## Mounir Tarek

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	The role of catechin in electroporation of pancreatic cancer cells – Effects on pore formation and multidrug resistance proteins. Bioelectrochemistry, 2022, 147, 108199.	2.4	4
2	Mechanisms of curcumin-based photodynamic therapy and its effects in combination with electroporation: An in vitro and molecular dynamics study. Bioelectrochemistry, 2021, 140, 107806.	2.4	14
3	Editorial: Molecular Mechanisms of Voltage-Gating in Ion Channels. Frontiers in Pharmacology, 2021, 12, 768153.	1.6	2
4	Molecular dynamics simulations of the effects of lipid oxidation on the permeability of cell membranes. Bioelectrochemistry, 2021, 141, 107869.	2.4	23
5	Oxidative Effects during Irreversible Electroporation of Melanoma Cells—In Vitro Study. Molecules, 2021, 26, 154.	1.7	28
6	Atorvastatin Modulates the Efficacy of Electroporation and Calcium Electrochemotherapy. International Journal of Molecular Sciences, 2021, 22, .	1.8	1
7	Atorvastatin Modulates the Efficacy of Electroporation and Calcium Electrochemotherapy. International Journal of Molecular Sciences, 2021, 22, 11245.	1.8	9
8	In Vitro Study of Calcium Microsecond Electroporation of Prostate Adenocarcinoma Cells. Molecules, 2020, 25, 5406.	1.7	11
9	Cepharanthine induces ROS stress in glioma and neuronal cells via modulation of VDAC permeability. Saudi Pharmaceutical Journal, 2020, 28, 1364-1373.	1.2	8
10	Lipid composition of the cancer cell membrane. Journal of Bioenergetics and Biomembranes, 2020, 52, 321-342.	1.0	190
11	Two-stage "Hand-and-Elbow―Gating Mechanism of a KV Channel. Biophysical Journal, 2020, 118, 113a.	0.2	0
12	New insights on the role of ROS in the mechanisms of sonoporation-mediated gene delivery. Ultrasonics Sonochemistry, 2020, 64, 104998.	3.8	16
13	Two-stage electro–mechanical coupling of a KV channel in voltage-dependent activation. Nature Communications, 2020, 11, 676.	5.8	46
14	The contribution of lipid peroxidation to membrane permeability in electropermeabilization: A molecular dynamics study. Bioelectrochemistry, 2019, 125, 46-57.	2.4	71
15	Membrane Electroporation and Electropermeabilization: Mechanisms and Models. Annual Review of Biophysics, 2019, 48, 63-91.	4.5	417
16	Effects of hydration on the protonation state of a lysine analog crossing a phospholipid bilayer – insights from molecular dynamics and free-energy calculations. Physical Chemistry Chemical Physics, 2018, 20, 9101-9107.	1.3	9
17	Studying Kv Channels Function using Computational Methods. Methods in Molecular Biology, 2018, 1684, 321-341.	0.4	4

