Yovani Marrero-Ponce

List of Publications by Year
in descending order

165 papers	4,000 citations	108046 37 h-index	198040 52 g-index
171 all docs	171 docs citations	171 times ranked	2244 citing authors

#	Article	IF	Citations
1	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. Molecular Diversity, 2022, 26, 1383-1397.	2.1	3
2	A Novel Network Science and Similarity-Searching-Based Approach for Discovering Potential Tumor-Homing Peptides from Antimicrobials. Antibiotics, 2022, 11, 401.	1.5	6
3	Emerging Computational Approaches for Antimicrobial Peptide Discovery. Antibiotics, 2022, 11, 936.	1.5	12
4	The minimal and the optimal size for two different types of encapsulated replicator systems. Chinese Journal of Physics, 2021, 71, 397-402.	2.0	1
5	LEGO-based generalized set of two linear algebraic 3D bio-macro-molecular descriptors: Theory and validation by QSARs. Journal of Theoretical Biology, 2020, 485, 110039.	0.8	7
6	Smoothed Spherical Truncation based on Fuzzy Membership Functions: Application to the Molecular Encoding. Journal of Computational Chemistry, 2020, 41, 203-217.	1.5	4
7	MuLiMs-MCoMPAs: A Novel Multiplatform Framework to Compute Tensor Algebra-Based Three-Dimensional Protein Descriptors. Journal of Chemical Information and Modeling, 2020, 60, 1042-1059.	2.5	7
8	When global and local molecular descriptors are more than the sum of its parts: Simple, But Not Simpler?. Molecular Diversity, 2020, 24, 913-932.	2.1	10
9	Automatic construction of molecular similarity networks for visual graph mining in chemical space of bioactive peptides: an unsupervised learning approach. Scientific Reports, 2020, 10, 18074.	1.6	29
10	Ensemble Models Based on QuBiLS-MAS Features and Shallow Learning for the Prediction of Drug-Induced Liver Toxicity: Improving Deep Learning and Traditional Approaches. Chemical Research in Toxicology, 2020, 33, 1855-1873.	1.7	26
11	Distributed and multicore QuBiLSâ€MIDAS software v2.0: Computing chiral, fuzzy, weighted and truncated geometrical molecular descriptors based on tensor algebra. Journal of Computational Chemistry, 2020, 41, 1209-1227.	1.5	9
12	Tensor Algebra-based Geometrical (3D) Biomacro-Molecular Descriptors for Protein Research: Theory, Applications and Comparison with other Methods. Scientific Reports, 2019, 9, 11391.	1.6	7
13	Enhancing Acute Oral Toxicity Predictions by using Consensus Modeling and Algebraic Form-Based 0D-to-2D Molecular Encodes. Chemical Research in Toxicology, 2019, 32, 1178-1192.	1.7	19
14	Graph-based data integration from bioactive peptide databases of pharmaceutical interest: toward an organized collection enabling visual network analysis. Bioinformatics, 2019, 35, 4739-4747.	1.8	39
15	Higher-Order and Mixed Discrete Derivatives such as a Novel Graph- Theoretical Invariant for Generating New Molecular Descriptors. Current Topics in Medicinal Chemistry, 2019, 19, 944-956.	1.0	2
16	Integration of algebra and chemistry concepts with molecular descriptors: A problem-based-learning exercise. Educacion Quimica, 2019, 30, 14.	0.1	0
17	Drug repositioning for novel antitrichomonas from known antiprotozoan drugs using hierarchical screening. Future Medicinal Chemistry, 2018, 10, 863-878.	1.1	7
18	QSRR prediction of gas chromatography retention indices of essential oil components. Chemical Papers, 2018, 72, 57-69.	1.0	16

