Antonino Lauria

List of Publications by Year
in descending order

102	2,888	136950	206112
papers	citations	32 h-index	48 g-index

114	114	114	3802
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	1,2,3â€Triazole in Heterocyclic Compounds, Endowed with Biological Activity, through 1,3â€Dipolar Cycloadditions. European Journal of Organic Chemistry, 2014, 2014, 3289-3306.	2.4	271
2	DNA-binding of nickel(II), copper(II) and zinc(II) complexes: Structureâ€“affinity relationships. Coordination Chemistry Reviews, 2013, 257, 2848-2862.	18.8	240
3	Nickel(ii), copper(ii) and zinc(ii) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation. Dalton Transactions, 2014, 43, 6108.	3.3	79
4	Selective G-quadruplex stabilizers: Schiff-base metal complexes with anticancer activity. RSC Advances, 2014, 4, 33245-33256.	3.6	78
5	Hsp60, a Novel Target for Antitumor Therapy: Structure-Function Features and Prospective Drugs Design. Current Pharmaceutical Design, 2013, 19, 2757-2764.	1.9	65
6	Pyrrolo[2,3-d][1,2,3]triazoles as Potential Antineoplastic Agents. Heterocycles, 1998, 48, 1229.	0.7	64
7	Melatonin reduces inflammatory response in human intestinal epithelial cells stimulated by interleukinâ€1Î². Journal of Pineal Research, 2019, 67, e12598.	7.4	64
8	Design and Synthesis of 4-Substituted Indolo[3,2-e][1,2,3]triazolo[1,5-a]pyrimidine Derivatives with Antitumor Activity. Journal of Medicinal Chemistry, 2008, 51, 2037-2046.	6.4	57
9	Pyrrolo[2,1-c][1,2,4]triazines from 2-diazopyrroles: synthesis and antiproliferative activity. European Journal of Medicinal Chemistry, 2002, 37, 267-272.	5.5	55
10	Molecular Modeling Approaches in the Discovery of New Drugs for Anti-Cancer Therapy: The Investigation of p53-MDM2 Interaction and its Inhibition by Small Molecules. Current Medicinal Chemistry, 2010, 17, 3142-3154.	2.4	55
11	Indolo[3,2- c]cinnolines with antiproliferative, antifungal, and antibacterial activity. Bioorganic and Medicinal Chemistry, 1999, 7, 1591-1596.	3.0	50
12	Derivatives of the New Ring System Indolo[1,2-c]benzo[1,2,3]triazine with Potent Antitumor and Antimicrobial Activity. Journal of Medicinal Chemistry, 1999, 42, 2561-2568.	6.4	50
13	The dimer-monomer equilibrium of SARS-CoV-2 main protease is affected by small molecule inhibitors. Scientific Reports, 2021, 11, 9283.	3.3	48
14	Intercalation of Daunomycin into Stacked DNA Base Pairs. DFT Study of an Anticancer Drug. Journal of Biomolecular Structure and Dynamics, 2008, 26, 115-129.	3.5	47
15	New annelated thieno[2,3- e][1,2,3]triazolo[1,5- a]pyrimidines, with potent anticancer activity, designed through VLAK protocol. European Journal of Medicinal Chemistry, 2013, 62, 416-424.	5.5	44
16	Quinoline anticancer agents active on DNA and DNA-interacting proteins: From classical to emerging therapeutic targets. European Journal of Medicinal Chemistry, 2021, 220, 113555.	5.5	42
17	G-quadruplex vs. duplex-DNA binding of nickel(II) and zinc(II) Schiff base complexes. Journal of Inorganic Biochemistry, 2016, 161, 115-121.	3.5	41
18	New tricyclic systems of biological interest. Annelated 1,2,3-triazolo[1,5-a]pyrimidines through domino reaction of 3-azidopyrroles and methylene active nitriles. Tetrahedron, 2002, 58, 9723-9727.	1.9	39

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19	IKK-Î² inhibitors: An analysis of drugâ€“receptor interaction by using Molecular Docking and Pharmacophore 3D-QSAR approaches. Journal of Molecular Graphics and Modelling, 2010, 29, 72-81.	2.4	39
