Stefano Alcaro

List of Publications by Year in Descending Order

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	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
226	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. *Pharmaceuticals*, **2022**, 15, 548	5.2	0
225	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
224	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. *European Journal of Medicinal Chemistry*, **2022**, 114507	6.8	
223	New Pyrimidine and Pyridine Derivatives as Multitarget Cholinesterase Inhibitors: Design, Synthesis, and and Evaluation. *ACS Chemical Neuroscience*, **2021**, 12, 4090-4112	5.7	2
222	4-Oxoquinolines and monoamine oxidase: When tautomerism matters. *European Journal of Medicinal Chemistry*, **2021**, 213, 113183	6.8	1
221	Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. *Molecules*, **2021**, 26,	4.8	2
220	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
219	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
218	Joining European Scientific Forces to Face Pandemics. *Trends in Microbiology*, **2021**, 29, 92-97	12.4	3
217	Insight on [1,3]thiazolo[4,5-e]isoindoles as tubulin polymerization inhibitors. *European Journal of Medicinal Chemistry*, **2021**, 212, 113122	6.8	14
216	Mapping Chromone-3-Phenylcarboxamide Pharmacophore: ?. *Journal of Medicinal Chemistry*, **2021**, 64, 11169-11182	8.3	3
215	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
214	Novel propargylamine-based inhibitors of cholinesterases and monoamine oxidases: Synthesis, biological evaluation and docking study. *Bioorganic Chemistry*, **2021**, 116, 105301	5.1	3
213	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
212	Current Updates on Naturally Occurring Compounds Recognizing SARS-CoV-2 Druggable Targets. *Molecules*, **2021**, 26,	4.8	12
211	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. *Molecules*, **2020**, 25,	4.8	5

210	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
209	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
208	12. Computer-based techniques for lead identification and optimization I: Basics **2020**, 311-332		1
207	13. Computer-based techniques for lead identification and optimization II: Advanced search methods **2020**, 333-360		
206	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
205	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. *Scientific Reports*, **2020**, 10, 3176	4.9	10
204	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
203	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
202	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. *European Journal of Medicinal Chemistry*, **2020**, 185, 111838	6.8	12
201	Pyrazolones Activate the Proteasome by Gating Mechanisms and Protect Neuronal Cells from β-Amyloid Toxicity. *ChemMedChem*, **2020**, 15, 302-316	3.7	8
200	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
199	Pyrrolo[2,3,4]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
198	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
197	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
196	Inside Perspective of the Synthetic and Computational Toolbox of JAK Inhibitors: Recent Updates. *Molecules*, **2020**, 25,	4.8	6
195	Improving the Treatment of Acute Lymphoblastic Leukemia. *Biochemistry*, **2020**, 59, 3193-3200	3.2	12
194	DJ-1 Proteoforms in Breast Cancer Cells: The Escape of Metabolic Epigenetic Misregulation. *Cells*, **2020**, 9,	7.9	9
193	In Silico Identification and Biological Evaluation of Antioxidant Food Components Endowed with IX and XII CA Inhibition. *Antioxidants*, **2020**, 9,	7.1	2

192	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
191	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
190	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
189	A drug repurposing screening reveals a novel epigenetic activity of hydroxychloroquine. *European Journal of Medicinal Chemistry*, **2019**, 183, 111715	6.8	17
188	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
187	Computer-based techniques for lead identification and optimization I: Basics. *Physical Sciences Reviews*, **2019**, 4,	1.4	10
186	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
185	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
184	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
183	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
182	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
181	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
180	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
179	The chemistry toolbox of multitarget-directed ligands for Alzheimer disease. *European Journal of Medicinal Chemistry*, **2019**, 181, 111572	6.8	38
178	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
177	Synthesis, Monoamine Oxidase Inhibition and Computational Analysis of Diversely Substituted N-Propargylated-1,3,5-triazines. *ChemistrySelect*, **2019**, 4, 8334-8337	1.8	4
176	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
175	ABCC Transporters Mediate the Vacuolar Accumulation of Crocins in Saffron Stigmas. *Plant Cell*, **2019**, 31, 2789-2804	11.6	26

