Humbert GonzÃ¡lez-DÃ-az

List of Publications by Year
in descending order

283 papers	8,932 citations	31949 53 h-index	74108 75 g-index
291 all docs	291 docs citations	291 times ranked	3505 citing authors

#	Article	IF	Citations
1	Medicinal Chemistry and Bioinformatics - Current Trends in Drugs Discovery with Networks Topological Indices. Current Topics in Medicinal Chemistry, 2007, 7, 1015-1029.	1.0	271
2	Proteomics, networks and connectivity indices. Proteomics, 2008, 8, 750-778.	1.3	207
3	Unified QSAR approach to antimicrobials. Part 3: First multi-tasking QSAR model for Input-Coded prediction, structural back-projection, and complex networks clustering of antiprotozoal compounds. Bioorganic and Medicinal Chemistry, 2008, 16, 5871-5880.	1.4	197
4	Predicting Antimicrobial Drugs and Targets with the MARCH-INSIDE Approach. Current Topics in Medicinal Chemistry, 2008, 8, 1676-1690.	1.0	142
5	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarinsâ€. Journal of Medicinal Chemistry, 2006, 49, 1149-1156.	2.9	140
6	Computational Tool for Risk Assessment of Nanomaterials: Novel QSTR-Perturbation Model for Simultaneous Prediction of Ecotoxicity and Cytotoxicity of Uncoated and Coated Nanoparticles under Multiple Experimental Conditions. Environmental Science & Technology, 2014, 48, 14686-14694.	4.6	124
7	Computer-aided nanotoxicology: assessing cytotoxicity of nanoparticles under diverse experimental conditions by using a novel QSTR-perturbation approach. Nanoscale, 2014, 6, 10623.	2.8	118
8	Quantitative Structureâ^'Activity Relationship and Complex Network Approach to Monoamine Oxidase A and B Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 6740-6751.	2.9	109
9	Multi-target spectral moment QSAR versus ANN for antiparasitic drugs against different parasite species. Bioorganic and Medicinal Chemistry, 2010, 18, 2225-2231.	1.4	109
10	Unified QSAR approach to antimicrobials. 4. Multi-target QSAR modeling and comparative multi-distance study of the giant components of antiviral drugâ€“drug complex networks. Bioorganic and Medicinal Chemistry, 2009, 17, 569-575.	1.4	106
11	Computational ecotoxicology: Simultaneous prediction of ecotoxic effects of nanoparticles under different experimental conditions. Environment International, 2014, 73, 288-294.	4.8	102
12	Novel 2D maps and coupling numbers for protein sequences. The first QSAR study of polygalacturonases; isolation and prediction of a novel sequence fromPsidium guajavaL.. FEBS Letters, 2006, 580, 723-730.	1.3	94
13	Unified QSAR and networkâ€based computational chemistry approach to antimicrobials, part 1: Multispecies activity models for antifungals. Journal of Computational Chemistry, 2008, 29, 656-667.	1.5	90
14	TOPS-MODE Based QSARs Derived from Heterogeneous Series of Compounds. Applications to the Design of New Herbicides. Journal of Chemical Information and Computer Sciences, 2003, 43, 1192-1199.	2.8	89
15	3D-MEDNEs:â€‰ An Alternative â€œIn Silicoâ€•Technique for Chemical Research in Toxicology. 1. Prediction of Chemically Induced Agranulocytosis. Chemical Research in Toxicology, 2003, 16, 1318-1327.	1.7	88
16	HP-Lattice QSAR for dynein proteins: Experimental proteomics (2D-electrophoresis, mass spectrometry) and theoretic study of a Leishmania infantum sequence. Bioorganic and Medicinal Chemistry, 2008, 16, 7770-7776.	1.4	88
17	Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer-aided molecular design I: discovery of anticancer compounds. Journal of Molecular Modeling, 2003, 9, 395-407.	0.8	87
18	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

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19	Alignment-Free Prediction of a Drugâ˜Target Complex Network Based on Parameters of Drug Connectivity and Protein Sequence of Receptors. Molecular Pharmaceutics, 2009, 6, 825-835.	2.3	83
