Francisco Torrens

List of Publications by Year
in descending order

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		159358	243296
217	3,513	30	44
papers	citations	h-index	g-index

222	222	222	1621
all docs	docs citations	times ranked	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	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
3	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
4	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
5	Revealing the relationship between vegetable oil composition and oxidative stability: A multifactorial approach. Journal of Food Composition and Analysis, 2018, 66, 221-229.	1.9	81
6	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
7	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
8	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
9	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
10	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
11	A new topological descriptors based model for predicting intestinal epithelial transport of drugs in Caco-2 cell culture. Journal of Pharmacy and Pharmaceutical Sciences, 2004, 7, 186-99.	0.9	58
12	New tyrosinase inhibitors selected by atomic linear indices-based classification models. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 324-330.	1.0	57
13	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
14	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
15	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
16	Prediction of Tyrosinase Inhibition Activity Using Atom-Based Bilinear Indices. ChemMedChem, 2007, 2, 449-478.	1.6	52
17	A novel approach to predict aquatic toxicity from molecular structure. Chemosphere, 2008, 73, 415-427.	4.2	50
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	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
24	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
25	Classification of flavonoid compounds by using entropy of information theory. Phytochemistry, 2013, 93, 182-191.	1.4	39
26	Tyrosinase Enzyme: 1. An Overview on a Pharmacological Target. Current Topics in Medicinal Chemistry, 2014, 14, 1494-1501.	1.0	38
27	New ligand-based approach for the discovery of antitrypanosomal compounds. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1898-1904.	1.0	36
28	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
29	Universal model for the calculation of all organic solventâ€“water partition coefficients. Journal of Chromatography A, 1998, 827, 345-358.	1.8	32
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	Conformational aspects of some asymmetric Diels-Alder reactions. A molecular mechanics + polarization study. Tetrahedron, 1992, 48, 5209-5218.	1.0	31
32	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
33	Vectorized TOPO program for the theoretical simulation of molecular shape. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1991, 88, 2435-2441.	0.2	30
34	Relations frequency hypermatrices in mutual, conditional, and joint entropyâ€based information indices. Journal of Computational Chemistry, 2013, 34, 259-274.	1.5	28
35	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
36	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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37	Universal Organic Solventâ^'Water Partition Coefficient Model. Journal of Chemical Information and Computer Sciences, 2000, 40, 236-240.	2.8	26
38	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
39	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
40	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
41	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
42	Incorporation of a dispersion energy term to Fraga's atomâ€“atom pair intermolecular potential. Application to benzene, s-tetrazine, and their mixed dimers. Journal of the Chemical Society Perkin Transactions II, 1987, , 943-950.	0.9	23
43	Interacting induced dipoles polarization model for molecular polarizabilities. Reference molecules, amino acids and model peptides. Computational and Theoretical Chemistry, 1999, 463, 27-39.	1.5	23
44	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
45	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
46	Information entropy-based classification of triterpenoids and steroids from Ganoderma. Phytochemistry, 2015, 116, 305-313.	1.4	23
47	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
48	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
49	Quantitative Structure-Antioxidant Activity Models of Isoflavonoids: A Theoretical Study. International Journal of Molecular Sciences, 2015, 16, 12891-12906.	1.8	22
50	Are most of the stationary points in a molecular association minima? Application of Fraga's potential to benzene-benzene. Journal of Computational Chemistry, 1993, 14, 647-654.	1.5	21
51	Pair potential calculation of molecular associations: a vectorized version. Computer Physics Communications, 1991, 66, 341-362.	3.0	20
52	Periodic Classification of Local Anaesthetics (Procaine Analogues). International Journal of Molecular Sciences, 2006, 7, 12-34.	1.8	20
53	Calculations of organic-solvent dispersions of single-wall carbon nanotubes. International Journal of Quantum Chemistry, 2006, 106, 712-718.	1.0	20
54	Effect of packing on the cluster nature of C nanotubes: An information entropy analysis. Microelectronics Journal, 2007, 38, 1109-1122.	1.1	20

