# Peter J Bond

List of Publications by Year
in descending order



| 150 | 7,325 | 53751 45 | 66879 78 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 169 | 169 | 169 | 9857 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The molecular basis for selective inhibition of unconventional mRNA splicing by an IRE1-binding small molecule. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E869-78. | 3.3 | 476 |
| 2 | Insertion and Assembly of Membrane Proteins via Simulation. Journal of the American Chemical Society, 2006, 128, 2697-2704. | 6.6 | 314 |
| 3 | Evidence that TLR4 Is Not a Receptor for Saturated Fatty Acids but Mediates Lipid-Induced Inflammation by Reprogramming Macrophage Metabolism. Cell Metabolism, 2018, 27, 1096-1110.e5. | 7.2 | 309 |
| 4 | Coarse-grained molecular dynamics simulations of membrane proteins and peptides. Journal of Structural Biology, 2007, 157, 593-605. | 1.3 | 303 |
| 5 | Computational Prediction of Metabolism: Sites, Products, SAR, P450 Enzyme Dynamics, and Mechanisms. Journal of Chemical Information and Modeling, 2012, 52, 617-648. | 2.5 | 246 |
| 6 | From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574. | 1.2 | 243 |
| 7 | Coarse-Grained MD Simulations of Membrane Protein-Bilayer Self-Assembly. Structure, 2008, 16, 621-630. | 1.6 | 199 |
| 8 | Interaction of the Antimicrobial Peptide Polymyxin B1 with Both Membranes of E. coli: A Molecular Dynamics Study. PLoS Computational Biology, 2015, 11, e1004180. | 1.5 | 134 |
| 9 | Membrane Protein Dynamics versus Environment: Simulations of OmpA in a Micelle and in a Bilayer. Journal of Molecular Biology, 2003, 329, 1035-1053. | 2.0 | 130 |
| 10 | Efficient Characterization of Protein Cavities within Molecular Simulation Trajectories: trj_cavity. Journal of Chemical Theory and Computation, 2014, 10, 2151-2164. | 2.3 | 129 |
| 11 | An Optical Technique for Mapping Microviscosity Dynamics in Cellular Organelles. ACS Nano, 2018, 12, 4398-4407. | 7.3 | 125 |
| 12 | SARS-CoV-2 spike protein binds to bacterial lipopolysaccharide and boosts proinflammatory activity. Journal of Molecular Cell Biology, 2021, 12, 916-932. | 1.5 | 121 |
| 13 | Coarse-grained simulation: a high-throughput computational approach to membrane proteins. Biochemical Society Transactions, 2008, 36, 27-32. | 1.6 | 117 |
| 14 | The antibiotic darobactin mimics a Î²-strand to inhibit outer membrane insertase. Nature, 2021, 593, 125-129. | 13.7 | 112 |
| 15 | Lipid-Protein Interactions of Integral Membrane Proteins: A Comparative Simulation Study. Biophysical Journal, 2004, 87, 3737-3749. | 0.2 | 104 |
| 16 | Structure mapping of dengue and Zika viruses reveals functional long-range interactions. Nature Communications, 2019, 10, 1408. | 5.8 | 104 |
| 17 | Bilayer deformation by the Kv channel voltage sensor domain revealed by self-assembly simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2631-2636. | 3.3 | 100 |
| 18 | SARS-CoV-2 S protein:ACE2 interaction reveals novel allosteric targets. ELife, 2021, 10, . | 2.8 | 100 |

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| 19 | Complete Ion-Coordination Structure in the Rotor Ring of Na+-Dependent F-ATP Synthases. Journal of Molecular Biology, 2009, 391, 498-507. | 2.0 | 98 |
| 20 | Minor pseudopilin self-assembly primes type II secretion pseudopilus elongation. EMBO Journal, 2012, 31, 1041-1053. | 3.5 | 94 |
