

# Alex Bunker

## List of Publications by Year in descending order

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75  
papers

2,522  
citations

186265

28  
h-index

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48  
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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. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183961.	2.6	4
2	Mechanistic Insight into How PEGylation Reduces the Efficacy of pH-Sensitive Liposomes from Molecular Dynamics Simulations. <i>Molecular Pharmaceutics</i> , 2021, 18, 2612-2621.	4.6	8
3	Mechanistic Understanding from Molecular Dynamics in Pharmaceutical Research 2: Lipid Membrane in Drug Design. <i>Pharmaceutics</i> , 2021, 14, 1062.	3.8	23
4	In Vitro and in Vivo Behavior of Liposomes Decorated with PEGs with Different Chemical Features. <i>Molecular Pharmaceutics</i> , 2020, 17, 472-487.	4.6	18
5	Mechanistic Understanding From Molecular Dynamics Simulation in Pharmaceutical Research 1: Drug Delivery. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 604770.	3.5	54
6	Rigorous Computational Study Reveals What Docking Overlooks: Double Trouble from Membrane Association in Protein Kinase C Modulators. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5624-5633.	5.4	6
7	Cholesterol Reduces Partitioning of Antifungal Drug Itraconazole into Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2139-2148.	2.6	12
8	Insight into the antimicrobial mechanism of action of 2,2-amino acid derivatives from molecular dynamics simulation: Dancing the can-can at the membrane surface. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 183028.	2.6	9
9	Determinants of Orexin Receptor Binding and Activationâ€”A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2609-2622.	2.6	6
10	Membrane bound COMT isoform is an interfacial enzyme: general mechanism and new drug design paradigm. <i>Chemical Communications</i> , 2018, 54, 3440-3443.	4.1	20
11	Lipid Architectonics for Superior Oral Bioavailability of Nelfinavir Mesylate: Comparative in vitro and in vivo Assessment. <i>AAPS PharmSciTech</i> , 2018, 19, 3584-3598.	3.3	9
12	Glycerol Monostearate: Probing the Self Assembly of a Lipid Amenable To Surface Modification for Hepatic Targeting. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22160-22169.	3.1	4
13	Characterization of membraneâ€”foulant interactions with novel combination of Raman spectroscopy, surface plasmon resonance and molecular dynamics simulation. <i>Separation and Purification Technology</i> , 2018, 205, 263-272.	7.9	23
14	The effect of light sensitizer localization on the stability of indocyanine green liposomes. <i>Journal of Controlled Release</i> , 2018, 284, 213-223.	9.9	43
15	Control of Peptide Aggregation and Fibrillation by Physical PEGylation. <i>Biomacromolecules</i> , 2018, 19, 3958-3969.	5.4	9
16	Comparison of timeâ€”gated surfaceâ€”enhanced raman spectroscopy (TGâ€”SERS) and classical SERS based monitoring of Escherichia coli cultivation samples. <i>Biotechnology Progress</i> , 2018, 34, 1533-1542.	2.6	10
17	Biophysical Characterization of Supported Lipid Bilayers Using Parallel Dual-Wavelength Surface Plasmon Resonance and Quartz Crystal Microbalance Measurements. <i>Langmuir</i> , 2018, 34, 8081-8091.	3.5	32
18	Effect of piroxicam on lipid membranes: Drug encapsulation and gastric toxicity aspects. <i>European Journal of Pharmaceutical Sciences</i> , 2017, 100, 116-125.	4.0	16

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19	Effects of Membrane PEGylation on Entry and Location of Antifungal Drug Itraconazole and Their Pharmacological Implications. <i>Molecular Pharmaceutics</i> , 2017, 14, 1057-1070.	4.6	19
20	A novel <i>in silico</i> framework to improve MHC-I epitopes and break the tolerance to melanoma. <i>Oncol Immunology</i> , 2017, 6, e1319028.	4.6	25
21	A computational study suggests that replacing PEG with PMOZ may increase exposure of hydrophobic targeting moiety. <i>European Journal of Pharmaceutical Sciences</i> , 2017, 103, 128-135.	4.0	17
22	Oligomerization Alters Binding Affinity between Amyloid Beta and a Modulator of Peptide Aggregation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23974-23987.	3.1	4
23	Influence of doxorubicin on model cell membrane properties: insights from in vitro and in silico studies. <i>Scientific Reports</i> , 2017, 7, 6343.	3.3	70
24	Interactions between Chloramphenicol, Carrier Polymers, and Bacteria—Implications for Designing Electrospun Drug Delivery Systems Countering Wound Infection. <i>Molecular Pharmaceutics</i> , 2017, 14, 4417-4430.	4.6	45
25	Stearylated cycloarginine nanosystems for intracellular delivery — simulations, formulation and proof of concept. <i>RSC Advances</i> , 2016, 6, 113538-113550.	3.6	17
26	642. Oncolytic Vaccines with Modified Tumor Epitopes for Cancer Immunotherapy. <i>Molecular Therapy</i> , 2016, 24, S254.	8.2	0
27	Design of cholesterol arabinogalactan anchored liposomes for asialoglycoprotein receptor mediated targeting to hepatocellular carcinoma: In silico modeling, in vitro and in vivo evaluation. <i>International Journal of Pharmaceutics</i> , 2016, 509, 149-158.	5.2	28
28	Indocyanine Green-Loaded Liposomes for Light-Triggered Drug Release. <i>Molecular Pharmaceutics</i> , 2016, 13, 2095-2107.	4.6	102
29	Detection of <i>Listeria innocua</i> on roll-to-roll produced SERS substrates with gold nanoparticles. <i>RSC Advances</i> , 2016, 6, 62981-62989.	3.6	23
30	Rational design of liposomal drug delivery systems, a review: Combined experimental and computational studies of lipid membranes, liposomes and their PEGylation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2334-2352.	2.6	146
31	Oncolytic adenoviruses coated with MHC-I tumor epitopes increase the antitumor immunity and efficacy against melanoma. <i>Oncol Immunology</i> , 2016, 5, e1105429.	4.6	70
32	PEGylated Liposomes as Carriers of Hydrophobic Porphyrins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6646-6657.	2.6	47
33	Hydrophobin Film Structure for HFBI and HFBII and Mechanism for Accelerated Film Formation. <i>PLoS Computational Biology</i> , 2014, 10, e1003745.	3.2	27
34	Effect of PEGylation on Drug Entry into Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2014, 118, 144-151.	2.6	26
35	Molecular Dynamics Simulation of Inverse-Phosphocholine Lipids. <i>Journal of Physical Chemistry C</i> , 2014, 118, 19444-19449.	3.1	14
36	Molecular Dynamics Simulation of PEGylated Membranes with Cholesterol: Building Toward the DOXIL Formulation. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15541-15549.	3.1	25

