Saraswathi Vishveshwara

List of Publications by Year
in descending order

79 papers	2,777 citations	257450 24 h-index	189892 50 g-index
80 all docs	80 docs citations	80 times ranked	2375 citing authors

#	Article	IF	Citations
1	A Network Representation of Protein Structures: Implications for Protein Stability. Biophysical Journal, 2005, 89, 4159-4170.	0.5	385
2	A study of communication pathways in methionyl- tRNA synthetase by molecular dynamics simulations and structure network analysis. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15711-15716.	7.1	222
3	Interaction Energy Based Protein Structure Networks. Biophysical Journal, 2010, 99, 3704-3715.	0.5	196
4	Intra and Inter-Molecular Communications Through Protein Structure Network. Current Protein and Peptide Science, 2009, 10, 146-160.	1.4	159
5	PROTEIN STRUCTURE: INSIGHTS FROM GRAPH THEORY. Journal of Theoretical and Computational Chemistry, 2002, 01, 187-211.	1.8	153
6	Oligomeric protein structure networks: insights into protein-protein interactions. BMC Bioinformatics, 2005, 6, 296.	2.6	92
7	Dynamics of Lysozyme Structure Network: Probing the Process of Unfolding. Biophysical Journal, 2007, 92, 2523-2535.	0.5	89
8	Geometry of prolineâ€containing alphaâ€helices in proteins. International Journal of Peptide and Protein Research, 1992, 39, 356-363.	0.1	82
9	Variations in Clique and Community Patterns in Protein Structures during Allosteric Communication: Investigation of Dynamically Equilibrated Structures of Methionyl tRNA Synthetase Complexes. Biochemistry, 2008, 47, 11398-11407.	2.5	78
10	Insights into Proteinâ€“DNA Interactions through Structure Network Analysis. PLoS Computational Biology, 2008, 4, e1000170.	3.2	71
11	Allosteric Communication in Cysteinyl tRNA Synthetase. Journal of Biological Chemistry, 2011, 286, 37721-37731.	3.4	68
12	Conformational studies on peptides with proline in the right-handed ?-helical region. Biopolymers, 1990, 30, 287-298.	2.4	66
13	Determinants of quaternary association in legume lectins. Protein Science, 2004, 13, 1735-1749.	7.6	66
14	Probing the Allosteric Mechanism in Pyrrolysyl-tRNA Synthetase Using Energy-Weighted Network Formalism. Biochemistry, 2011, 50, 6225-6236.	2.5	55
15	An automated approach to network features of protein structure ensembles. Protein Science, 2013, 22, 1399-1416.	7.6	55
16	Targeting the pregnane X receptor using microbial metabolite mimicry. EMBO Molecular Medicine, 2020, 12, e11621.	6.9	53
17	Protein Structure and Function: Looking through the Network of Side-Chain Interactions. Current Protein and Peptide Science, 2015, 17, 4-25.	1.4	51
18	Amino acid interaction preferences in proteins. Protein Science, 2010, 19, 603-616.	7.6	49

