Attilio V Vargiu

List of Publications by Year
in descending order

94 papers	3,330 citations	126907 33 h-index	161849 54 g-index
100 all docs	100 docs citations	100 times ranked	3538 citing authors

#	Article	IF	Citations
1	Molecular rationale for the impairment of the MexAB-OprM efflux pump by a single mutation in MexA. Computational and Structural Biotechnology Journal, 2022, 20, 252-260.	4.1	4
2	Pyridylpiperazine-based allosteric inhibitors of RND-type multidrug efflux pumps. Nature Communications, 2022, 13, 115.	12.8	28
3	Single-atom substitution enables supramolecular diversity from dipeptide building blocks. Soft Matter, 2022, 18, 2129-2136.	2.7	6
4	Molecular Insights Into Binding and Activation of the Human KCNQ2 Channel by Retigabine. Frontiers in Molecular Biosciences, 2022, 9, 839249.	3.5	1
5	AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials. Scientific Data, 2022, 9, 148.	5.3	6
6	The Structural and Functional Study of Efflux Pumps Belonging to the RND Transporters Family from Gram-Negative Bacteria. Antibiotics, 2022, 11, 429.	3.7	2
7	Recognition of quinolone antibiotics by the multidrug efflux transporter MexB ofPseudomonas aeruginosa. Physical Chemistry Chemical Physics, 2022, 24, 16566-16575.	2.8	9
8	Molecular insights into the Patched1 drug efflux inhibitory activity of panicein A hydroquinone: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 8013-8022.	2.8	2
9	Predictive Rules of Efflux Inhibition and Avoidance in Pseudomonas aeruginosa. MBio, 2021, 12, .	4.1	28
10	Nanoscale Assembly of Functional Peptides with Divergent Programming Elements. ACS Nano, 2021, 15, 3015-3025.	14.6	50
11	Bacterial efflux transportersâ€™ polyspecificity â€“ a gift and a curse?. Current Opinion in Microbiology, 2021, 61, 115-123.	5.1	23
12	Mechanistic Duality of Bacterial Efflux Substrates and Inhibitors: Example of Simple Substituted Cinnamoyl and Naphthyl Amides. ACS Infectious Diseases, 2021, 7, 2650-2665.	3.8	16
13	Native or Non-Native Proteinâ€“Protein Docking Models? Molecular Dynamics to the Rescue. Journal of Chemical Theory and Computation, 2021, 17, 5944-5954.	5.3	21
14	Structural and functional analysis of the promiscuous AcrB and AdeB efflux pumps suggests different drug binding mechanisms. Nature Communications, 2021, 12, 6919.	12.8	25
15	Coupling enhanced sampling of the apo-receptor with template-based ligand conformers selection: performance in pose prediction in the D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 149-162.	2.9	11
16	Binding and Transport of Carboxylated Drugs by the Multidrug Transporter AcrB. Journal of Molecular Biology, 2020, 432, 861-877.	4.2	37
17	Self-Assembling l-d-l-Tripeptides Dance the Twist. Synlett, 2020, 31, 434-438.	1.8	7
18	Heterochirality and Halogenation Control Phe-Phe Hierarchical Assembly. ACS Nano, 2020, 14, 16951-16961.	14.6	67