174	Computer-based techniques for lead identification and optimization II: Advanced search methods. *Physical Sciences Reviews*, **2019**, 5,	1.4	4
173	Towards the Modulation of RNA-Binding Proteins: New Compounds Targeting Protein HuR. *Proceedings (mdpi)*, **2019**, 22, 65	0.3	
172	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
171	Design and Development of Biomimetic Nanovesicles Using a Microfluidic Approach. *Advanced Materials*, **2018**, 30, e1702749	24	65
170	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
169	Pathway involving the N155H mutation in HIV-1 integrase leads to dolutegravir resistance. *Journal of Antimicrobial Chemotherapy*, **2018**, 73, 1158-1166	5.1	8
168	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
167	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
166	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
165	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
164	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
163	Indole and 2,4-Thiazolidinedione conjugates as potential anticancer modulators. *PeerJ*, **2018**, 6, e5386	3.1	19
162	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
161	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
160	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
159	Tuning the Dual Inhibition of Carbonic Anhydrase and Cyclooxygenase by Dihydrothiazole Benzensulfonamides. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1045-1050	4.3	14
158	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
157	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

156	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
155	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
154	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
153	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
152	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
151	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. *Journal of Medicinal Chemistry*, **2017**, 60, 7206-7212	8.3	35
150	-Acylbenzenesulfonamide Dihydro-1,3,4-oxadiazole Hybrids: Seeking Selectivity toward Carbonic Anhydrase Isoforms. *ACS Medicinal Chemistry Letters*, **2017**, 8, 792-796	4.3	22
149	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
148	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. *Molecules*, **2017**, 22,	4.8	15
147	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
146	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
145	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
144	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
143	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
142	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
141	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
140	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
139	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

138	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. *Oncotarget*, **2016**, 7, 29927-36	3.3	9
137	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
136	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
135	G-quadruplex Structure Prediction and integration in the GenData2020 data model **2016**,		1
134	(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
133	Exploring new chemical functionalities to improve aromatase inhibition of steroids. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 2823-31	3.4	11
132	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
131	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
130	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
129	(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
128	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
127	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
126	(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
125	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
124	Macrocyclic naphthalene diimides as G-quadruplex binders. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3819-30	3.4	28
123	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
122	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
121	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

120	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
119	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
118	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
117	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
116	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
115	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
114	Aryl ethynyl anthraquinones: a useful platform for targeting telomeric G-quadruplex structures. *Organic and Biomolecular Chemistry*, **2014**, 12, 3744-54	3.9	23
113	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
112	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
111	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
110	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
109	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
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. *Journal of Medicinal Chemistry*, **2014**, 57, 10455-63	8.3	50
107	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
106	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
105	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
104	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
103	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

102	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
101	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
100	Molecular interaction fields in drug discovery: recent advances and future perspectives. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 594-613	7.9	25
99	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
98	Molecular Recognition of Human Telomeric DNA by Phenanthroline-Based G-Quadruplex Ligands. *Open Journal of Medicinal Chemistry*, **2013**, 03, 41-49	0.1	11
97	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
96	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
95	Design, Synthesis, and Evaluation of New Tripeptides as COX-2 Inhibitors. *Journal of Amino Acids*, **2013**, 2013, 606282		2
94	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
93	Identification of new natural DNA G-quadruplex binders selected by a structure-based virtual screening approach. *Molecules*, **2013**, 18, 12051-70	4.8	18
92	Conformation and stability of intramolecular telomeric G-quadruplexes: sequence effects in the loops. *PLoS ONE*, **2013**, 8, e84113	3.7	27
91	Molecular aspects of the RT/drug interactions. Perspective of dual inhibitors. *Current Pharmaceutical Design*, **2013**, 19, 1850-9	3.3	39
90	Fhit delocalizes annexin a4 from plasma membrane to cytosol and sensitizes lung cancer cells to paclitaxel. *PLoS ONE*, **2013**, 8, e78610	3.7	13
89	Disrupting Protein–Protein Interfaces Using GRID Molecular Interaction Fields **2013**, 61-82		1
88	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
87	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
86	Structure-activity relationships of novel substituted naphthalene diimides as anticancer agents. *European Journal of Medicinal Chemistry*, **2012**, 57, 417-28	6.8	39
85	Hybrid ligand-alkylating agents targeting telomeric G-quadruplex structures. *Organic and Biomolecular Chemistry*, **2012**, 10, 2798-806	3.9	85

84	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
83	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
82	Theoretical and structural studies on mechanism of the Stec reaction. *Tetrahedron*, **2012**, 68, 5554-5563	2.4	1
81	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
80	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
79	The polymorphisms of DNA G-quadruplex investigated by docking experiments with telomestatin enantiomers. *Current Pharmaceutical Design*, **2012**, 18, 1873-9	3.3	22
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