Jeffrey Comer

List of Publications by Year
in descending order

71 papers	2,973 citations	159573 30 h-index	168376 53 g-index
72 all docs	72 docs citations	72 times ranked	3953 citing authors

#	Article	IF	Citations
1	Local immune checkpoint blockade therapy by an adenovirus encoding a novel PD-L1 inhibitory peptide inhibits the growth of colon carcinoma in immunocompetent mice. Translational Oncology, 2022, 16, 101337.	3.7	1
2	Oral Administration of Water Extract from Euglena gracilis Alters the Intestinal Microbiota and Prevents Lung Carcinoma Growth in Mice. Nutrients, 2022, 14, 678.	4.1	5
3	Organic contaminants and atmospheric nitrogen at the grapheneâ€“water interface: a simulation study. Nanoscale Advances, 2022, 4, 1741-1757.	4.6	4
4	Urea-Modified Self-Assembling Peptide Amphiphiles That Form Well-Defined Nanostructures and Hydrogels for Biomedical Applications. ACS Applied Bio Materials, 2022, 5, 4599-4610.	4.6	6
5	A Water Extract from Chlorella sorokiniana Cell Walls Stimulates Growth of Bone Marrow Cells and Splenocytes. Nutrients, 2022, 14, 2901.	4.1	1
6	Atomically resolved interfacial water structures on crystalline hydrophilic and hydrophobic surfaces. Nanoscale, 2021, 13, 5275-5283.	5.6	35
7	Beta-1,3 Oligoglucans Specifically Bind to Immune Receptor CD28 and May Enhance T Cell Activation. International Journal of Molecular Sciences, 2021, 22, 3124.	4.1	6
8	Extraction of Chlorobenzenes and PCBs from Water by ZnO Nanoparticles. Processes, 2021, 9, 1764.	2.8	0
9	Water extract from Euglena gracilis prevents lung carcinoma growth in mice by attenuation of the myeloid-derived cell population. Biomedicine and Pharmacotherapy, 2020, 127, 110166.	5.6	12
10	Structural Determinants of the Dopamine Transporter Regulation Mediated by G Proteins. Journal of Chemical Information and Modeling, 2020, 60, 3577-3586.	5.4	2
11	Cell Wall Membrane Fraction ofChlorella sorokinianaEnhances Host Antitumor Immunity and Inhibits Colon Carcinoma Growth in Mice. Integrative Cancer Therapies, 2020, 19, 153473541990055.	2.0	10
12	Potential of Matrix Metalloproteinase Inhibitors for the Treatment of Local Tissue Damage Induced by a Type P-I Snake Venom Metalloproteinase. Toxins, 2020, 12, 8.	3.4	7
13	A Structural Model of the Inactivation Gate of Voltage-Activated Potassium Channels. Biophysical Journal, 2019, 117, 377-387.	0.5	5
14	Affordable Membrane Permeability Calculations: Permeation of Short-Chain Alcohols through Pure-Lipid Bilayers and a Mammalian Cell Membrane. Journal of Chemical Theory and Computation, 2019, 15, 2913-2924.	5.3	27
15	Predicting the preferred morphology of hexagonal boron nitride domain structure on nickel from ReaxFF-based molecular dynamics simulations. Nanoscale, 2019, 11, 5607-5616.	5.6	20
16	Computational modeling of the adsorption of capping agent biomolecules to inorganic nanoparticles. , 2019, , 21-41.		0
17	Comparative Molecular Immunological Activity of Physiological Metal Oxide Nanoparticle and its Anticancer Peptide and RNA Complexes. Nanomaterials, 2019, 9, 1670.	4.1	12
18	Thermodynamics of Adsorption on Graphenic Surfaces from Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1302-1316.	5.3	41

