Adriano Martinelli

List of Publications by Year
in descending order

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110 papers	3,247 citations	117625 34 h-index	189892 50 g-index
117 all docs	117 docs citations	117 times ranked	4093 citing authors

#	Article	IF	Citations
1	Discovery of N-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
2	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
3	Synthesis and Î²-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 â€“ Part IX. European Journal of Medicinal Chemistry, 2000, 35, 815-826.	5.5	94
4	Cannabinoid CB2/CB1 Selectivity. Receptor Modeling and Automated Docking Analysis. Journal of Medicinal Chemistry, 2006, 49, 984-994.	6.4	93
5	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
6	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
7	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
8	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
9	New 1,8-naphthyridine and quinoline derivatives as CB2 selective agonists. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 6505-6510.	2.2	64
10	N-Hydroxyindole-based inhibitors of lactate dehydrogenase against cancer cell proliferation. European Journal of Medicinal Chemistry, 2011, 46, 5398-5407.	5.5	64
11	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
12	Synthesis and 3D QSAR of New Pyrazolo[3,4-b]pyridines:â€‰ Potent and Selective Inhibitors of A1 Adenosine Receptors. Journal of Medicinal Chemistry, 2005, 48, 7172-7185.	6.4	61
13	N-O-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
14	Protein Kinases: Docking and Homology Modeling Reliability. Journal of Chemical Information and Modeling, 2010, 50, 1432-1441.	5.4	58
15	Derivatives of 4-Amino-6-hydroxy-2-mercaptopyrimidine as Novel, Potent, and Selective A₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2008, 51, 1764-1770.	6.4	54
16	N-O-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
17	Dual Inhibitors of Matrix Metalloproteinases and Carbonic Anhydrases: Iminodiacetyl-Based Hydroxamateâ"Benzenesulfonamide Conjugates. Journal of Medicinal Chemistry, 2008, 51, 7968-7979.	6.4	52
18	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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19	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
20	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
21	Dual Targeting of the Warburg Effect with a Glucoseâ€Conjugated Lactate Dehydrogenase Inhibitor. ChemBioChem, 2013, 14, 2263-2267.	2.6	43
22	Identification and characterization of a new reversible MAGL inhibitor. Bioorganic and Medicinal Chemistry, 2014, 22, 3285-3291.	3.0	43
23	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
24	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
25	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
26	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
27	Phenylpropanoids and flavonoids from Phlomis kurdica as inhibitors of human lactate dehydrogenase. Phytochemistry, 2015, 116, 262-268.	2.9	40
28	Analysis of Human Carbonic Anhydrase II:â€‰ Docking Reliability and Receptor-Based 3D-QSAR Study. Journal of Chemical Information and Modeling, 2007, 47, 515-525.	5.4	39
29	Indoles and Related Compounds as Cannabinoid Ligands. Mini-Reviews in Medicinal Chemistry, 2008, 8, 370-387.	2.4	39
30	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
31	Molecular modeling of adenosine receptors: new results and trends. Medicinal Research Reviews, 2008, 28, 247-277.	10.5	38
32	Structural Evolutions of Salicylaldoximes as Selective Agonists for Estrogen Receptor Î². Journal of Medicinal Chemistry, 2009, 52, 858-867.	6.4	38
33	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
34	Synthesis, Modeling, and RET Protein Kinase Inhibitory Activity of 3- and 4-Substituted Î²-Carbolin-1-ones. Journal of Medicinal Chemistry, 2008, 51, 7777-7787.	6.4	36
35	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
36	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

