Stefano Alcaro

List of Publications by Citations

227 papers	6,116 citations	44 h-index	61 g-index
248 ext. papers	7,008 ext. citations	5.3 avg, IF	5.47 L-index

#	Paper	IF	Citations
227	Chalcones: a valid scaffold for monoamine oxidases inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 2818-24	8.3	137
226	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
225	Chromone, a privileged scaffold for the development of monoamine oxidase inhibitors. *Journal of Medicinal Chemistry*, **2011**, 54, 5165-73	8.3	124
224	The mechanisms of pharmacokinetic food-drug interactions - A perspective from the UNGAP group. *European Journal of Pharmaceutical Sciences*, **2019**, 134, 31-59	5.1	119
223	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
222	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
221	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. *Bioinformatics*, **2006**, 22, 1449-55	7.2	93
220	Inhibition of amine oxidases activity by 1-acetyl-3,5-diphenyl-4,5-dihydro-(1H)-pyrazole derivatives. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 3629-33	2.9	91
219	Hybrid ligand-alkylating agents targeting telomeric G-quadruplex structures. *Organic and Biomolecular Chemistry*, **2012**, 10, 2798-806	3.9	85
218	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
217	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
216	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
215	Homoisoflavonoids: natural scaffolds with potent and selective monoamine oxidase-B inhibition properties. *Journal of Medicinal Chemistry*, **2011**, 54, 2155-64	8.3	77
214	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
213	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
212	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
211	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

210	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
209	HCV genotypes are differently prone to the development of resistance to linear and macrocyclic protease inhibitors. *PLoS ONE*, **2012**, 7, e39652	3.7	74
208	Selective inhibitory activity against MAO and molecular modeling studies of 2-thiazolylhydrazone derivatives. *Journal of Medicinal Chemistry*, **2007**, 50, 707-12	8.3	73
207	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
206	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
205	Design and Development of Biomimetic Nanovesicles Using a Microfluidic Approach. *Advanced Materials*, **2018**, 30, e1702749	24	65
204	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
203	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
202	Inhibition of Human Monoamine Oxidase: Biological and Molecular Modeling Studies on Selected Natural Flavonoids. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 9004-9011	5.7	59
201	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
200	Non-coding RNAs in cancer: platforms and strategies for investigating the genomic "dark matter". *Journal of Experimental and Clinical Cancer Research*, **2020**, 39, 117	12.8	56
199	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint- and pharmacophore-based virtual screening approach. *European Journal of Medicinal Chemistry*, **2012**, 50, 216-29	6.8	55
198	Characterization and structural analysis of novel mutations in human immunodeficiency virus type 1 reverse transcriptase involved in the regulation of resistance to nonnucleoside inhibitors. *Journal of Virology*, **2007**, 81, 11507-19	6.6	55
197	New structure-activity relationships of A- and D-ring modified steroidal aromatase inhibitors: design, synthesis, and biochemical evaluation. *Journal of Medicinal Chemistry*, **2012**, 55, 3992-4002	8.3	54
196	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
195	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
194	Specific HIV-1 integrase polymorphisms change their prevalence in untreated versus antiretroviral-treated HIV-1-infected patients, all naive to integrase inhibitors. *Journal of Antimicrobial Chemotherapy*, **2010**, 65, 2305-18	5.1	53
193	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

