Dhananjay Bhattacharyya

List of Publications by Year
in descending order

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91	1,697	304743	345221
papers	citations	22 h-index	36 g-index

94	94	94	1362
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interaction of Nucleobases with Wrinkled Graphene Surface: Dispersion Corrected DFT and AFM Studies. Journal of Physical Chemistry C, 2012, 116, 4374-4379.	3.1	88
2	NUPARM and NUCGEN: software for analysis and generation of sequence dependent nucleic acid structures. Bioinformatics, 1995, 11, 281-287.	4.1	74
3	Role of Hydrogen Bonds in Proteinâ^'DNA Recognition:Â Effect of Nonplanar Amino Groups. Journal of Physical Chemistry B, 2005, 109, 10484-10492.	2.6	72
4	Non-Canonical Base Pairs and Higher Order Structures in Nucleic Acids: Crystal Structure Database Analysis. Journal of Biomolecular Structure and Dynamics, 2006, 24, 149-161.	3.5	60
5	RNA structure and dynamics: A base pairing perspective. Progress in Biophysics and Molecular Biology, 2013, 113, 264-283.	2.9	58
6	Local Variability and Base Sequence Effects in DNA Crystal Structures. Journal of Biomolecular Structure and Dynamics, 1990, 8, 539-572.	3.5	55
7	Trans Hoogsteen/Sugar Edge Base Pairing in RNA. Structures, Energies, and Stabilities from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2009, 113, 1743-1755.	2.6	55
8	Conformational specificity of non-canonical base pairs and higher order structures in nucleic acids: crystal structure database analysis. Journal of Computer-Aided Molecular Design, 2006, 20, 629-645.	2.9	54
9	Differential Interactions of the Mg2+Complexes of Chromomycin A3and Mithramycin with Poly(dG-dC)Â·Poly(dC-dG) and Poly(dG)Â·Poly(dC). Biochemistry, 1997, 36, 2291-2299.	2.5	51
10	Structure, Stability, and Dynamics of Canonical and Noncanonical Base Pairs:â€‰ Quantum Chemical Studies. Journal of Physical Chemistry B, 2008, 112, 3786-3796.	2.6	50
11	Quantum Chemical Studies of Structures and Binding in Noncanonical RNA Base pairs: The Trans Watson-Crick:Watson-Crick Family. Journal of Biomolecular Structure and Dynamics, 2008, 25, 709-732.	3.5	50
12	Structural basis of DNA recognition by anticancer antibiotics, chromomycin A3, and mithramycin: Roles of minor groove width and ligand flexibility. Biopolymers, 2000, 56, 85-95.	2.4	49
13	Theoretical analysis of noncanonical base pairing interactions in RNA molecules. Journal of Biosciences, 2007, 32, 809-825.	1.1	46
14	A Self-Consistent Formulation for Analysis and Generation of Non-Uniform DNA Structures. Journal of Biomolecular Structure and Dynamics, 1989, 6, 635-653.	3.5	45
15	Protonation of Base Pairs in RNA: Context Analysis and Quantum Chemical Investigations of Their Geometries and Stabilities. Journal of Physical Chemistry B, 2011, 115, 1469-1484.	2.6	44
16	Groove Width and Depth of B-DNA Structures Depend on Local Variation in Slide. Journal of Biomolecular Structure and Dynamics, 1992, 10, 213-226.	3.5	39
17	Feasibility of occurrence of different types of protonated base pairs in RNA: a quantum chemical study. Physical Chemistry Chemical Physics, 2014, 16, 18383-18396.	2.8	36
18	On the Role of the cis Hoogsteen:Sugar-Edge Family of Base Pairs in Platforms and Tripletsâ€"Quantum Chemical Insights into RNA Structural Biology. Journal of Physical Chemistry B, 2010, 114, 3307-3320.	2.6	33

