Francisco Torrens

List of Publications by Citations

200 papers	2,791 citations	27 h-index	40 g-index
221 ext. papers	3,019 ext. citations	3 avg, IF	5.06 L-index

#	Paper	IF	Citations
200	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**,	3.4	84
199	3D-chiral quadratic indices of the 'molecular pseudograph's atom adjacency matrix' and their application to central chirality codification: classification of ACE inhibitors and prediction of sigma-receptor antagonist activities. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 5331-42	3.4	79
198	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, 1483-503	3.4	68
197	Protein linear indices of the 'macromolecular pseudograph alpha-carbon atom adjacency matrix' 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, 3003-15	3.4	65
196	Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 2881-99	3.4	62
195	Dragon method for finding novel tyrosinase inhibitors: Biosilico identification and experimental in vitro assays. *European Journal of Medicinal Chemistry*, **2007**, 42, 1370-81	6.8	57
194	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	3.4	56
193	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, 1946-76	3.9	55
192	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, 615-34	4.2	54
191	Atom, atom-type, and total linear indices of the "molecular pseudograph's atom adjacency matrix": application to QSPR/QSAR studies of organic compounds. *Molecules*, **2004**, 9, 1100-23	4.8	52
190	Nucleic Acid Quadratic Indices of the Macromolecular Graph Nucleotides Adjacency Matrix Modeling of Footprints after the Interaction of Paromomycin with the HIV-1 RNA Packaging Region. *International Journal of Molecular Sciences*, **2004**, 5, 276-293	6.3	51
189	Revealing the relationship between vegetable oil composition and oxidative stability: A multifactorial approach. *Journal of Food Composition and Analysis*, **2018**, 66, 221-229	4.1	48
188	New tyrosinase inhibitors selected by atomic linear indices-based classification models. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 324-30	2.9	48
187	Predicting antitrichomonal activity: a computational screening using atom-based bilinear indices and experimental proofs. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 6502-24	3.4	48
186	Non-stochastic and stochastic linear indices of the molecular pseudograph's atom-adjacency matrix: a novel approach for computational in silico screening and "rational" selection of new lead antibacterial agents. *Journal of Molecular Modeling*, **2006**, 12, 255-71	2	48
185	A novel approach to predict aquatic toxicity from molecular structure. *Chemosphere*, **2008**, 73, 415-27	8.4	45
184	Prediction of tyrosinase inhibition activity using atom-based bilinear indices. *ChemMedChem*, **2007**, 2, 449-78	3.7	43

183	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	2.8	39
182	Protein quadratic indices of the "macromolecular pseudograph's alpha-carbon atom adjacency matrix". 1. Prediction of Arc repressor alanine-mutant's stability. *Molecules*, **2004**, 9, 1124-47	4.8	38
181	Non-stochastic quadratic fingerprints and LDA-based QSAR models in hit and lead generation through virtual screening: theoretical and experimental assessment of a promising method for the discovery of new antimalarial compounds. *European Journal of Medicinal Chemistry*, **2006**, 41, 483-93	6.8	36
180	New ligand-based approach for the discovery of antitrypanosomal compounds. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 1898-904	2.9	34
179	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, 2601-24	3.3	33
178	A computer-based approach to the rational discovery of new trichomonacidal drugs by atom-type linear indices. *Current Drug Discovery Technologies*, **2005**, 2, 245-65	1.5	33
177	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, 2398-408	3.4	32
176	Vectorized TOPO program for the theoretical simulation of molecular shape. *Journal De Chimie Physique Et De Physico-Chimie Biologique*, **1991**, 88, 2435-2441		30
175	Discovery of novel anti-inflammatory drug-like compounds by aligning in silico and in vivo screening: the nitroindazolinone chemotype. *European Journal of Medicinal Chemistry*, **2011**, 46, 5736-53	6.8	29
174	Classification of flavonoid compounds by using entropy of information theory. *Phytochemistry*, **2013**, 93, 182-91	4	28
173	Universal model for the calculation of all organic solvent□water partition coefficients. *Journal of Chromatography A*, **1998**, 827, 345-358	4.5	27
172	Conformational aspects of some asymmetric Diels-Alder reactions. A molecular mechanics + polarization study. *Tetrahedron*, **1992**, 48, 5209-5218	2.4	27
171	Tyrosinase enzyme: 1. An overview on a pharmacological target. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1494-501	3	26
170	Bond-based 2D quadratic fingerprints in QSAR studies: virtual and in vitro tyrosinase inhibitory activity elucidation. *Chemical Biology and Drug Design*, **2010**, 76, 538-45	2.9	25
169	Bond-based 3D-chiral linear indices: theory and QSAR applications to central chirality codification. *Journal of Computational Chemistry*, **2008**, 29, 2500-12	3.5	25
168	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, 30-6	5.1	24
167	Bond-based linear indices in QSAR: computational discovery of novel anti-trichomonal compounds. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 523-40	4.2	24
166	Relations frequency hypermatrices in mutual, conditional and joint entropy-based information indices. *Journal of Computational Chemistry*, **2013**, 34, 259-74	3.5	23