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55	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
56	Topological Charge-Transfer Indices: From Small Molecules to Proteins. Current Proteomics, 2009, 6, 204-213.	0.1	20
57	Calculation of partition coefficient and hydrophobic moment of the secondary structure of lysozyme. Journal of Chromatography A, 2001, 908, 215-221.	1.8	19
58	Molecular polarizability of semiconductor clusters and nanostructures. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 13, 67-71.	1.3	19
59	Molecular polarizability of fullerenes and endohedral metallofullerenes. Journal of Physical Organic Chemistry, 2002, 15, 742-749.	0.9	19
60	Calculations on solvents and co-solvents of single-wall carbon nanotubes: Cyclopyranoses. Computational and Theoretical Chemistry, 2005, 757, 183-191.	1.5	19
61	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
62	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
63	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
64	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
65	The use of â€œab initioâ€•net charges to improve Fraga's atom-atom pair potential for molecular association. Computational and Theoretical Chemistry, 1988, 166, 135-140.	1.5	18
66	Torsional effects on the molecular polarizabilities of the benzothiazole (A)-benzobisthiazole (B) oligomer A-B13-A. Journal of Molecular Graphics, 1996, 14, 245-259.	1.7	18
67	Polarization Force Fields for Peptides Implemented in ECEPP2 and MM2. Molecular Simulation, 2000, 24, 391-410.	0.9	18
68	Free energy of solvation of solutes and their partition coefficients in methanol-water binary mixtures. Chromatographia, 2001, 53, S199-S203.	0.7	18
69	Calculations on solvents and co-solvents of single-wall carbon nanotubes:cyclopyranoses. Nanotechnology, 2005, 16, S181-S189.	1.3	18
70	Molecular aggregation of polycyclic aromatic hydrocarbons. A theoretical modelling of coronene aggregation. Computational and Theoretical Chemistry, 1992, 254, 429-441.	1.5	17
71	Calculations on cyclopyranoses as co-solvents of single-wall carbon nanotubes. Molecular Simulation, 2005, 31, 107-114.	0.9	17
72	New Antitrichomonal Drug-like Chemicals Selected by Bond (Edge)-Based TOMOCOMD-CARDD Descriptors. Journal of Biomolecular Screening, 2008, 13, 785-794.	2.6	17

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73	(Co-)solvent selection for single-wall carbon nanotubes: best solvents, acids, superacids and guestâ€“host inclusion complexes. Nanoscale, 2011, 3, 2494.	2.8	17
74	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
75	Interacting induced dipoles polarization model for molecular polarizabilities: application to benzothiazole (A)-benzobisthiazole (B) oligomers Aî—¸B13î—¸A. Computational and Theoretical Chemistry, 1998, 426, 105-116.	1.5	16
76	A new topological index to elucidate apolar hydrocarbons. , 2001, 15, 709-719.		16
77	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. Nanotechnology, 2004, 15, S259-S264.	1.3	16
78	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
79	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. Journal of the Brazilian Chemical Society, 2015, , .	0.6	16
80	Theoretical characterization of iron and manganese porphyrins for catalyzed saturated alkane hydroxylations. Journal of Molecular Catalysis A, 1997, 119, 393-403.	4.8	15
81	Interaction of polyelectrolytes with oppositely charged micelles studied by fluorescence and liquid chromatography. European Polymer Journal, 2005, 41, 1439-1452.	2.6	15
82	Cluster Origin of the Solubility of Single-Wall Carbon Nanotubes. Computing Letters, 2005, 1, 331-336.	0.5	15
83	Negatively cooperative binding of melittin to neutral phospholipid vesicles. Journal of Molecular Structure, 2007, 834-836, 216-228.	1.8	15
84	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
85	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
86	New dimension indices for the characterization of the solvent-accessible surface. Journal of Computational Chemistry, 2001, 22, 477-487.	1.5	14
87	Table of Periodic Properties of Fullerenes Based on Structural Parameters. Journal of Chemical Information and Computer Sciences, 2004, 44, 60-67.	2.8	14
88	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
89	Identification In Silico and In Vitro of Novel Trypanosomicidal Drugâ€Like Compounds. Chemical Biology and Drug Design, 2012, 80, 38-45.	1.5	14
90	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

