Jordi Munoz-Muriedas

List of Publications by Year
in descending order

25 papers	703 citations	567281 15 h-index	580821 25 g-index
25 all docs	25 docs citations	25 times ranked	1081 citing authors

#	Article	IF	Citations
1	Large scale meta-analysis of preclinical toxicity data for target characterisation and hypotheses generation. PLoS ONE, 2021, 16, e0252533.	2.5	3
2	Investigation into Small Molecule Isomeric Glucuronide Metabolite Differentiation Using In Silico and Experimental Collision Cross-Section Values. Journal of the American Society for Mass Spectrometry, 2021, 32, 1976-1986.	2.8	11
3	Identification and Optimization of Novel Small c-Abl Kinase Activators Using Fragment and HTS Methodologies. Journal of Medicinal Chemistry, 2019, 62, 2154-2171.	6.4	21
4	Unveiling the photophysics of thiourea from CASPT2/CASSCF potential energy surfaces and singlet/triplet excited state molecular dynamics simulations. Computational and Theoretical Chemistry, 2019, 1151, 36-42.	2.5	2
5	Excited state dynamics of some nonsteroidal anti-inflammatory drugs: A surface-hopping investigation. Computational and Theoretical Chemistry, 2019, 1152, 20-27.	2.5	13
6	A pharma-wide approach to address the genotoxicity prediction of primary aromatic amines. Computational Toxicology, 2018, 7, 27-35.	3.3	20
7	Application of the quantum mechanical IEF/PCM-MST hydrophobic descriptors to selectivity in ligand binding. Journal of Molecular Modeling, 2016, 22, 136.	1.8	3
8	Development and validation of hydrophobic molecular fields derived from the quantum mechanical IEF/PCMâ€MST solvation models in 3Dâ€QSAR. Journal of Computational Chemistry, 2016, 37, 1147-1162.	3.3	8
9	Elucidation of Drug Metabolite Structural Isomers Using Molecular Modeling Coupled with Ion Mobility Mass Spectrometry. Analytical Chemistry, 2016, 88, 2273-2280.	6.5	43
10	Ensuring confidence in predictions: A scheme to assess the scientific validity of in silico models. Advanced Drug Delivery Reviews, 2015, 86, 101-111.	13.7	17
11	Evaluation of an in silico cardiac safety assay: Using ion channel screening data to predict QT interval changes in the rabbit ventricular wedge. Journal of Pharmacological and Toxicological Methods, 2013, 68, 88-96.	0.7	62
12	Enabling Lead Discovery for Histone Lysine Demethylases by High-Throughput RapidFire Mass Spectrometry. Journal of Biomolecular Screening, 2012, 17, 39-48.	2.6	89
13	Configuration of a High-Content Imaging Platform for Hit Identification and Pharmacological Assessment of JMJD3 Demethylase Enzyme Inhibitors. Journal of Biomolecular Screening, 2012, 17, 108-120.	2.6	18
14	Wavelet Approximation of GRID Fields: Application to Quantitative Structureâ€Activity Relationships. Molecular Informatics, 2010, 29, 603-620.	2.5	4
15	Sites of metabolic substitution: investigating metabolite structures utilising ion mobility and molecular modelling. Rapid Communications in Mass Spectrometry, 2010, 24, 3157-3162.	1.5	70
16	A hydrophobic similarity analysis of solvation effects on nucleic acid bases. Journal of Molecular Modeling, 2007, 13, 357-365.	1.8	8
17	Binding of 13-Amidohuprines to Acetylcholinesterase:Â Exploring the Ligand-Induced Conformational Change of the Gly117-Gly118 Peptide Bond in the Oxyanion Hole. Journal of Medicinal Chemistry, 2006, 49, 6833-6840.	6.4	19
18	Hydrophobic Molecular Similarity from MST Fractional Contributions to the Octanol/water Partition Coefficient. Journal of Computer-Aided Molecular Design, 2005, 19, 401-419.	2.9	9

#	Article	IF	Citations
19	Modulation of Binding Strength in Several Classes of Active Site Inhibitors of Acetylcholinesterase Studied by Comparative Binding Energy Analysis. Journal of Medicinal Chemistry, 2004, 47, 4471-4482.	6.4	19
20	Molecular Modelling Approaches to the Design of Acetylcholinesterase Inhibitors: New Challenges for the Treatment of Alzheimers Disease. Current Pharmaceutical Design, 2004, 10, 3131-3140.	1.9	29
21	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	2.8	89
22	Can Divalent Metal Cations Stabilize the Triplex Motif? Theoretical Study of the Interaction of the Hydrated Mg2+ Cation with the GâˆGÂ·C Triplet. Journal of Physical Chemistry B, 2002, 106, 8849-8857.	2.6	20
23	Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. Journal of Computational Chemistry, 2002, 23, 554-563.	3.3	18
24	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B, 2001, 105, 6051-6060.	2.6	95
25	Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. Physical Chemistry Chemical Physics, 2000, 2, 4897-4905.	2.8	13