Federico Fogolari

List of Publications by Year
in descending order

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129 papers	5,158 citations	109321 35 h-index	98798 67 g-index
129 all docs	129 docs citations	129 times ranked	6991 citing authors

#	Article	IF	Citations
1	Dimers of mitochondrial ATP synthase form the permeability transition pore. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5887-5892.	7.1	822
2	The Poisson-Boltzmann equation for biomolecular electrostatics: a tool for structural biology. Journal of Molecular Recognition, 2002, 15, 377-392.	2.1	469
3	Protocol for MM/PBSA Molecular Dynamics Simulations of Proteins. Biophysical Journal, 2003, 85, 159-166.	0.5	173
4	The Catalytic Site of Glutathione Peroxidases. Antioxidants and Redox Signaling, 2008, 10, 1515-1526.	5.4	151
5	Nucleotide diversity and linkage disequilibrium in Populus nigra cinnamyl alcohol dehydrogenase (CAD4) gene. Tree Genetics and Genomes, 2011, 7, 1011-1023.	1.6	138
6	Collagen Plays an Active Role in the Aggregation of Î²2-Microglobulin under Physiopathological Conditions of Dialysis-related Amyloidosis*. Journal of Biological Chemistry, 2006, 281, 16521-16529.	3.4	128
7	Biomolecular Electrostatics with the Linearized Poisson-Boltzmann Equation. Biophysical Journal, 1999, 76, 1-16.	0.5	122
8	Bovine Î²â€lactoglobulin: Interaction studies with palmitic acid. Protein Science, 2000, 9, 1347-1356.	7.6	105
9	Electrostatic and non-electrostatic contributions to the binding free energies of anthracycline antibiotics to DNA. Journal of Molecular Biology, 1997, 274, 253-267.	4.2	104
10	From ATP to PTP and Back. Circulation Research, 2015, 116, 1850-1862.	4.5	97
11	Quantitative Correlation of Solvent Polarity with the Î±-/310-Helix Equilibrium: A Heptapeptide Behaves as a Solvent-Driven Molecular Spring. Angewandte Chemie - International Edition, 2003, 42, 3388-3392.	13.8	91
12	The unique histidine in OSCP subunit of Fâ€ATP synthase mediates inhibition of the permeability transition pore by acidic pH. EMBO Reports, 2018, 19, 257-268.	4.5	91
13	Amino acid empirical contact energy definitions for fold recognition in the space of contact maps. BMC Bioinformatics, 2003, 4, 8.	2.6	88
14	Effect of Tetracyclines on the Dynamics of Formation and Destructuration of Î²2-Microglobulin Amyloid Fibrils. Journal of Biological Chemistry, 2011, 286, 2121-2131.	3.4	87
15	The Projection Analysis of NMR Chemical Shifts Reveals Extended EPAC Autoinhibition Determinants. Biophysical Journal, 2012, 102, 630-639.	0.5	83
16	The Controlling Roles of Trp60 and Trp95 in Î²2-Microglobulin Function, Folding and Amyloid Aggregation Properties. Journal of Molecular Biology, 2008, 378, 887-897.	4.2	82
17	Structure, Folding Dynamics, and Amyloidogenesis of D76N Î²2-Microglobulin. Journal of Biological Chemistry, 2013, 288, 30917-30930.	3.4	80
18	Probing the Influence of Citrate-Capped Gold Nanoparticles on an Amyloidogenic Protein. ACS Nano, 2015, 9, 2600-2613.	14.6	80

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19	SIRT1 gene expression upon genotoxic damage is regulated by APE1 through nCaRE-promoter elements. Molecular Biology of the Cell, 2014, 25, 532-547.	2.1	74
20	Bluues server: electrostatic properties of wild-type and mutated protein structures. Bioinformatics, 2012, 28, 2189-2190.	4.1	72
21	On the variational approach to Poissonâ€“Boltzmann free energies. Chemical Physics Letters, 1997, 281, 135-139.	2.6	68
22	Electrostatic properties of bovine ?-lactoglobulin. , 2000, 39, 317-330.		68
