

# Francesco Ortuso

## List of Publications by Citations

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133  
papers

3,970  
citations

37  
h-index

55  
g-index

141  
ext. papers

4,408  
ext. citations

5  
avg, IF

4.94  
L-index

#	Paper	IF	Citations
133	Chalcones: a valid scaffold for monoamine oxidases inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2009</b> , 52, 2818-24	8.3	137
132	Synthesis, molecular modeling, and selective inhibitory activity against human monoamine oxidases of 3-carboxamido-7-substituted coumarins. <i>Journal of Medicinal Chemistry</i> , <b>2009</b> , 52, 1935-42	8.3	126
131	Chromone, a privileged scaffold for the development of monoamine oxidase inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2011</b> , 54, 5165-73	8.3	124
130	Quercetin as the active principle of <i>Hypericum hircinum</i> exerts a selective inhibitory activity against MAO-A: extraction, biological analysis, and computational study. <i>Journal of Natural Products</i> , <b>2006</b> , 69, 945-9	4.9	108
129	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of 1-thiocarbonyl-3,5-diaryl-4,5-dihydro-(1H)-pyrazole derivatives. <i>Journal of Medicinal Chemistry</i> , <b>2005</b> , 48, 7113-22	8.3	98
128	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. <i>Bioinformatics</i> , <b>2006</b> , 22, 1449-55	7.2	93
127	Synthesis, biological evaluation, and molecular modeling of oleuropein and its semisynthetic derivatives as cyclooxygenase inhibitors. <i>Journal of Agricultural and Food Chemistry</i> , <b>2009</b> , 57, 11161-7	5.7	81
126	Synthesis and biological evaluation of N-substituted-3,5-diphenyl-2-pyrazoline derivatives as cyclooxygenase (COX-2) inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2010</b> , 45, 6135-8	6.8	81
125	A new series of flavones, thioflavones, and flavanones as selective monoamine oxidase-B inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 1273-9	3.4	78
124	Homoisoflavonoids: natural scaffolds with potent and selective monoamine oxidase-B inhibition properties. <i>Journal of Medicinal Chemistry</i> , <b>2011</b> , 54, 2155-64	8.3	77
123	Synthesis and selective human monoamine oxidase inhibition of 3-carbonyl, 3-acyl, and 3-carboxyhydrazido coumarin derivatives. <i>European Journal of Medicinal Chemistry</i> , <b>2011</b> , 46, 4846-52	6.8	77
122	Synthesis, stereochemical identification, and selective inhibitory activity against human monoamine oxidase-B of 2-methylcyclohexylidene-(4-arylthiazol-2-yl)hydrazones. <i>Journal of Medicinal Chemistry</i> , <b>2008</b> , 51, 4874-80	8.3	77
121	Inhibition of monoamine oxidases by coumarin-3-acyl derivatives: biological activity and computational study. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2004</b> , 14, 3697-703	2.9	77
120	Identification and characterization of new DNA G-quadruplex binders selected by a combination of ligand and structure-based virtual screening approaches. <i>Journal of Medicinal Chemistry</i> , <b>2013</b> , 56, 843-55	8.3	75
119	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, E2136-E2145	11.5	74
118	Selective inhibitory activity against MAO and molecular modeling studies of 2-thiazolyldiazone derivatives. <i>Journal of Medicinal Chemistry</i> , <b>2007</b> , 50, 707-12	8.3	73
117	Investigations on the 2-thiazolyldiazone scaffold: synthesis and molecular modeling of selective human monoamine oxidase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 5715-23	3.4	68

