Robert C Glen

List of Publications by Citations

48 papers	1,380 citations	19 h-index	36 g-index
49 ext. papers	1,804 ext. citations	10.9 avg, IF	4.5 L-index

#	Paper	IF	Citations
48	Predicting drug metabolism: experiment and/or computation?. *Nature Reviews Drug Discovery*, **2015**, 14, 387-404	64.1	255
47	Microbiome-host systems interactions: protective effects of propionate upon the blood-brain barrier. *Microbiome*, **2018**, 6, 55	16.6	170
46	Elabela/Toddler Is an Endogenous Agonist of the Apelin APJ Receptor in the Adult Cardiovascular System, and Exogenous Administration of the Peptide Compensates for the Downregulation of Its Expression in Pulmonary Arterial Hypertension. *Circulation*, **2017**, 135, 1160-1173	16.7	127
45	Design, characterization, and first-in-human study of the vascular actions of a novel biased apelin receptor agonist. *Hypertension*, **2015**, 65, 834-40	8.5	105
44	Deep learning and 3D-DESI imaging reveal the hidden metabolic heterogeneity of cancer. *Chemical Science*, **2017**, 8, 3500-3511	9.4	83
43	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. *Metabolomics*, **2017**, 13, 12	4.7	52
42	Pharmacological targeting of apelin impairs glioblastoma growth. *Brain*, **2017**, 140, 2939-2954	11.2	46
41	PhenoMeNal: processing and analysis of metabolomics data in the cloud. *GigaScience*, **2019**, 8,	7.6	41
40	Cardiac action of the first G protein biased small molecule apelin agonist. *Biochemical Pharmacology*, **2016**, 116, 63-72	6	40
39	Metabolic Fingerprinting Links Oncogenic PIK3CA with Enhanced Arachidonic Acid-Derived Eicosanoids. *Cell*, **2020**, 181, 1596-1611.e27	56.2	39
38	[Pyr]Apelin-13 Is a Biologically Active ACE2 Metabolite of the Endogenous Cardiovascular Peptide [Pyr]Apelin-13. *Frontiers in Neuroscience*, **2017**, 11, 92	5.1	36
37	International Union of Basic and Clinical Pharmacology. CVII. Structure and Pharmacology of the Apelin Receptor with a Recommendation that Elabela/Toddler Is a Second Endogenous Peptide Ligand. *Pharmacological Reviews*, **2019**, 71, 467-502	22.5	35
36	Development and Comparison of hERG Blocker Classifiers: Assessment on Different Datasets Yields Markedly Different Results. *Molecular Informatics*, **2011**, 30, 443-58	3.8	34
35	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. *Journal of Cheminformatics*, **2015**, 7, 45	8.6	31
34	Metrabase: a cheminformatics and bioinformatics database for small molecule transporter data analysis and (Q)SAR modeling. *Journal of Cheminformatics*, **2015**, 7, 31	8.6	27
33	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. *Journal of Cheminformatics*, **2014**, 6, 29	8.6	25
32	A multi-label approach to target prediction taking ligand promiscuity into account. *Journal of Cheminformatics*, **2015**, 7, 24	8.6	23

