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	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
2	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
3	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
4	Chirality Effects on Peptide Self-Assembly Unraveled from Molecules to Materials. CheM, 2018, 4, 1862-1876.	11.7	151
5	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
6	The Phe-Phe Motif for Peptide Self-Assembly in Nanomedicine. Molecules, 2015, 20, 19775-19788.	3.8	131
7	RND Efflux Pumps: Structural Information Translated into Function and Inhibition Mechanisms. Current Topics in Medicinal Chemistry, 2013, 13, 3079-3100.	2.1	122
8	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. PLoS Computational Biology, 2010, 6, e1000806.	3.2	83
9	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
10	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
11	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
12	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
13	Heterochirality and Halogenation Control Phe-Phe Hierarchical Assembly. ACS Nano, 2020, 14, 16951-16961.	14.6	67
14	Magnetic Coupling between Copper(II) Ions Mediated by Hydrogen-Bonded (Neutral) Water Molecules. Inorganic Chemistry, 2009, 48, 5473-5479.	4.0	62
15	The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFTâ˜'PCM Calculations. Journal of Physical Chemistry B, 2008, 112, 4401-4409.	2.6	60
16	Dissociation of minor groove binders from DNA: insights from metadynamics simulations. Nucleic Acids Research, 2008, 36, 5910-5921.	14.5	60
17	Folding and Self-Assembly of the TatA Translocation Pore Based on a Charge Zipper Mechanism. Cell, 2013, 152, 316-326.	28.9	59
18	Design of a hydrophobic tripeptide that self-assembles into amphiphilic superstructures forming a hydrogel biomaterial. Chemical Communications, 2016, 52, 5912-5915.	4.1	58

#	Article	IF	Citations
19	Molecular Rationale behind the Differential Substrate Specificity of Bacterial RND Multi-Drug Transporters. Scientific Reports, 2017, 7, 8075.	3.3	58
20	Chlorpromazine and Amitriptyline Are Substrates and Inhibitors of the AcrB Multidrug Efflux Pump. MBio, 2020, 11, .	4.1	54
21	Nanoscale Assembly of Functional Peptides with Divergent Programming Elements. ACS Nano, 2021, 15, 3015-3025.	14.6	50
22	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	3.8	48
23	Some Ligands Enhance the Efflux of Other Ligands by the Escherichia coli Multidrug Pump AcrB. Biochemistry, 2013, 52, 8342-8351.	2.5	42
24	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
25	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
26	Detecting DNA Mismatches with Metallo-Insertors: A Molecular Simulation Study. Inorganic Chemistry, 2012, 51, 2046-2057.	4.0	41
27	A Novel Dendrimeric Peptide with Antimicrobial Properties: Structure-Function Analysis of SB056. Biophysical Journal, 2012, 102, 1039-1048.	0.5	41
28	MOLECULAR DYNAMICS COMPUTER SIMULATIONS OF MULTIDRUG RND EFFLUX PUMPS. Computational and Structural Biotechnology Journal, 2013, 5, e201302008.	4.1	41
29	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
30	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
31	Structureâ€“Activity Relationship Study of Hydroxycoumarins and Mushroom Tyrosinase. Journal of Agricultural and Food Chemistry, 2015, 63, 7236-7244.	5.2	38
32	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
33	Molecular Determinants of the Promiscuity of MexB and MexY Multidrug Transporters of Pseudomonas aeruginosa. Frontiers in Microbiology, 2018, 9, 1144.	3.5	37
34	Binding and Transport of Carboxylated Drugs by the Multidrug Transporter AcrB. Journal of Molecular Biology, 2020, 432, 861-877.	4.2	37
35	Perturbed structural dynamics underlie inhibition and altered efflux of the multidrugÂresistance pump AcrB. Nature Communications, 2020, 11, 5565.	12.8	34
36	The challenge of intracellular antibiotic accumulation, a function of fluoroquinolone influx versus bacterial efflux. Communications Biology, 2020, 3, 198.	4.4	34

#	Article	IF	Citations
37	Molecular Mechanism of Viral Resistance to a Potent Non-nucleoside Inhibitor Unveiled by Molecular Simulations. Biochemistry, 2014, 53, 6941-6953.	2.5	33
38	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
39	Computer simulations of the activity of RND efflux pumps. Research in Microbiology, 2018, 169, 384-392.	2.1	32
40	Computational modelling of efflux pumps and their inhibitors. Essays in Biochemistry, 2017, 61, 141-156.	4.7	31
41	Predictive Rules of Efflux Inhibition and Avoidance in Pseudomonas aeruginosa. MBio, 2021, 12, .	4.1	28
42	Pyridylpiperazine-based allosteric inhibitors of RND-type multidrug efflux pumps. Nature Communications, 2022, 13, 115.	12.8	28
43	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
44	A New Critical Conformational Determinant of Multidrug Efflux by an MFS Transporter. Journal of Molecular Biology, 2018, 430, 1368-1385.	4.2	27
45	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
46	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
47	Atomisticâ€Ł evel Portrayal of Drugâ€“DNA Interplay: A History of Courtships and Meetings Revealed by Molecular Simulations. ChemMedChem, 2014, 9, 1966-1981.	3.2	25
48	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
49	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
50	Anthramycinâ^'DNA Binding Explored by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 24687-24695.	2.6	23
51	Bacterial efflux transportersâ€™ polyspecificity â€“ a gift and a curse?. Current Opinion in Microbiology, 2021, 61, 115-123.	5.1	23
52	HIV-1 Protease Dimerization Dynamics Reveals a Transient Druggable Binding Pocket at the Interface. Scientific Reports, 2016, 5, 18555.	3.3	21
53	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
54	Molecular recognition of DNA by ligands: Roughness and complexity of the free energy profile. Journal of Chemical Physics, 2013, 139, 145102.	3.0	20

