Angelica Mazzolari

List of Publications by Year
in descending order

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34	589	623734	642732
papers	citations	14 h-index	23 g-index

34	34	34	892
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hempseed (Cannabis sativa) Peptide H3 (IGFLIIWV) Exerts Cholesterol-Lowering Effects in Human Hepatic Cell Line. Nutrients, 2022, 14, 1804.	4.1	11
2	Cyclo(His-Pro) Exerts Protective Carbonyl Quenching Effects through Its Open Histidine Containing Dipeptides. Nutrients, 2022, 14, 1775.	4.1	4
3	GLORYx: Prediction of the Metabolites Resulting from Phase 1 and Phase 2 Biotransformations of Xenobiotics. Chemical Research in Toxicology, 2021, 34, 286-299.	3.3	51
4	The VEGA suite of programs: an versatile platform for cheminformatics and drug design projects. Bioinformatics, 2021, 37, 1174-1175.	4.1	90
5	MetaTREE, a Novel Database Focused on Metabolic Trees, Predicts an Important Detoxification Mechanism: The Glutathione Conjugation. Molecules, 2021, 26, 2098.	3.8	2
6	MetaClass, a Comprehensive Classification System for Predicting the Occurrence of Metabolic Reactions Based on the MetaQSAR Database. Molecules, 2021, 26, 5857.	3.8	4
7	Tree2C: A Flexible Tool for Enabling Model Deployment with Special Focus on Cheminformatics Applications. Applied Sciences (Switzerland), 2020, 10, 7704.	2.5	3
8	Repositioning Dequalinium as Potent Muscarinic Allosteric Ligand by Combining Virtual Screening Campaigns and Experimental Binding Assays. International Journal of Molecular Sciences, 2020, 21, 5961.	4.1	9
9	Unveiling the molecular mechanisms underpinning biorecognition of early-glycated human serum albumin and receptor for advanced glycation end products. Analytical and Bioanalytical Chemistry, 2020, 412, 4245-4259.	3.7	7
10	Carbachol dimers with primary carbamate groups as homobivalent modulators of muscarinic receptors. European Journal of Pharmacology, 2020, 883, 173183.	3.5	6
11	Impact of the Journal of Chemical Information and Modeling Special Issue on Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2020, 60, 3328-3330.	5.4	5
12	What Makes a Paper Be Highly Cited? 60 Years of the Journal of Chemical Information and Modeling. Journal of Chemical Information and Modeling, 2020, 60, 5866-5867.	5.4	1
13	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. Journal of Chemical Information and Modeling, 2019, 59, 3400-3412.	5.4	60
14	Rescoring and Linearly Combining: A Highly Effective Consensus Strategy for Virtual Screening Campaigns. International Journal of Molecular Sciences, 2019, 20, 2060.	4.1	17
15	Prediction of UGT-mediated Metabolism Using the Manually Curated MetaQSAR Database. ACS Medicinal Chemistry Letters, 2019, 10, 633-638.	2.8	10
16	MetaQSAR: An Integrated Database Engine to Manage and Analyze Metabolic Data. Journal of Medicinal Chemistry, 2018, 61, 1019-1030.	6.4	18
17	Prediction of the Formation of Reactive Metabolites by A Novel Classifier Approach Based on Enrichment Factor Optimization (EFO) as Implemented in the VEGA Program. Molecules, 2018, 23, 2955.	3.8	9
18	Approaching Pharmacological Space: Events and Components. Methods in Molecular Biology, 2018, 1800, 245-274.	0.9	1

#	Article	IF	Citations
19	A capture method based on the VC1 domain reveals new binding properties of the human receptor for advanced glycation end products (RAGE). Redox Biology, 2017, 11, 275-285.	9.0	16
20	Binding Space Concept: A New Approach To Enhance the Reliability of Docking Scores and Its Application to Predicting Butyrylcholinesterase Hydrolytic Activity. Journal of Chemical Information and Modeling, 2017, 57, 1691-1702.	5.4	31
21	Data from docking simulations to develop an efficient strategy able to evaluate the interactions between RAGE and MDA-induced albumin adducts. Data in Brief, 2017, 12, 656-661.	1.0	1
22	Quenching activity of carnosine derivatives towards reactive carbonyl species: Focus on Î±â^'(methylglyoxal) and Î²â^'(malondialdehyde) dicarbonyls. Biochemical and Biophysical Research Communications, 2017, 492, 487-492.	2.1	26
23	The replacement of the 2-methoxy substituent of N-((6,6-diphenyl-1,4-dioxan-2-yl)methyl)-2-(2-methoxyphenoxy)ethan-1-amine improves the selectivity for 5-HT1A receptor over Î±1-adrenoceptor andÂD2-like receptor subtypes. European Journal of Medicinal Chemistry, 2017, 125, 233-244.	5.5	17
24	Carbachol dimers as homobivalent modulators of muscarinic receptors. Biochemical Pharmacology, 2016, 108, 90-101.	4.4	8
25	Structural Effects of Some Relevant Missense Mutations on the MECP2â€ÐNA Binding: A MD Study Analyzed by Rescore+, a Versatile Rescoring Tool of the VEGA ZZ Program. Molecular Informatics, 2016, 35, 424-433.	2.5	18
26	Computational approaches in the rational design of improved carbonyl quenchers: focus on histidine containing dipeptides. Future Medicinal Chemistry, 2016, 8, 1721-1737.	2.3	21
27	Serum albumin as a probe for testing the selectivity of irreversible cysteine protease inhibitors: The case of vinyl sulfones. Journal of Pharmaceutical and Biomedical Analysis, 2016, 124, 294-302.	2.8	6
28	Enhancing the Reliability of GPCR Models by Accounting for Flexibility of Their Proâ€Containing Helices: the Case of the Human mAChR1 Receptor. Molecular Informatics, 2015, 34, 216-227.	2.5	2
29	Improvement of Topical Palmitoylethanolamide Anti-Inflammatory Activity by Pegylated Prodrugs. Molecular Pharmaceutics, 2015, 12, 3369-3379.	4.6	5
30	Mode of interaction of 1,4-dioxane agonists at the M2 and M3 muscarinic receptor orthosteric sites. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3255-3259.	2.2	10
31	Insights into the Structural Determinants Required for High-Affinity Binding of Chiral Cyclopropane-Containing Ligands to Î±4Î²2-Nicotinic Acetylcholine Receptors: An Integrated Approach to Behaviorally Active Nicotinic Ligands. Journal of Medicinal Chemistry, 2012, 55, 8028-8037.	6.4	24
32	Homology modeling and metabolism prediction of human carboxylesterase-2 using docking analyses by GriDock: a parallelized tool based on AutoDock 4.0. Journal of Computer-Aided Molecular Design, 2010, 24, 771-787.	2.9	40
33	In silico prediction of human carboxylesterase-1 (hCES1) metabolism combining docking analyses and MD simulations. Bioorganic and Medicinal Chemistry, 2010, 18, 320-329.	3.0	42
34	Influence of Ionization State on the Activation of Temocapril by hCES1: A Molecularâ€Dynamics Study. Chemistry and Biodiversity, 2009, 6, 2092-2100.	2.1	14