

Marc Delarue

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7527248/publications.pdf>

Version: 2024-02-01

104
papers

8,073
citations

101496

36
h-index

49868

87
g-index

107
all docs

107
docs citations

107
times ranked

5974
citing authors

#	ARTICLE	IF	CITATIONS
1	Partition of tRNA synthetases into two classes based on mutually exclusive sets of sequence motifs. <i>Nature</i> , 1990, 347, 203-206.	13.7	1,372
2	X-ray structure of a pentameric ligand-gated ion channel in an apparently open conformation. <i>Nature</i> , 2009, 457, 111-114.	13.7	644
3	An attempt to unify the structure of polymerases. <i>Protein Engineering, Design and Selection</i> , 1990, 3, 461-467.	1.0	616
4	X-ray structures of general anaesthetics bound to a pentameric ligand-gated ion channel. <i>Nature</i> , 2011, 469, 428-431.	13.7	407
5	Application of a Self-consistent Mean Field Theory to Predict Protein Side-chains Conformation and Estimate Their Conformational Entropy. <i>Journal of Molecular Biology</i> , 1994, 239, 249-275.	2.0	347
6	NOMAD-Ref: visualization, deformation and refinement of macromolecular structures based on all-atom normal mode analysis. <i>Nucleic Acids Research</i> , 2006, 34, W52-W56.	6.5	292
7	Simplified Normal Mode Analysis of Conformational Transitions in DNA-dependent Polymerases: the Elastic Network Model. <i>Journal of Molecular Biology</i> , 2002, 320, 1011-1024.	2.0	243
8	Structure and Pharmacology of Pentameric Receptor Channels: From Bacteria to Brain. <i>Structure</i> , 2012, 20, 941-956.	1.6	202
9	On the use of low-frequency normal modes to enforce collective movements in refining macromolecular structural models. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 6957-6962.	3.3	187
10	Normal Mode Analysis Suggests a Quaternary Twist Model for the Nicotinic Receptor Gating Mechanism. <i>Biophysical Journal</i> , 2005, 88, 3954-3965.	0.2	178
11	Crystal structures of a pentameric ligand-gated ion channel provide a mechanism for activation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 966-971.	3.3	175
12	One-microsecond molecular dynamics simulation of channel gating in a nicotinic receptor homologue. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 6275-6280.	3.3	159
13	Structure of phenylalanyl-tRNA synthetase from <i>Thermus thermophilus</i> . <i>Nature Structural Biology</i> , 1995, 2, 537-547.	9.7	145
14	Structural basis for ion permeation mechanism in pentameric ligand-gated ion channels. <i>EMBO Journal</i> , 2013, 32, 728-741.	3.5	140
15	Crystal structures of a template-independent DNA polymerase: murine terminal deoxynucleotidyltransferase. <i>EMBO Journal</i> , 2002, 21, 427-439.	3.5	138
16	A locally closed conformation of a bacterial pentameric proton-gated ion channel. <i>Nature Structural and Molecular Biology</i> , 2012, 19, 642-649.	3.6	135
17	Structural basis for potentiation by alcohols and anaesthetics in a ligand-gated ion channel. <i>Nature Communications</i> , 2013, 4, 1697.	5.8	126
18	Structural Insights into the Quinolone Resistance Mechanism of <i>Mycobacterium tuberculosis</i> DNA Gyrase. <i>PLoS ONE</i> , 2010, 5, e12245.	1.1	118

