U Deva Priyakumar

List of Publications by Year
in descending order

99 papers	2,627 citations	185998 28 h-index	233125 45 g-index
136 all docs	136 docs citations	136 times ranked	2894 citing authors

#	Article	IF	Citations
1	DeepPocket: Ligand Binding Site Detection and Segmentation using 3D Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 5069-5079.	2.5	41
2	MolGPT: Molecular Generation Using a Transformer-Decoder Model. Journal of Chemical Information and Modeling, 2022, 62, 2064-2076.	2.5	105
3	Modern machine learning for tackling inverse problems in chemistry: molecular design to realization. Chemical Communications, 2022, 58, 5316-5331.	2.2	18
4	COVID-19 Risk Stratification and Mortality Prediction in Hospitalized Indian Patients: Harnessing clinical data for public health benefits. PLoS ONE, 2022, 17, e0264785.	1.1	16
5	Benchmark study on deep neural network potentials for small organic molecules. Journal of Computational Chemistry, 2022, 43, 308-318.	1.5	4
6	Molecular representations for machine learning applications in chemistry. International Journal of Quantum Chemistry, 2022, 122, .	1.0	26
7	Artificial intelligence: machine learning for chemical sciences. Journal of Chemical Sciences, 2022, 134, 2.	0.7	32
8	BiRDS - Binding Residue Detection from Protein Sequences Using Deep ResNets. Journal of Chemical Information and Modeling, 2022, 62, 1809-1818.	2.5	6
9	Deep Reinforcement Learning for Molecular Inverse Problem of Nuclear Magnetic Resonance Spectra to Molecular Structure. Journal of Physical Chemistry Letters, 2022, 13, 4924-4933.	2.1	6
10	Synthesis and reactivity of NHC-coordinated phosphinidene oxide. Chemical Communications, 2021, 57, 9546-9549.	2.2	5
11	Learning Atomic Interactions through Solvation Free Energy Prediction Using Graph Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 689-698.	2.5	21
12	Multiscale Modeling of Wobble to Watsonâ€“Crick-Like Guanineâ€“Uracil Tautomerization Pathways in RNA. International Journal of Molecular Sciences, 2021, 22, 5411.	1.8	6
13	Machine Learning Based Clinical Decision Support System for Early COVID-19 Mortality Prediction. Frontiers in Public Health, 2021, 9, 626697.	1.3	72
14	Ion Selectivity and Permeation Mechanism in a Cyclodextrin-Based Channel. Journal of Physical Chemistry B, 2021, 125, 8028-8037.	1.2	1
15	Desolvation of Peptide Bond by O to S Substitution Impacts Protein Stability. Angewandte Chemie - International Edition, 2021, 60, 24870-24874.	7.2	9
16	Host metabolic reprogramming in response to SARS-CoV-2 infection: A systems biology approach. Microbial Pathogenesis, 2021, 158, 105114.	1.3	44
17	SCONES: Self-Consistent Neural Network for Protein Stability Prediction Upon Mutation. Journal of Physical Chemistry B, 2021, 125, 10657-10671.	1.2	14
18	MEMES: Machine learning framework for Enhanced MolEcular Screening. Chemical Science, 2021, 12, 11710-11721.	3.7	26