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19	Interactions between Triterpenes and a P-I Type Snake Venom Metalloproteinase: Molecular Simulations and Experiments. Toxins, 2018, 10, 397.	3.4	5
20	Inhibition of a Snake Venom Metalloproteinase by the Flavonoid Myricetin. Molecules, 2018, 23, 2662.	3.8	26
21	Link between Membrane Composition and Permeability to Drugs. Journal of Chemical Theory and Computation, 2018, 14, 2895-2909.	5.3	35
22	The influence of polyethylene glycol passivation on the surface plasmon resonance induced photothermal properties of gold nanorods. Nanoscale, 2018, 10, 13684-13693.	5.6	24
23	Chasing a Proteinâ€™s Tail: Detection of Polypeptide Translocation through Nanopores. Biophysical Journal, 2018, 114, 759-760.	0.5	4
24	Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. Environmental Science: Nano, 2018, 5, 2117-2128.	4.3	22
25	Experimental and Computational Characterization of the Interaction between Gold Nanoparticles and Polyamidoamine Dendrimers. Langmuir, 2018, 34, 10063-10072.	3.5	11
26	Comparative functional dynamics studies on the enzyme nano-bio interface. International Journal of Nanomedicine, 2018, Volume 13, 4523-4536.	6.7	7
27	Polymeric substances for the removal of ochratoxin A from red wine followed by computational modeling of the complexes formed. Food Chemistry, 2018, 265, 159-164.	8.2	10
28	Study of specific interactions in inclusion complexes of amine-terminated PAMAM dendrimer/flavonoids by experimental and computational methods. International Journal of Polymeric Materials and Polymeric Biomaterials, 2017, 66, 485-494.	3.4	4
29	Enzyme and Cancer Cell Selectivity of Nanoparticles: Inhibition of 3-D Metastatic Phenotype and Experimental Melanoma by Zinc Oxide. Journal of Biomedical Nanotechnology, 2017, 13, 221-231.	1.1	15
30	Permeability of a Fluid Lipid Bilayer to Short-Chain Alcohols from First Principles. Journal of Chemical Theory and Computation, 2017, 13, 2523-2532.	5.3	33
31	Determinants of Alanine Dipeptide Conformational Equilibria on Graphene and Hydroxylated Derivatives. Journal of Physical Chemistry B, 2017, 121, 3895-3907.	2.6	23
32	Novel specific peptides as superior surface stabilizers for silver nano structures: role of peptide chain length. Journal of Materials Chemistry B, 2017, 5, 8925-8928.	5.8	14
33	Understanding Noncovalent Interactions of Small Molecules with Carbon Nanotubes. Chemistry - A European Journal, 2017, 23, 12909-12916.	3.3	30
34	Iodide Binding in Sodium-Coupled Cotransporters. Journal of Chemical Information and Modeling, 2017, 57, 3043-3055.	5.4	12
35	Rose Bengal Binding to Collagen and Tissue Photobonding. ACS Omega, 2017, 2, 6646-6657.	3.5	41
36	Self-Assembly of Amphiphilic Dendrimers: The Role of Generation and Alkyl Chain Length in siRNA Interaction. Scientific Reports, 2016, 6, 29436.	3.3	30

