Simone Brogi

List of Publications by Year
in descending order

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109 papers	3,117 citations	126907 33 h-index	214800 47 g-index
116 all docs	116 docs citations	116 times ranked	4115 citing authors

#	Article	IF	Citations
1	Multitarget compounds bearing tacrine- and donepezil-like structural and functional motifs for the potential treatment of Alzheimer's disease. Progress in Neurobiology, 2017, 151, 4-34.	5.7	128
2	Editorial: In silico Methods for Drug Design and Discovery. Frontiers in Chemistry, 2020, 8, 612.	3.6	117
3	Improving Curcumin Bioavailability: Current Strategies and Future Perspectives. Pharmaceutics, 2021, 13, 1715.	4.5	88
4	Donepezil-like multifunctional agents: Design, synthesis, molecular modeling and biological evaluation. European Journal of Medicinal Chemistry, 2016, 121, 864-879.	5.5	80
5	Development and Pharmacological Characterization of Selective Blockers of 2-Arachidonoyl Glycerol Degradation with Efficacy in Rodent Models of Multiple Sclerosis and Pain. Journal of Medicinal Chemistry, 2016, 59, 2612-2632.	6.4	70
6	Old but Gold: Tracking the New Guise of Histone Deacetylase 6 (HDAC6) Enzyme as a Biomarker and Therapeutic Target in Rare Diseases. Journal of Medicinal Chemistry, 2020, 63, 23-39.	6.4	69
7	Dopamine D3 Receptor Antagonists as Potential Therapeutics for the Treatment of Neurological Diseases. Frontiers in Neuroscience, 2016, 10, 451.	2.8	66
8	Role of hydrogen sulfide in endothelial dysfunction: Pathophysiology and therapeutic approaches. Journal of Advanced Research, 2021, 27, 99-113.	9.5	64
9	Antiâ€inflammatory and antiviral roles of hydrogen sulfide: Rationale for considering H₂S donors in COVIDâ€19 therapy. British Journal of Pharmacology, 2020, 177, 4931-4941.	5.4	63
10	Mimicking the Intramolecular Hydrogen Bond: Synthesis, Biological Evaluation, and Molecular Modeling of Benzoxazines and Quinazolines as Potential Antimalarial Agents. Journal of Medicinal Chemistry, 2012, 55, 10387-10404.	6.4	58
11	Structure-based discovery of the first non-covalent inhibitors of Leishmania major tryparedoxin peroxidase by high throughput docking. Scientific Reports, 2015, 5, 9705.	3.3	58
12	Polypharmacology of dopamine receptor ligands. Progress in Neurobiology, 2016, 142, 68-103.	5.7	57
13	Computational Tool for Fast in silico Evaluation of hERG K+ Channel Affinity. Frontiers in Chemistry, 2017, 5, 7.	3.6	52
14	The Citrus Flavonoid Naringenin Protects the Myocardium from Ageing-Dependent Dysfunction: Potential Role of SIRT1. Oxidative Medicine and Cellular Longevity, 2020, 2020, 1-15.	4.0	52
15	Diseaseâ€Modifying Antiâ€Alzheimer's Drugs: Inhibitors of Human Cholinesterases Interfering with Î²â€Amyloid Aggregation. CNS Neuroscience and Therapeutics, 2014, 20, 624-632.	3.9	51
16	Organic Isothiocyanates as Hydrogen Sulfide Donors. Antioxidants and Redox Signaling, 2020, 32, 110-144.	5.4	51
17	Discovery and Cardioprotective Effects of the First Non-Peptide Agonists of the G Protein-Coupled Prokineticin Receptor-1. PLoS ONE, 2015, 10, e0121027.	2.5	50
18	Verbascoside Inhibits Promastigote Growth and Arginase Activity of Leishmania amazonensis. Journal of Natural Products, 2016, 79, 1459-1463.	3.0	47

