Francesco Ortuso

List of Publications by Year in Descending Order

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	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. *Pharmaceuticals*, **2022**, 15, 548	5.2	0
132	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. *European Journal of Medicinal Chemistry*, **2022**, 114507	6.8	
131	Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. *Molecules*, **2021**, 26,	4.8	2
130	From Homology Modeling to the Hit Identification and Drug Repurposing: A Structure-Based Approach in the Discovery of Novel Potential Anti-Obesity Compounds. *Methods in Molecular Biology*, **2021**, 2266, 263-277	1.4	1
129	Structural genetics of circulating variants affecting the SARS-CoV-2 spike/human ACE2 complex. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-11	3.6	21
128	Selective inhibition of carbonic anhydrase IX and XII by coumarin and psoralen derivatives. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 685-692	5.6	8
127	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. *Molecules*, **2020**, 25,	4.8	5
126	13. Computer-based techniques for lead identification and optimization II: Advanced search methods **2020**, 333-360		
125	New Dihydrothiazole Benzensulfonamides: Looking for Selectivity toward Carbonic Anhydrase Isoforms I, II, IX, and XII. *ACS Medicinal Chemistry Letters*, **2020**, 11, 852-856	4.3	2
124	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. *Scientific Reports*, **2020**, 10, 3176	4.9	10
123	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. *European Journal of Medicinal Chemistry*, **2020**, 185, 111838	6.8	12
122	Mediterranean products as promising source of multi-target agents in the treatment of metabolic syndrome. *European Journal of Medicinal Chemistry*, **2020**, 186, 111903	6.8	42
121	BOPC1 Enantiomers Preparation and HuR Interaction Study. From Molecular Modeling to a Curious DEEP-STD NMR Application. *ACS Medicinal Chemistry Letters*, **2020**, 11, 883-888	4.3	3
120	Natural Products Extracted from Fungal Species as New Potential Anti-Cancer Drugs: A Structure-Based Drug Repurposing Approach Targeting HDAC7. *Molecules*, **2020**, 25,	4.8	4
119	Benzo[]tiophen-3-ol derivatives as effective inhibitors of human monoamine oxidase: design, synthesis, and biological activity. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 1511-1525	5.6	7
118	Review about the multi-target profile of resveratrol and its implication in the SGK1 inhibition. *European Journal of Medicinal Chemistry*, **2019**, 183, 111675	6.8	15
117	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. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019** , 34, 1526-1533	5.6	5

116	Benzoic acid-derived nitrones: A new class of potential acetylcholinesterase inhibitors and neuroprotective agents. *European Journal of Medicinal Chemistry*, **2019**, 174, 116-129	6.8	19
115	4-(3-Nitrophenyl)thiazol-2-ylhydrazone derivatives as antioxidants and selective hMAO-B inhibitors: synthesis, biological activity and computational analysis. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 597-612	5.6	29
114	The Mediterranean Diet as source of bioactive compounds with multi-targeting anti-cancer profile. *European Journal of Medicinal Chemistry*, **2019**, 181, 111579	6.8	28
113	A computer-assisted discovery of novel potential anti-obesity compounds as selective carbonic anhydrase VA inhibitors. *European Journal of Medicinal Chemistry*, **2019**, 181, 111565	6.8	17
112	Computer-based techniques for lead identification and optimization II: Advanced search methods. *Physical Sciences Reviews*, **2019**, 5,	1.4	4
111	Novel natural non-nucleoside inhibitors of HIV-1 reverse transcriptase identified by shape- and structure-based virtual screening techniques. *European Journal of Medicinal Chemistry*, **2019**, 161, 1-10	6.8	23