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91	Cluster Origin of the Transfer Phenomena of Single-Wall Carbon Nanotubes. Journal of Computational and Theoretical Nanoscience, 2007, 4, 588-603.	0.4	14
92	Molecular polarizability of Scn, Cn and endohedral Scn@Cm clusters. Microelectronic Engineering, 2000, 51-52, 613-626.	1.1	13
93	Fractal Hybrid Orbitals Analysis of the Tertiary Structure of Protein Molecules. Molecules, 2002, 7, 26-37.	1.7	13
94	Calculation of organic solventâ€“water partition coefficients of ironâ€“sulfur protein models. Polyhedron, 2002, 21, 1357-1361.	1.0	13
95	Nature of FeIIIâ€“O2, FeIIâ€“CO and FeIIIâ€“CN complexes of hemoprotein models. Polyhedron, 2003, 22, 1091-1098.	1.0	13
96	Asymptotic Analysis of Coagulationâ€“Fragmentation Equations of Carbon Nanotube Clusters. Nanoscale Research Letters, 2007, 2, 337-349.	3.1	13
97	Stationaryâ€“mobile phase distribution coefficient for polystyrene standards. Separation Science and Technology, 2002, 37, 1653-1665.	1.3	12
98	Valence Topological Charge-Transfer Indices for Dipole Moments. Molecules, 2003, 8, 169-185.	1.7	12
99	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
100	QSPR Prediction of Retention Times of Phenylurea Herbicides by Biological Plastic Evolution. Current Drug Safety, 2012, 7, 262-268.	0.3	12
101	Molecular Classification of Pesticides Including Persistent Organic Pollutants, Phenylurea and Sulphonylurea Herbicides. Molecules, 2014, 19, 7388-7414.	1.7	12
102	Classification of stilbenoid compounds by entropy of artificial intelligence. Phytochemistry, 2014, 97, 62-69.	1.4	12
103	QSPR prediction of chromatographic retention times of pesticides: Partition and fractal indices. Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes, 2014, 49, 400-407.	0.7	12
104	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
105	Improved AMYR program: an algorithm for the theoretical simulation of molecular associations, including geometrical and topological characterization of the dimers. Journal of Molecular Graphics, 1991, 9, 254-256.	1.7	11
106	Characterizing cavities in model inclusion molecules: a comparative study. Journal of Molecular Graphics and Modelling, 1998, 16, 57-71.	1.3	11
107	Valence topological charge-transfer indices for dipole moments. Molecular Diversity, 2004, 8, 365-370.	2.1	11
108	Compatibility between polystyrene copolymers and polymers in solution via hydrogen bonding. European Polymer Journal, 2006, 42, 2807-2823.	2.6	11

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109	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
110	AMYR 2: A new version of a computer program for pair potential calculation of molecular associations. Computer Physics Communications, 1998, 115, 87-89.	3.0	10
111	Fractal Dimension of Different Structural-Type Zeolites and of the Active Sites. Topics in Catalysis, 2002, 18, 291-297.	1.3	10
112	Cluster nature of the solvent features of singleâ€wall carbon nanohorns. International Journal of Quantum Chemistry, 2010, 110, 563-570.	1.0	10
113	Prediction of Aquatic Toxicity of Benzene Derivatives to Tetrahymena pyriformis According to OECD Principles. Current Pharmaceutical Design, 2016, 22, 5085-5094.	0.9	10
114	Molecular polarizability of Scn, Cn and endohedral Scn@Cm clusters. Nanotechnology, 2002, 13, 433-438.	1.3	9
115	Characterizing cavity-like spaces in active-site models of zeolites. Computational Materials Science, 2003, 27, 96-101.	1.4	9
116	QSAR Modeling ANTI-HIV-1 Activities by Optimization of Correlation Weights of Local Graph Invariants. Molecular Simulation, 2004, 30, 691-696.	0.9	9
117	Binding of water-soluble, globular proteins to anionic model membranes. Journal of Molecular Structure, 2009, 924-926, 274-284.	1.8	9
118	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
119	Structural, Chemical Topological, Electrotopological and Electronic Structure Hypotheses. Combinatorial Chemistry and High Throughput Screening, 2003, 6, 801-809.	0.6	9
120	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
121	Valence Topological Charge-Transfer Indices for Dipole Moments: Percutaneous Enhancers. Molecules, 2004, 9, 1222-1235.	1.7	8
122	A Chemical Index Inspired by Biological Plastic Evolution:â€‰ Valence-Isoelectronic Series of Aromatics. Journal of Chemical Information and Computer Sciences, 2004, 44, 575-581.	2.8	8
123	Fractal Dimension of Transdermal-Delivery Drug Models: 4-Alkylanilines. Journal of Liquid Chromatography and Related Technologies, 2008, 31, 2337-2347.	0.5	8
124	Incorporation of Silica Nanospherical Particles into Epoxy-Amine Crosslinked Materials. Polymers and Polymer Composites, 2008, 16, 139-151.	1.0	8
125	Modelling of complex multicellular systems: tumour-immune cells competition. Chemistry Central Journal, 2009, 3, .	2.6	8
126	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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127	Polarization by the effect of a small torsional change in the benzothiazole (A)-benzobisthiazole (B) oligomer A-B13-A. Molecules, 1999, 4, 28-51.	1.7	7
128	Molecular Polarizability of Sc and C (Fullerene and Graphite) Clusters. Molecules, 2001, 6, 496-509.	1.7	7
129	Computing the KekulÃ© structure count for alternant hydrocarbons. International Journal of Quantum Chemistry, 2002, 88, 392-397.	1.0	7
130	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
131	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
132	<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
133	Electrically Conductive Phthalocyanine Assemblies. Structural and Non-Integer Oxidation Number Considerations. NATO ASI Series Series B: Physics, 1990, , 461-466.	0.2	7
134	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
135	Fractals for hybrid orbitals in protein models. , 0, , .		6
136	Fractal dimension of zeolite catalysts. Molecular Physics, 2002, 100, 3105-3109.	0.8	6
137	Valence topological charge-transfer indices for dipole moments. Computational and Theoretical Chemistry, 2003, 621, 37-42.	1.5	6
138	A Comparative Study of O2, CO and CN Binding to Heme IX Protein Models. Molecules, 2004, 9, 632-649.	1.7	6
139	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. Nanotechnology, 2006, 17, 1541-1541.	1.3	6
140	Solvent features of cluster single-wall C, BC2N and BN nanotubes, cones and horns. Microelectronic Engineering, 2013, 108, 127-133.	1.1	6
141	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
142	Classification of Complex Molecules. Studies in Computational Intelligence, 2009, , 243-315.	0.7	6
143	Computational Study of Nanosized Drug Delivery from Cyclodextrins, Crown Ethers and Hyaluronan in Pharmaceutical Formulations. Current Topics in Medicinal Chemistry, 2015, 15, 1901-1913.	1.0	6
144	Molecular polarizability of Si/Ge/GaAs semiconductors clusters. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 439-450.	0.1	6

