Nico P E Vermeulen

List of Publications by Year in Descending Order

271 papers	13,357 citations	52 h-index	106 g-index
288 ext. papers	14,239 ext. citations	5 avg, IF	6.24 L-index

#	Paper	IF	Citations
271	Critique of the "Comment" etitled "Pyrethroid exposure: Not so harmless after all" by Demeneix et al. (2020) published in the lancet diabetes endocrinology. *Toxicology Letters*, **2021**, 340, 1-3	4.4	
270	Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC Technical Report). *Pure and Applied Chemistry*, **2021**, 93, 273-403	2.1	1
269	The EU chemicals strategy for sustainability: in support of the BfR position. *Archives of Toxicology*, **2021**, 95, 3133-3136	5.8	2
268	Human multidrug resistance protein 4 (MRP4) is a cellular efflux transporter for paracetamol glutathione and cysteine conjugates. *Archives of Toxicology*, **2020**, 94, 3027-3032	5.8	3
267	Human exposure to synthetic endocrine disrupting chemicals (S-EDCs) is generally negligible as compared to natural compounds with higher or comparable endocrine activity. How to evaluate the risk of the S-EDCs?. *Journal of Toxicology and Environmental Health - Part A: Current Issues*, **2020**, 83, 485-494	3.2	7
266	A Comparative Linear Interaction Energy and MM/PBSA Study on SIRT1-Ligand Binding Free Energy Calculation. *Journal of Chemical Information and Modeling*, **2019**, 59, 4018-4033	6.1	34
265	Cytochrome P450 Protein Modeling and Ligand Docking **2019**, 435-470		
264	Characterization of kinetics of human cytochrome P450s involved in bioactivation of flucloxacillin: inhibition of CYP3A-catalysed hydroxylation by sulfaphenazole. *British Journal of Pharmacology*, **2019**, 176, 466-477	8.6	6
263	Drug toxicity profiling of a Saccharomyces cerevisiae deubiquitinase deletion panel shows that acetaminophen mimics tyrosine. *Toxicology in Vitro*, **2018**, 47, 259-268	3.6	4
262	Reduction and Scavenging of Chemically Reactive Drug Metabolites by NAD(P)H:Quinone Oxidoreductase 1 and NRH:Quinone Oxidoreductase 2 and Variability in Hepatic Concentrations. *Chemical Research in Toxicology*, **2018**, 31, 116-126	4	8
261	Binding free energy predictions of farnesoid X receptor (FXR) agonists using a linear interaction energy (LIE) approach with reliability estimation: application to the D3R Grand Challenge 2. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 239-249	4.2	12
260	A combined computational and experimental study on selective flucloxacillin hydroxylation by cytochrome P450 BM3 variants. *Journal of Inorganic Biochemistry*, **2018**, 184, 115-122	4.2	9
259	High-performance liquid chromatography-based assay for glutathione transferase theta 2 activity: Application to characterize interindividual variability in human liver fractions. *Journal of Pharmaceutical and Biomedical Analysis*, **2018**, 156, 181-188	3.5	1
258	Glutathione -Transferase P1 Protects Against Amodiaquine Quinoneimines-Induced Cytotoxicity but Does Not Prevent Activation of Endoplasmic Reticulum Stress in HepG2 Cells. *Frontiers in Pharmacology*, **2018**, 9, 388	5.6	5
257	Acetaminophen reduces the protein levels of high affinity amino acid permeases and causes tryptophan depletion. *Amino Acids*, **2018**, 50, 1377-1390	3.5	1
256	Linking cytochrome P450 enzymes from Mycobacterium tuberculosis to their cognate ferredoxin partners. *Applied Microbiology and Biotechnology*, **2018**, 102, 9231-9242	5.7	10
255	Inter-individual Variability in Activity of the Major Drug Metabolizing Enzymes in Liver Homogenates of 20 Individuals. *Current Drug Metabolism*, **2018**, 19, 370-381	3.5	12

254	Effect of UGT2B7*2 and CYP2C8*4 polymorphisms on diclofenac metabolism. *Toxicology Letters*, **2018**, 284, 70-78	4.4	28