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19	Linear Prediction Residual for Efficient Diagnosis of Parkinsonâ€™s Disease from Gait. Lecture Notes in Computer Science, 2021, , 614-623.	1.0	2
20	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.	1.3	7
21	Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems. Atoms, 2021, 9, 79.	0.7	3
22	A Model of Graph Transactional Coverage Patterns with Applications to Drug Discovery. , 2021, , .		0
23	MoleGuLAR: Molecule Generation Using Reinforcement Learning with Alternating Rewards. Journal of Chemical Information and Modeling, 2021, 61, 5815-5826.	2.5	22
24	BAND NN: A Deep Learning Framework for Energy Prediction and Geometry Optimization of Organic Small Molecules. Journal of Computational Chemistry, 2020, 41, 790-799.	1.5	26
25	Selectivity and transport in aquaporins from molecular simulation studies. Vitamins and Hormones, 2020, 112, 47-70.	0.7	7
26	Deep learning enabled inorganic material generator. Physical Chemistry Chemical Physics, 2020, 22, 26935-26943.	1.3	27
27	Machine Learning for Accurate Force Calculations in Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2020, 124, 6954-6967.	1.1	35
28	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.	3.6	21
29	Urea-water solvation of protein side chain models. Journal of Molecular Liquids, 2020, 311, 113191.	2.3	2
30	Transition between [R]- and [S]-stereoisomers without bond breaking. Physical Chemistry Chemical Physics, 2020, 22, 14983-14991.	1.3	11
31	Urea-aromatic interactions in biology. Biophysical Reviews, 2020, 12, 65-84.	1.5	18
32	Enantioseparation and chiral induction in Ag₂₉ nanoclusters with intrinsic chirality. Chemical Science, 2020, 11, 2394-2400.	3.7	37
33	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.	2.6	22
34	Goldâ€Palladium Nanocluster Catalysts for Homocoupling: Electronic Structure and Interface Dynamics. Chemical Record, 2019, 19, 947-959.	2.9	10
35	Energetic, Structural and Dynamic Properties of Nucleobase-Urea Interactions that Aid in Urea Assisted RNA Unfolding. Scientific Reports, 2019, 9, 8805.	1.6	8
36	Computational modeling of the catalytic mechanism of hydroxymethylbilane synthase. Physical Chemistry Chemical Physics, 2019, 21, 7932-7940.	1.3	4

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37	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
38	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.	0.7	2
39	A Probabilistic Framework for Constructing Temporal Relations in Replica Exchange Molecular Trajectories. Journal of Chemical Theory and Computation, 2018, 14, 3365-3380.	2.3	6
40	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.	6.6	47
41	pH-mediated gating and formate transport mechanism in the Escherichia coli formate channel. Molecular Simulation, 2017, 43, 1300-1306.	0.9	3
42	Microsecond simulation of human aquaporin 2 reveals structural determinants of water permeability and selectivity. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 10-16.	1.4	16
43	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.	1.2	5
44	Urea Mimics Nucleobases by Preserving the Helical Integrity of B-DNA Duplexes via Hydrogen Bonding and Stacking Interactions. Biochemistry, 2016, 55, 5653-5664.	1.2	14
45	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.	2.3	9
46	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.	1.5	26
47	Modeling the structure of SARS 3a transmembrane protein using a minimum unfavorable contact approach. Journal of Chemical Sciences, 2015, 127, 2159-2169.	0.7	3
48	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.	1.7	9
49	Sumoylation of Sir2 differentially regulates transcriptional silencing in yeast. Nucleic Acids Research, 2015, 43, gkv842.	6.5	26
50	Prediction of the structures of helical membrane proteins based on a minimum unfavorable contacts approach. Journal of Computational Chemistry, 2015, 36, 539-552.	1.5	3
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.	1.2	16
52	Dynamics Based Pharmacophore Models for Screening Potential Inhibitors of Mycobacterial Cyclopropane Synthase. Journal of Chemical Information and Modeling, 2015, 55, 848-860.	2.5	48
53	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.	1.3	3
54	Small-molecule inhibitors of ERK-mediated immediate early gene expression and proliferation of melanoma cells expressing mutated BRaf. Biochemical Journal, 2015, 467, 425-438.	1.7	35

