Josep LluÃ-s GelpÃ-

List of Publications by Year
in descending order

98 papers	8,983 citations	87843 38 h-index	43868 91 g-index
103 all docs	103 docs citations	103 times ranked	15284 citing authors

#	Article	IF	Citations
1	Whole-genome sequencing identifies recurrent mutations in chronic lymphocytic leukaemia. Nature, 2011, 475, 101-105.	13.7	1,364
2	Exome sequencing identifies recurrent mutations of the splicing factor SF3B1 gene in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 47-52.	9.4	893
3	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
4	Non-coding recurrent mutations in chronic lymphocytic leukaemia. Nature, 2015, 526, 519-524.	13.7	749
5	Epigenomic analysis detects widespread gene-body DNA hypomethylation in chronic lymphocytic leukemia. Nature Genetics, 2012, 44, 1236-1242.	9.4	525
6	PMUT: a web-based tool for the annotation of pathological mutations on proteins. Bioinformatics, 2005, 21, 3176-3178.	1.8	441
7	Molecular dynamics simulations: advances and applications. Advances and Applications in Bioinformatics and Chemistry, 2015, 8, 37.	1.6	409
8	A consensus view of protein dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 796-801.	3.3	223
9	PMut: a web-based tool for the annotation of pathological variants on proteins, 2017 update. Nucleic Acids Research, 2017, 45, W222-W228.	6.5	184
10	Obligatory Amino Acid Exchange via Systems bo,+-like and y+L-like. Journal of Biological Chemistry, 1996, 271, 17761-17770.	1.6	158
11	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. Bioinformatics, 2012, 28, 1278-1279.	1.8	153
12	Towards FAIR principles forÂresearchÂsoftware. Data Science, 2020, 3, 37-59.	0.7	144
13	Glutaryl-CoA Dehydrogenase Deficiency in Spain: Evidence of Two Groups of Patients, Genetically, and Biochemically Distinct. Pediatric Research, 2000, 48, 315-322.	1.1	127
14	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
15	SAR and 3D-QSAR Studies on Thiadiazolidinone Derivatives:â€‰ Exploration of Structural Requirements for Glycogen Synthase Kinase 3 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7103-7112.	2.9	114
16	Theoretical Study of the Truncated Hemoglobin HbN:Â Exploring the Molecular Basis of the NO Detoxification Mechanism. Journal of the American Chemical Society, 2005, 127, 4433-4444.	6.6	111
17	4D Genome Rewiring during Oncogene-Induced and Replicative Senescence. Molecular Cell, 2020, 78, 522-538.e9.	4.5	107
18	Interoperability with Moby 1.0–It's better than sharing your toothbrush!. Briefings in Bioinformatics, 2008, 9, 220-231.	3.2	91

