Giuliano Malloci

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5260371/publications.pdf

Version: 2024-02-01

92 papers	2,434 citations	159358 30 h-index	233125 45 g-index
95 all docs	95 docs citations	95 times ranked	2655 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.	1.9	4
2	Pyridylpiperazine-based allosteric inhibitors of RND-type multidrug efflux pumps. Nature Communications, 2022, 13, 115.	5.8	28
3	Inhibition of the drug efflux activity of Ptch1 as a promising strategy to overcome chemotherapy resistance in cancer cells. European Journal of Medicinal Chemistry, 2022, 236, 114306.	2.6	2
4	AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials. Scientific Data, 2022, 9, 148.	2.4	6
5	Recognition of quinolone antibiotics by the multidrug efflux transporter MexB ofPseudomonas aeruginosa. Physical Chemistry Chemical Physics, 2022, 24, 16566-16575.	1.3	9
6	Molecular insights into the Patched1 drug efflux inhibitory activity of panicein A hydroquinone: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 8013-8022.	1.3	2
7	Predictive Rules of Efflux Inhibition and Avoidance in Pseudomonas aeruginosa. MBio, 2021, 12, .	1.8	28
8	Bacterial efflux transportersâ€™ polyspecificity â€“ a gift and a curse?. Current Opinion in Microbiology, 2021, 61, 115-123.	2.3	23
9	Mechanistic Duality of Bacterial Efflux Substrates and Inhibitors: Example of Simple Substituted Cinnamoyl and Naphthyl Amides. ACS Infectious Diseases, 2021, 7, 2650-2665.	1.8	16
10	Structural and functional analysis of the promiscuous AcrB and AdeB efflux pumps suggests different drug binding mechanisms. Nature Communications, 2021, 12, 6919.	5.8	25
11	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.	1.3	11
12	Binding and Transport of Carboxylated Drugs by the Multidrug Transporter AcrB. Journal of Molecular Biology, 2020, 432, 861-877.	2.0	37
13	Time-Dependent Density Functional Theory Investigation on the Electronic and Optical Properties of Poly-C,Si,Ge-acenes. ACS Omega, 2020, 5, 16654-16663.	1.6	8
14	Perturbed structural dynamics underlie inhibition and altered efflux of the multidrugÂresistance pump AcrB. Nature Communications, 2020, 11, 5565.	5.8	34
15	Chlorpromazine and Amitriptyline Are Substrates and Inhibitors of the AcrB Multidrug Efflux Pump. MBio, 2020, 11, .	1.8	54
16	EDES: A Protocol to Generate Holo-Like and Druggable Protein Conformations Starting from the APO Structure. Biophysical Journal, 2020, 118, 44a.	0.2	0
17	Molecular Interactions of Carbapenem Antibiotics with the Multidrug Efflux Transporter AcrB of Escherichia coli. International Journal of Molecular Sciences, 2020, 21, 860.	1.8	11
18	The challenge of intracellular antibiotic accumulation, a function of fluoroquinolone influx versus bacterial efflux. Communications Biology, 2020, 3, 198.	2.0	34

#	Article	IF	Citations
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	Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. Journal of Physical Chemistry B, 2019, 123, 4625-4635.	1.2	18
21	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.	2.5	33
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	Identification and characterization of carbapenem binding sites within the RND-transporter AcrB. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 62-74.	1.4	18
24	Bacterial Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. Biophysical Journal, 2018, 114, 134a.	0.2	0
25	Computer simulations of the activity of RND efflux pumps. Research in Microbiology, 2018, 169, 384-392.	1.0	32
26	Water-mediated interactions enable smooth substrate transport in a bacterial efflux pump. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 836-845.	1.1	42
27	A New Critical Conformational Determinant of Multidrug Efflux by an MFS Transporter. Journal of Molecular Biology, 2018, 430, 1368-1385.	2.0	27
28	Molecular Modeling of Multidrug Properties of Resistance Nodulation Division (RND) Transporters. Methods in Molecular Biology, 2018, 1700, 179-219.	0.4	6
29	Molecular Determinants of the Promiscuity of MexB and MexY Multidrug Transporters of Pseudomonas aeruginosa. Frontiers in Microbiology, 2018, 9, 1144.	1.5	37
30	Rationalizing the permeation of polar antibiotics into Gram-negative bacteria. Journal of Physics Condensed Matter, 2017, 29, 113001.	0.7	22
31	Computational Study of the Interaction between Antimicrobial Compounds and Efflux Systems of Gram-Negative Bacteria. Biophysical Journal, 2017, 112, 274a.	0.2	0
32	Investigation of Siderophore-Monobactam Antibiotic Derivatives: Their Iron(III)-Complexes and Binding to Receptors. Biophysical Journal, 2017, 112, 551a-552a.	0.2	1
33	Molecular Rationale Behind the Differential Substrate Specificity of RND Transporters AcrB and AcrD. Biophysical Journal, 2017, 112, 274a.	0.2	0
34	Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. ACS Nano, 2017, 11, 5465-5473.	7.3	74
35	Transport Mechanism in the RND Transporter AcrD of E. coli. Biophysical Journal, 2017, 112, 274a.	0.2	0
36	Filtering with the Electric Field: A Story on Protein Channels Electrostatics. Biophysical Journal, 2017, 112, 417a.	0.2	0

