

U Deva Priyakumar

List of Publications by Year in descending order

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99
papers

2,627
citations

185998

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233125

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136
all docs

136
docs citations

136
times ranked

2894
citing authors

#	ARTICLE	IF	CITATIONS
1	Impact of 2-â€œhydroxyl sampling on the conformational properties of RNA: Update of the CHARMM all-atom additive force field for RNA. <i>Journal of Computational Chemistry</i> , 2011, 32, 1929-1943.	1.5	341
2	MolGPT: Molecular Generation Using a Transformer-Decoder Model. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2064-2076.	2.5	105
3	Computational Approaches for Investigating Base Flipping in Oligonucleotides. <i>Chemical Reviews</i> , 2006, 106, 489-505.	23.0	85
4	First ab Initio and Density Functional Study on the Structure, Bowl-to-Bowl Inversion Barrier, and Vibrational Spectra of the Elusive C _{3v} -Symmetric Buckybowl:â€œ Sumanene, C ₂₁ H ₁₂ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 4488-4494.	1.1	81
5	Exploration of C ₆ H ₆ Potential Energy Surface: A Computational Effort to Unravel the Relative Stabilities and Synthetic Feasibility of New Benzene Isomers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11433-11448.	1.1	80
6	Urea Destabilizes RNA by Forming Stacking Interactions and Multiple Hydrogen Bonds with Nucleic Acid Bases. <i>Journal of the American Chemical Society</i> , 2009, 131, 17759-17761.	6.6	73
7	Machine Learning Based Clinical Decision Support System for Early COVID-19 Mortality Prediction. <i>Frontiers in Public Health</i> , 2021, 9, 626697.	1.3	72
8	Heterobuckybowls: A Theoretical Study on the Structure, Bowl-to-Bowl Inversion Barrier, Bond Length Alternation, Structure-Inversion Barrier Relationship, Stability, and Synthetic Feasibility. <i>Journal of Organic Chemistry</i> , 2001, 66, 6523-6530.	1.7	70
9	Solvent-Induced Helical Assembly and Reversible Chiroptical Switching of Chiral Cyclic Dipeptide-Functionalized Naphthalenediimides. <i>Chemistry - A European Journal</i> , 2013, 19, 16615-16624.	1.7	61
10	Role of the Adenine Ligand on the Stabilization of the Secondary and Tertiary Interactions in the Adenine Riboswitch. <i>Journal of Molecular Biology</i> , 2010, 396, 1422-1438.	2.0	55
11	A Lipophilic Hexaporphyrin Assembly Supported on a Stannoxane Core. <i>Journal of the American Chemical Society</i> , 2005, 127, 2410-2411.	6.6	51
12	Dynamics Based Pharmacophore Models for Screening Potential Inhibitors of Mycobacterial Cyclopropane Synthase. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 848-860.	2.5	48
13	Base Flipping in a GCGC Containing DNA Dodecamer: A Comparative Study of the Performance of the Nucleic Acid Force Fields, CHARMM, AMBER, and BMS. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 187-200.	2.3	47
14	Role of Urea-Induced Aromatic Stacking Interactions in Stabilizing the Aromatic Residues of the Protein in Urea-Induced Denatured State. <i>Journal of the American Chemical Society</i> , 2017, 139, 14931-14946.	6.6	47
15	On the use of NICS criterion to evaluate aromaticity in heteroaromatics involving III and IV row main group elements. <i>Computational and Theoretical Chemistry</i> , 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. <i>Tetrahedron Letters</i> , 2004, 45, 1515-1517.	0.7	44
17	Host metabolic reprogramming in response to SARS-CoV-2 infection: A systems biology approach. <i>Microbial Pathogenesis</i> , 2021, 158, 105114.	1.3	44
18	A Theoretical Study of the Structures, Energetics, Stabilities, Reactivities, and Out-of-Plane Distortive Tendencies of Skeletally Substituted Benzenes (CH) ₅ XH and (CH) ₄ (XH) ₂ (X = B-, N+, Al-, Si, P+, Ga-, Ge-, and Tl). <i>Journal of Physical Chemistry A</i> , 2000, 104, 1000-1008.	0.0	41

