Megan L O'mara

List of Publications by Year
in descending order

82 papers	3,159 citations	186254 28 h-index	168376 53 g-index
86 all docs	86 docs citations	86 times ranked	4379 citing authors

#	Article	IF	Citations
1	Pore structure controls stability and molecular flux in engineered protein cages. Science Advances, 2022, 8, eabl7346.	10.3	30
2	Lipid-mediated antimicrobial resistance: a phantom menace or a new hope?. Biophysical Reviews, 2022, 14, 145-162.	3.2	10
3	Dynamics of the Acinetobacter baumannii inner membrane under exogenous polyunsaturated fatty acid stress. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183908.	2.6	3
4	PsiRESP: calculating RESP charges with Psi4. Journal of Open Source Software, 2022, 7, 4100.	4.6	0
5	The allosteric inhibition of glycine transporter 2 by bioactive lipid analgesics is controlled by penetration into a deep lipid cavity. Journal of Biological Chemistry, 2021, 296, 100282.	3.4	7
6	The role of plasmalogens, Forssman lipids, and sphingolipid hydroxylation in modulating the biophysical properties of the epithelial plasma membrane. Journal of Chemical Physics, 2021, 154, 095101.	3.0	12
7	Coordination of Substrate Binding and Protonation in the N.Âgonorrhoeae MtrD Efflux Pump Controls the Functionally Rotating Transport Mechanism. ACS Infectious Diseases, 2021, 7, 1833-1847.	3.8	5
8	Enzyme inspired polymer functionalized with an artificial catalytic triad. Polymer, 2021, 225, 123735.	3.8	9
9	The Membrane Composition Defines the Spatial Organization and Function of a Major Acinetobacter baumannii Drug Efflux System. MBio, 2021, 12, e0107021.	4.1	14
10	A Unique Sequence Is Essential for Efficient Multidrug Efflux Function of the MtrD Protein of Neisseria gonorrhoeae. MBio, 2021, 12, e0167521.	4.1	1
11	The structural basis of bacterial manganese import. Science Advances, 2021, 7, .	10.3	17
12	Effect of the Force Field on Molecular Dynamics Simulations of the Multidrug Efflux Protein P-Glycoprotein. Journal of Chemical Theory and Computation, 2021, 17, 6491-6508.	5.3	17
13	Investigating the lipid fingerprint of SLC6 neurotransmitter transporters: a comparison of dDAT, hDAT, hSERT, and GlyT2. BBA Advances, 2021, 1, 100010.	1.6	9
14	Site of Cholesterol Oxidation Impacts Its Localization and Domain Formation in the Neuronal Plasma Membrane. ACS Chemical Neuroscience, 2021, 12, 3873-3884.	3.5	4
15	Understanding the Link between Lipid Diversity and the Biophysical Properties of the Neuronal Plasma Membrane. Biochemistry, 2020, 59, 3010-3018.	2.5	23
16	Aryl urea substituted fatty acids: a new class of protonophoric mitochondrial uncoupler that utilises a synthetic anion transporter. Chemical Science, 2020, 11, 12677-12685.	7.4	14
17	Comparing Nonbonded Metal Ion Models in the Divalent Cation Binding Protein PsaA. Journal of Chemical Theory and Computation, 2020, 16, 1913-1923.	5.3	15
18	A multifunctional surfactant catalyst inspired by hydrolases. Science Advances, 2020, 6, eaaz0404.	10.3	41

