

# Francisco Torrens

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Machine learning approach to discovery of small molecules with potential inhibitory action against vasoactive metalloproteases. <i>Molecular Diversity</i> , <b>2021</b> , 1	3.1	1
199	Computational identification of chemical compounds with potential anti-Chagas activity using a classification tree. <i>SAR and QSAR in Environmental Research</i> , <b>2021</b> , 32, 71-83	3.5	1
198	Computational approach to the discovery of potential neprilysin inhibitors compounds for cardiovascular diseases treatment. <i>Medicinal Chemistry Research</i> , <b>2020</b> , 29, 897-909	2.2	0
197	Structure-Activity Relationships of Cytotoxic Lactones as Inhibitors and Mechanisms of Action. <i>Current Drug Discovery Technologies</i> , <b>2020</b> , 17, 166-182	1.5	0
196	Matter, Plasma, Quasi Two-Dimensional Au Film, Drug Products Quality, and Circular Economy <b>2020</b> , 55-72		
195	Thorough evaluation of OECD principles in modelling of 1-[(2-hydroxyethoxy)methyl]-6-(phenylthio)thymine derivatives using QSARINS. <i>SAR and QSAR in Environmental Research</i> , <b>2020</b> , 31, 741-759	3.5	1
194	Polarizability Characterization of Zeolitic Bnpnsted Acidic Sites <b>2019</b> , 555-556		3
193	An approach to identify new antihypertensive agents using Thermolysin as model: In silico study based on QSARINS and docking. <i>Arabian Journal of Chemistry</i> , <b>2019</b> , 12, 4861-4877	5.9	8
192	Revealing the relationship between vegetable oil composition and oxidative stability: A multifactorial approach. <i>Journal of Food Composition and Analysis</i> , <b>2018</b> , 66, 221-229	4.1	48
191	QSAR of Natural Sesquiterpene Lactones as Inhibitors of Myb-dependent Gene Expression. <i>Current Topics in Medicinal Chemistry</i> , <b>2018</b> , 17, 3256-3268	3	1
190	Computational Identification of Chemical Compounds with Potential Activity against Leishmania amazonensis using Nonlinear Machine Learning Techniques. <i>Current Topics in Medicinal Chemistry</i> , <b>2018</b> , 18, 2347-2354	3	9
189	QSPR Prediction of Retention Times of Methylxanthines and Cotinine by Bioplastic Evolution. <i>International Journal of Quantitative Structure-Property Relationships</i> , <b>2018</b> , 3, 74-87	1.2	2
188	Dry selection and wet evaluation for the rational discovery of new anthelmintics. <i>Molecular Physics</i> , <b>2017</b> , 115, 2300-2313	1.7	1
187	Machine learning-based models to predict modes of toxic action of phenols to Tetrahymena pyriformis. <i>SAR and QSAR in Environmental Research</i> , <b>2017</b> , 28, 735-747	3.5	9
186	State of the Art Review and Report of New Tool for Drug Discovery. <i>Current Topics in Medicinal Chemistry</i> , <b>2017</b> , 17, 2957-2976	3	6
185	Graphene and Fullenene Clusters. <i>Advances in Chemical and Materials Engineering Book Series</i> , <b>2017</b> , 569-599	6.2	
184	Generalized Molecular Descriptors Derived From Event-Based Discrete Derivative. <i>Current Pharmaceutical Design</i> , <b>2016</b> , 22, 5095-5113	3.3	4

183	Prediction of Aquatic Toxicity of Benzene Derivatives to <i>Tetrahymena pyriformis</i> According to OECD Principles. <i>Current Pharmaceutical Design</i> , <b>2016</b> , 22, 5085-5094	3.3	9
182	Cluster Origin of Solvation Features of C-Nanostructures in Organic Solvents. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , <b>2016</b> , 189-293	0.3	
181	Bond-based bilinear indices for computational discovery of novel trypanosomicidal drug-like compounds through virtual screening. <i>European Journal of Medicinal Chemistry</i> , <b>2015</b> , 96, 238-44	6.8	12
180	Molecular Classification of N-Aryloxazolidinone-5-carboxamides as Human Immunodeficiency Virus Protease Inhibitors <b>2015</b> , 69-97		
179	QuBiLS-MAS method in early drug discovery and rational drug identification of antifungal agents. <i>SAR and QSAR in Environmental Research</i> , <b>2015</b> , 26, 943-58	3.5	20
178	Quantitative Structure-Antioxidant Activity Models of Isoflavonoids: A Theoretical Study. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 12891-906	6.3	12
177	Information entropy-based classification of triterpenoids and steroids from <i>Ganoderma</i> . <i>Phytochemistry</i> , <b>2015</b> , 116, 305-313	4	13