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19	Allostery and conformational free energy changes in human tryptophanylâ€tRNA synthetase from essential dynamics and structure networks. Proteins: Structure, Function and Bioinformatics, 2010, 78, 506-517.	2.6	47
20	Metabolome Based Reaction Graphs of M. tuberculosis and M. leprae: A Comparative Network Analysis. PLoS ONE, 2007, 2, e881.	2.5	38
21	Understanding Protein Structure from a Percolation Perspective. Biophysical Journal, 2009, 97, 1787-1794.	0.5	37
22	Characterization of proline-containing Î±-helix (helix F model of bacteriorhodopsin) by molecular dynamics studies. Proteins: Structure, Function and Bioinformatics, 1993, 15, 26-41.	2.6	35
23	Identification of domains and domain interface residues in multidomain proteins from graph spectral method. Proteins: Structure, Function and Bioinformatics, 2005, 59, 616-626.	2.6	28
24	Stabilizing interactions in the dimer interface of Î±-subunit inEscherichia coliRNA polymerase: A graph spectral and point mutation study. Protein Science, 2001, 10, 46-54.	7.6	25
25	Random network behaviour of protein structures. Molecular BioSystems, 2010, 6, 391-398.	2.9	25
26	Interaction Signatures Stabilizing the NAD(P)-Binding Rossmann Fold: A Structure Network Approach. PLoS ONE, 2012, 7, e51676.	2.5	25
27	Insights into the Fold Organization of TIM Barrel from Interaction Energy Based Structure Networks. PLoS Computational Biology, 2012, 8, e1002505.	3.2	24
28	Ligand dependent intra and inter subunit communication in human tryptophanyl tRNA synthetase as deduced from the dynamics of structure networks. Molecular BioSystems, 2009, 5, 1860.	2.9	22
29	Comparative analysis of thermophilic and mesophilic proteins using Protein Energy Networks. BMC Bioinformatics, 2010, 11, S49.	2.6	22
30	Dynamics of ribonuclease A and ribonuclease S: Computational and experimental studies. Protein Science, 1996, 5, 2104-2114.	7.6	21
31	A graph spectral analysis of the structural similarity network of protein chains. Proteins: Structure, Function and Bioinformatics, 2005, 61, 152-163.	2.6	21
32	Cell Dynamics of Model Proteins. Physical Review Letters, 1996, 77, 3681-3684.	7.8	19
33	Elucidation of the conformational free energy landscape in H.pylori LuxS and its implications to catalysis. BMC Structural Biology, 2010, 10, 27.	2.3	19
34	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	3.3	19
35	From Quantum Chemistry to Networks in Biology: A Graph Spectral Approach to Protein Structure Analyses. Journal of Chemical Information and Modeling, 2019, 59, 1715-1727.	5.4	19
36	Network approach for capturing ligand-induced subtle global changes in protein structures. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 429-439.	2.5	18

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37	A Histidine Aspartate Ionic Lock Gates the Iron Passage in Miniferritins from Mycobacterium smegmatis. Journal of Biological Chemistry, 2014, 289, 11042-11058.	3.4	17
38	Effects of substrate binding on the dynamics of RNase A: Molecular dynamics simulations of UpA bound and native RNase A. Biopolymers, 1997, 42, 505-520.	2.4	16
39	Correlation of the Side-Chain Hubs with the Functional Residues in DNA Binding Protein Structures. Journal of Chemical Information and Modeling, 2006, 46, 123-129.	5.4	16
40	Ab initio studies on the tri- and diphosphate fragments of adenosine triphosphate. Biophysical Chemistry, 2006, 119, 127-136.	2.8	16
41	Structure networks of E. coli glutaminyl-tRNA synthetase: Effects of ligand binding. Proteins: Structure, Function and Bioinformatics, 2007, 68, 541-550.	2.6	16
42	Insight into the early stages of thermal unfolding of peanut agglutinin by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2007, 69, 32-42.	2.6	15
43	Network properties of protein-decoy structures. Journal of Biomolecular Structure and Dynamics, 2012, 29, 1110-1126.	3.5	15
44	Validation of protein structure models using network similarity score. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1759-1776.	2.6	14
45	Mechanism of Iron-Dependent Repressor (IdeR) Activation and DNA Binding: A Molecular Dynamics and Protein Structure Network Study. PLoS Computational Biology, 2015, 11, e1004500.	3.2	13
46	Belinostat, at Its Clinically Relevant Concentrations, Inhibits Rifampicin-Induced CYP3A4 and MDR1 Gene Expression. Molecular Pharmacology, 2019, 95, 324-334.	2.3	12
47	Ranking the quality of protein structure models using sidechain based network properties. F1000Research, 2014, 3, 17.	1.6	11
48	Effect of constraints by threonine on proline containing Î±-helixâ€"A molecular dynamics approach. Biophysical Chemistry, 1993, 46, 77-89.	2.8	10
49	Amino acid interaction preferences in helical membrane proteins. Protein Engineering, Design and Selection, 2011, 24, 579-588.	2.1	10
50	Exploration of the conformational landscape in pregnane X receptor reveals a new binding pocket. Protein Science, 2016, 25, 1989-2005.	7.6	10
51	Characterization of proline-containing right-handed Î±-helix by molecular dynamics studies. Biophysical Chemistry, 1991, 40, 97-108.	2.8	9
52	Functional correlation of bacterial LuxS with their quaternary associations: interface analysis of the structure networks. BMC Structural Biology, 2009, 9, 8.	2.3	9
53	Surveying the Side-Chain Network Approach to Protein Structure and Dynamics: The SARS-CoV-2 Spike Protein as an Illustrative Case. Frontiers in Molecular Biosciences, 2020, 7, 596945.	3.5	9
54	Structure-based design of model proteins. , 1998, 31, 10-20.		8