#	Article	IF	Citations
37	Binding of Antibiotics to the Multidrug Efflux Pump AcrB of E. coli Investigated by Molecular Docking. Biophysical Journal, 2017, 112, 493a-494a.	0.2	0
38	Tuning Optical Properties of Dibenzochrysenes by Functionalization: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry C, 2017, 121, 24480-24488.	1.5	18
39	Molecular Rationale behind the Differential Substrate Specificity of Bacterial RND Multi-Drug Transporters. Scientific Reports, 2017, 7, 8075.	1.6	58
40	Computational modelling of efflux pumps and their inhibitors. Essays in Biochemistry, 2017, 61, 141-156.	2.1	31
41	Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. Computation, 2016, 4, 5.	1.0	17
42	Computational investigation of the effects of perfluorination on the charge-transport properties of polyaromatic hydrocarbons. Chemical Physics, 2016, 478, 8-13.	0.9	13
43	Electronic and optical properties of functionalized polyaromatic hydrocarbons: a computational investigation on perfluorinated circumacenes. Proceedings of SPIE, 2016, , .	0.8	4
44	Electronic and optical properties of hexathiapentacene in the gas and crystal phases. Physical Review B, 2016, 93, .	1.1	29
45	Multidrug Efflux Pumps and Their Inhibitors Characterized by Computational Modeling. , 2016, , 797-831.		7
46	Exploiting the porin pathway for polar compound delivery into Gram-negative bacteria. Future Medicinal Chemistry, 2016, 8, 1047-1062.	1.1	16
47	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	1.7	48
48	Effects of TIPS-Functionalization and Perhalogenation on the Electronic, Optical, and Transport Properties of Angular and Compact Dibenzochrysene. Journal of Physical Chemistry A, 2014, 118, 5170-5177.	1.1	46
49	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. Advanced Energy Materials, 2014, 4, 1301694.	10.2	42
50	Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces. Thin Solid Films, 2014, 560, 34-38.	0.8	1
51	Electronic Properties and Quantum Confinement in Bi₂S₃ Ribbon-Like Nanostructures. Journal of Physical Chemistry C, 2013, 117, 21923-21929.	1.5	17
52	A (time-dependent) density functional theory study of the optoelectronic properties of bis-triisopropylsilylethynyl-functionalized acenes. Thin Solid Films, 2013, 543, 32-34.	0.8	10
53	Role of Molecular Thermodynamical Processes at Functionalized Polymer/Metaloxide Interfaces for Photovoltaics. Journal of Physical Chemistry C, 2013, 117, 13894-13901.	1.5	13
54	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 8741-8746.	1.5	41

