

# Anna Marabotti

## List of Publications by Year in descending order

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94  
papers

1,859  
citations

236925

25  
h-index

330143

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 Protein–Ligand Complexes. 1. Models without Explicit Constrained Water. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 2469-2483.	6.4	131
2	A review on drug repurposing applicable to COVID-19. <i>Briefings in Bioinformatics</i> , 2021, 22, 726-741.	6.5	117
3	Free Energy of Ligand Binding to Protein: Evaluation of the Contribution of Water Molecules by Computational Methods. <i>Current Medicinal Chemistry</i> , 2004, 11, 3093-3118.	2.4	89
4	Energetics of the protein-DNA-water interaction. <i>BMC Structural Biology</i> , 2007, 7, 4.	2.3	57
5	Environment, dysbiosis, immunity and sex-specific susceptibility: A translational hypothesis for regressive autism pathogenesis. <i>Nutritional Neuroscience</i> , 2015, 18, 145-161.	3.1	57
6	<i>Myosin-binding Protein C</i> DNA Variants in Domestic Cats ( <i>A</i> 31 <i>P</i> , <i>A</i> 74 <i>T</i> , <i>R</i> 820 <i>A</i> W) and their Association with Hypertrophic Cardiomyopathy. <i>Journal of Veterinary Internal Medicine</i> , 2013, 27, 275-285.	1.6	51
7	Energy-based prediction of amino acid–nucleotide base recognition. <i>Journal of Computational Chemistry</i> , 2008, 29, 1955-1969.	3.3	44
8	Homology Modeling Studies on Human Galactose-1-phosphate Uridyltransferase and on Its Galactosemia-Related Mutant Q188R Provide an Explanation of Molecular Effects of the Mutation on Homo- and Heterodimers. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 773-779.	6.4	43
9	Analysis of galactosemia-linked mutations of GALT enzyme using a computational biology approach. <i>Protein Engineering, Design and Selection</i> , 2010, 23, 103-113.	2.1	40
10	Crystal Structures of a New Class of Allosteric Effectors Complexed to Tryptophan Synthase. <i>Journal of Biological Chemistry</i> , 2002, 277, 10647-10652.	3.4	36
11	Homology modeling in tandem with 3D-QSAR analyses: A computational approach to depict the agonist binding site of the human CB2 receptor. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 4489-4505.	5.5	36
12	Study on the Association among Mycotoxins and other Variables in Children with Autism. <i>Toxins</i> , 2017, 9, 203.	3.4	36
13	Histological changes, apoptosis and metallothionein levels in <i>Triturus carnifex</i> (Amphibia, Urodela) exposed to environmental cadmium concentrations. <i>Aquatic Toxicology</i> , 2016, 173, 63-73.	4.0	33
14	Hydrophobic interactions and ionic networks play an important role in thermal stability and denaturation mechanism of the porcine odorant-binding protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 35-44.	2.6	32
15	A theoretical study on predicted protein targets of apple polyphenols and possible mechanisms of chemoprevention in colorectal cancer. <i>Scientific Reports</i> , 2016, 6, 32516.	3.3	32
16	Predicting the stability of mutant proteins by computational approaches: an overview. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	32
17	Binding of glutamine to glutamine-binding protein from <i>Escherichia coli</i> induces changes in protein structure and increases protein stability. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 80-87.	2.6	30
18	Modulation of the structural integrity of helix F in apomyoglobin by single amino acid replacements. <i>Protein Science</i> , 2004, 13, 1572-1585.	7.6	30

