

Megan L O'mara

List of Publications by Year in descending order

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Version: 2024-02-01

82
papers

3,159
citations

212478

28
h-index

190340

53
g-index

86
all docs

86
docs citations

86
times ranked

4888
citing authors

#	ARTICLE	IF	CITATIONS
1	Pore structure controls stability and molecular flux in engineered protein cages. <i>Science Advances</i> , 2022, 8, eabl7346.	4.7	30
2	Lipid-mediated antimicrobial resistance: a phantom menace or a new hope?. <i>Biophysical Reviews</i> , 2022, 14, 145-162.	1.5	10
3	Dynamics of the <i>Acinetobacter baumannii</i> inner membrane under exogenous polyunsaturated fatty acid stress. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183908.	1.4	3
4	PsiRESP: calculating RESP charges with Psi4. <i>Journal of Open Source Software</i> , 2022, 7, 4100.	2.0	0
5	The allosteric inhibition of glycine transporter 2 by bioactive lipid analgesics is controlled by penetration into a deep lipid cavity. <i>Journal of Biological Chemistry</i> , 2021, 296, 100282.	1.6	7
6	The role of plasmalogens, Forssman lipids, and sphingolipid hydroxylation in modulating the biophysical properties of the epithelial plasma membrane. <i>Journal of Chemical Physics</i> , 2021, 154, 095101.	1.2	12
7	Coordination of Substrate Binding and Protonation in the <i>N.Âgonorrhoeae</i> MtrD Efflux Pump Controls the Functionally Rotating Transport Mechanism. <i>ACS Infectious Diseases</i> , 2021, 7, 1833-1847.	1.8	5
8	Enzyme inspired polymer functionalized with an artificial catalytic triad. <i>Polymer</i> , 2021, 225, 123735.	1.8	9
9	The Membrane Composition Defines the Spatial Organization and Function of a Major <i>Acinetobacter baumannii</i> Drug Efflux System. <i>MBio</i> , 2021, 12, e0107021.	1.8	14
10	A Unique Sequence Is Essential for Efficient Multidrug Efflux Function of the MtrD Protein of <i>Neisseria gonorrhoeae</i> . <i>MBio</i> , 2021, 12, e0167521.	1.8	1
11	The structural basis of bacterial manganese import. <i>Science Advances</i> , 2021, 7, .	4.7	17
12	Effect of the Force Field on Molecular Dynamics Simulations of the Multidrug Efflux Protein P-Glycoprotein. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6491-6508.	2.3	17
13	Investigating the lipid fingerprint of SLC6 neurotransmitter transporters: a comparison of dDAT, hDAT, hSERT, and GlyT2. <i>BBA Advances</i> , 2021, 1, 100010.	0.7	9
14	Site of Cholesterol Oxidation Impacts Its Localization and Domain Formation in the Neuronal Plasma Membrane. <i>ACS Chemical Neuroscience</i> , 2021, 12, 3873-3884.	1.7	4
15	Understanding the Link between Lipid Diversity and the Biophysical Properties of the Neuronal Plasma Membrane. <i>Biochemistry</i> , 2020, 59, 3010-3018.	1.2	23
16	Aryl urea substituted fatty acids: a new class of protonophoric mitochondrial uncoupler that utilises a synthetic anion transporter. <i>Chemical Science</i> , 2020, 11, 12677-12685.	3.7	14
17	Comparing Nonbonded Metal Ion Models in the Divalent Cation Binding Protein PsaA. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1913-1923.	2.3	15
18	A multifunctional surfactant catalyst inspired by hydrolases. <i>Science Advances</i> , 2020, 6, eaaz0404.	4.7	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. <i>Journal of Structural Biology</i> , 2020, 211, 107513.	1.3	7
20	High resolution crystal structure of a KRAS promoter G-quadruplex reveals a dimer with extensive poly-A i€-stacking interactions for small-molecule recognition. <i>Nucleic Acids Research</i> , 2020, 48, 5766-5776.	6.5	34
21	The Fats of Life: Using Computational Chemistry to Characterise the Eukaryotic Cell Membrane. <i>Australian Journal of Chemistry</i> , 2020, 73, 85.	0.5	7
22	Is protein structure enough? A review of the role of lipids in SLC6 transporter function. <i>Neuroscience Letters</i> , 2019, 700, 64-69.	1.0	5
23	The effects of oxidised phospholipids and cholesterol on the biophysical properties of POPC bilayers. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 210-219.	1.4	25
24	Mutation p.R356Q in the Collybistin Phosphoinositide Binding Site Is Associated With Mild Intellectual Disability. <i>Frontiers in Molecular Neuroscience</i> , 2019, 12, 60.	1.4	10
25	Multidrug Resistance in <i>Neisseria gonorrhoeae</i> : Identification of Functionally Important Residues in the MtrD Efflux Protein. <i>MBio</i> , 2019, 10, .	1.8	26
26	Probing the Pharmacological Binding Sites of P-Glycoprotein Using Umbrella Sampling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2287-2298.	2.5	17
27	Lipid-Based Inhibitors Act Directly on GlyT2. <i>ACS Chemical Neuroscience</i> , 2019, 10, 1668-1678.	1.7	10
28	Identification of an allosteric binding site on the human glycine transporter, GlyT2, for bioactive lipid analgesics. <i>ELife</i> , 2019, 8, .	2.8	26
29	A potential new, stable state of the E-cadherin strand-swapped dimer in solution. <i>European Biophysics Journal</i> , 2018, 47, 59-67.	1.2	1
30	Molecular Determinants for Substrate Interactions with the Glycine Transporter GlyT2. <i>ACS Chemical Neuroscience</i> , 2018, 9, 603-614.	1.7	30
31	The reliability of molecular dynamics simulations of the multidrug transporter P-glycoprotein in a membrane environment. <i>PLoS ONE</i> , 2018, 13, e0191882.	1.1	35
32	Synthetically controlling dendrimer flexibility improves delivery of large plasmid DNA. <i>Chemical Science</i> , 2017, 8, 2923-2930.	3.7	101
33	Structure of a lipid A phosphoethanolamine transferase suggests how conformational changes govern substrate binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2218-2223.	3.3	113
34	Simple Design of an Enzyme-Inspired Supported Catalyst Based on a Catalytic Triad. <i>CheM</i> , 2017, 2, 732-745.	5.8	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. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1587-1597.	1.7	25
36	Simple Design of an Enzyme-Inspired Supported Catalyst Based on a Catalytic Triad. <i>CheM</i> , 2017, 2, 893-894.	5.8	2