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145	Aqueous coefficient calculations for chemicals and drugs. Toxicological and Environmental Chemistry, 1999, 73, 177-189.	0.6	5
146	Effect of size and deformation on polarizabilities of carbon nanotubes from atomic increments. Future Generation Computer Systems, 2004, 20, 763-772.	4.9	5
147	Nature of O2, CO, and CN binding to hemoprotein models. International Journal of Quantum Chemistry, 2004, 99, 963-971.	1.0	5
148	Fractal Dimension of Active-Site Models of Zeolite Catalysts. Journal of Nanomaterials, 2006, 2006, 1-9.	1.5	5
149	Resonance in Interacting Induced-Dipole Polarizing Force Fields: Application to Force-Field Derivatives. Algorithms, 2009, 2, 437-447.	1.2	5
150	Fullerite Crystal Thermodynamic Characteristics and the Law of Corresponding States. Journal of Nanoscience and Nanotechnology, 2010, 10, 1208-1222.	0.9	5
151	Using Chemical Structural Indicators for Periodic Classification of Local Anaesthetics. International Journal of Chemoinformatics and Chemical Engineering, 2011, 1, 15-35.	0.1	5
152	Binding of vinyl polymers to anionic model membranes. Cellular and Molecular Biology, 2003, 49, 991-8.	0.3	5
153	Characterizing Cavities in Model Inclusion Fullerenes: A Comparative Study. International Journal of Molecular Sciences, 2001, 2, 72-88.	1.8	4
154	New structural parameters of fullerenes for principal component analysis. Theoretical Chemistry Accounts, 2003, 110, 371-376.	0.5	4
155	Effect of Elliptical Deformation on Molecular Polarizabilities of Model Carbon Nanotubes from Atomic Increments. Journal of Nanoscience and Nanotechnology, 2003, 3, 313-318.	0.9	4
156	An Improved Force Field for O2, CO and CN Binding to Metalloporphyrins. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2004, 49, 37-46.	1.6	4
157	Valence Topological Charge-Transfer Indices for Reflecting Polarity: Correction for Heteromolecules. Molecules, 2005, 10, 334-345.	1.7	4
158	Study and comparison of interaction parameters and phase behavior of epoxy/polystyrene and epoxies copolymer polystyreneâ€bâ€poly(methyl methacrylate) blends. Polymer Composites, 2008, 29, 1337-1345.	2.3	4
159	Modeling Studies of the Phase Behavior of Monomer/Polymer/Disk Composites. Macromolecular Theory and Simulations, 2008, 17, 325-340.	0.6	4
160	Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites II. Polymers and Polymer Composites, 2009, 17, 313-324.	1.0	4
161	Comparative analysis of the electrostatics of the binding of cationic proteins to vesicles: Asymmetric location of anionic phospholipids. Analytica Chimica Acta, 2009, 654, 2-10.	2.6	4
162	Table of periodic properties of human immunodeficiency virus inhibitors. International Journal of Computational Intelligence in Bioinformatics and Systems Biology, 2010, 1, 246.	0.1	4

