Tiago Rodrigues

List of Publications by Year in descending order

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79 papers	3,345 citations	186265 28 h-index	149698 56 g-index
93 all docs	93 docs citations	93 times ranked	4756 citing authors

#	Article	IF	Citations
1	Deriving intuition in catalyst design with machine learning. CheM, 2022, 8, 15-17.	11.7	3
2	Evaluation guidelines for machine learning tools in the chemical sciences. Nature Reviews Chemistry, 2022, 6, 428-442.	30.2	49
3	Controlled masking and targeted release of redox-cycling ortho-quinones via a Câ€“C bond-cleaving 1,6-elimination. Nature Chemistry, 2022, 14, 754-765.	13.6	18
4	A special issue on artificial intelligence for drug discovery. Bioorganic and Medicinal Chemistry, 2022, , 116939.	3.0	0
5	Allosteric Antagonist Modulation of TRPV2 by Piperlongumine Impairs Glioblastoma Progression. ACS Central Science, 2021, 7, 868-881.	11.3	34
6	Exploration of Long-Chain Vitamin E Metabolites for the Discovery of a Highly Potent, Orally Effective, and Metabolically Stable 5-LOX Inhibitor that Limits Inflammation. Journal of Medicinal Chemistry, 2021, 64, 11496-11526.	6.4	7
7	Augmenting Adaptive Machine Learning with Kinetic Modeling for Reaction Optimization. Journal of Organic Chemistry, 2021, 86, 14192-14198.	3.2	9
8	Facts and Figures on Materials Science and Nanotechnology Progress and Investment. ACS Nano, 2021, 15, 15940-15952.	14.6	48
9	Combating small-molecule aggregation with machine learning. Cell Reports Physical Science, 2021, 2, 100573.	5.6	11
10	Machine learning for next-generation nanotechnology in healthcare. Matter, 2021, 4, 3078-3080.	10.0	5
11	Machine learning for target discovery in drug development. Current Opinion in Chemical Biology, 2020, 56, 16-22.	6.1	34
12	Adaptive Optimization of Chemical Reactions with Minimal Experimental Information. Cell Reports Physical Science, 2020, 1, 100247.	5.6	42
13	Structural and biophysical insights into the mode of covalent binding of rationally designed potent BMX inhibitors. RSC Chemical Biology, 2020, 1, 251-262.	4.1	6
14	The antidiabetic drug lobeglitazone has the potential to inhibit PTP1B activity. Bioorganic Chemistry, 2020, 100, 103927.	4.1	12
15	Brain-Sparing Sympathofacilitators Mitigate Obesity without Adverse Cardiovascular Effects. Cell Metabolism, 2020, 31, 1120-1135.e7.	16.2	18
16	11. Drug target prediction using chem- and bioinformatics. , 2020, , 291-310.		0
17	Evaluation of linker length effects on a BET bromodomain probe. Chemical Communications, 2019, 55, 10128-10131.	4.1	2
18	Synthetic organic chemistry driven by artificial intelligence. Nature Reviews Chemistry, 2019, 3, 589-604.	30.2	173

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19	Dissecting celastrol with machine learning to unveil dark pharmacology. Chemical Communications, 2019, 55, 6369-6372.	4.1	10
20	Computational advances in combating colloidal aggregation in drug discovery. Nature Chemistry, 2019, 11, 402-418.	13.6	51
21	Natural productâ€“drug conjugates for modulation of TRPV1-expressing tumors. Bioorganic and Medicinal Chemistry, 2019, 27, 2531-2536.	3.0	8
22	The good, the bad, and the ugly in chemical and biological data for machine learning. Drug Discovery Today: Technologies, 2019, 32-33, 3-8.	4.0	27
23	A Toolbox for the Identification of Modes of Action of Natural Products. Progress in the Chemistry of Organic Natural Products, 2019, 110, 73-97.	1.1	2
24	AntikÃ¶rpergerichtete Therapien: Quo vadis?. Angewandte Chemie, 2018, 130, 2050-2052.	2.0	0
25	Development of Antibodyâ€Directed Therapies: Quo Vadis?. Angewandte Chemie - International Edition, 2018, 57, 2032-2034.	13.8	22
26	Drug target prediction using chem- and bioinformatics. Physical Sciences Reviews, 2018, 3, .	0.8	2
27	Discovery of 2,4-dimethoxypyridines as novel autophagy inhibitors. Tetrahedron, 2018, 74, 4531-4537.	1.9	8
28	Machine intelligence decrypts Î²-lapachone as an allosteric 5-lipoxygenase inhibitor. Chemical Science, 2018, 9, 6899-6903.	7.4	64
29	Vinyl Ether/Tetrazine Pair for the Traceless Release of Alcohols in Cells. Angewandte Chemie - International Edition, 2017, 56, 243-247.	13.8	100
30	Harnessing the potential of natural products in drug discovery from a cheminformatics vantage point. Organic and Biomolecular Chemistry, 2017, 15, 9275-9282.	2.8	30
31	A Water-Bridged Cysteine-Cysteine Redox Regulation Mechanism in Bacterial Protein Tyrosine Phosphatases. CheM, 2017, 3, 665-677.	11.7	18
32	Chemoselective Installation of Amine Bonds on Proteins through Aza-Michael Ligation. Journal of the American Chemical Society, 2017, 139, 18365-18375.	13.7	74
33	Counting on natural products for drug design. Nature Chemistry, 2016, 8, 531-541.	13.6	879
34	Unveiling (â^')â€Englerinâ€…A as a Modulator of Lâ€Type Calcium Channels. Angewandte Chemie, 2016, 128, 11243-11247.	2.0	7
35	Designing Multiâ€target Compound Libraries with Gaussian Process Models. Molecular Informatics, 2016, 35, 192-198.	2.5	9
36	The missing link. Nature Chemistry, 2016, 8, 1088-1090.	13.6	7