#	ARTICLE	IF	CITATIONS
19	Crystal Structure of Cleaved Bovine Antithrombin III at 3Å ² Resolution. <i>Journal of Molecular Biology</i> , 1993, 232, 223-241.	2.0	110
20	Atomic structure and dynamics of pentameric ligand-gated ion channels: new insight from bacterial homologues. <i>Journal of Physiology</i> , 2010, 588, 565-572.	1.3	102
21	AquaSAXS: a web server for computation and fitting of SAXS profiles with non-uniformly hydrated atomic models. <i>Nucleic Acids Research</i> , 2011, 39, W184-W189.	6.5	91
22	Polar and nonpolar atomic environments in the protein core: Implications for folding and binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994, 20, 264-278.	1.5	86
23	Enzymatic and Structural Analysis of Inhibitors Designed against Mycobacterium tuberculosis Thymidylate Kinase. <i>Journal of Biological Chemistry</i> , 2003, 278, 4963-4971.	1.6	82
24	Mean-field minimization methods for biological macromolecules. <i>Current Opinion in Structural Biology</i> , 1996, 6, 222-226.	2.6	77
25	MinActionPath: maximum likelihood trajectory for large-scale structural transitions in a coarse-grained locally harmonic energy landscape. <i>Nucleic Acids Research</i> , 2007, 35, W477-W482.	6.5	76
26	Synthesis and Recognition of Aspartyl-adenylate by Thermus thermophilus Aspartyl-tRNA Synthetase. <i>Journal of Molecular Biology</i> , 1994, 244, 158-167.	2.0	73
27	Incorporating Dipolar Solvents with Variable Density in Poisson-Boltzmann Electrostatics. <i>Biophysical Journal</i> , 2008, 95, 5587-5605.	0.2	73
28	Refinement of docked protein-ligand and protein-DNA structures using low frequency normal mode amplitude optimization. <i>Nucleic Acids Research</i> , 2005, 33, 4496-4506.	6.5	62
29	PDB_Hydro: incorporating dipolar solvents with variable density in the Poisson-Boltzmann treatment of macromolecule electrostatics. <i>Nucleic Acids Research</i> , 2006, 34, W38-W42.	6.5	62
30	String method solution of the gating pathways for a pentameric ligand-gated ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E4158-E4167.	3.3	60
31	Allosteric and hyperekplexic mutant phenotypes investigated on an $\alpha 1$ glycine receptor transmembrane structure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 2865-2870.	3.3	56
32	Crystal Structure of the Extracellular Domain of a Bacterial Ligand-Gated Ion Channel. <i>Journal of Molecular Biology</i> , 2010, 395, 1114-1127.	2.0	52
33	An asymmetric underlying rule in the assignment of codons: Possible clue to a quick early evolution of the genetic code via successive binary choices. <i>Rna</i> , 2006, 13, 161-169.	1.6	47
34	Crystallographic studies of pharmacological sites in pentameric ligand-gated ion channels. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 511-523.	1.1	46
35	Structures of Intermediates along the Catalytic Cycle of Terminal Deoxynucleotidyltransferase: Dynamical Aspects of the Two-Metal Ion Mechanism. <i>Journal of Molecular Biology</i> , 2013, 425, 4334-4352.	2.0	41
36	Solution structural studies and low-resolution model of the Schizosaccharomyces pombe sap1 protein. <i>Journal of Molecular Biology</i> , 2000, 300, 563-574.	2.0	40

