Marianne Rooman

List of Publications by Year
in descending order

95 papers	5,075 citations	117625 34 h-index	98798 67 g-index
108 all docs	108 docs citations	108 times ranked	5847 citing authors

#	Article	IF	Citations
1	PoPMuSiC 2.1: a web server for the estimation of protein stability changes upon mutation and sequence optimality. BMC Bioinformatics, 2011, 12, 151.	2.6	435
2	Fast and accurate predictions of protein stability changes upon mutations using statistical potentials and neural networks: PoPMuSiC-2.0. Bioinformatics, 2009, 25, 2537-2543.	4.1	387
3	BeAtMuSiC: prediction of changes in proteinâ€“protein binding affinity on mutations. Nucleic Acids Research, 2013, 41, W333-W339.	14.5	275
4	Structural Classification of HTH DNA-binding Domains and Protein â€“ DNA Interaction Modes. Journal of Molecular Biology, 1996, 262, 294-313.	4.2	234
5	Contribution of cation-Ï€ interactions to the stability of protein-DNA complexes 1 1Edited by J. Thornton. Journal of Molecular Biology, 2000, 302, 393-408.	4.2	212
6	Predicting protein stability changes upon mutation using database-derived potentials: solvent accessibility determines the importance of local versus non-local interactions along the sequence. Journal of Molecular Biology, 1997, 272, 276-290.	4.2	206
7	Optimality of the genetic code with respect to protein stability and amino-acid frequencies. Genome Biology, 2001, 2, research0049.1.	9.6	164
8	Stability Changes upon Mutation of Solvent- accessible Residues in Proteins Evaluated by Database-derived Potentials. Journal of Molecular Biology, 1996, 257, 1112-1126.	4.2	159
9	PoPMuSiC, an algorithm for predicting protein mutant stability changes. Application to prion proteins. Protein Engineering, Design and Selection, 2000, 13, 849-856.	2.1	149
10	Enhancing the stability and solubility of TEV protease using in silico design. Protein Science, 2007, 16, 2360-2367.	7.6	141
11	Physical and molecular bases of protein thermal stability and cold adaptation. Current Opinion in Structural Biology, 2017, 42, 117-128.	5.7	124
12	Cationâ€“Ï€/H-bond Stair Motifs at Proteinâ€“DNA Interfaces. Journal of Molecular Biology, 2002, 319, 67-76.	4.2	119
13	DEOGEN2: prediction and interactive visualization of single amino acid variant deleteriousness in human proteins. Nucleic Acids Research, 2017, 45, W201-W206.	14.5	114
14	Histidineâˆ’Aromatic Interactions in Proteins and Proteinâˆ’Ligand Complexes:â€‰ Quantum Chemical Study of X-ray and Model Structures. Journal of Chemical Theory and Computation, 2005, 1, 472-483.	5.3	110
15	Quantification of biases in predictions of protein stability changes upon mutations. Bioinformatics, 2018, 34, 3659-3665.	4.1	110
16	Predicting protein thermal stability changes upon point mutations using statistical potentials: Introducing HoTMuSiC. Scientific Reports, 2016, 6, 23257.	3.3	96
17	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	2.6	87
18	SCooP: an accurate and fast predictor of protein stability curves as a function of temperature. Bioinformatics, 2017, 33, 3415-3422.	4.1	82

