# Martin Zacharias

List of Publications by Year
in descending order

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|---|---|---|---|
| 230 papers | 8,131 citations | 44069 48 h-index | 71685 76 g-index |

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|---|---|---|---|
| 247 all docs | 247 docs citations | 247 times ranked | 8338 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Separationâ€shifted scaling, a new scaling method for Lennardâ€Jones interactions in thermodynamic integration. Journal of Chemical Physics, 1994, 100, 9025-9031. | 3.0 | 472 |
| 2 | NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102. | 3.0 | 425 |
| 3 | Protein-protein docking with a reduced protein model accounting for side-chain flexibility. Protein Science, 2003, 12, 1271-1282. | 7.6 | 318 |
| 4 | Single-molecule dissection of stacking forces in DNA. Science, 2016, 353, . | 12.6 | 180 |
| 5 | A molecular mechanics/grid method for evaluation of ligand-receptor interactions. Journal of Computational Chemistry, 1995, 16, 454-464. | 3.3 | 175 |
| 6 | CHARMM-GUI supports the Amber force fields. Journal of Chemical Physics, 2020, 153, 035103. | 3.0 | 175 |
| 7 | Accounting for conformational changes during proteinâ€“protein docking. Current Opinion in Structural Biology, 2010, 20, 180-186. | 5.7 | 141 |
| 8 | Cryo-EM structure of a transthyretin-derived amyloid fibril from a patient with hereditary ATTR amyloidosis. Nature Communications, 2019, 10, 5008. | 12.8 | 127 |
| 9 | The interface of protein-protein complexes: Analysis of contacts and prediction of interactions. Cellular and Molecular Life Sciences, 2008, 65, 1059-1072. | 5.4 | 120 |
| 10 | Conformational Flexibility of the MHC Class I Î±1-Î±2 Domain in Peptide Bound and Free States: A Molecular Dynamics Simulation Study. Biophysical Journal, 2004, 87, 2203-2214. | 0.5 | 116 |
| 11 | Fully Blind Peptide-Protein Docking with pepATTRACT. Structure, 2015, 23, 1507-1515. | 3.3 | 112 |
| 12 | Multidomain structure and correlated dynamics determined by self-consistent FRET networks. Nature Methods, 2017, 14, 174-180. | 19.0 | 110 |
| 13 | Energy minimization in lowâ€frequency normal modes to efficiently allow for global flexibility during systematic proteinâ€“protein docking. Proteins: Structure, Function and Bioinformatics, 2008, 70, 794-809. | 2.6 | 109 |
| 14 | Computational prediction of proteinâ€“protein binding affinities. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1448. | 14.6 | 107 |
| 15 | Enhanced sampling of peptide and protein conformations using replica exchange simulations with a peptide backbone biasing-potential. Proteins: Structure, Function and Bioinformatics, 2006, 66, 697-706. | 2.6 | 102 |
| 16 | ATTRACT: Protein-protein docking in CAPRI using a reduced protein model. Proteins: Structure, Function and Bioinformatics, 2005, 60, 252-256. | 2.6 | 99 |
| 17 | Accounting for global protein deformability during proteinâ€“protein and proteinâ€“ligand docking. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1754, 225-231. | 2.3 | 95 |
| 18 | The Architecture of Talin1 Reveals an Autoinhibition Mechanism. Cell, 2019, 179, 120-131.e13. | 28.9 | 93 |

| # | Article | IF | Citations |
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| 19 | Proteinâ^'Ligand Docking Accounting for Receptor Side Chain and Global Flexibility in Normal Modes: Evaluation on Kinase Inhibitor Cross Docking. Journal of Medicinal Chemistry, 2008, 51, 3499-3506. | 6.4 | 86 |
