Alex Bunker

List of Publications by Year
in descending order

75 papers	2,522 citations	185998 28 h-index	205818 48 g-index
78 all docs	78 docs citations	78 times ranked	3768 citing authors

#	Article	IF	Citations
1	Insights into the behavior of unsaturated diacylglycerols in mixed lipid bilayers in relation to protein kinase C activationâ€"A molecular dynamics simulation study. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183961.	1.4	4
2	Mechanistic Insight into How PEGylation Reduces the Efficacy of pH-Sensitive Liposomes from Molecular Dynamics Simulations. Molecular Pharmaceutics, 2021, 18, 2612-2621.	2.3	8
3	Mechanistic Understanding from Molecular Dynamics in Pharmaceutical Research 2: Lipid Membrane in Drug Design. Pharmaceuticals, 2021, 14, 1062.	1.7	23
4	In Vitro and in Vivo Behavior of Liposomes Decorated with PEGs with Different Chemical Features. Molecular Pharmaceutics, 2020, 17, 472-487.	2.3	18
5	Mechanistic Understanding From Molecular Dynamics Simulation in Pharmaceutical Research 1: Drug Delivery. Frontiers in Molecular Biosciences, 2020, 7, 604770.	1.6	54
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	Cholesterol Reduces Partitioning of Antifungal Drug Itraconazole into Lipid Bilayers. Journal of Physical Chemistry B, 2020, 124, 2139-2148.	1.2	12
8	Insight into the antimicrobial mechanism of action of Î²2,2-amino acid derivatives from molecular dynamics simulation: Dancing the can-can at the membrane surface. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 183028.	1.4	9
9	Determinants of Orexin Receptor Binding and Activationâ€"A Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 2609-2622.	1.2	6
10	Membrane bound COMT isoform is an interfacial enzyme: general mechanism and new drug design paradigm. Chemical Communications, 2018, 54, 3440-3443.	2.2	20
11	Lipid Architectonics for Superior Oral Bioavailability of Nelfinavir Mesylate: Comparative in vitro and in vivo Assessment. AAPS PharmSciTech, 2018, 19, 3584-3598.	1.5	9
12	Glyceryl Monostearate: Probing the Self Assembly of a Lipid Amenable To Surface Modification for Hepatic Targeting. Journal of Physical Chemistry C, 2018, 122, 22160-22169.	1.5	4
13	Characterization of membraneâ€"foulant interactions with novel combination of Raman spectroscopy, surface plasmon resonance and molecular dynamics simulation. Separation and Purification Technology, 2018, 205, 263-272.	3.9	23
14	The effect of light sensitizer localization on the stability of indocyanine green liposomes. Journal of Controlled Release, 2018, 284, 213-223.	4.8	43
15	Control of Peptide Aggregation and Fibrillation by Physical PEGylation. Biomacromolecules, 2018, 19, 3958-3969.	2.6	9
16	Comparison of timeâ€gated surfaceâ€enhanced raman spectroscopy (TGâ€SERS) and classical SERS based monitoring of Escherichia coli cultivation samples. Biotechnology Progress, 2018, 34, 1533-1542.	1.3	10
17	Biophysical Characterization of Supported Lipid Bilayers Using Parallel Dual-Wavelength Surface Plasmon Resonance and Quartz Crystal Microbalance Measurements. Langmuir, 2018, 34, 8081-8091.	1.6	32
18	Effect of piroxicam on lipid membranes: Drug encapsulation and gastric toxicity aspects. European Journal of Pharmaceutical Sciences, 2017, 100, 116-125.	1.9	16