31	A novel cyclic biased agonist of the apelin receptor, MM07, is disease modifying in the rat monocrotaline model of pulmonary arterial hypertension. *British Journal of Pharmacology*, **2019**, 176, 1206-1221	8.6	21
30	Validating the validation: reanalyzing a large-scale comparison of deep learning and machine learning models for bioactivity prediction. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 717-730	4.2	21
29	Metabolomics: The Stethoscope for the Twenty-First Century. *Medical Principles and Practice*, **2021**, 30, 301-310	2.1	17
28	The nPYc-Toolbox, a Python module for the pre-processing, quality-control and analysis of metabolic profiling datasets. *Bioinformatics*, **2019**, 35, 5359-5360	7.2	11
27	A combination of computational and experimental approaches identifies DNA sequence constraints associated with target site binding specificity of the transcription factor CSL. *Nucleic Acids Research* , **2014**, 42, 10550-63	20.1	11
26	Regulation of blood-brain barrier integrity by microbiome-associated methylamines and cognition by trimethylamine N-oxide. *Microbiome*, **2021**, 9, 235	16.6	11
25	A Bone Morphogenetic Protein (BMP)-derived Peptide Based on the Type I Receptor-binding Site Modifies Cell-type Dependent BMP Signalling. *Scientific Reports*, **2019**, 9, 13446	4.9	10
24	Colocalization Features for Classification of Tumors Using Desorption Electrospray Ionization Mass Spectrometry Imaging. *Analytical Chemistry*, **2019**, 91, 6530-6540	7.8	10
23	Computer-aided design of multi-target ligands at AR, AR and PDE10A, key proteins in neurodegenerative diseases. *Journal of Cheminformatics*, **2017**, 9, 67	8.6	10
22	Chapter 9 Molecular Similarity: Advances in Methods, Applications and Validations in Virtual Screening and QSAR. *Annual Reports in Computational Chemistry*, **2006**, 2, 141-168	1.8	10
21	Complexity of classical dynamics of molecular systems. I. Methodology. *Journal of Chemical Physics*, **2002**, 117, 9611-9617	3.9	10
20	Molecular mechanism of a specific capsid binder resistance caused by mutations outside the binding pocket. *Antiviral Research*, **2015**, 123, 138-45	10.8	9
19	SPUTNIK: an R package for filtering of spatially related peaks in mass spectrometry imaging data. *Bioinformatics*, **2019**, 35, 178-180	7.2	9
18	Experimental validation of in silico target predictions on synergistic protein targets. *MedChemComm*, **2013**, 4, 278-288	5	7
17	Structure-based design of allosteric calpain-1 inhibitors populating a novel bioactivity space. *European Journal of Medicinal Chemistry*, **2018**, 157, 1264-1275	6.8	6
16	Complexity of classical dynamics of molecular systems. II. Finite statistical complexity of a water$Na+ system. *Journal of Chemical Physics*, **2002**, 117, 9618-9622	3.9	6
15	Probability Based hERG Blocker Classifiers. *Molecular Informatics*, **2012**, 31, 679-85	3.8	5
14	Apelin peptides linked to anti-serum albumin domain antibodies retain affinity in vitro and are efficacious receptor agonists in vivo. *Basic and Clinical Pharmacology and Toxicology*, **2020**, 126 Suppl 6, 96-103	3.1	5

13	Consequences of Lipid Remodeling of Adipocyte Membranes Being Functionally Distinct from Lipid Storage in Obesity. *Journal of Proteome Research*, **2020**, 19, 3919-3935	5.6	4
12	G392E neuroserpin causing the dementia FENIB is secreted from cells but is not synaptotoxic. *Scientific Reports*, **2021**, 11, 8766	4.9	4
11	The structural basis for membrane assembly of immunoreceptor signalling complexes. *Journal of Molecular Modeling*, **2019**, 25, 277	2	2
10	Extraction and Integration of Genetic Networks from Short-Profile Omic Data Sets. *Metabolites*, **2020**, 10,	5.6	2
9	Microbiome□host systems interactions: Protective effects of propionate upon the blood□brain barrier		2
8	Network analysis of mass spectrometry imaging data from colorectal cancer identifies key metabolites common to metastatic development		2
7	Analysis of Differential Efficacy and Affinity of GABA (□1/□2) Selective Modulators. *Molecular Pharmaceutics*, **2016**, 13, 4001-4012	5.6	2
6	Estimation of permutation-based metabolome-wide significance thresholds		1
5	Structure-based identification of dual ligands at the AR and PDE10A with anti-proliferative effects in lung cancer cell-lines. *Journal of Cheminformatics*, **2021**, 13, 17	8.6	1
4	The G Protein Biased Small Molecule Apelin Agonist CMF-019 is Disease Modifying in Endothelial Cell Apoptosis and Induces Vasodilatation Without Desensitisation. *Frontiers in Pharmacology*, **2020**, 11, 588669	5.6	1
3	Multiple-testing correction in metabolome-wide association studies. *BMC Bioinformatics*, **2021**, 22, 67	3.6	1
2	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
1	Shouldn□t enantiomeric purity be included in the □minimum information about a bioactive entity? Response from the MIABE group. *Nature Reviews Drug Discovery*, **2012**, 11, 730-730	64.1	