R Scott Obach

List of Publications by Year
in descending order

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49 papers	5,837 citations	186265 28 h-index	182427 51 g-index
54 all docs	54 docs citations	54 times ranked	5481 citing authors

#	Article	IF	Citations
1	An oral SARS-CoV-2 M ^{pro} inhibitor clinical candidate for the treatment of COVID-19. Science, 2021, 374, 1586-1593.	12.6	1,074
2	VALIDATED ASSAYS FOR HUMAN CYTOCHROME P450 ACTIVITIES. Drug Metabolism and Disposition, 2004, 32, 647-660.	3.3	484
3	Mechanism-Based Inactivation of Human Cytochrome P450 Enzymes and the Prediction of Drug-Drug Interactions. Drug Metabolism and Disposition, 2007, 35, 246-255.	3.3	425
4	The Utility of in Vitro Cytochrome P450 Inhibition Data in the Prediction of Drug-Drug Interactions. Journal of Pharmacology and Experimental Therapeutics, 2006, 316, 336-348.	2.5	415
5	Trend Analysis of a Database of Intravenous Pharmacokinetic Parameters in Humans for 670 Drug Compounds. Drug Metabolism and Disposition, 2008, 36, 1385-1405.	3.3	345
6	Aldehyde Oxidase: An Enzyme of Emerging Importance in Drug Discovery. Journal of Medicinal Chemistry, 2010, 53, 8441-8460.	6.4	311
7	The Conduct of in Vitro Studies to Address Time-Dependent Inhibition of Drug-Metabolizing Enzymes: A Perspective of the Pharmaceutical Research and Manufacturers of America. Drug Metabolism and Disposition, 2009, 37, 1355-1370.	3.3	279
8	Chemical and Computational Methods for the Characterization of Covalent Reactive Groups for the Prospective Design of Irreversible Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 10072-10079.	6.4	249
9	Prediction of Volume of Distribution Values in Humans for Neutral and Basic Drugs Using Physicochemical Measurements and Plasma Protein Binding Data. Journal of Medicinal Chemistry, 2002, 45, 2867-2876.	6.4	194
10	Can In Vitro Metabolism-Dependent Covalent Binding Data in Liver Microsomes Distinguish Hepatotoxic from Nonhepatotoxic Drugs? An Analysis of 18 Drugs with Consideration of Intrinsic Clearance and Daily Dose. Chemical Research in Toxicology, 2008, 21, 1814-1822.	3.3	194
11	Mechanism-Based Inactivation (MBI) of Cytochrome P450 Enzymes: Structureâ€“Activity Relationships and Discovery Strategies To Mitigate Drugâ€“Drug Interaction Risks. Journal of Medicinal Chemistry, 2012, 55, 4896-4933.	6.4	176
12	Prediction of Human Volume of Distribution Values for Neutral and Basic Drugs. 2. Extended Data Set and Leave-Class-Out Statistics. Journal of Medicinal Chemistry, 2004, 47, 1242-1250.	6.4	161
13	POTENT INHIBITION OF HUMAN LIVER ALDEHYDE OXIDASE BY RALOXIFENE. Drug Metabolism and Disposition, 2004, 32, 89-97.	3.3	149
14	A Hybrid Mixture Discriminant Analysisâ^'Random Forest Computational Model for the Prediction of Volume of Distribution of Drugs in Human. Journal of Medicinal Chemistry, 2006, 49, 2262-2267.	6.4	101
15	Metabolism-Directed Design of Oxetane-Containing Arylsulfonamide Derivatives as Î³-Secretase Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 7772-7783.	6.4	92
16	Trend Analysis of a Database of Intravenous Pharmacokinetic Parameters in Humans for 1352 Drug Compounds. Drug Metabolism and Disposition, 2018, 46, 1466-1477.	3.3	91
17	Comprehensive Assessment of Human Pharmacokinetic Prediction Based on In Vivo Animal Pharmacokinetic Data, Part 2: Clearance. Journal of Clinical Pharmacology, 2013, 53, 178-191.	2.0	76
18	Hydralazine As a Selective Probe Inactivator of Aldehyde Oxidase in Human Hepatocytes: Estimation of the Contribution of Aldehyde Oxidase to Metabolic Clearance. Drug Metabolism and Disposition, 2012, 40, 1441-1448.	3.3	68

