List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	The corona of protein–gold nanoparticle systems: the role of ionic strength. Physical Chemistry Chemical Physics, 2022, 24, 1630-1637.	2.8	5
2	Biallelic <i>ATOH1</i> Gene Variant in Siblings With Pontocerebellar Hypoplasia, Developmental Delay, and Hearing Loss. Neurology: Genetics, 2022, 8, e677.	1.9	2
3	Case Report: Novel Compound Heterozygous RNASEH2B Mutations Cause Aicardi–Goutières Syndrome. Frontiers in Immunology, 2021, 12, 672952.	4.8	1
4	Entropy of Two-Molecule Correlated Translational-Rotational Motions Using the <i>k</i> th Nearest Neighbor Method. Journal of Chemical Theory and Computation, 2021, 17, 3039-3051.	5.3	4
5	Structure of Nanobody Nb23. Molecules, 2021, 26, 3567.	3.8	6
6	Topologically non-trivial metal-organic assemblies inhibit β2-microglobulin amyloidogenesis. Cell Reports Physical Science, 2021, 2, 100477.	5.6	1
7	Optimal Relabeling of Water Molecules and Single-Molecule Entropy Estimation. Biophysica, 2021, 1, 279-296.	1.4	2
8	A novel de novo <i>HDAC8</i> missense mutation causing Cornelia de Lange syndrome. Molecular Genetics & Genomic Medicine, 2021, 9, e1612.	1.2	2
9	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
10	Amplifying the spectrum of SPAST gene mutations Acta Biomedica, 2021, 92, e2021220.	0.3	0
11	Insights into a Protein-Nanoparticle System by Paramagnetic Perturbation NMR Spectroscopy. Molecules, 2020, 25, 5187.	3.8	7
12	Generalized Born radii computation using linear models and neural networks. Bioinformatics, 2020, 36, 1757-1764.	4.1	4
13	Missense <i>NR2F1</i> variant in monozygotic twins affected with the Bosch–Boonstra–Schaaf optic atrophy syndrome. Molecular Genetics & Genomic Medicine, 2020, 8, e1278.	1.2	7
14	Exploring exchange processes in proteins by paramagnetic perturbation of NMR spectra. Physical Chemistry Chemical Physics, 2020, 22, 6247-6259.	2.8	5
15	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
16	Citrate stabilized gold nanoparticles interfere with amyloid fibril formation: D76N and ΔN6 β2-microglobulin variants. Nanoscale, 2018, 10, 4793-4806.	5.6	30
17	Interference of citrate-stabilized gold nanoparticles with β2-microglobulin oligomeric association. Chemical Communications, 2018, 54, 5422-5425.	4.1	11
18	The α4β1/EMILIN1 interaction discloses a novel and unique integrin-ligand type of engagement. Matrix Biology, 2018, 66, 50-66.	3.6	11

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19	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
20	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
21	Dynamics and Thermodynamics of Transthyretin Association from Molecular Dynamics Simulations. BioMed Research International, 2018, 2018, 1-14.	1.9	9
22	Free Energy, Enthalpy and Entropy from Implicit Solvent End-Point Simulations. Frontiers in Molecular Biosciences, 2018, 5, 11.	3.5	22
23	The interaction of β2-microglobulin with gold nanoparticles: impact of coating, charge and size. Journal of Materials Chemistry B, 2018, 6, 5964-5974.	5.8	7
24	PDB2ENTROPY and PDB2TRENT: Conformational and Translational–Rotational Entropy from Molecular Ensembles. Journal of Chemical Information and Modeling, 2018, 58, 1319-1324.	5.4	24
25	Citrate-stabilized gold nanoparticles hinder fibrillogenesis of a pathological variant of β ₂ -microglobulin. Nanoscale, 2017, 9, 3941-3951.	5.6	26
26	Automation of peak-tracking analysis of stepwise perturbed NMR spectra. Journal of Biomolecular NMR, 2017, 67, 121-134.	2.8	6
27	A specific nanobody prevents amyloidogenesis of D76N β2-microglobulin in vitro and modifies its tissue distribution in vivo. Scientific Reports, 2017, 7, 46711.	3.3	18
28	Molecular dynamics simulations of β2-microglobulin interaction with hydrophobic surfaces. Molecular BioSystems, 2017, 13, 2625-2637.	2.9	6
29	Short-Chain Alkanethiol Coating for Small-Size Gold Nanoparticles Supporting Protein Stability. Magnetochemistry, 2017, 3, 40.	2.4	4