20	General Theory for Multiple Input-Output Perturbations in Complex Molecular Systems. 1. Linear QSPR Electronegativity Models in Physical, Organic, and Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2013, 13, 1713-1741.	1.0	83
21	Designing Antibacterial Compounds through a Topological Substructural Approach. Journal of Chemical Information and Computer Sciences, 2004, 44, 515-521.	2.8	82
22	Stochastic-based descriptors studying peptides biological properties: modeling the bitter tasting threshold of dipeptides. Bioorganic and Medicinal Chemistry, 2004, 12, 4815-4822.	1.4	81
23	Prediction of Enzyme Classes from 3D Structure: A General Model and Examples of Experimental-Theoretic Scoring of Peptide Mass Fingerprints of Leishmania Proteins. Journal of Proteome Research, 2009, 8, 4372-4382.	1.8	81
24	Computational chemistry development of a unified free energy Markov model for the distribution of 1300 chemicals to 38 different environmental or biological systems. Journal of Computational Chemistry, 2007, 28, 1909-1923.	1.5	79
25	A Model for the Recognition of Protein Kinases Based on the Entropy of 3D van der Waals Interactions. Journal of Proteome Research, 2007, 6, 904-908.	1.8	78
26	Review of MARCH-INSIDE & Complex Networks Prediction of Drugs: ADMET, Anti-parasite Activity, Metabolizing Enzymes and Cardiotoxicity Proteome Biomarkers. Current Drug Metabolism, 2010, 11, 379-406.	0.7	76
27	MIND-BEST: Web Server for Drugs and Target Discovery; Design, Synthesis, and Assay of MAO-B Inhibitors and Theoreticalâ˜Experimental Study of G3PDH Protein fromTrichomonas gallinae. Journal of Proteome Research, 2011, 10, 1698-1718.	1.8	75
28	Markovian Backbone Negentropies: Molecular descriptors for protein research. I. Predicting protein stability in Arc repressor mutants. Proteins: Structure, Function and Bioinformatics, 2004, 56, 715-723.	1.5	74
29	QSAR-Co: An Open Source Software for Developing Robust Multitasking or Multitarget Classification-Based QSAR Models. Journal of Chemical Information and Modeling, 2019, 59, 2538-2544.	2.5	73
30	Multi-target QPDR classification model for human breast and colon cancer-related proteins using star graph topological indices. Journal of Theoretical Biology, 2009, 257, 303-311.	0.8	72
31	Unified QSAR approach to antimicrobials. Part 2: Predicting activity against more than 90 different species in order to halt antibacterial resistance. Bioorganic and Medicinal Chemistry, 2007, 15, 897-902.	1.4	70
32	Unify QSAR approach to antimicrobials. Part 1: Predicting antifungal activity against different species. Bioorganic and Medicinal Chemistry, 2006, 14, 5973-5980.	1.4	69
33	First computational chemistry multi-target model for anti-Alzheimer, anti-parasitic, anti-fungi, and anti-bacterial activity of GSK-3 inhibitors in vitro, in vivo, and in different cellular lines. Molecular Diversity, 2011, 15, 561-567.	2.1	68
34	Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer aided molecular design II: experimental and theoretical assessment of a novel method for virtual screening of fasciolicides. Journal of Molecular Modeling, 2002, 8, 237-245.	0.8	67
35	ANN-QSAR model for selection of anticancer leads from structurally heterogeneous series of compounds. European Journal of Medicinal Chemistry, 2007, 42, 580-585.	2.6	67
36	A network-QSAR model for prediction of genetic-component biomarkers in human colorectal cancer. Journal of Theoretical Biology, 2009, 261, 449-458.	0.8	67

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37	Multi-target spectral moments for QSAR and Complex Networks study of antibacterial drugs. European Journal of Medicinal Chemistry, 2009, 44, 4516-4521.	2.6	66
