Laura Goracci

List of Publications by Year
in descending order

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Version: 2024-02-01

81	2,644	126708	205818
papers	citations	33	48
		h-index	g-index

87	87	87	3908
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751.	2.9	141
2	LC/MS lipid profiling from human serum: a new method for global lipid extraction. Analytical and Bioanalytical Chemistry, 2014, 406, 7937-7948.	1.9	115
3	Small molecule inhibitors of influenza A and B viruses that act by disrupting subunit interactions of the viral polymerase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6247-6252.	3.3	114
4	Extending pKa prediction accuracy: High-throughput pKa measurements to understand pKa modulation of new chemical series. European Journal of Medicinal Chemistry, 2010, 45, 4270-4279.	2.6	107
5	A Broad Anti-influenza Hybrid Small Molecule That Potently Disrupts the Interaction of Polymerase Acidic Proteinâ€“Basic Protein 1 (PA-PB1) Subunits. Journal of Medicinal Chemistry, 2015, 58, 3830-3842.	2.9	81
6	Decarboxylation and Dephosphorylation in New Gemini Surfactants. Changes in Aggregate Structures. Langmuir, 2002, 18, 7821-7825.	1.6	78
7	GRID-Based Three-Dimensional Pharmacophores I: FLAPpharm, a Novel Approach for Pharmacophore Elucidation. Journal of Chemical Information and Modeling, 2012, 52, 2587-2598.	2.5	76
8	Lipostar, a Comprehensive Platform-Neutral Cheminformatics Tool for Lipidomics. Analytical Chemistry, 2017, 89, 6257-6264.	3.2	76
9	In silico pK_a Prediction and ADME Profiling. Chemistry and Biodiversity, 2009, 6, 1812-1821.	1.0	70
10	Understanding the Metabolism of Proteolysis Targeting Chimeras (PROTACs): The Next Step toward Pharmaceutical Applications. Journal of Medicinal Chemistry, 2020, 63, 11615-11638.	2.9	69
11	BioGPS: Navigating biological space to predict polypharmacology, off-targeting, and selectivity. Proteins: Structure, Function and Bioinformatics, 2015, 83, 517-532.	1.5	68
12	Indole Based Weapons to Fight Antibiotic Resistance: A Structureâ€“Activity Relationship Study. Journal of Medicinal Chemistry, 2016, 59, 867-891.	2.9	64
13	Optimization of Small-Molecule Inhibitors of Influenza Virus Polymerase: From Thiophene-3-Carboxamide to Polyamido Scaffolds. Journal of Medicinal Chemistry, 2014, 57, 4337-4350.	2.9	59
14	Use of lipidomics to investigate sebum dysfunction in juvenile acne. Journal of Lipid Research, 2016, 57, 1051-1058.	2.0	58
15	Prediction of retention time in reversed-phase liquid chromatography as a tool for steroid identification. Analytica Chimica Acta, 2016, 916, 8-16.	2.6	58
16	Structural Investigation of Cycloheptathiophene-3-carboxamide Derivatives Targeting Influenza Virus Polymerase Assembly. Journal of Medicinal Chemistry, 2013, 56, 10118-10131.	2.9	51
17	Structureâ€“metabolism relationships in human- AOX: Chemical insights from a large database of aza-aromatic and amide compounds. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E3178-E3187.	3.3	51
18	Nutritional and lipidomics biomarkers of docosahexaenoic acid-based multivitamin therapy in pediatric NASH. Scientific Reports, 2019, 9, 2045.	1.6	51

