U Deva Priyakumar

List of Publications by Year
in descending order

99	2,627	186265	233421
papers	citations	28 h-index	45 g-index

136	136	136	2894
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Impact of 2â€²â€hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM allâ€atom additive force field for RNA. Journal of Computational Chemistry, 2011, 32, 1929-1943.	3.3	341
2	MolGPT: Molecular Generation Using a Transformer-Decoder Model. Journal of Chemical Information and Modeling, 2022, 62, 2064-2076.	5.4	105
3	Computational Approaches for Investigating Base Flipping in Oligonucleotides. Chemical Reviews, 2006, 106, 489-505.	47.7	85
4	First ab Initio and Density Functional Study on the Structure, Bowl-to-Bowl Inversion Barrier, and Vibrational Spectra of the Elusive C3v-Symmetric Buckybowl:â€‰ Sumanene, C21H12. Journal of Physical Chemistry A, 2001, 105, 4488-4494.	2.5	81
5	Exploration of C6H6Potential Energy Surface:Â A Computational Effort to Unravel the Relative Stabilities and Synthetic Feasibility of New Benzene Isomersâ€. Journal of Physical Chemistry A, 2004, 108, 11433-11448.	2.5	80
6	Urea Destabilizes RNA by Forming Stacking Interactions and Multiple Hydrogen Bonds with Nucleic Acid Bases. Journal of the American Chemical Society, 2009, 131, 17759-17761.	13.7	73
7	Machine Learning Based Clinical Decision Support System for Early COVID-19 Mortality Prediction. Frontiers in Public Health, 2021, 9, 626697.	2.7	72
8	Heterobuckybowls:â€‰ A Theoretical Study on the Structure, Bowl-to-Bowl Inversion Barrier, Bond Length Alternation, Structure-Inversion Barrier Relationship, Stability, and Synthetic Feasibility. Journal of Organic Chemistry, 2001, 66, 6523-6530.	3.2	70
9	Solventâ€Induced Helical Assembly and Reversible Chiroptical Switching of Chiral Cyclicâ€Dipeptideâ€Functionalized Naphthalenediimides. Chemistry - A European Journal, 2013, 19, 16615-16624.	3.3	61
10	Role of the Adenine Ligand on the Stabilization of the Secondary and Tertiary Interactions in the Adenine Riboswitch. Journal of Molecular Biology, 2010, 396, 1422-1438.	4.2	55
11	A Lipophilic Hexaporphyrin Assembly Supported on a Stannoxane Core. Journal of the American Chemical Society, 2005, 127, 2410-2411.	13.7	51
12	Dynamics Based Pharmacophore Models for Screening Potential Inhibitors of Mycobacterial Cyclopropane Synthase. Journal of Chemical Information and Modeling, 2015, 55, 848-860.	5.4	48
13	Base Flipping in a GCGC Containing DNA Dodecamer:â€‰ A Comparative Study of the Performance of the Nucleic Acid Force Fields, CHARMM, AMBER, and BMS. Journal of Chemical Theory and Computation, 2006, 2, 187-200.	5.3	47
14	Role of Ureaâ€“Aromatic Stacking Interactions in Stabilizing the Aromatic Residues of the Protein in Urea-Induced Denatured State. Journal of the American Chemical Society, 2017, 139, 14931-14946.	13.7	47
15	On the use of NICS criterion to evaluate aromaticity in heteroaromatics involving III and IV row main group elements. Computational and Theoretical Chemistry, 2003, 663, 145-148.	1.5	45
16	A system with three contiguous planar tetracoordinate carbons is viable: a computational study on a C 6 H 6 2= isomer. Tetrahedron Letters, 2004, 45, 1515-1517.	1.4	44
17	Host metabolic reprogramming in response to SARS-CoV-2 infection: A systems biology approach. Microbial Pathogenesis, 2021, 158, 105114.	2.9	44
18	A Theoretical Study of the Structures, Energetics, Stabilities, Reactivities, and Out-of-Plane Distortive Tendencies of Skeletally Substituted Benzenes (CH)5XH and (CH)4(XH)2(X = B-, N+, Al-, Si, P+, Ga-, Ge, and) Tj ETQq0 0 0 rgBT /Overloc	3.1	41