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37	Computational Studies of Epidermal Growth Factor Receptor: Docking Reliability, Three-Dimensional Quantitative Structureâ"Activity Relationship Analysis, and Virtual Screening Studies. Journal of Medicinal Chemistry, 2009, 52, 964-975.	6.4	34
38	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
39	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
40	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
41	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
42	Synthesis of heterocycle-based analogs of resveratrol and their antitumor and vasorelaxing properties. Bioorganic and Medicinal Chemistry, 2010, 18, 6715-6724.	3.0	30
43	Discovery of long-chain salicylketoxime derivatives as monoacylglycerol lipase (MAGL) inhibitors. European Journal of Medicinal Chemistry, 2018, 157, 817-836.	5.5	30
44	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
45	Development of terphenyl-2-methyloxazol-5(4H)-one derivatives as selective reversible MAGL inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1240-1252.	5.2	27
46	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
47	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
48	Monoaryl-Substituted Salicylaldoximes as Ligands for Estrogen Receptor Î². Journal of Medicinal Chemistry, 2008, 51, 1344-1351.	6.4	26
49	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
50	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
51	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
52	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
53	Substituted Pyrazolo[3,4â€b]pyridines as Potent A₁ Adenosine Antagonists: Synthesis, Biological Evaluation, and Development of an A₁ Bovine Receptor Model. ChemMedChem, 2008, 3, 898-913.	3.2	24
54	Identification of New Fyn Kinase Inhibitors Using a FLAP-Based Approach. Journal of Chemical Information and Modeling, 2013, 53, 2538-2547.	5.4	24

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55	5-Amino-2-phenyl[1,2,3]triazolo[1,2-a][1,2,4]benzotriazin-1-one:â€‰ A Versatile Scaffold To Obtain Potent and Selective A3 Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2007, 50, 5676-5684.	6.4	22
56	Triazole-substituted N-hydroxyindol-2-carboxylates as inhibitors of isoform 5 of human lactate dehydrogenase (hLDH5). MedChemComm, 2011, 2, 638.	3.4	22
57	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
58	Highly Selective Salicylketoxime-Based Estrogen Receptor Î² Agonists Display Antiproliferative Activities in a Glioma Model. Journal of Medicinal Chemistry, 2015, 58, 1184-1194.	6.4	22
59	Conformational effects on the activity of drugs. 13. A revision of previously proposed models for the activation of .alpha.- and .beta.-adrenergic receptors. Journal of Medicinal Chemistry, 1992, 35, 1009-1018.	6.4	21
60	4-Aryliden-2-methyloxazol-5(4H)-one as a new scaffold for selective reversible MAGL inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 137-146.	5.2	21
61	The [(Methyloxy)imino]methyl Moiety as a Bioisoster of Aryl. A Novel Class of Completely Aliphatic .beta.-Adrenergic Receptor Antagonists. Journal of Medicinal Chemistry, 1994, 37, 1518-1525.	6.4	20
62	Extensive Reliability Evaluation of Docking-Based Target-Fishing Strategies. International Journal of Molecular Sciences, 2019, 20, 1023.	4.1	20
63	New Resorcinolâ^'Anandamide â€œHybridsâ€•as Potent Cannabinoid Receptor Ligands Endowed with Antinociceptive Activity in Vivo. Journal of Medicinal Chemistry, 2009, 52, 2506-2514.	6.4	19
64	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
65	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
66	A Theoretical Study To Investigate D2DAR/D4DAR Selectivity:â€‰ Receptor Modeling and Molecular Docking of Dopaminergic Ligands. Journal of Medicinal Chemistry, 2006, 49, 1397-1407.	6.4	18
67	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
68	Receptor-based virtual screening evaluation for the identification of estrogen receptorÎ²ligands. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 662-670.	5.2	18
69	A Virtual Screening Study for Lactate Dehydrogenase 5 Inhibitors by Using a Pharmacophoreâ€based Approach. Molecular Informatics, 2016, 35, 434-439.	2.5	18
70	VenomPred: A Machine Learning Based Platform for Molecular Toxicity Predictions. International Journal of Molecular Sciences, 2022, 23, 2105.	4.1	18
71	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
72	Pyrazole phenylcyclohexylcarbamates as inhibitors of human fatty acid amide hydrolases (FAAH). European Journal of Medicinal Chemistry, 2015, 97, 289-305.	5.5	17

