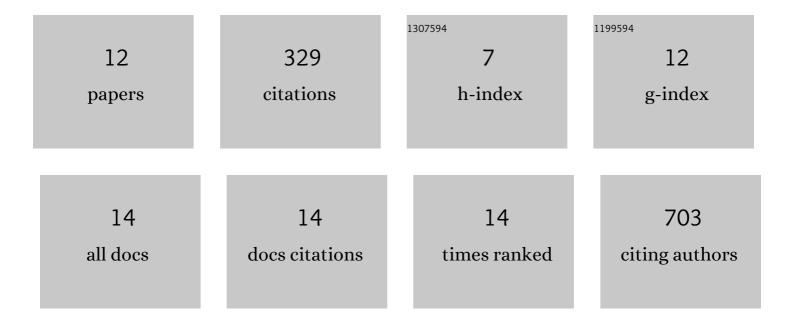
Leili Zhang

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3809344/publications.pdf

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