Ismael Zamora

List of Publications by Year
in descending order

51 papers	2,339 citations	186265 28 h-index	206112 48 g-index
56 all docs	56 docs citations	56 times ranked	2163 citing authors

#	Article	IF	Citations
1	pH-dependent bidirectional transport of weakly basic drugs across Caco-2 monolayers: implications for drug-drug interactions. Pharmaceutical Research, 2003, 20, 1141-1148.	3.5	179
2	Predicting Drug Metabolism:Â A Site of Metabolism Prediction Tool Applied to the Cytochrome P450 2C9. Journal of Medicinal Chemistry, 2003, 46, 2313-2324.	6.4	156
3	pH-Dependent passive and active transport of acidic drugs across Caco-2 cell monolayers. European Journal of Pharmaceutical Sciences, 2005, 25, 211-220.	4.0	127
4	Contribution of solid-state properties to the aqueous solubility of drugs. European Journal of Pharmaceutical Sciences, 2006, 29, 294-305.	4.0	122
5	Competitive CYP2C9 Inhibitors: Enzyme Inhibition Studies, Protein Homology Modeling, and Three-Dimensional Quantitative Structure-Activity Relationship Analysis. Molecular Pharmacology, 2001, 59, 909-919.	2.3	116
6	CYP2C9 Structureâ^'Metabolism Relationships:â€‰ Optimizing the Metabolic Stability of COX-2 Inhibitors. Journal of Medicinal Chemistry, 2007, 50, 4444-4452.	6.4	103
7	Analysis of Selective Regions in the Active Sites of Human Cytochromes P450, 2C8, 2C9, 2C18, and 2C19 Homology Models Using GRID/CPCA. Journal of Medicinal Chemistry, 2001, 44, 4072-4081.	6.4	84
8	Anchorâ^'GRIND:Â Filling the Gap between Standard 3D QSAR and the GRid-INdependent Descriptors. Journal of Medicinal Chemistry, 2005, 48, 2687-2694.	6.4	84
9	Pharmacokinetically Based Mapping Device for Chemical Space Navigation. ACS Combinatorial Science, 2002, 4, 258-266.	3.3	82
10	COMPARISON OF METHODS FOR THE PREDICTION OF THE METABOLIC SITES FOR CYP3A4-MEDIATED METABOLIC REACTIONS. Drug Metabolism and Disposition, 2006, 34, 976-983.	3.3	81
11	Enhanced metabolite identification with MS^E and a semi-automated software for structural elucidation. Rapid Communications in Mass Spectrometry, 2010, 24, 3127-3138.	1.5	78
12	SHOP:Â Scaffold HOPping by GRID-Based Similarity Searches. Journal of Medicinal Chemistry, 2007, 50, 2708-2717.	6.4	75
13	Brassinosteroids: A new way to define the structural requirements. Tetrahedron, 1996, 52, 2435-2448.	1.9	73
14	Surface Descriptors for Proteinâ^'Ligand Affinity Prediction. Journal of Medicinal Chemistry, 2003, 46, 25-33.	6.4	64
15	Conformer- and Alignment-Independent Model for Predicting Structurally Diverse Competitive CYP2C9 Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 907-914.	6.4	64
16	Virtual Screening and Scaffold Hopping Based on GRID Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2005, 45, 1313-1323.	5.4	56
17	Suitability of GRIND-Based Principal Properties for the Description of Molecular Similarity and Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 2129-2138.	5.4	55
18	New methods in predictive metabolism. Journal of Computer-Aided Molecular Design, 2002, 16, 403-413.	2.9	54