38	Markovian negentropies in bioinformatics. 1. A picture of footprints after the interaction of the HIV-1 Â-RNA packaging region with drugs. Bioinformatics, 2003, 19, 2079-2087.	1.8	65
39	Alignment-Free Prediction of Polygalacturonases with Pseudofolding Topological Indices: Experimental Isolation from Coffea arabica and Prediction of a New Sequence. Journal of Proteome Research, 2009, 8, 2122-2128.	1.8	65
40	A psychosocial analysis of parents' decisions for limiting their young child's screen time: An examination of attitudes, social norms and roles, and control perceptions. British Journal of Health Psychology, 2016, 21, 285-301.	1.9	64
41	Enzymes/non-enzymes classification model complexity based on composition, sequence, 3D and topological indices. Journal of Theoretical Biology, 2008, 254, 476-482.	0.8	63
42	Using the TOPS-MODE approach to fit multi-target QSAR models for tyrosine kinases inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 2185-2192.	2.6	62
43	3D-QSAR study for DNA cleavage proteins with a potential anti-tumor ATCUN-like motif. Journal of Inorganic Biochemistry, 2006, 100, 1290-1297.	1.5	61
44	Computational chemistry comparison of stable/nonstable protein mutants classification models based on 3D and topological indices. Journal of Computational Chemistry, 2007, 28, 1990-1995.	1.5	61
45	Trypano-PPI: A Web Server for Prediction of Unique Targets in Trypanosome Proteome by using Electrostatic Parameters of Proteinâ^'protein Interactions. Journal of Proteome Research, 2010, 9, 1182-1190.	1.8	61
46	A topological sub-structural approach for predicting human intestinal absorption of drugs. European Journal of Medicinal Chemistry, 2004, 39, 905-916.	2.6	60
47	A topological substructural approach applied to the computational prediction of rodent carcinogenicity. Bioorganic and Medicinal Chemistry, 2005, 13, 2477-2488.	1.4	60
48	Markov entropy backbone electrostatic descriptors for predicting proteins biological activity. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4691-4695.	1.0	59
49	Using entropy of drug and protein graphs to predict FDA drug-target network: Theoretic-experimental study of MAO inhibitors and hemoglobin peptides from Fasciola hepatica. European Journal of Medicinal Chemistry, 2011, 46, 1074-1094.	2.6	59
50	Brain-inspired cheminformatics of drug-target brain interactome, synthesis, and assay of TVP1022 derivatives. Neuropharmacology, 2016, 103, 270-278.	2.0	59
51	2D-RNA-coupling numbers: A new computational chemistry approach to link secondary structure topology with biological function. Journal of Computational Chemistry, 2007, 28, 1049-1056.	1.5	58
52	ANN Multiscale Model of Anti-HIV Drugs Activity vs AIDS Prevalence in the US at County Level Based on Information Indices of Molecular Graphs and Social Networks. Journal of Chemical Information and Modeling, 2014, 54, 744-755.	2.5	58
53	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
54	Computational chemistry approach to protein kinase recognition using 3D stochastic van der Waals spectral moments. Journal of Computational Chemistry, 2007, 28, 1042-1048.	1.5	56

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55	Quantitative structure-toxicity relationships using TOPS-MODE. 3. Structural factors influencing the permeability of commercial solvents through living human skin. SAR and QSAR in Environmental Research, 2003, 14, 145-163.	1.0	55
56	ANN multiplexing model of drugs effect on macrophages; theoretical and flow cytometry study on the cytotoxicity of the anti-microbial drug G1 in spleen. Bioorganic and Medicinal Chemistry, 2012, 20, 6181-6194.	1.4	55