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37	Cholesterol level affects surface charge of lipid membranes in saline solution. Scientific Reports, 2014, 4, 5005.	3.3	157
38	The Interactions of Dopamine and L-Dopa with Lipid Headgroup and its Implication for Neurotransmitters Metabolism. Biophysical Journal, 2013, 104, 498a.	0.5	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.	5.3	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.	2.6	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.	2.6	38
43	Strong preferences of dopamine and $\alpha$ -dopa towards lipid head group: importance of lipid composition and implication for neurotransmitter metabolism. Journal of Neurochemistry, 2012, 122, 681-690.	3.9	51
44	Molecular dynamics, crystallography and mutagenesis studies on the substrate gating mechanism of prolyl oligopeptidase. Biochimie, 2012, 94, 1398-1411.	2.6	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.	2.6	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.	9.4	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.	4.0	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.	9.9	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.	2.6	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.	3.5	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.	5.3	28
52	Effects of the Lipid Bilayer Phase State on the Water Membrane Interface. Journal of Physical Chemistry B, 2010, 114, 11784-11792.	2.6	58
53	Molecular dynamics study of prolyl oligopeptidase with inhibitor in binding cavity. SAR and QSAR in Environmental Research, 2009, 20, 595-609.	2.2	10
54	Multiscale modeling of emergent materials: biological and soft matter. Physical Chemistry Chemical Physics, 2009, 11, 1869.	2.8	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.	2.2	11
56	Glycolipid Membranes through Atomistic Simulations: Effect of Glucose and Galactose Head Groups on Lipid Bilayer Properties. Journal of Physical Chemistry B, 2007, 111, 10146-10154.	2.6	61
57	Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet. Computer Physics Communications, 2002, 147, 97-100.	7.5	1
58	Equation of State and Metal-Nonmetal Transition in Dense Hydrogen Fluid. , 2002, , 365-368.		0
59	Magnetic excitations and critical dynamics in RbMnF <sub>3</sub> : simulation versus theory and experiment. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 550-552.	2.3	2
60	Spin Dynamics Simulations. Progress of Theoretical Physics Supplement, 2000, 138, 423-432.	0.1	7
61	Classical ferromagnet with double-exchange interaction: High-resolution Monte Carlo simulations. Physical Review B, 2000, 62, 9458-9462.	3.2	26
62	Parallel excluded volume tempering for polymer melts. Physical Review E, 2000, 63, 016701.	2.1	45
63	Longitudinal Magnetic Excitations in Classical Spin Systems. Physical Review Letters, 2000, 85, 2601-2604.	7.8	19
64	Spin-dynamics simulations of the magnetic dynamics of RbMnF <sub>3</sub> and direct comparison with experiment. Physical Review B, 2000, 61, 333-342.	3.2	26
65	IMPROVED SPIN DYNAMICS SIMULATIONS OF MAGNETIC EXCITATIONS. International Journal of Modern Physics C, 1999, 10, 1541-1551.	1.7	10
66	Fast spin dynamics algorithms for classical spin systems. Computer Physics Communications, 1998, 111, 1-13.	7.5	79
67	Critical dynamics of the anisotropic BCC Heisenberg antiferromagnet. Journal of Magnetism and Magnetic Materials, 1998, 177-181, 161-162.	2.3	2
68	Dissociation and thermodynamics of dense fluid hydrogen. Physical Review B, 1997, 56, 3094-3098.	3.2	33
69	Dissociation and Thermodynamics in Dense Hydrogen Fluid. Contributions To Plasma Physics, 1997, 37, 115-128.	1.1	17
70	Critical dynamics of the body-centered-cubic classical Heisenberg antiferromagnet. Physical Review B, 1996, 54, 9259-9266.	3.2	28
71	SPIN DYNAMICS SIMULATIONS OF CLASSICAL, THREE-DIMENSIONAL HEISENBERG MAGNETS. International Journal of Modern Physics C, 1996, 07, 401-408.	1.7	3
72	Critical dynamics of the bcc classical Heisenberg magnets. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 1473-1474.	2.3	3

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73	Reply to “Comment on “Multiple-histogram Monte Carlo study of the Ising antiferromagnet on a stacked triangular lattice”” Physical Review B, 1995, 52, 1415-1416.	3.2	3
74	Multiple-histogram Monte Carlo study of the Ising antiferromagnet on a stacked triangular lattice. Physical Review B, 1993, 48, 15861-15872.	3.2	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.	2.5	27