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19	Cross-Species Comparison of the Metabolism and Excretion of Zoniporide: Contribution of Aldehyde Oxidase to Interspecies Differences. Drug Metabolism and Disposition, 2010, 38, 641-654.	3.3	66
20	Disposition of Nirmatrelvir, an Orally Bioavailable Inhibitor of SARS-CoV-2 3C-Like Protease, across Animals and Humans. Drug Metabolism and Disposition, 2022, 50, 576-590.	3.3	64
21	Comprehensive Assessment of Human Pharmacokinetic Prediction Based on In Vivo Animal Pharmacokinetic Data, Part 1: Volume of Distribution at Steady State. Journal of Clinical Pharmacology, 2013, 53, 167-177.	2.0	60
22	Biosynthesis of Drug Metabolites and Quantitation Using NMR Spectroscopy for Use in Pharmacologic and Drug Metabolism Studies. Drug Metabolism and Disposition, 2014, 42, 1627-1639.	3.3	55
23	Discovery of Azetidinyl Ketolides for the Treatment of Susceptible and Multidrug Resistant Community-Acquired Respiratory Tract Infections. Journal of Medicinal Chemistry, 2009, 52, 7446-7457.	6.4	51
24	Clearance Mechanism Assignment and Total Clearance Prediction in Human Based upon in Silico Models. Journal of Medicinal Chemistry, 2014, 57, 4397-4405.	6.4	51
25	Aldehyde Oxidase 1 (AOX1) in Human Liver Cytosols: Quantitative Characterization of AOX1 Expression Level and Activity Relationship. Drug Metabolism and Disposition, 2013, 41, 1797-1804.	3.3	48
26	Application of a Micropatterned Cocultured Hepatocyte System To Predict Preclinical and Human-Specific Drug Metabolism. Drug Metabolism and Disposition, 2016, 44, 172-179.	3.3	48
27	Intrinsic reactivity profile of electrophilic moieties to guide covalent drug design: N-Î±-acetyl-<scp>l</scp>-lysine as an amine nucleophile. MedChemComm, 2016, 7, 864-872.	3.4	43
28	An Automated High-Throughput Metabolic Stability Assay Using an Integrated High-Resolution Accurate Mass Method and Automated Data Analysis Software. Drug Metabolism and Disposition, 2016, 44, 1653-1661.	3.3	35
29	Design and optimization of selective azaindole amide M 1 positive allosteric modulators. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 650-655.	2.2	35
30	Late-Stage Microsomal Oxidation Reduces Drugâ€“Drug Interaction and Identifies Phosphodiesterase 2A Inhibitor PF-06815189. ACS Medicinal Chemistry Letters, 2018, 9, 68-72.	2.8	31
31	Enzalutamide and Apalutamide: In Vitro Chemical Reactivity Studies and Activity in a Mouse Drug Allergy Model. Chemical Research in Toxicology, 2020, 33, 211-222.	3.3	31
32	Statistical Methods for Analysis of Time-Dependent Inhibition of Cytochrome P450 Enzymes. Drug Metabolism and Disposition, 2012, 40, 2289-2296.	3.3	27
33	Lead Diversification at the Nanomole Scale Using Liver Microsomes and Quantitative Nuclear Magnetic Resonance Spectroscopy: Application to Phosphodiesterase 2 Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 3626-3640.	6.4	25
34	Effective Application of Metabolite Profiling in Drug Design and Discovery. Journal of Medicinal Chemistry, 2020, 63, 6387-6406.	6.4	25
35	Biosynthesis of Fluorinated Analogs of Drugs Using Human Cytochrome P450 Enzymes Followed by Deoxyfluorination and Quantitative Nuclear Magnetic Resonance Spectroscopy to Improve Metabolic Stability. Drug Metabolism and Disposition, 2016, 44, 634-646.	3.3	23
36	Mechanistic insights on clearance and inhibition discordance between liver microsomes and hepatocytes when clearance in liver microsomes is higher than in hepatocytes. European Journal of Pharmaceutical Sciences, 2020, 155, 105541.	4.0	22