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19	Effects of Membrane PEGylation on Entry and Location of Antifungal Drug Itraconazole and Their Pharmacological Implications. Molecular Pharmaceutics, 2017, 14, 1057-1070.	2.3	19
20	A novelin silicoframework to improve MHC-I epitopes and break the tolerance to melanoma. OncoImmunology, 2017, 6, e1319028.	2.1	25
21	A computational study suggests that replacing PEG with PMOZ may increase exposure of hydrophobic targeting moiety. European Journal of Pharmaceutical Sciences, 2017, 103, 128-135.	1.9	17
22	Oligomerization Alters Binding Affinity between Amyloid Beta and a Modulator of Peptide Aggregation. Journal of Physical Chemistry C, 2017, 121, 23974-23987.	1.5	4
23	Influence of doxorubicin on model cell membrane properties: insights from in vitro and in silico studies. Scientific Reports, 2017, 7, 6343.	1.6	70
24	Interactions between Chloramphenicol, Carrier Polymers, and Bacteriaâ€“Implications for Designing Electrospun Drug Delivery Systems Countering Wound Infection. Molecular Pharmaceutics, 2017, 14, 4417-4430.	2.3	45
25	Stearylated cycloarginine nanosystems for intracellular delivery â€“ simulations, formulation and proof of concept. RSC Advances, 2016, 6, 113538-113550.	1.7	17
26	642. Oncolytic Vaccines with Modified Tumor Epitopes for Cancer Immunotherapy. Molecular Therapy, 2016, 24, S254.	3.7	0
27	Design of cholesterol arabinogalactan anchored liposomes for asialoglycoprotein receptor mediated targeting to hepatocellular carcinoma: In silic o modeling, in vitro and in vivo evaluation. International Journal of Pharmaceutics, 2016, 509, 149-158.	2.6	28
28	Indocyanine Green-Loaded Liposomes for Light-Triggered Drug Release. Molecular Pharmaceutics, 2016, 13, 2095-2107.	2.3	102
29	Detection of Listeria innocua on roll-to-roll produced SERS substrates with gold nanoparticles. RSC Advances, 2016, 6, 62981-62989.	1.7	23
30	Rational design of liposomal drug delivery systems, a review: Combined experimental and computational studies of lipid membranes, liposomes and their PEGylation. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2334-2352.	1.4	146
31	Oncolytic adenoviruses coated with MHC-I tumor epitopes increase the antitumor immunity and efficacy against melanoma. OncoImmunology, 2016, 5, e1105429.	2.1	70
32	PEGylated Liposomes as Carriers of Hydrophobic Porphyrins. Journal of Physical Chemistry B, 2015, 119, 6646-6657.	1.2	47
33	Hydrophobin Film Structure for HFBI and HFBII and Mechanism for Accelerated Film Formation. PLoS Computational Biology, 2014, 10, e1003745.	1.5	27
34	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
35	Molecular Dynamics Simulation of Inverse-Phosphocholine Lipids. Journal of Physical Chemistry C, 2014, 118, 19444-19449.	1.5	14
36	Molecular Dynamics Simulation of PEGylated Membranes with Cholesterol: Building Toward the DOXIL Formulation. Journal of Physical Chemistry C, 2014, 118, 15541-15549.	1.5	25

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37	Cholesterol level affects surface charge of lipid membranes in saline solution. Scientific Reports, 2014, 4, 5005.	1.6	157
38	The Interactions of Dopamine and L-Dopa with Lipid Headgroup and its Implication for Neurotransmitters Metabolism. Biophysical Journal, 2013, 104, 498a.	0.2	0
39	Force Biased Molecular Dynamics Simulation Study of Effect of Dendrimer Generation on Interaction with DNA. Journal of Chemical Theory and Computation, 2013, 9, 722-729.	2.3	22
40	Study of Interaction Between PEG Carrier and Three Relevant Drug Molecules: Piroxicam, Paclitaxel, and Hematoporphyrin. Journal of Physical Chemistry B, 2012, 116, 7334-7341.	1.2	51
41	Poly(Ethylene Glycol) in Drug Delivery, Why Does it Work, and Can We do Better? All Atom Molecular Dynamics Simulation Provides Some Answers. Physics Procedia, 2012, 34, 24-33.	1.2	63
42	Molecular Dynamics Simulations of the Bacterial ABC Transporter SAV1866 in the Closed Form. Journal of Physical Chemistry B, 2012, 116, 2934-2942.	1.2	38
43	Strong preferences of dopamine and <scp>l</scp>â€dopa towards lipid head group: importance of lipid composition and implication for neurotransmitter metabolism. Journal of Neurochemistry, 2012, 122, 681-690.	2.1	51
44	Molecular dynamics, crystallography and mutagenesis studies on the substrate gating mechanism of prolyl oligopeptidase. Biochimie, 2012, 94, 1398-1411.	1.3	47
45	Molecular Dynamics Simulation of PEGylated Bilayer Interacting with Salt Ions: A Model of the Liposome Surface in the Bloodstream. Journal of Physical Chemistry B, 2012, 116, 4212-4219.	1.2	64
46	Fluid dynamics modeling for synchronizing surface plasmon resonance and quartz crystal microbalance as tools for biomolecular and targeted drug delivery studies. Journal of Colloid and Interface Science, 2012, 378, 251-259.	5.0	18
47	Analysis of cause of failure of new targeting peptide in PEGylated liposome: Molecular modeling as rational design tool for nanomedicine. European Journal of Pharmaceutical Sciences, 2012, 46, 121-130.	1.9	58
48	Tat(48-60) peptide amino acid sequence is not unique in its cell penetrating properties and cell-surface glycosaminoglycans inhibit its cellular uptake. Journal of Controlled Release, 2012, 158, 277-285.	4.8	33
49	Properties of the Membrane Binding Component of Catechol-O-methyltransferase Revealed by Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 13541-13550.	1.2	15
50	Study of PEGylated Lipid Layers as a Model for PEGylated Liposome Surfaces: Molecular Dynamics Simulation and Langmuir Monolayer Studies. Langmuir, 2011, 27, 7788-7798.	1.6	95
51	Use of Umbrella Sampling to Calculate the Entrance/Exit Pathway for Z-Pro-Prolinal Inhibitor in Prolyl Oligopeptidase. Journal of Chemical Theory and Computation, 2011, 7, 1583-1594.	2.3	28
52	Effects of the Lipid Bilayer Phase State on the Water Membrane Interface. Journal of Physical Chemistry B, 2010, 114, 11784-11792.	1.2	58
53	Molecular dynamics study of prolyl oligopeptidase with inhibitor in binding cavity. SAR and QSAR in Environmental Research, 2009, 20, 595-609.	1.0	10
54	Multiscale modeling of emergent materials: biological and soft matter. Physical Chemistry Chemical Physics, 2009, 11, 1869.	1.3	243