23	EF Loop Conformational Change Triggers Ligand Binding in Î²-Lactoglobulins. Journal of Biological Chemistry, 2003, 278, 38840-38846.	3.4	67
24	Constraint Logic Programming approach to protein structure prediction. BMC Bioinformatics, 2004, 5, 186.	2.6	57
25	Native-unlike Long-lived Intermediates along the Folding Pathway of the Amyloidogenic Protein Î²2-Microglobulin Revealed by Real-time Two-dimensional NMR. Journal of Biological Chemistry, 2010, 285, 5827-5835.	3.4	55
26	Bluues: a program for the analysis of the electrostatic properties of proteins based on generalized Born radii. BMC Bioinformatics, 2012, 13, S18.	2.6	52
27	NMR and circular dichroism studies of the lantibiotic nisin in non-aqueous environments. FEBS Letters, 1993, 319, 189-194.	2.8	50
28	NMR Dynamic Studies Suggest that Allosteric Activation Regulates Ligand Binding in Chicken Liver Bile Acid-binding Protein. Journal of Biological Chemistry, 2006, 281, 9697-9709.	3.4	50
29	NMR structural characterization of the reaction product between d(GpG) and the octahedral antitumor complex trans-RuCl2(DMSO)4. Biochemistry, 1992, 31, 7094-7103.	2.5	46
30	NMR structural determination of viscotoxin A3 from Viscum album L.. Biochemical Journal, 2000, 350, 569-577.	3.7	45
31	The Oligomycin-Sensitivity Conferring Protein of Mitochondrial ATP Synthase: Emerging New Roles in Mitochondrial Pathophysiology. International Journal of Molecular Sciences, 2014, 15, 7513-7536.	4.1	44
32	Application of MM/PBSA colony free energy to loop decoy discrimination: Toward correlation between energy and root mean square deviation. Protein Science, 2005, 14, 889-901.	7.6	41
33	Comparative molecular dynamics simulations of HIV-1 integrase and the T66I/M154I mutant: Binding modes and drug resistance to a diketo acid inhibitor. Proteins: Structure, Function and Bioinformatics, 2005, 59, 723-741.	2.6	41
34	Molecular Dynamics Simulation Suggests Possible Interaction Patterns at Early Steps of Î²2-Microglobulin Aggregation. Biophysical Journal, 2007, 92, 1673-1681.	0.5	39
35	Limiting-laws of polyelectrolyte solutions. Ionic distribution in mixed-valency counterions systems. I: The model. Biophysical Chemistry, 1991, 41, 73-80.	2.8	38
36	Role of Dynamics in the Autoinhibition and Activation of the Exchange Protein Directly Activated by Cyclic AMP (EPAC). Journal of Biological Chemistry, 2011, 286, 42655-42669.	3.4	38

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37	pKaShift Effects on Backbone Amide Base-Catalyzed Hydrogen Exchange Rates in Peptides. Journal of the American Chemical Society, 1998, 120, 3735-3738.	13.7	35
38	Folding and Fibrillogenesis: Clues from Î²2-Microglobulin. Journal of Molecular Biology, 2010, 401, 286-297.	4.2	35
39	Monitoring the Interaction between Î²2-Microglobulin and the Molecular Chaperone Î±B-crystallin by NMR and Mass Spectrometry. Journal of Biological Chemistry, 2013, 288, 17844-17858.	3.4	32
40	Distance-Based Configurational Entropy of Proteins from Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0132356.	2.5	32
41	OSCP subunit of mitochondrial ATP synthase: role in regulation of enzyme function and of its transition to a pore. British Journal of Pharmacology, 2019, 176, 4247-4257.	5.4	32
42	Molecular dynamics simulation of Î²₂â€microglobulin in denaturing and stabilizing conditions. Proteins: Structure, Function and Bioinformatics, 2011, 79, 986-1001.	2.6	31
43	NMR Solution Structure of Viscotoxin C1 from Viscum Album SpeciesColoratum ohwi:Â Toward a Structureâ^'Function Analysis of Viscotoxinsâ€. Biochemistry, 2003, 42, 12503-12510.	2.5	30