#	Article	IF	Citations
19	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	1.3	89
20	Four simple recommendations to encourage best practices in research software. F1000Research, 2017, 6, 876.	0.8	88
21	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	1.5	87
22	Long-timescale dynamics of the Drewâ€“Dickerson dodecamer. Nucleic Acids Research, 2016, 44, 4052-4066.	6.5	86
23	Risk variants for psoriasis vulgaris in a large caseâ€“control collection and association with clinical subphenotypes. Human Molecular Genetics, 2012, 21, 4549-4557.	1.4	79
24	Comprehensive characterization of complex structural variations in cancer by directly comparing genome sequence reads. Nature Biotechnology, 2014, 32, 1106-1112.	9.4	74
25	FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710.	1.8	72
26	Evidence for Transcript Networks Composed of Chimeric RNAs in Human Cells. PLoS ONE, 2012, 7, e28213.	1.1	61
27	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2009, 284, 14457-14468.	1.6	59
28	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. Nucleic Acids Research, 2016, 44, D272-D278.	6.5	57
29	Synthesis, Structural Analysis, and Biological Evaluation of Thioxoquinazoline Derivatives as Phosphodiesteraseâ€…7 Inhibitors. ChemMedChem, 2009, 4, 866-876.	1.6	56
30	Theoretical Study of the Mechanisms of Substrate Recognition by Catalase. Journal of the American Chemical Society, 2001, 123, 9665-9672.	6.6	50
31	Thienylhalomethylketones: Irreversible glycogen synthase kinase 3 inhibitors as useful pharmacological tools. Bioorganic and Medicinal Chemistry, 2009, 17, 6914-6925.	1.4	49
32	Cystinuria-specific rBAT(R365W) mutation reveals two translocation pathways in the amino acid transporter rBAT-b0,+AT. Biochemical Journal, 2004, 377, 665-674.	1.7	47
33	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	1.8	46
34	Identification of Risk Loci for Crohnâ€™s Disease Phenotypes Using a Genome-Wide Association Study. Gastroenterology, 2015, 148, 794-805.	0.6	46
35	NAFlex: a web server for the study of nucleic acid flexibility. Nucleic Acids Research, 2013, 41, W47-W55.	6.5	45
36	Genetic variation at the glycosaminoglycan metabolism pathway contributes to the risk of psoriatic arthritis but not psoriasis. Annals of the Rheumatic Diseases, 2019, 78, 355-364.	0.5	44

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37	Sequential Amino Acid Exchange across b0,+-like System in Chicken Brush Border Jejunum. Journal of Membrane Biology, 2001, 180, 213-220.	1.0	43
38	A genome-wide association study on a southern European population identifies a new Crohn's disease susceptibility locus atRBX1-EP300. Gut, 2013, 62, 1440-1445.	6.1	42
39	The Quest for Orthologs benchmark service and consensus calls in 2020. Nucleic Acids Research, 2020, 48, W538-W545.	6.5	41
40	Modulation of drug cytotoxicity by reintroduction of wild-type p53 gene (Ad5CMV-p53) in human pancreatic cancer. Cancer Gene Therapy, 2000, 7, 545-556.	2.2	40
41	Mutations in JMJD1C are involved in Rett syndrome and intellectual disability. Genetics in Medicine, 2016, 18, 378-385.	1.1	40
42	Properties of triple helices formed by parallel-stranded hairpins containing 8-aminopurines. Nucleic Acids Research, 2002, 30, 2609-2619.	6.5	39
43	A genome-wide association study identifies a novel locus at 6q22.1 associated with ulcerative colitis. Human Molecular Genetics, 2014, 23, 6927-6934.	1.4	39
44	Unconventional interactions between water and heterocyclic nitrogens in protein structures. Proteins: Structure, Function and Bioinformatics, 2004, 57, 1-8.	1.5	38
45	Functional and Structural Characterization of the First Prokaryotic Member of the L-Amino Acid Transporter (LAT) Family. Journal of Biological Chemistry, 2007, 282, 13270-13281.	1.6	38
46	BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. Scientific Data, 2019, 6, 169.	2.4	35
47	Adenovirus-mediated wt- p16 reintroduction induces cell cycle arrest or apoptosis in pancreatic cancer. Cancer Gene Therapy, 2001, 8, 740-750.	2.2	34
48	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. Journal of Molecular Biology, 2019, 431, 3845-3859.	2.0	34
49	Coarse-grained Representation of Protein Flexibility. Foundations, Successes, and Shortcomings. Advances in Protein Chemistry and Structural Biology, 2011, 85, 183-215.	1.0	33
50	Replacement of terminal cysteine with histidine in the metallothionein Î± and Î² domains maintains its binding capacity. FEBS Journal, 1999, 259, 519-527.	0.2	32
51	Four-Stranded DNA Structure Stabilized by a Novel G:C:A:T Tetrad. Journal of the American Chemical Society, 2003, 125, 5654-5662.	6.6	29
52	Finding Conformational Transition Pathways from Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4707-4718.	2.3	29
53	Effects of Cadmium and Mercury on the Upper Part of Skeletal Muscle Glycolysis in Mice. PLoS ONE, 2014, 9, e80018.	1.1	28
54	Construction of a stable dimer of Bacillus stearothermophilus lactate dehydrogenase. Biochemistry, 1992, 31, 8307-8314.	1.2	27