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19	Impact of Extracellular Protein Binding on Passive and Active Drug Transport Across Caco-2 Cells. Pharmaceutical Research, 2006, 23, 350-359.	3.5	54
20	Discriminant and quantitative PLS analysis of competitive CYP2C9 inhibitors versus non-inhibitors using alignment independent GRIND descriptors. Journal of Computer-Aided Molecular Design, 2002, 16, 443-458.	2.9	46
21	Virtual Screening for Novel Openers of Pancreatic KATPChannels. Journal of Medicinal Chemistry, 2007, 50, 2117-2126.	6.4	46
22	Model based on GRID-derived descriptors for estimating CYP3A4 enzyme stability of potential drug candidates. Journal of Computer-Aided Molecular Design, 2004, 18, 155-166.	2.9	41
23	High-throughput, computer assisted, specific MetID. A revolution for drug discovery. Drug Discovery Today: Technologies, 2013, 10, e199-e205.	4.0	41
24	Fragment-based design for the development of N-domain-selective angiotensin-1-converting enzyme inhibitors. Clinical Science, 2014, 126, 305-313.	4.3	36
25	CYP2C9 Structureâ^'Metabolism Relationships:â€‰ Substrates, Inhibitors, and Metabolites. Journal of Medicinal Chemistry, 2007, 50, 5382-5391.	6.4	34
26	Postâ€acquisition analysis of untargeted accurate mass quadrupole timeâ€ofâ€flight MS^E data for multiple collisionâ€induced neutral losses and fragment ions of glutathione conjugates. Rapid Communications in Mass Spectrometry, 2014, 28, 2695-2703.	1.5	30
27	Exploration of Enzymeâ^'Ligand Interactions in CYP2D6 & 3A4 Homology Models and Crystal Structures Using a Novel Computational Approach. Journal of Chemical Information and Modeling, 2007, 47, 1234-1247.	5.4	29
28	The challenges ofin silicocontributions to drug metabolism in lead optimization. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 851-861.	3.3	29
29	Characterization of Type II Ligands in CYP2C9 and CYP3A4. Journal of Medicinal Chemistry, 2008, 51, 1755-1763.	6.4	28
30	STRUCTURAL ANALYSIS OF CYP2C9 AND CYP2C5 AND AN EVALUATION OF COMMONLY USED MOLECULAR MODELING TECHNIQUES. Drug Metabolism and Disposition, 2004, 32, 1218-1229.	3.3	24
31	Software automation tools for increased throughput metabolic soft-spot identification in early drug discovery. Bioanalysis, 2013, 5, 1165-1179.	1.5	23
32	Synthesis and molecular modeling: Related approaches to progress in brassinosteroid research. Lipids, 1997, 32, 1341-1347.	1.7	19
33	SHOP: Receptor-Based Scaffold HOPping by GRID-Based Similarity Searches. Journal of Chemical Information and Modeling, 2009, 49, 658-669.	5.4	19
34	Enabling Efficient Lateâ€Stage Functionalization of Drugâ€Like Molecules with LCâ€MS and Reactionâ€Driven Data Processing. European Journal of Organic Chemistry, 2017, 2017, 7122-7126.	2.4	17
35	The Molecular Basis of CYP2D6-Mediated N-Dealkylation: Balance between Metabolic Clearance Routes and Enzyme Inhibition. Drug Metabolism and Disposition, 2008, 36, 2199-2210.	3.3	16
36	SHOP: A Method For Structureâ€Based Fragment and Scaffold Hopping. ChemMedChem, 2009, 4, 427-439.	3.2	15

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37	Combining pharmacophore and protein modeling to predict CYP450 inhibitors and substrates. Methods in Enzymology, 2002, 357, 133-144.	1.0	14
38	Rapid Classification of CYP3A4 Inhibition Potential Using Support Vector Machine Approach. Letters in Drug Design and Discovery, 2007, 4, 192-200.	0.7	14
39	Software-aided approach to investigate peptide structure and metabolic susceptibility of amide bonds in peptide drugs based on high resolution mass spectrometry. PLoS ONE, 2017, 12, e0186461.	2.5	14
40	Development, optimization and implementation of a centralized metabolic soft spot assay. Bioanalysis, 2017, 9, 541-552.	1.5	13
41	Update on hydrocodone metabolites in rats and dogs aided with a semi-automatic software for metabolite identification Mass-MetaSite. Xenobiotica, 2013, 43, 390-398.	1.1	10
42	Softwareâ€aided cytochrome P450 reaction phenotyping and kinetic analysis in early drug discovery. Rapid Communications in Mass Spectrometry, 2016, 30, 301-310.	1.5	10
43	Metabolite identification using an ion mobility enhanced dataâ€independent acquisition strategy and automated data processing. Rapid Communications in Mass Spectrometry, 2020, 34, e8792.	1.5	10
44	Softwareâ€aided structural elucidation in drug discovery. Rapid Communications in Mass Spectrometry, 2015, 29, 2083-2089.	1.5	8
45	Software-aided workflow for predicting protease-specific cleavage sites using physicochemical properties of the natural and unnatural amino acids in peptide-based drug discovery. PLoS ONE, 2019, 14, e0199270.	2.5	6
46	WebMetabase: cleavage sites analysis tool for natural and unnatural substrates from diverse data source. Bioinformatics, 2019, 35, 650-655.	4.1	5
47	Automatic Identification of Lansoprazole Degradants under Stress Conditions by LC-HRMS with MassChemSite and WebChembase. Journal of Chemical Information and Modeling, 2021, 61, 2706-2719.	5.4	5
48	New methods in predictive metabolism. Molecular Diversity, 2000, 5, 277-287.	3.9	4
49	Shaping the future of safer innovative drugs in Europe. Nature Biotechnology, 2011, 29, 789-790.	17.5	3
50	Modeling Organic Anion-Transporting Polypeptide 1B1 Inhibition to Elucidate Interaction Risks in Early Drug Design. Journal of Pharmaceutical Sciences, 2016, 105, 3214-3220.	3.3	2
51	Prediction of Site of Metabolism in Humans: Case Studies of Cytochromes P450 2C9, 2D6, and 3A4. , 0, , 367-379.		0