Orazio Nicolotti

List of Publications by Year
in descending order

144	4,421	100601	162838
papers	citations	38 h-index	57 g-index

146	146	146	5617
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Getting Insights into Structural and Energetic Properties of Reciprocal Peptideâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2022, 62, 1113-1125.	2.5	8
2	Praseodymium trivalent ion is an effective inhibitor of mitochondrial basic amino acids and carnitine/acylcarnitine carriers. Biochimica Et Biophysica Acta - Bioenergetics, 2022, 1863, 148557.	0.5	1
3	Rational Discovery of Antiviral Whey Protein-Derived Small Peptides Targeting the SARS-CoV-2 Main Protease. Biomedicines, 2022, 10, 1067.	1.4	7
4	PLATO: A Predictive Drug Discovery Web Platform for Efficient Target Fishing and Bioactivity Profiling of Small Molecules. International Journal of Molecular Sciences, 2022, 23, 5245.	1.8	15
5	Development of a Novel Class of Pyridazinone Derivatives as Selective MAO-B Inhibitors. Molecules, 2022, 27, 3801.	1.7	10
6	Assessing the Role of a Malonamide Linker in the Design of Potent Dual Inhibitors of Factor Xa and Cholinesterases. Molecules, 2022, 27, 4269.	1.7	7
7	Design, synthesis and biological evaluation of imidazole and triazole-based carbamates as novel aromatase inhibitors. European Journal of Medicinal Chemistry, 2021, 211, 113115.	2.6	28
8	Piperazine-substituted chalcones: a new class of MAO-B, AChE, and BACE-1 inhibitors for the treatment of neurological disorders. Environmental Science and Pollution Research, 2021, 28, 38855-38866.	2.7	26
9	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
10	Trimethoxylated Halogenated Chalcones as Dual Inhibitors of MAO-B and BACE-1 for the Treatment of Neurodegenerative Disorders. Pharmaceutics, 2021, 13, 850.	2.0	22
11	Synthesis of Nâ€²-(4-/3-/2-/Non-substituted benzylidene)-4-[(4-methylphenyl)sulfonyloxy] Benzohydrazides and Evaluation of Their Inhibitory Activities against Monoamine Oxidases and Î²-Secretase. Applied Sciences (Switzerland), 2021, 11, 5830.	1.3	4
12	Current Progress in Quinazoline Derivatives as Acetylcholinesterase and Monoamine Oxidase Inhibitors. ChemistrySelect, 2021, 6, 7162-7182.	0.7	12
13	Anticancer potential of novel Î±,Î²-unsaturated Î³-lactam derivatives targeting the PI3K/AKT signaling pathway. Biochemical Pharmacology, 2021, 190, 114659.	2.0	8
14	The Interaction of Hemin, a Porphyrin Derivative, with the Purified Rat Brain 2-Oxoglutarate Carrier. Biomolecules, 2021, 11, 1175.	1.8	3
15	Synthesis and biological evaluation of 3,5â€diarylâ€pyrazole derivatives as potential antiprostate cancer agents. Archiv Der Pharmazie, 2021, 354, e2100225.	2.1	4
16	First-in-Class Isonipecotamide-Based Thrombin and Cholinesterase Dual Inhibitors with Potential for Alzheimer Disease. Molecules, 2021, 26, 5208.	1.7	9
17	Design, Synthesis and Biological Evaluation of Aromatase Inhibitors Based on Sulfonates and Sulfonamides of Resveratrol. Pharmaceuticals, 2021, 14, 984.	1.7	16
18	Quantitative Polypharmacology Profiling Based on a Multifingerprint Similarity Predictive Approach. Journal of Chemical Information and Modeling, 2021, 61, 4868-4876.	2.5	18

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19	Synthesis, structure-activity relationships and molecular docking studies of phenyldiazenyl sulfonamides as aromatase inhibitors. European Journal of Medicinal Chemistry, 2021, 224, 113737.	2.6	14
20	Homobivalent Lamellarin-Like Schiff Bases: In Vitro Evaluation of Their Cancer Cell Cytotoxicity and Multitargeting Anti-Alzheimerâ€™s Disease Potential. Molecules, 2021, 26, 359.	1.7	7
