

# Thomas A Baillie

## List of Publications by Year in descending order

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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  | The resurgence of covalent drugs. <i>Nature Reviews Drug Discovery</i> , 2011, 10, 307-317.   | 46.4 | 1,384     |
| 2  | Drug-Protein Adducts: An Industry Perspective on Minimizing the Potential for Drug Bioactivation in Drug Discovery and Development. <i>Chemical Research in Toxicology</i> , 2004, 17, 3-16.  | 3.3  | 707       |
| 3  | 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. <i>Chemical Research in Toxicology</i> , 2011, 24, 1345-1410. | 3.3  | 569       |
| 4  | Managing the challenge of chemically reactive metabolites in drug development. <i>Nature Reviews Drug Discovery</i> , 2011, 10, 292-306.  | 46.4 | 382       |
| 5  | Targeted Covalent Inhibitors for Drug Design. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 13408-13421.   | 13.8 | 360       |
| 6  | Drug Metabolites in Safety Testing. <i>Toxicology and Applied Pharmacology</i> , 2002, 182, 188-196.  | 2.8  | 344       |
| 7  | Glucuronidation of Statins in Animals and Humans: A Novel Mechanism of Statin Lactonization. <i>Drug Metabolism and Disposition</i> , 2002, 30, 505-512.  | 3.3  | 317       |
| 8  | 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 Scission. <i>Chemical Research in Toxicology</i> , 2001, 14, 62-70.                                      | 3.3  | 316       |
| 9  | Mechanistic Studies on Metabolic Interactions between Gemfibrozil and Statins. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2002, 301, 1042-1051.   | 2.5  | 280       |
| 10 | Mass spectrometry in the analysis of glutathione conjugates. <i>Biological Mass Spectrometry</i> , 1993, 22, 319-325.   | 0.5  | 232       |
| 11 | Negative Ion Tandem Mass Spectrometry for the Detection of Glutathione Conjugates. <i>Chemical Research in Toxicology</i> , 2005, 18, 630-638.  | 3.3  | 210       |
| 12 | Biotransformation of the Naturally Occurring Isothiocyanate Sulforaphane in the Rat: Identification of Phase I Metabolites and Glutathione Conjugates. <i>Chemical Research in Toxicology</i> , 1997, 10, 1228-1233.  | 3.3  | 202       |
| 13 | Metabolism and Toxicity of Drugs. Two Decades of Progress in Industrial Drug Metabolism. <i>Chemical Research in Toxicology</i> , 2008, 21, 129-137.  | 3.3  | 193       |
| 14 | Cytochrome P450 3A4-Mediated Bioactivation of Raloxifene: Irreversible Enzyme Inhibition and Thiol Adduct Formation. <i>Chemical Research in Toxicology</i> , 2002, 15, 907-914.  | 3.3  | 169       |
| 15 | Future of Toxicology Metabolic Activation and Drug Design: Challenges and Opportunities in Chemical Toxicology. <i>Chemical Research in Toxicology</i> , 2006, 19, 889-893.   | 3.3  | 166       |
| 16 | Roles of Human Hepatic Cytochrome P450s 2C9 and 3A4 in the Metabolic Activation of Diclofenac. <i>Chemical Research in Toxicology</i> , 1999, 12, 192-199.  | 3.3  | 156       |
| 17 | Extrapolation of Diclofenac Clearance from in Vitro Microsomal Metabolism Data: Role of Acyl Glucuronidation and Sequential Oxidative Metabolism of the Acyl Glucuronide. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2002, 303, 969-978.  | 2.5  | 149       |
| 18 | Glutathione: a vehicle for the transport of chemically reactive metabolites in vivo. <i>Accounts of Chemical Research</i> , 1991, 24, 264-270.  | 15.6 | 139       |

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|----|--|------|-----------|
