Giulio Rastelli

List of Publications by Citations

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	Polypharmacology: challenges and opportunities in drug discovery. *Journal of Medicinal Chemistry*, **2014**, 57, 7874-87	8.3	571
120	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
119	The 1,2,3-triazole ring as a bioisostere in medicinal chemistry. *Drug Discovery Today*, **2017**, 22, 1572-1581	8.8	301
118	Molecular Docking: Shifting Paradigms in Drug Discovery. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	272
117	Crystal structure and molecular modeling of 17-DMAG in complex with human Hsp90. *Chemistry and Biology*, **2003**, 10, 361-8		163
116	Synthesis and biological activities of novel 17-aminogeldanamycin derivatives. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 5317-29	3.4	144
115	Activity of polyphenolic crude extracts as scavengers of superoxide radicals and inhibitors of xanthine oxidase. *Planta Medica*, **1992**, 58, 342-4	3.1	137
114	Diabetes complications and their potential prevention: aldose reductase inhibition and other approaches. *Medicinal Research Reviews*, **1999**, 19, 3-23	14.4	133
113	Histone deacetylases: structural determinants of inhibitor selectivity. *Drug Discovery Today*, **2015**, 20, 718-35	8.8	126
112	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
111	On the Integration of Drug Design Methods for Drug Repurposing. *Frontiers in Pharmacology*, **2017**, 8, 298	5.6	109
110	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
109	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
108	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
107	Docking and database screening reveal new classes of Plasmodium falciparum dihydrofolate reductase inhibitors. *Journal of Medicinal Chemistry*, **2003**, 46, 2834-45	8.3	84
106	1-Benzopyran-4-one antioxidants as aldose reductase inhibitors. *Journal of Medicinal Chemistry*, **1999**, 42, 1881-93	8.3	82
105	αC helix displacement as a general approach for allosteric modulation of protein kinases. *Drug Discovery Today*, **2013**, 18, 407-14	8.8	76

104	Structure-based design of potent aromatase inhibitors by high-throughput docking. *Journal of Medicinal Chemistry*, **2011**, 54, 4006-17	8.3	75
103	Pharmacological approaches to the treatment of diabetic complications. *Expert Opinion on Therapeutic Patents*, **2000**, 10, 1245-1262	6.8	65
102	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
101	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
100	Advances and applications of binding affinity prediction methods in drug discovery. *Biotechnology Advances*, **2012**, 30, 244-50	17.8	52
99	Discovery of new inhibitors of aldose reductase from molecular docking and database screening. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 1437-50	3.4	52
98	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
97	Molecular modeling and crystal structure of ERK2-hypothemycin complexes. *Journal of Structural Biology*, **2008**, 164, 18-23	3.4	50
96	Role of bifidobacteria in the hydrolysis of chlorogenic acid. *MicrobiologyOpen*, **2015**, 4, 41-52	3.4	44
95	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
94	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
93	Structure-based discovery of the first allosteric inhibitors of cyclin-dependent kinase 2. *Cell Cycle*, **2014**, 13, 2296-305	4.7	41
92	Dual Kinase-Bromodomain Inhibitors in Anticancer Drug Discovery: A Structural and Pharmacological Perspective. *Journal of Medicinal Chemistry*, **2016**, 59, 9305-9320	8.3	39
91	Design and discovery of plasmepsin II inhibitors using an automated workflow on large-scale grids. *ChemMedChem*, **2009**, 4, 1164-73	3.7	38
90	Structure-based design of 7-carbamate analogs of geldanamycin. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 5016-21	2.9	38
89	Computational polypharmacology comes of age. *Frontiers in Pharmacology*, **2015**, 6, 157	5.6	36
88	A rational approach to the design of flavones as xanthine oxidase inhibitors. *European Journal of Medicinal Chemistry*, **1996**, 31, 693-699	6.8	34
87	Structure-based and in silico design of Hsp90 inhibitors. *ChemMedChem*, **2009**, 4, 1399-409	3.7	33

