Ramasubbu Sankararamakrishnan

List of Publications by Year
in descending order

64 papers	2,035 citations	257450 24 h-index	243625 44 g-index
69 all docs	69 docs citations	69 times ranked	2346 citing authors

#	Article	IF	Citations
1	Genome-wide analysis of major intrinsic proteins in the tree plant Populus trichocarpa: Characterization of XIP subfamily of aquaporins from evolutionary perspective. BMC Plant Biology, 2009, 9, 134.	3.6	225
2	Water in channel-like cavities: structure and dynamics. Biophysical Journal, 1996, 70, 693-702.	0.5	128
3	Parallel helix bundles and ion channels: molecular modeling via simulated annealing and restrained molecular dynamics. Biophysical Journal, 1994, 67, 1501-1515.	0.5	115
4	Lone pair Â·Â·Â· Ï€ interactions between water oxygens and aromatic residues: Quantum chemical studies based on highâ€resolution protein structures and model compounds. Protein Science, 2009, 18, 595-605.	7.6	111
5	Molecular dynamics simulations of water within models of ion channels. Biophysical Journal, 1996, 70, 1643-1661.	0.5	97
6	Close Contacts between Carbonyl Oxygen Atoms and Aromatic Centers in Protein Structures:â€‰ Ï€Â·Â·Â·Ï€ or Lone-PairÂ·Â·Â·Ï€ Interactions?. Journal of Physical Chemistry B, 2007, 111, 8680-8683.	2.6	97
7	Homology modeling of major intrinsic proteins in rice, maize and Arabidopsis: comparative analysis of transmembrane helix association and aromatic/arginine selectivity filters. BMC Structural Biology, 2007, 7, 27.	2.3	94
8	Geometry of prolineâ€containing alphaâ€helices in proteins. International Journal of Peptide and Protein Research, 1992, 39, 356-363.	0.1	82
9	The pore domain of the nicotinic acetylcholine receptor: molecular modeling, pore dimensions, and electrostatics. Biophysical Journal, 1996, 71, 1659-1671.	0.5	72
10	ATCUN-like metal-binding motifs in proteins: Identification and characterization by crystal structure and sequence analysis. Proteins: Structure, Function and Bioinformatics, 2004, 58, 211-221.	2.6	62
11	Molecular Dynamics Simulations Predict a Tilted Orientation for the Helical Region of Dynorphin A(1â€“17) in Dimyristoylphosphatidylcholine Bilayers. Biophysical Journal, 2000, 79, 2331-2344.	0.5	47
12	Antiâ€apoptotic Bclâ€X_L protein in complex with BH3 peptides of proâ€apoptotic Bak, Bad, and Bim proteins: Comparative molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 73, 492-514.	2.6	44
13	Seven-helix bundles: molecular modeling via restrained molecular dynamics. Biophysical Journal, 1995, 68, 1295-1310.	0.5	39
14	New subfamilies of major intrinsic proteins in fungi suggest novel transport properties in fungal channels: implications for the host-fungal interactions. BMC Evolutionary Biology, 2014, 14, 173.	3.2	38
15	Unconventional N-Hâ€¦N Hydrogen Bonds Involving Proline Backbone Nitrogen in Protein Structures. Biophysical Journal, 2016, 110, 1967-1979.	0.5	38
16	A Survey of mRNA Sequences with a Non-AUG Start Codon in RefSeq Database. Journal of Biomolecular Structure and Dynamics, 2006, 24, 33-41.	3.5	37
17	Nâ€“HÂ·Â·Â·N Hydrogen Bonds Involving Histidine Imidazole Nitrogen Atoms: A New Structural Role for Histidine Residues in Proteins. Biochemistry, 2016, 55, 3774-3783.	2.5	36
18	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

