Syma Khalid

List of Publications by Year
in descending order

81 papers	4,008 citations	109137 35 h-index	133063 59 g-index
85 all docs	85 docs citations	85 times ranked	4980 citing authors

#	Article	IF	Citations
1	Coarse-grained molecular dynamics simulations of membrane proteins and peptides. Journal of Structural Biology, 2007, 157, 593-605.	1.3	303
2	Electroporation of the E. coli and S. Aureus Membranes: Molecular Dynamics Simulations of Complex Bacterial Membranes. Journal of Physical Chemistry B, 2011, 115, 13381-13388.	1.2	219
3	Coarse-Grained MD Simulations of Membrane Protein-Bilayer Self-Assembly. Structure, 2008, 16, 621-630.	1.6	199
4	Intramolecular DNA coiling mediated by metallo-supramolecular cylinders: Differential binding of P and M helical enantiomers. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 5069-5074.	3.3	194
5	Molecular Dynamics Simulations of Phosphatidylcholine Membranes: A Comparative Force Field Study. Journal of Chemical Theory and Computation, 2012, 8, 4593-4609.	2.3	176
6	Outer membrane protein G: Engineering a quiet pore for biosensing. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6272-6277.	3.3	160
7	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
8	Interaction of the Antimicrobial Peptide Polymyxin B1 with Both Membranes of E. coli: A Molecular Dynamics Study. PLoS Computational Biology, 2015, 11, e1004180.	1.5	134
9	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
10	Single-Stranded DNA within Nanopores: Conformational Dynamics and Implications for Sequencing; a Molecular Dynamics Simulation Study. Biophysical Journal, 2012, 103, 1028-1036.	0.2	104
11	An Accurate In Vitro Model of the E.â€...coli Envelope. Angewandte Chemie - International Edition, 2015, 54, 11952-11955.	7.2	91
12	OmpA: A Flexible Clamp for Bacterial Cell Wall Attachment. Structure, 2016, 24, 2227-2235.	1.6	76
13	Self-Assembly of a Simple Membrane Protein: Coarse-Grained Molecular Dynamics Simulations of the Influenza M2 Channel. Biophysical Journal, 2008, 95, 3790-3801.	0.2	69
14	A positively charged channel within the Smc1/Smc3 hinge required for sister chromatid cohesion. EMBO Journal, 2011, 30, 364-378.	3.5	69
15	Molecular Dynamics Simulations Predict the Pathways via Which Pristine Fullerenes Penetrate Bacterial Membranes. Journal of Physical Chemistry B, 2016, 120, 11170-11179.	1.2	68
16	Full-Length OmpA: Structure, Function, and Membrane Interactions Predicted by Molecular Dynamics Simulations. Biophysical Journal, 2016, 111, 1692-1702.	0.2	67
17	Conformational dynamics and membrane interactions of the E. coli outer membrane protein FecA: A molecular dynamics simulation study. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 284-293.	1.4	66
18	PyCGTOOL: Automated Generation of Coarse-Grained Molecular Dynamics Models from Atomistic Trajectories. Journal of Chemical Information and Modeling, 2017, 57, 650-656.	2.5	66

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19	DNA and lipid bilayers: self-assembly and insertion. Journal of the Royal Society Interface, 2008, 5, 241-250.	1.5	64
20	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	2.5	59
21	The Free Energy of Small Solute Permeation through the Escherichia coli Outer Membrane Has a Distinctly Asymmetric Profile. Journal of Physical Chemistry Letters, 2016, 7, 3446-3451.	2.1	57
22	Braunâ€™s Lipoprotein Facilitates OmpA Interaction with the Escherichia coli Cell Wall. Biophysical Journal, 2017, 113, 1496-1504.	0.2	55
23	OmpA: Gating and dynamics via molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1871-1880.	1.4	53
24	On the Ability of PAMAM Dendrimers and Dendrimer/DNA Aggregates To Penetrate POPC Model Biomembranes. Journal of Physical Chemistry B, 2010, 114, 7229-7244.	1.2	53
25	Structural basis for Mep2 ammonium transceptor activation by phosphorylation. Nature Communications, 2016, 7, 11337.	5.8	52
26	It Is Complicated: Curvature, Diffusion, and Lipid Sorting within the Two Membranes of Escherichia coli. Journal of Physical Chemistry Letters, 2017, 8, 5513-5518.	2.1	52
27	Enantiomeric resolution of supramolecular helicates with different surface topographies. Dalton Transactions, 2007, , 734-742.	1.6	51
28	Influence of surface shape on DNA binding of bimetallo helicates. Journal of Inorganic Biochemistry, 2007, 101, 1937-1945.	1.5	45
29	Role of O-Antigen in Response to Mechanical Stress of the E. coli Outer Membrane: Insights from Coarse-Grained MD Simulations. Journal of Physical Chemistry B, 2019, 123, 3567-3575.	1.2	43
30	Binding from Both Sides: TolR and Full-Length OmpA Bind and Maintain the Local Structure of the E.Âcoli Cell Wall. Structure, 2019, 27, 713-724.e2.	1.6	42
31	Atomistic and Coarse Grain Simulations of the Cell Envelope of Gram-Negative Bacteria: What Have We Learned?. Accounts of Chemical Research, 2019, 52, 180-188.	7.6	42
32	Molecular Dynamics Simulations of Inwardly Rectifying (Kir) Potassium Channels:Â A Comparative Studyâ€. Biochemistry, 2007, 46, 3643-3652.	1.2	40
33	DNA Lipoplexes: Formation of the Inverse Hexagonal Phase Observed by Coarse-Grained Molecular Dynamics Simulation. Langmuir, 2010, 26, 12119-12125.	1.6	39
34	Molecular Simulations of Gram-Negative Bacterial Membranes: A Vignette of Some Recent Successes. Biophysical Journal, 2015, 109, 461-468.	0.2	39
35	Through the Lipopolysaccharide Glass: A Potent Antimicrobial Peptide Induces Phase Changes in Membranes. Biochemistry, 2017, 56, 1672-1679.	1.2	39
36	Simulations of DNA Coiling around a Synthetic Supramolecular Cylinder That Binds in the DNA Major Groove. Chemistry - A European Journal, 2006, 12, 3493-3506.	1.7	37