| 21 | Design, Synthesis, and Biological Evaluation of an Allosteric Inhibitor of HSET that Targets Cancer Cells with Supernumerary Centrosomes. Chemistry and Biology, 2013, 20, 1399-1410. | 6.2 | 94 |
| 22 | Membrane Recognition and Dynamics of the RNA Degradosome. PLoS Genetics, 2015, 11, e1004961. | 1.5 | 93 |
| 23 | OmpA: A Pore or Not a Pore? Simulation and Modeling Studies. Biophysical Journal, 2002, 83, 763-775. | 0.2 | 92 |
| 24 | Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 783-791. | 1.5 | 92 |
| 25 | Coarse-Grained Molecular Dynamics Simulations of the Energetics of Helix Insertion into a Lipid Bilayer. Biochemistry, 2008, 47, 11321-11331. | 1.2 | 87 |
| 26 | MD Simulations of Spontaneous Membrane Protein/Detergent Micelle Formation. Journal of the American Chemical Society, 2004, 126, 15948-15949. | 6.6 | 85 |
| 27 | Activation of Toll-like receptors nucleates assembly of the MyDDosome signaling hub. ELife, 2018, 7, . | 2.8 | 83 |
| 28 | Helixâ^'Helix Interactions in Membrane Proteins: Coarse-Grained Simulations of Glycophorin A Helix Dimerization. Biochemistry, 2008, 47, 10503-10512. | 1.2 | 82 |
| 29 | Anionic Phospholipid Interactions with the Potassium Channel KcsA: Simulation Studies. Biophysical Journal, 2006, 90, 822-830. | 0.2 | 77 |
| 30 | OmpA: A Flexible Clamp for Bacterial Cell Wall Attachment. Structure, 2016, 24, 2227-2235. | 1.6 | 76 |
| 31 | Self-Assembly of a Simple Membrane Protein: Coarse-Grained Molecular Dynamics Simulations of the Influenza M2 Channel. Biophysical Journal, 2008, 95, 3790-3801. | 0.2 | 69 |
| 32 | Coarse-Grained Simulations of the Membrane-Active Antimicrobial Peptide Maculatin 1.1. Biophysical Journal, 2008, 95, 3802-3815. | 0.2 | 68 |
| 33 | Full-Length OmpA: Structure, Function, and Membrane Interactions Predicted by Molecular Dynamics Simulations. Biophysical Journal, 2016, 111, 1692-1702. | 0.2 | 67 |
| 34 | Transmembrane Helixâ^'Helix Interactions:â€‰ Comparative Simulations of the Glycophorin A Dimer. Biochemistry, 2006, 45, 14298-14310. | 1.2 | 65 |
| 35 | DNA and lipid bilayers: self-assembly and insertion. Journal of the Royal Society Interface, 2008, 5, 241-250. | 1.5 | 64 |
| 36 | The architecture of the OmpCâ€“MlaA complex sheds light on the maintenance of outer membrane lipid asymmetry in Escherichia coli. Journal of Biological Chemistry, 2018, 293, 11325-11340. | 1.6 | 64 |

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| 37 | The simulation approach to bacterial outer membrane proteins (Review). Molecular Membrane Biology, 2004, 21, 151-161. | 2.0 | 61 |
| 38 | Cysteine-scanning Mutagenesis and Disulfide Mapping Studies of the Conserved Domain of the Twin-arginine Translocase TatB Component*. Journal of Biological Chemistry, 2006, 281, 34072-34085. | 1.6 | 60 |
| 39 | Membrane protein structure quality in molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2005, 24, 157-165. | 1.3 | 58 |
| 40 | Structural and energetic basis for H+ versus Na+ binding selectivity in ATP synthase Fo rotors. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 763-772. | 0.5 | 58 |
| 41 | Lipid/Protein Interactions and the Membrane/Water Interfacial Region. Journal of the American Chemical Society, 2003, 125, 14966-14967. | 6.6 | 57 |
| 42 | Site-Specific Steric Control of SARS-CoV-2 Spike Glycosylation. Biochemistry, 2021, 60, 2153-2169. | 1.2 | 54 |
| 43 | OmpA: Gating and dynamics via molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1871-1880. | 1.4 | 53 |