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19	Modelling membrane proteins using structural restraints. Nature Structural Biology, 1995, 2, 624-631.	9.7	35
20	MIPModDB: a central resource for the superfamily of major intrinsic proteins. Nucleic Acids Research, 2012, 40, D362-D369.	14.5	33
21	Quantum Chemical Investigations on Intraresidue Carbonylâ‹¯Carbonyl Contacts in Aspartates of High-Resolution Protein Structures. Journal of Physical Chemistry B, 2010, 114, 1038-1049.	2.6	30
22	Controlling in Vitro Insulin Amyloidosis with Stable Peptide Conjugates: A Combined Experimental and Computational Study. Journal of Physical Chemistry B, 2015, 119, 15395-15406.	2.6	30
23	Recognition of GPCRs by Peptide Ligands and Membrane Compartments theory: Structural Studies of Endogenous Peptide Hormones in Membrane Environment. Bioscience Reports, 2006, 26, 131-158.	2.4	29
24	Solvation in simulated annealing and high-temperature molecular dynamics of proteins: A restrained water droplet model. International Journal of Quantum Chemistry, 2000, 77, 174-186.	2.0	25
25	Molecular dynamics simulations of pro-apoptotic BH3 peptide helices in aqueous medium: relationship between helix stability and their binding affinities to the anti-apoptotic protein Bcl-XL. Journal of Computer-Aided Molecular Design, 2011, 25, 413-426.	2.9	25
26	Hidden coding potential of eukaryotic genomes: nonAUG started ORFs. Journal of Biomolecular Structure and Dynamics, 2013, 31, 103-114.	3.5	25
27	Major Intrinsic Protein Superfamily. Methods in Enzymology, 2015, 557, 485-520.	1.0	25
28	Identification of Core Structural Residues in the Sequentially Diverse and Structurally Homologous Bcl-2 Family of Proteins. Biochemistry, 2010, 49, 2574-2584.	2.5	24
29	Anion-selective Formate/nitrite transporters: taxonomic distribution, phylogenetic analysis and subfamily-specific conservation pattern in prokaryotes. BMC Genomics, 2017, 18, 560.	2.8	24
30	Solvation, water permeation, and ionic selectivity of a putative model for the pore region of the voltage-gated sodium channel. Biophysical Journal, 1996, 71, 2276-2288.	0.5	23
31	Positioning and Stabilization of Dynorphin Peptides in Membrane Bilayers:â€‰ the Mechanistic Role of Aromatic and Basic Residues Revealed from Comparative MD Simulations. Journal of Physical Chemistry B, 2002, 106, 209-218.	2.6	23
32	Molecular modelling of Staphylococcal Î´-toxin ion channels by restrained molecular dynamics. Protein Engineering, Design and Selection, 1996, 9, 161-171.	2.1	22
33	Cooperativity in Plant Plasma Membrane Intrinsic Proteins (PIPs): Mechanism of Increased Water Transport in Maize PIP1 Channels in Hetero-tetramers. Scientific Reports, 2018, 8, 12055.	3.3	22
34	Structural features of isolated M2 helices of nicotinic receptors. Simulated annealing via molecular dynamics studies. Biophysical Chemistry, 1995, 55, 215-230.	2.8	21
35	Surface Tension Parameterization in Molecular Dynamics Simulations of a Phospholipid-bilayer Membrane:â€‰ Calibration and Effects. Journal of Physical Chemistry B, 2004, 108, 11802-11811.	2.6	21
36	Force field dependence of phospholipid headgroup and acyl chain properties: Comparative molecular dynamics simulations of DMPC bilayers. Journal of Computational Chemistry, 2010, 31, 266-277.	3.3	20

