Steve O'Hagan

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	A palette of fluorophores that are differentially accumulated by wild-type and mutant strains of Escherichia coli: surrogate ligands for profiling bacterial membrane transporters. Microbiology (United Kingdom), 2021, 167, .	1.8	15
2	An untargeted metabolomics strategy to measure differences in metabolite uptake and excretion by mammalian cell lines. Metabolomics, 2020, 16, 107.	3.0	26
3	Structural Similarities between Some Common Fluorophores Used in Biology, Marketed Drugs, Endogenous Metabolites, and Natural Products. Marine Drugs, 2020, 18, 582.	4.6	14
4	VAE-Sim: A Novel Molecular Similarity Measure Based on a Variational Autoencoder. Molecules, 2020, 25, 3446.	3.8	23
5	The role and robustness of the Gini coefficient as an unbiased tool for the selection of Gini genes for normalising expression profiling data. Scientific Reports, 2019, 9, 17960.	3.3	25
6	Generation of a Small Library of Natural Products Designed to Cover Chemical Space Inexpensively. , 2019, 1, e190005.		6
7	GeneGini: Assessment via the Gini Coefficient of Reference "Housekeeping―Genes and Diverse Human Transporter Expression Profiles. Cell Systems, 2018, 6, 230-244.e1.	6.2	61
8	Analysing and Navigating Natural Products Space for Generating Small, Diverse, But Representative Chemical Libraries. Biotechnology Journal, 2018, 13, 1700503.	3.5	25
9	Analysis of drug–endogenous human metabolite similarities in terms of their maximum common substructures. Journal of Cheminformatics, 2017, 9, 18.	6.1	25
10	Enhancing Drug Efficacy and Therapeutic Index through Cheminformatics-Based Selection of Small Molecule Binary Weapons That Improve Transporter-Mediated Targeting: A Cytotoxicity System Based on Gemcitabine. Frontiers in Pharmacology, 2017, 8, 155.	3.5	18
11	Consensus rank orderings of molecular fingerprints illustrate the most genuine similarities between marketed drugs and small endogenous human metabolites, but highlight exogenous natural products as the most important †natural' drug transporter substrates. ADMET and DMPK, 2017, 5, 85.	2.1	36
12	MetMaxStruct: A Tversky-Similarity-Based Strategy for Analysing the (Sub)Structural Similarities of Drugs and Endogenous Metabolites. Frontiers in Pharmacology, 2016, 7, 266.	3.5	26
13	The apparent permeabilities of Caco-2 cells to marketed drugs: magnitude, and independence from both biophysical properties and endogenite similarities. PeerJ, 2015, 3, e1405.	2.0	39
14	Understanding the foundations of the structural similarities between marketed drugs and endogenous human metabolites. Frontiers in Pharmacology, 2015, 6, 105.	3.5	27
15	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	3.0	140
16	Molecular phenotyping of a UK population: defining the human serum metabolome. Metabolomics, 2015, 11, 9-26.	3.0	202
17	Illuminating disease and enlightening biomedicine: Raman spectroscopy as a diagnostic tool. Analyst, The, 2013, 138, 3871.	3.5	163
18	Exploiting Genomic Knowledge in Optimising Molecular Breeding Programmes: Algorithms from Evolutionary Computing. PLoS ONE, 2012, 7, e48862.	2.5	15

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#	Article	IF	CITATIONS
19	Development of a Robust and Repeatable UPLCâ^'MS Method for the Long-Term Metabolomic Study of Human Serum. Analytical Chemistry, 2009, 81, 1357-1364.	6.5	447
20	Closed-Loop, Multiobjective Optimization of Two-Dimensional Gas Chromatography/Mass Spectrometry for Serum Metabolomics. Analytical Chemistry, 2007, 79, 464-476.	6.5	94
21	Direct infusion electrospray ionization mass spectra of crude cell extracts for microbial characterizations: influence of solvent conditions on the detection of proteins. Rapid Communications in Mass Spectrometry, 2006, 20, 21-30.	1.5	6
22	Closed-Loop, Multiobjective Optimization of Analytical Instrumentation:Â Gas Chromatography/Time-of-Flight Mass Spectrometry of the Metabolomes of Human Serum and of Yeast Fermentations. Analytical Chemistry, 2005, 77, 290-303.	6.5	136