| 44 | Hydrocarbons Are Essential for Optimal Cell Size, Division, and Growth of Cyanobacteria. Plant Physiology, 2016, 172, 1928-1940. | 2.3 | 53 |
| 45 | Systematic analysis of protein identity between Zika virus and other arthropod-borne viruses. Bulletin of the World Health Organization, 2017, 95, 517-525I. | 1.5 | 52 |
| 46 | Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. Scientific Reports, 2020, 10, 17501. | 1.6 | 52 |
| 47 | The Structural Basis for Endotoxin-induced Allosteric Regulation of the Toll-like Receptor 4 (TLR4) Innate Immune Receptor. Journal of Biological Chemistry, 2013, 288, 36215-36225. | 1.6 | 51 |
| 48 | Membrane Protein Simulations: Ion Channels And Bacterial Outer Membrane Proteins. Advances in Protein Chemistry, 2003, 66, 159-193. | 4.4 | 49 |
| 49 | Aggregation of thrombin-derived C-terminal fragments as a previously undisclosed host defense mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4213-E4222. | 3.3 | 49 |
| 50 | Understanding Dengue Virus Capsid Protein Disordered N-Terminus and pep14-23-Based Inhibition. ACS Chemical Biology, 2015, 10, 517-526. | 1.6 | 45 |
| 51 | Interaction of Monotopic Membrane Enzymes with a Lipid Bilayer: A Coarse-Grained MD Simulation Studyâ€. Biochemistry, 2009, 48, 2135-2145. | 1.2 | 44 |
| 52 | Somatic genetic rescue of a germline ribosome assembly defect. Nature Communications, 2021, 12, 5044. | 5.8 | 44 |
| 53 | Structural basis for endotoxin neutralisation and anti-inflammatory activity of thrombin-derived C-terminal peptides. Nature Communications, 2018, 9, 2762. | 5.8 | 43 |
| 54 | A-Ring Dihalogenation Increases the Cellular Activity of Combretastatin-Templated Tetrazoles. ACS Medicinal Chemistry Letters, 2012, 3, 177-181. | 1.3 | 42 |

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| 55 | Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. Structure, 2016, 24, 1410-1420. | 1.6 | 41 |
| 56 | Membrane protein dynamics and detergent interactions within a crystal: A simulation study of OmpA. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9518-9523. | 3.3 | 38 |
| 57 | The severity of hereditary porphyria is modulated by the porphyrin exporter and Lan antigen ABCB6. Nature Communications, 2016, 7, 12353. | 5.8 | 37 |
| 58 | Antimicrobial and Cell-Penetrating Peptides: Structure, Assembly and Mechanisms of Membrane Lysis via Atomistic and Coarse-Grained Molecular Dynamic Simulations. Protein and Peptide Letters, 2010, 17, 1313-1327. | 0.4 | 37 |
| 59 | Mechanism of Enhanced Immature Dengue Virus Attachment to Endosomal Membrane Induced by prM Antibody. Structure, 2019, 27, 253-267.e8. | 1.6 | 36 |
| 60 | Molecular Dynamics Simulations of GlpF in a Micelle vs in a Bilayer:Â Conformational Dynamics of a Membrane Protein as a Function of Environment. Journal of Physical Chemistry B, 2005, 109, 575-582. | 1.2 | 35 |
| 61 | Membrane Simulations of OpcA: Gating in the Loops?. Biophysical Journal, 2007, 92, L23-L25. | 0.2 | 34 |
| 62 | A Spring-Loaded Mechanism Governs the Clamp-like Dynamics of the Skp Chaperone. Structure, 2017, 25, 1079-1088.e3. | 1.6 | 34 |
| 63 | Progress in Molecular Dynamics Simulations of Gram-Negative Bacterial Cell Envelopes. Journal of Physical Chemistry Letters, 2017, 8, 2513-2518. | 2.1 | 33 |
| 64 | A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. Structure, 2018, 26, 1151-1161.e4. | 1.6 | 32 |
| 65 | A T164S mutation in the dengue virus NS1 protein is associated with greater disease severity in mice. Science Translational Medicine, 2019, 11, . | 5.8 | 32 |