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19	Perturbed structural dynamics underlie inhibition and altered efflux of the multidrugÂresistance pump AcrB. Nature Communications, 2020, 11, 5565.	12.8	34
20	Chlorpromazine and Amitriptyline Are Substrates and Inhibitors of the AcrB Multidrug Efflux Pump. MBio, 2020, 11, .	4.1	54
21	Cryo-EM Structure and Molecular Dynamics Analysis of the Fluoroquinolone Resistant Mutant of the AcrB Transporter from Salmonella. Microorganisms, 2020, 8, 943.	3.6	25
22	Molecular Interactions of Carbapenem Antibiotics with the Multidrug Efflux Transporter AcrB of Escherichia coli. International Journal of Molecular Sciences, 2020, 21, 860.	4.1	11
23	The challenge of intracellular antibiotic accumulation, a function of fluoroquinolone influx versus bacterial efflux. Communications Biology, 2020, 3, 198.	4.4	34
24	Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. Journal of Physical Chemistry B, 2019, 123, 4625-4635.	2.6	18
25	Molecular basis for the different interactions of congeneric substrates with the polyspecific transporter AcrB. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1397-1408.	2.6	11
26	Holo-like and Druggable Protein Conformations from Enhanced Sampling of Binding Pocket Volume and Shape. Journal of Chemical Information and Modeling, 2019, 59, 1515-1528.	5.4	33
27	Relevance of Ebola virus VP35 homo-dimerization on the type I interferon cascade inhibition. Antiviral Chemistry and Chemotherapy, 2019, 27, 204020661988922.	0.6	11
28	Identification and characterization of carbapenem binding sites within the RND-transporter AcrB. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 62-74.	2.6	18
29	Computer simulations of the activity of RND efflux pumps. Research in Microbiology, 2018, 169, 384-392.	2.1	32
30	Insights into the homo-oligomerization properties of N-terminal coiled-coil domain of Ebola virus VP35 protein. Virus Research, 2018, 247, 61-70.	2.2	14
31	Water-mediated interactions enable smooth substrate transport in a bacterial efflux pump. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 836-845.	2.4	42
32	A New Critical Conformational Determinant of Multidrug Efflux by an MFS Transporter. Journal of Molecular Biology, 2018, 430, 1368-1385.	4.2	27
33	Molecular Modeling of Multidrug Properties of Resistance Nodulation Division (RND) Transporters. Methods in Molecular Biology, 2018, 1700, 179-219.	0.9	6
34	Chirality Effects on Peptide Self-Assembly Unraveled from Molecules to Materials. CheM, 2018, 4, 1862-1876.	11.7	151
35	Molecular Determinants of the Promiscuity of MexB and MexY Multidrug Transporters of Pseudomonas aeruginosa. Frontiers in Microbiology, 2018, 9, 1144.	3.5	37
36	Computational Study of the Interaction between Antimicrobial Compounds and Efflux Systems of Gram-Negative Bacteria. Biophysical Journal, 2017, 112, 274a.	0.5	0

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37	Molecular Rationale Behind the Differential Substrate Specificity of RND Transporters AcrB and AcrD. Biophysical Journal, 2017, 112, 274a.	0.5	0
38	Molecular Insights into Compound-Transporter Interactions: The Case ofÂInhibitors of Gram-Negative Bacteria Efflux Pumps. Biophysical Journal, 2017, 112, 274a.	0.5	1
39	Transport Mechanism in the RND Transporter AcrD of E. coli. Biophysical Journal, 2017, 112, 274a.	0.5	0
40	Molecular Insights on the Recognition of Substrates by the Promiscuous Efflux Pump AcrB. Biophysical Journal, 2017, 112, 336a-337a.	0.5	0
41	Binding of Antibiotics to the Multidrug Efflux Pump AcrB of E. coli Investigated by Molecular Docking. Biophysical Journal, 2017, 112, 493a-494a.	0.5	0
42	Molecular Rationale behind the Differential Substrate Specificity of Bacterial RND Multi-Drug Transporters. Scientific Reports, 2017, 7, 8075.	3.3	58
43	Computational modelling of efflux pumps and their inhibitors. Essays in Biochemistry, 2017, 61, 141-156.	4.7	31
44	Editorial: Bad Bugs in the XXIst Century: Resistance Mediated by Multi-Drug Efflux Pumps in Gram-Negative Bacteria. Frontiers in Microbiology, 2016, 7, 833.	3.5	26
45	Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. Computation, 2016, 4, 5.	2.0	17
46	HIV-1 Protease Dimerization Dynamics Reveals a Transient Druggable Binding Pocket at the Interface. Scientific Reports, 2016, 5, 18555.	3.3	21
47	Multidrug Efflux Pumps and Their Inhibitors Characterized by Computational Modeling. , 2016, , 797-831.		7
48	Effect of site-directed mutations in multidrug efflux pump AcrB examined by quantitative efflux assays. Biochemical and Biophysical Research Communications, 2016, 480, 552-557.	2.1	18
49	Aminoacyl Î²-naphthylamides as substrates and modulators of AcrB multidrug efflux pump. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1405-1410.	7.1	69
50	Design of a hydrophobic tripeptide that self-assembles into amphiphilic superstructures forming a hydrogel biomaterial. Chemical Communications, 2016, 52, 5912-5915.	4.1	58
51	Molecular basis for inhibition of AcrB multidrug efflux pump by novel and powerful pyranopyridine derivatives. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 3509-3514.	7.1	172
52	The Phe-Phe Motif for Peptide Self-Assembly in Nanomedicine. Molecules, 2015, 20, 19775-19788.	3.8	131
53	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	3.8	48
54	Computational Study of Correlated Domain Motions in the AcrB Efflux Transporter. BioMed Research International, 2015, 2015, 1-12.	1.9	14