| 20 | Between inflammation and thrombosis: endothelial cells in COVID-19. European Respiratory Journal, 2021, 58, 2100377. | 6.7 | 86 |
| 21 | The pepATTRACT web server for blind, large-scale peptideâ€"protein docking. Nucleic Acids Research, 2017, 45, W361-W364. | 14.5 | 84 |
| 22 | A Web Interface for Easy Flexible Protein-Protein Docking with ATTRACT. Biophysical Journal, 2015, 108, 462-465. | 0.5 | 82 |
| 23 | Rapid protein-ligand docking using soft modes from molecular dynamics simulations to account for protein deformability: Binding of FK506 to FKBP. Proteins: Structure, Function and Bioinformatics, 2004, 54, 759-767. | 2.6 | 79 |
| 24 | PEP-SiteFinder: a tool for the blind identification of peptide binding sites on protein surfaces. Nucleic Acids Research, 2014, 42, W221-W226. | 14.5 | 79 |
| 25 | Accounting for loop flexibility during protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2005, 62, 956-969. | 2.6 | 78 |
| 26 | In Silico Prediction of Binding Sites on Proteins. Current Medicinal Chemistry, 2010, 17, 1550-1562. | 2.4 | 77 |
| 27 | Dynamics of Seeded AÎ²<sub>40</sub>-Fibril Growth from Atomistic Molecular Dynamics Simulations: Kinetic Trapping and Reduced Water Mobility in the Locking Step. Journal of the American Chemical Society, 2016, 138, 527-539. | 13.7 | 77 |
| 28 | Harmonic modes as variables to approximately account for receptor flexibility in ligand-receptor docking simulations: Application to DNA minor groove ligand complex. Journal of Computational Chemistry, 1999, 20, 287-300. | 3.3 | 69 |
| 29 | Poisson-Boltzmann analysis of the lambda repressor-operator interaction. Biophysical Journal, 1992, 63, 1280-1285. | 0.5 | 68 |
| 30 | Tapasin and other chaperones: models of the MHC class I loading complex. Biological Chemistry, 2004, 385, 763-78. | 2.5 | 68 |
| 31 | Empty peptide-receptive MHC class I molecules for efficient detection of antigen-specific T cells. Science Immunology, 2019, 4, . | 11.9 | 64 |
| 32 | Advanced replica-exchange sampling to study the flexibility and plasticity of peptides and proteins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 847-853. | 2.3 | 62 |
| 33 | Binding site prediction and improved scoring during flexible proteinâ€"protein docking with ATTRACT. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3131-3139. | 2.6 | 61 |
| 34 | Tapasin dependence of major histocompatibility complex class I molecules correlates with their conformational flexibility. FASEB Journal, 2011, 25, 3989-3998. | 0.5 | 61 |
| 35 | Free energy analysis and mechanism of base pair stacking in nicked DNA. Nucleic Acids Research, 2016, 44, gkw607. | 14.5 | 60 |
| 36 | B-DNA Under Stress: Over- and Untwisting of DNA during Molecular Dynamics Simulations. Biophysical Journal, 2006, 91, 2956-2965. | 0.5 | 58 |

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| 37 | Flexible docking and refinement with a coarseâ€grained protein model using ATTRACT. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2167-2174. | 2.6 | 57 |
| 38 | iATTRACT: Simultaneous global and local interface optimization for proteinâ€“protein docking refinement. Proteins: Structure, Function and Bioinformatics, 2015, 83, 248-258. | 2.6 | 57 |
| 39 | Comparative molecular dynamics analysis of tapasin-dependent and -independent MHC class I alleles. Protein Science, 2006, 16, 299-308. | 7.6 | 56 |
| 40 | Folding of a DNA Hairpin Loop Structure in Explicit Solvent Using Replica-Exchange Molecular Dynamics Simulations. Biophysical Journal, 2007, 93, 3218-3228. | 0.5 | 56 |