116	N-myristoylation determines dual targeting of mammalian NADH-cytochrome b5 reductase to ER and mitochondrial outer membranes by a mechanism of kinetic partitioning. <i>Journal of Cell Biology</i> , <b>2005</b> , 168, 735-45	7.3	66
115	Discovery of New Chemical Entities for Old Targets: Insights on the Lead Optimization of Chromone-Based Monoamine Oxidase B (MAO-B) Inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2016</b> , 59, 5879-93	8.3	65
114	Monoamine oxidase isoform-dependent tautomeric influence in the recognition of 3,5-diaryl pyrazole inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2007</b> , 50, 425-8	8.3	61
113	Further studies on the interaction of the 5-hydroxytryptamine <sub>3</sub> (5-HT <sub>3</sub> ) receptor with arylpiperazine ligands. development of a new 5-HT <sub>3</sub> receptor ligand showing potent acetylcholinesterase inhibitory properties. <i>Journal of Medicinal Chemistry</i> , <b>2005</b> , 48, 3564-75	8.3	59
112	Synthesis, biological evaluation and 3D-QSAR of 1,3,5-trisubstituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase A inhibitors. <i>Current Medicinal Chemistry</i> , <b>2006</b> , 13, 1411-28	4.3	54
111	The beta1/betaIII-tubulin isoforms and their complexes with antimitotic agents. Docking and molecular dynamics studies. <i>FEBS Journal</i> , <b>2006</b> , 273, 3301-10	5.7	54
110	SGK1, the New Player in the Game of Resistance: Chemo-Radio Molecular Target and Strategy for Inhibition. <i>Cellular Physiology and Biochemistry</i> , <b>2016</b> , 39, 1863-1876	3.9	53
109	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 2256-74	6.1	52
108	N-Methyl-N-((1-methyl-5-(3-(1-(2-methylbenzyl)piperidin-4-yl)propoxy)-1H-indol-2-yl)methyl)prop-2-yn-1-amine, a new cholinesterase and monoamine oxidase dual inhibitor. <i>Journal of Medicinal Chemistry</i> , <b>2014</b> , 57, 10455-63	8.3	50
107	Modeling and biological evaluation of 3,3S(1,2-ethanediy)bis[2-(4-methoxyphenyl)-thiazolidin-4-one], a new synthetic cyclooxygenase-2 inhibitor. <i>European Journal of Pharmacology</i> , <b>2002</b> , 448, 71-80	5.3	48
106	Preclinical model in HCC: the SGK1 kinase inhibitor SI113 blocks tumor progression in vitro and in vivo and synergizes with radiotherapy. <i>Oncotarget</i> , <b>2015</b> , 6, 37511-25	3.3	47
105	Synthesis, molecular modeling studies and selective inhibitory activity against MAO of N1-propanoyl-3,5-diphenyl-4,5-dihydro-(1H)-pyrazole derivatives. <i>European Journal of Medicinal Chemistry</i> , <b>2008</b> , 43, 2262-7	6.8	43
104	Preparation, characterization, molecular modeling and in vitro activity of paclitaxel-cyclodextrin complexes. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2002</b> , 12, 1637-41	2.9	43
103	SI113, a SGK1 inhibitor, potentiates the effects of radiotherapy, modulates the response to oxidative stress and induces cytotoxic autophagy in human glioblastoma multiforme cells. <i>Oncotarget</i> , <b>2016</b> , 7, 15868-84	3.3	43
102	SI113, a specific inhibitor of the Sgk1 kinase activity that counteracts cancer cell proliferation. <i>Cellular Physiology and Biochemistry</i> , <b>2015</b> , 35, 2006-18	3.9	42
101	Mediterranean products as promising source of multi-target agents in the treatment of metabolic syndrome. <i>European Journal of Medicinal Chemistry</i> , <b>2020</b> , 186, 111903	6.8	42
100	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 5063-70	3.4	41
99	Chromone-2- and -3-carboxylic acids inhibit differently monoamine oxidases A and B. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2010</b> , 20, 2709-12	2.9	41