192	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
191	3-Acetyl-2,5-diaryl-2,3-dihydro-1,3,4-oxadiazoles: a new scaffold for the selective inhibition of monoamine oxidase B. *Journal of Medicinal Chemistry*, **2011**, 54, 6394-8	8.3	51
190	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
189	Modeling and biological evaluation of 3,3Q(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
188	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
187	New raltegravir resistance pathways induce broad cross-resistance to all currently used integrase inhibitors. *Journal of Antimicrobial Chemotherapy*, **2014**, 69, 2118-22	5.1	46
186	New insights into the biological properties of Crocus sativus L.: chemical modifications, human monoamine oxidases inhibition and molecular modeling studies. *European Journal of Medicinal Chemistry*, **2014**, 82, 164-71	6.8	46
185	Bioactive compounds of Crocus sativus L. and their semi-synthetic derivatives as promising anti-Helicobacter pylori, anti-malarial and anti-leishmanial agents. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2015**, 30, 1027-33	5.6	44
184	Current status of antivirals and druggable targets of SARS CoV-2 and other human pathogenic coronaviruses. *Drug Resistance Updates*, **2020**, 53, 100721	23.2	44
183	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
182	Preparation, characterization, molecular modeling and in vitro activity of paclitaxel-cyclodextrin complexes. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 1637-41	2.9	43
181	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
180	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
179	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
178	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
177	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
176	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
175	Structure-activity relationships of novel substituted naphthalene diimides as anticancer agents. *European Journal of Medicinal Chemistry*, **2012**, 57, 417-28	6.8	39

174	Molecular aspects of the RT/drug interactions. Perspective of dual inhibitors. *Current Pharmaceutical Design*, **2013**, 19, 1850-9	3.3	39
173	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
172	The chemistry toolbox of multitarget-directed ligands for Alzheimer's disease. *European Journal of Medicinal Chemistry*, **2019**, 181, 111572	6.8	38
171	A molecular model for DNA cross-linking by the antitumor agent azinomycin B. *Journal of Medicinal Chemistry*, **2000**, 43, 2783-8	8.3	38
170	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
169	Kaempferol as Selective Human MAO-A Inhibitor: Analytical Detection in Calabrian Red Wines, Biological and Molecular Modeling Studies. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 1394-400	5.7	36
168	(3Z)-3-(2-[4-(aryl)-1,3-thiazol-2-yl]hydrazin-1-ylidene)-2,3-dihydro-1H-indol-2-one derivatives as dual inhibitors of HIV-1 reverse transcriptase. *European Journal of Medicinal Chemistry*, **2015**, 93, 452-60	6.8	35
167	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. *Journal of Medicinal Chemistry*, **2017**, 60, 7206-7212	8.3	35
166	Ribonuclease H/DNA Polymerase HIV-1 Reverse Transcriptase Dual Inhibitor: Mechanistic Studies on the Allosteric Mode of Action of Isatin-Based Compound RMNC6. *PLoS ONE*, **2016**, 11, e0147225	3.7	35
165	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
164	Specific enfuvirtide-associated mutational pathways in HIV-1 Gp41 are significantly correlated with an increase in CD4(+) cell count, despite virological failure. *Journal of Infectious Diseases*, **2008**, 197, 1408-18	7	34
163	Rational design, synthesis, biophysical and antiproliferative evaluation of fluorenone derivatives with DNA G-quadruplex binding properties. *ChemMedChem*, **2010**, 5, 575-83	3.7	33
162	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
161	New conformationally locked bicyclic N,O-nucleoside analogues of antiviral drugs. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 545-50	2.9	31
160	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
159	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
158	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
157	Different evolution of genotypic resistance profiles to emtricitabine versus lamivudine in tenofovir-containing regimens. *Journal of Acquired Immune Deficiency Syndromes (1999)*, **2010**, 55, 336-44	3.1	29

