Giovanni Bottegoni

List of Publications by Year
in descending order

62	3,756	147566 31	128067 60
papers	citations	h-index	g-index

68	68	68	8134
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dopamine D3 receptor ligands: a patent review (2014â€“2020). Expert Opinion on Therapeutic Patents, 2022, 32, 605-627.	2.4	1
2	The multitarget FAAH inhibitor/D3 partial agonist ARN15381 decreases nicotine self-administration in male rats. European Journal of Pharmacology, 2022, 928, 175088.	1.7	4
3	Discovery and SAR Evolution of Pyrazole Azabicyclo[3.2.1]octane Sulfonamides as a Novel Class of Non-Covalent N-Acylethanolamine-Hydrolyzing Acid Amidase (NAAA) Inhibitors for Oral Administration. Journal of Medicinal Chemistry, 2021, 64, 13327-13355.	2.9	6
4	Inflammation causes remodeling of mitochondrial cytochrome c oxidase mediated by the bifunctional gene C15orf48. Science Advances, 2021, 7, eabl5182.	4.7	29
5	Multi-target dopamine D3 receptor modulators: Actionable knowledge for drug design from molecular dynamics and machine learning. European Journal of Medicinal Chemistry, 2020, 188, 111975.	2.6	19
6	Multitarget Compounds for Bipolar Disorder: From Rational Design to Preliminary Pharmacokinetic Evaluation. ChemMedChem, 2020, 15, 949-954.	1.6	4
7	A Triazolotriazineâ€Based Dual GSKâ€3Î²/CKâ€1Î´ Ligand as a Potential Neuroprotective Agent Presenting Two Different Mechanisms of Enzymatic Inhibition. ChemMedChem, 2019, 14, 310-314.	1.6	22
8	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 219-224.	2.5	48
9	Structure of the complement C5a receptor bound to the extra-helical antagonist NDT9513727. Nature, 2018, 553, 111-114.	13.7	110
10	BACE-1 Inhibitors: From Recent Single-Target Molecules to Multitarget Compounds for Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2018, 61, 619-637.	2.9	90
11	Design, Synthesis, Structureâ€“Activity Relationship Studies, and Three-Dimensional Quantitative Structureâ€“Activity Relationship (3D-QSAR) Modeling of a Series of O-Biphenyl Carbamates as Dual Modulators of Dopamine D3 Receptor and Fatty Acid Amide Hydrolase. Journal of Medicinal Chemistry, 2017, 60, 2287-2304.	2.9	28
12	Multitarget drug design strategy in Alzheimer's disease: focus on cholinergic transmission and amyloid-Î² aggregation. Future Medicinal Chemistry, 2017, 9, 953-963.	1.1	19
13	Computational Methods in Multitarget Drug Discovery. , 2017, , 239-258.		3
14	Molecular Dynamics Simulations and Kinetic Measurements to Estimate and Predict Proteinâ€“Ligand Residence Times. Journal of Medicinal Chemistry, 2016, 59, 7167-7176.	2.9	81
15	Development and Application of a Virtual Screening Protocol for the Identification of Multitarget Fragments. ChemMedChem, 2016, 11, 1259-1263.	1.6	18
16	Pyrazole-Based Acid Ceramidase Inhibitors: Design, Synthesis, and Structureâ€“Activity Relationships. Synthesis, 2016, 48, 2739-2756.	1.2	4
17	Role of Molecular Dynamics and Related Methods in Drug Discovery. Journal of Medicinal Chemistry, 2016, 59, 4035-4061.	2.9	797
18	Aryl and heteroaryl N-[4-[4-(2,3-substituted-phenyl)piperazine-1-yl]alkyl]carbamates with improved physico-chemical properties as dual modulators of dopamine D3 receptor and fatty acid amide hydrolase. MedChemComm, 2016, 7, 537-541.	3.5	4

