Marc Baaden

List of Publications by Year
in descending order

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127 papers	5,139 citations	87888 38 h-index	98798 67 g-index
137 all docs	137 docs citations	137 times ranked	5362 citing authors

#	Article	IF	Citations
1	X-ray structure of a pentameric ligand-gated ion channel in an apparently open conformation. Nature, 2009, 457, 111-114.	27.8	644
2	X-ray structures of general anaesthetics bound to a pentameric ligand-gated ion channel. Nature, 2011, 469, 428-431.	27.8	407
3	Game On, Science - How Video Game Technology May Help Biologists Tackle Visualization Challenges. PLoS ONE, 2013, 8, e57990.	2.5	242
4	One-microsecond molecular dynamics simulation of channel gating in a nicotinic receptor homologue. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 6275-6280.	7.1	159
5	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. Chemical Society Reviews, 2014, 43, 4871-4893.	38.1	147
6	Structural basis for ion permeation mechanism in pentameric ligand-gated ion channels. EMBO Journal, 2013, 32, 728-741.	7.8	140
7	A locally closed conformation of a bacterial pentameric proton-gated ion channel. Nature Structural and Molecular Biology, 2012, 19, 642-649.	8.2	135
8	Coarse-grain modelling of proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 878-886.	5.7	124
9	TBP at the Waterâ"Oil Interface:â€‰ The Effect of TBP Concentration and Water Acidity Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2001, 105, 11131-11141.	2.6	122
10	Salt-Excluding Artificial Water Channels Exhibiting Enhanced Dipolar Water and Proton Translocation. Journal of the American Chemical Society, 2016, 138, 5403-5409.	13.7	111
11	Atomic structure and dynamics of pentameric ligand-gated ion channels: new insight from bacterial homologues. Journal of Physiology, 2010, 588, 565-572.	2.9	102
12	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 783-791.	2.6	92
13	Nothing to Sneeze At: A Dynamic and Integrative Computational Model of an Influenza A Virion. Structure, 2015, 23, 584-597.	3.3	90
14	Epock: rapid analysis of protein pocket dynamics. Bioinformatics, 2015, 31, 1478-1480.	4.1	81
15	Molecular Dynamics Study of the Uranyl Extraction by Tri-n-butylphosphate (TBP):Â Demixing of Water/â€œOilâ€TBP Solutions with a Comparison of Supercritical CO2and Chloroform. Journal of Physical Chemistry B, 2002, 106, 434-441.	2.6	80
16	Controlling Redox Enzyme Orientation at Planar Electrodes. Catalysts, 2018, 8, 192.	3.5	78
17	Photocontrol of Protein Activity in Cultured Cells and Zebrafish with Oneâ€•and Twoâ€Photon Illumination. ChemBioChem, 2010, 11, 653-663.	2.6	72
18	M3+Lanthanide Cation Solvation by Acetonitrile:Â The Role of Cation Size, Counterions, and Polarization Effects Investigated by Molecular Dynamics and Quantum Mechanical Simulations. Journal of Physical Chemistry A, 2000, 104, 7659-7671.	2.5	69

