Waldemar Kulig

List of Publications by Year
in descending order

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42 papers	1,465 citations	411340 20 h-index	371746 37 g-index
44 all docs	44 docs citations	44 times ranked	2322 citing authors

#	Article	IF	Citations
1	Dimerization of the pulmonary surfactant protein C in a membrane environment. PLoS ONE, 2022, 17, e0267155.	1.1	5
2	Maturation of the SARS-CoV-2 virus is regulated by dimerization of its main protease. Computational and Structural Biotechnology Journal, 2022, 20, 3336-3346.	1.9	5
3	A cholesterol analog stabilizes the human Î² ₂ -adrenergic receptor nonlinearly with temperature. Science Signaling, 2022, 15, .	1.6	8
4	Mcl-1 and Bok transmembrane domains: Unexpected players in the modulation of apoptosis. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27980-27988.	3.3	19
5	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. Langmuir, 2020, 36, 10438-10447.	1.6	24
6	Rigorous Computational Study Reveals What Docking Overlooks: Double Trouble from Membrane Association in Protein Kinase C Modulators. Journal of Chemical Information and Modeling, 2020, 60, 5624-5633.	2.5	6
7	Functionalization of the Parylene C Surface Enhances the Nucleation of Calcium Phosphate: Combined Experimental and Molecular Dynamics Simulations Approach. ACS Applied Materials & Interfaces, 2020, 12, 12426-12435.	4.0	12
8	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. PLoS Computational Biology, 2019, 15, e1007033.	1.5	25
9	Multiscale Simulations of Biological Membranes: The Challenge To Understand Biological Phenomena in a Living Substance. Chemical Reviews, 2019, 119, 5607-5774.	23.0	209
10	Complex Behavior of Phosphatidylcholineâ€“Phosphatidic Acid Bilayers and Monolayers: Effect of Acyl Chain Unsaturation. Langmuir, 2019, 35, 5944-5956.	1.6	27
11	Physiologically-relevant levels of sphingomyelin, but not GM1, induces a Î²-sheet-rich structure in the amyloid-Î²(1-42) monomer. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1709-1720.	1.4	22
12	Bobbing of Oxysterols: Molecular Mechanism for Translocation of Tail-Oxidized Sterols through Biological Membranes. Journal of Physical Chemistry Letters, 2018, 9, 1118-1123.	2.1	24
13	Cholesterol Protects the Oxidized Lipid Bilayer from Water Injury: An All-Atom Molecular Dynamics Study. Journal of Membrane Biology, 2018, 251, 521-534.	1.0	12
14	How to minimize dye-induced perturbations while studying biomembrane structure and dynamics: PEG linkers as a rational alternative. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2436-2445.	1.4	31
15	Molecular Dynamics Insights into Waterâ€“Parylene C Interface: Relevance of Oxygen Plasma Treatment for Biocompatibility. ACS Applied Materials & Interfaces, 2017, 9, 16685-16693.	4.0	10
16	The Effect of Membrane Polyunsaturated Fatty Acids on Receptor Partitioning to Ordered Domains. Biophysical Journal, 2017, 112, 230a-231a.	0.2	0
17	Oxysterols Versus Cholesterol in Model Neuronal Membrane. I. The Case of 7-Ketocholesterol. The Langmuir Monolayer Study. Journal of Membrane Biology, 2017, 250, 553-564.	1.0	23
18	The role of hydrophobic matching on transmembrane helix packing in cells. Cell Stress, 2017, 1, 90-106.	1.4	37

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19	Cholesterol oxidation products and their biological importance. Chemistry and Physics of Lipids, 2016, 199, 144-160.	1.5	130
20	Cis and trans unsaturated phosphatidylcholine bilayers: A molecular dynamics simulation study. Chemistry and Physics of Lipids, 2016, 195, 12-20.	1.5	69
21	Mechanism of allosteric regulation of Î²2-adrenergic receptor by cholesterol. ELife, 2016, 5, .	2.8	115
22	Cholesterol under oxidative stressâ€"How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. Free Radical Biology and Medicine, 2015, 84, 30-41.	1.3	57
23	Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study. Journal of Physical Chemistry B, 2015, 119, 10042-10051.	1.2	20
24	How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: Î²₂-Adrenergic Receptor in the Spotlight. Journal of Chemical Theory and Computation, 2015, 11, 3432-3445.	2.3	16
25	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	1.2	109
26	Topologies, structures and parameter files for lipid simulations in GROMACS with the OPLS-aa force field: DPPC, POPC, DOPC, PEPC, and cholesterol. Data in Brief, 2015, 5, 333-336.	0.5	65
27	Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 422-432.	1.4	45
28	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. Journal of Molecular Modeling, 2014, 20, 2121.	0.8	44
29	Both Zundel and Eigen Isomers Contribute to the IR Spectrum of the Gas-Phase H₉O₄⁺ Cluster. Journal of Physical Chemistry B, 2014, 118, 278-286.	1.2	56
30	Deciphering the infrared spectrum of the protonated water pentamer and the hybrid Eigenâ€"Zundel cation. Physical Chemistry Chemical Physics, 2014, 16, 4933.	1.3	29
31	A â€˜clusters-in-liquidâ€™ method for calculating infrared spectra identifies the proton-transfer mode in acidic aqueous solutions. Nature Chemistry, 2013, 5, 29-35.	6.6	109
32	Excited-state polarizability in crystalline sexithiophene: Charge-transfer and vibronic effects. Chemical Physics Letters, 2012, 529, 27-30.	1.2	4
33	Steric and Electronic Effects in the Hostâ"Guest Hydrogen Bonding in Clathrate Hydrates. Journal of Physical Chemistry A, 2011, 115, 6149-6154.	1.1	20
34	Intermediate vibronic coupling in charge transfer states: Comprehensive calculation of electronic excitations in sexithiophene crystal. Journal of Chemical Physics, 2011, 134, 224505.	1.2	14
35	Vibronic coupling in Frenkel and chargeâ€transfer states of oligothiophene crystals. Physica Status Solidi (B): Basic Research, 2011, 248, 408-411.	0.7	2
36	Absorption profile and femtosecond intraband relaxation of the intense upper Davydov component in oligothiophenes. Physica Status Solidi (B): Basic Research, 2011, 248, 412-415.	0.7	0

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37	Spectral shape of intense exciton absorption in oligothiophene crystals. Physical Review B, 2009, 79, .	1.1	12
38	Intraband relaxation of Frenkel excitons in sexithiophene crystals. Physical Review B, 2009, 80, .	1.1	6
39	Unusual features of the quaterthiophene electroâ€absorption spectrum. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 85-88.	0.8	2
40	Unbound excitonâ€“phonon states in oligothiophene crystals â€“ A model approach for spectroscopic purposes. Chemical Physics, 2008, 343, 100-106.	0.9	10
41	Reactivity of a sodium atom in vibrationally excited water clusters: An ab initio molecular dynamics study. Chemical Physics Letters, 2008, 460, 112-115.	1.2	6
42	A sodium atom in a large water cluster: Electron delocalization and infrared spectra. Journal of Chemical Physics, 2008, 128, 154306.	1.2	24