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19	Versatility of the Curcumin Scaffold: Discovery of Potent and Balanced Dual BACE-1 and GSK-3Î² Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 531-544.	2.9	100
20	Kinetic and Structural Insights into the Mechanism of Binding of Sulfonamides to Human Carbonic Anhydrase by Computational and Experimental Studies. Journal of Medicinal Chemistry, 2016, 59, 4245-4256.	2.9	60
21	Mapping Cholesterol Interaction Sites on Serotonin Transporter through Coarse-Grained Molecular Dynamics. PLoS ONE, 2016, 11, e0166196.	1.1	29
22	Diaryl Urea: A Privileged Structure in Anticancer Agents. Current Medicinal Chemistry, 2016, 23, 1528-1548.	1.2	47
23	The ligand binding mechanism to purine nucleoside phosphorylase elucidated via molecular dynamics and machine learning. Nature Communications, 2015, 6, 6155.	5.8	98
24	Dual inhibition of REV-ERBÎ² and autophagy as a novel pharmacological approach to induce cytotoxicity in cancer cells. Oncogene, 2015, 34, 2597-2608.	2.6	100
25	3,4-Dihydro-1,3,5-triazin-2(1H)-ones as the First Dual BACE-1/GSK-3Î² Fragment Hits against Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2015, 6, 1665-1682.	1.7	54
26	Structure-Based Predictions of Activity Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 1062-1076.	2.5	34
27	Modeling lipid raft domains containing a mono-unsaturated phosphatidylethanolamine species. RSC Advances, 2015, 5, 37102-37111.	1.7	6
28	Multitarget Drug Discovery for Alzheimer's Disease: Triazinones as BACEâ€1 and GSKâ€3Î² Inhibitors. Angewandte Chemie - International Edition, 2015, 54, 1578-1582.	7.2	107
29	Multi-Kinase Inhibitors. Current Medicinal Chemistry, 2015, 22, 695-712.	1.2	61
30	Fluorinated benzophenone derivatives: Balanced multipotent agents for Alzheimer's disease. European Journal of Medicinal Chemistry, 2014, 78, 157-166.	2.6	21
31	Describing the Conformational Landscape of Small Organic Molecules through Gaussian Mixtures in Dihedral Space. Journal of Chemical Theory and Computation, 2014, 10, 2557-2568.	2.3	10
32	Synthesis, Biological Evaluation, and 3D QSAR Study of 2-Methyl-4-oxo-3-oxetanylcarbamic Acid Esters as N-Acylethanolamine Acid Amidase (NAAA) Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 10101-10111.	2.9	13
33	Applying a multitarget rational drug design strategy: the first set of modulators with potent and balanced activity toward dopamine D3 receptor and fatty acid amide hydrolase. Chemical Communications, 2014, 50, 4904-4907.	2.2	23
34	Benzimidazole Derivatives as Kinase Inhibitors. Current Medicinal Chemistry, 2014, 21, 2284-2298.	1.2	21
35	Discovery of a New Class of Highly Potent Inhibitors of Acid Ceramidase: Synthesis and Structureâ€“Activity Relationship (SAR). Journal of Medicinal Chemistry, 2013, 56, 3518-3530.	2.9	41
36	Anandamide transport inhibition by <scp>ARN</scp>272 attenuates nauseaâ€induced behaviour in rats, and vomiting in shrews (<scp>S</scp>uncus murinus). British Journal of Pharmacology, 2013, 170, 1130-1136.	2.7	12