165	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, 1014-24		23
164	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	2.1	21
163	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	4.2	21
162	QuBiLs-MAS method in early drug discovery and rational drug identification of antifungal agents. *SAR and QSAR in Environmental Research*, **2015**, 26, 943-58	3.5	20
161	Atom-based non-stochastic and stochastic bilinear indices: Application to QSPR/QSAR studies of organic compounds. *Chemical Physics Letters*, **2008**, 464, 107-112	2.5	20
160	Universal organic solvent-water partition coefficient model. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 236-40		20
159	Incorporation of a dispersion energy term to Fraga's atom□atom pair intermolecular potential. Application to benzene, s-tetrazine, and their mixed dimers. *Journal of the Chemical Society Perkin Transactions II*, **1987**, 943-950		20
158	A review of QSAR studies to discover new drug-like compounds actives against leishmaniasis and trypanosomiasis. *Current Topics in Medicinal Chemistry*, **2012**, 12, 852-65	3	19
157	Pair potential calculation of molecular associations: a vectorized version. *Computer Physics Communications*, **1991**, 66, 341-362	4.2	19
156	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	3.5	19
155	Shannon's, mutual, conditional and joint entropy information indices: generalization of global indices defined from local vertex invariants. *Current Computer-Aided Drug Design*, **2013**, 9, 164-83	1.4	19
154	Ligand-based discovery of novel trypanosomicidal drug-like compounds: in silico identification and experimental support. *European Journal of Medicinal Chemistry*, **2011**, 46, 3324-30	6.8	18
153	Bond-based 2D TOMOCOMD-CARDD approach for drug discovery: aiding decision-making in 'in silico' selection of new lead tyrosinase inhibitors. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 167-88	4.2	18
152	Interacting induced dipoles polarization model for molecular polarizabilities. Reference molecules, amino acids and model peptides. *Computational and Theoretical Chemistry*, **1999**, 463, 27-39		18
151	The use of □b initio□net charges to improve Fraga's atom-atom pair potential for molecular association. *Computational and Theoretical Chemistry*, **1988**, 166, 135-140		18
150	Periodic Classification of Local Anaesthetics (Procaine Analogues). *International Journal of Molecular Sciences*, **2006**, 7, 12-34	6.3	17
149	Calculations of organic-solvent dispersions of single-wall carbon nanotubes. *International Journal of Quantum Chemistry*, **2006**, 106, 712-718	2.1	17
148	Molecular polarizability of semiconductor clusters and nanostructures. *Physica E: Low-Dimensional Systems and Nanostructures*, **2002**, 13, 67-71	3	17