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19	DeepPocket: Ligand Binding Site Detection and Segmentation using 3D Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 5069-5079.	5.4	41
20	Crenarchaeal chromatin proteins Cren7 and Sul7 compact DNA by inducing rigid bends. Nucleic Acids Research, 2013, 41, 196-205.	14.5	39
21	NMR Imino Proton Exchange Experiments on Duplex DNA Primarily Monitor the Opening of Purine Bases. Journal of the American Chemical Society, 2006, 128, 678-679.	13.7	38
22	Enantioseparation and chiral induction in Ag₂₉ nanoclusters with intrinsic chirality. Chemical Science, 2020, 11, 2394-2400.	7.4	37
23	Small-molecule inhibitors of ERK-mediated immediate early gene expression and proliferation of melanoma cells expressing mutated BRaf. Biochemical Journal, 2015, 467, 425-438.	3.7	35
24	Machine Learning for Accurate Force Calculations in Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2020, 124, 6954-6967.	2.5	35
25	Artificial intelligence: machine learning for chemical sciences. Journal of Chemical Sciences, 2022, 134, 2.	1.5	32
26	Theoretical Study of Silabenzene and Its Valence Isomers. Organometallics, 2002, 21, 1493-1499.	2.3	29
27	Molecular Dynamics Study of the Structure, Flexibility, and Hydrophilicity of PETIM Dendrimers: A Comparison with PAMAM Dendrimers. Journal of Physical Chemistry B, 2015, 119, 12990-13001.	2.6	29
28	Structures, Energetics, Relative Stabilities, and Out-of-Plane Distortivities of Skeletally Disubstituted Benzenes, (CH)4X2 (X = N, P, C-, Si-, O+, and S+):â€‰ An ab Initio and DFT Study. Journal of the American Chemical Society, 2000, 122, 11173-11181.	13.7	28
29	Deep learning enabled inorganic material generator. Physical Chemistry Chemical Physics, 2020, 22, 26935-26943.	2.8	27
30	Theoretical studies on the effect of sequential benzannulation to corannulene. Computational and Theoretical Chemistry, 2001, 543, 1-10.	1.5	26
31	Sumoylation of Sir2 differentially regulates transcriptional silencing in yeast. Nucleic Acids Research, 2015, 43, gkv842.	14.5	26
32	Structure, Interaction, and Dynamics of Au/Pd Bimetallic Nanoalloys Dispersed in Aqueous Ethylpyrrolidone, a Monomeric Moiety of Polyvinylpyrrolidone. Journal of Physical Chemistry C, 2016, 120, 17454-17464.	3.1	26
33	BAND NN: A Deep Learning Framework for Energy Prediction and Geometry Optimization of Organic Small Molecules. Journal of Computational Chemistry, 2020, 41, 790-799.	3.3	26
34	MEMES: Machine learning framework for Enhanced MolEcular Screening. Chemical Science, 2021, 12, 11710-11721.	7.4	26
35	Molecular representations for machine learning applications in chemistry. International Journal of Quantum Chemistry, 2022, 122, .	2.0	26
36	A computational study of the valence isomers of benzene and their group V hetero analogs. New Journal of Chemistry, 2002, 26, 347-353.	2.8	25

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37	Conformational Determinants of Tandem GU Mismatches in RNA:â€‰ Insights from Molecular Dynamics Simulations and Quantum Mechanical Calculations. Biochemistry, 2005, 44, 1433-1443.	2.5	24
38	Structural and Energetic Determinants of Thermal Stability and Hierarchical Unfolding Pathways of Hyperthermophilic Proteins, Sac7d and Sso7d. Journal of Physical Chemistry B, 2010, 114, 1707-1718.	2.6	24