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19	DeepPocket: Ligand Binding Site Detection and Segmentation using 3D Convolutional Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5069-5079.	2.5	41
20	Crenarchaeal chromatin proteins Cren7 and Sul7 compact DNA by inducing rigid bends. <i>Nucleic Acids Research</i> , 2013, 41, 196-205.	6.5	39
21	NMR Imino Proton Exchange Experiments on Duplex DNA Primarily Monitor the Opening of Purine Bases. <i>Journal of the American Chemical Society</i> , 2006, 128, 678-679.	6.6	38
22	Enantioseparation and chiral induction in Ag ₂₉ nanoclusters with intrinsic chirality. <i>Chemical Science</i> , 2020, 11, 2394-2400.	3.7	37
23	Small-molecule inhibitors of ERK-mediated immediate early gene expression and proliferation of melanoma cells expressing mutated BRAf. <i>Biochemical Journal</i> , 2015, 467, 425-438.	1.7	35
24	Machine Learning for Accurate Force Calculations in Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6954-6967.	1.1	35
25	Artificial intelligence: machine learning for chemical sciences. <i>Journal of Chemical Sciences</i> , 2022, 134, 2.	0.7	32
26	Theoretical Study of Silabenzene and Its Valence Isomers. <i>Organometallics</i> , 2002, 21, 1493-1499.	1.1	29
27	Molecular Dynamics Study of the Structure, Flexibility, and Hydrophilicity of PETIM Dendrimers: A Comparison with PAMAM Dendrimers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12990-13001.	1.2	29
28	Structures, Energetics, Relative Stabilities, and Out-of-Plane Distortivities of Skeletally Disubstituted Benzenes, (CH) ₄ X ₂ (X = N, P, C-, Si-, O+, and S+): An ab Initio and DFT Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 11173-11181.	6.6	28
29	Deep learning enabled inorganic material generator. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26935-26943.	1.3	27
30	Theoretical studies on the effect of sequential benzannulation to corannulene. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 1-10.	1.5	26
31	Sumoylation of Sir2 differentially regulates transcriptional silencing in yeast. <i>Nucleic Acids Research</i> , 2015, 43, gkv842.	6.5	26
32	Structure, Interaction, and Dynamics of Au/Pd Bimetallic Nanoalloys Dispersed in Aqueous Ethylpyrrolidone, a Monomeric Moiety of Polyvinylpyrrolidone. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17454-17464.	1.5	26
33	BAND NN: A Deep Learning Framework for Energy Prediction and Geometry Optimization of Organic Small Molecules. <i>Journal of Computational Chemistry</i> , 2020, 41, 790-799.	1.5	26
34	MEMES: Machine learning framework for Enhanced MolEcular Screening. <i>Chemical Science</i> , 2021, 12, 11710-11721.	3.7	26
35	Molecular representations for machine learning applications in chemistry. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	26
36	A computational study of the valence isomers of benzene and their group V hetero analogs. <i>New Journal of Chemistry</i> , 2002, 26, 347-353.	1.4	25

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37	Conformational Determinants of Tandem GU Mismatches in RNA: Insights from Molecular Dynamics Simulations and Quantum Mechanical Calculations. <i>Biochemistry</i> , 2005, 44, 1433-1443.	1.2	24
38	Structural and Energetic Determinants of Thermal Stability and Hierarchical Unfolding Pathways of Hyperthermophilic Proteins, Sac7d and Sso7d. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1707-1718.	1.2	24
39	Structures, Dynamics, and Stabilities of Fully Modified Locked Nucleic Acid (\hat{I}^2 -LNA and) Tj ETQq1 1 0.784314 rgBT /Ov Chemistry B, 2013, 117, 5556-5564.	1.2	23
40	Isomers of Disilabenzene (C4Si2H6): A Computational Study. <i>Organometallics</i> , 2002, 21, 4823-4832.	1.1	22
41	Cholic Acid-Derived Amphiphile which Combats Gram-Positive Bacteria-Mediated Infections via Disintegration of Lipid Clusters. <i>ACS Biomaterials Science and Engineering</i> , 2019, 5, 4764-4775.	2.6	22
42	MoleGuLAR: Molecule Generation Using Reinforcement Learning with Alternating Rewards. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5815-5826.	2.5	22
43	Chemically Interpretable Graph Interaction Network for Prediction of Pharmacokinetic Properties of Drug-Like Molecules. <i>Proceedings of the AAAI Conference on Artificial Intelligence</i> , 2020, 34, 873-880.	3.6	21
44	Learning Atomic Interactions through Solvation Free Energy Prediction Using Graph Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 689-698.	2.5	21
45	Role of Hydrophobic Core on the Thermal Stability of Proteins Molecular Dynamics Simulations on a Single Point Mutant of Sso7d. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 29, 961-971.	2.0	20
46	Molecular Dynamics Simulations Reveal the HIV-1 Vpu Transmembrane Protein to Form Stable Pentamers. <i>PLoS ONE</i> , 2013, 8, e79779.	1.1	20
47	Atomic Detail Investigation of the Structure and Dynamics of DNA-RNA Hybrids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1515-1524.	1.2	19
48	DNA-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. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18148-18155.	1.3	19
49	Urea-aromatic interactions in biology. <i>Biophysical Reviews</i> , 2020, 12, 65-84.	1.5	18
50	Modern machine learning for tackling inverse problems in chemistry: molecular design to realization. <i>Chemical Communications</i> , 2022, 58, 5316-5331.	2.2	18
51	Dispersion Interactions between Urea and Nucleobases Contribute to the Destabilization of RNA by Urea in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3755-3761.	1.2	16
52	Microsecond simulation of human aquaporin 2 reveals structural determinants of water permeability and selectivity. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 10-16.	1.4	16
53	COVID-19 Risk Stratification and Mortality Prediction in Hospitalized Indian Patients: Harnessing clinical data for public health benefits. <i>PLoS ONE</i> , 2022, 17, e0264785.	1.1	16
54	Atomistic Investigation of the Effect of Incremental Modification of Deoxyribose Sugars by Locked Nucleic Acid (\hat{I}^2 -LNA and \hat{I}^{\pm} -LNA) Moieties on the Structures and Thermodynamics of DNA-RNA Hybrid Duplexes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5853-5863.	1.2	15

