Gerardo M CasaÃ±ola-MartÃ-n

List of Publications by Year
in descending order

37 papers	772 citations	516561 16 h-index	526166 27 g-index
37 all docs	37 docs citations	37 times ranked	588 citing authors

#	Article	IF	Citations
1	Machine Learning Study of Metabolic NetworksvsChEMBL Data of Antibacterial Compounds. Molecular Pharmaceutics, 2022, 19, 2151-2163.	2.3	3
2	Machine Learning Applications in Nanomedicine and Nanotoxicology. , 2022, , 38-45.		1
3	Predicting Metabolic Reaction Networks with Perturbation-Theory Machine Learning (PTML) Models. Current Topics in Medicinal Chemistry, 2021, 21, 819-827.	1.0	10
4	Beyond model interpretability using <scp>LDA</scp> and decision trees for Î±â€amylase and Î±â€glucosidase inhibitor classification studies. Chemical Biology and Drug Design, 2019, 94, 1414-1421.	1.5	11
5	Machine Learning Applications in Nanomedicine and Nanotoxicology. International Journal of Applied Nanotechnology Research, 2019, 4, 1-7.	1.1	3
6	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
7	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
8	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
9	Carbon Nanotubesâ€™ Effect on Mitochondrial Oxygen Flux Dynamics: Polarography Experimental Study and Machine Learning Models using Star Graph Trace Invariants of Raman Spectra. Nanomaterials, 2017, 7, 386.	1.9	14
10	A Two QSAR Way for Antidiabetic Agents Targeting Using Î±-Amylase and Î±-Glucosidase Inhibitors: Model Parameters Settings in Artificial Intelligence Techniques. Letters in Drug Design and Discovery, 2017, 14, .	0.4	13
11	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
12	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
13	Prediction of Aquatic Toxicity of Benzene Derivatives to Tetrahymena pyriformis According to OECD Principles. Current Pharmaceutical Design, 2016, 22, 5085-5094.	0.9	10
14	Multi-output model with Boxâ€“Jenkins operators of linear indices to predict multi-target inhibitors of ubiquitinâ€“proteasome pathway. Molecular Diversity, 2015, 19, 347-356.	2.1	25
15	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
16	A Rational Workflow for Sequential Virtual Screening of Chemical Libraries on Searching for New Tyrosinase Inhibitors. Current Topics in Medicinal Chemistry, 2014, 14, 1473-1485.	1.0	8
17	Tyrosinase Enzyme: 1. An Overview on a Pharmacological Target. Current Topics in Medicinal Chemistry, 2014, 14, 1494-1501.	1.0	38
18	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

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19	Retrained Classification of Tyrosinase Inhibitors and â€œIn Silicoâ€•Potency Estimation by Using Atom-Type Linear Indices. International Journal of Chemoinformatics and Chemical Engineering, 2012, 2, 42-144.	0.1	0
20	QSAR-Based CMs and TOMOCOMD-CARD Approach for the Discovery of New Tyrosinase Inhibitor Chemicals. , 2012, , 298-341.		1
21	Vanilloid Derivatives as Tyrosinase Inhibitors Driven by Virtual Screeningâ€Based QSAR Models. Drug Testing and Analysis, 2011, 3, 176-181.	1.6	26
22	Novel coumarin-based tyrosinase inhibitors discovered by OECD principles-validated QSAR approach from an enlarged, balanced database. Molecular Diversity, 2011, 15, 507-520.	2.1	22
23	Bondâ€extended stochastic and nonstochastic bilinear indices. I. QSPR/QSAR applications to the description of properties/activities of smallâ€medium size organic compounds. International Journal of Quantum Chemistry, 2011, 111, 8-34.	1.0	2
24	A Comparative Study of Nonlinear Machine Learning for the â€œIn Silicoâ€•Depiction of Tyrosinase Inhibitory Activity from Molecular Structure. Molecular Informatics, 2011, 30, 527-537.	1.4	9
25	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
26	QSAR models for tyrosinase inhibitory activity description applying modern statistical classification techniques: A comparative study. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 249-259.	1.8	7
27	Bondâ€Based 2D Quadratic Fingerprints in QSAR Studies: Virtual and In vitro Tyrosinase Inhibitory Activity Elucidation. Chemical Biology and Drug Design, 2010, 76, 538-545.	1.5	41
28	Ligand-Based Computer-Aided Discovery of Tyrosinase Inhibitors. Applications of the TOMOCOMD-CARDD Method to the Elucidation of New Compounds. Current Pharmaceutical Design, 2010, 16, 2601-2624.	0.9	42
29	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
30	Atom- and Bond-Based 2D TOMOCOMD-CARDD Approach and Ligand-Based Virtual Screening for the Drug Discovery of New Tyrosinase Inhibitors. Journal of Biomolecular Screening, 2008, 13, 1014-1024.	2.6	32
31	Prediction of Tyrosinase Inhibition Activity Using Atom-Based Bilinear Indices. ChemMedChem, 2007, 2, 449-478.	1.6	52
32	TOMOCOMD-CARDD descriptors-based virtual screening of tyrosinase inhibitors: Evaluation of different classification model combinations using bond-based linear indices. Bioorganic and Medicinal Chemistry, 2007, 15, 1483-1503.	1.4	85
33	Dragon method for finding novel tyrosinase inhibitors: Biosilico identification and experimental in vitro assays. European Journal of Medicinal Chemistry, 2007, 42, 1370-1381.	2.6	64
34	Atom-Based 2D Quadratic Indices in Drug Discovery of Novel Tyrosinase Inhibitors: Results ofIn Silico Studies Supported by Experimental Results. QSAR and Combinatorial Science, 2007, 26, 469-487.	1.5	12
35	Bond-based 2D TOMOCOMD-CARDD approach for drug discovery: aiding decision-making in â€˜in silicoâ€™ selection of new lead tyrosinase inhibitors. Journal of Computer-Aided Molecular Design, 2007, 21, 167-188.	1.3	26
36	New tyrosinase inhibitors selected by atomic linear indices-based classification models. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 324-330.	1.0	57

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37	Retrained Classification of Tyrosinase Inhibitors and â€œIn Silicoâ€•Potency Estimation by Using Atom-Type Linear Indices. , 0, , 322-427.		0