Adriano Martinelli

List of Publications by Year in descending order

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110 papers 3,247 citations

34 h-index 50 g-index

117 all docs

117 docs citations

117 times ranked

4093 citing authors

#	Article	IF	CITATIONS
1	From Anti-infective Agents to Cancer Therapy: A Drug Repositioning Study Revealed a New Use for Nitrofuran Derivatives. Medicinal Chemistry, 2022, 18, 249-259.	1.5	2
2	VenomPred: A Machine Learning Based Platform for Molecular Toxicity Predictions. International Journal of Molecular Sciences, 2022, 23, 2105.	4.1	18
3	Development of a cheminformatics platform for selectivity analyses of carbonic anhydrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 365-371.	5.2	11
4	Extensive Reliability Evaluation of Docking-Based Target-Fishing Strategies. International Journal of Molecular Sciences, 2019, 20, 1023.	4.1	20
5	Discovery of 1,5-Diphenylpyrazole-3-Carboxamide Derivatives as Potent, Reversible, and Selective Monoacylglycerol Lipase (MAGL) Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 1340-1354.	6.4	43
6	Rational Development of MAGL Inhibitors. Methods in Molecular Biology, 2018, 1824, 335-346.	0.9	2
7	Development of a Fingerprint-Based Scoring Function for the Prediction of the Binding Mode of Carbonic Anhydrase II Inhibitors. International Journal of Molecular Sciences, 2018, 19, 1851.	4.1	12
8	Discovery of long-chain salicylketoxime derivatives as monoacylglycerol lipase (MAGL) inhibitors. European Journal of Medicinal Chemistry, 2018, 157, 817-836.	5 . 5	30
9	Identification of Lactate Dehydrogenase 5 Inhibitors using Pharmacophore- Driven Consensus Docking. Current Bioactive Compounds, 2018, 14, 197-204.	0.5	5
10	Identification of Transthyretin Fibril Formation Inhibitors Using Structureâ€Based Virtual Screening. ChemMedChem, 2017, 12, 1327-1334.	3.2	6
11	Development of terphenyl-2-methyloxazol-5(4 <i>H</i>)-one derivatives as selective reversible MAGL inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1240-1252.	5.2	27
12	A Virtual Screening Study for Lactate Dehydrogenase 5 Inhibitors by Using a Pharmacophoreâ€based Approach. Molecular Informatics, 2016, 35, 434-439.	2.5	18
13	Targeting Different Transthyretin Binding Sites with Unusual Natural Compounds. ChemMedChem, 2016, 11, 1865-1874.	3.2	16
14	Structural Optimization of 4-Chlorobenzoylpiperidine Derivatives for the Development of Potent, Reversible, and Selective Monoacylglycerol Lipase (MAGL) Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 10299-10314.	6.4	42
15	Reliability analysis and optimization of the consensus docking approach for the development of virtual screening studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 167-173.	5.2	63
16	4-Aryliden-2-methyloxazol-5(4 <i>H</i>)-one as a new scaffold for selective reversible MACL inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 137-146.	5.2	21
17	Identification of a new STAT3 dimerization inhibitor through a pharmacophore-based virtual screening approach. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1011-1017.	5.2	33
18	Development and Validation of a Docking-Based Virtual Screening Platform for the Identification of New Lactate Dehydrogenase Inhibitors. Molecules, 2015, 20, 8772-8790.	3.8	22

