Carmen Domene

List of Publications by Year
in descending order

132 papers	3,800 citations	117619 34 h-index	155644 55 g-index
132 all docs	132 docs citations	132 times ranked	4715 citing authors

#	Article	IF	Citations
1	Ion conduction mechanism as a fingerprint of potassium channels. Biophysical Journal, 2022, 121, 388a.	0.5	1
2	Selective Anticancer Therapy Based on a HA-CD44 Interaction Inhibitor Loaded on Polymeric Nanoparticles. Pharmaceutics, 2022, 14, 788.	4.5	4
3	A Potential Route of Capsaicin to Its Binding Site in the TRPV1 Ion Channel. Journal of Chemical Information and Modeling, 2022, 62, 2481-2489.	5.4	8
4	The ligand-bound state of a G protein-coupled receptor stabilizes the interaction of functional cholesterol molecules. Journal of Lipid Research, 2021, 62, 100059.	4.2	17
5	Structure based analysis of KATP channel with a DEND syndrome mutation in murine skeletal muscle. Scientific Reports, 2021, 11, 6668.	3.3	4
6	Ion Conduction Mechanism as a Fingerprint of Potassium Channels. Journal of the American Chemical Society, 2021, 143, 12181-12193.	13.7	14
7	Multiple Interactions of Glucose with the Extra-Membranous Loops of GLUT1 Aid Transport. Journal of Chemical Information and Modeling, 2021, 61, 3559-3570.	5.4	5
8	An Integrated Mass Spectrometry and Molecular Dynamics Simulations Approach Reveals the Spatial Organization Impact of Metal-Binding Sites on the Stability of Metal-Depleted Metallothionein-2 Species. Journal of the American Chemical Society, 2021, 143, 16486-16501.	13.7	26
9	The Bilayer Collective Properties Govern the Interaction of an HIV-1 Antibody with the Viral Membrane. Biophysical Journal, 2020, 118, 44-56.	0.5	6
10	Insights into the Mechanisms of K⁺ Permeation in K⁺ Channels from Computer Simulations. Journal of Chemical Theory and Computation, 2020, 16, 794-799.	5.3	6
11	Critical Assessment of Common Force Fields for Molecular Dynamics Simulations of Potassium Channels. Journal of Chemical Theory and Computation, 2020, 16, 7148-7159.	5.3	24
12	Differential Stability of Aurein 1.2 Pores in Model Membranes of Two Probiotic Strains. Journal of Chemical Information and Modeling, 2020, 60, 5142-5152.	5.4	5
13	Conduction and Gating Properties of the TRAAK Channel from Molecular Dynamics Simulations with Different Force Fields. Journal of Chemical Information and Modeling, 2020, 60, 6532-6543.	5.4	12
14	Affinity for the Interface Underpins Potency of Antibodies Operating In Membrane Environments. Cell Reports, 2020, 32, 108037.	6.4	10
15	Effect of anionic lipids on ion permeation through the KcsA K+-channel. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183406.	2.6	3
16	Mechanism of Molecular Oxygen Diffusion in a Hypoxia-Sensing Prolyl Hydroxylase Using Multiscale Simulation. Journal of the American Chemical Society, 2020, 142, 2253-2263.	13.7	19
17	Modulation of the potassium channel KcsA by anionic phospholipids: Role of arginines at the non-annular lipid binding sites. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 183029.	2.6	22
18	Combining Structural Data with Computational Methodologies to Investigate Structureâ€“Function Relationships in TRP Channels. Methods in Molecular Biology, 2019, 1987, 65-82.	0.9	5