253	Engineering a self-sufficient Mycobacterium tuberculosis CYP130 by gene fusion with the reductase-domain of CYP102A1 from Bacillus megaterium. *Journal of Inorganic Biochemistry*, **2018**, 180, 47-53	4.2	5
252	Generic method for the absolute quantification of glutathione S-conjugates: Application to the conjugates of acetaminophen, clozapine and diclofenac. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2017**, 1046, 185-194	3.2	3
251	Human glutathione S-transferases- and NAD(P)H:quinone oxidoreductase 1-catalyzed inactivation of reactive quinoneimines of amodiaquine and N-desethylamodiaquine: Possible implications for susceptibility to amodiaquine-induced liver toxicity. *Toxicology Letters*, **2017**, 275, 83-91	4.4	8
250	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
249	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. *Journal of Cheminformatics*, **2017**, 9, 58	8.6	6
248	Direct comparison of UDP-glucuronosyltransferase and cytochrome P450 activities in human liver microsomes, plated and suspended primary human hepatocytes from five liver donors. *European Journal of Pharmaceutical Sciences*, **2017**, 109, 96-110	5.1	3
247	Comprehensive and Automated Linear Interaction Energy Based Binding-Affinity Prediction for Multifarious Cytochrome P450 Aromatase Inhibitors. *Journal of Chemical Information and Modeling*, **2017**, 57, 2294-2308	6.1	16
246	Characterization of human cytochrome P450 mediated bioactivation of amodiaquine and its major metabolite N-desethylamodiaquine. *British Journal of Clinical Pharmacology*, **2017**, 83, 572-583	3.8	20
245	The effect of acetaminophen on ubiquitin homeostasis in Saccharomyces cerevisiae. *PLoS ONE*, **2017**, 12, e0173573	3.7	3
244	Evidence-based selection of training compounds for use in the mechanism-based integrated prediction of drug-induced liver injury in man. *Archives of Toxicology*, **2016**, 90, 2979-3003	5.8	34
243	Different Reactive Metabolites of Nevirapine Require Distinct Glutathione S-Transferase Isoforms for Bioinactivation. *Chemical Research in Toxicology*, **2016**, 29, 2136-2144	4	15
242	Insights into regioselective metabolism of mefenamic acid by cytochrome P450 BM3 mutants through crystallography, docking, molecular dynamics, and free energy calculations. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 383-96	4.2	25
241	Application of a cocktail approach to screen cytochrome P450 BM3 libraries for metabolic activity and diversity. *Analytical and Bioanalytical Chemistry*, **2016**, 408, 1425-43	4.4	4
240	Improving the iterative Linear Interaction Energy approach using automated recognition of configurational transitions. *Journal of Molecular Modeling*, **2016**, 22, 31	2	10
239	Inter-donor variability of phase I/phase II metabolism of three reference drugs in cryopreserved primary human hepatocytes in suspension and monolayer. *Toxicology in Vitro*, **2016**, 33, 71-9	3.6	33
238	Simulation of interindividual differences in inactivation of reactive para-benzoquinone imine metabolites of diclofenac by glutathione S-transferases in human liver cytosol. *Toxicology Letters*, **2016**, 255, 52-62	4.4	18
237	Characterization of cytochrome P450 isoforms involved in sequential two-step bioactivation of diclofenac to reactive p-benzoquinone imines. *Toxicology Letters*, **2016**, 253, 46-54	4.4	24

236	Mass spectrometric identification of isocyanate-induced modifications of keratins in human skin. *Chemico-Biological Interactions*, **2015**, 237, 141-50	5	9
235	Application of a Continuous-Flow Bioassay to Investigate the Organic Solvent Tolerability of Cytochrome P450 BM3 Mutants. *Journal of Biomolecular Screening*, **2015**, 20, 1246-55		5