#	Article	IF	Citations
55	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
56	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
57	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
58	Identification and characterization of carbapenem binding sites within the RND-transporter AcrB. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 62-74.	2.6	18
59	Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. Computation, 2016, 4, 5.	2.0	17
60	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
61	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
62	Computational Study of Correlated Domain Motions in the AcrB Efflux Transporter. BioMed Research International, 2015, 2015, 1-12.	1.9	14
63	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
64	A kinetic Monte Carlo approach to investigate antibiotic translocation through bacterial porins. Journal of Physics Condensed Matter, 2012, 24, 104012.	1.8	13
65	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
66	Relevance of Ebola virus VP35 homo-dimerization on the type I interferon cascade inhibition. Antiviral Chemistry and Chemotherapy, 2019, 27, 204020661988922.	0.6	11
67	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
68	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
69	Recognition of quinolone antibiotics by the multidrug efflux transporter MexB ofPseudomonas aeruginosa. Physical Chemistry Chemical Physics, 2022, 24, 16566-16575.	2.8	9
70	Multidrug Efflux Pumps and Their Inhibitors Characterized by Computational Modeling. , 2016, , 797-831.		7
71	Self-Assembling l-d-l-Tripeptides Dance the Twist. Synlett, 2020, 31, 434-438.	1.8	7
72	Molecular Modeling of Multidrug Properties of Resistance Nodulation Division (RND) Transporters. Methods in Molecular Biology, 2018, 1700, 179-219.	0.9	6

#	Article	IF	Citations
73	Single-atom substitution enables supramolecular diversity from dipeptide building blocks. Soft Matter, 2022, 18, 2129-2136.	2.7	6
74	AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials. Scientific Data, 2022, 9, 148.	5.3	6
75	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
76	Functional Rotation of the Transporter AcrB: The Essentials of Peristaltic Motion and Subsequent Substrate Extrusion. Biophysical Journal, 2010, 98, 685a.	0.5	2
77	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
78	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
79	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. Biophysical Journal, 2010, 98, 628a.	0.5	1
80	Point Mutation I261M Affects the Dynamics of BVDV and its Interaction with Benzimidazole Antiviral 227G. Biophysical Journal, 2011, 100, 395a-396a.	0.5	1
81	Multidrug Binding Properties of the AcrB Efflux Pump Characterized by Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 285a-286a.	0.5	1
82	Molecular Insights into Compound-Transporter Interactions: The Case ofÂInhibitors of Gram-Negative Bacteria Efflux Pumps. Biophysical Journal, 2017, 112, 274a.	0.5	1
83	Molecular Insights Into Binding and Activation of the Human KCNQ2 Channel by Retigabine. Frontiers in Molecular Biosciences, 2022, 9, 839249.	3.5	1
84	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
85	Simulating Efflux Pumps: The Extrusion Mechanism of Substrates. Biophysical Journal, 2009, 96, 381a-382a.	0.5	0
86	Simulations of Copper-1,10-Phenanthroline Complexes Binding the DNA. Biophysical Journal, 2009, 96, 577a.	0.5	0
87	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
88	Effects of Point Mutations on the Activity of AcrB. Biophysical Journal, 2012, 102, 247a.	0.5	0
89	Modeling Assembly of the Tata Pore Forming Complex using an Implicit Membrane Model. Biophysical Journal, 2013, 104, 288a.	0.5	0
90	Computational Study of the Interaction between Antimicrobial Compounds and Efflux Systems of Gram-Negative Bacteria. Biophysical Journal, 2017, 112, 274a.	0.5	0

#	Article	IF	Citations
91	Molecular Rationale Behind the Differential Substrate Specificity of RND Transporters AcrB and AcrD. Biophysical Journal, 2017, 112, 274a.	0.5	0
92	Transport Mechanism in the RND Transporter AcrD of E. coli. Biophysical Journal, 2017, 112, 274a.	0.5	0
93	Molecular Insights on the Recognition of Substrates by the Promiscuous Efflux Pump AcrB. Biophysical Journal, 2017, 112, 336a-337a.	0.5	0
94	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