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19	Pyrazole phenylcyclohexylcarbamates as inhibitors of human fatty acid amide hydrolases (FAAH). European Journal of Medicinal Chemistry, 2015, 97, 289-305.	5.5	17
20	Highly Selective Salicylketoxime-Based Estrogen Receptor \hat{l}^2 Agonists Display Antiproliferative Activities in a Glioma Model. Journal of Medicinal Chemistry, 2015, 58, 1184-1194.	6.4	22
21	Synthesis and biological evaluation of non-glucose glycoconjugated N-hydroyxindole class LDH inhibitors as anticancer agents. RSC Advances, 2015, 5, 19944-19954.	3.6	19
22	Application of a FLAP-Consensus Docking Mixed Strategy for the Identification of New Fatty Acid Amide Hydrolase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 667-675.	5.4	25
23	Phenylpropanoids and flavonoids from Phlomis kurdica as inhibitors of human lactate dehydrogenase. Phytochemistry, 2015, 116, 262-268.	2.9	40
24	$\langle i \rangle N \langle i \rangle - \langle i \rangle O \langle i \rangle$ -Isopropyl Sulfonamido-Based Hydroxamates as Matrix Metalloproteinase Inhibitors: Hit Selection and in Vivo Antiangiogenic Activity. Journal of Medicinal Chemistry, 2015, 58, 7224-7240.	6.4	54
25	Receptor-based virtual screening evaluation for the identification of estrogen receptor b>βligands. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 662-670.	5.2	18
26	Identification and characterization of a new reversible MAGL inhibitor. Bioorganic and Medicinal Chemistry, 2014, 22, 3285-3291.	3.0	43
27	Extensive Consensus Docking Evaluation for Ligand Pose Prediction and Virtual Screening Studies. Journal of Chemical Information and Modeling, 2014, 54, 2980-2986.	5.4	89
28	Molecular Modeling of Adenosine Receptors. Methods in Enzymology, 2013, 522, 37-59.	1.0	5
29	Identification of New Fyn Kinase Inhibitors Using a FLAP-Based Approach. Journal of Chemical Information and Modeling, 2013, 53, 2538-2547.	5.4	24
30	Immune-Modulation and Properties of Absorption and Blood Brain Barrier Permeability of 1,8-Naphthyridine Derivatives. Journal of NeuroImmune Pharmacology, 2013, 8, 1077-1086.	4.1	13
31	Assessing the differential action on cancer cells of LDH-A inhibitors based on the N-hydroxyindole-2-carboxylate (NHI) and malonic (Mal) scaffolds. Organic and Biomolecular Chemistry, 2013, 11, 6588.	2.8	44
32	Oxime-based inhibitors of glucose transporter 1 displaying antiproliferative effects in cancer cells. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6923-6927.	2.2	42
33	Salicylaldoxime derivatives as new leads for the development of carbonic anhydrase inhibitors. Bioorganic and Medicinal Chemistry, 2013, 21, 1511-1515.	3.0	12
34	Dual Targeting of the Warburg Effect with a Glucoseâ€Conjugated Lactate Dehydrogenase Inhibitor. ChemBioChem, 2013, 14, 2263-2267.	2.6	43
35	Computational Studies on Translocator Protein (TSPO) and its Ligands. Current Topics in Medicinal Chemistry, 2012, 12, 352-359.	2.1	8
36	Rational design, synthesis and anti-proliferative properties of new CB2 selective cannabinoid receptor ligands: An investigation of the 1,8-naphthyridin-2(1H)-one scaffold. European Journal of Medicinal Chemistry, 2012, 52, 284-294.	5.5	50