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19	Ligand-, structure- and pharmacophore-based molecular fingerprints: a case study on adenosine A1, A2A, A2B, and A3 receptor antagonists. Journal of Computer-Aided Molecular Design, 2012, 26, 1247-1266.	1.3	46
20	Modeling Phospholipidosis Induction: Reliability and Warnings. Journal of Chemical Information and Modeling, 2013, 53, 1436-1446.	2.5	46
21	Indomethacin-based PROTACs as pan-coronavirus antiviral agents. European Journal of Medicinal Chemistry, 2021, 226, 113814.	2.6	46
22	Surfactant-Based Photorheological Fluids: Effect of the Surfactant Structure. Langmuir, 2009, 25, 5467-5475.	1.6	45
23	Polymerase Acidic Proteinâ€“Basic Protein 1 (PAâ€“PB1) Proteinâ€“Protein Interaction as a Target for Next-Generation Anti-influenza Therapeutics. Journal of Medicinal Chemistry, 2016, 59, 7699-7718.	2.9	43
24	New linezolid-like 1,2,4-oxadiazoles active against Gram-positive multiresistant pathogens. European Journal of Medicinal Chemistry, 2013, 65, 533-545.	2.6	42
25	Hoechst 33258 as a pH-Sensitive Probe to Study the Interaction of Amine Oxide Surfactants with DNA. ChemBioChem, 2005, 6, 197-203.	1.3	40
26	Exposition and reactivity optimization to predict sites of metabolism in chemicals. Drug Discovery Today: Technologies, 2013, 10, e155-e165.	4.0	40
27	Flavin Monooxygenase Metabolism: Why Medicinal Chemists Should Matter. Journal of Medicinal Chemistry, 2014, 57, 6183-6196.	2.9	39
28	A novel small-molecule inhibitor of the human papillomavirus E6-p53 interaction that reactivates p53 function and blocks cancer cells growth. Cancer Letters, 2020, 470, 115-125.	3.2	39
29	Human Cytomegalovirus Inhibitor AL18 Also Possesses Activity against Influenza A and B Viruses. Antimicrobial Agents and Chemotherapy, 2012, 56, 6009-6013.	1.4	38
30	Exploring the cycloheptathiophene-3-carboxamide scaffold to disrupt the interactions of the influenza polymerase subunits and obtain potent anti-influenza activity. European Journal of Medicinal Chemistry, 2017, 138, 128-139.	2.6	38
31	Dehydrogenation of Amines to Nitriles in Aqueous Micelles. European Journal of Organic Chemistry, 2005, 2005, 3060-3063.	1.2	36
32	Computational solutions in redox lipidomics â€“ Current strategies and future perspectives. Free Radical Biology and Medicine, 2019, 144, 110-123.	1.3	36
33	Anomalous Behavior of Amine Oxide Surfactants at the Air/Water Interface. Langmuir, 2007, 23, 10525-10532.	1.6	35
34	A Rational Approach for the Identification of Non-Hydroxamate HDAC6-Selective Inhibitors. Scientific Reports, 2016, 6, 29086.	1.6	33
35	Improved Potency of Indole-Based NorA Efflux Pump Inhibitors: From Serendipity toward Rational Design and Development. Journal of Medicinal Chemistry, 2017, 60, 517-523.	2.9	33
36	Efficient and regioselective one-step synthesis of 7-aryl-5-methyl- and 5-aryl-7-methyl-2-amino-[1,2,4]triazolo[1,5-a]pyrimidine derivatives. Organic and Biomolecular Chemistry, 2017, 15, 7944-7955.	1.5	31

