Venkata S K Mattaparthi

List of Publications by Year
in descending order

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47	649	932766 10	610482 24
papers	citations	h-index	g-index

49	49	49	1098
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Chemical system biology approach to identify multi-targeting FDA inhibitors for treating COVID-19 and associated health complications. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9543-9567.	2.0	19
2	Computational investigation on the effect of Oleuropein aglycone on the Î±-synuclein aggregation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1259-1270.	2.0	14
3	Effect of CTerm of human albumin on the aggregation propensity of AÎ²1-42 peptide: a potential of mean force study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1334-1342.	2.0	1
4	Computational Investigation on the MDM2-Idasanutlin Interaction using the Potential of Mean Force method. Current Chemical Biology, 2021, 15, .	0.2	0
5	Bis- and mixed-ligand copper(II) complexes of nalidixic acid the antibacterial drug: Mode of nalidixate coordination determines DNA binding and cleavage and cytotoxicity. Inorganica Chimica Acta, 2020, 504, 119450.	1.2	15
6	Computational Investigation on the p53â€“MDM2 Interaction Using the Potential of Mean Force Study. ACS Omega, 2020, 5, 8449-8462.	1.6	8
7	Effect of Ionic Strength on the Aggregation Propensity of AÎ²1-42 Peptide: An In-silico Study. Current Chemical Biology, 2020, 14, 216-226.	0.2	0
8	Structure-Based Virtual Screening of High-Affinity ATP-Competitive Inhibitors Against Human Lemur Tyrosine Kinase-3 (LMTK3) Domain: A Novel Therapeutic Target for Breast Cancer. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 527-541.	2.2	10
9	1Î±, 25-dihydroxy Vitamin D3 containing fractions of Catharanthus roseus leaf aqueous extract inhibit preadipocyte differentiation and induce lipolysis in 3T3-L1 cells. BMC Complementary and Alternative Medicine, 2019, 19, 338.	3.7	12
10	Investigation of the probable homo-dimer model of the Xeroderma pigmentosum complementation group A (XPA) protein to represent the DNA-binding core. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3322-3336.	2.0	4
11	Consequences of Heterogeneous Crowding on an Enzymatic Reaction: A Residence Time Monte Carlo Approach. ACS Omega, 2019, 4, 727-736.	1.6	8
12	Computational Study on the Role of Î³-Synuclein in Inhibiting the Î±-Synuclein Aggregation. Central Nervous System Agents in Medicinal Chemistry, 2019, 19, 24-30.	0.5	4
13	In silico investigation on the inhibition of AÎ²₄₂ aggregation by AÎ²₄₀ peptide by potential of mean force study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 741-752.	2.0	10
14	Computational investigation on the effects of H50Q and G51D mutations on the Î±-Synuclein aggregation propensity. Journal of Biomolecular Structure and Dynamics, 2018, 36, 2224-2236.	2.0	6
15	Structural dynamics and interactions of Xeroderma pigmentosum complementation group A (XPA_{98â€“210}) with damaged DNA. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3341-3353.	2.0	3
16	Unveiling the Transient Protein-Protein Interactions that Regulate the Activity of Human Lemur Tyrosine Kinase-3 (LMTK3) Domain by Cyclin Dependent Kinase 5 (CDK5) in Breast Cancer: An in silico Study. Current Proteomics, 2018, 15, .	0.1	5
17	Characterizing the Binding Interactions between DNA-Binding Proteins, XPA and XPE: A Molecular Dynamics Approach. ACS Omega, 2018, 3, 15442-15454.	1.6	4
18	A Comparative Study to Elucidate the Inhibitory Mechanism of a 6-Mer Fragment of Amyloid-Beta 42 Peptide as a Potential Therapeutic in Alzheimerâ€™s Disease:Insights from Molecular Dynamics Simulations. Current Science, 2018, 114, 1207.	0.4	3

