

Jakob P Ulmschneider

List of Publications by Year in descending order

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32
papers

1,536
citations

331670

21
h-index

434195

31
g-index

34
all docs

34
docs citations

34
times ranked

1786
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular dynamics of ion transport through the open conformation of a bacterial voltage-gated sodium channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6364-6369.	7.1	149
2	United Atom Lipid Parameters for Combination with the Optimized Potentials for Liquid Simulations All-Atom Force Field. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1803-1813.	5.3	104
3	Spontaneous formation of structurally diverse membrane channel architectures from a single antimicrobial peptide. <i>Nature Communications</i> , 2016, 7, 13535.	12.8	99
4	Molecular Dynamics Simulations Are Redefining Our View of Peptides Interacting with Biological Membranes. <i>Accounts of Chemical Research</i> , 2018, 51, 1106-1116.	15.6	94
5	In Silico Partitioning and Transmembrane Insertion of Hydrophobic Peptides under Equilibrium Conditions. <i>Journal of the American Chemical Society</i> , 2011, 133, 15487-15495.	13.7	92
6	Spontaneous transmembrane helix insertion thermodynamically mimics translocon-guided insertion. <i>Nature Communications</i> , 2014, 5, 4863.	12.8	91
7	Charged Antimicrobial Peptides Can Translocate across Membranes without Forming Channel-like Pores. <i>Biophysical Journal</i> , 2017, 113, 73-81.	0.5	91
8	How reliable are molecular dynamics simulations of membrane active antimicrobial peptides?. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 2280-2288.	2.6	83
9	Mechanism and Kinetics of Peptide Partitioning into Membranes from All-Atom Simulations of Thermostable Peptides. <i>Journal of the American Chemical Society</i> , 2010, 132, 3452-3460.	13.7	80
10	Simulation-Guided Rational <i>de Novo</i> Design of a Small Pore-Forming Antimicrobial Peptide. <i>Journal of the American Chemical Society</i> , 2019, 141, 4839-4848.	13.7	80
11	A Generalized Born Implicit-Membrane Representation Compared to Experimental Insertion Free Energies. <i>Biophysical Journal</i> , 2007, 92, 2338-2349.	0.5	74
12	Reorientation and Dimerization of the Membrane-Bound Antimicrobial Peptide PGLa from Microsecond All-Atom MD Simulations. <i>Biophysical Journal</i> , 2012, 103, 472-482.	0.5	51
13	Monte Carlo vs Molecular Dynamics for All-Atom Polypeptide Folding Simulations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16733-16742.	2.6	49
14	Conformational States of Melittin at a Bilayer Interface. <i>Biophysical Journal</i> , 2013, 104, L12-L14.	0.5	48
15	Understanding and modelling the interactions of peptides with membranes: from partitioning to self-assembly. <i>Current Opinion in Structural Biology</i> , 2020, 61, 160-166.	5.7	31
16	Folding Simulations of the Transmembrane Helix of Virus Protein U in an Implicit Membrane Model. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2335-2346.	5.3	30
17	Folding Peptides into Lipid Bilayer Membranes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1807-1809.	5.3	28
18	Peptide Partitioning Properties from Direct Insertion Studies. <i>Biophysical Journal</i> , 2010, 98, L60-L62.	0.5	26

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19	Insights from Micro-second Atomistic Simulations of Melittin in Thin Lipid Bilayers. <i>Journal of Membrane Biology</i> , 2015, 248, 497-503.	2.1	26
20	Sampling efficiency in explicit and implicit membrane environments studied by peptide folding simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 586-597.	2.6	25
21	Determining Peptide Partitioning Properties via Computer Simulation. <i>Journal of Membrane Biology</i> , 2011, 239, 15-26.	2.1	25
22	Computed Free Energies of Peptide Insertion into Bilayers are Independent of Computational Method. <i>Journal of Membrane Biology</i> , 2018, 251, 345-356.	2.1	22
23	Monte carlo folding of trans-membrane helical peptides in an implicit generalized Born membrane. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 297-308.	2.6	21
24	Transmembrane helices containing a charged arginine are thermodynamically stable. <i>European Biophysics Journal</i> , 2017, 46, 627-637.	2.2	21
25	Membrane adsorption, folding, insertion and translocation of synthetic trans-membrane peptides. <i>Molecular Membrane Biology</i> , 2008, 25, 245-257.	2.0	20
26	Peptide Partitioning and Folding into Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2202-2205.	5.3	17
27	The importance of the membrane interface as the reference state for membrane protein stability. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2539-2548.	2.6	13
28	Role of the Interaction Motif in Maintaining the Open Gate of an Open Sodium Channel. <i>Biophysical Journal</i> , 2018, 115, 1920-1930.	0.5	13
29	Tuning of a Membrane-Perforating Antimicrobial Peptide to Selectively Target Membranes of Different Lipid Composition. <i>Journal of Membrane Biology</i> , 2021, 254, 75-96.	2.1	13
30	Mechanisms of a Small Membrane-Active Antimicrobial Peptide from <i>Hyla punctata</i> . <i>Australian Journal of Chemistry</i> , 2020, 73, 236.	0.9	12
31	Integrated Design of a Membrane-Lytic Peptide-Based Intravenous Nanotherapeutic Suppresses Triple-Negative Breast Cancer. <i>Advanced Science</i> , 2022, 9, e2105506.	11.2	7
32	Predicting Membrane-Active Peptide Dynamics in Fluidic Lipid Membranes. <i>Methods in Molecular Biology</i> , 2022, 2405, 115-136.	0.9	0