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19	Choquet integral-based fuzzy molecular characterizations: when global definitions are computed from the dependency among atom/bond contributions (LOVIs/LOEIs). Journal of Cheminformatics, 2018, 10, 51.	2.8	7
20	GOWAWA Aggregation Operatorâ€based Global Molecular Characterizations: Weighting Atom/bond Contributions (LOVIs/LOEIs) According to their Influence in the Molecular Encoding. Molecular Informatics, 2018, 37, e1800039.	1.4	10
21	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
22	Anti-Inflammatory Activity and Cheminformatics Analysis of New Poten t 2-Substituted 1-Methyl-5-Nitroindazolinones. Current Topics in Medicinal Chemistry, 2018, 17, 3236-3248.	1.0	1
23	Conformation-dependent QSAR approach for the prediction of inhibitory activity of bromodomain modulators. SAR and QSAR in Environmental Research, 2017, 28, 41-58.	1.0	18
24	QuBiLS-MAS, open source multi-platform software for atom- and bond-based topological (2D) and chiral (2.5D) algebraic molecular descriptors computations. Journal of Cheminformatics, 2017, 9, 35.	2.8	56
25	Exploring the QSARâ€™s predictive truthfulness of the novel N-tuple discrete derivative indices on benchmark datasets. SAR and QSAR in Environmental Research, 2017, 28, 367-389.	1.0	6
26	Discovering key residues of dengue virus NS2b-NS3-protease: New binding sites for antiviral inhibitors design. Biochemical and Biophysical Research Communications, 2017, 492, 631-642.	1.0	12
27	Dry selection and wet evaluation for the rational discovery of new anthelmintics. Molecular Physics, 2017, 115, 2300-2313.	0.8	2
28	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
29	Tensor algebra-based geometric methodology to codify central chirality on organic molecules. SAR and QSAR in Environmental Research, 2017, 28, 541-556.	1.0	3
30	Novel â€œextended sequonsâ€•of human N-glycosylation sites improve the precision of qualitative predictions: an alignment-free study of pattern recognition using ProtDCal protein features. Amino Acids, 2017, 49, 317-325.	1.2	10
31	Fishing Anti-Inflammatories from Known Drugs: In Silico Repurposing, Design, Synthesis and Biological Evaluation of Bisacodyl Analogues. Current Topics in Medicinal Chemistry, 2017, 17, .	1.0	5
32	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
33	QSPR/QSAR Studies of 2-Furylethylenes Using Bond-Level Quadratic Indices and Comparison with Other Computational Approaches. Journal of the Mexican Chemical Society, 2017, 57, .	0.2	0
34	Physico-Chemical and Structural Interpretation of Discrete Derivative Indices on N-Tuples Atoms. International Journal of Molecular Sciences, 2016, 17, 812.	1.8	7
35	N-tuple topological/geometric cutoffs for 3D N-linear algebraic molecular codifications: variability, linear independence and QSAR analysis. SAR and QSAR in Environmental Research, 2016, 27, 949-975.	1.0	11
36	Orthotropic Piezoelectricity in 2D Nanocellulose. Scientific Reports, 2016, 6, 34616.	1.6	32

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37	Examining the predictive accuracy of the novel 3D N-linear algebraic molecular codifications on benchmark datasets. Journal of Cheminformatics, 2016, 8, 10.	2.8	17
38	A new type of quinoxalinone derivatives affects viability, invasion, and intracellular growth of Toxoplasma gondii tachyzoites in vitro. Parasitology Research, 2016, 115, 2081-2096.	0.6	11
39	Relational Agreement Measures for Similarity Searching of Cheminformatic Data Sets. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2016, 13, 158-167.	1.9	6
40	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. Current Pharmaceutical Design, 2016, 22, 5095-5113.	0.9	4
41	Multi-output Model with Box-Jenkins Operators of Quadratic Indices for Prediction of Malaria and Cancer Inhibitors Targeting Ubiquitin- Proteasome Pathway (UPP) Proteins. Current Protein and Peptide Science, 2016, 17, 220-227.	0.7	14
42	Digital Communication and Chemical Structure Codification. , 2016, , 1-28.		0
43	Structural and Physicochemical Interpretation of GT-STAF Information Theory-Based Indices. Bulletin of the Chemical Society of Japan, 2015, 88, 97-109.	2.0	6
44	Towards Better BBB Passage Prediction Using an Extensive and Curated Data Set. Molecular Informatics, 2015, 34, 308-330.	1.4	33
45	Computational fishing of new DNA methyltransferase inhibitors from natural products. Journal of Molecular Graphics and Modelling, 2015, 60, 43-54.	1.3	25
46	Novel 3D bio-macromolecular bilinear descriptors for protein science: Predicting protein structural classes. Journal of Theoretical Biology, 2015, 374, 125-137.	0.8	20
47	Multiâ€Server Approach for Highâ€Throughput Molecular Descriptors Calculation based on Multiâ€Linear Algebraic Maps. Molecular Informatics, 2015, 34, 60-69.	1.4	13
48	IMMAN: free software for information theory-based chemometric analysis. Molecular Diversity, 2015, 19, 305-319.	2.1	44
49	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
50	Novel global and local 3D atom-based linear descriptors of the Minkowski distance matrix: theory, diversityâ€“variability analysis and QSPR applications. Journal of Mathematical Chemistry, 2015, 53, 2028-2064.	0.7	9
51	ProtDCal: A program to compute general-purpose-numerical descriptors for sequences and 3D-structures of proteins. BMC Bioinformatics, 2015, 16, 162.	1.2	58
52	Overlap and diversity in antimicrobial peptide databases: compiling a non-redundant set of sequences. Bioinformatics, 2015, 31, 2553-2559.	1.8	42
53	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
54	QuBiLs-MAS method in early drug discovery and rational drug identification of antifungal agents. SAR and QSAR in Environmental Research, 2015, 26, 943-958.	1.0	27

