Miguel-Ãngel Cabrera-PÃ©rez

List of Publications by Year
in descending order

56 papers	1,678 citations	236612 25 h-index	288905 40 g-index
57 all docs	57 docs citations	57 times ranked	1391 citing authors

#	Article	IF	Citations
1	TOPS-MODE Based QSARs Derived from Heterogeneous Series of Compounds. Applications to the Design of New Herbicides. Journal of Chemical Information and Computer Sciences, 2003, 43, 1192-1199.	2.8	89
2	3D-MEDNEs:â€‰ An Alternative â€œIn Silicoâ€•Technique for Chemical Research in Toxicology. 1. Prediction of Chemically Induced Agranulocytosis. Chemical Research in Toxicology, 2003, 16, 1318-1327.	1.7	88
3	Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer-aided molecular design I: discovery of anticancer compounds. Journal of Molecular Modeling, 2003, 9, 395-407.	0.8	87
4	Provisional Classification and in Silico Study of Biopharmaceutical System Based on Caco-2 Cell Permeability and Dose Number. Molecular Pharmaceutics, 2013, 10, 2445-2461.	2.3	78
5	In Silico Prediction of Cacoâ€2 Cell Permeability by a Classification QSAR Approach. Molecular Informatics, 2011, 30, 376-385.	1.4	76
6	Application of the replacement method as a novel variable selection strategy in QSAR. 1. Carcinogenic potential. Chemometrics and Intelligent Laboratory Systems, 2006, 81, 180-187.	1.8	61
7	A topological sub-structural approach for predicting human intestinal absorption of drugs. European Journal of Medicinal Chemistry, 2004, 39, 905-916.	2.6	60
8	A topological substructural approach applied to the computational prediction of rodent carcinogenicity. Bioorganic and Medicinal Chemistry, 2005, 13, 2477-2488.	1.4	60
9	Quantitative structure carcinogenicity relationship for detecting structural alerts in nitroso-compounds. Toxicology and Applied Pharmacology, 2007, 221, 189-202.	1.3	59
10	Total and Local Quadratic Indices of the â€œMolecular Pseudographâ€™s Atom Adjacency Matrixâ€• Application to Prediction of Caco-2 Permeability of Drugs. International Journal of Molecular Sciences, 2003, 4, 512-536.	1.8	55
11	Quantitative structure activity relationship for the computational prediction of nitrocompounds carcinogenicity. Toxicology, 2006, 220, 51-62.	2.0	54
12	A topological substructural approach for the prediction of P-glycoprotein substrates. Journal of Pharmaceutical Sciences, 2006, 95, 589-606.	1.6	53
13	A novel approach to determining physicochemical and absorption properties of 6-fluoroquinolone derivatives: experimental assessment. European Journal of Pharmaceutics and Biopharmaceutics, 2002, 53, 317-325.	2.0	45
14	Unified Markov thermodynamics based on stochastic forms to classify drugs considering molecular structure, partition system, and biological species:. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 551-557.	1.0	45
15	A novel approach to predict a toxicological property of aromatic compounds in the Tetrahymena pyriformis. Bioorganic and Medicinal Chemistry, 2004, 12, 735-744.	1.4	44
16	Quantitative Structureâ^'Carcinogenicity Relationship for Detecting Structural Alerts in Nitroso Compounds: Species, Rat; Sex, Female; Route of Administration, Gavage. Chemical Research in Toxicology, 2008, 21, 633-642.	1.7	42
17	The Use of Ruleâ€Based and QSPR Approaches in ADME Profiling: A Case Study on Cacoâ€2 Permeability. Molecular Informatics, 2013, 32, 459-479.	1.4	42
18	TOPSâ€MODE Approach for the Prediction of Bloodâ€“Brain Barrier Permeation. Journal of Pharmaceutical Sciences, 2004, 93, 1701-1717.	1.6	40