147	Calculations on solvents and co-solvents of single-wall carbon nanotubes: Cyclopyranoses. *Computational and Theoretical Chemistry*, **2005**, 757, 183-191		17
146	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	3.5	16
145	Effect of packing on the cluster nature of C nanotubes: An information entropy analysis. *Microelectronics Journal*, **2007**, 38, 1109-1122	1.8	16
144	Free energy of solvation of solutes and their partition coefficients in methanol-water binary mixtures. *Chromatographia*, **2001**, 53, S199-S203	2.1	16
143	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	2.1	15
142	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. *Nanotechnology*, **2004**, 15, S259-S264	3.4	15
141	Molecular polarizability of fullerenes and endohedral metallofullerenes. *Journal of Physical Organic Chemistry*, **2002**, 15, 742-749	2.1	15
140	Calculations on solvents and co-solvents of single-wall carbon nanotubes:cyclopyranoses. *Nanotechnology*, **2005**, 16, S181-S189	3.4	15
139	Calculations on cyclopyranoses as co-solvents of single-wall carbon nanotubes. *Molecular Simulation*, **2005**, 31, 107-114	2	15
138	Calculation of partition coefficient and hydrophobic moment of the secondary structure of lysozyme. *Journal of Chromatography A*, **2001**, 908, 215-21	4.5	15
137	Polarization Force Fields for Peptides Implemented in ECEPP2 and MM2. *Molecular Simulation*, **2000**, 24, 391-410	2	15
136	Comparative study to predict toxic modes of action of phenols from molecular structures. *SAR and QSAR in Environmental Research*, **2013**, 24, 235-51	3.5	14
135	New antitrichomonal drug-like chemicals selected by bond (edge)-based TOMOCOMD-CARDD descriptors. *Journal of Biomolecular Screening*, **2008**, 13, 785-94		14
134	Negatively cooperative binding of melittin to neutral phospholipid vesicles. *Journal of Molecular Structure*, **2007**, 834-836, 216-228	3.4	14
133	Interaction of polyelectrolytes with oppositely charged micelles studied by fluorescence and liquid chromatography. *European Polymer Journal*, **2005**, 41, 1439-1452	5.2	14
132	Torsional effects on the molecular polarizabilities of the benzothiazole (A)-benzobisthiazole (B) oligomer A-B13-A. *Journal of Molecular Graphics*, **1996**, 14, 245-59, 277		14
131	Molecular aggregation of polycyclic aromatic hydrocarbons. A theoretical modelling of coronene aggregation. *Computational and Theoretical Chemistry*, **1992**, 254, 429-441		14
130	Information entropy-based classification of triterpenoids and steroids from Ganoderma. *Phytochemistry*, **2015**, 116, 305-313	4	13

129	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, 1229-46	4.2	13
128	Novel coumarin-based tyrosinase inhibitors discovered by OECD principles-validated QSAR approach from an enlarged, balanced database. *Molecular Diversity*, **2011**, 15, 507-20	3.1	13
127	Discovery of Novel Trichomonacidals Using LDA-Driven QSAR Models and Bond-Based Bilinear Indices as Molecular Descriptors. *QSAR and Combinatorial Science*, **2009**, 28, 9-26		13
126	Interacting induced dipoles polarization model for molecular polarizabilities: application to benzothiazole (A)-benzobisthiazole (B) oligomers A?B13?A. *Computational and Theoretical Chemistry*, **1998**, 426, 105-116		13
125	Table of periodic properties of fullerenes based on structural parameters. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 60-7		13
124	Cluster Origin of the Solubility of Single-Wall Carbon Nanotubes. *Computing Letters*, **2005**, 1, 331-336		13
123	Bond-based bilinear indices for computational discovery of novel trypanosomicidal drug-like compounds through virtual screening. *European Journal of Medicinal Chemistry*, **2015**, 96, 238-44	6.8	12
122	Quantitative Structure-Antioxidant Activity Models of Isoflavonoids: A Theoretical Study. *International Journal of Molecular Sciences*, **2015**, 16, 12891-906	6.3	12
121	(Co-)solvent selection for single-wall carbon nanotubes: best solvents, acids, superacids and guest-host inclusion complexes. *Nanoscale*, **2011**, 3, 2494-510	7.7	12
120	Theoretical characterization of iron and manganese porphyrins for catalyzed saturated alkane hydroxylations. *Journal of Molecular Catalysis A*, **1997**, 119, 393-403		12
119	Asymptotic Analysis of Coagulation□Fragmentation Equations of Carbon Nanotube Clusters. *Nanoscale Research Letters*, **2007**, 2, 337-349	5	12
118	A new topological index to elucidate apolar hydrocarbons. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 709-19	4.2	12
117	Cluster Origin of the Transfer Phenomena of Single-Wall Carbon Nanotubes. *Journal of Computational and Theoretical Nanoscience*, **2007**, 4, 588-603	0.3	12
116	Topological Charge-Transfer Indices: From Small Molecules to Proteins. *Current Proteomics*, **2009**, 6, 204-213	0.7	11
115	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, 731-53	3.1	11
114	Atom-Based 2D Quadratic Indices in Drug Discovery of Novel Tyrosinase Inhibitors: Results of In Silico Studies Supported by Experimental Results. *QSAR and Combinatorial Science*, **2007**, 26, 469-487		11
113	Nature of Fe^{III}□O2, Fe^{II}□CO and Fe^{III}□CN complexes of hemoprotein models. *Polyhedron*, **2003**, 22, 1091-1098	2.7	11
112	Molecular polarizability of Scn, Cn and endohedral Scn@Cm clusters. *Microelectronic Engineering*, **2000**, 51-52, 613-626	2.5	11