176	Computational Study of Nanosized Drug Delivery from Cyclodextrins, Crown Ethers and Hyaluronan in Pharmaceutical Formulations. <i>Current Topics in Medicinal Chemistry</i> , <b>2015</b> , 15, 1901-13	3	4
175	Prediction of Caco-2 Cell Permeability Using Bilinear Indices and Multiple Linear Regression. <i>Letters in Drug Design and Discovery</i> , <b>2015</b> , 13, 161-169	0.8	9
174	In silico Antibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. <i>Journal of the Brazilian Chemical Society</i> , <b>2015</b> ,	1.5	3
173	QSPR prediction of chromatographic retention times of pesticides: partition and fractal indices. <i>Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes</i> , <b>2014</b> , 49, 400-7	2.2	7
172	Cluster solvation models of carbon nanostructures: extension to fullerenes, tubes, and buds. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2263	2	2
171	Discrete Derivatives for Atom-Pairs as a Novel Graph-Theoretical Invariant for Generating New Molecular Descriptors: Orthogonality, Interpretation and QSARs/QSPRs on Benchmark Databases. <i>Molecular Informatics</i> , <b>2014</b> , 33, 343-68	3.8	9
170	Molecular classification of pesticides including persistent organic pollutants, phenylurea and sulphonylurea herbicides. <i>Molecules</i> , <b>2014</b> , 19, 7388-414	4.8	6
169	Classification of stilbenoid compounds by entropy of artificial intelligence. <i>Phytochemistry</i> , <b>2014</b> , 97, 62-9	4	8
168	Tyrosinase enzyme: 1. An overview on a pharmacological target. <i>Current Topics in Medicinal Chemistry</i> , <b>2014</b> , 14, 1494-501	3	26
167	Analysis of Proteasome Inhibition Prediction Using Atom-Based Quadratic Indices Enhanced by Machine Learning Classification Techniques. <i>Letters in Drug Design and Discovery</i> , <b>2014</b> , 11, 705-711	0.8	3
166	Lacosamide derivatives with anticonvulsant activity as carbonic anhydrase inhibitors. Molecular modeling, docking and QSAR analysis. <i>Current Computer-Aided Drug Design</i> , <b>2014</b> , 10, 160-7	1.4	4

165	Nanostructures Cluster Models in Solution. <i>Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series</i> , <b>2014</b> , 221-253	0.4	1
164	Classification of flavonoid compounds by using entropy of information theory. <i>Phytochemistry</i> , <b>2013</b> , 93, 182-91	4	28
163	Solvent features of cluster single-wall C, BC2N and BN nanotubes, cones and horns. <i>Microelectronic Engineering</i> , <b>2013</b> , 108, 127-133	2.5	4
162	Comparative study to predict toxic modes of action of phenols from molecular structures. <i>SAR and QSAR in Environmental Research</i> , <b>2013</b> , 24, 235-51	3.5	14
161	Relations frequency hypermatrices in mutual, conditional and joint entropy-based information indices. <i>Journal of Computational Chemistry</i> , <b>2013</b> , 34, 259-74	3.5	23
160	Event-based criteria in GT-STAF information indices: theory, exploratory diversity analysis and QSPR applications. <i>SAR and QSAR in Environmental Research</i> , <b>2013</b> , 24, 3-34	3.5	16
159	Shannon's, mutual, conditional and joint entropy information indices: generalization of global indices defined from local vertex invariants. <i>Current Computer-Aided Drug Design</i> , <b>2013</b> , 9, 164-83	1.4	19
158	Information theoretic entropy for molecular classification: oxadiazolamines as potential therapeutic agents. <i>Current Computer-Aided Drug Design</i> , <b>2013</b> , 9, 241-53	1.4	1
157	Bundlet Model of Single- Wall Carbon, BC2N and BN Nanotubes, Cones and Horns in Organic Solvents. <i>Journal of Nanomaterials &amp; Molecular Nanotechnology</i> , <b>2013</b> , 02,		3
156	Complexity, Emergence and Molecular Diversity via Information Theory <b>2013</b> , 196-208		1
155	Molecular Classification of 5-Amino-2-Aroylquinolines and 4-Aroyl-6,7,8-Trimethoxyquinolines as Highly Potent Tubulin Polymerization Inhibitors. <i>International Journal of Chemoinformatics and Chemical Engineering</i> , <b>2013</b> , 3, 1-26	0.3	1
154	Identification in silico and in vitro of novel trypanosomicidal drug-like compounds. <i>Chemical Biology and Drug Design</i> , <b>2012</b> , 80, 38-45	2.9	9