#	ARTICLE	IF	CITATIONS
37	Shared active site architecture between archaeal PolD and multi-subunit RNA polymerases revealed by X-ray crystallography. <i>Nature Communications</i> , 2016, 7, 12227.	5.8	40
38	Atomic Environment Energies in Proteins Defined from Statistics of Accessible and Contact Surface Areas. <i>Journal of Molecular Biology</i> , 1995, 249, 675-690.	2.0	36
39	Aspartyl tRNA-synthetase from <i>Escherichia coli</i> : flexibility and adaptability to the substrates. <i>Journal of Molecular Biology</i> , 2000, 299, 1157-1164.	2.0	36
40	Molecular Recognition of Canonical and Deaminated Bases by P. abyssii Family B DNA Polymerase. <i>Journal of Molecular Biology</i> , 2012, 423, 315-336.	2.0	36
41	Computational Assembly of Polymorphic Amyloid Fibrils Reveals Stable Aggregates. <i>Biophysical Journal</i> , 2013, 104, 683-693.	0.2	36
42	Identification of a pre-active conformation of a pentameric channel receptor. <i>ELife</i> , 2017, 6, .	2.8	36
43	Sites of Anesthetic Inhibitory Action on a Cationic Ligand-Gated Ion Channel. <i>Structure</i> , 2016, 24, 595-605.	1.6	35
44	Cryophotolysis of caged compounds: a technique for trapping intermediate states in protein crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 607-614.	2.5	34
45	An updated structural classification of replicative DNA polymerases. <i>Biochemical Society Transactions</i> , 2019, 47, 239-249.	1.6	34
46	Structural basis for the increased processivity of D-family DNA polymerases in complex with PCNA. <i>Nature Communications</i> , 2020, 11, 1591.	5.8	34
47	Enhanced Amino Acid Selection in Fully Evolved Tryptophanyl-tRNA Synthetase, Relative to Its Urzyme, Requires Domain Motion Sensed by the D1 Switch, a Remote Dynamic Packing Motif. <i>Journal of Biological Chemistry</i> , 2014, 289, 4367-4376.	1.6	33
48	Structural Basis for a Bimodal Allosteric Mechanism of General Anesthetic Modulation in Pentameric Ligand-Gated Ion Channels. <i>Cell Reports</i> , 2018, 23, 993-1004.	2.9	33
49	Structural Basis for Xenon Inhibition in a Cationic Pentameric Ligand-Gated Ion Channel. <i>PLoS ONE</i> , 2016, 11, e0149795.	1.1	31
50	Crystallization and X-ray Crystallographic Analysis of Recombinant Chicken Poly (ADP-ribose) Polymerase Catalytic Domain Produced in Sf9 Insect Cells. <i>Journal of Molecular Biology</i> , 1994, 244, 114-116.	2.0	30
51	Electrostatics, proton sensor, and networks governing the gating transition in GLIC, a proton-gated pentameric ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E12172-E12181.	3.3	30
52	Structure of the DP1â€“DP2 PolD complex bound with DNA and its implications for the evolutionary history of DNA and RNA polymerases. <i>PLoS Biology</i> , 2019, 17, e3000122.	2.6	30
53	Independent saturation of three TrpRS subsites generates a partially assembled state similar to those observed in molecular simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 1790-1795.	3.3	28
54	Conferring a template-dependent polymerase activity to terminal deoxynucleotidyltransferase by mutations in the Loop1 region. <i>Nucleic Acids Research</i> , 2009, 37, 4642-4656.	6.5	28