| 66 | Full-length, Oligomeric Structure of Wzz Determined by Cryoelectron Microscopy Reveals Insights into Membrane-Bound States. Structure, 2017, 25, 806-815.e3. | 1.6 | 31 |
| 67 | Multiscale molecular dynamics simulation approaches to the structure and dynamics of viruses. Progress in Biophysics and Molecular Biology, 2017, 128, 121-132. | 1.4 | 31 |
| 68 | Coarseâ€Grain Simulations of the Râ€SNARE Fusion Protein in its Membrane Environment Detect Longâ€Lived Conformational Subâ€States. ChemPhysChem, 2009, 10, 1548-1552. | 1.0 | 30 |
| 69 | The disordered plant dehydrin Lti30 protects the membrane during water-related stress by cross-linking lipids. Journal of Biological Chemistry, 2019, 294, 6468-6482. | 1.6 | 30 |
| 70 | Extending the Martini Coarse-Grained Force Field to N-Glycans. Journal of Chemical Information and Modeling, 2020, 60, 3864-3883. | 2.5 | 30 |
| 71 | Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. PLoS ONE, 2016, 11, e0156963. | 1.1 | 28 |
| 72 | Modeling and simulations of a bacterial outer membrane protein: OprF from Pseudomonas aeruginosa. Proteins: Structure, Function and Bioinformatics, 2006, 63, 6-15. | 1.5 | 27 |

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| 73 | Molecular Dynamics Simulations of Membrane Proteins. Methods in Molecular Biology, 2008, 443, 147-160. | 0.4 | 26 |
| 74 | Molecular Dynamics Simulations of DNA within a Nanopore: Argincâ˜Phosphate Tethering and a Binding/Sliding Mechanism for Translocation. Biochemistry, 2011, 50, 3777-3783. | 1.2 | 26 |
| 75 | Selective inhibition of the unfolded protein response: targeting catalytic sites for Schiff base modification. Molecular BioSystems, 2013, 9, 2408. | 2.9 | 26 |
| 76 | Structural Basis of Pullulanase Membrane Binding and Secretion Revealed by X-Ray Crystallography, Molecular Dynamics and Biochemical Analysis. Structure, 2016, 24, 92-104. | 1.6 | 26 |
| 77 | Multiscale modelling and simulation of viruses. Current Opinion in Structural Biology, 2020, 61, 146-152. | 2.6 | 26 |
| 78 | Energetics of Endotoxin Recognition in the Toll-Like Receptor 4 Innate Immune Response. Scientific Reports, 2015, 5, 17997. | 1.6 | 25 |
| 79 | Influence of pH on the activity of thrombin-derived antimicrobial peptides. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2374-2384. | 1.4 | 25 |
| 80 | Molecular basis of dengue virus serotype 2 morphological switch from 29Â°C to 37Â°C. PLoS Pathogens, 2019, 15, e1007996. | 2.1 | 25 |
| 81 | The role of proteinâ€“protein interactions in Toll-like receptor function. Progress in Biophysics and Molecular Biology, 2015, 119, 72-83. | 1.4 | 24 |
| 82 | Thrombin-derived C-terminal fragments aggregate and scavenge bacteria and their proinflammatory products. Journal of Biological Chemistry, 2020, 295, 3417-3430. | 1.6 | 24 |
| 83 | Allosteric perspective on the mutability and druggability of the SARS-CoV-2 Spike protein. Structure, 2022, 30, 590-607.e4. | 1.6 | 24 |
| 84 | Impairing Cohesin Smc1/3 Head Engagement Compensates for the Lack of Eco1 Function. Structure, 2016, 24, 1991-1999. | 1.6 | 23 |
| 85 | Not all therapeutic antibody isotypes are equal: the case of IgM versus IgG in Pertuzumab and Trastuzumab. Chemical Science, 2020, 11, 2843-2854. | 3.7 | 23 |
| 86 | Infectivity of Dengue Virus Serotypes 1 and 2 Is Correlated with E-Protein Intrinsic Dynamics but Not to Envelope Conformations. Structure, 2019, 27, 618-630.e4. | 1.6 | 23 |
