Juan A Castillo-Garit

List of Publications by Year
in descending order

50 papers	1,227 citations	331259 21 h-index	377514 34 g-index
50 all docs	50 docs citations	50 times ranked	799 citing authors

#	Article	IF	Citations
1	Atom, atom-type and total molecular linear indices as a promising approach for bioorganic and medicinal chemistry: theoretical and experimental assessment of a novel method for virtual screening and rational design of new lead anthelmintic. Bioorganic and Medicinal Chemistry, 2005, 13, 1005-1020.	1.4	97
2	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
3	Estimation of ADME Properties in Drug Discovery: Predicting Caco-2 Cell Permeability Using Atom-Based Stochastic and Non-stochastic Linear Indices. Journal of Pharmaceutical Sciences, 2008, 97, 1946-1976.	1.6	72
4	Protein linear indices of the â€˜macromolecular pseudograph Î±-carbon atom adjacency matrixâ€™ in bioinformatics. Part 1: Prediction of protein stability effects of a complete set of alanine substitutions in Arc repressor. Bioorganic and Medicinal Chemistry, 2005, 13, 3003-3015.	1.4	70
5	Atom, Atom-Type, and Total Linear Indices of the â€œMolecular Pseudographâ€™s Atom Adjacency Matrixâ€: Application to QSPR/QSAR Studies of Organic Compounds. Molecules, 2004, 9, 1100-1123.	1.7	64
6	Tomocomd-Cardd, a novel approach for computer-aided ? rational? drug design: I. Theoretical and experimental assessment of a promising method for computational screening and in silico design of new anthelmintic compounds. Journal of Computer-Aided Molecular Design, 2004, 18, 615-634.	1.3	62
7	Predicting antitrichomonal activity: A computational screening using atom-based bilinear indices and experimental proofs. Bioorganic and Medicinal Chemistry, 2006, 14, 6502-6524.	1.4	53
8	A novel approach to predict aquatic toxicity from molecular structure. Chemosphere, 2008, 73, 415-427.	4.2	50
9	Atom-based stochastic and non-stochastic 3D-chiral bilinear indices and their applications to central chirality codification. Journal of Molecular Graphics and Modelling, 2007, 26, 32-47.	1.3	45
10	Linear indices of the â€˜macromolecular graphâ€™s nucleotides adjacency matrixâ€™ as a promising approach for bioinformatics studies. Part 1: Prediction of paromomycinâ€™s affinity constant with HIV-1 Î¨-RNA packaging region. Bioorganic and Medicinal Chemistry, 2005, 13, 3397-3404.	1.4	44
11	Tyrosinase Enzyme: 1. An Overview on a Pharmacological Target. Current Topics in Medicinal Chemistry, 2014, 14, 1494-1501.	1.0	38
12	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
13	3D-chiral Atom, Atom-type, and Total Non-stochastic and Stochastic Molecular Linear Indices and their Applications to Central Chirality Codification. Journal of Computer-Aided Molecular Design, 2005, 19, 369-383.	1.3	35
14	Atom-based 3D-chiral quadratic indices. Part 2: Prediction of the corticosteroid-binding globulinbinding affinity of the 31 benchmark steroids data set. Bioorganic and Medicinal Chemistry, 2006, 14, 2398-2408.	1.4	34
15	Prediction of acute toxicity of phenol derivatives using multiple linear regression approach for Tetrahymena pyriformis contaminant identification in a median-size database. Chemosphere, 2016, 165, 434-441.	4.2	28
16	A Review of QSAR studies to Discover New Drug-like Compounds Actives Against Leishmaniasis and Trypanosomiasis. Current Topics in Medicinal Chemistry, 2012, 12, 852-865.	1.0	27
17	Bondâ€based 3Dâ€chiral linear indices: Theory and QSAR applications to central chirality codification. Journal of Computational Chemistry, 2008, 29, 2500-2512.	1.5	26
18	Computational discovery of novel trypanosomicidal drug-like chemicals by using bond-based non-stochastic and stochastic quadratic maps and linear discriminant analysis. European Journal of Pharmaceutical Sciences, 2010, 39, 30-36.	1.9	26

