Stefano Alcaro

List of Publications by Year in descending order

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242 papers	7,787 citations	38738 50 h-index	88628 70 g-index

248 all docs	248 docs citations	248 times ranked	9878 citing authors

#	Article	IF	Citations
1	The mechanisms of pharmacokinetic food-drug interactions â€“ A perspective from the UNGAP group. European Journal of Pharmaceutical Sciences, 2019, 134, 31-59.	4.0	224
2	Chalcones: A Valid Scaffold for Monoamine Oxidases Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 2818-2824.	6.4	162
3	Synthesis, Molecular Modeling, and Selective Inhibitory Activity against Human Monoamine Oxidases of 3-Carboxamido-7-Substituted Coumarins. Journal of Medicinal Chemistry, 2009, 52, 1935-1942.	6.4	152
4	Chromone, a Privileged Scaffold for the Development of Monoamine Oxidase Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 5165-5173.	6.4	140
5	Non-coding RNAs in cancer: platforms and strategies for investigating the genomic â€œdark matterâ€• Journal of Experimental and Clinical Cancer Research, 2020, 39, 117.	8.6	137
6	Quercetin as the Active Principle ofHypericumhircinumExerts a Selective Inhibitory Activity against MAO-A:Â Extraction, Biological Analysis, and Computational Study. Journal of Natural Products, 2006, 69, 945-949.	3.0	118
7	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, 7113-7122.	6.4	112
8	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, 6135-6138.	5.5	103
9	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. Bioinformatics, 2006, 22, 1449-1455.	4.1	102
10	Design and Development of Biomimetic Nanovesicles Using a Microfluidic Approach. Advanced Materials, 2018, 30, e1702749.	21.0	100
11	Inhibition of amine oxidases activity by 1-acetyl-3,5-diphenyl-4,5-dihydro-(1H)-pyrazole derivatives. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 3629-3633.	2.2	98
12	Synthesis, Biological Evaluation, and Molecular Modeling of Oleuropein and Its Semisynthetic Derivatives as Cyclooxygenase Inhibitors. Journal of Agricultural and Food Chemistry, 2009, 57, 11161-11167.	5.2	96
13	Hybrid ligandâ€“alkylating agents targeting telomeric G-quadruplex structures. Organic and Biomolecular Chemistry, 2012, 10, 2798.	2.8	94
14	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.	7.1	91
15	Inhibition of monoamine oxidases by coumarin-3-acyl derivatives: biological activity and computational study. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 3697-3703.	2.2	89
16	Homoisoflavonoids: Natural Scaffolds with Potent and Selective Monoamine Oxidase-B Inhibition Properties. Journal of Medicinal Chemistry, 2011, 54, 2155-2164.	6.4	89
17	Synthesis and selective human monoamine oxidase inhibition of 3-carbonyl, 3-acyl, and 3-carboxyhydrazido coumarin derivatives. European Journal of Medicinal Chemistry, 2011, 46, 4846-4852.	5.5	88
18	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, 5879-5893.	6.4	87

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19	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, 4874-4880.	6.4	86
20	A new series of flavones, thioflavones, and flavanones as selective monoamine oxidase-B inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 1273-1279.	3.0	83
21	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, 843-855.	6.4	81
22	Current status of antivirals and druggable targets of SARS CoV-2 and other human pathogenic coronaviruses. Drug Resistance Updates, 2020, 53, 100721.	14.4	80
23	Selective Inhibitory Activity against MAO and Molecular Modeling Studies of 2-Thiazolylhydrazone Derivatives. Journal of Medicinal Chemistry, 2007, 50, 707-712.	6.4	79
24	HCV Genotypes Are Differently Prone to the Development of Resistance to Linear and Macrocyclic Protease Inhibitors. PLoS ONE, 2012, 7, e39652.	2.5	78
25	Investigations on the 2-thiazolylhydrazyne scaffold: Synthesis and molecular modeling of selective human monoamine oxidase inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 5715-5723.	3.0	76
26	Inhibition of Human Monoamine Oxidase: Biological and Molecular Modeling Studies on Selected Natural Flavonoids. Journal of Agricultural and Food Chemistry, 2016, 64, 9004-9011.	5.2	74
27	N-myristoylation determines dual targeting of mammalian NADH-cytochrome b(5) reductase to ER and mitochondrial outer membranes by a mechanism of kinetic partitioning. Journal of Cell Biology, 2005, 168, 735-745.	5.2	72
28	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.	1.6	72
29	Mediterranean products as promising source of multi-target agents in the treatment of metabolic syndrome. European Journal of Medicinal Chemistry, 2020, 186, 111903.	5.5	66
30	Monoamine Oxidase Isoform-Dependent Tautomeric Influence in the Recognition of 3,5-Diaryl Pyrazole Inhibitors. Journal of Medicinal Chemistry, 2007, 50, 425-428.	6.4	65
31	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	5.4	65
32	Further Studies on the Interaction of the 5-Hydroxytryptamine3(5-HT3) Receptor with Arylpiperazine Ligands. Development of a New 5-HT3Receptor Ligand Showing Potent Acetylcholinesterase Inhibitory Properties. Journal of Medicinal Chemistry, 2005, 48, 3564-3575.	6.4	64
33	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, 216-229.	5.5	63
34	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, 11507-11519.	3.4	62
35	New Structureâ€“Activity Relationships of A- and D-Ring Modified Steroidal Aromatase Inhibitors: Design, Synthesis, and Biochemical Evaluation. Journal of Medicinal Chemistry, 2012, 55, 3992-4002.	6.4	60
36	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, 1411-1428.	2.4	58