234	Selective whole-cell biosynthesis of the designer drug metabolites 15- or 16-betahydroxynorethisterone by engineered Cytochrome P450 BM3 mutants. *Journal of Molecular Catalysis B: Enzymatic*, **2015**, 121, 64-74		9
233	Biosynthesis of a steroid metabolite by an engineered Rhodococcus erythropolis strain expressing a mutant cytochrome P450 BM3 enzyme. *Applied Microbiology and Biotechnology*, **2015**, 99, 4713-21	5.7	22
232	Mini-dialysis tubes as tools to prepare drug-protein adducts of P450-dependent reactive drug metabolites. *Journal of Pharmaceutical and Biomedical Analysis*, **2015**, 103, 17-25	3.5	1
231	Activation of the anticancer drugs cyclophosphamide and ifosfamide by cytochrome P450 BM3 mutants. *Toxicology Letters*, **2015**, 232, 182-92	4.4	14
230	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. *Molecular Informatics*, **2015**, 34, 477-84	3.8	17
229	Linear Interaction Energy Based Prediction of Cytochrome P450 1A2 Binding Affinities with Reliability Estimation. *PLoS ONE*, **2015**, 10, e0142232	3.7	22
228	Characterization of human cytochrome P450s involved in the bioactivation of tri-ortho-cresyl phosphate (ToCP). *Chemical Research in Toxicology*, **2015**, 28, 711-21	4	10
227	Principles of Pharmacology and Toxicology Also Govern Effects of Chemicals on the Endocrine System. *Toxicological Sciences*, **2015**, 146, 11-5	4.4	19
226	Biotransformation of endocrine disrupting compounds by selected phase I and phase II enzymes--formation of estrogenic and chemically reactive metabolites by cytochromes P450 and sulfotransferases. *Current Medicinal Chemistry*, **2015**, 22, 500-27	4.3	19
225	Effect of human glutathione S-transferase hGSTP1-1 polymorphism on the detoxification of reactive metabolites of clozapine, diclofenac and acetaminophen. *Toxicology Letters*, **2014**, 224, 272-81	4.4	18
224	Human NAD(P)H:quinone oxidoreductase 1 (NQO1)-mediated inactivation of reactive quinoneimine metabolites of diclofenac and mefenamic acid. *Chemical Research in Toxicology*, **2014**, 27, 576-86	4	26
223	One-electron oxidation of diclofenac by human cytochrome P450s as a potential bioactivation mechanism for formation of 2P(glutathion-S-yl)-deschloro-diclofenac. *Chemico-Biological Interactions*, **2014**, 207, 32-40	5	10
222	Application of engineered cytochrome P450 mutants as biocatalysts for the synthesis of benzylic and aromatic metabolites of fenamic acid NSAIDs. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 5613-20	3.4	27
221	Towards automated binding affinity prediction using an iterative linear interaction energy approach. *International Journal of Molecular Sciences*, **2014**, 15, 798-816	6.3	18
220	Cytochrome P450-mediated bioactivation of mefenamic acid to quinoneimine intermediates and inactivation by human glutathione S-transferases. *Chemical Research in Toxicology*, **2014**, 27, 2071-81	4	23
219	Combination of biotransformation by P450 BM3 mutants with on-line post-column bioaffinity and mass spectrometric profiling as a novel strategy to diversify and characterize p38 kinase inhibitors. *MedChemComm*, **2013**, 4, 371-377	5	11

218	Urinary lipid and protein oxidation products upon halothane, isoflurane, or sevoflurane anesthesia in humans: potential biomarkers for a subclinical nephrotoxicity. *Biomarkers*, **2013**, 18, 73-81	2.6	7
217	Characterization of human cytochrome P450s involved in the bioactivation of clozapine. *Drug Metabolism and Disposition*, **2013**, 41, 651-8	4	38
216	Reconstitution of the interplay between cytochrome P450 and human glutathione S-transferases in clozapine metabolism in yeast. *Toxicology Letters*, **2013**, 222, 247-56	4.4	4