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19	Targeting Dopamine D3 and Serotonin 5-HT1A and 5-HT2A Receptors for Developing Effective Antipsychotics: Synthesis, Biological Characterization, and Behavioral Studies. Journal of Medicinal Chemistry, 2014, 57, 9578-9597.	6.4	46
20	Optimization of 4-Aminoquinoline/Clotrimazole-Based Hybrid Antimalarials: Further Structureâ€“Activity Relationships, in Vivo Studies, and Preliminary Toxicity Profiling. Journal of Medicinal Chemistry, 2012, 55, 6948-6967.	6.4	43
21	Novel Analgesic/Anti-Inflammatory Agents: 1,5-Diarylpyrrole Nitrooxyalkyl Ethers and Related Compounds as Cyclooxygenase-2 Inhibiting Nitric Oxide Donors. Journal of Medicinal Chemistry, 2013, 56, 3191-3206.	6.4	43
22	Development of Potent Inhibitors of the Mycobacterium tuberculosis Virulence Factor Zmp1 and Evaluation of Their Effect on Mycobacterial Survival inside Macrophages. ChemMedChem, 2018, 13, 422-430.	3.2	43
23	An integrated in silico screening strategy for identifying promising disruptors of p53-MDM2 interaction. Computational Biology and Chemistry, 2019, 83, 107105.	2.3	42
24	Multifunctional Cholinesterase and Amyloid Beta Fibrillization Modulators. Synthesis and Biological Investigation. ACS Medicinal Chemistry Letters, 2013, 4, 1178-1182.	2.8	40
25	Synthetic spirocyclic endoperoxides: new antimalarial scaffolds. MedChemComm, 2015, 6, 357-362.	3.4	39
26	Identification of novel fluorescent probes preventing PrP Sc replication in prion diseases. European Journal of Medicinal Chemistry, 2017, 127, 859-873.	5.5	39
27	Novel spiroindoline HDAC inhibitors: Synthesis, molecular modelling and biological studies. European Journal of Medicinal Chemistry, 2018, 157, 127-138.	5.5	39
28	The Structural Evolution of β-Secretase Inhibitors: A Focus on the Development of Small-Molecule Inhibitors. Current Topics in Medicinal Chemistry, 2013, 13, 1787-1807.	2.1	39
29	Characterization of COR627 and COR628, Two Novel Positive Allosteric Modulators of the GABA_B Receptor. Journal of Pharmacology and Experimental Therapeutics, 2012, 340, 529-538.	2.5	38
30	Rational design of the first difluorostatone-based PfSUB1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3582-3586.	2.2	38
31	iPSC-derived neurons profiling reveals GABAergic circuit disruption and acetylated Î±-tubulin defect which improves after iHDAC6 treatment in Rett syndrome. Experimental Cell Research, 2018, 368, 225-235.	2.6	36
32	Computational Approaches for Drug Discovery. Molecules, 2019, 24, 3061.	3.8	36
33	Structural characterization of Giardia duodenalis thioredoxin reductase (g TrxR) and computational analysis of its interaction with NBDHEX. European Journal of Medicinal Chemistry, 2017, 135, 479-490.	5.5	35
34	Role of hydrogen sulfide in cardiovascular ageing. Pharmacological Research, 2020, 160, 105125.	7.1	35
35	A Repurposing Approach for Uncovering the Anti-Tubercular Activity of FDA-Approved Drugs with Potential Multi-Targeting Profiles. Molecules, 2019, 24, 4373.	3.8	34
36	First dual AK/GSK-3Î² inhibitors endowed with antioxidant properties as multifunctional, potential neuroprotective agents. European Journal of Medicinal Chemistry, 2017, 138, 438-457.	5.5	33