#	Article	IF	Citations
55	Optoelectronic properties of (ZnO)60 isomers. Physical Chemistry Chemical Physics, 2012, 14, 14293.	1.3	14
56	The effect of selective interactions at the interface of polymerâ€“oxide hybrid solar cells. Energy and Environmental Science, 2012, 5, 9068.	15.6	42
57	Electronic Properties of Hybrid Zinc Oxideâ€“Oligothiophene Nanostructures. Journal of Physical Chemistry C, 2012, 116, 8174-8180.	1.5	13
58	Zinc Oxideâ€“Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448.	1.5	36
59	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. Journal of Physical Chemistry C, 2011, 115, 9651-9655.	1.5	30
60	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. Chemical Physics, 2011, 384, 19-27.	0.9	139
61	Search for far-IR PAH bands with Herschel: modelling and observational approaches. EAS Publications Series, 2011, 46, 123-130.	0.3	10
62	Polycyclic Aromatic Hydrocarbons and the Extinction Curve. EAS Publications Series, 2011, 46, 327-340.	0.3	2
63	Visible photodissociation spectroscopy of PAH cations and derivatives in the PIRENEA experiment. Chemical Physics, 2010, 371, 16-23.	0.9	40
64	Modelling peculiar extinction curves. Monthly Notices of the Royal Astronomical Society, 2010, , no-no.	1.6	5
65	Large prebiotic molecules in space: photophysics of acetic acid and its isomers. Monthly Notices of the Royal Astronomical Society, 2010, 402, 1667-1674.	1.6	14
66	Search for corannulene (C₂₀H₁₀) in the Red Rectangle. Monthly Notices of the Royal Astronomical Society, 2009, 397, 1053-1060.	1.6	39
67	Electronic excitations of oligoacenes: A time dependent density functional theory study. Superlattices and Microstructures, 2009, 46, 14-18.	1.4	33
68	High-resolution infrared absorption spectroscopy of thermally excited naphthalene. Measurements and calculations of anharmonic parameters and vibrational interactions. Physical Chemistry Chemical Physics, 2009, 11, 3443.	1.3	57
69	Testing the attribution of selected DIBs to dehydrogenated coronene cations. Proceedings of the International Astronomical Union, 2008, 4, 67-68.	0.0	0
70	Dehydrogenated coronene cations and interstellar extinction. Proceedings of the International Astronomical Union, 2008, 4, 75-76.	0.0	0
71	The role of the charge state of PAHs in ultraviolet extinction. Astronomy and Astrophysics, 2008, 486, L25-L29.	2.1	54
72	Dehydrogenated polycyclic aromatic hydrocarbons and UV bump. Astronomy and Astrophysics, 2008, 489, 1183-1187.	2.1	44

#	Article	IF	Citations
73	Theoretical evaluation of PAH dication properties. Astronomy and Astrophysics, 2007, 462, 627-635.	2.1	61
74	Efficient calculation of van der Waals dispersion coefficients with time-dependent density functional theory in real time: Application to polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2007, 127, 014107.	1.2	31
75	On-line database of the spectral properties of polycyclic aromatic hydrocarbons. Chemical Physics, 2007, 332, 353-359.	0.9	164
76	Time-dependent density functional study of the electronic spectra of oligoacenes in the charge states â^'1, 0, +1, and +2. Chemical Physics, 2007, 340, 43-58.	0.9	100
77	A general model for the identification of specific PAHs in the far-IR. Astronomy and Astrophysics, 2006, 460, 93-104.	2.1	53
78	Diagnostics for specific PAHs in the far-IR: searching neutral naphthalene and anthracene in the Red Rectangle. Astronomy and Astrophysics, 2006, 456, 161-169.	2.1	42
79	Estimated IR and phosphorescence emission fluxes for specific polycyclic aromatic hydrocarbons in the Red Rectangle. Astronomy and Astrophysics, 2006, 446, 537-549.	2.1	32
80	Identifyingspecificinterstellar polycyclic aromatic hydrocarbons. Journal of Physics: Conference Series, 2005, 6, 217-222.	0.3	1
81	Theoretical electron affinities of PAHs and electronic absorption spectra of their mono-anions. Astronomy and Astrophysics, 2005, 432, 585-594.	2.1	57
82	Theoretical spectral properties of PAHs: towards a detailed model of their photophysics in the ISM. Journal of Physics: Conference Series, 2005, 6, 178-184.	0.3	3
83	Modelling photoluminescence from interstellar dust. Journal of Physics: Conference Series, 2005, 6, 185-190.	0.3	0
84	Electronic excitations of stable fullerene-like GaP clusters. Materials Research Society Symposia Proceedings, 2004, 854, U3.4.1.	0.1	0
85	Quasiparticle effects and optical absorption in small fullerenelike GaP clusters. Physical Review B, 2004, 70, .	1.1	24
86	Rotational profiles of molecular absorption bands in astrophysically relevant conditions: ab-initio approach. Computational Materials Science, 2004, 30, 92-97.	1.4	0
87	Electronic absorption spectra of PAHs up to vacuum UV. Astronomy and Astrophysics, 2004, 426, 105-117.	2.1	112
88	Modelling photoluminescence from small particles. Astronomy and Astrophysics, 2004, 420, 809-820.	2.1	5
89	Modelling photoluminescence from small particles. Astronomy and Astrophysics, 2004, 420, 921-927.	2.1	6
90	Testing the â€œstrongâ€•PAHs hypothesis. Astronomy and Astrophysics, 2003, 410, 623-637.	2.1	21

#	Article	IF	Citations
91	Testing the â€œstrongâ€•PAHs hypothesis. Astronomy and Astrophysics, 2003, 410, 639-648.	2.1	22
92	Zâ€Selective Synthesis of Î±â€Sulfanyl Carbonyl Compounds from Internal Alkynes and Thiols via Photoredox Catalysis. Advanced Synthesis and Catalysis, 0, , .	2.1	3