Rituraj Purohit

List of Publications by Year
in descending order

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106	4,015	61857	143772
papers	citations	43 h-index	57 g-index

107	107	107	3073
all docs	docs citations	times ranked	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.	2.0	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.	1.5	72
3	Improving the catalytic efficiency and dimeric stability of Cu,Zn superoxide dismutase by combining structure-guided consensus approach with site-directed mutagenesis. Biochimica Et Biophysica Acta - Bioenergetics, 2022, 1863, 148505.	0.5	7
4	Identification and comparison of plant-derived scaffolds as selective CDK5 inhibitors against standard molecules: Insights from umbrella sampling simulations. Journal of Molecular Liquids, 2022, 348, 118015.	2.3	11
5	Evaluation of plant-derived semi-synthetic molecules against BRD3-BD2 protein: a computational strategy to combat breast cancer. Molecular Systems Design and Engineering, 2022, 7, 381-391.	1.7	12
6	Identification of 11Î²-HSD1 inhibitors through enhanced sampling methods. Chemical Communications, 2022, 58, 5005-5008.	2.2	48
7	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.	1.2	57
8	Mechanistic behavior and subtle key events during DNA clamp opening and closing in T4 bacteriophage. International Journal of Biological Macromolecules, 2022, 208, 11-19.	3.6	54
9	Screening and reckoning of potential therapeutic agents against DprE1 protein of Mycobacterium tuberculosis. Journal of Molecular Liquids, 2022, 358, 119101.	2.3	14
10	A lesson for the maestro of the replication fork: Targeting the proteinâ€binding interface of proliferating cell nuclear antigen for anticancer therapy. Journal of Cellular Biochemistry, 2022, 123, 1091-1102.	1.2	50
11	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.	3.9	28
12	Kutkin, Iridoid glycosides enriched fraction of Picrorrhiza kurroa promotes insulin sensitivity and enhances glucose uptake by activating PI3K/Akt signaling in 3T3-L1 adipocytes. Phytomedicine, 2022, , 154204.	2.3	6
13	Computational targeting of allosteric site of MEK1 by quinolineâ€based molecules. Cell Biochemistry and Function, 2022, 40, 481-490.	1.4	51
14	Identification of bioactive molecules from tea plant as SARS-CoV-2 main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3449-3458.	2.0	216
15	Identification of naturally originated molecules as Î³-aminobutyric acid receptor antagonist. Journal of Biomolecular Structure and Dynamics, 2021, 39, 911-922.	2.0	33
16	Discovery and in silico evaluation of aminoarylbenzosuberene molecules as novel checkpoint kinase 1 inhibitor determinants. Genomics, 2021, 113, 707-715.	1.3	58
17	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.	3.9	90
18	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.	2.0	53

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19	New ecdysone receptor agonists: a computational approach for rational discovery of insecticides for crop protection. Molecular Systems Design and Engineering, 2021, 6, 936-945.	1.7	7
20	Computer simulation to identify selective inhibitor for human phosphodiesterase10A. Journal of Molecular Liquids, 2021, 328, 115419.	2.3	14
21	Bioactive Molecules of Tea as Potential Inhibitors for RNA-Dependent RNA Polymerase of SARS-CoV-2. Frontiers in Medicine, 2021, 8, 684020.	1.2	48
22	Himalayan bioactive molecules as potential entry inhibitors for the human immunodeficiency virus. Food Chemistry, 2021, 347, 128932.	4.2	55
23	Plant-based analogues identified as potential inhibitor against tobacco mosaic virus: A biosimulation approach. Pesticide Biochemistry and Physiology, 2021, 175, 104858.	1.6	15
24	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.	4.2	125
25	Benzosuberene-sulfone analogues synthesis from Cedrus deodara oil and their therapeutic evaluation by computational analysis to treat type 2 diabetes. Bioorganic Chemistry, 2021, 112, 104860.	2.0	9
26	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.	3.9	60
27	Identification of potential plant bioactive as SARS-CoV-2 Spike protein and human ACE2 fusion inhibitors. Computers in Biology and Medicine, 2021, 136, 104631.	3.9	75
28	Amelioration of cognitive deficit in zebrafish by an undescribed anthraquinone from Juglans regia L.: An in-silico, in-vitro and in-vivo approach. European Journal of Pharmacology, 2021, 906, 174234.	1.7	9
29	Taming the ringmaster of the genome (PCNA): Phytomolecules for anticancer therapy against a potential non-oncogenic target. Journal of Molecular Liquids, 2021, 337, 116437.	2.3	10
30	Site-directed mutagenesis (P61G) of copper, zinc superoxide dismutase enhances its kinetic properties and tolerance to inactivation by H2O2. Plant Physiology and Biochemistry, 2021, 168, 221-229.	2.8	6
31	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.	2.3	20
32	Recognition of distinct chemical molecules as inhibitors for KIT receptor mutants D816H/Y/V: A simulation approach. Journal of Molecular Liquids, 2021, 339, 116317.	2.3	8
33	Targeting the protein-protein interface pocket of Aurora-A-TPX2 complex: rational drug design and validation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3882-3891.	2.0	80
34	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.	3.9	54
35	Computational investigation on effect of mutations in PCNA resulting in structural perturbations and inhibition of mismatch repair pathway. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1963-1974.	2.0	59
36	Iodine(iii) promoted ring-rearrangement reaction of 1-arylamino-2-oxocyclopentane-1-carbonitriles to synthesize N-aryl-Î´-valerolactams. Organic and Biomolecular Chemistry, 2020, 18, 745-749.	1.5	10