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19	Cross-linking, DEER-spectroscopy and molecular dynamics confirm the inward facing state of P-glycoprotein in a lipid membrane. Journal of Structural Biology, 2020, 211, 107513.	2.8	7
20	High resolution crystal structure of a KRAS promoter G-quadruplex reveals a dimer with extensive poly-A Ï€-stacking interactions for small-molecule recognition. Nucleic Acids Research, 2020, 48, 5766-5776.	14.5	34
21	The Fats of Life: Using Computational Chemistry to Characterise the Eukaryotic Cell Membrane. Australian Journal of Chemistry, 2020, 73, 85.	0.9	7
22	Is protein structure enough? A review of the role of lipids in SLC6 transporter function. Neuroscience Letters, 2019, 700, 64-69.	2.1	5
23	The effects of oxidised phospholipids and cholesterol on the biophysical properties of POPC bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 210-219.	2.6	25
24	Mutation p.R356Q in the Collybistin Phosphoinositide Binding Site Is Associated With Mild Intellectual Disability. Frontiers in Molecular Neuroscience, 2019, 12, 60.	2.9	10
25	Multidrug Resistance in Neisseria gonorrhoeae: Identification of Functionally Important Residues in the MtrD Efflux Protein. MBio, 2019, 10, .	4.1	26
26	Probing the Pharmacological Binding Sites of P-Glycoprotein Using Umbrella Sampling Simulations. Journal of Chemical Information and Modeling, 2019, 59, 2287-2298.	5.4	17
27	Lipid-Based Inhibitors Act Directly on GlyT2. ACS Chemical Neuroscience, 2019, 10, 1668-1678.	3.5	10
28	Identification of an allosteric binding site on the human glycine transporter, GlyT2, for bioactive lipid analgesics. ELife, 2019, 8, .	6.0	26
29	A potential new, stable state of the E-cadherin strand-swapped dimer in solution. European Biophysics Journal, 2018, 47, 59-67.	2.2	1
30	Molecular Determinants for Substrate Interactions with the Glycine Transporter GlyT2. ACS Chemical Neuroscience, 2018, 9, 603-614.	3.5	30
31	The reliability of molecular dynamics simulations of the multidrug transporter P-glycoprotein in a membrane environment. PLoS ONE, 2018, 13, e0191882.	2.5	35
32	Synthetically controlling dendrimer flexibility improves delivery of large plasmid DNA. Chemical Science, 2017, 8, 2923-2930.	7.4	101
33	Structure of a lipid A phosphoethanolamine transferase suggests how conformational changes govern substrate binding. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2218-2223.	7.1	113
34	Simple Design of an Enzyme-Inspired Supported Catalyst Based on a Catalytic Triad. CheM, 2017, 2, 732-745.	11.7	44
35	Hydrogen bondâ€Driven Selfâ€“Assembly between Amidinium Cations and Carboxylate Anions: A Combined Molecular Dynamics, NMR Spectroscopy, and Single Crystal Xâ€ray Diffraction Study. Chemistry - an Asian Journal, 2017, 12, 1587-1597.	3.3	25
36	Simple Design of an Enzyme-Inspired Supported Catalyst Based on a Catalytic Triad. CheM, 2017, 2, 893-894.	11.7	2

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37	Method for Developing Optical Sensors Using a Synthetic Dye-Fluorescent Protein FRET Pair and Computational Modeling and Assessment. Methods in Molecular Biology, 2017, 1596, 89-99.	0.9	2
38	Capturing the Dynamics of a Spring-Loaded Protein. Structure, 2017, 25, 963-964.	3.3	1
39	Location of contact residues in pharmacologically distinct drug binding sites on P-glycoprotein. Biochemical Pharmacology, 2017, 123, 19-28.	4.4	29
40	Thylakoid Ultrastructure: Visualizing the Photosynthetic Machinery. Microbiology Monographs, 2017, , 149-191.	0.6	0
41	Structural and dynamic perspectives on the promiscuous transport activity of P-glycoprotein. Neurochemistry International, 2016, 98, 146-152.	3.8	35
42	Rv2074 is a novel F 420 H 2 â€dependent biliverdin reductase in Mycobacterium tuberculosis. Protein Science, 2016, 25, 1692-1709.	7.6	31
43	Hydrophobic Shielding Drives Catalysis of Hydride Transfer in a Family of F₄₂₀H₂-Dependent Enzymes. Biochemistry, 2016, 55, 6908-6918.	2.5	15
44	Rangefinder: A Semisynthetic FRET Sensor Design Algorithm. ACS Sensors, 2016, 1, 1286-1290.	7.8	11
45	Mechanism of JAK2 Activation by the Archetype Class I Cytokine Receptor, the Growth Hormone Receptor. Biophysical Journal, 2016, 110, 31a.	0.5	0
46	Understanding the accumulation of P-glycoprotein substrates within cells: The effect of cholesterol on membrane partitioning. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 776-782.	2.6	15
47	Identification of a 3rd Na+ Binding Site of the Glycine Transporter, GlyT2. PLoS ONE, 2016, 11, e0157583.	2.5	28
48	Identification of Possible Binding Sites for Morphine and Nicardipine on the Multidrug Transporter P-Glycoprotein Using Umbrella Sampling Techniques. Journal of Chemical Information and Modeling, 2015, 55, 1202-1217.	5.4	29
49	Dysregulation of transition metal ion homeostasis is the molecular basis for cadmium toxicity in Streptococcus pneumoniae. Nature Communications, 2015, 6, 6418.	12.8	117
50	Characterizing the conformational dynamics of metal-free PsaA using molecular dynamics simulations and electron paramagnetic resonance spectroscopy. Biophysical Chemistry, 2015, 207, 51-60.	2.8	8
51	Molecular Basis for the Interaction of the Mammalian Amino Acid Transporters B0AT1 and B0AT3 with Their Ancillary Protein Collectrin. Journal of Biological Chemistry, 2015, 290, 24308-24325.	3.4	51
52	Structural Characterization of Two Metastable ATP-Bound States of P-Glycoprotein. PLoS ONE, 2014, 9, e91916.	2.5	26
53	<scp>AdcA</scp> and <scp>AdcAII</scp> employ distinct zinc acquisition mechanisms and contribute additively to zinc homeostasis in <scp>S</scp>treptococcus pneumoniae. Molecular Microbiology, 2014, 91, 834-851.	2.5	108
54	The central cavity of <scp>ABCB</scp>1 undergoes alternating access during <scp>ATP</scp> hydrolysis. FEBS Journal, 2014, 281, 2190-2201.	4.7	35