30	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
31	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
32	Accurate Estimation of the Entropy of Rotation–Translation Probability Distributions. Journal of Chemical Theory and Computation, 2016, 12, 1-8.	5.3	21
33	Chelating effect in short polymers for the design of bidentate binders of increased affinity and selectivity. Scientific Reports, 2015, 5, 15633.	3.3	6
34	Distance-Based Configurational Entropy of Proteins from Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0132356.	2.5	32
35	From ATP to PTP and Back. Circulation Research, 2015, 116, 1850-1862.	4.5	97
36	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

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37	Accuracy assessment of the linear <scp>P</scp> oisson– <scp>B</scp> oltzmann equation and reparametrization of the <scp>OBC</scp> generalized <scp>B</scp> orn model for nucleic acids and nucleic acid–protein complexes. Journal of Computational Chemistry, 2015, 36, 585-596.	3.3	9
38	Probing the Influence of Citrate-Capped Gold Nanoparticles on an Amyloidogenic Protein. ACS Nano, 2015, 9, 2600-2613.	14.6	80
39	The Accuracy of Generalized Born Forces. , 2015, , 143-155.		1
40	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
41	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
42	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
43	Transcriptomic Analysis Unveils Correlations between Regulative Apoptotic Caspases and Genes of Cholesterol Homeostasis in Human Brain. PLoS ONE, 2014, 9, e110610.	2.5	8
44	Structure, Folding Dynamics, and Amyloidogenesis of D76N β2-Microglobulin. Journal of Biological Chemistry, 2013, 288, 30917-30930.	3.4	80
45	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
46	A new germline <i><scp>VHL</scp></i> gene mutation in three patients with apparently sporadic pheochromocytoma. Clinical Endocrinology, 2013, 78, 391-397.	2.4	5
47	A differential equation for the Generalized Born radii. Physical Chemistry Chemical Physics, 2013, 15, 9783.	2.8	1
48	Generalized Born forces: Surface integral formulation. Journal of Chemical Physics, 2013, 138, 054112.	3.0	8
49	Reduction of conformational mobility and aggregation in W60G β ₂ â€microglobulin: assessment by ¹⁵ N NMR relaxation. Magnetic Resonance in Chemistry, 2013, 51, 795-807.	1.9	10
50	Monitoring the Interaction between β2-Microglobulin and the Molecular Chaperone αB-crystallin by NMR and Mass Spectrometry. Journal of Biological Chemistry, 2013, 288, 17844-17858.	3.4	32
51	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
52	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
53	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
54	Studying Interactions by Molecular Dynamics Simulations at High Concentration. Journal of Biomedicine and Biotechnology, 2012, 2012, 1-9.	3.0	16

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55	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
56	Bluues server: electrostatic properties of wild-type and mutated protein structures. Bioinformatics, 2012, 28, 2189-2190.	4.1	72
57	Single-shot NMR measurement of protein unfolding landscapes. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 842-849.	2.3	7
58	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
59	The Projection Analysis of NMR Chemical Shifts Reveals Extended EPAC Autoinhibition Determinants. Biophysical Journal, 2012, 102, 630-639.	0.5	83
60	Fast structure similarity searches among protein models: efficient clustering of protein fragments. Algorithms for Molecular Biology, 2012, 7, 16.	1.2	5
61	Rapid oligomer formation of human muscle acylphosphatase induced by heparan sulfate. Nature Structural and Molecular Biology, 2012, 19, 547-554.	8.2	28
62	Nucleotide diversity and linkage disequilibrium in Populus nigra cinnamyl alcohol dehydrogenase (CAD4) gene. Tree Genetics and Genomes, 2011, 7, 1011-1023.	1.6	138