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37	Unveiling (â˜†)â€Englerinâ€...A as a Modulator of Lâ€Type Calcium Channels. Angewandte Chemie - International Edition, 2016, 55, 11077-11081.	13.8	37
38	Von komplexen Naturstoffen zu synthetisch leicht zugÃnglichen Mimetika mithilfe von computergestÃ¼tztem Deâ€novoâ€Design. Angewandte Chemie, 2016, 128, 6901-6904.	2.0	11
39	From Complex Natural Products to Simple Synthetic Mimetics by Computational De Novo Design. Angewandte Chemie - International Edition, 2016, 55, 6789-6792.	13.8	42
40	Natural product modulators of transient receptor potential (TRP) channels as potential anti-cancer agents. Chemical Society Reviews, 2016, 45, 6130-6137.	38.1	57
41	De Novo Fragment Design for Drug Discovery and Chemical Biology. Angewandte Chemie - International Edition, 2015, 54, 15079-15083.	13.8	30
42	Fragmentâ€Based Deâ€...Novo Design Reveals a Smallâ€Molecule Inhibitor of Helicobacter Pylori HtrA. Angewandte Chemie - International Edition, 2015, 54, 10244-10248.	13.8	37
43	Revealing the Macromolecular Targets of Fragmentâ€Like Natural Products. Angewandte Chemie - International Edition, 2015, 54, 10516-10520.	13.8	54
44	Multidimensional Deâ€...Novo Design Reveals 5â€HT_{2B} Receptorâ€Selective Ligands. Angewandte Chemie - International Edition, 2015, 54, 1551-1555.	13.8	39
45	In Silico Screening. , 2015, , 141-160.		1
46	Repurposing de novo designed entities reveals phosphodiesterase 3B and cathepsin L modulators. Chemical Communications, 2015, 51, 7478-7481.	4.1	10
47	Flashback Forward: Reaction-Driven De Novo Design of Bioactive Compounds. Synlett, 2014, 25, 170-178.	1.8	14
48	Coping with Polypharmacology by Computational Medicinal Chemistry. Chimia, 2014, 68, 648.	0.6	6
49	Identifying the macromolecular targets of de novo-designed chemical entities through self-organizing map consensus. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4067-4072.	7.1	196
50	Combining Onâ€Chip Synthesis of a Focused Combinatorial Library with Computational Target Prediction Reveals Imidazopyridine GPCR Ligands. Angewandte Chemie - International Edition, 2014, 53, 582-585.	13.8	66
51	Accessing New Chemical Entities through Microfluidic Systems. Angewandte Chemie - International Edition, 2014, 53, 5750-5758.	13.8	86
52	Antiplasmodial Drugs in the Gas Phase: A CID and DFT Study of Quinolon-4(1H)-Imine Derivatives. Journal of the American Society for Mass Spectrometry, 2014, 25, 1650-1661.	2.8	2
53	Revealing the macromolecular targets of complex natural products. Nature Chemistry, 2014, 6, 1072-1078.	13.6	114
54	Multiâ€Objective Molecular De Novo Design by Adaptive Fragment Prioritization. Angewandte Chemie - International Edition, 2014, 53, 4244-4248.	13.8	76