39	Structures, Dynamics, and Stabilities of Fully Modified Locked Nucleic Acid (Î²-<scp>d</scp>-LNA and) Tj ETQq1 1 0.784314 rgBT /Ov Chemistry B, 2013, 117, 5556-5564.	2.6	23
40	Isomers of Disilabenzene (C4Si2H6):Â A Computational Study. Organometallics, 2002, 21, 4823-4832.	2.3	22
41	Cholic Acid-Derived Amphiphile which Combats Gram-Positive Bacteria-Mediated Infections via Disintegration of Lipid Clusters. ACS Biomaterials Science and Engineering, 2019, 5, 4764-4775.	5.2	22
42	MoleGuLAR: Molecule Generation Using Reinforcement Learning with Alternating Rewards. Journal of Chemical Information and Modeling, 2021, 61, 5815-5826.	5.4	22
43	Chemically Interpretable Graph Interaction Network for Prediction of Pharmacokinetic Properties of Drug-Like Molecules. Proceedings of the AAAI Conference on Artificial Intelligence, 2020, 34, 873-880.	4.9	21
44	Learning Atomic Interactions through Solvation Free Energy Prediction Using Graph Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 689-698.	5.4	21
45	Role of Hydrophobic Core on the Thermal Stability of Proteinsâ€”Molecular Dynamics Simulations on a Single Point Mutant of Sso7d. Journal of Biomolecular Structure and Dynamics, 2012, 29, 961-971.	3.5	20
46	Molecular Dynamics Simulations Reveal the HIV-1 Vpu Transmembrane Protein to Form Stable Pentamers. PLoS ONE, 2013, 8, e79779.	2.5	20
47	Atomic Detail Investigation of the Structure and Dynamics of DNAâ€¢RNA Hybrids:â€‰ A Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 1515-1524.	2.6	19
48	DNAâ€“RNA hybrid duplexes with decreasing pyrimidine content in the DNA strand provide structural snapshots for the A- to B-form conformational transition of nucleic acids. Physical Chemistry Chemical Physics, 2014, 16, 18148-18155.	2.8	19
49	Urea-aromatic interactions in biology. Biophysical Reviews, 2020, 12, 65-84.	3.2	18
50	Modern machine learning for tackling inverse problems in chemistry: molecular design to realization. Chemical Communications, 2022, 58, 5316-5331.	4.1	18
51	Dispersion Interactions between Urea and Nucleobases Contribute to the Destabilization of RNA by Urea in Aqueous Solution. Journal of Physical Chemistry B, 2015, 119, 3755-3761.	2.6	16
52	Microsecond simulation of human aquaporin 2 reveals structural determinants of water permeability and selectivity. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 10-16.	2.6	16
53	COVID-19 Risk Stratification and Mortality Prediction in Hospitalized Indian Patients: Harnessing clinical data for public health benefits. PLoS ONE, 2022, 17, e0264785.	2.5	16
54	Atomistic Investigation of the Effect of Incremental Modification of Deoxyribose Sugars by Locked Nucleic Acid (Î²-<scp>d</scp>-LNA and Î±-<scp>l</scp>-LNA) Moieties on the Structures and Thermodynamics of DNAâ€“RNA Hybrid Duplexes. Journal of Physical Chemistry B, 2014, 118, 5853-5863.	2.6	15

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55	Silaaromaticity in Polycyclic Systems: A Computational Study. Journal of Organic Chemistry, 2003, 68, 1168-1171.	3.2	14
56	Urea Mimics Nucleobases by Preserving the Helical Integrity of B-DNA Duplexes via Hydrogen Bonding and Stacking Interactions. Biochemistry, 2016, 55, 5653-5664.	2.5	14
57	SCONES: Self-Consistent Neural Network for Protein Stability Prediction Upon Mutation. Journal of Physical Chemistry B, 2021, 125, 10657-10671.	2.6	14
58	Molecular Simulations on the Thermal Stabilization of DNA by Hyperthermophilic Chromatin Protein Sac7d, and Associated Conformational Transitions. Journal of Physical Chemistry B, 2010, 114, 16548-16557.	2.6	13