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19	Visualization of Biomolecular Structures: State of the Art Revisited. Computer Graphics Forum, 2017, 36, 178-204.	3.0	69
20	Oriented chiral water wires in artificial transmembrane channels. Science Advances, 2018, 4, eaao5603.	10.3	69
21	The major Î²-catenin/E-cadherin junctional binding site is a primary molecular mechano-transductor of differentiation in vivo. ELife, 2018, 7, .	6.0	62
22	How Cations Can Assist DNase I in DNA Binding and Hydrolysis. PLoS Computational Biology, 2010, 6, e1001000.	3.2	60
23	String method solution of the gating pathways for a pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4158-E4167.	7.1	60
24	Membrane protein structure quality in molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2005, 24, 157-165.	2.4	58
25	Extending the Structure of an ABC Transporter to Atomic Resolution:â€‰ Modeling and Simulation Studies of MsbA. Biochemistry, 2003, 42, 3666-3673.	2.5	56
26	Allosteric and hyperekplexic mutant phenotypes investigated on an Î± ₁ glycine receptor transmembrane structure. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2865-2870.	7.1	56
27	GPUâ€accelerated atom and dynamic bond visualization using hyperballs: A unified algorithm for balls, sticks, and hyperboloids. Journal of Computational Chemistry, 2011, 32, 2924-2935.	3.3	55
28	Understanding small biomoleculeâ€biomaterial interactions: A review of fundamental theoretical and experimental approaches for biomolecule interactions with inorganic surfaces. Journal of Biomedical Materials Research - Part A, 2013, 101A, 1210-1222.	4.0	54
29	Formation of Raft-Like Assemblies within Clusters of Influenza Hemagglutinin Observed by MD Simulations. PLoS Computational Biology, 2013, 9, e1003034.	3.2	53
30	Three-dimensional representations of complex carbohydrates and polysaccharides--SweetUnityMol: A video game-based computer graphic software. Glycobiology, 2015, 25, 483-491.	2.5	50
31	OmpT: Molecular Dynamics Simulations of an Outer Membrane Enzyme. Biophysical Journal, 2004, 87, 2942-2953.	0.5	49
32	Calix[4]arenes as Selective Extracting Agents. An NMR Dynamic and Conformational Investigation of the Lanthanide(III) and Thorium(IV) Complexes. Inorganic Chemistry, 2000, 39, 2033-2041.	4.0	47
33	Visual Analysis of Biomolecular Cavities: State of the Art. Computer Graphics Forum, 2016, 35, 527-551.	3.0	46
34	Microseconds Dynamics Simulations of the Outer-Membrane Protease T. Biophysical Journal, 2008, 94, 71-78.	0.5	43
35	Mixing Atomistic and Coarse Grain Solvation Models for MD Simulations: Let WT4 Handle the Bulk. Journal of Chemical Theory and Computation, 2012, 8, 3880-3894.	5.3	43
36	A Molecular Dynamics Investigation of Mono and Dimeric States of the Outer Membrane Enzyme OMPLA. Journal of Molecular Biology, 2003, 331, 177-189.	4.2	42

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37	Molecular Graphics: Bridging Structural Biologists and Computer Scientists. Structure, 2019, 27, 1617-1623.	3.3	42
38	Interactive Molecular Dynamics: Scaling up to Large Systems. Procedia Computer Science, 2013, 18, 20-29.	2.0	40
39	Complex molecular assemblies at hand via interactive simulations. Journal of Computational Chemistry, 2009, 30, 2375-2387.	3.3	39
40	Glutathionylation primes soluble glyceraldehyde-3-phosphate dehydrogenase for late collapse into insoluble aggregates. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26057-26065.	7.1	39
41	Molecular simulations and visualization: introduction and overview. Faraday Discussions, 2014, 169, 9-22.	3.2	38
42	GPU-powered tools boost molecular visualization. Briefings in Bioinformatics, 2011, 12, 689-701.	6.5	37
43	Sites of Anesthetic Inhibitory Action on a Cationic Ligand-Gated Ion Channel. Structure, 2016, 24, 595-605.	3.3	35
44	The chloroform / TBP / aqueous nitric acid interfacial system: a molecular dynamics investigation. Journal of Molecular Liquids, 2001, 90, 1-9.	4.9	34
45	Biomimetic Approach for Highly Selective Artificial Water Channels Based on Tubular Pillar[5]arene Dimers. Angewandte Chemie - International Edition, 2020, 59, 23213-23219.	13.8	32
46	Lanthanide cation binding to a phosphoryl-calix[4]arene: the importance of solvent and counterions investigated by molecular dynamics and quantum mechanical simulations. Physical Chemistry Chemical Physics, 2001, 3, 1317-1325.	2.8	31
47	Modeling the early stage of DNA sequence recognition within RecA nucleoprotein filaments. Nucleic Acids Research, 2010, 38, 6313-6323.	14.5	31
48	The weak, fluctuating, dipole moment of membrane-bound hydrogenase from Aquifex aeolicus accounts for its adaptability to charged electrodes. Physical Chemistry Chemical Physics, 2014, 16, 11318-11322.	2.8	31
49	Visualizing biomolecular electrostatics in virtual reality with UnityMolâ€APBS. Protein Science, 2020, 29, 237-246.	7.6	31
50	Coarseâ€Grain Simulations of the Râ€SNARE Fusion Protein in its Membrane Environment Detect Longâ€Lived Conformational Subâ€States. ChemPhysChem, 2009, 10, 1548-1552.	2.1	30
51	Water permeation across artificial I-quartet membrane channels: from structure to disorder. Faraday Discussions, 2018, 209, 125-148.	3.2	29
52	Hydroxy Channelsâ€“Adaptive Pathways for Selective Water Cluster Permeation. Journal of the American Chemical Society, 2021, 143, 4224-4233.	13.7	27
53	Interactions between Neuronal Fusion Proteins Explored by Molecular Dynamics. Biophysical Journal, 2008, 94, 3436-3446.	0.5	26
54	Multiscale Simulations Give Insight into the Hydrogen In and Out Pathways of [NiFe]-Hydrogenases from Aquifex aeolicus and Desulfovibrio fructosovorans. Journal of Physical Chemistry B, 2014, 118, 13800-13811.	2.6	26