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19	Self-Complementarity within Proteins: Bridging the Gap between Binding and Folding. Biophysical Journal, 2012, 102, 2605-2614.	0.5	32
20	Characterization of Unfolding Mechanism of Human Lamin A Ig Fold by Single-Molecule Force Spectroscopyâ€"Implications in EDMD. Biochemistry, 2014, 53, 7247-7258.	2.5	27
21	Comparative analysis of 16S rRNA signature sequences of the genus Idiomarina and Idiomarina woesei sp. nov., a novel marine bacterium isolated from the Andaman Sea. Research in Microbiology, 2014, 165, 501-507.	2.1	27
22	The role of N7 protonation of guanine in determining the structure, stability and function of RNA base pairs. Physical Chemistry Chemical Physics, 2015, 17, 26249-26263.	2.8	27
23	Sequence Directed Flexibility of DNA and the Role of Cross-strand Hydrogen Bonds. Journal of Biomolecular Structure and Dynamics, 1999, 17, 289-300.	3.5	25
24	Analysis of stacking overlap in nucleic acid structures: algorithm and application. Journal of Computer-Aided Molecular Design, 2014, 28, 851-867.	2.9	24
25	HD-RNAS: An Automated Hierarchical Database of RNA Structures. Frontiers in Genetics, 2012, 3, 59.	2.3	23
26	Influence of divalent magnesium ion on DNA: molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2013, 31, 896-912.	3.5	22
27	Structure and Energy of Non-Canonical Basepairs: Comparison of Various Computational Chemistry Methods with Crystallographic Ensembles. Journal of Biomolecular Structure and Dynamics, 2011, 29, 541-556.	3.5	21
28	Estimating Strengths of Individual Hydrogen Bonds in RNA Base Pairs: Toward a Consensus between Different Computational Approaches. ACS Omega, 2019, 4, 7354-7368.	3.5	21
29	Structural properties of polymeric DNA from molecular dynamics simulations. Journal of Chemical Physics, 2009, 130, 115103.	3.0	20
30	Skeletal Muscle Dystrophy mutant of lamin A alters the structure and dynamics of the Ig fold domain. Scientific Reports, 2018, 8, 13793.	3.3	20
31	Consequences of Mg²⁺ binding on the geometry and stability of RNA base pairs. Physical Chemistry Chemical Physics, 2018, 20, 21934-21948.	2.8	20
32	Engineered Histidine-Enriched Facial Lipopeptides for Enhanced Intracellular Delivery of Functional siRNA to Triple Negative Breast Cancer Cells. ACS Applied Materials & Interfaces, 2019, 11, 4719-4736.	8.0	20
33	Structural Stability of Tandemly Occurring Noncanonical Basepairs within Double Helical Fragments: Molecular Dynamics Studies of Functional RNA. Journal of Physical Chemistry B, 2010, 114, 14028-14040.	2.6	19
34	Structure dependent hydrophobic and hydrophilic interactions between nickel(II) Schiff base complexes and serum albumins: Spectroscopic and docking studies. Journal of Luminescence, 2016, 171, 85-97.	3.1	18
35	Role of mg2+ in chromomycin a3 - DNA interaction: a molecular modeling study. Journal of Biological Physics, 2000, 26, 203-218.	1.5	17
36	Why Does Substitution of Thymine by 6-Ethynylpyridone Increase the Thermostability of DNA Double Helices?. Journal of Physical Chemistry B, 2014, 118, 6586-6596.	2.6	17