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55	AcrB drug-binding pocket substitution confers clinically relevant resistance and altered substrate specificity. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3511-3516.	7.1	165
56	Structureâ€“Activity Relationship Study of Hydroxycoumarins and Mushroom Tyrosinase. Journal of Agricultural and Food Chemistry, 2015, 63, 7236-7244.	5.2	38
57	Higher and lower supramolecular orders for the design of self-assembled heterochiral tripeptide hydrogel biomaterials. Journal of Materials Chemistry B, 2015, 3, 8123-8132.	5.8	79
58	Atomisticâ€Level Portrayal of Drugâ€“DNA Interplay: A History of Courtships and Meetings Revealed by Molecular Simulations. ChemMedChem, 2014, 9, 1966-1981.	3.2	25
59	Molecular Mechanism of Viral Resistance to a Potent Non-nucleoside Inhibitor Unveiled by Molecular Simulations. Biochemistry, 2014, 53, 6941-6953.	2.5	33
60	Molecular Mechanism of MBX2319 Inhibition of Escherichia coli AcrB Multidrug Efflux Pump and Comparison with Other Inhibitors. Antimicrobial Agents and Chemotherapy, 2014, 58, 6224-6234.	3.2	137
61	Ru[(bpy)₂(dppz)]²⁺ and Rh[(bpy)₂(chrysi)]³⁺ Targeting Double Strand DNA: The Shape of the Intercalating Ligand Tunes the Free Energy Landscape of Deintercalation. Inorganic Chemistry, 2014, 53, 7999-8008.	4.0	27
62	Modeling Assembly of the Tata Pore Forming Complex using an Implicit Membrane Model. Biophysical Journal, 2013, 104, 288a.	0.5	0
63	Folding and Self-Assembly of the TatA Translocation Pore Based on a Charge Zipper Mechanism. Cell, 2013, 152, 316-326.	28.9	59
64	Multidrug Binding Properties of the AcrB Efflux Pump Characterized by Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 285a-286a.	0.5	1
65	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.	2.5	37
66	Some Ligands Enhance the Efflux of Other Ligands by the Escherichia coli Multidrug Pump AcrB. Biochemistry, 2013, 52, 8342-8351.	2.5	42
67	MOLECULAR DYNAMICS COMPUTER SIMULATIONS OF MULTIDRUG RND EFFLUX PUMPS. Computational and Structural Biotechnology Journal, 2013, 5, e201302008.	4.1	41
68	Molecular recognition of DNA by ligands: Roughness and complexity of the free energy profile. Journal of Chemical Physics, 2013, 139, 145102.	3.0	20
69	RND Efflux Pumps: Structural Information Translated into Function and Inhibition Mechanisms. Current Topics in Medicinal Chemistry, 2013, 13, 3079-3100.	2.1	122
70	Multidrug binding properties of the AcrB efflux pump characterized by molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 20637-20642.	7.1	208
71	Recognition of Imipenem and Meropenem by the RND-Transporter MexB Studied by Computer Simulations. Journal of the American Chemical Society, 2012, 134, 19146-19158.	13.7	41
72	Detecting DNA Mismatches with Metallo-Insertors: A Molecular Simulation Study. Inorganic Chemistry, 2012, 51, 2046-2057.	4.0	41