110	Design, synthesis and biochemical evaluation of novel multi-target inhibitors as potential anti-Parkinson agents. *European Journal of Medicinal Chemistry*, **2018**, 143, 1543-1552	6.8	27
109	Identification of Piperidinyl-amine Derivatives as Novel Dual Binders of Oncogene c-myc/c-Kit G-quadruplexes. *ACS Medicinal Chemistry Letters*, **2018**, 9, 848-853	4.3	13
108	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. *Frontiers in Chemistry*, **2018**, 6, 130	5	6
107	Targeting Tumor Associated Carbonic Anhydrases IX and XII: Highly Isozyme Selective Coumarin and Psoralen Inhibitors. *ACS Medicinal Chemistry Letters*, **2018**, 9, 725-729	4.3	27
106	Tuning the Dual Inhibition of Carbonic Anhydrase and Cyclooxygenase by Dihydrothiazole Benzensulfonamides. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1045-1050	4.3	14
105	Multi-target-directed ligands for Alzheimer's disease: Discovery of chromone-based monoamine oxidase/cholinesterase inhibitors. *European Journal of Medicinal Chemistry*, **2018**, 158, 781-800	6.8	40
104	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E2136-E2145	11.5	74
103	Molecular recognition of a carboxy pyridostatin toward G-quadruplex structures: Why does it prefer RNA?. *Chemical Biology and Drug Design*, **2017**, 90, 919-925	2.9	18
102	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 1329-1340	4	25
101	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. *Journal of Medicinal Chemistry*, **2017**, 60, 7206-7212	8.3	35
100	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. *Molecules*, **2017**, 22,	4.8	15
99	Discovery of New Chemical Entities for Old Targets: Insights on the Lead Optimization of Chromone-Based Monoamine Oxidase B (MAO-B) Inhibitors. *Journal of Medicinal Chemistry*, **2016**, 59, 5879-93	8.3	65

98	Drug design, synthesis, in vitro and in silico evaluation of selective monoaminoxidase B inhibitors based on 3-acetyl-2-dichlorophenyl-5-aryl-2,3-dihydro-1,3,4-oxadiazole chemical scaffold. *European Journal of Medicinal Chemistry*, **2016**, 108, 542-552	6.8	26
97	SI113, a SGK1 inhibitor, potentiates the effects of radiotherapy, modulates the response to oxidative stress and induces cytotoxic autophagy in human glioblastoma multiforme cells. *Oncotarget*, **2016**, 7, 15868-84	3.3	43
96	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. *Oncotarget*, **2016**, 7, 29927-36	3.3	9
95	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. *ChemMedChem*, **2016**, 11, 1721-33	3.7	13
94	SGK1, the New Player in the Game of Resistance: Chemo-Radio Molecular Target and Strategy for Inhibition. *Cellular Physiology and Biochemistry*, **2016**, 39, 1863-1876	3.9	53
93	(E)-3-Heteroarylidenechroman-4-ones as potent and selective monoamine oxidase-B inhibitors. *European Journal of Medicinal Chemistry*, **2016**, 117, 292-300	6.8	25
92	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of G-quadruplex DNA c-myc and bcl-2 Sequences. *Molecular Informatics*, **2016**, 35, 391-402	3.8	12
91	SI113, a specific inhibitor of the Sgk1 kinase activity that counteracts cancer cell proliferation. *Cellular Physiology and Biochemistry*, **2015**, 35, 2006-18	3.9	42
90	Molecular clefts of Rebek revisited: potential application as drug carriers for the antiviral acyclovir. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2015**, 83, 203-208	1.7	2
89	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. *Journal of Chemical Information and Modeling*, **2015**, 55, 2256-74	6.1	52
88	Preclinical model in HCC: the SGK1 kinase inhibitor SI113 blocks tumor progression in vitro and in vivo and synergizes with radiotherapy. *Oncotarget*, **2015**, 6, 37511-25	3.3	47