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37	Triazole-substituted N-hydroxyindol-2-carboxylates as inhibitors of isoform 5 of human lactate dehydrogenase (hLDH5). MedChemComm, 2011, 2, 638.	3.4	22
38	Novel 1-Hydroxypiperazine-2,6-diones as New Leads in the Inhibition of Metalloproteinases. Journal of Medicinal Chemistry, 2011, 54, 8289-8298.	6.4	16
39	Discovery of <i>N</i> -Hydroxyindole-Based Inhibitors of Human Lactate Dehydrogenase Isoform A (LDH-A) as Starvation Agents against Cancer Cells. Journal of Medicinal Chemistry, 2011, 54, 1599-1612.	6.4	195
40	Substituted pyrazolo[3,4-b]pyridines as human A1 adenosine antagonists: Developments in understanding the receptor stereoselectivity. Organic and Biomolecular Chemistry, 2011, 9, 4448.	2.8	19
41	Novel Folate-Hydroxamate Based Antimetabolites: Synthesis and Biological Evaluation. Medicinal Chemistry, 2011, 7, 265-274.	1.5	8
42	N-Hydroxyindole-based inhibitors of lactate dehydrogenase against cancer cell proliferation. European Journal of Medicinal Chemistry, 2011, 46, 5398-5407.	5 . 5	64
43	Synthesis of sulfonamide-containing N-hydroxyindole-2-carboxylates as inhibitors of human lactate dehydrogenase-isoform 5. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7331-7336.	2.2	26
44	Selective and potent agonists for estrogen receptor beta derived from molecular refinements of salicylaldoximes. European Journal of Medicinal Chemistry, 2011, 46, 2453-2462.	5 . 5	25
45	Protein Kinase Homology Models: Recent Developments and Results. Current Medicinal Chemistry, 2011, 18, 2848-2853.	2.4	9
46	Editorial [Hot topic: Adenosine Receptor Ligands: Where Are We, and Where Are We Going? (Guest) Tj ETQq0 0 941-941.	0 rgBT /Ον 2.1	verlock 10 Tf 0
47	Editorial [Hot topic: Adenosine Receptor Ligands: Where Are We, and Where Are We Going? (Guest) Tj ETQq1 1 859-859.	0.784314 2.1	rgBT /Overlo O
48	Spirotetrahydronaphthalene analogues of sympathomimetic catecholamines. Synthesis and adrenergic activity of 5,6- and 6,7-dihydroxy-3,4-dihydrospiro[naphthalen-1(2H)-3â \in 2 -piperidines]. Journal of Pharmacy and Pharmacology, 2010, 54, 649-660.	2.4	0
49	New Tris(hydroxypyridinones) as Iron and Aluminium Sequestering Agents: Synthesis, Complexation and In Vivo Studies. Chemistry - A European Journal, 2010, 16, 10535-10545.	3.3	41
50	Synthesis of heterocycle-based analogs of resveratrol and their antitumor and vasorelaxing properties. Bioorganic and Medicinal Chemistry, 2010, 18, 6715-6724.	3.0	30
51	Interaction of aminoadamantane derivatives with the influenza A virus M2 channel-Docking using a pore blocking model. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4182-4187.	2.2	12
52	Protein Kinases: Docking and Homology Modeling Reliability. Journal of Chemical Information and Modeling, 2010, 50, 1432-1441.	5.4	58
53	Different Binding Modes of Structurally Diverse Ligands for Human D3DAR. Journal of Chemical Information and Modeling, 2010, 50, 2162-2175.	5.4	3
54	A Virtual Screening Study of the 18 kDa Translocator Protein using Pharmacophore Models Combined with 3Dâ€QSAR Studies. ChemMedChem, 2009, 4, 1686-1694.	3.2	7