153	Derivatives in discrete mathematics: a novel graph-theoretical invariant for generating new 2/3D molecular descriptors. I. Theory and QSPR application. <i>Journal of Computer-Aided Molecular Design</i> , <b>2012</b> , 26, 1229-46	4.2	13
152	Modelling Monomer/Disc Composites Phase Behaviour. <i>Macromolecular Symposia</i> , <b>2012</b> , 311, 49-56	0.8	
151	Retrained Classification of Tyrosinase Inhibitors and In Silico Potency Estimation by Using Atom-Type Linear Indices. <i>International Journal of Chemoinformatics and Chemical Engineering</i> , <b>2012</b> , 2, 42-144	0.3	
150	A review of QSAR studies to discover new drug-like compounds actives against leishmaniasis and trypanosomiasis. <i>Current Topics in Medicinal Chemistry</i> , <b>2012</b> , 12, 852-65	3	19
149	QSPR prediction of retention times of phenylurea herbicides by biological plastic evolution. <i>Current Drug Safety</i> , <b>2012</b> , 7, 262-8	1.4	8
148	Revisã da literatura sobre orãmento em cinco periãdicos internacionais no anos de 2000 atã 2009. <i>REGE Revista De Gestã</i> , <b>2012</b> , 19, 107-123	1.6	3

147	Bundlet Model for Single-Wall Carbon Nanotubes, Nanocones and Nanohorns. <i>International Journal of Chemoinformatics and Chemical Engineering</i> , <b>2012</b> , 2, 48-98	0.3	2
146	(Co-)solvent selection for single-wall carbon nanotubes: best solvents, acids, superacids and guest-host inclusion complexes. <i>Nanoscale</i> , <b>2011</b> , 3, 2494-510	7.7	12
145	Using Chemical Structural Indicators for Periodic Classification of Local Anaesthetics. <i>International Journal of Chemoinformatics and Chemical Engineering</i> , <b>2011</b> , 1, 15-35	0.3	4
144	Discovery of novel anti-inflammatory drug-like compounds by aligning in silico and in vivo screening: the nitroindazolinone chemotype. <i>European Journal of Medicinal Chemistry</i> , <b>2011</b> , 46, 5736-53	6.8	29
143	Novel coumarin-based tyrosinase inhibitors discovered by OECD principles-validated QSAR approach from an enlarged, balanced database. <i>Molecular Diversity</i> , <b>2011</b> , 15, 507-20	3.1	13
142	A Comparative Study of Nonlinear Machine Learning for the "In Silico" Depiction of Tyrosinase Inhibitory Activity from Molecular Structure. <i>Molecular Informatics</i> , <b>2011</b> , 30, 527-37	3.8	5
141	Ligand-based discovery of novel trypanosomicidal drug-like compounds: in silico identification and experimental support. <i>European Journal of Medicinal Chemistry</i> , <b>2011</b> , 46, 3324-30	6.8	18
140	Cooperativity of protein binding to vesicles. <i>Advances in Experimental Medicine and Biology</i> , <b>2011</b> , 696, 271-8	3.6	
139	Bond-based 2D quadratic fingerprints in QSAR studies: virtual and in vitro tyrosinase inhibitory activity elucidation. <i>Chemical Biology and Drug Design</i> , <b>2010</b> , 76, 538-45	2.9	25
138	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. <i>FEBS Journal</i> , <b>2010</b> , 277, 3118-46	5.7	5
137	Experimental Studies for Modelling the Phase Behaviour of Monomer/Polymer/Disc Composites. <i>Macromolecular Symposia</i> , <b>2010</b> , 296, 557-565	0.8	1
136	Ligand-based computer-aided discovery of tyrosinase inhibitors. Applications of the TOMOCOMD-CARDD method to the elucidation of new compounds. <i>Current Pharmaceutical Design</i> , <b>2010</b> , 16, 2601-24	3.3	33
135	Fullerite crystal thermodynamic characteristics and the law of corresponding states. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2010</b> , 10, 1208-22	1.3	5
134	Table of periodic properties of human immunodeficiency virus inhibitors. <i>International Journal of Computational Intelligence in Bioinformatics and Systems Biology</i> , <b>2010</b> , 1, 246	0	1
133	Bond-based linear indices of the non-stochastic and stochastic edge-adjacency matrix. 1. Theory and modeling of ChemPhys properties of organic molecules. <i>Molecular Diversity</i> , <b>2010</b> , 14, 731-53	3.1	11
132	Computational discovery of novel trypanosomicidal drug-like chemicals by using bond-based non-stochastic and stochastic quadratic maps and linear discriminant analysis. <i>European Journal of Pharmaceutical Sciences</i> , <b>2010</b> , 39, 30-6	5.1	24
