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	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	6.4	140
2	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
3	Computational chemistry approach for the early detection of drugâ€induced idiosyncratic liver toxicity. Journal of Computational Chemistry, 2008, 29, 533-549.	3.3	50
4	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
5	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
6	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
7	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
8	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
9	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
10	Efficient and biologically relevant consensus strategy for Parkinsonâ€™s disease gene prioritization. BMC Medical Genomics, 2016, 9, 12.	1.5	29
11	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. Drug Discovery Today, 2017, 22, 994-1007.	6.4	28
12	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	6.4	28
13	Evolutionary Computation and QSAR Research. Current Computer-Aided Drug Design, 2013, 9, 206-225.	1.2	28
14	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
15	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
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. BMC Medical Genomics, 2017, 10, 50.	1.5	18
24	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
25	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
26	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
27	Desirability-Based Multi-Objective QSAR in Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2012, 12, 920-935.	2.4	13
28	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
29	Multidimensional Drug Design: Simultaneous Analysis of Binding and Relative Efficacy Profiles of N⁶â€substituted4â€²â€thioadenosines A₃ Adenosine Receptor Agonists. Chemical Biology and Drug Design, 2010, 75, 607-618.	3.2	12
30	Chemoinformatics Profiling of Ionic Liquidsâ€"Uncovering Structure-Cytotoxicity Relationships With Network-like Similarity Graphs. Toxicological Sciences, 2014, 138, 191-204.	3.1	12
31	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
32	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
33	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
34	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
35	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. Current Topics in Medicinal Chemistry, 2019, 19, 957-969.	2.1	8
36	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

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37	Complex Networks and Machine Learning: From Molecular to Social Sciences. Applied Sciences (Switzerland), 2019, 9, 4493.	2.5	5
38	Quantitative Structure-Epigenetic Activity Relationships. Challenges and Advances in Computational Chemistry and Physics, 2017, , 303-338.	0.6	4
39	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
40	Desirability-based Multi-criteria Virtual Screening of Selective Antimicrobial Cyclic Î²-Hairpin Cationic Peptidomimetics. Current Pharmaceutical Design, 2013, 19, 2148-2163.	1.9	2
41	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