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55	Multi-scale simulations of biological systems using the OPEP coarse-grained model. Biochemical and Biophysical Research Communications, 2018, 498, 296-304.	2.1	26
56	A membrane-inserted structural model of the yeast mitofusin Fzo1. Scientific Reports, 2017, 7, 10217.	3.3	25
57	MinOmics, an Integrative and Immersive Tool for Multi-Omics Analysis. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	25
58	Advances in Human-Protein Interaction - Interactive and Immersive Molecular Simulations. , 2012, , .		23
59	From Virtual Reality to Immersive Analytics in Bioinformatics. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	23
60	Outer membrane proteins: comparing X-ray and NMR structures by MD simulations in lipid bilayers. European Biophysics Journal, 2008, 37, 131-141.	2.2	22
61	Functional Modes and Residue Flexibility Control the Anisotropic Response of Guanylate Kinase to Mechanical Stress. Biophysical Journal, 2010, 99, 3412-3419.	0.5	22
62	Modelling lipid systems in fluid with Lattice Boltzmann Molecular Dynamics simulations and hydrodynamics. Scientific Reports, 2019, 9, 16450.	3.3	22
63	Electrostatically-driven fast association and perdeuteration allow detection of transferred cross-relaxation for G protein-coupled receptor ligands with equilibrium dissociation constants in the high-to-low nanomolar range. Journal of Biomolecular NMR, 2011, 50, 191-195.	2.8	21
64	UnityMol: Interactive scientific visualization for integrative biology. , 2014, , .		20
65	Semantics for an Integrative and Immersive Pipeline Combining Visualization and Analysis of Molecular Data. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	20
66	Ten simple rules to create a serious game, illustrated with examples from structural biology. PLoS Computational Biology, 2018, 14, e1005955.	3.2	20
67	Innovative interactive flexible docking method for multi-scale reconstruction elucidates dystrophin molecular assembly. Faraday Discussions, 2014, 169, 45-62.	3.2	19
68	Dystrophin's central domain forms a complex filament that becomes disorganized by in-frame deletions. Journal of Biological Chemistry, 2018, 293, 6637-6646.	3.4	19
69	Characterization of Î²-turns by electronic circular dichroism spectroscopy: a coupled molecular dynamics and time-dependent density functional theory computational study. Physical Chemistry Chemical Physics, 2020, 22, 1611-1623.	2.8	19
70	Visualizing Biological Membrane Organization and Dynamics. Journal of Molecular Biology, 2019, 431, 1889-1919.	4.2	18
71	The Molecular Recognition Mechanism for Superoxide Dismutase Presequence Binding to the Mitochondrial Protein Import Receptor Tom20 from Oryza sativa Involves an LRTLA Motif. Journal of Physical Chemistry B, 2010, 114, 13839-13846.	2.6	17
72	Enzyme Closure and Nucleotide Binding Structurally Lock Guanylate Kinase. Biophysical Journal, 2011, 101, 1440-1449.	0.5	16