| 19 | Integration of Knowledge-Based Metabolic Predictions with Liquid Chromatography Data-Dependent Tandem Mass Spectrometry for Drug Metabolism Studies: An Application to Studies on the Biotransformation of Indinavir. <i>Analytical Chemistry</i> , 2004, 76, 823-832. | 6.5  | 133       |
| 20 | Metabolism of the Chemoprotective Agent Diallyl Sulfide to Glutathione Conjugates in Rats. <i>Chemical Research in Toxicology</i> , 1997, 10, 318-327.   | 3.3  | 127       |
| 21 | Biotransformation of methyl isocyanate in the rat. Evidence for glutathione conjugation as a major pathway of metabolism and implications for isocyanate-mediated toxicities. <i>Chemical Research in Toxicology</i> , 1991, 4, 157-161.                               | 3.3  | 122       |
| 22 | Comparative pharmacology in the rat of ketamine and its two principal metabolites, norketamine and (Z)-6-hydroxynorketamine. <i>Journal of Medicinal Chemistry</i> , 1986, 29, 2396-2399.  | 6.4  | 117       |
| 23 | Role of Biotransformation in Drug-Induced Toxicity: Influence of Intra- and Inter-Species Differences in Drug Metabolism. <i>Drug Metabolism and Pharmacokinetics</i> , 2011, 26, 15-29.   | 2.2  | 114       |
| 24 | Effects of polytherapy with phenytoin, carbamazepine, and stiripentol on formation of 4-ene-valproate, a hepatotoxic metabolite of valproic acid. <i>Clinical Pharmacology and Therapeutics</i> , 1990, 48, 225-235.   | 4.7  | 113       |
| 25 | High-throughput, accurate mass liquid chromatography/tandem mass spectrometry on a quadrupole time-of-flight system as a first-line approach for metabolite identification studies. <i>Rapid Communications in Mass Spectrometry</i> , 2008, 22, 1053-1061.            | 1.5  | 108       |
| 26 | A Kinetic Model for the Metabolic Interaction of Two Substrates at the Active Site of Cytochrome P450 3A4. <i>Journal of Biological Chemistry</i> , 2001, 276, 2256-2262.  | 3.4  | 107       |
| 27 | Organic Chemistry in Drug Discovery. <i>Science</i> , 2004, 303, 1810-1813.  | 12.6 | 107       |
| 28 | Enzyme Kinetics of Cytochrome P450-Mediated Reactions. <i>Current Drug Metabolism</i> , 2012, 2, 17-36.  | 1.2  | 100       |
| 29 | Metabolic interactions between mibefradil and HMG-CoA reductase inhibitors: an in vitro investigation with human liver preparations. <i>British Journal of Clinical Pharmacology</i> , 1999, 47, 291-298.  | 2.4  | 96        |
| 30 | Metabolic activation of valproic acid and drug-mediated hepatotoxicity. Role of the terminal olefin, 2-n-propyl-4-pentenoic acid. <i>Chemical Research in Toxicology</i> , 1988, 1, 195-199.   | 3.3  | 92        |
| 31 | An Inducible Cytochrome P450 3A4-Dependent Vitamin D Catabolic Pathway. <i>Molecular Pharmacology</i> , 2012, 81, 498-509.   | 2.3  | 87        |
| 32 | Inhibition of medium-chain fatty acid $\beta$ -oxidation in vitro by valproic acid and its unsaturated metabolite, 2-n-propyl-4-pentenoic acid. <i>Biochemical and Biophysical Research Communications</i> , 1985, 132, 245-252.                                       | 2.1  | 83        |
| 33 | Complicating factors in safety testing of drug metabolites: Kinetic differences between generated and preformed metabolites. <i>Toxicology and Applied Pharmacology</i> , 2006, 217, 143-152.  | 2.8  | 81        |
| 34 | In Vitro Studies on the Metabolic Activation of the Furanopyridine L-754,394, a Highly Potent and Selective Mechanism-Based Inhibitor of Cytochrome P450 3A4. <i>Chemical Research in Toxicology</i> , 1996, 9, 1007-1012.   | 3.3  | 79        |
| 35 | S-(N-Methylcarbamoyl)glutathione: A reactive S-linked metabolite of methyl isocyanate. <i>Biochemical and Biophysical Research Communications</i> , 1990, 166, 245-250.  | 2.1  | 74        |