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37	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.	5.5	58
38	Modeling and biological evaluation of 3,3â€²-(1,2-ethanediyl)bis[2-(4-methoxyphenyl)-thiazolidin-4-one], a new synthetic cyclooxygenase-2 inhibitor. European Journal of Pharmacology, 2002, 448, 71-80.	3.5	57
39	The Î²I/Î²IIIâ€tubulin isoforms and their complexes with antimitotic agents. FEBS Journal, 2006, 273, 3301-3310.	4.7	57
40	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, 2305-2318.	3.0	57
41	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, 10455-10463.	6.4	56
42	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, 1394-1400.	5.2	56
43	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, 6394-6398.	6.4	55
44	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, 164-171.	5.5	55
45	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, 1027-1033.	5.2	55
46	Preclinical model in HCC: the SGK1 kinase inhibitor SI113 blocks tumor progressionin vitroandin vivoand synergizes with radiotherapy. Oncotarget, 2015, 6, 37511-37525.	1.8	55
47	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, 15868-15884.	1.8	54
48	SI113, a Specific Inhibitor of the Sgk1 Kinase Activity that Counteracts Cancer Cell Proliferation. Cellular Physiology and Biochemistry, 2015, 35, 2006-2018.	1.6	53
49	The Mediterranean Diet as source of bioactive compounds with multi-targeting anti-cancer profile. European Journal of Medicinal Chemistry, 2019, 181, 111579.	5.5	51
50	Preparation, characterization, molecular modeling and In vitro activity of paclitaxelâ€“cyclodextrin complexes. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 1637-1641.	2.2	50
51	New raltegravir resistance pathways induce broad cross-resistance to all currently used integrase inhibitors. Journal of Antimicrobial Chemotherapy, 2014, 69, 2118-2122.	3.0	50
52	The chemistry toolbox of multitarget-directed ligands for Alzheimer's disease. European Journal of Medicinal Chemistry, 2019, 181, 111572.	5.5	49
53	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.	5.5	48
54	Chromone-2- and -3-carboxylic acids inhibit differently monoamine oxidases A and B. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2709-2712.	2.2	47

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55	(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, 452-460.	5.5	47
56	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. Journal of Medicinal Chemistry, 2017, 60, 7206-7212.	6.4	47
57	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, 2262-2267.	5.5	46
58	New Insight into the Central Benzodiazepine Receptorâ€“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, 5694-5711.	6.4	45
59	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.	2.5	45
60	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 5063-5070.	3.0	44
61	Structureâ€“activity relationships of novel substituted naphthalene diimides as anticancer agents. European Journal of Medicinal Chemistry, 2012, 57, 417-428.	5.5	44
62	Pyrrolo[2â€²,3â€²:3,4]cyclohepta[1,2-d][1,2]oxazoles, a New Class of Antimitotic Agents Active against Multiple Malignant Cell Types. Journal of Medicinal Chemistry, 2020, 63, 12023-12042.	6.4	43
63	A Molecular Model for DNA Cross-Linking by the Antitumor Agent Azinomycin B. Journal of Medicinal Chemistry, 2000, 43, 2783-2788.	6.4	42
64	DNA Cross-Linking by Azinomycin B:â€‰ Monte Carlo Simulations in the Evaluation of Sequence Selectivity. Journal of Medicinal Chemistry, 2002, 45, 861-870.	6.4	42
65	Molecular Aspects of the RT/drug Interactions. Perspective of Dual Inhibitors. Current Pharmaceutical Design, 2013, 19, 1850-1859.	1.9	42
66	Design, synthesis and biochemical evaluation of novel multi-target inhibitors as potential anti-Parkinson agents. European Journal of Medicinal Chemistry, 2018, 143, 1543-1552.	5.5	40
67	Targeting Tumor Associated Carbonic Anhydrases IX and XII: Highly Isozyme Selective Coumarin and Psoralen Inhibitors. ACS Medicinal Chemistry Letters, 2018, 9, 725-729.	2.8	39
68	Specific Enfuvirtideâ€Associated Mutational Pathways in HIVâ€1 Gp41 Are Significantly Correlated With an Increase in CD4+Cell Count, Despite Virological Failure. Journal of Infectious Diseases, 2008, 197, 1408-1418.	4.0	38
69	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.	5.2	37
70	GRID-Based Three-Dimensional Pharmacophores II: PharmBench, a Benchmark Data Set for Evaluating Pharmacophore Elucidation Methods. Journal of Chemical Information and Modeling, 2012, 52, 2599-2608.	5.4	36
71	Molecular interaction fields in drug discovery: recent advances and future perspectives. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 594-613.	14.6	36
72	ABCC transporters mediate the vacuolar accumulation of crocins in saffron stigmas. Plant Cell, 2019, 31, tpc.00193.2019.	6.6	36

