

Syma Khalid

List of Publications by Year in descending order

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81
papers

4,008
citations

109264

35
h-index

133188

59
g-index

85
all docs

85
docs citations

85
times ranked

4980
citing authors

#	ARTICLE	IF	CITATIONS
1	Simulations of the spike: molecular dynamics and SARS-CoV-2. <i>Nature Reviews Microbiology</i> , 2022, 20, 192-192.	13.6	11
2	Lipid bilayers as potential ice nucleating agents. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6476-6491.	1.3	3
3	Translocation of flexible and tensioned ssDNA through <i>in silico</i> designed hydrophobic nanopores with two constrictions. <i>Nanoscale</i> , 2021, 13, 1673-1679.	2.8	1
4	The hitchhiker's guide to the periplasm: Unexpected molecular interactions of polymyxin B1 in <i>E. coli</i> . <i>Structure</i> , 2021, 29, 444-456.e2.	1.6	20
5	Structural Basis for Silicic Acid Uptake by Higher Plants. <i>Journal of Molecular Biology</i> , 2021, 433, 167226.	2.0	18
6	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 831-839.	2.5	59
7	Polymyxin B1 within the <i>E. coli</i> cell envelope: insights from molecular dynamics simulations. <i>Biophysical Reviews</i> , 2021, 13, 1061-1070.	1.5	7
8	A Computational Swiss Army Knife Approach to Unraveling the Secrets of Proton Movement through SERCA. <i>Biophysical Journal</i> , 2020, 119, 890-891.	0.2	0
9	Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling?. <i>Journal of Chemical Physics</i> , 2020, 153, 044122.	1.2	10
10	To infect or not to infect: molecular determinants of bacterial outer membrane vesicle internalization by host membranes. <i>Journal of Molecular Biology</i> , 2020, 432, 1251-1264.	2.0	21
11	Distinct Intramolecular Hydrogen Bonding Dictates Antimicrobial Action of Membrane-Targeting Amphiphiles. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 754-760.	2.1	22
12	Outer Membrane Proteins OmpA, FhuA, OmpF, EstA, BtuB, and OmpX Have Unique Lipopolysaccharide Fingerprints. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2608-2619.	2.3	34
13	Movement of Arginine through OprD: The Energetics of Permeation and the Role of Lipopolysaccharide in Directing Arginine to the Protein. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2824-2832.	1.2	20
14	Details of hydrophobic entanglement between small molecules and Braun's lipoprotein within the cavity of the bacterial chaperone LolA. <i>Scientific Reports</i> , 2019, 9, 3717.	1.6	11
15	Role of O-Antigen in Response to Mechanical Stress of the <i>E. coli</i> Outer Membrane: Insights from Coarse-Grained MD Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3567-3575.	1.2	43
16	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1393.	6.2	110
17	Binding from Both Sides: TolR and Full-Length OmpA Bind and Maintain the Local Structure of the <i>E. coli</i> Cell Wall. <i>Structure</i> , 2019, 27, 713-724.e2.	1.6	42
18	Atomistic and Coarse Grain Simulations of the Cell Envelope of Gram-Negative Bacteria: What Have We Learned?. <i>Accounts of Chemical Research</i> , 2019, 52, 180-188.	7.6	42

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19	Communication between the leaflets of asymmetric membranes revealed from coarse-grain molecular dynamics simulations. <i>Scientific Reports</i> , 2018, 8, 1805.	1.6	24
20	Prediction of the Closed Conformation and Insights into the Mechanism of the Membrane Enzyme LpxR. <i>Biophysical Journal</i> , 2018, 115, 1445-1456.	0.2	4
21	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018, 251, 609-631.	1.0	33
22	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. <i>Structure</i> , 2018, 26, 1151-1161.e4.	1.6	32
23	The role of the jaw subdomain of peptidoglycan glycosyltransferases for lipid II polymerization. <i>Cell Surface</i> , 2018, 2, 54-66.	1.5	8
24	Directional Porin Binding of Intrinsically Disordered Protein Sequences Promotes Colicin Epitope Display in the Bacterial Periplasm. <i>Biochemistry</i> , 2018, 57, 4374-4381.	1.2	12
25	Electric-Field-Driven Translocation of ssDNA through Hydrophobic Nanopores. <i>ACS Nano</i> , 2018, 12, 8208-8213.	7.3	13
26	Through the Lipopolysaccharide Glass: A Potent Antimicrobial Peptide Induces Phase Changes in Membranes. <i>Biochemistry</i> , 2017, 56, 1672-1679.	1.2	39
27	Progress in Molecular Dynamics Simulations of Gram-Negative Bacterial Cell Envelopes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2513-2518.	2.1	33
28	PyCGTOOL: Automated Generation of Coarse-Grained Molecular Dynamics Models from Atomistic Trajectories. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 650-656.	2.5	66
29	Braunâ€™s Lipoprotein Facilitates OmpA Interaction with the <i>Escherichia coli</i> Cell Wall. <i>Biophysical Journal</i> , 2017, 113, 1496-1504.	0.2	55
30	It Is Complicated: Curvature, Diffusion, and Lipid Sorting within the Two Membranes of <i>Escherichia coli</i> . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5513-5518.	2.1	52
31	Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. <i>PLoS ONE</i> , 2016, 11, e0156963.	1.1	28
32	Molecular Dynamics Simulations Reveal the Conformational Flexibility of Lipid II and Its Loose Association with the Defensin Plectasin in the <i>Staphylococcus aureus</i> Membrane. <i>Biochemistry</i> , 2016, 55, 3303-3314.	1.2	18
33	Molecular Dynamics Simulations Predict the Pathways via Which Pristine Fullerenes Penetrate Bacterial Membranes. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11170-11179.	1.2	68
34	The Free Energy of Small Solute Permeation through the <i>Escherichia coli</i> Outer Membrane Has a Distinctly Asymmetric Profile. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3446-3451.	2.1	57
35	OmpA: A Flexible Clamp for Bacterial Cell Wall Attachment. <i>Structure</i> , 2016, 24, 2227-2235.	1.6	76
36	Full-Length OmpA: Structure, Function, and Membrane Interactions Predicted by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2016, 111, 1692-1702.	0.2	67

