Matteo Ceccarelli

List of Publications by Year
in descending order

123 papers	3,820 citations	117453 34 h-index	138251 58 g-index
131 all docs	131 docs citations	131 times ranked	3745 citing authors

#	Article	IF	Citations
1	Current Methods to Unravel the Functional Properties of Lysosomal Ion Channels and Transporters. Cells, 2022, 11, 921.	1.8	7
2	Diffusion of molecules through nanopores under confinement: Time-scale bridging and crowding effects via Markov state model. Biomolecular Concepts, 2022, 13, 207-219.	1.0	5
3	The Optimal Permeation of Cyclic Boronates to Cross the Outer Membrane via the Porin Pathway. Antibiotics, 2022, 11, 840.	1.5	3
4	Computational methods and theory for ion channel research. Advances in Physics: X, 2022, 7, .	1.5	8
5	The key role of the central cavity in sodium transport through ligand-gated two-pore channels. Physical Chemistry Chemical Physics, 2021, 23, 18461-18474.	1.3	7
6	Ab Initio Spectroscopic Investigation of Pharmacologically Relevant Chiral Molecules: The Cases of Avibactam, Cephems, and Idelalisib as Benchmarks for Antibiotics and Anticancer Drugs. Symmetry, 2021, 13, 601.	1.1	2
7	New Perspectives for Neutron Capture Radiation Therapy with ⁷Be. The Chemistry and Biochemistry Gap. Journal of Nanoscience and Nanotechnology, 2021, 21, 2939-2942.	0.9	3
8	The Influence of Permeability through Bacterial Porins in Whole-Cell Compound Accumulation. Antibiotics, 2021, 10, 635.	1.5	11
9	The Discovery of Naringenin as Endolysosomal Two-Pore Channel Inhibitor and Its Emerging Role in SARS-CoV-2 Infection. Cells, 2021, 10, 1130.	1.8	20
10	Structural analysis of the architecture and in situ localization of the main S-layer complex in Deinococcus radiodurans. Structure, 2021, 29, 1279-1285.e3.	1.6	18
11	Patient Perceptions and Knowledge of Ionizing Radiation From Medical Imaging. JAMA Network Open, 2021, 4, e2128561.	2.8	22
12	Porins and small-molecule translocation across the outer membrane of Gram-negative bacteria. Nature Reviews Microbiology, 2020, 18, 164-176.	13.6	225
13	Permeation of Î²-Lactamase Inhibitors through the General Porins of Gram-Negative Bacteria. Molecules, 2020, 25, 5747.	1.7	8
14	Kanamycin Uptake into Escherichia coli Is Facilitated by OmpF and OmpC Porin Channels Located in the Outer Membrane. ACS Infectious Diseases, 2020, 6, 1855-1865.	1.8	38
15	Rationalizing the Transport of Trojan Horse Compounds for Crossing the Outer Membrane of Gram-Bacteria. Biophysical Journal, 2020, 118, 161a.	0.2	0
16	The mechanism and energetics of a ligand-controlled hydrophobic gate in a mammalian two pore channel. Physical Chemistry Chemical Physics, 2020, 22, 15664-15674.	1.3	13
17	Structural insights into the main S-layer unit of Deinococcus radiodurans reveal a massive protein complex with porin-like features. Journal of Biological Chemistry, 2020, 295, 4224-4236.	1.6	21
18	A perspective on the modulation of plant and animal two pore channels (TPCs) by the flavonoid naringenin. Biophysical Chemistry, 2019, 254, 106246.	1.5	21

