Anna Marabotti

List of Publications by Year
in descending order

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94 papers	1,859 citations	236612 25 h-index	329751 37 g-index
119 all docs	119 docs citations	119 times ranked	2309 citing authors

#	Article	IF	Citations
1	Simple, Intuitive Calculations of Free Energy of Binding for Proteinâ˜Ligand Complexes. 1. Models without Explicit Constrained Water. Journal of Medicinal Chemistry, 2002, 45, 2469-2483.	2.9	131
2	A review on drug repurposing applicable to COVID-19. Briefings in Bioinformatics, 2021, 22, 726-741.	3.2	117
3	Free Energy of Ligand Binding to Protein: Evaluation of the Contribution of Water Molecules by Computational Methods. Current Medicinal Chemistry, 2004, 11, 3093-3118.	1.2	89
4	Energetics of the protein-DNA-water interaction. BMC Structural Biology, 2007, 7, 4.	2.3	57
5	Environment, dysbiosis, immunity and sex-specific susceptibility: A translational hypothesis for regressive autism pathogenesis. Nutritional Neuroscience, 2015, 18, 145-161.	1.5	57
6	Myosinâ€Binding Protein C <scp>DNA</scp> Variants in Domestic Cats (<scp>A</scp>31<scp>P</scp>,<scp> A</scp>74<scp>T</scp>,<scp> R</scp>820<scp>W</scp>) and their Association with Hypertrophic Cardiomyopathy. Journal of Veterinary Internal Medicine, 2013, 27, 275-285.	0.6	51
7	Energyâ€based prediction of amino acidâ€nucleotide base recognition. Journal of Computational Chemistry, 2008, 29, 1955-1969.	1.5	44
8	Homology Modeling Studies on Human Galactose-1-phosphate Uridylyltransferase and on Its Galactosemia-Related Mutant Q188R Provide an Explanation of Molecular Effects of the Mutation on Homo- and Heterodimers. Journal of Medicinal Chemistry, 2005, 48, 773-779.	2.9	43
9	Analysis of galactosemia-linked mutations of GALT enzyme using a computational biology approach. Protein Engineering, Design and Selection, 2010, 23, 103-113.	1.0	40
10	Crystal Structures of a New Class of Allosteric Effectors Complexed to Tryptophan Synthase. Journal of Biological Chemistry, 2002, 277, 10647-10652.	1.6	36
11	Homology modeling in tandem with 3D-QSAR analyses: A computational approach to depict the agonist binding site of the human CB2 receptor. European Journal of Medicinal Chemistry, 2011, 46, 4489-4505.	2.6	36
12	Study on the Association among Mycotoxins and other Variables in Children with Autism. Toxins, 2017, 9, 203.	1.5	36
13	Histological changes, apoptosis and metallothionein levels in Triturus carnifex (Amphibia, Urodela) exposed to environmental cadmium concentrations. Aquatic Toxicology, 2016, 173, 63-73.	1.9	33
14	Hydrophobic interactions and ionic networks play an important role in thermal stability and denaturation mechanism of the porcine odorantâ€binding protein. Proteins: Structure, Function and Bioinformatics, 2008, 71, 35-44.	1.5	32
15	A theoretical study on predicted protein targets of apple polyphenols and possible mechanisms of chemoprevention in colorectal cancer. Scientific Reports, 2016, 6, 32516.	1.6	32
16	Predicting the stability of mutant proteins by computational approaches: an overview. Briefings in Bioinformatics, 2021, 22, .	3.2	32
17	Binding of glutamine to glutamine-binding protein from Escherichia coli induces changes in protein structure and increases protein stability. Proteins: Structure, Function and Bioinformatics, 2004, 58, 80-87.	1.5	30
18	Modulation of the structural integrity of helix F in apomyoglobin by single amino acid replacements. Protein Science, 2004, 13, 1572-1585.	3.1	30