87	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. *Journal of Chromatography A*, **2014**, 1324, 51-7	4.5	16
86	Identification of the stereochemical requirements in the 4-aryl-2-cycloalkylidenhydrazinylthiazole scaffold for the design of selective human monoamine oxidase B inhibitors. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 2887-95	3.4	20
85	Design, synthesis, and biological evaluation of 1,3-diarylpropenones as dual inhibitors of HIV-1 reverse transcriptase. *ChemMedChem*, **2014**, 9, 1869-79	3.7	20
84	In silico identification and biological evaluation of novel selective serum/glucocorticoid-inducible kinase 1 inhibitors based on the pyrazolo-pyrimidine scaffold. *Journal of Chemical Information and Modeling*, **2014**, 54, 1828-32	6.1	31
83	Targeting unimolecular G-quadruplex nucleic acids: a new paradigm for the drug discovery?. *Expert Opinion on Drug Discovery*, **2014**, 9, 1167-87	6.2	28
82	Structure-based virtual screening of novel natural alkaloid derivatives as potential binders of h-telo and c-myc DNA G-quadruplex conformations. *Molecules*, **2014**, 20, 206-23	4.8	22
81	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. *Journal of Medicinal Chemistry*, **2014**, 57, 10455-63	8.3	50

80	Discovery of PTPRJ agonist peptides that effectively inhibit in vitro cancer cell proliferation and tube formation. *ACS Chemical Biology*, **2013**, 8, 1497-506	4.9	23
79	Toward the design of new DNA G-quadruplex ligands through rational analysis of polymorphism and binding data. *European Journal of Medicinal Chemistry*, **2013**, 68, 139-49	6.8	20
78	Detecting and understanding genetic and structural features in HIV-1 B subtype V3 underlying HIV-1 co-receptor usage. *Bioinformatics*, **2013**, 29, 451-60	7.2	15
77	Antioxidant efficiency of oxovitisin, a new class of red wine pyranoanthocyanins, revealed through quantum mechanical investigations. *Journal of Chemical Information and Modeling*, **2013**, 53, 66-75	6.1	16
76	1,5-Diphenylpenta-2,4-dien-1-ones as potent and selective monoamine oxidase-B inhibitors. *European Journal of Medicinal Chemistry*, **2013**, 59, 91-100	6.8	22
75	Identification and characterization of new DNA G-quadruplex binders selected by a combination of ligand and structure-based virtual screening approaches. *Journal of Medicinal Chemistry*, **2013**, 56, 843-55	8.3	75
74	Molecular interaction fields in drug discovery: recent advances and future perspectives. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 594-613	7.9	25
73	Exploring 4-substituted-2-thiazolylhydrazones from 2-, 3-, and 4-acetylpyridine as selective and reversible hMAO-B inhibitors. *European Journal of Medicinal Chemistry*, **2013**, 66, 221-7	6.8	20
72	Molecular Recognition of Human Telomeric DNA by Phenanthroline-Based G-Quadruplex Ligands. *Open Journal of Medicinal Chemistry*, **2013**, 03, 41-49	0.1	11
71	Design, Synthesis, and Evaluation of New Tripeptides as COX-2 Inhibitors. *Journal of Amino Acids*, **2013**, 2013, 606282		2
70	State-of-the-art and dissemination of computational tools for drug-design purposes: a survey among Italian academics and industrial institutions. *Future Medicinal Chemistry*, **2013**, 5, 907-27	4.1	5
69	Identification of new natural DNA G-quadruplex binders selected by a structure-based virtual screening approach. *Molecules*, **2013**, 18, 12051-70	4.8	18
68	Fhit delocalizes annexin a4 from plasma membrane to cytosol and sensitizes lung cancer cells to paclitaxel. *PLoS ONE*, **2013**, 8, e78610	3.7	13
67	Disrupting Protein–Protein Interfaces Using GRID Molecular Interaction Fields **2013**, 61-82		1
66	Synthesis and biological assessment of novel 2-thiazolylhydrazones and computational analysis of their recognition by monoamine oxidase B. *European Journal of Medicinal Chemistry*, **2012**, 48, 284-95	6.8	29