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55	Genome-Wide Pathway Analysis Identifies Genetic Pathways Associated with Psoriasis. Journal of Investigative Dermatology, 2016, 136, 593-602.	0.3	27
56	How accurate can molecular dynamics/linear response and Poisson-Boltzmann/solvent accessible surface calculations be for predicting relative binding affinities? Acetylcholinesterase huprine inhibitors as a test case. Theoretical Chemistry Accounts, 2001, 106, 2-9.	0.5	25
57	Dissection of the Recognition Properties of p38 MAP Kinase. Determination of the Binding Mode of a New Pyridinylâ^'Heterocycle Inhibitor Family. Journal of Medicinal Chemistry, 2007, 50, 283-293.	2.9	24
58	Inntags: small self-structured epitopes for innocuous protein tagging. Nature Methods, 2015, 12, 955-958.	9.0	22
59	D-2-Hydroxy-4-Methylvalerate Dehydrogenase from Lactobacillus Delbrueckii Subsp. Bulgaricus- II. Mutagenic analysis of catalytically important residues. FEBS Journal, 1997, 244, 213-219.	0.2	20
60	Can Divalent Metal Cations Stabilize the Triplex Motif? Theoretical Study of the Interaction of the Hydrated Mg2+ Cation with the Gâ^'GÂ·C Triplet. Journal of Physical Chemistry B, 2002, 106, 8849-8857.	1.2	20
61	Structural and energetic study of cationâ€“Ï€â€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861.	1.3	19
62	Î±-thalassaemia due to a single codon deletion in the Î±-1-globin gene. Computational structural analysis of the new Î±-chain variant. Human Mutation, 1998, 11, 412-412.	1.1	18
63	A deletion atADAMTS9-MAGI1locus is associated with psoriatic arthritis risk. Annals of the Rheumatic Diseases, 2015, 74, 1875-1881.	0.5	18
64	The Multiple Roles of Waters in Protein Solvation. Journal of Physical Chemistry B, 2017, 121, 3636-3643.	1.2	17
65	Surviving the deluge of biosimulation data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1449.	6.2	16
66	Efficient aminoacylation of the tRNAAla acceptor stem: Dependence on the 2:71 base pair. Rna, 2002, 8, 659-670.	1.6	14
67	Exploring Early Stages of the Chemical Unfolding of Proteins at the Proteome Scale. PLoS Computational Biology, 2013, 9, e1003393.	1.5	14
68	PACSAB: Coarse-Grained Force Field for the Study of Proteinâ€“Protein Interactions and Conformational Sampling in Multiprotein Systems. Journal of Chemical Theory and Computation, 2015, 11, 5929-5938.	2.3	14
69	A genome-wide association study identifiesSLC8A3as a susceptibility locus for ACPA-positive rheumatoid arthritis. Rheumatology, 2016, 55, 1106-1111.	0.9	14
70	Genome-wide pathway analysis identifies VEGF pathway association with oral ulceration in systemic lupus erythematosus. Arthritis Research and Therapy, 2017, 19, 138.	1.6	14
71	Efficient Relaxation of Proteinâ€“Protein Interfaces by Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1222-1229.	2.3	13
72	Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. Nucleic Acids Research, 2019, 47, 9511-9523.	6.5	12

