Domenico Alberga

List of Publications by Year
in descending order

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Version: 2024-02-01

95 papers	3,640 citations	117571 34 h-index	155592 55 g-index
95 all docs	95 docs citations	95 times ranked	4636 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	Structural Characterization of the Full-Length Anti-CD20 Antibody Rituximab. Frontiers in Molecular Biosciences, 2022, 9, 823174.	1.6	10
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	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
6	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
7	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
8	First-in-Class Isonipecotamide-Based Thrombin and Cholinesterase Dual Inhibitors with Potential for Alzheimer Disease. Molecules, 2021, 26, 5208.	1.7	9
9	Quantitative Polypharmacology Profiling Based on a Multifingerprint Similarity Predictive Approach. Journal of Chemical Information and Modeling, 2021, 61, 4868-4876.	2.5	18
10	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
11	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
12	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
13	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
14	Human ether-Ã-go-go-related potassium channel: exploring SAR to improve drug design. Drug Discovery Today, 2020, 25, 344-366.	3.2	33
15	(Hetero-)(arylidene)arylhydrazides as Multitarget-Directed Monoamine Oxidase Inhibitors. ACS Combinatorial Science, 2020, 22, 592-599.	3.8	5
16	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
17	Theoretical insights on acceptorâ€“donor dyads for organic photovoltaics. Physical Chemistry Chemical Physics, 2020, 22, 27413-27424.	1.3	1
18	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

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19	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
20	Bcr-Abl Allosteric Inhibitors: Where We Are and Where We Are Going to. Molecules, 2020, 25, 4210.	1.7	13
21	Design of enamides as new selective monoamine oxidase-B inhibitors. Journal of Pharmacy and Pharmacology, 2020, 72, 916-926.	1.2	18
22	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
23	Bcr-Abl Tyrosine Kinase Inhibitors in the Treatment of Pediatric CML. International Journal of Molecular Sciences, 2020, 21, 4469.	1.8	19
24	Enhancing the Sensitivity of Biotinylated Surfaces by Tailoring the Design of the Mixed Self-Assembled Monolayer Synthesis. ACS Omega, 2020, 5, 16762-16771.	1.6	22
25	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
26	Novel Class of Chalcone Oxime Ethers as Potent Monoamine Oxidase-B and Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 2356.	1.7	35
27	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
28	Design, synthesis and biological evaluation of oxygenated chalcones as potent and selective MAO-B inhibitors. Bioorganic Chemistry, 2019, 93, 103335.	2.0	49
29	Accelerating Drug Discovery by Early Protein Drug Target Prediction Based on a Multi-Fingerprint Similarity Search â€. Molecules, 2019, 24, 2233.	1.7	34
30	Prediction of Acute Oral Systemic Toxicity Using a Multifingerprint Similarity Approach. Toxicological Sciences, 2019, 167, 484-495.	1.4	26
31	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
32	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
33	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
34	Persulfate Reaction in a Hairâ€Bleaching Formula: Unveiling the Unconventional Reactivity of 1,13â€Diaminoâ€4,7,10â€Trioxatridecane. ChemistryOpen, 2018, 7, 319-322.	0.9	4
35	Optoeletronic properties of poly(Nâ€alkenylâ€carbazole)s driven by polymer stereoregularity. Journal of Polymer Science Part A, 2018, 56, 242-251.	2.5	20
36	Revealing the Origins of Mechanically Induced Fluorescence Changes in Organic Molecular Crystals. Advanced Materials, 2018, 30, e1800817.	11.1	82

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37	Molecular Docking for Predictive Toxicology. Methods in Molecular Biology, 2018, 1800, 181-197.	0.4	11
38	Ion Channels in Drug Discovery and Safety Pharmacology. Methods in Molecular Biology, 2018, 1800, 313-326.	0.4	15
39	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
40	Single-molecule detection with a millimetre-sized transistor. Nature Communications, 2018, 9, 3223.	5.8	184
41	Design, Synthesis, and Biological Evaluation of Tetrahydroâ€Î²â€carboline Derivatives as Selective Subâ€Nanomolar Gelatinase Inhibitors. ChemMedChem, 2018, 13, 1343-1352.	1.6	4
42	A rational approach to elucidate human monoamine oxidase molecular selectivity. European Journal of Pharmaceutical Sciences, 2017, 101, 90-99.	1.9	29
43	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
44	Effects of Substituents on Transport Properties of Molecular Materials for Organic Solar Cells: A Theoretical Investigation. Chemistry of Materials, 2017, 29, 673-681.	3.2	31
45	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	3.2	28
46	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
47	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
48	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
49	Effects of Anthryl Groups on the Charge Transport and Photovoltaic Properties of Small Triarylamineâ€Based Donorâ€Acceptor Molecules: A Joint Experimental and Theoretical Study. ChemistrySelect, 2017, 2, 6296-6303.	0.7	8
50	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
51	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
52	Applicability Domain for QSAR Models. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 45-63.	1.1	130
53	Human Aquaporin-4 and Molecular Modeling: Historical Perspective and View to the Future. International Journal of Molecular Sciences, 2016, 17, 1119.	1.8	12
54	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