57	Symmetry considerations in Markovian chemicals â€˜in silicoâ€™ design (MARCH-INSIDE) I: central chirality codification, classification of ACE inhibitors and prediction of Ïƒ-receptor antagonist activities. Computational Biology and Chemistry, 2003, 27, 217-227.	1.1	54
58	Predicting Drugs and Proteins in Parasite Infections with Topological Indices of Complex Networks: Theoretical Backgrounds, Applications and Legal Issues. Current Pharmaceutical Design, 2010, 16, 2737-2764.	0.9	54
59	Markovian chemicals â€œin silicoâ€•design (MARCH-INSIDE), a promising approach for computer-aided molecular design III: 2.5D indices for the discovery of antibacterials. Journal of Molecular Modeling, 2005, 11, 116-123.	0.8	53
60	Multi-target spectral moment: QSAR for antifungal drugs vs. different fungi species. European Journal of Medicinal Chemistry, 2009, 44, 4051-4056.	2.6	53
61	Modeling Diamagnetic and Magnetooptic Properties of Organic Compounds with the TOSS-MODE Approachâ€. Journal of Chemical Information and Computer Sciences, 2000, 40, 1386-1399.	2.8	52
62	What Are the Limits of Applicability for Graph Theoretic Descriptors in QSPR/QSAR? Modeling Dipole Moments of Aromatic Compounds with TOPS-MODE Descriptors. Journal of Chemical Information and Computer Sciences, 2003, 43, 75-84.	2.8	52
63	Predicting stability of Arc repressor mutants with protein stochastic moments. Bioorganic and Medicinal Chemistry, 2005, 13, 323-331.	1.4	52
64	Computational chemistry study of 3Dâ€structureâ€function relationships for enzymes based on Markov models for protein electrostatic, HINT, and van der Waals potentials. Journal of Computational Chemistry, 2009, 30, 1510-1520.	1.5	52
65	3D entropy and moments prediction of enzyme classes and experimental-theoretic study of peptide fingerprints in Leishmania parasites. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1784-1794.	1.1	52
66	2D MI-DRAGON: A new predictor for proteinâ€“ligands interactions and theoretic-experimental studies of US FDA drug-target network, oxoisoaporphine inhibitors for MAO-A and human parasite proteins. European Journal of Medicinal Chemistry, 2011, 46, 5838-5851.	2.6	52
67	Model for High-Throughput Screening of Multitarget Drugs in Chemical Neurosciences: Synthesis, Assay, and Theoretic Study of Rasagiline Carbamates. ACS Chemical Neuroscience, 2013, 4, 1393-1403.	1.7	50
68	Recognition of stable protein mutants with 3D stochastic average electrostatic potentials. FEBS Letters, 2005, 579, 4297-4301.	1.3	48
69	QSAR model for alignmentâ€free prediction of human breast cancer biomarkers based on electrostatic potentials of protein pseudofolding HPâ€lattice networks. Journal of Computational Chemistry, 2008, 29, 2613-2622.	1.5	48
70	TOPS-MODE model of multiplexing neuroprotective effects of drugs and experimental-theoretic study of new 1,3-rasagiline derivatives potentially useful in neurodegenerative diseases. Bioorganic and Medicinal Chemistry, 2013, 21, 1870-1879.	1.4	48
71	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. Bioorganic and Medicinal Chemistry, 2005, 13, 1119-1129.	1.4	47
72	Review of QSAR Models for Enzyme Classes of Drug Targets: Theoretical Background and Applications in Parasites, Hosts and Other Organisms. Current Pharmaceutical Design, 2010, 16, 2710-2723.	0.9	47

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73	A novel approach to determining physicochemical and absorption properties of 6-fluoroquinolone derivatives: experimental assessment. European Journal of Pharmaceutics and Biopharmaceutics, 2002, 53, 317-325.	2.0	45
74	Unified Markov thermodynamics based on stochastic forms to classify drugs considering molecular structure, partition system, and biological species:. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 551-557.	1.0	45
