Therese E Malliavin

List of Publications by Year
in descending order

86	2,769	270111	214428
papers	citations	25 h-index	50 g-index

91	91	91	4042
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tandem domain structure determination based on a systematic enumeration of conformations. Scientific Reports, 2021, 11, 16925.	1.6	2
2	Conformational Insights into the Control of CNF1 Toxin Activity by Peptidyl-Prolyl Isomerization: A Molecular Dynamics Perspective. International Journal of Molecular Sciences, 2021, 22, 10129.	1.8	1
3	Computational and biochemical analysis of type IV pilus dynamics and stability. Structure, 2021, 29, 1397-1409.e6.	1.6	5
4	Secondary structure assignment of proteins in the absence of sequence information. Bioinformatics Advances, 2021, 1, .	0.9	1
5	Analyzing In Silico the Relationship Between the Activation of the Edema Factor and Its Interaction With Calmodulin. Frontiers in Molecular Biosciences, 2020, 7, 586544.	1.6	0
6	Systematic Exploration of Protein Conformational Space Using a Distance Geometry Approach. Journal of Chemical Information and Modeling, 2019, 59, 4486-4503.	2.5	25
7	Structural Biology and Molecular Modeling to Analyze the Entry of Bacterial Toxins and Virulence Factors into Host Cells. Toxins, 2019, 11, 369.	1.5	5
8	Minimal NMR distance information for rigidity of protein graphs. Discrete Applied Mathematics, 2019, 256, 91-104.	0.5	26
9	Ordering Protein Contact Matrices. Computational and Structural Biotechnology Journal, 2018, 16, 140-156.	1.9	0
10	Tuning interval Branch-and-Prune for protein structure determination. Journal of Global Optimization, 2018, 72, 109-127.	1.1	19
11	Conformational sampling of CpxA: Connecting HAMP motions to the histidine kinase function. PLoS ONE, 2018, 13, e0207899.	1.1	1
12	Closed-Locked and Apo-Resting State Structures of the Human Î±7 Nicotinic Receptor: A Computational Study. Journal of Chemical Information and Modeling, 2018, 58, 2278-2293.	2.5	6
13	re-TAMD: exploring interactions between H3 peptide and YEATS domain using enhanced sampling. BMC Structural Biology, 2018, 18, 4.	2.3	7
14	A possible desensitized state conformation of the human Î± 7 nicotinic receptor: A molecular dynamics study. Biophysical Chemistry, 2017, 229, 99-109.	1.5	14
15	Molecular Modeling of the Catalytic Domain of CyaA Deepened the Knowledge of Its Functional Dynamics. Toxins, 2017, 9, 199.	1.5	5
16	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	1.8	95
17	Modification in hydrophobic packing of HAMP domain induces a destabilization of the autoâ€phosphorylation site in the histidine kinase CpxA. Biopolymers, 2016, 105, 670-682.	1.2	2
18	Building Graphs To Describe Dynamics, Kinetics, and Energetics in the <scp>d</scp>-ALa:<scp>d</scp>-Lac Ligase VanA. Journal of Chemical Information and Modeling, 2016, 56, 1762-1775.	2.5	9

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19	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	0.9	10
20	Applications of proteochemometrics - from species extrapolation to cell line sensitivity modelling. BMC Bioinformatics, 2015, 16, .	1.2	4
21	Comparing the Influence of Simulated Experimental Errors on 12 Machine Learning Algorithms in Bioactivity Modeling Using 12 Diverse Data Sets. Journal of Chemical Information and Modeling, 2015, 55, 1413-1425.	2.5	28
22	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. Journal of Cheminformatics, 2015, 7, 1.	2.8	138
23	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. Journal of Chemical Theory and Computation, 2015, 11, 3446-3454.	2.3	12
24	Improved reliability, accuracy and quality in automated NMR structure calculation with ARIA. Journal of Biomolecular NMR, 2015, 62, 425-438.	1.6	34
25	An algorithm to enumerate all possible protein conformations verifying a set of distance constraints. BMC Bioinformatics, 2015, 16, 23.	1.2	42
26	Identification of binding sites and favorable ligand binding moieties by virtual screening and self-organizing map analysis. BMC Bioinformatics, 2015, 16, 93.	1.2	16
27	Proteochemometric modelling coupled to in silico target prediction: an integrated approach for the simultaneous prediction of polypharmacology and binding affinity/potency of small molecules. Journal of Cheminformatics, 2015, 7, 15.	2.8	29
28	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. Molecular Informatics, 2015, 34, 357-366.	1.4	26
29	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. Journal of Cheminformatics, 2015, 7, 45.	2.8	32
30	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.5	109
31	A Structural Model of the Human Î±7 Nicotinic Receptor in an Open Conformation. PLoS ONE, 2015, 10, e0133011.	1.1	11
32	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	1.1	19
33	Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. Integrative Biology (United Kingdom), 2014, 6, 1023-1033.	0.6	26
34	Proteochemometric modeling in a Bayesian framework. Journal of Cheminformatics, 2014, 6, 35.	2.8	37
35	Stabilization of the integraseâ€ÐNA complex by Mg²⁺ ions and prediction of key residues for binding HIVâ€1 integrase inhibitors. Proteins: Structure, Function and Bioinformatics, 2014, 82, 466-478.	1.5	19
36	Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2483-2496.	1.5	12