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37	Structural basis for Mep2 ammonium transceptor activation by phosphorylation. <i>Nature Communications</i> , 2016, 7, 11337.	5.8	52
38	Encapsulated membrane proteins: A simplified system for molecular simulation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2549-2557.	1.4	25
39	An Accurate In Vitro Model of the <i>E. coli</i> Envelope. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11952-11955.	7.2	91
40	The membranes of Gram-negative bacteria: progress in molecular modelling and simulation. <i>Biochemical Society Transactions</i> , 2015, 43, 162-167.	1.6	23
41	DNA sequencing with MspA: Molecular Dynamics simulations reveal free-energy differences between sequencing and non-sequencing mutants. <i>Scientific Reports</i> , 2015, 5, 12783.	1.6	6
42	The Nucleotide Capture Region of Alpha Hemolysin: Insights into Nanopore Design for DNA Sequencing from Molecular Dynamics Simulations. <i>Nanomaterials</i> , 2015, 5, 144-153.	1.9	10
43	Free-Energy Calculations Reveal the Subtle Differences in the Interactions of DNA Bases with β -Hemolysin. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 810-816.	2.3	4
44	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. <i>Journal of Membrane Biology</i> , 2015, 248, 611-640.	1.0	157
45	Molecular Simulations of Gram-Negative Bacterial Membranes: A Vignette of Some Recent Successes. <i>Biophysical Journal</i> , 2015, 109, 461-468.	0.2	39
46	Interaction between the NS4B amphipathic helix, AH2, and charged lipid headgroups alters membrane morphology and AH2 oligomeric state – Implications for the Hepatitis C virus life cycle. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015, 1848, 1671-1677.	1.4	15
47	Interaction of the Antimicrobial Peptide Polymyxin B1 with Both Membranes of <i>E. coli</i> : A Molecular Dynamics Study. <i>PLoS Computational Biology</i> , 2015, 11, e1004180.	1.5	134
48	Atomistic Molecular-Dynamics Simulations Enable Prediction of the Arginine Permeation Pathway through OccD1/OprD from <i>Pseudomonas aeruginosa</i> . <i>Biophysical Journal</i> , 2014, 107, 1853-1861.	0.2	23
49	The NorM MATE Transporter from <i>N. gonorrhoeae</i> : Insights into Drug and Ion Binding from Atomistic Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2014, 107, 460-468.	0.2	20
50	Conformational dynamics and membrane interactions of the <i>E. coli</i> outer membrane protein FecA: A molecular dynamics simulation study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2013, 1828, 284-293.	1.4	66
51	Molecular Dynamics Simulations of Phosphatidylcholine Membranes: A Comparative Force Field Study. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4593-4609.	2.3	176
52	Single-Stranded DNA within Nanopores: Conformational Dynamics and Implications for Sequencing; a Molecular Dynamics Simulation Study. <i>Biophysical Journal</i> , 2012, 103, 1028-1036.	0.2	104
53	Probing the oligomeric state and interaction surfaces of Fukutin-I in dilauroylphosphatidylcholine bilayers. <i>European Biophysics Journal</i> , 2012, 41, 199-207.	1.2	13
54	Electroporation of the <i>E. coli</i> and <i>S. Aureus</i> Membranes: Molecular Dynamics Simulations of Complex Bacterial Membranes. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13381-13388.	1.2	219