| 36 | 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. <i>Chemical Research in Toxicology</i> , 1991, 4, 436-444.                         | 3.3  | 73        |

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|----|--|------|-----------|
| 37 | The Generation, Detection, and Effects of Reactive Drug Metabolites. <i>Medicinal Research Reviews</i> , 2013, 33, 985-1080.   | 10.5 | 73        |
| 38 | Metabolism of the nigrostriatal toxin 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine by liver homogenate fractions. <i>Journal of Medicinal Chemistry</i> , 1985, 28, 997-1001.  | 6.4  | 72        |
| 39 | Addressing Metabolic Activation as an Integral Component of Drug Design. <i>Drug Metabolism Reviews</i> , 2006, 38, 641-649.   | 3.6  | 72        |
| 40 | Zafirlukast Metabolism by Cytochrome P450 3A4 Produces an Electrophilic $\hat{\pm}$ , $\hat{2}$ -Unsaturated Iminium Species That Results in the Selective Mechanism-Based Inactivation of the Enzyme. <i>Chemical Research in Toxicology</i> , 2005, 18, 1427-1437.                   | 3.3  | 69        |
| 41 | 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. <i>Chemical Research in Toxicology</i> , 1994, 7, 526-533.             | 3.3  | 68        |
| 42 | 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. <i>Drug Metabolism and Disposition</i> , 2004, 32, 1254-1259.                                     | 3.3  | 68        |
| 43 | In Vitro Bioactivation of Dihydrobenzoxathiin Selective Estrogen Receptor Modulators by Cytochrome P450 3A4 in Human Liver Microsomes: Formation of Reactive Iminium and Quinone Type Metabolites. <i>Chemical Research in Toxicology</i> , 2005, 18, 675-685.                         | 3.3  | 68        |
| 44 | Monoacetylhydrazine as a metabolite of isoniazid in man. <i>Clinical Pharmacology and Therapeutics</i> , 1977, 22, 602-608.  | 4.7  | 67        |
| 45 | Matrix-assisted laser desorption ionization for rapid determination of the sequences of biologically active peptides isolated from support-bound combinatorial peptide libraries. <i>Rapid Communications in Mass Spectrometry</i> , 1994, 8, 77-81.                                   | 1.5  | 63        |
| 46 | Metabolic activation of unsaturated derivatives of valproic acid. Identification of novel glutathione adducts formed through coenzyme A-dependent and -independent processes. <i>Chemico-Biological Interactions</i> , 1994, 90, 253-275.  | 4.0  | 62        |
| 47 | 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. <i>Drug Metabolism and Disposition</i> , 2006, 34, 145-151.  | 3.3  | 57        |
| 48 | The unanticipated loss of SO <sub>2</sub> from sulfonamides in collision-induced dissociation. <i>Rapid Communications in Mass Spectrometry</i> , 2003, 17, 81-86.   | 1.5  | 55        |
| 49 | Identification in Rat Bile of Glutathione Conjugates of Fluoromethyl 2,2-Difluoro-1-(trifluoromethyl)vinyl Ether, a Nephrotoxic Degradate of the Anesthetic Agent Sevoflurane. <i>Chemical Research in Toxicology</i> , 1996, 9, 555-561.  | 3.3  | 54        |
| 50 | Approaches to the Assessment of Stable and Chemically Reactive Drug Metabolites in Early Clinical Trials. <i>Chemical Research in Toxicology</i> , 2009, 22, 263-266.  | 3.3  | 54        |
| 51 | Bridging cheminformatic metabolite prediction and tandem mass spectrometry. <i>Drug Discovery Today</i> , 2005, 10, 711-717.   | 6.4  | 52        |
| 52 | Electrospray tandem mass spectrometry in the diagnosis of organic acidemias. <i>Rapid Communications in Mass Spectrometry</i> , 1994, 8, 129-133.  | 1.5  | 51        |