75	A novel approach to predict a toxicological property of aromatic compounds in the Tetrahymena pyriformis. Bioorganic and Medicinal Chemistry, 2004, 12, 735-744.	1.4	44
76	MMM-QSAR Recognition of Ribonucleases without Alignment:â€‰ Comparison with an HMM Model and Isolation from Schizosaccharomyces pombe, Prediction, and Experimental Assay of a New Sequence. Journal of Chemical Information and Modeling, 2008, 48, 434-448.	2.5	44
77	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
78	Simple stochastic fingerprints towards mathematical modelling in biology and medicine. 1. The treatment of coccidiosis. Bulletin of Mathematical Biology, 2004, 66, 1285-1311.	0.9	43
79	NL MIND-BEST: A web server for ligands and proteins discoveryâ€”Theoretic-experimental study of proteins of Giardia lamblia and new compounds active against Plasmodium falciparum. Journal of Theoretical Biology, 2011, 276, 229-249.	0.8	43
80	3D-MEDNEs: An Alternative â€œin Silicoâ€•Technique for Chemical Research in Toxicology. 2. Quantitative Proteomeâ^'Toxicity Relationships (QPTR) based on Mass Spectrum Spiral Entropy. Chemical Research in Toxicology, 2008, 21, 619-632.	1.7	42
81	Complex Network Spectral Moments for ATCUN Motif DNA Cleavage: First Predictive Study on Proteins of Human Pathogen Parasites. Journal of Proteome Research, 2009, 8, 5219-5228.	1.8	42
82	Editorial [Hot topic: Network Topological Indices, Drug Metabolism, and Distribution (Guest Editor:) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.7	42
83	Generalized lattice graphs for 2D-visualization of biological information. Journal of Theoretical Biology, 2009, 261, 136-147.	0.8	41
84	Model for high-throughput screening of drug immunotoxicity â€“ Study of the anti-microbial G1 over peritoneal macrophages using flow cytometry. European Journal of Medicinal Chemistry, 2014, 72, 206-220.	2.6	41
85	PTML Model for Proteome Mining of B-Cell Epitopes and Theoreticalâ€“Experimental Study of Bm86 Protein Sequences from Colima, Mexico. Journal of Proteome Research, 2017, 16, 4093-4103.	1.8	41
86	Stochastic molecular descriptors for polymers. 1. Modelling the properties of icosahedral viruses with 3D-Markovian negentropies. Polymer, 2004, 45, 3845-3853.	1.8	40
87	Vibrational Markovian modelling of footprints after the interaction of antibiotics with the packaging region of HIV Type 1. Bulletin of Mathematical Biology, 2003, 65, 991-1002.	0.9	39
88	A TOPS-MODE approach to predict permeability coefficients. Polymer, 2004, 45, 2073-2079.	1.8	39
89	QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1651-1657.	1.0	39
90	Natural/random protein classification models based on star network topological indices. Journal of Theoretical Biology, 2008, 254, 775-783.	0.8	39

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91	New Markovâ€“Shannon Entropy models to assess connectivity quality in complex networks: From molecular to cellular pathway, Parasiteâ€“Host, Neural, Industry, and Legalâ€“Social networks. Journal of Theoretical Biology, 2012, 293, 174-188.	0.8	39
92	Modeling Antibacterial Activity with Machine Learning and Fusion of Chemical Structure Information with Microorganism Metabolic Networks. Journal of Chemical Information and Modeling, 2019, 59, 1109-1120.	2.5	39
93	Proteins Markovian 3D-QSAR with spherically-truncated average electrostatic potentials. Bioorganic and Medicinal Chemistry, 2005, 13, 3641-3647.	1.4	38
94	Comparative Study of Topological Indices of Macro/Supramolecular RNA Complex Networks. Journal of Chemical Information and Modeling, 2008, 48, 2265-2277.	2.5	38
95	Editorial [Hot topic: QSAR and Complex Networks in Pharmaceutical Design, Microbiology, Parasitology, Toxicology, Cancer and Neurosciences (Executive Editor: Humberto Gonzalez-Diaz)]. Current Pharmaceutical Design, 2010, 16, 2598-2600.	0.9	38