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73	Holding the Nucleosome Together: A Quantitative Description of the DNAâ€“Histone Interface in Solution. Journal of Chemical Theory and Computation, 2018, 14, 1045-1058.	5.3	16
74	Visualizing protein structures â€” tools and trends. Biochemical Society Transactions, 2020, 48, 499-506.	3.4	16
75	Theoretical Studies on Lanthanide Cation Extraction by Picolinamides: Ligandâ€“Cation Interactions and Interfacial Behavior. Solvent Extraction and Ion Exchange, 2003, 21, 199-220.	2.0	15
76	Modeling complex biological systems: From solution chemistry to membranes and channels. Pure and Applied Chemistry, 2012, 85, 1-13.	1.9	15
77	Cation coordination by calix[4]arenes bearing amide and/or phosphine oxide pendant groups: how many arms are needed to bind Li+ vs. Na+? A combined NMR and molecular dynamics study. Perkin Transactions II RSC, 2000, , 1315-1322.	1.1	14
78	A VR framework for interacting with molecular simulations. , 2008, , .		13
79	Taming molecular flexibility to tackle rare diseases. Biochimie, 2015, 113, 54-58.	2.6	13
80	UnityMol prototype for FAIR sharing of molecular-visualization experiences: from pictures in the cloud to collaborative virtual reality exploration in immersive 3D environments. Acta Crystallographica Section D: Structural Biology, 2021, 77, 746-754.	2.3	13
81	Interactive visual analytics of molecular data in immersive environments via a semantic definition of the content and the context. , 2016, , .		12
82	Physics-based oligomeric models of the yeast mitofusin Fzo1 at the molecular scale in the context of membrane docking. Mitochondrion, 2019, 49, 234-244.	3.4	12
83	A Molecular Perspective on Mitochondrial Membrane Fusion: From the Key Players to Oligomerization and Tethering of Mitofusin. Journal of Membrane Biology, 2019, 252, 293-306.	2.1	12
84	ExaViz: a flexible framework to analyse, steer and interact with molecular dynamics simulations. Faraday Discussions, 2014, 169, 119-142.	3.2	11
85	Molecular modelling as the spark for active learning approaches for interdisciplinary biology teaching. Interface Focus, 2019, 9, 20180065.	3.0	11
86	Biomimetic water channels: general discussion. Faraday Discussions, 2018, 209, 205-229.	3.2	10
87	What Can Human-Guided Simulations Bring to RNA Folding?. Biophysical Journal, 2017, 113, 302-312.	0.5	8
88	Implicit Modeling of the Impact of Adsorption on Solid Surfaces for Protein Mechanics and Activity with a Coarse-Grained Representation. Journal of Physical Chemistry B, 2020, 124, 8516-8523.	2.6	8
89	Three hydrolases and a transferase: Comparative analysis of active-site dynamics via the BioSimGrid database. Journal of Molecular Graphics and Modelling, 2007, 25, 896-902.	2.4	7
90	UnityMol: interactive and ludic visual manipulation of coarse-grained RNA and other biomolecules. , 2015, , .		7

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91	Residues of Alpha Helix H3 Determine Distinctive Features of Transforming Growth Factor Î²3. Journal of Physical Chemistry B, 2017, 121, 5483-5498.	2.6	7
92	A Cooperative Mechanism of Clotrimazoles in P450 Revealed by the Dissociation Picture of Clotrimazole from P450. Journal of Chemical Information and Modeling, 2014, 54, 1218-1225.	5.4	6
93	Biomimetic Approach for Highly Selective Artificial Water Channels Based on Tubular Pillar[5]arene Dimers. Angewandte Chemie, 2020, 132, 23413-23419.	2.0	6
94	Analyzing protein topology based on Laguerre tessellation of a pore-traversing water network. Scientific Reports, 2018, 8, 13540.	3.3	5
95	Molecular dynamics simulations reveal statistics and microscopic mechanisms of water permeation in membrane-embedded artificial water channel nanoconstructs. Journal of Chemical Physics, 2021, 154, 184102.	3.0	5
96	Wielding the power of interactive molecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	5
97	MULTI-RESOLUTION APPROACH FOR INTERACTIVELY LOCATING FUNCTIONALLY LINKED ION BINDING SITES BY STEERING SMALL MOLECULES INTO ELECTROSTATIC POTENTIAL MAPS USING A HAPTIC DEVICE. , 2009, , 205-215.		4
98	Content and task based navigation for structural biology in 3D environments. , 2015, , .		4
99	Structure and function of natural proteins for water transport: general discussion. Faraday Discussions, 2018, 209, 83-95.	3.2	4
100	Applications to water transport systems: general discussion. Faraday Discussions, 2018, 209, 389-414.	3.2	4
101	Structural dataset from microsecond-long simulations of yeast mitofusin Fzo1 in the context of membrane docking. Data in Brief, 2019, 26, 104460.	1.0	4
102	Conformational Dynamics in a Nicotinic Receptor Homologue Probed by Simulations. Biophysical Journal, 2011, 100, 272a.	0.5	3
103	Highlights from the Faraday Discussion on Artificial Water Channels, Glasgow, UK. Chemical Communications, 2019, 55, 3853-3858.	4.1	3
104	Mechanistic Insights on Heme-to-Heme Transmembrane Electron Transfer Within NADPH Oxydases From Atomistic Simulations. Frontiers in Chemistry, 2021, 9, 650651.	3.6	3
105	Lessons learned from urgent computing in Europe: Tackling the COVID-19 pandemic. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	3
106	Design â€“ a new way to look at old molecules. Journal of Integrative Bioinformatics, 2022, 19, .	1.5	3
107	The modelling and enhancement of water hydrodynamics: general discussion. Faraday Discussions, 2018, 209, 273-285.	3.2	2
108	Using Computer Simulations and Virtual Reality to Understand, Design and Optimize Artificial Water Channels. Lecture Notes in Bioengineering, 2020, , 78-99.	0.4	2

