Thomas A Baillie

List of Publications by Year
in descending order

88 papers	9,841 citations	41344 49 h-index	46799 89 g-index
91 all docs	91 docs citations	91 times ranked	8026 citing authors

#	Article	IF	Citations
1	Approaches to mitigate the risk of serious adverse reactions in covalent drug design. Expert Opinion on Drug Discovery, 2021, 16, 275-287.	5.0	17
2	Drugâ€“protein adducts: past, present, and future. Medicinal Chemistry Research, 2020, 29, 1093-1104.	2.4	14
3	Pharmacokinetic and Metabolic Profile of Deutetrabenazine (TEVâ€50717) Compared With Tetrabenazine in Healthy Volunteers. Clinical and Translational Science, 2020, 13, 707-717.	3.1	25
4	Managing Metabolic Activation Issues in Drug Discovery. , 2019, , 577-603.		1
5	Safety Assessment of Acyl Glucuronidesâ€”A Simplified Paradigm. Drug Metabolism and Disposition, 2018, 46, 908-912.	3.3	34
6	Zielgerichtete kovalente Inhibitoren fÃ¼r das Wirkstoffdesign. Angewandte Chemie, 2016, 128, 13606-13619.	2.0	39
7	Targeted Covalent Inhibitors for Drug Design. Angewandte Chemie - International Edition, 2016, 55, 13408-13421.	13.8	360
8	Biotransformation and bioactivation reactions â€“ 2015 literature highlights. Drug Metabolism Reviews, 2016, 48, 113-138.	3.6	14
9	The contributions of Sidney D. Nelson to drug metabolism research. Drug Metabolism Reviews, 2015, 47, 4-11.	3.6	6
10	The Generation, Detection, and Effects of Reactive Drug Metabolites. Medicinal Research Reviews, 2013, 33, 985-1080.	10.5	73
11	Enzyme Kinetics of Cytochrome P450-Mediated Reactions. Current Drug Metabolism, 2012, 2, 17-36.	1.2	100
12	An Inducible Cytochrome P450 3A4-Dependent Vitamin D Catabolic Pathway. Molecular Pharmacology, 2012, 81, 498-509.	2.3	87
13	Managing the challenge of chemically reactive metabolites in drug development. Nature Reviews Drug Discovery, 2011, 10, 292-306.	46.4	382
14	The resurgence of covalent drugs. Nature Reviews Drug Discovery, 2011, 10, 307-317.	46.4	1,384
15	Structural Alert/Reactive Metabolite Concept as Applied in Medicinal Chemistry to Mitigate the Risk of Idiosyncratic Drug Toxicity: A Perspective Based on the Critical Examination of Trends in the Top 200 Drugs Marketed in the United States. Chemical Research in Toxicology, 2011, 24, 1345-1410.	3.3	569
16	Role of Biotransformation in Drug-Induced Toxicity: Influence of Intra- and Inter-Species Differences in Drug Metabolism. Drug Metabolism and Pharmacokinetics, 2011, 26, 15-29.	2.2	114
17	Approaches for Minimizing Metabolic Activation of New Drug Candidates in Drug Discovery. Handbook of Experimental Pharmacology, 2010, , 511-544.	1.8	21
18	Approaches to the Assessment of Stable and Chemically Reactive Drug Metabolites in Early Clinical Trials. Chemical Research in Toxicology, 2009, 22, 263-266.	3.3	54

