

Peter J Bond

List of Publications by Year in descending order

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150
papers

7,325
citations

61687

45
h-index

75989

78
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169
all docs

169
docs citations

169
times ranked

10968
citing authors

#	ARTICLE	IF	CITATIONS
1	Glycosylation and Serological Reactivity of an Expression-enhanced SARS-CoV-2 Viral Spike Mimetic. <i>Journal of Molecular Biology</i> , 2022, 434, 167332.	2.0	22
2	Allosteric perspective on the mutability and druggability of the SARS-CoV-2 Spike protein. <i>Structure</i> , 2022, 30, 590-607.e4.	1.6	24
3	Bridging the N-terminal and middle domains in FlIG of the flagellar rotor. <i>Current Research in Structural Biology</i> , 2022, 4, 59-67.	1.1	2
4	What have molecular simulations contributed to understanding of Gram-negative bacterial cell envelopes?. <i>Microbiology (United Kingdom)</i> , 2022, 168, .	0.7	10
5	Motional clustering in supra- β -sheet structures influences NOE cross-relaxation rate. <i>Journal of Magnetic Resonance</i> , 2022, 338, 107196.	1.2	4
6	Uncovering cryptic pockets in the SARS-CoV-2 spike glycoprotein. <i>Structure</i> , 2022, 30, 1062-1074.e4.	1.6	21
7	Antibacterial and Anti-Inflammatory Effects of Apolipoprotein E. <i>Biomedicines</i> , 2022, 10, 1430.	1.4	8
8	Computational modelling of flavivirus dynamics: The ins and outs. <i>Methods</i> , 2021, 185, 28-38.	1.9	9
9	SARS-CoV-2 spike protein binds to bacterial lipopolysaccharide and boosts proinflammatory activity. <i>Journal of Molecular Cell Biology</i> , 2021, 12, 916-932.	1.5	121
10	A second shell residue modulates a conserved ATP-binding site with radically different affinities for ATP. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021, 1865, 129766.	1.1	4
11	The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 330-342.	1.9	7
12	Antibody affinity versus dengue morphology influences neutralization. <i>PLoS Pathogens</i> , 2021, 17, e1009331.	2.1	8
13	SARS-CoV-2 S protein:ACE2 interaction reveals novel allosteric targets. <i>ELife</i> , 2021, 10, .	2.8	100
14	The antibiotic darobactin mimics a β -strand to inhibit outer membrane insertase. <i>Nature</i> , 2021, 593, 125-129.	13.7	112
15	Site-Specific Steric Control of SARS-CoV-2 Spike Glycosylation. <i>Biochemistry</i> , 2021, 60, 2153-2169.	1.2	54
16	Somatic genetic rescue of a germline ribosome assembly defect. <i>Nature Communications</i> , 2021, 12, 5044.	5.8	44
17	Manipulating turn residues on de novo designed β -hairpin peptides for selectivity against drug-resistant bacteria. <i>Acta Biomaterialia</i> , 2021, 135, 214-224.	4.1	6
18	The nanotube express: Delivering a stapled peptide to the cell surface. <i>Journal of Colloid and Interface Science</i> , 2021, 604, 670-679.	5.0	3