63	Molecular dynamics simulation of β ₂ â€microglobulin in denaturing and stabilizing conditions. Proteins: Structure, Function and Bioinformatics, 2011, 79, 986-1001.	2.6	31
64	Effect of Tetracyclines on the Dynamics of Formation and Destructuration of β2-Microglobulin Amyloid Fibrils. Journal of Biological Chemistry, 2011, 286, 2121-2131.	3.4	87
65	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
66	CLP-based protein fragment assembly. Theory and Practice of Logic Programming, 2010, 10, 709-724.	1.5	10
67	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
68	Native-unlike Long-lived Intermediates along the Folding Pathway of the Amyloidogenic Protein β2-Microglobulin Revealed by Real-time Two-dimensional NMR. Journal of Biological Chemistry, 2010, 285, 5827-5835.	3.4	55
69	Folding and Fibrillogenesis: Clues from β2-Microglobulin. Journal of Molecular Biology, 2010, 401, 286-297.	4.2	35
70	Electric dipole reorientation in the interaction of botulinum neurotoxins with neuronal membranes. FEBS Letters, 2009, 583, 2321-2325.	2.8	17
71	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
72	Molecular models for intrastrand DNA G-quadruplexes. BMC Structural Biology, 2009, 9, 64.	2.3	18

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73	Conformational stability of neuroglobin helix F – possible effects on the folding pathway within the globin family. FEBS Journal, 2009, 276, 5177-5190.	4.7	8
74	Equilibrium Unfolding Thermodynamics of β2-Microglobulin Analyzed through Native-State H/D Exchange. Biophysical Journal, 2009, 96, 169-179.	0.5	20
75	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
76	Helix mobility and recognition function of the rat thyroid transcription factor 1 homeodomain – hints from ¹⁵ Nâ€NMR relaxation studies. FEBS Journal, 2008, 275, 435-448.	4.7	7
77	The Controlling Roles of Trp60 and Trp95 in \hat{I}^2 2-Microglobulin Function, Folding and Amyloid Aggregation Properties. Journal of Molecular Biology, 2008, 378, 887-897.	4.2	82
78	The Catalytic Site of Glutathione Peroxidases. Antioxidants and Redox Signaling, 2008, 10, 1515-1526.	5.4	151
79	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
80	Molecular Dynamics Simulation Suggests Possible Interaction Patterns at Early Steps of β2-Microglobulin Aggregation. Biophysical Journal, 2007, 92, 1673-1681.	0.5	39
81	Agent-based protein structure prediction. Multiagent and Grid Systems, 2007, 3, 183-197.	0.9	12
82	Scoring predictive models using a reduced representation of proteins: model and energy definition. BMC Structural Biology, 2007, 7, 15.	2.3	25
83	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
84	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
85	Molecular analysis of a human PAX6 homeobox mutant. European Journal of Human Genetics, 2006, 14, 744-751.	2.8	9
86	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
87	Collagen Plays an Active Role in the Aggregation of β2-Microglobulin under Physiopathological Conditions of Dialysis-related Amyloidosis*. Journal of Biological Chemistry, 2006, 281, 16521-16529.	3.4	128
88	Solution structure of β2-microglobulin and insights into fibrillogenesis. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1753, 76-84.	2.3	25
89	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
90	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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91	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
92	MM/PBSA analysis of molecular dynamics simulations of bovine β-lactoglobulin: Free energy gradients in conformational transitions?. Proteins: Structure, Function and Bioinformatics, 2005, 59, 91-103.	2.6	28
93	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
94	Protein Folding Simulation in CCP. Lecture Notes in Computer Science, 2004, , 452-453.	1.3	4
95	Constraint Logic Programming approach to protein structure prediction. BMC Bioinformatics, 2004, 5, 186.	2.6	57
