

Simon J F Macdonald

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

48
papers

2,382
citations

23
h-index

48
g-index

51
ext. papers

2,730
ext. citations

8.9
avg, IF

5.2
L-index

#	Paper	IF	Citations
48	The impact of aromatic ring count on compound developability--are too many aromatic rings a liability in drug design?. <i>Drug Discovery Today</i> , 2009 , 14, 1011-20	8.8	512
47	The impact of aromatic ring count on compound developability: further insights by examining carbo- and hetero-aromatic and -aliphatic ring types. <i>Drug Discovery Today</i> , 2011 , 16, 164-71	8.8	286
46	Factors determining the selection of organic reactions by medicinal chemists and the use of these reactions in arrays (small focused libraries). <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 8082-91	16.4	208
45	Dissecting fibrosis: therapeutic insights from the small-molecule toolbox. <i>Nature Reviews Drug Discovery</i> , 2015 , 14, 693-720	64.1	141
44	The developability of heteroaromatic and heteroaliphatic rings --do some have a better pedigree as potential drug molecules than others?. <i>MedChemComm</i> , 2012 , 3, 1062	5	128
43	Dimeric zanamivir conjugates with various linking groups are potent, long-lasting inhibitors of influenza neuraminidase including H5N1 avian influenza. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 2964-71	8.3	76
42	Potent and long-acting dimeric inhibitors of influenza virus neuraminidase are effective at a once-weekly dosing regimen. <i>Antimicrobial Agents and Chemotherapy</i> , 2004 , 48, 4542-9	5.9	71
41	An RGD Integrin Inhibitor Toolbox: Drug Discovery Insight, Challenges and Opportunities. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 3298-3321	16.4	64
40	An Invitation to Open Innovation in Malaria Drug Discovery: 47 Quality Starting Points from the TCAMS. <i>ACS Medicinal Chemistry Letters</i> , 2011 , 2, 741-6	4.3	61
39	Physicochemical descriptors of aromatic character and their use in drug discovery. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 7206-15	8.3	58
38	Highly potent and long-acting trimeric and tetrameric inhibitors of influenza virus neuraminidase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004 , 14, 1589-92	2.9	52
37	Analysis of the calculated physicochemical properties of respiratory drugs: can we design for inhaled drugs yet?. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1025-32	6.1	49
36	Faktoren für die Auswahl organischer Reaktionen in der medizinischen Chemie und die Anwendung dieser Reaktionen in Arrays (kleinen fokussierten Bibliotheken). <i>Angewandte Chemie</i> , 2010 , 122, 8258-8267	3.6	48
35	Development of Autotaxin Inhibitors: An Overview of the Patent and Primary Literature. <i>Journal of Medicinal Chemistry</i> , 2016 , 59, 5604-21	8.3	46
34	Increasing small molecule drug developability in sub-optimal chemical space. <i>MedChemComm</i> , 2013 , 4, 673	5	46
33	How drug-like are TuglyTdrugs: do drug-likeness metrics predict ADME behaviour in humans?. <i>Drug Discovery Today</i> , 2014 , 19, 489-95	8.8	43
32	Medicinal chemistry in drug discovery in big pharma: past, present and future. <i>Drug Discovery Today</i> , 2018 , 23, 219-234	8.8	41