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55	A Hookeׂ³s law-based approach to protein folding rate. Journal of Theoretical Biology, 2015, 364, 407-417.	0.8	9
56	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
57	Optimum Search Strategies or Novel 3D Molecular Descriptors: is there a Stalemate?. Current Bioinformatics, 2015, 10, 533-564.	0.7	15
58	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. Journal of the Brazilian Chemical Society, 2015, , .	0.6	16
59	Digital Communication and Chemical Structure Codification. , 2015, , 1-28.		0
60	Multi-Criteria Decision Making: the Best Choice for the Modeling of Chemicals against Hyper-Pigmentation?. Current Bioinformatics, 2015, 10, 520-532.	0.7	1
61	A sequential procedure for rapid and accurate identification of putative trichomonacidal agents. Journal of Microbiological Methods, 2014, 105, 162-167.	0.7	8
62	A physics-based scoring function for protein structural decoys: Dynamic testing on targets of CASP-ROLL. Chemical Physics Letters, 2014, 610-611, 135-140.	1.2	7
63	Trends in information theory-based chemical structure codification. Molecular Diversity, 2014, 18, 673-686.	2.1	34
64	Discrete Derivatives for Atomâ€Pairs as a Novel Graphâ€Theoretical Invariant for Generating New Molecular Descriptors: Orthogonality, Interpretation and QSARs/QSPRs on Benchmark Databases. Molecular Informatics, 2014, 33, 343-368.	1.4	15
65	Antiprotozoan lead discovery by aligning dry and wet screening: Prediction, synthesis, and biological assay of novel quinoxalinones. Bioorganic and Medicinal Chemistry, 2014, 22, 1568-1585.	1.4	11
66	QuBiLSâ€MIDAS: A parallel freeâ€software for molecular descriptors computation based on multilinear algebraic maps. Journal of Computational Chemistry, 2014, 35, 1395-1409.	1.5	42
67	N-Linear Algebraic Maps for Chemical Structure Codification: A Suitable Generalization for Atom-pair Approaches?. Current Drug Metabolism, 2014, 15, 441-469.	0.7	24
68	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
69	Tyrosinase Enzyme: 1. An Overview on a Pharmacological Target. Current Topics in Medicinal Chemistry, 2014, 14, 1494-1501.	1.0	38
70	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
71	Integration of ligand and structure-based virtual screening for identification of leading anabolic steroids. Journal of Steroid Biochemistry and Molecular Biology, 2013, 138, 348-358.	1.2	3
72	In vivo genotoxicity and cytotoxicity assessment of a novel quinoxalinone with trichomonacide activity. Journal of Applied Toxicology, 2013, 33, 1493-1499.	1.4	5