21	Away from Flatness: Unprecedented Nitrogen-Bridged Cyclopenta[a]indene Derivatives as Novel Anti-Alzheimer Multitarget Agents. ACS Chemical Neuroscience, 2021, 12, 340-353.	1.7	8
22	Morpholine-based chalcones as dual-acting monoamine oxidase-B and acetylcholinesterase inhibitors: synthesis and biochemical investigations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 188-197.	2.5	24
23	Selected Class of Enamides Bearing Nitro Functionality as Dual-Acting with Highly Selective Monoamine Oxidase-B and BACE1 Inhibitors. Molecules, 2021, 26, 6004.	1.7	7
24	Halogenated Coumarinâ€“Chalcones as Multifunctional Monoamine Oxidase-B and Butyrylcholinesterase Inhibitors. ACS Omega, 2021, 6, 28182-28193.	1.6	26
25	17Î²-Hydroxysteroid Dehydrogenase Type 1 Inhibition: A Potential Treatment Option for Non-Small Cell Lung Cancer. ACS Medicinal Chemistry Letters, 2021, 12, 1920-1924.	1.3	3
26	Design and synthesis of fluorescent ligands for the detection of cannabinoid type 2 receptor (CB2R). European Journal of Medicinal Chemistry, 2020, 188, 112037.	2.6	14
27	Structure-Based Identification and Design of Angiotensin Converting Enzyme-Inhibitory Peptides from Whey Proteins. Journal of Agricultural and Food Chemistry, 2020, 68, 541-548.	2.4	18
28	Exploring the role of elongation Factor-Like 1 (EFL1) in Shwachman-Diamond syndrome through molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5219-5229.	2.0	3
29	Human ether-Ã-go-go-related potassium channel: exploring SAR to improve drug design. Drug Discovery Today, 2020, 25, 344-366.	3.2	33
30	Selected 1,3â€Benzodioxineâ€Containing Chalcones as Multipotent Oxidase and Acetylcholinesterase Inhibitors. ChemMedChem, 2020, 15, 2257-2263.	1.6	11
31	(Hetero-)(arylidene)arylhydrazides as Multitarget-Directed Monoamine Oxidase Inhibitors. ACS Combinatorial Science, 2020, 22, 592-599.	3.8	5
32	Design, Synthesis, and Biological Evaluation of Pyridazinones Containing the (2-Fluorophenyl) Piperazine Moiety as Selective MAO-B Inhibitors. Molecules, 2020, 25, 5371.	1.7	11
33	Design, synthesis and biological evaluation of 3,5-diaryl isoxazole derivatives as potential anticancer agents. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127427.	1.0	13
34	De Novo Drug Design of Targeted Chemical Libraries Based on Artificial Intelligence and Pair-Based Multiobjective Optimization. Journal of Chemical Information and Modeling, 2020, 60, 4582-4593.	2.5	55
35	Bcr-Abl Allosteric Inhibitors: Where We Are and Where We Are Going to. Molecules, 2020, 25, 4210.	1.7	13
36	Pharmacophore Modeling and 3D-QSAR Study of Indole and Isatin Derivatives as Antiamyloidogenic Agents Targeting Alzheimerâ€™s Disease. Molecules, 2020, 25, 5773.	1.7	9

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37	Design of enamides as new selective monoamine oxidase-B inhibitors. Journal of Pharmacy and Pharmacology, 2020, 72, 916-926.	1.2	18
38	A New Potent and Selective Monoamine Oxidaseâ€B Inhibitor with Extended Conjugation in a Chalcone Framework: 1â€[4â€(Morpholinâ€4â€yl)phenyl]â€5â€phenylpentaâ€2,4â€dienâ€1â€one. ChemMedChem, 2020, 15, 1629-1633.	1.6	11
39	Bcr-Abl Tyrosine Kinase Inhibitors in the Treatment of Pediatric CML. International Journal of Molecular Sciences, 2020, 21, 4469.	1.8	19
40	Chiral Separation, X-ray Structure, and Biological Evaluation of a Potent and Reversible Dual Binding Site AChE Inhibitor. ACS Medicinal Chemistry Letters, 2020, 11, 869-876.	1.3	7
41	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
