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	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	1.2	446
2	Water Rotational Relaxation and Diffusion in Hydrated Lysozyme. Journal of the American Chemical Society, 2002, 124, 6787-6791.	6.6	232
3	Porins and small-molecule translocation across the outer membrane of Gram-negative bacteria. Nature Reviews Microbiology, 2020, 18, 164-176.	13.6	225
4	Interaction of Zwitterionic Penicillins with the OmpF Channel Facilitates Their Translocation. Biophysical Journal, 2006, 90, 1617-1627.	0.2	146
5	Getting Drugs into Gram-Negative Bacteria: Rational Rules for Permeation through General Porins. ACS Infectious Diseases, 2018, 4, 1487-1498.	1.8	117
6	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
7	Microscopic Mechanism of Antibiotics Translocation through a Porin. Biophysical Journal, 2004, 87, 58-64.	0.2	92
8	Molecular Basis of Enrofloxacin Translocation through OmpF, an Outer Membrane Channel of Escherichia coli - When Binding Does Not Imply Translocation. Journal of Physical Chemistry B, 2010, 114, 5170-5179.	1.2	88
9	Anab initio force field for the cofactors of bacterial photosynthesis. Journal of Computational Chemistry, 2003, 24, 129-142.	1.5	79
10	Dynamics of hydration in hen egg white lysozyme. Journal of Molecular Biology, 2001, 311, 409-419.	2.0	78
11	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
12	Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. ACS Nano, 2017, 11, 5465-5473.	7.3	74
13	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
14	The Gating Mechanism of the Human Aquaporin 5 Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e59897.	1.1	64
15	The complex of ferric-enterobactin with its transporter from Pseudomonas aeruginosa suggests a two-site model. Nature Communications, 2019, 10, 3673.	5.8	62
16	A concerted variational strategy for investigating rare events. Journal of Chemical Physics, 2003, 118, 2025-2032.	1.2	61
17	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
18	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

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19	Molecular Simulations Reveal the Mechanism and the Determinants for Ampicillin Translocation through OmpF. Journal of Physical Chemistry B, 2010, 114, 9608-9616.	1.2	54
20	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
21	Exploring the Gating Mechanism in the ClC Chloride Channel via Metadynamics. Journal of Molecular Biology, 2006, 361, 390-398.	2.0	53
22	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
23	Filtering with Electric Field: The Case of <i>E. coli</i> Porins. Journal of Physical Chemistry Letters, 2015, 6, 1807-1812.	2.1	51
24	CO escape from myoglobin with metadynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1231-1236.	1.5	50
25	Implication of Porins in Î²-Lactam Resistance of Providencia stuartii. Journal of Biological Chemistry, 2010, 285, 32273-32281.	1.6	49
26	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	1.7	48
27	Toward Screening for Antibiotics with Enhanced Permeation Properties through Bacterial Porins. Biochemistry, 2010, 49, 6928-6935.	1.2	47
28	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
29	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
30	Preacinetobactin not acinetobactin is essential for iron uptake by the BauA transporter of the pathogen Acinetobacter baumannii. ELife, 2018, 7, .	2.8	41
31	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
32	Kanamycin Uptake into <i>Escherichia coli</i> Is Facilitated by OmpF and OmpC Porin Channels Located in the Outer Membrane. ACS Infectious Diseases, 2020, 6, 1855-1865.	1.8	38
33	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
34	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
35	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
36	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

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37	Breathing Motions of a Respiratory Protein Revealed by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 11825-11832.	6.6	34
38	Physical Insights into Permeation of and Resistance to Antibiotics in Bacteria. Current Drug Targets, 2008, 9, 779-788.	1.0	33
39	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
40	Simulation and Modeling of theRhodobactersphaeroidesBacterial Reaction Center:Â Structure and Interactions. Journal of Physical Chemistry B, 2003, 107, 1423-1431.	1.2	31
41	A Density Functional Normal Mode Calculation of a Bacteriochlorophyll a Derivative. Journal of the American Chemical Society, 2000, 122, 3532-3533.	6.6	30
42	Structural and dynamical properties of the porins OmpF and OmpC: insights from molecular simulations. Journal of Physics Condensed Matter, 2010, 22, 454125.	0.7	29
43	The Microscopic Switching Mechanism of a [2]Catenane. Journal of Physical Chemistry B, 2005, 109, 17094-17099.	1.2	27
44	Nonperiodic boundary conditions for solvated systems. Journal of Chemical Physics, 2005, 123, 044103.	1.2	27
45	Macroscopic electric field inside water-filled biological nanopores. Physical Chemistry Chemical Physics, 2016, 18, 8855-8864.	1.3	25
46	Getting Drugs through Small Pores: Exploiting the Porins Pathway in <i>Pseudomonas aeruginosa</i>. ACS Infectious Diseases, 2018, 4, 1519-1528.	1.8	25
47	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
48	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
49	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
50	Analysis of fast channel blockage: revealing substrate binding in the microsecond range. Analyst, The, 2015, 140, 4820-4827.	1.7	22
51	Rationalizing the permeation of polar antibiotics into Gram-negative bacteria. Journal of Physics Condensed Matter, 2017, 29, 113001.	0.7	22
52	Unusual Constriction Zones in the Major Porins OmpU and OmpT from Vibrio cholerae. Structure, 2018, 26, 708-721.e4.	1.6	22
53	Patient Perceptions and Knowledge of Ionizing Radiation From Medical Imaging. JAMA Network Open, 2021, 4, e2128561.	2.8	22
54	yVDAC2, the second mitochondrial porin isoform of Saccharomyces cerevisiae. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 270-279.	0.5	21