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73	Benzoic acid-derived nitrones: A new class of potential acetylcholinesterase inhibitors and neuroprotective agents. European Journal of Medicinal Chemistry, 2019, 174, 116-129.	5.5	35
74	New conformationally locked bicyclic N,O-nucleoside analogues of antiviral drugs. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 545-550.	2.2	34
75	Rational Design, Synthesis, Biophysical and Antiproliferative Evaluation of Fluorenone Derivatives with DNA Gâ€Quadruplex Binding Properties. ChemMedChem, 2010, 5, 575-583.	3.2	34
76	Towards the Discovery of a Novel Class of Monoamine Oxidase Inhibitors: Structureâ€“Propertyâ€“Activity and Docking Studies on Chromone Amides. ChemMedChem, 2011, 6, 628-632.	3.2	34
77	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, 1828-1832.	5.4	34
78	Macrocyclic naphthalene diimides as G-quadruplex binders. Bioorganic and Medicinal Chemistry, 2015, 23, 3819-3830.	3.0	34
79	Drug design, synthesis, inÂvitro 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.	5.5	34
80	Editorial: Multi-Target-Directed Ligands (MTDL) as Challenging Research Tools in Drug Discovery: From Design to Pharmacological Evaluation. Frontiers in Chemistry, 2019, 7, 71.	3.6	34
81	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, 284-295.	5.5	33
82	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1329-1340.	2.4	33
83	AMBER force field implementation of the boronate function to simulate the inhibition of Î²-lactamases by alkyl and aryl boronic acids. European Journal of Medicinal Chemistry, 2005, 40, 1134-1142.	5.5	32
84	Different Evolution of Genotypic Resistance Profiles to Emtricitabine Versus Lamivudine in Tenofovir-Containing Regimens. Journal of Acquired Immune Deficiency Syndromes (1999), 2010, 55, 336-344.	2.1	32
85	Isolation and Functional Characterization of Peptide Agonists of PTPRJ, a Tyrosine Phosphatase Receptor Endowed with Tumor Suppressor Activity. ACS Chemical Biology, 2012, 7, 1666-1676.	3.4	32
86	Conformation and Stability of Intramolecular Telomeric G-Quadruplexes: Sequence Effects in the Loops. PLoS ONE, 2013, 8, e84113.	2.5	32
87	Indole and 2,4-Thiazolidinedione conjugates as potential anticancer modulators. PeerJ, 2018, 6, e5386.	2.0	32
88	N-1,2,3-triazole-isatin derivatives for cholinesterase and Î²-amyloid aggregation inhibition: A comprehensive bioassay study. Bioorganic Chemistry, 2020, 98, 103753.	4.1	32
89	New deferiprone derivatives as multi-functional cholinesterase inhibitors: design, synthesis and inÂvitro evaluation. European Journal of Medicinal Chemistry, 2020, 198, 112350.	5.5	32
90	Aryl ethynyl anthraquinones: a useful platform for targeting telomeric G-quadruplex structures. Organic and Biomolecular Chemistry, 2014, 12, 3744-3754.	2.8	31