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73	Global stability of protein folding from an empirical free energy function. Journal of Theoretical Biology, 2013, 321, 44-53.	0.8	13
74	Biological assay of a novel quinoxalinone with antimalarial efficacy on Plasmodium yoelii yoelii. Parasitology Research, 2013, 112, 1523-1527.	0.6	14
75	Extended GT-STAF information indices based on Markov approximation models. Chemical Physics Letters, 2013, 570, 147-152.	1.2	9
76	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
77	Relations frequency hypermatrices in mutual, conditional, and joint entropyâ€based information indices. Journal of Computational Chemistry, 2013, 34, 259-274.	1.5	28
78	Event-based criteria in GT-STAF information indices: theory, exploratory diversity analysis and QSPR applications. SAR and QSAR in Environmental Research, 2013, 24, 3-34.	1.0	19
79	Shannonâ€™s, Mutual, Conditional and Joint Entropy Information Indices: Generalization of Global Indices Defined from Local Vertex Invariants. Current Computer-Aided Drug Design, 2013, 9, 164-183.	0.8	23
80	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
81	Synthesis, biological evaluation and chemometric analysis of indazole derivatives. 1,2-Disubstituted 5-nitroindazolinones, new prototypes of antichagasic drug. European Journal of Medicinal Chemistry, 2012, 58, 214-227.	2.6	45
82	Derivatives in discrete mathematics: a novel graph-theoretical invariant for generating new 2/3D molecular descriptors. I. Theory and QSPR application. Journal of Computer-Aided Molecular Design, 2012, 26, 1229-1246.	1.3	17
83	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
84	Dunnâ€™s index for cluster tendency assessment of pharmacological data sets. Canadian Journal of Physiology and Pharmacology, 2012, 90, 425-433.	0.7	14
85	Identification In Silico and In Vitro of Novel Trypanosomicidal Drugâ€Like Compounds. Chemical Biology and Drug Design, 2012, 80, 38-45.	1.5	14
86	QSAR-Based CMs and TOMOCOMD-CARD Approach for the Discovery of New Tyrosinase Inhibitor Chemicals. , 2012, , 298-341.		1
87	Comparison of Combinatorial Clustering Methods on Pharmacological Data Sets Represented by Machine Learning-Selected Real Molecular Descriptors. Journal of Chemical Information and Modeling, 2011, 51, 3036-3049.	2.5	25
88	Anabolic and androgenic activities of 19-nor-testosterone steroids: QSAR study using quantum and physicochemical molecular descriptors. Journal of Steroid Biochemistry and Molecular Biology, 2011, 126, 35-45.	1.2	7
89	Discovery of novel anti-inflammatory drug-like compounds by aligning in silico and inÂvivo screening: The nitroindazolinone chemotype. European Journal of Medicinal Chemistry, 2011, 46, 5736-5753.	2.6	39
90	Vanilloid Derivatives as Tyrosinase Inhibitors Driven by Virtual Screeningâ€Based QSAR Models. Drug Testing and Analysis, 2011, 3, 176-181.	1.6	26

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91	Thermodynamics of Solution, Interaction with Calf Thymus DNA and Anticancer Activity ofÂPhenylhydrazone Derivatives. Journal of Solution Chemistry, 2011, 40, 26-39.	0.6	3
92	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
93	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
94	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
95	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
96	Experimental and Theoretical Determination ofÂtheÂLimiting Partial Molar Volume of Indole in CCl4, Tetrahydrofuran and Acetonitrile at 293.15ÂK: AÂComparative Study with Benzimidazole andÂBenzothiophene. Journal of Solution Chemistry, 2010, 39, 277-290.	0.6	2
97	Solubility of Thiophene-, Furan- andÂPyrrole-2-Carboxaldehyde Phenylhydrazone Derivatives in 2.82Âmolâ‹…Lâ^'1 Aqueous DMSO at 298.15 K, Inhibition of Lymphoproliferation and Tubulin Polymerization: AÂStudy Based on the Scaled Particle Theory. Journal of Solution Chemistry, 2010, 39, 1099-1112.	0.6	8
98	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
99	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
100	New set of 2D/3D thermodynamic indices for proteins. A formalism based on â€œMolten Globuleâ€•theory. Physics Procedia, 2010, 8, 63-72.	1.2	8
101	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
102	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
103	<scp>tomocomdâ€camps</scp> and protein bilinear indices â€“ novel bioâ€macromolecular descriptors for protein research: I. Predicting protein stability effects of a complete set of alanine substitutions in the Arc repressor. FEBS Journal, 2010, 277, 3118-3146.	2.2	7
104	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
105	Discovery of Novel Trichomonacidals Using LDAâ€Driven QSAR Models and Bondâ€Based Bilinear Indices as Molecular Descriptors. QSAR and Combinatorial Science, 2009, 28, 9-26.	1.5	14
106	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
107	Nucleotide's bilinear indices: Novel bio-macromolecular descriptors for bioinformatics studies of nucleic acids. I. Prediction of paromomycin's affinity constant with HIV-1 Î¨-RNA packaging region. Journal of Theoretical Biology, 2009, 259, 229-241.	0.8	7
108	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