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19	Stair Motifs at Proteinâ^'DNA Interfaces:Â Nonadditivity of H-Bond, Stacking, and Cationâ^'Ï€ Interactions. Journal of the American Chemical Society, 2004, 126, 6220-6221.	13.7	81
20	Free-Energy Calculations of Proteinâ^'Ligand Cationâ^'Ï€ and Aminoâ^'Ï€ Interactions: From Vacuum to Proteinlike Environments. Journal of the American Chemical Society, 2003, 125, 13988-13994.	13.7	79
21	Probing the Energetic and Structural Role of Amino Acid/Nucleobase Cation-Ï€ Interactions in Protein-Ligand Complexes. Journal of Biological Chemistry, 2002, 277, 40816-40822.	3.4	75
22	The first peptides: The evolutionary transition between prebiotic amino acids and early proteins. Journal of Theoretical Biology, 2009, 261, 531-539.	1.7	74
23	Specificity and Phenetic Relationships of Iron- and Manganese-containing Superoxide Dismutases on the Basis of Structure and Sequence Comparisons. Journal of Biological Chemistry, 2004, 279, 9248-9254.	3.4	71
24	Thermostability of Salt Bridges versus Hydrophobic Interactions in Proteins Probed by Statistical Potentials. Journal of Chemical Information and Modeling, 2008, 48, 119-127.	5.4	64
25	Prediction and interpretation of deleterious coding variants in terms of protein structural stability. Scientific Reports, 2018, 8, 4480.	3.3	64
26	Thermo- and Mesostabilizing Protein Interactions Identified by Temperature-Dependent Statistical Potentials. Biophysical Journal, 2010, 98, 667-677.	0.5	51
27	Single Mutations in the Transmembrane Domains of Maize Plasma Membrane Aquaporins Affect the Activity of Monomers within a Heterotetramer. Molecular Plant, 2016, 9, 986-1003.	8.3	51
28	Cationâ€“Ï€, aminoâ€“Ï€, Ï€â€“Ï€, and Hâ€bond interactions stabilize antigenâ€“antibody interfaces. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1734-1746.	2.6	50
29	Protein Thermostability Prediction within Homologous Families Using Temperature-Dependent Statistical Potentials. PLoS ONE, 2014, 9, e91659.	2.5	50
30	Computational analysis of the amino acid interactions that promote or decrease protein solubility. Scientific Reports, 2018, 8, 14661.	3.3	48
31	Sequence-structure Signals of 3D Domain Swapping in Proteins. Journal of Molecular Biology, 2003, 330, 1215-1225.	4.2	45
32	Basis Set and Electron Correlation Effects on ab Initio Calculations of Cation-Ï€/H-Bond Stair Motifs. Journal of Physical Chemistry A, 2003, 107, 6249-6258.	2.5	45
33	Artificial intelligence challenges for predicting the impact of mutations on protein stability. Current Opinion in Structural Biology, 2022, 72, 161-168.	5.7	45
34	SOLart: a structure-based method to predict protein solubility and aggregation. Bioinformatics, 2020, 36, 1445-1452.	4.1	44
35	Structure-based mutant stability predictions on proteins of unknown structure. Journal of Biotechnology, 2012, 161, 287-293.	3.8	40
36	A comprehensive computational study of amino acid interactions in membrane proteins. Scientific Reports, 2019, 9, 12043.	3.3	40

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37	Inhibition of aquaporin-1 prevents myocardial remodeling by blocking the transmembrane transport of hydrogen peroxide. Science Translational Medicine, 2020, 12, .	12.4	39
38	High-quality Thermodynamic Data on the Stability Changes of Proteins Upon Single-site Mutations. Journal of Physical and Chemical Reference Data, 2016, 45, .	4.2	38
39	In Vitro and In Silico Design of Î±1-antitrypsin Mutants with Different Conformational Stabilities. Journal of Molecular Biology, 2003, 325, 581-589.	4.2	36
40	Flanking domain stability modulates the aggregation kinetics of a polyglutamine disease protein. Protein Science, 2011, 20, 1675-1681.	7.6	35
41	Sequence and conformation effects on ionization potential and charge distribution of homo-nucleobase stacks using M06-2X hybrid density functional theory calculations. Journal of Biomolecular Structure and Dynamics, 2014, 32, 532-545.	3.5	35
42	SEPIa, a knowledge-driven algorithm for predicting conformational B-cell epitopes from the amino acid sequence. BMC Bioinformatics, 2017, 18, 95.	2.6	34
43	Revisiting the correlation between proteins' thermoresistance and organisms' thermophilicity. Protein Engineering, Design and Selection, 2008, 21, 275-278.	2.1	32
44	Stability Curve Prediction of Homologous Proteins Using Temperature-Dependent Statistical Potentials. PLoS Computational Biology, 2014, 10, e1003689.	3.2	32
45	Multilevel biological characterization of exomic variants at the protein level significantly improves the identification of their deleterious effects. Bioinformatics, 2016, 32, 1797-1804.	4.1	32
46	Different derivations of knowledge-based potentials and analysis of their robustness and context-dependent predictive power. FEBS Journal, 1998, 254, 135-143.	0.2	29
47	Evidence that Interaction between Conserved Residues in Transmembrane Helices 2, 3, and 7 Are Crucial for Human VPAC₁ Receptor Activation. Molecular Pharmacology, 2010, 78, 394-401.	2.3	29
48	Symmetry Principles in Optimization Problems: an application to Protein Stability Prediction. IFAC-PapersOnLine, 2015, 48, 458-463.	0.9	29
49	Mn/Fe superoxide dismutase interaction fingerprints and prediction of oligomerization and metal cofactor from sequence. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1564-1577.	2.6	23
50	Prediction and Evolution of the Molecular Fitness of SARS-CoV-2 Variants: Introducing SpikePro. Viruses, 2021, 13, 935.	3.3	22
51	Quantifying Renin-Angiotensin-System Alterations in COVID-19. Cells, 2021, 10, 2755.	4.1	21
52	Prediction of stability changes upon single-site mutations using database-derived potentials. Theoretical Chemistry Accounts, 1999, 101, 46-50.	1.4	20
53	Development of Novel Statistical Potentials Describing Cationâ^Ï€ Interactions in Proteins and Comparison with Semiempirical and Quantum Chemistry Approaches. Journal of Chemical Information and Modeling, 2006, 46, 884-893.	5.4	20
54	Towards an accurate prediction of the thermal stability of homologous proteins. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1132-1142.	3.5	19

