1140. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12530-12539.	1.3	27
27	Hydrogen Bond Flexibility Correlates with Stokes Shift in mPlum Variants. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2940-2948.	1.2	26
28	Microfluidics-based selection of red-fluorescent proteins with decreased rates of photobleaching. <i>Integrative Biology (United Kingdom)</i> , 2015, 7, 263-273.	0.6	25
29	Significance of the RBD mutations in the SARS-CoV-2 omicron: from spike opening to antibody escape and cell attachment. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9123-9129.	1.3	24
30	Interdomain salt-bridges in the Ebola virus protein VP40 and their role in domain association and plasma membrane localization. <i>Protein Science</i> , 2016, 25, 1648-1658.	3.1	21
31	Discovery of novel bacterial topoisomerase I inhibitors by use of in silico docking and in vitro assays. <i>Scientific Reports</i> , 2018, 8, 1437.	1.6	21
32	Identification of HMGA2 inhibitors by AlphaScreen-based ultra-high-throughput screening assays. <i>Scientific Reports</i> , 2020, 10, 18850.	1.6	20
33	Molecular Structure and Regulation of P2X Receptors With a Special Emphasis on the Role of P2X ₂ in the Auditory System. <i>Journal of Cellular Physiology</i> , 2016, 231, 1656-1670.	2.0	19
34	ELMOD3, a novel causative gene, associated with human autosomal dominant nonsyndromic and progressive hearing loss. <i>Human Genetics</i> , 2018, 137, 329-342.	1.8	19
35	Graphene-VP40 interactions and potential disruption of the Ebola virus matrix filaments. <i>Biochemical and Biophysical Research Communications</i> , 2017, 493, 176-181.	1.0	18
36	Excluded volume entropic effects on protein unfolding times and intermediary stability. <i>Journal of Chemical Physics</i> , 2004, 120, 2475-2481.	1.2	16

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37	Removal of kinetic traps and enhanced protein folding by strategic substitution of amino acids in a model α -helical hairpin peptide. <i>Biopolymers</i> , 2006, 81, 167-178.	1.2	16
38	Plasma membrane association facilitates conformational changes in the Marburg virus protein VP40 dimer. <i>RSC Advances</i> , 2017, 7, 22741-22748.	1.7	15
39	Kinetics of peptide secondary structure conversion during amyloid β -protein fibrillogenesis. <i>Journal of Theoretical Biology</i> , 2012, 301, 95-102.	0.8	14
40	Characterization of molecular interactions between <i>Escherichia coli</i> RNA polymerase and topoisomerase I by molecular simulations. <i>FEBS Letters</i> , 2016, 590, 2844-2851.	1.3	14
41	Fluorescence from Multiple Chromophore Hydrogen-Bonding States in the Far-Red Protein TagRFP675. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3046-3051.	2.1	14
42	Genetic basis of hearing loss in Spanish, Hispanic and Latino populations. <i>Gene</i> , 2018, 647, 297-305.	1.0	14
43	Investigating molecular interactions between oxidized neuroglobin and cytochrome c. <i>Scientific Reports</i> , 2018, 8, 10557.	1.6	14
44	Sampling of states for estimating the folding funnel entropy and energy landscape of a model α -helical hairpin peptide. <i>Journal of Chemical Physics</i> , 2007, 127, 075103.	1.2	13
45	Membrane pore formation and ion selectivity of the Ebola virus delta peptide. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5578-5585.	1.3	13
46	Lipid-specific oligomerization of the Marburg virus matrix protein VP40 is regulated by two distinct interfaces for virion assembly. <i>Journal of Biological Chemistry</i> , 2021, 296, 100796.	1.6	13
