Giulio Rastelli

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/3580223/giulio-rastelli-publications-by-year.pdf
Version: 2024-04-09

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

121 papers	4,882 citations	34 h-index	67 g-index
152 ext. papers	5,754 ext. citations	5 avg, IF	6.07 L-index

#	Paper	IF	Citations
121	Synthesis of potent and selective HDAC6 inhibitors led to unexpected opening of a quinazoline ring.. *RSC Advances*, **2022**, 12, 11548-11556	3.7	0
120	Design and Synthesis of Hsp90 Inhibitors with B-Raf and PDHK1 Multi-Target Activity. *ChemistryOpen*, **2021**, 10, 1177-1185	2.3	3
119	Prediction of activity and selectivity profiles of human Carbonic Anhydrase inhibitors using machine learning classification models. *Journal of Cheminformatics*, **2021**, 13, 18	8.6	3
118	Antifungal Activity and DNA Topoisomerase Inhibition of Hydrolysable Tannins from L. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	5
117	LigAdvisor: a versatile and user-friendly web-platform for drug design. *Nucleic Acids Research*, **2021**, 49, W326-W335	20.1	4
116	Promising Non-cytotoxic Monosubstituted Chalcones to Target Monoamine Oxidase-B. *ACS Medicinal Chemistry Letters*, **2021**, 12, 1151-1158	4.3	6
115	Investigation of the effect of different linker chemotypes on the inhibition of histone deacetylases (HDACs). *Bioorganic Chemistry*, **2021**, 106, 104462	5.1	4
114	Inhibitors of histone deacetylase 6 based on a novel 3-hydroxy-isoxazole zinc binding group. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 2080-2086	5.6	3
113	Drug Repurposing and Polypharmacology to Fight SARS-CoV-2 Through Inhibition of the Main Protease. *Frontiers in Pharmacology*, **2021**, 12, 636989	5.6	17
112	Chemoinformatics Analyses of Tau Ligands Reveal Key Molecular Requirements for the Identification of Potential Drug Candidates against Tauopathies. *Molecules*, **2021**, 26,	4.8	1
111	Hydroxamic Acid Derivatives: From Synthetic Strategies to Medicinal Chemistry Applications. *ACS Omega*, **2021**, 6, 21843-21849	3.9	9
110	Design of Dual Inhibitors of Histone Deacetylase 6 and Heat Shock Protein 90. *ACS Omega*, **2020**, 5, 11473-11488	3.9	18
109	Identification of Target Associations for Polypharmacology from Analysis of Crystallographic Ligands of the Protein Data Bank. *Journal of Chemical Information and Modeling*, **2020**, 60, 372-390	6.1	9
108	Molecular Docking: Shifting Paradigms in Drug Discovery. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	272
107	In Silico Repositioning of Cannabigerol as a Novel Inhibitor of the Enoyl Acyl Carrier Protein (ACP) Reductase (InhA). *Molecules*, **2019**, 24,	4.8	17
106	2-Phenyloxazole-4-carboxamide as a Scaffold for Selective Inhibition of Human Monoamine Oxidase B. *ChemMedChem*, **2019**, 14, 1641-1652	3.7	4
105	Refinement and Rescoring of Virtual Screening Results. *Frontiers in Chemistry*, **2019**, 7, 498	5	27

