

Simone Brogi

List of Publications by Year in descending order

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109
papers

3,117
citations

126708

33
h-index

214527

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. <i>Progress in Neurobiology</i> , 2017, 151, 4-34.	2.8	128
2	Editorial: In silico Methods for Drug Design and Discovery. <i>Frontiers in Chemistry</i> , 2020, 8, 612.	1.8	117
3	Improving Curcumin Bioavailability: Current Strategies and Future Perspectives. <i>Pharmaceutics</i> , 2021, 13, 1715.	2.0	88
4	Donepezil-like multifunctional agents: Design, synthesis, molecular modeling and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2016, 121, 864-879.	2.6	80
5	Development and Pharmacological Characterization of Selective Blockers of 2-Arachidonoyl Glycerol Degradation with Efficacy in Rodent Models of Multiple Sclerosis and Pain. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 2612-2632.	2.9	70
6	Old but Gold: Tracking the New Guise of Histone Deacetylase 6 (HDAC6) Enzyme as a Biomarker and Therapeutic Target in Rare Diseases. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 23-39.	2.9	69
7	Dopamine D3 Receptor Antagonists as Potential Therapeutics for the Treatment of Neurological Diseases. <i>Frontiers in Neuroscience</i> , 2016, 10, 451.	1.4	66
8	Role of hydrogen sulfide in endothelial dysfunction: Pathophysiology and therapeutic approaches. <i>Journal of Advanced Research</i> , 2021, 27, 99-113.	4.4	64
9	Anti-inflammatory and antiviral roles of hydrogen sulfide: Rationale for considering H ₂ S donors in COVID-19 therapy. <i>British Journal of Pharmacology</i> , 2020, 177, 4931-4941.	2.7	63
10	Mimicking the Intramolecular Hydrogen Bond: Synthesis, Biological Evaluation, and Molecular Modeling of Benzoxazines and Quinazolines as Potential Antimalarial Agents. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 10387-10404.	2.9	58
11	Structure-based discovery of the first non-covalent inhibitors of <i>Leishmania major</i> trypanothione peroxidase by high throughput docking. <i>Scientific Reports</i> , 2015, 5, 9705.	1.6	58
12	Polypharmacology of dopamine receptor ligands. <i>Progress in Neurobiology</i> , 2016, 142, 68-103.	2.8	57
13	Computational Tool for Fast in silico Evaluation of hERG K ⁺ Channel Affinity. <i>Frontiers in Chemistry</i> , 2017, 5, 7.	1.8	52
14	The Citrus Flavonoid Naringenin Protects the Myocardium from Ageing-Dependent Dysfunction: Potential Role of SIRT1. <i>Oxidative Medicine and Cellular Longevity</i> , 2020, 2020, 1-15.	1.9	52
15	Disease-Modifying Anti-Alzheimer's Drugs: Inhibitors of Human Cholinesterases Interfering with Amyloid Aggregation. <i>CNS Neuroscience and Therapeutics</i> , 2014, 20, 624-632.	1.9	51
16	Organic Isothiocyanates as Hydrogen Sulfide Donors. <i>Antioxidants and Redox Signaling</i> , 2020, 32, 110-144.	2.5	51
17	Discovery and Cardioprotective Effects of the First Non-Peptide Agonists of the G Protein-Coupled Prokineticin Receptor-1. <i>PLoS ONE</i> , 2015, 10, e0121027.	1.1	50
18	Verbascoside Inhibits Promastigote Growth and Arginase Activity of <i>Leishmania amazonensis</i> . <i>Journal of Natural Products</i> , 2016, 79, 1459-1463.	1.5	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. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9578-9597.	2.9	46
