Harish Vashisth

List of Publications by Year
in descending order

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52	1,028	567144 15	477173 29
papers	citations	h-index	g-index

54	54	54	1358
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structures and interactions of insulinâ€like peptides from cone snail venom. Proteins: Structure, Function and Bioinformatics, 2022, 90, 680-690.	1.5	5
2	Cover Image, Volume 90, Issue 3. Proteins: Structure, Function and Bioinformatics, 2022, 90, .	1.5	0
3	Molecular interactions and inhibition of the SARSâ€CoVâ€2 main protease by a thiadiazolidinone derivative. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1896-1907.	1.5	3
4	Role of conformational heterogeneity in ligand recognition by viral RNA molecules. Physical Chemistry Chemical Physics, 2021, 23, 11211-11223.	1.3	8
5	Reaction Coordinate and Thermodynamics of Base Flipping in RNA. Journal of Chemical Theory and Computation, 2021, 17, 1914-1921.	2.3	9
6	Allosteric Pathways Originating at Cysteine Residues in Regulators of G-Protein Signaling Proteins. Biophysical Journal, 2021, 120, 517-526.	0.2	5
7	Enhanced Porosity in Self-Assembled Morphologies Mediated by Charged Lobes on Patchy Particles. Journal of Physical Chemistry B, 2021, 125, 3208-3215.	1.2	5
8	Design of Functionalized Lobed Particles for Porous Self-Assemblies. Jom, 2021, 73, 2413-2422.	0.9	5
9	Liposome-based measurement of light-driven chloride transport kinetics of halorhodopsin. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183637.	1.4	4
10	Role of salt-bridging interactions in recognition of viral RNA by arginine-rich peptides. Biophysical Journal, 2021, 120, 5060-5073.	0.2	7
11	Self-Assembly of Porous Structures From a Binary Mixture of Lobed Patchy Particles. Frontiers in Physics, 2021, 9, .	1.0	3
12	Water Dynamics in a Peptide-appended Pillar[5]arene Artificial Channel in Lipid and Biomimetic Membranes. Frontiers in Chemistry, 2021, 9, 753635.	1.8	3
13	Conformational dynamics and energetics of viral RNA recognition by lab-evolved proteins. Physical Chemistry Chemical Physics, 2021, 23, 24773-24779.	1.3	8
14	Self-assembly of lobed particles into amorphous and crystalline porous structures. Soft Matter, 2020, 16, 1142-1147.	1.2	15
15	Structural Analysis of the Regulatory GAF Domains of cGMP Phosphodiesterase Elucidates the Allosteric Communication Pathway. Journal of Molecular Biology, 2020, 432, 5765-5783.	2.0	6
16	Role of Entropy in Colloidal Self-Assembly. Entropy, 2020, 22, 877.	1.1	19
17	Self-assembly behavior of experimentally realizable lobed patchy particles. Soft Matter, 2020, 16, 8101-8107.	1.2	11
18	Functional Nanoassemblies with Mirror-Image Chiroptical Properties Templated by a Single Homochiral DNA Strand. Chemistry of Materials, 2020, 32, 2272-2281.	3.2	10