| 41 | Prediction of Protein-Protein Interaction Sites Using Electrostatic Desolvation Profiles. Biophysical Journal, 2010, 98, 1921-1930. | 0.5 | 55 |
| 42 | A coarse-grained force field for Proteinâ€“RNA docking. Nucleic Acids Research, 2011, 39, 9118-9129. | 14.5 | 55 |
| 43 | Dipeptides promote folding and peptide binding of MHC class I molecules. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15383-15388. | 7.1 | 55 |
| 44 | The temperature dependence of the helical twist of DNA. Nucleic Acids Research, 2018, 46, 7998-8009. | 14.5 | 55 |
| 45 | Holonomic constraint contributions to free energy differences from thermodynamic integration molecular dynamics simulations. Chemical Physics Letters, 1992, 196, 297-302. | 2.6 | 54 |
| 46 | RNA Kink-Turns as Molecular Elbows: Hydration, Cation Binding, and Large-Scale Dynamics. Structure, 2006, 14, 825-835. | 3.3 | 54 |
| 47 | Simulation of the structure and dynamics of nonhelical RNA motifs. Current Opinion in Structural Biology, 2000, 10, 311-317. | 5.7 | 51 |
| 48 | DAPI binding to the DNA minor groove: a continuum solvent analysis. Journal of Molecular Recognition, 2002, 15, 209-220. | 2.1 | 51 |
| 49 | Folding simulations of Trpâ€cage mini protein in explicit solvent using biasing potential replicaâ€exchange molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2009, 76, 448-460. | 2.6 | 50 |
| 50 | Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632. | 2.6 | 50 |
| 51 | Explaining the striking difference in twist-stretch coupling between DNA and RNA: A comparative molecular dynamics analysis. Nucleic Acids Research, 2015, 43, gkv1028. | 14.5 | 50 |
| 52 | Combined Conformational Search and Finite-Difference Poisson?Boltzmann Approach for Flexible Docking. Journal of Molecular Biology, 1994, 238, 455-465. | 4.2 | 49 |
| 53 | Continuum Solvent Modeling of Nonpolar Solvation:â€‰ Improvement by Separating Surface Area Dependent Cavity and Dispersion Contributions. Journal of Physical Chemistry A, 2003, 107, 3000-3004. | 2.5 | 47 |
| 54 | Evaluation of Predicted Proteinâ€“Protein Complexes by Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2019, 15, 2071-2086. | 5.3 | 46 |

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| 55 | Extracellular interface between APP and Nicastrin regulates AÎ² length and response to Î³â€secretase modulators. EMBO Journal, 2019, 38, . | 7.8 | 45 |
| 56 | ATTRACT-EM: A New Method for the Computational Assembly of Large Molecular Machines Using Cryo-EM Maps. PLoS ONE, 2012, 7, e49733. | 2.5 | 45 |
| 57 | Proteinâ€"protein docking in CAPRI using ATTRACT to account for global and local flexibility. Proteins: Structure, Function and Bioinformatics, 2007, 69, 774-780. | 2.6 | 44 |
| 58 | Minor Groove Deformability of DNA: A Molecular Dynamics Free Energy Simulation Study. Biophysical Journal, 2006, 91, 882-891. | 0.5 | 42 |
| 59 | The structure and oxidation of the eye lens chaperone Î±A-crystallin. Nature Structural and Molecular Biology, 2019, 26, 1141-1150. | 8.2 | 42 |
| 60 | Simulation of DNA double-strand dissociation and formation during replica-exchange molecular dynamics simulations. Physical Chemistry Chemical Physics, 2009, 11, 10589. | 2.8 | 41 |
| 61 | SAXS Data Alone can Generate High-Quality Models of Protein-Protein Complexes. Structure, 2016, 24, 1387-1397. | 3.3 | 40 |
| 62 | Structures of peptide-free and partially loaded MHC class I molecules reveal mechanisms of peptide selection. Nature Communications, 2020, 11, 1314. | 12.8 | 40 |