44	Citrate stabilized gold nanoparticles interfere with amyloid fibril formation: D76N and Î”N6 Î²2-microglobulin variants. Nanoscale, 2018, 10, 4793-4806.	5.6	30
45	MM/PBSA analysis of molecular dynamics simulations of bovine Î²-lactoglobulin: Free energy gradients in conformational transitions?. Proteins: Structure, Function and Bioinformatics, 2005, 59, 91-103.	2.6	28
46	Rapid oligomer formation of human muscle acylphosphatase induced by heparan sulfate. Nature Structural and Molecular Biology, 2012, 19, 547-554.	8.2	28
47	Structural comparison between retro-inverso and parent peptides: Molecular basis for the biological activity of a retro-inverso analogue of the immunodominant fragment of VP1 coat protein from foot-and-mouth disease virus. , 1997, 41, 569-590.		27
48	The BR domain of PsrP interacts with extracellular DNA to promote bacterial aggregation; structural insights into pneumococcal biofilm formation. Scientific Reports, 2016, 6, 32371.	3.3	27
49	Analysis of the Solution Structure of the Homeodomain of Rat Thyroid Transcription Factor 1 by 1H-NMR Spectroscopy and Restrained Molecular Mechanics. FEBS Journal, 1996, 241, 101-113.	0.2	26
50	Citrate-stabilized gold nanoparticles hinder fibrillogenesis of a pathological variant of Î²₂-microglobulin. Nanoscale, 2017, 9, 3941-3951.	5.6	26
51	Solution structure of Î²2-microglobulin and insights into fibrillogenesis. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1753, 76-84.	2.3	25
52	Scoring predictive models using a reduced representation of proteins: model and energy definition. BMC Structural Biology, 2007, 7, 15.	2.3	25
53	Comparison of the structural and functional properties of RNase A and BSâ€RNase: A stepwise mutagenesis approach. Biopolymers, 2009, 91, 1009-1017.	2.4	24
54	PDB2ENTROPY and PDB2TRENT: Conformational and Translationalâ€“Rotational Entropy from Molecular Ensembles. Journal of Chemical Information and Modeling, 2018, 58, 1319-1324.	5.4	24

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55	Structural and Dynamics Characteristics of Acylphosphatase from Sulfolobus solfataricus in the Monomeric State and in the Initial Native-like Aggregates. Journal of Biological Chemistry, 2010, 285, 14689-14700.	3.4	23
56	Absolute Quantification of Choline-Related Biomarkers in Breast Cancer Biopsies by Liquid Chromatography Electrospray Ionization Mass Spectrometry. Analytical Cellular Pathology, 2013, 36, 71-83.	1.4	23
57	Role of Dynamics in the Autoinhibition and Activation of the Hyperpolarization-activated Cyclic Nucleotide-modulated (HCN) Ion Channels. Journal of Biological Chemistry, 2015, 290, 17642-17654.	3.4	23
58	The TTTT B lymphocyte stimulator promoter haplotype is associated with good response to rituximab therapy in seropositive rheumatoid arthritis resistant to tumor necrosis factor blockers. Arthritis and Rheumatism, 2013, 65, 88-97.	6.7	22
59	Free Energy, Enthalpy and Entropy from Implicit Solvent End-Point Simulations. Frontiers in Molecular Biosciences, 2018, 5, 11.	3.5	22
60	The Solution Structure of DNA-free Pax-8 Paired Box Domain Accounts for Redox Regulation of Transcriptional Activity in the Pax Protein Family. Journal of Biological Chemistry, 2008, 283, 33321-33328.	3.4	21
61	Accurate Estimation of the Entropy of Rotationâ€“Translation Probability Distributions. Journal of Chemical Theory and Computation, 2016, 12, 1-8.	5.3	21
62	Peptide Models of Folding Initiation Sites of Bovine Î²-Lactoglobulin:Â Identification of Nativelike Hydrophobic Interactions Involving G and H Strandsâ€. Biochemistry, 2002, 41, 2786-2796.	2.5	20