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37	Relationship between helix stability and binding affinities: molecular dynamics simulations of Bfl-1/A1-binding pro-apoptotic BH3 peptide helices in explicit solvent. Journal of Biomolecular Structure and Dynamics, 2013, 31, 65-77.	3.5	16
38	Comparison of metal-binding strength between methionine and cysteine residues: Implications for the design of metal-binding motifs in proteins. Biophysical Chemistry, 2017, 224, 32-39.	2.8	16
39	Prediction of translation initiation sites in human mRNA sequences with AUG start codon in weak Kozak context: A neural network approach. Biochemical and Biophysical Research Communications, 2008, 369, 1166-1168.	2.1	15
40	Intra-helical salt-bridge and helix destabilizing residues within the same helical turn: Role of functionally important loop E half-helix in channel regulation of major intrinsic proteins. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1436-1449.	2.6	13
41	Imidazole Nitrogens of Two Histidine Residues Participating in Nâ€“HÂ·Â·Â·N Hydrogen Bonds in Protein Structures: Structural Bioinformatics Approach Combined with Quantum Chemical Calculations. Journal of Physical Chemistry B, 2018, 122, 1205-1212.	2.6	13
42	Self-contacts in Asx and Glx residues of high-resolution protein structures: Role of local environment and tertiary interactions. Journal of Molecular Graphics and Modelling, 2008, 27, 20-33.	2.4	12
43	Behavior of Solvent-Exposed Hydrophobic Groove in the Anti-Apoptotic Bcl-XL Protein: Clues for Its Ability to Bind Diverse BH3 Ligands from MD Simulations. PLoS ONE, 2013, 8, e54397.	2.5	10
44	Binding affinity of pro-apoptotic BH3 peptides for the anti-apoptotic Mcl-1 and A1 proteins: Molecular dynamics simulations of Mcl-1 and A1 in complex with six different BH3 peptides. Journal of Molecular Graphics and Modelling, 2017, 73, 115-128.	2.4	10
45	Characterization of proline-containing right-handed Î±-helix by molecular dynamics studies. Biophysical Chemistry, 1991, 40, 97-108.	2.8	9
46	Dynamics of Noncovalent Interactions in All-Î± and All-Î² Class Proteins: Implications for the Stability of Amyloid Aggregates. Journal of Chemical Information and Modeling, 2011, 51, 3208-3216.	5.4	8
47	Computational Design of BH3-Mimetic Peptide Inhibitors That Can Bind Specifically to Mcl-1 or Bcl-X_L: Role of Non-Hot Spot Residues. Biochemistry, 2020, 59, 4379-4394.	2.5	8
48	Designing BH3-Mimetic Peptide Inhibitors for the Viral Bcl-2 Homologues A179L and BHRF1: Importance of Long-Range Electrostatic Interactions. ACS Omega, 2021, 6, 26976-26989.	3.5	8
49	dbSWEET: An Integrated Resource for SWEET Superfamily to Understand, Analyze and Predict the Function of Sugar Transporters in Prokaryotes and Eukaryotes. Journal of Molecular Biology, 2018, 430, 2203-2211.	4.2	7
50	Antiapoptotic Bclâ€2 homolog CEDâ€9 in Caenorhabditis elegans: Dynamics of BH3 and CEDâ€4 binding regions and comparison with mammalian antiapoptotic Bclâ€2 proteins. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1035-1047.	2.6	6
51	Oxygenâ€“aromatic contacts in intra-strand base pairs: Analysis of high-resolution DNA crystal structures and quantum chemical calculations. Journal of Structural Biology, 2014, 187, 49-57.	2.8	6
52	End-to-end and end-to-middle interhelical interactions: new classes of interacting helix pairs in protein structures. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 1032-1041.	2.5	4
53	Presence of Intra-helical Salt-Bridge in Loop E Half-Helix Can Influence the Transport Properties of AQP1 and GlpF Channels: Molecular Dynamics Simulations of In Silico Mutants. Journal of Membrane Biology, 2019, 252, 17-29.	2.1	4
54	Simplified Models of the Pore Domain of the Nicotinic Acetylcholine Receptor. Biochemical Society Transactions, 1994, 22, 158S-158S.	3.4	3

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55	Is the E.Âcoli Homolog of the Formate/Nitrite Transporter Family an Anion Channel? A Computational Study. Biophysical Journal, 2020, 118, 846-860.	0.5	3
56	The Structures of Bacteriorhodopsin With Different Retinal-Schiff Base Orientations - Computer Modeling And Energy Minimization Studies. Journal of Biomolecular Structure and Dynamics, 1992, 9, 1073-1095.	3.5	2
57	Molecular Dynamics Studies of M2 Helices of Nicotinic Acetylcholine Receptors. Biochemical Society Transactions, 1994, 22, 156S-156S.	3.4	2
58	Molecular Dynamics Simulations of C-Terminal Decapeptide of Gastrin-Releasing Peptide in DMPC Bilayers: Structure, Stability and Orientation of the Peptide Hormone Within the Bilayers. Protein and Peptide Letters, 2007, 14, 590-596.	0.9	2
59	Distinguishing Features of Aquaglyceroporin in Plasmodium Falciparum: Comparative Molecular Dynamics Simulations of Three Aquaporins. Biophysical Journal, 2012, 102, 452a.	0.5	1
60	PLASTICITY OF BH3 DOMAIN-BINDING HYDROPHOBIC GROOVES IN THE ANTI-APOPTOTIC MCL-1 AND A1 PROTEINS. , 2013, , 468-481.		1
61	Non-Covalent Interactions Involving Aromatic Residues in Protein Structures: Stability and Dynamics in Membrane and Globular Proteins using Molecular Dynamics Simulations. Biophysical Journal, 2010, 98, 635a-636a.	0.5	0
62	Differential Binding Affinities of Anti-Apoptotic MCL-1 and A1 Proteins for the Pro-Apoptotic BH3 Peptides: Understanding the Molecular Basis using MD Simulations. Biophysical Journal, 2011, 100, 396a.	0.5	0
63	Affinities of Selective-Serotonin Reuptake Inhibitor (SSRI) for Human Transporters: Molecular Modeling and Quantum Chemical Studies. Biophysical Journal, 2014, 106, 255a.	0.5	0
64	Molecular Dynamics Simulations of Wild-Type and Mutant AQP6 Channels: Investigation of Anion Transport in Human AQP6. Biophysical Journal, 2015, 108, 373a-374a.	0.5	0