

# Alexandra M Antunes

## List of Publications by Year in descending order

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82  
papers

1,310  
citations

361296

20  
h-index

414303

32  
g-index

93  
all docs

93  
docs citations

93  
times ranked

1903  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Motions in Amorphous Ibuprofen As Studied by Broadband Dielectric Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11087-11099.	1.2	152
2	Selenium-Containing Chrysin and Quercetin Derivatives: Attractive Scaffolds for Cancer Therapy. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 4250-4265.	2.9	82
3	Synthesis and evaluation of diaryl sulfides and diaryl selenide compounds for antitubulin and cytotoxic activity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 4669-4673.	1.0	67
4	Palladium(ii)-promoted aziridination of olefins with bromamine T as the nitrogen transfer reagent. <i>Chemical Communications</i> , 2001, , 405-406.	2.2	53
5	Scavenging activity of aminoantipyridines against hydroxyl radical. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 2258-2264.	2.6	42
6	Protein Adducts As Prospective Biomarkers of Nevirapine Toxicity. <i>Chemical Research in Toxicology</i> , 2010, 23, 1714-1725.	1.7	42
7	Novel Antibacterial Azelaic Acid BioMOFs. <i>Crystal Growth and Design</i> , 2020, 20, 370-382.	1.4	37
8	Evidence for nevirapine bioactivation in man: Searching for the first step in the mechanism of nevirapine toxicity. <i>Toxicology</i> , 2012, 301, 33-39.	2.0	35
9	Mg- and Mn-MOFs Boost the Antibiotic Activity of Nalidixic Acid. <i>ACS Applied Bio Materials</i> , 2019, 2, 2347-2354.	2.3	35
10	Amino Acid Adduct Formation by the Nevirapine Metabolite, 12-Hydroxynevirapine—A Possible Factor in Nevirapine Toxicity. <i>Chemical Research in Toxicology</i> , 2010, 23, 888-899.	1.7	34
11	Targeting Glutathione and Cystathionine $\hat{I}^2$ -Synthase in Ovarian Cancer Treatment by Selenium—Chrysin Polyurea Dendrimer Nanoformulation. <i>Nutrients</i> , 2019, 11, 2523.	1.7	33
12	Reactive Aldehyde Metabolites from the Anti-HIV Drug Abacavir: Amino Acid Adducts as Possible Factors in Abacavir Toxicity. <i>Chemical Research in Toxicology</i> , 2011, 24, 2129-2141.	1.7	31
13	Packing Interactions and Physicochemical Properties of Novel Multicomponent Crystal Forms of the Anti-Inflammatory Azelaic Acid Studied by X-ray and Solid-State NMR. <i>Crystal Growth and Design</i> , 2016, 16, 154-166.	1.4	30
14	Synthesis and Characterization of DNA Adducts from the HIV Reverse Transcriptase Inhibitor Nevirapine. <i>Chemical Research in Toxicology</i> , 2008, 21, 1443-1456.	1.7	27
15	Genotoxic and Epigenotoxic Alterations in the Lung and Liver of Mice Induced by Acrylamide: A 28 Day Drinking Water Study. <i>Chemical Research in Toxicology</i> , 2019, 32, 869-877.	1.7	27
16	New insights into the molecular mechanisms of chemical carcinogenesis: In vivo adduction of histone H2B by a reactive metabolite of the chemical carcinogen furan. <i>Toxicology Letters</i> , 2016, 264, 106-113.	0.4	26
17	Hepatocyte spheroids as a competent in vitro system for drug biotransformation studies: nevirapine as a bioactivation case study. <i>Archives of Toxicology</i> , 2017, 91, 1199-1211.	1.9	25
18	Bioactivation to an aldehyde metabolite—Possible role in the onset of toxicity induced by the anti-HIV drug abacavir. <i>Toxicology Letters</i> , 2014, 224, 416-423.	0.4	23