98	Multi-target-directed ligands for Alzheimer's disease: Discovery of chromone-based monoamine oxidase/cholinesterase inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2018</b> , 158, 781-800	6.8	40
97	DNA cross-linking by azinomycin B: Monte Carlo simulations in the evaluation of sequence selectivity. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 861-70	8.3	39
96	New insight into the central benzodiazepine receptor-ligand interactions: design, synthesis, biological evaluation, and molecular modeling of 3-substituted 6-phenyl-4H-imidazo[1,5-a][1,4]benzodiazepines and related compounds. <i>Journal of Medicinal Chemistry</i> , <b>2011</b> , 54, 5694-711	8.3	37
95	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. <i>Journal of Medicinal Chemistry</i> , <b>2017</b> , 60, 7206-7212	8.3	35
94	GRID-based three-dimensional pharmacophores II: PharmBench, a benchmark data set for evaluating pharmacophore elucidation methods. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 2599-608	6.1	34
93	Rational design, synthesis, biophysical and antiproliferative evaluation of fluorenone derivatives with DNA G-quadruplex binding properties. <i>ChemMedChem</i> , <b>2010</b> , 5, 575-83	3.7	33
92	In silico identification and biological evaluation of novel selective serum/glucocorticoid-inducible kinase 1 inhibitors based on the pyrazolo-pyrimidine scaffold. <i>Journal of Chemical Information and Modeling</i> , <b>2014</b> , 54, 1828-32	6.1	31
91	New conformationally locked bicyclic N,O-nucleoside analogues of antiviral drugs. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2005</b> , 15, 545-50	2.9	31
90	Towards the discovery of a novel class of monoamine oxidase inhibitors: structure-property-activity and docking studies on chromone amides. <i>ChemMedChem</i> , <b>2011</b> , 6, 628-32	3.7	30
89	4-(3-Nitrophenyl)thiazol-2-ylhydrazones derivatives as antioxidants and selective hMAO-B inhibitors: synthesis, biological activity and computational analysis. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2019</b> , 34, 597-612	5.6	29
88	Synthesis and biological assessment of novel 2-thiazolyhydrazones and computational analysis of their recognition by monoamine oxidase B. <i>European Journal of Medicinal Chemistry</i> , <b>2012</b> , 48, 284-95	6.8	29
87	The Mediterranean Diet as source of bioactive compounds with multi-targeting anti-cancer profile. <i>European Journal of Medicinal Chemistry</i> , <b>2019</b> , 181, 111579	6.8	28
86	Targeting unimolecular G-quadruplex nucleic acids: a new paradigm for the drug discovery?. <i>Expert Opinion on Drug Discovery</i> , <b>2014</b> , 9, 1167-87	6.2	28
85	Design, synthesis and biochemical evaluation of novel multi-target inhibitors as potential anti-Parkinson agents. <i>European Journal of Medicinal Chemistry</i> , <b>2018</b> , 143, 1543-1552	6.8	27
84	Targeting Tumor Associated Carbonic Anhydrases IX and XII: Highly Isozyme Selective Coumarin and Psoralen Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , <b>2018</b> , 9, 725-729	4.3	27
83	Isolation and functional characterization of peptide agonists of PTPRJ, a tyrosine phosphatase receptor endowed with tumor suppressor activity. <i>ACS Chemical Biology</i> , <b>2012</b> , 7, 1666-76	4.9	27
82	Drug design, synthesis, in vitro and in silico evaluation of selective monoaminooxidase B inhibitors based on 3-acetyl-2-dichlorophenyl-5-aryl-2,3-dihydro-1,3,4-oxadiazole chemical scaffold. <i>European Journal of Medicinal Chemistry</i> , <b>2016</b> , 108, 542-552	6.8	26
81	Design, synthesis, and SAR analysis of novel selective sigma1 ligands. <i>Bioorganic and Medicinal Chemistry</i> , <b>2007</b> , 15, 771-83	3.4	26

