

Nilesh K Banavali

List of Publications by Year in descending order

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49
papers

3,268
citations

279778

23
h-index

214788

47
g-index

55
all docs

55
docs citations

55
times ranked

4264
citing authors

#	ARTICLE	IF	CITATIONS
1	Development and current status of the CHARMM force field for nucleic acids. <i>Biopolymers</i> , 2000, 56, 257-265.	2.4	923
2	All-atom empirical force field for nucleic acids: II. Application to molecular dynamics simulations of DNA and RNA in solution. <i>Journal of Computational Chemistry</i> , 2000, 21, 105-120.	3.3	701
3	Existing drugs as broad-spectrum and potent inhibitors for Zika virus by targeting NS2B-NS3 interaction. <i>Cell Research</i> , 2017, 27, 1046-1064.	12.0	153
4	Free Energy and Structural Pathways of Base Flipping in a DNA GCGC Containing Sequence. <i>Journal of Molecular Biology</i> , 2002, 319, 141-160.	4.2	151
5	Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 68-73.	7.1	128
6	Free Energy Landscape of A-DNA to B-DNA Conversion in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2005, 127, 6866-6876.	13.7	122
7	Mapping the conformational transition in Src activation by cumulating the information from multiple molecular dynamics trajectories. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 3776-3781.	7.1	106
8	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11026-11035.	2.6	69
9	Novel Broad Spectrum Inhibitors Targeting the Flavivirus Methyltransferase. <i>PLoS ONE</i> , 2015, 10, e0130062.	2.5	58
10	Post-translational environmental switch of RadA activity by exteinâ€“intein interactions in protein splicing. <i>Nucleic Acids Research</i> , 2015, 43, 6631-6648.	14.5	54
11	Use of Oligodeoxyribonucleotides with Conformationally Constrained Abasic Sugar Targets To Probe the Mechanism of Base Flipping by HhaI DNA (Cytosine C5)-methyltransferase. <i>Journal of the American Chemical Society</i> , 2000, 122, 12422-12434.	13.7	51
12	Insertion domain within mammalian mitochondrial translation initiation factor 2 serves the role of eubacterial initiation factor 1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 3918-3923.	7.1	51
13	Selective inhibition of the West Nile virus methyltransferase by nucleoside analogs. <i>Antiviral Research</i> , 2013, 97, 232-239.	4.1	51
14	Identification and Characterization of Novel Broad-Spectrum Inhibitors of the Flavivirus Methyltransferase. <i>ACS Infectious Diseases</i> , 2015, 1, 340-349.	3.8	51
15	The N-Terminal End of the Catalytic Domain of Src Kinase Hck Is a Conformational Switch Implicated in Long-Range Allosteric Regulation. <i>Structure</i> , 2005, 13, 1715-1723.	3.3	45
16	Caught in the act: visualization of an intermediate in the DNA base-flipping pathway induced by HhaI methyltransferase. <i>Nucleic Acids Research</i> , 2004, 32, 3877-3886.	14.5	43
17	Anatomy of a structural pathway for activation of the catalytic domain of Src kinase Hck. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 1096-1112.	2.6	39
18	Flexibility and charge asymmetry in the activation loop of Src tyrosine kinases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 378-389.	2.6	38