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55	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
56	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
57	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
58	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
59	Sensing Single Molecule Penetration into Nanopores: Pushing the Time Resolution to the Diffusion Limit. ACS Sensors, 2017, 2, 1184-1190.	4.0	19
60	Diffusion of large particles through small pores: From entropic to enthalpic transport. Journal of Chemical Physics, 2019, 150, 211102.	1.2	18
61	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
62	Exploiting the porin pathway for polar compound delivery into Gram-negative bacteria. Future Medicinal Chemistry, 2016, 8, 1047-1062.	1.1	16
63	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
64	Simulation of a Protein Crystal at Constant Pressure. Journal of Physical Chemistry B, 1997, 101, 2105-2108.	1.2	14
65	A kinetic model for molecular diffusion through pores. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1772-1777.	1.4	14
66	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
67	Molecular dynamics simulation of POPC at low hydration near the liquid crystal phase transition. Biochimie, 1998, 80, 415-419.	1.3	13
68	Structure-Function Relationship in a Variant Hemoglobin: A Combined Computational-Experimental Approach. Biophysical Journal, 2006, 91, 3529-3541.	0.2	13
69	A kinetic Monte Carlo approach to investigate antibiotic translocation through bacterial porins. Journal of Physics Condensed Matter, 2012, 24, 104012.	0.7	13
70	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
71	Investigating reaction pathways in rare events simulations of antibiotics diffusion through protein channels. Journal of Molecular Modeling, 2010, 16, 1701-1708.	0.8	12
72	Free energy calculations and molecular properties of substrate translocation through OccAB porins. Physical Chemistry Chemical Physics, 2018, 20, 8533-8546.	1.3	11

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73	The Influence of Permeability through Bacterial Porins in Whole-Cell Compound Accumulation. Antibiotics, 2021, 10, 635.	1.5	11
74	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
75	Exploring Binding Properties of Agonists Interacting with a Î´-Opioid Receptor. PLoS ONE, 2012, 7, e52633.	1.1	8
76	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
77	Permeation of Î²-Lactamase Inhibitors through the General Porins of Gram-Negative Bacteria. Molecules, 2020, 25, 5747.	1.7	8
78	Computational methods and theory for ion channel research. Advances in Physics: X, 2022, 7, .	1.5	8
79	Exploring free-energy profiles through ion channels: Comparison on a test case. Journal of Computational Electronics, 2007, 6, 373-376.	1.3	7
80	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
81	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
82	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
83	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
84	Current Methods to Unravel the Functional Properties of Lysosomal Ion Channels and Transporters. Cells, 2022, 11, 921.	1.8	7
85	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
86	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
87	Simulating transport properties through bacterial channels. Frontiers in Bioscience - Landmark, 2009, Volume, 3222.	3.0	4
88	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
89	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
90	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

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91	The Optimal Permeation of Cyclic Boronates to Cross the Outer Membrane via the Porin Pathway. Antibiotics, 2022, 11, 840.	1.5	3
92	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
93	MD simulations of plant hemoglobins: the hexa- to penta-coordinate structural transition. Theoretical Chemistry Accounts, 2011, 130, 1105-1114.	0.5	2
94	How to Get Large Drugs through Small Pores? Exploiting the Porins Pathway in Pseudomonas Aeruginosa. Biophysical Journal, 2017, 112, 416a.	0.2	2
95	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
96	Point Mutation I261M Affects the Dynamics of BVDV and its Interaction with Benzimidazole Antiviral 227G. Biophysical Journal, 2011, 100, 395a-396a.	0.2	1
97	Structural and Functional Characterization of a New Double Variant Haemoglobin		

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109	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
110	MD Simulations of Plant Hemoglobins: the Hexa- to Penta-Coordinate Structural Transition. Biophysical Journal, 2012, 102, 465a.	0.2	0
111	Transport Properties of the Human Aquaporin HsAQP5. Biophysical Journal, 2012, 102, 661a.	0.2	0
112	Role of Antibiotic Side Chains in Uptake Through OmpPst1 Channel from Providencia Stuartii. Biophysical Journal, 2014, 106, 556a-557a.	0.2	0
113	The Open State of Human VDAC Isoforms Compared through MD Simulations. Biophysical Journal, 2014, 106, 760a-761a.	0.2	0
114	Transport of Antibiotics through the Substrate Specific OprD Channel of Pseudomonas Aeruginosa. Biophysical Journal, 2014, 106, 338a.	0.2	0
115	Antibiotic Transport through Porins. Biophysical Journal, 2014, 106, 557a.	0.2	0
116	Preliminary Characterization of VDAC3, an Elusive Member of the Outer Mitochondrial Membrane Pore Family. Biophysical Journal, 2015, 108, 311a.	0.2	0
117	Understanding the Translocation of Fluoroquinolones through OmpC using the Metadynamics. Biophysical Journal, 2015, 108, 443a.	0.2	0
118	Internal Electric Field of GRAM- Unspecific Porins Directs the Choreography of Antibiotic Translocation. Biophysical Journal, 2016, 110, 115a.	0.2	0
119	Unexpected Modifications of Cysteines in VDAC3: Indication that VDAC3 may Signal the Mitochondrial Intermembrane Redox State. Biophysical Journal, 2016, 110, 19a.	0.2	0
120	Towards In-Silica Screening of Molecule Permeation through Outer Membrane Channels in Gramm-Negative Bacteria. Biophysical Journal, 2017, 112, 291a.	0.2	0
121	Filtering with the Electric Field: A Story on Protein Channels Electrostatics. Biophysical Journal, 2017, 112, 417a.	0.2	0
122	Bacterial Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. Biophysical Journal, 2018, 114, 134a.	0.2	0
123	Rationalizing the Transport of Trojan Horse Compounds for Crossing the Outer Membrane of Gram-Bacteria. Biophysical Journal, 2020, 118, 161a.	0.2	0