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37	Contribution of phenylalanine side chain intercalation to the TATA-box binding proteinâ€“DNA interaction: molecular dynamics and dispersion-corrected density functional theory studies. Journal of Molecular Modeling, 2014, 20, 2499.	1.8	15
38	RNABP COGEST: a resource for investigating functional RNAs. Database: the Journal of Biological Databases and Curation, 2015, 2015, .	3.0	15
39	Stacking interactions in RNA and DNA: Rollâ€slide energy hyperspace for ten unique dinucleotide steps. Biopolymers, 2015, 103, 134-147.	2.4	14
40	Structural Variations of Single and Tandem Mismatches in RNA Duplexes: A Joint MD Simulation and Crystal Structure Database Analysis. Journal of Physical Chemistry B, 2012, 116, 11845-11856.	2.6	13
41	Effect of temperature on DNA double helix: An insight from molecular dynamics simulation. Journal of Biosciences, 2012, 37, 445-455.	1.1	13
42	Twistâ€dependent stacking energy of baseâ€pair steps in Bâ€DNA geometry: A density functional theory approach. International Journal of Quantum Chemistry, 2008, 108, 1173-1180.	2.0	12
43	Sequence dependent variations in RNA duplex are related to non-canonical hydrogen bond interactions in dinucleotide steps. BMC Research Notes, 2014, 7, 83.	1.4	12
44	Equilibrium unfolding of cyclophilin from Leishmania donovani: Characterization of intermediate states. International Journal of Biological Macromolecules, 2014, 69, 353-360.	7.5	12
45	Stability and softening of a lipid monolayer in the presence of a pain-killer drug. Colloids and Surfaces B: Biointerfaces, 2015, 132, 34-44.	5.0	12
46	How Does Mg 2+ Modulate the RNA Folding Mechanism: A Case Study of the G:C W:W Trans Basepair. Biophysical Journal, 2017, 113, 277-289.	0.5	12
47	Energy hyperspace for stacking interaction in AU/AU dinucleotide step: Dispersionâ€corrected density functional theory study. Biopolymers, 2014, 101, 107-120.	2.4	11
48	Role of Mg²⁺in the Interaction of Anticancer Antibiotic, Chromomycin A₃with DNA: Does Neutral Antibiotic Bind DNA in Absence of the Metal Ion?. Journal of Biomolecular Structure and Dynamics, 2000, 18, 209-218.	3.5	10
49	Going beyond base-pairs: topology-based characterization of base-multiplets in RNA. Rna, 2019, 25, 573-589.	3.5	10
50	Plausible blockers of Spike RBD in SARS-CoV2â€”molecular design and underlying interaction dynamics from high-level structural descriptors. Journal of Molecular Modeling, 2021, 27, 191.	1.8	10
51	A comparison of four different conformations adopted by human telomeric Gâ€quadruplex using computer simulations. Biopolymers, 2016, 105, 83-99.	2.4	9
52	Application of multilayered strategy for variable selection in QSAR modeling of PET and SPECT imaging agents as diagnostic agents for Alzheimerâ€™s disease. Structural Chemistry, 2019, 30, 2429-2445.	2.0	9
53	Effect of Neighboring Bases on Base-Pair Stacking Orientation: A Molecular Dynamics Study. Journal of Biomolecular Structure and Dynamics, 2000, 18, 29-43.	3.5	8
54	Capturing state-dependent dynamic events of GABA_A-receptors: a microscopic look into the structural and functional insights. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1818-1837.	3.5	8

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55	RNAHelix: computational modeling of nucleic acid structures with Watsonâ€“Crick and non-canonical base pairs. Journal of Computer-Aided Molecular Design, 2017, 31, 219-235.	2.9	8
56	Engineering Ionophore Gramicidinâ€Inspired Selfâ€Assembled Peptides for Drug Delivery and Cancer Nanotherapeutics. Advanced Therapeutics, 2018, 1, 1800018.	3.2	8
57	Evidence for Hidden Involvement of N3-Protonated Guanine in RNA Structure and Function. ACS Omega, 2019, 4, 699-709.	3.5	8
58	Stacking geometry for nonâ€canonical G:U wobble base pair containing dinucleotide sequences in RNA: dispersionâ€corrected DFTâ€D study. Biopolymers, 2015, 103, 328-338.	2.4	7
59	Exploration of nitroimidazoles as radiosensitizers: application of multilayered feature selection approach in QSAR modeling. Structural Chemistry, 2020, 31, 1043-1055.	2.0	7
60	Temperature effect on poly(dA).poly(dT): molecular dynamics simulation studies of polymeric and oligomeric constructs. Journal of Computer-Aided Molecular Design, 2014, 28, 735-749.	2.9	6
61	Stacking interactions involving non-Watsonâ€“Crick basepairs: dispersion corrected density functional theory studies. Physical Chemistry Chemical Physics, 2017, 19, 28718-28730.	2.8	6
62	Exploring the major cross-talking edges of competitive endogenous RNA networks in human Chronic and Acute Myeloid Leukemia. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1883-1892.	2.4	6
63	Structural properties and influence of solvent on the stability of telomeric four-stranded i-motif DNA. Physical Chemistry Chemical Physics, 2019, 21, 21549-21560.	2.8	6
64	Sequence specificity in DNAâ€“drug intercalation: MD simulation and density functional theory approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 83-95.	2.9	6
65	Can the jigsaw puzzle model of protein folding reâ€assemble a hydrophobic core?. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1390-1412.	2.6	6
66	The Unfolding MD Simulations of Cyclophilin: Analyzed by Surface Contact Networks and Their Associated Metrics. PLoS ONE, 2015, 10, e0142173.	2.5	5
67	Engineered isopeptide bond stabilized fibrin inspired nanoscale peptide based sealants for efficient blood clotting. Scientific Reports, 2017, 7, 6509.	3.3	5
68	Melting of polymeric DNA double helix at elevated temperature: a molecular dynamics approach. Journal of Molecular Modeling, 2017, 23, 226.	1.8	5
69	Cross-talk between allosteric and orthosteric binding sites of Î³-amino butyric acid type A receptors (GABA_A-Rs): A computational study revealing the structural basis of selectivity. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3065-3080.	3.5	5
70	Contact networks in RNA: a structural bioinformatics study with a new tool. Journal of Computer-Aided Molecular Design, 2022, 36, 131.	2.9	4
71	Ab initio QM/MM study of excited state electron transfer between pyrene and 4,4?-bis(dimethylamino)-diphenylmethane with different solvent systems: Role of hydrogen bonding within solvent molecules. International Journal of Quantum Chemistry, 2005, 102, 368-378.	2.0	3
72	Ab initio studies on excited state intramolecular electron transfer in 4-amino-N-methylphthalimide and 3-amino-N-methylphthalimide. International Journal of Quantum Chemistry, 2006, 106, 913-927.	2.0	3