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55	Silaaromaticity in Polycyclic Systems: A Computational Study. <i>Journal of Organic Chemistry</i> , 2003, 68, 1168-1171.	1.7	14
56	Urea Mimics Nucleobases by Preserving the Helical Integrity of B-DNA Duplexes via Hydrogen Bonding and Stacking Interactions. <i>Biochemistry</i> , 2016, 55, 5653-5664.	1.2	14
57	SCONES: Self-Consistent Neural Network for Protein Stability Prediction Upon Mutation. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10657-10671.	1.2	14
58	Molecular Simulations on the Thermal Stabilization of DNA by Hyperthermophilic Chromatin Protein Sac7d, and Associated Conformational Transitions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16548-16557.	1.2	13
59	Atomistic Details of the Ligand Discrimination Mechanism of S ⁺ MK ⁺ /SAM-III Riboswitch. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9920-9925.	1.2	12
60	C21H9Z (Z=+3 to +3): a theoretical study on the redox behaviour of C3 symmetric fragment of C60. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 69-75.	1.5	11
61	Transition between [R]- and [S]-stereoisomers without bond breaking. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14983-14991.	1.3	11
62	Basis set and method dependence of the relative energies of C2S2H2 isomers. <i>Chemical Physics Letters</i> , 2004, 383, 192-197.	1.2	10
63	Gold-Palladium Nanocluster Catalysts for Homocoupling: Electronic Structure and Interface Dynamics. <i>Chemical Record</i> , 2019, 19, 947-959.	2.9	10
64	The effect of bulky group substitution on the skeleton, geometries, relative energies and the reactivities of silabenzene valence isomers. <i>Computational and Theoretical Chemistry</i> , 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. <i>RSC Advances</i> , 2015, 5, 49408-49419.	1.7	9
66	Ion Hydration Dynamics in Conjunction with a Hydrophobic Gating Mechanism Regulates Ion Permeation in p7 Viroporin from Hepatitis C Virus. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6204-6210.	1.2	9
67	Urea-Aromatic Stacking and Concerted Urea Transport: Conserved Mechanisms in Urea Transporters Revealed by Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5190-5200.	2.3	9
68	Desolvation of Peptide Bond by O to S Substitution Impacts Protein Stability. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24870-24874.	7.2	9
69	Computational investigation of the effect of thermal perturbation on the mechanical unfolding of titin I27. <i>Journal of Molecular Modeling</i> , 2012, 18, 2823-2829.	0.8	8
70	Atomistic Detailed Mechanism and Weak Cation-Conducting Activity of HIV-1 Vpu Revealed by Free Energy Calculations. <i>PLoS ONE</i> , 2014, 9, e112983.	1.1	8
71	Energetic, Structural and Dynamic Properties of Nucleobase-Urea Interactions that Aid in Urea Assisted RNA Unfolding. <i>Scientific Reports</i> , 2019, 9, 8805.	1.6	8
72	Transannular Diels-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. <i>Journal of Organic Chemistry</i> , 2012, 77, 5371-5380.	1.7	7