20	Optimization of 4-Aminoquinoline/Clotrimazole-Based Hybrid Antimalarials: Further Structure-Activity Relationships, in Vivo Studies, and Preliminary Toxicity Profiling. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6948-6967.	2.9	43
21	Novel Analgesic/Anti-Inflammatory Agents: 1,5-Diarylpyrrole Nitrooxyalkyl Ethers and Related Compounds as Cyclooxygenase-2 Inhibiting Nitric Oxide Donors. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 3191-3206.	2.9	43
22	Development of Potent Inhibitors of the <i>Mycobacterium tuberculosis</i> Virulence Factor Zmp1 and Evaluation of Their Effect on Mycobacterial Survival inside Macrophages. <i>ChemMedChem</i> , 2018, 13, 422-430.	1.6	43
23	An integrated in silico screening strategy for identifying promising disruptors of p53-MDM2 interaction. <i>Computational Biology and Chemistry</i> , 2019, 83, 107105.	1.1	42
24	Multifunctional Cholinesterase and Amyloid Beta Fibrillization Modulators. Synthesis and Biological Investigation. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 1178-1182.	1.3	40
25	Synthetic spirocyclic endoperoxides: new antimalarial scaffolds. <i>MedChemComm</i> , 2015, 6, 357-362.	3.5	39
26	Identification of novel fluorescent probes preventing PrP Sc replication in prion diseases. <i>European Journal of Medicinal Chemistry</i> , 2017, 127, 859-873.	2.6	39
27	Novel spiroindoline HDAC inhibitors: Synthesis, molecular modelling and biological studies. <i>European Journal of Medicinal Chemistry</i> , 2018, 157, 127-138.	2.6	39
28	The Structural Evolution of β -Secretase Inhibitors: A Focus on the Development of Small-Molecule Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 1787-1807.	1.0	39
29	Characterization of COR627 and COR628, Two Novel Positive Allosteric Modulators of the GABA _B Receptor. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2012, 340, 529-538.	1.3	38
30	Rational design of the first difluorostatone-based PfSUB1 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014, 24, 3582-3586.	1.0	38
31	iPSC-derived neurons profiling reveals GABAergic circuit disruption and acetylated β -tubulin defect which improves after iHDAC6 treatment in Rett syndrome. <i>Experimental Cell Research</i> , 2018, 368, 225-235.	1.2	36
32	Computational Approaches for Drug Discovery. <i>Molecules</i> , 2019, 24, 3061.	1.7	36
33	Structural characterization of <i>Giardia duodenalis</i> thioredoxin reductase (g TrxR) and computational analysis of its interaction with NBDHEX. <i>European Journal of Medicinal Chemistry</i> , 2017, 135, 479-490.	2.6	35
34	Role of hydrogen sulfide in cardiovascular ageing. <i>Pharmacological Research</i> , 2020, 160, 105125.	3.1	35
35	A Repurposing Approach for Uncovering the Anti-Tubercular Activity of FDA-Approved Drugs with Potential Multi-Targeting Profiles. <i>Molecules</i> , 2019, 24, 4373.	1.7	34
36	First dual AK/GSK-3 β inhibitors endowed with antioxidant properties as multifunctional, potential neuroprotective agents. <i>European Journal of Medicinal Chemistry</i> , 2017, 138, 438-457.	2.6	33