215	Effect of human glutathione S-transferases on glutathione-dependent inactivation of cytochrome P450-dependent reactive intermediates of diclofenac. *Chemical Research in Toxicology*, **2013**, 26, 1632-41	4	17
214	A single active site mutation inverts stereoselectivity of 16-hydroxylation of testosterone catalyzed by engineered cytochrome P450 BM3. *ChemBioChem*, **2012**, 13, 520-3	3.8	43
213	Differential involvement of mitochondrial dysfunction, cytochrome P450 activity, and active transport in the toxicity of structurally related NSAIDs. *Toxicology in Vitro*, **2012**, 26, 197-205	3.6	27
212	Mass spectrometric characterization of protein adducts of multiple P450-dependent reactive intermediates of diclofenac to human glutathione-S-transferase P1-1. *Chemical Research in Toxicology*, **2012**, 25, 2532-41	4	25
211	Regio- and Stereoselective Hydroxylation of Optically Active Ionone Enantiomers by Engineered Cytochrome P450 BM3 Mutants. *Advanced Synthesis and Catalysis*, **2012**, 354, 2172-2184	5.6	29
210	Free energy calculations give insight into the stereoselective hydroxylation of Ionones by engineered cytochrome P450 BM3 mutants. *Journal of Chemical Information and Modeling*, **2012**, 52, 2139-48	6.1	13
209	Interactions of organophosphates with keratins in the cornified epithelium of human skin. *Chemico-Biological Interactions*, **2012**, 197, 93-102	5	17
208	Yeast as a humanized model organism for biotransformation-related toxicity. *Current Drug Metabolism*, **2012**, 13, 1464-75	3.5	20
207	The role of protein plasticity in computational rationalization studies on regioselectivity in testosterone hydroxylation by cytochrome P450 BM3 mutants. *Current Drug Metabolism*, **2012**, 13, 155-66	3.5	10
206	Malleability and versatility of cytochrome P450 active sites studied by molecular simulations. *Current Drug Metabolism*, **2012**, 13, 190-6	3.5	16
205	Application of CYP102A1M11H as a tool for the generation of protein adducts of reactive drug metabolites. *Chemical Research in Toxicology*, **2011**, 24, 1263-74	4	18
204	Metabolism related toxicity of diclofenac in yeast as model system. *Toxicology Letters*, **2011**, 200, 162-8	4.4	37
203	Managing the challenge of chemically reactive metabolites in drug development. *Nature Reviews Drug Discovery*, **2011**, 10, 292-306	64.1	348
202	Identification of CYP1A2 ligands by structure-based and ligand-based virtual screening. *MedChemComm*, **2011**, 2, 853	5	6
201	Role of residue 87 in substrate selectivity and regioselectivity of drug-metabolizing cytochrome P450 CYP102A1 M11. *Journal of Biological Inorganic Chemistry*, **2011**, 16, 899-912	3.7	42

200	Diclofenac inhibits tumor necrosis factor-induced nuclear factor-B activation causing synergistic hepatocyte apoptosis. *Hepatology*, **2011**, 53, 2027-41	11.2	76
199	Molecular dynamics simulations and free energy calculations on the enzyme 4-hydroxyphenylpyruvate dioxygenase. *Journal of Computational Chemistry*, **2011**, 32, 2160-9	3.5	5
198	Application of a fluorescence-based continuous-flow bioassay to screen for diversity of cytochrome P450 BM3 mutant libraries. *Journal of Biomolecular Screening*, **2011**, 16, 239-50		14
197	Subunits Rip1p and Cox9p of the respiratory chain contribute to diclofenac-induced mitochondrial dysfunction. *Microbiology (United Kingdom)*, **2011**, 157, 685-694	2.9	20
196	Efficient screening of cytochrome P450 BM3 mutants for their metabolic activity and diversity toward a wide set of drug-like molecules in chemical space. *Drug Metabolism and Disposition*, **2011**, 39, 1568-76	4	33