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163	QSPR Prediction of Retention Times of Methylxanthines and Cotinine by Bioplastic Evolution. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 74-87.	1.1	4
164	Polarizability Characterization of Zeolitic Bnpnsted Acidic Sites. , 2019, , 555-556.		4
165	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. Current Pharmaceutical Design, 2016, 22, 5095-5113.	0.9	4
166	QSAR of Natural Sesquiterpene Lactones as Inhibitors of Myb-dependent Gene Expression. Current Topics in Medicinal Chemistry, 2018, 17, 3256-3268.	1.0	4
167	Lacosamide Derivatives with Anticonvulsant Activity as Carbonic Anhydrase Inhibitors. Molecular Modeling, Docking and QSAR Analysis. Current Computer-Aided Drug Design, 2014, 10, 160-167.	0.8	4
168	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
169	QSPR Modeling of Hydrocarbon Dipole Moments by Means of Correlation Weighting of Local Graph Invariants. Journal of Theoretical and Computational Chemistry, 2003, 02, 139-146.	1.8	3
170	Net charge and polarizability of zeolitic BrÃ¸nsted acidic sites. International Journal of Quantum Chemistry, 2007, 107, 2378-2383.	1.0	3
171	Incorporation of Silica Nanospherical Particles in Epoxyâ€“Amine Crosslinked Materials II. Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites. Polymers and Polymer Composites, 2009, 17, 457-465.	1.0	3
172	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. Molecular Diversity, 2022, 26, 1383-1397.	2.1	3
173	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
174	Structure-Activity Relationships of Cytotoxic Lactones as Inhibitors and Mechanisms of Action. Current Drug Discovery Technologies, 2020, 17, 166-182.	0.6	3
175	Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones and Nanohorns. , 0, , 228-284.		3
176	Bundlet Model of Single- Wall Carbon, BC2N and BN Nanotubes, Cones and Horns in Organic Solvents. Journal of Nanomaterials & Molecular Nanotechnology, 2013, 02, .	0.1	3
177	RevisÃ£o da literatura sobre orÃ§amento em cinco periÃ³dicos internacionais no anos de 2000 atÃ© 2009. REGE Revista De GestÃ£o, 2012, 19, 107-123.	1.0	3
178	Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones and Nanohorns. International Journal of Chemoinformatics and Chemical Engineering, 2012, 2, 48-98.	0.1	3
179	Complexity, Emergence and Molecular Diversity via Information Theory. , 2013, , 196-208.		3
180	Treatment of poly(styrene-co-methacrylic acid)/poly(4-vinylpyridine) blends in solution under liquidâ€“liquid phase-separation conditions. A new method for phase-separation data attainment from viscosity measurements. Journal of Applied Polymer Science, 2006, 102, 5039-5049.	1.3	2