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55	A graph spectral-based scoring scheme for network comparison. Journal of Complex Networks, 0, , cnw016.	1.8	8
56	A Search for Energy Minimized Sequences of Proteins. PLoS ONE, 2009, 4, e6684.	2.5	8
57	A Hydrogen Bonded Chain in Bactereorhodopsin by Computer Modelling Approach. Journal of Biomolecular Structure and Dynamics, 1989, 7, 187-205.	3.5	6
58	Comparison of the dynamics of bovine and human angiogenin: a molecular dynamics study. , 1999, 49, 131-144.		6
59	Identification of crucial elements for network integrity: a perturbation approach through graph spectral method. International Journal of Advances in Engineering Sciences and Applied Mathematics, 2019, 11, 91-104.	1.1	6
60	Network Re-Wiring During Allostery and Protein-Protein Interactions: A Graph Spectral Approach. Methods in Molecular Biology, 2021, 2253, 89-112.	0.9	6
61	Understanding structural variability in proteins using protein structural networks. Current Research in Structural Biology, 2022, 4, 134-145.	2.2	6
62	Modeling of Angiogenin - 3â€²-NMP Complex. Journal of Biomolecular Structure and Dynamics, 1998, 16, 715-722.	3.5	5
63	Inter-helical Interactions in Membrane Proteins: Analysis Based on the Local Backbone Geometry and the Side Chain Interactions. Journal of Biomolecular Structure and Dynamics, 2009, 26, 719-729.	3.5	5
64	Quantum clustering and network analysis of MD simulation trajectories to probe the conformational ensembles of proteinâ€“ligand interactions. Molecular BioSystems, 2011, 7, 2320.	2.9	5
65	The stability of transmembrane helices: A molecular dynamics study on the isolated helices of bacteriorhodopsin. Biopolymers, 1996, 38, 401-422.	2.4	5
66	Binding of active site directed ligands to phospholipase A2: Implications on the molecular constraints and catalytic mechanism. Journal of Chemical Sciences, 1994, 106, 1177-1189.	1.5	5
67	The stability of transmembrane helices: A molecular dynamics study on the isolated helices of bacteriorhodopsin. Biopolymers, 1998, 38, 401-422.	2.4	4
68	Stability of dimeric interface in banana lectin: Insight from molecular dynamics simulations. IUBMB Life, 2009, 61, 252-260.	3.4	4
69	A model for transmembrane helix with acis-Proline in the middle. FEBS Letters, 1995, 374, 21-24.	2.8	3
70	Impact of theoretical chemistry on chemical and biological sciences. Resonance, 2014, 19, 347-367.	0.3	3
71	Molecular mechanism of facilitated transport by carrier ionophores:a study of energetics. Journal of Biosciences, 1987, 12, 175-189.	1.1	2
72	Stability and Dynamics of Domain-Swapped Bovine-Seminal Ribonuclease. Chemistry and Biodiversity, 2004, 1, 802-818.	2.1	2

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73	Characterization of the backbone geometry of protein native state structures. Proteins: Structure, Function and Bioinformatics, 2006, 64, 992-1000.	2.6	2
74	Protein structure and folding â€“ simplicity within complexity. Journal of Biomolecular Structure and Dynamics, 2013, 31, 973-975.	3.5	2
75	Structureâ€based design of model proteins. Proteins: Structure, Function and Bioinformatics, 1998, 31, 10-20.	2.6	2
76	Insights into Mechanisms and Models for Studying Neurological Adverse Events Mediated by Pharmacokinetic Interactions between Clinical Drugs and Illicit Substances of Herbal and Fungal Origin. , 2021, , 137-158.		1
77	Effect of the valine-threonine constraint on the dynamics of the proline helix â€” A molecular dynamics study. Journal of Chemical Sciences, 1994, 106, 579-589.	1.5	1
78	Energy expressions for atomic configurations in theL-S coupling scheme. International Journal of Quantum Chemistry, 1986, 30, 783-790.	2.0	0
79	Inferring biochemical routes from biochemical networks. , 2013, , .		0