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37	Telomerase-based Cancer Therapeutics: A Review on their Clinical Trials. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 433-457.	1.0	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. <i>Frontiers in Chemistry</i> , 2019, 7, 574.	1.8	32
39	Dietary polyphenols rutin, taxifolin and quercetin related compounds target <i>Leishmania amazonensis</i> arginase. <i>Food and Function</i> , 2019, 10, 3172-3180.	2.1	32
40	Three-dimensional quantitative structure–selectivity relationships analysis guided rational design of a highly selective ligand for the cannabinoid receptor 2. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 547-555.	2.6	31
41	Discovery of GPCR ligands for probing signal transduction pathways. <i>Frontiers in Pharmacology</i> , 2014, 5, 255.	1.6	31
42	Structure-activity relationships, biological evaluation and structural studies of novel pyrrolonaphthoxazepines as antitumor agents. <i>European Journal of Medicinal Chemistry</i> , 2019, 162, 290-320.	2.6	31
43	Pharmacophore Modeling for Qualitative Prediction of Antiestrogenic Activity. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2489-2497.	2.5	30
44	Tetrahydrofuran Acetogenins from <i>Laurencia glandulifera</i> . <i>Journal of Natural Products</i> , 2009, 72, 190-193.	1.5	28
45	Quinolyldrazones as novel inhibitors of Plasmodium falciparum serine protease PfSUB1. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 5317-5321.	1.0	28
46	Synthesis and structure–activity relationship studies in serotonin 5-HT1A receptor agonists based on fused pyrrolidone scaffolds. <i>European Journal of Medicinal Chemistry</i> , 2013, 63, 85-94.	2.6	28
47	3D-QSAR using pharmacophore-based alignment and virtual screening for discovery of novel MCF-7 cell line inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2013, 67, 344-351.	2.6	28
48	Structure-activity relationships study of isothiocyanates for H2S releasing properties: 3-Pyridyl-isothiocyanate as a new promising cardioprotective agent. <i>Journal of Advanced Research</i> , 2021, 27, 41-53.	4.4	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. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5391-5402.	2.9	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. <i>European Journal of Medicinal Chemistry</i> , 2016, 109, 99-106.	2.6	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. <i>European Journal of Medicinal Chemistry</i> , 2018, 150, 698-718.	2.6	27
52	Allosteric Modulation of Ionotropic Glutamate Receptors: An Outlook on New Therapeutic Approaches To Treat Central Nervous System Disorders. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 228-236.	1.3	27
53	Development of novel cyclic peptides as pro-apoptotic agents. <i>European Journal of Medicinal Chemistry</i> , 2016, 117, 301-320.	2.6	26
54	Screening and Phenotypical Characterization of <i>Schistosoma mansoni</i> Histone Deacetylase 8 (HDAC8) Inhibitors as Multistage Antischistosomal Agents. <i>ACS Infectious Diseases</i> , 2020, 6, 100-113.	1.8	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. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 9960-9988.	2.9	26
56	Synthesis and Antiplasmodial Activity of Bicyclic Dioxanes as Simplified Dihydroplakortin Analogues. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 5949-5953.	2.9	25
57	Spiroindoline-Capped Selective HDAC6 Inhibitors: Design, Synthesis, Structural Analysis, and Biological Evaluation. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 2268-2276.	1.3	23
58	Novel quinolone-based potent and selective HDAC6 inhibitors: Synthesis, molecular modeling studies and biological investigation. <i>European Journal of Medicinal Chemistry</i> , 2021, 212, 112998.	2.6	22
59	Discovery of novel hit compounds as potential HDAC1 inhibitors: The case of ligand- and structure-based virtual screening. <i>Computers in Biology and Medicine</i> , 2021, 137, 104808.	3.9	22
60	Synthesis, Molecular Modelling and Biological Studies of 3-hydroxypyran-4-one and 3-hydroxy-pyridine-4-one Derivatives as HIV-1 Integrase Inhibitors. <i>Medicinal Chemistry</i> , 2019, 15, 755-770.	0.7	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. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 115045.	1.4	21
62	Amyloid β 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. <i>Food and Function</i> , 2020, 11, 8122-8132.	2.1	21
63	(<i>S</i>)-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. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 2124-2130.	2.9	20