| 87 | Outer membrane proteins: comparing X-ray and NMR structures by MD simulations in lipid bilayers. European Biophysics Journal, 2008, 37, 131-141. | 1.2 | 22 |
| 88 | Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit Î´. Journal of Structural Biology, 2019, 207, 199-208. | 1.3 | 22 |
| 89 | Glycosylation and Serological Reactivity of an Expression-enhanced SARS-CoV-2 Viral Spike Mimetic. Journal of Molecular Biology, 2022, 434, 167332. | 2.0 | 22 |
| 90 | Uncovering cryptic pockets in the SARS-CoV-2 spike glycoprotein. Structure, 2022, 30, 1062-1074.e4. | 1.6 | 21 |

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| 91 | Free Energy Predictions of Ligand Binding to an Î±-Helix Using Steered Molecular Dynamics and Umbrella Sampling Simulations. Journal of Chemical Information and Modeling, 2014, 54, 2093-2104. | 2.5 | 19 |
| 92 | MD Simulations of Mistic:â€‰ Conformational Stability in Detergent Micelles and Water. Biochemistry, 2006, 45, 9053-9058. | 1.2 | 18 |
| 93 | Increased endothelial cell selectivity of triazole-bridged dihalogenated A-ring analogues of combretastatin Aâ€“1. Bioorganic and Medicinal Chemistry, 2012, 20, 1749-1759. | 1.4 | 18 |
| 94 | Polar N-terminal Residues Conserved in Type 2 Secretion Pseudopilins Determine Subunit Targeting and Membrane Extraction Steps during Fibre Assembly. Journal of Molecular Biology, 2017, 429, 1746-1765. | 2.0 | 18 |
| 95 | Partial Intrinsic Disorder Governs the Dengue Capsid Protein Conformational Ensemble. ACS Chemical Biology, 2018, 13, 1621-1630. | 1.6 | 18 |
| 96 | Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. Scientific Reports, 2016, 6, 19160. | 1.6 | 17 |
| 97 | Molecular Mechanism of Selective Recruitment of Syk Kinases by the Membrane Antigen-Receptor Complex. Journal of Biological Chemistry, 2011, 286, 25872-25881. | 1.6 | 16 |
| 98 | Multiscale Molecular Dynamics Simulations of Membrane Proteins. Methods in Molecular Biology, 2013, 924, 635-657. | 0.4 | 16 |
| 99 | Dynamics of the Antigen-binding Grooves in CD1 Proteins. Journal of Biological Chemistry, 2013, 288, 19528-19536. | 1.6 | 16 |
| 100 | Energetics and Dynamics Across the Bcl-2-Regulated Apoptotic Pathway Reveal Distinct Evolutionary Determinants of Specificity and Affinity. Structure, 2016, 24, 2024-2033. | 1.6 | 16 |
| 101 | On the ion coupling mechanism of the MATE transporter ClbM. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183137. | 1.4 | 16 |
| 102 | Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. Diagnostics, 2020, 10, 11. | 1.3 | 16 |
| 103 | Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. Pharmacological Research, 2019, 147, 104372. | 3.1 | 15 |
| 104 | Molecular Dynamics Simulations of Membrane Proteins. Methods in Molecular Biology, 2015, 1215, 91-108. | 0.4 | 13 |
| 105 | Revisiting the Interaction between the Chaperone Skp and Lipopolysaccharide. Biophysical Journal, 2015, 108, 1516-1526. | 0.2 | 12 |
| 106 | A polar SxxS motif drives assembly of the transmembrane domains of Toll-like receptor 4. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2086-2095. | 1.4 | 12 |
| 107 | The Structural Basis for Activation and Inhibition of ZAP-70 Kinase Domain. PLoS Computational Biology, 2015, 11, e1004560. | 1.5 | 12 |
| 108 | Predicted structural basis for CD1c presentation of mycobacterial branched polyketides and long lipopeptide antigens. Molecular Immunology, 2009, 47, 253-260. | 1.0 | 11 |