42	Development of a Rapid Mass Spectrometric Determination of AMP and Cyclic AMP for PDE3 Activity Study: Application and Computational Analysis for Evaluating the Effect of a Novel 2-oxo-1,2-dihydropyridine-3-carbonitrile Derivative as PDE-3 Inhibitor. Molecules, 2020, 25, 1817.	1.7	3
43	Novel Class of Chalcone Oxime Ethers as Potent Monoamine Oxidase-B and Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 2356.	1.7	35
44	Strategies of Virtual Screening in Medicinal Chemistry. , 2020, , 194-225.		1
45	Early Prediction of Ecotoxicological Side Effects of Pharmaceutical Impurities Based on Open-Source Non-testing Approaches. Methods in Pharmacology and Toxicology, 2020, , 235-269.	0.1	1
46	Design, synthesis and biological evaluation of oxygenated chalcones as potent and selective MAO-B inhibitors. Bioorganic Chemistry, 2019, 93, 103335.	2.0	49
47	Accelerating Drug Discovery by Early Protein Drug Target Prediction Based on a Multi-Fingerprint Similarity Search â€. Molecules, 2019, 24, 2233.	1.7	34
48	Ethoxylated Head of Chalcones as a New Class of Multiâ€Targeted MAO Inhibitors. ChemistrySelect, 2019, 4, 6614-6619.	0.7	22
49	Prediction of Acute Oral Systemic Toxicity Using a Multifingerprint Similarity Approach. Toxicological Sciences, 2019, 167, 484-495.	1.4	26
50	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel proteinâ€“protein interaction inhibitors. Drug Discovery Today, 2019, 24, 551-559.	3.2	20
51	A New Approach for Drug Target and Bioactivity Prediction: The Multifingerprint Similarity Search Algorithm (MuSSeL). Journal of Chemical Information and Modeling, 2019, 59, 586-596.	2.5	56
52	Ethyl Acetohydroxamate Incorporated Chalcones: Unveiling a Novel Class of Chalcones for Multitarget Monoamine Oxidase-B Inhibitors Against Alzheimerâ€™s Disease. CNS and Neurological Disorders - Drug Targets, 2019, 18, 643-654.	0.8	27
53	Automated identification of structurally heterogeneous and patentable antiproliferative hits as potential tubulin inhibitors. Chemical Biology and Drug Design, 2018, 92, 1161-1170.	1.5	3
54	Strategies of Virtual Screening in Medicinal Chemistry. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 134-160.	1.1	12

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55	Molecular Docking for Predictive Toxicology. Methods in Molecular Biology, 2018, 1800, 181-197.	0.4	11
56	Multitarget Drug Design for Neurodegenerative Diseases. Methods in Pharmacology and Toxicology, 2018, , 93-105.	0.1	2
57	Nitazoxanide inhibits paramyxovirus replication by targeting the Fusion protein folding: role of glycoprotein-specific thiol oxidoreductase ERp57. Scientific Reports, 2018, 8, 10425.	1.6	54
58	Design, Synthesis, and Biological Evaluation of Tetrahydroâ€Î²â€carboline Derivatives as Selective Subâ€Nanomolar Gelatinase Inhibitors. ChemMedChem, 2018, 13, 1343-1352.	1.6	4
59	A rational approach to elucidate human monoamine oxidase molecular selectivity. European Journal of Pharmaceutical Sciences, 2017, 101, 90-99.	1.9	29
60	Comparative molecular dynamics study of neuromyelitis optica-immunoglobulin G binding to aquaporin-4 extracellular domains. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1326-1334.	1.4	9
61	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	3.2	28
62	Supramolecular Anchoring of NCNâ€Pincer Palladium Complexes into a Î²â€Barrel Protein Host: Molecularâ€Docking and Reactivity Insights. European Journal of Inorganic Chemistry, 2017, 2017, 3622-3634.	1.0	11
63	Pharmacovigilance database search discloses ClCâ€K channels as a novel target of the AT₁ receptor blockers valsartan and olmesartan. British Journal of Pharmacology, 2017, 174, 1972-1983.	2.7	16
