Catherine Etchebest

List of Publications by Year
in descending order

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93 papers	3,974 citations	126708 33 h-index	128067 60 g-index
96 all docs	96 docs citations	96 times ranked	3743 citing authors

#	Article	IF	Citations
1	A New Approach to the Rapid Determination of Protein Side Chain Conformations. Journal of Biomolecular Structure and Dynamics, 1991, 8, 1267-1289.	2.0	320
2	Bayesian probabilistic approach for predicting backbone structures in terms of protein blocks. Proteins: Structure, Function and Bioinformatics, 2000, 41, 271-287.	1.5	254
3	A Model for the Photosystem II Reaction Center Core Including the Structure of the Primary Donor P680â€‚â€¡. Biochemistry, 1996, 35, 14486-14502.	1.2	209
4	Amphipathic Lipid Packing Sensor Motifs: Probing Bilayer Defects with Hydrophobic Residues. Biophysical Journal, 2013, 104, 575-584.	0.2	171
5	Determining membrane protein structures: still a challenge!. Trends in Biochemical Sciences, 2007, 32, 259-270.	3.7	164
6	Conical Lipids in Flat Bilayers Induce Packing Defects Similar to that Induced by Positive Curvature. Biophysical Journal, 2013, 104, 585-593.	0.2	149
7	Describing protein structure: A general algorithm yielding complete helicoidal parameters and a unique overall axis. Proteins: Structure, Function and Bioinformatics, 1989, 6, 46-60.	1.5	129
8	Comparison of three algorithms for the assignment of secondary structure in proteins: the advantages of a consensus assignment. Protein Engineering, Design and Selection, 1993, 6, 377-382.	1.0	117
9	A short survey on protein blocks. Biophysical Reviews, 2010, 2, 137-145.	1.5	107
10	Predicting protein flexibility through the prediction of local structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 839-852.	1.5	107
11	Unraveling Proteins: A Molecular Mechanics Study. Biophysical Journal, 1999, 76, 2760-2768.	0.2	103
12	Dynamical Properties of the MscL of Escherichia coli: A Normal Mode Analysis. Journal of Molecular Biology, 2003, 332, 657-674.	2.0	101
13	A structural alphabet for local protein structures: Improved prediction methods. Proteins: Structure, Function and Bioinformatics, 2005, 59, 810-827.	1.5	98
14	On the Orientation of a Designed Transmembrane Peptide:â€‰Toward the Right Tilt Angle?. Journal of the American Chemical Society, 2007, 129, 15174-15181.	6.6	96
15	A reduced amino acid alphabet for understanding and designing protein adaptation to mutation. European Biophysics Journal, 2007, 36, 1059-1069.	1.2	78
16	PredyFlexy: flexibility and local structure prediction from sequence. Nucleic Acids Research, 2012, 40, W317-W322.	6.5	78
17	Protein flexibility in the light of structural alphabets. Frontiers in Molecular Biosciences, 2015, 2, 20.	1.6	71
18	A structural model of a seven-transmembrane helix receptor: The Duffy antigen/receptor for chemokine (DARC). Biochimica Et Biophysica Acta - General Subjects, 2005, 1724, 288-306.	1.1	68