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19	A Simple Method to Predict Blood-Brain Barrier Permeability of Drug- Like Compounds Using Classification Trees. Medicinal Chemistry, 2017, 13, 664-669.	0.7	25
20	3D-chiral (2.5) atom-based TOMOCOMD-CARDD descriptors: theory and QSAR applications to central chirality codification. Journal of Mathematical Chemistry, 2008, 44, 755-786.	0.7	23
21	Atom-based non-stochastic and stochastic bilinear indices: Application to QSPR/QSAR studies of organic compounds. Chemical Physics Letters, 2008, 464, 107-112.	1.2	23
22	Ligand-based discovery of novel trypanosomicidal drug-like compounds: In silico identification and experimental support. European Journal of Medicinal Chemistry, 2011, 46, 3324-3330.	2.6	19
23	Comparative study to predict toxic modes of action of phenols from molecular structures. SAR and QSAR in Environmental Research, 2013, 24, 235-251.	1.0	19
24	An approach to identify new antihypertensive agents using Thermolysin as model: In silico study based on QSARINS and docking. Arabian Journal of Chemistry, 2019, 12, 4861-4877.	2.3	19
25	Bond-based bilinear indices for computational discovery of novel trypanosomicidal drug-like compounds through virtual screening. European Journal of Medicinal Chemistry, 2015, 96, 238-244.	2.6	16
26	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. Journal of the Brazilian Chemical Society, 2015, , .	0.6	16
27	Bond-based linear indices of the non-stochastic and stochastic edge-adjacency matrix. 1. Theory and modeling of ChemPhys properties of organic molecules. Molecular Diversity, 2010, 14, 731-753.	2.1	15
28	Identification In Silico and In Vitro of Novel Trypanosomicidal Drugâ€Like Compounds. Chemical Biology and Drug Design, 2012, 80, 38-45.	1.5	14
29	Machine learning-based models to predict modes of toxic action of phenols to Tetrahymena pyriformis. SAR and QSAR in Environmental Research, 2017, 28, 735-747.	1.0	14
30	Discrete Fourier Transform-Based Multivariate Image Analysis: Application to Modeling of Aromatase Inhibitory Activity. ACS Combinatorial Science, 2018, 20, 75-81.	3.8	14
31	Computational Identification of Chemical Compounds with Potential Activity against Leishmania amazonensis using Nonlinear Machine Learning Techniques. Current Topics in Medicinal Chemistry, 2019, 18, 2347-2354.	1.0	12
32	Applications of Bondâ€Based 3Dâ€Chiral Quadratic Indices in QSAR Studies Related to Central Chirality Codification. QSAR and Combinatorial Science, 2009, 28, 1465-1477.	1.5	11
33	Prediction of aquatic toxicity of benzene derivatives using molecular descriptor from atomic weighted vectors. Environmental Toxicology and Pharmacology, 2017, 56, 314-321.	2.0	11
34	Prediction of Aquatic Toxicity of Benzene Derivatives to Tetrahymena pyriformis According to OECD Principles. Current Pharmaceutical Design, 2016, 22, 5085-5094.	0.9	10
35	Prediction of Caco-2 Cell Permeability Using Bilinear Indices and Multiple Linear Regression. Letters in Drug Design and Discovery, 2015, 13, 161-169.	0.4	9
36	State of the Art Review and Report of New Tool for Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2957-2976.	1.0	8

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37	Larvicidal activity prediction against mosquito using computational tools. Journal of Vector Borne Diseases, 2017, 54, 164-171.	0.1	8
38	Analysis of Proteasome Inhibition Prediction Using Atom-Based Quadratic Indices Enhanced by Machine Learning Classification Techniques. Letters in Drug Design and Discovery, 2014, 11, 705-711.	0.4	7
39	Undersampling: case studies of flaviviral inhibitory activities. Journal of Computer-Aided Molecular Design, 2019, 33, 997-1008.	1.3	6
40	Thorough evaluation of OECD principles in modelling of 1-[(2-hydroxyethoxy)methyl]-6-(phenylthio)thymine derivatives using QSARINS. SAR and QSAR in Environmental Research, 2020, 31, 741-759.	1.0	6
41	Learning from Multiple Classifier Systems: Perspectives for Improving Decision Making of QSAR Models in Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2018, 17, 3269-3288.	1.0	5
42	Evolutionary algorithm-based generation of optimum peptide sequences with dengue virus inhibitory activity. Future Medicinal Chemistry, 2021, 13, 993-1000.	1.1	4
43	Ligand-based discovery of new potential acetylcholinesterase inhibitors for Alzheimerâ€™s disease treatment. SAR and QSAR in Environmental Research, 2022, 33, 49-61.	1.0	4
44	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. Molecular Diversity, 2022, 26, 1383-1397.	2.1	3
45	Computational identification of chemical compounds with potential anti-Chagas activity using a classification tree. SAR and QSAR in Environmental Research, 2021, 32, 71-83.	1.0	3
46	A Review of Computational Approaches Targeting SARS-CoV-2 Main Protease to the Discovery of New Potential Antiviral Compounds. Current Topics in Medicinal Chemistry, 2023, 23, 3-16.	1.0	3
47	Dry selection and wet evaluation for the rational discovery of new anthelmintics. Molecular Physics, 2017, 115, 2300-2313.	0.8	2
48	Atom based linear index descriptors in QSAR-machine learning classifiers for the prediction of ubiquitin-proteasome pathway activity. Medicinal Chemistry Research, 2018, 27, 695-704.	1.1	1
49	Computational approach to the discovery of potential neprilysin inhibitors compounds for cardiovascular diseases treatment. Medicinal Chemistry Research, 2020, 29, 897-909.	1.1	1
50	Computational Modeling of Aldose Reductase Inhibitory Activity of Flavonoids Derivatives for Diabetic Complications Treatment. Letters in Drug Design and Discovery, 2021, 18, .	0.4	0