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55	Mechanism of Activation of Protein Kinase JAK2 by the Growth Hormone Receptor. Science, 2014, 344, 1249783.	12.6	340
56	Imperfect coordination chemistry facilitates metal ion release in the Psa permease. Nature Chemical Biology, 2014, 10, 35-41.	8.0	137
57	The ryanodine receptor store-sensing gate controls Ca2+ waves and Ca2+-triggered arrhythmias. Nature Medicine, 2014, 20, 184-192.	30.7	172
58	Vancomycin: ligand recognition, dimerization and superâ€complex formation. FEBS Journal, 2013, 280, 1294-1307.	4.7	41
59	Intestinal peptidases form functional complexes with the neutral amino acid transporter B0AT1. Biochemical Journal, 2012, 446, 135-148.	3.7	61
60	The Effect of Environment on the Structure of a Membrane Protein: P-Glycoprotein under Physiological Conditions. Journal of Chemical Theory and Computation, 2012, 8, 3964-3976.	5.3	47
61	Molecular Dynamics Simulations of Membrane Proteins: Building Starting Structures and Example Applications. Current Physical Chemistry, 2012, 2, 363-378.	0.2	3
62	The Effect of Environment on the Recognition and Binding of Vancomycin to Native and Resistant Forms of Lipid II. Biophysical Journal, 2011, 101, 2684-2692.	0.5	36
63	Effect of Poly(ethylene glycol) (PEG) Spacers on the Conformational Properties of Small Peptides: A Molecular Dynamics Study. Langmuir, 2011, 27, 296-303.	3.5	35
64	Orientation of Î¼-Conotoxin PIIIA in a Sodium Channel Vestibule, Based on Voltage Dependence of Its Binding. Molecular Pharmacology, 2011, 80, 219-227.	2.3	23
65	Transmembrane helixâ€ƒ12 plays a pivotal role in coupling energy provision and drug binding in ABCB1. FEBS Journal, 2010, 277, 3974-3985.	4.7	22
66	ABC transporters: a riddle wrapped in a mystery inside an enigma. Trends in Biochemical Sciences, 2009, 34, 520-531.	7.5	160
67	Transmembrane Helix 12 Modulates Progression of the ATP Catalytic Cycle in ABCB1. Biochemistry, 2009, 48, 6249-6258.	2.5	27
68	Structural arrangement of the transmission interface in the antigen ABC transport complex TAP. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 5551-5556.	7.1	86
69	The mechanism of ABC transporters: general lessons from structural and functional studies of an antigenic peptide transporter. FASEB Journal, 2009, 23, 1287-1302.	0.5	155
70	Cytosolic Region of TM6 in P-Glycoprotein: Topographical Analysis and Functional Perturbation by Site Directed Labeling. Biochemistry, 2008, 47, 3615-3624.	2.5	18
71	Structure-based interpretation of the mutagenesis database for the nucleotide binding domains of P-glycoprotein. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 376-391.	2.6	29
72	ATP-binding cassette transporters in Escherichia coli. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1757-1771.	2.6	139

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73	Non-linear intramolecular interactions and voltage sensitivity of a KV1 family potassium channel fromPolyorchis penicillatus(Eschscholtz 1829). Journal of Experimental Biology, 2008, 211, 3442-3453.	1.7	8
74	Pâ€glycoprotein models of the apo and ATPâ€bound states based on homology with Sav1866 and MalK. FEBS Letters, 2007, 581, 4217-4222.	2.8	80
75	Residue G346 in Transmembrane Segment Six is Involved in Inter-Domain Communication in P-Glycoprotein. Biochemistry, 2007, 46, 9899-9910.	2.5	41
76	Computer simulations of ABC transporter componentsThis paper is one of a selection of papers published in this Special Issue, entitled CSBMCB â€" Membrane Proteins in Health and Disease.. Biochemistry and Cell Biology, 2006, 84, 900-911.	2.0	12
77	Mechanism and Putative Structure of B0-like Neutral Amino Acid Transporters. Journal of Membrane Biology, 2006, 213, 111-118.	2.1	23
78	Homology Model of the GABAA Receptor Examined Using Brownian Dynamics. Biophysical Journal, 2005, 88, 3286-3299.	0.5	58
79	Permeation dynamics of chloride ions in the ClC-0 and ClC-1 channels. Chemical Physics Letters, 2004, 386, 233-238.	2.6	9
80	Conduction Mechanisms of Chloride Ions in ClC-Type Channels. Biophysical Journal, 2004, 86, 846-860.	0.5	71
81	A model of the glycine receptor deduced from Brownian dynamics studies. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 4310-4315.	7.1	27
82	Polymerâ€"solvent interactions as a tool to engineer material properties. Molecular Systems Design and Engineering, 0, , .	3.4	1