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37	Telomerase-based Cancer Therapeutics: A Review on their Clinical Trials. Current Topics in Medicinal Chemistry, 2020, 20, 433-457.	2.1	33
38	Identification of Novel 3-Hydroxy-pyran-4-One Derivatives as Potent HIV-1 Integrase Inhibitors Using in silico Structure-Based Combinatorial Library Design Approach. Frontiers in Chemistry, 2019, 7, 574.	3.6	32
39	Dietary polyphenols rutin, taxifolin and quercetin related compounds target Leishmania amazonensis arginase. Food and Function, 2019, 10, 3172-3180.	4.6	32
40	Three-dimensional quantitative structureâ€“selectivity relationships analysis guided rational design of a highly selective ligand for the cannabinoid receptor 2. European Journal of Medicinal Chemistry, 2011, 46, 547-555.	5.5	31
41	Discovery of GPCR ligands for probing signal transduction pathways. Frontiers in Pharmacology, 2014, 5, 255.	3.5	31
42	Structure-activity relationships, biological evaluation and structural studies of novel pyrrolonaphthoxazepines as antitumor agents. European Journal of Medicinal Chemistry, 2019, 162, 290-320.	5.5	31
43	Pharmacophore Modeling for Qualitative Prediction of Antiestrogenic Activity. Journal of Chemical Information and Modeling, 2009, 49, 2489-2497.	5.4	30
44	Tetrahydrofuran Acetogenins from Laurencia glandulifera. Journal of Natural Products, 2009, 72, 190-193.	3.0	28
45	Quinolylhydrazones as novel inhibitors of Plasmodium falciparum serine protease PfSUB1. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5317-5321.	2.2	28
46	Synthesis and structureâ€“activity relationship studies in serotonin 5-HT1A receptor agonists based on fused pyrrolidone scaffolds. European Journal of Medicinal Chemistry, 2013, 63, 85-94.	5.5	28
47	3D-QSAR using pharmacophore-based alignment and virtual screening for discovery of novel MCF-7 cell line inhibitors. European Journal of Medicinal Chemistry, 2013, 67, 344-351.	5.5	28
48	Structure-activity relationships study of isothiocyanates for H2S releasing properties: 3-Pyridyl-isothiocyanate as a new promising cardioprotective agent. Journal of Advanced Research, 2021, 27, 41-53.	9.5	28
49	Design, Synthesis, and Pharmacological Characterization of Indol-3-ylacetamides, Indol-3-yloxoacetamides, and Indol-3-ylcarboxamides: Potent and Selective CB2 Cannabinoid Receptor Inverse Agonists. Journal of Medicinal Chemistry, 2012, 55, 5391-5402.	6.4	27
50	Synthesis and biological evaluation of fluorinated 1,5-diarylpyrrole-3-alkoxyethyl ether derivatives as selective COX-2 inhibitors endowed with anti-inflammatory activity. European Journal of Medicinal Chemistry, 2016, 109, 99-106.	5.5	27
51	Antimalarial agents against both sexual and asexual parasites stages: structure-activity relationships and biological studies of the Malaria Box compound 1-[5-(4-bromo-2-chlorophenyl)furan-2-yl]-N-[(piperidin-4-yl)methyl]methanamine (MMV019918) and analogues. European Journal of Medicinal Chemistry, 2018, 150, 698-718.	5.5	27
52	Allosteric Modulation of Ionotropic Glutamate Receptors: An Outlook on New Therapeutic Approaches To Treat Central Nervous System Disorders. ACS Medicinal Chemistry Letters, 2019, 10, 228-236.	2.8	27
53	Development of novel cyclic peptides as pro-apoptotic agents. European Journal of Medicinal Chemistry, 2016, 117, 301-320.	5.5	26
54	Screening and Phenotypical Characterization of Schistosoma mansoni Histone Deacetylase 8 (SmHDAC8) Inhibitors as Multistage Antischistosomal Agents. ACS Infectious Diseases, 2020, 6, 100-113.	3.8	26

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55	Harnessing the Role of HDAC6 in Idiopathic Pulmonary Fibrosis: Design, Synthesis, Structural Analysis, and Biological Evaluation of Potent Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 9960-9988.	6.4	26
56	Synthesis and Antiplasmodial Activity of Bicyclic Dioxanes as Simplified Dihydroplakortin Analogues. Journal of Medicinal Chemistry, 2011, 54, 5949-5953.	6.4	25
57	Spiroindoline-Capped Selective HDAC6 Inhibitors: Design, Synthesis, Structural Analysis, and Biological Evaluation. ACS Medicinal Chemistry Letters, 2020, 11, 2268-2276.	2.8	23
58	Novel quinolone-based potent and selective HDAC6 inhibitors: Synthesis, molecular modeling studies and biological investigation. European Journal of Medicinal Chemistry, 2021, 212, 112998.	5.5	22
59	Discovery of novel hit compounds as potential HDAC1 inhibitors: The case of ligand- and structure-based virtual screening. Computers in Biology and Medicine, 2021, 137, 104808.	7.0	22
60	Synthesis, Molecular Modelling and Biological Studies of 3-hydroxypyrane- 4-one and 3-hydroxy-pyridine-4-one Derivatives as HIV-1 Integrase Inhibitors. Medicinal Chemistry, 2019, 15, 755-770.	1.5	22
61	Synthesis, biological evaluation and molecular modeling of novel selective COX-2 inhibitors: sulfide, sulfoxide, and sulfone derivatives of 1,5-diarylpyrrol-3-substituted scaffold. Bioorganic and Medicinal Chemistry, 2019, 27, 115045.	3.0	21
62	Amyloid Î² fibril disruption by oleuropein aglycone: long-time molecular dynamics simulation to gain insight into the mechanism of action of this polyphenol from extra virgin olive oil. Food and Function, 2020, 11, 8122-8132.	4.6	21
63	(S)-2-Amino-3-(5-methyl-3-hydroxyisoxazol-4-yl)propanoic Acid (AMPA) and Kainate Receptor Ligands: Further Exploration of Bioisosteric Replacements and Structural and Biological Investigation. Journal of Medicinal Chemistry, 2018, 61, 2124-2130.	6.4	20
64	Cinnamic acids derived compounds with antileishmanial activity target Leishmania amazonensis arginase. Chemical Biology and Drug Design, 2019, 93, 139-146.	3.2	20
65	Targeting clinically-relevant metallo-Î²-lactamases: from high-throughput docking to broad-spectrum inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 98-109.	5.2	19
66	Phenylpyrrole-based HDAC inhibitors: synthesis, molecular modeling and biological studies. Future Medicinal Chemistry, 2016, 8, 1573-1587.	2.3	19
67	Development of Potent Inhibitors of Fatty Acid Amide Hydrolase Useful for the Treatment of Neuropathic Pain. ChemMedChem, 2018, 13, 2090-2103.	3.2	19
68	Harnessing the pyrroloquinoxaline scaffold for FAAH and MAGL interaction: definition of the structural determinants for enzyme inhibition. RSC Advances, 2016, 6, 64651-64664.	3.6	19
69	A stereoselective approach to peptidomimetic BACE1 inhibitors. European Journal of Medicinal Chemistry, 2013, 70, 233-247.	5.5	17
70	In silico study of subtilisin-like protease 1 (SUB1) from different Plasmodium species in complex with peptidyl-difluorostatones and characterization of potent pan-SUB1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 64, 121-130.	2.4	17
71	MicroRNA-Based Multitarget Approach for Alzheimerâ€™s Disease: Discovery of the First-In-Class Dual Inhibitor of Acetylcholinesterase and MicroRNA-15b Biogenesis. Journal of Medicinal Chemistry, 2020, 63, 9695-9704.	6.4	17
72	H2S donating corticosteroids: Design, synthesis and biological evaluation in a murine model of asthma. Journal of Advanced Research, 2022, 35, 267-277.	9.5	17