64	Cinnamic acids derived compounds with antileishmanial activity target <i>Leishmania amazonensis</i> arginase. <i>Chemical Biology and Drug Design</i> , 2019, 93, 139-146.	1.5	20
65	Targeting clinically-relevant metallo- β -lactamases: from high-throughput docking to broad-spectrum inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 98-109.	2.5	19
66	Phenylpyrrole-based HDAC inhibitors: synthesis, molecular modeling and biological studies. <i>Future Medicinal Chemistry</i> , 2016, 8, 1573-1587.	1.1	19
67	Development of Potent Inhibitors of Fatty Acid Amide Hydrolase Useful for the Treatment of Neuropathic Pain. <i>ChemMedChem</i> , 2018, 13, 2090-2103.	1.6	19
68	Harnessing the pyrroloquinoxaline scaffold for FAAH and MAGL interaction: definition of the structural determinants for enzyme inhibition. <i>RSC Advances</i> , 2016, 6, 64651-64664.	1.7	19
69	A stereoselective approach to peptidomimetic BACE1 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2013, 70, 233-247.	2.6	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. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 64, 121-130.	1.3	17
71	MicroRNA-Based Multitarget Approach for Alzheimer's Disease: Discovery of the First-In-Class Dual Inhibitor of Acetylcholinesterase and MicroRNA-15b Biogenesis. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 9695-9704.	2.9	17
72	H2S donating corticosteroids: Design, synthesis and biological evaluation in a murine model of asthma. <i>Journal of Advanced Research</i> , 2022, 35, 267-277.	4.4	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. <i>Molecules</i> , 2022, 27, 2561.	1.7	17
74	<i>Plasmodium falciparum</i> subtilisin-like protease 1: discovery of potent difluorostatone-based inhibitors. <i>RSC Advances</i> , 2015, 5, 22431-22448.	1.7	15
75	Exploring clotrimazole-based pharmacophore: 3D-QSAR studies and synthesis of novel antiplasmodial agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 5412-5418.	1.0	15
76	Synthesis and Biological Evaluation of Novel Neuroprotective Pyridazine Derivatives as Excitatory Amino Acid Transporter 2 (EAAT2) Activators. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5216-5221.	2.9	15
77	Cinnamides Target <i>Leishmania amazonensis</i> Arginase Selectively. <i>Molecules</i> , 2020, 25, 5271.	1.7	15
78	Computer-Driven Development of an in Silico Tool for Finding Selective Histone Deacetylase 1 Inhibitors. <i>Molecules</i> , 2020, 25, 1952.	1.7	15
79	Synthesis and biological evaluation of a new class of benzothiazines as neuroprotective agents. <i>European Journal of Medicinal Chemistry</i> , 2017, 126, 614-630.	2.6	14
80	Development of novel multipotent compounds modulating endocannabinoid and dopaminergic systems. <i>European Journal of Medicinal Chemistry</i> , 2019, 183, 111674.	2.6	14
81	From (+)-epigallocatechin gallate to a simplified synthetic analogue as a cytoadherence inhibitor for <i>P. falciparum</i> . <i>RSC Advances</i> , 2014, 4, 4769-4781.	1.7	13
82	Activation of the Wnt Pathway by Small Peptides: Rational Design, Synthesis and Biological Evaluation. <i>ChemMedChem</i> , 2017, 12, 2074-2085.	1.6	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). <i>Bioorganic Chemistry</i> , 2019, 89, 103020.	2.0	13
84	Selective Fatty Acid Amide Hydrolase Inhibitors as Potential Novel Antiepileptic Agents. <i>ACS Chemical Neuroscience</i> , 2021, 12, 1716-1736.	1.7	12
85	Development of HuperTacrines as Non-Toxic, Cholinesterase Inhibitors for the Potential Treatment of Alzheimer's Disease. <i>Mini-Reviews in Medicinal Chemistry</i> , 2015, 15, 648-658.	1.1	12
86	Virtual Combinatorial Library Screening of Quinadoline B Derivatives against SARS-CoV-2 RNA-Dependent RNA Polymerase. <i>Computation</i> , 2022, 10, 7.	1.0	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. <i>European Journal of Medicinal Chemistry</i> , 2022, 238, 114409.	2.6	11
88	Dealing with schistosomiasis: Current drug discovery strategies. <i>Annual Reports in Medicinal Chemistry</i> , 2019, 53, 107-138.	0.5	10
89	Myxobacterial depsipeptide chondramides interrupt SARS-CoV-2 entry by targeting its broad, cell tropic spike protein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12209-12220.	2.0	10
90	In silico analysis of RNA-dependent RNA polymerase of the SARS-CoV-2 and therapeutic potential of existing antiviral drugs. <i>Computers in Biology and Medicine</i> , 2021, 135, 104591.	3.9	9