156	AMBER force field implementation of the boronate function to simulate the inhibition of beta-lactamases by alkyl and aryl boronic acids. *European Journal of Medicinal Chemistry*, **2005**, 40, 1134-42	6.8	29
155	Eriocitrin and Apigenin as New Carbonic Anhydrase VA Inhibitors from a Virtual Screening of Calabrian Natural Products. *Planta Medica*, **2015**, 81, 533-40	3.1	28
154	(Thiazol-2-yl)hydrazone derivatives from acetylpyridines as dual inhibitors of MAO and AChE: synthesis, biological evaluation and molecular modeling studies. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2015**, 30, 908-19	5.6	28
153	Macrocyclic naphthalene diimides as G-quadruplex binders. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3819-30	3.4	28
152	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
151	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
150	Natural product-inspired esters and amides of ferulic and caffeic acid as dual inhibitors of HIV-1 reverse transcriptase. *European Journal of Medicinal Chemistry*, **2017**, 130, 248-260	6.8	27
149	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
148	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
147	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
146	Conformation and stability of intramolecular telomeric G-quadruplexes: sequence effects in the loops. *PLoS ONE*, **2013**, 8, e84113	3.7	27
145	Active Components of Essential Oils as Anti-Obesity Potential Drugs Investigated by in Silico Techniques. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 5295-300	5.7	26
144	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
143	ABCC Transporters Mediate the Vacuolar Accumulation of Crocins in Saffron Stigmas. *Plant Cell*, **2019**, 31, 2789-2804	11.6	26
142	Design, synthesis, and SAR analysis of novel selective sigma1 ligands. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 771-83	3.4	26
141	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of N,N′-bis[2-oxo-2H-benzopyran]-3-carboxamides. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 4135-40	2.9	26
140	Molecular Modeling of the Antitumor Agents Azinomycins A and B: Force-Field Parametrization and DNA Cross-Linking-Based Filtering. *Journal of Organic Chemistry*, **1998**, 63, 4620-4625	4.2	26
139	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

138	Molecular interaction fields in drug discovery: recent advances and future perspectives. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 594-613	7.9	25
137	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
136	(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
135	Aryl ethynyl anthraquinones: a useful platform for targeting telomeric G-quadruplex structures. *Organic and Biomolecular Chemistry*, **2014**, 12, 3744-54	3.9	23
134	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
133	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
132	Tetraplex DNA specific ligands based on the fluorenone-carboxamide scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 2509-14	2.9	23
131	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
130	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
129	-Acylbenzenesulfonamide Dihydro-1,3,4-oxadiazole Hybrids: Seeking Selectivity toward Carbonic Anhydrase Isoforms. *ACS Medicinal Chemistry Letters*, **2017**, 8, 792-796	4.3	22
128	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
127	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
126	The polymorphisms of DNA G-quadruplex investigated by docking experiments with telomestatin enantiomers. *Current Pharmaceutical Design*, **2012**, 18, 1873-9	3.3	22
125	Hit identification and biological evaluation of anticancer pyrazolopyrimidines endowed with anti-inflammatory activity. *ChemMedChem*, **2010**, 5, 1242-6	3.7	22
124	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
123	C-6 vs C-7 Substituted Steroidal Aromatase Inhibitors: Which Is Better? Synthesis, Biochemical Evaluation, Docking Studies, and Structure-Activity Relationships. *Journal of Medicinal Chemistry*, **2019**, 62, 3636-3657	8.3	21
122	N-Alkyl dien- and trienamides from the roots of Otanthus maritimus with binding affinity for opioid and cannabinoid receptors. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 7074-82	3.4	21
121	Conformational studies and solvent-accessible surface area analysis of known selective DNA G-Quadruplex binders. *Biochimie*, **2011**, 93, 1267-74	4.6	21