131	QSAR models for tyrosinase inhibitory activity description applying modern statistical classification techniques: A comparative study. <i>Chemometrics and Intelligent Laboratory Systems</i> , <b>2010</b> , 104, 249-259	3.8	6
130	Protein negative/positively cooperative binding to zwitterionic/anionic vesicles. <i>Journal of Cheminformatics</i> , <b>2010</b> , 2,	8.6	1

129	Cluster nature of the solvent features of single-wall carbon nanohorns. <i>International Journal of Quantum Chemistry</i> , <b>2010</b> , 110, 563-570	2.1	9
128	Resonance in Interacting Induced-Dipole Polarizing Force Fields: Application to Force-Field Derivatives. <i>Algorithms</i> , <b>2009</b> , 2, 437-447	1.8	3
127	Topological Charge-Transfer Indices: From Small Molecules to Proteins. <i>Current Proteomics</i> , <b>2009</b> , 6, 204-213	2.1	11
126	Discovery of Novel Trichomonacids Using LDA-Driven QSAR Models and Bond-Based Bilinear Indices as Molecular Descriptors. <i>QSAR and Combinatorial Science</i> , <b>2009</b> , 28, 9-26		13
125	Applications of Bond-Based 3D-Chiral Quadratic Indices in QSAR Studies Related to Central Chirality Codification. <i>QSAR and Combinatorial Science</i> , <b>2009</b> , 28, 1465-1477		8
124	Modelling of complex multicellular systems: tumour-immune cells competition. <i>Chemistry Central Journal</i> , <b>2009</b> , 3,		1
123	Binding of water-soluble, globular proteins to anionic model membranes. <i>Journal of Molecular Structure</i> , <b>2009</b> , 924-926, 274-284	3.4	8
122	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. <i>Journal of Theoretical Biology</i> , <b>2009</b> , 259, 229-41	2.3	6
121	Comparative analysis of the electrostatics of the binding of cationic proteins to vesicles: asymmetric location of anionic phospholipids. <i>Analytica Chimica Acta</i> , <b>2009</b> , 654, 2-10	6.6	3
120	Incorporation of Silica Nanospherical Particles in Epoxy-Amine Crosslinked Materials II. Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites. <i>Polymers and Polymer Composites</i> , <b>2009</b> , 17, 457-465	0.8	2
119	Dynamic Mechanical Measurements of Epoxy Matrix-Silica Nanocomposites II. <i>Polymers and Polymer Composites</i> , <b>2009</b> , 17, 313-324	0.8	2
118	Classification of Complex Molecules. <i>Studies in Computational Intelligence</i> , <b>2009</b> , 243-315	0.8	3
117	A novel approach to predict aquatic toxicity from molecular structure. <i>Chemosphere</i> , <b>2008</b> , 73, 415-27	8.4	45
116	Improvement of charge-transfer indices for multifunctional amino acids: application to lysozyme. <i>SAR and QSAR in Environmental Research</i> , <b>2008</b> , 19, 643-54	3.5	1
115	Atom- and bond-based 2D TOMOCOMD-CARDD approach and ligand-based virtual screening for the drug discovery of new tyrosinase inhibitors. <i>Journal of Biomolecular Screening</i> , <b>2008</b> , 13, 1014-24		23
114	New antitrichomonal drug-like chemicals selected by bond (edge)-based TOMOCOMD-CARDD descriptors. <i>Journal of Biomolecular Screening</i> , <b>2008</b> , 13, 785-94		14
113	Fractal Dimension of Transdermal-Delivery Drug Models: 4-Alkylanilines. <i>Journal of Liquid Chromatography and Related Technologies</i> , <b>2008</b> , 31, 2337-2347	1.3	4
112	Incorporation of Silica Nanospherical Particles into Epoxy-Amine Crosslinked Materials. <i>Polymers and Polymer Composites</i> , <b>2008</b> , 16, 139-151	0.8	6

111	3D-chiral (2.5) atom-based TOMOCOMD-CARDD descriptors: theory and QSAR applications to central chirality codification. <i>Journal of Mathematical Chemistry</i> , <b>2008</b> , 44, 755-786	2.1	21
110	Novel 2D TOMOCOMD-CARDD molecular descriptors: atom-based stochastic and non-stochastic bilinear indices and their QSPR applications. <i>Journal of Mathematical Chemistry</i> , <b>2008</b> , 44, 650-673	2.1	15
109	Bond-based linear indices in QSAR: computational discovery of novel anti-trichomonal compounds. <i>Journal of Computer-Aided Molecular Design</i> , <b>2008</b> , 22, 523-40	4.2	24
108	Study and comparison of interaction parameters and phase behavior of epoxy/polystyrene and epoxies copolymer polystyrene-b-poly(methyl methacrylate) blends. <i>Polymer Composites</i> , <b>2008</b> , 29, 1337 <sup>2</sup> 1345 <sup>2</sup>		