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37	Allosteric Activation of Bordetella pertussis Adenylyl Cyclase by Calmodulin. Journal of Biological Chemistry, 2014, 289, 21131-21141.	1.6	18
38	Functional Motions Modulating VanA Ligand Binding Unraveled by Self-Organizing Maps. Journal of Chemical Information and Modeling, 2014, 54, 289-301.	2.5	14
39	Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics. PLoS ONE, 2014, 9, e88555.	1.1	16
40	Identification of Cinnamic Acid Derivatives As Novel Antagonists of the Prokaryotic Proton-Gated Ion Channel GLIC. Journal of Medicinal Chemistry, 2013, 56, 4619-4630.	2.9	28
41	Distance Geometry in Structural Biology: New Perspectives. , 2013, , 329-350.		16
42	Molecular Motions as a Drug Target: Mechanistic Simulations of Anthrax Toxin Edema Factor Function Led to the Discovery of Novel Allosteric Inhibitors. Toxins, 2012, 4, 580-604.	1.5	18
43	Lobeline Docking on AChBP and Nicotinic Receptors: Discriminating Importance of the Pocket Geometry and of the Ligand Configuration. Letters in Drug Design and Discovery, 2012, 9, 54-62.	0.4	2
44	Differential role of calmodulin and calcium ions in the stabilization of the catalytic domain of adenyl cyclase CyaA from Bordetella pertussis. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1028-1040.	1.5	14
45	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 2012, 20, 227-236.	1.6	75
46	ARIA for Solution and Solid-State NMR. Methods in Molecular Biology, 2012, 831, 453-483.	0.4	54
47	Discrimination of agonists versus antagonists of nicotinic ligands based on docking onto AChBP structures. Journal of Molecular Graphics and Modelling, 2011, 30, 100-109.	1.3	17
48	The redundancy of NMR restraints can be used to accelerate the unfolding behavior of an SH3 domain during molecular dynamics simulations. BMC Structural Biology, 2011, 11, 46.	2.3	1
49	Bayesian estimation of NMR restraint potential and weight: A validation on a representative set of protein structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1525-1537.	1.5	23
50	Mechanism of reactant and product dissociation from the anthrax edema factor: A locally enhanced sampling and steered molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1649-1661.	1.5	7
51	Grid computing for improving conformational sampling in NMR structurecalculation. Bioinformatics, 2011, 27, 1713-1714.	1.8	2
52	Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems. Lecture Notes in Computer Science, 2011, , 206-217.	1.0	12
53	Simultaneous use of solution, solid-state NMR and X-ray crystallography to study the conformational landscape of the Crh protein during oligomerization and crystallization. Advances and Applications in Bioinformatics and Chemistry, 2010, 3, 25.	1.6	0
54	Use of allostery to identify inhibitors of calmodulin-induced activation of Bacillus anthracis edema factor. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 11277-11282.	3.3	65