111	Calculation of organic solvent–water partition coefficients of iron–sulfur protein models. *Polyhedron*, **2002**, 21, 1357-1361	2.7	10
110	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, 254-6		10
109	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	3.5	9
108	Discrete Derivatives for Atom-Pairs as a Novel Graph-Theoretical Invariant for Generating New Molecular Descriptors: Orthogonality, Interpretation and QSARs/QSPRs on Benchmark Databases. *Molecular Informatics*, **2014**, 33, 343-68	3.8	9
107	Identification in silico and in vitro of novel trypanosomicidal drug-like compounds. *Chemical Biology and Drug Design*, **2012**, 80, 38-45	2.9	9
106	Cluster nature of the solvent features of single-wall carbon nanohorns. *International Journal of Quantum Chemistry*, **2010**, 110, 563-570	2.1	9
105	Characterizing cavities in model inclusion molecules: a comparative study. *Journal of Molecular Graphics and Modelling*, **1998**, 16, 57-71	2.8	9
104	Valence Topological Charge-Transfer Indices for Dipole Moments. *Molecules*, **2003**, 8, 169-185	4.8	9
103	Fractal Hybrid Orbitals Analysis of the Tertiary Structure of Protein Molecules. *Molecules*, **2002**, 7, 26-37	4.8	9
102	New dimension indices for the characterization of the solvent-accessible surface. *Journal of Computational Chemistry*, **2001**, 22, 477-487	3.5	9
101	Stationary–mobile phase distribution coefficient for polystyrene standards. *Separation Science and Technology*, **2002**, 37, 1653-1665	2.5	9
100	Prediction of Aquatic Toxicity of Benzene Derivatives to Tetrahymena pyriformis According to OECD Principles. *Current Pharmaceutical Design*, **2016**, 22, 5085-5094	3.3	9
99	Computational Identification of Chemical Compounds with Potential Activity against Leishmania amazonensis using Nonlinear Machine Learning Techniques. *Current Topics in Medicinal Chemistry*, **2018**, 18, 2347-2354	3	9
98	Prediction of Caco-2 Cell Permeability Using Bilinear Indices and Multiple Linear Regression. *Letters in Drug Design and Discovery*, **2015**, 13, 161-169	0.8	9
97	Classification of stilbenoid compounds by entropy of artificial intelligence. *Phytochemistry*, **2014**, 97, 62-9	4	8
96	Applications of Bond-Based 3D-Chiral Quadratic Indices in QSAR Studies Related to Central Chirality Codification. *QSAR and Combinatorial Science*, **2009**, 28, 1465-1477		8
95	Binding of water-soluble, globular proteins to anionic model membranes. *Journal of Molecular Structure*, **2009**, 924-926, 274-284	3.4	8
94	QSPR prediction of retention times of phenylurea herbicides by biological plastic evolution. *Current Drug Safety*, **2012**, 7, 262-8	1.4	8