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19	A critical comparison of search algorithms applied to the optimization of protein side-chain conformations. Journal of Computational Chemistry, 1993, 14, 790-798.	1.5	66
20	Antioxidant and Membrane Binding Properties of Serotonin Protect Lipids from Oxidation. Biophysical Journal, 2017, 112, 1863-1873.	0.2	66
21	New insights into GluT1 mechanics during glucose transfer. Scientific Reports, 2019, 9, 998.	1.6	60
22	Extension of a local backbone description using a structural alphabet: A new approach to the sequence-structure relationship. Protein Science, 2009, 11, 2871-2886.	3.1	54
23	Structural and Dynamical Insights into the Opening Mechanism of P. aeruginosa OprM Channel. Structure, 2010, 18, 507-517.	1.6	53
24	Prediction of protein side chain conformations: a study on the influence of backbone accuracy on conformation stability in the rotamer space. Protein Engineering, Design and Selection, 1997, 10, 361-372.	1.0	49
25	Genome adaptation to chemical stress: clues from comparative transcriptomics in Saccharomyces cerevisiae and Candida glabrata. Genome Biology, 2008, 9, R164.	13.9	48
26	Insights into Brain Glycogen Metabolism. Journal of Biological Chemistry, 2016, 291, 18072-18083.	1.6	43
27	The gramicidin A channel: the energy profile for single and double occupancy in a head-to-head Î²6.3 3,3 -helical dimer backbone. FEBS Letters, 1983, 163, 199-202.	1.3	42
28	The gramicidin A channel: comparison of the energy profiles of Na+ , K+ and Cs+. FEBS Letters, 1984, 173, 301-306.	1.3	42
29	Multisensory VR interaction for protein-docking in the CoRSAIRe project. Virtual Reality, 2009, 13, 273-293.	4.1	42
30	Assessing a novel approach for predicting local 3D protein structures from sequence. Proteins: Structure, Function and Bioinformatics, 2005, 62, 865-880.	1.5	40
31	Structural Model of the Anion Exchanger 1 (SLC4A1) and Identification of Transmembrane Segments Forming the Transport Site. Journal of Biological Chemistry, 2013, 288, 26372-26384.	1.6	40
32	Mg2+ in the Major Groove Modulates B-DNA Structure and Dynamics. PLoS ONE, 2012, 7, e41704.	1.1	37
33	The Effect of the Amino-Acid Side Chains on the Energy Profiles for Ion Transport in the Gramicidin A Channel. Journal of Biomolecular Structure and Dynamics, 1985, 2, 859-870.	2.0	36
34	Amphipathic-Lipid-Packing-Sensor interactions with lipids assessed by atomistic molecular dynamics. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 2119-2127.	1.4	35
35	Conformational and helicoidal analysis of the molecular dynamics of proteins: â€œCurves,â€•dials and windows for a 50 psec dynamic trajectory of BPTI. Proteins: Structure, Function and Bioinformatics, 1990, 8, 179-193.	1.5	34
36	The gramicidin A channel. FEBS Letters, 1984, 170, 191-195.	1.3	33

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37	Prediction of the positioning of the seven transmembrane Î±-helices of bacteriorhodopsin. Journal of Molecular Biology, 1994, 236, 1105-1122.	2.0	32
38	The Gramicidin A Channel: Energetics and Structural Characteristics of the Progression of a Sodium Ion in the Presence of Water. Journal of Biomolecular Structure and Dynamics, 1986, 3, 805-825.	2.0	29
39	A new prediction strategy for long local protein structures using an original description. Proteins: Structure, Function and Bioinformatics, 2009, 76, 570-587.	1.5	29
40	Local backbone structure prediction of proteins. In Silico Biology, 2004, 4, 381-6.	0.4	29
41	Calculation of the molecular electrostatic potential from a multipole expansion based on localized orbitals. Chemical Physics Letters, 1982, 85, 266-270.	1.2	28
42	â€œPinning strategyâ€• a novel approach for predicting the backbone structure in terms of protein blocks from sequence. Journal of Biosciences, 2007, 32, 51-70.	0.5	28
43	Energetic and Molecular Water Permeation Mechanisms of the Human Red Blood Cell Urea Transporter B. PLoS ONE, 2013, 8, e82338.	1.1	27
44	The calculation of molecular electrostatic potential from a multipole expansion based on localized orbitals and developed at their centroids: Accuracy and applicability for macromolecular computations. Theoretica Chimica Acta, 1982, 62, 17-28.	0.9	26
45	A theoretical study of the selective alkali and alkaline-earth cation binding properties of valinomycin. International Journal of Quantum Chemistry, 1981, 20, 109-116.	1.0	25
46	Aminopeptidase B, a glucagon-processing enzyme: site directed mutagenesis of the Zn2+-binding motif and molecular modelling. BMC Biochemistry, 2007, 8, 21.	4.4	25
47	Theoretical model of human apolipoprotein B100 tertiary structure. Proteins: Structure, Function and Bioinformatics, 2006, 66, 342-358.	1.5	22
48	Insights into the ZIKV NS1 Virology from Different Strains through a Fine Analysis of Physicochemical Properties. ACS Omega, 2018, 3, 16212-16229.	1.6	22
49	Structure and dynamics of bacteriorhodopsin. FEBS Letters, 1993, 327, 256-260.	1.3	20
50	Decoding the structural events in substrateâ€gating mechanism of eukaryotic prolyl oligopeptidase using normal mode analysis and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1428-1443.	1.5	20
51	An Isozyme-specific Redox Switch in Human Brain Glycogen Phosphorylase Modulates Its Allosteric Activation by AMP. Journal of Biological Chemistry, 2016, 291, 23842-23853.	1.6	20
52	Discrete analyses of protein dynamics. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2988-3002.	2.0	20
53	Identification of Electrostatic Epitopes in Flavivirus by Computer Simulations: The PROCEEDpKa Method. Journal of Chemical Information and Modeling, 2020, 60, 944-963.	2.5	20
54	New insights of membrane environment effects on MscL channel mechanics from theoretical approaches. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1183-1196.	1.5	18