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19	Synthesis and oxidation of 2-hydroxynevirapine, a metabolite of the HIV reverse transcriptase inhibitor nevirapine. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7822.	1.5	22
20	Synthesis and Biological Activity of 6-Selenocaffeine: Potential Modulator of Chemotherapeutic Drugs in Breast Cancer Cells. <i>Molecules</i> , 2013, 18, 5251-5264.	1.7	22
21	Differences in nevirapine biotransformation as a factor for its sex-dependent dimorphic profile of adverse drug reactions. <i>Journal of Antimicrobial Chemotherapy</i> , 2014, 69, 476-482.	1.3	21
22	Unmasking efavirenz neurotoxicity: Time matters to the underlying mechanisms. <i>European Journal of Pharmaceutical Sciences</i> , 2017, 105, 47-54.	1.9	21
23	Monitoring abacavir bioactivation in humans: Screening for an aldehyde metabolite. <i>Toxicology Letters</i> , 2013, 219, 59-64.	0.4	20
24	Palladium(II) mediated aziridination of olefins with bromamine-T as the nitrogen source: scope and mechanism. <i>Tetrahedron</i> , 2007, 63, 7009-7017.	1.0	19
25	Chlorinated Polycyclic Aromatic Hydrocarbons Associated with Drinking Water Disinfection: Synthesis, Formation under Aqueous Chlorination Conditions and Genotoxic Effects. <i>Polycyclic Aromatic Compounds</i> , 2014, 34, 356-371.	1.4	19
26	<i>N</i> -terminal valine adduct from the anti-HIV drug abacavir in rat haemoglobin as evidence for abacavir metabolism to a reactive aldehyde <i>in vivo</i> . <i>British Journal of Pharmacology</i> , 2012, 167, 1353-1361.	2.7	17
27	Mass Spectrometry-Based Methodologies for Targeted and Untargeted Identification of Protein Covalent Adducts (Adductomics): Current Status and Challenges. <i>High-Throughput</i> , 2019, 8, 9.	4.4	17
28	Mercapturate Pathway in the Tubulocentric Perspective of Diabetic Kidney Disease. <i>Nephron</i> , 2019, 143, 17-23.	0.9	17
29	Use of In Vivo <sup>13</sup> C Nuclear Magnetic Resonance Spectroscopy To Elucidate -Arabinose Metabolism in Yeasts. <i>Applied and Environmental Microbiology</i> , 2008, 74, 1845-1855.	1.4	15
30	Bioactivity of Isostructural Hydrogen Bonding Frameworks Built from Pipemidic Acid Metal Complexes. <i>Molecules</i> , 2020, 25, 2374.	1.7	14
31	The role of competitive binding to human serum albumin on efavirenz-warfarin interaction: a nuclear magnetic resonance study. <i>International Journal of Antimicrobial Agents</i> , 2013, 42, 443-446.	1.1	13
32	Quantification of the arylesterase activity of paraoxonase-1 in human blood. <i>Analytical Methods</i> , 2014, 6, 289-294.	1.3	13
33	The phenolic metabolites of the anti-HIV drug efavirenz: Evidence for distinct reactivities upon oxidation with Frémy's salt. <i>European Journal of Medicinal Chemistry</i> , 2014, 74, 7-11.	2.6	13
34	Severe Acute Kidney Injury and Double Tubulopathy Due to Dual Toxicity Caused by Combination Antiretroviral Therapy. <i>Kidney International Reports</i> , 2019, 4, 494-499.	0.4	13
35	Metabolic Profile of Four Selected Cathinones in Microsome Incubations: Identification of Phase I and II Metabolites by Liquid Chromatography High Resolution Mass Spectrometry. <i>Frontiers in Chemistry</i> , 2020, 8, 609251.	1.8	13
36	Electronic Communication in Linear Oligo(azobenzene) Radical Anions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14056-14064.	1.1	12