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19	Highâ€throughput, accurate mass liquid chromatography/tandem mass spectrometry on a quadrupole timeâ€ofâ€flight system as a â€˜firstâ€lineâ€™ approach for metabolite identification studies. Rapid Communications in Mass Spectrometry, 2008, 22, 1053-1061.	1.5	108
20	Fractional mass filtering as a means to assess circulating metabolites in early human clinical studies. Rapid Communications in Mass Spectrometry, 2008, 22, 3510-3516.	1.5	40
21	Metabolism and Toxicity of Drugs. Two Decades of Progress in Industrial Drug Metabolism. Chemical Research in Toxicology, 2008, 21, 129-137.	3.3	193
22	In Vitro Metabolic Activation of Lumiracoxib in Rat and Human Liver Preparations. Drug Metabolism and Disposition, 2008, 36, 469-473.	3.3	50
23	Minimizing metabolic activation during pharmaceutical lead optimization: progress, knowledge gaps and future directions. Current Opinion in Drug Discovery & Development, 2008, 11, 43-52.	1.9	14
24	Addressing Metabolic Activation as an Integral Component of Drug Design. Drug Metabolism Reviews, 2006, 38, 641-649.	3.6	72
25	Future of ToxicologyMetabolic Activation and Drug Design:Â Challenges and Opportunities in Chemical Toxicology. Chemical Research in Toxicology, 2006, 19, 889-893.	3.3	166
26	Complicating factors in safety testing of drug metabolites: Kinetic differences between generated and preformed metabolites. Toxicology and Applied Pharmacology, 2006, 217, 143-152.	2.8	81
27	EVIDENCE FOR THE BIOACTIVATION OF ZOMEPIRAC AND TOLMETIN BY AN OXIDATIVE PATHWAY: IDENTIFICATION OF GLUTATHIONE ADDUCTS IN VITRO IN HUMAN LIVER MICROSOMES AND IN VIVO IN RATS. Drug Metabolism and Disposition, 2006, 34, 145-151.	3.3	57
28	Bridging cheminformatic metabolite prediction and tandem mass spectrometry. Drug Discovery Today, 2005, 10, 711-717.	6.4	52
29	Metabolic Activation of a 1,3-Disubstituted Piperazine Derivative:Â Evidence for a Novel Ring Contraction to an Imidazoline. Chemical Research in Toxicology, 2005, 18, 271-276.	3.3	45
30	In Vitro Bioactivation of Dihydrobenzoxathiin Selective Estrogen Receptor Modulators by Cytochrome P450 3A4 in Human Liver Microsomes:â€‰ Formation of Reactive Iminium and Quinone Type Metabolites. Chemical Research in Toxicology, 2005, 18, 675-685.	3.3	68
31	Zafirlukast Metabolism by Cytochrome P450 3A4 Produces an Electrophilic Î±,Î²-Unsaturated Iminium Species That Results in the Selective Mechanism-Based Inactivation of the Enzyme. Chemical Research in Toxicology, 2005, 18, 1427-1437.	3.3	69
32	Negative Ion Tandem Mass Spectrometry for the Detection of Glutathione Conjugates. Chemical Research in Toxicology, 2005, 18, 630-638.	3.3	210
33	Minimizing the potential for metabolic activation as an integral part of drug design. Current Opinion in Drug Discovery & Development, 2005, 8, 44-50.	1.9	7
34	EVALUATION OF MICRODOSING STRATEGIES FOR STUDIES IN PRECLINICAL DRUG DEVELOPMENT: DEMONSTRATION OF LINEAR PHARMACOKINETICS IN DOGS OF A NUCLEOSIDE ANALOG OVER A 50-FOLD DOSE RANGE. Drug Metabolism and Disposition, 2004, 32, 1254-1259.	3.3	68
35	Integration of Knowledge-Based Metabolic Predictions with Liquid Chromatography Data-Dependent Tandem Mass Spectrometry for Drug Metabolism Studies:Â Application to Studies on the Biotransformation of Indinavir. Analytical Chemistry, 2004, 76, 823-832.	6.5	133
36	Drugâ^'Protein Adducts:Â An Industry Perspective on Minimizing the Potential for Drug Bioactivation in Drug Discovery and Development. Chemical Research in Toxicology, 2004, 17, 3-16.	3.3	707