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37	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	5.4	174
38	DNA sequence-dependent ionic currents in ultra-small solid-state nanopores. Nanoscale, 2016, 8, 9600-9613.	5.6	29
39	Subdiffusion in Membrane Permeation of Small Molecules. Scientific Reports, 2016, 6, 35913.	3.3	63
40	Understanding the Interaction between Biomolecules and Silver Nanoparticles. Biophysical Journal, 2016, 110, 341a.	0.5	3
41	New Insights into Peptideâ€“Silver Nanoparticle Interaction: Deciphering the Role of Cysteine and Lysine in the Peptide Sequence. Langmuir, 2016, 32, 265-273.	3.5	49
42	Is Sodium Monocarboxylate Transporter (SMCT1) A Protein Involved in the Apical Iodide Transport?. Biophysical Journal, 2016, 110, 139a.	0.5	0
43	Molecular Dynamics Simulations of Membrane Translocation of Dendrimers. Biophysical Journal, 2016, 110, 571a.	0.5	0
44	Sonoporation at Small and Large Length Scales: Effect of Cavitation Bubble Collapse on Membranes. Journal of Physical Chemistry Letters, 2015, 6, 413-418.	4.6	41
45	Molecular Determinants of Phosphatidylinositol 4,5-Bisphosphate (PI(4,5)P2) Binding to Transient Receptor Potential V1 (TRPV1) Channels. Journal of Biological Chemistry, 2015, 290, 2086-2098.	3.4	65
46	Predicting Adsorption Affinities of Small Molecules on Carbon Nanotubes Using Molecular Dynamics Simulation. ACS Nano, 2015, 9, 11761-11774.	14.6	89
47	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. Journal of Physical Chemistry B, 2015, 119, 1129-1151.	2.6	351
48	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	2.0	23
49	Multiple-Replica Strategies for Free-Energy Calculations in NAMD: Multiple-Walker Adaptive Biasing Force and Walker Selection Rules. Journal of Chemical Theory and Computation, 2014, 10, 5276-5285.	5.3	66
50	In situ and in silico evaluation of amine- and folate-terminated dendrimers as nanocarriers of anesthetics. European Journal of Medicinal Chemistry, 2014, 73, 250-257.	5.5	17
51	Close encounters with DNA. Journal of Physics Condensed Matter, 2014, 26, 413101.	1.8	46
52	Calculation of Lipid-Bilayer Permeabilities Using an Average Force. Journal of Chemical Theory and Computation, 2014, 10, 554-564.	5.3	57
53	Diffusive Models of Membrane Permeation with Explicit Orientational Freedom. Journal of Chemical Theory and Computation, 2014, 10, 2710-2718.	5.3	43
54	Dangerous Liaisons between Detergents and Membrane Proteins. The Case of Mitochondrial Uncoupling Protein 2. Journal of the American Chemical Society, 2013, 135, 15174-15182.	13.7	86

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55	Paclitaxel-PHBV nanoparticles and their toxicity to endometrial and primary ovarian cancer cells. Biomaterials, 2013, 34, 4098-4108.	11.4	87
56	Calculating Position-Dependent Diffusivity in Biased Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 876-882.	5.3	64
57	Computationally Efficient Methodology for Atomic-Level Characterization of Dendrimerâ€"Drug Complexes: A Comparison of Amine- and Acetyl-Terminated PAMAM. Journal of Physical Chemistry B, 2013, 117, 6801-6813.	2.6	80
58	Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803.	3.1	30
59	Toward detection of DNAâ€bound proteins using solidâ€state nanopores: Insights from computer simulations. Electrophoresis, 2012, 33, 3466-3479.	2.4	14
60	Assessing Graphene Nanopores for Sequencing DNA. Nano Letters, 2012, 12, 4117-4123.	9.1	237
61	DNA Base-Calling from a Nanopore Using a Viterbi Algorithm. Biophysical Journal, 2012, 102, L37-L39.	0.5	75
62	Predicting the DNA Sequence Dependence of Nanopore Ion Current Using Atomic-Resolution Brownian Dynamics. Journal of Physical Chemistry C, 2012, 116, 3376-3393.	3.1	90
63	Modeling Pressure-Driven Transport of Proteins Through a Nanochannel. IEEE Nanotechnology Magazine, 2011, 10, 75-82.	2.0	25
64	Microscopic Perspective on the Adsorption Isotherm of a Heterogeneous Surface. Journal of Physical Chemistry Letters, 2011, 2, 1804-1807.	4.6	32
65	Atoms-to-microns model for small solute transport through sticky nanochannels. Lab on A Chip, 2011, 11, 3766.	6.0	19
66	Lipid bilayer coated Al2O3 nanopore sensors: towards a hybrid biological solid-state nanopore. Biomedical Microdevices, 2011, 13, 671-682.	2.8	52
67	Slowing the translocation of double-stranded DNA using a nanopore smaller than the double helix. Nanotechnology, 2010, 21, 395501.	2.6	74
68	Analyzing the forces binding a restriction endonuclease to DNA using a synthetic nanopore. Nucleic Acids Research, 2009, 37, 4170-4179.	14.5	39
69	Microscopic Mechanics of Hairpin DNA Translocation through Synthetic Nanopores. Biophysical Journal, 2009, 96, 593-608.	0.5	84
70	Detection of DNA Sequences Using an Alternating Electric Field in a Nanopore Capacitor. Nano Letters, 2008, 8, 56-63.	9.1	162
71	Stretching and unzipping nucleic acid hairpins using a synthetic nanopore. Nucleic Acids Research, 2008, 36, 1532-1541.	14.5	65