96	Protein Folding in CLP(\$mathcal{FD}\$) with Empirical Contact Energies. Lecture Notes in Computer Science, 2004, , 250-265.	1.3	4
97	Amino acid empirical contact energy definitions for fold recognition in the space of contact maps. BMC Bioinformatics, 2003, 4, 8.	2.6	88
98	Quantitative Correlation of Solvent Polarity with the α-/310-Helix Equilibrium: A Heptapeptide Behaves as a Solvent-Driven Molecular Spring. Angewandte Chemie - International Edition, 2003, 42, 3388-3392.	13.8	91
99	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
100	Investigations of Sso7d Catalytic Residues by NMR Titration Shifts and Electrostatic Calculationsâ€. Biochemistry, 2003, 42, 1421-1429.	2.5	20
101	Protocol for MM/PBSA Molecular Dynamics Simulations of Proteins. Biophysical Journal, 2003, 85, 159-166.	0.5	173
102	EF Loop Conformational Change Triggers Ligand Binding in Î ² -Lactoglobulins. Journal of Biological Chemistry, 2003, 278, 38840-38846.	3.4	67
103	Peptide Models of Folding Initiation Sites of Bovine β-Lactoglobulin: Identification of Nativelike Hydrophobic Interactions Involving G and H Strandsâ€. Biochemistry, 2002, 41, 2786-2796.	2.5	20
104	The Poisson-Boltzmann equation for biomolecular electrostatics: a tool for structural biology. Journal of Molecular Recognition, 2002, 15, 377-392.	2.1	469
105	Using Secondary Structure Information for Protein Folding in CLP(FD)1 1The work is partially supported by MIUR project: Automatic Aggregate –and number– Reasoning for Computing Electronic Notes in Theoretical Computer Science, 2002, 76, 83-98.	0.9	8
106	Dimerization, stability and electrostatic properties of porcine β-lactoglobulin. FEBS Journal, 2001, 268, 4477-4488.	0.2	16
107	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
108	NMR structural determination of viscotoxin A3 from Viscum album L Biochemical Journal, 2000, 350, 569.	3.7	12

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109	NMR structural determination of viscotoxin A3 from Viscum album L Biochemical Journal, 2000, 350, 569-577.	3.7	45
110	Electrostatic properties of bovine ?-lactoglobulin. , 2000, 39, 317-330.		68
111	Simulation of electrostatic effects in Fab-antigen complex formation. FEBS Journal, 2000, 267, 4861-4869.	0.2	10
112	Bovine βâ€lactoglobulin: Interaction studies with palmitic acid. Protein Science, 2000, 9, 1347-1356.	7.6	105
113	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
114	Biomolecular Electrostatics with the Linearized Poisson-Boltzmann Equation. Biophysical Journal, 1999, 76, 1-16.	0.5	122
115	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
116	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
117	Hydrogen-deuterium exchange studies of the rat thyroid transcription factor 1 homeodomain. Journal of Biomolecular NMR, 1997, 9, 397-407.	2.8	1
118	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
119	On the variational approach to Poisson–Boltzmann free energies. Chemical Physics Letters, 1997, 281, 135-139.	2.6	68
120	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
121	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
122	Analysis of the conformation and stability of rat TTF-1 homeodomain by circular dichroism. FEBS Letters, 1994, 354, 293-296.	2.8	19
123	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
124	NMR and circular dichroism studies of the lantibiotic nisin in non-aqueous environments. FEBS Letters, 1993, 319, 189-194.	2.8	50
125	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
126	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

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127	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
128	Limiting-laws of polyelectrolyte solutions. Ionic distribution in mixed-valency counterions systems. I: The model. Biophysical Chemistry, 1991, 41, 73-80.	2.8	38
129	Secondary structure effects on the interaction of different polynucleotides with Ca2+. Biopolymers, 1990, 30, 325-333.	2.4	11