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37	High resolution mass spectrometry-based methodologies for identification of Etravirine bioactivation to reactive metabolites: In vitro and in vivo approaches. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 119, 70-82.	1.9	12
38	New Syntheses of DNA Adducts from Methylated Anilines Present in Tobacco Smoke. <i>Chemical Research in Toxicology</i> , 1999, 12, 1223-1233.	1.7	11
39	Differentiation of isomeric C8-substituted alkyylaniline adducts of guanine by electrospray ionization and tandem quadrupole ion trap mass spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2003, 14, 1488-1492.	1.2	11
40	Gabapentin Coordination Networks: Mechanochemical Synthesis and Behavior under Shelf Conditions. <i>Crystal Growth and Design</i> , 2013, 13, 5007-5017.	1.4	11
41	Nevirapine Biotransformation Insights: An Integrated In Vitro Approach Unveils the Biocompetence and Glutathiolomic Profile of a Human Hepatocyte-Like Cell 3D Model. <i>International Journal of Molecular Sciences</i> , 2020, 21, 3998.	1.8	10
42	Singularities of nevirapine metabolism: from sex-dependent differences to idiosyncratic toxicity. <i>Drug Metabolism Reviews</i> , 2019, 51, 76-90.	1.5	10
43	Cysteine as a Multifaceted Player in Kidney, the Cysteine-Related Thiols and Its Implications for Precision Medicine. <i>Molecules</i> , 2022, 27, 1416.	1.7	10
44	Development and validation of an HPLC-UV method for quantifying nevirapine and its main phase I metabolites in human blood. <i>Analytical Methods</i> , 2014, 6, 1575.	1.3	9
45	The first-line antiepileptic drug carbamazepine: Reaction with biologically relevant free radicals. <i>Free Radical Biology and Medicine</i> , 2018, 129, 559-568.	1.3	9
46	Identification of gallotannins and ellagitannins in aged wine spirits: A new perspective using alternative ageing technology and high-resolution mass spectrometry. <i>Food Chemistry</i> , 2022, 382, 132322.	4.2	9
47	Integration of cellular and molecular endpoints to assess the toxicity of polycyclic aromatic hydrocarbons in HepG2 cell line. <i>Environmental Toxicology and Chemistry</i> , 2017, 36, 3404-3414.	2.2	8
48	Oxidation of 2-Hydroxynevirapine, a Phenolic Metabolite of the Anti-HIV Drug Nevirapine: Evidence for an Unusual Pyridine Ring Contraction. <i>Molecules</i> , 2012, 17, 2616-2627.	1.7	7
49	Efavirenz biotransformation as an up-stream event of mood changes in HIV-infected patients. <i>Toxicology Letters</i> , 2016, 260, 28-35.	0.4	7
50	Nevirapine modulation of paraoxonase-1 in the liver: An in vitro three-model approach. <i>European Journal of Pharmaceutical Sciences</i> , 2016, 82, 147-153.	1.9	7
51	The mercapturomic profile of health and non-communicable diseases. <i>High-Throughput</i> , 2019, 8, 10.	4.4	7
52	Biomimetic oxidation of aromatic xenobiotics: synthesis of the phenolic metabolites from the anti-HIV drug efavirenz. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4554.	1.5	6
53	2'-Deoxythymidine Adducts from the Anti-HIV Drug Nevirapine. <i>Molecules</i> , 2013, 18, 4955-4971.	1.7	6
54	A Metabolomics-Inspired Strategy for the Identification of Protein Covalent Modifications. <i>Frontiers in Chemistry</i> , 2019, 7, 532.	1.8	6