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73	A Novel Dendrimeric Peptide with Antimicrobial Properties: Structure-Function Analysis of SB056. Biophysical Journal, 2012, 102, 1039-1048.	0.5	41
74	A kinetic Monte Carlo approach to investigate antibiotic translocation through bacterial porins. Journal of Physics Condensed Matter, 2012, 24, 104012.	1.8	13
75	Effects of Point Mutations on the Activity of AcrB. Biophysical Journal, 2012, 102, 247a.	0.5	0
76	Effect of the F610A Mutation on Substrate Extrusion in the AcrB Transporter: Explanation and Rationale by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 10704-10707.	13.7	79
77	Point Mutation I261M Affects the Dynamics of BVDV and its Interaction with Benzimidazole Antiviral 227G. Biophysical Journal, 2011, 100, 395a-396a.	0.5	1
78	Folding and Self-Assembly of the Pore-Forming Unit Tat-A of the Bacterial Twin-Arginine Translocase. Biophysical Journal, 2011, 100, 345a.	0.5	0
79	Role of Water during the Extrusion of Substrates by the Efflux Transporter AcrB. Journal of Physical Chemistry B, 2011, 115, 8278-8287.	2.6	38
80	Molecular motions in drug design: the coming age of the metadynamics method. Journal of Computer-Aided Molecular Design, 2011, 25, 395-402.	2.9	38
81	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. PLoS Computational Biology, 2010, 6, e1000806.	3.2	83
82	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. Biophysical Journal, 2010, 98, 628a.	0.5	1
83	Functional Rotation of the Transporter AcrB: The Essentials of Peristaltic Motion and Subsequent Substrate Extrusion. Biophysical Journal, 2010, 98, 685a.	0.5	2
84	Magnetic Coupling between Copper(II) Ions Mediated by Hydrogen-Bonded (Neutral) Water Molecules. Inorganic Chemistry, 2009, 48, 5473-5479.	4.0	62
85	Molecular Recognition Routes Of DNA By Anticancer Ligands: Mechanisms and Free Energies Explored Via Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 84a.	0.5	0
86	Copperâ^'1,10-Phenanthroline Complexes Binding to DNA: Structural Predictions from Molecular Simulations. Journal of Physical Chemistry B, 2009, 113, 10881-10890.	2.6	78
87	Simulating Efflux Pumps: The Extrusion Mechanism of Substrates. Biophysical Journal, 2009, 96, 381a-382a.	0.5	0
88	Simulations of Copper-1,10-Phenanthroline Complexes Binding the DNA. Biophysical Journal, 2009, 96, 577a.	0.5	0
89	Waterâ^'Chloride and Waterâ^'Bromide Hydrogen-Bonded Networks: Influence of the Nature of the Halide Ions on the Stability of the Supramolecular Assemblies. Journal of Physical Chemistry A, 2009, 113, 8626-8634.	2.5	19
90	Sliding of Alkylating Anticancer Drugs along the Minor Groove of DNA: New Insights on Sequence Selectivity. Biophysical Journal, 2008, 94, 550-561.	0.5	25

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91	The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFTâˆ’PCM Calculations. Journal of Physical Chemistry B, 2008, 112, 4401-4409.	2.6	60
92	Dissociation of minor groove binders from DNA: insights from metadynamics simulations. Nucleic Acids Research, 2008, 36, 5910-5921.	14.5	60
93	Anthramycinâ€“DNA Binding Explored by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 24687-24695.	2.6	23
94	Molecular dynamics simulations of outer-membrane protease T fromE. colibased on a hybrid coarse-grained/atomistic potential. Journal of Physics Condensed Matter, 2006, 18, S347-S355.	1.8	14