| 53 | In Vitro Metabolic Activation of Lumiracoxib in Rat and Human Liver Preparations. <i>Drug Metabolism and Disposition</i> , 2008, 36, 469-473.  | 3.3  | 50        |
| 54 | 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. <i>Chemical Research in Toxicology</i> , 1993, 6, 376-383. | 3.3  | 48        |

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|----|--|-----|-----------|
| 55 | Metabolic Activation of a 1,3-Disubstituted Piperazine Derivative: Evidence for a Novel Ring Contraction to an Imidazoline. <i>Chemical Research in Toxicology</i> , 2005, 18, 271-276.  | 3.3 | 45        |
| 56 | Fractional mass filtering as a means to assess circulating metabolites in early human clinical studies. <i>Rapid Communications in Mass Spectrometry</i> , 2008, 22, 3510-3516.  | 1.5 | 40        |
| 57 | 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. <i>Chemico-Biological Interactions</i> , 1988, 68, 99-116.                                   | 4.0 | 39        |
| 58 | Zielgerichtete kovalente Inhibitoren für das Wirkstoffdesign. <i>Angewandte Chemie</i> , 2016, 128, 13606-13619.   | 2.0 | 39        |
| 59 | Binding of flexible ligands to proteins: Valproic acid and its interaction with cytochrome P450cam. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 161-180.   | 2.0 | 36        |
| 60 | Safety Assessment of Acyl Glucuronides – A Simplified Paradigm. <i>Drug Metabolism and Disposition</i> , 2018, 46, 908-912.  | 3.3 | 34        |
| 61 | Metabolism of valproate to hepatotoxic intermediates. <i>Pharmaceutisch Weekblad Scientific Edition</i> , 1992, 14, 122-125.   | 0.9 | 32        |
| 62 | Applications of tandem mass spectrometry to the characterization of derivatized glutathione conjugates. Studies with S-(N-Methylcarbamoyl)-glutathione, a metabolite of the antineoplastic agent N-methylformamide. <i>Biological Mass Spectrometry</i> , 1988, 16, 51-56. | 0.5 | 29        |
| 63 | Reversibility in Glutathione-Conjugate Formation. <i>Advances in Pharmacology</i> , 1994, 27, 163-181.   | 2.0 | 27        |
| 64 | Pharmacokinetic and Metabolic Profile of Deutetrabenazine (TEV-50717) Compared With Tetrabenazine in Healthy Volunteers. <i>Clinical and Translational Science</i> , 2020, 13, 707-717.  | 3.1 | 25        |
| 65 | Recent Advances in the Use of Stable Isotopes in Drug Metabolism Research. <i>Journal of Clinical Pharmacology</i> , 1986, 26, 481-484.  | 2.0 | 23        |
| 66 | Valproate hydroxylation by human fetal tissues and embryotoxicity of metabolites. <i>Clinical Pharmacology and Therapeutics</i> , 1986, 40, 172-177.   | 4.7 | 22        |
| 67 | Approaches for Minimizing Metabolic Activation of New Drug Candidates in Drug Discovery. <i>Handbook of Experimental Pharmacology</i> , 2010, , 511-544.   | 1.8 | 21        |
| 68 | The use of alkoxy carbonyl derivatives for the mass spectral analysis of drug-thioether metabolites. Studies with the cysteine, mercapturic acid and glutathione conjugates of acetaminophen. <i>Biomedical &amp; Environmental Mass Spectrometry</i> , 1988, 15, 637-647. | 1.6 | 17        |
| 69 | Toxicity of the methyl isocyanate metabolite S-(N-methylcarbamoyl)GSH on mouse embryos in culture. <i>Teratology</i> , 1992, 46, 61-67.  | 1.6 | 17        |
| 70 | Approaches to mitigate the risk of serious adverse reactions in covalent drug design. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 275-287.   | 5.0 | 17        |
| 71 | Application of liquid chromatography/thermospray mass spectrometry to studies on the formation of glutathione and cysteine conjugates from monomethylcarbamate metabolites of bambuterol. <i>Rapid Communications in Mass Spectrometry</i> , 1989, 3, 360-363.             | 1.5 | 16        |
