Rahul Singh

List of Publications by Year
in descending order

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20 papers	1,203 citations	430874 18 h-index	752698 20 g-index
20 all docs	20 docs citations	20 times ranked	950 citing authors

#	Article	IF	Citations
1	Identification of selective cyclin-dependent kinase 2 inhibitor from the library of pyrrolone-fused benzosuberene compounds: an in silico exploration. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7693-7701.	3.5	40
2	In-silico evaluation of bioactive compounds from tea as potential SARS-CoV-2 nonstructural protein 16 inhibitors. Journal of Traditional and Complementary Medicine, 2022, 12, 35-43.	2.7	72
3	Identification of 11Î²-HSD1 inhibitors through enhanced sampling methods. Chemical Communications, 2022, 58, 5005-5008.	4.1	48
4	Identification of acridinedione scaffolds as potential inhibitor of DENVâ€2 C protein: An in silico strategy to combat dengue. Journal of Cellular Biochemistry, 2022, 123, 935-946.	2.6	57
5	Benchmarking the ability of novel compounds to inhibit SARS-CoV-2 main protease using steered molecular dynamics simulations. Computers in Biology and Medicine, 2022, 146, 105572.	7.0	28
6	Identification of bioactive molecules from tea plant as SARS-CoV-2 main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3449-3458.	3.5	216
7	Discovery and in silico evaluation of aminoarylbenzosuberene molecules as novel checkpoint kinase 1 inhibitor determinants. Genomics, 2021, 113, 707-715.	2.9	58
8	Evaluation of acridinedione analogs as potential SARS-CoV-2 main protease inhibitors and their comparison with repurposed anti-viral drugs. Computers in Biology and Medicine, 2021, 128, 104117.	7.0	90
9	Identification of a novel binding mechanism of Quinoline based molecules with lactate dehydrogenase of Plasmodium falciparum. Journal of Biomolecular Structure and Dynamics, 2021, 39, 348-356.	3.5	53
10	New ecdysone receptor agonists: a computational approach for rational discovery of insecticides for crop protection. Molecular Systems Design and Engineering, 2021, 6, 936-945.	3.4	7
11	Bioactive Molecules of Tea as Potential Inhibitors for RNA-Dependent RNA Polymerase of SARS-CoV-2. Frontiers in Medicine, 2021, 8, 684020.	2.6	48
12	An in-silico evaluation of different bioactive molecules of tea for their inhibition potency against non structural protein-15 of SARS-CoV-2. Food Chemistry, 2021, 346, 128933.	8.2	125
13	A computational approach for rational discovery of inhibitors for non-structural protein 1 of SARS-CoV-2. Computers in Biology and Medicine, 2021, 135, 104555.	7.0	60
14	Identification of potential plant bioactive as SARS-CoV-2 Spike protein and human ACE2 fusion inhibitors. Computers in Biology and Medicine, 2021, 136, 104631.	7.0	75
15	Explicit-solvent molecular dynamics simulations revealed conformational regain and aggregation inhibition of I113T SOD1 by Himalayan bioactive molecules. Journal of Molecular Liquids, 2021, 339, 116798.	4.9	20
16	Potential of turmeric-derived compounds against RNAâ€dependent RNA polymerase of SARSâ€CoVâ€2: An in-silico approach. Computers in Biology and Medicine, 2021, 139, 104965.	7.0	54
17	Elimination of bitter-off taste of stevioside through structure modification and computational interventions. Journal of Theoretical Biology, 2020, 486, 110094.	1.7	26
18	Natural analogues inhibiting selective cyclin-dependent kinase protein isoforms: a computational perspective. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5126-5135.	3.5	54

#	Article	IF	Citations
19	Identification of novel and selective agonists for ABA receptor PYL3. Plant Physiology and Biochemistry, 2020, 154, 387-395.	5.8	18
20	Structural based study to identify new potential inhibitors for dual specificity tyrosine-phosphorylation- regulated kinase. Computer Methods and Programs in Biomedicine, 2020, 194, 105494.	4.7	54