| 63 | Tackling the challenges posed by target flexibility in drug design. Expert Opinion on Drug Discovery, 2010, 5, 347-359. | 5.0 | 38 |
| 64 | Inversion of receptor binding preferences by mutagenesis: Free energy thermodynamic integration studies on sugar binding to L-arabinose binding proteins. Biochemistry, 1993, 32, 7428-7434. | 2.5 | 37 |
| 65 | Enhanced conformational sampling of nucleic acids by a new Hamiltonian replica exchange molecular dynamics approach. Journal of Chemical Physics, 2009, 130, 104110. | 3.0 | 37 |
| 66 | Accurate modeling of DNA conformational flexibility by a multivariate Ising model. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 35 |
| 67 | Altered fibrin clot structure and dysregulated fibrinolysis contribute toÂthrombosis risk in severe COVID-19. Blood Advances, 2022, 6, 1074-1087. | 5.2 | 35 |
| 68 | Atomic resolution model of the antibody Fc interaction with the complement C1q component. Molecular Immunology, 2012, 51, 66-72. | 2.2 | 34 |
| 69 | From AÎ² Filament to Fibril: Molecular Mechanism of Surface-Activated Secondary Nucleation from All-Atom MD Simulations. Journal of Physical Chemistry B, 2017, 121, 671-682. | 2.6 | 34 |
| 70 | Combining Elastic Network Analysis and Molecular Dynamics Simulations by Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2008, 4, 477-487. | 5.3 | 33 |
| 71 | Bulk tumour cell migration in lung carcinomas might be more common than epithelial-mesenchymal transition and be differently regulated. BMC Cancer, 2018, 18, 717. | 2.6 | 33 |
| 72 | Tethered multifluorophore motion reveals equilibrium transition kinetics of single DNA double helices. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7512-E7521. | 7.1 | 33 |

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| 73 | Fatal amyloid formation in a patientâ€™s antibody light chain is caused by a single point mutation. ELife, 2020, 9, . | 6.0 | 33 |
| 74 | The Impact of Prolonged Inflammation on Wound Healing. Biomedicines, 2022, 10, 856. | 3.2 | 33 |
| 75 | PTools: an opensource molecular docking library. BMC Structural Biology, 2009, 9, 27. | 2.3 | 32 |
| 76 | Proteinâ€“Ligand Docking Using Hamiltonian Replica Exchange Simulations with Soft Core Potentials. Journal of Chemical Information and Modeling, 2014, 54, 1669-1675. | 5.4 | 32 |
| 77 | A folding switch regulates interleukin 27 biogenesis and secretion of its Î±-subunit as a cytokine. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1585-1590. | 7.1 | 32 |
| 78 | Bovine Serum Albumin and Lysozyme Adsorption on Calcium Phosphate Particles. Advanced Engineering Materials, 2010, 12, B53. | 3.5 | 31 |
| 79 | Application of biasingâ€potential replicaâ€exchange simulations for loop modeling and refinement of proteins in explicit solvent. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2809-2819. | 2.6 | 31 |
| 80 | Protein-DNA docking with a coarse-grained force field. BMC Bioinformatics, 2012, 13, 228. | 2.6 | 31 |
| 81 | Elastic Network Models of Nucleic Acids Flexibility. Journal of Chemical Theory and Computation, 2013, 9, 5460-5470. | 5.3 | 29 |
| 82 | Î³-Secretase Studied by Atomistic Molecular Dynamics Simulations: Global Dynamics, Enzyme Activation, Water Distribution and Lipid Binding. Frontiers in Chemistry, 2018, 6, 640. | 3.6 | 29 |
| 83 | Hamiltonian replicaâ€exchange simulations with adaptive biasing of peptide backbone and side chain dihedral angles. Journal of Computational Chemistry, 2014, 35, 150-158. | 3.3 | 28 |
| 84 | Concerted regulation of ISWI by an autoinhibitory domain and the H4 N-terminal tail. ELife, 2017, 6, . | 6.0 | 28 |
