

Tsjerk A Wassenaar

List of Publications by Year in Descending Order

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Version: 2024-04-27

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

46 papers	3,913 citations	21 h-index	50 g-index
50 ext. papers	5,123 ext. citations	6.2 avg, IF	5.34 L-index

#	Paper	IF	Citations
46	Martini 3: a general purpose force field for coarse-grained molecular dynamics. <i>Nature Methods</i> , 2021 , 18, 382-388	21.6	124
45	Asymmetric CorA Gating Mechanism as Observed by Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2407-2417	6.1	1
44	General Protocol for Constructing Molecular Models of Nanodiscs. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2869-2883	6.1	1
43	Retinyl esters form lipid droplets independently of triacylglycerol and seipin. <i>Journal of Cell Biology</i> , 2021 , 220,	7.3	3
42	Competing Roles of Ca and Nonmuscle Myosin IIA on the Dynamics of the Metastasis-Associated Protein S100A4. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 10059-10071	3.4	1
41	Backmapping triangulated surfaces to coarse-grained membrane models. <i>Nature Communications</i> , 2020 , 11, 2296	17.4	25
40	Charge-dependent interactions of monomeric and filamentous actin with lipid bilayers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 5861-5872	11.5	12
39	Lipid-dependent conformational landscape of the ErbB2 growth factor receptor dimers. <i>Chemistry and Physics of Lipids</i> , 2020 , 230, 104911	3.7	2
38	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 21083-21093	3.6	4
37	LION/web: a web-based ontology enrichment tool for lipidomic data analysis. <i>GigaScience</i> , 2019 , 8,	7.6	51
36	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. <i>ACS Central Science</i> , 2018 , 4, 709-717	16.8	139
35	Statistical efficiency of methods for computing free energy of hydration. <i>Journal of Chemical Physics</i> , 2018 , 149, 144111	3.9	14
34	Dopamine transporter oligomerization involves the scaffold domain, but spares the bundle domain. <i>PLoS Computational Biology</i> , 2018 , 14, e1006229	5	13
33	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. <i>Journal of Cheminformatics</i> , 2017 , 9, 58	8.6	6
32	A MoS2-Based Capacitive Displacement Sensor for DNA Sequencing. <i>ACS Nano</i> , 2016 , 10, 9009-16	16.7	35
31	Nucleobase-functionalized graphene nanoribbons for accurate high-speed DNA sequencing. <i>Nanoscale</i> , 2016 , 8, 1861-7	7.7	43
30	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. <i>PLoS Computational Biology</i> , 2016 , 12, e1005169	5	61

29	Spontaneous adsorption of coiled-coil model peptides K and E to a mixed lipid bilayer. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4396-408	3.4	24
28	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015 , 1848, 1319-30	3.8	94
27	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2144-55	6.4	504
26	Thermodynamic and kinetic characterization of transmembrane helix association. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 1390-8	3.6	17
25	Activation of the bacterial thermosensor DesK involves a serine zipper dimerization motif that is modulated by bilayer thickness. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 6353-8	11.5	37
24	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2278-91	6.4	73
23	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2015 , 109, 760-71	2.9	17
22	Molecular dynamics study of the effect of active site protonation on Helicobacter pylori 5methylthioadenosine/S-adenosylhomocysteine nucleosidase. <i>European Biophysics Journal</i> , 2015 , 44, 685-96	1.9	5
21	Probing binding sites and mechanisms of action of an I(Ks) activator by computations and experiments. <i>Biophysical Journal</i> , 2015 , 108, 62-75	2.9	17
20	Molecular dynamics investigation of Helicobacter pylori chemotactic protein CheY1 and two mutants. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2212	2	3
19	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 676-90	6.4	378
18	X-ray structure, thermodynamics, elastic properties and MD simulations of cardiolipin/dimyristoylphosphatidylcholine mixed membranes. <i>Chemistry and Physics of Lipids</i> , 2014 , 178, 1-10	3.7	34
17	Lipid organization of the plasma membrane. <i>Journal of the American Chemical Society</i> , 2014 , 136, 14554-26.4	26.4	519
16	The effect of triple glutamic mutations E9Q/E194Q/E204Q on the structural stability of bacteriorhodopsin. <i>FEBS Journal</i> , 2014 , 281, 1181-95	5.7	3
15	Improved Parameters for the Martini Coarse-Grained Protein Force Field. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 687-97	6.4	782
14	Mixing MARTINI: electrostatic coupling in hybrid atomistic-coarse-grained biomolecular simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 3516-30	3.4	117
13	Molecular dynamics simulations of membrane proteins. <i>Methods in Molecular Biology</i> , 2013 , 1033, 85-101.4	1.4	19
12	WeNMR: Structural Biology on the Grid. <i>Journal of Grid Computing</i> , 2012 , 10, 743-767	4.2	142

11	SQUEEZE-E: The Optimal Solution for Molecular Simulations with Periodic Boundary Conditions. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3618-27	6.4	5
10	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3463-72	6.4	25
9	The eNMR platform for structural biology. <i>Journal of Structural and Functional Genomics</i> , 2010 , 11, 1-8		17
8	Calcium binding to the purple membrane: A molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 74, 669-81	4.2	5
7	The conformation of the extracellular binding domain of Death Receptor 5 in the presence and absence of the activating ligand TRAIL: a molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 70, 333-43	4.2	14
6	How sensitive are nanosecond molecular dynamics simulations of proteins to changes in the force field?. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 6015-25	3.4	16
5	HADDOCK versus HADDOCK: new features and performance of HADDOCK2.0 on the CAPRI targets. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 69, 726-33	4.2	462
4	The effect of box shape on the dynamic properties of proteins simulated under periodic boundary conditions. <i>Journal of Computational Chemistry</i> , 2006 , 27, 316-25	3.5	28
3	A method to obtain a near-minimal-volume molecular simulation of a macromolecule, using periodic boundary conditions and rotational constraints. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1037-46	3.5	13
2	Lecithin:Retinol Acyl Transferase (LRAT) induces the formation of lipid droplets		4
1	Molecular architecture of SARS-CoV-2 envelope by integrative modeling		3