

Leili Zhang

List of Publications by Year in descending order

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12
papers

329
citations

1307594

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1199594

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14
docs citations

14
times ranked

703
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural Basis of the Potential Binding Mechanism of Remdesivir to SARS-CoV-2 RNA-Dependent RNA Polymerase. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6955-6962.	2.6	105
2	Graphene Oxide Nanosheets Retard Cellular Migration via Disruption of Actin Cytoskeleton. <i>Small</i> , 2017, 13, 1602133.	10.0	68
3	Emerging β -Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. <i>Journal of the American Chemical Society</i> , 2017, 139, 8820-8827.	13.7	43
4	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1176-1184.	2.6	29
5	Modeling and Structural Characterization of the Sweet Taste Receptor Heterodimer. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4579-4592.	3.5	18
6	Molecular Mechanism of Stabilizing the Helical Structure of Huntingtin N17 in a Micellar Environment. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4713-4721.	2.6	11
7	Parameterization of Molybdenum Disulfide Interacting with Water Using the Free Energy Perturbation Method. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7243-7252.	2.6	11
8	Dynamics-Based Peptide-MHC Binding Optimization by a Convolutional Variational Autoencoder: A Use-Case Model for CASTELO. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7962-7971.	5.3	7
9	Dioxybenzone triggers enhanced estrogenic effect via metabolic activation: in silico, in vitro and in vivo investigation. <i>Environmental Pollution</i> , 2021, 268, 115766.	7.5	6
10	Exploring the binding mechanism between human profilin (PFN1) and polyproline-10 through binding mode screening. <i>Journal of Chemical Physics</i> , 2019, 150, 015102.	3.0	4
11	CASTELO: clustered atom subtypes aided lead optimization—a combined machine learning and molecular modeling method. <i>BMC Bioinformatics</i> , 2021, 22, 338.	2.6	4
12	Possible Co-Evolution of Polyglutamine and Polyproline in Huntingtin Protein: Proline-Rich Domain as Transient Folding Chaperone. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6331-6341.	4.6	3