#	ARTICLE	IF	CITATIONS
55	Structural Basis for a New Templated Activity by Terminal Deoxynucleotidyl Transferase: Implications for V(D)J Recombination. <i>Structure</i> , 2016, 24, 1452-1463.	1.6	28
56	Terminal deoxynucleotidyltransferase: the story of an untemplated DNA polymerase capable of DNA bridging and templated synthesis across strands. <i>Current Opinion in Structural Biology</i> , 2018, 53, 22-31.	2.6	27
57	Crystal structures of a pentameric ion channel gated by alkaline pH show a widely open pore and identify a cavity for modulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E3959-E3968.	3.3	26
58	Computing Ion Solvation Free Energies Using the Dipolar Poisson Model. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5694-5697.	1.2	25
59	Genuine open form of the pentameric ligand-gated ion channel GLIC. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 454-460.	2.5	25
60	New Nucleotide-Competitive Non-Nucleoside Inhibitors of Terminal Deoxynucleotidyl Transferase: Discovery, Characterization, and Crystal Structure in Complex with the Target. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 7431-7441.	2.9	24
61	How cyanophage S-2L rejects adenine and incorporates 2-aminoadenine to saturate hydrogen bonding in its DNA. <i>Nature Communications</i> , 2021, 12, 2420.	5.8	24
62	Full mutational mapping of titratable residues helps to identify proton-sensors involved in the control of channel gating in the <i>Gloeobacter violaceus</i> pentameric ligand-gated ion channel. <i>PLoS Biology</i> , 2017, 15, e2004470.	2.6	24
63	Structure of the Archaeal Pab87 Peptidase Reveals a Novel Self-Compartmentalizing Protease Family. <i>PLoS ONE</i> , 2009, 4, e4712.	1.1	23
64	<i>Ab initio</i> sampling of transition paths by conditioned Langevin dynamics. <i>Journal of Chemical Physics</i> , 2017, 147, 152703.	1.2	22
65	Three Dimensional Structure and Implications for the Catalytic Mechanism of 6-Phosphogluconolactonase from <i>Trypanosoma brucei</i> . <i>Journal of Molecular Biology</i> , 2007, 366, 868-881.	2.0	21
66	Structural basis for a novel mechanism of DNA bridging and alignment in eukaryotic DSB DNA repair. <i>EMBO Journal</i> , 2015, 34, 1126-1142.	3.5	21
67	Extracting Dynamical Correlations and Identifying Key Residues for Allosteric Communication in Proteins by <i>correlationplus</i> . <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4832-4838.	2.5	21
68	Dealing with structural variability in molecular replacement and crystallographic refinement through normal-mode analysis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2008, 64, 40-48.	2.5	20
69	Barbiturates Bind in the GLIC Ion Channel Pore and Cause Inhibition by Stabilizing a Closed State. <i>Journal of Biological Chemistry</i> , 2017, 292, 1550-1558.	1.6	19
70	Structural basis for allosteric transitions of a multidomain pentameric ligand-gated ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 13437-13446.	3.3	18
71	Insights Into the Enzymatic Mechanism of 6-Phosphogluconolactonase from <i>Trypanosoma brucei</i> Using Structural Data and Molecular Dynamics Simulation. <i>Journal of Molecular Biology</i> , 2009, 388, 1009-1021.	2.0	16
72	The Renormalization Group and Its Applications to Generating Coarse-Grained Models of Large Biological Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1424-1438.	2.3	16

#	ARTICLE	IF	CITATIONS
73	Enzymatic synthesis of random sequences of RNA and RNA analogues by DNA polymerase theta mutants for the generation of aptamer libraries. <i>Nucleic Acids Research</i> , 2018, 46, 6271-6284.	6.5	16
74	Partition of aminoacyl-tRNA synthetases in two different structural classes dating back to early metabolism: Implications for the origin of the genetic code and the nature of protein sequences. <i>Journal of Molecular Evolution</i> , 1995, 41, 703-11.	0.8	15
75	Characterization of a triad of genes in cyanophage S-2L sufficient to replace adenine by 2-aminoadenine in bacterial DNA. <i>Nature Communications</i> , 2021, 12, 4710.	5.8	15
76	Building protein lattice models using self-consistent mean field theory. <i>Journal of Chemical Physics</i> , 1998, 108, 9540-9549.	1.2	14
77	Modified Poisson-Boltzmann equations for characterizing biomolecular solvation. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1440001.	1.8	13
78	Comparative Normal Mode Analysis of the Dynamics of DENV and ZIKV Capsids. <i>Frontiers in Molecular Biosciences</i> , 2016, 3, 85.	1.6	11
79	Statistical Physics Approach to the Optimal Transport Problem. <i>Physical Review Letters</i> , 2019, 123, 040603.	2.9	11
80	Parameterizing elastic network models to capture the dynamics of proteins. <i>Journal of Computational Chemistry</i> , 2021, 42, 1643-1661.	1.5	11
81	Three-dimensional structure of phenylalanyl-transfer RNA synthetase from <i>Thermus thermophilus</i> HB8 at 0.6-nm resolution. <i>FEBS Journal</i> , 1992, 208, 411-417.	0.2	9
82	2'-Deoxyribonucleoside Phosphoramidate Triphosphate Analogues as Alternative Substrates for <i>E. coli</i> Polymerase III. <i>ChemBioChem</i> , 2012, 13, 2439-2444.	1.3	9
83	Combined approaches from physics, statistics, and computer science for ab initio protein structure prediction: ex univates vires (unity is strength)? <i>F1000Research</i> , 2018, 7, 1125.	0.8	9
84	Optimal transport at finite temperature. <i>Physical Review E</i> , 2019, 100, 013310.	0.8	8
85	Structural evidence for an in trans base selection mechanism involving Loop1 in polymerase β at an NHEJ double-strand break junction. <i>Journal of Biological Chemistry</i> , 2019, 294, 10579-10595.	1.6	7
86	Structural Studies of HNA Substrate Specificity in Mutants of an Archaeal DNA Polymerase Obtained by Directed Evolution. <i>Biomolecules</i> , 2020, 10, 1647.	1.8	7
87	Physics approach to the variable-mass optimal-transport problem. <i>Physical Review E</i> , 2021, 103, 012113.	0.8	6
88	Structural evidence for the binding of monocarboxylates and dicarboxylates at pharmacologically relevant extracellular sites of a pentameric ligand-gated ion channel. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 668-675.	1.1	6
89	General formalism for phase combination and phase refinement: a statistical thermodynamics approach in reciprocal space. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2000, 56, 562-574.	0.3	5
90	Fast and efficient purification of SARS-CoV-2 RNA dependent RNA polymerase complex expressed in <i>Escherichia coli</i> . <i>PLoS ONE</i> , 2021, 16, e0250610.	1.1	5