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19	On the ion coupling mechanism of the MATE transporter ClbM. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183137.	1.4	16
20	Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. <i>Diagnostics</i> , 2020, 10, 11.	1.3	16
21	Extending the Martini Coarse-Grained Force Field to <i>N</i> -Glycans. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3864-3883.	2.5	30
22	Concentration- and pH-Dependent Oligomerization of the Thrombin-Derived C-Terminal Peptide TCP-25. <i>Biomolecules</i> , 2020, 10, 1572.	1.8	9
23	Characterizing the Hydration Properties of Proton Binding Sites in the ATP Synthase c-Rings of <i>Bacillus</i> Species. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7176-7183.	1.2	5
24	Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling?. <i>Journal of Chemical Physics</i> , 2020, 153, 044122.	1.2	10
25	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. <i>Scientific Reports</i> , 2020, 10, 17501.	1.6	52
26	A Benzene-Mapping Approach for Uncovering Cryptic Pockets in Membrane-Bound Proteins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5948-5959.	2.3	6
27	An Alternative HIV-1 Non-Nucleoside Reverse Transcriptase Inhibition Mechanism: Targeting the p51 Subunit. <i>Molecules</i> , 2020, 25, 5902.	1.7	5
28	3D reconstruction and flexibility of the hybrid engine <i>Acetobacterium woodii</i> F-ATP synthase. <i>Biochemical and Biophysical Research Communications</i> , 2020, 527, 518-524.	1.0	1
29	How Ligand Binding Affects the Dynamical Transition Temperature in Proteins. <i>ChemPhysChem</i> , 2020, 21, 916-926.	1.0	3
30	The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase μ Subunit. <i>ChemBioChem</i> , 2020, 21, 3249-3254.	1.3	5
31	Thrombin-derived C-terminal fragments aggregate and scavenge bacteria and their proinflammatory products. <i>Journal of Biological Chemistry</i> , 2020, 295, 3417-3430.	1.6	24
32	Not all therapeutic antibody isotypes are equal: the case of IgM versus IgG in Pertuzumab and Trastuzumab. <i>Chemical Science</i> , 2020, 11, 2843-2854.	3.7	23
33	Multiscale modelling and simulation of viruses. <i>Current Opinion in Structural Biology</i> , 2020, 61, 146-152.	2.6	26
34	Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. <i>Pharmacological Research</i> , 2019, 147, 104372.	3.1	15
35	A T164S mutation in the dengue virus NS1 protein is associated with greater disease severity in mice. <i>Science Translational Medicine</i> , 2019, 11, .	5.8	32
36	Linker length affects photostability of protein-targeted sensor of cellular microviscosity. <i>Methods and Applications in Fluorescence</i> , 2019, 7, 044004.	1.1	8

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37	The structural basis for membrane assembly of immunoreceptor signalling complexes. <i>Journal of Molecular Modeling</i> , 2019, 25, 277.	0.8	3
38	Molecular basis of dengue virus serotype 2 morphological switch from 29Å°C to 37Å°C. <i>PLoS Pathogens</i> , 2019, 15, e1007996.	2.1	25
39	Directing GDNF-mediated neuronal signaling with proactively programmable cell-surface saccharide-free glycosaminoglycan mimetics. <i>Chemical Communications</i> , 2019, 55, 1259-1262.	2.2	0
40	Multiscale Modeling and Simulation Approaches to Lipid-Protein Interactions. <i>Methods in Molecular Biology</i> , 2019, 2003, 1-30.	0.4	7
41	Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit f ₁ . <i>Journal of Structural Biology</i> , 2019, 207, 199-208.	1.3	22
42	The disordered plant dehydrin Lti30 protects the membrane during water-related stress by cross-linking lipids. <i>Journal of Biological Chemistry</i> , 2019, 294, 6468-6482.	1.6	30
43	Insights into water accessible pathways and the inactivation mechanism of proton translocation by the membrane-embedded domain of V-type ATPases. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 1004-1010.	1.4	10
44	Structure mapping of dengue and Zika viruses reveals functional long-range interactions. <i>Nature Communications</i> , 2019, 10, 1408.	5.8	104
45	Single-molecule studies of flavivirus envelope dynamics: Experiment and computation. <i>Progress in Biophysics and Molecular Biology</i> , 2019, 143, 38-51.	1.4	9
46	Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 245-261.	2.5	4
47	Mechanism of Enhanced Immature Dengue Virus Attachment to Endosomal Membrane Induced by prM Antibody. <i>Structure</i> , 2019, 27, 253-267.e8.	1.6	36
48	Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices. <i>Structure</i> , 2019, 27, 302-314.e4.	1.6	11
49	Infectivity of Dengue Virus Serotypes 1 and 2 Is Correlated with E-Protein Intrinsic Dynamics but Not to Envelope Conformations. <i>Structure</i> , 2019, 27, 618-630.e4.	1.6	23
50	Evidence that TLR4 Is Not a Receptor for Saturated Fatty Acids but Mediates Lipid-Induced Inflammation by Reprogramming Macrophage Metabolism. <i>Cell Metabolism</i> , 2018, 27, 1096-1110.e5.	7.2	309
51	An Optical Technique for Mapping Microviscosity Dynamics in Cellular Organelles. <i>ACS Nano</i> , 2018, 12, 4398-4407.	7.3	125
52	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. <i>Structure</i> , 2018, 26, 1151-1161.e4.	1.6	32
53	The architecture of the OmpC-MlaA complex sheds light on the maintenance of outer membrane lipid asymmetry in <i>Escherichia coli</i> . <i>Journal of Biological Chemistry</i> , 2018, 293, 11325-11340.	1.6	64
54	Partial Intrinsic Disorder Governs the Dengue Capsid Protein Conformational Ensemble. <i>ACS Chemical Biology</i> , 2018, 13, 1621-1630.	1.6	18

