

# Angelica Mazzolari

## List of Publications by Year in descending order

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34  
papers

589  
citations

623734

14  
h-index

642732

23  
g-index

34  
all docs

34  
docs citations

34  
times ranked

892  
citing authors

#	ARTICLE	IF	CITATIONS
1	The VEGA suite of programs: an versatile platform for cheminformatics and drug design projects. <i>Bioinformatics</i> , 2021, 37, 1174-1175.	4.1	90
2	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3400-3412.	5.4	60
3	GLORYx: Prediction of the Metabolites Resulting from Phase 1 and Phase 2 Biotransformations of Xenobiotics. <i>Chemical Research in Toxicology</i> , 2021, 34, 286-299.	3.3	51
4	In silico prediction of human carboxylesterase-1 (hCES1) metabolism combining docking analyses and MD simulations. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 320-329.	3.0	42
5	Homology modeling and metabolism prediction of human carboxylesterase-2 using docking analyses by GriDock: a parallelized tool based on AutoDock 4.0. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 771-787.	2.9	40
6	Binding Space Concept: A New Approach To Enhance the Reliability of Docking Scores and Its Application to Predicting Butyrylcholinesterase Hydrolytic Activity. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1691-1702.	5.4	31
7	Quenching activity of carnosine derivatives towards reactive carbonyl species: Focus on $\alpha$ -methylglyoxal and $\alpha$ -malondialdehyde dicarbonyls. <i>Biochemical and Biophysical Research Communications</i> , 2017, 492, 487-492.	2.1	26
8	Insights into the Structural Determinants Required for High-Affinity Binding of Chiral Cyclopropane-Containing Ligands to $\alpha$ 2-Nicotinic Acetylcholine Receptors: An Integrated Approach to Behaviorally Active Nicotinic Ligands. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 8028-8037.	6.4	24
9	Computational approaches in the rational design of improved carbonyl quenchers: focus on histidine containing dipeptides. <i>Future Medicinal Chemistry</i> , 2016, 8, 1721-1737.	2.3	21
10	Structural Effects of Some Relevant Missense Mutations on the MECP2-DNA Binding: A MD Study Analyzed by Rescore+, a Versatile Rescoring Tool of the VEGA ZZ Program. <i>Molecular Informatics</i> , 2016, 35, 424-433.	2.5	18
11	MetaQSAR: An Integrated Database Engine to Manage and Analyze Metabolic Data. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 1019-1030.	6.4	18
12	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 $\alpha$ 1-adrenoceptor and $\beta$ 2-like receptor subtypes. <i>European Journal of Medicinal Chemistry</i> , 2017, 125, 233-244.	5.5	17
13	Rescoring and Linearly Combining: A Highly Effective Consensus Strategy for Virtual Screening Campaigns. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2060.	4.1	17
14	A capture method based on the VC1 domain reveals new binding properties of the human receptor for advanced glycation end products (RAGE). <i>Redox Biology</i> , 2017, 11, 275-285.	9.0	16
15	Influence of Ionization State on the Activation of Temocapril by hCES1: A Molecular Dynamics Study. <i>Chemistry and Biodiversity</i> , 2009, 6, 2092-2100.	2.1	14
16	Hempseed ( <i>Cannabis sativa</i> ) Peptide H3 (IGFLIIVV) Exerts Cholesterol-Lowering Effects in Human Hepatic Cell Line. <i>Nutrients</i> , 2022, 14, 1804.	4.1	11
17	Mode of interaction of 1,4-dioxane agonists at the M2 and M3 muscarinic receptor orthosteric sites. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014, 24, 3255-3259.	2.2	10
18	Prediction of UGT-mediated Metabolism Using the Manually Curated MetaQSAR Database. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 633-638.	2.8	10

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19	Prediction of the Formation of Reactive Metabolites by A Novel Classifier Approach Based on Enrichment Factor Optimization (EFO) as Implemented in the VEGA Program. <i>Molecules</i> , 2018, 23, 2955.	3.8	9
20	Repositioning Dequalinium as Potent Muscarinic Allosteric Ligand by Combining Virtual Screening Campaigns and Experimental Binding Assays. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5961.	4.1	9
21	Carbachol dimers as homobivalent modulators of muscarinic receptors. <i>Biochemical Pharmacology</i> , 2016, 108, 90-101.	4.4	8
22	Unveiling the molecular mechanisms underpinning biorecognition of early-glycated human serum albumin and receptor for advanced glycation end products. <i>Analytical and Bioanalytical Chemistry</i> , 2020, 412, 4245-4259.	3.7	7
23	Serum albumin as a probe for testing the selectivity of irreversible cysteine protease inhibitors: The case of vinyl sulfones. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2016, 124, 294-302.	2.8	6
24	Carbachol dimers with primary carbamate groups as homobivalent modulators of muscarinic receptors. <i>European Journal of Pharmacology</i> , 2020, 883, 173183.	3.5	6
25	Improvement of Topical Palmitoylethanolamide Anti-Inflammatory Activity by Pegylated Prodrugs. <i>Molecular Pharmaceutics</i> , 2015, 12, 3369-3379.	4.6	5
26	Impact of the <i>Journal of Chemical Information and Modeling</i> Special Issue on Women in Computational Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3328-3330.	5.4	5
27	MetaClass, a Comprehensive Classification System for Predicting the Occurrence of Metabolic Reactions Based on the MetaQSAR Database. <i>Molecules</i> , 2021, 26, 5857.	3.8	4
28	Cyclo(His-Pro) Exerts Protective Carbonyl Quenching Effects through Its Open Histidine Containing Dipeptides. <i>Nutrients</i> , 2022, 14, 1775.	4.1	4
29	Tree2C: A Flexible Tool for Enabling Model Deployment with Special Focus on Cheminformatics Applications. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 7704.	2.5	3
30	Enhancing the Reliability of GPCR Models by Accounting for Flexibility of Their Proline-Containing Helices: the Case of the Human mAChR1 Receptor. <i>Molecular Informatics</i> , 2015, 34, 216-227.	2.5	2
31	MetaTREE, a Novel Database Focused on Metabolic Trees, Predicts an Important Detoxification Mechanism: The Glutathione Conjugation. <i>Molecules</i> , 2021, 26, 2098.	3.8	2
32	Data from docking simulations to develop an efficient strategy able to evaluate the interactions between RAGE and MDA-induced albumin adducts. <i>Data in Brief</i> , 2017, 12, 656-661.	1.0	1
33	Approaching Pharmacological Space: Events and Components. <i>Methods in Molecular Biology</i> , 2018, 1800, 245-274.	0.9	1
34	What Makes a Paper Be Highly Cited? 60 Years of the <i>Journal of Chemical Information and Modeling</i> . <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5866-5867.	5.4	1