

Deborah K Shoemark

List of Publications by Year in descending order

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Version: 2024-02-01

37
papers

3,576
citations

516710

16
h-index

377865

34
g-index

52
all docs

52
docs citations

52
times ranked

8209
citing authors

#	ARTICLE	IF	CITATIONS
1	The fatty acid site is coupled to functional motifs in the SARS-CoV-2 spike protein and modulates spike allosteric behaviour. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 139-147.	4.1	19
2	Structural insights in cell-type specific evolution of intra-host diversity by SARS-CoV-2. <i>Nature Communications</i> , 2022, 13, 222.	12.8	23
3	Identification and validation of novel microtubule suppressors with an imidazopyridine scaffold through structure-based virtual screening and docking. <i>RSC Medicinal Chemistry</i> , 2022, 13, 929-943.	3.9	6
4	ESCPE-1 mediates retrograde endosomal sorting of the SARS-CoV-2 host factor Neuropilin-1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	17
5	Query-guided protein-protein interaction inhibitor discovery. <i>Chemical Science</i> , 2021, 12, 4753-4762.	7.4	5
6	Identification of β^2 -strand mediated protein-protein interaction inhibitors using ligand-directed fragment ligation. <i>Chemical Science</i> , 2021, 12, 2286-2293.	7.4	3
7	De Novo Designed Peptide and Protein Hairpins Self-Assemble into Sheets and Nanoparticles. <i>Small</i> , 2021, 17, e2100472.	10.0	18
8	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7098-7110.	13.8	77
9	Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein**. <i>Angewandte Chemie</i> , 2021, 133, 7174-7186.	2.0	6
10	A conserved arginine with non-conserved function is a key determinant of agonist selectivity in β_7 nicotinic ACh receptors. <i>British Journal of Pharmacology</i> , 2021, 178, 1651-1668.	5.4	6
11	Frontispiz: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein. <i>Angewandte Chemie</i> , 2021, 133, .	2.0	7
12	Frontispiece: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands of the Free Fatty Acid Pocket of the SARS-CoV-2 Spike Protein. <i>Angewandte Chemie - International Edition</i> , 2021, 60, .	13.8	0
13	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. <i>Biophysical Journal</i> , 2021, 120, 983-993.	0.5	43
14	Discovery of SARS-CoV-2 M ^{pro} peptide inhibitors from modelling substrate and ligand binding. <i>Chemical Science</i> , 2021, 12, 13686-13703.	7.4	54
15	Characterization and evolutionary origin of novel C ₂ H ₂ zinc finger protein (ZNF648) required for both erythroid and megakaryocyte differentiation in humans. <i>Haematologica</i> , 2021, 106, 2859-2873.	3.5	4
16	Neuropilin-1 is a host factor for SARS-CoV-2 infection. <i>Science</i> , 2020, 370, 861-865.	12.6	1,015
17	Small-residue packing motifs modulate the structure and function of a minimal de novo membrane protein. <i>Scientific Reports</i> , 2020, 10, 15203.	3.3	5
18	Characterisation of the transcriptome and proteome of SARS-CoV-2 reveals a cell passage induced in-frame deletion of the furin-like cleavage site from the spike glycoprotein. <i>Genome Medicine</i> , 2020, 12, 68.	8.2	386

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19	Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein. <i>Science</i> , 2020, 370, 725-730.	12.6	348
20	Modelling the early evolution of extracellular matrix from modern Ctenophores and Sponges. <i>Essays in Biochemistry</i> , 2019, 63, 389-405.	4.7	11
21	The dynamical interplay between a megadalton peptide nanocage and solutes probed by microsecond atomistic MD; implications for design. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 137-147.	2.8	5
22	Identification of the Initial Steps in Signal Transduction in the $\alpha 4\beta 2$ Nicotinic Receptor: Insights from Equilibrium and Nonequilibrium Simulations. <i>Structure</i> , 2019, 27, 1171-1183.e3.	3.3	24
23	Guiding Biomolecular Interactions in Cells Using <i>de Novo</i> Protein-Protein Interfaces. <i>ACS Synthetic Biology</i> , 2019, 8, 1284-1293.	3.8	35
24	Emergence of a Thrombospondin Superfamily at the Origin of Metazoans. <i>Molecular Biology and Evolution</i> , 2019, 36, 1220-1238.	8.9	5
25	Antiproliferative and Antimigratory Effects of a Novel YAP-TEAD Interaction Inhibitor Identified Using <i>Silico</i> Molecular Docking. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1291-1305.	6.4	66
26	Intraring allostery controls the function and assembly of a heterooligomeric class II chaperonin. <i>FASEB Journal</i> , 2018, 32, 2223-2234.	0.5	1
27	The <i>de novo</i> design of a biocompatible and functional integral membrane protein using minimal sequence complexity. <i>Scientific Reports</i> , 2018, 8, 14564.	3.3	16
28	Unlocking Nicotinic Selectivity via Direct C-H Functionalization of α -Cytisine. <i>CheM</i> , 2018, 4, 1710-1725.	11.7	31
29	ACTN1 variants associated with thrombocytopenia. <i>Platelets</i> , 2017, 28, 625-627.	2.3	18
30	Beyond icosahedral symmetry in packings of proteins in spherical shells. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 9014-9019.	7.1	36
31	Decorating Self-Assembled Peptide Cages with Proteins. <i>ACS Nano</i> , 2017, 11, 7901-7914.	14.6	55
32	16S rRNA Next Generation Sequencing Analysis Shows Bacteria in Alzheimer's Post-Mortem Brain. <i>Frontiers in Aging Neuroscience</i> , 2017, 9, 195.	3.4	234
33	The Microbiome and Disease: Reviewing the Links between the Oral Microbiome, Aging, and Alzheimer's Disease. <i>Journal of Alzheimer's Disease</i> , 2014, 43, 725-738.	2.6	175
34	GDNF, NGF and BDNF as therapeutic options for neurodegeneration. , 2013, 138, 155-175.		624
35	Identification of novel small molecule TGF- $\beta 2$ antagonists using structure-based drug design. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 365-372.	2.9	7
36	Structure of Bacterial Glutathione-S-Transferase Maleyl Pyruvate Isomerase and Implications for Mechanism of Isomerisation. <i>Journal of Molecular Biology</i> , 2008, 384, 165-177.	4.2	20

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37	Enzymatic properties of the lactate dehydrogenase enzyme from Plasmodium falciparum. FEBS Journal, 2007, 274, 2738-2748.	4.7	49