# 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 | Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388. | 9.0 | 557 |
| 2 | Frontier Bonds in QM/MM Methods: A Comparison of Different Approaches. Journal of Physical Chemistry A, 2000, 104, 1720-1735. | 1.1 | 367 |
| 3 | 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 |
| 4 | Proliferating cell nuclear antigen acts as a cytoplasmic platform controlling human neutrophil survival. Journal of Experimental Medicine, 2010, 207, 2631-2645. | 4.2 | 144 |
| 5 | Normal mode analysis for proteins. Computational and Theoretical Chemistry, 2009, 898, 42-48. | 1.5 | 111 |
| 6 | Measuring and comparing structural fluctuation patterns in large protein datasets. Bioinformatics, 2012, 28, 2431-2440. | 1.8 | 111 |
| 7 | 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 |
| 8 | Orexins and their receptors: structural aspects and role in peripheral tissues. Cellular and Molecular Life Sciences, 2003, 60, 72-87. | 2.4 | 107 |
| 9 | 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 |
| 10 | WEBnm@: a web application for normal mode analyses of proteins. BMC Bioinformatics, 2005, 6, 52. | 1.2 | 103 |
| 11 | 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 |
| 12 | Biochemical and cellular analysis of Ogden syndrome reveals downstream Nt-acetylation defects. Human Molecular Genetics, 2015, 24, 1956-1976. | 1.4 | 97 |
| 13 | WEBnm@ v2.0: Web server and services for comparing protein flexibility. BMC Bioinformatics, 2014, 15, 427. | 1.2 | 95 |
| 14 | 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 |
| 15 | Transconformations of the SERCA1 Ca-ATPase: A Normal Mode Study. Biophysical Journal, 2003, 85, 2186-2197. | 0.2 | 65 |
| 16 | Structures of human proteinaseâ€ƒ3 and neutrophil elastaseâ€ƒâ€“â€ƒso similar yet so different. FEBS Journal, 2010, 277, 2238-2254. | 2.2 | 65 |
| 17 | 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 |
| 18 | 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 |

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|---|---|---|---|
| 19 | Evolution of oligomeric state through allosteric pathways that mimic ligand binding. Science, 2014, 346, 1254346. | 6.0 | 62 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | Visual cavity analysis in molecular simulations. BMC Bioinformatics, 2013, 14, S4. | 1.2 | 52 |
| 25 | A Role for Weak Electrostatic Interactions in Peripheral Membrane Protein Binding. Biophysical Journal, 2016, 110, 1367-1378. | 0.2 | 47 |
| 26 | 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 |
| 27 | 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 |
| 28 | PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542. | 6.5 | 46 |
| 29 | Molecular Dynamics Simulations of Mixed Acidic/Zwitterionic Phospholipid Bilayers. Biophysical Journal, 2010, 99, 825-833. | 0.2 | 45 |
| 30 | 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 |
| 31 | Improving the Force Field Description of Tyrosineâ€“Choline Cationâ‹¯Ï€ Interactions: QM Investigation of Phenolâ€“N(Me)<sub>4</sub><sup>+</sup> Interactions. Journal of Chemical Theory and Computation, 2016, 12, 5585-5595. | 2.3 | 39 |
| 32 | 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 |
| 33 | Theoretical study of arginineâ€“carboxylate interactions. Computational and Theoretical Chemistry, 1999, 463, 81-90. | 1.5 | 37 |
| 34 | Dynamics, flexibility and ligand-induced conformational changes in biological macromolecules: a computational approach. Future Medicinal Chemistry, 2011, 3, 2079-2100. | 1.1 | 37 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Capturing Cholineâ€“Aromatics Cationâˆ’Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560. | 2.3 | 35 |
| 38 | Two-Level Approach to Efficient Visualization of Protein Dynamics. IEEE Transactions on Visualization and Computer Graphics, 2007, 13, 1616-1623. | 2.9 | 34 |
| 39 | Molecular determinants of the N-terminal acetyltransferase Naa60 anchoring to the Golgi membrane. Journal of Biological Chemistry, 2017, 292, 6821-6837. | 1.6 | 33 |
| 40 | 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 |
| 41 | Evaluation of models for the evolution of protein sequences and functions under structural constraint. Biophysical Chemistry, 2006, 124, 134-144. | 1.5 | 26 |
| 42 | A model for hydrophobic protrusions on peripheral membrane proteins. PLoS Computational Biology, 2018, 14, e1006325. | 1.5 | 26 |
| 43 | 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 |
| 44 | Exploring the factors determining the dynamics of different protein folds. Protein Science, 2011, 20, 197-209. | 3.1 | 25 |
| 45 | Search and Subvert: Minimalist Bacterial Phosphatidylinositol-Specific Phospholipase C Enzymes. Chemical Reviews, 2018, 118, 8435-8473. | 23.0 | 25 |
| 46 | Interactive Visual Analysis of Temporal Cluster Structures. Computer Graphics Forum, 2011, 30, 711-720. | 1.8 | 24 |
| 47 | 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 |
| 48 | Interfacial Aromatics Mediating Cationâˆ’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 |
| 49 | Comparing aminoglycoside binding sites in bacterial ribosomal RNA and aminoglycoside modifying enzymes. Proteins: Structure, Function and Bioinformatics, 2013, 81, 63-80. | 1.5 | 23 |
| 50 | A novel locust (Schistocerca gregaria) serine protease inhibitor with a high affinity for neutrophil elastase. Biochemical Journal, 2006, 400, 467-476. | 1.7 | 21 |
| 51 | Membrane Docking of the Synaptotagmin 7 C2A Domain: Computation Reveals Interplay between Electrostatic and Hydrophobic Contributions. Biochemistry, 2015, 54, 5696-5711. | 1.2 | 21 |
| 52 | Differences in the substrate binding sites of murine and human proteinase 3 and neutrophil elastase. FEBS Letters, 2007, 581, 5685-5690. | 1.3 | 19 |
| 53 | How does Proteinase 3 interact with lipid bilayers?. Physical Chemistry Chemical Physics, 2010, 12, 7487. | 1.3 | 18 |
| 54 | 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 |