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37	Late-Stage Lead Diversification Coupled with Quantitative Nuclear Magnetic Resonance Spectroscopy to Identify New Structureâ€“Activity Relationship Vectors at Nanomole-Scale Synthesis: Application to Loratadine, a Human Histamine H₁ Receptor Inverse Agonist. Journal of Medicinal Chemistry, 2020, 63, 7268-7292.	6.4	21
38	Static and Dynamic Projections of Drug-Drug Interactions Caused by Cytochrome P450 3A Time-Dependent Inhibitors Measured in Human Liver Microsomes and Hepatocytes. Drug Metabolism and Disposition, 2021, 49, 947-960.	3.3	17
39	Cytochrome P450 3A Time-Dependent Inhibition Assays Are Too Sensitive for Identification of Drugs Causing Clinically Significant Drug-Drug Interactions: A Comparison of Human Liver Microsomes and Hepatocytes and Definition of Boundaries for Inactivation Rate Constants. Drug Metabolism and Disposition, 2021, 49, 442-450.	3.3	15
40	Metabolism and Excretion of Nirmatrelvir in Humans Using Quantitative Fluorine Nuclear Magnetic Resonance Spectroscopy: A Novel Approach for Accelerating Drug Development. Clinical Pharmacology and Therapeutics, 2022, 112, 1201-1206.	4.7	15
41	Development of Robust Quantitative Structure-Activity Relationship Models for CYP2C9, CYP2D6, and CYP3A4 Catalysis and Inhibition. Drug Metabolism and Disposition, 2021, 49, 822-832.	3.3	14
42	Role of Molybdenum-Containing Enzymes in the Biotransformation of the Novel Ghrelin Receptor Inverse Agonist PF-5190457: A Reverse Translational Bed-to-Bench Approach. Drug Metabolism and Disposition, 2019, 47, 874-882.	3.3	11
43	Metabolism of a 5HT₆ Antagonist, 2-Methyl-1-(Phenylsulfonyl)-4-(Piperazin-1-yl)-1H-Benzo[d]imidazole (SAM-760): Impact of Sulfonamide Metabolism on Diminution of a Ketoconazole-Mediated Clinical Drug-Drug Interaction. Drug Metabolism and Disposition, 2018, 46, 934-942.	3.3	7
44	Identification and quantitation of enzyme and transporter contributions to hepatic clearance for the assessment of potential drug-drug interactions. Drug Metabolism and Pharmacokinetics, 2020, 35, 18-29.	2.2	6
45	An exposureâ€“response analysis based on rifampin suggests CYP3A4 induction is driven by AUC: an in vitro investigation. Xenobiotica, 2017, 47, 673-681.	1.1	5
46	Unbiased Scanning Method and Data Banking Approach Using Ultra-High Performance Liquid Chromatography Coupled with High-Resolution Mass Spectrometry for Quantitative Comparison of Metabolite Exposure in Plasma across Species Analyzed at Different Dates. Analytical Chemistry, 2015, 87, 11771-11776.	6.5	3
47	Production of active recombinant human aldehyde oxidase (AOX) in the baculovirus expression vector system (BEVS) and deployment in a pre-clinical fraction-of-control AOX compound exposure assay. Protein Expression and Purification, 2021, 177, 105749.	1.3	3
48	Prediction of Metaboliteâ€toâ€Parent Drug Exposure: Derivation and Application of a Mechanistic Static Model. Clinical and Translational Science, 2020, 13, 520-528.	3.1	3
49	Consideration of the Unbound Drug Concentration in Enzyme Kinetics. Methods in Molecular Biology, 2021, 2342, 113-145.	0.9	2