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91	Targeting unimolecular G-quadruplex nucleic acids: a new paradigm for the drug discovery?. Expert Opinion on Drug Discovery, 2014, 9, 1167-1187.	5.0	31
92	Eriocitrin and Apigenin as New Carbonic Anhydrase VA Inhibitors from a Virtual Screening of Calabrian Natural Products. Planta Medica, 2015, 81, 533-540.	1.3	31
93	(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, 908-919.	5.2	31
94	Active Components of Essential Oils as Anti-Obesity Potential Drugs Investigated by in Silico Techniques. Journal of Agricultural and Food Chemistry, 2016, 64, 5295-5300.	5.2	31
95	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, .	2.0	31
96	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.	5.5	31
97	Design, synthesis, and SAR analysis of novel selective Ïƒ1 ligands. Bioorganic and Medicinal Chemistry, 2007, 15, 771-783.	3.0	30
98	(E)-3-Heteroarylidenechroman-4-ones as potent and selective monoamine oxidase-B inhibitors. European Journal of Medicinal Chemistry, 2016, 117, 292-300.	5.5	30
99	Improving the Treatment of Acute Lymphoblastic Leukemia. Biochemistry, 2020, 59, 3193-3200.	2.5	30
100	Insight on [1,3]thiazolo[4,5-e]isoindoles as tubulin polymerization inhibitors. European Journal of Medicinal Chemistry, 2021, 212, 113122.	5.5	30
101	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, 1751-1761.	5.4	29
102	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of N,Nâ€²-bis[2-oxo-2H-benzopyran]-3-carboxamides. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 4135-4140.	2.2	28
103	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.	5.5	28
104	Molecular Modeling of the Antitumor Agents Azinomycins A and B:Â Force-Field Parametrization and DNA Cross-Linking-Based Filtering. Journal of Organic Chemistry, 1998, 63, 4620-4625.	3.2	27
105	Discovery of PTPRJ Agonist Peptides That Effectively Inhibit in Vitro Cancer Cell Proliferation and Tube Formation. ACS Chemical Biology, 2013, 8, 1497-1506.	3.4	27
106	N-Acylbenzenesulfonamide Dihydro-1,3,4-oxadiazole Hybrids: Seeking Selectivity toward Carbonic Anhydrase Isoforms. ACS Medicinal Chemistry Letters, 2017, 8, 792-796.	2.8	27
107	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.	5.5	27
108	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, 206-214.	3.2	26

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109	Hit Identification and Biological Evaluation of Anticancer Pyrazolopyrimidines Endowed with Antiâ€inflammatory Activity. ChemMedChem, 2010, 5, 1242-1246.	3.2	25
110	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 (Supplementary Material). Current Medicinal Chemistry, 2010, 17, 290-308.	2.4	25
111	Structure-Based Virtual Screening of Novel Natural Alkaloid Derivatives as Potential Binders of h-telo and c-myc DNA G-Quadruplex Conformations. Molecules, 2015, 20, 206-223.	3.8	25
112	Molecular recognition of a carboxy pyridostatin toward Gâ€quadruplex structures: Why does it prefer <scp>RNA</scp>?. Chemical Biology and Drug Design, 2017, 90, 919-925.	3.2	25
113	C-6Î±- vs C-7Î±-Substituted Steroidal Aromatase Inhibitors: Which Is Better? Synthesis, Biochemical Evaluation, Docking Studies, and Structureâ€"Activity Relationships. Journal of Medicinal Chemistry, 2019, 62, 3636-3657.	6.4	25
114	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, 7074-7082.	3.0	24
115	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, 221-227.	5.5	24
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, 2887-2895.	3.0	24
117	Tetraplex DNA specific ligands based on the fluorenone-carboxamide scaffold. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2509-2514.	2.2	23
118	Unusually high enantioselectivity in high-performance liquid chromatography using cellulose tris(4-methylbenzoate) as a chiral stationary phase. Journal of Chromatography A, 2009, 1216, 4673-4678.	3.7	23
119	Conformational studies and solvent-accessible surface area analysis of known selective DNA G-Quadruplex binders. Biochimie, 2011, 93, 1267-1274.	2.6	23
120	Identification and Structural Characterization of Novel Genetic Elements in the HIV-1 V3 Loop Regulating Coreceptor Usage. Antiviral Therapy, 2011, 16, 1035-1045.	1.0	23
121	The Polymorphisms of DNA G-Quadruplex Investigated by Docking Experiments with Telomestatin Enantiomers. Current Pharmaceutical Design, 2012, 18, 1873-1879.	1.9	23
122	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, 649-654.	5.4	23
123	Toward the design of new DNA G-quadruplex ligands through rational analysis of polymorphism and binding data. European Journal of Medicinal Chemistry, 2013, 68, 139-149.	5.5	23
124	Identification of New Natural DNA G-Quadruplex Binders Selected by a Structure-Based Virtual Screening Approach. Molecules, 2013, 18, 12051-12070.	3.8	23
125	Design, Synthesis, and Biological Evaluation of 1,3â€Diarylpropenones as Dual Inhibitors of HIVâ€1 Reverse Transcriptase. ChemMedChem, 2014, 9, 1869-1879.	3.2	23
126	A computer-assisted discovery of novel potential anti-obesity compounds as selective carbonic anhydrase VA inhibitors. European Journal of Medicinal Chemistry, 2019, 181, 111565.	5.5	23