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55	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.	1.2	9
56	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.	1.2	29
57	Nucleobases tagged to gold nanoclusters cause a mechanistic crossover in the oxidation of CO. Physical Chemistry Chemical Physics, 2015, 17, 24275-24281.	1.3	7
58	Atomistic Detailed Mechanism and Weak Cation-Conducting Activity of HIV-1 Vpu Revealed by Free Energy Calculations. PLoS ONE, 2014, 9, e112983.	1.1	8
59	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.	1.3	19
60	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.	1.7	6
61	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.	1.2	15
62	Role of conformational properties on the transannular Dielsâ€“Alder reactivity of macrocyclic trienes with varying linker lengths. RSC Advances, 2013, 3, 15892.	1.7	1
63	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.	1.0	0
64	Structures, Dynamics, and Stabilities of Fully Modified Locked Nucleic Acid (Î²-<scp>d</scp>-LNA and) Tj ETQq0 0 0 rgBT /Overlock 10 T Chemistry B, 2013, 117, 5556-5564.	1.2	23
65	Crenarchaeal chromatin proteins Cren7 and Sul7 compact DNA by inducing rigid bends. Nucleic Acids Research, 2013, 41, 196-205.	6.5	39
66	Solventâ€Induced Helical Assembly and Reversible Chiroptical Switching of Chiral Cyclicâ€Dipeptideâ€Functionalized Naphthalenediimides. Chemistry - A European Journal, 2013, 19, 16615-16624.	1.7	61
67	Molecular Dynamics Simulations Reveal the HIV-1 Vpu Transmembrane Protein to Form Stable Pentamers. PLoS ONE, 2013, 8, e79779.	1.1	20
68	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.	1.7	7
69	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.	2.0	20
70	Computational investigation of the effect of thermal perturbation on the mechanical unfolding of titin I27. Journal of Molecular Modeling, 2012, 18, 2823-2829.	0.8	8
71	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.	0.8	2
72	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.	1.5	341

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73	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.	1.2	24
74	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.	1.2	13
75	Atomistic Details of the Ligand Discrimination Mechanism of S_{MK}/SAM-III Riboswitch. Journal of Physical Chemistry B, 2010, 114, 9920-9925.	1.2	12
76	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.	2.0	55
77	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.	6.6	73
78	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.	1.2	19
79	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.	2.3	47
80	Computational Approaches for Investigating Base Flipping in Oligonucleotides. Chemical Reviews, 2006, 106, 489-505.	23.0	85
81	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.	6.6	38
82	Conformational Determinants of Tandem GU Mismatches in RNA:â€‰ Insights from Molecular Dynamics Simulations and Quantum Mechanical Calculations. Biochemistry, 2005, 44, 1433-1443.	1.2	24
83	A Lipophilic Hexaporphyrin Assembly Supported on a Stannoxane Core. Journal of the American Chemical Society, 2005, 127, 2410-2411.	6.6	51
84	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.	0.7	44
85	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
86	Facile valence isomerization among bis(silacyclopropenyl), disila(Dewar benzene) and disilabenzvalene. Journal of Organometallic Chemistry, 2004, 689, 1284-1287.	0.8	6
87	Basis set and method dependence of the relative energies of C2S2H2 isomers. Chemical Physics Letters, 2004, 383, 192-197.	1.2	10
88	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.	1.1	80
89	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
90	Silaaromaticity in Polycyclic Systems: A Computational Study. Journal of Organic Chemistry, 2003, 68, 1168-1171.	1.7	14

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91	Theoretical Study of Silabenzene and Its Valence Isomers. Organometallics, 2002, 21, 1493-1499.	1.1	29
92	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 ETQq1 0 0 rgBT /Overloc	1.7	81
93	Isomers of Disilabenzene (C4Si2H6):Â A Computational Study. Organometallics, 2002, 21, 4823-4832.	1.1	22
94	A computational study of the valence isomers of benzene and their group V hetero analogs. New Journal of Chemistry, 2002, 26, 347-353.	1.4	25
95	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
96	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.	1.7	70
97	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.	1.1	81
98	Theoretical studies on the effect of sequential benzannulation to corannulene. Computational and Theoretical Chemistry, 2001, 543, 1-10.	1.5	26
99	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.	6.6	28