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19	Influence of Cholesterol and Its Stereoisomers on Members of the Serotonin Receptor Family. Journal of Molecular Biology, 2019, 431, 1633-1649.	4.2	12
20	Antibiotic resistance and host immune evasion in Staphylococcus aureus mediated by a metabolic adaptation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3722-3727.	7.1	69
21	Regulation of KcsA by Anionic Phospholipids. Biophysical Journal, 2019, 116, 221a.	0.5	0
22	Capturing the Molecular Mechanism of Anesthetic Action by Simulation Methods. Chemical Reviews, 2019, 119, 5998-6014.	47.7	14
23	El efecto de la educaciÃ³n en el cuidado paliativo por parejas en el manejo del dolor en pacientes con cÃ¡ncer. Apuntes Universitarios, 2019, 10, 88-100.	0.2	0
24	Role of Zinc and Magnesium Ions in the Modulation of Phosphoryl Transfer in Protein Tyrosine Phosphatase 1B. Journal of the American Chemical Society, 2018, 140, 4446-4454.	13.7	23
25	Exposure of the HIV-1 broadly neutralizing antibody 10E8 MPER epitope on the membrane surface by gp41 transmembrane domain scaffolds. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1259-1271.	2.6	4
26	Oxytocin Modulates Nociception as a Direct Agonist of Pain-Sensing TRPV1. Biophysical Journal, 2018, 114, 396a.	0.5	0
27	Stereospecific Interactions of Cholesterol in a Model Cell Membrane: Implications for the Membrane Dipole Potential. Journal of Membrane Biology, 2018, 251, 507-519.	2.1	7
28	2-Oxoglutarate regulates binding of hydroxylated hypoxia-inducible factor to prolyl hydroxylase domain 2. Chemical Communications, 2018, 54, 3130-3133.	4.1	29
29	Modulation of Membrane Proteins by Lipids. Biophysical Journal, 2018, 114, 609a.	0.5	1
30	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. Journal of Membrane Biology, 2018, 251, 609-631.	2.1	33
31	Location and Character of Volatile General Anesthetics Binding Sites in the Transmembrane Domain of TRPV1. Molecular Pharmaceutics, 2018, 15, 3920-3930.	4.6	9
32	Ion-triggered selectivity in bacterial sodium channels. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5450-5455.	7.1	24
33	Ribonucleotide Reductase Requires Subunit Switching in Hypoxia to Maintain DNA Replication. Molecular Cell, 2017, 66, 206-220.e9.	9.7	71
34	Computational Characterisation of the Modulation of Membrane Proteins by Lipids. Biophysical Journal, 2017, 112, 386a.	0.5	0
35	Computational Approaches to the Study of TRPV Channel Activation and Modulation. Biophysical Journal, 2017, 112, 169a.	0.5	0
36	Membrane Phase-Dependent Occlusion of Intramolecular GLUT1 Cavities Demonstrated by Simulations. Biophysical Journal, 2017, 112, 1176-1184.	0.5	12

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37	Functional mapping of the N-terminal arginine cluster and C-terminal acidic residues of Kir6.2 channel fused to a G protein-coupled receptor. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2144-2153.	2.6	2
38	Computer Simulations of Membrane Proteins. Springer Series in Biophysics, 2017, , 351-374.	0.4	1
39	Oxytocin Modulates Nociception as an Agonist of Pain-Sensing TRPV1. Cell Reports, 2017, 21, 1681-1691.	6.4	95
40	¹³C-Carbamylation as a mechanistic probe for the inhibition of class D Î²-lactamases by avibactam and halide ions. Organic and Biomolecular Chemistry, 2017, 15, 6024-6032.	2.8	19
41	Novel Insights into Membrane Transport from Computational Methodologies. Chemical Biology, 2017, , 247-280.	0.2	1
42	The Use of Multiscale Molecular Simulations in Understanding a Relationship between the Structure and Function of Biological Systems of the Brain: The Application to Monoamine Oxidase Enzymes. Frontiers in Neuroscience, 2016, 10, 327.	2.8	32
43	Lateral Fenestrations in K⁺-Channels Explored Using Molecular Dynamics Simulations. Molecular Pharmaceutics, 2016, 13, 2263-2273.	4.6	21
44	A perspective on structural and computational work on collagen. Physical Chemistry Chemical Physics, 2016, 18, 24802-24811.	2.8	30
45	Energetics of Ion Permeation in an Open-Activated TRPV1 Channel. Biophysical Journal, 2016, 111, 1214-1222.	0.5	21
46	Exploring the Dynamics of the TWIK-1 Channel. Biophysical Journal, 2016, 111, 775-784.	0.5	7
47	Structural basis for oxygen degradation domain selectivity of the HIF prolyl hydroxylases. Nature Communications, 2016, 7, 12673.	12.8	109
48	Voltage-Gated Sodium Channels. Current Topics in Membranes, 2016, 78, 183-214.	0.9	7
49	Computational studies of transport in ion channels using metadynamics. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1733-1740.	2.6	31
50	Chapter 2. Molecular Dynamics Simulations: Principles and Applications for the Study of Membrane Proteins. RSC Theoretical and Computational Chemistry Series, 2016, , 19-58.	0.7	0
51	Permeation and Dynamics of an Open-Activated TRPV1 Channel. Biophysical Journal, 2015, 108, 37a.	0.5	0
52	Conduction and Selectivity in Na+ Channels Analyzed by Bias-Exchange Metadynamics Simulations. Biophysical Journal, 2015, 108, 490a.	0.5	1
53	In Silico Identification of PAP-1 Binding Sites in the Kv1.2 Potassium Channel. Molecular Pharmaceutics, 2015, 12, 1299-1307.	4.6	16
54	Quantifying the Binding Interaction between the Hypoxia-Inducible Transcription Factor and the von Hippelâ€“Lindau Suppressor. Journal of Chemical Theory and Computation, 2015, 11, 3946-3954.	5.3	2

