Maykel Cruz-Monteagudo

List of Publications by Year
in descending order

41 papers	1,001 citations	430874 18 h-index	454955 30 g-index
42 all docs	42 docs citations	42 times ranked	1092 citing authors

#	Article	IF	Citations
1	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. Current Topics in Medicinal Chemistry, 2019, 19, 957-969.	2.1	8
2	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.	5.4	20
3	Complex Networks and Machine Learning: From Molecular to Social Sciences. Applied Sciences (Switzerland), 2019, 9, 4493.	2.5	5
4	A desirability-based multi objective approach for the virtual screening discovery of broad-spectrum anti-gastric cancer agents. PLoS ONE, 2018, 13, e0192176.	2.5	15
5	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. Drug Discovery Today, 2017, 22, 994-1007.	6.4	28
6	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	6.4	28
7	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. BMC Medical Genomics, 2017, 10, 50.	1.5	18
8	Quantitative Structure-Epigenetic Activity Relationships. Challenges and Advances in Computational Chemistry and Physics, 2017, , 303-338.	0.6	4
9	Fusing Docking Scoring Functions Improves the Virtual Screening Performance for Discovering Parkinson's Disease Dual Target Ligands. Current Neuropharmacology, 2017, 15, 1107-1116.	2.9	11
10	Efficient and biologically relevant consensus strategy for Parkinsonâ€™s disease gene prioritization. BMC Medical Genomics, 2016, 9, 12.	1.5	29
11	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A_{2A} Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. Current Pharmaceutical Design, 2016, 22, 3082-3096.	1.9	13
12	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. Current Pharmaceutical Design, 2016, 22, 5043-5056.	1.9	7
13	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, 2094-2110.	5.4	20
14	Chemoinformatics Profiling of Ionic Liquidsâ€"Uncovering Structure-Cytotoxicity Relationships With Network-like Similarity Graphs. Toxicological Sciences, 2014, 138, 191-204.	3.1	12
15	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. Molecular Diversity, 2014, 18, 637-654.	3.9	8
16	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	6.4	140
17	Chemoinformatics Profiling of Ionic Liquidsâ€"Automatic and Chemically Interpretable Cytotoxicity Profiling, Virtual Screening, and Cytotoxicophore Identification. Toxicological Sciences, 2013, 136, 548-565.	3.1	19
18	Desirability-based Multi-criteria Virtual Screening of Selective Antimicrobial Cyclic Î²-Hairpin Cationic Peptidomimetics. Current Pharmaceutical Design, 2013, 19, 2148-2163.	1.9	2

#	Article	IF	Citations
19	Recent Advances on QSAR-Based Profiling of Agonist and Antagonist A3 Adenosine Receptor Ligands. Current Topics in Medicinal Chemistry, 2013, 13, 1048-1068.	2.1	4
20	Evolutionary Computation and QSAR Research. Current Computer-Aided Drug Design, 2013, 9, 206-225.	1.2	28
21	Editorial [Hot Topic ; Special Issue: Multi-Criteria Approaches in Computer-Aided Drug Discovery]. Mini-Reviews in Medicinal Chemistry, 2012, 12, 905-906.	2.4	0
22	Desirability-Based Multi-Objective QSAR in Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2012, 12, 920-935.	2.4	13
23	Jointly Handling Potency and Toxicity of Antimicrobial Peptidomimetics by Simple Rules from Desirability Theory and Chemoinformatics. Journal of Chemical Information and Modeling, 2011, 51, 3060-3077.	5.4	21
24	Prioritizing Hits with Appropriate Tradeâ€Offs Between HIVâ€1 Reverse Transcriptase Inhibitory Efficacy and MT4 Blood Cells Toxicity Through Desirabilityâ€Based Multiobjective Optimization and Ranking. Molecular Informatics, 2010, 29, 303-321.	2.5	19
25	Multidimensional Drug Design: Simultaneous Analysis of Binding and Relative Efficacy Profiles of N⁶â€substitutedâ€4â€²â€thioadenosines A₃ Adenosine Receptor Agonists. Chemical Biology and Drug Design, 2010, 75, 607-618.	3.2	12
26	Global Antifungal Profile Optimization of Chlorophenyl Derivatives against Botrytis cinerea and Colletotrichum gloeosporioides. Journal of Agricultural and Food Chemistry, 2009, 57, 4838-4843.	5.2	10
27	Computational chemistry approach for the early detection of drugâ€induced idiosyncratic liver toxicity. Journal of Computational Chemistry, 2008, 29, 533-549.	3.3	50
28	Desirabilityâ€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, 2445-2459.	3.3	49
29	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.	3.8	27
30	Quantitative Proteomeâ€“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, 9684-9693.	3.0	18
31	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.	3.5	13
32	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.	3.3	46
33	3D-MEDNEs: An Alternative â€œin Silicoâ€•Technique for Chemical Research in Toxicology. 2. Quantitative Proteomeâ€“Toxicity Relationships (QPTR) based on Mass Spectrum Spiral Entropy. Chemical Research in Toxicology, 2008, 21, 619-632.	3.3	42
34	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, 1909-1923.	3.3	79
35	Computational modeling tools for the design of potent antimalarial bisbenzamidines: Overcoming the antimalarial potential of pentamidine. Bioorganic and Medicinal Chemistry, 2007, 15, 5322-5339.	3.0	18
36	Chemometrics for QSAR with low sequence homology: Mycobacterial promoter sequences recognition with 2D-RNA entropies. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 20-26.	3.5	30

#	Article	IF	Citations
37	Simple Stochastic Fingerprints Towards Mathematical Modeling in Biology and Medicine 2. Unifying Markov Model for Drugs Side Effects. Bulletin of Mathematical Biology, 2006, 68, 1527-1554.	1.9	9
38	Simple stochastic fingerprints towards mathematical modeling in biology and medicine. 3. ocular irritability classification model. Bulletin of Mathematical Biology, 2006, 68, 1555-1572.	1.9	14
39	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. Bioorganic and Medicinal Chemistry, 2005, 13, 1119-1129.	3.0	47
40	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, 1651-1657.	2.2	39
41	Unified drugâ€“target interaction thermodynamic Markov model using stochastic entropies to predict multiple drugs side effects. European Journal of Medicinal Chemistry, 2005, 40, 1030-1041.	5.5	26