#	ARTICLE	IF	CITATIONS
91	Structural dynamics and determinants of 2-aminoadenine specificity in DNA polymerase DpoZ of vibriophage ϕ VC8. <i>Nucleic Acids Research</i> , 2021, 49, 11974-11985.	6.5	5
92	[40] Converting sequence block alignments into structural insights. <i>Methods in Enzymology</i> , 1996, 266, 662-680.	0.4	4
93	Determination of dihedral ϕ angles in large proteins by combining NHN/C β H β dipole/dipole cross-correlation and chemical shifts. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 931-939.	1.5	4
94	Meet-U: Educating through research immersion. <i>PLoS Computational Biology</i> , 2018, 14, e1005992.	1.5	4
95	Beyond Poisson-Boltzmann: Numerical Sampling of Charge Density Fluctuations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6270-6277.	1.2	3
96	Coarse-grained dynamics of supramolecules: Conformational changes in outer shells of Dengue viruses. <i>Progress in Biophysics and Molecular Biology</i> , 2019, 143, 20-37.	1.4	3
97	Cloning and characterisation of a gene from <i>Plasmodium vivax</i> and <i>P. knowlesi</i> : homology with valine-tRNA synthetase. <i>Gene</i> , 1996, 173, 137-145.	1.0	2
98	Resolution of the phase-ambiguity problem in the centrosymmetric $P\{1\}$ space group by Monte Carlo methods. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2000, 56, 554-561.	0.3	2
99	Numerical Encodings of Amino Acids in Multivariate Gaussian Modeling of Protein Multiple Sequence Alignments. <i>Molecules</i> , 2019, 24, 104.	1.7	2
100	Rapid enzymatic synthesis of long RNA polymers: A simple protocol to generate RNA libraries with random sequences. <i>Methods</i> , 2019, 161, 83-90.	1.9	1
101	Simultaneous Identification of Multiple Binding Sites in Proteins: A Statistical Mechanics Approach. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5052-5067.	1.2	1
102	Structural Basis for Allosteric Transitions in the GLIC Pentameric Proton-Gated Ion Channel. <i>Biophysical Journal</i> , 2014, 106, 343a.	0.2	0
103	Barbiturates Bind in the GLIC Ion Channel Pore and Cause Inhibition by Stabilizing a Shut State. <i>Biophysical Journal</i> , 2017, 112, 553a.	0.2	0
104	Secret From the ABYSS: Structures of the D-Family DNA Polymerase (POLD) Reveal that DNA Replication and DNA Transcription Share a Joint Evolutionary History in Archaea. <i>Biophysical Journal</i> , 2018, 114, 218a.	0.2	0