## Tsjerk A Wassenaar

List of Publications by Year in descending order

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45 6,121 papers citations

279798 23 h-index 45 g-index

50 all docs

50 does citations

50 times ranked 6867 citing authors

#	Article	IF	CITATIONS
1	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
2	Asymmetric CorA Gating Mechanism as Observed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 2407-2417.	5.4	10
3	General Protocol for Constructing Molecular Models of Nanodiscs. Journal of Chemical Information and Modeling, 2021, 61, 2869-2883.	5.4	11
4	Retinyl esters form lipid droplets independently of triacylglycerol and seipin. Journal of Cell Biology, 2021, 220, .	5.2	22
5	Competing Roles of Ca2+ and Nonmuscle Myosin IIA on the Dynamics of the Metastasis-Associated Protein S100A4. Journal of Physical Chemistry B, 2021, 125, 10059-10071.	2.6	2
6	Sequential Voxel-Based Leaflet Segmentation of Complex Lipid Morphologies. Journal of Chemical Theory and Computation, 2021, 17, 7873-7885.	5.3	8
7	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093.	2.8	14
8	Backmapping triangulated surfaces to coarse-grained membrane models. Nature Communications, 2020, 11, 2296.	12.8	86
9	Charge-dependent interactions of monomeric and filamentous actin with lipid bilayers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5861-5872.	7.1	35
10	Lipid-dependent conformational landscape of the ErbB2 growth factor receptor dimers. Chemistry and Physics of Lipids, 2020, 230, 104911.	3.2	7
11	LION/web: a web-based ontology enrichment tool for lipidomic data analysis. GigaScience, 2019, 8, .	6.4	128
12	Statistical efficiency of methods for computing free energy of hydration. Journal of Chemical Physics, 2018, 149, 144111.	3.0	16
13	Dopamine transporter oligomerization involves the scaffold domain, but spares the bundle domain. PLoS Computational Biology, 2018, 14, e1006229.	3.2	20
14	Lipid–Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	11.3	274
15	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. Journal of Cheminformatics, 2017, 9, 58.	6.1	7
16	A MoS <sub>2</sub> -Based Capacitive Displacement Sensor for DNA Sequencing. ACS Nano, 2016, 10, 9009-9016.	14.6	40
17	Nucleobase-functionalized graphene nanoribbons for accurate high-speed DNA sequencing. Nanoscale, 2016, 8, 1861-1867.	<b>5.</b> 6	52
18	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. PLoS Computational Biology, 2016, 12, e1005169.	3.2	75

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19	Molecular dynamics study of the effect of active site protonation on Helicobacter pylori $5\hat{a}\in^2$ -methylthioadenosine/S-adenosylhomocysteine nucleosidase. European Biophysics Journal, 2015, 44, 685-696.	2.2	6
20	Probing Binding Sites and Mechanisms of Action of an I Ks Activator by Computations and Experiments. Biophysical Journal, 2015, 108, 62-75.	0.5	35
21	Spontaneous Adsorption of Coiled-Coil Model Peptides K and E to a Mixed Lipid Bilayer. Journal of Physical Chemistry B, 2015, 119, 4396-4408.	2.6	29
22	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1319-1330.	2.6	120
23	Computational Lipidomics with <i>insane</i> : A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	5.3	847
24	Thermodynamic and kinetic characterization of transmembrane helix association. Physical Chemistry Chemical Physics, 2015, 17, 1390-1398.	2.8	25
25	Activation of the bacterial thermosensor DesK involves a serine zipper dimerization motif that is modulated by bilayer thickness. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6353-6358.	7.1	44
26	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. Journal of Chemical Theory and Computation, 2015, 11, 2278-2291.	5.3	94
27	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. Biophysical Journal, 2015, 109, 760-771.	0.5	22
28	The effect of triple glutamic mutations E9Q/E194Q/E204Q on the structural stability of bacteriorhodopsin. FEBS Journal, 2014, 281, 1181-1195.	4.7	4
29	Molecular dynamics investigation of Helicobacter pylori chemotactic protein CheY1 and two mutants. Journal of Molecular Modeling, 2014, 20, 2212.	1.8	3
30	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. Journal of Chemical Theory and Computation, 2014, 10, 676-690.	5.3	566
31	X-ray structure, thermodynamics, elastic properties and MD simulations of cardiolipin/dimyristoylphosphatidylcholine mixed membranes. Chemistry and Physics of Lipids, 2014, 178, 1-10.	3.2	42
32	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	13.7	734
33	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	5.3	1,181
34	Mixing MARTINI: Electrostatic Coupling in Hybrid Atomistic–Coarse-Grained Biomolecular Simulations. Journal of Physical Chemistry B, 2013, 117, 3516-3530.	2.6	145
35	Molecular Dynamics Simulations of Membrane Proteins. Methods in Molecular Biology, 2013, 1033, 85-101.	0.9	26
36	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	3.9	170

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37	SQUEEZE-E: The Optimal Solution for Molecular Simulations with Periodic Boundary Conditions. Journal of Chemical Theory and Computation, 2012, 8, 3618-3627.	5.3	6
38	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	5.3	32
39	The eNMR platform for structural biology. Journal of Structural and Functional Genomics, 2010, 11, 1-8.	1.2	18
40	Calcium binding to the purple membrane: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2009, 74, 669-681.	2.6	5
41	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. Proteins: Structure, Function and Bioinformatics, 2008, 70, 333-343.	2.6	15
42	How Sensitive Are Nanosecond Molecular Dynamics Simulations of Proteins to Changes in the Force Field?. Journal of Physical Chemistry B, 2007, 111, 6015-6025.	2.6	16
43	HADDOCK versus HADDOCK: New features and performance of HADDOCK2.0 on the CAPRI targets. Proteins: Structure, Function and Bioinformatics, 2007, 69, 726-733.	2.6	504
44	The effect of box shape on the dynamic properties of proteins simulated under periodic boundary conditions. Journal of Computational Chemistry, 2006, 27, 316-325.	3.3	33
45	A method to obtain a near-minimal-volume molecular simulation of a macromolecule, using periodic boundary conditions and rotational constraints. Journal of Computational Chemistry, 2004, 25, 1037-1046.	3.3	16