Simon J F Macdonald

List of Publications by Year
in descending order

49	3,098	218381	189595
papers	citations	26 h-index	50 g-index

51	51	51	4077
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The impact of aromatic ring count on compound developability â€“ are too many aromatic rings a liability in drug design?. Drug Discovery Today, 2009, 14, 1011-1020.	3.2	637
2	The impact of aromatic ring count on compound developability: further insights by examining carbo- and hetero-aromatic and -aliphatic ring types. Drug Discovery Today, 2011, 16, 164-171.	3.2	333
3	Factors Determining the Selection of Organic Reactions by Medicinal Chemists and the Use of These Reactions in Arrays (Small Focused Libraries). Angewandte Chemie - International Edition, 2010, 49, 8082-8091.	7.2	248
4	Emerging therapeutic opportunities for integrin inhibitors. Nature Reviews Drug Discovery, 2022, 21, 60-78.	21.5	191
5	Dissecting fibrosis: therapeutic insights from the small-molecule toolbox. Nature Reviews Drug Discovery, 2015, 14, 693-720.	21.5	181
6	The developability of heteroaromatic and heteroaliphatic rings â€“ do some have a better pedigree as potential drug molecules than others?. MedChemComm, 2012, 3, 1062.	3.5	144
7	An Î±vâ€RGD Integrin Inhibitor Toolbox: Drug Discovery Insight, Challenges and Opportunities. Angewandte Chemie - International Edition, 2018, 57, 3298-3321.	7.2	94
8	Dimeric Zanamivir Conjugates with Various Linking Groups Are Potent, Long-Lasting Inhibitors of Influenza Neuraminidase Including H5N1 Avian Influenza. Journal of Medicinal Chemistry, 2005, 48, 2964-2971.	2.9	82
9	Potent and Long-Acting Dimeric Inhibitors of Influenza Virus Neuraminidase Are Effective at a Once-Weekly Dosing Regimen. Antimicrobial Agents and Chemotherapy, 2004, 48, 4542-4549.	1.4	81
10	Physicochemical Descriptors of Aromatic Character and Their Use in Drug Discovery. Journal of Medicinal Chemistry, 2014, 57, 7206-7215.	2.9	74
11	An Invitation to Open Innovation in Malaria Drug Discovery: 47 Quality Starting Points from the TCAMS. ACS Medicinal Chemistry Letters, 2011, 2, 741-746.	1.3	69
12	Increasing small molecule drug developability in sub-optimal chemical space. MedChemComm, 2013, 4, 673.	3.5	67
13	Translational pharmacology of an inhaled small molecule Î±vÎ²6 integrin inhibitor for idiopathic pulmonary fibrosis. Nature Communications, 2020, 11, 4659.	5.8	65
14	Medicinal chemistry in drug discovery in big pharma: past, present and future. Drug Discovery Today, 2018, 23, 219-234.	3.2	61
15	Development of Autotaxin Inhibitors: An Overview of the Patent and Primary Literature. Journal of Medicinal Chemistry, 2016, 59, 5604-5621.	2.9	59
16	Analysis of the Calculated Physicochemical Properties of Respiratory Drugs: Can We Design for Inhaled Drugs Yet?. Journal of Chemical Information and Modeling, 2009, 49, 1025-1032.	2.5	58
17	Highly potent and long-acting trimeric and tetrameric inhibitors of influenza virus neuraminidase. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1589-1592.	1.0	56
18	How drug-like are â€˜uglyâ€™ drugs: do drug-likeness metrics predict ADME behaviour in humans?. Drug Discovery Today, 2014, 19, 489-495.	3.2	56