20	3D-QSAR pharmacophore modeling and in silico screening of new Bcl-xl inhibitors. European Journal of Medicinal Chemistry, 2010, 45, 4774-4782.	5.5	38
21	Virtual lock-and-key approach: The in silico revival of Fischer model by means of molecular descriptors. European Journal of Medicinal Chemistry, 2011, 46, 4274-4280.	5.5	38
22	Lead optimization through VLAK protocol: New annelated pyrrolo-pyrimidine derivatives as antitumor agents. European Journal of Medicinal Chemistry, 2012, 55, 375-383.	5.5	38
23	Synthesis, antiproliferative activity, and in silico insights of new 3-benzoylamino-benzo[b]thiophene derivatives. European Journal of Medicinal Chemistry, 2015, 90, 537-546.	5.5	38
24	Curcumin-like compounds designed to modify amyloid beta peptide aggregation patterns. RSC Advances, 2017, 7, 31714-31724.	3.6	38
25	Vaccinium macrocarpon (Cranberry)-Based Dietary Supplements: Variation in Mass Uniformity, Proanthocyanidin Dosage and Anthocyanin Profile Demonstrates Quality Control Standard Needed. Nutrients, 2020, 12, 992.	4.1	37
26	A General Treatment of Solubility. 3. Principal Component Analysis (PCA) of the Solubilities of Diverse Solutes in Diverse Solvents. Journal of Chemical Information and Modeling, 2005, 45, 913-923.	5.4	36
27	DNA Minor Groove Binders: an Overview on Molecular Modeling and QSAR Approaches. Current Medicinal Chemistry, 2007, 14, 2136-2160.	2.4	35
28	Pyrrolo[2,3-h]quinolinones: synthesis and photochemotherapic activity. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2809-2811.	2.2	34
29	Isoindolo[2,1-c]benzo[1,2,4]triazines: A new ring system with antiproliferative activity. Bioorganic and Medicinal Chemistry, 2007, 15, 343-349.	3.0	34
30	Principal component analysis on molecular descriptors as an alternative point of view in the search of new Hsp90 inhibitors. Computational Biology and Chemistry, 2009, 33, 386-390.	2.3	34
31	Quinoline-Based Molecules Targeting c-Met, EGF, and VEGF Receptors and the Proteins Involved in Related Carcinogenic Pathways. Molecules, 2020, 25, 4279.	3.8	34
32	Heterocyclic Scaffolds for the Treatment of Alzheimer's Disease. Current Pharmaceutical Design, 2016, 22, 3971-3995.	1.9	34
33	Pyrrolo[1,2-f]phenanthridines and related non-rigid analogues as antiviral agents. European Journal of Medicinal Chemistry, 2002, 37, 3-10.	5.5	33
34	Kinase Inhibitors in Multitargeted Cancer Therapy. Current Medicinal Chemistry, 2017, 24, 1671-1686.	2.4	33
35	Zinc complexes as fluorescent chemosensors for nucleic acids: new perspectives for a â€œboringâ€• element. Dalton Transactions, 2015, 44, 3527-3535.	3.3	32
36	Pyrrolo[2,1-d][1,2,3,5]tetrazine-4(3h)-ones, a new class of azolotetrazines with potent antitumor activity. Bioorganic and Medicinal Chemistry, 2003, 11, 2371-2380.	3.0	30

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37	A New Tetracyclic Ring System of Biological Interest. Indolo[3,2-e][1,2,3]triazolo[1,5-a]pyrimidines through Domino Reactions of 2-Azidoindole. Heterocycles, 2003, 60, 2669.	0.7	29
38	Inside the Hsp90 inhibitors binding mode through induced fit docking. Journal of Molecular Graphics and Modelling, 2009, 27, 712-722.	2.4	29
39	The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA. Journal of Inorganic Biochemistry, 2018, 178, 106-114.	3.5	29
40	Molecular docking approach on the Topoisomerase I inhibitors series included in the NCI anti-cancer agents mechanism database. Journal of Molecular Modeling, 2007, 13, 393-400.	1.8	28