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55	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
56	Kidney CLC-K chloride channels inhibitors. Journal of Hypertension, 2016, 34, 981-992.	0.3	22
57	Mind the Gap! A Journey towards Computational Toxicology. Molecular Informatics, 2016, 35, 294-308.	1.4	25
58	Permeability Coefficients of Lipophilic Compounds Estimated by Computer Simulations. Journal of Chemical Theory and Computation, 2016, 12, 4093-4099.	2.3	22
59	Organic bioelectronics probing conformational changes in surface confined proteins. Scientific Reports, 2016, 6, 28085.	1.6	27
60	A Round Trip from Medicinal Chemistry to Predictive Toxicology. Methods in Molecular Biology, 2016, 1425, 461-473.	0.4	0
61	Multidisciplinary study of a new ClCâ€1 mutation causing myotonia congenita: a paradigm to understand and treat ion channelopathies. FASEB Journal, 2016, 30, 3285-3295.	0.2	24
62	Understanding complexity of physiology by combined molecular simulations and experiments: anion channels as a proof of concept. Journal of Physiology, 2016, 594, 2777-2778.	1.3	2
63	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
64	ClCâ€1 mutations in myotonia congenita patients: insights into molecular gating mechanisms and genotypeâ€“phenotype correlation. Journal of Physiology, 2015, 593, 4181-4199.	1.3	24
65	Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data. Chemistry Central Journal, 2015, 9, 62.	2.6	35
66	Morphological and charge transport properties of amorphous and crystalline P3HT and PBTTT: insights from theory. Physical Chemistry Chemical Physics, 2015, 17, 18742-18750.	1.3	50
67	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
68	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
69	Theoretical Investigation of Hole Transporter Materials for Energy Devices. Journal of Physical Chemistry C, 2015, 119, 23890-23898.	1.5	44
70	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. Future Medicinal Chemistry, 2015, 7, 1921-1936.	1.1	30
71	Effects of Different Self-Assembled Monolayers on Thin-Film Morphology: A Combined DFT/MD Simulation Protocol. Langmuir, 2015, 31, 10693-10701.	1.6	15
72	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

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73	A generalizable definition of chemical similarity for read-across. Journal of Cheminformatics, 2014, 6, 39.	2.8	75
74	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
75	REACH and in silico methods: an attractive opportunity for medicinal chemists. Drug Discovery Today, 2014, 19, 1757-1768.	3.2	70
76	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
77	Effects of Annealing and Residual Solvents on Amorphous P3HT and PBTTT Films. Journal of Physical Chemistry C, 2014, 118, 8641-8655.	1.5	32
78	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
79	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	3.2	140
80	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
81	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
82	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
83	Integration of QSAR models for bioconcentration suitable for REACH. Science of the Total Environment, 2013, 456-457, 325-332.	3.9	27
84	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
85	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
86	Strategies of multi-objective optimization in drug discovery and development. Expert Opinion on Drug Discovery, 2011, 6, 871-884.	2.5	31
87	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
88	Analysis of X-ray Structures of Matrix Metalloproteinases via Chaotic Map Clustering. BMC Bioinformatics, 2010, 11, 500.	1.2	10
89	Improving Quantitative Structureâ^'Activity Relationships through Multiobjective Optimization. Journal of Chemical Information and Modeling, 2009, 49, 2290-2302.	2.5	48
90	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

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91	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
92	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
93	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
94	QSAR and QSPR Studies of a Highly Structured Physicochemical Domain. Journal of Chemical Information and Modeling, 2006, 46, 264-276.	2.5	56
95	Multiobjective Optimization in Quantitative Structureâ^'Activity Relationships:Â Deriving Accurate and Interpretable QSARs. Journal of Medicinal Chemistry, 2002, 45, 5069-5080.	2.9	96