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37	Low molecular weight, non-peptidic agonists of TrkA receptor with NGF-mimetic activity. Cell Death and Disease, 2012, 3, e339-e339.	2.7	48
38	Combining Galantamine and Memantine in Multitargeted, New Chemical Entities Potentially Useful in Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2012, 55, 9708-9721.	2.9	129
39	A catalytically silent FAAH-1 variant drives anandamide transport in neurons. Nature Neuroscience, 2012, 15, 64-69.	7.1	150
40	Polo-Like Kinases Inhibitors. Current Medicinal Chemistry, 2012, 19, 3937-3948.	1.2	26
41	Combining Dyad Protonation and Active Site Plasticity in BACE-1 Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2012, 52, 1079-1085.	2.5	22
42	The role of fragment-based and computational methods in polypharmacology. Drug Discovery Today, 2012, 17, 23-34.	3.2	110
43	Application of Conformational Clustering in Proteinâ€“Ligand Docking. Methods in Molecular Biology, 2012, 819, 169-186.	0.4	7
44	SERAPhiC: A Benchmark for in Silico Fragment-Based Drug Design. Journal of Chemical Information and Modeling, 2011, 51, 2882-2896.	2.5	20
45	Cyclin-dependent kinases: bridging their structure and function through computations. Future Medicinal Chemistry, 2011, 3, 1551-1559.	1.1	19
46	Synthesis of Monomeric Derivatives To Probe Memoquinâ€™s Bivalent Interactions. Journal of Medicinal Chemistry, 2011, 54, 8299-8304.	2.9	27
47	Systematic Exploitation of Multiple Receptor Conformations for Virtual Ligand Screening. PLoS ONE, 2011, 6, e18845.	1.1	82
48	Protein-ligand docking. Frontiers in Bioscience - Landmark, 2011, 16, 2289.	3.0	17
49	Benzophenone-based derivatives: A novel series of potent and selective dual inhibitors of acetylcholinesterase and acetylcholinesterase-induced beta-amyloid aggregation. European Journal of Medicinal Chemistry, 2011, 46, 1682-1693.	2.6	43
50	Irreversible Protein Kinase Inhibitors. Current Medicinal Chemistry, 2011, 18, 2981-2994.	1.2	67
51	Recipes for the Selection of Experimental Protein Conformations for Virtual Screening. Journal of Chemical Information and Modeling, 2010, 50, 186-193.	2.5	160
52	Non-ATP Competitive Protein Kinase Inhibitors. Current Medicinal Chemistry, 2010, 17, 2804-2821.	1.2	108
53	Small Molecule Aurora Kinases Inhibitors. Current Medicinal Chemistry, 2009, 16, 1949-1963.	1.2	42
54	Consistent Improvement of Cross-Docking Results Using Binding Site Ensembles Generated with Elastic Network Normal Modes. Journal of Chemical Information and Modeling, 2009, 49, 716-725.	2.5	106

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55	Four-Dimensional Docking: A Fast and Accurate Account of Discrete Receptor Flexibility in Ligand Docking. Journal of Medicinal Chemistry, 2009, 52, 397-406.	2.9	172
56	A new method for ligand docking to flexible receptors by dual alanine scanning and refinement (SCARE). Journal of Computer-Aided Molecular Design, 2008, 22, 311-325.	1.3	74
57	A Comparative Study on the Application of Hierarchicalâ^'Agglomerative Clustering Approaches to Organize Outputs of Reiterated Docking Runs. Journal of Chemical Information and Modeling, 2006, 46, 852-862.	2.5	52
58	AClAP, Autonomous hierarchical agglomerative Cluster Analysis based protocol to partition conformational datasets. Bioinformatics, 2006, 22, e58-e65.	1.8	41
59	(38) Computational approaches to the study of dual-site and peripheral site binding ache inhibitors. Chemico-Biological Interactions, 2005, 157-158, 414-415.	1.7	0
60	Role of phosphorylated Thr160 for the activation of the CDK2/Cyclin A complex. Proteins: Structure, Function and Bioinformatics, 2005, 62, 89-98.	1.5	16
61	In silico antitarget screening. Drug Discovery Today: Technologies, 2004, 1, 209-215.	4.0	24
62	A Computational Study of the Binding of Propidium to the Peripheral Anionic Site of Human Acetylcholinesterase. Journal of Medicinal Chemistry, 2004, 47, 3991-3999.	2.9	61