Parimal Kar

List of Publications by Year
in descending order

51 papers	1,210 citations	331538 21 h-index	414303 32 g-index
58 all docs	58 docs citations	58 times ranked	1118 citing authors

#	Article	IF	Citations
1	Conformational preferences of triantennary and tetraantennary hybrid N-glycans in aqueous solution: Insights from 20 Î¼s long atomistic molecular dynamic simulations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3305-3320.	2.0	8
2	Plant-derived active compounds as a potential nucleocapsid protein inhibitor of SARS-CoV-2: anin-silicostudy. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4770-4785.	2.0	6
3	A comparative study of structural and conformational properties of WNK kinase isoforms bound to an inhibitor: insights from molecular dynamic simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1400-1415.	2.0	19
4	Investigating the mechanism of recognition and structural dynamics of nucleoprotein-RNA complex from Peste des petits ruminants virus via Gaussian accelerated molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2302-2315.	2.0	22
5	Mining of Ebola virus genome for the construction of multi-epitope vaccine to combat its infection. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4815-4831.	2.0	9
6	Finding potent inhibitors against SARS-CoV-2 main protease through virtual screening, ADMET, and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6556-6568.	2.0	20
7	Finding potential inhibitors against RNA-dependent RNA polymerase (RdRp) of bovine ephemeral fever virus (BEFV): an in-silico study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10403-10421.	2.0	3
8	Decoding the Hostâ€“Parasite Protein Interactions Involved in Cerebral Malaria Through Glares of Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2022, 126, 387-402.	1.2	8
9	Discovery of potential competitive inhibitors against With-No-Lysine kinase 1 for treating hypertension by virtual screening, inverse pharmacophore-based lead optimization, and molecular dynamics simulations. SAR and QSAR in Environmental Research, 2022, 33, 63-87.	1.0	4
10	Unraveling the Molecular Mechanism of Recognition of Selected Next-Generation Antirheumatoid Arthritis Inhibitors by Janus Kinase 1. ACS Omega, 2022, 7, 6195-6209.	1.6	11
11	Identification of novel efflux pump inhibitors for Neisseria gonorrhoeae via multiple ligand-based pharmacophores, e-pharmacophore, molecular docking, density functional theory, and molecular dynamics approaches. Computational Biology and Chemistry, 2022, 98, 107682.	1.1	3
12	Phosphorylation-Induced Conformational Dynamics and Inhibition of Janus Kinase 1 by Suppressors of Cytokine Signaling 1. Journal of Physical Chemistry B, 2022, 126, 3224-3239.	1.2	4
13	Comparative Structural Dynamics of Isoforms of Helicobacter pylori Adhesin BabA Bound to Lewis b Hexasaccharide via Multiple Replica Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 2022, 9, 852895.	1.6	4
14	Effect of Sulfation on the Conformational Dynamics of Dermatan Sulfate Glycosaminoglycan: A Gaussian Accelerated Molecular Dynamics Study. Journal of Physical Chemistry B, 2022, 126, 3852-3866.	1.2	7
15	Structure-based design and synthesis of a novel long-chain 4â€²â€²-alkyl ether derivative of EGCG as potent EGFR inhibitor: in vitro and in silico studies. RSC Advances, 2022, 12, 17821-17836.	1.7	12
16	Role of Doxorubicin on the Loading Efficiency of ICG within Silk Fibroin Nanoparticles. ACS Biomaterials Science and Engineering, 2022, 8, 3054-3065.	2.6	1
17	A plausible contributor to multiple sclerosis; presentation of antigenic myelin protein epitopes by major histocompatibility complexes. Computers in Biology and Medicine, 2022, 148, 105856.	3.9	9
18	Plant-derived natural polyphenols as potential antiviral drugs against SARS-CoV-2 via RNAâ€dependent RNA polymerase (RdRp) inhibition: an in-silico analysis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6249-6264.	2.0	101

