

Nilesh K Banavali

List of Publications by Year in descending order

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49
papers

3,268
citations

279798

23
h-index

214800

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. Biopolymers, 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. Journal of Computational Chemistry, 2000, 21, 105-120.	3.3	701
3	Existing drugs as broad-spectrum and potent inhibitors for Zika virus by targeting NS2B-NS3 interaction. Cell Research, 2017, 27, 1046-1064.	12.0	153
4	Free Energy and Structural Pathways of Base Flipping in a DNA GCGC Containing Sequence. Journal of Molecular Biology, 2002, 319, 141-160.	4.2	151
5	Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 68-73.	7.1	128
6	Free Energy Landscape of A-DNA to B-DNA Conversion in Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 6866-6876.	13.7	122
7	Mapping the conformational transition in Src activation by cumulating the information from multiple molecular dynamics trajectories. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3776-3781.	7.1	106
8	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. Journal of Physical Chemistry B, 2002, 106, 11026-11035.	2.6	69
9	Novel Broad Spectrum Inhibitors Targeting the Flavivirus Methyltransferase. PLoS ONE, 2015, 10, e0130062.	2.5	58
10	Post-translational environmental switch of RadA activity by exteinâ€“intein interactions in protein splicing. Nucleic Acids Research, 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. Journal of the American Chemical Society, 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. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3918-3923.	7.1	51
13	Selective inhibition of the West Nile virus methyltransferase by nucleoside analogs. Antiviral Research, 2013, 97, 232-239.	4.1	51
14	Identification and Characterization of Novel Broad-Spectrum Inhibitors of the Flavivirus Methyltransferase. ACS Infectious Diseases, 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. Structure, 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. Nucleic Acids Research, 2004, 32, 3877-3886.	14.5	43
17	Anatomy of a structural pathway for activation of the catalytic domain of Src kinase Hck. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1096-1112.	2.6	39
18	Flexibility and charge asymmetry in the activation loop of Src tyrosine kinases. Proteins: Structure, Function and Bioinformatics, 2009, 74, 378-389.	2.6	38

#	ARTICLE	IF	CITATIONS
19	Electrostatic free energy calculations using the generalized solvent boundary potential method. Journal of Chemical Physics, 2002, 117, 7381-7388.	3.0	37
20	Reevaluation of Stereoelectronic Contributions to the Conformational Properties of the Phosphodiester and N3'-Phosphoramidate Moieties of Nucleic Acids. Journal of the American Chemical Society, 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. Nature Communications, 2020, 11, 3830.	12.8	36
22	Spliceosomal Prp8 intein at the crossroads of protein and RNA splicing. PLoS Biology, 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. Molecular Microbiology, 2017, 105, 294-308.	2.5	26
24	Conditional Protein Splicing Switch in Hyperthermophiles through an Intein-Extein Partnership. MBio, 2018, 9, .	4.1	26
25	Mycobacterial DnaB helicase intein as oxidative stress sensor. Nature Communications, 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. Nucleosides, Nucleotides and Nucleic Acids, 2001, 20, 451-459.	1.1	21
27	S-Adenosyl-Homocysteine Is a Weakly Bound Inhibitor for a Flaviviral Methyltransferase. PLoS ONE, 2013, 8, e76900.	2.5	18
28	Molecular Evidence for β -tubulin Neofunctionalization in Retaria (Foraminifera and Radiolarians). Molecular Biology and Evolution, 2013, 30, 2487-2493.	8.9	16
29	Ribosome hibernation: a new molecular framework for targeting nonreplicating persisters of mycobacteria. Microbiology (United Kingdom), 2021, 167, .	1.8	16
30	Partial Base Flipping Is Sufficient for Strand Slippage near DNA Duplex Termini. Journal of the American Chemical Society, 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. Journal of Physical Chemistry B, 2006, 110, 10997-11004.	2.6	12
32	A Low Affinity Ground State Conformation for the Dynein Microtubule Binding Domain. Journal of Biological Chemistry, 2010, 285, 15994-16002.	3.4	12
33	Modeling a Ryanodine Receptor N-terminal Domain Connecting the Central Vestibule and the Corner Clamp Region. Journal of Biological Chemistry, 2013, 288, 903-914.	3.4	10
34	Sterol A-ring plasticity in hedgehog protein cholesterolysis supports a primitive substrate selectivity mechanism. Chemical Communications, 2019, 55, 1829-1832.	4.1	10
35	The Mechanism of Cholesterol Modification of Hedgehog Ligand. Journal of Computational Chemistry, 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