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19	4-Nonylphenol reduces cell viability and induces apoptosis and ER-stress in a human epithelial intestinal cell line. Toxicology in Vitro, 2015, 29, 1436-1444.	1.1	30
20	Allosteric Communication of Tryptophan Synthase. Journal of Biological Chemistry, 2001, 276, 17747-17753.	1.6	28
21	Crystal Structure of the Î²Ser178 â†' Pro Mutant of Tryptophan Synthase. Journal of Biological Chemistry, 2002, 277, 10653-10660.	1.6	28
22	Detection and molecular characterization of a novel BRAF activated domain mutation in follicular variant of papillary thyroid carcinoma. Human Pathology, 2009, 40, 827-833.	1.1	28
23	Stability and Dynamics of the Porcine Odorant-Binding Protein. Biochemistry, 2007, 46, 11120-11127.	1.2	27
24	Static and dynamic interactions between GALK enzyme and known inhibitors: Guidelines to design new drugs for galactosemic patients. European Journal of Medicinal Chemistry, 2013, 63, 423-434.	2.6	27
25	Interaction of human chymase with ginkgolides, terpene trilactones of Ginkgo biloba investigated by molecular docking simulations. Biochemical and Biophysical Research Communications, 2016, 473, 449-454.	1.0	27
26	The Odd Couple(s): An Overview of Beta-Lactam Antibiotics Bearing More Than One Pharmacophoric Group. International Journal of Molecular Sciences, 2021, 22, 617.	1.8	27
27	Theoretical model of the three-dimensional structure of a sugar-binding protein from Pyrococcus horikoshii: structural analysis and sugar-binding simulations. Biochemical Journal, 2004, 380, 677-684.	1.7	25
28	Binding of Glucose to the d-Galactose/d-Glucoseâ€"Binding Protein from Escherichia coli Restores the Native Protein Secondary Structure and Thermostability That Are Lost upon Calcium Depletion. Journal of Biochemistry, 2006, 139, 213-221.	0.9	25
29	Mutation spectrum in the French cohort of galactosemic patients and structural simulation of 27 novel missense variations. Molecular Genetics and Metabolism, 2012, 107, 438-447.	0.5	25
30	Correlation assessment among clinical phenotypes, expression analysis and molecular modeling of 14 novel variations in the human galactose-1-phosphate uridylyltransferase gene. Human Mutation, 2012, 33, 1107-1115.	1.1	25
31	GALK inhibitors for classic galactosemia. Future Medicinal Chemistry, 2014, 6, 1003-1015.	1.1	24
32	Clinical and molecular spectra in galactosemic patients from neonatal screening in northeastern Italy: Structural and functional characterization of new variations in the galactose-1-phosphate uridyltransferase (GALT) gene. Gene, 2015, 559, 112-118.	1.0	23
33	Searching for Chymase Inhibitors among Chamomile Compounds Using a Computational-Based Approach. Biomolecules, 2019, 9, 5.	1.8	23
34	Performance of Web tools for predicting changes in protein stability caused by mutations. BMC Bioinformatics, 2021, 22, 345.	1.2	23
35	In silico approach to find chymase inhibitors among biogenic compounds. Future Medicinal Chemistry, 2016, 8, 841-851.	1.1	22
36	Novel allosteric effectors of the tryptophan synthase Î±2Î²2 complex identified by computer-assisted molecular modeling. BBA - Proteins and Proteomics, 2000, 1476, 287-299.	2.1	20

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37	D-Trehalose/D-maltose-binding protein from the hyperthermophilic archaeon Thermococcus litoralis: The binding of trehalose and maltose results in different protein conformational states. Proteins: Structure, Function and Bioinformatics, 2006, 63, 754-767.	1.5	20
38	Amino acid transport in thermophiles: characterization of an arginine-binding protein in Thermotoga maritima. 2. Molecular organization and structural stability. Molecular BioSystems, 2010, 6, 687.	2.9	20
39	The Tryptophan Phosphorescence of Porcine and Mutant Bovine Odorant-Binding Proteins: A Probe for the Local Protein Structure and Dynamics. Journal of Proteome Research, 2008, 7, 1151-1158.	1.8	19
40	GALT Protein Database, a Bioinformatics Resource for the Management and Analysis of Structural Features of a Galactosemia-related Protein and Its Mutants. Genomics, Proteomics and Bioinformatics, 2009, 7, 71-76.	3.0	19
41	GALT Protein Database: Querying Structural and Functional Features of GALT Enzyme. Human Mutation, 2014, 35, 1060-1067.	1.1	19
42	Ochratoxin A as possible factor trigging autism and its male prevalence via epigenetic mechanism. Nutritional Neuroscience, 2016, 19, 43-46.	1.5	19
43	Human aryl-hydrocarbon receptor and its interaction with dioxin and physiological ligands investigated by molecular modelling and docking simulations. Biochemical and Biophysical Research Communications, 2011, 413, 176-181.	1.0	18
44	Galactoseâ€1â€phosphate uridyltransferase deficiency: A literature review of the putative mechanisms of short and longâ€term complications and allelic variants. Clinical Genetics, 2018, 93, 206-215.	1.0	18
45	Structure and Stability of a Rat Odorant-Binding Protein: Another Brick in the Wall. Journal of Proteome Research, 2009, 8, 4005-4013.	1.8	17
46	Wild-Type and Mutant Bovine Odorant-Binding Proteins To Probe the Role of the Quaternary Structure Organization in the Protein Thermal Stability. Journal of Proteome Research, 2008, 7, 5221-5229.	1.8	16
47	Association Analysis of Noncoding Variants in Neuroligins 3 and 4X Genes with Autism Spectrum Disorder in an Italian Cohort. International Journal of Molecular Sciences, 2016, 17, 1765.	1.8	16
48	Structure and Dynamics of Cold-Adapted Enzymes as Investigated by Phosphorescence Spectroscopy and Molecular Dynamics Studies. 2. The Case of an Esterase from Pseudoalteromonas haloplanktis. Journal of Physical Chemistry B, 2009, 113, 13171-13178.	1.2	15
49	Structure and Dynamics of Cold-Adapted Enzymes as Investigated by FT-IR Spectroscopy and MD. The Case of an Esterase from Pseudoalteromonas haloplanktis. Journal of Physical Chemistry B, 2009, 113, 7753-7761.	1.2	15
50	A Thermostable Sugar-Binding Protein from the Archaeon Pyrococcus horikoshii as a Probe for the Development of a Stable Fluorescence Biosensor for Diabetic Patients. Biotechnology Progress, 2004, 20, 1572-1577.	1.3	14
51	Binding of mycotoxins to proteins involved in neuronal plasticity: a combined in silico/wet investigation. Scientific Reports, 2017, 7, 15156.	1.6	14
52	HINT predictive analysis of binding between retinol binding protein and hydrophobic ligands. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2129-2132.	1.0	13
53	Mutant bovine odorantâ€binding protein: Temperature affects the protein stability and dynamics as revealed by infrared spectroscopy and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 72, 769-778.	1.5	13
54	Celiac Anti-Type 2 Transglutaminase Antibodies Induce Phosphoproteome Modification in Intestinal Epithelial Caco-2 Cells. PLoS ONE, 2013, 8, e84403.	1.1	13