64	Predictive Structure-Based Toxicology Approaches To Assess the Androgenic Potential of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 2874-2884.	2.5	24
65	Ligand efficiency metrics in drug discovery: the pros and cons from a practical perspective. Expert Opinion on Drug Discovery, 2017, 12, 1087-1104.	2.5	75
66	Novel chemotypes targeting tubulin at the colchicine binding site and unbiasing P-glycoprotein. European Journal of Medicinal Chemistry, 2017, 139, 792-803.	2.6	37
67	Mannich base approach to 5-methoxyisatin 3-(4-isopropylphenyl)hydrazone: A water-soluble prodrug for a multitarget inhibition of cholinesterases, beta-amyloid fibrillization and oligomer-induced cytotoxicity. European Journal of Pharmaceutical Sciences, 2017, 109, 381-388.	1.9	33
68	A novel KCNA1 mutation in a patient with paroxysmal ataxia, myokymia, painful contractures and metabolic dysfunctions. Molecular and Cellular Neurosciences, 2017, 83, 6-12.	1.0	23
69	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
70	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
71	Applicability Domain for QSAR Models. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 45-63.	1.1	130
72	Human Aquaporin-4 and Molecular Modeling: Historical Perspective and View to the Future. International Journal of Molecular Sciences, 2016, 17, 1119.	1.8	12

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73	Searching for Multi-Targeting Neurotherapeutics against Alzheimerâ€™s: Discovery of Potent AChE-MAO B Inhibitors through the Decoration of the 2H-Chromen-2-one Structural Motif. Molecules, 2016, 21, 362.	1.7	43
74	Design, synthesis, biological evaluation, <scp>NMR</scp> and <scp>DFT</scp> studies of structurally simplified trimethoxy benzamides as selective Pâ€glycoprotein inhibitors: the role of molecular flatness. Chemical Biology and Drug Design, 2016, 88, 820-831.	1.5	3
75	Kidney CLC-K chloride channels inhibitors. Journal of Hypertension, 2016, 34, 981-992.	0.3	22
76	Mind the Gap! A Journey towards Computational Toxicology. Molecular Informatics, 2016, 35, 294-308.	1.4	25
77	A Round Trip from Medicinal Chemistry to Predictive Toxicology. Methods in Molecular Biology, 2016, 1425, 461-473.	0.4	0
78	Multidisciplinary study of a new CICâ€1 mutation causing myotonia congenita: a paradigm to understand and treat ion channelopathies. FASEB Journal, 2016, 30, 3285-3295.	0.2	24
79	Exploring Basic Tail Modifications of Coumarin-Based Dual Acetylcholinesterase-Monoamine Oxidase B Inhibitors: Identification of Water-Soluble, Brain-Permeant Neuroprotective Multitarget Agents. Journal of Medicinal Chemistry, 2016, 59, 6791-6806.	2.9	76
80	Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data. Chemistry Central Journal, 2015, 9, 62.	2.6	35
81	Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). Environmental Research, 2015, 137, 398-409.	3.7	42
82	Challenging AQP4 druggability for NMO-IgG antibody binding using molecular dynamics and molecular interaction fields. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1462-1471.	1.4	25
83	Structure-Based Design and Optimization of Multitarget-Directed 2H-Chromen-2-one Derivatives as Potent Inhibitors of Monoamine Oxidase B and Cholinesterases. Journal of Medicinal Chemistry, 2015, 58, 5561-5578.	2.9	89
84	Studies on the antiplatelet and antithrombotic profile of anti-inflammatory coumarin derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 925-933.	2.5	33
85	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. Future Medicinal Chemistry, 2015, 7, 1921-1936.	1.1	30
86	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. Journal of Chemical Information and Modeling, 2015, 55, 2094-2110.	2.5	20