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37	Metabolism of JWH-015, JWH-098, JWH-251, and JWH-307 in silico and in vitro: a pilot study for the detection of unknown synthetic cannabinoids metabolites. Analytical and Bioanalytical Chemistry, 2014, 406, 3621-3636.	1.9	29
38	Evaluating the risk of phospholipidosis using a new multidisciplinary pipeline approach. European Journal of Medicinal Chemistry, 2015, 92, 49-63.	2.6	29
39	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. Journal of Medicinal Chemistry, 2018, 61, 360-371.	2.9	29
40	Pharmacophoreâ€based discovery of inhibitors of a novel drug/proton antiporter in human brain endothelial hCMEC/D3 cell line. British Journal of Pharmacology, 2015, 172, 4888-4904.	2.7	28
41	Modeling, design and synthesis of new heteroaryl ethylenes active against the MCF-7 breast cancer cell-line. Molecular BioSystems, 2013, 9, 2426.	2.9	26
42	Challenging AQP4 druggability for NMO-IgG antibody binding using molecular dynamics and molecular interaction fields. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1462-1471.	1.4	25
43	Enhanced triacylglycerol catabolism by carboxylesterase 1 promotes aggressive colorectal carcinoma. Journal of Clinical Investigation, 2021, 131, .	3.9	25
44	New potent antibacterials against Gram-positive multiresistant pathogens: Effects of side chain modification and chirality in linezolid-like 1,2,4-oxadiazoles. Bioorganic and Medicinal Chemistry, 2014, 22, 6814-6825.	1.4	21
45	Interaction between DNA and Cationic Amphiphiles: A Multi-Technique Study. Langmuir, 2010, 26, 7885-7892.	1.6	19
46	Cyto- and enzyme toxicities of ionic liquids modelled on the basis of VolSurf+ descriptors and their principal properties. SAR and QSAR in Environmental Research, 2016, 27, 221-244.	1.0	19
47	Modelling the aquatic toxicity of ionic liquids by means of VolSurfin silicodescriptors. SAR and QSAR in Environmental Research, 2016, 27, 1-15.	1.0	18
48	Premicellar Accelerated Decarboxylation of 6-Nitrobenzisoxazole-3-carboxylate Ion and Its 5-Tetradecyloxy Derivative. Langmuir, 2007, 23, 436-442.	1.6	17
49	Enabling Efficient Lateâ€Stage Functionalization of Drugâ€Like Molecules with LCâ€MS and Reactionâ€Driven Data Processing. European Journal of Organic Chemistry, 2017, 2017, 7122-7126.	1.2	17
50	Delving into the Polar Lipidome by Optimized Chromatographic Separation, High-Resolution Mass Spectrometry, and Comprehensive Identification with Lipostar: Microalgae as Case Study. Analytical Chemistry, 2018, 90, 12230-12238.	3.2	17
51	Synthesis and characterization of 1,2,4-triazolo[1,5-a]pyrimidine-2-carboxamide-based compounds targeting the PA-PB1 interface of influenza A virus polymerase. European Journal of Medicinal Chemistry, 2021, 209, 112944.	2.6	17
52	Are carboxylic esters really refractory to DAST? On the fluorination of Î±-hydroxyesters with DAST. Journal of Fluorine Chemistry, 2015, 171, 82-91.	0.9	16
53	Some considerations on the predictions of pharmacokinetic alterations in subjects with liver disease. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 1397-1408.	1.5	15
54	A role for the autophagy regulator Transcription Factor EB in amiodarone-induced phospholipidosis. Biochemical Pharmacology, 2015, 95, 201-209.	2.0	14