18 Electrical Conductance of Lipid Pores. , 2017, , 219-233.

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19	Notice of Removal: New insights in the role of reactive oxygen species in mechanisms of sonoporation: In-vitro validation and molecular dynamic simulations. , 2017, , .		1
20	Atomistic Simulations of Electroporation of Model Cell Membranes. Advances in Anatomy, Embryology and Cell Biology, 2017, 227, 1-15.	1.0	3
21	A molecular insight into the electro-transfer of small molecules through electropores driven by electric fields. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2278-2289.	1.4	66
22	In-Silico Electrophysiology: On the Activation of Voltage-Gated Ion Channels using Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 107a.	0.2	1
23	Properties of lipid electropores II: Comparison of continuum-level modeling of pore conductance to molecular dynamics simulations. Bioelectrochemistry, 2016, 112, 112-124.	2.4	25
24	Properties of lipid electropores I: Molecular dynamics simulations of stabilized pores by constant charge imbalance. Bioelectrochemistry, 2016, 109, 108-116.	2.4	42
25	Electrical Conductance of Lipid Pores. , 2016, , 1-15.		0
26	Molecular Determinants of Voltage Sensor Domain Activation. Biophysical Journal, 2015, 108, 427a.	0.2	0
27	PIP2 Modifies the Free Energy of the Kv1.2 Voltage-Sensor Activation. Biophysical Journal, 2015, 108, 120a.	0.2	0
28	PIP2-dependent coupling is prominent in Kv7.1 due to weakened interactions between S4-S5 and S6. Scientific Reports, 2015, 5, 7474.	1.6	53
29	Free-energy landscape of ion-channel voltage-sensor–domain activation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 124-129.	3.3	63
30	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
31	The Mechanism of KCNE1 Modulation of KCNQ1 Channels. Biophysical Journal, 2015, 108, 349a.	0.2	0
32	Electroporation Threshold of POPC Lipid Bilayers with Incorporated Polyoxyethylene Glycol (C <sub>12</sub> E <sub>8</sub> ). Journal of Physical Chemistry B, 2015, 119, 192-200.	1.2	17
33	Functional interaction between S1 and S4 segments in voltage-gated sodium channels revealed by human channelopathies. Channels, 2014, 8, 414-420.	1.5	7
34	Prerequisites to proton transport in the bacterial ClC-ec1 Clâ^'/H+exchanger: Fig. 1 Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1668-1669.	3.3	2
35	State-Dependent Lipid Interactions Couple the Conformations of the Voltage-Sensing and Pore-Gate Domains. Biophysical Journal, 2014, 106, 742a.	0.2	0
36	Investigation of Ion Permeation through the Cx26 Hemichannel. Biophysical Journal, 2014, 106, 556a.	0.2	0

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37	Voltage-gated ion channel modulation by lipids: Insights from molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1322-1331.	1.4	32
38	Electroporation of archaeal lipid membranes using MD simulations. Bioelectrochemistry, 2014, 100, 18-26.	2.4	56
39	A molecular dynamic study of cholesterol rich lipid membranes: comparison of electroporation protocols. Bioelectrochemistry, 2014, 100, 11-17.	2.4	75
40	Structural Properties of Archaeal Lipid Bilayers: Small-Angle X-ray Scattering and Molecular Dynamics Simulation Study. Langmuir, 2014, 30, 8308-8315.	1.6	24
41	On the Coupling between the Collective Dynamics of Proteins and Their Hydration Water. Journal of Physical Chemistry Letters, 2014, 5, 1181-1186.	2.1	59
42	Evidence of Conducting Hydrophobic Nanopores Across Membranes in Response to an Electric Field. Journal of Physical Chemistry C, 2014, 118, 6752-6757.	1.5	38
43	Multi-Dimensional Free Energy Landscape of Voltage Sensor Domain Activation. Biophysical Journal, 2014, 106, 233a.	0.2	Ο