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55	Antimicrobial peptide dendrimer interacts with phosphocholine membranes in a fluidity dependent manner: A neutron reflection study combined with molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2075-2084.	2.6	26
56	Bias-Exchange Metadynamics Simulations: An Efficient Strategy for the Analysis of Conduction and Selectivity in Ion Channels. Journal of Chemical Theory and Computation, 2015, 11, 1896-1906.	5.3	43
57	Blocking the Passage: C₆₀ Geometrically Clogs K⁺ Channels. ACS Nano, 2015, 9, 4827-4834.	14.6	41
58	Molecular Dynamics Simulations and Neutron Reflectivity as an Effective Approach To Characterize Biological Membranes and Related Macromolecular Assemblies. Journal of Chemical Theory and Computation, 2015, 11, 4875-4884.	5.3	22
59	Surfactin at the Water/Air Interface and in Solution. Langmuir, 2015, 31, 11097-11104.	3.5	16
60	Binding of Capsaicin to the TRPV1 Ion Channel. Molecular Pharmaceutics, 2015, 12, 4454-4465.	4.6	71
61	Permeation and Dynamics of an Open-Activated TRPV1 Channel. Journal of Molecular Biology, 2015, 427, 537-549.	4.2	39
62	DNA Recognition Process of the Lactose Repressor Protein Studied via Metadynamics and Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2014, 118, 13059-13065.	2.6	7
63	Structure and Immunogenicity of a Peptide Vaccine, Including the Complete HIV-1 gp41 2F5 Epitope. Journal of Biological Chemistry, 2014, 289, 6565-6580.	3.4	26
64	Cholesterol-Dependent Membrane Fusion Induced by the gp41 Membrane-Proximal External Regionâ€"Transmembrane Domain Connection Suggests a Mechanism for Broad HIV-1 Neutralization. Journal of Virology, 2014, 88, 13367-13377.	3.4	39
65	Effects of the Protonation States of the EEEE Motif of a Bacterial Na+-Channel on Conduction and Pore Structure. Biophysical Journal, 2014, 106, 130a.	0.5	1
66	The Gp41 Sequence Connecting Mper and Tm Domains Constitutes a Distinct HIV-1 â€œFusion Peptideâ€• Targeted by Neutralizing Antibodies. Biophysical Journal, 2014, 106, 708a-709a.	0.5	0
67	Development of GoSlo-SR-5-69, a potent activator of large conductance Ca2+-activated K+ (BK) channels. European Journal of Medicinal Chemistry, 2014, 75, 426-437.	5.5	23
68	Effects of the Protonation State of the EEEE Motif of a Bacterial Na+-channel on Conduction and Pore Structure. Biophysical Journal, 2014, 106, 2175-2183.	0.5	27
69	On Conduction and Permeation in a Bacterial Sodium Channel. Biophysical Journal, 2013, 104, 135a.	0.5	0
70	K+ and Na+ Conduction in Selective and Nonselective Ion Channels Via Molecular Dynamics Simulations. Biophysical Journal, 2013, 105, 1737-1745.	0.5	38
71	Fusogenic Activity of the HIV-1 Gp41 MPER-TMD Region: Mechanism and Targeting by Immunogens and Inhibitors. Biophysical Journal, 2013, 104, 90a.	0.5	0
72	Strong and weak zinc binding sites in human zincâ€Î±2â€glycoprotein. FEBS Letters, 2013, 587, 3949-3954.	2.8	15

