Nathalie Reuter

List of Publications by Year
in descending order

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93 papers	4,134 citations	126708 33 h-index	128067 60 g-index
99 all docs	99 docs citations	99 times ranked	4923 citing authors

#	Article	IF	Citations
1	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
2	Specificity of Loxosceles Î± clade phospholipase D enzymes for choline-containing lipids: Role of a conserved aromatic cage. PLoS Computational Biology, 2022, 18, e1009871.	1.5	6
3	Standard Binding Free Energy and Membrane Desorption Mechanism for a Phospholipase C. Journal of Chemical Information and Modeling, 2022, 62, 6602-6613.	2.5	8
4	Membrane models for molecular simulations of peripheral membrane proteins. Advances in Physics: X, 2021, 6, 1932589.	1.5	3
5	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
6	Phospholipids in Motion: High-Resolution ³¹P NMR Field Cycling Studies. Journal of Physical Chemistry B, 2021, 125, 8827-8838.	1.2	5
7	Dynamics-function relationship in the catalytic domains of N-terminal acetyltransferases. Computational and Structural Biotechnology Journal, 2020, 18, 532-547.	1.9	8
8	Capturing Cholineâ€“Aromatics Cationâ˜Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	2.3	35
9	The Arabidopsis (ASHH2) CW domain binds monomethylated K4 of the histone H3 tail through conformational selection. FEBS Journal, 2020, 287, 4458-4480.	2.2	4
10	Visual exploration of large normal mode spaces to study protein flexibility. Computers and Graphics, 2020, 90, 73-83.	1.4	4
11	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. PLoS Computational Biology, 2020, 16, e1007988.	1.5	7
12	Levels of proteinase 3 and neutrophil elastase in plasma, BAL and biopsies in COPD. , 2020, , .		0
13	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0
14	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0
15	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0
16	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0
17	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0
18	Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988.		0

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19	Interfacial Aromatics Mediating Cationâ˜Ï€ Interactions with Choline-Containing Lipids Can Contribute as Much to Peripheral Protein Affinity for Membranes as Aromatics Inserted below the Phosphates. Journal of Physical Chemistry Letters, 2019, 10, 3972-3977.	2.1	24
20	Peptidomimetic inhibitors targeting the membrane-binding site of the neutrophil proteinase 3. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1502-1509.	1.4	4
21	Cation-Ï€ Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2019, 15, 7-12.	2.3	58
22	Conservation of intrinsic dynamics in proteins â€" what have computational models taught us?. Current Opinion in Structural Biology, 2018, 50, 75-81.	2.6	38
23	d-Peptides as inhibitors of PR3-membrane interactions. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 458-466.	1.4	4
24	A model for hydrophobic protrusions on peripheral membrane proteins. PLoS Computational Biology, 2018, 14, e1006325.	1.5	26
25	Search and Subvert: Minimalist Bacterial Phosphatidylinositol-Specific Phospholipase C Enzymes. Chemical Reviews, 2018, 118, 8435-8473.	23.0	25
26	Molecular determinants of the N-terminal acetyltransferase Naa60 anchoring to the Golgi membrane. Journal of Biological Chemistry, 2017, 292, 6821-6837.	1.6	33
27	Interactions stabilizing the C-terminal helix of human phospholipid scramblase 1 in lipid bilayers: A computational study. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1200-1210.	1.4	8
28	Improving the Force Field Description of Tyrosineâ€"Choline Cationâ˜Ï€ Interactions: QM Investigation of Phenolâ€"N(Me)₄⁺ Interactions. Journal of Chemical Theory and Computation, 2016, 12, 5585-5595.	2.3	39
29	A Role for Weak Electrostatic Interactions in Peripheral Membrane Protein Binding. Biophysical Journal, 2016, 110, 1367-1378.	0.2	47
30	Proteinase 3 Is a Phosphatidylserine-binding Protein That Affects the Production and Function of Microvesicles. Journal of Biological Chemistry, 2016, 291, 10476-10489.	1.6	46
31	Similarity in Shape Dictates Signature Intrinsic Dynamics Despite No Functional Conservation in TIM Barrel Enzymes. PLoS Computational Biology, 2016, 12, e1004834.	1.5	18
32	Membrane Docking of the Synaptotagmin 7 C2A Domain: Computation Reveals Interplay between Electrostatic and Hydrophobic Contributions. Biochemistry, 2015, 54, 5696-5711.	1.2	21
33	Comparing the intrinsic dynamics of multiple protein structures using elastic network models. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 911-922.	1.1	68
34	Biochemical and cellular analysis of Ogden syndrome reveals downstream Nt-acetylation defects. Human Molecular Genetics, 2015, 24, 1956-1976.	1.4	97
35	Quantifying Transient Interactions between Bacillus Phosphatidylinositol-Specific Phospholipase-C and Phosphatidylcholine-Rich Vesicles. Journal of the American Chemical Society, 2015, 137, 14-17.	6.6	24
36	Specific Transient Interactions Between a Bacillus Virulence Factor and Phosphatidylcholine in Membranes. FASEB Journal, 2015, 29, 568.9.	0.2	0