195	Role of residue 87 in the activity and regioselectivity of clozapine metabolism by drug-metabolizing CYP102A1 M11H: application for structural characterization of clozapine GSH conjugates. *Drug Metabolism and Disposition*, **2011**, 39, 2411-20	4	13
194	Involvement of the pleiotropic drug resistance response, protein kinase C signaling, and altered zinc homeostasis in resistance of Saccharomyces cerevisiae to diclofenac. *Applied and Environmental Microbiology*, **2011**, 77, 5973-80	4.8	11
193	Application of cytochrome P450 BM3 mutants as biocatalysts for the profiling of estrogen receptor binding metabolites of the mycotoxin zearalenone. *Xenobiotica*, **2011**, 41, 59-70	2	12
192	Conventional and novel approaches in generating and characterization of reactive intermediates from drugs/drug candidates. *Current Drug Metabolism*, **2011**, 12, 383-94	3.5	17
191	Computational prediction of binding affinity for CYP1A2-ligand complexes using empirical free energy calculations. *Drug Metabolism and Disposition*, **2010**, 38, 1347-54	4	31
190	The role of water molecules in computational drug design. *Current Topics in Medicinal Chemistry*, **2010**, 10, 55-66	3	138
189	Role of human glutathione S-transferases in the inactivation of reactive metabolites of clozapine. *Chemical Research in Toxicology*, **2010**, 23, 1467-76	4	52
188	Comparison of murine and human estrogen sulfotransferase inhibition in vitro and in silico--implications for differences in activity, subunit dimerization and substrate inhibition. *Molecular and Cellular Endocrinology*, **2010**, 317, 127-40	4.4	15
187	Endocrine disrupting chemicals-Linking internal exposure to vitellogenin levels and ovotestis in Abramis brama from Dutch surface waters. *Environmental Toxicology and Pharmacology*, **2010**, 30, 209-23	5.8	11
186	Determination and identification of estrogenic compounds generated with biosynthetic enzymes using hyphenated screening assays, high resolution mass spectrometry and off-line NMR. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2010**, 878, 667-74	3.2	36
185	Classification of cytochrome P450 1A2 inhibitors and noninhibitors by machine learning techniques. *Drug Metabolism and Disposition*, **2009**, 37, 658-64	4	81
184	Virtual screening and prediction of site of metabolism for cytochrome P450 1A2 ligands. *Journal of Chemical Information and Modeling*, **2009**, 49, 43-52	6.1	71
183	Application of drug metabolising mutants of cytochrome P450 BM3 (CYP102A1) as biocatalysts for the generation of reactive metabolites. *Chemico-Biological Interactions*, **2008**, 171, 96-107	5	80

182	Interactions between cytochromes P450, glutathione S-transferases and Ghanaian medicinal plants. *Food and Chemical Toxicology*, **2008**, 46, 3598-603	4.7	28
181	Computational prediction of drug binding and rationalisation of selectivity towards cytochromes P450. *Expert Opinion on Drug Metabolism and Toxicology*, **2008**, 4, 513-27	5.5	60
180	Trimethoprim: novel reactive intermediates and bioactivation pathways by cytochrome p450s. *Chemical Research in Toxicology*, **2008**, 21, 2181-7	4	36
179	Reversed-phase liquid chromatography coupled on-line to estrogen receptor bioaffinity detection based on fluorescence polarization. *Analytical and Bioanalytical Chemistry*, **2008**, 390, 1987-98	4.4	16
178	Active-site structure, binding and redox activity of the heme-thiolate enzyme CYP2D6 immobilized on coated Ag electrodes: a surface-enhanced resonance Raman scattering study. *Journal of Biological Inorganic Chemistry*, **2008**, 13, 85-96	3.7	14
177	Glutathione-S-transferase pi as a model protein for the characterisation of chemically reactive metabolites. *Proteomics*, **2008**, 8, 301-15	4.8	29