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55	<i>N-O-</i> Isopropyl Sulfonamido-Based Hydroxamates: Design, Synthesis and Biological Evaluation of Selective Matrix Metalloproteinase-13 Inhibitors as Potential Therapeutic Agents for Osteoarthritis. Journal of Medicinal Chemistry, 2009, 52, 4757-4773.	6.4	60
56	Multitemplate Alignment Method for the Development of a Reliable 3D-QSAR Model for the Analysis of MMP3 Inhibitors. Journal of Chemical Information and Modeling, 2009, 49, 1715-1724.	5.4	18
57	Design, Synthesis, Biological Evaluation, and NMR Studies of a New Series of Arylsulfones As Selective and Potent Matrix Metalloproteinase-12 Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 6347-6361.	6.4	49
58	Docking of Hydroxamic Acids into HDAC1 and HDAC8: A Rationalization of Activity Trends and Selectivities. Journal of Chemical Information and Modeling, 2009, 49, 2774-2785.	5.4	37
59	New Resorcinolâ^'Anandamide "Hybrids―as Potent Cannabinoid Receptor Ligands Endowed with Antinociceptive Activity in Vivo. Journal of Medicinal Chemistry, 2009, 52, 2506-2514.	6.4	19
60	Rational Design, Synthesis, and Pharmacological Properties of New 1,8-Naphthyridin-2(1H)-on-3-Carboxamide Derivatives as Highly Selective Cannabinoid-2 Receptor Agonists. Journal of Medicinal Chemistry, 2009, 52, 3644-3651.	6.4	36
61	Structural Evolutions of Salicylaldoximes as Selective Agonists for Estrogen Receptor \hat{l}^2 . Journal of Medicinal Chemistry, 2009, 52, 858-867.	6.4	38
62	Computational Studies of Epidermal Growth Factor Receptor: Docking Reliability, Three-Dimensional Quantitative Structurea [^] Activity Relationship Analysis, and Virtual Screening Studies. Journal of Medicinal Chemistry, 2009, 52, 964-975.	6.4	34
63	Molecular modeling of adenosine receptors: new results and trends. Medicinal Research Reviews, 2008, 28, 247-277.	10.5	38
64	Substituted Pyrazolo[3,4â€∢i>b)pyridines as Potent A ₁ Adenosine Antagonists: Synthesis, Biological Evaluation, and Development of an A ₁ Bovine Receptor Model. ChemMedChem, 2008, 3, 898-913.	3.2	24
65	Development of a receptor-based 3D-QSAR study for the analysis of MMP2, MMP3, and MMP9 inhibitors. Bioorganic and Medicinal Chemistry, 2008, 16, 7749-7758.	3.0	25
66	Structure–activity relationship studies of a new series of imidazo[2,1-f]purinones as potent and selective A3 adenosine receptor antagonists. Bioorganic and Medicinal Chemistry, 2008, 16, 10281-10294.	3.0	16
67	Dual Inhibitors of Matrix Metalloproteinases and Carbonic Anhydrases: Iminodiacetyl-Based Hydroxamateâ^Benzenesulfonamide Conjugates. Journal of Medicinal Chemistry, 2008, 51, 7968-7979.	6.4	52
68	Synthesis, Modeling, and RET Protein Kinase Inhibitory Activity of 3- and 4-Substituted \hat{l}^2 -Carbolin-1-ones. Journal of Medicinal Chemistry, 2008, 51, 7777-7787.	6.4	36
69	Derivatives of 4-Amino-6-hydroxy-2-mercaptopyrimidine as Novel, Potent, and Selective A ₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2008, 51, 1764-1770.	6.4	54
70	Monoaryl-Substituted Salicylaldoximes as Ligands for Estrogen Receptor \hat{l}^2 . Journal of Medicinal Chemistry, 2008, 51, 1344-1351.	6.4	26
71	Indoles and Related Compounds as Cannabinoid Ligands. Mini-Reviews in Medicinal Chemistry, 2008, 8, 370-387.	2.4	39
72	Structure-Based Virtual Screening: Identification of Novel CB2 Receptor Ligands. Letters in Drug Design and Discovery, 2007, 4, 15-19.	0.7	3