120	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
119	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
118	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
117	Design, synthesis and antiviral evaluation of novel heteroarylcarbothioamide derivatives as dual inhibitors of HIV-1 reverse transcriptase-associated RNase H and RDDP functions. *Pathogens and Disease*, **2017**, 75,	4.2	20
116	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
115	Identification and structural characterization of novel genetic elements in the HIV-1 V3 loop regulating coreceptor usage. *Antiviral Therapy*, **2011**, 16, 1035-45	1.6	20
114	Pyrrolo[2Q3C3,4]cyclohepta[1,2-][1,2]oxazoles, a New Class of Antimitotic Agents Active against Multiple Malignant Cell Types. *Journal of Medicinal Chemistry*, **2020**, 63, 12023-12042	8.3	20
113	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
112	Indole and 2,4-Thiazolidinedione conjugates as potential anticancer modulators. *PeerJ*, **2018**, 6, e5386	3.1	19
111	Synthesis and molecular modelling studies of prenylated pyrazolines as MAO-B inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 6479-82	2.9	19
110	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
109	Identification of new natural DNA G-quadruplex binders selected by a structure-based virtual screening approach. *Molecules*, **2013**, 18, 12051-70	4.8	18
108	A drug repurposing screening reveals a novel epigenetic activity of hydroxychloroquine. *European Journal of Medicinal Chemistry*, **2019**, 183, 111715	6.8	17
107	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
106	Methoxyflavones from Stachys glutinosa with binding affinity to opioid receptors: in silico, in vitro, and in vivo studies. *Journal of Natural Products*, **2015**, 78, 69-76	4.9	17
105	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
104	Cyclodextrin interactions with three drugs used in inflammatory pathologies: An experimental and theoretical study. *Chemical Physics Letters*, **2008**, 454, 374-381	2.5	17
103	New 4-[(3-cyclohexyl-4-aryl-2,3-dihydro-1,3-thiazol-2-ylidene)amino]benzene-1-sulfonamides, synthesis and inhibitory activity toward carbonic anhydrase I, II, IX, XII. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 3281-4	2.9	16

102	N-1,2,3-triazole-isatin derivatives for cholinesterase and β-amyloid aggregation inhibition: A comprehensive bioassay study. *Bioorganic Chemistry*, **2020**, 98, 103753	5.1	16
101	Chromenone derivatives as a versatile scaffold with dual mode of inhibition of HIV-1 reverse transcriptase-associated Ribonuclease H function and integrase activity. *European Journal of Medicinal Chemistry*, **2019**, 182, 111617	6.8	16
100	A chromatographic and computational study on the driving force operating in the exceptionally large enantioseparation of N-thiocarbamoyl-3-(4-biphenyl)-5-phenyl-4,5-dihydro-(1H) pyrazole on a 4-methylbenzoate cellulose-based chiral stationary phase. *Journal of Chromatography A*, **2014**, 1324, 71-7	4.5	16
99	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
98	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
97	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
96	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. *Molecules*, **2017**, 22,	4.8	15
95	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
94	Naphthalene diimide-polyamine hybrids as antiproliferative agents: Focus on the architecture of the polyamine chains. *European Journal of Medicinal Chemistry*, **2017**, 128, 107-122	6.8	14
93	Identification of new anti-Candida compounds by ligand-based pharmacophore virtual screening. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 1703-6	5.6	14
92	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
91	Insight on [1,3]thiazolo[4,5-e]isoindoles as tubulin polymerization inhibitors. *European Journal of Medicinal Chemistry*, **2021**, 212, 113122	6.8	14
90	Tuning the Dual Inhibition of Carbonic Anhydrase and Cyclooxygenase by Dihydrothiazole Benzensulfonamides. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1045-1050	4.3	14
89	Optimized Virtual Screening Workflow for the Identification of Novel G-Quadruplex Ligands. *Journal of Chemical Information and Modeling*, **2016**, 56, 484-500	6.1	13
88	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
87	Enantioselective chromatography and absolute configuration of N,N-dimethyl-3-(naphthalen-2-yl)-butan-1-amines: potential sigma1 ligands. *Chirality*, **2006**, 18, 245-53	2.1	13
86	Enantioselective recognition of 2,3-benzodiazepin-4-one derivatives with anticonvulsant activity on several polysaccharide chiral stationary phases. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2006**, 838, 56-62	3.2	13
85	Fhit delocalizes annexin a4 from plasma membrane to cytosol and sensitizes lung cancer cells to paclitaxel. *PLoS ONE*, **2013**, 8, e78610	3.7	13