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55	In Silico Studies on DARC. Infectious Disorders - Drug Targets, 2009, 9, 289-303.	0.4	18
56	Rotational orientation of transmembrane Î±-helices in bacteriorhodopsin. Journal of Molecular Biology, 1994, 236, 1093-1104.	2.0	17
57	Protein Peeling 2: a web server to convert protein structures into series of protein units. Nucleic Acids Research, 2006, 34, W75-W78.	6.5	16
58	The gramicidin A channel: theoretical energy profile computed for single occupancy by a divalent cation, Ca2+. Biochimica Et Biophysica Acta - Biomembranes, 1985, 818, 23-30.	1.4	15
59	Experimental and theoretical study of gramicidin P, an analog of gramicidin A with a methylamine C-terminal. FEBS Letters, 1987, 216, 11-16.	1.3	15
60	In silico prediction of protein flexibility with local structure approach. Biochimie, 2019, 165, 150-155.	1.3	15
61	How the Strain Origin of Zika Virus NS1 Protein Impacts Its Dynamics and Implications to Their Differential Virulence. Journal of Chemical Information and Modeling, 2021, 61, 1516-1530.	2.5	15
62	The Reconstruction of Condition-Specific Transcriptional Modules Provides New Insights in the Evolution of Yeast AP-1 Proteins. PLoS ONE, 2011, 6, e20924.	1.1	14
63	Construction and validation of an atomic model for bacterial TSPO from electron microscopy density, evolutionary constraints, and biochemical and biophysical data. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 568-580.	1.4	14
64	Multiple interests in structural models of DARC transmembrane protein. Transfusion Clinique Et Biologique, 2010, 17, 184-196.	0.2	13
65	The gramicidin A channel. FEBS Letters, 1986, 204, 261-265.	1.3	12
66	A Procedure for Refining a Coiled Coil Protein Structure Using X-Ray Fiber Diffraction and Modeling. Biophysical Journal, 2002, 83, 1774-1783.	0.2	12
67	Cloning and modeling of CD8 Î² in the amphibian ambystoma Mexicanum. Evolutionary conserved structures for interactions with major histocompatibility complex (MHC) class I molecules. Gene, 2002, 288, 95-102.	1.0	10
68	Taking advantage of local structure descriptors to analyze interresidue contacts in protein structures and protein complexes. Proteins: Structure, Function and Bioinformatics, 2008, 73, 672-689.	1.5	10
69	Mutation in the substrate-binding site of aminopeptidase B confers new enzymatic properties. Biochimie, 2011, 93, 730-741.	1.3	10
70	Dynamics and deformability of Î±-, 310- and Ï€-helices. Archives of Biological Sciences, 2018, 70, 21-31.	0.2	10
71	VHH Structural Modelling Approaches: A Critical Review. International Journal of Molecular Sciences, 2022, 23, 3721.	1.8	9
72	Sequenceâ€“structure relationship study in all-Î± transmembrane proteins using an unsupervised learning approach. Amino Acids, 2015, 47, 2303-2322.	1.2	8