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109	Novel 2D TOMOCOMD-CARDD molecular descriptors: atom-based stochastic and non-stochastic bilinear indices and their QSPR applications. Journal of Mathematical Chemistry, 2008, 44, 650-673.	0.7	20
110	Bond-based linear indices in QSAR: computational discovery of novel anti-trichomonal compounds. Journal of Computer-Aided Molecular Design, 2008, 22, 523-540.	1.3	31
111	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
112	Applying pattern recognition methods plus quantum and physicoâ€chemical molecular descriptors to analyze the anabolic activity of structurally diverse steroids. Journal of Computational Chemistry, 2008, 29, 317-333.	1.5	19
113	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
114	Activity of a hydroxybibenzyl bryophyte constituent against Leishmania spp. and Trypanosoma cruzi: In silico, in vitro and in vivo activity studies. European Journal of Medicinal Chemistry, 2008, 43, 1797-1807.	2.6	66
115	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
116	Chemometric and chemoinformatic analyses of anabolic and androgenic activities of testosterone and dihydrotestosterone analogues. Bioorganic and Medicinal Chemistry, 2008, 16, 6448-6459.	1.4	12
117	In SilicoFasciolicide Activity of Three Experimental Compounds in Sheep. Annals of the New York Academy of Sciences, 2008, 1149, 183-185.	1.8	9
118	A novel approach to predict aquatic toxicity from molecular structure. Chemosphere, 2008, 73, 415-427.	4.2	50
119	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
120	New Antitrichomonal Drug-like Chemicals Selected by Bond (Edge)-Based TOMOCOMD-CARDD Descriptors. Journal of Biomolecular Screening, 2008, 13, 785-794.	2.6	17
121	Prediction of Tyrosinase Inhibition Activity Using Atom-Based Bilinear Indices. ChemMedChem, 2007, 2, 449-478.	1.6	52
122	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
123	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
124	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
125	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
126	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

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127	Experimental Determination of the Electronic Polarizability of Quinoline and Isoquinoline in Solution by Three New Strategies. Journal of Solution Chemistry, 2007, 36, 1139-1155.	0.6	2
128	Quantitative Structureâ€“Activity Relationship of the 4,5Î±-Dihydrotestosterone Steroid Family. QSAR and Combinatorial Science, 2006, 25, 881-894.	1.5	11
129	Non-stochastic quadratic fingerprints andÂLDA-based QSAR models inÂhit andÂlead generation through virtual screening: theoretical andÂexperimental assessment ofÂaÂpromising method forÂtheÂdiscovery ofÂnew antimalarial compounds. European Journal of Medicinal Chemistry, 2006, 41, 483-493.	2.6	40
130	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
131	New ligand-based approach for the discovery of antitrypanosomal compounds. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1898-1904.	1.0	36
132	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
133	Bond-based global and local (bond, group and bond-type) quadratic indices and their applications to computer-aided molecular design. 1. QSPR studies of diverse sets of organic chemicals. Journal of Computer-Aided Molecular Design, 2006, 20, 685-701.	1.3	24
134	Non-stochastic and stochastic linear indices of the molecular pseudographâ€™s atom-adjacency matrix: a novel approach for computational in silico screening and â€œrationalâ€•selection of new lead antibacterial agents. Journal of Molecular Modeling, 2006, 12, 255-271.	0.8	54
135	New tyrosinase inhibitors selected by atomic linear indices-based classification models. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 324-330.	1.0	57
136	Non-stochastic and stochastic linear indices of the â€˜molecular pseudographâ€™s atom adjacency matrixâ€™: application to â€˜in silicoâ€™ studies for the rational discovery of new antimalarial compounds. Bioorganic and Medicinal Chemistry, 2005, 13, 1293-1304.	1.4	68
137	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
138	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
139	Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity. Bioorganic and Medicinal Chemistry, 2005, 13, 2881-2899.	1.4	90
140	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
141	A novel non-stochastic quadratic fingerprints-based approach for the â€˜in silicoâ€™ discovery of new antitrypanosomal compounds. Bioorganic and Medicinal Chemistry, 2005, 13, 6264-6275.	1.4	51
142	Quadratic indices of the â€˜molecular pseudograph's atom adjacency matrixâ€™ and their stochastic forms: a novel approach for virtual screening and in silico discovery of new lead paramphistomicide drugs-like compounds. Computational and Theoretical Chemistry, 2005, 717, 67-79.	1.5	40
143	A linear discrimination analysis based virtual screening of trichomonacidal lead-like compounds: Outcomes of in silico studies supported by experimental results. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3838-3843.	1.0	61
144	Linear Indices of the â€œMolecular Pseudographâ€²s Atom Adjacency Matrixâ€: Definition, Significance-Interpretation, and Application to QSAR Analysis of Flavone Derivatives as HIV-1 Integrase Inhibitors.. ChemInform, 2005, 36, no.	0.1	0