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55	Activation of Toll-like receptors nucleates assembly of the MyDDosome signaling hub. <i>ELife</i> , 2018, 7, .	2.8	83
56	Structural basis for endotoxin neutralisation and anti-inflammatory activity of thrombin-derived C-terminal peptides. <i>Nature Communications</i> , 2018, 9, 2762.	5.8	43
57	Facile saccharide-free mimetics that recapitulate key features of glycosaminoglycan sulfation patterns. <i>Chemical Science</i> , 2018, 9, 7940-7947.	3.7	10
58	A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3920-3932.	2.3	9
59	Influence of pH on the activity of thrombin-derived antimicrobial peptides. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2374-2384.	1.4	25
60	Single mutations in the $\hat{\mu}$ subunit from thermophilic <i>Bacillus</i> PS3 generate a high binding affinity site for ATP. <i>PeerJ</i> , 2018, 6, e5505.	0.9	3
61	Selective inhibitors of trypanosomal uridylyl transferase RET1 establish druggability of RNA post-transcriptional modifications. <i>RNA Biology</i> , 2017, 14, 611-619.	1.5	5
62	Full-length, Oligomeric Structure of Wzz Determined by Cryoelectron Microscopy Reveals Insights into Membrane-Bound States. <i>Structure</i> , 2017, 25, 806-815.e3.	1.6	31
63	Aggregation of thrombin-derived C-terminal fragments as a previously undisclosed host defense mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E4213-E4222.	3.3	49
64	Progress in Molecular Dynamics Simulations of Gram-Negative Bacterial Cell Envelopes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2513-2518.	2.1	33
65	A Spring-Loaded Mechanism Governs the Clamp-like Dynamics of the Skp Chaperone. <i>Structure</i> , 2017, 25, 1079-1088.e3.	1.6	34
66	Polar N-terminal Residues Conserved in Type 2 Secretion Pseudopilins Determine Subunit Targeting and Membrane Extraction Steps during Fibre Assembly. <i>Journal of Molecular Biology</i> , 2017, 429, 1746-1765.	2.0	18
67	A polar SxxS motif drives assembly of the transmembrane domains of Toll-like receptor 4. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2086-2095.	1.4	12
68	Editorial. <i>Progress in Biophysics and Molecular Biology</i> , 2017, 128, 1-2.	1.4	0
69	Multiscale molecular dynamics simulation approaches to the structure and dynamics of viruses. <i>Progress in Biophysics and Molecular Biology</i> , 2017, 128, 121-132.	1.4	31
70	Systematic analysis of protein identity between Zika virus and other arthropod-borne viruses. <i>Bulletin of the World Health Organization</i> , 2017, 95, 517-525l.	1.5	52
71	Protein-protein interactions in paralogues: Electrostatics modulates specificity on a conserved steric scaffold. <i>PLoS ONE</i> , 2017, 12, e0185928.	1.1	7
72	Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. <i>PLoS ONE</i> , 2016, 11, e0156963.	1.1	28