87	Effects of Different Self-Assembled Monolayers on Thin-Film Morphology: A Combined DFT/MD Simulation Protocol. Langmuir, 2015, 31, 10693-10701.	1.6	15
88	Discovery of new 7-substituted-4-imidazolylmethyl coumarins and 4â€²-substituted-2-imidazolyl acetophenones open analogues as potent and selective inhibitors of steroid-11Î²-hydroxylase. European Journal of Medicinal Chemistry, 2015, 89, 106-114.	2.6	22
89	In silico design of novel 2H-chromen-2-one derivatives as potent and selective MAO-B inhibitors. European Journal of Medicinal Chemistry, 2015, 89, 98-105.	2.6	55
90	QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585.	0.2	10

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91	A generalizable definition of chemical similarity for read-across. Journal of Cheminformatics, 2014, 6, 39.	2.8	75
92	Building up QSAR model for toxicity of psychotropic drugs by the Monte Carlo method. Structural Chemistry, 2014, 25, 1067-1073.	1.0	7
93	Identification of a Point Mutation Impairing the Binding between Aquaporin-4 and Neuromyelitis Optica Autoantibodies. Journal of Biological Chemistry, 2014, 289, 30578-30589.	1.6	26
94	REACH and in silico methods: an attractive opportunity for medicinal chemists. Drug Discovery Today, 2014, 19, 1757-1768.	3.2	70
95	Trimethoxybenzanilide-Based P-Glycoprotein Modulators: An Interesting Case of Lipophilicity Tuning by Intramolecular Hydrogen Bonding. Journal of Medicinal Chemistry, 2014, 57, 6403-6418.	2.9	23
96	A new gating site in human aquaporin-4: Insights from molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 3052-3060.	1.4	46
97	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	3.2	140
98	An alternative QSAR-based approach for predicting the bioconcentration factor for regulatory purposes. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 23-36.	0.9	41
99	A k-NN algorithm for predicting oral sub-chronic toxicity in the rat. ALTEX: Alternatives To Animal Experimentation, 2014, 31, 423-432.	0.9	13
100	Discovery, Biological Evaluation, and Structureâ€“Activity and â˜Selectivity Relationships of 6â€²-Substituted (E)-2-(Benzofuran-3(2H)-ylidene)-N-methylacetamides, a Novel Class of Potent and Selective Monoamine Oxidase Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 2651-2664.	2.9	56
101	Multivariate analysis of quaternary carbamazepineâ€“saccharin mixtures by X-ray diffraction and infrared spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2013, 78-79, 269-279.	1.4	34
102	Fine molecular tuning at position 4 of 2H-chromen-2-one derivatives in the search of potent and selective monoamine oxidase B inhibitors. European Journal of Medicinal Chemistry, 2013, 70, 723-739.	2.6	41
103	Design, synthesis and biological evaluation of coumarin alkylamines as potent and selective dual binding site inhibitors of acetylcholinesterase. Bioorganic and Medicinal Chemistry, 2013, 21, 146-152.	1.4	80
104	Integration of QSAR models for bioconcentration suitable for REACH. Science of the Total Environment, 2013, 456-457, 325-332.	3.9	27
105	Computational methods for the design of potent aromatase inhibitors. Expert Opinion on Drug Discovery, 2013, 8, 395-409.	2.5	28
106	Potent Galloyl-Based Selective Modulators Targeting Multidrug Resistance Associated Protein 1 and P-glycoprotein. Journal of Medicinal Chemistry, 2012, 55, 424-436.	2.9	34
107	Design, synthesis and biological evaluation of 5-hydroxy, 5-substituted-pyrimidine-2,4,6-triones as potent inhibitors of gelatinases MMP-2 and MMP-9. European Journal of Medicinal Chemistry, 2012, 58, 368-376.	2.6	42