176	Structural rationalization of novel drug metabolizing mutants of cytochrome P450 BM3. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 336-52	4.2	37
175	Structure-activity relationships for the inhibition of recombinant human cytochromes P450 by curcumin analogues. *European Journal of Medicinal Chemistry*, **2008**, 43, 1621-31	6.8	34
174	In vitro bioactivation of 3-(N-phenylamino)propane-1,2-diol by human and rat liver microsomes and recombinant P450 enzymes. Implications for toxic oil syndrome. *Chemical Research in Toxicology*, **2007**, 20, 1218-24	4	4
173	Metabolic profiling of endocrine-disrupting compounds by on-line cytochrome p450 bioreaction coupled to on-line receptor affinity screening. *Chemical Research in Toxicology*, **2007**, 20, 1825-32	4	19
172	Identification of critical residues in novel drug metabolizing mutants of cytochrome P450 BM3 using random mutagenesis. *Journal of Medicinal Chemistry*, **2007**, 50, 455-61	8.3	95
171	Cytochrome P450 bio-affinity detection coupled to gradient HPLC: on-line screening of affinities to cytochrome P4501A2 and 2D6. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2007**, 858, 49-58	3.2	13
170	Automated detection of covalent adducts to human serum albumin by immunoaffinity chromatography, on-line solution phase digestion and liquid chromatography-mass spectrometry. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2007**, 859, 147-56	3.2	16
169	Surface-enhanced resonance Raman scattering of cytochrome P450-2D6 on coated silver hydrosols. *Langmuir*, **2007**, 23, 1860-6	4	9
168	Combining substrate dynamics, binding statistics, and energy barriers to rationalize regioselective hydroxylation of octane and lauric acid by CYP102A1 and mutants. *Protein Science*, **2007**, 16, 420-31	6.3	33
167	An on-line post-column detection system for the detection of reactive-oxygen-species-producing compounds and antioxidants in mixtures. *Analytical and Bioanalytical Chemistry*, **2007**, 388, 871-9	4.4	13
166	Free energies of binding of R- and S-propranolol to wild-type and F483A mutant cytochrome P450 2D6 from molecular dynamics simulations. *European Biophysics Journal*, **2007**, 36, 589-99	1.9	19
165	Altered spin state equilibrium in the T309V mutant of cytochrome P450 2D6: a spectroscopic and computational study. *Journal of Biological Inorganic Chemistry*, **2007**, 12, 645-54	3.7	9

164	Inhibition of human recombinant cytochrome P450s by curcumin and curcumin decomposition products. *Toxicology*, **2007**, 235, 83-91	4.4	117
163	Molecular modeling-guided site-directed mutagenesis of cytochrome P450 2D6. *Current Drug Metabolism*, **2007**, 8, 59-77	3.5	39
162	A flow-through fluorescence polarization detection system for measuring GPCR-mediated modulation of cAMP production. *Journal of Biomolecular Screening*, **2007**, 12, 1074-83		7
161	Online biochemical detection of glutathione-S-transferase P1-specific inhibitors in complex mixtures. *Journal of Biomolecular Screening*, **2007**, 12, 396-405		19
160	Development of three parallel cytochrome P450 enzyme affinity detection systems coupled on-line to gradient high-performance liquid chromatography. *Drug Metabolism and Disposition*, **2007**, 35, 640-8	4	18
159	Liquid chromatography/tandem mass spectrometry detection of covalent binding of acetaminophen to human serum albumin. *Drug Metabolism and Disposition*, **2007**, 35, 1408-17	4	58
158	Screening the oxidative potential of several mono- and di-halogenated biphenyls and biphenyl ethers in rat hepatocytes. *Combinatorial Chemistry and High Throughput Screening*, **2006**, 9, 449-54	1.3	6