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73	Nucleobases tagged to gold nanoclusters cause a mechanistic crossover in the oxidation of CO. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24275-24281.	1.3	7
74	Selectivity and transport in aquaporins from molecular simulation studies. <i>Vitamins and Hormones</i> , 2020, 112, 47-70.	0.7	7
75	DART: deep learning enabled topological interaction model for energy prediction of metal clusters and its application in identifying unique low energy isomers. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21995-22003.	1.3	7
76	Facile valence isomerization among bis(silacyclopropenyl), disila(Dewar benzene) and disilabenzvalene. <i>Journal of Organometallic Chemistry</i> , 2004, 689, 1284-1287.	0.8	6
77	Modulation of structural, energetic and electronic properties of DNA and size-expanded DNA bases upon binding to gold clusters. <i>RSC Advances</i> , 2014, 4, 29642-29651.	1.7	6
78	A Probabilistic Framework for Constructing Temporal Relations in Replica Exchange Molecular Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3365-3380.	2.3	6
79	Multiscale Modeling of Wobble to Watson-Crick-Like Guanine-Uracil Tautomerization Pathways in RNA. <i>International Journal of Molecular Sciences</i> , 2021, 22, 5411.	1.8	6
80	BiRDS - Binding Residue Detection from Protein Sequences Using Deep ResNets. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1809-1818.	2.5	6
81	Deep Reinforcement Learning for Molecular Inverse Problem of Nuclear Magnetic Resonance Spectra to Molecular Structure. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4924-4933.	2.1	6
82	Cooperation of Hydrophobic Gating, Knock-on Effect, and Ion Binding Determines Ion Selectivity in the p7 Channel. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4351-4356.	1.2	5
83	Synthesis and reactivity of NHC-coordinated phosphinidene oxide. <i>Chemical Communications</i> , 2021, 57, 9546-9549.	2.2	5
84	Computational modeling of the catalytic mechanism of hydroxymethylbilane synthase. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7932-7940.	1.3	4
85	Benchmark study on deep neural network potentials for small organic molecules. <i>Journal of Computational Chemistry</i> , 2022, 43, 308-318.	1.5	4
86	Modeling the structure of SARS 3a transmembrane protein using a minimum unfavorable contact approach. <i>Journal of Chemical Sciences</i> , 2015, 127, 2159-2169.	0.7	3
87	Prediction of the structures of helical membrane proteins based on a minimum unfavorable contacts approach. <i>Journal of Computational Chemistry</i> , 2015, 36, 539-552.	1.5	3
88	Inclusion of methoxy groups inverts the thermodynamic stabilities of DNA-RNA hybrid duplexes: A molecular dynamics simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 61, 150-159.	1.3	3
89	pH-mediated gating and formate transport mechanism in the <i>Escherichia coli</i> formate channel. <i>Molecular Simulation</i> , 2017, 43, 1300-1306.	0.9	3
90	Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems. <i>Atoms</i> , 2021, 9, 79.	0.7	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. <i>Journal of Molecular Modeling</i> , 2012, 18, 3181-3197.	0.8	2
92	Quantum mechanical investigation of the nature of nucleobase-urea stacking interaction, a crucial driving force in RNA unfolding in aqueous urea. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	2
93	Urea-water solvation of protein side chain models. <i>Journal of Molecular Liquids</i> , 2020, 311, 113191.	2.3	2
94	Linear Prediction Residual for Efficient Diagnosis of Parkinson's Disease from Gait. <i>Lecture Notes in Computer Science</i> , 2021, , 614-623.	1.0	2
95	Role of conformational properties on the transannular Diels-Alder reactivity of macrocyclic trienes with varying linker lengths. <i>RSC Advances</i> , 2013, 3, 15892.	1.7	1
96	Recent Advancements in Computing Reliable Binding Free Energies in Drug Discovery Projects. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 221-246.	0.6	1
97	Ion Selectivity and Permeation Mechanism in a Cyclodextrin-Based Channel. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8028-8037.	1.2	1
98	Synthesis and Reactivity Studies of Dicationic Dihydrogen Complexes Bearing Sulfur Donor Ligands: A Combined Experimental and Computational Study. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 1434-1443.	1.0	0
99	A Model of Graph Transactional Coverage Patterns with Applications to Drug Discovery. , 2021, , .		0