

Parimal Kar

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1653966/publications.pdf>

Version: 2024-02-01

51
papers

1,210
citations

331670

21
h-index

414414

32
g-index

58
all docs

58
docs citations

58
times ranked

1118
citing authors

#	ARTICLE	IF	CITATIONS
1	Plant-derived natural polyphenols as potential antiviral drugs against SARS-CoV-2 <i>via</i> RNA-dependent RNA polymerase (RdRp) inhibition: an <i>in-silico</i> analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 6249-6264.	3.5	101
2	PRIMO: A Transferable Coarse-Grained Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3769-3788.	5.3	87
3	Elucidating biophysical basis of binding of inhibitors to SARS-CoV-2 main protease by using molecular dynamics simulations and free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 3649-3661.	3.5	62
4	Origin of Decrease in Potency of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Compared to HIV-1 Protease. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2605-2614.	2.6	53
5	Energetic basis for drug resistance of HIV-1 protease mutants against amprenavir. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 215-232.	2.9	49
6	Importance of Polar Solvation and Configurational Entropy for Design of Antiretroviral Drugs Targeting HIV-1 Protease. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5793-5805.	2.6	48
7	Recent Advances in Transferable Coarse-Grained Modeling of Proteins. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 143-180.	2.3	46
8	Investigating Phosphorylation-Induced Conformational Changes in WNK1 Kinase by Molecular Dynamics Simulations. <i>ACS Omega</i> , 2019, 4, 17404-17416.	3.5	46
9	Importance of Polar Solvation for Cross-Reactivity of Antibody and Its Variants with Steroids. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7661-7669.	2.6	38
10	Computational Investigation of Structural Dynamics of SARS-CoV-2 Methyltransferase-Stimulatory Factor Heterodimer nsp16/nsp10 Bound to the Cofactor SAM. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 590165.	3.5	33
11	Investigating Conformational Dynamics of Lewis Y Oligosaccharides and Elucidating Blood Group Dependency of Cholera Using Molecular Dynamics. <i>ACS Omega</i> , 2020, 5, 3932-3942.	3.5	33
12	Exploring the potency of currently used drugs against HIV-1 protease of subtype D variant by using multiscale simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 988-1003.	3.5	32
13	An <i>in-silico</i> study on selected organosulfur compounds as potential drugs for SARS-CoV-2 infection via binding multiple drug targets. <i>Chemical Physics Letters</i> , 2021, 763, 138193.	2.6	32
14	Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helix-Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3459-3472.	5.3	31
15	Mutation-Induced Loop Opening and Energetics for Binding of Tamiflu to Influenza N8 Neuraminidase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6137-6149.	2.6	30
16	Dispersion Terms and Analysis of Size- and Charge Dependence in an Enhanced Poisson-Boltzmann Approach. <i>Journal of Physical Chemistry B</i> , 2007, 111, 8910-8918.	2.6	29
17	Hybrid All-Atom/Coarse-Grained Simulations of Proteins by Direct Coupling of CHARMM and PRIMO Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5753-5765.	5.3	29
18	Investigating specificity of the anti-hypertensive inhibitor WNK463 against With-No-Lysine kinase family isoforms via multiscale simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 1306-1321.	3.5	28