| 85 | Efficient inclusion of receptor flexibility in gridâ€based proteinâ€“ligand docking*. Journal of Computational Chemistry, 2011, 32, 3433-3439. | 3.3 | 27 |
| 86 | Exploring biomolecular dynamics and interactions using advanced sampling methods. Journal of Physics Condensed Matter, 2015, 27, 323101. | 1.8 | 27 |
| 87 | Unwinding Induced Melting of Double-Stranded DNA Studied by Free Energy Simulations. Journal of Physical Chemistry B, 2017, 121, 11019-11030. | 2.6 | 27 |
| 88 | Prediction of proteinâ€“protein complexes using replica exchange with repulsive scaling. Journal of Computational Chemistry, 2020, 41, 1436-1447. | 3.3 | 27 |
| 89 | Molecular and Spectroscopic Characterization of Green and Red Cyanine Fluorophores from the Alexa Fluor and AF Series**. ChemPhysChem, 2021, 22, 1566-1583. | 2.1 | 27 |
| 90 | Modelling ion binding to AA platform motifs in RNA: a continuum solvent study including conformational adaptation. Nucleic Acids Research, 2001, 29, 3910-3918. | 14.5 | 26 |

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| 91 | Elbow Flexibility of the kt38 RNA Kink-Turn Motif Investigated by Free-Energy Molecular Dynamics Simulations. Biophysical Journal, 2009, 97, 2004-2013. | 0.5 | 26 |
| 92 | Role of Tryptophan Side Chain Dynamics on the Trp-Cage Mini-Protein Folding Studied by Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e88383. | 2.5 | 26 |
| 93 | Structural Modeling of Î³-Secretase AÎ²<sub>n</sub> Complex Formation and Substrate Processing. ACS Chemical Neuroscience, 2019, 10, 1826-1840. | 3.5 | 25 |
| 94 | Analysis of the stability of looped-out and stacked-in conformations of an adenine bulge in DNA using a continuum model for solvent and ions. Biophysical Journal, 1997, 73, 2990-3003. | 0.5 | 24 |
| 95 | Combining coarseâ€grained nonbonded and atomistic bonded interactions for protein modeling. Proteins: Structure, Function and Bioinformatics, 2013, 81, 81-92. | 2.6 | 24 |
| 96 | Enhanced conformational sampling of carbohydrates by Hamiltonian replica-exchange simulation. Glycobiology, 2014, 24, 70-84. | 2.5 | 24 |
| 97 | Application of Enhanced Sampling Monte Carlo Methods for High-Resolution Protein-Protein Docking in Rosetta. PLoS ONE, 2015, 10, e0125941. | 2.5 | 24 |
| 98 | Multiscale Simulation of Receptorâ€“Drug Association Kinetics: Application to Neuraminidase Inhibitors. Journal of Chemical Theory and Computation, 2017, 13, 5097-5105. | 5.3 | 24 |
| 99 | Adaptive Biasing Combined with Hamiltonian Replica Exchange to Improve Umbrella Sampling Free Energy Simulations. Journal of Chemical Theory and Computation, 2014, 10, 703-710. | 5.3 | 23 |
| 100 | RAID3 - An interleukin-6 receptor-binding aptamer with post-selective modification-resistant affinity. RNA Biology, 2015, 12, 1043-1053. | 3.1 | 23 |
| 101 | Optical control of a receptor-linked guanylyl cyclase using a photoswitchable peptidic hormone. Chemical Science, 2017, 8, 4644-4653. | 7.4 | 23 |
| 102 | Molecular mechanism of amyloidogenic mutations in hypervariable regions of antibody light chains. Journal of Biological Chemistry, 2021, 296, 100334. | 3.4 | 22 |
| 103 | The Antibody Light-Chain Linker Is Important for Domain Stability and Amyloid Formation. Journal of Molecular Biology, 2015, 427, 3572-3586. | 4.2 | 21 |
| 104 | Uncovering the Binding Mode of Î³ -Secretase Inhibitors. ACS Chemical Neuroscience, 2019, 10, 3398-3403. | 3.5 | 21 |
| 105 | How methylâ€“sugar interactions determine DNA structure and flexibility. Nucleic Acids Research, 2019, 47, 1132-1140. | 14.5 | 21 |