104	Evaluation of Amides, Carbamates, Sulfonamides, and Ureas of 4-Prop-2-ynylidenecycloalkylamine as Potent, Selective, and Bioavailable Negative Allosteric Modulators of Metabotropic Glutamate Receptor 5. *Journal of Medicinal Chemistry*, **2019**, 62, 1246-1273	8.3	4
103	Identification of 4-aryl-1H-pyrrole[2,3-b]pyridine derivatives for the development of new B-Raf inhibitors. *Chemical Biology and Drug Design*, **2018**, 92, 1382-1386	2.9	1
102	Exploration and Comparison of the Geometrical and Physicochemical Properties of an Allosteric Pocket in the Structural Kinome. *Journal of Chemical Information and Modeling*, **2018**, 58, 1094-1103	6.1	6
101	Selection of protein conformations for structure-based polypharmacology studies. *Drug Discovery Today*, **2018**, 23, 1889-1896	8.8	16
100	Structure-Activity Relationships of Hexahydrocyclopenta[c]quinoline Derivatives as Allosteric Inhibitors of CDK2 and EGFR. *ChemMedChem*, **2018**, 13, 2627-2634	3.7	15
99	Investigating the Selectivity of Allosteric Inhibitors for Mutant T790M EGFR over Wild Type Using Molecular Dynamics and Binding Free Energy Calculations. *ACS Omega*, **2018**, 3, 16556-16562	3.9	5
98	Identification of small-molecule EGFR allosteric inhibitors by high-throughput docking. *Future Medicinal Chemistry*, **2018**, 10, 1545-1553	4.1	17
97	Promiscuity of inhibitors of human protein kinases at varying data confidence levels and test frequencies. *RSC Advances*, **2017**, 7, 41265-41271	3.7	20
96	Heat shock protein 90 and serine/threonine kinase B-Raf inhibitors have overlapping chemical space. *RSC Advances*, **2017**, 7, 31069-31074	3.7	12
95	The 1,2,3-triazole ring as a bioisostere in medicinal chemistry. *Drug Discovery Today*, **2017**, 22, 1572-1581	8.8	301
94	Probing an Allosteric Pocket of CDK2 with Small Molecules. *ChemMedChem*, **2017**, 12, 33-41	3.7	16
93	Synthesis and Biological Evaluation of Migrastatin Macrotriazoles. *European Journal of Organic Chemistry*, **2017**, 2017, 60-69	3.2	10
92	Virtual Screening for Dual Hsp90/B-Raf Inhibitors. *Methods in Pharmacology and Toxicology*, **2017**, 355-365		1
91	On the Integration of Drug Design Methods for Drug Repurposing. *Frontiers in Pharmacology*, **2017**, 8, 298	5.6	109
90	Dual Kinase-Bromodomain Inhibitors in Anticancer Drug Discovery: A Structural and Pharmacological Perspective. *Journal of Medicinal Chemistry*, **2016**, 59, 9305-9320	8.3	39
89	Exploiting computationally derived out-of-the-box protein conformations for drug design. *Future Medicinal Chemistry*, **2016**, 8, 1887-1897	4.1	6
88	Novel and less explored chemotypes of natural origin for the inhibition of Hsp90. *MedChemComm*, **2016**, 7, 2063-2075	5	1
87	An unexpected reversal in the pharmacological stereoselectivity of benzothiadiazine AMPA positive allosteric modulators. *MedChemComm*, **2016**, 7, 2410-2417	5	4

86	Molecular Dynamics Simulations and Classical Multidimensional Scaling Unveil New Metastable States in the Conformational Landscape of CDK2. *PLoS ONE*, **2016**, 11, e0154066	3.7	20
85	G48A, a New KRAS Mutation Found in Lung Adenocarcinoma. *Journal of Thoracic Oncology*, **2016**, 11, 1170-5	8.9	3
84	Analytical and Simulation-Based Models for Drug Release and Gel-Degradation in a Tetra-PEG Hydrogel Drug-Delivery System. *Macromolecules*, **2015**, 48, 7359-7369	5.5	22
83	Role of bifidobacteria in the hydrolysis of chlorogenic acid. *MicrobiologyOpen*, **2015**, 4, 41-52	3.4	44
82	Computational polypharmacology comes of age. *Frontiers in Pharmacology*, **2015**, 6, 157	5.6	36
81	Discovery of Multitarget Antivirals Acting on Both the Dengue Virus NS5-NS3 Interaction and the Host Src/Fyn Kinases. *Journal of Medicinal Chemistry*, **2015**, 58, 4964-75	8.3	44
80	Insights into the interaction of negative allosteric modulators with the metabotropic glutamate receptor 5: discovery and computational modeling of a new series of ligands with nanomolar affinity. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3040-58	3.4	14
79	Computational polypharmacology analysis of the heat shock protein 90 interactome. *Journal of Chemical Information and Modeling*, **2015**, 55, 676-86	6.1	25
78	Histone deacetylases: structural determinants of inhibitor selectivity. *Drug Discovery Today*, **2015**, 20, 718-35	8.8	126
77	Polypharmacology: challenges and opportunities in drug discovery. *Journal of Medicinal Chemistry*, **2014**, 57, 7874-87	8.3	571
76	Dimerization hot spots in the structure of human Hsp90. *MedChemComm*, **2014**, 5, 797-801	5	1
75	Structure-based discovery of the first allosteric inhibitors of cyclin-dependent kinase 2. *Cell Cycle*, **2014**, 13, 2296-305	4.7	41
74	Emerging topics in structure-based virtual screening. *Pharmaceutical Research*, **2013**, 30, 1458-63	4.5	15
73	Enrichment factor analyses on G-protein coupled receptors with known crystal structure. *Journal of Chemical Information and Modeling*, **2013**, 53, 739-43	6.1	19
72	αC helix displacement as a general approach for allosteric modulation of protein kinases. *Drug Discovery Today*, **2013**, 18, 407-14	8.8	76
71	Advances and applications of binding affinity prediction methods in drug discovery. *Biotechnology Advances*, **2012**, 30, 244-50	17.8	52
70	Application of a post-docking procedure based on MM-PBSA and MM-GBSA on single and multiple protein conformations. *European Journal of Medicinal Chemistry*, **2012**, 58, 431-40	6.8	57
69	Structure-based design of potent aromatase inhibitors by high-throughput docking. *Journal of Medicinal Chemistry*, **2011**, 54, 4006-17	8.3	75