41	A3 adenosine receptor: Homology modeling and 3D-QSAR studies. Journal of Molecular Graphics and Modelling, 2013, 42, 60-72.	2.4	28
42	An unexpected Dimroth rearrangement leading to annelated thieno[3,2-d][1,2,3]triazolo[1,5-a]pyrimidines with potent antitumor activity. European Journal of Medicinal Chemistry, 2013, 65, 381-388.	5.5	26
43	Annelated pyrrolo-pyrimidines from amino-cyanopyrroles and BMMAs as leads for new DNA-interactive ring systems. Bioorganic and Medicinal Chemistry, 2005, 13, 1545-1553.	3.0	25
44	New benzothieno[3,2-d]-1,2,3-triazines with antiproliferative activity: Synthesis, spectroscopic studies, and biological activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3291-3297.	2.2	25
45	Pyrrolo[3,4â€e][1,2,3]triazolo[1,5â€a]pyrimidine and pyrrolo[3,4â€d][1,2,3]triazolo[1,5â€a]pyrimidine. New tricyclic ring systems of biological interest. Journal of Heterocyclic Chemistry, 2000, 37, 747-750.	2.6	24
46	Combined Use of PCA and QSAR/QSPR to Predict the Drugs Mechanism of Action. An Application to the NCI ACAM Database. QSAR and Combinatorial Science, 2009, 28, 387-395.	1.4	24
47	Multivariate analysis in the identification of biological targets for designed molecular structures: The BIOTA protocol. European Journal of Medicinal Chemistry, 2014, 75, 106-110.	5.5	24
48	Receptor-guided 3D-QSAR approach for the discovery of c-kit tyrosine kinase inhibitors. Journal of Molecular Modeling, 2012, 18, 2885-2895.	1.8	23
49	A synthetic approach to new polycyclic ring system of biological interest through domino reaction: indolo[2,3-e][1,2,3]triazolo[1,5-a]pyrimidine. Tetrahedron Letters, 2006, 47, 2187-2190.	1.4	22
50	Pyrazolo[3,4-d][1,2,3]triazolo[1,5-a]pyrimidine: a new ring system through Dimroth rearrangement. Tetrahedron Letters, 2008, 49, 5125-5128.	1.4	22
51	Synthesis and Biological Activities of a New Class of Heat Shock Protein 90 Inhibitors, Designed by Energy-Based Pharmacophore Virtual Screening. Journal of Medicinal Chemistry, 2013, 56, 3424-3428.	6.4	22
52	Bioactive Triterpenes of Protium heptaphyllum Gum Resin Extract Display Cholesterol-Lowering Potential. International Journal of Molecular Sciences, 2021, 22, 2664.	4.1	22
53	Docking and multivariate methods to explore HIV-1 drug-resistance: a comparative analysis. Journal of Computer-Aided Molecular Design, 2008, 22, 287-297.	2.9	21
54	Synthesis and antiproliferative activity of [1,2,3,5]tetrazino[5,4-a]indoles, a new class of azolo-tetrazinones. Bioorganic and Medicinal Chemistry, 2005, 13, 295-300.	3.0	20

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55	Molecular dynamics studies on Mdm2 complexes: An analysis of the inhibitor influence. Biochemical and Biophysical Research Communications, 2012, 424, 341-347.	2.1	20
56	DRUDIT: web-based DRUgs DIscovery Tools to design small molecules as modulators of biological targets. Bioinformatics, 2019, 36, 1562-1569.	4.1	20
57	Exploring the anticancer potential of pyrazolo[1,2-a]benzo[1,2,3,4]tetrazin-3-one derivatives: The effect on apoptosis induction, cell cycle and proliferation. European Journal of Medicinal Chemistry, 2013, 64, 345-356.	5.5	19
58	Drugs Polypharmacology by In Silico Methods: New Opportunities in Drug Discovery. Current Pharmaceutical Design, 2016, 22, 3073-3081.	1.9	19
59	The Repurposing of Old Drugs or Unsuccessful Lead Compounds by in Silico Approaches: New Advances and Perspectives. Current Topics in Medicinal Chemistry, 2016, 16, 2088-2106.	2.1	19