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19	Effect of C-terminal truncations on the aggregation propensity of A53E, a familial mutant of Î±-Synuclein: An Insilico Study. International Journal for Computational Biology, 2018, 7, 16.	0.1	0
20	Dimerization of C-terminal Truncations of Î±-synuclein and its Effect on the Aggregation Propensity: A Potential of Mean Force Study. Current Chemical Biology, 2018, 12, 191-200.	0.2	1
21	Salient Structural Features of Human Lemur Tyrosine Kinase 3 (LMTK3) Domain from Molecular Dynamics Simulation Study. Current Biotechnology, 2018, 7, 309-316.	0.2	0
22	Anin silicoapproach to understand the structureâ€“function properties of a serine protease (Bacifrinase) fromBacillus cereusand experimental evidence to support the interaction of Bacifrinase with fibrinogen and thrombin. Journal of Biomolecular Structure and Dynamics, 2017, 35, 622-644.	2.0	7
23	Inhibition of AÎ²_{1â€“42} peptide aggregation using short ss-oligonucleotide as polyions: an in silico approach. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1401-1406.	2.0	4
24	Potential of mean force and molecular dynamics study on the transient interactions between Î± and Î² synuclein that drive inhibition of Î±-synuclein aggregation. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3342-3353.	2.0	11
25	Comparative Study on the Binding Affinity of Methimazole and Propylthiouracil to Thyroid Peroxidase as an Anti-Thyroid Drug: An Insilico Approach. Journal of Molecular Imaging & Dynamics, 2017, 07, .	0.2	3
26	Structural Characterization of Amyloid Î²17-42 Dimer by Potential of Mean Force Analysis: Insights from Molecular Dynamics Simulations. Protein and Peptide Letters, 2017, 24, 650-660.	0.4	1
27	Computational Investigation on Tyrosine to Alanine Mutations Delaying the Early Stage of Î±-Synuclein Aggregation. Current Proteomics, 2017, 14, 31-41.	0.1	5
28	Investigation on the Molecular Interactions Stabilizing the Structure of Î±-synuclein Fibril: An In silico Study. Central Nervous System Agents in Medicinal Chemistry, 2017, 17, 209-218.	0.5	8
29	Cross-Seeding Interaction Between Amyloid Î² and Tau Protein can Enhance Aggregation. Current Biotechnology, 2017, 6, .	0.2	3
30	Effect of C-Terminal Truncations on the Aggregation Propensity of Î³- Synuclein - A Potential of Mean Force Study. Journal of Molecular Imaging & Dynamics, 2017, 07, .	0.2	1
31	Unveiling the Transient Protein-Protein Interactions that Modulate the Activity of Estrogen Receptor(ER)-Î± by Human Lemur Tyrosine Kinase-3 (LMTK3) Domain: An In Silico Study. Current Proteomics, 2017, 14, 157-164.	0.1	1
32	Computational Study of Intermolecular Interactions between α-Synuclein Fibrils and Tau Protein Propagating Tau Aggregation. Current Science, 2017, 112, 2219.	0.4	0
33	Kaempferol attenuates COX-2 expression in IL-6-induced macrophages and carrageenan-induced mouse paw edema by targeting STAT3 and NF-κB. Canadian Journal of Biotechnology, 2017, 1, 163-163.	0.3	0
34	Daboxin P, a Major Phospholipase A2 Enzyme from the Indian Daboia russelii russelii Venom Targets Factor X and Factor Xa for Its Anticoagulant Activity. PLoS ONE, 2016, 11, e0153770.	1.1	26
35	Excellent N-fixing and P-solubilizing traits in earthworm gut-isolated bacteria: A vermicompost based assessment with vegetable market waste and rice straw feed mixtures. Bioresource Technology, 2016, 222, 165-174.	4.8	92
36	Investigations on the Structural Characteristics that Seed the Aggregation of Amyloid-Î²1-42 Peptide: Insights from Molecular Dynamics Simulations. Current Proteomics, 2016, 13, 172-178.	0.1	0

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37	Structural insight into the binding interactions of modeled structure ofArabidopsis thalianaurease with urea: anin silicostudy. Journal of Biomolecular Structure and Dynamics, 2015, 33, 845-851.	2.0	6
38	Interchain hydrophobic clustering promotes rigidity in HIV-1 protease flap dynamics: new insights from Molecular Dynamics. Journal of Biomolecular Structure and Dynamics, 2014, 32, 899-915.	2.0	3
39	DNA Assisted Self-Assembly of PAMAM Dendrimers. Journal of Physical Chemistry B, 2014, 118, 11805-11815.	1.2	14
40	PAMAM Dendrimerâ€"Drug Interactions: Effect of pH on the Binding and Release Pattern. Journal of Physical Chemistry B, 2012, 116, 4370-4376.	1.2	100
41	CONFORMATIONAL DYNAMICS OF HIV-1 PROTEASE: A COMPARATIVE MOLECULAR DYNAMICS SIMULATION STUDY WITH MULTIPLE AMBER FORCE FIELDS. Journal of Bioinformatics and Computational Biology, 2012, 10, 1250018.	0.3	3
42	Structure of DNA-functionalized dendrimer nanoparticles. Soft Matter, 2012, 8, 1893-1900.	1.2	10
43	Interaction studies of E. coli uracil phosphoribosyltransferase with 5-fluorouracil for potent anti cancer activity. Medicinal Chemistry Research, 2012, 21, 1149-1155.	1.1	2
44	Lysozyme. Advances in Protein Chemistry and Structural Biology, 2011, 84, 63-111.	1.0	205
45	A novel approach to segregate and identify functional loop regions in protein structures using their Ramachandran maps. Proteins: Structure, Function and Bioinformatics, 2010, 78, 900-916.	1.5	7
46	Molecular dynamics simulation of HIV-protease with polarizable and non-polarizable force fields. Indian Journal of Physics, 2009, 83, 81-90.	0.9	7
47	Pressure Induced Conformational Dynamics of HIV-1 Protease: A Molecular Dynamics Simulation Study. , 2008, , .		1