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|---|---|---|---|
| 55 | Similarity in Shape Dictates Signature Intrinsic Dynamics Despite No Functional Conservation in TIM Barrel Enzymes. PLoS Computational Biology, 2016, 12, e1004834. | 1.5 | 18 |
| 56 | Modeling enzyme-inhibitor interactions in serine proteases. , 1999, 74, 299-314. | | 17 |
| 57 | Implicit surfaces for interactive graph based cavity analysis of molecular simulations. , 2012, , . | | 17 |
| 58 | Reversible Ketomethylene-Based Inhibitors of Human Neutrophil Proteinase 3. Journal of Medicinal Chemistry, 2014, 57, 9396-9408. | 2.9 | 17 |
| 59 | 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 |
| 60 | 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 |
| 61 | 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 |
| 62 | 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 |
| 63 | Does Changing the Predicted Dynamics of a Phospholipase C Alter Activity and Membrane Binding?. Biophysical Journal, 2013, 104, 185-195. | 0.2 | 11 |
| 64 | Integrating cluster formation and cluster evaluation in interactive visual analysis. , 2013, , . | | 8 |
| 65 | 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 |
| 66 | Dynamics-function relationship in the catalytic domains of N-terminal acetyltransferases. Computational and Structural Biotechnology Journal, 2020, 18, 532-547. | 1.9 | 8 |
| 67 | 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 |
| 68 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. PLoS Computational Biology, 2020, 16, e1007988. | 1.5 | 7 |
| 69 | The Nature of the Lowâ€Frequency Normal Modes of the E1Ca Form of the SERCA1 Ca<sup>2+</sup>â€ATPase. Annals of the New York Academy of Sciences, 2003, 986, 344-346. | 1.8 | 6 |
| 70 | 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 |
| 71 | 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 |
| 72 | The search for a new model structure of beta-factor XIIa. Journal of Computer-Aided Molecular Design, 2001, 15, 309-322. | 1.3 | 5 |

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|---|---|---|---|
| 73 | Specificity and Versatility of Substrate Binding Sites in Four Catalytic Domains of Human N-Terminal Acetyltransferases. PLoS ONE, 2012, 7, e52642. | 1.1 | 5 |
| 74 | Phospholipids in Motion: High-Resolution <sup>31</sup>P NMR Field Cycling Studies. Journal of Physical Chemistry B, 2021, 125, 8827-8838. | 1.2 | 5 |
| 75 | A Quantum Chemical Approach to Reactions in Biomolecules. Molecular Engineering, 1997, 7, 349-365. | 0.2 | 4 |
| 76 | d-Peptides as inhibitors of PR3-membrane interactions. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 458-466. | 1.4 | 4 |
| 77 | Peptidomimetic inhibitors targeting the membrane-binding site of the neutrophil proteinase 3. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1502-1509. | 1.4 | 4 |
| 78 | 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 |
| 79 | Visual exploration of large normal mode spaces to study protein flexibility. Computers and Graphics, 2020, 90, 73-83. | 1.4 | 4 |
| 80 | Membrane models for molecular simulations of peripheral membrane proteins. Advances in Physics: X, 2021, 6, 1932589. | 1.5 | 3 |
| 81 | TMM@: a web application for the analysis of transmembrane helix mobility. BMC Bioinformatics, 2007, 8, 232. | 1.2 | 2 |
| 82 | Examining the Flexibility of Tim Barrel Proteins Based on their Structural Topology. Biophysical Journal, 2013, 104, 227a-228a. | 0.2 | 1 |
| 83 | The Functional Role of Membrane Bound Proteinase 3. Biophysical Journal, 2010, 98, 569a. | 0.2 | 0 |
| 84 | Anchoring of PI-PLC to DMPC Bilayers Involves Specific Cation-PI Interactions. Biophysical Journal, 2012, 102, 78a-79a. | 0.2 | 0 |
| 85 | Proliferating cell nuclear antigen acts as a cytoplasmic platform controlling human neutrophil survival. Journal of Cell Biology, 2010, 191, i6-i6. | 2.3 | 0 |
| 86 | Specific Transient Interactions Between a Bacillus Virulence Factor and Phosphatidylcholine in Membranes. FASEB Journal, 2015, 29, 568.9. | 0.2 | 0 |
| 87 | Levels of proteinase 3 and neutrophil elastase in plasma, BAL and biopsies in COPD. , 2020, , . | | 0 |
| 88 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |
| 89 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |
| 90 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |

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| 91 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |
| 92 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |
| 93 | Classification and phylogeny for the annotation of novel eukaryotic GNAT acetyltransferases. , 2020, 16, e1007988. | | 0 |