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List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9260328/publications.pdf

Version: 2024-02-01

22	490	840119 11	713013 21
papers	citations	h-index	g-index

28	28	28	410
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Investigating Phosphorylation-Induced Conformational Changes in WNK1 Kinase by Molecular Dynamics Simulations. ACS Omega, 2019, 4, 17404-17416.	1.6	46
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	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
21	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
22	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