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73	Simulating the Pyrolysis of Polyazides: a Mechanistic Case Study of the [P(N₃)₆]^{â^'} Anion. Inorganic Chemistry, 2013, 52, 1747-1754.	4.0	3
74	DNA-recognition process described by MD simulations of the lactose repressor protein on a specific and a non-specific DNA sequence. Nucleic Acids Research, 2013, 41, 3963-3972.	14.5	49
75	On Conduction in a Bacterial Sodium Channel. PLoS Computational Biology, 2012, 8, e1002476.	3.2	79
76	Dynamics of a bacterial multidrug ABC transporter in the inward- and outward-facing conformations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10832-10836.	7.1	99
77	Voltage-sensor cycle fully described. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 8362-8363.	7.1	4
78	Nonselective Conduction in a Mutated NaK Channel with Three Cation-Binding Sites. Biophysical Journal, 2012, 103, 2106-2114.	0.5	17
79	Effects of point mutations in pVHL on the binding of HIFâ€1Î±. Proteins: Structure, Function and Bioinformatics, 2012, 80, 733-746.	2.6	15
80	Molecular Dynamics Simulations of the TrkH Membrane Protein. Biochemistry, 2012, 51, 1559-1565.	2.5	24
81	On Conduction and Gating in K+-Channels. Biophysical Journal, 2011, 100, 579a.	0.5	0
82	Gating at the Selectivity Filter of Ion Channels that Conduct Na+ and K+ Ions. Biophysical Journal, 2011, 101, 1623-1631.	0.5	19
83	Selectivity and Permeation of Alkali Metal Ions in K+-channels. Journal of Molecular Biology, 2011, 409, 867-878.	4.2	30
84	Structural and biochemical analyses reveal how ornithine acetyl transferase binds acidic and basic amino acid substrates. Organic and Biomolecular Chemistry, 2011, 9, 6219.	2.8	5
85	On ionic conduction in potassium channels. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, E128; author reply E129.	7.1	3
86	A Multiscale Model To Analyze the Sliding Movement of Repressor Proteins on DNA. Biophysical Journal, 2010, 98, 72a.	0.5	0
87	Chiral Phosphineâ^'Phosphite Ligands with a Substituted Ethane Backbone. Influence of Conformational Effects in Rhodium-Catalyzed Asymmetric Olefin Hydrogenation and Hydroformylation Reactions. Organometallics, 2010, 29, 5791-5804.	2.3	38
88	Computational Studies on Polarization Effects and Selectivity in K⁺ Channels. Journal of Chemical Theory and Computation, 2010, 6, 3780-3792.	5.3	26
89	Insights into the Sliding Movement of the Lac Repressor Nonspecifically Bound to DNA. Journal of Physical Chemistry B, 2010, 114, 2238-2245.	2.6	27
90	Chemical Basis for the Selectivity of the von Hippel Lindau Tumor Suppressor pVHL for Prolyl-Hydroxylated HIF-1Î±. Biochemistry, 2010, 49, 6936-6944.	2.5	16

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91	Computational Studies on the Interactions of Inhalational Anesthetics with Proteins. Accounts of Chemical Research, 2010, 43, 103-110.	15.6	35
92	Examining Ion Channel Properties Using Free-Energy Methods. Methods in Enzymology, 2009, 466, 155-177.	1.0	15
93	Many-body effects and simulations of potassium channels. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2009, 465, 1701-1716.	2.1	37
94	Structural Basis for Binding of Hypoxia-Inducible Factor to the Oxygen-Sensing Prolyl Hydroxylases. Structure, 2009, 17, 981-989.	3.3	205
95	Permeation of water through the KcsA K⁺ channel. Proteins: Structure, Function and Bioinformatics, 2009, 74, 437-448.	2.6	28
96	Atypical mechanism of conduction in potassium channels. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 16074-16077.	7.1	102
97	Anatomy of a Simple Acyl Intermediate in Enzyme Catalysis: Combined Biophysical and Modeling Studies on Ornithine Acetyl Transferase. Journal of the American Chemical Society, 2009, 131, 749-757.	13.7	14
98	Dynamics, Energetics, and Selectivity of the Low-K+ KcsA Channel Structure. Journal of Molecular Biology, 2009, 389, 637-645.	4.2	38
99	Interaction of Anesthetics with Open and Closed Conformations of a Potassium Channel Studied via Molecular Dynamics and Normal Mode Analysis. Biophysical Journal, 2008, 94, 4260-4269.	0.5	23
100	Model-Based Prediction of the Î±-Hemolysin Structure in the Hexameric State. Biophysical Journal, 2008, 95, 2265-2274.	0.5	24
101	The Role of Conformation in Ion Permeation in a K⁺ Channel. Journal of the American Chemical Society, 2008, 130, 3389-3398.	13.7	32
102	Conformational Changes and Gating at the Selectivity Filter of Potassium Channels. Journal of the American Chemical Society, 2008, 130, 9474-9480.	13.7	61
103	On the Lack of Ring-Current Aromaticity of (Heteroatom) [N]Radialenes and their Dianions. Chemistry - A European Journal, 2007, 13, 269-276.	3.3	29
104	Molecular dynamics simulations of potassium channels. Open Chemistry, 2007, 5, 635-671.	1.9	7
105	Anionic Phospholipid Interactions with the Potassium Channel KcsA: Simulation Studies. Biophysical Journal, 2006, 90, 822-830.	0.5	77
106	Role of Aromatic Localization in the Gating Process of a Potassium Channel. Biophysical Journal, 2006, 90, L01-L03.	0.5	35
107	Aromaticity of anthranil and its isomers, 1,2-benzisoxazole and benzoxazole. Tetrahedron Letters, 2005, 46, 4077-4080.	1.4	18
108	Two Different Conformational States of the KirBac3.1 Potassium Channel Revealed by Electron Crystallography. Structure, 2005, 13, 1463-1472.	3.3	100