84	New deferiprone derivatives as multi-functional cholinesterase inhibitors: design, synthesis and in vitro evaluation. *European Journal of Medicinal Chemistry*, **2020**, 198, 112350	6.8	13
83	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
82	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
81	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
80	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. *European Journal of Medicinal Chemistry*, **2020**, 185, 111838	6.8	12
79	Improving the Treatment of Acute Lymphoblastic Leukemia. *Biochemistry*, **2020**, 59, 3193-3200	3.2	12
78	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
77	Current Updates on Naturally Occurring Compounds Recognizing SARS-CoV-2 Druggable Targets. *Molecules*, **2021**, 26,	4.8	12
76	Novel Compounds Targeting the RNA-Binding Protein HuR. Structure-Based Design, Synthesis, and Interaction Studies. *ACS Medicinal Chemistry Letters*, **2019**, 10, 615-620	4.3	11
75	Molecular Recognition of Human Telomeric DNA by Phenanthroline-Based G-Quadruplex Ligands. *Open Journal of Medicinal Chemistry*, **2013**, 03, 41-49	0.1	11
74	Effect of the human immunodeficiency virus type 1 reverse transcriptase polymorphism Leu-214 on replication capacity and drug susceptibility. *Journal of Virology*, **2009**, 83, 7434-9	6.6	11
73	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
72	Exploring new chemical functionalities to improve aromatase inhibition of steroids. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 2823-31	3.4	11
71	Through scaffold modification to 3,5-diaryl-4,5-dihydroisoxazoles: new potent and selective inhibitors of monoamine oxidase B. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 264-270	5.6	10
70	Computer-based techniques for lead identification and optimization I: Basics. *Physical Sciences Reviews*, **2019**, 4,	1.4	10
69	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. *Scientific Reports*, **2020**, 10, 3176	4.9	10
68	Targeting multiple G-quadruplex-forming DNA sequences: Design, biophysical and biological evaluations of indolo-naphthyridine scaffold derivatives. *European Journal of Medicinal Chemistry*, **2019**, 182, 111627	6.8	10
67	A chromatographic study on the exceptional enantioselectivity of cellulose tris(4-methylbenzoate) towards C5-chiral 4,5-dihydro-(1H)-pyrazole derivatives. *Journal of Chromatography A*, **2011**, 1218, 5653-7	4.5	10

66	Dependence of DNA sequence selectivity and cell cytotoxicity on azinomycin A and B epoxyamide stereochemistry. *Organic Letters*, **2007**, 9, 1891-4	6.2	10
65	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
64	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. *Oncotarget*, **2016**, 7, 29927-36	3.3	9
63	9-Fluorenon-4-carboxamides: synthesis, conformational analysis, anti-HSV-2, and immunomodulatory evaluation. Note II. *Arkivoc*, **2004**, 2004, 334-348	0.9	9
62	DJ-1 Proteoforms in Breast Cancer Cells: The Escape of Metabolic Epigenetic Misregulation. *Cells*, **2020**, 9,	7.9	9
61	Incomplete APOBEC3G/F Neutralization by HIV-1 Vif Mutants Facilitates the Genetic Evolution from CCR5 to CXCR4 Usage. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 4870-81	5.9	8
60	Pathway involving the N155H mutation in HIV-1 integrase leads to dolutegravir resistance. *Journal of Antimicrobial Chemotherapy*, **2018**, 73, 1158-1166	5.1	8
59	Structural modifications induced by specific HIV-1 protease-compensatory mutations have an impact on the virological response to a first-line lopinavir/ritonavir-containing regimen. *Journal of Antimicrobial Chemotherapy*, **2013**, 68, 2205-9	5.1	8
58	Enantioselective semi-preparative HPLC of two 2-arylpropionic acids on glycopeptides containing chiral stationary phases. *Tetrahedron: Asymmetry*, **2002**, 13, 69-75		8
57	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
56	Pyrazolones Activate the Proteasome by Gating Mechanisms and Protect Neuronal Cells from Amyloid Toxicity. *ChemMedChem*, **2020**, 15, 302-316	3.7	8
55	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
54	Benzo[]thiophen-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
53	Identification of a rare mutation at reverse transcriptase Lys65 (K65E) in HIV-1-infected patients failing on nucleos(t)ide reverse transcriptase inhibitors. *Journal of Antimicrobial Chemotherapy*, **2013**, 68, 2199-204	5.1	7
52	Simple choline esters as potential anti-Alzheimer agents. *Current Pharmaceutical Design*, **2010**, 16, 692-7	3.3	7
51	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
50	Microwave assisted synthesis of chiral pyrrolines with biological activity. *Tetrahedron: Asymmetry*, **2004**, 15, 3601-3608		7
49	Extended Naphthalene Diimides with Donor/Acceptor Hydrogen-Bonding Properties Targeting G-Quadruplex Nucleic Acids. *European Journal of Organic Chemistry*, **2016**, 2016, 4824-4833	3.2	7