| 72 | In vitro and in vivo investigations of dihydropyridine-based chemical delivery systems for anticonvulsants. <i>Pharmaceutical Research</i> , 1991, 08, 690-697.  | 3.5 | 15        |

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|----|---|-----|-----------|
| 73 | Biotransformation and bioactivation reactions – 2015 literature highlights. <i>Drug Metabolism Reviews</i> , 2016, 48, 113-138.   | 3.6 | 14        |
| 74 | Drug-protein adducts: past, present, and future. <i>Medicinal Chemistry Research</i> , 2020, 29, 1093-1104.   | 2.4 | 14        |
| 75 | Minimizing metabolic activation during pharmaceutical lead optimization: progress, knowledge gaps and future directions. <i>Current Opinion in Drug Discovery &amp; Development</i> , 2008, 11, 43-52.  | 1.9 | 14        |
| 76 | Studies on the formation of reactive intermediates from the antineoplastic agent N,N-Bis(2-chloroethyl)-N-nitrosourea (BCNU) in vitro and in vivo. Characterization of novel glutathione adducts by ionspray tandem mass spectrometry. <i>Journal of Mass Spectrometry</i> , 1995, 30, 57-68. | 1.6 | 13        |
| 77 | Metabolism of a Thiazole Benzenesulfonamide Derivative, a Potent and Selective Agonist of the Human $\beta_3$ -Adrenergic Receptor, in Rats: Identification of a Novel Isethionic Acid Conjugate. <i>Drug Metabolism and Disposition</i> , 2002, 30, 778-787.                                 | 3.3 | 13        |
| 78 | Studies on the biotransformation of ketamine. – quantitative significance of the N-demethylation pathway in rats in vivo determined by a novel stable isotope technique. <i>Biomedical &amp; Environmental Mass Spectrometry</i> , 1989, 18, 401-404.   | 1.6 | 12        |
| 79 | Identification of S-(n-Butylcarbamoyl)glutathione, a Reactive Carbamoylating Agent, as a Biliary Metabolite of Benomyl in the Rat. <i>Journal of Agricultural and Food Chemistry</i> , 1994, 42, 2953-2957.   | 5.2 | 12        |
| 80 | Recognition of quaternary ammonium compounds using mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 1994, 8, 65-70.  | 1.5 | 11        |
| 81 | 2-acetamido-p-benzoquinone: A reactive arylating metabolite of 3'-hydroxyacetanilide. <i>Biochemical Pharmacology</i> , 1985, 34, 2871-2876.  | 4.4 | 9         |
| 82 | Drug Biotransformation: Mechanistic Studies With Stable Isotopes. <i>Journal of Clinical Pharmacology</i> , 1986, 26, 448-451.  | 2.0 | 9         |
| 83 | Evidence for the in vitro metabolism of allylisopropylacetamide to reactive intermediates. Mechanistic studies with oxygen-18. <i>Biomedical Mass Spectrometry</i> , 1984, 11, 320-331.   | 1.9 | 8         |
| 84 | Minimizing the potential for metabolic activation as an integral part of drug design. <i>Current Opinion in Drug Discovery &amp; Development</i> , 2005, 8, 44-50.  | 1.9 | 7         |
| 85 | Synthesis and characterization of isotopically-labelled cysteine- and glutathione conjugates of methylisocyanate. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 1989, 27, 1371-1382.  | 1.0 | 6         |
| 86 | The contributions of Sidney D. Nelson to drug metabolism research. <i>Drug Metabolism Reviews</i> , 2015, 47, 4-11.   | 3.6 | 6         |
| 87 | Improved detection of glucuronide and glutathione conjugates with thermospray ionization following esterification. <i>Rapid Communications in Mass Spectrometry</i> , 1994, 8, 371-376.   | 1.5 | 3         |
| 88 | Managing Metabolic Activation Issues in Drug Discovery. , 2019, , 577-603.  |     | 1         |