63	Investigations of Sso7d Catalytic Residues by NMR Titration Shifts and Electrostatic Calculationsâ€. Biochemistry, 2003, 42, 1421-1429.	2.5	20
64	Equilibrium Unfolding Thermodynamics of Î²2-Microglobulin Analyzed through Native-State H/D Exchange. Biophysical Journal, 2009, 96, 169-179.	0.5	20
65	Analysis of the conformation and stability of rat TTF-1 homeodomain by circular dichroism. FEBS Letters, 1994, 354, 293-296.	2.8	19
66	Molecular models for intrastrand DNA G-quadruplexes. BMC Structural Biology, 2009, 9, 64.	2.3	18
67	A specific nanobody prevents amyloidogenesis of D76N Î²2-microglobulin in vitro and modifies its tissue distribution in vivo. Scientific Reports, 2017, 7, 46711.	3.3	18
68	Electric dipole reorientation in the interaction of botulinum neurotoxins with neuronal membranes. FEBS Letters, 2009, 583, 2321-2325.	2.8	17
69	Dimerization, stability and electrostatic properties of porcine Î²-lactoglobulin. FEBS Journal, 2001, 268, 4477-4488.	0.2	16
70	Studying Interactions by Molecular Dynamics Simulations at High Concentration. Journal of Biomedicine and Biotechnology, 2012, 2012, 1-9.	3.0	16
71	Absolute quantification of choline-related biomarkers in breast cancer biopsies by liquid chromatography electrospray ionization mass spectrometry. Analytical Cellular Pathology, 2013, 36, 71-83.	1.4	15
72	A decoy set for the thermostable subdomain from chicken villin headpiece, comparison of different free energy estimators. BMC Bioinformatics, 2005, 6, 301.	2.6	14

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73	Structural study of rat thyroid transcription factor 1 homeodomain (TTF-1 HD) by nuclear magnetic resonance. FEBS Letters, 1993, 336, 397-402.	2.8	13
74	Monitoring folding/unfolding transitions of proteins by capillary zone electrophoresis: Measurement ofG and its variation along the pH scale. Electrophoresis, 2001, 22, 3728-3735.	2.4	13
75	NMR structural determination of viscotoxin A3 from Viscum album L.. Biochemical Journal, 2000, 350, 569.	3.7	12
76	Functional analysis of a novel RUNX2 missense mutation found in a family with cleidocranial dysplasia. Journal of Human Genetics, 2005, 50, 679-683.	2.3	12
77	Agent-based protein structure prediction. Multiagent and Grid Systems, 2007, 3, 183-197.	0.9	12
78	Secondary structure effects on the interaction of different polynucleotides with Ca2+. Biopolymers, 1990, 30, 325-333.	2.4	11
79	Interference of citrate-stabilized gold nanoparticles with Î²2-microglobulin oligomeric association. Chemical Communications, 2018, 54, 5422-5425.	4.1	11
80	The Î±4Î²1/EMILIN1 interaction discloses a novel and unique integrin-ligand type of engagement. Matrix Biology, 2018, 66, 50-66.	3.6	11
81	Simulation of electrostatic effects in Fab-antigen complex formation. FEBS Journal, 2000, 267, 4861-4869.	0.2	10
82	CLP-based protein fragment assembly. Theory and Practice of Logic Programming, 2010, 10, 709-724.	1.5	10
83	Reduction of conformational mobility and aggregation in W60G Î²₂â€microglobulin: assessment by ¹⁵N NMR relaxation. Magnetic Resonance in Chemistry, 2013, 51, 795-807.	1.9	10
84	Conformational study of a short Pertussis toxin T cell epitope incorporated in a multiple antigen peptide template by CD and two-dimensional NMR. Analysis of the structural effects on the activity of synthetic immunogens. FEBS Journal, 1993, 217, 171-187.	0.2	9
85	Molecular analysis of a human PAX6 homeobox mutant. European Journal of Human Genetics, 2006, 14, 744-751.	2.8	9