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55	Molecular dynamics simulations of the enzyme Catechol-O-Methyltransferase: methodological issues. SAR and QSAR in Environmental Research, 2008, 19, 179-189.	1.0	11
56	Glycolipid Membranes through Atomistic Simulations:â€‰ Effect of Glucose and Galactose Head Groups on Lipid Bilayer Properties. Journal of Physical Chemistry B, 2007, 111, 10146-10154.	1.2	61
57	Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet. Computer Physics Communications, 2002, 147, 97-100.	3.0	1
58	Equation of State and Metal-Nonmetal Transition in Dense Hydrogen Fluid. , 2002, , 365-368.		0
59	Magnetic excitations and critical dynamics in RbMnF3: simulation versus theory and experiment. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 550-552.	1.0	2
60	Spin Dynamics Simulations. Progress of Theoretical Physics Supplement, 2000, 138, 423-432.	0.2	7
61	Classical ferromagnet with double-exchange interaction: High-resolution Monte Carlo simulations. Physical Review B, 2000, 62, 9458-9462.	1.1	26
62	Parallel excluded volume tempering for polymer melts. Physical Review E, 2000, 63, 016701.	0.8	45
63	Longitudinal Magnetic Excitations in Classical Spin Systems. Physical Review Letters, 2000, 85, 2601-2604.	2.9	19
64	Spin-dynamics simulations of the magnetic dynamics ofRbMnF3and direct comparison with experiment. Physical Review B, 2000, 61, 333-342.	1.1	26
65	IMPROVED SPIN DYNAMICS SIMULATIONS OF MAGNETIC EXCITATIONS. International Journal of Modern Physics C, 1999, 10, 1541-1551.	0.8	10
66	Fast spin dynamics algorithms for classical spin systems. Computer Physics Communications, 1998, 111, 1-13.	3.0	79
67	Critical dynamics of the anisotropic BCC Heisenberg antiferromagnet. Journal of Magnetism and Magnetic Materials, 1998, 177-181, 161-162.	1.0	2
68	Dissociation and thermodynamics of dense fluid hydrogen. Physical Review B, 1997, 56, 3094-3098.	1.1	33
69	Dissociation and Thermodynamics in Dense Hydrogen Fluid. Contributions To Plasma Physics, 1997, 37, 115-128.	0.5	17
70	Critical dynamics of the body-centered-cubic classical Heisenberg antiferromagnet. Physical Review B, 1996, 54, 9259-9266.	1.1	28
71	SPIN DYNAMICS SIMULATIONS OF CLASSICAL, THREE-DIMENSIONAL HEISENBERG MAGNETS. International Journal of Modern Physics C, 1996, 07, 401-408.	0.8	3
72	Critical dynamics of the bcc classical Heisenberg magnets. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 1473-1474.	1.0	3

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73	Reply to â€˜â€˜Comment on â€˜Multiple-histogram Monte Carlo study of the Ising antiferromagnet on a stacked triangular latticeâ€™ â€™â€™. Physical Review B, 1995, 52, 1415-1416.	1.1	3
74	Multiple-histogram Monte Carlo study of the Ising antiferromagnet on a stacked triangular lattice. Physical Review B, 1993, 48, 15861-15872.	1.1	35
75	Electron-positron pair creation with capture and ionization in relativistic heavy-ion collisions by the finite-difference method. Physical Review A, 1992, 46, 2607-2612.	1.0	27