48	Exploration of ligand binding modes towards the identification of compounds targeting HuR: a combined STD-NMR and Molecular Modelling approach. *Scientific Reports*, **2018**, 8, 13780	4.9	7
47	Real-life 3D therapy failure: Analysis of NS5A 93H RAS plus 108 K polymorphism in complex with ombitasvir by molecular modeling. *Journal of Medical Virology*, **2018**, 90, 1257-1263	19.7	6
46	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
45	Chiral arylpyrrolidinols: preparation and biological profile. *Bioorganic and Medicinal Chemistry*, **2005** , 13, 3117-26	3.4	6
44	Inside Perspective of the Synthetic and Computational Toolbox of JAK Inhibitors: Recent Updates. *Molecules*, **2020**, 25,	4.8	6
43	Key genetic elements, single and in clusters, underlying geographically dependent SARS-CoV-2 genetic adaptation and their impact on binding affinity for drugs and immune control. *Journal of Antimicrobial Chemotherapy*, **2021**, 76, 396-412	5.1	6
42	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
41	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. *Molecules*, **2020**, 25,	4.8	5
40	TCL1A interacts with TP63 and enhances the survival of Raji Burkitt lymphoma cell line. *British Journal of Haematology*, **2018**, 183, 509-512	4.5	5
39	Structural Modeling of New Polymorphism Clusters of HCV Polymerase Isolated from Direct-Acting Antiviral Naïve Patients: Focus on Dasabuvir and Setrobuvir Binding Affinity. *ChemistrySelect*, **2018**, 3, 6009-6017	1.8	5
38	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
37	Synthesis of 2H-Imidazo[2,1-*b*][1,3]thiazolo[4,5-*e*]isoindol-8-yl-phenylureas with promising therapeutic features for the treatment of acute myeloid leukemia (AML) with FLT3/ITD mutations.. *European Journal of Medicinal Chemistry*, **2022**, 235, 114292	6.8	5
36	Synthesis, Monoamine Oxidase Inhibition and Computational Analysis of Diversely Substituted N-Propargylated-1,3,5-triazines. *ChemistrySelect*, **2019**, 4, 8334-8337	1.8	4
35	Synthesis and pharmacological evaluation of new N-methyl-arylpyrrolidinols with analgesic activity. *Il Farmaco*, **2003**, 58, 939-46		4
34	Computer-based techniques for lead identification and optimization II: Advanced search methods. *Physical Sciences Reviews*, **2019**, 5,	1.4	4
33	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
32	Probing Substituents in the 1- and 3-Position: Tetrahydropyrazino-Annelated Water-Soluble Xanthine Derivatives as Multi-Target Drugs With Potent Adenosine Receptor Antagonistic Activity. *Frontiers in Chemistry*, **2018**, 6, 206	5	3
31	GRID-based Pharmacophore Models: Concept and Application Examples. *Methods and Principles in Medicinal Chemistry*, **2006**, 151-170	0.4	3