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127	A drug repurposing screening reveals a novel epigenetic activity of hydroxychloroquine. European Journal of Medicinal Chemistry, 2019, 183, 111715.	5.5	23
128	DJ-1 Proteoforms in Breast Cancer Cells: The Escape of Metabolic Epigenetic Misregulation. Cells, 2020, 9, 1968.	4.1	23
129	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. Molecules, 2017, 22, 1571.	3.8	22
130	Current Updates on Naturally Occurring Compounds Recognizing SARS-CoV-2 Druggable Targets. Molecules, 2021, 26, 632.	3.8	22
131	Synthesis and molecular modelling studies of prenylated pyrazolines as MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6479-6482.	2.2	21
132	Methoxyflavones fromStachys glutinosawith Binding Affinity to Opioid Receptors: In Silico, in Vitro, and in Vivo Studies. Journal of Natural Products, 2015, 78, 69-76.	3.0	21
133	Novel Compounds Targeting the RNA-Binding Protein HuR. Structure-Based Design, Synthesis, and Interaction Studies. ACS Medicinal Chemistry Letters, 2019, 10, 615-620.	2.8	21
134	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. Scientific Reports, 2020, 10, 3176.	3.3	21
135	A chromatographic and computational study on the driving force operating in the exceptionally large enantioseparation of N-thiocarbamoyl-3-(4â€²-biphenyl)-5-phenyl-4,5-dihydro-(1H) pyrazole on a 4-methylbenzoate cellulose-based chiral stationary phase. Journal of Chromatography A, 2014, 1324, 71-77.	3.7	20
136	Review about the multi-target profile of resveratrol and its implication in the SGK1 inhibition. European Journal of Medicinal Chemistry, 2019, 183, 111675.	5.5	20
137	Inside Perspective of the Synthetic and Computational Toolbox of JAK Inhibitors: Recent Updates. Molecules, 2020, 25, 3321.	3.8	20
138	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, 3281-3284.	2.2	19
139	Identification of new anti-Candida compounds by ligand-based pharmacophore virtual screening. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1703-1706.	5.2	19
140	In Silico 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.	2.8	19
141	Tuning the Dual Inhibition of Carbonic Anhydrase and Cyclooxygenase by Dihydrothiazole Benzensulfonamides. ACS Medicinal Chemistry Letters, 2018, 9, 1045-1050.	2.8	18
142	Benzo[b]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.	5.2	18
143	Selective inhibition of carbonic anhydrase IX and XII by coumarin and psoralen derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 685-692.	5.2	18
144	Fhit Delocalizes Annexin A4 from Plasma Membrane to Cytosol and Sensitizes Lung Cancer Cells to Paclitaxel. PLoS ONE, 2013, 8, e78610.	2.5	18