157	Rapid on-line profiling of estrogen receptor binding metabolites of tamoxifen. *Journal of Medicinal Chemistry*, **2006**, 49, 3287-92	8.3	33
156	Bioactivation of N-substituted NP(4-imidazole-ethyl)thioureas by human FMO1 and FMO3. *Xenobiotica*, **2006**, 36, 645-57	2	4
155	Enantioselective substrate binding in a monooxygenase protein model by molecular dynamics and docking. *Biophysical Journal*, **2006**, 91, 3206-16	2.9	24
154	Are automated molecular dynamics simulations and binding free energy calculations realistic tools in lead optimization? An evaluation of the linear interaction energy (LIE) method. *Journal of Chemical Information and Modeling*, **2006**, 46, 1972-83	6.1	56
153	Catalytic site prediction and virtual screening of cytochrome P450 2D6 substrates by consideration of water and rescoring in automated docking. *Journal of Medicinal Chemistry*, **2006**, 49, 2417-30	8.3	124
152	Topological role of cytochrome P450 2D6 active site residues. *Archives of Biochemistry and Biophysics*, **2006**, 447, 53-8	4.1	13
151	Binding of bufuralol, dextromethorphan, and 3,4-methylenedioxymethylamphetamine to wild-type and F120A mutant cytochrome P450 2D6 studied by resonance Raman spectroscopy. *Biochemical and Biophysical Research Communications*, **2006**, 343, 772-9	3.4	17
150	Heterotropic and homotropic cooperativity by a drug-metabolising mutant of cytochrome P450 BM3. *Biochemical and Biophysical Research Communications*, **2006**, 346, 810-8	3.4	84
149	Application of lipid peroxidation and protein oxidation biomarkers for oxidative damage in mammalian cells. A comparison with two fluorescent probes. *Toxicology in Vitro*, **2006**, 20, 1005-13	3.6	22
148	Binding of 7-methoxy-4-(aminomethyl)-coumarin to wild-type and W128F mutant cytochrome P450 2D6 studied by time-resolved fluorescence spectroscopy. *Biochemical Journal*, **2006**, 393, 635-43	3.8	10
147	Development and validation of a fluorescence HPLC-based screening assay for inhibition of human estrogen sulfotransferase. *Analytical Biochemistry*, **2006**, 357, 85-92	3.1	20

146	Binding mode prediction of cytochrome p450 and thymidine kinase protein-ligand complexes by consideration of water and rescoring in automated docking. *Journal of Medicinal Chemistry*, **2005**, 48, 2308-18	8.3	110
145	Metabolic regio- and stereoselectivity of cytochrome P450 2D6 towards 3,4-methylenedioxy-N-alkylamphetamines: in silico predictions and experimental validation. *Journal of Medicinal Chemistry*, **2005**, 48, 6117-27	8.3	56
144	Bioactivation of dibrominated biphenyls by cytochrome P450 activity to metabolites with estrogenic activity and estrogen sulfotransferase inhibition capacity. *Chemical Research in Toxicology*, **2005**, 18, 1691-700	4	17
143	Cytochrome p450 in silico: an integrative modeling approach. *Journal of Medicinal Chemistry*, **2005**, 48, 2725-55	8.3	187
142	Role of the conserved threonine 309 in mechanism of oxidation by cytochrome P450 2D6. *Biochemical and Biophysical Research Communications*, **2005**, 338, 1065-74	3.4	33
141	Formation of estrogenic metabolites of benzo[a]pyrene and chrysene by cytochrome P450 activity and their combined and supra-maximal estrogenic activity. *Environmental Toxicology and Pharmacology*, **2005**, 19, 41-55	5.8	63
140	A novel microplate reader-based high-throughput assay for estrogen receptor binding. *International Journal of Environmental Analytical Chemistry*, **2005**, 85, 149-161	1.8	8
139	Evaluation of alkoxyresorufins as fluorescent substrates for cytochrome P450 BM3 and site-directed mutants. *Analytical Biochemistry*, **2005**, 341, 148-55	3.1	53