107	Estimation of ADME properties in drug discovery: predicting Caco-2 cell permeability using atom-based stochastic and non-stochastic linear indices. <i>Journal of Pharmaceutical Sciences</i> , <b>2008</b> , 97, 1946-76	3.9	55
106	Modeling Studies of the Phase Behavior of Monomer/Polymer/Disk Composites. <i>Macromolecular Theory and Simulations</i> , <b>2008</b> , 17, 325-340	1.5	3
105	Bond-based 3D-chiral linear indices: theory and QSAR applications to central chirality codification. <i>Journal of Computational Chemistry</i> , <b>2008</b> , 29, 2500-12	3.5	25
104	Atom-based non-stochastic and stochastic bilinear indices: Application to QSPR/QSAR studies of organic compounds. <i>Chemical Physics Letters</i> , <b>2008</b> , 464, 107-112	2.5	20
103	Prediction of tyrosinase inhibition activity using atom-based bilinear indices. <i>ChemMedChem</i> , <b>2007</b> , 2, 449-78	3.7	43
102	TOMOCOMD-CARDD descriptors-based virtual screening of tyrosinase inhibitors: evaluation of different classification model combinations using bond-based linear indices. <i>Bioorganic and Medicinal Chemistry</i> , <b>2007</b> , 15, 1483-503	3.4	68
101	Dragon method for finding novel tyrosinase inhibitors: Biosilico identification and experimental in vitro assays. <i>European Journal of Medicinal Chemistry</i> , <b>2007</b> , 42, 1370-81	6.8	57
100	Effect of packing on the cluster nature of C nanotubes: An information entropy analysis. <i>Microelectronics Journal</i> , <b>2007</b> , 38, 1109-1122	1.8	16
99	Negatively cooperative binding of melittin to neutral phospholipid vesicles. <i>Journal of Molecular Structure</i> , <b>2007</b> , 834-836, 216-228	3.4	14
98	Atom-based stochastic and non-stochastic 3D-chiral bilinear indices and their applications to central chirality codification. <i>Journal of Molecular Graphics and Modelling</i> , <b>2007</b> , 26, 32-47	2.8	39
97	Atom-Based 2D Quadratic Indices in Drug Discovery of Novel Tyrosinase Inhibitors: Results of In Silico Studies Supported by Experimental Results. <i>QSAR and Combinatorial Science</i> , <b>2007</b> , 26, 469-487		11
96	Net charge and polarizability of zeolitic Brønsted acidic sites. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 2378-2383	2.1	3
95	Bond-based 2D TOMOCOMD-CARDD approach for drug discovery: aiding decision-making in 'in silico' selection of new lead tyrosinase inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , <b>2007</b> , 21, 167-88	4.2	18
94	Asymptotic Analysis of Coagulation-Fragmentation Equations of Carbon Nanotube Clusters. <i>Nanoscale Research Letters</i> , <b>2007</b> , 2, 337-349	5	12

93	Cluster Origin of the Transfer Phenomena of Single-Wall Carbon Nanotubes. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2007</b> , 4, 588-603	0.3	12
92	New tyrosinase inhibitors selected by atomic linear indices-based classification models. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2006</b> , 16, 324-30	2.9	48
91	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. <i>Journal of Applied Polymer Science</i> , <b>2006</b> , 102, 5039-5049	2.9	1
90	Effect of Packing on Cluster Solvation of Nanotubes <b>2006</b> ,		1
89	Periodic Classification of Local Anaesthetics (Procaine Analogues). <i>International Journal of Molecular Sciences</i> , <b>2006</b> , 7, 12-34	6.3	17
88	Fractal Dimension of Active-Site Models of Zeolite Catalysts. <i>Journal of Nanomaterials</i> , <b>2006</b> , 2006, 1-9	3.2	4
87	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. <i>Nanotechnology</i> , <b>2006</b> , 17, 1541-1541	3.4	6
86	Calculations of organic-solvent dispersions of single-wall carbon nanotubes. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 712-718	2.1	17
85	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. <i>European Journal of Medicinal Chemistry</i> , <b>2006</b> , 41, 483-93	6.8	36
84	Compatibility between polystyrene copolymers and polymers in solution via hydrogen bonding. <i>European Polymer Journal</i> , <b>2006</b> , 42, 2807-2823	5.2	7
83	Predicting antitrichomonal activity: a computational screening using atom-based bilinear indices and experimental proofs. <i>Bioorganic and Medicinal Chemistry</i> , <b>2006</b> , 14, 6502-24	3.4	48
82	New ligand-based approach for the discovery of antitrypanosomal compounds. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2006</b> , 16, 1898-904	2.9	34