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19	The complex of ferric-enterobactin with its transporter from Pseudomonas aeruginosa suggests a two-site model. Nature Communications, 2019, 10, 3673.	5.8	62
20	Diffusion of large particles through small pores: From entropic to enthalpic transport. Journal of Chemical Physics, 2019, 150, 211102.	1.2	18
21	Glucose transport via the pseudomonad porin OprB: implications for the design of Trojan Horse anti-infectives. Physical Chemistry Chemical Physics, 2019, 21, 8457-8463.	1.3	7
22	Complexes formed by the siderophore-based monosulfactam antibiotic BAL30072 and their interaction with the outer membrane receptor PiuA of P. aeruginosa. BioMetals, 2019, 32, 155-170.	1.8	8
23	Free energy calculations and molecular properties of substrate translocation through OccAB porins. Physical Chemistry Chemical Physics, 2018, 20, 8533-8546.	1.3	11
24	Unusual Constriction Zones in the Major Porins OmpU and OmpT from Vibrio cholerae. Structure, 2018, 26, 708-721.e4.	1.6	22
25	Bacterial Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. Biophysical Journal, 2018, 114, 134a.	0.2	0
26	yVDAC2, the second mitochondrial porin isoform of Saccharomyces cerevisiae. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 270-279.	0.5	21
27	Folded Structure and Membrane Affinity of the N-Terminal Domain of the Three Human Isoforms of the Mitochondrial Voltage-Dependent Anion-Selective Channel. ACS Omega, 2018, 3, 11415-11425.	1.6	7
28	Effects of amphipathic profile regularization on structural order and interaction with membrane models of two highly cationic branched peptides with Î²-sheet propensity. Peptides, 2018, 105, 28-36.	1.2	3
29	Getting Drugs into Gram-Negative Bacteria: Rational Rules for Permeation through General Porins. ACS Infectious Diseases, 2018, 4, 1487-1498.	1.8	117
30	Getting Drugs through Small Pores: Exploiting the Porins Pathway in Pseudomonas aeruginosa. ACS Infectious Diseases, 2018, 4, 1519-1528.	1.8	25
31	Preacinetobactin not acinetobactin is essential for iron uptake by the BauA transporter of the pathogen Acinetobacter baumannii. ELife, 2018, 7, .	2.8	41
32	Rationalizing the permeation of polar antibiotics into Gram-negative bacteria. Journal of Physics Condensed Matter, 2017, 29, 113001.	0.7	22
33	Investigation of Siderophore-Monobactam Antibiotic Derivatives: Their Iron(III)-Complexes and Binding to Receptors. Biophysical Journal, 2017, 112, 551a-552a.	0.2	1
34	How to Get Large Drugs through Small Pores? Exploiting the Porins Pathway in Pseudomonas Aeruginosa. Biophysical Journal, 2017, 112, 416a.	0.2	2
35	General Method to Determine the Flux of Charged Molecules through Nanopores Applied to Î²-Lactamase Inhibitors and OmpF. Journal of Physical Chemistry Letters, 2017, 8, 1295-1301.	2.1	53
36	Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. ACS Nano, 2017, 11, 5465-5473.	7.3	74