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37	Method for Developing Optical Sensors Using a Synthetic Dye-Fluorescent Protein FRET Pair and Computational Modeling and Assessment. <i>Methods in Molecular Biology</i> , 2017, 1596, 89-99.	0.4	2
38	Capturing the Dynamics of a Spring-Loaded Protein. <i>Structure</i> , 2017, 25, 963-964.	1.6	1
39	Location of contact residues in pharmacologically distinct drug binding sites on P-glycoprotein. <i>Biochemical Pharmacology</i> , 2017, 123, 19-28.	2.0	29
40	Thylakoid Ultrastructure: Visualizing the Photosynthetic Machinery. <i>Microbiology Monographs</i> , 2017, , 149-191.	0.3	0
41	Structural and dynamic perspectives on the promiscuous transport activity of P-glycoprotein. <i>Neurochemistry International</i> , 2016, 98, 146-152.	1.9	35
42	Rv2074 is a novel F ₄₂₀ H ₂ -dependent biliverdin reductase in <i>Mycobacterium tuberculosis</i> . <i>Protein Science</i> , 2016, 25, 1692-1709.	3.1	31
43	Hydrophobic Shielding Drives Catalysis of Hydride Transfer in a Family of F ₄₂₀ H ₂ -Dependent Enzymes. <i>Biochemistry</i> , 2016, 55, 6908-6918.	1.2	15
44	Rangefinder: A Semisynthetic FRET Sensor Design Algorithm. <i>ACS Sensors</i> , 2016, 1, 1286-1290.	4.0	11
45	Mechanism of JAK2 Activation by the Archetype Class I Cytokine Receptor, the Growth Hormone Receptor. <i>Biophysical Journal</i> , 2016, 110, 31a.	0.2	0
46	Understanding the accumulation of P-glycoprotein substrates within cells: The effect of cholesterol on membrane partitioning. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 776-782.	1.4	15
47	Identification of a 3rd Na ⁺ Binding Site of the Glycine Transporter, GlyT2. <i>PLoS ONE</i> , 2016, 11, e0157583.	1.1	28
48	Identification of Possible Binding Sites for Morphine and Nicardipine on the Multidrug Transporter P-Glycoprotein Using Umbrella Sampling Techniques. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1202-1217.	2.5	29
49	Dysregulation of transition metal ion homeostasis is the molecular basis for cadmium toxicity in <i>Streptococcus pneumoniae</i> . <i>Nature Communications</i> , 2015, 6, 6418.	5.8	117
50	Characterizing the conformational dynamics of metal-free PsaA using molecular dynamics simulations and electron paramagnetic resonance spectroscopy. <i>Biophysical Chemistry</i> , 2015, 207, 51-60.	1.5	8
51	Molecular Basis for the Interaction of the Mammalian Amino Acid Transporters B0AT1 and B0AT3 with Their Ancillary Protein Collectrin. <i>Journal of Biological Chemistry</i> , 2015, 290, 24308-24325.	1.6	51
52	Structural Characterization of Two Metastable ATP-Bound States of P-Glycoprotein. <i>PLoS ONE</i> , 2014, 9, e91916.	1.1	26
53	<sc>AdcA</sc> and <sc>AdcAll</sc> employ distinct zinc acquisition mechanisms and contribute additively to zinc homeostasis in <sc>S</sc><i>treptococcus pneumoniae</i>. <i>Molecular Microbiology</i> , 2014, 91, 834-851.	1.2	108
54	The central cavity of <sc>ABCB</sc>1 undergoes alternating access during <sc>ATP</sc> hydrolysis. <i>FEBS Journal</i> , 2014, 281, 2190-2201.	2.2	35