#	Article	IF	Citations
145	Synthesis of 2H-Imidazo[2â€²,1':2,3] [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.	5.5	18
146	Î²-Cyclodextrin interactions with three drugs used in inflammatory pathologies: An experimental and theoretical study. Chemical Physics Letters, 2008, 454, 374-381.	2.6	17
147	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.	5.4	17
148	Naphthalene diimide-polyamine hybrids as antiproliferative agents: Focus on the architecture of the polyamine chains. European Journal of Medicinal Chemistry, 2017, 128, 107-122.	5.5	17
149	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. European Journal of Medicinal Chemistry, 2020, 185, 111838.	5.5	17
150	Detecting and understanding genetic and structural features in HIV-1 B subtype V3 underlying HIV-1 co-receptor usage. Bioinformatics, 2013, 29, 451-460.	4.1	16
151	Computer-based techniques for lead identification and optimization I: Basics. Physical Sciences Reviews, 2019, 4, .	0.8	16
152	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.	3.0	16
153	A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. Oncotarget, 2016, 7, 29927-29936.	1.8	16
154	New Pyrimidine and Pyridine Derivatives as Multitarget Cholinesterase Inhibitors: Design, Synthesis, and In Vitro and In Cellulo Evaluation. ACS Chemical Neuroscience, 2021, 12, 4090-4112.	3.5	16
155	Tn5 transposase as a useful platform to simulate HIV-1 integrase inhibitor binding mode. Biochemical and Biophysical Research Communications, 2007, 363, 554-560.	2.1	15
156	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of Gâ€quadruplex DNA câ€myc and bclâ€2 Sequences. Molecular Informatics, 2016, 35, 391-402.	2.5	15
157	Targeting multiple G-quadruplexâ€“forming DNA sequences: Design, biophysical and biological evaluations of indolo-naphthyridine scaffold derivatives. European Journal of Medicinal Chemistry, 2019, 182, 111627.	5.5	15
158	Pyrazolones Activate the Proteasome by Gating Mechanisms and Protect Neuronal Cells from Î²â€Amyloid Toxicity. ChemMedChem, 2020, 15, 302-316.	3.2	15
159	Molecular Modeling of DNA Cross-linking Analogues Based on the Azinomycin Scaffold. Journal of Chemical Information and Modeling, 2005, 45, 602-609.	5.4	14
160	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.	2.3	14
161	Enantioselective chromatography and absolute configuration ofN,N-dimethyl-3-(naphthalen-2-yl)-butan-1-amines: Potential sigma1 ligands. Chirality, 2006, 18, 245-253.	2.6	14
162	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, 141-149.	14.4	14

#	Article	IF	Citations
163	Docking Analysis and Resistance Evaluation of Clinically Relevant Mutations Associated with the HIVâ€1 Nonâ€nucleoside Reverse Transcriptase Inhibitors Nevirapine, Efavirenz and Etravirine. ChemMedChem, 2011, 6, 2203-2213.	3.2	14
164	Hit Identification of a Novel Dual Binder for hâ€telo/câ€myc Gâ€Quadruplex by a Combination of Pharmacophore Structureâ€Based Virtual Screening and Docking Refinement. ChemMedChem, 2016, 11, 1721-1733.	3.2	14
165	Optimized Virtual Screening Workflow for the Identification of Novel G-Quadruplex Ligands. Journal of Chemical Information and Modeling, 2016, 56, 484-500.	5.4	14
166	Biocatalysed synthesis of Î²-O-glucosides from 9-fluorenon-2-carbohydroxyesters. Part 3: IFN-inducing and anti-HSV-2 properties. Bioorganic and Medicinal Chemistry, 2005, 13, 3371-3378.	3.0	13
167	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, 5653-5657.	3.7	13
168	Exploring new chemical functionalities to improve aromatase inhibition of steroids. Bioorganic and Medicinal Chemistry, 2016, 24, 2823-2831.	3.0	13
169	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.	5.2	13
170	Pathway involving the N155H mutation in HIV-1 integrase leads to dolutegravir resistance. Journal of Antimicrobial Chemotherapy, 2018, 73, 1158-1166.	3.0	13
171	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. Frontiers in Chemistry, 2018, 6, 130.	3.6	13
172	Molecular Modeling, Synthesis, and Preliminary Biological Evaluation of Glutathione-S-Transferase Inhibitors as Potential Therapeutic Agents. Journal of Medicinal Chemistry, 2005, 48, 6084-6089.	6.4	12
173	Effect of the Human Immunodeficiency Virus Type 1 Reverse Transcriptase Polymorphism Leu-214 on Replication Capacity and Drug Susceptibility. Journal of Virology, 2009, 83, 7434-7439.	3.4	12
174	Simple Choline Esters as Potential Anti-Alzheimer Agents. Current Pharmaceutical Design, 2010, 16, 692-697.	1.9	12
175	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.	3.3	12
176	Microwave assisted synthesis of chiral pyrrolines with biological activity. Tetrahedron: Asymmetry, 2004, 15, 3601-3608.	1.8	11
177	Molecular Recognition of Human Telomeric DNA by Phenanthroline-Based G-Quadruplex Ligands. Open Journal of Medicinal Chemistry, 2013, 03, 41-49.	0.7	11
178	Novel propargylamine-based inhibitors of cholinesterases and monoamine oxidases: Synthesis, biological evaluation and docking study. Bioorganic Chemistry, 2021, 116, 105301.	4.1	11
179	Mediterranean Diet: The Beneficial Effects of Lycopene in Non-Alcoholic Fatty Liver Disease. Journal of Clinical Medicine, 2022, 11, 3477.	2.4	11
180	Enantioselective semi-preparative HPLC of two 2-arylpropionic acids on glycopeptides containing chiral stationary phases. Tetrahedron: Asymmetry, 2002, 13, 69-75.	1.8	10