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73	A theoretical approach to the discrimination and characterization of the different classes of reversible inhibitors. Journal of Chemical Education, 1993, 70, 805.	1.1	11
74	Contribution of engineered electrostatic interactions to the stability of cytosolic malate dehydrogenase. Protein Engineering, Design and Selection, 2001, 14, 911-917.	1.0	11
75	Butler enables rapid cloud-based analysis of thousands of human genomes. Nature Biotechnology, 2020, 38, 288-292.	9.4	11
76	D-2-Hydroxy-4-Methylvalerate Dehydrogenase from Lactobacillus Delbrueckii Subsp. Bulgaricus- I. Kinetic Mechanism and pH Dependence of Kinetic Parameters, Coenzyme Binding and Substrate Inhibition. FEBS Journal, 1997, 244, 203-212.	0.2	10
77	Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up In Silico Drug Discovery. Journal of Chemical Theory and Computation, 2020, 16, 6586-6597.	2.3	10
78	Identifying causative mechanisms linking early-life stress to psycho-cardio-metabolic multi-morbidity: The EarlyCause project. PLoS ONE, 2021, 16, e0245475.	1.1	9
79	Continuum and discrete calculation of fractional contributions to solvation free energy. Journal of Computational Chemistry, 2003, 24, 1610-1623.	1.5	8
80	Linear response theory: An alternative to PB and GB methods for the analysis of molecular dynamics trajectories?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 458-467.	1.5	8
81	Partition of protein solvation into group contributions from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 58, 101-109.	1.5	8
82	Electrostatic interaction energies in lactate dehydrogenase catalysis. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2707.	1.7	7
83	Cloning, sequencing and functional expression of a DNA encoding pig cytosolic malate dehydrogenase: purification and characterization of the recombinant enzyme. Gene, 1996, 172, 303-308.	1.0	7
84	Effect of several anions on the activity of mitochondrial malate dehydrogenase from pig heart. Journal of Molecular Catalysis B: Enzymatic, 2001, 11, 743-755.	1.8	7
85	BioExcel Building Blocks Workflows (BioBB-Wfs), an integrated web-based platform for biomolecular simulations. Nucleic Acids Research, 2022, 50, W99-W107.	6.5	7
86	Highâ€throughput molecular dynamics simulations: toward a dynamic view of macromolecular structure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 364-377.	6.2	6
87	Identification of IRX1 as a Risk Locus for Rheumatoid Factor Positivity in Rheumatoid Arthritis in a Genomeâ€Wide Association Study. Arthritis and Rheumatology, 2016, 68, 1384-1391.	2.9	6
88	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	6
89	BioSWR â€“ Semantic Web Services Registry for Bioinformatics. PLoS ONE, 2014, 9, e107889.	1.1	4
90	A fast method for the determination of fractional contributions to solvation in proteins. Protein Science, 2006, 15, 2525-2533.	3.1	3

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91	Enabling HMMER for the Grid with COMP Superscalar. Procedia Computer Science, 2010, 1, 2629-2638.	1.2	3
92	Unveiling Caseâ€Control Relationships in Designing a Simple and Powerful Method for Detecting Geneâ€Gene Interactions. Genetic Epidemiology, 2012, 36, 710-716.	0.6	3
93	ATM germline variants in a young adult with chronic lymphocytic leukemia: 8â€‰years of genomic evolution. Blood Cancer Journal, 2022, 12, .	2.8	2
94	Purification of malate dehydrogenase from chicken liver mitochondria. existence of a small quantity of cytosolic isoenzyme. International Journal of Biochemistry & Cell Biology, 1988, 20, 989-996.	0.8	1
95	Comparison of the kinetic behaviour of lactate dehydrogenase and cytosolic and mitochondrial malate dehydrogenase from guinea pig skeletal muscle. Journal of Molecular Catalysis, 1990, 58, 269-275.	1.2	1
96	Comparative Analysis of the Reduction of Oxaloacetate by Human Hepatoma and Normal Liver Extracts. Tumor Biology, 1990, 11, 120-128.	0.8	0
97	Nature of artifactual bands in the electropherograms of malate dehydrogenase isoenzymes. Biochemical Education, 1990, 18, 200-202.	0.1	0
98	Comparative analysis of the binding of multiple forms of mitochondrial malate dehydrogenase to the inner membrane of the mitochondria. Biochemical Society Transactions, 1991, 19, 73S-73S.	1.6	0