59	Atomistic Details of the Ligand Discrimination Mechanism of S_{MK}/SAM-III Riboswitch. Journal of Physical Chemistry B, 2010, 114, 9920-9925.	2.6	12
60	C21H9Z (Z=â¯3 to +3): a theoretical study on the redox behaviour of C3 symmetric fragment of C60. Computational and Theoretical Chemistry, 2004, 674, 69-75.	1.5	11
61	Transition between [R]- and [S]-stereoisomers without bond breaking. Physical Chemistry Chemical Physics, 2020, 22, 14983-14991.	2.8	11
62	Basis set and method dependence of the relative energies of C2S2H2 isomers. Chemical Physics Letters, 2004, 383, 192-197.	2.6	10
63	Goldâ€Palladium Nanocluster Catalysts for Homocoupling: Electronic Structure and Interface Dynamics. Chemical Record, 2019, 19, 947-959.	5.8	10
64	The effect of bulky group substitution on the skeleton, geometries, relative energies and the reactivities of silabenzene valence isomers. Computational and Theoretical Chemistry, 2002, 618, 173-179.	1.5	9
65	Binding to gold nanoclusters alters the hydrogen bonding interactions and electronic properties of canonical and size-expanded DNA base pairs. RSC Advances, 2015, 5, 49408-49419.	3.6	9
66	Ion Hydration Dynamics in Conjunction with a Hydrophobic Gating Mechanism Regulates Ion Permeation in p7 Viroporin from Hepatitis C Virus. Journal of Physical Chemistry B, 2015, 119, 6204-6210.	2.6	9
67	Ureaâ€“Aromatic Stacking and Concerted Urea Transport: Conserved Mechanisms in Urea Transporters Revealed by Molecular Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 5190-5200.	5.3	9
68	Desolvation of Peptide Bond by O to S Substitution Impacts Protein Stability. Angewandte Chemie - International Edition, 2021, 60, 24870-24874.	13.8	9
69	Computational investigation of the effect of thermal perturbation on the mechanical unfolding of titin I27. Journal of Molecular Modeling, 2012, 18, 2823-2829.	1.8	8
70	Atomistic Detailed Mechanism and Weak Cation-Conducting Activity of HIV-1 Vpu Revealed by Free Energy Calculations. PLoS ONE, 2014, 9, e112983.	2.5	8
71	Energetic, Structural and Dynamic Properties of Nucleobase-Urea Interactions that Aid in Urea Assisted RNA Unfolding. Scientific Reports, 2019, 9, 8805.	3.3	8
72	Transannular Dielsâ€“Alder Reactivities of 14-Membered Macrocylic Trienes and Their Relationship with the Conformational Preferences of the Reactants: A Combined Quantum Chemical and Molecular Dynamics Study. Journal of Organic Chemistry, 2012, 77, 5371-5380.	3.2	7

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73	Nucleobases tagged to gold nanoclusters cause a mechanistic crossover in the oxidation of CO. Physical Chemistry Chemical Physics, 2015, 17, 24275-24281.	2.8	7
74	Selectivity and transport in aquaporins from molecular simulation studies. Vitamins and Hormones, 2020, 112, 47-70.	1.7	7
75	DART: deep learning enabled topological interaction model for energy prediction of metal clusters and its application in identifying unique low energy isomers. Physical Chemistry Chemical Physics, 2021, 23, 21995-22003.	2.8	7
76	Facile valence isomerization among bis(silacyclopropenyl), disila(Dewar benzene) and disilabenzvalene. Journal of Organometallic Chemistry, 2004, 689, 1284-1287.	1.8	6
77	Modulation of structural, energetic and electronic properties of DNA and size-expanded DNA bases upon binding to gold clusters. RSC Advances, 2014, 4, 29642-29651.	3.6	6
78	A Probabilistic Framework for Constructing Temporal Relations in Replica Exchange Molecular Trajectories. Journal of Chemical Theory and Computation, 2018, 14, 3365-3380.	5.3	6