93	QSAR Modeling ANTI-HIV-1 Activities by Optimization of Correlation Weights of Local Graph Invariants. *Molecular Simulation*, **2004**, 30, 691-696	2	8
92	Molecular polarizability of Scn, Cn and endohedral Scn@Cm clusters. *Nanotechnology*, **2002**, 13, 433-438	3.4	8
91	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	5.9	8
90	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, 400-7	2.2	7
89	AMYR 2: A new version of a computer program for pair potential calculation of molecular associations. *Computer Physics Communications*, **1998**, 115, 87-89	4.2	7
88	Compatibility between polystyrene copolymers and polymers in solution via hydrogen bonding. *European Polymer Journal*, **2006**, 42, 2807-2823	5.2	7
87	Valence topological charge-transfer indices for dipole moments. *Molecular Diversity*, **2004**, 8, 365-70	3.1	7
86	Fractal Dimension of Different Structural-Type Zeolites and of the Active Sites. *Topics in Catalysis*, **2002**, 18, 291-297	2.3	7
85	Structural, chemical topological, electrotopological and electronic structure hypotheses. *Combinatorial Chemistry and High Throughput Screening*, **2003**, 6, 801-9	1.3	7
84	Molecular classification of pesticides including persistent organic pollutants, phenylurea and sulphonylurea herbicides. *Molecules*, **2014**, 19, 7388-414	4.8	6
83	Nucleotide's bilinear indices: novel bio-macromolecular descriptors for bioinformatics studies of nucleic acids. I. Prediction of paromomycin's affinity constant with HIV-1 Psi-RNA packaging region. *Journal of Theoretical Biology*, **2009**, 259, 229-41	2.3	6
82	QSAR models for tyrosinase inhibitory activity description applying modern statistical classification techniques: A comparative study. *Chemometrics and Intelligent Laboratory Systems*, **2010**, 104, 249-259	3.8	6
81	Incorporation of Silica Nanospherical Particles into Epoxy-Amine Crosslinked Materials. *Polymers and Polymer Composites*, **2008**, 16, 139-151	0.8	6
80	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. *Nanotechnology*, **2006**, 17, 1541-1541	3.4	6
79	A chemical index inspired by biological plastic evolution: valence-isoelectronic series of aromatics. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 575-81		6
78	Characterizing cavity-like spaces in active-site models of zeolites. *Computational Materials Science*, **2003**, 27, 96-101	3.2	6
77	Molecular Polarizability of Sc and C (Fullerene and Graphite) Clusters. *Molecules*, **2001**, 6, 496-509	4.8	6
76	State of the Art Review and Report of New Tool for Drug Discovery. *Current Topics in Medicinal Chemistry*, **2017**, 17, 2957-2976	3	6

75	A Comparative Study of Nonlinear Machine Learning for the "In Silico" Depiction of Tyrosinase Inhibitory Activity from Molecular Structure. *Molecular Informatics*, **2011**, 30, 527-37	3.8	5
74	TOMOCOMD-CAMPS and protein bilinear indices--novel bio-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, 3118-46	5.7	5
73	Fullerite crystal thermodynamic characteristics and the law of corresponding states. *Journal of Nanoscience and Nanotechnology*, **2010**, 10, 1208-22	1.3	5
72	Valence topological charge-transfer indices for dipole moments: percutaneous enhancers. *Molecules*, **2004**, 9, 1222-35	4.8	5
71	Effect of size and deformation on polarizabilities of carbon nanotubes from atomic increments. *Future Generation Computer Systems*, **2004**, 20, 763-772	7.5	5
70	Computing the Kekul structure count for alternant hydrocarbons. *International Journal of Quantum Chemistry*, **2002**, 88, 392-397	2.1	5
69	Valence topological charge-transfer indices for dipole moments. *Computational and Theoretical Chemistry*, **2003**, 621, 37-42		5
68	Fractal dimension of zeolite catalysts. *Molecular Physics*, **2002**, 100, 3105-3109	1.7	5
67	Polarization by the effect of a small torsional change in the benzothiazole (A)-benzobisthiazole (B) oligomer A-B13-A. *Molecules*, **1999**, 4, 28-51	4.8	5
66	Molecular polarizability of Si/Ge/GaAs semiconductors clusters. *Journal of Computational Methods in Sciences and Engineering*, **2004**, 4, 439-450	0.3	5
65	Binding of vinyl polymers to anionic model membranes. *Cellular and Molecular Biology*, **2003**, 49, 991-8	1.1	5
64	Solvent features of cluster single-wall C, BC2N and BN nanotubes, cones and horns. *Microelectronic Engineering*, **2013**, 108, 127-133	2.5	4
63	Using Chemical Structural Indicators for Periodic Classification of Local Anaesthetics. *International Journal of Chemoinformatics and Chemical Engineering*, **2011**, 1, 15-35	0.3	4
62	Fractal Dimension of Transdermal-Delivery Drug Models: 4-Alkylanilines. *Journal of Liquid Chromatography and Related Technologies*, **2008**, 31, 2337-2347	1.3	4
61	Fractal Dimension of Active-Site Models of Zeolite Catalysts. *Journal of Nanomaterials*, **2006**, 2006, 1-9	3.2	4
60	A comparative study of O2, CO and CN binding to heme IX protein models. *Molecules*, **2004**, 9, 632-49	4.8	4
59	New structural parameters of fullerenes for principal component analysis. *Theoretical Chemistry Accounts*, **2003**, 110, 371-376	1.9	4
58	Aqueous coefficient calculations for chemicals and drugs. *Toxicological and Environmental Chemistry*, **1999**, 73, 177-189	1.4	4