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73	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
74	Structureâ€“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
75	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
76	Targeting Different Transthyretin Binding Sites with Unusual Natural Compounds. ChemMedChem, 2016, 11, 1865-1874.	3.2	16
77	Adenosine receptor modelling. A1/A2a selectivity. European Journal of Medicinal Chemistry, 2006, 41, 321-329.	5.5	15
78	1,2-Disubstituted cyclohexane derived tripeptide aldehydes as novel selective thrombin inhibitors. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 1249-1254.	2.2	13
79	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
80	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
81	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
82	Salicylaldoxime derivatives as new leads for the development of carbonic anhydrase inhibitors. Bioorganic and Medicinal Chemistry, 2013, 21, 1511-1515.	3.0	12
83	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
84	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
85	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
86	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
87	An overview of recent developments in GPCR modelling: methods and validation. Expert Opinion on Drug Discovery, 2006, 1, 459-476.	5.0	10
88	The [(methyloxy)imino]methyl moiety (MOIMM) in the design of a new type of Î²-adrenergic blocking agent. European Journal of Medicinal Chemistry, 1999, 34, 283-291.	5.5	9
89	Protein Kinase Homology Models: Recent Developments and Results. Current Medicinal Chemistry, 2011, 18, 2848-2853.	2.4	9
90	Novel Folate-Hydroxamate Based Antimetabolites: Synthesis and Biological Evaluation. Medicinal Chemistry, 2011, 7, 265-274.	1.5	8

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91	Computational Studies on Translocator Protein (TSPO) and its Ligands. Current Topics in Medicinal Chemistry, 2012, 12, 352-359.	2.1	8
92	Computational Approaches on Angiotensin Receptors and Their Ligands: Recent Developments and Results. Current Medicinal Chemistry, 2007, 14, 3105-3121.	2.4	7
93	A Virtual Screening Study of the 18â€…kDa Translocator Protein using Pharmacophore Models Combined with 3Dâ€QSAR Studies. ChemMedChem, 2009, 4, 1686-1694.	3.2	7
94	Synthesis and Î±-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
95	Identification of Transthyretin Fibril Formation Inhibitors Using Structureâ€Based Virtual Screening. ChemMedChem, 2017, 12, 1327-1334.	3.2	6
96	Synthesis and aldose reductase inhibitory activity of new N-(benzyloxy) glycine derivatives. Il Farmaco, 1998, 53, 369-373.	0.9	5
97	Synthesis and Î²-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 Î²-Blocking Agents. Bioorganic and Medicinal Chemistry, 1998, 6, 2151-2160.	3.0	5
98	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
99	Molecular Modeling of Adenosine Receptors. Methods in Enzymology, 2013, 522, 37-59.	1.0	5
100	Identification of Lactate Dehydrogenase 5 Inhibitors using Pharmacophore- Driven Consensus Docking. Current Bioactive Compounds, 2018, 14, 197-204.	0.5	5
101	Conformationally restrained analogues of sympathomimetic catecholamines. European Journal of Medicinal Chemistry, 2002, 37, 11-22.	5.5	4
102	Structure-Based Virtual Screening: Identification of Novel CB2 Receptor Ligands. Letters in Drug Design and Discovery, 2007, 4, 15-19.	0.7	3
103	Different Binding Modes of Structurally Diverse Ligands for Human D3DAR. Journal of Chemical Information and Modeling, 2010, 50, 2162-2175.	5.4	3
104	Rational Development of MAGL Inhibitors. Methods in Molecular Biology, 2018, 1824, 335-346.	0.9	2
105	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
106	QSAR Studies of MMP Inhibitors. , 0, , 647-671.		0
107	QSAR of Carbonic Anhydrase Inhibitors and Their Impact on Drug Design. , 0, , 375-397.		0
108	Editorial [Hot topic: Adenosine Receptor Ligands: Where Are We, and Where Are We Going? (Guest) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 941-941.	2.1	0

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109	Editorial [Hot topic: Adenosine Receptor Ligands: Where Are We, and Where Are We Going? (Guest) Tj ETQq1 1 0.784314 rgBT /Over 859-859.	2.1	0
110	Spirotetrahydronaphthalene analogues of sympathomimetic catecholamines. Synthesis and adrenergic activity of 5,6- and 6,7-dihydroxy-3,4-dihydrospiro[naphthalen-1(2H)-3â€² -piperidines]. Journal of Pharmacy and Pharmacology, 2010, 54, 649-660.	2.4	0