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37	Antimicrobial and Cell-Penetrating Peptides: Structure, Assembly and Mechanisms of Membrane Lysis via Atomistic and Coarse-Grained Molecular Dynamic Simulations. Protein and Peptide Letters, 2010, 17, 1313-1327.	0.4	37
38	Molecular dynamics simulations of a bacterial autotransporter: NalP fromNeisseria meningitidis. Molecular Membrane Biology, 2006, 23, 499-508.	2.0	35
39	Outer Membrane Proteins OmpA, FhuA, OmpF, EstA, BtuB, and OmpX Have Unique Lipopolysaccharide Fingerprints. Journal of Chemical Theory and Computation, 2019, 15, 2608-2619.	2.3	34
40	Progress in Molecular Dynamics Simulations of Gram-Negative Bacterial Cell Envelopes. Journal of Physical Chemistry Letters, 2017, 8, 2513-2518.	2.1	33
41	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. Journal of Membrane Biology, 2018, 251, 609-631.	1.0	33
42	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. Structure, 2018, 26, 1151-1161.e4.	1.6	32
43	Both Interaction Surfaces within Cohesin's Hinge Domain Are Essential for Its Stable Chromosomal Association. Current Biology, 2010, 20, 279-289.	1.8	28
44	Dynamics of Crowded Vesicles: Local and Global Responses to Membrane Composition. PLoS ONE, 2016, 11, e0156963.	1.1	28
45	Modeling and simulations of a bacterial outer membrane protein: OprF from Pseudomonas aeruginosa. Proteins: Structure, Function and Bioinformatics, 2006, 63, 6-15.	1.5	27
46	Molecular Dynamics Simulations of DNA within a Nanopore: Argincâ˜Phosphate Tethering and a Binding/Sliding Mechanism for Translocation. Biochemistry, 2011, 50, 3777-3783.	1.2	26
47	Encapsulated membrane proteins: A simplified system for molecular simulation. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2549-2557.	1.4	25
48	Stability and Membrane Orientation of the Fukutin Transmembrane Domain: A Combined Multiscale Molecular Dynamics and Circular Dichroism Study. Biochemistry, 2010, 49, 10796-10802.	1.2	24
49	Communication between the leaflets of asymmetric membranes revealed from coarse-grain molecular dynamics simulations. Scientific Reports, 2018, 8, 1805.	1.6	24
50	Atomistic Molecular-Dynamics Simulations Enable Prediction of the Arginine Permeation Pathway through OccD1/OprD from PseudomonasÂaeruginosa. Biophysical Journal, 2014, 107, 1853-1861.	0.2	23
51	The membranes of Gram-negative bacteria: progress in molecular modelling and simulation. Biochemical Society Transactions, 2015, 43, 162-167.	1.6	23
52	Distinct Intramolecular Hydrogen Bonding Dictates Antimicrobial Action of Membrane-Targeting Amphiphiles. Journal of Physical Chemistry Letters, 2019, 10, 754-760.	2.1	22
53	To infect or not to infect: molecular determinants of bacterial outer membrane vesicle internalization by host membranes. Journal of Molecular Biology, 2020, 432, 1251-1264.	2.0	21
54	The NorM MATE Transporter from N.Âgonorrhoeae: Insights into Drug and Ion Binding from Atomistic Molecular Dynamics Simulations. Biophysical Journal, 2014, 107, 460-468.	0.2	20

