

# Maykel Cruz-Monteagudo

## List of Publications by Year in descending order

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41  
papers

1,001  
citations

430442

18  
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454577

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42  
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42  
docs citations

42  
times ranked

1092  
citing authors

#	ARTICLE	IF	CITATIONS
1	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 957-969.	1.0	8
2	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.	2.5	20
3	Complex Networks and Machine Learning: From Molecular to Social Sciences. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 4493.	1.3	5
4	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.	1.1	15
5	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. <i>Drug Discovery Today</i> , 2017, 22, 994-1007.	3.2	28
6	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. <i>Drug Discovery Today</i> , 2017, 22, 1489-1502.	3.2	28
7	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. <i>BMC Medical Genomics</i> , 2017, 10, 50.	0.7	18
8	Quantitative Structure-Epigenetic Activity Relationships. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2017, , 303-338.	0.6	4
9	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.	1.4	11
10	Efficient and biologically relevant consensus strategy for Parkinson's disease gene prioritization. <i>BMC Medical Genomics</i> , 2016, 9, 12.	0.7	29
11	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A <sub>2A</sub> Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. <i>Current Pharmaceutical Design</i> , 2016, 22, 3082-3096.	0.9	13
12	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.	0.9	7
13	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, 2094-2110.	2.5	20
14	Chemoinformatics Profiling of Ionic Liquids—Uncovering Structure-Cytotoxicity Relationships With Network-like Similarity Graphs. <i>Toxicological Sciences</i> , 2014, 138, 191-204.	1.4	12
15	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. <i>Molecular Diversity</i> , 2014, 18, 637-654.	2.1	8
16	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. <i>Drug Discovery Today</i> , 2014, 19, 1069-1080.	3.2	140
17	Chemoinformatics Profiling of Ionic Liquids—Automatic and Chemically Interpretable Cytotoxicity Profiling, Virtual Screening, and Cytotoxicophore Identification. <i>Toxicological Sciences</i> , 2013, 136, 548-565.	1.4	19
18	Desirability-based Multi-criteria Virtual Screening of Selective Antimicrobial Cyclic Î <sup>2</sup> -Hairpin Cationic Peptidomimetics. <i>Current Pharmaceutical Design</i> , 2013, 19, 2148-2163.	0.9	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.	1.0	4
20	Evolutionary Computation and QSAR Research. Current Computer-Aided Drug Design, 2013, 9, 206-225.	0.8	28
21	Editorial[Hot Topic ; Special Issue: Multi-Criteria Approaches in Computer-Aided Drug Discovery]. Mini-Reviews in Medicinal Chemistry, 2012, 12, 905-906.	1.1	0
22	Desirability-Based Multi-Objective QSAR in Drug Discovery. Mini-Reviews in Medicinal Chemistry, 2012, 12, 920-935.	1.1	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.	2.5	21
24	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, 303-321.	1.4	19
25	Multidimensional Drug Design: Simultaneous Analysis of Binding and Relative Efficacy Profiles of N <sup>6</sup> -substituted 4- $\epsilon$ -thioadenosines A <sub>3</sub> Adenosine Receptor Agonists. Chemical Biology and Drug Design, 2010, 75, 607-618.	1.5	12
26	Global Antifungal Profile Optimization of Chlorophenyl Derivatives against <i>Botrytis cinerea</i> and <i>Colletotrichum gloeosporioides</i> . Journal of Agricultural and Food Chemistry, 2009, 57, 4838-4843.	2.4	10
27	Computational chemistry approach for the early detection of drug-induced idiosyncratic liver toxicity. Journal of Computational Chemistry, 2008, 29, 533-549.	1.5	50
28	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, 2445-2459.	1.5	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.	1.8	27
30	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, 9684-9693.	1.4	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.	1.8	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 $\epsilon$ -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, 619-632.	1.7	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.	1.5	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.	1.4	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.	1.8	30

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37	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, 1527-1554.	0.9	9
38	Simple stochastic fingerprints towards mathematical modeling in biology and medicine. 3. ocular irritability classification model. <i>Bulletin of Mathematical Biology</i> , 2006, 68, 1555-1572.	0.9	14
39	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 1119-1129.	1.4	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 1651-1657.	1.0	39
41	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, 1030-1041.	2.6	26