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37	Elimination of bitter-off taste of stevioside through structure modification and computational interventions. Journal of Theoretical Biology, 2020, 486, 110094.	0.8	26
38	Natural analogues inhibiting selective cyclin-dependent kinase protein isoforms: a computational perspective. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5126-5135.	2.0	54
39	Structural changes induced by substitution of amino acid 129 in the coat protein of Cucumber mosaic virus. Genomics, 2020, 112, 3729-3738.	1.3	22
40	AV2 protein of tomato leaf curl Palampur virus interacts with F-box Kelch protein of tomato and enhances phenylalanine ammonia-lyase activity during virus infection. Physiological and Molecular Plant Pathology, 2020, 110, 101479.	1.3	3
41	Identification of novel and selective agonists for ABA receptor PYL3. Plant Physiology and Biochemistry, 2020, 154, 387-395.	2.8	18
42	A new insight into protein-protein interactions and the effect of conformational alterations in PCNA. International Journal of Biological Macromolecules, 2020, 148, 999-1009.	3.6	49
43	Conformational behavior of coat protein in plants and association with coat protein-mediated resistance against TMV. Brazilian Journal of Microbiology, 2020, 51, 893-908.	0.8	12
44	Hesperidin Interacts With CREB-BDNF Signaling Pathway to Suppress Pentylenetetrazole-Induced Convulsions in Zebrafish. Frontiers in Pharmacology, 2020, 11, 607797.	1.6	26
45	Structural based study to identify new potential inhibitors for dual specificity tyrosine-phosphorylation- regulated kinase. Computer Methods and Programs in Biomedicine, 2020, 194, 105494.	2.6	54
46	Phloretin and phloridzin improve insulin sensitivity and enhance glucose uptake by subverting PPARÎ³/Cdk5 interaction in differentiated adipocytes. Experimental Cell Research, 2019, 383, 111480.	1.2	43
47	Molecular mechanics and quantum chemical calculations unveil the combating effect of baicalein on human islet amyloid polypeptide aggregates. Molecular Simulation, 2019, 45, 1538-1548.	0.9	5
48	Structural Perturbations due to Mutation (H1047R) in Phosphoinositide-3-kinase (PI3KÎ±) and Its Involvement in Oncogenesis: An in Silico Insight. ACS Omega, 2019, 4, 15815-15823.	1.6	21
49	Target identification, screening and in vivo evaluation of pyrrolone-fused benzosuberene compounds against human epilepsy using Zebrafish model of pentylenetetrazol-induced seizures. Scientific Reports, 2019, 9, 7904.	1.6	58
50	Molecular dynamic (MD) studies on Gln233Arg (rs1137101) polymorphism of leptin receptor gene and associated variations in the anthropometric and metabolic profiles of Saudi women. PLoS ONE, 2019, 14, e0211381.	1.1	16
51	Gain of native conformation of Aurora A S155R mutant by small molecules. Journal of Cellular Biochemistry, 2019, 120, 11104-11114.	1.2	36
52	Styryl-cinnamate hybrid inhibits glioma by alleviating translation, bioenergetics and other key cellular responses leading to apoptosis. Experimental Cell Research, 2019, 375, 11-21.	1.2	0
53	Evaluation of Antiplasmodial Potential of C2 and C8 Modified Quinolines: in vitro and in silico Study. Medicinal Chemistry, 2019, 15, 790-800.	0.7	9
54	Screening of Potential Inhibitor against Coat Protein of Apple Chlorotic Leaf Spot Virus. Cell Biochemistry and Biophysics, 2018, 76, 273-278.	0.9	11