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55	Digenic inheritance of human primary microcephaly delineates centrosomal and nonâ€centrosomal pathways. Human Mutation, 2020, 41, 512-524.	2.5	19
56	Database-Derived Potentials Dependent on Protein Size for In Silico Folding and Design. Biophysical Journal, 2004, 87, 171-181.	0.5	18
57	Improved insights into protein thermal stability: from the molecular to the structurome scale. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160141.	3.4	18
58	Stability strengths and weaknesses in protein structures detected by statistical potentials: Application to bovine seminal ribonuclease. Proteins: Structure, Function and Bioinformatics, 2016, 84, 143-158.	2.6	16
59	Identification and ab initio simulations of early folding units in proteins. Proteins: Structure, Function and Bioinformatics, 2001, 42, 164-176.	2.6	15
60	Modeling the Molecular Impact of SARS-CoV-2 Infection on the Renin-Angiotensin System. Viruses, 2020, 12, 1367.	3.3	15
61	Protein Thermal Stability Engineering Using HoTMuSiC. Methods in Molecular Biology, 2020, 2112, 59-73.	0.9	15
62	What is Paradoxical about Levinthal Paradox?. Journal of Biomolecular Structure and Dynamics, 2002, 20, 327-329.	3.5	14
63	SODa: An Mn/Fe superoxide dismutase prediction and design server. BMC Bioinformatics, 2008, 9, 257.	2.6	13
64	Conformations Consistent with Charge Migration Observed in DNA and RNA X-ray Structures. Journal of Biomolecular Structure and Dynamics, 2011, 28, 949-954.	3.5	13
65	SWOTein: a structure-based approach to predict stability Strengths and Weaknesses of prOTEINs. Bioinformatics, 2021, 37, 1963-1971.	4.1	13
66	Dynamic modeling of gene expression in prokaryotes: application to glucose-lactose diauxie in Escherichia coli. Systems and Synthetic Biology, 2011, 5, 33-43.	1.0	11
67	Gene expression model (in)validation by Fourier analysis. BMC Systems Biology, 2010, 4, 123.	3.0	10
68	NPTX1 mutations trigger endoplasmic reticulum stress and cause autosomal dominant cerebellar ataxia. Brain, 2022, 145, 1519-1534.	7.6	10
69	Stochastic noise reduction upon complexification: Positively correlated birth-death type systems. Journal of Theoretical Biology, 2014, 354, 113-123.	1.7	9
70	Role of salt bridges in homeodomains investigated by structural analyses and molecular dynamics simulations. Biopolymers, 2001, 59, 145-159.	2.4	8
71	Relation between DNA ionization potentials, single base substitutions and pathogenic variants. BMC Genomics, 2019, 20, 551.	2.8	7
72	Large-scale in silico mutagenesis experiments reveal optimization of genetic code and codon usage for protein mutational robustness. BMC Biology, 2020, 18, 146.	3.8	7