65	Isolation and functional characterization of peptide agonists of PTPRJ, a tyrosine phosphatase receptor endowed with tumor suppressor activity. *ACS Chemical Biology*, **2012**, 7, 1666-76	4.9	27
64	GRID-based three-dimensional pharmacophores II: PharmBench, a benchmark data set for evaluating pharmacophore elucidation methods. *Journal of Chemical Information and Modeling*, **2012**, 52, 2599-608	6.1	34
63	Computer-aided molecular design of asymmetric pyrazole derivatives with exceptional enantioselective recognition toward the Chiralcel OJ-H stationary phase. *Journal of Chemical Information and Modeling*, **2012**, 52, 649-54	6.1	17

62	The polymorphisms of DNA G-quadruplex investigated by docking experiments with telomestatin enantiomers. *Current Pharmaceutical Design*, **2012**, 18, 1873-9	3.3	22
61	Homoisoflavonoids: natural scaffolds with potent and selective monoamine oxidase-B inhibition properties. *Journal of Medicinal Chemistry*, **2011**, 54, 2155-64	8.3	77
60	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. *Journal of Medicinal Chemistry*, **2011**, 54, 5694-711	8.3	37
59	Chromone, a privileged scaffold for the development of monoamine oxidase inhibitors. *Journal of Medicinal Chemistry*, **2011**, 54, 5165-73	8.3	124
58	Conformational studies and solvent-accessible surface area analysis of known selective DNA G-Quadruplex binders. *Biochimie*, **2011**, 93, 1267-74	4.6	21
57	Molecular and structural aspects of clinically relevant mutations related to the approved non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Drug Resistance Updates*, **2011**, 14, 141-9	23.2	14
56	Synthesis and selective human monoamine oxidase inhibition of 3-carbonyl, 3-acyl, and 3-carboxyhydrazido coumarin derivatives. *European Journal of Medicinal Chemistry*, **2011**, 46, 4846-52	6.8	77
55	Towards the discovery of a novel class of monoamine oxidase inhibitors: structure-property-activity and docking studies on chromone amides. *ChemMedChem*, **2011**, 6, 628-32	3.7	30
54	Docking analysis and resistance evaluation of clinically relevant mutations associated with the HIV-1 non-nucleoside reverse transcriptase inhibitors nevirapine, efavirenz and etravirine. *ChemMedChem*, **2011**, 6, 2203-13	3.7	12
53	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. *Current Medicinal Chemistry*, **2010**, 17, 290-308	4.3	25
52	Simple choline esters as potential anti-Alzheimer agents. *Current Pharmaceutical Design*, **2010**, 16, 692-7	3.3	7
51	Synthesis and biological evaluation of N-substituted-3,5-diphenyl-2-pyrazoline derivatives as cyclooxygenase (COX-2) inhibitors. *European Journal of Medicinal Chemistry*, **2010**, 45, 6135-8	6.8	81
50	Investigations on the 2-thiazolylhydrazyne scaffold: synthesis and molecular modeling of selective human monoamine oxidase inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5715-23	3.4	68
49	Rational design, synthesis, biophysical and antiproliferative evaluation of fluorenone derivatives with DNA G-quadruplex binding properties. *ChemMedChem*, **2010**, 5, 575-83	3.7	33
48	Hit identification and biological evaluation of anticancer pyrazolopyrimidines endowed with anti-inflammatory activity. *ChemMedChem*, **2010**, 5, 1242-6	3.7	22
47	A new series of flavones, thioflavones, and flavanones as selective monoamine oxidase-B inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 1273-9	3.4	78
46	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5063-70	3.4	41
45	Chromone-2- and -3-carboxylic acids inhibit differently monoamine oxidases A and B. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 2709-12	2.9	41