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55	Human Cystathionine $\hat{3}$ -Lyase Is Inhibited by s-Nitrosation: A New Crosstalk Mechanism between NO and H <sub>2</sub> S. <i>Antioxidants</i> , 2021, 10, 1391.	2.2	6
56	Sex differences in hepatic and intestinal contributions to nevirapine biotransformation in rats. <i>Chemico-Biological Interactions</i> , 2015, 233, 115-121.	1.7	5
57	Product ion studies of some novel arylamine adducts of deoxyguanosine by matrix-assisted laser desorption/ionization and post-source decay. , 1999, 13, 2004-2010.		4
58	Quinoid derivatives of the nevirapine metabolites 2-hydroxy- and 3-hydroxy-nevirapine: activation pathway to amino acid adducts. <i>Toxicology Research</i> , 2015, 4, 1565-1577.	0.9	4
59	16 $\hat{1}$ -Hydroxyestrone: Mass Spectrometry-Based Methodologies for the Identification of Covalent Adducts Formed with Blood Proteins. <i>Chemical Research in Toxicology</i> , 2020, 33, 2147-2156.	1.7	4
60	Covalent Histone Modification by an Electrophilic Derivative of the Anti-HIV Drug Nevirapine. <i>Molecules</i> , 2021, 26, 1349.	1.7	4
61	Synthetic Red Blood Cell-Specific Glycolytic Intermediate 2,3-Diphosphoglycerate (2,3-DPG) Inhibits <i>Plasmodium falciparum</i> Development In Vitro. <i>Frontiers in Cellular and Infection Microbiology</i> , 2022, 12, 840968.	1.8	4
62	Glycidamide and cis-2-butene-1,4-dial (BDA) as potential carcinogens and promoters of liver cancer - An in vitro study. <i>Food and Chemical Toxicology</i> , 2022, 166, 113251.	1.8	4
63	Insights into the Role of Bioactivation Mechanisms in the Toxic Events Elicited by Non-nucleoside Reverse Transcriptase Inhibitors. <i>Advances in Molecular Toxicology</i> , 2012, 6, 1-39.	0.4	3
64	Tryptophan-Derived Oxazolopyrrolidone Lactams as Potential Anticancer Agents against Gastric Adenocarcinoma. <i>Pharmaceuticals</i> , 2021, 14, 208.	1.7	3
65	A Mechanistic-Based and Non-invasive Approach to Quantify the Capability of Kidney to Detoxify Cysteine-Disulfides. <i>Advances in Experimental Medicine and Biology</i> , 2021, 1306, 109-120.	0.8	3
66	Sex differences in apolipoprotein A1 and nevirapine-induced toxicity. <i>Journal of the International AIDS Society</i> , 2014, 17, 19575.	1.2	2
67	Anti-histone antibodies in HIV-infected patients on Nevirapine-containing ANTIRETROVIRAL THERAPY. <i>Clinical Therapeutics</i> , 2015, 37, e142.	1.1	1
68	Special Issue "Adductomics: Elucidating the Environmental Causes of Disease". <i>High-Throughput</i> , 2019, 8, 17.	4.4	1
69	The 2-hydroxy-nevirapine metabolite as a candidate for boosting apolipoprotein A1 and for modulating anti-HDL antibodies. <i>Pharmacological Research</i> , 2021, 165, 105446.	3.1	1
70	A simple method to measure sulfonation in man using paracetamol as probe drug. <i>Scientific Reports</i> , 2021, 11, 9036.	1.6	1
71	Isonothoapiol: A New Phenylpropenoid from <i>Ammi huntii</i> . <i>Natural Product Research</i> , 1997, 11, 77-80.	0.4	0
72	Post-source decay production studies of aniline and methylaniline adducts of deoxyguanosine. <i>Analytica Chimica Acta</i> , 1999, 397, 257-265.	2.6	0

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73	Protein adduct formation: A possible factor in hypersensitivity reactions induced by the anti HIV drug abacavir. Toxicology Letters, 2010, 196, S110.	0.4	0
74	Thiol status in HIV-infected patients: The effect of nevirapine metabolism. Toxicology Letters, 2014, 229, S95.	0.4	0
75	An animal model to explore efavirenz toxicokinetics and its relation to neurological phenotype. Toxicology Letters, 2014, 229, S244.	0.4	0
76	Sex differences in hepatic and intestinal contributions for nevirapine biotransformation. Toxicology Letters, 2014, 229, S240-S241.	0.4	0
77	First in vitro evidence for a catechol metabolite from the anti-HIV drug efavirenz – A plausible role in toxicity. Toxicology Letters, 2015, 238, S360.	0.4	0
78	Toxic events induced by the antiepileptic drug carbamazepine: Is bioactivation really involved?. Toxicology Letters, 2017, 280, S241.	0.4	0
79	Phenotyping SULT in Man: a Simple Metric Using Paracetamol as Probe. FASEB Journal, 2021, 35, .	0.2	0
80	Oxidation of The Nevirapine Metabolite, 2-Hydroxy-Nevirapine, With FrÃ©my's Salt: Unusual Pyridine Ring Contraction. , 0, , .		0
81	Enantiopure oxazoloisoindolinones: Promising small molecules for p53-based therapy with potential anticancer properties. , 0, , .		0
82	Tryptophan-derived oxazoloisoindolinones: Novel small molecule p53 activators with promising antitumor activity. , 0, , .		0