86	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
85	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
84	Structural bases for the inhibition of aldose reductase by phenolic compounds. *Bioorganic and Medicinal Chemistry*, **2000**, 8, 1151-8	3.4	30
83	Aldose reductase does catalyse the reduction of glyceraldehyde through a stoichiometric oxidation of NADPH. *Experimental Eye Research*, **2000**, 71, 515-21	3.7	30
82	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
81	BEAR, a novel virtual screening methodology for drug discovery. *Journal of Biomolecular Screening*, **2011**, 16, 129-33		28
80	Refinement and Rescoring of Virtual Screening Results. *Frontiers in Chemistry*, **2019**, 7, 498	5	27
79	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
78	Computational polypharmacology analysis of the heat shock protein 90 interactome. *Journal of Chemical Information and Modeling*, **2015**, 55, 676-86	6.1	25
77	Exploring the binding site of C-terminal hsp90 inhibitors. *Journal of Chemical Information and Modeling*, **2010**, 50, 1522-8	6.1	24
76	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
75	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
74	WISDOM-II: screening against multiple targets implicated in malaria using computational grid infrastructures. *Malaria Journal*, **2009**, 8, 88	3.6	22
73	Promiscuity of inhibitors of human protein kinases at varying data confidence levels and test frequencies. *RSC Advances*, **2017**, 7, 41265-41271	3.7	20
72	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
71	Nitrophenyl derivatives as aldose reductase inhibitors. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 3923-31	3.4	20
70	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
69	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

68	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
67	Oxidative modification of aldose reductase induced by copper ion. Factors and conditions affecting the process. *Biochemistry*, **1998**, 37, 14167-74	3.2	18
66	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
65	Design of Dual Inhibitors of Histone Deacetylase 6 and Heat Shock Protein 90. *ACS Omega*, **2020**, 5, 11473-11480	3.9	18
64	In Silico Repositioning of Cannabigerol as a Novel Inhibitor of the Enoyl Acyl Carrier Protein (ACP) Reductase (InhA). *Molecules*, **2019**, 24,	4.8	17
63	Synthesis and aldose reductase inhibitory activity of a new series of benz[h]cinnolinone derivatives. *Il Farmaco*, **2000**, 55, 544-52		17
62	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
61	Drug Repurposing and Polypharmacology to Fight SARS-CoV-2 Through Inhibition of the Main Protease. *Frontiers in Pharmacology*, **2021**, 12, 636989	5.6	17
60	Identification of small-molecule EGFR allosteric inhibitors by high-throughput docking. *Future Medicinal Chemistry*, **2018**, 10, 1545-1553	4.1	17
59	Selection of protein conformations for structure-based polypharmacology studies. *Drug Discovery Today*, **2018**, 23, 1889-1896	8.8	16
58	Probing an Allosteric Pocket of CDK2 with Small Molecules. *ChemMedChem*, **2017**, 12, 33-41	3.7	16
57	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
56	Virtual screening on large scale grids. *Parallel Computing*, **2007**, 33, 289-301	1	16
55	Theoretical and experimental study of flavones as inhibitors of xanthine oxidase. *European Journal of Medicinal Chemistry*, **1995**, 30, 141-146	6.8	16
54	Molecular orbital study of the nitrogen basicity of prazosin analogues in relation to their α1-adrenoceptor binding affinity. *Computational and Theoretical Chemistry*, **1991**, 233, 343-351		16
53	Emerging topics in structure-based virtual screening. *Pharmaceutical Research*, **2013**, 30, 1458-63	4.5	15
52	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
51	Structure-Activity Relationships of Hexahydrocyclopenta[c]quinoline Derivatives as Allosteric Inhibitors of CDK2 and EGFR. *ChemMedChem*, **2018**, 13, 2627-2634	3.7	15

50	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
49	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
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	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
46	QSAR Analysis in 2,4-Diamino-6,7-dimethoxy Quinoline Derivatives □-Adrenoceptor Antagonists □Using the Partial Least Squares (PLS) Method and Theoretical Molecular Descriptors. *QSAR and Combinatorial Science*, **1990**, 9, 340-345		13
45	Heat shock protein 90 and serine/threonine kinase B-Raf inhibitors have overlapping chemical space. *RSC Advances*, **2017**, 7, 31069-31074	3.7	12
44	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
43	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
42	Inhibitory activity of flavonols towards the xanthine oxidase enzyme. *International Journal of Pharmaceutics*, **1992**, 86, 17-23	6.5	11
41	Anthocyanidines as inhibitors of xanthine oxidase. *Die Pharmazie*, **1995**, 50, 573-4	1.5	11
40	Synthesis and Biological Evaluation of Migrastatin Macrotriazoles. *European Journal of Organic Chemistry*, **2017**, 2017, 60-69	3.2	10
39	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
38	Fruits of ribes, rubus, vaccinium and prunus genus. Metal contents and genome. *Freseniusr Journal of Analytical Chemistry*, **1998**, 361, 353-354		9
37	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
36	Hydroxamic Acid Derivatives: From Synthetic Strategies to Medicinal Chemistry Applications. *ACS Omega*, **2021**, 6, 21843-21849	3.9	9
35	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
34	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
33	Synthesis and cytotoxicity of bis(benzo[g]indole-3-carboxamides) and related compounds. *Archiv Der Pharmazie*, **2001**, 334, 337-44	4.3	7