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37	WEBnm@ v2.0: Web server and services for comparing protein flexibility. BMC Bioinformatics, 2014, 15, 427.	1.2	95
38	Evolution of oligomeric state through allosteric pathways that mimic ligand binding. Science, 2014, 346, 1254346.	6.0	62
39	Two homologous neutrophil serine proteases bind to POPC vesicles with different affinities: When aromatic amino acids matter. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 3191-3202.	1.4	16
40	Reversible Ketomethylene-Based Inhibitors of Human Neutrophil Proteinase 3. Journal of Medicinal Chemistry, 2014, 57, 9396-9408.	2.9	17
41	In Silico Design, Synthesis, and Assays of Specific Substrates for Proteinase 3: Influence of Fluorogenic and Charged Groups. Journal of Medicinal Chemistry, 2014, 57, 1111-1115.	2.9	12
42	Characterization of Immunological Cross-Reactivity between Enterotoxigenic Escherichia coli Heat-Stable Toxin and Human Guanylin and Uroguanylin. Infection and Immunity, 2014, 82, 2913-2922.	1.0	18
43	Examining the Flexibility of Tim Barrel Proteins Based on their Structural Topology. Biophysical Journal, 2013, 104, 227a-228a.	0.2	1
44	Does Changing the Predicted Dynamics of a Phospholipase C Alter Activity and Membrane Binding?. Biophysical Journal, 2013, 104, 185-195.	0.2	11
45	Visual cavity analysis in molecular simulations. BMC Bioinformatics, 2013, 14, S4.	1.2	52
46	Cationâ^'Ï€ Interactions As Lipid-Specific Anchors for Phosphatidylinositol-Specific Phospholipase C. Journal of the American Chemical Society, 2013, 135, 5740-5750.	6.6	62
47	Evaluation of Protein Elastic Network Models Based on an Analysis of Collective Motions. Journal of Chemical Theory and Computation, 2013, 9, 5618-5628.	2.3	65
48	Comparing aminoglycoside binding sites in bacterial ribosomal RNA and aminoglycoside modifying enzymes. Proteins: Structure, Function and Bioinformatics, 2013, 81, 63-80.	1.5	23
49	Integrating cluster formation and cluster evaluation in interactive visual analysis. , 2013, , .		8
50	Implicit surfaces for interactive graph based cavity analysis of molecular simulations. , 2012, , .		17
51	Nuclear-to-cytoplasmic Relocalization of the Proliferating Cell Nuclear Antigen (PCNA) during Differentiation Involves a Chromosome Region Maintenance 1 (CRM1)-dependent Export and Is a Prerequisite for PCNA Antiapoptotic Activity in Mature Neutrophils. Journal of Biological Chemistry, 2012, 287, 33812-33825.	1.6	53
52	Measuring and comparing structural fluctuation patterns in large protein datasets. Bioinformatics, 2012, 28, 2431-2440.	1.8	111
53	Anchoring of PI-PLC to DMPC Bilayers Involves Specific Cation-PI Interactions. Biophysical Journal, 2012, 102, 78a-79a.	0.2	0
54	Specificity and Versatility of Substrate Binding Sites in Four Catalytic Domains of Human N-Terminal Acetyltransferases. PLoS ONE, 2012, 7, e52642.	1.1	5

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55	A dynamic model of longâ€range conformational adaptations triggered by nucleotide binding in GroELâ€GroES. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2333-2346.	1.5	6
56	Dynamics, flexibility and ligand-induced conformational changes in biological macromolecules: a computational approach. Future Medicinal Chemistry, 2011, 3, 2079-2100.	1.1	37
57	Interactive Visual Analysis of Temporal Cluster Structures. Computer Graphics Forum, 2011, 30, 711-720.	1.8	24
58	Principal component and normal mode analysis of proteins; a quantitative comparison using the GroEL subunit. Proteins: Structure, Function and Bioinformatics, 2011, 79, 232-243.	1.5	107
59	Exploring the factors determining the dynamics of different protein folds. Protein Science, 2011, 20, 197-209.	3.1	25
60	Molecular analysis of the membrane insertion domain of proteinase 3, the WegenerËˆs autoantigen, in RBL cells: implication for its pathogenic activity. Journal of Leukocyte Biology, 2011, 90, 941-950.	1.5	35
61	Conformational Sampling and Nucleotide-Dependent Transitions of the GroEL Subunit Probed by Unbiased Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1002004.	1.5	27
62	Interaction of proteinase 3 with its associated partners: implications in the pathogenesis of Wegener's granulomatosis. Current Opinion in Rheumatology, 2010, 22, 1-7.	2.0	43
63	Structures of human proteinaseâ€ƒ3 and neutrophil elastaseâ€ƒâ€“â€ƒso similar yet so different. FEBS Journal, 2010, 277, 2238-2254.	2.2	65
64	Molecular Dynamics Simulations of Mixed Acidic/Zwitterionic Phospholipid Bilayers. Biophysical Journal, 2010, 99, 825-833.	0.2	45
65	Proliferating cell nuclear antigen acts as a cytoplasmic platform controlling human neutrophil survival. Journal of Experimental Medicine, 2010, 207, 2631-2645.	4.2	144
66	How does Proteinase 3 interact with lipid bilayers?. Physical Chemistry Chemical Physics, 2010, 12, 7487.	1.3	18
67	The Functional Role of Membrane Bound Proteinase 3. Biophysical Journal, 2010, 98, 569a.	0.2	0
68	Proliferating cell nuclear antigen acts as a cytoplasmic platform controlling human neutrophil survival. Journal of Cell Biology, 2010, 191, i6-i6.	2.3	0
69	Normal mode analysis for proteins. Computational and Theoretical Chemistry, 2009, 898, 42-48.	1.5	111
70	Challenges in pKa Predictions for Proteins: The case of Asp213 in Human Proteinase 3. Journal of Physical Chemistry A, 2009, 113, 11783-11792.	1.1	12
71	Computational prediction of the binding site of proteinase 3 to the plasma membrane. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1655-1669.	1.5	46
72	Influence of Charge Distribution at the Active Site Surface on the Substrate Specificity of Human Neutrophil Protease 3 and Elastase. Journal of Biological Chemistry, 2007, 282, 1989-1997.	1.6	56