44	Molecular Insights into Electroporation and Electrotransfer through Model Cell Membranes. Biophysical Journal, 2014, 106, 291a.	0.2	0
45	Molecular dynamics simulation of short-wavelength collective dynamics of phospholipid membranes. Physical Review E, 2014, 89, 050301.	0.8	24
46	Lipid Peroxidation in Membranes: The Peroxyl Radical Does Not "Float― Journal of Physical Chemistry Letters, 2014, 5, 1653-1658.	2.1	67
47	High-Yield Nontoxic Gene Transfer through Conjugation of the CM <sub>18</sub> -Tat <sub>11</sub> Chimeric Peptide with Nanosecond Electric Pulses. Molecular Pharmaceutics, 2014, 11, 2466-2474.	2.3	23
48	Domain–domain interactions determine the gating, permeation, pharmacology, and subunit modulation of the IKs ion channel. ELife, 2014, 3, e03606.	2.8	81
49	On the Electroporation Thresholds of Lipid Bilayers: Molecular Dynamics Simulation Investigations. Journal of Membrane Biology, 2013, 246, 843-850.	1.0	54
50	How do functionalized carbon nanotubes land on, bind to and pierce through model and plasma membranes. Nanoscale, 2013, 5, 10242.	2.8	61
51	Voltage Gated Cation Channels Activation: Towards an Ab-Initio Kinetic Model. Biophysical Journal, 2013, 104, 279a.	0.2	0
52	Dual Effect of PIP2 on Shaker K+ Channels. Biophysical Journal, 2013, 104, 464a.	0.2	1
53	Vibrational excitations of proteins and their hydration water in the far-infrared range. Chemical Physics, 2013, 424, 80-83.	0.9	8
54	Omega Currents in Voltage-Gated Ion Channels: What Can We Learn from Uncovering the Voltage-Sensing Mechanism Using MD Simulations?. Accounts of Chemical Research, 2013, 46, 2755-2762.	7.6	20

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55	Effects of Phospholipid Composition on the Transfer of a Small Cationic Peptide Across a Model Biological Membrane. Journal of Chemical Theory and Computation, 2013, 9, 5675-5684.	2.3	25
56	Computational tools to investigate genetic cardiac channelopathies. Frontiers in Physiology, 2013, 4, 390.	1.3	6
57	Dual effect of phosphatidylinositol (4,5)-bisphosphate PIP2 on Shaker K+ channels Journal of Biological Chemistry, 2013, 288, 10951.	1.6	2
58	Mechanisms of Ion Channels Voltage-Dependency: All about Molecular Sensors, Gates, Levers, Locks, and Grease. Frontiers in Pharmacology, 2012, 3, 174.	1.6	2
59	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. Journal of General Physiology, 2012, 140, 587-594.	0.9	179
60	Cell membrane electroporation- Part 1: The phenomenon. IEEE Electrical Insulation Magazine, 2012, 28, 14-23.	1.1	375
61	Dual Effect of Phosphatidyl (4,5)-Bisphosphate PIP2 on Shaker K+ Channels. Journal of Biological Chemistry, 2012, 287, 36158-36167.	1.6	37
62	Transport of siRNA through Lipid Membranes Driven by Nanosecond Electric Pulses: An Experimental and Computational Study. Journal of the American Chemical Society, 2012, 134, 13938-13941.	6.6	85
63	Molecular-Level Characterization of Lipid Membrane Electroporation using Linearly Rising Current. Journal of Membrane Biology, 2012, 245, 651-659.	1.0	36
64	Molecular Dynamics Simulations of Voltage-Gated Cation Channels: Insights on Voltage-Sensor Domain Function and Modulation. Frontiers in Pharmacology, 2012, 3, 97.	1.6	26
65	Molecular Dynamics Simulations of Lipid Membrane Electroporation. Journal of Membrane Biology, 2012, 245, 531-543.	1.0	158
66	Insertion of Short Amino-Functionalized Single-Walled Carbon Nanotubes into Phospholipid Bilayer Occurs by Passive Diffusion. PLoS ONE, 2012, 7, e40703.	1.1	67
67	Intermediate states of the Kv1.2 voltage sensor from atomistic molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6109-6114.	3.3	171