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73	Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. <i>Structure</i> , 2016, 24, 1410-1420.	1.6	41
74	Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. <i>Scientific Reports</i> , 2016, 6, 19160.	1.6	17
75	Impairing Cohesin Smc1/3 Head Engagement Compensates for the Lack of Eco1 Function. <i>Structure</i> , 2016, 24, 1991-1999.	1.6	23
76	Hydrocarbons Are Essential for Optimal Cell Size, Division, and Growth of Cyanobacteria. <i>Plant Physiology</i> , 2016, 172, 1928-1940.	2.3	53
77	OmpA: A Flexible Clamp for Bacterial Cell Wall Attachment. <i>Structure</i> , 2016, 24, 2227-2235.	1.6	76
78	Full-Length OmpA: Structure, Function, and Membrane Interactions Predicted by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2016, 111, 1692-1702.	0.2	67
79	The severity of hereditary porphyria is modulated by the porphyrin exporter and Lan antigen ABCB6. <i>Nature Communications</i> , 2016, 7, 12353.	5.8	37
80	Energetics and Dynamics Across the Bcl-2-Regulated Apoptotic Pathway Reveal Distinct Evolutionary Determinants of Specificity and Affinity. <i>Structure</i> , 2016, 24, 2024-2033.	1.6	16
81	Bioinformatics and systems biology research update from the 15th International Conference on Bioinformatics (InCoB2016). <i>BMC Bioinformatics</i> , 2016, 17, 524.	1.2	3
82	Structural Basis of Pullulanase Membrane Binding and Secretion Revealed by X-Ray Crystallography, Molecular Dynamics and Biochemical Analysis. <i>Structure</i> , 2016, 24, 92-104.	1.6	26
83	The Structural Basis for Lipid and Endotoxin Binding in RP105-MD-1, and Consequences for Regulation of Host Lipopolysaccharide Sensitivity. <i>Structure</i> , 2016, 24, 200-211.	1.6	11
84	Energetics of Endotoxin Recognition in the Toll-Like Receptor 4 Innate Immune Response. <i>Scientific Reports</i> , 2015, 5, 17997.	1.6	25
85	Interaction of the Antimicrobial Peptide Polymyxin B1 with Both Membranes of <i>E. coli</i> : A Molecular Dynamics Study. <i>PLoS Computational Biology</i> , 2015, 11, e1004180.	1.5	134
86	The role of protein-protein interactions in Toll-like receptor function. <i>Progress in Biophysics and Molecular Biology</i> , 2015, 119, 72-83.	1.4	24
87	Membrane Recognition and Dynamics of the RNA Degradosome. <i>PLoS Genetics</i> , 2015, 11, e1004961.	1.5	93
88	Revisiting the Interaction between the Chaperone Skp and Lipopolysaccharide. <i>Biophysical Journal</i> , 2015, 108, 1516-1526.	0.2	12
89	Understanding Dengue Virus Capsid Protein Disordered N-Terminus and pep14-23-Based Inhibition. <i>ACS Chemical Biology</i> , 2015, 10, 517-526.	1.6	45
90	Molecular Dynamics Simulations of Membrane Proteins. <i>Methods in Molecular Biology</i> , 2015, 1215, 91-108.	0.4	13

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91	The Structural Basis for Activation and Inhibition of ZAP-70 Kinase Domain. <i>PLoS Computational Biology</i> , 2015, 11, e1004560.	1.5	12
92	Ab Initio Folding of Glycophorin A and Acetylcholine M2 Transmembrane Segments Via Simplified Environment Molecular Simulations. , 2015, , 115-139.		0
93	A Study on Fe ²⁺ α -Helical-Rich Keratin Complex Formation Using Isothermal Titration Calorimetry and Molecular Dynamics Simulation. <i>Journal of Pharmaceutical Sciences</i> , 2014, 103, 1224-1232.	1.6	8
94	Free Energy Predictions of Ligand Binding to an α -Helix Using Steered Molecular Dynamics and Umbrella Sampling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2093-2104.	2.5	19
95	Efficient Characterization of Protein Cavities within Molecular Simulation Trajectories: <i>trj_cavity</i> . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2151-2164.	2.3	129
96	Molecular and thermodynamic basis for EGCG-Keratin interaction—part II: Experimental investigation. <i>AIChE Journal</i> , 2013, 59, 4824-4827.	1.8	9
97	Molecular and thermodynamic basis for EGCG-Keratin interaction—part I: Molecular dynamics simulations. <i>AIChE Journal</i> , 2013, 59, 4816-4823.	1.8	9
98	Selective inhibition of the unfolded protein response: targeting catalytic sites for Schiff base modification. <i>Molecular BioSystems</i> , 2013, 9, 2408.	2.9	26
99	Multiscale Molecular Dynamics Simulations of Membrane Proteins. <i>Methods in Molecular Biology</i> , 2013, 924, 635-657.	0.4	16
100	Design, Synthesis, and Biological Evaluation of an Allosteric Inhibitor of HSET that Targets Cancer Cells with Supernumerary Centrosomes. <i>Chemistry and Biology</i> , 2013, 20, 1399-1410.	6.2	94
101	The Structural Basis for Endotoxin-induced Allosteric Regulation of the Toll-like Receptor 4 (TLR4) Innate Immune Receptor. <i>Journal of Biological Chemistry</i> , 2013, 288, 36215-36225.	1.6	51
102	The Simulation Approach to Lipid-Protein Interactions. <i>Methods in Molecular Biology</i> , 2013, 974, 435-455.	0.4	4
103	Dynamics of the Antigen-binding Grooves in CD1 Proteins. <i>Journal of Biological Chemistry</i> , 2013, 288, 19528-19536.	1.6	16
104	Minor pseudopilin self-assembly primes type II secretion pseudopilus elongation. <i>EMBO Journal</i> , 2012, 31, 1041-1053.	3.5	94
105	The molecular basis for selective inhibition of unconventional mRNA splicing by an IRE1-binding small molecule. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, E869-78.	3.3	476
106	A-Ring Dihalogenation Increases the Cellular Activity of Combretastatin-Templated Tetrazoles. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 177-181.	1.3	42
107	Computational Prediction of Metabolism: Sites, Products, SAR, P450 Enzyme Dynamics, and Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 617-648.	2.5	246
108	Increased endothelial cell selectivity of triazole-bridged dihalogenated A-ring analogues of combretastatin 1. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 1749-1759.	1.4	18