86	Identification of DNA-binding protein target sequences by physical effective energy functions, free energy analysis of lambda repressor-DNA complexes. BMC Structural Biology, 2007, 7, 61.	2.3	9
87	Determining the Energy Landscape of Proteins by a Fast Isotope Exchange NMR Approach. Journal of the American Chemical Society, 2012, 134, 4457-4460.	13.7	9
88	Accuracy assessment of the linear <scp>P</scp>oissonâ€“<scp>B</scp>oltzmann equation and reparametrization of the <scp>OBC</scp> generalized <scp>B</scp>orn model for nucleic acids and nucleic acidâ€“protein complexes. Journal of Computational Chemistry, 2015, 36, 585-596.	3.3	9
89	Dynamics and Thermodynamics of Transthyretin Association from Molecular Dynamics Simulations. BioMed Research International, 2018, 2018, 1-14.	1.9	9
90	NMRâ€Based Analysis of Nanobodies to SARSâ€CoVâ€2 Nsp9 Reveals a Possible Antiviral Strategy Against COVIDâ€19. Advanced Biology, 2021, 5, e2101113.	2.5	9

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91	Using Secondary Structure Information for Protein Folding in CLP(FD)1 1The work is partially supported by MIUR project: Automatic Aggregate â€“and numberâ€“ Reasoning for Computing.. Electronic Notes in Theoretical Computer Science, 2002, 76, 83-98.	0.9	8
92	Conformational stability of neuroglobin helix F â€“ possible effects on the folding pathway within the globin family. FEBS Journal, 2009, 276, 5177-5190.	4.7	8
93	NMR-based homology model for the solution structure of the C-terminal globular domain of EMILIN1. Journal of Biomolecular NMR, 2009, 43, 79-96.	2.8	8
94	Generalized Born forces: Surface integral formulation. Journal of Chemical Physics, 2013, 138, 054112.	3.0	8
95	Transcriptomic Analysis Unveils Correlations between Regulative Apoptotic Caspases and Genes of Cholesterol Homeostasis in Human Brain. PLoS ONE, 2014, 9, e110610.	2.5	8
96	Helix mobility and recognition function of the rat thyroid transcription factorâ€ƒ1 homeodomainâ€ƒâ€“â€ƒhints from ¹⁵Nâ€NMR relaxation studies. FEBS Journal, 2008, 275, 435-448.	4.7	7
97	Single-shot NMR measurement of protein unfolding landscapes. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 842-849.	2.3	7
98	The interaction of Î²2-microglobulin with gold nanoparticles: impact of coating, charge and size. Journal of Materials Chemistry B, 2018, 6, 5964-5974.	5.8	7
99	Insights into a Protein-Nanoparticle System by Paramagnetic Perturbation NMR Spectroscopy. Molecules, 2020, 25, 5187.	3.8	7
100	Missense NR2F1 variant in monozygotic twins affected with the Boschâ€“Boonstraâ€“Schaaf optic atrophy syndrome. Molecular Genetics & Genomic Medicine, 2020, 8, e1278.	1.2	7
101	Chelating effect in short polymers for the design of bidentate binders of increased affinity and selectivity. Scientific Reports, 2015, 5, 15633.	3.3	6
102	Automation of peak-tracking analysis of stepwise perturbed NMR spectra. Journal of Biomolecular NMR, 2017, 67, 121-134.	2.8	6
103	Molecular dynamics simulations of Î²2-microglobulin interaction with hydrophobic surfaces. Molecular BioSystems, 2017, 13, 2625-2637.	2.9	6
104	Structure of Nanobody Nb23. Molecules, 2021, 26, 3567.	3.8	6
105	Improved Processing of Selective NMR Spectra of Biopolymers by Separation of Noise and Signal Subspaces through Singular-Value Decomposition. Journal of Magnetic Resonance Series B, 1996, 113, 160-166.	1.6	5
106	Comparative stability analysis of the thyroid transcription factor 1 and Antennapedia homeodomains: evidence for residue 54 in controlling the structural stability of the recognition helix. International Journal of Biochemistry and Cell Biology, 1999, 31, 1339-1353.	2.8	5