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37	Organic Chemistry in Drug Discovery. Science, 2004, 303, 1810-1813.	12.6	107
38	The unanticipated loss of SO2 from sulfonamides in collision-induced dissociation. Rapid Communications in Mass Spectrometry, 2003, 17, 81-86.	1.5	55
39	Mechanistic Studies on Metabolic Interactions between Gemfibrozil and Statins. Journal of Pharmacology and Experimental Therapeutics, 2002, 301, 1042-1051.	2.5	280
40	Metabolism of a Thiazole Benzenesulfonamide Derivative, a Potent and Selective Agonist of the Human Î²3-Adrenergic Receptor, in Rats: Identification of a Novel Isethionic Acid Conjugate. Drug Metabolism and Disposition, 2002, 30, 778-787.	3.3	13
41	Glucuronidation of Statins in Animals and Humans: A Novel Mechanism of Statin Lactonization. Drug Metabolism and Disposition, 2002, 30, 505-512.	3.3	317
42	Extrapolation of Diclofenac Clearance from in Vitro Microsomal Metabolism Data: Role of Acyl Glucuronidation and Sequential Oxidative Metabolism of the Acyl Glucuronide. Journal of Pharmacology and Experimental Therapeutics, 2002, 303, 969-978.	2.5	149
43	Cytochrome P450 3A4-Mediated Bioactivation of Raloxifene:â€‰ Irreversible Enzyme Inhibition and Thiol Adduct Formation. Chemical Research in Toxicology, 2002, 15, 907-914.	3.3	169
44	Drug Metabolites in Safety Testing. Toxicology and Applied Pharmacology, 2002, 182, 188-196.	2.8	344
45	Studies on the Metabolism of Troglitazone to Reactive Intermediates in Vitro and in Vivo. Evidence for Novel Biotransformation Pathways Involving Quinone Methide Formation and Thiazolidinedione Ring Scissionâ€. Chemical Research in Toxicology, 2001, 14, 62-70.	3.3	316
46	A Kinetic Model for the Metabolic Interaction of Two Substrates at the Active Site of Cytochrome P450 3A4. Journal of Biological Chemistry, 2001, 276, 2256-2262.	3.4	107
47	Metabolic interactions between mibefradil and HMGâ€CoA reductase inhibitors: an in vitro investigation with human liver preparations. British Journal of Clinical Pharmacology, 1999, 47, 291-298.	2.4	96
48	Roles of Human Hepatic Cytochrome P450s 2C9 and 3A4 in the Metabolic Activation of Diclofenacâ€. Chemical Research in Toxicology, 1999, 12, 192-199.	3.3	156
49	Biotransformation of the Naturally Occurring Isothiocyanate Sulforaphane in the Rat:Â Identification of Phase I Metabolites and Glutathione Conjugates. Chemical Research in Toxicology, 1997, 10, 1228-1233.	3.3	202
50	Metabolism of the Chemoprotective Agent Diallyl Sulfide to Glutathione Conjugates in Rats. Chemical Research in Toxicology, 1997, 10, 318-327.	3.3	127
51	Identification in Rat Bile of Glutathione Conjugates of Fluoromethyl 2,2-Difluoro-1-(trifluoromethyl)vinyl Ether, a Nephrotoxic Degradate of the Anesthetic Agent Sevoflurane. Chemical Research in Toxicology, 1996, 9, 555-561.	3.3	54
52	In VitroStudies on the Metabolic Activation of the Furanopyridine L-754,394, a Highly Potent and Selective Mechanism-Based Inhibitor of Cytochrome P450 3A4. Chemical Research in Toxicology, 1996, 9, 1007-1012.	3.3	79
53	Studies on the formation of reactive intermediates from the antineoplastic agentN,Nâ€²Bis(2-chloroethyl)-N-nitrosourea (BCNU)in vitro andin Vivo. Characterization of novel glutathione adducts by ionspray tandem mass spectrometry. Journal of Mass Spectrometry, 1995, 30, 57-68.	1.6	13
54	Reversibility in Glutathione-Conjugate Formation. Advances in Pharmacology, 1994, 27, 163-181.	2.0	27

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55	Recognition of quaternary ammonium compounds using mass spectrometry. Rapid Communications in Mass Spectrometry, 1994, 8, 65-70.	1.5	11
56	Matrix-assisted laser desorption ionization for rapid determination of the sequences of biologically active peptides isolated from support-bound combinatorial peptide libraries. Rapid Communications in Mass Spectrometry, 1994, 8, 77-81.	1.5	63
57	Electrospray tandem mass spectrometry in the diagnosis of organic acidemias. Rapid Communications in Mass Spectrometry, 1994, 8, 129-133.	1.5	51
58	Improved detection of glucuronide and glutathione conjugates with thermospray ionization following esterification. Rapid Communications in Mass Spectrometry, 1994, 8, 371-376.	1.5	3
59	Metabolic activation of unsaturated derivatives of valproic acid. Identification of novel glutathione adducts formed through coenzyme A-dependent and -independent processes. Chemico-Biological Interactions, 1994, 90, 253-275.	4.0	62
60	Identification of Novel Glutathione Conjugates of Disulfiram and Diethyldithiocarbamate in Rat Bile by Liquid Chromatography-Tandem Mass Spectrometry. Evidence for Metabolic Activation of Disulfiram in vivo. Chemical Research in Toxicology, 1994, 7, 526-533.	3.3	68
61	Identification of S-(n-Butylcarbamoyl)glutathione, a Reactive Carbamoylating Agent, as a Biliary Metabolite of Benomyl in the Rat. Journal of Agricultural and Food Chemistry, 1994, 42, 2953-2957.	5.2	12
62	Mass spectrometry in the analysis of glutathione conjugates. Biological Mass Spectrometry, 1993, 22, 319-325.	0.5	232
63	Binding of flexible ligands to proteins: Valproic acid and its interaction with cytochrome P450cam. International Journal of Quantum Chemistry, 1993, 48, 161-180.	2.0	36
64	Glutathione and N-acetylcysteine conjugates of 2-chloroethyl isocyanate. Identification as metabolites of N,N'-bis(2-chloroethyl)-N-nitrosourea in the rat and inhibitory properties toward glutathione reductase in vitro. Chemical Research in Toxicology, 1993, 6, 376-383.	3.3	48
65	Toxicity of the methyl isocyanate metabolite S-(N-methylcarbamoyl)GSH on mouse embryos in culture. Teratology, 1992, 46, 61-67.	1.6	17
66	Metabolism of valproate to hepatotoxic intermediates. Pharmaceutisch Weekblad Scientific Edition, 1992, 14, 122-125.	0.9	32
67	Glutathione: a vehicle for the transport of chemically reactive metabolites in vivo. Accounts of Chemical Research, 1991, 24, 264-270.	15.6	139
68	Carbamoylation of peptides and proteins in vitro by S-(N-methylcarbamoyl)glutathione and S-(N-methylcarbamoyl)cysteine, two electrophilic S-linked conjugates of methyl isocyanate. Chemical Research in Toxicology, 1991, 4, 436-444.	3.3	73
69	Biotransformation of methyl isocyanate in the rat. Evidence for glutathione conjugation as a major pathway of metabolism and implications for isocyanate-mediated toxicities. Chemical Research in Toxicology, 1991, 4, 157-161.	3.3	122
70	In vitro and in vivo investigations of dihydropyridine-based chemical delivery systems for anticonvulsants. Pharmaceutical Research, 1991, 08, 690-697.	3.5	15
71	Effects of polytherapy with phenytoin, carbamazepine, and stiripentol on formation of 4-ene-valproate, a hepatotoxic metabolite of valproic acid. Clinical Pharmacology and Therapeutics, 1990, 48, 225-235.	4.7	113
72	S-(N-Methylcarbamoyl)glutathione: A reactive S-linked metabolite of methyl isocyanate. Biochemical and Biophysical Research Communications, 1990, 166, 245-250.	2.1	74