68	Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. *Chemical Biology and Drug Design*, **2011**, 78, 252-9	2.9	26
67	BEAR, a novel virtual screening methodology for drug discovery. *Journal of Biomolecular Screening*, **2011**, 16, 129-33		28
66	Exploring the binding site of C-terminal hsp90 inhibitors. *Journal of Chemical Information and Modeling*, **2010**, 50, 1522-8	6.1	24
65	Fast and accurate predictions of binding free energies using MM-PBSA and MM-GBSA. *Journal of Computational Chemistry*, **2010**, 31, 797-810	3.5	377
64	A computational workflow for the design of irreversible inhibitors of protein kinases. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 183-94	4.2	9
63	Design and discovery of plasmepsin II inhibitors using an automated workflow on large-scale grids. *ChemMedChem*, **2009**, 4, 1164-73	3.7	38
62	Structure-based and in silico design of Hsp90 inhibitors. *ChemMedChem*, **2009**, 4, 1399-409	3.7	33
61	Binding estimation after refinement, a new automated procedure for the refinement and rescoring of docked ligands in virtual screening. *Chemical Biology and Drug Design*, **2009**, 73, 283-6	2.9	87
60	Activity prediction and structural insights of extracellular signal-regulated kinase 2 inhibitors with molecular dynamics simulations. *Chemical Biology and Drug Design*, **2009**, 74, 630-5	2.9	12
59	WISDOM-II: screening against multiple targets implicated in malaria using computational grid infrastructures. *Malaria Journal*, **2009**, 8, 88	3.6	22
58	Molecular modeling and crystal structure of ERK2-hypothemycin complexes. *Journal of Structural Biology*, **2008**, 164, 18-23	3.4	50
57	In vitro effects of Plasmodium falciparum dihydrofolate reductase inhibitors on normal and cancer cell proliferation. *ChemMedChem*, **2008**, 3, 421-4	3.7	1
56	Structural models and binding site prediction of the C-terminal domain of human Hsp90: a new target for anticancer drugs. *Chemical Biology and Drug Design*, **2008**, 71, 420-433	2.9	20
55	Validation of an automated procedure for the prediction of relative free energies of binding on a set of aldose reductase inhibitors. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 7865-77	3.4	87
54	Relationship between quantum-chemical descriptors of proton dissociation and experimental acidity constants of various hydroxylated coumarins. Identification of the biologically active species for xanthine oxidase inhibition. *European Journal of Medicinal Chemistry*, **2007**, 42, 1028-31	6.8	30
53	Virtual screening on large scale grids. *Parallel Computing*, **2007**, 33, 289-301	1	16
52	Grid-Enabled High Throughput Virtual Screening **2007**, 45-59		1
51	Structure-based design of 7-carbamate analogs of geldanamycin. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 5016-21	2.9	38