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55	The evolution of a Web resource: The Galactosemia Proteins Database 2.0. Human Mutation, 2018, 39, 52-60.	1.1	13
56	The differences in the microenvironment of the two tryptophan residues of the glutamineâ€binding protein from Escherichia coli shed light on the binding properties and the structural dynamics of the protein. Proteins: Structure, Function and Bioinformatics, 2008, 71, 743-750.	1.5	11
57	Pyrimidineâ€specific ribonucleoside hydrolase from the archaeon Sulfolobusâ€ƒsolfataricusâ€“ biochemical characterization and homology modeling. FEBS Journal, 2008, 275, 1900-1914.	2.2	11
58	Biochemical characterization and homology modeling of a purine-specific ribonucleoside hydrolase from the archaeon Sulfolobus solfataricus: Insights into mechanisms of protein stabilization. Archives of Biochemistry and Biophysics, 2009, 483, 55-65.	1.4	11
59	Pressure Affects the Structure and the Dynamics of thed-Galactose/d-Glucose-Binding Protein fromEscherichia coliby Perturbing the C-Terminal Domain of the Proteinâ€. Biochemistry, 2006, 45, 11885-11894.	1.2	10
60	Molecular adaptation strategies to high temperature and thermal denaturation mechanism of the D-trehalose/D-maltose-binding protein from the hyperthermophilic archaeon Thermococcus litoralis. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1002-1009.	1.5	9
61	Molecular strategies for protein stabilization: The case of a trehalose/maltoseâ€binding protein from Thermus thermophilus. Proteins: Structure, Function and Bioinformatics, 2008, 73, 839-850.	1.5	8
62	Under Pressure That Splits a Family in Two. The Case of Lipocalin Family. PLoS ONE, 2012, 7, e50489.	1.1	8
63	Investigating the Effects of Amino Acid Variations in Human Menin. Molecules, 2022, 27, 1747.	1.7	8
64	Computational methods to assist in the discovery of pharmacological chaperones for rare diseases. Briefings in Bioinformatics, 2022, 23, .	3.2	8
65	Pressure effect on the stability and the conformational dynamics of the D-Galactose/D-Glucose-binding protein from Escherichia coli. Proteins: Structure, Function and Bioinformatics, 2005, 62, 193-201.	1.5	7
66	Assessment of the conformational features of vasoactive intestinal peptide in solution by limited proteolysis experiments. Biopolymers, 2006, 81, 110-119.	1.2	7
67	Synthesis and biological evaluation of the progenitor of a new class of cephalosporin analogues, with a particular focus on structure-based computational analysis. PLoS ONE, 2017, 12, e0181563.	1.1	7
68	When it comes to homology, bad habits die hard. Trends in Biochemical Sciences, 2009, 34, 98-99.	3.7	6
69	New compounds for a good old class: Synthesis of two Î²-lactam bearing cephalosporins and their evaluation with a multidisciplinary approach. Bioorganic and Medicinal Chemistry, 2020, 28, 115302.	1.4	6
70	Site-directed mutagenesis gives insights into substrate specificity of Sulfolobus solfataricus purine-specific nucleoside hydrolase. Annals of Microbiology, 2012, 62, 881-887.	1.1	5
71	Analysis of the Structure-Function-Dynamics Relationships of GALT Enzyme and of Its Pathogenic Mutant p.Q188R: A Molecular Dynamics Simulation Study in Different Experimental Conditions. Molecules, 2021, 26, 5941.	1.7	5
72	Efficient Fludarabineâ€Activating PNP From Archaea as a Guidance for Redesign the Active Site of E. Coli PNP. Journal of Cellular Biochemistry, 2016, 117, 1126-1135.	1.2	4