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19	Exploring the conformational changes of the ATP binding site of gyrase B from Escherichia coli complexed with different established inhibitors by using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2011, 29, 726-739.	1.3	40
20	Computational modeling of human oral bioavailability: what will be next?. Expert Opinion on Drug Discovery, 2018, 13, 509-521.	2.5	39
21	In Silico Assessment of ADME Properties: Advances in Caco-2 Cell Monolayer Permeability Modeling. Current Topics in Medicinal Chemistry, 2019, 18, 2209-2229.	1.0	38
22	A radial-distribution-function approach for predicting rodent carcinogenicity. Journal of Molecular Modeling, 2006, 12, 769-780.	0.8	33
23	Quantitative structure carcinogenicity relationship for detecting structural alerts in nitroso-compoundsâ˜†Species: Rat; Sex: Male; Route of administration: Water. Toxicology and Applied Pharmacology, 2008, 231, 197-207.	1.3	33
24	Quantitative structureâ€“activity relationship to predict toxicological properties of benzene derivative compounds. Bioorganic and Medicinal Chemistry, 2005, 13, 1775-1781.	1.4	31
25	ADME Prediction with KNIME: Development and Validation of a Publicly Available Workflow for the Prediction of Human Oral Bioavailability. Journal of Chemical Information and Modeling, 2020, 60, 2660-2667.	2.5	31
26	GA(M)E-QSAR: A Novel, Fully Automatic Genetic-Algorithm-(Meta)-Ensembles Approach for Binary Classification in Ligand-Based Drug Design. Journal of Chemical Information and Modeling, 2012, 52, 2366-2386.	2.5	23
27	QSAR modeling of the rodent carcinogenicity of nitrocompounds. Bioorganic and Medicinal Chemistry, 2008, 16, 3395-3407.	1.4	22
28	In silico prediction of central nervous system activity of compounds. Identification of potential pharmacophores by the TOPSâ€“MODE approach. Bioorganic and Medicinal Chemistry, 2004, 12, 5833-5843.	1.4	21
29	FDA-approved Drugs Selected Using Virtual Screening Bind Specifically to G-quadruplex DNA. Current Pharmaceutical Design, 2013, 19, 2164-2173.	0.9	21
30	The Prediction of Carcinogenicity from Molecular Structure. Current Computer-Aided Drug Design, 2005, 1, 237-255.	0.8	21
31	QSPR in Oral Bioavailability: Specificity or Integrality?. Mini-Reviews in Medicinal Chemistry, 2012, 12, 534-550.	1.1	20
32	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.	2.5	20
33	Biowaiver or Bioequivalence: Ambiguity in Sildenafil Citrate BCS Classification. AAPS PharmSciTech, 2018, 19, 1693-1698.	1.5	20
34	Bacterial β-Ketoacyl-Acyl Carrier Protein Synthase III (FabH): An Attractive Target for the Design of New Broad-Spectrum Antimicrobial Agents. Mini-Reviews in Medicinal Chemistry, 2008, 8, 36-45.	1.1	18
35	Molecular dynamics and docking simulations as a proof of high flexibility in E. coli FabH and its relevance for accurate inhibitor modeling. Journal of Computer-Aided Molecular Design, 2011, 25, 371-393.	1.3	17
36	A topological-substructural molecular design (TOPS-MODE) approach to determining pharmacokinetics and pharmacological properties of 6-fluoroquinolone derivatives. European Journal of Pharmaceutics and Biopharmaceutics, 2003, 56, 197-206.	2.0	16

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37	Integrating theoretical and experimental permeability estimations for provisional biopharmaceutical classification: Application to the WHO essential medicines. Biopharmaceutics and Drug Disposition, 2018, 39, 354-368.	1.1	15
38	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
39	Combining molecular docking and QSAR studies for modelling the antigyrase activity of cyclothialidine derivatives. European Journal of Medicinal Chemistry, 2011, 46, 2736-2747.	2.6	13
40	Prediction of telomerase inhibitory activity for acridinic derivatives based on chemical structure. European Journal of Medicinal Chemistry, 2009, 44, 4826-4840.	2.6	11
41	Exploring different strategies for imbalanced ADME data problem: case study on Caco-2 permeability modeling. Molecular Diversity, 2016, 20, 93-109.	2.1	11
42	ADME Prediction with KNIME: In silico aqueous solubility models based on supervised recursive machine learning approaches. ADMET and DMPK, 2020, 8, 251-273.	1.1	11
43	Importance and applications of cell- and tissue-based in vitro models for drug permeability screening in early stages of drug development. , 2016, , 3-29.		10
44	The efficacy of 2-nitrovinylfuran derivatives againstLeishmania in vitro and in vivo. Memorias Do Instituto Oswaldo Cruz, 2015, 110, 166-173.	0.8	9
45	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. Molecular Diversity, 2014, 18, 637-654.	2.1	8
46	A Novel Automated Framework for QSAR Modeling of Highly Imbalanced Leishmania High-Throughput Screening Data. Journal of Chemical Information and Modeling, 2021, 61, 3213-3231.	2.5	8
47	Computational Tools in the Discovery of New G-Quadruplex Ligands with Potential Anticancer Activity. Current Topics in Medicinal Chemistry, 2013, 12, 2843-2856.	1.0	7
48	Telomerase Inhibitory Activity of Acridinic Derivatives: A 3Dâ€QSAR Approach. QSAR and Combinatorial Science, 2009, 28, 526-536.	1.5	5
49	Thermodynamic computational approach to capture molecular recognition in the binding of different inhibitors to the DNA gyrase B subunit from Escherichia coli. Journal of Molecular Modeling, 2013, 19, 3187-3200.	0.8	3
50	Policy of Multisource Drug Products in Latin America: Opportunities and Challenges on the Application of Bioequivalence In Vitro Assays. Therapeutic Innovation and Regulatory Science, 2021, 55, 65-81.	0.8	3
51	ADME prediction with KNIME: A retrospective contribution to the second â€œSolubility Challengeâ€. ADMET and DMPK, 2021, 9, 209-218.	1.1	3
52	Bacterial FabH: Towards the Discovery of New Broad-Spectrum Antibiotics. , 2014, , 131-158.		1
53	ICH Guideline for Biopharmaceutics Classification System-Based Biowaiver (M9): Toward Harmonization in Latin American Countries. Pharmaceutics, 2021, 13, 363.	2.0	1
54	QSAR modeling for predicting carcinogenic potency of nitroso-compounds using 0D-2D molecular descriptors. , 0, , .		1

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55	Bacterial FabH: Towards the Discovery of New Broad-Spectrum Antibiotics. , 2014, , 131-158.		0
56	Integration of In Silico, In Vitro and In Situ Tools for the Preformulation and Characterization of a Novel Cardio-Neuroprotective Compound during the Early Stages of Drug Development. Pharmaceutics, 2022, 14, 182.	2.0	0