50	Synthesis and biological activities of novel 17-aminogeldanamycin derivatives. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 5317-29	3.4	144
49	Three-dimensional quantitative structure-activity relationship analysis of a set of Plasmodium falciparum dihydrofolate reductase inhibitors using a pharmacophore generation approach. *Journal of Medicinal Chemistry*, **2004**, 47, 4258-67	8.3	42
48	Structure of Plasmodium vivax dihydrofolate reductase determined by homology modeling and molecular dynamics refinement. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 3257-60	2.9	14
47	ortho-Halogen naphthaleins as specific inhibitors of Lactobacillus casei thymidylate synthase. Conformational properties and biological activity. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 951-63	3.4	7
46	Crystal structure and molecular modeling of 17-DMAG in complex with human Hsp90. *Chemistry and Biology*, **2003**, 10, 361-8		163
45	Docking and database screening reveal new classes of Plasmodium falciparum dihydrofolate reductase inhibitors. *Journal of Medicinal Chemistry*, **2003**, 46, 2834-45	8.3	84
44	Mutational analysis of Plasmodium falciparum dihydrofolate reductase: the role of aspartate 54 and phenylalanine 223 on catalytic activity and antifolate binding. *Molecular and Biochemical Parasitology*, **2002**, 121, 185-93	1.9	14
43	Binding of 1-benzopyran-4-one derivatives to aldose reductase: a free energy perturbation study. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 1427-36	3.4	8
42	Discovery of new inhibitors of aldose reductase from molecular docking and database screening. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 1437-50	3.4	52
41	Nitrophenyl derivatives as aldose reductase inhibitors. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 3923-31	3.4	20
40	Oxidative modification of aldose reductase induced by copper ion. Definition of the metal-protein interaction mechanism. *Journal of Biological Chemistry*, **2002**, 277, 42017-27	5.4	51
39	7-Hydroxy-2-substituted-4-H-1-benzopyran-4-one derivatives as aldose reductase inhibitors: a SAR study. *European Journal of Medicinal Chemistry*, **2001**, 36, 697-703	6.8	18
38	Synthesis and cytotoxicity of bis(benzo[g]indole-3-carboxamides) and related compounds. *Archiv Der Pharmazie*, **2001**, 334, 337-44	4.3	7
37	Preparation of thieno[3,2-h]cinnolinones as matrix metalloproteinase inhibitors. *Archiv Der Pharmazie*, **2000**, 333, 37-47	4.3	4
36	A series of diarylsubstituted oximes as potential substrate for new aldose reductase inhibitors. *Journal of Heterocyclic Chemistry*, **2000**, 37, 1089-1096	1.9	7
35	Interaction of pyrimethamine, cycloguanil, WR99210 and their analogues with Plasmodium falciparum dihydrofolate reductase: structural basis of antifolate resistance. *Bioorganic and Medicinal Chemistry*, **2000**, 8, 1117-28	3.4	118
34	Structural bases for the inhibition of aldose reductase by phenolic compounds. *Bioorganic and Medicinal Chemistry*, **2000**, 8, 1151-8	3.4	30
33	Synthesis and aldose reductase inhibitory activity of a new series of benz[h]cinnolinone derivatives. *Il Farmaco*, **2000**, 55, 544-52		17