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73	Construction and Validation of a RET TK Catalytic Domain by Homology Modeling. Journal of Chemical Information and Modeling, 2007, 47, 644-655.	5.4	38
74	Analysis of Human Carbonic Anhydrase II:  Docking Reliability and Receptor-Based 3D-QSAR Study. Journal of Chemical Information and Modeling, 2007, 47, 515-525.	5.4	39
75	Computational Approaches on Angiotensin Receptors and Their Ligands: Recent Developments and Results. Current Medicinal Chemistry, 2007, 14, 3105-3121.	2.4	7
76	Homology Modeling and Receptor-Based 3D-QSAR Study of Carbonic Anhydrase IX. Journal of Chemical Information and Modeling, 2007, 47, 2253-2262.	5.4	26
77	5-Amino-2-phenyl[1,2,3]triazolo[1,2-a][1,2,4]benzotriazin-1-one:  A Versatile Scaffold To Obtain Potent and Selective A3 Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2007, 50, 5676-5684.	6.4	22
78	Design, synthesis, binding, and molecular modeling studies of new potent ligands of cannabinoid receptors. Bioorganic and Medicinal Chemistry, 2007, 15, 5406-5416.	3.0	16
79	New 1,8-naphthyridine and quinoline derivatives as CB2 selective agonists. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 6505-6510.	2.2	64
80	Cannabinoid CB2/CB1 Selectivity. Receptor Modeling and Automated Docking Analysis. Journal of Medicinal Chemistry, 2006, 49, 984-994.	6.4	93
81	Proposal of a New Binding Orientation for Non-Peptide AT1 Antagonists:Â Homology Modeling, Docking and Three-Dimensional Quantitative Structureâ 'Activity Relationship Analysis. Journal of Medicinal Chemistry, 2006, 49, 4305-4316.	6.4	72
82	Pharmacophore Based Receptor Modeling:Â The Case of Adenosine A3Receptor Antagonists. An Approach to the Optimization of Protein Models. Journal of Medicinal Chemistry, 2006, 49, 4085-4097.	6.4	32
83	A Theoretical Study To Investigate D2DAR/D4DAR Selectivity:  Receptor Modeling and Molecular Docking of Dopaminergic Ligands. Journal of Medicinal Chemistry, 2006, 49, 1397-1407.	6.4	18
84	Design, Synthesis, and Biological Evaluation of New 1,8-Naphthyridin-4(1H)-on-3-carboxamide and Quinolin-4(1H)-on-3-carboxamide Derivatives as CB2Selective Agonists. Journal of Medicinal Chemistry, 2006, 49, 5947-5957.	6.4	66
85	Synthesis of Anthranylaldoxime Derivatives as Estrogen Receptor Ligands and Computational Prediction of Binding Modes. Journal of Medicinal Chemistry, 2006, 49, 5001-5012.	6.4	27
86	An overview of recent developments in GPCR modelling: methods and validation. Expert Opinion on Drug Discovery, 2006, 1 , 459-476.	5.0	10
87	Adenosine receptor modelling. A1/A2a selectivity. European Journal of Medicinal Chemistry, 2006, 41, 321-329.	5.5	15
88	Amber force field implementation, molecular modelling study, synthesis and MMP-1/MMP-2 inhibition profile of (R)- and (S)-N-hydroxy-2-(N-isopropoxybiphenyl-4-ylsulfonamido)-3-methylbutanamides. Bioorganic and Medicinal Chemistry, 2006, 14, 4260-4276.	3.0	78
89	Synthesis of Stable Analogues of Geranylgeranyl Diphosphate Possessing a (Z,E,E)-Geranylgeranyl Side Chain, Docking Analysis, and Biological Assays for Prenyl Protein Transferase Inhibition. ChemMedChem, 2006, 1, 218-224.	3.2	5
90	1,8-Naphthyridin-4-one derivatives as new ligands of A2A adenosine receptors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 4604-4610.	2.2	11