#	ARTICLE	IF	CITATIONS
19	Identification of Potential Inhibitors against Epstein-Barr Virus Nuclear Antigen 1 (EBNA1): An Insight from Docking and Molecular Dynamic Simulations. <i>ACS Chemical Neuroscience</i> , 2021, 12, 3060-3072.	3.5	28
20	Energetics of Mutation-Induced Changes in Potency of Lersivirine against HIV-1 Reverse Transcriptase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6269-6278.	2.6	26
21	Exploring the energetic basis of binding of currently used drugs against HIV-1 subtype CRF01_AE protease via molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-18.	3.5	26
22	Anti-Hemagglutinin Antibody Derived Lead Peptides for Inhibitors of Influenza Virus Binding. <i>PLoS ONE</i> , 2016, 11, e0159074.	2.5	25
23	Systematic study of the boundary composition in Poisson Boltzmann calculations. <i>Journal of Computational Chemistry</i> , 2007, 28, 2538-2544.	3.3	23
24	Investigating the mechanism of recognition and structural dynamics of nucleoprotein-RNA complex from Peste des petits ruminants virus via Gaussian accelerated molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2302-2315.	3.5	22
25	Microcanonical replica exchange molecular dynamics simulation of proteins. <i>Physical Review E</i> , 2009, 80, 056703.	2.1	20
26	Theoretical mimicry of biomembranes. <i>FEBS Letters</i> , 2009, 583, 1909-1915.	2.8	20
27	Finding potent inhibitors against SARS-CoV-2 main protease through virtual screening, ADMET, and molecular dynamics simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 6556-6568.	3.5	20
28	A comparative study of structural and conformational properties of WNK kinase isoforms bound to an inhibitor: insights from molecular dynamic simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 1400-1415.	3.5	19
29	Characterizing an allosteric inhibitor-induced inactive state in with-no-lysine kinase 1 using Gaussian accelerated molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7343-7358.	2.8	19
30	Elucidating specificity of an allosteric inhibitor WNK476 among With-no-lysine kinase isoforms using molecular dynamic simulations. <i>Chemical Biology and Drug Design</i> , 2021, 98, 405-420.	3.2	13
31	Identification of Food Compounds as inhibitors of SARS-CoV-2 main protease using molecular docking and molecular dynamics simulations. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 217, 104394.	3.5	13
32	Unraveling the Molecular Mechanism of Recognition of Human Interferon-Stimulated Gene Product 15 by Coronavirus Papain-Like Proteases: A Multiscale Simulation Study. <i>Journal of Chemical Information and Modeling</i> , 2021, , .	5.4	12
33	Structure-based design and synthesis of a novel long-chain 4-alkyl ether derivative of EGCC as potent EGFR inhibitor: <i>in vitro</i> and <i>in silico</i> studies. <i>RSC Advances</i> , 2022, 12, 17821-17836.	3.6	12
34	Unraveling the Molecular Mechanism of Recognition of Selected Next-Generation Antirheumatoid Arthritis Inhibitors by Janus Kinase 1. <i>ACS Omega</i> , 2022, 7, 6195-6209.	3.5	11
35	The Evolutionarily Conserved C-terminal Domains in the Mammalian Retinoblastoma Tumor Suppressor Family Serve as Dual Regulators of Protein Stability and Transcriptional Potency. <i>Journal of Biological Chemistry</i> , 2015, 290, 14462-14475.	3.4	10
36	Mining of Ebola virus genome for the construction of multi-epitope vaccine to combat its infection. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 4815-4831.	3.5	9

#	ARTICLE	IF	CITATIONS
37	A plausible contributor to multiple sclerosis; presentation of antigenic myelin protein epitopes by major histocompatibility complexes. <i>Computers in Biology and Medicine</i> , 2022, 148, 105856.	7.0	9
38	Decoding the Host-Parasite Protein Interactions Involved in Cerebral Malaria Through Glares of Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2022, 126, 387-402.	2.6	8
39	Conformational preferences of triantennary and tetraantennary hybrid N-glycans in aqueous solution: Insights from 20 μ s long atomistic molecular dynamic simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 3305-3320.	3.5	8
40	Effect of Sulfation on the Conformational Dynamics of Dermatan Sulfate Glycosaminoglycan: A Gaussian Accelerated Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3852-3866.	2.6	7
41	Investigating potency of TMC-126 against wild-type and mutant variants of HIV-1 protease: a molecular dynamics and free energy study. <i>SAR and QSAR in Environmental Research</i> , 2021, 32, 941-962.	2.2	6
42	Plant-derived active compounds as a potential nucleocapsid protein inhibitor of SARS-CoV-2: an <i>in-silico</i> study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 4770-4785.	3.5	6
43	Ethyl Pyruvate as a Potential Defense Intervention against Cytokine Storm in COVID-19?. <i>ACS Omega</i> , 2021, 6, 7754-7760.	3.5	5
44	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. <i>SAR and QSAR in Environmental Research</i> , 2022, 33, 63-87.	2.2	4
45	Phosphorylation-Induced Conformational Dynamics and Inhibition of Janus Kinase 1 by Suppressors of Cytokine Signaling 1. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3224-3239.	2.6	4
46	Comparative Structural Dynamics of Isoforms of Helicobacter pylori Adhesin BabA Bound to Lewis b Hexasaccharide via Multiple Replica Molecular Dynamics Simulations. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 852895.	3.5	4
47	Finding potential inhibitors against RNA-dependent RNA polymerase (RdRp) of bovine ephemeral fever virus (BEFV): an <i>in-silico</i> study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10403-10421.	3.5	3
48	Molecular Mechanism of Inhibiting WNK Binding to OSR1 by Targeting the Allosteric Pocket of the OSR1-CCT Domain with Potential Antihypertensive Inhibitors: An <i>In Silico</i> Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9115-9129.	2.6	3
49	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. <i>Computational Biology and Chemistry</i> , 2022, 98, 107682.	2.3	3
50	Role of Doxorubicin on the Loading Efficiency of ICG within Silk Fibroin Nanoparticles. <i>ACS Biomaterials Science and Engineering</i> , 2022, 8, 3054-3065.	5.2	1
51	PRIMO-M: An Extension of the Coarse-Grained Force Field Primo to the Membrane Environment. <i>Biophysical Journal</i> , 2014, 106, 462a.	0.5	0