81	Atom-based 3D-chiral quadratic indices. Part 2: prediction of the corticosteroid-binding globulin-binding affinity of the 31 benchmark steroids data set. <i>Bioorganic and Medicinal Chemistry</i> , <b>2006</b> , 14, 2398-408	3.4	32
80	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. <i>Journal of Computer-Aided Molecular Design</i> , <b>2006</b> , 20, 685-701	4.2	21
79	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. <i>Journal of Molecular Modeling</i> , <b>2006</b> , 12, 255-71	2	48
78	Partition of Solvents and Co-Solvents of Nanotubes: Proteins and Cyclopyranoses. <i>Frontiers in Medicinal Chemistry</i> , <b>2005</b> , 1, 231-266		1
77	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 1005-20	3.4	84
76	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 3003-15	3.4	65



75	Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising approach for modeling of antibacterial activity. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 2881-99	3.4	62
74	Interaction of polyelectrolytes with oppositely charged micelles studied by fluorescence and liquid chromatography. <i>European Polymer Journal</i> , <b>2005</b> , 41, 1439-1452	5.2	14
73	Calculations on solvents and co-solvents of single-wall carbon nanotubes: Cyclopyranoses. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 757, 183-191		17
72	Valence topological charge-transfer indices for reflecting polarity: correction for heteromolecules. <i>Molecules</i> , <b>2005</b> , 10, 334-45	4.8	2
71	A computer-based approach to the rational discovery of new trichomonacidal drugs by atom-type linear indices. <i>Current Drug Discovery Technologies</i> , <b>2005</b> , 2, 245-65	1.5	33
70	Calculations on solvents and co-solvents of single-wall carbon nanotubes:cyclopyranoses. <i>Nanotechnology</i> , <b>2005</b> , 16, S181-S189	3.4	15
69	Calculations on cyclopyranoses as co-solvents of single-wall carbon nanotubes. <i>Molecular Simulation</i> , <b>2005</b> , 31, 107-114	2	15
68	Cluster Origin of the Solubility of Single-Wall Carbon Nanotubes. <i>Computing Letters</i> , <b>2005</b> , 1, 331-336		13
67	Protein quadratic indices of the "macromolecular pseudograph's alpha-carbon atom adjacency matrix". 1. Prediction of Arc repressor alanine-mutant's stability. <i>Molecules</i> , <b>2004</b> , 9, 1124-47	4.8	38
66	Nucleic Acid Quadratic Indices of the Macromolecular Graph's Nucleotides Adjacency Matrix Modeling of Footprints after the Interaction of Paromomycin with the HIV-1 RNA Packaging Region. <i>International Journal of Molecular Sciences</i> , <b>2004</b> , 5, 276-293	6.3	51
65	A comparative study of O <sub>2</sub> , CO and CN binding to heme IX protein models. <i>Molecules</i> , <b>2004</b> , 9, 632-49	4.8	4
64	Atom, atom-type, and total linear indices of the "molecular pseudograph's atom adjacency matrix": application to QSPR/QSAR studies of organic compounds. <i>Molecules</i> , <b>2004</b> , 9, 1100-23	4.8	52
63	Valence topological charge-transfer indices for dipole moments: percutaneous enhancers. <i>Molecules</i> , <b>2004</b> , 9, 1222-35	4.8	5
62	An Improved Force Field for O <sub>2</sub> , CO and CN Binding to Metalloporphyrins. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , <b>2004</b> , 49, 37-46		3
61	Valence topological charge-transfer indices for dipole moments. <i>Molecular Diversity</i> , <b>2004</b> , 8, 365-70	3.1	7
60	Effect of size and deformation on polarizabilities of carbon nanotubes from atomic increments. <i>Future Generation Computer Systems</i> , <b>2004</b> , 20, 763-772	7.5	5
59	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. <i>Journal of Computer-Aided Molecular Design</i> , <b>2004</b> , 18, 615-34	4.2	54
58	Nature of O <sub>2</sub> , CO, and CN binding to hemoprotein models. <i>International Journal of Quantum Chemistry</i> , <b>2004</b> , 99, 963-971	2.1	3

57	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2004</b> , 12, 5331-42	3.4	79
56	QSAR Modeling ANTI-HIV-1 Activities by Optimization of Correlation Weights of Local Graph Invariants. <i>Molecular Simulation</i> , <b>2004</b> , 30, 691-696	2	8