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37	Towards In-Silica Screening of Molecule Permeation through Outer Membrane Channels in Gramm-Negative Bacteria. Biophysical Journal, 2017, 112, 291a.	0.2	0
38	Filtering with the Electric Field: A Story on Protein Channels Electrostatics. Biophysical Journal, 2017, 112, 417a.	0.2	0
39	Sensing Single Molecule Penetration into Nanopores: Pushing the Time Resolution to the Diffusion Limit. ACS Sensors, 2017, 2, 1184-1190.	4.0	19
40	Porin flexibility in Providencia stuartii: cell-surface-exposed loops L5 and L7 are markers of Providencia porin OmpPst1. Research in Microbiology, 2017, 168, 685-699.	1.0	7
41	Internal Electric Field of GRAM- Unspecific Porins Directs the Choreography of Antibiotic Translocation. Biophysical Journal, 2016, 110, 115a.	0.2	0
42	A kinetic model for molecular diffusion through pores. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1772-1777.	1.4	14
43	A computational study of ion current modulation in hVDAC3 induced by disulfide bonds. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 813-823.	1.4	15
44	Unexpected Modifications of Cysteines in VDAC3: Indication that VDAC3 may Signal the Mitochondrial Intermembrane Redox State. Biophysical Journal, 2016, 110, 19a.	0.2	0
45	MOMP from Campylobacter jejuni Is a Trimer of 18-Stranded Î²-Barrel Monomers with a Ca 2+ Ion Bound at the Constriction Zone. Journal of Molecular Biology, 2016, 428, 4528-4543.	2.0	36
46	The singular behavior of a Î²-type semi-synthetic two branched polypeptide: three-dimensional structure and mode of action. Physical Chemistry Chemical Physics, 2016, 18, 30998-31011.	1.3	14
47	Exploiting the porin pathway for polar compound delivery into Gram-negative bacteria. Future Medicinal Chemistry, 2016, 8, 1047-1062.	1.1	16
48	Molecular Basis of Filtering Carbapenems by Porins from Î²-Lactam-resistant Clinical Strains of Escherichia coli. Journal of Biological Chemistry, 2016, 291, 2837-2847.	1.6	65
49	Water-Based Screening of Antibiotics Permeability. Biophysical Journal, 2016, 110, 115a-116a.	0.2	1
50	Macroscopic electric field inside water-filled biological nanopores. Physical Chemistry Chemical Physics, 2016, 18, 8855-8864.	1.3	25
51	VDAC3 as a sensor of oxidative state of the intermembrane space of mitochondria: the putative role of cysteine residue modifications. Oncotarget, 2016, 7, 2249-2268.	0.8	78
52	Preliminary Characterization of VDAC3, an Elusive Member of the Outer Mitochondrial Membrane Pore Family. Biophysical Journal, 2015, 108, 311a.	0.2	0
53	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	1.7	48
54	Analysis of fast channel blockage: revealing substrate binding in the microsecond range. Analyst, The, 2015, 140, 4820-4827.	1.7	22

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55	Physical methods to quantify small antibiotic molecules uptake into Gram-negative bacteria. European Journal of Pharmaceutics and Biopharmaceutics, 2015, 95, 63-67.	2.0	41
56	Filtering with Electric Field: The Case of E. coli Porins. Journal of Physical Chemistry Letters, 2015, 6, 1807-1812.	2.1	51
57	Small-Molecule Transport by CarO, an Abundant Eight-Stranded Î²-Barrel Outer Membrane Protein from Acinetobacter baumannii. Journal of Molecular Biology, 2015, 427, 2329-2339.	2.0	54
58	Understanding the Translocation of Fluoroquinolones through OmpC using the Metadynamics. Biophysical Journal, 2015, 108, 443a.	0.2	0
59	The N-Terminal Peptides of the Three Human Isoforms of the Mitochondrial Voltage-Dependent Anion Channel Have Different Helical Propensities. Biochemistry, 2015, 54, 5646-5656.	1.2	19
60	Molecular basis of substrate translocation through the outer membrane channel OprD of Pseudomonas aeruginosa. Physical Chemistry Chemical Physics, 2015, 17, 23867-23876.	1.3	23
61	Charged Residues Distribution Modulates Selectivity of the Open State of Human Isoforms of the Voltage Dependent Anion-Selective Channel. PLoS ONE, 2014, 9, e103879.	1.1	45
62	Role of Antibiotic Side Chains in Uptake Through OmpPst1 Channel from Providencia Stuartii. Biophysical Journal, 2014, 106, 556a-557a.	0.2	0
63	The Open State of Human VDAC Isoforms Compared through MD Simulations. Biophysical Journal, 2014, 106, 760a-761a.	0.2	0
64	Transport of Antibiotics through the Substrate Specific OprD Channel of Pseudomonas Aeruginosa. Biophysical Journal, 2014, 106, 338a.	0.2	0
65	Antibiotic Transport through Porins. Biophysical Journal, 2014, 106, 557a.	0.2	0
66	Aquaporins within a Tetramer Exhibit Different Structural Conformations: An in Silico Study of the Human Aquaporin 5. Biophysical Journal, 2013, 104, 409a.	0.2	1
67	Deletion of Î²-strands 9 and 10 converts VDAC1 voltage-dependence in an asymmetrical process. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 793-805.	0.5	32
68	Structureâ€“Function Paradigm in Human Myoglobin: How a Single-Residue Substitution Affects NO Reactivity at Low pO2. Journal of the American Chemical Society, 2013, 135, 7534-7544.	6.6	6
69	Different Molecular Mechanisms of Inhibition of Bovine Viral Diarrhea Virus and Hepatitis C Virus RNA-Dependent RNA Polymerases by a Novel Benzimidazole. Biochemistry, 2013, 52, 3752-3764.	1.2	37
70	The Gating Mechanism of the Human Aquaporin 5 Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e59897.	1.1	64
71	MD Simulations of Plant Hemoglobins: the Hexa- to Penta-Coordinate Structural Transition. Biophysical Journal, 2012, 102, 465a.	0.2	0
72	Transport Properties of the Human Aquaporin HsAQP5. Biophysical Journal, 2012, 102, 661a.	0.2	0

