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	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
2	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
3	WebMetabase: cleavage sites analysis tool for natural and unnatural substrates from diverse data source. Bioinformatics, 2019, 35, 650-655.	4.1	5
4	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
5	Development, optimization and implementation of a centralized metabolic soft spot assay. Bioanalysis, 2017, 9, 541-552.	1.5	13
6	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
7	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
8	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
9	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
10	Softwareâ€aided structural elucidation in drug discovery. Rapid Communications in Mass Spectrometry, 2015, 29, 2083-2089.	1.5	8
11	Fragment-based design for the development of N-domain-selective angiotensin-1-converting enzyme inhibitors. Clinical Science, 2014, 126, 305-313.	4.3	36
12	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
13	High-throughput, computer assisted, specific MetID. A revolution for drug discovery. Drug Discovery Today: Technologies, 2013, 10, e199-e205.	4.0	41
14	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
15	Software automation tools for increased throughput metabolic soft-spot identification in early drug discovery. Bioanalysis, 2013, 5, 1165-1179.	1.5	23
16	Shaping the future of safer innovative drugs in Europe. Nature Biotechnology, 2011, 29, 789-790.	17.5	3
17	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
18	The challenges ofin silicocontributions to drug metabolism in lead optimization. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 851-861.	3.3	29

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19	SHOP: A Method For Structureâ€Based Fragment and Scaffold Hopping. ChemMedChem, 2009, 4, 427-439.	3.2	15
20	SHOP: Receptor-Based Scaffold HOPping by GRID-Based Similarity Searches. Journal of Chemical Information and Modeling, 2009, 49, 658-669.	5.4	19
21	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
22	Characterization of Type II Ligands in CYP2C9 and CYP3A4. Journal of Medicinal Chemistry, 2008, 51, 1755-1763.	6.4	28
23	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
24	Rapid Classification of CYP3A4 Inhibition Potential Using Support Vector Machine Approach. Letters in Drug Design and Discovery, 2007, 4, 192-200.	0.7	14
25	CYP2C9 Structureâ^'Metabolism Relationships:â€‰ Substrates, Inhibitors, and Metabolites. Journal of Medicinal Chemistry, 2007, 50, 5382-5391.	6.4	34
26	Virtual Screening for Novel Openers of Pancreatic KATPChannels. Journal of Medicinal Chemistry, 2007, 50, 2117-2126.	6.4	46
27	SHOP:Â Scaffold HOPping by GRID-Based Similarity Searches. Journal of Medicinal Chemistry, 2007, 50, 2708-2717.	6.4	75
28	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
29	CYP2C9 Structureâ^'Metabolism Relationships:â€‰ Optimizing the Metabolic Stability of COX-2 Inhibitors. Journal of Medicinal Chemistry, 2007, 50, 4444-4452.	6.4	103
30	Impact of Extracellular Protein Binding on Passive and Active Drug Transport Across Caco-2 Cells. Pharmaceutical Research, 2006, 23, 350-359.	3.5	54
31	Contribution of solid-state properties to the aqueous solubility of drugs. European Journal of Pharmaceutical Sciences, 2006, 29, 294-305.	4.0	122
32	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
33	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
34	Virtual Screening and Scaffold Hopping Based on GRID Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2005, 45, 1313-1323.	5.4	56
35	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
36	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

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37	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
38	Conformer- and Alignment-Independent Model for Predicting Structurally Diverse Competitive CYP2C9 Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 907-914.	6.4	64
39	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
40	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
41	Surface Descriptors for Proteinâ~Ligand Affinity Prediction. Journal of Medicinal Chemistry, 2003, 46, 25-33.	6.4	64
42	Combining pharmacophore and protein modeling to predict CYP450 inhibitors and substrates. Methods in Enzymology, 2002, 357, 133-144.	1.0	14
43	Pharmacokinetically Based Mapping Device for Chemical Space Navigation. ACS Combinatorial Science, 2002, 4, 258-266.	3.3	82
44	New methods in predictive metabolism. Journal of Computer-Aided Molecular Design, 2002, 16, 403-413.	2.9	54
45	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
46	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
47	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
48	New methods in predictive metabolism. Molecular Diversity, 2000, 5, 277-287.	3.9	4
49	Synthesis and molecular modeling: Related approaches to progress in brassinosteroid research. Lipids, 1997, 32, 1341-1347.	1.7	19
50	Brassinosteroids: A new way to define the structural requirements. Tetrahedron, 1996, 52, 2435-2448.	1.9	73
51	Prediction of Site of Metabolism in Humans: Case Studies of Cytochromes P450 2C9, 2D6, and 3A4. , 0, , 367-379.		0