| 106 | Tumuc1: A New Accurate DNA Force Field Consistent with High-Level Quantum Chemistry. Journal of Chemical Theory and Computation, 2021, 17, 7096-7105. | 5.3 | 21 |
| 107 | Folding of Trp-cage Mini Protein Using Temperature and Biasing Potential Replicaâ€”Exchange Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2009, 10, 1121-1137. | 4.1 | 20 |
| 108 | Influence of 8-Oxoguanosine on the Fine Structure of DNA Studied with Biasing-Potential Replica Exchange Simulations. Biophysical Journal, 2013, 104, 1089-1097. | 0.5 | 20 |

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| 109 | gp130 activation is regulated by D2â€“D3 interdomain connectivity. Biochemical Journal, 2013, 450, 487-496. | 3.7 | 20 |
| 110 | Structure and target interaction of a G-quadruplex RNA-aptamer. RNA Biology, 2016, 13, 973-987. | 3.1 | 20 |
| 111 | Fragment-based modelling of single stranded RNA bound to RNA recognition motif containing proteins. Nucleic Acids Research, 2016, 44, 4565-4580. | 14.5 | 20 |
| 112 | A Stable Mutant Predisposes Antibody Domains to Amyloid Formation through Specific Non-Native Interactions. Journal of Molecular Biology, 2016, 428, 1315-1332. | 4.2 | 20 |
| 113 | Determinants of the assembly and function of antibody variable domains. Scientific Reports, 2017, 7, 12276. | 3.3 | 20 |
| 114 | Prognostic value of cyclin A2 and B1 expression in lung carcinoids. Pathology, 2019, 51, 481-486. | 0.6 | 20 |
| 115 | Efficient Refinement and Free Energy Scoring of Predicted Proteinâ€“Protein Complexes Using Replica Exchange with Repulsive Scaling. Journal of Chemical Information and Modeling, 2020, 60, 5552-5562. | 5.4 | 20 |
| 116 | Base-Pairing and Base-Stacking Contributions to Double-Stranded DNA Formation. Journal of Physical Chemistry B, 2020, 124, 10345-10352. | 2.6 | 20 |
| 117 | Refinement of protein cores and proteinâ€“peptide interfaces using a potential scaling approach. Protein Engineering, Design and Selection, 2005, 18, 465-476. | 2.1 | 19 |
| 118 | How to Efficiently Include Receptor Flexibility During Computational Docking. Current Computer-Aided Drug Design, 2008, 4, 143-153. | 1.2 | 19 |
| 119 | How global DNA unwinding causes non-uniform stress distribution and melting of DNA. PLoS ONE, 2020, 15, e0232976. | 2.5 | 19 |
| 120 | The dynamics of Î³-secretase and its substrates. Seminars in Cell and Developmental Biology, 2020, 105, 86-101. | 5.0 | 19 |
| 121 | Binding Site Identification and Flexible Docking of Single Stranded RNA to Proteins Using a Fragment-Based Approach. PLoS Computational Biology, 2016, 12, e1004697. | 3.2 | 19 |
| 122 | Influence of a fluorobenzene nucleobase analogue on the conformational flexibility of RNA studied by molecular dynamics simulations. Nucleic Acids Research, 2004, 32, 6304-6311. | 14.5 | 18 |
| 123 | Hydration in Discrete Water. A Mean Field, Cellular Automata Based Approach to Calculating Hydration Free Energies. Journal of Physical Chemistry B, 2010, 114, 8667-8675. | 2.6 | 18 |
| 124 | ATTRACT and PTOOLS: Open Source Programs for Proteinâ€“Protein Docking. Methods in Molecular Biology, 2012, 819, 221-232. | 0.9 | 18 |
| 125 | Efficient calculation of relative binding free energies by umbrella sampling perturbation. Journal of Computational Chemistry, 2014, 35, 2256-2262. | 3.3 | 18 |
| 126 | Evaluation of Generalized Born Model Accuracy for Absolute Binding Free Energy Calculations. Journal of Physical Chemistry B, 2014, 118, 7467-7474. | 2.6 | 18 |