60	Synthesis and photochemotherapeutic activity of thiopyrano[2,3-e]indol-2-ones. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 2291-2294.	2.2	18
61	In-silico screening of new potential Bcl-2/Bcl-xl inhibitors as apoptosis modulators. Journal of Molecular Modeling, 2009, 15, 349-355.	1.8	16
62	2-Triazenopyrroles: synthesis and biological activity. European Journal of Medicinal Chemistry, 1999, 34, 353-360.	5.5	15
63	Reactivity of asymmetric benzo-condensed diazines with nitrilimine dipoles in the 1,3-dipolar cycloaddition reactions. Tetrahedron Letters, 2009, 50, 7333-7336.	1.4	14
64	Molecular dynamics, dynamic site mapping, and highthroughput virtual screening on leptin and the Ob receptor as anti-obesity target. Journal of Molecular Modeling, 2014, 20, 2247.	1.8	14
65	Protonation of Aminoindoles. Tetrahedron, 2000, 56, 5177-5183.	1.9	13
66	A Multivariate Analysis of HIV-1 Protease Inhibitors and Resistance Induced by Mutation. Journal of Chemical Information and Modeling, 2006, 46, 168-179.	5.4	13
67	Molecular dynamics studies on HIV-1 protease: a comparison of the flap motions between wild type protease and the M46I/G51D double mutant. Journal of Molecular Modeling, 2007, 13, 1151-1156.	1.8	13
68	In Silico Insights into the SARS CoV-2 Main Protease Suggest NADH Endogenous Defences in the Control of the Pandemic Coronavirus Infection. Viruses, 2020, 12, 805.	3.3	13
69	Does Ligand Symmetry Play a Role in the Stabilization of DNA G-Quadruplex Host-Guest Complexes?. Current Medicinal Chemistry, 2014, 21, 2665-2690.	2.4	13
70	Bis-1,2,4-triazolo[4,3-a:3â€²,4â€²-c]quinoxalines of pharmaceutical interest from 1,3-dipolar cycloaddition. Tetrahedron Letters, 2008, 49, 1847-1850.	1.4	12
71	In vitro and in silico studies of polycondensed diazine systems as anti-parasitic agents. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1000-1004.	2.2	12
72	In Silico Identification of Small Molecules as New Cdc25 Inhibitors through the Correlation between Chemosensitivity and Protein Expression Pattern. International Journal of Molecular Sciences, 2021, 22, 3714.	4.1	12

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73	1-Methyl-3H-pyrazolo[1,2-a]benzo[1,2,3,4]tetrazin-3-ones. Design, Synthesis, and Biological Activity of New Antitumor Agents. Journal of Medicinal Chemistry, 2005, 48, 2859-2866.	6.4	11
74	Molecular Modelling and QSAR in the Discovery of HIV-1 Integrase Inhibitors. Current Computer-Aided Drug Design, 2007, 3, 214-233.	1.2	11
75	Synthesis, biological evaluation, and in silico studies of novel chalcone- and pyrazoline-based 1,3,5-triazines as potential anticancer agents. RSC Advances, 2020, 10, 34114-34129.	3.6	11
76	Pyrrolo[3,2â€c][1,2,5]benzotriazocine: A new ring system. Journal of Heterocyclic Chemistry, 1998, 35, 1535-1537.	2.6	10
77	In Silico, Spectroscopic, and Biological Insights on Annelated Pyrrolo[3,2- e]Pyrimidines with Antiproliferative Activity. Letters in Drug Design and Discovery, 2013, 11, 15-26.	0.7	10
78	Leptin and the Ob-Receptor as Anti-Obesity Target: Recent In Silico Advances in the Comprehension of the Protein-Protein Interaction and Rational Drug Design of Anti- Obesity Lead Compounds. Current Pharmaceutical Design, 2014, 20, 136-145.	1.9	9
79	Docking of indolo- and pyrrolo-pyrimidines to DNA. New DNA-interactive polycycles from amino-indoles/pyrroles and BMMA. Arkivoc, 2004, 2004, 263-271.	0.5	9
80	The influence of substitution in the quinoxaline nucleus on 1,3-dipolar cycloaddition reactions: A DFT study. Computational and Theoretical Chemistry, 2013, 1013, 116-122.	2.5	8
