Sirish Kaushik Lakkaraju

List of Publications by Year
in descending order

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15	489	840776 11	996975 15
papers	citations	h-index	g-index

15	15	15	494
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insights into Glucose-6-phosphate Allosteric Activation of Î²-Glucosidase A. Journal of Chemical Information and Modeling, 2021, 61, 1931-1941.	5.4	4
2	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. Journal of Chemical Information and Modeling, 2019, 59, 3018-3035.	5.4	47
3	Exploring proteinâ€protein interactions using the siteâ€identification by ligand competitive saturation methodology. Proteins: Structure, Function and Bioinformatics, 2019, 87, 289-301.	2.6	21
4	Determination of Ionic Hydration Free Energies with Grand Canonical Monte Carlo/Molecular Dynamics Simulations in Explicit Water. Journal of Chemical Theory and Computation, 2018, 14, 5290-5302.	5.3	17
5	Estimation of relative free energies of binding using preâ€computed ensembles based on the singleâ€step free energy perturbation and the siteâ€identification by Ligand competitive saturation approaches. Journal of Computational Chemistry, 2017, 38, 1238-1251.	3.3	26
6	<scp>DIRECTâ€D</scp>: An automated method to identify and quantify conformational variationsâ€”application to Î²₂â€adrenergic <scp>GPCR</scp>. Journal of Computational Chemistry, 2016, 37, 416-425.	3.3	13
7	Characterization of Mg²⁺ Distributions around RNA in Solution. ACS Omega, 2016, 1, 680-688.	3.5	40
8	Conformational Heterogeneity of Intracellular Loop 3 of the Î¼-opioid G-protein Coupled Receptor. Journal of Physical Chemistry B, 2016, 120, 11897-11904.	2.6	8
9	Pharmacophore Modeling Using Site-Identification by Ligand Competitive Saturation (SILCS) with Multiple Probe Molecules. Journal of Chemical Information and Modeling, 2015, 55, 407-420.	5.4	62
10	Mapping Functional Group Free Energy Patterns at Protein Occluded Sites: Nuclear Receptors and G-Protein Coupled Receptors. Journal of Chemical Information and Modeling, 2015, 55, 700-708.	5.4	48
11	Acyl-2-aminobenzimidazoles: A novel class of neuroprotective agents targeting mGluR5. Bioorganic and Medicinal Chemistry, 2015, 23, 2211-2220.	3.0	21
12	Cyclopropyl-containing positive allosteric modulators of metabotropic glutamate receptor subtype 5. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2275-2279.	2.2	9
13	Sampling of Organic Solutes in Aqueous and Heterogeneous Environments Using Oscillating Excess Chemical Potentials in Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2281-2290.	5.3	69
14	Estimation of Ligand Efficacies of Metabotropic Glutamate Receptors from Conformational Forces Obtained from Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2013, 53, 1337-1349.	5.4	3
15	Inclusion of Multiple Fragment Types in the Site Identification by Ligand Competitive Saturation (SILCS) Approach. Journal of Chemical Information and Modeling, 2013, 53, 3384-3398.	5.4	101