# Simon J F Macdonald

## List of Publications by Year in Descending Order



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| 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 | Emerging therapeutic opportunities for integrin inhibitors. *Nature Reviews Drug Discovery*, **2021**, | 64.1 | 30 |
| 47 | Molecular Simulation of □□ Integrin Inhibitors. *Journal of Chemical Information and Modeling*, **2020**, 60, 5487-5498 | 6.1 | 1 |
| 46 | Late-Stage Functionalization by Chan-Lam Amination: Rapid Access to Potent and Selective Integrin Inhibitors. *Chemistry - A European Journal*, **2020**, 26, 7678-7684 | 4.8 | 10 |
| 45 | Sprinkling the pixie dust: reflections on innovation and innovators in medicinal chemistry and drug discovery. *Drug Discovery Today*, **2020**, 25, 599-609 | 8.8 | 3 |
| 44 | Writing Your Next Medicinal Chemistry Article: Journal Bibliometrics and Guiding Principles for Industrial Authors. *Journal of Medicinal Chemistry*, **2020**, 63, 14336-14356 | 8.3 | 2 |
| 43 | Translational pharmacology of an inhaled small molecule □□ integrin inhibitor for idiopathic pulmonary fibrosis. *Nature Communications*, **2020**, 11, 4659 | 17.4 | 23 |
| 42 | Discovery of an Orally Bioavailable Pan □ Integrin Inhibitor for Idiopathic Pulmonary Fibrosis. *Journal of Medicinal Chemistry*, **2019**, 62, 8796-8808 | 8.3 | 3 |
| 41 | The Design of Potent, Selective and Drug-Like RGD □□ Small-Molecule Inhibitors Derived from non-RGD □□ Antagonists. *ChemMedChem*, **2019**, 14, 1315-1320 | 3.7 | 3 |
| 40 | 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. *Journal of Medicinal Chemistry*, **2019**, 62, 7543-7556 | 8.3 | 4 |
| 39 | Medicinal chemistry in drug discovery in big pharma: past, present and future. *Drug Discovery Today* , **2018**, 23, 219-234 | 8.8 | 41 |
| 38 | An □-RGD Integrin Inhibitor Toolbox: Drug Discovery Insight, Challenges and Opportunities. *Angewandte Chemie - International Edition*, **2018**, 57, 3298-3321 | 16.4 | 64 |
| 37 | 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. *Journal of Medicinal Chemistry*, **2018**, 61, 8417-8443 | 8.3 | 23 |
| 36 | Emergence of Small-Molecule Non-RGD-Mimetic Inhibitors for RGD Integrins. *Journal of Medicinal Chemistry*, **2017**, 60, 3241-3251 | 8.3 | 37 |
| 35 | Rational Design of Autotaxin Inhibitors by Structural Evolution of Endogenous Modulators. *Journal of Medicinal Chemistry*, **2017**, 60, 2006-2017 | 8.3 | 19 |
| 34 | Unusual Undergraduate Training in Medicinal Chemistry in Collaboration between Academia and Industry. *Journal of Medicinal Chemistry*, **2017**, 60, 7958-7964 | 8.3 | 7 |
| 33 | Structure-Activity Relationships of Small Molecule Autotaxin Inhibitors with a Discrete Binding Mode. *Journal of Medicinal Chemistry*, **2017**, 60, 722-748 | 8.3 | 19 |
| 32 | The Discovery of Novel Antimalarial Aminoxadiazoles as a Promising Nonendoperoxide Scaffold. *Journal of Medicinal Chemistry*, **2017**, 60, 6880-6896 | 8.3 | 8 |