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19	4-Nonylphenol reduces cell viability and induces apoptosis and ER-stress in a human epithelial intestinal cell line. <i>Toxicology in Vitro</i> , 2015, 29, 1436-1444.	2.4	30
20	Allosteric Communication of Tryptophan Synthase. <i>Journal of Biological Chemistry</i> , 2001, 276, 17747-17753.	3.4	28
21	Crystal Structure of the $\hat{I}^2$ Ser178 $\hat{A}^*$ Pro Mutant of Tryptophan Synthase. <i>Journal of Biological Chemistry</i> , 2002, 277, 10653-10660.	3.4	28
22	Detection and molecular characterization of a novel BRAF activated domain mutation in follicular variant of papillary thyroid carcinoma. <i>Human Pathology</i> , 2009, 40, 827-833.	2.0	28
23	Stability and Dynamics of the Porcine Odorant-Binding Protein. <i>Biochemistry</i> , 2007, 46, 11120-11127.	2.5	27
24	Static and dynamic interactions between GALK enzyme and known inhibitors: Guidelines to design new drugs for galactosemic patients. <i>European Journal of Medicinal Chemistry</i> , 2013, 63, 423-434.	5.5	27
25	Interaction of human chymase with ginkgolides, terpene trilactones of Ginkgo biloba investigated by molecular docking simulations. <i>Biochemical and Biophysical Research Communications</i> , 2016, 473, 449-454.	2.1	27
26	The Odd Couple(s): An Overview of Beta-Lactam Antibiotics Bearing More Than One Pharmacophoric Group. <i>International Journal of Molecular Sciences</i> , 2021, 22, 617.	4.1	27
27	Theoretical model of the three-dimensional structure of a sugar-binding protein from <i>Pyrococcus horikoshii</i> : structural analysis and sugar-binding simulations. <i>Biochemical Journal</i> , 2004, 380, 677-684.	3.7	25
28	Binding of Glucose to the d-Galactose/d-Glucose-binding Protein from <i>Escherichia coli</i> Restores the Native Protein Secondary Structure and Thermostability That Are Lost upon Calcium Depletion. <i>Journal of Biochemistry</i> , 2006, 139, 213-221.	1.7	25
29	Mutation spectrum in the French cohort of galactosemic patients and structural simulation of 27 novel missense variations. <i>Molecular Genetics and Metabolism</i> , 2012, 107, 438-447.	1.1	25
30	Correlation assessment among clinical phenotypes, expression analysis and molecular modeling of 14 novel variations in the human galactose-1-phosphate uridylyltransferase gene. <i>Human Mutation</i> , 2012, 33, 1107-1115.	2.5	25
31	GALK inhibitors for classic galactosemia. <i>Future Medicinal Chemistry</i> , 2014, 6, 1003-1015.	2.3	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 uridylyltransferase (GALT) gene. <i>Gene</i> , 2015, 559, 112-118.	2.2	23
33	Searching for Chymase Inhibitors among Chamomile Compounds Using a Computational-Based Approach. <i>Biomolecules</i> , 2019, 9, 5.	4.0	23
34	Performance of Web tools for predicting changes in protein stability caused by mutations. <i>BMC Bioinformatics</i> , 2021, 22, 345.	2.6	23
35	<i>In silico</i> approach to find chymase inhibitors among biogenic compounds. <i>Future Medicinal Chemistry</i> , 2016, 8, 841-851.	2.3	22
36	Novel allosteric effectors of the tryptophan synthase $\hat{I}^2$ complex identified by computer-assisted molecular modeling. <i>BBA - Proteins and Proteomics</i> , 2000, 1476, 287-299.	2.1	20