31	Emergence of Small-Molecule Non-RGD-Mimetic Inhibitors for RGD Integrins. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 3241-3251	8.3	37
30	Emerging therapeutic opportunities for integrin inhibitors. <i>Nature Reviews Drug Discovery</i> , 2021 ,	64.1	30
29	Cyclopropyl Carboxamides: A New Oral Antimalarial Series Derived from the Tres Cantos Anti-Malarial Set (TCAMS). <i>ACS Medicinal Chemistry Letters</i> , 2011 , 2, 840-4	4.3	26
28	Non-steroidal glucocorticoid agonists: the discovery of aryl pyrazoles as A-ring mimetics. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007 , 17, 4737-45	2.9	26
27	Analysis of neighborhood behavior in lead optimization and array design. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 195-208	6.1	25
26	Lead optimization in 12 months? True confessions of a chemistry team. <i>Drug Discovery Today</i> , 2001 , 6, 947-953	8.8	25
25	Translational pharmacology of an inhaled small molecule $\alpha_5\beta_1$ integrin inhibitor for idiopathic pulmonary fibrosis. <i>Nature Communications</i> , 2020 , 11, 4659	17.4	23
24	Discovery of (S)-3-(3-(3,5-Dimethyl-1 H-pyrazol-1-yl)phenyl)-4-((R)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)ethyl)pyrrolidin-1-yl)butanoic Acid, a Nonpeptidic Integrin Inhibitor for the Inhaled Treatment of Idiopathic Pulmonary Fibrosis. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 8417-8443	8.3	23
23	A direct route to triazole boronic esters and their application in the synthesis of small molecule arrays. <i>Tetrahedron Letters</i> , 2009 , 50, 5539-5541	2	22
22	Synthesis and determination of absolute configuration of a non-peptidic $\alpha_5\beta_1$ integrin antagonist for the treatment of idiopathic pulmonary fibrosis. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 5992-6009	3.0	21
21	Structure Activity Relationships of α_5 Integrin Antagonists for Pulmonary Fibrosis by Variation in Aryl Substituents. <i>ACS Medicinal Chemistry Letters</i> , 2014 , 5, 1207-12	4.3	20
20	Aryl aminopyrazole benzamides as oral non-steroidal selective glucocorticoid receptor agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009 , 19, 158-62	2.9	20
19	Rational Design of Autotaxin Inhibitors by Structural Evolution of Endogenous Modulators. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 2006-2017	8.3	19
18	Structure-Activity Relationships of Small Molecule Autotaxin Inhibitors with a Discrete Binding Mode. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 722-748	8.3	19
17	Heterocyclic replacements for benzene: Maximising ADME benefits by considering individual ring isomers. <i>European Journal of Medicinal Chemistry</i> , 2016 , 124, 1057-1068	6.8	15
16	Asymmetric Rhodium-Catalysed Addition of Arylboronic Acids to Acyclic Unsaturated Esters Containing a Basic β Amino Group. <i>Synlett</i> , 2012 , 23, 2817-2821	2.2	14
15	A practical drug discovery project at the undergraduate level. <i>Drug Discovery Today</i> , 2013 , 18, 1158-72	8.8	11
14	Late-Stage Functionalization by Chan-Lam Amination: Rapid Access to Potent and Selective Integrin Inhibitors. <i>Chemistry - A European Journal</i> , 2020 , 26, 7678-7684	4.8	10

13	Passing on the medicinal chemistry baton: training undergraduates to be industry-ready through research projects between the University of Nottingham and GlaxoSmithKline. <i>Drug Discovery Today</i> , 2016 , 21, 880-7	8.8	9
12	Highly tractable, sub-nanomolar non-steroidal glucocorticoid receptor agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009 , 19, 4846-50	2.9	9
11	The Discovery of Novel Antimalarial Aminoxadiazoles as a Promising Nonendoperoxide Scaffold. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 6880-6896	8.3	8
10	Unusual Undergraduate Training in Medicinal Chemistry in Collaboration between Academia and Industry. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 7958-7964	8.3	7
9	Efficient synthesis of an α -trifluoromethyl- β -silyloxymethyl epoxide enabling stepwise double functionalisation to afford CF ₃ -substituted tertiary alcohols. <i>Tetrahedron Letters</i> , 2008 , 49, 5101-5104	2	7
8	Identification of a novel class of autotaxin inhibitors through cross-screening. <i>MedChemComm</i> , 2015 , 6, 1149-1155	5	6
7	Profile of a Highly Selective Quaternized Pyrrolidine Betaine Integrin Inhibitor-(3)-3-(3-(3,5-Dimethyl-1-pyrazol-1-yl)phenyl)-4-((1 and 1,3)-1-methyl-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)ethyl)pyrrolidin-1-ium-1-yl)butanoate Synthesized by Stereoselective Methylation. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 7543-7556	8.3	4
6	Discovery of an Orally Bioavailable Pan α Integrin Inhibitor for Idiopathic Pulmonary Fibrosis. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 8796-8808	8.3	3
5	The Design of Potent, Selective and Drug-Like RGD α Small-Molecule Inhibitors Derived from non-RGD α Antagonists. <i>ChemMedChem</i> , 2019 , 14, 1315-1320	3.7	3
4	Sprinkling the pixie dust: reflections on innovation and innovators in medicinal chemistry and drug discovery. <i>Drug Discovery Today</i> , 2020 , 25, 599-609	8.8	3
3	Relative binding affinities of integrin antagonists by equilibrium dialysis and liquid chromatography-mass spectrometry. <i>ACS Medicinal Chemistry Letters</i> , 2015 , 6, 221-4	4.3	3
2	Writing Your Next Medicinal Chemistry Article: Journal Bibliometrics and Guiding Principles for Industrial Authors. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 14336-14356	8.3	2
1	Molecular Simulation of α Integrin Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5487-5498	6.1	1