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| 31 | Heterocyclic replacements for benzene: Maximising ADME benefits by considering individual ring isomers. *European Journal of Medicinal Chemistry*, **2016**, 124, 1057-1068 | 6.8 | 15 |
| 30 | 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, 880-7 | 8.8 | 9 |
| 29 | Development of Autotaxin Inhibitors: An Overview of the Patent and Primary Literature. *Journal of Medicinal Chemistry*, **2016**, 59, 5604-21 | 8.3 | 46 |
| 28 | Synthesis and determination of absolute configuration of a non-peptidic αvβ6 integrin antagonist for the treatment of idiopathic pulmonary fibrosis. *Organic and Biomolecular Chemistry*, **2016**, 14, 5992-6009 | 3.9 | 21 |
| 27 | Identification of a novel class of autotaxin inhibitors through cross-screening. *MedChemComm*, **2015**, 6, 1149-1155 | 5 | 6 |
| 26 | Dissecting fibrosis: therapeutic insights from the small-molecule toolbox. *Nature Reviews Drug Discovery*, **2015**, 14, 693-720 | 64.1 | 141 |
| 25 | Relative binding affinities of integrin antagonists by equilibrium dialysis and liquid chromatography-mass spectrometry. *ACS Medicinal Chemistry Letters*, **2015**, 6, 221-4 | 4.3 | 3 |
| 24 | How drug-like are ‘ugly’ drugs: do drug-likeness metrics predict ADME behaviour in humans?. *Drug Discovery Today*, **2014**, 19, 489-95 | 8.8 | 43 |
| 23 | Structure Activity Relationships of αvβ6 Integrin Antagonists for Pulmonary Fibrosis by Variation in Aryl Substituents. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1207-12 | 4.3 | 20 |
| 22 | Physicochemical descriptors of aromatic character and their use in drug discovery. *Journal of Medicinal Chemistry*, **2014**, 57, 7206-15 | 8.3 | 58 |
| 21 | Increasing small molecule drug developability in sub-optimal chemical space. *MedChemComm*, **2013**, 4, 673 | 5 | 46 |
| 20 | A practical drug discovery project at the undergraduate level. *Drug Discovery Today*, **2013**, 18, 1158-72 | 8.8 | 11 |
| 19 | The developability of heteroaromatic and heteroaliphatic rings – do some have a better pedigree as potential drug molecules than others?. *MedChemComm*, **2012**, 3, 1062 | 5 | 128 |
| 18 | Asymmetric Rhodium-Catalysed Addition of Arylboronic Acids to Acyclic Unsaturated Esters Containing a Basic Amino Group. *Synlett*, **2012**, 23, 2817-2821 | 2.2 | 14 |
| 17 | An Invitation to Open Innovation in Malaria Drug Discovery: 47 Quality Starting Points from the TCAMS. *ACS Medicinal Chemistry Letters*, **2011**, 2, 741-6 | 4.3 | 61 |
| 16 | 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, 164-71 | 8.8 | 286 |
| 15 | Cyclopropyl Carboxamides: A New Oral Antimalarial Series Derived from the Tres Cantos Anti-Malarial Set (TCAMS). *ACS Medicinal Chemistry Letters*, **2011**, 2, 840-4 | 4.3 | 26 |
| 14 | Faktoren für die Auswahl organischer Reaktionen in der medizinischen Chemie und die Anwendung dieser Reaktionen in Arrays (kleinen fokussierten Bibliotheken). *Angewandte Chemie*, **2010**, 122, 8258-8267 | 3.6 | 48 |

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| 13 | 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, 8082-91 | 16.4 | 208 |
| 12 | The impact of aromatic ring count on compound developability--are too many aromatic rings a liability in drug design?. *Drug Discovery Today*, **2009**, 14, 1011-20 | 8.8 | 512 |
| 11 | A direct route to triazole boronic esters and their application in the synthesis of small molecule arrays. *Tetrahedron Letters*, **2009**, 50, 5539-5541 | 2 | 22 |
| 10 | Aryl aminopyrazole benzamides as oral non-steroidal selective glucocorticoid receptor agonists. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 158-62 | 2.9 | 20 |
| 9 | Highly tractable, sub-nanomolar non-steroidal glucocorticoid receptor agonists. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 4846-50 | 2.9 | 9 |
| 8 | Analysis of neighborhood behavior in lead optimization and array design. *Journal of Chemical Information and Modeling*, **2009**, 49, 195-208 | 6.1 | 25 |
| 7 | Analysis of the calculated physicochemical properties of respiratory drugs: can we design for inhaled drugs yet?. *Journal of Chemical Information and Modeling*, **2009**, 49, 1025-32 | 6.1 | 49 |
| 6 | Efficient synthesis of an □trifluoromethyl-□tosyloxymethyl epoxide enabling stepwise double functionalisation to afford CF3-substituted tertiary alcohols. *Tetrahedron Letters*, **2008**, 49, 5101-5104 | 2 | 7 |
| 5 | Non-steroidal glucocorticoid agonists: the discovery of aryl pyrazoles as A-ring mimetics. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 4737-45 | 2.9 | 26 |
| 4 | 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, 2964-71 | 8.3 | 76 |
| 3 | Potent and long-acting dimeric inhibitors of influenza virus neuraminidase are effective at a once-weekly dosing regimen. *Antimicrobial Agents and Chemotherapy*, **2004**, 48, 4542-9 | 5.9 | 71 |
| 2 | Highly potent and long-acting trimeric and tetrameric inhibitors of influenza virus neuraminidase. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 1589-92 | 2.9 | 52 |
| 1 | Lead optimization in 12 months? True confessions of a chemistry team. *Drug Discovery Today*, **2001**, 6, 947-953 | 8.8 | 25 |