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19	Elucidating biophysical basis of binding of inhibitors to SARS-CoV-2 main protease by using molecular dynamics simulations and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3649-3661.	2.0	62
20	Exploring the potency of currently used drugs against HIV-1 protease of subtype D variant by using multiscale simulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 988-1003.	2.0	32
21	An in-silico study on selected organosulfur compounds as potential drugs for SARS-CoV-2 infection via binding multiple drug targets. Chemical Physics Letters, 2021, 763, 138193.	1.2	32
22	Characterizing an allosteric inhibitor-induced inactive state in with-no-lysine kinase 1 using Gaussian accelerated molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 7343-7358.	1.3	19
23	Ethyl Pyruvate as a Potential Defense Intervention against Cytokine Storm in COVID-19?. ACS Omega, 2021, 6, 7754-7760.	1.6	5
24	Elucidating specificity of an allosteric inhibitor WNK476 among Withâ€Noâ€Lysine kinase isoforms using molecular dynamic simulations. Chemical Biology and Drug Design, 2021, 98, 405-420.	1.5	13
25	Identification of Potential Inhibitors against Epsteinâ€“Barr Virus Nuclear Antigen 1 (EBNA1): An Insight from Docking and Molecular Dynamic Simulations. ACS Chemical Neuroscience, 2021, 12, 3060-3072.	1.7	28
26	Molecular Mechanism of Inhibiting WNK Binding to OSR1 by Targeting the Allosteric Pocket of the OSR1-CCT Domain with Potential Antihypertensive Inhibitors: An In Silico Study. Journal of Physical Chemistry B, 2021, 125, 9115-9129.	1.2	3
27	Identification of Food Compounds as inhibitors of SARS-CoV-2 main protease using molecular docking and molecular dynamics simulations. Chemometrics and Intelligent Laboratory Systems, 2021, 217, 104394.	1.8	13
28	Unraveling the Molecular Mechanism of Recognition of Human Interferon-Stimulated Gene Product 15 by Coronavirus Papain-Like Proteases: A Multiscale Simulation Study. Journal of Chemical Information and Modeling, 2021, , .	2.5	12
29	Investigating potency of TMC-126 against wild-type and mutant variants of HIV-1 protease: a molecular dynamics and free energy study. SAR and QSAR in Environmental Research, 2021, 32, 941-962.	1.0	6
30	Investigating specificity of the anti-hypertensive inhibitor WNK463 against With-No-Lysine kinase family isoforms via multiscale simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1306-1321.	2.0	28
31	Exploring the energetic basis of binding of currently used drugs against HIV-1 subtype CRF01_AE protease via molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-18.	2.0	26
32	Computational Investigation of Structural Dynamics of SARS-CoV-2 Methyltransferase-Stimulatory Factor Heterodimer nsp16/nsp10 Bound to the Cofactor SAM. Frontiers in Molecular Biosciences, 2020, 7, 590165.	1.6	33
33	Investigating Conformational Dynamics of Lewis Y Oligosaccharides and Elucidating Blood Group Dependency of Cholera Using Molecular Dynamics. ACS Omega, 2020, 5, 3932-3942.	1.6	33
34	Investigating Phosphorylation-Induced Conformational Changes in WNK1 Kinase by Molecular Dynamics Simulations. ACS Omega, 2019, 4, 17404-17416.	1.6	46
35	Hybrid All-Atom/Coarse-Grained Simulations of Proteins by Direct Coupling of CHARMM and PRIMO Force Fields. Journal of Chemical Theory and Computation, 2017, 13, 5753-5765.	2.3	29
36	Anti-Hemagglutinin Antibody Derived Lead Peptides for Inhibitors of Influenza Virus Binding. PLoS ONE, 2016, 11, e0159074.	1.1	25

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37	The Evolutionarily Conserved C-terminal Domains in the Mammalian Retinoblastoma Tumor Suppressor Family Serve as Dual Regulators of Protein Stability and Transcriptional Potency. Journal of Biological Chemistry, 2015, 290, 14462-14475.	1.6	10
38	Recent Advances in Transferable Coarse-Grained Modeling of Proteins. Advances in Protein Chemistry and Structural Biology, 2014, 96, 143-180.	1.0	46
39	Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helixâ€“Helix Association. Journal of Chemical Theory and Computation, 2014, 10, 3459-3472.	2.3	31
40	PRIMO-M: An Extension of the Coarse-Grained Force Field Primo to the Membrane Environment. Biophysical Journal, 2014, 106, 462a.	0.2	0
41	PRIMO: A Transferable Coarse-Grained Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 3769-3788.	2.3	87
42	Importance of Polar Solvation and Configurational Entropy for Design of Antiretroviral Drugs Targeting HIV-1 Protease. Journal of Physical Chemistry B, 2013, 117, 5793-5805.	1.2	48
43	Origin of Decrease in Potency of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Compared to HIV-1 Protease. Journal of Physical Chemistry B, 2012, 116, 2605-2614.	1.2	53
44	Mutation-Induced Loop Opening and Energetics for Binding of Tamiflu to Influenza N8 Neuraminidase. Journal of Physical Chemistry B, 2012, 116, 6137-6149.	1.2	30
45	Energetics of Mutation-Induced Changes in Potency of Lersivirine against HIV-1 Reverse Transcriptase. Journal of Physical Chemistry B, 2012, 116, 6269-6278.	1.2	26
46	Energetic basis for drug resistance of HIV-1 protease mutants against amprenavir. Journal of Computer-Aided Molecular Design, 2012, 26, 215-232.	1.3	49
47	Importance of Polar Solvation for Cross-Reactivity of Antibody and Its Variants with Steroids. Journal of Physical Chemistry B, 2011, 115, 7661-7669.	1.2	38
48	Microcanonical replica exchange molecular dynamics simulation of proteins. Physical Review E, 2009, 80, 056703.	0.8	20
49	Theoretical mimicry of biomembranes. FEBS Letters, 2009, 583, 1909-1915.	1.3	20
50	Dispersion Terms and Analysis of Size- and Charge Dependence in an Enhanced Poissonâ^'Boltzmann Approach. Journal of Physical Chemistry B, 2007, 111, 8910-8918.	1.2	29
51	Systematic study of the boundary composition in Poisson Boltzmann calculations. Journal of Computational Chemistry, 2007, 28, 2538-2544.	1.5	23