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109	Between Two Walls: Modeling the Adsorption Behavior of Î²-Glucosidase A on Bare and SAM-Functionalized Gold Surfaces. Langmuir, 2022, 38, 1313-1323.	3.5	2
110	Building Biological Relevance Into Integrative Modelling of Macromolecular Assemblies. Frontiers in Molecular Biosciences, 2022, 9, 826136.	3.5	2
111	A Zoom on Membrane Fusion through Coarse-Grained, Atomistic and Hybrid Molecular Dynamics of SNARE Proteins. Biophysical Journal, 2013, 104, 32a.	0.5	1
112	Gating Pathways for a Pentameric Ligand-Gated Ion Channel Solved by Atomistic String Method Simulations. Biophysical Journal, 2017, 112, 475a.	0.5	1
113	Protein-Lipid Interactions in a Full-Scale Influenza a Virion: Insight into Flu Seasonality. Biophysical Journal, 2013, 104, 412a.	0.5	0
114	Study of the Interaction between General Anesthetics and a Bacterial Homologue to the Human Nicotinic Receptor. Biophysical Journal, 2013, 104, 623a.	0.5	0
115	Molecular Modeling of Hydrogenase Enzymes for Biofuel Cell Design. Biophysical Journal, 2013, 104, 335a.	0.5	0
116	Structural Basis for Ion Permeation Mechanism in Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2013, 104, 67a.	0.5	0
117	Probing Pentameric Ligand-Gated Ion Channels with Bromoform Reveals Many Interconnected Anesthetic Binding Sites. Biophysical Journal, 2014, 106, 342a.	0.5	0
118	Foundations of Biomolecular Simulations: A Critical Introduction to Homology Modeling, Molecular Dynamics Simulations, and Free Energy Calculations of Membrane Proteins. , 2014, , 347-392.		0
119	The Dipolar Solvent Model and Its Applications to the Structural Analysis of Low-(SAXS) and High-(CRYSTALLOGRAPHY) Resolution X-Ray Data. Biophysical Journal, 2014, 106, 663a.	0.5	0
120	Game on, Science - How Video Game Technology may Help Biophysicists Tackle Visualization Challenges. Biophysical Journal, 2014, 106, 809a.	0.5	0
121	Nothing to Sneeze at: A Full-Scale Computational Model of the Human Influenza Virion. Biophysical Journal, 2015, 108, 31a.	0.5	0
122	Allosteric Gating Pathways for the Pentameric Ligand-Gated Ion ChannelÂGlic. Biophysical Journal, 2016, 110, 456a.	0.5	0
123	Mitochondrial Membrane Fusion: Computational Modeling of Mitofusins. Biophysical Journal, 2016, 110, 571a.	0.5	0
124	Deciphering Anesthetic Action of Noble Gases through their Modulation of Membrane Protein and Lipid Bilayer Properties. Biophysical Journal, 2017, 112, 553a-554a.	0.5	0
125	Advancing Multi-Scale Simulation Methods for Biological Membrane Systems. Biophysical Journal, 2019, 116, 373a-374a.	0.5	0
126	The never-ending quest to understand the shapes and motions of molecules. Biochemist, 0, , .	0.5	0

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127	Computer Simulations Provide Guidance for Molecular Medicine Through Insights on Dynamics and Mechanisms at the Atomic Scale. IFMBE Proceedings, 2020, , 261-265.	0.3	0