57	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. *Current Pharmaceutical Design*, **2016**, 22, 5095-5113	3.3	4
56	Computational Study of Nanosized Drug Delivery from Cyclodextrins, Crown Ethers and Hyaluronan in Pharmaceutical Formulations. *Current Topics in Medicinal Chemistry*, **2015**, 15, 1901-13	3	4
55	Lacosamide derivatives with anticonvulsant activity as carbonic anhydrase inhibitors. Molecular modeling, docking and QSAR analysis. *Current Computer-Aided Drug Design*, **2014**, 10, 160-7	1.4	4
54	Electrically Conductive Phthalocyanine Assemblies. Structural and Non-Integer Oxidation Number Considerations. *NATO ASI Series Series B: Physics*, **1990**, 461-466		4
53	Resonance in Interacting Induced-Dipole Polarizing Force Fields: Application to Force-Field Derivatives. *Algorithms*, **2009**, 2, 437-447	1.8	3
52	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	6.6	3
51	Net charge and polarizability of zeolitic Br□sted acidic sites. *International Journal of Quantum Chemistry*, **2007**, 107, 2378-2383	2.1	3
50	Modeling Studies of the Phase Behavior of Monomer/Polymer/Disk Composites. *Macromolecular Theory and Simulations*, **2008**, 17, 325-340	1.5	3
49	Effect of elliptical deformation on molecular polarizabilities of model carbon nanotubes from atomic increments. *Journal of Nanoscience and Nanotechnology*, **2003**, 3, 313-8	1.3	3
48	An Improved Force Field for O2, CO and CN Binding to Metalloporphyrins. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2004**, 49, 37-46		3
47	Nature of O2, CO, and CN binding to hemoprotein models. *International Journal of Quantum Chemistry*, **2004**, 99, 963-971	2.1	3
46	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
45	Characterizing Cavities in Model Inclusion Fullerenes: A Comparative Study. *International Journal of Molecular Sciences*, **2001**, 2, 72-88	6.3	3
44	Polarizability Characterization of Zeolitic Bnpnsted Acidic Sites **2019**, 555-556		3
43	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	0.8	3
42	Bundlet Model of Single- Wall Carbon, BC2N and BN Nanotubes, Cones and Horns in Organic Solvents. *Journal of Nanomaterials & Molecular Nanotechnology*, **2013**, 02,		3
41	Revis□ da literatura sobre or□amento em cinco peri□dicos internacionais no anos de 2000 at□ 2009. *REGE Revista De Gest□*, **2012**, 19, 107-123	1.6	3
40	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. *Journal of the Brazilian Chemical Society*, **2015**,	1.5	3

