

Maykel Cruz-Monteagudo

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

39
papers

785
citations

16
h-index

27
g-index

42
ext. papers

858
ext. citations

4
avg, IF

3.69
L-index

#	Paper	IF	Citations
39	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. <i>Drug Discovery Today</i> , 2014 , 19, 1069-80	8.8	103
38	Computational chemistry development of a unified free energy Markov model for the distribution of 1300 chemicals to 38 different environmental or biological systems. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1909-23	3.5	67
37	Computational chemistry approach for the early detection of drug-induced idiosyncratic liver toxicity. <i>Journal of Computational Chemistry</i> , 2008 , 29, 533-49	3.5	42
36	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. <i>Bioorganic and Medicinal Chemistry</i> , 2005 , 13, 1119-29	3.4	41
35	Desirability-based methods of multiobjective optimization and ranking for global QSAR studies. Filtering safe and potent drug candidates from combinatorial libraries. <i>ACS Combinatorial Science</i> , 2008 , 10, 897-913		40
34	Desirability-based multiobjective optimization for global QSAR studies: application to the design of novel NSAIDs with improved analgesic, antiinflammatory, and ulcerogenic profiles. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2445-59	3.5	40
33	3D-MEDNEs: an alternative "in silico" technique for chemical research in toxicology. 2. quantitative proteome-toxicity relationships (QPTR) based on mass spectrum spiral entropy. <i>Chemical Research in Toxicology</i> , 2008 , 21, 619-32	4	35
32	QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005 , 15, 1651-7	2.9	34
31	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. <i>Drug Discovery Today</i> , 2017 , 22, 994-1007	8.8	25
30	Chemometrics for QSAR with low sequence homology: Mycobacterial promoter sequences recognition with 2D-RNA entropies. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007 , 85, 20-26	3.8	23
29	Unified drug-target interaction thermodynamic Markov model using stochastic entropies to predict multiple drugs side effects. <i>European Journal of Medicinal Chemistry</i> , 2005 , 40, 1030-41	6.8	23
28	Stochastic molecular descriptors for polymers. 4. Study of complex mixtures with topological indices of mass spectra spiral and star networks: The blood proteome case. <i>Polymer</i> , 2008 , 49, 5575-5587	3.9	22
27	Evolutionary computation and QSAR research. <i>Current Computer-Aided Drug Design</i> , 2013 , 9, 206-25	1.4	22
26	Jointly handling potency and toxicity of antimicrobial peptidomimetics by simple rules from desirability theory and chemoinformatics. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 3060-77	6.7	21
25	Chemoinformatics profiling of ionic liquids--automatic and chemically interpretable cytotoxicity profiling, virtual screening, and cytotoxicophore identification. <i>Toxicological Sciences</i> , 2013 , 136, 548-65	4.4	19
24	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. <i>Drug Discovery Today</i> , 2017 , 22, 1489-1502	8.8	17
23	Efficient and biologically relevant consensus strategy for Parkinson's disease gene prioritization. <i>BMC Medical Genomics</i> , 2016 , 9, 12	3.7	15

22	Computational modeling tools for the design of potent antimalarial bisbenzamidines: overcoming the antimalarial potential of pentamidine. <i>Bioorganic and Medicinal Chemistry</i> , 2007 , 15, 5322-39	3.4	15
21	CompScore: Boosting Structure-Based Virtual Screening Performance by Incorporating Docking Scoring Function Components into Consensus Scoring. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3655-3666	6.1	14
20	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2094-110	6.1	14
19	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. <i>BMC Medical Genomics</i> , 2017 , 10, 50	3.7	14
18	Quantitative Proteome-Property Relationships (QPPRs). Part 1: finding biomarkers of organic drugs with mean Markov connectivity indices of spiral networks of blood mass spectra. <i>Bioorganic and Medicinal Chemistry</i> , 2008 , 16, 9684-93	3.4	13
17	Prioritizing Hits with Appropriate Trade-Offs Between HIV-1 Reverse Transcriptase Inhibitory Efficacy and MT4 Blood Cells Toxicity Through Desirability-Based Multiobjective Optimization and Ranking. <i>Molecular Informatics</i> , 2010 , 29, 303-21	3.8	12
16	Desirability-based multi-objective QSAR in drug discovery. <i>Mini-Reviews in Medicinal Chemistry</i> , 2012 , 12, 920-35	3.2	11
15	A desirability-based multi objective approach for the virtual screening discovery of broad-spectrum anti-gastric cancer agents. <i>PLoS ONE</i> , 2018 , 13, e0192176	3.7	11
14	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A2A Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. <i>Current Pharmaceutical Design</i> , 2016 , 22, 3082-96	3.3	10
13	Cheminformatics profiling of ionic liquids--uncovering structure-cytotoxicity relationships with network-like similarity graphs. <i>Toxicological Sciences</i> , 2014 , 138, 191-204	4.4	9
12	Simple stochastic fingerprints towards mathematical modeling in biology and medicine 2. Unifying Markov model for drugs side effects. <i>Bulletin of Mathematical Biology</i> , 2006 , 68, 1527-54	2.1	9
11	Simple stochastic fingerprints towards mathematical modeling in biology and medicine. 3. Ocular irritability classification model. <i>Bulletin of Mathematical Biology</i> , 2006 , 68, 1555-72	2.1	9
10	Multidimensional drug design: simultaneous analysis of binding and relative efficacy profiles of N(6)-substituted-4Pthioadenosines A3 adenosine receptor agonists. <i>Chemical Biology and Drug Design</i> , 2010 , 75, 607-18	2.9	8
9	Global antifungal profile optimization of chlorophenyl derivatives against <i>Botrytis cinerea</i> and <i>Colletotrichum gloeosporioides</i> . <i>Journal of Agricultural and Food Chemistry</i> , 2009 , 57, 4838-43	5.7	7
8	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 957-969	3	6
7	Multi-target QSPR assemble of a Complex Network for the distribution of chemicals to biphasic systems and biological tissues. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2008 , 94, 160-165	3.8	6
6	Fusing Docking Scoring Functions Improves the Virtual Screening Performance for Discovering Parkinson's Disease Dual Target Ligands. <i>Current Neuropharmacology</i> , 2017 , 15, 1107-1116	7.6	6
5	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. <i>Molecular Diversity</i> , 2014 , 18, 637-54	3.1	5

4	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. <i>Current Pharmaceutical Design</i> , 2016 , 22, 5043-5056	3-3	5
3	Recent advances on QSAR-based profiling of agonist and antagonist A3 adenosine receptor ligands. <i>Current Topics in Medicinal Chemistry</i> , 2013 , 13, 1048-68	3	4
2	Quantitative Structure-Epigenetic Activity Relationships. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2017 , 303-338	0-7	4
1	Desirability-based multi-criteria virtual screening of selective antimicrobial cyclic hairpin cationic peptidomimetics. <i>Current Pharmaceutical Design</i> , 2013 , 19, 2148-63	3-3	2