Pratul K Agarwal

List of Publications by Year
in descending order

78 papers	3,510 citations	249298 26 h-index	169272 56 g-index
85 all docs	85 docs citations	85 times ranked	3987 citing authors

#	Article	IF	Citations
1	Mechanism of nucleotide discrimination by the translesion synthesis polymerase Rev1. Nature Communications, 2022, 13, .	5.8	4
2	On the Case of the Misplaced Hydrogens. ChemBioChem, 2021, 22, 288-297.	1.3	14
3	Altered APE1 activity on abasic ribonucleotides is mediated by changes in the nucleoside sugar pucker. Computational and Structural Biotechnology Journal, 2021, 19, 3293-3302.	1.9	6
4	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	2.8	44
5	Modulating Enzyme Function via Dynamic Allostery within Biliverdin Reductase B. Frontiers in Molecular Biosciences, 2021, 8, 691208.	1.6	5
6	Insights into Structural and Dynamical Changes Experienced by Human RNase 6 upon Ligand Binding. Biochemistry, 2020, 59, 755-765.	1.2	6
7	Application health monitoring for extremeâ€scale resiliency using cooperative fault management. Concurrency Computation Practice and Experience, 2020, 32, e5449.	1.4	2
8	Visualizing Rev1 catalyze protein-template DNA synthesis. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 25494-25504.	3.3	15
9	Myelin Basic Protein Phospholipid Complexation Likely Competes with Deimination in Experimental Autoimmune Encephalomyelitis Mouse Model. ACS Omega, 2020, 5, 15454-15467.	1.6	7
10	Structure, dynamics and function of the evolutionarily changing biliverdin reductase B family. Journal of Biochemistry, 2020, 168, 191-202.	0.9	9
11	AP-endonuclease 1 sculpts DNA through an anchoring tyrosine residue on the DNA intercalating loop. Nucleic Acids Research, 2020, 48, 7345-7355.	6.5	15
12	Enzyme Dynamics: Looking Beyond a Single Structure. ChemCatChem, 2020, 12, 4704-4720.	1.8	31
13	Electrostatic Switching Controls Channel Dynamics of the Sensor Protein VirB10 in A. tumefaciens Type IV Secretion System. ACS Omega, 2020, 5, 3271-3281.	1.6	6
14	Engineering Dynamic Surface Peptide Networks on Butyrylcholinesterase_{G117H} for Enhanced Organophosphosphorus Anticholinesterase Catalysis. Chemical Research in Toxicology, 2019, 32, 1801-1810.	1.7	3
15	Lowâ€Barrier and Canonical Hydrogen Bonds Modulate Activity and Specificity of a Catalytic Triad. Angewandte Chemie, 2019, 131, 16406-16412.	1.6	3
16	Lowâ€Barrier and Canonical Hydrogen Bonds Modulate Activity and Specificity of a Catalytic Triad. Angewandte Chemie - International Edition, 2019, 58, 16260-16266.	7.2	20
17	Evolution Conserves the Network of Coupled Residues in Dihydrofolate Reductase. Biochemistry, 2019, 58, 3861-3868.	1.2	3
18	Nucleotide substrate binding characterization in human pancreatic-type ribonucleases. PLoS ONE, 2019, 14, e0220037.	1.1	4