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73	Synthesis and characterization of isotopically-labelled cysteine- and glutathione conjugates of methylisocyanate. Journal of Labelled Compounds and Radiopharmaceuticals, 1989, 27, 1371-1382.	1.0	6
74	Studies on the biotransformation of ketamine. Ilâ€"quantitative significance of theN-demethylation pathway in ratsin vivo determined by a novel stable isotope technique. Biomedical & Environmental Mass Spectrometry, 1989, 18, 401-404.	1.6	12
75	Application of liquid chromatography/thermospray mass spectrometry to studies on the formation of glutathione and cysteine conjugates from monomethylcarbamate metabolites of bambuterol. Rapid Communications in Mass Spectrometry, 1989, 3, 360-363.	1.5	16
76	The use of alkoxycarbonyl derivatives for the mass spectral analysis of drug-thioether metabolites. Studies with the cysteine, mercapturic acid and glutathione conjugates of acetaminophen. Biomedical & Environmental Mass Spectrometry, 1988, 15, 637-647.	1.6	17
77	Applications of tandem mass spectrometry to the characterization of derivatized glutathione conjugates. Studies withS-(N-Methylcarbamoyl)-glutathione, a metabolite of the antineoplastic agentN-methylformamide. Biological Mass Spectrometry, 1988, 16, 51-56.	0.5	29
78	Covalent binding of acetaminophen to mouse hemoglobin. Identification of major and minor adducts formed in vivo and implications for the nature of the arylating metabolites. Chemico-Biological Interactions, 1988, 68, 99-116.	4.0	39
79	Metabolic activation of valproic acid and drug-mediated hepatotoxicity. Role of the terminal olefin, 2-n-propyl-4-pentenoic acid. Chemical Research in Toxicology, 1988, 1, 195-199.	3.3	92
80	Comparative pharmacology in the rat of ketamine and its two principal metabolites, norketamine and (Z)-6-hydroxynorketamine. Journal of Medicinal Chemistry, 1986, 29, 2396-2399.	6.4	117
81	Drug Biotransformation: Mechanistic Studies With Stable Isotopes. Journal of Clinical Pharmacology, 1986, 26, 448-451.	2.0	9
82	Recent Advances in the Use of Stable Isotopes in Drug Metabolism Research. Journal of Clinical Pharmacology, 1986, 26, 481-484.	2.0	23
83	Valproate hydroxylation by human fetal tissues and embryotoxicity of metabolites. Clinical Pharmacology and Therapeutics, 1986, 40, 172-177.	4.7	22
84	Metabolism of the nigrostriatal toxin 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine by liver homogenate fractions. Journal of Medicinal Chemistry, 1985, 28, 997-1001.	6.4	72
85	Inhibition of medium-chain fatty acid Î²-oxidationinvitro by valproic acid and its unsaturated metabolite, 2-n-propyl-4-pentenoic acid. Biochemical and Biophysical Research Communications, 1985, 132, 245-252.	2.1	83
86	2-acetamido-p-benzoquinone: A reactive arylating metabolite of 3'-hydroxyacetanilide. Biochemical Pharmacology, 1985, 34, 2871-2876.	4.4	9
87	Evidence for thein vitro metabolism of allylisopropylacetamide to reactive intermediates. Mechanistic studies with oxygen-18. Biomedical Mass Spectrometry, 1984, 11, 320-331.	1.9	8
88	Monoacetylhydrazine as a metabolite of isoniazid in man. Clinical Pharmacology and Therapeutics, 1977, 22, 602-608.	4.7	67