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| 127 | Coupling between side chain interactions and binding pocket flexibility in HLA-B*44:02 molecules investigated by molecular dynamics simulations. Molecular Immunology, 2015, 63, 312-319. | 2.2 | 18 |
| 128 | Origin of Ion Specificity of Telomeric DNA G-Quadruplexes Investigated by Free-Energy Simulations. Biophysical Journal, 2017, 112, 2280-2290. | 0.5 | 18 |
| 129 | Proteinâ€protein and peptideâ€protein docking and refinement using ATTRACT in CAPRI. Proteins: Structure, Function and Bioinformatics, 2017, 85, 391-398. | 2.6 | 18 |
| 130 | Occurrence of SARS-CoV-2 in the intraocular milieu. Experimental Eye Research, 2020, 201, 108273. | 2.6 | 18 |
| 131 | Covalent dye attachment influences the dynamics and conformational properties of flexible peptides. PLoS ONE, 2017, 12, e0177139. | 2.5 | 18 |
| 132 | Effect of 8-Oxoguanine on DNA Structure and Deformability. Journal of Physical Chemistry B, 2013, 117, 11617-11622. | 2.6 | 17 |
| 133 | Substrate Binding Specifically Modulates Domain Arrangements in Adenylate Kinase. Biophysical Journal, 2015, 109, 1978-1985. | 0.5 | 17 |
| 134 | Comparison of molecular dynamics and harmonic mode calculations on RNA. Biopolymers, 2000, 54, 547-560. | 2.4 | 16 |
| 135 | Rapid in silico Design of Potential Cyclic Peptide Binders Targeting Protein-Protein Interfaces. Frontiers in Chemistry, 2020, 8, 573259. | 3.6 | 16 |
| 136 | Compensatory Mechanisms in Temperature Dependence of DNA Double Helical Structure: Bending and Elongation. Journal of Chemical Theory and Computation, 2020, 16, 2857-2863. | 5.3 | 16 |
| 137 | Efficient evaluation of sampling quality of molecular dynamics simulations by clustering of dihedral torsion angles and Sammon mapping. Journal of Computational Chemistry, 2009, 30, 479-492. | 3.3 | 15 |
| 138 | A Residue-specific Shift in Stability and Amyloidogenicity of Antibody Variable Domains. Journal of Biological Chemistry, 2014, 289, 26829-26846. | 3.4 | 15 |
| 139 | Monte Carlo replica-exchange based ensemble docking of protein conformations. Proteins: Structure, Function and Bioinformatics, 2017, 85, 924-937. | 2.6 | 15 |
| 140 | Modeling large proteinâ€“glycosaminoglycan complexes using a fragmentâ€based approach. Journal of Computational Chemistry, 2019, 40, 1429-1439. | 3.3 | 15 |
| 141 | Specificity of AMPylation of the human chaperone BiP is mediated by TPR motifs of FICD. Nature Communications, 2021, 12, 2426. | 12.8 | 15 |
| 142 | Cryo-EM demonstrates the in vitro proliferation of an ex vivo amyloid fibril morphology by seeding. Nature Communications, 2022, 13, 85. | 12.8 | 15 |
| 143 | Combining geometric pocket detection and desolvation properties to detect putative ligand binding sites on proteins. Journal of Structural Biology, 2012, 180, 546-550. | 2.8 | 14 |
| 144 | Cryo-EM Data Are Superior to Contact and Interface Information in Integrative Modeling. Biophysical Journal, 2016, 110, 785-797. | 0.5 | 14 |

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| 145 | How Mutations Perturb Î³-Secretase Active Site Studied by Free Energy Simulations. ACS Chemical Neuroscience, 2020, 11, 3321-3332. | 3.5 | 14 |
| 146 | Rapid Antigen Test for Postmortem Evaluation of SARS-CoV-2 Carriage. Emerging Infectious Diseases, 2021, 27, 1734-1737. | 4.3 | 14 |
| 147 | Modeling Proteinâ€“Glycosaminoglycan Complexes: Does the Size Matter?. Journal of Chemical Information and Modeling, 2021, 61, 4475-4485. | 5.4 | 14 |