138	Development and validation of a microsomal online cytochrome P450 bioreactor coupled to solid-phase extraction and reversed-phase liquid chromatography. *Journal of Chromatography A*, **2005**, 1075, 205-12	4.5	13
137	The role of phenylalanine 483 in cytochrome P450 2D6 is strongly substrate dependent. *Biochemical Pharmacology*, **2005**, 70, 1253-61	6	32
136	Development of a novel cytochrome p450 bioaffinity detection system coupled online to gradient reversed-phase high-performance liquid chromatography. *Journal of Biomolecular Screening*, **2005**, 10, 427-36		26
135	The role and application of in silico docking in chemical genomics research. *Methods in Molecular Biology*, **2005**, 310, 63-91	1.4	1
134	Influence of phenylalanine 120 on cytochrome P450 2D6 catalytic selectivity and regiospecificity: crucial role in 7-methoxy-4-(aminomethyl)-coumarin metabolism. *Biochemical Pharmacology*, **2004**, 68, 2263-71	6	42
133	Enzyme-catalyzed activation of anticancer prodrugs. *Pharmacological Reviews*, **2004**, 56, 53-102	22.5	402
132	Comparative cytotoxicity of N-substituted NP(4-imidazole-ethyl)thiourea in precision-cut rat liver slices. *Toxicology*, **2004**, 197, 81-91	4.4	27
131	Simultaneous determination of tyrosine, phenylalanine and deoxyguanosine oxidation products by liquid chromatography-tandem mass spectrometry as non-invasive biomarkers for oxidative damage. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*,	3.2	107
130	Evaluation of a multi-parameter biomarker set for oxidative damage in man: increased urinary excretion of lipid, protein and DNA oxidation products after one hour of exercise. *Free Radical Research*, **2004**, 38, 1269-79	4	77
129	In vitro biotransformation of 3,4-dihydro-6-hydroxy-2,2-dimethyl-7-methoxy-1(2H)-benzopyran (CR-6), a potent lipid peroxidation inhibitor and nitric oxide scavenger, in rat liver microsomes. *Chemical Research in Toxicology*, **2004**, 17, 904-13	4	9

128	Prediction of ligand binding affinity and orientation of xenoestrogens to the estrogen receptor by molecular dynamics simulations and the linear interaction energy method. *Journal of Medicinal Chemistry*, **2004**, 47, 1018-30	8.3	82
127	Prediction of drug metabolism: the case of cytochrome P450 2D6. *Current Topics in Medicinal Chemistry*, **2003**, 3, 1227-39	3	51
126	Modeling and molecular dynamics of glutamine transaminase K/cysteine conjugate beta-lyase. *Journal of Molecular Graphics and Modelling*, **2003**, 22, 55-70	2.8	
125	Homology modeling of rat and human cytochrome P450 2D (CYP2D) isoforms and computational rationalization of experimental ligand-binding specificities. *Journal of Medicinal Chemistry*, **2003**, 46, 74-86	8.3	104
124	Fish bioaccumulation and biomarkers in environmental risk assessment: a review. *Environmental Toxicology and Pharmacology*, **2003**, 13, 57-149	5.8	3086
123	Induction of glutathione-S-transferase mRNA levels by chemopreventive selenocysteine Se-conjugates. *Biochemical Pharmacology*, **2002**, 63, 1843-9	6	32
122	Tissue distribution of cytosolic beta-elimination reactions of selenocysteine Se-conjugates in rat and human. *Chemico-Biological Interactions*, **2002**, 140, 243-64	5	19
121	Selection of effective antisense oligodeoxynucleotides with a green fluorescent protein-based assay. Discovery of selective and potent inhibitors of glutathione S-transferase Mu expression. *FEBS Journal*, **2002**, 269, 2574-83		9
120	Beta-lyase-dependent attenuation of cisplatin-mediated toxicity by selenocysteine Se-conjugates in renal tubular cell lines. *Journal of Pharmacology and Experimental Therapeutics*, **2002**, 301, 884-92	4.7	14
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