#	Article	IF	Citations
181	Dependence of DNA Sequence Selectivity and Cell Cytotoxicity on Azinomycin A and B Epoxyamide Stereochemistry. Organic Letters, 2007, 9, 1891-1894.	4.6	10
182	Incomplete APOBEC3G/F Neutralization by HIV-1 Vif Mutants Facilitates the Genetic Evolution from CCR5 to CXCR4 Usage. Antimicrobial Agents and Chemotherapy, 2015, 59, 4870-4881.	3.2	10
183	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. Molecules, 2020, 25, 2174.	3.8	10
184	Realâ€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.	5.0	9
185	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.	5.2	9
186	Mapping Chromone-3-Phenylcarboxamide Pharmacophore: Quid Est Veritas?. Journal of Medicinal Chemistry, 2021, 64, 11169-11182.	6.4	9
187	Peptide Platform as a Powerful Tool in the Fight against COVID-19. Viruses, 2021, 13, 1667.	3.3	9
188	9-Fluorenon-4-carboxamides: synthesis, conformational analysis, anti-HSV-2, and immunomodulatory evaluation. Note II. Arkivoc, 2004, 2004, 334-348.	0.5	9
189	Anti-Multiple Myeloma Potential of Secondary Metabolites from Hibiscus sabdariffaâ€”Part 2. Molecules, 2021, 26, 6596.	3.8	9
190	Molecular modeling and enzymatic studies of the interaction of a choline analogue and acetylcholinesterase. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 2899-2905.	2.2	8
191	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.	2.2	8
192	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, 2205-2209.	3.0	8
193	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.	3.6	8
194	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.	2.8	8
195	Natural Products Extracted from Fungal Species as New Potential Anti-Cancer Drugs: A Structure-Based Drug Repurposing Approach Targeting HDAC7. Molecules, 2020, 25, 5524.	3.8	8
196	4-Oxoquinolines and monoamine oxidase: When tautomerism matters. European Journal of Medicinal Chemistry, 2021, 213, 113183.	5.5	8
197	Identification of Compounds Targeting HuD. Another Brick in the Wall of Neurodegenerative Disease Treatment. Journal of Medicinal Chemistry, 2021, 64, 9989-10000.	6.4	8
198	Computer-based techniques for lead identification and optimization II: Advanced search methods. Physical Sciences Reviews, 2020, 5, .	0.8	8

#	Article	IF	Citations
199	Presynaptic Release-Regulating Alpha2 Autoreceptors: Potential Molecular Target for Ellagic Acid Nutraceutical Properties. Antioxidants, 2021, 10, 1759.	5.1	8
200	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, 2199-2204.	3.0	7
201	Extended Naphthalene Diimides with Donor/Acceptor Hydrogenâ€Bonding Properties Targeting Gâ€Quadruplex Nucleic Acids. European Journal of Organic Chemistry, 2016, 2016, 4824-4833.	2.4	7
202	Structural Modeling of New Polymorphism Clusters of HCV Polymerase Isolated from Directâ€Acting Antiviral NaÃ¯ve Patients: Focus on Dasabuvir and Setrobuvir Binding Affinity. ChemistrySelect, 2018, 3, 6009-6017.	1.5	7
203	Synthesis, Monoamine Oxidase Inhibition and Computational Analysis of Diversely Substituted Nâ€Propargylatedâ€1,3,5â€triazines. ChemistrySelect, 2019, 4, 8334-8337.	1.5	7
204	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. Pharmaceuticals, 2022, 15, 548.	3.8	7
205	Chiral arylpyrrolidinols: preparation and biological profile. Bioorganic and Medicinal Chemistry, 2005, 13, 3117-3126.	3.0	6
206	<scp>TCL</scp>1A interacts with <scp>TP</scp>63 and enhances the survival of Raji Burkitt lymphoma cell line. British Journal of Haematology, 2018, 183, 509-512.	2.5	6
207	New Dihydrothiazole Benzensulfonamides: Looking for Selectivity toward Carbonic Anhydrase Isoforms I, II, IX, and XII. ACS Medicinal Chemistry Letters, 2020, 11, 852-856.	2.8	6
208	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. European Journal of Medicinal Chemistry, 2022, 239, 114507.	5.5	6
209	Synthesis and pharmacological evaluation of new N-methyl-arylpyrrolidinols with analgesic activity. Il Farmaco, 2003, 58, 939-946.	0.9	5
210	Editorial [Hot Topic: The Impact of the G-Quadruplex Conformation in the Development of Novel Therapeutic and Diagnostic Agents Executive (Guest Editor: Stefano Alcaro)]. Current Pharmaceutical Design, 2012, 18, 1865-1866.	1.9	5
211	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, 907-927.	2.3	5
212	In Silico Identification and Biological Evaluation of Antioxidant Food Components Endowed with Human Carbonic Anhydrase IX and XII Inhibition. Antioxidants, 2020, 9, 775.	5.1	5
213	Joining European Scientific Forces to Face Pandemics. Trends in Microbiology, 2021, 29, 92-97.	7.7	5
214	Design, Synthesis, and Evaluation of New Tripeptides as COX-2 Inhibitors. Journal of Amino Acids, 2013, 2013, 1-7.	5.8	4
215	Exploring New Scaffolds for the Dual Inhibition of HIV-1 RT Polymerase and Ribonuclease Associated Functions. Molecules, 2021, 26, 3821.	3.8	4
216	Molecular Modeling and Experimental Evaluation of Non-Chiral Components of Bergamot Essential Oil with Inhibitory Activity against Human Monoamine Oxidases. Molecules, 2022, 27, 2467.	3.8	4