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73	Covalent Reversible Inhibitors of Cysteine Proteases Containing the Nitrile Warhead: Recent Advancement in the Field of Viral and Parasitic Diseases. Molecules, 2022, 27, 2561.	3.8	17
74	Plasmodium falciparum subtilisin-like protease 1: discovery of potent difluorostatone-based inhibitors. RSC Advances, 2015, 5, 22431-22448.	3.6	15
75	Exploring clotrimazole-based pharmacophore: 3D-QSAR studies and synthesis of novel antiplasmodial agents. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5412-5418.	2.2	15
76	Synthesis and Biological Evaluation of Novel Neuroprotective Pyridazine Derivatives as Excitatory Amino Acid Transporter 2 (EAAT2) Activators. Journal of Medicinal Chemistry, 2017, 60, 5216-5221.	6.4	15
77	Cinnamides Target Leishmania amazonensis Arginase Selectively. Molecules, 2020, 25, 5271.	3.8	15
78	Computer-Driven Development of an in Silico Tool for Finding Selective Histone Deacetylase 1 Inhibitors. Molecules, 2020, 25, 1952.	3.8	15
79	Synthesis and biological evaluation of a new class of benzothiazines as neuroprotective agents. European Journal of Medicinal Chemistry, 2017, 126, 614-630.	5.5	14
80	Development of novel multipotent compounds modulating endocannabinoid and dopaminergic systems. European Journal of Medicinal Chemistry, 2019, 183, 111674.	5.5	14
81	From (+)-epigallocatechin gallate to a simplified synthetic analogue as a cytoadherence inhibitor for P. falciparum. RSC Advances, 2014, 4, 4769-4781.	3.6	13
82	Activation of the Wnt Pathway by Small Peptides: Rational Design, Synthesis and Biological Evaluation. ChemMedChem, 2017, 12, 2074-2085.	3.2	13
83	Bridged bicyclic 2,3-dioxabicyclo[3.3.1]nonanes as antiplasmodial agents: Synthesis, structure-activity relationships and studies on their biomimetic reaction with Fe(II). Bioorganic Chemistry, 2019, 89, 103020.	4.1	13
84	Selective Fatty Acid Amide Hydrolase Inhibitors as Potential Novel Antiepileptic Agents. ACS Chemical Neuroscience, 2021, 12, 1716-1736.	3.5	12
85	Development of HuperTacrines as Non-Toxic, Cholinesterase Inhibitors for the Potential Treatment of Alzheimerâ€™s Disease. Mini-Reviews in Medicinal Chemistry, 2015, 15, 648-658.	2.4	12
86	Virtual Combinatorial Library Screening of Quinadoline B Derivatives against SARS-CoV-2 RNA-Dependent RNA Polymerase. Computation, 2022, 10, 7.	2.0	12
87	Azetidin-2-one-based small molecules as dual hHDAC6/HDAC8 inhibitors: Investigation of their mechanism of action and impact of dual inhibition profile on cell viability. European Journal of Medicinal Chemistry, 2022, 238, 114409.	5.5	11
88	Dealing with schistosomiasis: Current drug discovery strategies. Annual Reports in Medicinal Chemistry, 2019, 53, 107-138.	0.9	10
89	Myxobacterial depsipeptide chondramides interrupt SARS-CoV-2 entry by targeting its broad, cell tropic spike protein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12209-12220.	3.5	10
90	In silico analysis of RNA-dependent RNA polymerase of the SARS-CoV-2 and therapeutic potential of existing antiviral drugs. Computers in Biology and Medicine, 2021, 135, 104591.	7.0	9