44	Synthesis and molecular modelling studies of prenylated pyrazolines as MAO-B inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 6479-82	2.9	19
43	Unusually high enantioselectivity in high-performance liquid chromatography using cellulose tris(4-methylbenzoate) as a chiral stationary phase. *Journal of Chromatography A*, **2009**, 1216, 4673-8	4.5	22
42	Chalcones: a valid scaffold for monoamine oxidases inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 2818-24	8.3	137
41	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. *Journal of Chemical Information and Modeling*, **2009**, 49, 1751-61	6.1	23
40	Synthesis, biological evaluation, and molecular modeling of oleuropein and its semisynthetic derivatives as cyclooxygenase inhibitors. *Journal of Agricultural and Food Chemistry*, **2009**, 57, 11161-7	5.7	81
39	Synthesis, molecular modeling, and selective inhibitory activity against human monoamine oxidases of 3-carboxamido-7-substituted coumarins. *Journal of Medicinal Chemistry*, **2009**, 52, 1935-42	8.3	126
38	Synthesis, stereochemical identification, and selective inhibitory activity against human monoamine oxidase-B of 2-methylcyclohexylidene-(4-arylthiazol-2-yl)hydrazones. *Journal of Medicinal Chemistry* , **2008**, 51, 4874-80	8.3	77
37	Computational methods applied to the discovery of stem cell factor ligands. *Theoretical Chemistry Accounts*, **2008**, 120, 523-531	1.9	1
36	Synthesis, molecular modeling studies and selective inhibitory activity against MAO of N1-propanoyl-3,5-diphenyl-4,5-dihydro-(1H)-pyrazole derivatives. *European Journal of Medicinal Chemistry*, **2008**, 43, 2262-7	6.8	43
35	Cyclodextrin interactions with three drugs used in inflammatory pathologies: An experimental and theoretical study. *Chemical Physics Letters*, **2008**, 454, 374-381	2.5	17
34	Molecular modelling and enzymatic studies of acetylcholinesterase and butyrylcholinesterase recognition with paraquat and related compounds. *SAR and QSAR in Environmental Research*, **2007**, 18, 595-602	3.5	7
33	Dependence of DNA sequence selectivity and cell cytotoxicity on azinomycin A and B epoxyamide stereochemistry. *Organic Letters*, **2007**, 9, 1891-4	6.2	10
32	Selective inhibitory activity against MAO and molecular modeling studies of 2-thiazolylhydrazone derivatives. *Journal of Medicinal Chemistry*, **2007**, 50, 707-12	8.3	73
31	Design, synthesis, and SAR analysis of novel selective sigma1 ligands. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 771-83	3.4	26
30	Tetraplex DNA specific ligands based on the fluorenone-carboxamide scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 2509-14	2.9	23
29	Conformational behavior of antineoplastic peptides Dolastatin 10 and Dolastatin 15 from Monte Carlo and molecular dynamics simulations. *International Journal of Quantum Chemistry*, **2007**, 107, 318-325	2.1	1
28	Tn5 transposase as a useful platform to simulate HIV-1 integrase inhibitor binding mode. *Biochemical and Biophysical Research Communications*, **2007**, 363, 554-60	3.4	15
27	An approach to address Candida rugosa lipase regioselectivity in the acylation reactions of trytilated glucosides. *Journal of Biotechnology*, **2007**, 128, 908-18	3.7	17

26	Monoamine oxidase isoform-dependent tautomeric influence in the recognition of 3,5-diaryl pyrazole inhibitors. *Journal of Medicinal Chemistry*, **2007**, 50, 425-8	8.3	61
25	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. *Current Medicinal Chemistry*, **2006**, 13, 1411-28	4.3	54
24	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. *Bioinformatics*, **2006**, 22, 1449-55	7.2	93
23	GRID-based Pharmacophore Models: Concept and Application Examples. *Methods and Principles in Medicinal Chemistry*, **2006**, 151-170	0.4	3