80	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of N,NSbis[2-oxo-2H-benzopyran]-3-carboxamides. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2006</b> , 16, 4135-40	2.9	26
79	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2017</b> , 1861, 1329-1340	4	25
78	Molecular interaction fields in drug discovery: recent advances and future perspectives. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2013</b> , 3, 594-613	7.9	25
77	Computational analysis of Human Immunodeficiency Virus (HIV) Type-1 reverse transcriptase crystallographic models based on significant conserved residues found in Highly Active Antiretroviral Therapy (HAART)-treated patients. <i>Current Medicinal Chemistry</i> , <b>2010</b> , 17, 290-308	4.3	25
76	(E)-3-Heteroarylidenechroman-4-ones as potent and selective monoamine oxidase-B inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2016</b> , 117, 292-300	6.8	25
75	Discovery of PTPRJ agonist peptides that effectively inhibit in vitro cancer cell proliferation and tube formation. <i>ACS Chemical Biology</i> , <b>2013</b> , 8, 1497-506	4.9	23
74	Molecular dynamics and free energy studies on the wild-type and mutated HIV-1 protease complexed with four approved drugs: mechanism of binding and drug resistance. <i>Journal of Chemical Information and Modeling</i> , <b>2009</b> , 49, 1751-61	6.1	23
73	Tetraplex DNA specific ligands based on the fluorenone-carboxamide scaffold. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2007</b> , 17, 2509-14	2.9	23
72	Novel natural non-nucleoside inhibitors of HIV-1 reverse transcriptase identified by shape- and structure-based virtual screening techniques. <i>European Journal of Medicinal Chemistry</i> , <b>2019</b> , 161, 1-10	6.8	23
71	1,5-Diphenylpenta-2,4-dien-1-ones as potent and selective monoamine oxidase-B inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2013</b> , 59, 91-100	6.8	22
70	Structure-based virtual screening of novel natural alkaloid derivatives as potential binders of h-telo and c-myc DNA G-quadruplex conformations. <i>Molecules</i> , <b>2014</b> , 20, 206-23	4.8	22
69	Unusually high enantioselectivity in high-performance liquid chromatography using cellulose tris(4-methylbenzoate) as a chiral stationary phase. <i>Journal of Chromatography A</i> , <b>2009</b> , 1216, 4673-8	4.5	22
68	The polymorphisms of DNA G-quadruplex investigated by docking experiments with telomestatin enantiomers. <i>Current Pharmaceutical Design</i> , <b>2012</b> , 18, 1873-9	3.3	22
67	Hit identification and biological evaluation of anticancer pyrazolopyrimidines endowed with anti-inflammatory activity. <i>ChemMedChem</i> , <b>2010</b> , 5, 1242-6	3.7	22
66	Synthesis and molecular modelling of novel substituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase-A inhibitors. <i>Chemical Biology and Drug Design</i> , <b>2006</b> , 67, 206-14	2.9	22
65	Conformational studies and solvent-accessible surface area analysis of known selective DNA G-Quadruplex binders. <i>Biochimie</i> , <b>2011</b> , 93, 1267-74	4.6	21
64	Structural genetics of circulating variants affecting the SARS-CoV-2 spike/human ACE2 complex. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-11	3.6	21
63	Identification of the stereochemical requirements in the 4-aryl-2-cycloalkylidenhydrazinylthiazole scaffold for the design of selective human monoamine oxidase B inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2014</b> , 22, 2887-95	3.4	20

62	Design, synthesis, and biological evaluation of 1,3-diarylpropenones as dual inhibitors of HIV-1 reverse transcriptase. <i>ChemMedChem</i> , <b>2014</b> , 9, 1869-79	3.7	20
61	Toward the design of new DNA G-quadruplex ligands through rational analysis of polymorphism and binding data. <i>European Journal of Medicinal Chemistry</i> , <b>2013</b> , 68, 139-49	6.8	20
60	Exploring 4-substituted-2-thiazolylhydrazones from 2-, 3-, and 4-acetylpyridine as selective and reversible hMAO-B inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2013</b> , 66, 221-7	6.8	20
59	Benzoic acid-derived nitrones: A new class of potential acetylcholinesterase inhibitors and neuroprotective agents. <i>European Journal of Medicinal Chemistry</i> , <b>2019</b> , 174, 116-129	6.8	19
58	Synthesis and molecular modelling studies of prenylated pyrazolines as MAO-B inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2010</b> , 20, 6479-82	2.9	19
57	Molecular recognition of a carboxy pyridostatin toward G-quadruplex structures: Why does it prefer RNA?. <i>Chemical Biology and Drug Design</i> , <b>2017</b> , 90, 919-925	2.9	18
56	Identification of new natural DNA G-quadruplex binders selected by a structure-based virtual screening approach. <i>Molecules</i> , <b>2013</b> , 18, 12051-70	4.8	18
55	A computer-assisted discovery of novel potential anti-obesity compounds as selective carbonic anhydrase VA inhibitors. <i>European Journal of Medicinal Chemistry</i> , <b>2019</b> , 181, 111565	6.8	17
54	Computer-aided molecular design of asymmetric pyrazole derivatives with exceptional enantioselective recognition toward the Chiralcel OJ-H stationary phase. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 649-54	6.1	17
53	βCyclodextrin interactions with three drugs used in inflammatory pathologies: An experimental and theoretical study. <i>Chemical Physics Letters</i> , <b>2008</b> , 454, 374-381	2.5	17
52	An approach to address <i>Candida rugosa</i> lipase regioselectivity in the acylation reactions of trytilated glucosides. <i>Journal of Biotechnology</i> , <b>2007</b> , 128, 908-18	3.7	17
51	A chromatographic and computational study on the driving force operating in the exceptionally large enantioseparation of N-thiocarbamoyl-3-(4Sbiphenyl)-5-phenyl-4,5-dihydro-(1H) pyrazole on a 4-methylbenzoate cellulose-based chiral stationary phase. <i>Journal of Chromatography A</i> , <b>2014</b> , 1284, 71-7	4.5	16
50	Antioxidant efficiency of oxovitisin, a new class of red wine pyranoanthocyanins, revealed through quantum mechanical investigations. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 66-75	6.1	16
49	Review about the multi-target profile of resveratrol and its implication in the SGK1 inhibition. <i>European Journal of Medicinal Chemistry</i> , <b>2019</b> , 183, 111675	6.8	15
48	Detecting and understanding genetic and structural features in HIV-1 B subtype V3 underlying HIV-1 co-receptor usage. <i>Bioinformatics</i> , <b>2013</b> , 29, 451-60	7.2	15
47	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. <i>Molecules</i> , <b>2017</b> , 22,	4.8	15
46	Tn5 transposase as a useful platform to simulate HIV-1 integrase inhibitor binding mode. <i>Biochemical and Biophysical Research Communications</i> , <b>2007</b> , 363, 554-60	3.4	15
45	Molecular and structural aspects of clinically relevant mutations related to the approved non-nucleoside inhibitors of HIV-1 reverse transcriptase. <i>Drug Resistance Updates</i> , <b>2011</b> , 14, 141-9	23.2	14