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91	Synthesis and 3D QSAR of New Pyrazolo[3,4-b]pyridines:  Potent and Selective Inhibitors of A1 Adenosine Receptors. Journal of Medicinal Chemistry, 2005, 48, 7172-7185.	6.4	61
92	Study on Affinity Profile toward Native Human and Bovine Adenosine Receptors of a Series of 1,8-Naphthyridine Derivatives. Journal of Medicinal Chemistry, 2004, 47, 3019-3031.	6.4	31
93	Synthesis of heteroaromatic analogues of (2-aryl-1-cyclopentenyl-1-alkylidene)-(arylmethyloxy)amine COX-2 inhibitors: effects on the inhibitory activity of the replacement of the cyclopentene central core with pyrazole, thiophene or isoxazole ring. European Journal of Medicinal Chemistry, 2003, 38, 157-168.	5.5	35
94	Synthesis, Antifungal Activity, and Molecular Modeling Studies of New Inverted Oxime Ethers of Oxiconazole. Journal of Medicinal Chemistry, 2002, 45, 4903-4912.	6.4	111
95	Conformationally restrained analogues of sympathomimetic catecholamines. European Journal of Medicinal Chemistry, 2002, 37, 11-22.	5.5	4
96	Synthesis and β-blocking activity of (R,S)-(E)-oximeethers of 2,3-dihydro-1,8-naphthyridine and 2,3-dihydrothiopyrano[2,3-b]pyridine:potential antihypertensive agents – Part IX. European Journal of Medicinal Chemistry, 2000, 35, 815-826.	5 . 5	94
97	Selective inhibition of human erythrocyte Na+/K+ ATPase by cardiac glycosides and by a mammalian digitalis like factor. Life Sciences, 2000, 67, 1921-1928.	4.3	26
98	A Novel Class of Highly Potent and Selective A1Adenosine Antagonists:Â Structureâ 'Affinity Profile of a Series of 1,8-Naphthyridine Derivatives. Journal of Medicinal Chemistry, 2000, 43, 2814-2823.	6.4	30
99	The [(methyloxy)imino]methyl moiety (MOIMM) in the design of a new type of \hat{I}^2 -adrenergic blocking agent. European Journal of Medicinal Chemistry, 1999, 34, 283-291.	5 . 5	9
100	Synthesis and HIV-1 inhibitory properties of new tetrahydrobenzoquinazolinedione and tetrahydrobenzocycloheptenuracil derivatives and of their thioxo analogues. Il Farmaco, 1999, 54, 242-247.	0.9	10
101	Synthesis and aldose reductase inhibitory activity of new N-(benzyloxy) glycine derivatives. Il Farmaco, 1998, 53, 369-373.	0.9	5
102	1,2-Disubstituted cyclohexane derived tripeptide aldehydes as novel selective thrombin inhibitors. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 1249-1254.	2.2	13
103	Synthesis and \hat{I}^2 -Adrenergic Properties of (Z)-N-[3-(Alkylamino)-2-hydroxypropylidene] (aryl-methyloxy)amines: Effects of the Configuration Around the Methyloxyiminomethyl (MOIM) Double Bond on the Biopharmacological Properties of MOIM-type \hat{I}^2 -Blocking Agents, Bioorganic and Medicinal Chemistry, 1998, 6, 2151-2160.	3.0	5
104	Synthesis and \hat{l}_{\pm} -adrenergic and I1-imidazoline activity of 3-phenylpiperidines dimethyl-substituted on the phenyl ring. European Journal of Medicinal Chemistry, 1998, 33, 911-919.	5 . 5	6
105	N-n-Propyl-Substituted 3-(Dimethylphenyl)piperidines Display Novel Discriminative Properties between Dopamine Receptor Subtypes:Â Synthesis and Receptor Binding Studies1. Journal of Medicinal Chemistry, 1998, 41, 4933-4938.	6.4	12
106	The [(Methyloxy)imino]methyl Moiety as a Bioisoster of Aryl. A Novel Class of Completely Aliphatic .betaAdrenergic Receptor Antagonists. Journal of Medicinal Chemistry, 1994, 37, 1518-1525.	6.4	20
107	Conformationally restrained analogs of sympathomimetic catecholamines. Synthesis, conformational analysis and adrenergic activity of isochroman derivatives. Journal of Medicinal Chemistry, 1993, 36, 3077-3086.	6.4	17
108	Conformational effects on the activity of drugs. 13. A revision of previously proposed models for the activation of .alpha and .betaadrenergic receptors. Journal of Medicinal Chemistry, 1992, 35, 1009-1018.	6.4	21

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109	QSAR Studies of MMP Inhibitors. , 0, , 647-671.		O
110	QSAR of Carbonic Anhydrase Inhibitors and Their Impact on Drug Design. , 0, , 375-397.		0