

Maykel Cruz-Monteagudo

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9116709/publications.pdf>

Version: 2024-02-01

41
papers

1,001
citations

430442

18
h-index

454577

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?. <i>Drug Discovery Today</i> , 2014, 19, 1069-1080.	3.2	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. <i>Journal of Computational Chemistry</i> , 2007, 28, 1909-1923.	1.5	79
3	Computational chemistry approach for the early detection of drug-induced idiosyncratic liver toxicity. <i>Journal of Computational Chemistry</i> , 2008, 29, 533-549.	1.5	50
4	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, 2445-2459.	1.5	49
5	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
6	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.	3.3	46
7	3D-MEDNEs: An Alternative α -in Silico α -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, 619-632.	1.7	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 1651-1657.	1.0	39
9	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.	1.8	30
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	Systemic QSAR and phenotypic virtual screening: chasing butterflies in drug discovery. <i>Drug Discovery Today</i> , 2017, 22, 994-1007.	3.2	28
12	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. <i>Drug Discovery Today</i> , 2017, 22, 1489-1502.	3.2	28
13	Evolutionary Computation and QSAR Research. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 206-225.	0.8	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. <i>Polymer</i> , 2008, 49, 5575-5587.	1.8	27
15	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
16	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, 3060-3077.	2.5	21
17	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
18	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

#	ARTICLE	IF	CITATIONS
19	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, 303-321.	1.4	19
20	Cheminformatics 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
21	Computational modeling tools for the design of potent antimalarial bisbenzamidines: Overcoming the antimalarial potential of pentamidine. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 5322-5339.	1.4	18
22	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, 9684-9693.	1.4	18
23	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. <i>BMC Medical Genomics</i> , 2017, 10, 50.	0.7	18
24	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
25	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
26	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.	1.8	13
27	Desirability-Based Multi-Objective QSAR in Drug Discovery. <i>Mini-Reviews in Medicinal Chemistry</i> , 2012, 12, 920-935.	1.1	13
28	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A _{2A} Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. <i>Current Pharmaceutical Design</i> , 2016, 22, 3082-3096.	0.9	13
29	Multidimensional Drug Design: Simultaneous Analysis of Binding and Relative Efficacy Profiles of N ⁶ -substituted- ϵ -thioadenosines A ₃ Adenosine Receptor Agonists. <i>Chemical Biology and Drug Design</i> , 2010, 75, 607-618.	1.5	12
30	Cheminformatics Profiling of Ionic Liquids—Uncovering Structure-Cytotoxicity Relationships With Network-like Similarity Graphs. <i>Toxicological Sciences</i> , 2014, 138, 191-204.	1.4	12
31	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
32	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, 4838-4843.	2.4	10
33	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
34	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
35	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 957-969.	1.0	8
36	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

#	ARTICLE	IF	CITATIONS
37	Complex Networks and Machine Learning: From Molecular to Social Sciences. Applied Sciences (Switzerland), 2019, 9, 4493.	1.3	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.	1.0	4
40	Desirability-based Multi-criteria Virtual Screening of Selective Antimicrobial Cyclic Î²-Hairpin Cationic Peptidomimetics. Current Pharmaceutical Design, 2013, 19, 2148-2163.	0.9	2
41	Editorial[Hot Topic ; Special Issue: Multi-Criteria Approaches in Computer-Aided Drug Discovery]. Mini-Reviews in Medicinal Chemistry, 2012, 12, 905-906.	1.1	0