# 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 | Role of Molecular Dynamics and Related Methods in Drug Discovery. Journal of Medicinal Chemistry, 2016, 59, 4035-4061. | 2.9 | 797 |
| 2 | 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 |
| 3 | Recipes for the Selection of Experimental Protein Conformations for Virtual Screening. Journal of Chemical Information and Modeling, 2010, 50, 186-193. | 2.5 | 160 |
| 4 | A catalytically silent FAAH-1 variant drives anandamide transport in neurons. Nature Neuroscience, 2012, 15, 64-69. | 7.1 | 150 |
| 5 | 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 |
| 6 | The role of fragment-based and computational methods in polypharmacology. Drug Discovery Today, 2012, 17, 23-34. | 3.2 | 110 |
| 7 | Structure of the complement C5a receptor bound to the extra-helical antagonist NDT9513727. Nature, 2018, 553, 111-114. | 13.7 | 110 |
| 8 | Non-ATP Competitive Protein Kinase Inhibitors. Current Medicinal Chemistry, 2010, 17, 2804-2821. | 1.2 | 108 |
| 9 | 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 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | The ligand binding mechanism to purine nucleoside phosphorylase elucidated via molecular dynamics and machine learning. Nature Communications, 2015, 6, 6155. | 5.8 | 98 |
| 14 | 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 |
| 15 | Systematic Exploitation of Multiple Receptor Conformations for Virtual Ligand Screening. PLoS ONE, 2011, 6, e18845. | 1.1 | 82 |
| 16 | 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 |
| 17 | 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 |
| 18 | Irreversible Protein Kinase Inhibitors. Current Medicinal Chemistry, 2011, 18, 2981-2994. | 1.2 | 67 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Multi-Kinase Inhibitors. Current Medicinal Chemistry, 2015, 22, 695-712. | 1.2 | 61 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | Low molecular weight, non-peptidic agonists of TrkA receptor with NGF-mimetic activity. Cell Death and Disease, 2012, 3, e339-e339. | 2.7 | 48 |
| 25 | 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 |
| 26 | Diaryl Urea: A Privileged Structure in Anticancer Agents. Current Medicinal Chemistry, 2016, 23, 1528-1548. | 1.2 | 47 |
| 27 | 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 |
| 28 | Small Molecule Aurora Kinases Inhibitors. Current Medicinal Chemistry, 2009, 16, 1949-1963. | 1.2 | 42 |
| 29 | ACIAP, Autonomous hierarchical agglomerative Cluster Analysis based protocol to partition conformational datasets. Bioinformatics, 2006, 22, e58-e65. | 1.8 | 41 |
| 30 | 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 |
| 31 | Structure-Based Predictions of Activity Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 1062-1076. | 2.5 | 34 |
| 32 | Mapping Cholesterol Interaction Sites on Serotonin Transporter through Coarse-Grained Molecular Dynamics. PLoS ONE, 2016, 11, e0166196. | 1.1 | 29 |
| 33 | Inflammation causes remodeling of mitochondrial cytochrome c oxidase mediated by the bifunctional gene C15orf48. Science Advances, 2021, 7, eabl5182. | 4.7 | 29 |
| 34 | 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 |
| 35 | Synthesis of Monomeric Derivatives To Probe Memoquinâ€™s Bivalent Interactions. Journal of Medicinal Chemistry, 2011, 54, 8299-8304. | 2.9 | 27 |
| 36 | Polo-Like Kinases Inhibitors. Current Medicinal Chemistry, 2012, 19, 3937-3948. | 1.2 | 26 |

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|---|---|---|---|
| 37 | In silico antitarget screening. Drug Discovery Today: Technologies, 2004, 1, 209-215. | 4.0 | 24 |
| 38 | 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 |
| 39 | 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 |
| 40 | 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 |
| 41 | Fluorinated benzophenone derivatives: Balanced multipotent agents for Alzheimer's disease. European Journal of Medicinal Chemistry, 2014, 78, 157-166. | 2.6 | 21 |
| 42 | Benzimidazole Derivatives as Kinase Inhibitors. Current Medicinal Chemistry, 2014, 21, 2284-2298. | 1.2 | 21 |
| 43 | SERAPhiC: A Benchmark for in Silico Fragment-Based Drug Design. Journal of Chemical Information and Modeling, 2011, 51, 2882-2896. | 2.5 | 20 |
| 44 | Cyclin-dependent kinases: bridging their structure and function through computations. Future Medicinal Chemistry, 2011, 3, 1551-1559. | 1.1 | 19 |
| 45 | 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 |
| 46 | 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 |
| 47 | Development and Application of a Virtual Screening Protocol for the Identification of Multitarget Fragments. ChemMedChem, 2016, 11, 1259-1263. | 1.6 | 18 |
| 48 | Protein-ligand docking. Frontiers in Bioscience - Landmark, 2011, 16, 2289. | 3.0 | 17 |
| 49 | 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 |
| 50 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | Application of Conformational Clustering in Proteinâ€“Ligand Docking. Methods in Molecular Biology, 2012, 819, 169-186. | 0.4 | 7 |
| 54 | Modeling lipid raft domains containing a mono-unsaturated phosphatidylethanolamine species. RSC Advances, 2015, 5, 37102-37111. | 1.7 | 6 |

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|---|---|---|---|
| 55 | 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 |
| 56 | Pyrazole-Based Acid Ceramidase Inhibitors: Design, Synthesis, and Structureâ€“Activity Relationships. Synthesis, 2016, 48, 2739-2756. | 1.2 | 4 |
| 57 | 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 |
| 58 | Multitarget Compounds for Bipolar Disorder: From Rational Design to Preliminary Pharmacokinetic Evaluation. ChemMedChem, 2020, 15, 949-954. | 1.6 | 4 |
| 59 | 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 |
| 60 | Computational Methods in Multitarget Drug Discovery. , 2017, , 239-258. | | 3 |
| 61 | Dopamine D3 receptor ligands: a patent review (2014â€“2020). Expert Opinion on Therapeutic Patents, 2022, 32, 605-627. | 2.4 | 1 |
| 62 | (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 |