# Jordi Munoz-Muriedas

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836. | 2.8 | 89 |
| 3 | Enabling Lead Discovery for Histone Lysine Demethylases by High-Throughput RapidFire Mass Spectrometry. Journal of Biomolecular Screening, 2012, 17, 39-48. | 2.6 | 89 |
| 4 | 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 |
| 5 | 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 |
| 6 | Elucidation of Drug Metabolite Structural Isomers Using Molecular Modeling Coupled with Ion Mobility Mass Spectrometry. Analytical Chemistry, 2016, 88, 2273-2280. | 6.5 | 43 |
| 7 | 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 |
| 8 | 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 |
| 9 | Can Divalent Metal Cations Stabilize the Triplex Motif? Theoretical Study of the Interaction of the Hydrated Mg2+ Cation with the Gâ^'GÂ·C Triplet. Journal of Physical Chemistry B, 2002, 106, 8849-8857. | 2.6 | 20 |
| 10 | A pharma-wide approach to address the genotoxicity prediction of primary aromatic amines. Computational Toxicology, 2018, 7, 27-35. | 3.3 | 20 |
| 11 | 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 |
| 12 | 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 |
| 13 | Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. Journal of Computational Chemistry, 2002, 23, 554-563. | 3.3 | 18 |
| 14 | 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 |
| 15 | 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 |
| 16 | Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. Physical Chemistry Chemical Physics, 2000, 2, 4897-4905. | 2.8 | 13 |
| 17 | Excited state dynamics of some nonsteroidal anti-inflammatory drugs: A surface-hopping investigation. Computational and Theoretical Chemistry, 2019, 1152, 20-27. | 2.5 | 13 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | A hydrophobic similarity analysis of solvation effects on nucleic acid bases. Journal of Molecular Modeling, 2007, 13, 357-365. | 1.8 | 8 |
| 21 | 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 |
| 22 | Wavelet Approximation of GRID Fields: Application to Quantitative Structureâ€Activity Relationships. Molecular Informatics, 2010, 29, 603-620. | 2.5 | 4 |
| 23 | 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 |
| 24 | Large scale meta-analysis of preclinical toxicity data for target characterisation and hypotheses generation. PLoS ONE, 2021, 16, e0252533. | 2.5 | 3 |
| 25 | 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 |