39	Classification of Complex Molecules. *Studies in Computational Intelligence*, **2009**, 243-315	0.8	3
38	Cluster solvation models of carbon nanostructures: extension to fullerenes, tubes, and buds. *Journal of Molecular Modeling*, **2014**, 20, 2263	2	2
37	Incorporation of Silica Nanospherical Particles in Epoxy−Amine Crosslinked Materials II. Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites. *Polymers and Polymer Composites*, **2009**, 17, 457-465	0.8	2
36	Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites II. *Polymers and Polymer Composites*, **2009**, 17, 313-324	0.8	2
35	Study and comparison of interaction parameters and phase behavior of epoxy/polystyrene and epoxies copolymer polystyrene-b-poly(methyl methacrylate) blends. *Polymer Composites*, **2008**, 29, 1337-1345	2	2
34	Valence topological charge-transfer indices for reflecting polarity: correction for heteromolecules. *Molecules*, **2005**, 10, 334-45	4.8	2
33	Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones and Nanohorns228-284		2
32	Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones and Nanohorns. *International Journal of Chemoinformatics and Chemical Engineering*, **2012**, 2, 48-98	0.3	2
31	QSPR Prediction of Retention Times of Methylxanthines and Cotinine by Bioplastic Evolution. *International Journal of Quantitative Structure-Property Relationships*, **2018**, 3, 74-87	1.2	2
30	Dry selection and wet evaluation for the rational discovery of new anthelmintics. *Molecular Physics*, **2017**, 115, 2300-2313	1.7	1
29	Experimental Studies for Modelling the Phase Behaviour of Monomer/Polymer/Disc Composites. *Macromolecular Symposia*, **2010**, 296, 557-565	0.8	1
28	Modelling of complex multicellular systems: tumour-immune cells competition. *Chemistry Central Journal*, **2009**, 3,		1
27	Table of periodic properties of human immunodeficiency virus inhibitors. *International Journal of Computational Intelligence in Bioinformatics and Systems Biology*, **2010**, 1, 246	0	1
26	Protein negative/positively cooperative binding to zwitterionic/anionic vesicles. *Journal of Cheminformatics*, **2010**, 2,	8.6	1
25	Improvement of charge-transfer indices for multifunctional amino acids: application to lysozyme. *SAR and QSAR in Environmental Research*, **2008**, 19, 643-54	3.5	1
24	Treatment of poly(styrene-co-methacrylic acid)/poly(4-vinylpyridine) blends in solution under liquid−liquid phase-separation conditions. A new method for phase-separation data attainment from viscosity measurements. *Journal of Applied Polymer Science*, **2006**, 102, 5039-5049	2.9	1
23	Effect of Packing on Cluster Solvation of Nanotubes **2006**,		1
22	Partition of Solvents and Co-Solvents of Nanotubes: Proteins and Cyclopyranoses. *Frontiers in Medicinal Chemistry*, **2005**, 1, 231-266		1

21	Structural Classification of Complex Molecules by Artificial Intelligence Techniques25-91		1
20	QSAR of Natural Sesquiterpene Lactones as Inhibitors of Myb-dependent Gene Expression. *Current Topics in Medicinal Chemistry*, **2018**, 17, 3256-3268	3	1
19	Information theoretic entropy for molecular classification: oxadiazolamines as potential therapeutic agents. *Current Computer-Aided Drug Design*, **2013**, 9, 241-53	1.4	1
18	Complexity, Emergence and Molecular Diversity via Information Theory **2013**, 196-208		1
17	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	0.3	1
16	Nanostructures Cluster Models in Solution. *Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series*, **2014**, 221-253	0.4	1
15	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	3.5	1
14	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. *Molecular Diversity*, **2021**, 1	3.1	1
13	Computational identification of chemical compounds with potential anti-Chagas activity using a classification tree. *SAR and QSAR in Environmental Research*, **2021**, 32, 71-83	3.5	1
12	Computational approach to the discovery of potential neprilysin inhibitors compounds for cardiovascular diseases treatment. *Medicinal Chemistry Research*, **2020**, 29, 897-909	2.2	0
11	Structure-Activity Relationships of Cytotoxic Lactones as Inhibitors and Mechanisms of Action. *Current Drug Discovery Technologies*, **2020**, 17, 166-182	1.5	0
10	Molecular Classification of N-Aryloxazolidinone-5-carboxamides as Human Immunodeficiency Virus Protease Inhibitors **2015**, 69-97		
9	Modelling Monomer/Disc Composites Phase Behaviour. *Macromolecular Symposia*, **2012**, 311, 49-56	0.8	
8	Retrained Classification of Tyrosinase Inhibitors and In Silico Potency Estimation by Using Atom-Type Linear Indices. *International Journal of Chemoinformatics and Chemical Engineering*, **2012**, 2, 42-144	0.3	
7	Cluster Origin of Solvent Features of Fullerenes, Single-Wall Carbon Nanotubes, Nanocones, and Nanohorns1-57		
6	Using Chemical Structural Indicators for Periodic Classification of Local Anaesthetics117-137		
5	Cluster Origin of Solvent Features of Fullerenes, Single-Wall Carbon Nanotubes, Nanocones, and Nanohorns262-318		
4	Matter, Plasma, Quasi Two-Dimensional Au Film, Drug Products Quality, and Circular Economy **2020**, 55-72		

3	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
2	Graphene and Fullenene Clusters. *Advances in Chemical and Materials Engineering Book Series*, **2017**, 569-599	0.2
1	Cooperativity of protein binding to vesicles. *Advances in Experimental Medicine and Biology*, **2011**, 696, 271-8	3.6