55	Table of periodic properties of fullerenes based on structural parameters. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2004</b> , 44, 60-7		13
54	A chemical index inspired by biological plastic evolution: valence-iso-electronic series of aromatics. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2004</b> , 44, 575-81		6
53	Effect of type, size and deformation on the polarizability of carbon nanotubes from atomic increments. <i>Nanotechnology</i> , <b>2004</b> , 15, S259-S264	3.4	15
52	Molecular polarizability of Si/Ge/GaAs semiconductors clusters. <i>Journal of Computational Methods in Sciences and Engineering</i> , <b>2004</b> , 4, 439-450	0.3	5
51	A new topological descriptors based model for predicting intestinal epithelial transport of drugs in Caco-2 cell culture. <i>Journal of Pharmacy and Pharmaceutical Sciences</i> , <b>2004</b> , 7, 186-99	3.4	56
50	Effect of elliptical deformation on molecular polarizabilities of model carbon nanotubes from atomic increments. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2003</b> , 3, 313-8	1.3	3
49	Valence Topological Charge-Transfer Indices for Dipole Moments. <i>Molecules</i> , <b>2003</b> , 8, 169-185	4.8	9
48	New structural parameters of fullerenes for principal component analysis. <i>Theoretical Chemistry Accounts</i> , <b>2003</b> , 110, 371-376	1.9	4
47	Valence topological charge-transfer indices for dipole moments. <i>Computational and Theoretical Chemistry</i> , <b>2003</b> , 621, 37-42		5
46	Nature of FeIII $\mu$ O <sub>2</sub> , FeIII $\mu$ O and FeIII $\mu$ N complexes of hemoprotein models. <i>Polyhedron</i> , <b>2003</b> , 22, 1091-1098	4.8	11
45	Characterizing cavity-like spaces in active-site models of zeolites. <i>Computational Materials Science</i> , <b>2003</b> , 27, 96-101	3.2	6
44	QSPR Modeling of Hydrocarbon Dipole Moments by Means of Correlation Weighting of Local Graph Invariants. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2003</b> , 02, 139-146	1.8	3
43	Structural, chemical topological, electrotopological and electronic structure hypotheses. <i>Combinatorial Chemistry and High Throughput Screening</i> , <b>2003</b> , 6, 801-9	1.3	7
42	Binding of vinyl polymers to anionic model membranes. <i>Cellular and Molecular Biology</i> , <b>2003</b> , 49, 991-8	1.1	5
41	Fractal Hybrid Orbitals Analysis of the Tertiary Structure of Protein Molecules. <i>Molecules</i> , <b>2002</b> , 7, 26-37	4.8	9
40	Molecular polarizability of semiconductor clusters and nanostructures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2002</b> , 13, 67-71	3	17

39	Calculation of organic solvent-water partition coefficients of iron-sulfur protein models. <i>Polyhedron</i> , <b>2002</b> , 21, 1357-1361	2.7	10
38	Molecular polarizability of fullerenes and endohedral metallofullerenes. <i>Journal of Physical Organic Chemistry</i> , <b>2002</b> , 15, 742-749	2.1	15
37	Computing the Kekulé structure count for alternant hydrocarbons. <i>International Journal of Quantum Chemistry</i> , <b>2002</b> , 88, 392-397	2.1	5
36	Fractal Dimension of Different Structural-Type Zeolites and of the Active Sites. <i>Topics in Catalysis</i> , <b>2002</b> , 18, 291-297	2.3	7
35	Stationary/mobile phase distribution coefficient for polystyrene standards. <i>Separation Science and Technology</i> , <b>2002</b> , 37, 1653-1665	2.5	9
34	Molecular polarizability of Sc <sub>n</sub> , C <sub>n</sub> and endohedral Sc <sub>n</sub> @C <sub>m</sub> clusters. <i>Nanotechnology</i> , <b>2002</b> , 13, 433-438	3.4	8
33	Fractal dimension of zeolite catalysts. <i>Molecular Physics</i> , <b>2002</b> , 100, 3105-3109	1.7	5
32	Free energy of solvation of solutes and their partition coefficients in methanol-water binary mixtures. <i>Chromatographia</i> , <b>2001</b> , 53, S199-S203	2.1	16
31	New dimension indices for the characterization of the solvent-accessible surface. <i>Journal of Computational Chemistry</i> , <b>2001</b> , 22, 477-487	3.5	9
30	Calculation of partition coefficient and hydrophobic moment of the secondary structure of lysozyme. <i>Journal of Chromatography A</i> , <b>2001</b> , 908, 215-21	4.5	15
29	A new topological index to elucidate apolar hydrocarbons. <i>Journal of Computer-Aided Molecular Design</i> , <b>2001</b> , 15, 709-19	4.2	12