22	The betaI/betaIII-tubulin isoforms and their complexes with antimitotic agents. Docking and molecular dynamics studies. *FEBS Journal*, **2006**, 273, 3301-10	5.7	54
21	Synthesis and molecular modelling of novel substituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase-A inhibitors. *Chemical Biology and Drug Design*, **2006**, 67, 206-14	2.9	22
20	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of N,NSbis[2-oxo-2H-benzopyran]-3-carboxamides. *Bioorganic and Medicinal Chemistry Letters*, **2006** , 16, 4135-40	2.9	26
19	Quercetin as the active principle of Hypericum hircinum exerts a selective inhibitory activity against MAO-A: extraction, biological analysis, and computational study. *Journal of Natural Products*, **2006**, 69, 945-9	4.9	108
18	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of 1-thiocarbamoyl-3,5-diaryl-4,5-dihydro-(1H)- pyrazole derivatives. *Journal of Medicinal Chemistry*, **2005**, 48, 7113-22	8.3	98
17	Molecular modeling, synthesis, and preliminary biological evaluation of glutathione-S-transferase inhibitors as potential therapeutic agents. *Journal of Medicinal Chemistry*, **2005**, 48, 6084-9	8.3	10
16	Further studies on the interaction of the 5-hydroxytryptamine3 (5-HT3) receptor with arylpiperazine ligands. development of a new 5-HT3 receptor ligand showing potent acetylcholinesterase inhibitory properties. *Journal of Medicinal Chemistry*, **2005**, 48, 3564-75	8.3	59
15	Molecular modeling of DNA cross-linking analogues based on the azinomycin scaffold. *Journal of Chemical Information and Modeling*, **2005**, 45, 602-9	6.1	12
14	Biocatalysed synthesis of beta-O-glucosides from 9-fluorenon-2-carbohydroxyesters. Part 3: IFN-inducing and anti-HSV-2 properties. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 3371-8	3.4	11
13	New conformationally locked bicyclic N,O-nucleoside analogues of antiviral drugs. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 545-50	2.9	31
12	N-myristoylation determines dual targeting of mammalian NADH-cytochrome b5 reductase to ER and mitochondrial outer membranes by a mechanism of kinetic partitioning. *Journal of Cell Biology*, **2005**, 168, 735-45	7.3	66
11	Conformational search of antisense nucleotides. Part 2. *Il Farmaco*, **2004**, 59, 169-73		
10	Inhibition of monoamine oxidases by coumarin-3-acyl derivatives: biological activity and computational study. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 3697-703	2.9	77
9	9-Fluorenon-4-carboxamides: synthesis, conformational analysis, anti-HSV-2, and immunomodulatory evaluation. Note II. *Arkivoc*, **2004**, 2004, 334-348	0.9	9

8	Docking experiments showing similar recognition patterns of paclitaxel when interacting with different macromolecular targets. *Il Farmaco*, **2003**, 58, 691-8		1
7	Modeling and biological evaluation of 3,3S(1,2-ethanediyl)bis[2-(4-methoxyphenyl)-thiazolidin-4-one], a new synthetic cyclooxygenase-2 inhibitor. *European Journal of Pharmacology*, **2002**, 448, 71-80	5.3	48
6	Preparation, characterization, molecular modeling and in vitro activity of paclitaxel-cyclodextrin complexes. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 1637-41	2.9	43
5	Molecular modeling and enzymatic studies of the interaction of a choline analogue and acetylcholinesterase. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 2899-905	2.9	8
4	DNA cross-linking by azinomycin B: Monte Carlo simulations in the evaluation of sequence selectivity. *Journal of Medicinal Chemistry*, **2002**, 45, 861-70	8.3	39
3	Conformational search of antisense nucleotides. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 2273-7	2.9	2
2	Rational Approaches to Anticancer Drug Design/in silico Drug Development29-46		1
1	Structural Genetics of circulating variants affecting the SARS-CoV-2 Spike / human ACE2 complex		3