| 148 | An Integrative Approach to the Study of Filamentous Oligomeric Assemblies, with Application to RecA. PLoS ONE, 2015, 10, e0116414. | 2.5 | 14 |
| 149 | Accelerated flexible protein-ligand docking using Hamiltonian replica exchange with a repulsive biasing potential. PLoS ONE, 2017, 12, e0172072. | 2.5 | 14 |
| 150 | Role of the closing base pair for d(GCA) hairpin stability: free energy analysis and folding simulations. Nucleic Acids Research, 2011, 39, 8271-8280. | 14.5 | 13 |
| 151 | Stabilization of duplex DNA and RNA by dangling ends studied by free energy simulations. Biopolymers, 2014, 101, 418-427. | 2.4 | 13 |
| 152 | Adenylylation of Tyr77 stabilizes Rab1b GTPase in an active state: A molecular dynamics simulation analysis. Scientific Reports, 2016, 6, 19896. | 3.3 | 13 |
| 153 | Both DNA global deformation and repair enzyme contacts mediate flipping of thymine dimer damage. Scientific Reports, 2017, 7, 41324. | 3.3 | 13 |
| 154 | Global deformation facilitates flipping of damaged 8-oxo-guanine and guanine in DNA. Nucleic Acids Research, 2016, 44, gkw827. | 14.5 | 12 |
| 155 | From monomer to fibril: Abetaâ€amyloid binding to Aducanumab antibody studied by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1592-1606. | 2.6 | 12 |
| 156 | Altered Hinge Conformations in APP Transmembrane Helix Mutants May Affect Enzymeâ€“Substrate Interactions of Î³-Secretase. ACS Chemical Neuroscience, 2020, 11, 4426-4433. | 3.5 | 12 |
| 157 | Coarseâ€grained and atomic resolution biomolecular docking with the ATTRACT approach. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1018-1028. | 2.6 | 12 |
| 158 | Proteolysis of Rab32 by Salmonella GtgE induces an inactive GTPase conformation. IScience, 2021, 24, 101940. | 4.1 | 12 |
| 159 | Structural Architecture of the Nucleosome Remodeler ISWI Determined from Cross-Linking, Mass Spectrometry, SAXS, and Modeling. Structure, 2018, 26, 282-294.e6. | 3.3 | 11 |
| 160 | Scoring optimisation of unbound proteinâ€“protein docking including protein binding site predictions. Journal of Molecular Recognition, 2012, 25, 15-23. | 2.1 | 10 |
| 161 | Role of tyrosine hotâ€spot residues at the interface of colicin E9 and immunity protein 9: A comparative free energy simulation study. Proteins: Structure, Function and Bioinformatics, 2013, 81, 461-468. | 2.6 | 10 |
| 162 | Hamiltonian replica exchange combined with elastic network analysis to enhance global domain motions in atomistic molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3410-3419. | 2.6 | 10 |

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| 163 | An Interspecies Analysis Reveals Molecular Construction Principles of Interleukin 27. Journal of Molecular Biology, 2019, 431, 2383-2393. | 4.2 | 10 |
| 164 | The N-Terminal Segment of the Voltage-Dependent Anion Channel: A Possible Membrane-Bound Intermediate in Pore Unbinding. Journal of Molecular Biology, 2019, 431, 223-243. | 4.2 | 10 |
| 165 | ReFlexIn: A Flexible Receptor Protein-Ligand Docking Scheme Evaluated on HIV-1 Protease. PLoS ONE, 2012, 7, e48008. | 2.5 | 10 |
| 166 | An internal docking site stabilizes substrate binding to Î³-secretase: Analysis by molecular dynamics simulations. Biophysical Journal, 2022, 121, 2330-2344. | 0.5 | 10 |
| 167 | Rationalizing perhydrolase activity of aryl-esterase and subtilisin Carlsberg mutants by molecular dynamics simulations of the second tetrahedral intermediate state. Theoretical Chemistry Accounts, 2010, 125, 375-386. | 1.4 | 9 |
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