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91	Offâ€target ACE2 ligands: Possible therapeutic option for CoVidâ€19?. British Journal of Clinical Pharmacology, 2020, 86, 1178-1179.	2.4	8
92	Ionotropic Glutamate Receptor GluA2 in Complex with Bicyclic Pyrimidinedione-Based Compounds: When Small Compound Modifications Have Distinct Effects on Binding Interactions. ACS Chemical Neuroscience, 2020, 11, 1791-1800.	3.5	8
93	HCV-targeted Antivirals: Current Status and Future Challenges. Current Pharmaceutical Design, 2014, 20, 3445-3464.	1.9	8
94	A light in the dark: state of the art and perspectives in optogenetics and optopharmacology for restoring vision. Future Medicinal Chemistry, 2019, 11, 463-487.	2.3	7
95	Design and synthesis of multifunctional microtubule targeting agents endowed with dual pro-apoptotic and anti-autophagic efficacy. European Journal of Medicinal Chemistry, 2022, 235, 114274.	5.5	6
96	Development of a practical and scalable route for the preparation of the deacetoxytubuvaline (dTuv) fragment of pretubulysin and analogs. Tetrahedron Letters, 2016, 57, 920-923.	1.4	5
97	A Jocic-type approach for a practical and scalable synthesis of pyrrolonaphthoxazepine (PNOX)-based potent proapoptotic agents. Tetrahedron Letters, 2018, 59, 4466-4470.	1.4	5
98	Development of In Vitro Corneal Models: Opportunity for Pharmacological Testing. Methods and Protocols, 2020, 3, 74.	2.0	5
99	Identification of novel SIRT1 activators endowed with cardioprotective profile. European Journal of Pharmaceutical Sciences, 2021, 165, 105930.	4.0	5
100	Design, synthesis and biological evaluation of 7-substituted 4-phenyl-6H-imidazo[1,5-a]thieno[3,2-f][1,4]diazepines as safe anxiolytic agents. European Journal of Medicinal Chemistry, 2020, 200, 112405.	5.5	4
101	Computer-Based Approaches for Determining the Pharmacological Profile of 5-(3-Nitro-Arylidene)-Thiazolidine-2,4-Dione. Biointerface Research in Applied Chemistry, 2021, 11, 13806-13828.	1.0	3
102	Design and Synthesis of New Oligopeptidic Parvulin Inhibitors. ChemMedChem, 2022, , .	3.2	3
103	In Silico Analysis of Peptide-Based Derivatives Containing Bifunctional Warheads Engaging Prime and Non-Prime Subsites to Covalent Binding SARS-CoV-2 Main Protease (Mpro). Computation, 2022, 10, 69.	2.0	3
104	Artificial Intelligence in Translational Medicine. International Journal of Translational Medicine, 2021, 1, 223-285.	0.4	2
105	Pro-Apoptotic Activity of the Marine Sponge Dactylospongia elegans Metabolites Pelorol and 5-epi-Ilimaquinone on Human 501Mel Melanoma Cells. Marine Drugs, 2022, 20, 427.	4.6	2
106	Synthetic studies toward bicyclic endoperoxides presenting polar side chains. Tetrahedron Letters, 2018, 59, 4330-4333.	1.4	1
107	Breakthroughs in Computational Approaches for Drug Discovery. Journal of Drug Research and Development, 2017, 3, .	0.2	1
108	Abstract 411: Discovery and Cardioprotective Effects of the First Non-peptide Agonists of Prokineticin Receptor-1. Circulation Research, 2015, 117, .	4.5	0

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109	Discovery of Iminobenzimidazole Derivatives as Novel Cytotoxic Agents. Open Medicinal Chemistry Journal, 2018, 12, 74-83.	2.4	0