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| 109 | The Structural Basis for Lipid and Endotoxin Binding in RP105-MD-1, and Consequences for Regulation of Host Lipopolysaccharide Sensitivity. Structure, 2016, 24, 200-211. | 1.6 | 11 |
| 110 | Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices. Structure, 2019, 27, 302-314.e4. | 1.6 | 11 |
| 111 | Facile saccharide-free mimetics that recapitulate key features of glycosaminoglycan sulfation patterns. Chemical Science, 2018, 9, 7940-7947. | 3.7 | 10 |
| 112 | Insights into water accessible pathways and the inactivation mechanism of proton translocation by the membrane-embedded domain of V-type ATPases. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1004-1010. | 1.4 | 10 |
| 113 | Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling?. Journal of Chemical Physics, 2020, 153, 044122. | 1.2 | 10 |
| 114 | What have molecular simulations contributed to understanding of Gram-negative bacterial cell envelopes?. Microbiology (United Kingdom), 2022, 168, . | 0.7 | 10 |
| 115 | Molecular and thermodynamic basis for EGCGâ€Keratin interactionâ€part II: Experimental investigation. AICHE Journal, 2013, 59, 4824-4827. | 1.8 | 9 |
| 116 | Molecular and thermodynamic basis for EGCGâ€Keratin interactionâ€part I: Molecular dynamics simulations. AICHE Journal, 2013, 59, 4816-4823. | 1.8 | 9 |
| 117 | A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. Journal of Chemical Theory and Computation, 2018, 14, 3920-3932. | 2.3 | 9 |
| 118 | Single-molecule studies of flavivirus envelope dynamics: Experiment and computation. Progress in Biophysics and Molecular Biology, 2019, 143, 38-51. | 1.4 | 9 |
| 119 | Concentration- and pH-Dependent Oligomerization of the Thrombin-Derived C-Terminal Peptide TCP-25. Biomolecules, 2020, 10, 1572. | 1.8 | 9 |
| 120 | Computational modelling of flavivirus dynamics: The ins and outs. Methods, 2021, 185, 28-38. | 1.9 | 9 |
| 121 | A Study on Fe2+Ââ€“ Î±-Helical-Rich Keratin Complex Formation Using Isothermal Titration Calorimetry and Molecular Dynamics Simulation. Journal of Pharmaceutical Sciences, 2014, 103, 1224-1232. | 1.6 | 8 |
| 122 | Linker length affects photostability of protein-targeted sensor of cellular microviscosity. Methods and Applications in Fluorescence, 2019, 7, 044004. | 1.1 | 8 |
| 123 | Antibody affinity versus dengue morphology influences neutralization. PLoS Pathogens, 2021, 17, e1009331. | 2.1 | 8 |
| 124 | Antibacterial and Anti-Inflammatory Effects of Apolipoprotein E. Biomedicines, 2022, 10, 1430. | 1.4 | 8 |
| 125 | Protein-protein interactions in paralogues: Electrostatics modulates specificity on a conserved steric scaffold. PLoS ONE, 2017, 12, e0185928. | 1.1 | 7 |
| 126 | Multiscale Modeling and Simulation Approaches to Lipidâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2003, 1-30. | 0.4 | 7 |

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| 127 | The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. Computational and Structural Biotechnology Journal, 2021, 19, 330-342. | 1.9 | 7 |
| 128 | Exploring the conformational dynamics and membrane interactions of PorB from C. glutamicum: A multi-scale molecular dynamics simulation study. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1746-1752. | 1.4 | 6 |
| 129 | A Benzene-Mapping Approach for Uncovering Cryptic Pockets in Membrane-Bound Proteins. Journal of Chemical Theory and Computation, 2020, 16, 5948-5959. | 2.3 | 6 |