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37	D-Trehalose/D-maltose-binding protein from the hyperthermophilic archaeon <i>Thermococcus litoralis</i> : The binding of trehalose and maltose results in different protein conformational states. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 754-767.	2.6	20
38	Amino acid transport in thermophiles: characterization of an arginine-binding protein in <i>Thermotoga maritima</i> . 2. Molecular organization and structural stability. <i>Molecular BioSystems</i> , 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. <i>Journal of Proteome Research</i> , 2008, 7, 1151-1158.	3.7	19
40	GALT Protein Database, a Bioinformatics Resource for the Management and Analysis of Structural Features of a Galactosemia-related Protein and Its Mutants. <i>Genomics, Proteomics and Bioinformatics</i> , 2009, 7, 71-76.	6.9	19
41	GALT Protein Database: Querying Structural and Functional Features of GALT Enzyme. <i>Human Mutation</i> , 2014, 35, 1060-1067.	2.5	19
42	Ochratoxin A as possible factor triggering autism and its male prevalence <i>via</i> epigenetic mechanism. <i>Nutritional Neuroscience</i> , 2016, 19, 43-46.	3.1	19
43	Human aryl-hydrocarbon receptor and its interaction with dioxin and physiological ligands investigated by molecular modelling and docking simulations. <i>Biochemical and Biophysical Research Communications</i> , 2011, 413, 176-181.	2.1	18
44	Galactose-4-epi-phosphate uridylyltransferase deficiency: A literature review of the putative mechanisms of short and long-term complications and allelic variants. <i>Clinical Genetics</i> , 2018, 93, 206-215.	2.0	18
45	Structure and Stability of a Rat Odorant-Binding Protein: Another Brick in the Wall. <i>Journal of Proteome Research</i> , 2009, 8, 4005-4013.	3.7	17
46	Wild-Type and Mutant Bovine Odorant-Binding Proteins To Probe the Role of the Quaternary Structure Organization in the Protein Thermal Stability. <i>Journal of Proteome Research</i> , 2008, 7, 5221-5229.	3.7	16
47	Association Analysis of Noncoding Variants in <i>Neurologins 3</i> and <i>4X</i> Genes with Autism Spectrum Disorder in an Italian Cohort. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1765.	4.1	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 <i>Pseudoalteromonas haloplanktis</i> . <i>Journal of Physical Chemistry B</i> , 2009, 113, 13171-13178.	2.6	15
49	Structure and Dynamics of Cold-Adapted Enzymes as Investigated by FT-IR Spectroscopy and MD. The Case of an Esterase from <i>Pseudoalteromonas haloplanktis</i> . <i>Journal of Physical Chemistry B</i> , 2009, 113, 7753-7761.	2.6	15
50	A Thermostable Sugar-Binding Protein from the Archaeon <i>Pyrococcus horikoshii</i> as a Probe for the Development of a Stable Fluorescence Biosensor for Diabetic Patients. <i>Biotechnology Progress</i> , 2004, 20, 1572-1577.	2.6	14
51	Binding of mycotoxins to proteins involved in neuronal plasticity: a combined <i>in silico</i> / <i>wet</i> investigation. <i>Scientific Reports</i> , 2017, 7, 15156.	3.3	14
52	HINT predictive analysis of binding between retinol binding protein and hydrophobic ligands. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2000, 10, 2129-2132.	2.2	13
53	Mutant bovine odorant-binding protein: Temperature affects the protein stability and dynamics as revealed by infrared spectroscopy and molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 72, 769-778.	2.6	13
54	Celiac Anti-Type 2 Transglutaminase Antibodies Induce Phosphoproteome Modification in Intestinal Epithelial Caco-2 Cells. <i>PLoS ONE</i> , 2013, 8, e84403.	2.5	13

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55	The evolution of a Web resource: The Galactosemia Proteins Database 2.0. <i>Human Mutation</i> , 2018, 39, 52-60.	2.5	13
56	The differences in the microenvironment of the two tryptophan residues of the glutamine-binding protein from <i>Escherichia coli</i> shed light on the binding properties and the structural dynamics of the protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 743-750.	2.6	11
57	Pyrimidine-specific ribonucleoside hydrolase from the archaeon <i>Sulfolobus solfataricus</i> : biochemical characterization and homology modeling. <i>FEBS Journal</i> , 2008, 275, 1900-1914.	4.7	11
58	Biochemical characterization and homology modeling of a purine-specific ribonucleoside hydrolase from the archaeon <i>Sulfolobus solfataricus</i> : Insights into mechanisms of protein stabilization. <i>Archives of Biochemistry and Biophysics</i> , 2009, 483, 55-65.	3.0	11
59	Pressure Affects the Structure and the Dynamics of the D-Galactose/D-Glucose-Binding Protein from <i>Escherichia coli</i> by Perturbing the C-Terminal Domain of the Protein. <i>Biochemistry</i> , 2006, 45, 11885-11894.	2.5	10
60	Molecular adaptation strategies to high temperature and thermal denaturation mechanism of the D-trehalose/D-maltose-binding protein from the hyperthermophilic archaeon <i>Thermococcus litoralis</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 1002-1009.	2.6	9
61	Molecular strategies for protein stabilization: The case of a trehalose/maltose-binding protein from <i>Thermus thermophilus</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 839-850.	2.6	8
62	Under Pressure That Splits a Family in Two. The Case of Lipocalin Family. <i>PLoS ONE</i> , 2012, 7, e50489.	2.5	8
63	Investigating the Effects of Amino Acid Variations in Human Menin. <i>Molecules</i> , 2022, 27, 1747.	3.8	8
64	Computational methods to assist in the discovery of pharmacological chaperones for rare diseases. <i>Briefings in Bioinformatics</i> , 2022, 23, .	6.5	8
65	Pressure effect on the stability and the conformational dynamics of the D-Galactose/D-Glucose-binding protein from <i>Escherichia coli</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 193-201.	2.6	7
66	Assessment of the conformational features of vasoactive intestinal peptide in solution by limited proteolysis experiments. <i>Biopolymers</i> , 2006, 81, 110-119.	2.4	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. <i>PLoS ONE</i> , 2017, 12, e0181563.	2.5	7
68	When it comes to homology, bad habits die hard. <i>Trends in Biochemical Sciences</i> , 2009, 34, 98-99.	7.5	6
69	New compounds for a good old class: Synthesis of two $\beta$ -lactam bearing cephalosporins and their evaluation with a multidisciplinary approach. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115302.	3.0	6
70	Site-directed mutagenesis gives insights into substrate specificity of <i>Sulfolobus solfataricus</i> purine-specific nucleoside hydrolase. <i>Annals of Microbiology</i> , 2012, 62, 881-887.	2.6	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. <i>Molecules</i> , 2021, 26, 5941.	3.8	5
72	Efficient Fludarabine-Activating PNP From <i>Archaea</i> as a Guidance for Redesign the Active Site of <i>E. Coli</i> PNP. <i>Journal of Cellular Biochemistry</i> , 2016, 117, 1126-1135.	2.6	4