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19	Ligand Recognition in Viral RNA Necessitates Rare Conformational Transitions. Journal of Physical Chemistry Letters, 2020, 11, 5426-5432.	2.1	12
20	Phase space and collective variable based simulation methods for studies of rare events. Molecular Simulation, 2019, 45, 1273-1284.	0.9	18
21	Conformational dynamics and interfacial interactions of peptide-appended pillar[5]arene water channels in biomimetic membranes. Physical Chemistry Chemical Physics, 2019, 21, 22711-22721.	1.3	5
22	Cover Image, Volume 87, Issue 2. Proteins: Structure, Function and Bioinformatics, 2019, 87, C1.	1.5	0
23	Pharmacological and molecular dynamics analyses of differences in inhibitor binding to human and nematode PDE4: Implications for management of parasitic nematodes. PLoS ONE, 2019, 14, e0214554.	1.1	7
24	An Interhelical Salt Bridge Controls Flexibility and Inhibitor Potency for Regulators of G-protein Signaling Proteins 4, 8, and 19. Molecular Pharmacology, 2019, 96, 683-691.	1.0	8
25	Interplay of cysteine exposure and global protein dynamics in smallâ€molecule recognition by a regulator of Gâ€protein signaling protein. Proteins: Structure, Function and Bioinformatics, 2019, 87, 146-156.	1.5	13
26	Differential Protein Dynamics of Regulators of G-Protein Signaling: Role in Specificity of Small-Molecule Inhibitors. Journal of the American Chemical Society, 2018, 140, 3454-3460.	6.6	21
27	Parameterization and atomistic simulations of biomimetic membranes. Faraday Discussions, 2018, 209, 161-178.	1.6	8
28	Diffusion network of CO in FeFe-Hydrogenase. Journal of Chemical Physics, 2018, 149, 204108.	1.2	4
29	The modelling and enhancement of water hydrodynamics: general discussion. Faraday Discussions, 2018, 209, 273-285.	1.6	2
30	Structure and function of natural proteins for water transport: general discussion. Faraday Discussions, 2018, 209, 83-95.	1.6	4
31	Interpreting Hydrogenâ€“Deuterium Exchange Events in Proteins Using Atomistic Simulations: Case Studies on Regulators of G-Protein Signaling Proteins. Journal of Physical Chemistry B, 2018, 122, 9314-9323.	1.2	30
32	Biomimetic water channels: general discussion. Faraday Discussions, 2018, 209, 205-229.	1.6	10
33	Achieving high permeability and enhanced selectivity for Angstrom-scale separations using artificial water channel membranes. Nature Communications, 2018, 9, 2294.	5.8	95
34	Insulin mimetic peptide S371 folds into a helical structure. Journal of Computational Chemistry, 2017, 38, 1158-1166.	1.5	9
35	Pathways and Thermodynamics of Oxygen Diffusion in [FeFe]-Hydrogenase. Journal of Physical Chemistry B, 2017, 121, 10007-10017.	1.2	11
36	Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review. Current Topics in Medicinal Chemistry, 2017, 17, 2626-2641.	1.0	44

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37	All-Atom Structural Models of the Transmembrane Domains of Insulin and Type 1 Insulin-Like Growth Factor Receptors. Frontiers in Endocrinology, 2016, 7, 68.	1.5	12
38	Theoretical and Computational Studies of Peptides and Receptors of the Insulin Family. Membranes, 2015, 5, 48-83.	1.4	8
39	Flexibility in the Insulin Receptor Ectodomain Enables Docking of Insulin in Crystallographic Conformation Observed in a Hormone-Bound Microreceptor. Membranes, 2014, 4, 730-746.	1.4	7
40	Collective Variable Approaches for Single Molecule Flexible Fitting and Enhanced Sampling. Chemical Reviews, 2014, 114, 3353-3365.	23.0	25
41	Conformational Dynamics of a Regulator of G-Protein Signaling Protein Reveals a Mechanism of Allosteric Inhibition by a Small Molecule. ACS Chemical Biology, 2013, 8, 2778-2784.	1.6	33
42	Allâ€atom structural models of insulin binding to the insulin receptor in the presence of a tandem hormoneâ€binding element. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1017-1030.	1.5	36
43	Enhanced Sampling and Overfitting Analyses in Structural Refinement of Nucleic Acids into Electron Microscopy Maps. Journal of Physical Chemistry B, 2013, 117, 3738-3746.	1.2	12
44	Conformational Sampling of Maltose-Transporter Components in Cartesian Collective Variables Is Governed by the Low-Frequency Normal Modes. Journal of Physical Chemistry Letters, 2012, 3, 3379-3384.	2.1	31
45	â€œDFG-Flipâ€•in the Insulin Receptor Kinase Is Facilitated by a Helical Intermediate State of the Activation Loop. Biophysical Journal, 2012, 102, 1979-1987.	0.2	50
46	Using Enhanced Sampling and Structural Restraints to Refine Atomic Structures into Low-Resolution Electron Microscopy Maps. Structure, 2012, 20, 1453-1462.	1.6	39
47	Ribosome Assembly Factors Prevent Premature Translation Initiation by 40 S Assembly Intermediates. Science, 2011, 333, 1449-1453.	6.0	199
48	Docking of insulin to a structurally equilibrated insulin receptor ectodomain. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1531-1543.	1.5	16
49	All-Atom Structural Models for Complexes of Insulin-Like Growth Factors IGF1 and IGF2 with Their Cognate Receptor. Journal of Molecular Biology, 2010, 400, 645-658.	2.0	21
50	Ligand Escape Pathways and (Un)Binding Free Energy Calculations for the Hexameric Insulin-Phenol Complex. Biophysical Journal, 2008, 95, 4193-4204.	0.2	82
51	Progress in Simulation Studies of Insulin Structure and Function. Frontiers in Endocrinology, 0, 13, .	1.5	10
52	Role of Mutations in Differential Recognition of Viral RNA Molecules by Peptides. Journal of Chemical Information and Modeling, 0, , .	2.5	4