108	Inactivation of the glutamine/amino acid transporter ASCT2 by 1,2,3-dithiazoles: proteoliposomes as a tool to gain insights in the molecular mechanism of action and of antitumor activity. Toxicology and Applied Pharmacology, 2012, 265, 93-102.	1.3	64

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109	A Chemocentric Approach to the Identification of Cancer Targets. PLoS ONE, 2012, 7, e35582.	1.1	19
110	Toward a fragment-based approach to MMPs inhibitors: an expedite and efficient synthesis of N-hydroxylactams. Tetrahedron Letters, 2012, 53, 4114-4116.	0.7	8
111	Design, Synthesis, and Biological Evaluation of Imidazolyl Derivatives of 4,7-Disubstituted Coumarins as Aromatase Inhibitors Selective over 17-Î±-Hydroxylase/C17â^'20 Lyase. Journal of Medicinal Chemistry, 2011, 54, 1613-1625.	2.9	78
112	D184E mutation in aquaporin-4 gene impairs water permeability and links to deafness. Neuroscience, 2011, 197, 80-88.	1.1	31
113	Strategies of multi-objective optimization in drug discovery and development. Expert Opinion on Drug Discovery, 2011, 6, 871-884.	2.5	31
114	Insights into the Complex Formed by Matrix Metalloproteinase-2 and Alloxan Inhibitors: Molecular Dynamics Simulations and Free Energy Calculations. PLoS ONE, 2011, 6, e25597.	1.1	12
115	Biarylmethoxy isonipecotanilides as potent and selective inhibitors of blood coagulation factor Xa. European Journal of Pharmaceutical Sciences, 2011, 42, 180-191.	1.9	16
116	Homodimeric Bis-Quaternary Heterocyclic Ammonium Salts as Potent Acetyl- and Butyrylcholinesterase Inhibitors: A Systematic Investigation of the Influence of Linker and Cationic Heads over Affinity and Selectivity. Journal of Medicinal Chemistry, 2011, 54, 2627-2645.	2.9	42
117	Quinolizidinyl derivatives of bi- and tricyclic systems as potent inhibitors of acetyl- and butyrylcholinesterase with potential in Alzheimerâ€™s disease. European Journal of Medicinal Chemistry, 2011, 46, 2170-2184.	2.6	56
118	Discovery of a Potent and Selective Heteroâ€Bivalent AChE Inhibitor via Bioisosteric Replacement. Molecular Informatics, 2011, 30, 133-136.	1.4	8
119	Design, synthesis and pharmacobiological evaluation of novel acrylic acid derivatives acting as lipoxygenase and cyclooxygenase-1 inhibitors with antioxidant and anti-inflammatory activities. European Journal of Medicinal Chemistry, 2011, 46, 191-200.	2.6	64
120	BCR-ABL Inhibitors in Chronic Myeloid Leukemia: Process Chemistry and Biochemical Profile. Current Medicinal Chemistry, 2011, 18, 2943-2959.	1.2	12
121	Screening of benzamidine-based thrombin inhibitors via a linear interaction energy in continuum electrostatics model. Journal of Computer-Aided Molecular Design, 2010, 24, 117-129.	1.3	7
122	Analysis of X-ray Structures of Matrix Metalloproteinases via Chaotic Map Clustering. BMC Bioinformatics, 2010, 11, 500.	1.2	10
123	Design, Synthesis, and Biological Evaluation of Coumarin Derivatives Tethered to an Edrophoniumâ€like Fragment as Highly Potent and Selective Dual Binding Site Acetylcholinesterase Inhibitors. ChemMedChem, 2010, 5, 1616-1630.	1.6	58
124	Solid phase synthesis of a molecular library of pyrimidines, pyrazoles, and isoxazoles with biological potential. Tetrahedron Letters, 2010, 51, 1702-1705.	0.7	18
125	Investigating Enzyme Selectivity and Hit Enrichment by Automatically Interfacing Ligandâ€•and Structureâ€Based Molecular Design. QSAR and Combinatorial Science, 2009, 28, 861-864.	1.5	2
126	1,3-Dialkyl-8-N-substituted benzyloxycarbonylamino-9-deazaxanthines as potent adenosine receptor ligands: Design, synthesis, structureâ€“affinity and structureâ€“selectivity relationships. Bioorganic and Medicinal Chemistry, 2009, 17, 3618-3629.	1.4	12