44	Tuning the Dual Inhibition of Carbonic Anhydrase and Cyclooxygenase by Dihydrothiazole Benzensulfonamides. <i>ACS Medicinal Chemistry Letters</i> , <b>2018</b> , 9, 1045-1050	4.3	14
43	Identification of Piperidiny-amine Derivatives as Novel Dual Binders of Oncogene c-myc/c-Kit G-quadruplexes. <i>ACS Medicinal Chemistry Letters</i> , <b>2018</b> , 9, 848-853	4.3	13
42	Fhit delocalizes annexin a4 from plasma membrane to cytosol and sensitizes lung cancer cells to paclitaxel. <i>PLoS ONE</i> , <b>2013</b> , 8, e78610	3.7	13
41	Hit Identification of a Novel Dual Binder for h-telo/c-myc G-Quadruplex by a Combination of Pharmacophore Structure-Based Virtual Screening and Docking Refinement. <i>ChemMedChem</i> , <b>2016</b> , 11, 1721-33	3.7	13
40	Docking analysis and resistance evaluation of clinically relevant mutations associated with the HIV-1 non-nucleoside reverse transcriptase inhibitors nevirapine, efavirenz and etravirine. <i>ChemMedChem</i> , <b>2011</b> , 6, 2203-13	3.7	12
39	Molecular modeling of DNA cross-linking analogues based on the azinomycin scaffold. <i>Journal of Chemical Information and Modeling</i> , <b>2005</b> , 45, 602-9	6.1	12
38	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. <i>European Journal of Medicinal Chemistry</i> , <b>2020</b> , 185, 111838	6.8	12
37	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of G-quadruplex DNA c-myc and bcl-2 Sequences. <i>Molecular Informatics</i> , <b>2016</b> , 35, 391-402	3.8	12
36	Molecular Recognition of Human Telomeric DNA by Phenanthroline-Based G-Quadruplex Ligands. <i>Open Journal of Medicinal Chemistry</i> , <b>2013</b> , 03, 41-49	0.1	11
35	Biocatalysed synthesis of beta-O-glucosides from 9-fluorenon-2-carbohydroxyesters. Part 3: IFN-inducing and anti-HSV-2 properties. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 3371-8	3.4	11
34	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. <i>Scientific Reports</i> , <b>2020</b> , 10, 3176	4.9	10
33	Dependence of DNA sequence selectivity and cell cytotoxicity on azinomycin A and B epoxyamide stereochemistry. <i>Organic Letters</i> , <b>2007</b> , 9, 1891-4	6.2	10
32	Molecular modeling, synthesis, and preliminary biological evaluation of glutathione-S-transferase inhibitors as potential therapeutic agents. <i>Journal of Medicinal Chemistry</i> , <b>2005</b> , 48, 6084-9	8.3	10
31	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. <i>Oncotarget</i> , <b>2016</b> , 7, 29927-36	3.3	9
30	9-Fluorenon-4-carboxamides: synthesis, conformational analysis, anti-HSV-2, and immunomodulatory evaluation. Note II. <i>Arkivoc</i> , <b>2004</b> , 2004, 334-348	0.9	9
29	Molecular modeling and enzymatic studies of the interaction of a choline analogue and acetylcholinesterase. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2002</b> , 12, 2899-905	2.9	8
28	Selective inhibition of carbonic anhydrase IX and XII by coumarin and psoralen derivatives. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2021</b> , 36, 685-692	5.6	8
27	Benzo[ <i>b</i> ]tiophen-3-ol derivatives as effective inhibitors of human monoamine oxidase: design, synthesis, and biological activity. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2019</b> , 34, 1511-1525	5.6	7