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73	Detection of Perturbation Phases and Developmental Stages in Organisms from DNA Microarray Time Series Data. PLoS ONE, 2011, 6, e27948.	2.5	7
74	Prelude&Fugue, predicting local protein structure, early folding regions and structural weaknesses. Bioinformatics, 2006, 22, 1800-1802.	4.1	6
75	Modeling the temporal evolution of theDrosophilagene expression from DNA microarray time series. Physical Biology, 2009, 6, 016004.	1.8	6
76	Robust non-linear differential equation models of gene expression evolution across Drosophila development. BMC Research Notes, 2012, 5, 46.	1.4	6
77	Probability distributions for multimeric systems. Journal of Mathematical Biology, 2016, 72, 157-169.	1.9	6
78	Rational antibiotic design: in silico structural comparison of the functional cavities of penicillin-binding proteins and ÃŸ-lactamases. Journal of Biomolecular Structure and Dynamics, 2019, 37, 65-74.	3.5	6
79	Design Principles of a Genetic Alarm Clock. PLoS ONE, 2012, 7, e47256.	2.5	5
80	Perturbing dimer interactions and allosteric communication modulates the immunosuppressive activity of human galectin-7. Journal of Biological Chemistry, 2021, 297, 101308.	3.4	5
81	Analysis of the Neutralizing Activity of Antibodies Targeting Open or Closed SARS-CoV-2 Spike Protein Conformations. International Journal of Molecular Sciences, 2022, 23, 2078.	4.1	5
82	Ab initio structure predictions using a hierarchical approach applied to 434 cro and the Drosophila homeodomain. Theoretical Chemistry Accounts, 2001, 106, 69-75.	1.4	4
83	In Silico Analysis of the Molecular-Level Impact of SMPD1 Variants on Niemann-Pick Disease Severity. International Journal of Molecular Sciences, 2021, 22, 4516.	4.1	4
84	Is the Cell Nucleus a Necessary Component in Precise Temporal Patterning?. PLoS ONE, 2015, 10, e0134239.	2.5	3
85	Lexicon Visualization Library and JavaScript for Scientific Data Visualization. Computing in Science and Engineering, 2018, 20, 50-65.	1.2	3
86	DISCOPOLIS: an algorithm for uniform sampling of metabolic flux distributions via iterative sequences of linear programs. IFAC-PapersOnLine, 2019, 52, 269-274.	0.9	3
87	BRANEart: Identify Stability Strength and Weakness Regions in Membrane Proteins. Frontiers in Bioinformatics, 2021, 1, .	2.1	3
88	Using metagenomic data to boost protein structure prediction and discovery. Computational and Structural Biotechnology Journal, 2022, 20, 434-442.	4.1	3
89	Intrinsic noise modulation in closed oligomerization-type systems âž âžFP and MR are research assistant and research director, respectively, at the Belgian Fund for scientific research (FNRS).. IFAC-PapersOnLine, 2018, 51, 649-654.	0.9	2
90	Insights into noise modulation in oligomerization systems of increasing complexity. Physical Review E, 2018, 98, 012137.	2.1	2

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91	MutaFrameâ€"an interpretative visualization framework for deleteriousness prediction of missense variants in the human exome. Bioinformatics, 2021, 38, 265-266.	4.1	2
92	Deciphering noise amplification and reduction in open chemical reaction networks. Journal of the Royal Society Interface, 2018, 15, 20180805.	3.4	1
93	Modeling the Drosophila Gene Cluster Regulation Network for Muscle Development. PLoS ONE, 2014, 9, e90285.	2.5	1
94	Detection of Developmental and Perturbation Stages from DNA Microarray Time Series and Robust Modeling of Gene Expression Evolution. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2012, 45, 635-640.	0.4	0
95	DISCOPOLIS 2.0: a new recursive version of the algorithm for uniform sampling of metabolic flux distributions with linear programming. IFAC-PapersOnLine, 2021, 54, 300-305.	0.9	0