81	A Multivariate Analysis on Non-nucleoside HIV-1 Reverse Transcriptase Inhibitors and Resistance Induced by Mutation. QSAR and Combinatorial Science, 2003, 22, 984-996.	1.4	7
82	2-Diazo-2H-indoles. Helvetica Chimica Acta, 2001, 84, 2212-2219.	1.6	6
83	Design of antitumor drugs targeting c-kit receptor by a new mixed ligand-structure based method. Journal of Molecular Graphics and Modelling, 2020, 100, 107666.	2.4	6
84	A QSAR study investigating the potential anti-HIV-1 effect of some Acyclovir and Ganciclovir analogs. Arkivoc, 2009, 2009, 85-94.	0.5	6
85	Study of the role of "gatekeeper" mutations V654A and T670I of c-kit kinase in the interaction with inhibitors by means mixed molecular dynamics/docking approach. Bioinformation, 2011, 7, 296-298.	0.5	6
86	2-Diazoindoles: building blocks for the synthesis of antineoplastic agents. Il Farmaco, 2002, 57, 97-100.	0.9	5
87	Design, synthesis, and biological evaluation of a new class of benzo[b]furan derivatives as antiproliferative agents, with in silico predicted antitubulin activity. Chemical Biology and Drug Design, 2018, 91, 39-49.	3.2	5
88	Off-Target-Based Design of Selective HIV-1 PROTEASE Inhibitors. International Journal of Molecular Sciences, 2021, 22, 6070.	4.1	5
89	Identification of an LPS-Induced Chemo-Attractive Peptide from Ciona robusta. Marine Drugs, 2020, 18, 209.	4.6	4
90	Pyrrolo[2,3-b][1,4]benzothiazine. A New Ring System from Azidopyrroles. Heterocycles, 1999, 51, 2103.	0.7	3

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91	MADoSPRO: a new approach to molecular modelling studies on a series of DNA minor groove binders. QSAR and Combinatorial Science, 2006, 25, 252-262.	1.4	3
92	Docking and synthesis of pyrrolopyrimidodiazepinone derivatives (PPDs) and their precursors: New scaffolds for DNA-interacting agents. Computational and Theoretical Chemistry, 2007, 819, 26-31.	1.5	3
93	Study of Reactivity in the 1,3-Dipolar Cycloaddition Reactions Leading to New Triazolopyrrolopyrazine Ring Systems. Synlett, 2010, 2010, 2067-2070.	1.8	3
94	Pyrrolo[2,1-d][1,2,3,5]tetrazinones deaza analogues of temozolomide with potent antitumor activity. Il Farmaco, 2000, 55, 200-201.	0.9	1
95	New insights into the mechanism of action of pyrazolo[1,2â€a]benzo[1,2,3,4]tetrazinâ€3â€one derivatives endowed with anticancer potential. Chemical Biology and Drug Design, 2018, 91, 463-477.	3.2	1
96	Identification of biological targets through the correlation between cell line chemosensitivity and protein expression pattern. Drug Discovery Today, 2021, 26, 2431-2438.	6.4	1
97	New Tetracyclic Ring System of Biological Interest Indolo[3,2-e][1,2,3]triazolo[1,5-a]pyrimidine through domino reactions of 2-azidoindole. , 2003, , 224.		1
98	New Tricyclic Systems of Biological Interest. Anellated 1,2,3-Triazolo[1,5-a]pyrimidines Through Domino Reaction of 3-Azidopyrroles and Methylene Active Nitriles.. ChemInform, 2003, 34, no.	0.0	0
99	Pyrrolo[2,3-h]quinolinones: Synthesis and Photochemotherapic Activity.. ChemInform, 2003, 34, no.	0.0	0
100	Antiproliferative Properties and G-Quadruplex-Binding of Symmetrical Naphtho[1,2-b:8,7-bâ€™]dithiophene Derivatives. Molecules, 2021, 26, 4309.	3.8	0
101	Pyrimido[5,4-c]pyrrolo[2,1-a]isoquinoline: a new potential DNA-interactive ring system. Arkivoc, 2003, 2002, 264-273.	0.5	0
102	Isoindolo[2,1-c]benzo[1,2,4]triazine: a New Ring System with Potential Antitumor Activity. , 2003, , 284.		0