68	Uptake and Translocation Mechanisms of Cationic Amino Derivatives Functionalized on Pristine C60 by Lipid Membranes: A Molecular Dynamics Simulation Study. ACS Nano, 2011, 5, 8571-8578.	7.3	36
69	Structural, hydration, and phase transition properties of phosphatidylcholine from salmon heads. European Journal of Lipid Science and Technology, 2011, 113, 744-755.	1.0	6
70	Ethanol enhances collective dynamics of lipid membranes. Physical Review E, 2011, 83, 050907.	0.8	21
71	Influence of multiple double bonds on the structural and dynamical properties of a multi-component PC membrane extracted from Salmon heads. Chemistry and Physics of Lipids, 2010, 163, S30.	1.5	0
72	On the Antibacterial Action of Cyclic Peptides: Insights from Coarse-Grained MD Simulations. Journal of Physical Chemistry B, 2010, 114, 2676-2684.	1.2	42

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73	Effect of Sensor Domain Mutations on the Properties of Voltage-Gated Ion Channels: Molecular Dynamics Studies of the Potassium Channel Kv1.2. Biophysical Journal, 2010, 99, L72-L74.	0.2	48
74	Affinity of C <sub>60</sub> Neat Fullerenes with Membrane Proteins: A Computational Study on Potassium Channels. ACS Nano, 2010, 4, 4158-4164.	7.3	63
75	Water and Membranes. , 2010, , 139-164.		0
76	Initial Response of the Potassium Channel Voltage Sensor to a Transmembrane Potential. Journal of the American Chemical Society, 2009, 131, 2107-2109.	6.6	55
77	Self assembly of peptides near or within membranes using coarse grained MD simulations. Chemical Physics, 2009, 358, 161-170.	0.9	28
78	Hydration dynamics of purple membranes. Faraday Discussions, 2009, 141, 99-116.	1.6	31
79	The role of protein–solvent hydrogen bond dynamics in the structural relaxation of a protein in glycerol versus water. European Biophysics Journal, 2008, 37, 701-709.	1.2	23
80	Modeling Membranes under a Transmembrane Potential. Journal of Physical Chemistry B, 2008, 112, 5547-5550.	1.2	94
81	Gating Motions in Voltage-Gated Potassium Channels Revealed by Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 3277-3282.	1.2	64
82	Fingerprints of Amorphous Icelike Behavior in the Vibrational Density of States of Protein Hydration Water. Physical Review Letters, 2008, 101, 148104.	2.9	45
83	Energetics of Ion Transport in a Peptide Nanotube. Journal of Physical Chemistry B, 2007, 111, 10633-10635.	1.2	49
84	Large-scale molecular dynamics of a G protein-coupled receptor, the human 5-HT4 serotonin receptor, in a lipid bilayer. Computational and Theoretical Chemistry, 2007, 817, 19-26.	1.5	37
85	Probing a Model of a GPCR/Ligand Complex in an Explicit Membrane Environment: The Human Cholecystokinin-1 Receptor. Biophysical Journal, 2006, 90, 1232-1240.	0.2	57
86	Environment of the Gating Charges in the Kv1.2 Shaker Potassium Channel. Biophysical Journal, 2006, 90, L64-L66.	0.2	90
87	K+ Conduction in the Selectivity Filter of Potassium Channels Is Monitored by the Charge Distribution along Their Sequence. Biophysical Journal, 2006, 91, L81-L83.	0.2	30
88	Molecular Restraints in the Permeation Pathway of Ion Channels. Biophysical Journal, 2006, 91, L26-L28.	0.2	31
89	Interaction of a peptide nanotube with a water–membrane interface. Physical Biology, 2006, 3, S20-S25.	0.8	22

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91	Membrane Electroporation: A Molecular Dynamics Simulation. Biophysical Journal, 2005, 88, 4045-4053.	0.2	438
92	Methyl Group Dynamics as a Probe of the Protein Dynamical Transition. Journal of the American Chemical Society, 2004, 126, 15928-15929.	6.6	43
93	Coupled Motions between Pore and Voltage-Sensor Domains: A Model for Shaker B, a Voltage-Gated Potassium Channel. Biophysical Journal, 2004, 87, 2365-2379.	0.2	45