| 130 | Manipulating turn residues on de novo designed Î²-hairpin peptides for selectivity against drug-resistant bacteria. Acta Biomaterialia, 2021, 135, 214-224. | 4.1 | 6 |
| 131 | Selective inhibitors of trypanosomal uridylyl transferase RET1 establish druggability of RNA post-transcriptional modifications. RNA Biology, 2017, 14, 611-619. | 1.5 | 5 |
| 132 | Characterizing the Hydration Properties of Proton Binding Sites in the ATP Synthase c-Rings of Bacillus Species. Journal of Physical Chemistry B, 2020, 124, 7176-7183. | 1.2 | 5 |
| 133 | An Alternative HIV-1 Non-Nucleoside Reverse Transcriptase Inhibition Mechanism: Targeting the p51 Subunit. Molecules, 2020, 25, 5902. | 1.7 | 5 |
| 134 | The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase Ïµ Subunit. ChemBioChem, 2020, 21, 3249-3254. | 1.3 | 5 |
| 135 | The Simulation Approach to Lipidâ€“Protein Interactions. Methods in Molecular Biology, 2013, 974, 435-455. | 0.4 | 4 |
| 136 | Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway. Journal of Chemical Information and Modeling, 2019, 59, 245-261. | 2.5 | 4 |
| 137 | A second shell residue modulates a conserved ATP-binding site with radically different affinities for ATP. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129766. | 1.1 | 4 |
| 138 | Motional clustering in supra-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si29.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ï„</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="normal">c</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> conformational exchange influences NOE cross-relaxation rate. Journal of Magnetic Resonance, 2022, 338, 107196. | 1.2 | 4 |
| 139 | Bioinformatics and systems biology research update from the 15th International Conference on Bioinformatics (InCoB2016). BMC Bioinformatics, 2016, 17, 524. | 1.2 | 3 |
| 140 | The structural basis for membrane assembly of immunoreceptor signalling complexes. Journal of Molecular Modeling, 2019, 25, 277. | 0.8 | 3 |
| 141 | How Ligand Binding Affects the Dynamical Transition Temperature in Proteins. ChemPhysChem, 2020, 21, 916-926. | 1.0 | 3 |
| 142 | The nanotube express: Delivering a stapled peptide to the cell surface. Journal of Colloid and Interface Science, 2021, 604, 670-679. | 5.0 | 3 |
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| 144 | Bridging the N-terminal and middle domains in FliG of the flagellar rotor. Current Research in Structural Biology, 2022, 4, 59-67. | 1.1 | 2 |

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| 145 | 3D reconstruction and flexibility of the hybrid engine Acetobacterium woodii F-ATP synthase. Biochemical and Biophysical Research Communications, 2020, 527, 518-524. | 1.0 | 1 |
| 146 | Editorial. Progress in Biophysics and Molecular Biology, 2017, 128, 1-2. | 1.4 | 0 |
| 147 | Directing GDNF-mediated neuronal signaling with proactively programmable cell-surface saccharide-free glycosaminoglycan mimetics. Chemical Communications, 2019, 55, 1259-1262. | 2.2 | 0 |
| 148 | Ab Initio Folding of Glycophorin A and Acetylcholine M2 Transmembrane Segments Via Simplified Environment Molecular Simulations. , 2015, , 115-139. | | 0 |
| 149 | Infectivity of Dengue Virus Serotypes 1 and 2 is Correlated to E Protein Intrinsic Dynamics But Not to Envelope Conformations. SSRN Electronic Journal, 0, , . | 0.4 | 0 |
| 150 | Membrane Protein Simulations: Modelling a Complex Environment. , 2006, , 3-20. | | 0 |