#	Article	IF	Citations
217	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.	2.2	3
218	New resistance mutations to nucleoside reverse transcriptase inhibitors at codon 184 of <scp>HIV</scp>â€1 reverse transcriptase (M184L and M184T). Chemical Biology and Drug Design, 2019, 93, 50-59.	3.2	3
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.	0.9	3
220	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.	3.8	3
221	Conformational search of antisense nucleotides. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 2273-2277.	2.2	2
222	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.	2.0	2
223	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.	1.6	2
224	12. Computer-based techniques for lead identification and optimization I: Basics. , 2020, , 311-332.		2
225	Docking experiments showing similar recognition patterns of paclitaxel when interacting with different macromolecular targets. Il Farmaco, 2003, 58, 691-698.	0.9	1
226	Inhibition of Amine Oxidases Activity by 1-Acetyl-3,5-diphenyl-4,5-dihydro-(1H)-pyrazole Derivatives.. ChemInform, 2003, 34, no.	0.0	1
227	Computational methods applied to the discovery of stem cell factor ligands. Theoretical Chemistry Accounts, 2008, 120, 523-531.	1.4	1
228	Rational Approaches to Anticancer Drug Design/in silico Drug Development. , 0, , 29-46.		1
229	Theoretical and structural studies on mechanism of the Stec reaction. Tetrahedron, 2012, 68, 5554-5563.	1.9	1
230	G-quadruplex Structure Prediction and integration in the GenData2020 data model. , 2016, , .		1
231	Disrupting Proteinâ€“Protein Interfaces Using GRID Molecular Interaction Fields. , 2013, , 61-82.		1
232	Conformational search of antisense nucleotides. Part 2. Il Farmaco, 2004, 59, 169-173.	0.9	0
233	Inhibition of Monoamine Oxidases by Coumarin-3-acyl Derivatives: Biological Activity and Computational Study.. ChemInform, 2004, 35, no.	0.0	0
234	Microwave-Assisted Synthesis of Chiral Pyrrolines with Biological Activity.. ChemInform, 2005, 36, no.	0.0	0

#	Article	IF	Citations
235	Molecular Modeling of DNA Cross-Linking Analogues Based on the Azinomycin Scaffold.. ChemInform, 2005, 36, no.	0.0	0
236	Towards the Modulation of RNA-Binding Proteins: New Compounds Targeting Protein HuR. Proceedings (mdpi), 2019, 22, .	0.2	0
237	In Silico Food-Drug Interaction: A Case Study of Eluxadoline and Fatty Meal. International Journal of Molecular Sciences, 2020, 21, 9127.	4.1	0
238	13. Computer-based techniques for lead identification and optimization II: Advanced search methods. , 2020, , 333-360.		0
239	Abstract 4796: EG-011 is a novel small molecule within vitroandin vivoanti-tumor activity against lymphoma. , 2019, , .		0
240	Abstract B122: The CD98hc oncoprotein as a target of new anticancer therapy. , 2019, , .		0
241	Identification of SET/EED dual binders as innovative PRC2 inhibitors. Future Medicinal Chemistry, 2022, , .	2.3	0
242	Abstract 4796: EG-011 is a novel small molecule within vitroandin vivoanti-tumor activity against lymphoma. , 2019, , .		0