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127	Improving Quantitative Structureâ^'Activity Relationships through Multiobjective Optimization. Journal of Chemical Information and Modeling, 2009, 49, 2290-2302.	2.5	48
128	Discovery of a Novel Class of Potent Coumarin Monoamine Oxidase B Inhibitors: Development and Biopharmacological Profiling of 7-[(3-Chlorobenzyl)oxy]-4-[(methylamino)methyl]-2H-chromen-2-one Methanesulfonate (NW-1772) as a Highly Potent, Selective, Reversible, and Orally Active Monoamine Oxidase B Inhibitor. Journal of Medicinal Chemistry, 2009, 52, 6685-6706.	2.9	100
129	Homo- and hetero-bivalent edrophonium-like ammonium salts as highly potent, dual binding site AChE inhibitors. Bioorganic and Medicinal Chemistry, 2008, 16, 7450-7456.	1.4	60
130	1,3-Dialkyl-8-(hetero)aryl-9-OH-9-deazaxanthines as potent A2B adenosine receptor antagonists: Design, synthesis, structureâ€"affinity and structureâ€"selectivity relationships. Bioorganic and Medicinal Chemistry, 2008, 16, 9780-9789.	1.4	24
131	An Integrated Approach to Ligand- and Structure-Based Drug Design: Development and Application to a Series of Serine Protease Inhibitors. Journal of Chemical Information and Modeling, 2008, 48, 1211-1226.	2.5	47
132	Screening of Matrix Metalloproteinases Available from the Protein Data Bank:â€‰ Insights into Biological Functions, Domain Organization, and Zinc Binding Groups. Journal of Chemical Information and Modeling, 2007, 47, 2439-2448.	2.5	41
133	Solid-Phase Synthesis and Insights into Structureâ^'Activity Relationships of Safinamide Analogues as Potent and Selective Inhibitors of Type B Monoamine Oxidase. Journal of Medicinal Chemistry, 2007, 50, 4909-4916.	2.9	49
134	Structural Insights into Monoamine Oxidase Inhibitory Potency and Selectivity of 7-Substituted Coumarins from Ligand- and Target-Based Approaches. Journal of Medicinal Chemistry, 2006, 49, 4912-4925.	2.9	104
135	QSAR and QSPR Studies of a Highly Structured Physicochemical Domain. Journal of Chemical Information and Modeling, 2006, 46, 264-276.	2.5	56
136	8-Substituted-9-deazaxanthines as Adenosine Receptor Ligands: Design, Synthesis and Structure-Affinity Relationships at A2B.. ChemInform, 2005, 36, no.	0.1	0
137	Alpha2-Adrenergic Receptors in Intestinal Epithelial Cells: Mechanisms of Signaling, Role, and Regulation. Medicinal Chemistry Research, 2004, 13, 170-189.	1.1	2
138	8-Substituted-9-deazaxanthines as adenosine receptor ligands: design, synthesis and structure-affinity relationships at A2B. European Journal of Medicinal Chemistry, 2004, 39, 879-887.	2.6	26
139	Neuronal Nicotinic Acetylcholine Receptor Agonists: Pharmacophores, Evolutionary QSAR and 3D-QSAR models. Current Topics in Medicinal Chemistry, 2004, 4, 335-360.	1.0	17
140	Multiobjective Optimization in Quantitative Structureâ^'Activity Relationships:Â Deriving Accurate and Interpretable QSARs. Journal of Medicinal Chemistry, 2002, 45, 5069-5080.	2.9	96
141	Cytisine derivatives as high affinity nAChR ligands: synthesis and comparative molecular field analysis. Il Farmaco, 2002, 57, 469-478.	0.9	44
142	Title is missing!. Journal of Computer-Aided Molecular Design, 2001, 15, 1153-1153.	1.3	1
143	Neuronal nicotinic receptor agonists: a multi-approach development of the pharmacophore. Journal of Computer-Aided Molecular Design, 2001, 15, 859-872.	1.3	20
144	Evaluation of reactant-based and product-based approaches to the design of combinatorial libraries. , 2000, 20, 265-287.		25