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91	Off-target ACE2 ligands: Possible therapeutic option for COVID-19?. <i>British Journal of Clinical Pharmacology</i> , 2020, 86, 1178-1179.	1.1	8
92	Ionotropic Glutamate Receptor GluA2 in Complex with Bicyclic Pyrimidinedione-Based Compounds: When Small Compound Modifications Have Distinct Effects on Binding Interactions. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1791-1800.	1.7	8
93	HCV-targeted Antivirals: Current Status and Future Challenges. <i>Current Pharmaceutical Design</i> , 2014, 20, 3445-3464.	0.9	8
94	A light in the dark: state of the art and perspectives in optogenetics and optopharmacology for restoring vision. <i>Future Medicinal Chemistry</i> , 2019, 11, 463-487.	1.1	7
95	Design and synthesis of multifunctional microtubule targeting agents endowed with dual pro-apoptotic and anti-autophagic efficacy. <i>European Journal of Medicinal Chemistry</i> , 2022, 235, 114274.	2.6	6
96	Development of a practical and scalable route for the preparation of the deacetyltubuvaine (dTuv) fragment of pretubulysin and analogs. <i>Tetrahedron Letters</i> , 2016, 57, 920-923.	0.7	5
97	A Jovic-type approach for a practical and scalable synthesis of pyrrolonaphthoxazepine (PNOX)-based potent proapoptotic agents. <i>Tetrahedron Letters</i> , 2018, 59, 4466-4470.	0.7	5
98	Development of In Vitro Corneal Models: Opportunity for Pharmacological Testing. <i>Methods and Protocols</i> , 2020, 3, 74.	0.9	5
99	Identification of novel SIRT1 activators endowed with cardioprotective profile. <i>European Journal of Pharmaceutical Sciences</i> , 2021, 165, 105930.	1.9	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. <i>European Journal of Medicinal Chemistry</i> , 2020, 200, 112405.	2.6	4
101	Computer-Based Approaches for Determining the Pharmacological Profile of 5-(3-Nitro-Arylidene)-Thiazolidine-2,4-Dione. <i>Biointerface Research in Applied Chemistry</i> , 2021, 11, 13806-13828.	1.0	3
102	Design and Synthesis of New Oligopeptidic Parvulin Inhibitors. <i>ChemMedChem</i> , 2022, , .	1.6	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). <i>Computation</i> , 2022, 10, 69.	1.0	3
104	Artificial Intelligence in Translational Medicine. <i>International Journal of Translational Medicine</i> , 2021, 1, 223-285.	0.1	2
105	Pro-Apoptotic Activity of the Marine Sponge <i>Dactylospongia elegans</i> Metabolites Pelorol and 5-epi-llimaquinone on Human 501Mel Melanoma Cells. <i>Marine Drugs</i> , 2022, 20, 427.	2.2	2
106	Synthetic studies toward bicyclic endoperoxides presenting polar side chains. <i>Tetrahedron Letters</i> , 2018, 59, 4330-4333.	0.7	1
107	Breakthroughs in Computational Approaches for Drug Discovery. <i>Journal of Drug Research and Development</i> , 2017, 3, .	0.2	1
108	Abstract 411: Discovery and Cardioprotective Effects of the First Non-peptide Agonists of Prokineticin Receptor-1. <i>Circulation Research</i> , 2015, 117, .	2.0	0

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109	Discovery of Iminobenzimidazole Derivatives as Novel Cytotoxic Agents. Open Medicinal Chemistry Journal, 2018, 12, 74-83.	0.9	0