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55	AV2 protein of tomato leaf curl Palampur virus promotes systemic necrosis in Nicotiana benthamiana and interacts with host Catalase2. Scientific Reports, 2018, 8, 1273.	1.6	37
56	Mutational Analysis on Membrane Associated Transporter Protein (MATP) and Their Structural Consequences in Oculocutaeous Albinism Type 4 (OCA4)â€"A Molecular Dynamics Approach. Journal of Cellular Biochemistry, 2016, 117, 2608-2619.	1.2	46
57	Biophysical Aspect of Huntingtin Protein During polyQ: An In Silico Insight. Cell Biochemistry and Biophysics, 2016, 74, 129-139.	0.9	17
58	Impact of point mutation P29S in RAC1 on tumorigenesis. Tumor Biology, 2016, 37, 15293-15304.	0.8	88
59	Biophysical aspect of phosphatidylinositol 3-kinase and role of oncogenic mutants (E542K &) Tj ETQq1 1 0.784314 rgBT /Overlock	2.0	30
60	Computational investigation of molecular mechanism and neuropathological implications in Huntington disease. Molecular and Cellular Biochemistry, 2015, 409, 1-11.	1.4	17
61	Mutational analysis of FUS gene and its structural and functional role in amyotrophic lateral sclerosis 6. Journal of Biomolecular Structure and Dynamics, 2015, 33, 834-844.	2.0	46
62	Single Nucleotide Polymorphisms in MicroRNA Binding Sites: Implications in Colorectal Cancer. Scientific World Journal, The, 2014, 2014, 1-10.	0.8	24
63	Use of Long Term Molecular Dynamics Simulation in Predicting Cancer Associated SNPs. PLoS Computational Biology, 2014, 10, e1003318.	1.5	103
64	Mutational Analysis of Oculocutaneous Albinism: A Compact Review. BioMed Research International, 2014, 2014, 1-10.	0.9	112
65	Computational SNP Analysis: Current Approaches and Future Prospects. Cell Biochemistry and Biophysics, 2014, 68, 233-239.	0.9	42
66	Computational Screening of Disease-Associated Mutations in OCA2 Gene. Cell Biochemistry and Biophysics, 2014, 68, 97-109.	0.9	53
67	Role of ELA region in auto-activation of mutant KIT receptor: a molecular dynamics simulation insight. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1033-1046.	2.0	99
68	Relationship between a point mutation S97C in CK1Î´ protein and its affect on ATP-binding affinity. Journal of Biomolecular Structure and Dynamics, 2014, 32, 394-405.	2.0	21
69	In Silico Analysis of miRNA-Mediated Gene Regulation in OCA and OA Genes. Cell Biochemistry and Biophysics, 2014, 70, 1923-1932.	0.9	23
70	Mutations in microRNA Binding Sites of CEP Genes Involved in Cancer. Cell Biochemistry and Biophysics, 2014, 70, 1933-1942.	0.9	30
71	Role of Centrosome in Regulating Immune Response. Current Drug Targets, 2014, 15, 558-563.	1.0	2
72	Evolution driven structural changes in CENP-E motor domain. Interdisciplinary Sciences, Computational Life Sciences, 2013, 5, 102-111.	2.2	5