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55	Movement of Arginine through OprD: The Energetics of Permeation and the Role of Lipopolysaccharide in Directing Arginine to the Protein. Journal of Physical Chemistry B, 2019, 123, 2824-2832.	1.2	20
56	The hitchhiker's guide to the periplasm: Unexpected molecular interactions of polymyxin B1 in E. coli. Structure, 2021, 29, 444-456.e2.	1.6	20
57	A multidomain outer membrane protein from Pasteurella multocida: Modelling and simulation studies of PmOmpA. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 2831-2840.	1.4	19
58	Molecular Dynamics Simulations Reveal the Conformational Flexibility of Lipid II and Its Loose Association with the Defensin Plectasin in the Staphylococcus aureus Membrane. Biochemistry, 2016, 55, 3303-3314.	1.2	18
59	Structural Basis for Silicic Acid Uptake by Higher Plants. Journal of Molecular Biology, 2021, 433, 167226.	2.0	18
60	Conformational dynamics of the mitochondrial ADP/ATP carrier: a simulation study. Molecular Membrane Biology, 2008, 25, 506-517.	2.0	17
61	Interaction between the NS4B amphipathic helix, AH2, and charged lipid headgroups alters membrane morphology and AH2 oligomeric state â€" Implications for the Hepatitis C virus life cycle. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1671-1677.	1.4	15
62	Probing the oligomeric state and interaction surfaces of Fukutin-I in dilauroylphosphatidylcholine bilayers. European Biophysics Journal, 2012, 41, 199-207.	1.2	13
63	Electric-Field-Driven Translocation of ssDNA through Hydrophobic Nanopores. ACS Nano, 2018, 12, 8208-8213.	7.3	13
64	Directional Porin Binding of Intrinsically Disordered Protein Sequences Promotes Colicin Epitope Display in the Bacterial Periplasm. Biochemistry, 2018, 57, 4374-4381.	1.2	12
65	Details of hydrophobic entanglement between small molecules and Braunâ€™s lipoprotein within the cavity of the bacterial chaperone LolA. Scientific Reports, 2019, 9, 3717.	1.6	11
66	Simulations of the spike: molecular dynamics and SARS-CoV-2. Nature Reviews Microbiology, 2022, 20, 192-192.	13.6	11
67	The Nucleotide Capture Region of Alpha Hemolysin: Insights into Nanopore Design for DNA Sequencing from Molecular Dynamics Simulations. Nanomaterials, 2015, 5, 144-153.	1.9	10
68	Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling?. Journal of Chemical Physics, 2020, 153, 044122.	1.2	10
69	Theoretical Aspects of the Enantiomeric Resolution of Dimetallo Helicates with Different Surface Topologies on Cellulose Columns. Journal of Liquid Chromatography and Related Technologies, 2005, 28, 2995-3003.	0.5	9
70	The role of the jaw subdomain of peptidoglycan glycosyltransferases for lipid II polymerization. Cell Surface, 2018, 2, 54-66.	1.5	8
71	Polymyxin B1 within the E. coli cell envelope: insights from molecular dynamics simulations. Biophysical Reviews, 2021, 13, 1061-1070.	1.5	7
72	Bookshelf: a simple curation system for the storage of biomolecular simulation data. Database: the Journal of Biological Databases and Curation, 2010, 2010, baq033-baq033.	1.4	6

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73	Exploring the conformational dynamics and membrane interactions of PorB from C. glutamicum: A multi-scale molecular dynamics simulation study. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1746-1752.	1.4	6
74	DNA sequencing with MspA: Molecular Dynamics simulations reveal free-energy differences between sequencing and non-sequencing mutants. Scientific Reports, 2015, 5, 12783.	1.6	6
75	Free-Energy Calculations Reveal the Subtle Differences in the Interactions of DNA Bases with Î±-Hemolysin. Journal of Chemical Theory and Computation, 2015, 11, 810-816.	2.3	4
76	Prediction of the Closed Conformation and Insights into the Mechanism of the Membrane Enzyme LpxR. Biophysical Journal, 2018, 115, 1445-1456.	0.2	4
77	Shape effects on the activity of synthetic major-groove binding ligands. Journal of Molecular Graphics and Modelling, 2007, 25, 794-800.	1.3	3
78	Lipid bilayers as potential ice nucleating agents. Physical Chemistry Chemical Physics, 2022, 24, 6476-6491.	1.3	3
79	Molecular Dynamics Simulations of Dna and Its Complexes. Progress in Reaction Kinetics and Mechanism, 2004, 29, 167-186.	1.1	2
80	Translocation of flexible and tensioned ssDNA through in silico designed hydrophobic nanopores with two constrictions. Nanoscale, 2021, 13, 1673-1679.	2.8	1
81	A Computational Swiss Army Knife Approach toÂUnraveling the Secrets of Proton Movement through SERCA. Biophysical Journal, 2020, 119, 890-891.	0.2	0