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73	The C Terminus of Rotavirus VP4 Protein Contains an Actin Binding Domain Which Requires Cooperation with the Coiled-Coil Domain for Actin Remodeling. Journal of Virology, 2019, 93, .	1.5	8
74	Energy Profile of Cs+in Gramicidin A in the Presence of Water. Problem of the Ion Selectivity of the Channel. Journal of Biomolecular Structure and Dynamics, 1988, 5, 1111-1125.	2.0	7
75	Versatile Dimerisation Process of Translocator Protein (TSPO) Revealed by an Extensive Sampling Based on a Coarse-Grained Dynamics Study. Journal of Chemical Information and Modeling, 2020, 60, 3944-3957.	2.5	7
76	Clustering of protein domains for functional and evolutionary studies. BMC Bioinformatics, 2009, 10, 335.	1.2	6
77	Influence of assignment on the prediction of transmembrane helices in protein structures. Amino Acids, 2010, 39, 1241-1254.	1.2	6
78	Self-association features of NS1 proteins from different flaviviruses. Virus Research, 2022, 318, 198838.	1.1	6
79	Repository of Enriched Structures of Proteins Involved in the Red Blood Cell Environment (RESPIRE). PLoS ONE, 2019, 14, e0211043.	1.1	5
80	Linear Gramicidins : Influence of the Nature of the Aromatic Side Chains of the Channel Conductance. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1988, , 147-165.	0.2	5
81	Critical Review of General Guidelines for Membrane Proteins Model Building and Analysis. Methods in Molecular Biology, 2010, 654, 363-385.	0.4	3
82	The Gramicidin a Channel: Left Versus Right-Handed Helix. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1988, , 167-185.	0.2	3
83	TMPL: a database of experimental and theoretical transmembrane protein models positioned in the lipid bilayer. Database: the Journal of Biological Databases and Curation, 2017, 2017, .	1.4	2
84	Urea and Water Permeation across the Human Red Blood Cell Membrane. New Insights into Transport Mechanisms. Biophysical Journal, 2013, 104, 112a-113a.	0.2	1
85	Molecular Dynamics Study of a Protein Motif that Senses Packing Defects Induced by Membrane Curvature. Biophysical Journal, 2013, 104, 662a.	0.2	1
86	Direct minimization: Alternative to the traditional L2 norm to derive partial atomic charges. Computational and Theoretical Chemistry, 2015, 1074, 50-57.	1.1	1
87	Hydrophobic neighboring homology (HNH) dotplot: an approach for assessing structurally similar motifs in proteins. Computer Methods and Programs in Biomedicine, 1994, 45, 265-282.	2.6	0
88	Modelling of transmembrane ?-helix bundles. Molecular Engineering, 1995, 5, 1-9.	0.2	0
89	Efficient Protein Structure Alignment Methods Based on a Structural Alphabet. Biophysical Journal, 2014, 106, 54a.	0.2	0
90	Effect of Serotonin on Membranes Properties Studied by Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 805a.	0.2	0

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91	Molecular Modeling of Transporters: From Low Resolution Cryo-Electron Microscopy Map to Conformational Exploration. The Example of TSPO. Methods in Molecular Biology, 2017, 1635, 383-416.	0.4	0
92	Steps Towards Predicting the Structure of Membrane Proteins. NATO ASI Series Series B: Physics, 1994, , 239-252.	0.2	0
93	Modelling of Transmembrane Î±-Helix Bundles. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 1-9.	0.2	0