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19	Crowders Steal Dihydrofolate Reductase Ligands through Quinary Interactions. Biochemistry, 2019, 58, 1198-1213.	1.2	4
20	A Biophysical Perspective on Enzyme Catalysis. Biochemistry, 2019, 58, 438-449.	1.2	104
21	Functionally Important Conformational Subâ€States in Human Ribonuclease Family. FASEB Journal, 2019, 33, .	0.2	0
22	Conservation of Dynamics Associated with Biological Function in an Enzyme Superfamily. Structure, 2018, 26, 426-436.e3.	1.6	52
23	Differential Substrate Recognition by Maltose Binding Proteins Influenced by Structure and Dynamics. Biochemistry, 2018, 57, 5864-5876.	1.2	20
24	Ligand-Induced Variations in Structural and Dynamical Properties Within an Enzyme Superfamily. Frontiers in Molecular Biosciences, 2018, 5, 54.	1.6	30
25	Modulating Enzyme Activity by Altering Protein Dynamics with Solvent. Biochemistry, 2018, 57, 4263-4275.	1.2	26
26	CONFORMATIONAL FLUCTUATIONS RELATED TO CATALYSIS IN HUMAN RIBONUCLEASE SUPERFAMILY. FASEB Journal, 2018, 32, 527.1.	0.2	0
27	Oxygen Activation at the Active Site of a Fungal Lytic Polysaccharide Monooxygenase. Angewandte Chemie, 2017, 129, 785-788.	1.6	9
28	Applications of NMR and computational methodologies to study protein dynamics. Archives of Biochemistry and Biophysics, 2017, 628, 71-80.	1.4	30
29	Synthetic, Switchable Enzymes. Journal of Molecular Microbiology and Biotechnology, 2017, 27, 117-127.	1.0	419
30	Sequence-specific backbone resonance assignments and microsecond timescale molecular dynamics simulation of human eosinophil-derived neurotoxin. Biomolecular NMR Assignments, 2017, 11, 143-149.	0.4	6
31	Oxygen Activation at the Active Site of a Fungal Lytic Polysaccharide Monooxygenase. Angewandte Chemie - International Edition, 2017, 56, 767-770.	7.2	78
32	Innentitelbild: Oxygen Activation at the Active Site of a Fungal Lytic Polysaccharide Monooxygenase (Angew. Chem. 3/2017). Angewandte Chemie, 2017, 129, 674-674.	1.6	0
33	Small Angle Neutron Scattering Studies of R67 Dihydrofolate Reductase, a Tetrameric Protein with Intrinsically Disordered N-Termini. Biochemistry, 2017, 56, 5886-5899.	1.2	6
34	Periplasmic Binding Protein Dimer Has a Second Allosteric Event Tied to Ligand Binding. Biochemistry, 2017, 56, 5328-5337.	1.2	14
35	Tales of Dihydrofolate Binding to R67 Dihydrofolate Reductase. Biochemistry, 2016, 55, 133-145.	1.2	8
36	Ligand Binding Enhances Millisecond Conformational Exchange in Xylanase B2 from Streptomyces lividans. Biochemistry, 2016, 55, 4184-4196.	1.2	22

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37	Aspects of Weak Interactions between Folate and Glycine Betaine. Biochemistry, 2016, 55, 6282-6294.	1.2	6
38	Perturbation of the Conformational Dynamics of an Active-Site Loop Alters Enzyme Activity. Structure, 2015, 23, 2256-2266.	1.6	54
39	Protein Conformational Populations and Functionally Relevant Substates. Accounts of Chemical Research, 2014, 47, 149-156.	7.6	86
40	Performance modeling of microsecond scale biological molecular dynamics simulations on heterogeneous architectures. Concurrency Computation Practice and Experience, 2013, 25, 1356-1375.	1.4	15
41	Role of protein motions in function. Physics of Life Reviews, 2013, 10, 35-36.	1.5	4
42	Engineering a Hyper-catalytic Enzyme by Photoactivated Conformation Modulation. Journal of Physical Chemistry Letters, 2012, 3, 1142-1146.	2.1	33
43	Event detection and subâ€state discovery from biomolecular simulations using higherâ€order statistics: Application to enzyme adenylate kinase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2536-2551.	1.5	27
44	Nanoscale Ferroelectricity in Crystalline Î³â€Glycine. Advanced Functional Materials, 2012, 22, 2996-3003.	7.8	119
45	Quasi-anharmonic analysis reveals intermediate states in the nuclear co-activator receptor binding domain ensemble. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2012, , 70-81.	0.7	6
46	Redox-Promoting Protein Motions in Rubredoxin. Journal of Physical Chemistry B, 2011, 115, 8925-8936.	1.2	14
47	Discovering Conformational Sub-States Relevant to Protein Function. PLoS ONE, 2011, 6, e15827.	1.1	61
48	Evolutionarily Conserved Linkage between Enzyme Fold, Flexibility, and Catalysis. PLoS Biology, 2011, 9, e1001193.	2.6	107
49	Realization of User Level Fault Tolerant Policy Management through a Holistic Approach for Fault Correlation. , 2011, , .		6
50	QAARM: quasi-anharmonic autoregressive model reveals molecular recognition pathways in ubiquitin. Bioinformatics, 2011, 27, i52-i60.	1.8	16
51	Towards microsecond biological molecular dynamics simulations on hybrid processors. , 2010, , .		10
52	An Online Approach for Mining Collective Behaviors from Molecular Dynamics Simulations. Journal of Computational Biology, 2010, 17, 309-324.	0.8	27
53	Energy efficient biomolecular simulations with FPGA-based reconfigurable computing. , 2010, , .		4
54	The Tail Wagging the Dog: Insights into Catalysis in R67 Dihydrofolate Reductase. Biochemistry, 2010, 49, 9078-9088.	1.2	23