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55	Molecular Dynamics Simulations of DNA within a Nanopore: Arginine~Phosphate Tethering and a Binding/Sliding Mechanism for Translocation. <i>Biochemistry</i> , 2011, 50, 3777-3783.	1.2	26
56	Exploring the conformational dynamics and membrane interactions of PorB from <i>C. glutamicum</i> : A multi-scale molecular dynamics simulation study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1746-1752.	1.4	6
57	A positively charged channel within the Smc1/Smc3 hinge required for sister chromatid cohesion. <i>EMBO Journal</i> , 2011, 30, 364-378.	3.5	69
58	DNA Lipoplexes: Formation of the Inverse Hexagonal Phase Observed by Coarse-Grained Molecular Dynamics Simulation. <i>Langmuir</i> , 2010, 26, 12119-12125.	1.6	39
59	Both Interaction Surfaces within Cohesin's Hinge Domain Are Essential for Its Stable Chromosomal Association. <i>Current Biology</i> , 2010, 20, 279-289.	1.8	28
60	Bookshelf: a simple curation system for the storage of biomolecular simulation data. <i>Database: the Journal of Biological Databases and Curation</i> , 2010, 2010, baq033-baq033.	1.4	6
61	Stability and Membrane Orientation of the Fukutin Transmembrane Domain: A Combined Multiscale Molecular Dynamics and Circular Dichroism Study. <i>Biochemistry</i> , 2010, 49, 10796-10802.	1.2	24
62	On the Ability of PAMAM Dendrimers and Dendrimer/DNA Aggregates To Penetrate POPC Model Biomembranes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7229-7244.	1.2	53
63	Antimicrobial and Cell-Penetrating Peptides: Structure, Assembly and Mechanisms of Membrane Lysis via Atomistic and Coarse-Grained Molecular Dynamic Simulations. <i>Protein and Peptide Letters</i> , 2010, 17, 1313-1327.	0.4	37
64	DNA and lipid bilayers: self-assembly and insertion. <i>Journal of the Royal Society Interface</i> , 2008, 5, 241-250.	1.5	64
65	Coarse-Grained MD Simulations of Membrane Protein-Bilayer Self-Assembly. <i>Structure</i> , 2008, 16, 621-630.	1.6	199
66	Self-Assembly of a Simple Membrane Protein: Coarse-Grained Molecular Dynamics Simulations of the Influenza M2 Channel. <i>Biophysical Journal</i> , 2008, 95, 3790-3801.	0.2	69
67	OmpA: Gating and dynamics via molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2008, 1778, 1871-1880.	1.4	53
68	Outer membrane protein C: Engineering a quiet pore for biosensing. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 6272-6277.	3.3	160
69	Conformational dynamics of the mitochondrial ADP/ATP carrier: a simulation study. <i>Molecular Membrane Biology</i> , 2008, 25, 506-517.	2.0	17
70	A multidomain outer membrane protein from <i>Pasteurella multocida</i> : Modelling and simulation studies of PmOmpA. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2007, 1768, 2831-2840.	1.4	19
71	Coarse-grained molecular dynamics simulations of membrane proteins and peptides. <i>Journal of Structural Biology</i> , 2007, 157, 593-605.	1.3	303
72	Enantiomeric resolution of supramolecular helicates with different surface topographies. <i>Dalton Transactions</i> , 2007, , 734-742.	1.6	51

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73	Molecular Dynamics Simulations of Inwardly Rectifying (Kir) Potassium Channels: A Comparative Study. <i>Biochemistry</i> , 2007, 46, 3643-3652.	1.2	40
74	Shape effects on the activity of synthetic major-groove binding ligands. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 25, 794-800.	1.3	3
75	Influence of surface shape on DNA binding of bimetallo helicates. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 1937-1945.	1.5	45
76	Modeling and simulations of a bacterial outer membrane protein: OprF from <i>Pseudomonas aeruginosa</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 6-15.	1.5	27
77	Simulations of DNA Coiling around a Synthetic Supramolecular Cylinder That Binds in the DNA Major Groove. <i>Chemistry - A European Journal</i> , 2006, 12, 3493-3506.	1.7	37
78	Molecular dynamics simulations of a bacterial autotransporter: NalP from <i>Neisseria meningitidis</i> . <i>Molecular Membrane Biology</i> , 2006, 23, 499-508.	2.0	35
79	Theoretical Aspects of the Enantiomeric Resolution of Dimetallo Helicates with Different Surface Topologies on Cellulose Columns. <i>Journal of Liquid Chromatography and Related Technologies</i> , 2005, 28, 2995-3003.	0.5	9
80	Molecular Dynamics Simulations of Dna and Its Complexes. <i>Progress in Reaction Kinetics and Mechanism</i> , 2004, 29, 167-186.	1.1	2
81	Intramolecular DNA coiling mediated by metallo-supramolecular cylinders: Differential binding of P and M helical enantiomers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 5069-5074.	3.3	194