## Markéta PaloncýovÃ;

List of Publications by Year in descending order

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Version: 2024-02-01

27 papers

1,140 citations

331259 21 h-index 27 g-index

27 all docs

27 docs citations

27 times ranked

1488 citing authors

#	Article	IF	Citations
1	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924.	2.3	57
2	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
3	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
4	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
5	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
6	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
7	Influence of Membrane Phase on the Optical Properties of DPH. Molecules, 2020, 25, 4264.	1.7	4
8	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
9	Dermal Delivery of Selected Polyphenols from Silybum marianum. Theoretical and Experimental Study. Molecules, 2019, 24, 61.	1.7	16
10	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
11	Structural Dynamics of Carbon Dots in Water and $\langle i \rangle N \langle  i \rangle, \langle i \rangle N \langle  i \rangle$ -Dimethylformamide Probed by All-Atom Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 2076-2083.	2.3	41
12	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
13	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
14	In silico pharmacology: Drug membrane partitioning and crossing. Pharmacological Research, 2016, 111, 471-486.	3.1	50
15	Effect of Lipid Charge on Membrane Immersion of Cytochrome P450 3A4. Journal of Physical Chemistry B, 2016, 120, 11205-11213.	1.2	24
16	The Role of Protein-Protein and Protein-Membrane Interactions on P450 Function. Drug Metabolism and Disposition, 2016, 44, 576-590.	1.7	39
17	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
18	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

#	Article	IF	CITATIONS
19	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
20	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
21	Rationalization of Reduced Penetration of Drugs through Ceramide Gel Phase Membrane. Langmuir, 2014, 30, 13942-13948.	1.6	28
22	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
23	Benchmarking of Force Fields for Molecule–Membrane Interactions. Journal of Chemical Theory and Computation, 2014, 10, 4143-4151.	2.3	73
24	Behavior of Human Cytochromes P450 on Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11556-11564.	1.2	94
25	Molecular Insight into Affinities of Drugs and Their Metabolites to Lipid Bilayers. Journal of Physical Chemistry B, 2013, 117, 2403-2410.	1.2	50
26	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
27	Convergence of Free Energy Profile of Coumarin in Lipid Bilayer. Journal of Chemical Theory and Computation, 2012, 8, 1200-1211.	2.3	102