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55	Activation of the Edema Factor of Bacillus anthracis by Calmodulin: Evidence of an Interplay between the EF-Calmodulin Interaction andÂCalcium Binding. Biophysical Journal, 2010, 99, 2264-2272.	0.2	16
56	Influence of different assignment conditions on the determination of symmetric homodimeric structures with ARIA. Proteins: Structure, Function and Bioinformatics, 2009, 75, 569-585.	1.5	33
57	ATP conformations and ion binding modes in the active site of anthrax edema factor: A computational analysis. Proteins: Structure, Function and Bioinformatics, 2009, 77, 971-983.	1.5	13
58	CASD-NMR: critical assessment of automated structure determination by NMR. Nature Methods, 2009, 6, 625-626.	9.0	80
59	Dynamics and Energetics: A Consensus Analysis of the Impact of Calcium on EF-CaM Protein Complex. Biophysical Journal, 2009, 96, 1249-1263.	0.2	12
60	Graphical analysis of NMR structural quality and interactive contact map of NOE assignments in ARIA. BMC Structural Biology, 2008, 8, 30.	2.3	5
61	The conformational plasticity of calmodulin upon calcium complexation gives a model of its interaction with the oedema factor of Bacillus anthracis. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1813-1829.	1.5	23
62	Accurate NMR Structures Through Minimization of an Extended Hybrid Energy. Structure, 2008, 16, 1305-1312.	1.6	58
63	3D Structure Determination of the Crh Protein from Highly Ambiguous Solid-State NMR Restraints. Journal of the American Chemical Society, 2008, 130, 3579-3589.	6.6	135
64	Structural Biology by NMR: Structure, Dynamics, and Interactions. PLoS Computational Biology, 2008, 4, e1000168.	1.5	120
65	Virtual Screening of the Guanylate Monophosphate Kinase (GMPK) Family: Investigating the Rules of Ligand Specificity. Letters in Drug Design and Discovery, 2008, 5, 319-326.	0.4	0
66	ARIA2: Automated NOE assignment and data integration in NMR structure calculation. Bioinformatics, 2007, 23, 381-382.	1.8	506
67	The Conformational Landscape of the Ribosomal Protein S15 and Its Influence on the Protein Interaction with 16S RNA. Biophysical Journal, 2007, 92, 2647-2665.	0.2	7
68	A general algorithm for peak-tracking in multi-dimensional NMR experiments. Journal of Biomolecular NMR, 2007, 37, 265-275.	1.6	6
69	Comparison of Different Torsion Angle Approaches for NMR Structure Determination. Journal of Biomolecular NMR, 2006, 34, 153-166.	1.6	7
70	Quantitative Analysis of Biomolecular NMR Spectra: A Prerequisite for the Determination of the Structure and Dynamics of Biomolecules. Current Organic Chemistry, 2006, 10, 555-568.	0.9	3
71	From NMR chemical shifts to amino acid types: Investigation of the predictive power carried by nuclei. Journal of Biomolecular NMR, 2004, 30, 47-60.	1.6	20
72	Molecular dynamics simulations of HPr under hydrostatic pressure. Biopolymers, 2004, 74, 377-388.	1.2	8

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73	The NMR structure of [Xd(C2)]4 investigated by molecular dynamics simulations. Magnetic Resonance in Chemistry, 2003, 41, 18-25.	1.1	9
74	Stability of the I-motif Structure Is Related to the Interactions between Phosphodiester Backbones. Biophysical Journal, 2003, 84, 3838-3847.	0.2	37
75	Analysis of peptide rotational diffusion by homonuclear NMR. Biopolymers, 2002, 63, 335-342.	1.2	2
76	FIRE: predicting the spatial proximity of protein residues from 3D NOESY-HSQC. Theoretical Chemistry Accounts, 2001, 106, 91-97.	0.5	7
77	Refined solution structure and backbone dynamics of 15N-labeled C12A-p8MTCP1 studied by NMR relaxation. Journal of Biomolecular NMR, 1999, 15, 271-288.	1.6	34
78	Maximum Entropy Processing of DOSY NMR Spectra. Analytical Chemistry, 1998, 70, 2146-2148.	3.2	173
79	The DOSY experiment provides insights into the protegrin-lipid interaction. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1998, 95, 178-186.	0.2	8
80	Gifa V. 4: A complete package for NMR data set processing. Journal of Biomolecular NMR, 1996, 8, 445-52.	1.6	192
81	Use of the Cadzow procedure in 2D NMR for the reduction of t1 noise. Journal of Biomolecular NMR, 1995, 6, 361-5.	1.6	20
82	An estimate of spin diffusion in a spin subset: Application to iterative distance calculation from 3D 15N NOESY-HMQC. Journal of Biomolecular NMR, 1995, 5, 193-201.	1.6	2
83	Accurate estimation of inter-atomic distances in large proteins by NMR. Biochimie, 1992, 74, 809-813.	1.3	3
84	Computation of relaxation matrix elements from incomplete NOESY data sets. Journal of Biomolecular NMR, 1992, 2, 349-360.	1.6	14
85	Compression of multidimensional NMR data sets. Journal of Magnetic Resonance, 1991, 93, 630-634.	0.5	0
86	Insight into protein nuclear magnetic resonance research. Biochimie, 1990, 72, 531-535.	1.3	3