47	Differentiating Parallel and Antiparallel DNA Duplexes in the Gas Phase Using Trapped Ion Mobility Spectrometry. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6855-6861.	1.2	11
48	In-silico identification of the vaccine candidate epitopes against the Lassa virus hemorrhagic fever. <i>Scientific Reports</i> , 2020, 10, 7667.	1.6	11
49	Cysteine Mutations in the Ebolavirus Matrix Protein VP40 Promote Phosphatidylserine Binding by Increasing the Flexibility of a Lipid-Binding Loop. <i>Viruses</i> , 2021, 13, 1375.	1.5	11
50	Ca^{2+} and Mg^{2+} modulate conformational dynamics and stability of downstream regulatory element antagonist modulator. <i>Protein Science</i> , 2015, 24, 741-751.	3.1	10
51	Cooperative structural transitions in amyloid-like aggregation. <i>Journal of Chemical Physics</i> , 2017, 146, 135103.	1.2	10
52	In Silico Investigations of Calcium Phosphate Mineralization in Extracellular Vesicles. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3782-3789.	1.2	9
53	Lattice model simulation of interchain protein interactions and the folding dynamics and dimerization of the GCN4 Leucine zipper. <i>Journal of Chemical Physics</i> , 2008, 128, 045106.	1.2	8
54	Domain rearrangement and denaturation in Ebola virus protein VP40. <i>AIP Advances</i> , 2018, 8, 125129.	0.6	8

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55	A cylindrical assembly model and dynamics of the Ebola virus VP40 structural matrix. <i>Scientific Reports</i> , 2018, 8, 9776.	1.6	8
56	A Conserved Tryptophan in the Ebola Virus Matrix Protein C-Terminal Domain Is Required for Efficient Virus-Like Particle Formation. <i>Pathogens</i> , 2020, 9, 402.	1.2	8
57	Finite size scaling of structural transitions in a simulated protein with secondary and tertiary structure. <i>Journal of Chemical Physics</i> , 2003, 119, 1174-1180.	1.2	7
58	The trigger sequence in the GCN4 leucine zipper: α -helical propensity and multistate dynamics of folding and dimerization. <i>Journal of Chemical Physics</i> , 2008, 129, 175103.	1.2	7
59	Structural propensities and entropy effects in peptide helix-coil transitions. <i>Physical Review E</i> , 2012, 86, 031915.	0.8	7
60	Direct observation of a 91 bp LacI-mediated, negatively supercoiled \langle scp \rangle DNA \rangle loop by atomic force microscope. <i>FEBS Letters</i> , 2016, 590, 613-618.	1.3	7
61	Amino acid 118 in the deafness causing (DFNA20/26) ACTG1 gene is a mutational hot spot. <i>Gene Reports</i> , 2018, 11, 264-269.	0.4	7
62	Conformational Flexibility of the Protein-Protein Interfaces of the Ebola Virus VP40 Structural Matrix Filament. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9045-9053.	1.2	7
63	Covalent Complex of DNA and Bacterial Topoisomerase: Implications in Antibacterial Drug Development. <i>ChemMedChem</i> , 2020, 15, 623-631.	1.6	7
64	Characterization of ATPase Activity of P2RX2 Cation Channel. <i>Frontiers in Physiology</i> , 2016, 7, 186.	1.3	6
65	Role of K-Loop Cysteine Residues in the Marburg Virus Protein VP24-Human Keap1 Complex. <i>ACS Omega</i> , 2018, 3, 18639-18645.	1.6	6
66	Mutation of Hydrophobic Residues in the C-Terminal Domain of the Marburg Virus Matrix Protein VP40 Disrupts Trafficking to the Plasma Membrane. <i>Viruses</i> , 2020, 12, 482.	1.5	6
67	AT-hook peptides bind the major and minor groove of AT-rich DNA duplexes. <i>Nucleic Acids Research</i> , 2022, 50, 2431-2439.	6.5	6
68	Immunomodulatory LncRNA on antisense strand of ICAM-1 augments SARS-CoV-2 infection-associated airway mucoinflammatory phenotype. <i>IScience</i> , 2022, 25, 104685.	1.9	6