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73	Differences in the substrate binding sites of murine and human proteinase 3 and neutrophil elastase. FEBS Letters, 2007, 581, 5685-5690.	1.3	19
74	Two-Level Approach to Efficient Visualization of Protein Dynamics. IEEE Transactions on Visualization and Computer Graphics, 2007, 13, 1616-1623.	2.9	34
75	TMM@: a web application for the analysis of transmembrane helix mobility. BMC Bioinformatics, 2007, 8, 232.	1.2	2
76	Inspection of the Binding Sites of Proteinase3 for the Design of a Highly Specific Substrate. Journal of Medicinal Chemistry, 2006, 49, 1248-1260.	2.9	36
77	A novel locust (Schistocerca gregaria) serine protease inhibitor with a high affinity for neutrophil elastase. Biochemical Journal, 2006, 400, 467-476.	1.7	21
78	Evaluation of models for the evolution of protein sequences and functions under structural constraint. Biophysical Chemistry, 2006, 124, 134-144.	1.5	26
79	WEBnm@: a web application for normal mode analyses of proteins. BMC Bioinformatics, 2005, 6, 52.	1.2	103
80	Cleavage of p21/WAF1/CIP1 by Proteinase 3 Modulates Differentiation of a Monocytic Cell Line. Journal of Biological Chemistry, 2005, 280, 30242-30253.	1.6	25
81	Normal Mode-Based Fitting of Atomic Structure into Electron Density Maps: Application to Sarcoplasmic Reticulum Ca-ATPase. Biophysical Journal, 2005, 88, 818-827.	0.2	97
82	Orexins and their receptors: structural aspects and role in peripheral tissues. Cellular and Molecular Life Sciences, 2003, 60, 72-87.	2.4	107
83	The Nature of the Lowâ€Frequency Normal Modes of the E1Ca Form of the SERCA1 Ca²⁺â€ATPase. Annals of the New York Academy of Sciences, 2003, 986, 344-346.	1.8	6
84	Transconformations of the SERCA1 Ca-ATPase: A Normal Mode Study. Biophysical Journal, 2003, 85, 2186-2197.	0.2	65
85	The Elusive Oxidant Species of Cytochrome P450 Enzymes:â€‰ Characterization by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Calculations. Journal of the American Chemical Society, 2002, 124, 8142-8151.	6.6	290
86	Green Fluorescent Proteins:Â Empirical Force Field for the Neutral and Deprotonated Forms of the Chromophore. Molecular Dynamics Simulations of the Wild Type and S65T Mutant. Journal of Physical Chemistry B, 2002, 106, 6310-6321.	1.2	110
87	The vibrational overtones of SiH4 isotopomers: experimental wavenumbers, assignment, ab initio dipole moment surfaces and intensities. Physical Chemistry Chemical Physics, 2001, 3, 3506-3517.	1.3	14
88	The search for a new model structure of beta-factor XIIa. Journal of Computer-Aided Molecular Design, 2001, 15, 309-322.	1.3	5
89	Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. Journal of Physical Chemistry A, 2000, 104, 10923-10931.	1.1	54
90	Frontier Bonds in QM/MM Methods: A Comparison of Different Approaches. Journal of Physical Chemistry A, 2000, 104, 1720-1735.	1.1	367

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91	Theoretical study of arginineâ€“carboxylate interactions. Computational and Theoretical Chemistry, 1999, 463, 81-90.	1.5	37
92	Modeling enzyme-inhibitor interactions in serine proteases. , 1999, 74, 299-314.		17
93	A Quantum Chemical Approach to Reactions in Biomolecules. Molecular Engineering, 1997, 7, 349-365.	0.2	4