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List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Membrane-attached mammalian cytochromes P450: An overview of the membrane's effects on structure, drug binding, and interactions with redox partners. Journal of Inorganic Biochemistry, 2018, 183, 117-136.	1.5	117
2	Convergence of Free Energy Profile of Coumarin in Lipid Bilayer. Journal of Chemical Theory and Computation, 2012, 8, 1200-1211.	2.3	102
3	Behavior of Human Cytochromes P450 on Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11556-11564.	1.2	94
4	Amphiphilic Drug-Like Molecules Accumulate in a Membrane below the Head Group Region. Journal of Physical Chemistry B, 2014, 118, 1030-1039.	1.2	89
5	Benchmarking of Force Fields for Molecule–Membrane Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4143-4151.	2.3	73
6	Synergism of antioxidant action of vitamins E, C and quercetin is related to formation of molecular associations in biomembranes. Chemical Communications, 2015, 51, 7713-7716.	2.2	62
7	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	2.3	57
8	Molecular Insight into Affinities of Drugs and Their Metabolites to Lipid Bilayers. Journal of Physical Chemistry B, 2013, 117, 2403-2410.	1.2	50
9	In silico pharmacology: Drug membrane partitioning and crossing. Pharmacological Research, 2016, 111, 471-486.	3.1	50
10	Structural Changes in Ceramide Bilayers Rationalize Increased Permeation through Stratum Corneum Models with Shorter Acyl Tails. Journal of Physical Chemistry B, 2015, 119, 9811-9819.	1.2	46
11	Role of Enzyme Flexibility in Ligand Access and Egress to Active Site: Bias-Exchange Metadynamics Study of 1,3,7-Trimethyluric Acid in Cytochrome P450 3A4. Journal of Chemical Theory and Computation, 2016, 12, 2101-2109.	2.3	44
12	Structural Dynamics of Carbon Dots in Water and <i>N</i> , <i>N</i> -Dimethylformamide Probed by All-Atom Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 2076-2083.	2.3	41
13	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. Drug Metabolism and Disposition, 2016, 44, 576-590.	1.7	39
14	Carbon Dots Detect Water-to-Ice Phase Transition and Act as Alcohol Sensors <i>via</i> Fluorescence Turn-Off/On Mechanism. ACS Nano, 2021, 15, 6582-6593.	7.3	34
15	Rationalization of Reduced Penetration of Drugs through Ceramide Gel Phase Membrane. Langmuir, 2014, 30, 13942-13948.	1.6	28
16	Role of Ionizable Lipids in SARS-CoV-2 Vaccines As Revealed by Molecular Dynamics Simulations: From Membrane Structure to Interaction with mRNA Fragments. Journal of Physical Chemistry Letters, 2021, 12, 11199-11205.	2.1	26
17	Effect of Cholesterol on the Structure of Membrane-Attached Cytochrome P450 3A4. Journal of Chemical Information and Modeling, 2015, 55, 628-635.	2.5	25
18	Conformational Behavior and Optical Properties of a Fluorophore Dimer as a Model of Luminescent Centers in Carbon Dots. Journal of Physical Chemistry C, 2020, 124, 14327-14337.	1.5	25

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19	Effect of Lipid Charge on Membrane Immersion of Cytochrome P450 3A4. Journal of Physical Chemistry B, 2016, 120, 11205-11213.	1.2	24
20	Molecular Fluorophores Self-Organize into C-Dot Seeds and Incorporate into C-Dot Structures. Journal of Physical Chemistry Letters, 2020, 11, 8252-8258.	2.1	24
21	Lipid Bilayer Membrane Affinity Rationalizes Inhibition of Lipid Peroxidation by a Natural Lignan Antioxidant. Journal of Physical Chemistry B, 2013, 117, 5043-5049.	1.2	22
22	Dermal Delivery of Selected Polyphenols from Silybum marianum. Theoretical and Experimental Study. Molecules, 2019, 24, 61.	1.7	16
23	Atomistic Picture of Fluorescent Probes with Hydrocarbon Tails in Lipid Bilayer Membranes: An Investigation of Selective Affinities and Fluorescent Anisotropies in Different Environmental Phases. Langmuir, 2018, 34, 9072-9084.	1.6	15
24	Orientational distribution of DPH in lipid membranes: a comparison of molecular dynamics calculations and experimental time-resolved anisotropy experiments. Physical Chemistry Chemical Physics, 2019, 21, 7594-7604.	1.3	13
25	Molecular insights into the role of a distal F240A mutation that alters CYP1A1 activity towards persistent organic pollutants. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2852-2860.	1.1	12
26	Cyanine dyes with tail length asymmetry enhance photoselection: AÂmultiscale study on DiD probes in a liquid disordered membrane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117329.	2.0	8
27	Influence of Membrane Phase on the Optical Properties of DPH. Molecules, 2020, 25, 4264.	1.7	4