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73	Computational analysis of the interactions of a novel cephalosporin derivative with $\beta$ -lactamases. <i>BMC Structural Biology</i> , 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. <i>Briefings in Bioinformatics</i> , 2021, 22, .	6.5	4
75	Modeling the Conformation of Side Chains in Proteins: Approaches, Problems and Possible Developments. <i>Current Chemical Biology</i> , 2008, 2, 200-214.	0.5	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. <i>Molecules</i> , 2021, 26, 6061.	3.8	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. <i>International Journal on Disability and Human Development</i> , 2007, 6, .	0.2	2
78	New computational strategy to analyze the interactions of ER $\alpha$ and ER $\beta$ with different ERE sequences. <i>Journal of Computational Chemistry</i> , 2007, 28, 1031-1041.	3.3	2
79	Correlation Spectroscopy and Molecular Dynamics Simulations to Study the Structural Features of Proteins. <i>PLoS ONE</i> , 2013, 8, e64840.	2.5	2
80	Correlation between fluorescence and structure in the orange-emitting GFP-like protein, monomeric Kusabira Orange. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2014, 138, 223-229.	3.8	2
81	Assessment of haptoglobin alleles in autism spectrum disorders. <i>Scientific Reports</i> , 2020, 10, 7758.	3.3	2
82	Critical Assessment of Side Chain Conformation Prediction in Modelling of Single Point Amino Acid Mutation. <i>Advances in Experimental Medicine and Biology</i> , 2010, 680, 283-289.	1.6	2
83	Modeling the Conformation of Side Chains in Proteins: Approaches, Problems and Possible Developments. <i>Current Chemical Biology</i> , 2008, 2, 200-214.	0.5	1
84	Pressure Effects on the Structure and Stability of the Hyperthermophilic Trehalose/Maltose-Binding Protein from <i>Thermococcus litoralis</i> . <i>Journal of Physical Chemistry B</i> , 2009, 113, 12804-12808.	2.6	1
85	Unraveling the structural and functional differences between purine nucleoside phosphorylase and 5'-deoxy-5'-methylthioadenosine phosphorylase from the archaeon <i>Pyrococcus furiosus</i> . <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1358-1366.	2.3	1
86	Solving Biclustering with a GRASP-Like Metaheuristic: Two Case-Studies on Gene Expression Analysis. <i>Lecture Notes in Computer Science</i> , 2012, , 253-267.	1.3	1
87	Statistical Analysis of Protein Structural Features: Relationships and PCA Grouping. <i>Lecture Notes in Computer Science</i> , 2015, , 33-43.	1.3	1
88	Erratum to "Detection and molecular characterization of a novel BRAF activated domain mutation in follicular variant of papillary thyroid carcinoma" [Hum Pathol 40 (2009) 827-833]. <i>Human Pathology</i> , 2009, 40, 1212.	2.0	0
89	The misuse of terms in scientific literature. <i>Bioinformatics</i> , 2010, 26, 2498-2498.	4.1	0
90	Preface: BITS2014, the annual meeting of the Italian Society of Bioinformatics. <i>BMC Bioinformatics</i> , 2015, 16, S1.	2.6	0

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91	Editorial: Computational Proteomics and Integration of Data Resources for Advanced Studies in Life Sciences. <i>Frontiers in Genetics</i> , 2021, 12, 729013.	2.3	0
92	Application of computational methods for structural and functional characterization of mutants of GALT enzyme. <i>EMBnet Journal</i> , 2012, 18, 116.	0.6	0
93	Identification of molecular targets for mycotoxins related to autism development. <i>EMBnet Journal</i> , 2012, 18, 118.	0.6	0
94	New metaheuristics approaches for biclustering of gene expression Data. <i>EMBnet Journal</i> , 2012, 18, 68.	0.6	0