30	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
29	Joining European Scientific Forces to Face Pandemics. *Trends in Microbiology*, **2021**, 29, 92-97	12.4	3
28	Mapping Chromone-3-Phenylcarboxamide Pharmacophore: ?. *Journal of Medicinal Chemistry*, **2021**, 64, 11169-11182	8.3	3
27	Novel propargylamine-based inhibitors of cholinesterases and monoamine oxidases: Synthesis, biological evaluation and docking study. *Bioorganic Chemistry*, **2021**, 116, 105301	5.1	3
26	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
25	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
24	New resistance mutations to nucleoside reverse transcriptase inhibitors at codon 184 of HIV-1 reverse transcriptase (M184L and M184T). *Chemical Biology and Drug Design*, **2019**, 93, 50-59	2.9	2
23	Design, Synthesis, and Evaluation of New Tripeptides as COX-2 Inhibitors. *Journal of Amino Acids*, **2013**, 2013, 606282		2
22	Conformational search of antisense nucleotides. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 2273-7	2.9	2
21	New Pyrimidine and Pyridine Derivatives as Multitarget Cholinesterase Inhibitors: Design, Synthesis, and and Evaluation. *ACS Chemical Neuroscience*, **2021**, 12, 4090-4112	5.7	2
20	In Silico Identification and Biological Evaluation of Antioxidant Food Components Endowed with IX and XII CA Inhibition. *Antioxidants*, **2020**, 9,	7.1	2
19	Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. *Molecules*, **2021**, 26,	4.8	2
18	The HIV-1 reverse transcriptase polymorphism A98S improves the response to tenofovir disoproxil fumarate+emtricitabine-containing HAART both in vivo and in vitro. *Journal of Global Antimicrobial Resistance*, **2016**, 7, 1-7	3.4	2
17	12. Computer-based techniques for lead identification and optimization I: Basics **2020**, 311-332		1
16	Theoretical and structural studies on mechanism of the Stec reaction. *Tetrahedron*, **2012**, 68, 5554-5563	2.4	1
15	Rational Approaches to Anticancer Drug Design/in silico Drug Development29-46		1
14	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
13	Computational methods applied to the discovery of stem cell factor ligands. *Theoretical Chemistry Accounts*, **2008**, 120, 523-531	1.9	1

12	Docking experiments showing similar recognition patterns of paclitaxel when interacting with different macromolecular targets. *Il Farmaco*, **2003**, 58, 691-8		1
11	Disrupting Protein-Protein Interfaces Using GRID Molecular Interaction Fields **2013**, 61-82		1
10	4-Oxoquinolines and monoamine oxidase: When tautomerism matters. *European Journal of Medicinal Chemistry*, **2021**, 213, 113183	6.8	1
9	G-quadruplex Structure Prediction and integration in the GenData2020 data model **2016**,		1
8	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
7	Identification of Compounds Targeting HuD. Another Brick in the Wall of Neurodegenerative Disease Treatment. *Journal of Medicinal Chemistry*, **2021**, 64, 9989-10000	8.3	0
6	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. *Pharmaceuticals*, **2022**, 15, 548	5.2	0
5	Design, Synthesis, and In Vitro, In Silico and In Cellulo Evaluation of New Pyrimidine and Pyridine Amide and Carbamate Derivatives as Multi-Functional Cholinesterase Inhibitors. *Pharmaceuticals*, **2022**, 15, 673	5.2	0
4	13. Computer-based techniques for lead identification and optimization II: Advanced search methods **2020**, 333-360		
3	Conformational search of antisense nucleotides. Part 2. *Il Farmaco*, **2004**, 59, 169-73		
2	Towards the Modulation of RNA-Binding Proteins: New Compounds Targeting Protein HuR. *Proceedings (mdpi)*, **2019**, 22, 65	0.3	
1	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. *European Journal of Medicinal Chemistry*, **2022**, 114507	6.8	