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19	Electrostatic free energy calculations using the generalized solvent boundary potential method. <i>Journal of Chemical Physics</i> , 2002, 117, 7381-7388.	3.0	37
20	Reevaluation of Stereoelectronic Contributions to the Conformational Properties of the Phosphodiester and N ³ -Phosphoramidate Moieties of Nucleic Acids. <i>Journal of the American Chemical Society</i> , 2001, 123, 6747-6755.	13.7	36
21	Structures of the human mitochondrial ribosome bound to EF-G1 reveal distinct features of mitochondrial translation elongation. <i>Nature Communications</i> , 2020, 11, 3830.	12.8	36
22	Spliceosomal Prp8 intein at the crossroads of protein and RNA splicing. <i>PLoS Biology</i> , 2019, 17, e3000104.	5.6	28
23	Chemical activation of adenylyl cyclase Rv1625c inhibits growth of <i>Mycobacterium tuberculosis</i> on cholesterol and modulates intramacrophage signaling. <i>Molecular Microbiology</i> , 2017, 105, 294-308.	2.5	26
24	Conditional Protein Splicing Switch in Hyperthermophiles through an Intein-Extein Partnership. <i>MBio</i> , 2018, 9, .	4.1	26
25	<i>Mycobacterium</i> DnaB helicase intein as oxidative stress sensor. <i>Nature Communications</i> , 2018, 9, 4363.	12.8	26
26	INHIBITION OF (CYTOSINE C5)-METHYLTRANSFERASE BY OLIGONUCLEOTIDES CONTAINING FLEXIBLE (CYCLOPENTANE) AND CONFORMATIONALLY CONSTRAINED (BICYCLO[3.1.0]HEXANE) ABASIC SITES. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2001, 20, 451-459.	1.1	21
27	S-Adenosyl-Homocysteine Is a Weakly Bound Inhibitor for a Flaviviral Methyltransferase. <i>PLoS ONE</i> , 2013, 8, e76900.	2.5	18
28	Molecular Evidence for β -tubulin Neofunctionalization in Retaria (Foraminifera and Radiolarians). <i>Molecular Biology and Evolution</i> , 2013, 30, 2487-2493.	8.9	16
29	Ribosome hibernation: a new molecular framework for targeting nonreplicating persisters of mycobacteria. <i>Microbiology (United Kingdom)</i> , 2021, 167, .	1.8	16
30	Partial Base Flipping Is Sufficient for Strand Slippage near DNA Duplex Termini. <i>Journal of the American Chemical Society</i> , 2013, 135, 8274-8282.	13.7	14
31	Conserved Patterns in Backbone Torsional Changes Allow for Single Base Flipping from Duplex DNA with Minimal Distortion of the Double Helix. <i>Journal of Physical Chemistry B</i> , 2006, 110, 10997-11004.	2.6	12
32	A Low Affinity Ground State Conformation for the Dynein Microtubule Binding Domain. <i>Journal of Biological Chemistry</i> , 2010, 285, 15994-16002.	3.4	12
33	Modeling a Ryanodine Receptor N-terminal Domain Connecting the Central Vestibule and the Corner Clamp Region. <i>Journal of Biological Chemistry</i> , 2013, 288, 903-914.	3.4	10
34	Sterol A-ring plasticity in hedgehog protein cholesterolysis supports a primitive substrate selectivity mechanism. <i>Chemical Communications</i> , 2019, 55, 1829-1832.	4.1	10
35	The Mechanism of Cholesterol Modification of Hedgehog Ligand. <i>Journal of Computational Chemistry</i> , 2020, 41, 520-527.	3.3	10
36	Insights into Structural Basis of Mammalian Mitochondrial Translation. , 2013, , 1-28.		9

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37	<scp>RNA</scp> approaches the <scp>B</scp>â€œform in stacked single strand dinucleotide contexts. Biopolymers, 2016, 105, 65-82.	2.4	7
38	Distinct mechanisms of the human mitoribosome recycling and antibiotic resistance. Nature Communications, 2021, 12, 3607.	12.8	7
39	Development and current status of the CHARMM force field for nucleic acids. , 0, .		7
40	Characterizing Structural Transitions Using Localized Free Energy Landscape Analysis. PLoS ONE, 2009, 4, e5525.	2.5	7
41	Geometric Patterns for Neighboring Bases Near the Stacked State in Nucleic Acid Strands. Biochemistry, 2017, 56, 1426-1443.	2.5	6
42	General Base Swap Preserves Activity and Expands Substrate Tolerance in Hedgehog Autoprocessing. Journal of the American Chemical Society, 2019, 141, 18380-18384.	13.7	6
43	DNA bending induced by carbocyclic sugar analogs constrained to the north conformation. Biopolymers, 2007, 85, 438-449.	2.4	5
44	Cytosine Unstacking and Strand Slippage at an Insertionâ€œDeletion Mutation Sequence in an Overhang-Containing DNA Duplex. Biochemistry, 2014, 53, 3807-3816.	2.5	5
45	Maintenance of electrostatic stabilization in altered tubulin lateral contacts may facilitate formation of helical filaments in foraminifera. Scientific Reports, 2016, 6, 31723.	3.3	5
46	Computational Exploration of Structural Hypotheses for an Additional Sequence in a Mammalian Mitochondrial Protein. PLoS ONE, 2011, 6, e21871.	2.5	5
47	Analyzing the Relationship between Single Base Flipping and Strand Slippage near DNA Duplex Termini. Journal of Physical Chemistry B, 2013, 117, 14320-14328.	2.6	4
48	Structural Articulation of Biochemical Reactions Using Restrained Geometries and Topology Switching. Journal of Chemical Information and Modeling, 2018, 58, 453-463.	5.4	3
49	SufB intein splicing in <i>Mycobacterium tuberculosis</i> is influenced by two remote conserved N-extein histidines. Bioscience Reports, 2022, 42, .	2.4	1