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55	Optimal Utilization of Heterogeneous Resources for Biomolecular Simulations. , 2010, , .		12
56	Computational Identification of Slow Conformational Fluctuations in Proteins. Journal of Physical Chemistry B, 2009, 113, 16669-16680.	1.2	45
57	An Online Approach for Mining Collective Behaviors from Molecular Dynamics Simulations. Lecture Notes in Computer Science, 2009, , 138-154.	1.0	6
58	Performance characteristics of biomolecular simulations on high-end systems with multi-core processors. Parallel Computing, 2008, 34, 640-651.	1.3	5
59	Implementation methodology for emerging reconfigurable systems. , 2008, , .		0
60	Impact of multicores on large-scale molecular dynamics simulations. Parallel and Distributed Processing Symposium (IPDPS), Proceedings of the International Conference on, 2008, , .	1.0	6
61	On the Path to Enable Multi-scale Biomolecular Simulations on PetaFLOPS Supercomputer with Multi-core Processors. , 2007, , .		7
62	Performance Evaluation of a Scalable Molecular Dynamics Simulation Framework on a Massively-Parallel System. , 2007, , .		0
63	Using FPGA Devices to Accelerate Biomolecular Simulations. Computer, 2007, 40, 66-73.	1.2	56
64	Simulating Biomolecules on the Petascale Supercomputers. Chapman & Hall/CRC Computational Science, 2007, , 211-235.	0.5	0
65	Enzymes: An integrated view of structure, dynamics and function. Microbial Cell Factories, 2006, 5, 2.	1.9	134
66	Computational challenges for modeling and simulating biomacromolecular assemblies. Journal of Physics: Conference Series, 2006, 46, 311-315.	0.3	1
67	Performance characterization of molecular dynamics techniques for biomolecular simulations. , 2006, , .		14
68	Biomolecular simulations on petascale: promises and challenges. Journal of Physics: Conference Series, 2006, 46, 327-333.	0.3	10
69	Role of Protein Dynamics in Reaction Rate Enhancement by Enzymes. Journal of the American Chemical Society, 2005, 127, 15248-15256.	6.6	175
70	Cis/trans isomerization in HIV-1 capsid protein catalyzed by cyclophilin A: Insights from computational and theoretical studies. Proteins: Structure, Function and Bioinformatics, 2004, 56, 449-463.	1.5	57
71	Protein Dynamics and Enzymatic Catalysis:â€‰Investigating the Peptidylâ^'Prolyl Cisâ^'Trans Isomerization Activity of Cyclophilin A. Biochemistry, 2004, 43, 10605-10618.	1.2	71
72	Effect of Mutation on Enzyme Motion in Dihydrofolate Reductase. Journal of the American Chemical Society, 2003, 125, 3745-3750.	6.6	112

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73	Nuclear Quantum Effects and Enzyme Dynamics in Dihydrofolate Reductase Catalysis. Journal of Physical Chemistry B, 2002, 106, 3283-3293.	1.2	178
74	Network of coupled promoting motions in enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 2794-2799.	3.3	448
75	Hydride Transfer in Liver Alcohol Dehydrogenase:â€‰ Quantum Dynamics, Kinetic Isotope Effects, and Role of Enzyme Motion. Journal of the American Chemical Society, 2001, 123, 11262-11272.	6.6	179
76	Hybrid approach for including electronic and nuclear quantum effects in molecular dynamics simulations of hydrogen transfer reactions in enzymes. Journal of Chemical Physics, 2001, 114, 6925-6936.	1.2	121
77	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. Journal of the American Chemical Society, 2000, 122, 4803-4812.	6.6	168
78	Combining Electronic Structure Methods with the Calculation of Hydrogen Vibrational Wavefunctions:Â Application to Hydride Transfer in Liver Alcohol Dehydrogenase. Journal of Physical Chemistry B, 2000, 104, 8884-8894.	1.2	54