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73	Evidence of Colorectal Cancer-Associated Mutation in MCAK: A Computational Report. Cell Biochemistry and Biophysics, 2013, 67, 837-851.	0.9	37
74	Computational Investigation of Cancer-Associated Molecular Mechanism in Aurora A (S155R) Mutation. Cell Biochemistry and Biophysics, 2013, 66, 787-796.	0.9	19
75	CEP proteins: the knights of centrosome dynasty. Protoplasma, 2013, 250, 965-983.	1.0	75
76	Inter-individual variation in nucleotide excision repair pathway is modulated by non-synonymous polymorphisms in ERCC4 and MBD4 genes. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2013, 751-752, 49-54.	0.4	10
77	Identifying novel oncogenes: A machine learning approach. Interdisciplinary Sciences, Computational Life Sciences, 2013, 5, 241-246.	2.2	15
78	In-silico screening of cancer associated mutation on PLK1 protein and its structural consequences. Journal of Molecular Modeling, 2013, 19, 5587-5599.	0.8	31
79	Roadmap to determine the point mutations involved in cardiomyopathy disorder: A Bayesian approach. Gene, 2013, 519, 34-40.	1.0	16
80	Computational evaluation of small molecule inhibitors of RGS4 to regulate the dopaminergic control of striatal LTD. Egyptian Journal of Medical Human Genetics, 2013, 14, 135-142.	0.5	1
81	Insight into Nek2A activity regulation and its pharmacological prospects. Egyptian Journal of Medical Human Genetics, 2013, 14, 213-219.	0.5	3
82	Investigation of Binding Phenomenon of NSP3 and p130Cas Mutants and Their Effect on Cell Signalling. Cell Biochemistry and Biophysics, 2013, 67, 623-633.	0.9	25
83	Sequencing Closterium moniliferum: Future prospects in nuclear waste disposal. Egyptian Journal of Medical Human Genetics, 2013, 14, 113-115.	0.5	2
84	Mutational analysis of TYR gene and its structural consequences in OCA1A. Gene, 2013, 513, 184-195.	1.0	47
85	In SilicoScreening and Molecular Dynamics Simulation of Disease-Associated nsSNP in TYRP1 Gene and Its Structural Consequences in OCA3. BioMed Research International, 2013, 2013, 1-13.	0.9	69
86	In-silico analysis of Betaine Aldehyde Dehydrogenase2 ofOryza sativaand significant mutations responsible for fragrance. Journal of Plant Interactions, 2013, 8, 321-333.	1.0	9
87	Cancer Associated E17K Mutation Causes Rapid Conformational Drift in AKT1 Pleckstrin Homology (PH) Domain. PLoS ONE, 2013, 8, e64364.	1.1	49
88	Evolutionary Reconstruction and Population Genetics Analysis of Aurora Kinases. PLoS ONE, 2013, 8, e75763.	1.1	3
89	AKT Kinase Pathway: A Leading Target in Cancer Research. Scientific World Journal, The, 2013, 2013, 1-6.	0.8	62
90	Molecular Dynamic Simulation Reveals Damaging Impact of RAC1 F28L Mutation in the Switch I Region. PLoS ONE, 2013, 8, e77453.	1.1	40

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91	In silico prediction of a diseaseâ€associated STIL mutant and its affect on the recruitment of centromere protein J (CENPJ). FEBS Open Bio, 2012, 2, 285-293.	1.0	53
92	Computational investigation of pathogenic nsSNPs in CEP63 protein. Gene, 2012, 503, 75-82.	1.0	47
93	Computational centrosomics: An approach to understand the dynamic behaviour of centrosome. Gene, 2012, 511, 125-126.	1.0	16
94	Computational screening and molecular dynamics simulation of disease associated nsSNPs in CENP-E. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2012, 738-739, 28-37.	0.4	62
95	Structure based energy calculation to determine the regulation of G protein signalling by RGS and RGS-G protein interaction specificity. Interdisciplinary Sciences, Computational Life Sciences, 2012, 4, 173-182.	2.2	4
96	In silico investigation of molecular mechanism of laminopathy caused by a point mutation (R482W) in lamin A/C protein. Amino Acids, 2012, 43, 603-615.	1.2	164
97	Relationship between mutation of serine residue at 315th position in M. tuberculosis catalase-peroxidase enzyme and Isoniazid susceptibility: An in silico analysis. Journal of Molecular Modeling, 2011, 17, 869-877.	0.8	66
98	Studies on Adaptability of Binding Residues Flap Region of TMC-114 Resistance HIV-1 Protease Mutants. Journal of Biomolecular Structure and Dynamics, 2011, 29, 137-152.	2.0	61
99	Effect of Flap Mutation I54L/M in Inhibition of Human Immunodeficiency Virus Type 1 Protease: Relationship to Drug Resistance. Journal of Computer Science and Systems Biology, 2010, 03, .	0.0	2
100	Structural basis for the resilience of Darunavir (TMC114) resistance major flap mutations of HIV-1 protease. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 320-328.	2.2	48
101	A novel computational and structural analysis of nsSNPs in CFTR gene. Genomic Medicine, 2008, 2, 23-32.	0.6	48
102	Analysis of binding residues between scorpion neurotoxins and D2 dopamine receptor: A computational docking study. Computers in Biology and Medicine, 2008, 38, 1056-1067.	3.9	6
103	Identification and structural comparison of deleterious mutations in nsSNPs of ABL1 gene in chronic myeloid leukemia: A bio-informatics study. Journal of Biomedical Informatics, 2008, 41, 607-612.	2.5	17
104	Studies on flexibility and binding affinity of Asp25 of HIV-1 protease mutants. International Journal of Biological Macromolecules, 2008, 42, 386-391.	3.6	49
105	Effect of deleterious nsSNP on the HER2 receptor based on stability and binding affinity with herceptin: A computational approach. Comptes Rendus - Biologies, 2008, 331, 409-417.	0.1	33
106	Investigations on the interactions of scorpion neurotoxins with the predicted structure of D1 dopamine receptor by proteinâ€“protein docking method. A bioinformatics approach. Comptes Rendus - Biologies, 2008, 331, 489-499.	0.1	3