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55	Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation. Journal of Cheminformatics, 2014, 6, .	6.1	1
56	Targeting flexibility: a structure-based computational study revealing allosteric HIV-1 protease inhibitors. Journal of Cheminformatics, 2014, 6, .	6.1	1
57	Go with the flow: de-orphaning focused combinatorial libraries. Journal of Cheminformatics, 2014, 6, .	6.1	0
58	Targeting Dynamic Pockets of HIV-1 Protease by Structure-Based Computational Screening for Allosteric Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 987-991.	5.4	29
59	Combinatorial chemistry by ant colony optimization. Future Medicinal Chemistry, 2014, 6, 267-280.	2.3	16
60	Exploring the Molecular Basis of Q_obc₁ Complex Inhibitors Activity to Find Novel Antimalarials Hits. Molecular Informatics, 2013, 32, 659-670.	2.5	11
61	Steering Target Selectivity and Potency by Fragmentâ€Based De Novo Drug Design. Angewandte Chemie - International Edition, 2013, 52, 10006-10009.	13.8	23
62	Drugs by Numbers: Reactionâ€Driven De Novo Design of Potent and Selective Anticancer Leads. Angewandte Chemie - International Edition, 2013, 52, 4676-4681.	13.8	22
63	De novo design and optimization of Aurora A kinase inhibitors. Chemical Science, 2013, 4, 1229.	7.4	23
64	Quinolin-4(1H)-imines are Potent Antiplasmodial Drugs Targeting the Liver Stage of Malaria. Journal of Medicinal Chemistry, 2013, 56, 4811-4815.	6.4	21
65	Flavones as isosteres of 4(1H)-quinolones: Discovery of ligand efficient and dual stage antimalarial lead compounds. European Journal of Medicinal Chemistry, 2013, 69, 872-880.	5.5	13
66	Chemically Advanced Template Search (CATS) for Scaffoldâ€Hopping and Prospective Target Prediction for â€˜Orphanâ€™ Molecules. Molecular Informatics, 2013, 32, 133-138.	2.5	132
67	Drug Screen Targeted at Plasmodium Liver Stages Identifies a Potent Multistage Antimalarial Drug. Journal of Infectious Diseases, 2012, 205, 1278-1286.	4.0	97
68	Significance estimation for sequence-based chemical similarity searching (PhAST) and application to AuroraA kinase inhibitors. Future Medicinal Chemistry, 2012, 4, 1897-1906.	2.3	5
69	Targeting the Liver Stage of Malaria Parasites: A Yet Unmet Goal. Journal of Medicinal Chemistry, 2012, 55, 995-1012.	6.4	73
70	Microwave-Assisted Wittig Reaction of Semistabilized Nitro-Substituted Benzyltriphenyl-Phosphorous Ylides with Aldehydes in Phase-Transfer Conditions. Synthetic Communications, 2012, 42, 747-755.	2.1	5
71	From Virtual Screening to Bioactive Compounds by Visualizing and Clustering of Chemical Space. Molecular Informatics, 2012, 31, 21-26.	2.5	12
72	Identification of new antimalarial leads by use of virtual screening against cytochrome bc1. Bioorganic and Medicinal Chemistry, 2011, 19, 6302-6308.	3.0	10

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73	A quantum mechanical study of novel potential inhibitors of cytochrome bc₁ as antimalarial compounds. International Journal of Quantum Chemistry, 2011, 111, 1196-1207.	2.0	16
74	New hope in the fight against malaria?. Future Medicinal Chemistry, 2011, 3, 1-3.	2.3	31
75	Design, synthesis and structureâ€“activity relationships of (1H-pyridin-4-ylidene)amines as potential antimalarials. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3476-3480.	2.2	29
76	Bis{(E)-3-[(diethylmethylammonio)methyl]-N-[3-(N,N-dimethylsulfamoyl)-1-methylpyridin-4-ylidene]-4-metho tetraiodide pentahydrate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o283-o284.	0.2	4
77	Unanticipated Acyloxymethylation of Sumatriptan Indole Nitrogen Atom and its Implications in Prodrug Design. Archiv Der Pharmazie, 2008, 341, 344-350.	4.1	2
78	Allosteric Antagonist Modulation of TRPV2 by Piperlongumine Impairs Glioblastoma Progression. SSRN Electronic Journal, 0, , .	0.4	1
79	Nuisance small molecules under a machine-learning lens. , 0, , .		2