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55	Proteolysis targeting chimeras in antiviral research. Future Medicinal Chemistry, 2022, 14, 459-462.	1.1	14
56	Metabolism study and biological evaluation of bosentan derivatives. European Journal of Medicinal Chemistry, 2016, 121, 658-670.	2.6	13
57	Esterification of Unprotected α-Amino Acids in Ionic Liquids as the Reaction Media. Letters in Organic Chemistry, 2010, 7, 39-44.	0.2	11
58	BioGPS: The Music for the Chemoâ€•and Bioinformatics Walzer. Molecular Informatics, 2014, 33, 446-453.	1.4	11
59	Role of mitochondria and cardiolipins in growth inhibition of breast cancer cells by retinoic acid. Journal of Experimental and Clinical Cancer Research, 2019, 38, 436.	3.5	11
60	Discovery of novel SARS-CoV-2 inhibitors targeting the main protease Mpro by virtual screenings and hit optimization. Antiviral Research, 2022, 204, 105350.	1.9	11
61	A Novel Lipidomics-Based Approach to Evaluating the Risk of Clinical Hepatotoxicity Potential of Drugs in 3D Human Microtissues. Chemical Research in Toxicology, 2020, 33, 258-270.	1.7	10
62	Synthesis of new indole-based bisphosphonates and evaluation of their chelating ability in PE/CA-PJ15 cells. European Journal of Medicinal Chemistry, 2015, 102, 403-412.	2.6	9
63	Targeting Nsp9 as an anti-SARS-CoV-2 strategy. New Journal of Chemistry, 2021, 45, 522-525.	1.4	9
64	Efficient Hydrolysis of Nitriles to Amides with Hydroperoxide Anion in Aqueous Surfactant Solutions as Reaction Medium. Letters in Organic Chemistry, 2009, 6, 175-179.	0.2	8
65	Phospholipidosis effect of drugs by adsorption into lipid monolayers. Colloids and Surfaces B: Biointerfaces, 2015, 136, 175-184.	2.5	8
66	Use of the Distribution Coefficient in Brain Polar Lipids for the Assessment of Drug-Induced Phospholipidosis Risk. Chemical Research in Toxicology, 2017, 30, 1145-1156.	1.7	7
67	Pharmacophore-Based Discovery of Substrates of a Novel Drug/Proton-Antiporter in the Human Brain Endothelial hCMEC/D3 Cell Line. Pharmaceutics, 2022, 14, 255.	2.0	6
68	Temperature effects upon aqueous micellar-assisted decarboxylation of 6-nitrobenzisoxazole-3-carboxylate and its 5-methyl derivative. Journal of Colloid and Interface Science, 2006, 298, 426-431.	5.0	5
69	Automatic Identification of Lansoprazole Degradants under Stress Conditions by LC-HRMS with MassChemSite and WebChembase. Journal of Chemical Information and Modeling, 2021, 61, 2706-2719.	2.5	5
70	Î±-Chymotrypsin superactivity in quaternary ammonium salt solution: kinetic and computational studies. RSC Advances, 2016, 6, 46202-46211.	1.7	4
71	Modeling from Theory and Modeling from Data: Complementary or Alternative Approaches? The Case of Ionic Liquids. ChemistryOpen, 2017, 6, 90-101.	0.9	4
72	CROMATIC: Cross-Relationship Map of Cavities from Coronaviruses. Journal of Chemical Information and Modeling, 0, , .	2.5	4

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73	Easy and Efficient Procedure for Preparation of Symmetric Organic Carbonates in Ionic Liquid. Letters in Organic Chemistry, 2006, 3, 530-533.	0.2	3
74	Passive Intestinal Absorption of Representative Plant Secondary Metabolites: A Physicochemical Study. Planta Medica, 2017, 83, 718-726.	0.7	3
75	Synthesis and phospholipidosis effect of a series of cationic amphiphilic compounds: a case study to evaluate in silico and in vitro assays. Medicinal Chemistry Research, 2018, 27, 679-692.	1.1	3
76	Role of cardiolipins, mitochondria, and autophagy in the differentiation process activated by all-trans retinoic acid in acute promyelocytic leukemia. Cell Death and Disease, 2022, 13, 30.	2.7	3
77	Synthesis and biological activity of cyclopropyl Î”7-dafachronic acids as DAF-12 receptor ligands. Organic and Biomolecular Chemistry, 2021, 19, 5403-5412.	1.5	2
78	Refining the model to design Î±-chymotrypsin superactivators: the role of the binding mode of quaternary ammonium salts. New Journal of Chemistry, 2020, 44, 20823-20833.	1.4	1
79	Dehydrogenation of Amines of Nitriles in Aqueous Micelles.. ChemInform, 2005, 36, no.	0.1	0
80	Integrating Crystallography into Early Metabolism Studies. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 63-77.	0.5	0
81	Non animal methodologies (NAMs): Research, testing, assessment and applications â€“ ecopa Symposium 2019. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 317-320.	0.9	0