28	Molecular Polarizability of Sc and C (Fullerene and Graphite) Clusters. <i>Molecules</i> , <b>2001</b> , 6, 496-509	4.8	6
27	Characterizing Cavities in Model Inclusion Fullerenes: A Comparative Study. <i>International Journal of Molecular Sciences</i> , <b>2001</b> , 2, 72-88	6.3	3
26	Polarization Force Fields for Peptides Implemented in ECEPP2 and MM2. <i>Molecular Simulation</i> , <b>2000</b> , 24, 391-410	2	15
25	Molecular polarizability of Sc <sub>n</sub> , C <sub>n</sub> and endohedral Sc <sub>n</sub> @C <sub>m</sub> clusters. <i>Microelectronic Engineering</i> , <b>2000</b> , 51-52, 613-626	2.5	11
24	Universal organic solvent-water partition coefficient model. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2000</b> , 40, 236-40		20
23	Polarization by the effect of a small torsional change in the benzothiazole (A)-benzobisthiazole (B) oligomer A-B13-A. <i>Molecules</i> , <b>1999</b> , 4, 28-51	4.8	5
22	Aqueous coefficient calculations for chemicals and drugs. <i>Toxicological and Environmental Chemistry</i> , <b>1999</b> , 73, 177-189	1.4	4

21	Interacting induced dipoles polarization model for molecular polarizabilities. Reference molecules, amino acids and model peptides. <i>Computational and Theoretical Chemistry</i> , <b>1999</b> , 463, 27-39		18
20	AMYR 2: A new version of a computer program for pair potential calculation of molecular associations. <i>Computer Physics Communications</i> , <b>1998</b> , 115, 87-89	4.2	7
19	Universal model for the calculation of all organic solvent-water partition coefficients. <i>Journal of Chromatography A</i> , <b>1998</b> , 827, 345-358	4.5	27
18	Interacting induced dipoles polarization model for molecular polarizabilities: application to benzothiazole (A)-benzobisthiazole (B) oligomers A <sub>n</sub> B <sub>13-n</sub> A. <i>Computational and Theoretical Chemistry</i> , <b>1998</b> , 426, 105-116		13
17	Characterizing cavities in model inclusion molecules: a comparative study. <i>Journal of Molecular Graphics and Modelling</i> , <b>1998</b> , 16, 57-71	2.8	9
16	Theoretical characterization of iron and manganese porphyrins for catalyzed saturated alkane hydroxylations. <i>Journal of Molecular Catalysis A</i> , <b>1997</b> , 119, 393-403		12
15	Torsional effects on the molecular polarizabilities of the benzothiazole (A)-benzobisthiazole (B) oligomer A-B <sub>13</sub> -A. <i>Journal of Molecular Graphics</i> , <b>1996</b> , 14, 245-59, 277		14
14	Are most of the stationary points in a molecular association minima? Application of Fraga's potential to benzene-Benzene. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 647-654	3.5	19
13	Conformational aspects of some asymmetric Diels-Alder reactions. A molecular mechanics + polarization study. <i>Tetrahedron</i> , <b>1992</b> , 48, 5209-5218	2.4	27
12	Molecular aggregation of polycyclic aromatic hydrocarbons. A theoretical modelling of coronene aggregation. <i>Computational and Theoretical Chemistry</i> , <b>1992</b> , 254, 429-441		14
11	Improved AMYR program: an algorithm for the theoretical simulation of molecular associations, including geometrical and topological characterization of the dimers. <i>Journal of Molecular Graphics</i> , <b>1991</b> , 9, 254-6		10
10	Pair potential calculation of molecular associations: a vectorized version. <i>Computer Physics Communications</i> , <b>1991</b> , 66, 341-362	4.2	19
9	Vectorized TOPO program for the theoretical simulation of molecular shape. <i>Journal De Chimie Physique Et De Physico-Chimie Biologique</i> , <b>1991</b> , 88, 2435-2441		30
8	Electrically Conductive Phthalocyanine Assemblies. Structural and Non-Integer Oxidation Number Considerations. <i>NATO ASI Series Series B: Physics</i> , <b>1990</b> , 461-466		4
7	The use of electrostatic charges to improve Fraga's atom-atom pair potential for molecular association. <i>Computational and Theoretical Chemistry</i> , <b>1988</b> , 166, 135-140		18
6	Incorporation of a dispersion energy term to Fraga's atom-atom pair intermolecular potential. Application to benzene, s-tetrazine, and their mixed dimers. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1987</b> , 943-950		20
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