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73	Specific DNA sequences allosterically enhance proteinâ€“protein interaction in a transcription factor through modulation of protein dynamics: implications for specificity of gene regulation. Physical Chemistry Chemical Physics, 2017, 19, 14781-14792.	2.8	3
74	Stacking geometry between two sheared Watson-Crick basepairs: Computational chemistry and bioinformatics based prediction. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129600.	2.4	3
75	Energetics of Left and Right Handed Models of DNA. Journal of Biomolecular Structure and Dynamics, 1987, 4, 1027-1040.	3.5	2
76	Oxidative Tearing of Graphene Sheets: Insights into the Probable Situations by Computational and Experimental Studies. Journal of Physical Chemistry C, 2015, 119, 951-959.	3.1	2
77	Conformational selection underpins recognition of multiple DNA sequences by proteins and consequent functional actions. Physical Chemistry Chemical Physics, 2016, 18, 21618-21628.	2.8	2
78	Hybrid simulation approach incorporating microscopic interaction along with rigid body degrees of freedom for stacking between base pairs. Biopolymers, 2016, 105, 212-226.	2.4	2
79	DNA base sequence specificity through partial intercalation: DFT-D based energy analysis of molecular dynamics snapshots. Journal of Molecular Graphics and Modelling, 2020, 101, 107722.	2.4	2
80	Chemometric modeling of PET imaging agents for diagnosis of Parkinsonâ€™s disease: a QSAR approach. Structural Chemistry, 2020, 31, 1969-1981.	2.0	2
81	Maturation of siRNA by strand separation: Steered molecular dynamics study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13682-13692.	3.5	2
82	Structural basis of DNA flexibility. Indian Journal of Biochemistry and Biophysics, 2001, 38, 16-9.	0.0	2
83	RNABPDB: Molecular Modeling of RNA Structureâ€”From Base Pair Analysis in Crystals to Structure Prediction. Interdisciplinary Sciences, Computational Life Sciences, 2022, 14, 759-774.	3.6	2
84	Excited state hydrogen bonding fluorescent probe: Role of structure and environment. Journal of Luminescence, 2016, 173, 105-112.	3.1	1
85	Identification of a suitable promoter for the sigma factor of Mycobacterium tuberculosis. Molecular BioSystems, 2017, 13, 2370-2378.	2.9	1
86	Understanding the role of nonâ€Watsonâ€Crick base pairs in DNAâ€“protein recognition: Structural and energetic aspects using crystallographic database analysis and quantum chemical calculation. Biopolymers, 0, , .	2.4	1
87	MetBP: a software tool for detection of interaction between metal ionâ€“RNA base pairs. Bioinformatics, 2022, 38, 3833-3834.	4.1	1
88	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
89	Intrinsic structural variability in GNRA-like tetraloops: insight from molecular dynamics simulation. Journal of Molecular Modeling, 2017, 23, 300.	1.8	0
90	Effect of single-residue bulges on RNA double-helical structures: crystallographic database analysis and molecular dynamics simulation studies. Journal of Molecular Modeling, 2017, 23, 311.	1.8	0

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91	Peptidyl transferase activity of tRNA: a quantum chemical study. Indian Journal of Biochemistry and Biophysics, 2001, 38, 48-52.	0.0	0