26	Simple choline esters as potential anti-Alzheimer agents. <i>Current Pharmaceutical Design</i> , <b>2010</b> , 16, 692-733	7
25	Molecular modelling and enzymatic studies of acetylcholinesterase and butyrylcholinesterase recognition with paraquat and related compounds. <i>SAR and QSAR in Environmental Research</i> , <b>2007</b> , 18, 595-602	3.5 7
24	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 130	5 6
23	Exploring new structural features of the 4-[(3-methyl-4-aryl-2,3-dihydro-1,3-thiazol-2-ylidene)amino]benzenesulphonamide scaffold for the inhibition of human carbonic anhydrases. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2019</b> , 34, 1526-1533	5.6 5
22	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. <i>Molecules</i> , <b>2020</b> , 25,	4.8 5
21	State-of-the-art and dissemination of computational tools for drug-design purposes: a survey among Italian academics and industrial institutions. <i>Future Medicinal Chemistry</i> , <b>2013</b> , 5, 907-27	4.1 5
20	Computer-based techniques for lead identification and optimization II: Advanced search methods. <i>Physical Sciences Reviews</i> , <b>2019</b> , 5,	1.4 4
19	Natural Products Extracted from Fungal Species as New Potential Anti-Cancer Drugs: A Structure-Based Drug Repurposing Approach Targeting HDAC7. <i>Molecules</i> , <b>2020</b> , 25,	4.8 4
18	GRID-based Pharmacophore Models: Concept and Application Examples. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2006</b> , 151-170	0.4 3
17	Structural Genetics of circulating variants affecting the SARS-CoV-2 Spike / human ACE2 complex	3
16	BOPC1 Enantiomers Preparation and HuR Interaction Study. From Molecular Modeling to a Curious DEEP-STD NMR Application. <i>ACS Medicinal Chemistry Letters</i> , <b>2020</b> , 11, 883-888	4.3 3
15	Molecular clefts of Rebek revisited: potential application as drug carriers for the antiviral acyclovir. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , <b>2015</b> , 83, 203-208	1.7 2
14	New Dihydrothiazole Benzensulfonamides: Looking for Selectivity toward Carbonic Anhydrase Isoforms I, II, IX, and XII. <i>ACS Medicinal Chemistry Letters</i> , <b>2020</b> , 11, 852-856	4.3 2
13	Design, Synthesis, and Evaluation of New Tripeptides as COX-2 Inhibitors. <i>Journal of Amino Acids</i> , <b>2013</b> , 2013, 606282	2
12	Conformational search of antisense nucleotides. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2001</b> , 11, 2273-7	2.9 2
11	Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. <i>Molecules</i> , <b>2021</b> , 26,	4.8 2
10	Rational Approaches to Anticancer Drug Design/in silico Drug Development	29-46 1
9	Conformational behavior of antineoplastic peptides Dolastatin 10 and Dolastatin 15 From Monte Carlo and molecular dynamics simulations. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 318-325 <sup>1</sup>	1



8	Computational methods applied to the discovery of stem cell factor ligands. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 120, 523-531	1.9	1
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6	Disrupting Protein-Protein Interfaces Using GRID Molecular Interaction Fields <b>2013</b> , 61-82		1
5	From Homology Modeling to the Hit Identification and Drug Repurposing: A Structure-Based Approach in the Discovery of Novel Potential Anti-Obesity Compounds. <i>Methods in Molecular Biology</i> , <b>2021</b> , 2266, 263-277	1.4	1
4	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. <i>Pharmaceuticals</i> , <b>2022</b> , 15, 548	5.2	0
3	13. Computer-based techniques for lead identification and optimization II: Advanced search methods <b>2020</b> , 333-360		
2	Conformational search of antisense nucleotides. Part 2. <i>Il Farmaco</i> , <b>2004</b> , 59, 169-73		
1	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. <i>European Journal of Medicinal Chemistry</i> , <b>2022</b> , 114507	6.8	