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73	Antibiotic Permeation across the OmpF Channel: Modulation of the Affinity Site in the Presence of Magnesium. Journal of Physical Chemistry B, 2012, 116, 4433-4438.	1.2	60
74	A kinetic Monte Carlo approach to investigate antibiotic translocation through bacterial porins. Journal of Physics Condensed Matter, 2012, 24, 104012.	0.7	13
75	Exploring Binding Properties of Agonists Interacting with a Î´-Opioid Receptor. PLoS ONE, 2012, 7, e52633.	1.1	8
76	Point Mutation I261M Affects the Dynamics of BVDV and its Interaction with Benzimidazole Antiviral 227G. Biophysical Journal, 2011, 100, 395a-396a.	0.2	1
77	Pathways to Exit a Receptor: Agonists and Delta-Oppioid Studied via Computer Simulations. Biophysical Journal, 2011, 100, 544a.	0.2	0
78	Human Myoglobin: Two Isoforms that Differ at Single Residue. Their Different Dynamics Suggest Distinct and Complementary Role. Biophysical Journal, 2011, 100, 194a.	0.2	0
79	Structural characterization of recombinant human myoglobin isoforms by 1H and 129Xe NMR and molecular dynamics simulations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1919-1929.	1.1	2
80	Altered Antibiotic Transport in OmpC Mutants Isolated from a Series of Clinical Strains of Multi-Drug Resistant E. coli. PLoS ONE, 2011, 6, e25825.	1.1	98
81	MD simulations of plant hemoglobins: the hexa- to penta-coordinate structural transition. Theoretical Chemistry Accounts, 2011, 130, 1105-1114.	0.5	2
82	Structural and Functional Characterization of a New Double Variant Haemoglobin		

