Tsjerk A Wassenaar

List of Publications by Year
in descending order

45	6,121	279798	233421
papers	citations	23 h-index	45 g-index

50	50	50	6867
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	5.3	1,181
2	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	5.3	847
3	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	13.7	734
4	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
5	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
6	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
7	Lipidâ€“Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	11.3	274
8	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	3.9	170
9	Mixing MARTINI: Electrostatic Coupling in Hybrid Atomisticâ€“Coarse-Grained Biomolecular Simulations. Journal of Physical Chemistry B, 2013, 117, 3516-3530.	2.6	145
10	LION/web: a web-based ontology enrichment tool for lipidomic data analysis. GigaScience, 2019, 8, .	6.4	128
11	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
12	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
13	Backmapping triangulated surfaces to coarse-grained membrane models. Nature Communications, 2020, 11, 2296.	12.8	86
14	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. PLoS Computational Biology, 2016, 12, e1005169.	3.2	75
15	Nucleobase-functionalized graphene nanoribbons for accurate high-speed DNA sequencing. Nanoscale, 2016, 8, 1861-1867.	5.6	52
16	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
17	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
18	A MoS₂-Based Capacitive Displacement Sensor for DNA Sequencing. ACS Nano, 2016, 10, 9009-9016.	14.6	40

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19	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
20	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
21	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
22	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	5.3	32
23	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
24	Molecular Dynamics Simulations of Membrane Proteins. Methods in Molecular Biology, 2013, 1033, 85-101.	0.9	26
25	Thermodynamic and kinetic characterization of transmembrane helix association. Physical Chemistry Chemical Physics, 2015, 17, 1390-1398.	2.8	25
26	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. Biophysical Journal, 2015, 109, 760-771.	0.5	22
27	Retinyl esters form lipid droplets independently of triacylglycerol and seipin. Journal of Cell Biology, 2021, 220, .	5.2	22
28	Dopamine transporter oligomerization involves the scaffold domain, but spares the bundle domain. PLoS Computational Biology, 2018, 14, e1006229.	3.2	20
29	The eNMR platform for structural biology. Journal of Structural and Functional Genomics, 2010, 11, 1-8.	1.2	18
30	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
31	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
32	Statistical efficiency of methods for computing free energy of hydration. Journal of Chemical Physics, 2018, 149, 144111.	3.0	16
33	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
34	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093.	2.8	14
35	General Protocol for Constructing Molecular Models of Nanodiscs. Journal of Chemical Information and Modeling, 2021, 61, 2869-2883.	5.4	11
36	Asymmetric CorA Gating Mechanism as Observed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 2407-2417.	5.4	10

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37	Sequential Voxel-Based Leaflet Segmentation of Complex Lipid Morphologies. Journal of Chemical Theory and Computation, 2021, 17, 7873-7885.	5.3	8
38	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. Journal of Cheminformatics, 2017, 9, 58.	6.1	7
39	Lipid-dependent conformational landscape of the ErbB2 growth factor receptor dimers. Chemistry and Physics of Lipids, 2020, 230, 104911.	3.2	7
40	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
41	Molecular dynamics study of the effect of active site protonation on Helicobacter pylori 5â€²-methylthioadenosine/S-adenosylhomocysteine nucleosidase. European Biophysics Journal, 2015, 44, 685-696.	2.2	6
42	Calcium binding to the purple membrane: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2009, 74, 669-681.	2.6	5
43	The effect of triple glutamic mutations E9Q/E194Q/E204Q on the structural stability of bacteriorhodopsin. FEBS Journal, 2014, 281, 1181-1195.	4.7	4
44	Molecular dynamics investigation of Helicobacter pylori chemotactic protein CheY1 and two mutants. Journal of Molecular Modeling, 2014, 20, 2212.	1.8	3
45	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