32	Aldose reductase does catalyse the reduction of glyceraldehyde through a stoichiometric oxidation of NADPH. *Experimental Eye Research*, **2000**, 71, 515-21	3.7	30
31	Pharmacological approaches to the treatment of diabetic complications. *Expert Opinion on Therapeutic Patents*, **2000**, 10, 1245-1262	6.8	65
30	Diabetes complications and their potential prevention: aldose reductase inhibition and other approaches. *Medicinal Research Reviews*, **1999**, 19, 3-23	14.4	133
29	1-Benzopyran-4-one antioxidants as aldose reductase inhibitors. *Journal of Medicinal Chemistry*, **1999**, 42, 1881-93	8.3	82
28	Isoxazolo-[3,4-d]-pyridazin-7-(6H)-one as a potential substrate for new aldose reductase inhibitors. *Journal of Medicinal Chemistry*, **1999**, 42, 1894-900	8.3	30
27	Free energy perturbation studies on binding of the inhibitor 5,6-dihydrobenzo[h]cinnolin-3(2H)one-2-acetic acid and its methoxylated analogs to aldose reductase. *Tetrahedron*, **1998**, 54, 9415-9428	2.4	11
26	Fruits of ribes, rubus, vaccinium and prunus genus. Metal contents and genome. *Freseniusr Journal of Analytical Chemistry*, **1998**, 361, 353-354		9
25	Molecular dynamics simulations of the structure of aldose reductase complexed with the inhibitor tolrestat. *Bioorganic and Medicinal Chemistry Letters*, **1998**, 8, 641-6	2.9	16
24	Oxidative modification of aldose reductase induced by copper ion. Factors and conditions affecting the process. *Biochemistry*, **1998**, 37, 14167-74	3.2	18
23	New aldose reductase inhibitors as potential agents for the prevention of long-term diabetic complications. *Expert Opinion on Therapeutic Patents*, **1997**, 7, 843-858	6.8	55
22	A Model of the Interaction of Substrates and Inhibitors with Xanthine Oxidase. *Journal of the American Chemical Society*, **1997**, 119, 3007-3016	16.4	33
21	Structure-based design of an inhibitor modeled at the substrate active site of aldose reductase. *Bioorganic and Medicinal Chemistry Letters*, **1997**, 7, 1897-1902	2.9	24
20	Synthesis, activity, and molecular modeling of a new series of tricyclic pyridazinones as selective aldose reductase inhibitors. *Journal of Medicinal Chemistry*, **1996**, 39, 4396-405	8.3	85
19	Conformational analysis of phthalein derivatives acting as thymidylate synthase inhibitors by means of 1H NMR and quantum chemical calculations. *Bioorganic and Medicinal Chemistry*, **1996**, 4, 1783-94	3.4	13
18	A rational approach to the design of flavones as xanthine oxidase inhibitors. *European Journal of Medicinal Chemistry*, **1996**, 31, 693-699	6.8	34
17	Natural polyhydroxylated compounds as inhibitors of xanthine oxidase. *Die Pharmazie*, **1996**, 51, 994-5	1.5	4
16	Theoretical and experimental study of flavones as inhibitors of xanthine oxidase. *European Journal of Medicinal Chemistry*, **1995**, 30, 141-146	6.8	16
15	Theoretical analysis of the addition of hydroxylamine to uracil and 5-fluorouracil as a model for the thymidylate synthase reaction. *Computational and Theoretical Chemistry*, **1995**, 343, 1-9		4

14	Insight into the specificity of thymidylate synthase from molecular dynamics and free energy perturbation calculations. *Journal of the American Chemical Society*, **1995**, 117, 7213-7227	16.4	15
13	Quantitative measurement of proton dissociation and tautomeric constants of apigeninidin. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 227		6
12	Anthocyanidines as inhibitors of xanthine oxidase. *Die Pharmazie*, **1995**, 50, 573-4	1.5	11
11	Solvent effects on the tautomerism of apigeninidin. *Tetrahedron Letters*, **1994**, 35, 9751-9754	2	1
10	Physico-chemical properties of anthocyanidins. Part 1. Theoretical evaluation of the stability of the neutral and anionic tautomeric forms. *Computational and Theoretical Chemistry*, **1993**, 279, 157-166		17
9	Activity of polyphenolic crude extracts as scavengers of superoxide radicals and inhibitors of xanthine oxidase. *Planta Medica*, **1992**, 58, 342-4	3.1	137
8	Antilipoperoxidant Activity of Polyphenolic Crude Extracts of some Edible Fruits. *Planta Medica*, **1992**, 58, 662-663	3.1	1
7	Inhibitory activity of flavonols towards the xanthine oxidase enzyme. *International Journal of Pharmaceutics*, **1992**, 86, 17-23	6.5	11
6	Molecular orbital study of the nitrogen basicity of prazosin analogues in relation to their 1-adrenoceptor binding affinity. *Computational and Theoretical Chemistry*, **1991**, 233, 343-351		16
5	Conformational analysis, molecular modeling and quantitative structure-activity relationship studies of 2,4-diamino-6,7-dimethoxy-2-substituted quinazoline 1-adrenergic antagonists. *Computational and Theoretical Chemistry*, **1991**, 251, 307-318		20
4	QSAR Analysis in 2,4-Diamino-6,7-dimethoxy Quinoline Derivatives 1-Adrenoceptor Antagonists Using the Partial Least Squares (PLS) Method and Theoretical Molecular Descriptors. *QSAR and Combinatorial Science*, **1990**, 9, 340-345		13
3	Drug repurposing and polypharmacology to fight SARS-CoV-2 through the inhibition of the main protease		2
2	Identification of potential biological targets of oxindole scaffolds via in silico repositioning strategies. *F1000Research*,11, 217	3.6	
1	Identification of potential biological targets of oxindole scaffolds via in silico repositioning strategies. *F1000Research*,11, 217	3.6	