#	Article	IF	Citations
19	Emergence of Small-Molecule Non-RGD-Mimetic Inhibitors for RGD Integrins. Journal of Medicinal Chemistry, 2017, 60, 3241-3251.	2.9	40
20	Rational Design of Autotaxin Inhibitors by Structural Evolution of Endogenous Modulators. Journal of Medicinal Chemistry, 2017, 60, 2006-2017.	2.9	34
21	Discovery of (S)-3-(3-(3,5-Dimethyl-1H-pyrazol-1-yl)phenyl)-4-((R)-3-(2-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)ethyl)pyrrolidin-1 Acid, a Nonpeptidic Î±_vÎ²₆ Integrin Inhibitor for the Inhaled Treatment of Idiopathic Pulmonary Fibrosis. Journal of Medicinal Chemistry, 2018, 61, 8417-8443.	2.9	31
22	Structureâ€“Activity Relationships of Small Molecule Autotaxin Inhibitors with a Discrete Binding Mode. Journal of Medicinal Chemistry, 2017, 60, 722-748.	2.9	29
23	Non-steroidal glucocorticoid agonistsâ€”The discovery of aryl pyrazoles as A-ring mimetics. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4737-4745.	1.0	28
24	Lead optimization in 12 months? True confessions of a chemistry team. Drug Discovery Today, 2001, 6, 947-953.	3.2	27
25	Analysis of Neighborhood Behavior in Lead Optimization and Array Design. Journal of Chemical Information and Modeling, 2009, 49, 195-208.	2.5	26
26	Cyclopropyl Carboxamides: A New Oral Antimalarial Series Derived from the Tres Cantos Anti-Malarial Set (TCAMS). ACS Medicinal Chemistry Letters, 2011, 2, 840-844.	1.3	26
27	A direct route to triazole boronic esters and their application in the synthesis of small molecule arrays. Tetrahedron Letters, 2009, 50, 5539-5541.	0.7	25
28	Synthesis and determination of absolute configuration of a non-peptidic Î±_vÎ²₆ integrin antagonist for the treatment of idiopathic pulmonary fibrosis. Organic and Biomolecular Chemistry, 2016, 14, 5992-6009.	1.5	22
29	Structure Activity Relationships of Î±_v Integrin Antagonists for Pulmonary Fibrosis by Variation in Aryl Substituents. ACS Medicinal Chemistry Letters, 2014, 5, 1207-1212.	1.3	21
30	Aryl aminopyrazole benzamides as oral non-steroidal selective glucocorticoid receptor agonists. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 158-162.	1.0	20
31	Heterocyclic replacements for benzene: Maximising ADME benefits by considering individual ring isomers. European Journal of Medicinal Chemistry, 2016, 124, 1057-1068.	2.6	17
32	Asymmetric Rhodium-Catalysed Addition of Arylboronic Acids to Acyclic Unsaturated Esters Containing a Basic Î²-Amino Group. Synlett, 2012, 23, 2817-2821.	1.0	16
33	A practical drug discovery project at the undergraduate level. Drug Discovery Today, 2013, 18, 1158-1172.	3.2	12
34	Lateâ€Stage Functionalization by Chanâ€“Lam Amination: Rapid Access to Potent and Selective Integrin Inhibitors. Chemistry - A European Journal, 2020, 26, 7678-7684.	1.7	12
35	The Discovery of Novel Antimalarial Aminoxadiazoles as a Promising Nonendoperoxide Scaffold. Journal of Medicinal Chemistry, 2017, 60, 6880-6896.	2.9	11
36	Efficient synthesis of an Î±-trifluoromethyl-Î±-tosyloxymethyl epoxide enabling stepwise double functionalisation to afford CF3-substituted tertiary alcohols. Tetrahedron Letters, 2008, 49, 5101-5104.	0.7	10

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37	Highly tractable, sub-nanomolar non-steroidal glucocorticoid receptor agonists. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4846-4850.	1.0	10
38	Passing on the medicinal chemistry baton: training undergraduates to be industry-ready through research projects between the University of Nottingham and GlaxoSmithKline. Drug Discovery Today, 2016, 21, 880-887.	3.2	9
39	Unusual Undergraduate Training in Medicinal Chemistry in Collaboration between Academia and Industry. Journal of Medicinal Chemistry, 2017, 60, 7958-7964.	2.9	9
40	Identification of a novel class of autotaxin inhibitors through cross-screening. MedChemComm, 2015, 6, 1149-1155.	3.5	7
41	Discovery of an Orally Bioavailable Pan Î±v Integrin Inhibitor for Idiopathic Pulmonary Fibrosis. Journal of Medicinal Chemistry, 2019, 62, 8796-8808.	2.9	7
42	Molecular Simulation of Î±vÎ²6 Integrin Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 5487-5498.	2.5	7
43	The Design of Potent, Selective and Drugâ€Like RGD Î±vÎ²1 Smallâ€Molecule Inhibitors Derived from nonâ€RGD Î±4Î²1 Antagonists. ChemMedChem, 2019, 14, 1315-1320.	1.6	6
44	Structure-Based Design of a Novel Class of Autotaxin Inhibitors Based on Endogenous Allosteric Modulators. Journal of Medicinal Chemistry, 2022, 65, 6338-6351.	2.9	6
45	Relative Binding Affinities of Integrin Antagonists by Equilibrium Dialysis and Liquid Chromatographyâ€“Mass Spectrometry. ACS Medicinal Chemistry Letters, 2015, 6, 221-224.	1.3	5
46	Profile of a Highly Selective Quaternized Pyrrolidine Betaine Î±_vÎ²₆ Integrin Inhibitorâ€”(3S)-3-(3-(3,5-Dimethyl-1H-pyrazol-1-yl)phenyl)-4-((1S and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 382 T Synthesized by Stereoselective Methylation. Journal of Medicinal Chemistry, 2019, 62, 7543-7556.	2.9	5
47	Writing Your Next Medicinal Chemistry Article: Journal Bibliometrics and Guiding Principles for Industrial Authors. Journal of Medicinal Chemistry, 2020, 63, 14336-14356.	2.9	5
48	Sprinkling the pixie dust: reflections on innovation and innovators in medicinal chemistry and drug discovery. Drug Discovery Today, 2020, 25, 599-609.	3.2	5
49	How Diverse Is Medicinal Chemistry? Insights into Race, Ethnicity, Origin, Gender, and Geography. Journal of Medicinal Chemistry, 2022, 65, 37-57.	2.9	2