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145	Ligand-Based Virtual Screening and in Silico Design of New Antimalarial Compounds Using Nonstochastic and Stochastic Total and Atom-Type Quadratic Maps.. ChemInform, 2005, 36, no.	0.1	0
146	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
147	A novel in-silico approach for QSAR Studies of Anabolic and Androgenic Activities in the 17Î²-hydroxy-5Î±-androstane Steroid Family. QSAR and Combinatorial Science, 2005, 24, 218-226.	1.5	22
148	A Computer-Based Approach to the Rational Discovery of New Trichomonacidal Drugs by Atom-Type Linear Indices. Current Drug Discovery Technologies, 2005, 2, 245-265.	0.6	40
149	Ligand-Based Virtual Screening and in Silico Design of New Antimalarial Compounds Using Nonstochastic and Stochastic Total and Atom-Type Quadratic Maps. Journal of Chemical Information and Modeling, 2005, 45, 1082-1100.	2.5	83
150	Protein Quadratic Indices of the â€œMacromolecular Pseudographâ€™s Î±-Carbon Atom Adjacency Matrixâ€• 1. Prediction of Arc Repressor Alanine-mutantâ€™s Stability. Molecules, 2004, 9, 1124-1147.	1.7	43
151	Nucleic Acid Quadratic Indices of the â€œMacromolecular Graphâ€™s Nucleotides Adjacency Matrixâ€• Modeling of Footprints after the Interaction of Paromomycin with the HIV-1 Î¨-RNA Packaging Region. International Journal of Molecular Sciences, 2004, 5, 276-293.	1.8	56
152	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
153	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
154	3D-Chiral quadratic indices of the â€˜molecular pseudographâ€™s atom adjacency matrixâ€™ and their application to central chirality codification: classification of ACE inhibitors and prediction of Ïƒ-receptor antagonist activities. Bioorganic and Medicinal Chemistry, 2004, 12, 5331-5342.	1.4	87
155	Total and local (atom and atom type) molecular quadratic indices: significance interpretation, comparison to other molecular descriptors, and QSPR/QSAR applications. Bioorganic and Medicinal Chemistry, 2004, 12, 6351-6369.	1.4	67
156	Linear Indices of the â€œMolecular Pseudograph's Atom Adjacency Matrixâ€•â€‰ Definition, Significance-Interpretation, and Application to QSAR Analysis of Flavone Derivatives as HIV-1 Integrase Inhibitors. Journal of Chemical Information and Computer Sciences, 2004, 44, 2010-2026.	2.8	87
157	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
158	Total and Local Quadratic Indices of the Molecular Pseudograph's Atom Adjacency Matrix: Applications to the Prediction of Physical Properties of Organic Compounds. Molecules, 2003, 8, 687-726.	1.7	77
159	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
160	Molecular simulation of the (GPx)-like antioxidant activity of ebselen derivatives through machine learning techniques. Molecular Simulation, 0, , 1-9.	0.9	1
161	Identification <i>In Silico</i> and <i>In Vitro</i> of Novel Trypanosomicidal Drug-like Compounds. , 0, , .		0
162	QSAR Models and Virtual Screening for Discovery of New Analgesic Leads. , 0, , .		0

#	Article	IF	Citations
163	Molecular descriptor from atomic weighted vectors to predict aquatic toxicity. , 0, , .		0
164	New tool useful for drug discovery validated through benchmark datasets. , 0, , .		0
165	Retrained Classification of Tyrosinase Inhibitors and â€œIn Silicoâ€•Potency Estimation by Using Atom-Type Linear Indices. , 0, , 322-427.		0