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73	Computational analysis of the interactions of a novel cephalosporin derivative with Î²-lactamases. BMC Structural Biology, 2018, 18, 13.	2.3	4
74	A multiple network-based bioinformatics pipeline for the study of molecular mechanisms in oncological diseases for personalized medicine. Briefings in Bioinformatics, 2021, 22, .	3.2	4
75	Modeling the Conformation of Side Chains in Proteins: Approaches, Problems and Possible Developments. Current Chemical Biology, 2008, 2, 200-214.	0.2	4
76	Simulation of the Interactions of Arginine with Wild-Type GALT Enzyme and the Classic Galactosemia-Related Mutant p.Q188R by a Computational Approach. Molecules, 2021, 26, 6061.	1.7	3
77	Identification of a novel point mutation in the ligand-binding domain of the human glucocorticoid receptor (hGR) in a patient with glucocorticoid resistance. International Journal on Disability and Human Development, 2007, 6, .	0.2	2
78	New computational strategy to analyze the interactions of ERÎ± and ERÎ² with different ERE sequences. Journal of Computational Chemistry, 2007, 28, 1031-1041.	1.5	2
79	Correlation Spectroscopy and Molecular Dynamics Simulations to Study the Structural Features of Proteins. PLoS ONE, 2013, 8, e64840.	1.1	2
80	Correlation between fluorescence and structure in the orange-emitting GFP-like protein, monomeric Kusabira Orange. Journal of Photochemistry and Photobiology B: Biology, 2014, 138, 223-229.	1.7	2
81	Assessment of haptoglobin alleles in autism spectrum disorders. Scientific Reports, 2020, 10, 7758.	1.6	2
82	Critical Assessment of Side Chain Conformation Prediction in Modelling of Single Point Amino Acid Mutation. Advances in Experimental Medicine and Biology, 2010, 680, 283-289.	0.8	2
83	Modeling the Conformation of Side Chains in Proteins: Approaches, Problems and Possible Developments. Current Chemical Biology, 2008, 2, 200-214.	0.2	1
84	Pressure Effects on the Structure and Stability of the Hyperthermophilic Trehalose/Maltose-Binding Protein from Thermococcus litoralis. Journal of Physical Chemistry B, 2009, 113, 12804-12808.	1.2	1
85	Unraveling the structural and functional differences between purine nucleoside phosphorylase and 5â€²-deoxy-5â€²-methylthioadenosine phosphorylase from the archaeon Pyrococcus furiosus. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1358-1366.	1.1	1
86	Solving Biclustering with a GRASP-Like Metaheuristic: Two Case-Studies on Gene Expression Analysis. Lecture Notes in Computer Science, 2012, , 253-267.	1.0	1
87	Statistical Analysis of Protein Structural Features: Relationships and PCA Grouping. Lecture Notes in Computer Science, 2015, , 33-43.	1.0	1
88	Erratum to â€œDetection and molecular characterization of a novel BRAF activated domain mutation in follicular variant of papillary thyroid carcinomaâ€•[Hum Pathol 40 (2009) 827-833]. Human Pathology, 2009, 40, 1212.	1.1	0
89	The misuse of terms in scientific literature. Bioinformatics, 2010, 26, 2498-2498.	1.8	0
90	Preface: BITS2014, the annual meeting of the Italian Society of Bioinformatics. BMC Bioinformatics, 2015, 16, S1.	1.2	0

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91	Editorial: Computational Proteomics and Integration of Data Resources for Advanced Studies in Life Sciences. Frontiers in Genetics, 2021, 12, 729013.	1.1	0
92	Application of computational methods for structural and functional characterization of mutants of GALT enzyme. EMBnet Journal, 2012, 18, 116.	0.2	0
93	Identification of molecular targets for mycotoxins related to autism development. EMBnet Journal, 2012, 18, 118.	0.2	0
94	New metaheuristics approaches for biclustering of gene expression Data. EMBnet Journal, 2012, 18, 68.	0.2	0