Laura Goracci

List of Publications by Year
in descending order

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81	2,644	126858	206029
papers	citations	33 h-index	48 g-index

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

#	Article	IF	Citations
1	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
2	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
3	Proteolysis targeting chimeras in antiviral research. Future Medicinal Chemistry, 2022, 14, 459-462.	1.1	14
4	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
5	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
6	Targeting Nsp9 as an anti-SARS-CoV-2 strategy. New Journal of Chemistry, 2021, 45, 522-525.	1.4	9
7	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
8	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
9	Enhanced triacylglycerol catabolism by carboxylesterase 1 promotes aggressive colorectal carcinoma. Journal of Clinical Investigation, 2021, 131, .	3.9	25
10	Indomethacin-based PROTACs as pan-coronavirus antiviral agents. European Journal of Medicinal Chemistry, 2021, 226, 113814.	2.6	46
11	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
12	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
13	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
14	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
15	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
16	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
17	Computational solutions in redox lipidomics â€“ Current strategies and future perspectives. Free Radical Biology and Medicine, 2019, 144, 110-123.	1.3	36
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	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
20	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
21	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
22	Modeling from Theory and Modeling from Data: Complementary or Alternative Approaches? The Case of Ionic Liquids. ChemistryOpen, 2017, 6, 90-101.	0.9	4
23	Passive Intestinal Absorption of Representative Plant Secondary Metabolites: A Physicochemical Study. Planta Medica, 2017, 83, 718-726.	0.7	3
24	Lipostar, a Comprehensive Platform-Neutral Cheminformatics Tool for Lipidomics. Analytical Chemistry, 2017, 89, 6257-6264.	3.2	76
25	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
26	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
27	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
28	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
29	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
30	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
31	A Rational Approach for the Identification of Non-Hydroxamate HDAC6-Selective Inhibitors. Scientific Reports, 2016, 6, 29086.	1.6	33
32	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
33	Use of lipidomics to investigate sebum dysfunction in juvenile acne. Journal of Lipid Research, 2016, 57, 1051-1058.	2.0	58
34	Î±-Chymotrypsin superactivity in quaternary ammonium salt solution: kinetic and computational studies. RSC Advances, 2016, 6, 46202-46211.	1.7	4
35	Metabolism study and biological evaluation of bosentan derivatives. European Journal of Medicinal Chemistry, 2016, 121, 658-670.	2.6	13
36	Indole Based Weapons to Fight Antibiotic Resistance: A Structureâ€“Activity Relationship Study. Journal of Medicinal Chemistry, 2016, 59, 867-891.	2.9	64

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37	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
38	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
39	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
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	BioGPS: Navigating biological space to predict polypharmacology, off-targeting, and selectivity. Proteins: Structure, Function and Bioinformatics, 2015, 83, 517-532.	1.5	68
42	Evaluating the risk of phospholipidosis using a new multidisciplinary pipeline approach. European Journal of Medicinal Chemistry, 2015, 92, 49-63.	2.6	29
43	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
44	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
45	A role for the autophagy regulator Transcription Factor EB in amiodarone-induced phospholipidosis. Biochemical Pharmacology, 2015, 95, 201-209.	2.0	14
46	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
47	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
48	Phospholipidosis effect of drugs by adsorption into lipid monolayers. Colloids and Surfaces B: Biointerfaces, 2015, 136, 175-184.	2.5	8
49	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
50	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
51	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
52	BioGPS: The Music for the Chemoâ€and Bioinformatics Walzer. Molecular Informatics, 2014, 33, 446-453.	1.4	11
53	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
54	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

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55	Flavin Monooxygenase Metabolism: Why Medicinal Chemists Should Matter. Journal of Medicinal Chemistry, 2014, 57, 6183-6196.	2.9	39
56	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
57	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
58	Structural Investigation of Cycloheptathiophene-3-carboxamide Derivatives Targeting Influenza Virus Polymerase Assembly. Journal of Medicinal Chemistry, 2013, 56, 10118-10131.	2.9	51
59	Exposition and reactivity optimization to predict sites of metabolism in chemicals. Drug Discovery Today: Technologies, 2013, 10, e155-e165.	4.0	40
60	Modeling Phospholipidosis Induction: Reliability and Warnings. Journal of Chemical Information and Modeling, 2013, 53, 1436-1446.	2.5	46
61	Human Cytomegalovirus Inhibitor AL18 Also Possesses Activity against Influenza A and B Viruses. Antimicrobial Agents and Chemotherapy, 2012, 56, 6009-6013.	1.4	38
62	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
63	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
64	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
65	A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751.	2.9	141
66	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
67	Esterification of Unprotected α-Amino Acids in Ionic Liquids as the Reaction Media. Letters in Organic Chemistry, 2010, 7, 39-44.	0.2	11
68	Interaction between DNA and Cationic Amphiphiles: A Multi-Technique Study. Langmuir, 2010, 26, 7885-7892.	1.6	19
69	In silico pK_a Prediction and ADME Profiling. Chemistry and Biodiversity, 2009, 6, 1812-1821.	1.0	70
70	Surfactant-Based Photorheological Fluids: Effect of the Surfactant Structure. Langmuir, 2009, 25, 5467-5475.	1.6	45
71	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
72	Integrating Crystallography into Early Metabolism Studies. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 63-77.	0.5	0

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73	Premicellar Accelerated Decarboxylation of 6-Nitrobenzisoxazole-3-carboxylate Ion and Its 5-Tetradecyloxy Derivative. Langmuir, 2007, 23, 436-442.	1.6	17
74	Anomalous Behavior of Amine Oxide Surfactants at the Air/Water Interface. Langmuir, 2007, 23, 10525-10532.	1.6	35
75	Easy and Efficient Procedure for Preparation of Symmetric Organic Carbonates in Ionic Liquid. Letters in Organic Chemistry, 2006, 3, 530-533.	0.2	3
76	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
77	Dehydrogenation of Amines to Nitriles in Aqueous Micelles. European Journal of Organic Chemistry, 2005, 2005, 3060-3063.	1.2	36
78	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
79	Dehydrogenation of Amines of Nitriles in Aqueous Micelles.. ChemInform, 2005, 36, no.	0.1	0
80	Decarboxylation and Dephosphorylation in New Gemini Surfactants. Changes in Aggregate Structures. Langmuir, 2002, 18, 7821-7825.	1.6	78
81	CROMATIC: Cross-Relationship Map of Cavities from Coronaviruses. Journal of Chemical Information and Modeling, 0, , .	2.5	4