32	A series of diarylsubstituted oximes as potential substrate for new aldose reductase inhibitors. *Journal of Heterocyclic Chemistry*, **2000**, 37, 1089-1096	1.9	7
31	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
30	Exploiting computationally derived out-of-the-box protein conformations for drug design. *Future Medicinal Chemistry*, **2016**, 8, 1887-1897	4.1	6
29	Quantitative measurement of proton dissociation and tautomeric constants of apigeninidin. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 227		6
28	Promising Non-cytotoxic Monosubstituted Chalcones to Target Monoamine Oxidase-B. *ACS Medicinal Chemistry Letters*, **2021**, 12, 1151-1158	4.3	6
27	Antifungal Activity and DNA Topoisomerase Inhibition of Hydrolysable Tannins from L. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	5
26	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
25	An unexpected reversal in the pharmacological stereoselectivity of benzothiadiazine AMPA positive allosteric modulators. *MedChemComm*, **2016**, 7, 2410-2417	5	4
24	2-Phenyloxazole-4-carboxamide as a Scaffold for Selective Inhibition of Human Monoamine Oxidase B. *ChemMedChem*, **2019**, 14, 1641-1652	3.7	4
23	Preparation of thieno[3,2-h]cinnolinones as matrix metalloproteinase inhibitors. *Archiv Der Pharmazie*, **2000**, 333, 37-47	4.3	4
22	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
21	LigAdvisor: a versatile and user-friendly web-platform for drug design. *Nucleic Acids Research*, **2021**, 49, W326-W335	20.1	4
20	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
19	Investigation of the effect of different linker chemotypes on the inhibition of histone deacetylases (HDACs). *Bioorganic Chemistry*, **2021**, 106, 104462	5.1	4
18	Natural polyhydroxylated compounds as inhibitors of xanthine oxidase. *Die Pharmazie*, **1996**, 51, 994-5	1.5	4
17	Design and Synthesis of Hsp90 Inhibitors with B-Raf and PDHK1 Multi-Target Activity. *ChemistryOpen*, **2021**, 10, 1177-1185	2.3	3
16	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
15	G48A, a New KRAS Mutation Found in Lung Adenocarcinoma. *Journal of Thoracic Oncology*, **2016**, 11, 1170-5	8.9	3

14	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
13	Drug repurposing and polypharmacology to fight SARS-CoV-2 through the inhibition of the main protease		2
12	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
11	Novel and less explored chemotypes of natural origin for the inhibition of Hsp90. *MedChemComm*, **2016**, 7, 2063-2075	5	1
10	Dimerization hot spots in the structure of human Hsp90. *MedChemComm*, **2014**, 5, 797-801	5	1
9	In vitro effects of Plasmodium falciparum dihydrofolate reductase inhibitors on normal and cancer cell proliferation. *ChemMedChem*, **2008**, 3, 421-4	3.7	1
8	Solvent effects on the tautomerism of apigeninidin. *Tetrahedron Letters*, **1994**, 35, 9751-9754	2	1
7	Antilipoperoxidant Activity of Polyphenolic Crude Extracts of some Edible Fruits. *Planta Medica*, **1992**, 58, 662-663	3.1	1
6	Grid-Enabled High Throughput Virtual Screening **2007**, 45-59		1
5	Chemoinformatics Analyses of Tau Ligands Reveal Key Molecular Requirements for the Identification of Potential Drug Candidates against Tauopathies. *Molecules*, **2021**, 26,	4.8	1
4	Synthesis of potent and selective HDAC6 inhibitors led to unexpected opening of a quinazoline ring.. *RSC Advances*, **2022**, 12, 11548-11556	3.7	0
3	Virtual Screening for Dual Hsp90/B-Raf Inhibitors. *Methods in Pharmacology and Toxicology*, **2017**, 355-365	1.1	
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	