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91	Bridging Timescales and Length Scales: From Macroscopic Flux to the Molecular Mechanism of Antibiotic Diffusion through Porins. Biophysical Journal, 2010, 98, 569-575.	0.2	40
92	Heme Proteins: The Role of Solvent in the Dynamics of Gates and Portals. Journal of the American Chemical Society, 2010, 132, 5156-5163.	6.6	23
93	Breathing Motions of a Respiratory Protein Revealed by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 11825-11832.	6.6	34
94	The Biophysics Of Antibiotics Translocation Through OmpF Revealed By Computer Simulations. Biophysical Journal, 2009, 96, 41a.	0.2	0
95	The Porin passport control - Conductance measurements and biological relevance. Biophysical Journal, 2009, 96, 148a-149a.	0.2	0
96	Simulating Efflux Pumps: The Extrusion Mechanism of Substrates. Biophysical Journal, 2009, 96, 381a-382a.	0.2	0
97	A Molecular Approach to Ligand-Receptor Interaction. Biophysical Journal, 2009, 96, 600a.	0.2	0
98	Structural Analysis of Hemoglobins and Myoglobins Using MD Simulations. Biophysical Journal, 2009, 96, 558a.	0.2	0
99	Simulating transport properties through bacterial channels. Frontiers in Bioscience - Landmark, 2009, Volume, 3222.	3.0	4
100	CO escape from myoglobin with metadynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1231-1236.	1.5	50
101	Biased Molecular Simulations for Free-Energy Mapping:â€‰ A Comparison on the KcsA Channel as a Test Case. Journal of Chemical Theory and Computation, 2008, 4, 173-183.	2.3	34
102	Evidences of Xenon-Induced Structural Changes in the Active Site of Cyano-MetMyoglobins: A ¹H NMR Study. Journal of Physical Chemistry B, 2008, 112, 15856-15866.	1.2	9
103	Facilitated Permeation of Antibiotics across Membrane Channels â^' Interaction of the Quinolone Moxifloxacin with the OmpF Channel. Journal of the American Chemical Society, 2008, 130, 13301-13309.	6.6	57
104	Physical Insights into Permeation of and Resistance to Antibiotics in Bacteria. Current Drug Targets, 2008, 9, 779-788.	1.0	33
105	Exploring free-energy profiles through ion channels: Comparison on a test case. Journal of Computational Electronics, 2007, 6, 373-376.	1.3	7
106	Interaction of Zwitterionic Penicillins with the OmpF Channel Facilitates Their Translocation. Biophysical Journal, 2006, 90, 1617-1627.	0.2	146
107	Structure-Function Relationship in a Variant Hemoglobin: A Combined Computational-Experimental Approach. Biophysical Journal, 2006, 91, 3529-3541.	0.2	13
108	Exploring the Gating Mechanism in the ClC Chloride Channel via Metadynamics. Journal of Molecular Biology, 2006, 361, 390-398.	2.0	53

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109	The Microscopic Switching Mechanism of a [2]Catenane. Journal of Physical Chemistry B, 2005, 109, 17094-17099.	1.2	27
110	Nonperiodic boundary conditions for solvated systems. Journal of Chemical Physics, 2005, 123, 044103.	1.2	27
111	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	1.2	446
112	Microscopic Mechanism of Antibiotics Translocation through a Porin. Biophysical Journal, 2004, 87, 58-64.	0.2	92
113	Anab initio force field for the cofactors of bacterial photosynthesis. Journal of Computational Chemistry, 2003, 24, 129-142.	1.5	79
114	Simulation and Modeling of theRhodobacter sphaeroidesBacterial Reaction Center II:Â Primary Charge Separation. Journal of Physical Chemistry B, 2003, 107, 5630-5641.	1.2	36
115	Simulation and Modeling of theRhodobactersphaeroidesBacterial Reaction Center:Â Structure and Interactions. Journal of Physical Chemistry B, 2003, 107, 1423-1431.	1.2	31
116	Linear Response and Electron Transfer in Complex Biomolecular Systems and a Reaction Center Protein. Journal of Physical Chemistry B, 2003, 107, 11208-11215.	1.2	22
117	A concerted variational strategy for investigating rare events. Journal of Chemical Physics, 2003, 118, 2025-2032.	1.2	61
118	Water Rotational Relaxation and Diffusion in Hydrated Lysozyme. Journal of the American Chemical Society, 2002, 124, 6787-6791.	6.6	232
119	Dynamics of hydration in hen egg white lysozyme. Journal of Molecular Biology, 2001, 311, 409-419.	2.0	78
120	Empirical force field for the simulation of a class of chromophores in a photosynthetic center. Computational Materials Science, 2001, 20, 318-324.	1.4	3
121	A Density Functional Normal Mode Calculation of a Bacteriochlorophyll a Derivative. Journal of the American Chemical Society, 2000, 122, 3532-3533.	6.6	30
122	Molecular dynamics simulation of POPC at low hydration near the liquid crystal phase transition. Biochimie, 1998, 80, 415-419.	1.3	13
123	Simulation of a Protein Crystal at Constant Pressure. Journal of Physical Chemistry B, 1997, 101, 2105-2108.	1.2	14