94	Characterization of sub-nanosecond dynamics of the molten globule state of α-lactalbumin using quasielastic neutron scattering and molecular dynamics simulations. Chemical Physics, 2003, 292, 435-443.	0.9	17
95	Influence of Anesthetic and Nonimmobilizer Molecules on the Physical Properties of a Polyunsaturated Lipid Bilayer. Journal of Physical Chemistry B, 2003, 107, 14500-14508.	1.2	41
96	Molecular Dynamics Investigation of an Oriented Cyclic Peptide Nanotube in DMPC Bilayers. Biophysical Journal, 2003, 85, 2287-2298.	0.2	87
97	Membrane Structural Perturbations Caused by Anesthetics and Nonimmobilizers: A Molecular Dynamics Investigation. Biophysical Journal, 2001, 81, 3339-3345.	0.2	46
98	Intermolecular Interactions and the Structure of Fatty Acidâ~'Soap Crystals. Journal of Physical Chemistry B, 2001, 105, 552-561.	1.2	39
99	Effects of solvent damping on side chain and backbone contributions to the protein boson peak. Journal of Chemical Physics, 2001, 115, 1607-1612.	1.2	54
100	Molecular Dynamics Study of the Poly(oxyethylene) Surfactant C12E2and Water. Langmuir, 2000, 16, 942-946.	1.6	64
101	The Dynamics of Protein Hydration Water: A Quantitative Comparison of Molecular Dynamics Simulations and Neutron-scattering Experiments. Biophysical Journal, 2000, 79, 3244-3257.	0.2	295
102	Distribution of Halothane in a Dipalmitoylphosphatidylcholine Bilayer from Molecular Dynamics Calculations. Biophysical Journal, 2000, 78, 800-811.	0.2	104
103	Amplitudes and Frequencies of Protein Dynamics:Â Analysis of Discrepancies between Neutron Scattering and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2000, 122, 10450-10451.	6.6	52
104	Molecular Dynamics Study of a Lipidâ^'DNA Complex. Journal of Physical Chemistry B, 1999, 103, 10075-10080.	1.2	97
105	Molecular Dynamics Simulations of Supported Phospholipid/Alkanethiol Bilayers on a Gold(111) Surface. Biophysical Journal, 1999, 77, 964-972.	0.2	49
106	Environmental Dependence of the Dynamics of Protein Hydration Water. Journal of the American Chemical Society, 1999, 121, 9740-9741.	6.6	63
107	Surfactant Aggregation at a Hydrophobic Surface. Journal of Physical Chemistry B, 1998, 102, 6318-6322.	1.2	81
108	Computer simulation studies of amphiphilic interfaces. Current Opinion in Colloid and Interface Science, 1998, 3, 242-246.	3.4	25

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109	Molecular dynamics studies of aqueous surfactants systems. Journal of Molecular Liquids, 1998, 78, 1-6.	2.3	40
110	Effects of Anesthetics on the Structure of a Phospholipid Bilayer: Molecular Dynamics Investigation of Halothane in the Hydrated Liquid Crystal Phase of Dipalmitoylphosphatidylcholine. Biophysical Journal, 1998, 75, 2123-2134.	0.2	86
111	Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution. Molecular Physics, 1998, 95, 377-384.	0.8	20
112	Molecular Dynamics Study of Two-Component Systems:Â The Shape and Surface Structure of Water/Ethanol Droplets. Journal of Physical Chemistry A, 1997, 101, 8639-8642.	1.1	29
113	Molecular dynamics investigation of the surface/bulk equilibrium in an ethanol–water solution. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 559-563.	1.7	64
114	Molecular dynamics investigation of an ethanol-water solution. Physica A: Statistical Mechanics and Its Applications, 1996, 231, 117-122.	1.2	38
115	Modelization of experimental isotherms of n-alkanes in NaX zeolite. Zeolites, 1995, 15, 67-72.	0.9	30
116	Molecular Dynamics Simulation of Tetradecyltrimethylammonium Bromide Monolayers at the Air/Water Interface. The Journal of Physical Chemistry, 1995, 99, 1393-1402.	2.9	120