107	Fast structure similarity searches among protein models: efficient clustering of protein fragments. Algorithms for Molecular Biology, 2012, 7, 16.	1.2	5
108	A new germline <scp>VHL</scp> gene mutation in three patients with apparently sporadic pheochromocytoma. Clinical Endocrinology, 2013, 78, 391-397.	2.4	5

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109	Exploring exchange processes in proteins by paramagnetic perturbation of NMR spectra. Physical Chemistry Chemical Physics, 2020, 22, 6247-6259.	2.8	5
110	The corona of proteinâ€“gold nanoparticle systems: the role of ionic strength. Physical Chemistry Chemical Physics, 2022, 24, 1630-1637.	2.8	5
111	Free Energies Calculated According to Manning's Polyelectrolyte Model Compared with Poisson Boltzmann Predictions. Journal of Biomolecular Structure and Dynamics, 1993, 11, 629-635.	3.5	4
112	Protein Folding Simulation in CCP. Lecture Notes in Computer Science, 2004, , 452-453.	1.3	4
113	Short-Chain Alkanethiol Coating for Small-Size Gold Nanoparticles Supporting Protein Stability. Magnetochemistry, 2017, 3, 40.	2.4	4
114	Generalized Born radii computation using linear models and neural networks. Bioinformatics, 2020, 36, 1757-1764.	4.1	4
115	Entropy of Two-Molecule Correlated Translational-Rotational Motions Using the kth Nearest Neighbor Method. Journal of Chemical Theory and Computation, 2021, 17, 3039-3051.	5.3	4
116	Protein Folding in CLP($mathcal{FD}$) with Empirical Contact Energies. Lecture Notes in Computer Science, 2004, , 250-265.	1.3	4
117	Similarity Measures Based on the Overlap of Ranked Genes Are Effective for Comparison and Classification of Microarray Data. Journal of Computational Biology, 2016, 23, 603-614.	1.6	3
118	Estimation of $$^{3}J_{HNhbox{-}Halpha}$$ and $$^{3}J_{Halphahbox{-}Heta}$$ coupling constants from heteronuclear TOCSY spectra. Journal of Biomolecular NMR, 2007, 39, 213-222.	2.8	2
119	Optimal Relabeling of Water Molecules and Single-Molecule Entropy Estimation. Biophysica, 2021, 1, 279-296.	1.4	2
120	A novel de novo HDAC8 missense mutation causing Cornelia de Lange syndrome. Molecular Genetics & Genomic Medicine, 2021, 9, e1612.	1.2	2
121	Biallelic ATOH1 Gene Variant in Siblings With Pontocerebellar Hypoplasia, Developmental Delay, and Hearing Loss. Neurology: Genetics, 2022, 8, e677.	1.9	2
122	Hydrogen-deuterium exchange studies of the rat thyroid transcription factor 1 homeodomain. Journal of Biomolecular NMR, 1997, 9, 397-407.	2.8	1
123	A differential equation for the Generalized Born radii. Physical Chemistry Chemical Physics, 2013, 15, 9783.	2.8	1
124	Case Report: Novel Compound Heterozygous RNASEH2B Mutations Cause Aicardiâ€“GoutiÃ¨res Syndrome. Frontiers in Immunology, 2021, 12, 672952.	4.8	1
125	Topologically non-trivial metal-organic assemblies inhibit Î²2-microglobulin amyloidogenesis. Cell Reports Physical Science, 2021, 2, 100477.	5.6	1
126	The Accuracy of Generalized Born Forces. , 2015, , 143-155.		1

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127	Modulation of F-ATP synthase by pH: Role of His112 protonation of OSCP. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, e12-e13.	1.0	0
128	Effect of anions on Cyclophilin D binding to F-ATP synthase: Implications for the permeability transition pore. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, e111-e112.	1.0	0
129	Amplifying the spectrum of SPAST gene mutations.. Acta Biomedica, 2021, 92, e2021220.	0.3	0