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109	A Unified Orbital Model of Delocalised and Localised Currents in Monocycles, from Annulenes to Azabora-heterocycles. Chemistry - A European Journal, 2005, 11, 1257-1266.	3.3	59
110	Molecular Dynamics Simulation Approaches to K Channels: Conformational Flexibility and Physiological Function. IEEE Transactions on Nanobioscience, 2005, 4, 112-120.	3.3	20
111	Conformational Dynamics of M2 Helices in KirBac Channels:Â Helix Flexibility in Relation to Gating via Molecular Dynamics Simulationsâ€. Biochemistry, 2005, 44, 14586-14594.	2.5	52
112	Modeling of an Ion Channel in Its Open Conformation. Biophysical Journal, 2005, 89, L01-L03.	0.5	35
113	KcsA closed and open: modelling and simulation studies. European Biophysics Journal, 2004, 33, 238-46.	2.2	25
114	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 783-791.	2.6	92
115	Filter Flexibility and Distortion in a Bacterial Inward Rectifier K+ Channel: Simulation Studies of KirBac1.1. Biophysical Journal, 2004, 87, 256-267.	0.5	60
116	Lipid-Protein Interactions of Integral Membrane Proteins: A Comparative Simulation Study. Biophysical Journal, 2004, 87, 3737-3749.	0.5	104
117	Calculation of Dipole-Shielding Polarizabilities (Ïƒ(±)(²)(³)):â€‰ The Influence of Uniform Electric Field Effects on the Shielding of Backbone Nuclei in Proteins. Journal of the American Chemical Society, 2003, 125, 9556-9557.	13.7	16
118	Lipid/Protein Interactions and the Membrane/Water Interfacial Region. Journal of the American Chemical Society, 2003, 125, 14966-14967.	13.7	57
119	Ion channel gating: insights via molecular simulations. FEBS Letters, 2003, 555, 85-90.	2.8	119
120	Potassium Channel, Ions, and Water: Simulation Studies Based on the High Resolution X-Ray Structure of KcsA. Biophysical Journal, 2003, 85, 2787-2800.	0.5	107
121	Membrane Protein Simulations: Ion Channels And Bacterial Outer Membrane Proteins. Advances in Protein Chemistry, 2003, 66, 159-193.	4.4	49
122	Ion channel structures: a review of recent progress. Current Opinion in Drug Discovery & Development, 2003, 6, 611-9.	1.9	5
123	A transferable representation of the induced multipoles in ionic crystals. Molecular Physics, 2002, 100, 3847-3865.	1.7	14
124	Nuclear Quadrupole Coupling of17O and33S in Ionic Solids:Â Invalidation of the Sternheimer Model by Short-Range Corrections. Journal of Physical Chemistry B, 2002, 106, 10342-10348.	2.6	7
125	Short-Range Contributions to the Polarization of Cations. Journal of Physical Chemistry A, 2001, 105, 4136-4142.	2.5	26
126	Overlap-model and ab initio cluster calculations of ion properties in distorted environments. Chemical Physics Letters, 2001, 333, 403-412.	2.6	35

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127	Dipole-induced-dipole polarizabilities of symmetric clusters. Molecular Physics, 2000, 98, 1391-1407.	1.7	6
128	Overlap model and ab initio cluster calculations of polarisabilities of ions in solids. Chemical Physics Letters, 1999, 314, 158-167.	2.6	19
129	Application of density functional theory to calculation of in-crystal anionic polarizability. Chemical Physics Letters, 1999, 299, 51-56.	2.6	25
130	Pentagon adjacency as a determinant of fullerene stability. Physical Chemistry Chemical Physics, 1999, 1, 2913-2918.	2.8	178
131	Partition Coefficients of Indoles and Betacarbolines. Journal of Pharmaceutical Sciences, 1997, 86, 106-109.	3.3	11
132	Role of geometrical relaxation in solution of simple molecules exhibiting anomeric effects. Computational and Theoretical Chemistry, 1996, 371, 245-256.	1.5	17