#	Article	IF	Citations
181	Improvement of charge-transfer indices for multifunctional amino acids: Application to lysozyme. SAR and QSAR in Environmental Research, 2008, 19, 643-654.	1.0	2
182	Experimental Studies for Modelling the Phase Behaviour of Monomer/Polymer/Disc Composites. Macromolecular Symposia, 2010, 296, 557-565.	0.4	2
183	Cluster solvation models of carbon nanostructures: extension to fullerenes, tubes, and buds. Journal of Molecular Modeling, 2014, 20, 2263.	0.8	2
184	Dry selection and wet evaluation for the rational discovery of new anthelmintics. Molecular Physics, 2017, 115, 2300-2313.	0.8	2
185	QSRP Prediction of Retention Times of Chlorogenic Acids in Coffee by Bioplastic Evolution. , 0, , .		2
186	Information Theoretic Entropy for Molecular Classification: Oxadiazolamines as Potential Therapeutic Agents. Current Computer-Aided Drug Design, 2013, 9, 241-253.	0.8	2
187	Molecular Classification of 5-Amino-2-Aroylquinolines and 4-Aroyl-6,7,8-Trimethoxyquinolines as Highly Potent Tubulin Polymerization Inhibitors. International Journal of Chemoinformatics and Chemical Engineering, 2013, 3, 1-26.	0.1	2
188	Structural Classification of Complex Molecules by Artificial Intelligence Techniques. , 0, , 25-91.		2
189	Partition of Solvents and Co-Solvents of Nanotubes: Proteins and Cyclopyranoses. Frontiers in Medicinal Chemistry, 2005, 1, 231-266.	0.2	1
190	Effect of Packing on Cluster Solvation of Nanotubes. , 2006, , .		1
191	Protein negative/positively cooperative binding to zwitterionic/anionic vesicles. Journal of Cheminformatics, 2010, 2, .	2.8	1
192	Modelling Monomer/Disc Composites Phase Behaviour. Macromolecular Symposia, 2012, 311, 49-56.	0.4	1
193	Computational approach to the discovery of potential neprilysin inhibitors compounds for cardiovascular diseases treatment. Medicinal Chemistry Research, 2020, 29, 897-909.	1.1	1
194	QSAR-Based CMs and TOMOCOMD-CARD Approach for the Discovery of New Tyrosinase Inhibitor Chemicals. , 2012, , 298-341.		1
195	Calculations on Solvents and Co Solvents of Single-Wall Carbon Nanotubes: Cyclopyranoses. , 0, , .		1
196	Nanostructures Cluster Models in Solution. Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series, 2014, , 221-253.	0.5	1
197	Mucoadhesive Polymer Hyaluronan as Biodegradable Cationic/Zwitterionic-Drug Delivery Vehicle. ADMET and DMPK, 2015, 2, .	1.1	1
198	Table of Periodic Properties of Fullerenes Based on Structural Parameters.. ChemInform, 2004, 35, no.	0.1	0

#	Article	IF	Citations
199	A Chemical Index Inspired by Biological Plastic Evolution: Valence-Isoelectronic Series of Aromatics.. ChemInform, 2004, 35, no.	0.1	0
200	Effect of Packing on Cluster Solvation of Nanotubes. , 0, , .		0
201	Asymptotic Coagulation-Fragmentation Equations. , 2008, , .		0
202	CLUSTER NATURE OF C-NANOHORN SOLVENT FEATURES. , 2009, , .		0
203	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
204	Molecular Classification of N-Aryloxazolidinone-5-carboxamides as Human Immunodeficiency Virus Protease Inhibitors. , 2015, , 69-97.		0
205	Molecular Classification of Antitubulin Agents with Indole Ring Binding at Colchicine-Binding Site. , 2018, , .		0
206	QSPR Prediction of Chromatographic Retention Times of Tea Compounds by Bioplastic Evolution. , 2018, , .		0
207	Classification of Congeneric and QSAR of Homologous Antileukemic Sâ€“Alkylcysteine Ketones. Molecules, 2021, 26, 235.	1.7	0
208	Cooperativity of Protein Binding to Vesicles. Advances in Experimental Medicine and Biology, 2011, 696, 271-278.	0.8	0
209	MOTIVAÃ‡ÃƒO E RESISTÃŠNCIA AO USO DA TECNOLOGIA DA INFORMAÃ‡ÃƒO: UM ESTUDO ENTRE PROFESSORES. AdministraÃ§Ã£o: Ensino E Pesquisa, 2012, 13, 301.	0.1	0
210	Valence-Topological Charge-Transfer Indices, Dipole, Isoelectric Point and Fractal: From Homo/Heterocycles to Proteins. Current Organic Chemistry, 2015, 19, 205-218.	0.9	0
211	Ideas in the History of Nano/Miniaturization and (Quantum) Simulators: Feynman, Education and Research Reorientation in Translational Science. , 0, , .		0
212	Cluster Origin of Solvation Features of C-Nanostructures in Organic Solvents. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 189-293.	0.3	0
213	Graphene and Fullenene Clusters. Advances in Chemical and Materials Engineering Book Series, 2017, , 569-599.	0.2	0
214	Matter, Plasma, Quasi Two-Dimensional Au Film, Drug Products Quality, and Circular Economy. , 2020, , 55-72.		0
215	Cluster Origin of Solvent Features of Fullerenes, Single-Wall Carbon Nanotubes, Nanocones, and Nanohorns. , 0, , 1-57.		0
216	Using Chemical Structural Indicators for Periodic Classification of Local Anaesthetics. , 0, , 117-137.		0

#	Article	IF	Citations
217	Cluster Origin of Solvent Features of Fullerenes, Single-Wall Carbon Nanotubes, Nanocones, and Nanohorns. , 0, , 262-318.		0