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109	Molecular Dynamics Simulations of DNA within a Nanopore: Arginine ⁺ Phosphate Tethering and a Binding/Sliding Mechanism for Translocation. <i>Biochemistry</i> , 2011, 50, 3777-3783.	1.2	26
110	Exploring the conformational dynamics and membrane interactions of PorB from <i>C. glutamicum</i> : A multi-scale molecular dynamics simulation study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1746-1752.	1.4	6
111	From in silico target prediction to multi-target drug design: Current databases, methods and applications. <i>Journal of Proteomics</i> , 2011, 74, 2554-2574.	1.2	243
112	Molecular Mechanism of Selective Recruitment of Syk Kinases by the Membrane Antigen-Receptor Complex. <i>Journal of Biological Chemistry</i> , 2011, 286, 25872-25881.	1.6	16
113	Structural and energetic basis for H ⁺ versus Na ⁺ binding selectivity in ATP synthase Fo rotors. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2010, 1797, 763-772.	0.5	58
114	Antimicrobial and Cell-Penetrating Peptides: Structure, Assembly and Mechanisms of Membrane Lysis via Atomistic and Coarse-Grained Molecular Dynamic Simulations. <i>Protein and Peptide Letters</i> , 2010, 17, 1313-1327.	0.4	37
115	Coarse-Grain Simulations of the α -SNARE Fusion Protein in its Membrane Environment Detect Long-Lived Conformational Substates. <i>ChemPhysChem</i> , 2009, 10, 1548-1552.	1.0	30
116	Complete Ion-Coordination Structure in the Rotor Ring of Na ⁺ -Dependent F-ATP Synthases. <i>Journal of Molecular Biology</i> , 2009, 391, 498-507.	2.0	98
117	Predicted structural basis for CD1c presentation of mycobacterial branched polyketides and long lipopeptide antigens. <i>Molecular Immunology</i> , 2009, 47, 253-260.	1.0	11
118	Interaction of Monotopic Membrane Enzymes with a Lipid Bilayer: A Coarse-Grained MD Simulation Study. <i>Biochemistry</i> , 2009, 48, 2135-2145.	1.2	44
119	Outer membrane proteins: comparing X-ray and NMR structures by MD simulations in lipid bilayers. <i>European Biophysics Journal</i> , 2008, 37, 131-141.	1.2	22
120	DNA and lipid bilayers: self-assembly and insertion. <i>Journal of the Royal Society Interface</i> , 2008, 5, 241-250.	1.5	64
121	Coarse-Grained MD Simulations of Membrane Protein-Bilayer Self-Assembly. <i>Structure</i> , 2008, 16, 621-630.	1.6	199
122	Molecular Dynamics Simulations of Membrane Proteins. <i>Methods in Molecular Biology</i> , 2008, 443, 147-160.	0.4	26
123	Coarse-Grained Molecular Dynamics Simulations of the Energetics of Helix Insertion into a Lipid Bilayer. <i>Biochemistry</i> , 2008, 47, 11321-11331.	1.2	87
124	Coarse-Grained Simulations of the Membrane-Active Antimicrobial Peptide Maculatin 1.1. <i>Biophysical Journal</i> , 2008, 95, 3802-3815.	0.2	68
125	Self-Assembly of a Simple Membrane Protein: Coarse-Grained Molecular Dynamics Simulations of the Influenza M2 Channel. <i>Biophysical Journal</i> , 2008, 95, 3790-3801.	0.2	69
126	OmpA: Gating and dynamics via molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008, 1778, 1871-1880.	1.4	53