79	Multiscale Modeling of Wobble to Watsonâ€“Crick-Like Guanineâ€“Uracil Tautomerization Pathways in RNA. International Journal of Molecular Sciences, 2021, 22, 5411.	4.1	6
80	BiRDS - Binding Residue Detection from Protein Sequences Using Deep ResNets. Journal of Chemical Information and Modeling, 2022, 62, 1809-1818.	5.4	6
81	Deep Reinforcement Learning for Molecular Inverse Problem of Nuclear Magnetic Resonance Spectra to Molecular Structure. Journal of Physical Chemistry Letters, 2022, 13, 4924-4933.	4.6	6
82	Cooperation of Hydrophobic Gating, Knock-on Effect, and Ion Binding Determines Ion Selectivity in the p7 Channel. Journal of Physical Chemistry B, 2016, 120, 4351-4356.	2.6	5
83	Synthesis and reactivity of NHC-coordinated phosphinidene oxide. Chemical Communications, 2021, 57, 9546-9549.	4.1	5
84	Computational modeling of the catalytic mechanism of hydroxymethylbilane synthase. Physical Chemistry Chemical Physics, 2019, 21, 7932-7940.	2.8	4
85	Benchmark study on deep neural network potentials for small organic molecules. Journal of Computational Chemistry, 2022, 43, 308-318.	3.3	4
86	Modeling the structure of SARS 3a transmembrane protein using a minimum unfavorable contact approach. Journal of Chemical Sciences, 2015, 127, 2159-2169.	1.5	3
87	Prediction of the structures of helical membrane proteins based on a minimum unfavorable contacts approach. Journal of Computational Chemistry, 2015, 36, 539-552.	3.3	3
88	Inclusion of methoxy groups inverts the thermodynamic stabilities of DNAâ€“RNA hybrid duplexes: A molecular dynamics simulation study. Journal of Molecular Graphics and Modelling, 2015, 61, 150-159.	2.4	3
89	pH-mediated gating and formate transport mechanism in the Escherichia coli formate channel. Molecular Simulation, 2017, 43, 1300-1306.	2.0	3
90	Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems. Atoms, 2021, 9, 79.	1.6	3

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91	Inter- versus intra-molecular cyclization of tripeptides containing tetrahydrofuran amino acids: a density functional theory study on kinetic control. Journal of Molecular Modeling, 2012, 18, 3181-3197.	1.8	2
92	Quantum mechanical investigation of the nature of nucleobase-urea stacking interaction, a crucial driving force in RNA unfolding in aqueous urea. Journal of Chemical Sciences, 2018, 130, 1.	1.5	2
93	Urea-water solvation of protein side chain models. Journal of Molecular Liquids, 2020, 311, 113191.	4.9	2
94	Linear Prediction Residual for Efficient Diagnosis of Parkinsonâ€™s Disease from Gait. Lecture Notes in Computer Science, 2021, , 614-623.	1.3	2
95	Role of conformational properties on the transannular Dielsâ€“Alder reactivity of macrocyclic trienes with varying linker lengths. RSC Advances, 2013, 3, 15892.	3.6	1
96	Recent Advancements in Computing Reliable Binding Free Energies in Drug Discovery Projects. Challenges and Advances in Computational Chemistry and Physics, 2019, , 221-246.	0.6	1
97	Ion Selectivity and Permeation Mechanism in a Cyclodextrin-Based Channel. Journal of Physical Chemistry B, 2021, 125, 8028-8037.	2.6	1
98	Synthesis and Reactivity Studies of Dicationic Dihydrogen Complexes Bearing Sulfurâ€Donor Ligands: A Combined Experimental and Computational Study. European Journal of Inorganic Chemistry, 2013, 2013, 1434-1443.	2.0	0
99	A Model of Graph Transactional Coverage Patterns with Applications to Drug Discovery. , 2021, , .		0