Maykel Cruz-Monteagudo

List of Publications by Year in Descending Order

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	CompScore: Boosting Structure-Based Virtual Screening Performance by Incorporating Docking Scoring Function Components into Consensus Scoring. *Journal of Chemical Information and Modeling*, **2019**, 59, 3655-3666	6.1	14
38	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. *Current Topics in Medicinal Chemistry*, **2019**, 19, 957-969	3	6
37	A desirability-based multi objective approach for the virtual screening discovery of broad-spectrum anti-gastric cancer agents. *PLoS ONE*, **2018**, 13, e0192176	3.7	11
36	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. *Drug Discovery Today*, **2017**, 22, 994-1007	8.8	25
35	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. *Drug Discovery Today*, **2017**, 22, 1489-1502	8.8	17
34	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. *BMC Medical Genomics*, **2017**, 10, 50	3.7	14
33	Fusing Docking Scoring Functions Improves the Virtual Screening Performance for Discovering Parkinson's Disease Dual Target Ligands. *Current Neuropharmacology*, **2017**, 15, 1107-1116	7.6	6
32	Quantitative Structure-Epigenetic Activity Relationships. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 303-338	0.7	4
31	Efficient and biologically relevant consensus strategy for Parkinson disease gene prioritization. *BMC Medical Genomics*, **2016**, 9, 12	3.7	15
30	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A2AAdenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. *Current Pharmaceutical Design*, **2016**, 22, 3082-96	3.3	10
29	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. *Current Pharmaceutical Design*, **2016**, 22, 5043-5056	3.3	5
28	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. *Journal of Chemical Information and Modeling*, **2015**, 55, 2094-110	6.1	14
27	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. *Molecular Diversity*, **2014**, 18, 637-54	3.1	5
26	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. *Drug Discovery Today*, **2014**, 19, 1069-80	8.8	103
25	Chemoinformatics profiling of ionic liquids--uncovering structure-cytotoxicity relationships with network-like similarity graphs. *Toxicological Sciences*, **2014**, 138, 191-204	4.4	9
24	Chemoinformatics profiling of ionic liquids--automatic and chemically interpretable cytotoxicity profiling, virtual screening, and cytotoxicophore identification. *Toxicological Sciences*, **2013**, 136, 548-65	4.4	19
23	Desirability-based multi-criteria virtual screening of selective antimicrobial cyclic -hairpin cationic peptidomimetics. *Current Pharmaceutical Design*, **2013**, 19, 2148-63	3.3	2

22	Recent advances on QSAR-based profiling of agonist and antagonist A3 adenosine receptor ligands. *Current Topics in Medicinal Chemistry*, **2013**, 13, 1048-68	3	4
21	Evolutionary computation and QSAR research. *Current Computer-Aided Drug Design*, **2013**, 9, 206-25	1.4	22
20	Desirability-based multi-objective QSAR in drug discovery. *Mini-Reviews in Medicinal Chemistry*, **2012**, 12, 920-35	3.2	11
19	Jointly handling potency and toxicity of antimicrobial peptidomimetics by simple rules from desirability theory and chemoinformatics. *Journal of Chemical Information and Modeling*, **2011**, 51, 3060-77	4.1	21
18	Multidimensional drug design: simultaneous analysis of binding and relative efficacy profiles of N(6)-substituted-4'thioadenosines A3 adenosine receptor agonists. *Chemical Biology and Drug Design*, **2010**, 75, 607-18	2.9	8
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. *Molecular Informatics*, **2010**, 29, 303-21	3.8	12
16	Global antifungal profile optimization of chlorophenyl derivatives against Botrytis cinerea and Colletotrichum gloeosporioides. *Journal of Agricultural and Food Chemistry*, **2009**, 57, 4838-43	5.7	7
15	Desirability-based methods of multiobjective optimization and ranking for global QSAR studies. Filtering safe and potent drug candidates from combinatorial libraries. *ACS Combinatorial Science*, **2008**, 10, 897-913		40
14	3D-MEDNEs: an alternative "in silico" technique for chemical research in toxicology. 2. quantitative proteome-toxicity relationships (QPTR) based on mass spectrum spiral entropy. *Chemical Research in Toxicology*, **2008**, 21, 619-32	4	35
13	Computational chemistry approach for the early detection of drug-induced idiosyncratic liver toxicity. *Journal of Computational Chemistry*, **2008**, 29, 533-49	3.5	42
12	Desirability-based multiobjective optimization for global QSAR studies: application to the design of novel NSAIDs with improved analgesic, antiinflammatory, and ulcerogenic profiles. *Journal of Computational Chemistry*, **2008**, 29, 2445-59	3.5	40
11	Stochastic molecular descriptors for polymers. 4. Study of complex mixtures with topological indices of mass spectra spiral and star networks: The blood proteome case. *Polymer*, **2008**, 49, 5575-5587	3.9	22
10	Quantitative Proteome-Property Relationships (QPPRs). Part 1: finding biomarkers of organic drugs with mean Markov connectivity indices of spiral networks of blood mass spectra. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 9684-93	3.4	13
9	Multi-target QSPR assemble of a Complex Network for the distribution of chemicals to biphasic systems and biological tissues. *Chemometrics and Intelligent Laboratory Systems*, **2008**, 94, 160-165	3.8	6
8	Computational chemistry development of a unified free energy Markov model for the distribution of 1300 chemicals to 38 different environmental or biological systems. *Journal of Computational Chemistry*, **2007**, 28, 1909-23	3.5	67
7	Computational modeling tools for the design of potent antimalarial bisbenzamidines: overcoming the antimalarial potential of pentamidine. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 5322-39	3.4	15
6	Chemometrics for QSAR with low sequence homology: Mycobacterial promoter sequences recognition with 2D-RNA entropies. *Chemometrics and Intelligent Laboratory Systems*, **2007**, 85, 20-26	3.8	23
5	Simple stochastic fingerprints towards mathematical modeling in biology and medicine 2. Unifying Markov model for drugs side effects. *Bulletin of Mathematical Biology*, **2006**, 68, 1527-54	2.1	9

4	Simple stochastic fingerprints towards mathematical modeling in biology and medicine. 3. Ocular irritability classification model. *Bulletin of Mathematical Biology*, **2006**, 68, 1555-72	2.1	9
3	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 1119-29	3.4	41
2	QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 1651-7	2.9	34
1	Unified drug-target interaction thermodynamic Markov model using stochastic entropies to predict multiple drugs side effects. *European Journal of Medicinal Chemistry*, **2005**, 40, 1030-41	6.8	23