69	Stabilization of Native and Non-native Structures by Salt Bridges in a Lattice Model of the GCN4 Leucine Dimer. <i>Journal of Physical Chemistry B</i> , 2010, 114, 796-803.	1.2	5
70	Structural insights into the repair mechanism of AGT for methyl-induced DNA damage. <i>Biological Chemistry</i> , 2021, 402, 1203-1211.	1.2	5
71	Ebola virus protein \langle scp \rangle VP40 \rangle binding to Sec24c for transport to the plasma membrane. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 340-350.	1.5	5
72	Lipid II Binding and Transmembrane Properties of Various Antimicrobial Lanthipeptides. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 516-525.	2.3	5

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73	Exploring the Conformational and Binding Dynamics of HMG A2-DNA Complexes Using Trapped Ion Mobility Spectrometry-Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 1103-1112.	1.2	4
74	Pairwise amino acid secondary structural propensities. <i>Physical Review E</i> , 2015, 91, 042709.	0.8	3
75	Single-stranded DNA structural diversity: TAGGGT from monomers to dimers to tetramer formation. <i>Rapid Communications in Mass Spectrometry</i> , 2019, 33, 60-65.	0.7	3
76	Incorporation of 5 TM ,8-cyclo-2 TM deoxyadenosines by DNA repair polymerases via base excision repair. <i>DNA Repair</i> , 2022, 109, 103258.	1.3	3
77	Detecting Individual Proteins and Their Surface Charge Variations in Solution by the Potentiometric Nanoimpact Method. <i>ACS Sensors</i> , 2022, 7, 555-563.	4.0	3
78	Self-Organizing Dynamics in Protein Folding. <i>Progress in Molecular Biology and Translational Science</i> , 2008, 84, 1-37.	0.9	2
79	Free-energy landscapes and thermodynamic parameters of complex molecules from nonequilibrium simulation trajectories. <i>Physical Review E</i> , 2011, 83, 061905.	0.8	2
80	Lattice model simulations of the effects of the position of a peptide trigger segment on helix folding and dimerization. <i>Journal of Chemical Physics</i> , 2012, 137, 105103.	1.2	1
81	Computational Simulations of Protein Folding to Engineer Amino Acid Sequences to Encourage Desired Supersecondary Structure Formation. <i>Methods in Molecular Biology</i> , 2012, 932, 191-204.	0.4	1
82	Inhibition of Aminoglycoside 6 ² -N-acetyltransferase Type Ib (AAC(6 ²)-Ib): Structure-Activity Relationship of Substituted Pyrrolidine Pentamine Derivatives as Inhibitors. <i>Biomedicines</i> , 2021, 9, 1218.	1.4	1
83	Hydrogen Bond Flexibility and Water Dynamics in the Far Red Fluorescent Protein TagRFP675. <i>Biophysical Journal</i> , 2015, 108, 469a.	0.2	0
84	Publisher's Note: Pairwise amino acid secondary structural propensities [Phys. Rev. E91, 042709 (2015)]. <i>Physical Review E</i> , 2015, 91, .	0.8	0
85	Covalent Complex Model of DNA Topoisomerase and DNA for Molecular Dynamics Simulation. <i>Biophysical Journal</i> , 2018, 114, 340a.	0.2	0
86	Molecular Dynamics Simulations of Conformational Conversions in Transformer Proteins. <i>Methods in Molecular Biology</i> , 2019, 1958, 297-311.	0.4	0
87	EF-hands in Neuronal Calcium Sensor Downstream Regulatory Element Antagonist Modulator Demonstrate Submillimolar Affinity for Li ⁺ : A New Prospect for Li ⁺ Therapy. <i>ACS Chemical Neuroscience</i> , 2020, 11, 2543-2548.	1.7	0
88	Effects of G198R Mutation in the Ebola VP40 Matrix Protein: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2021, 120, 303a.	0.2	0
89	Alternating access switching in molecular dynamics simulations of PfMATE transporter. <i>Biophysical Journal</i> , 2022, 121, 250a-251a.	0.2	0
90	Effects of sidechain isomerism on polymer-based non-covalent protein delivery. <i>Chemical Communications</i> , 0, , .	2.2	0