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55	Mechanism of Activation of Protein Kinase JAK2 by the Growth Hormone Receptor. <i>Science</i> , 2014, 344, 1249783.	6.0	340
56	Imperfect coordination chemistry facilitates metal ion release in the Psa permease. <i>Nature Chemical Biology</i> , 2014, 10, 35-41.	3.9	137
57	The ryanodine receptor store-sensing gate controls Ca ²⁺ waves and Ca ²⁺ -triggered arrhythmias. <i>Nature Medicine</i> , 2014, 20, 184-192.	15.2	172
58	Vancomycin: ligand recognition, dimerization and supercomplex formation. <i>FEBS Journal</i> , 2013, 280, 1294-1307.	2.2	41
59	Intestinal peptidases form functional complexes with the neutral amino acid transporter BOAT1. <i>Biochemical Journal</i> , 2012, 446, 135-148.	1.7	61
60	The Effect of Environment on the Structure of a Membrane Protein: P-Glycoprotein under Physiological Conditions. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3964-3976.	2.3	47
61	Molecular Dynamics Simulations of Membrane Proteins: Building Starting Structures and Example Applications. <i>Current Physical Chemistry</i> , 2012, 2, 363-378.	0.1	3
62	The Effect of Environment on the Recognition and Binding of Vancomycin to Native and Resistant Forms of Lipid II. <i>Biophysical Journal</i> , 2011, 101, 2684-2692.	0.2	36
63	Effect of Poly(ethylene glycol) (PEG) Spacers on the Conformational Properties of Small Peptides: A Molecular Dynamics Study. <i>Langmuir</i> , 2011, 27, 296-303.	1.6	35
64	Orientation of $\frac{1}{4}$ -Conotoxin P111A in a Sodium Channel Vestibule, Based on Voltage Dependence of Its Binding. <i>Molecular Pharmacology</i> , 2011, 80, 219-227.	1.0	23
65	Transmembrane helix 12 plays a pivotal role in coupling energy provision and drug binding in ABCB1. <i>FEBS Journal</i> , 2010, 277, 3974-3985.	2.2	22
66	ABC transporters: a riddle wrapped in a mystery inside an enigma. <i>Trends in Biochemical Sciences</i> , 2009, 34, 520-531.	3.7	160
67	Transmembrane Helix 12 Modulates Progression of the ATP Catalytic Cycle in ABCB1. <i>Biochemistry</i> , 2009, 48, 6249-6258.	1.2	27
68	Structural arrangement of the transmission interface in the antigen ABC transport complex TAP. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 5551-5556.	3.3	86
69	The mechanism of ABC transporters: general lessons from structural and functional studies of an antigenic peptide transporter. <i>FASEB Journal</i> , 2009, 23, 1287-1302.	0.2	155
70	Cytosolic Region of TM6 in P-Glycoprotein: Topographical Analysis and Functional Perturbation by Site Directed Labeling. <i>Biochemistry</i> , 2008, 47, 3615-3624.	1.2	18
71	Structure-based interpretation of the mutagenesis database for the nucleotide binding domains of P-glycoprotein. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008, 1778, 376-391.	1.4	29
72	ATP-binding cassette transporters in Escherichia coli. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008, 1778, 1757-1771.	1.4	139

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73	Non-linear intramolecular interactions and voltage sensitivity of a KV1 family potassium channel from <i>Polyorchis penicillatus</i> (Eschscholtz 1829). <i>Journal of Experimental Biology</i> , 2008, 211, 3442-3453.	0.8	8
74	P-glycoprotein models of the apo and ATP-bound states based on homology with Sav1866 and MalK. <i>FEBS Letters</i> , 2007, 581, 4217-4222.	1.3	80
75	Residue G346 in Transmembrane Segment Six is Involved in Inter-Domain Communication in P-Glycoprotein. <i>Biochemistry</i> , 2007, 46, 9899-9910.	1.2	41
76	Computer simulations of ABC transporter components This paper is one of a selection of papers published in this Special Issue, entitled CSBMCB "Membrane Proteins in Health and Disease". <i>Biochemistry and Cell Biology</i> , 2006, 84, 900-911.	0.9	12
77	Mechanism and Putative Structure of BO-like Neutral Amino Acid Transporters. <i>Journal of Membrane Biology</i> , 2006, 213, 111-118.	1.0	23
78	Homology Model of the GABAA Receptor Examined Using Brownian Dynamics. <i>Biophysical Journal</i> , 2005, 88, 3286-3299.	0.2	58
79	Permeation dynamics of chloride ions in the ClC-0 and ClC-1 channels. <i>Chemical Physics Letters</i> , 2004, 386, 233-238.	1.2	9
80	Conduction Mechanisms of Chloride Ions in ClC-Type Channels. <i>Biophysical Journal</i> , 2004, 86, 846-860.	0.2	71
81	A model of the glycine receptor deduced from Brownian dynamics studies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 4310-4315.	3.3	27
82	Polymer-solvent interactions as a tool to engineer material properties. <i>Molecular Systems Design and Engineering</i> , 0, , .	1.7	1