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127	Helix-Helix Interactions in Membrane Proteins: Coarse-Grained Simulations of Glycophorin A Helix Dimerization. <i>Biochemistry</i> , 2008, 47, 10503-10512.	1.2	82
128	Coarse-grained simulation: a high-throughput computational approach to membrane proteins. <i>Biochemical Society Transactions</i> , 2008, 36, 27-32.	1.6	117
129	Bilayer deformation by the Kv channel voltage sensor domain revealed by self-assembly simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 2631-2636.	3.3	100
130	Coarse-grained molecular dynamics simulations of membrane proteins and peptides. <i>Journal of Structural Biology</i> , 2007, 157, 593-605.	1.3	303
131	Membrane Simulations of OpcA: Gating in the Loops?. <i>Biophysical Journal</i> , 2007, 92, L23-L25.	0.2	34
132	MD Simulations of Mistic: Conformational Stability in Detergent Micelles and Water. <i>Biochemistry</i> , 2006, 45, 9053-9058.	1.2	18
133	Anionic Phospholipid Interactions with the Potassium Channel KcsA: Simulation Studies. <i>Biophysical Journal</i> , 2006, 90, 822-830.	0.2	77
134	Transmembrane Helix-Helix Interactions: Comparative Simulations of the Glycophorin A Dimer. <i>Biochemistry</i> , 2006, 45, 14298-14310.	1.2	65
135	Modeling and simulations of a bacterial outer membrane protein: OprF from <i>Pseudomonas aeruginosa</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 6-15.	1.5	27
136	Insertion and Assembly of Membrane Proteins via Simulation. <i>Journal of the American Chemical Society</i> , 2006, 128, 2697-2704.	6.6	314
137	Membrane protein dynamics and detergent interactions within a crystal: A simulation study of OmpA. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 9518-9523.	3.3	38
138	Cysteine-scanning Mutagenesis and Disulfide Mapping Studies of the Conserved Domain of the Twin-arginine Translocase TatB Component*. <i>Journal of Biological Chemistry</i> , 2006, 281, 34072-34085.	1.6	60
139	Membrane Protein Simulations: Modelling a Complex Environment. , 2006, , 3-20.		0
140	Membrane protein structure quality in molecular dynamics simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 24, 157-165.	1.3	58
141	Molecular Dynamics Simulations of GlpF in a Micelle vs in a Bilayer: Conformational Dynamics of a Membrane Protein as a Function of Environment. <i>Journal of Physical Chemistry B</i> , 2005, 109, 575-582.	1.2	35
142	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 783-791.	1.5	92
143	Lipid-Protein Interactions of Integral Membrane Proteins: A Comparative Simulation Study. <i>Biophysical Journal</i> , 2004, 87, 3737-3749.	0.2	104
144	MD Simulations of Spontaneous Membrane Protein/Detergent Micelle Formation. <i>Journal of the American Chemical Society</i> , 2004, 126, 15948-15949.	6.6	85

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145	The simulation approach to bacterial outer membrane proteins (Review). <i>Molecular Membrane Biology</i> , 2004, 21, 151-161.	2.0	61
146	Lipid/Protein Interactions and the Membrane/Water Interfacial Region. <i>Journal of the American Chemical Society</i> , 2003, 125, 14966-14967.	6.6	57
147	Membrane Protein Dynamics versus Environment: Simulations of OmpA in a Micelle and in a Bilayer. <i>Journal of Molecular Biology</i> , 2003, 329, 1035-1053.	2.0	130
148	Membrane Protein Simulations: Ion Channels And Bacterial Outer Membrane Proteins. <i>Advances in Protein Chemistry</i> , 2003, 66, 159-193.	4.4	49
149	OmpA: A Pore or Not a Pore? Simulation and Modeling Studies. <i>Biophysical Journal</i> , 2002, 83, 763-775.	0.2	92
150	Infectivity of Dengue Virus Serotypes 1 and 2 is Correlated to E Protein Intrinsic Dynamics But Not to Envelope Conformations. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0