96	Perturbation Theory/Machine Learning Model of ChEMBL Data for Dopamine Targets: Docking, Synthesis, and Assay of New <scp>l</scp>-Prolyl-<scp>l</scp>-leucyl-glycinamide Peptidomimetics. ACS Chemical Neuroscience, 2018, 9, 2572-2587.	1.7	38
97	TOPS-MODE based QSARs derived from heterogeneous series of compounds. Applications to the design of new anti-inflammatory compounds. Bioorganic and Medicinal Chemistry, 2004, 12, 4467-4475.	1.4	36
98	Proteins QSAR with Markov average electrostatic potentials. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5088-5094.	1.0	36
99	Alignment-free prediction of mycobacterial DNA promoters based on pseudo-folding lattice network or star-graph topological indices. Journal of Theoretical Biology, 2009, 256, 458-466.	0.8	36
100	PTML Combinatorial Model of ChEMBL Compounds Assays for Multiple Types of Cancer. ACS Combinatorial Science, 2018, 20, 621-632.	3.8	36
101	OncoOmics approaches to reveal essential genes in breast cancer: a panoramic view from pathogenesis to precision medicine. Scientific Reports, 2020, 10, 5285.	1.6	36
102	QSAR study for mycobacterial promoters with low sequence homology. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 547-553.	1.0	35
103	From QSAR models of Drugs to Complex Networks: State-of-Art Review and Introduction of New Markov-Spectral Moments Indices. Current Topics in Medicinal Chemistry, 2012, 12, 927-960.	1.0	35
104	Perturbation-Theory and Machine Learning (PTML) Model for High-Throughput Screening of Parham Reactions: Experimental and Theoretical Studies. Journal of Chemical Information and Modeling, 2018, 58, 1384-1396.	2.5	35
105	Using spectral moments of spiral networks based on PSA/mass spectra outcomes to derive quantitative proteomeâ€“disease relationships (QPDRs) and predicting prostate cancer. Biochemical and Biophysical Research Communications, 2008, 372, 320-325.	1.0	34
106	Unified QSAR & networkâ€based computational chemistry approach to antimicrobials. II. Multiple distance and triadic census analysis of antiparasitic drugs complex networks. Journal of Computational Chemistry, 2010, 31, 164-173.	1.5	34
107	Diagnosing Human Anisakiasis: Recombinant Ani s 1 and Ani s 7 Allergens versus the UniCAP 100 Fluorescence Enzyme Immunoassay. Vaccine Journal, 2010, 17, 496-502.	3.2	33
108	2D RNA-QSAR: assigning ACC oxidase family membership with stochastic molecular descriptors; isolation and prediction of a sequence from Psidium guajava L. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 2932-2937.	1.0	32

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109	Multi-target spectral moment: QSAR for antiviral drugs vs. different viral species. Analytica Chimica Acta, 2009, 651, 159-164.	2.6	32
110	Entropy multi-target QSAR model for prediction of antiviral drug complex networks. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 227-233.	1.8	32
111	Experimentalâ€“Computational Study of Carbon Nanotube Effects on Mitochondrial Respiration: In Silico Nano-QSPR Machine Learning Models Based on New Raman Spectra Transform with Markovâ€“Shannon Entropy Invariants. Journal of Chemical Information and Modeling, 2017, 57, 1029-1044.	2.5	32
112	Entropy Model for Multiplex Drug-Target Interaction Endpoints of Drug Immunotoxicity. Current Topics in Medicinal Chemistry, 2013, 13, 1636-1649.	1.0	32
113	Stochastic molecular descriptors for polymers. 2. Spherical truncation of electrostatic interactions on entropy based polymers 3D-QSAR. Polymer, 2005, 46, 2791-2798.	1.8	31
114	Biopolymer stochastic moments. I. Modeling human rhinovirus cellular recognition with protein surface electrostatic moments. Biopolymers, 2005, 77, 296-303.	1.2	30
115	Chemometrics for QSAR with low sequence homology: Mycobacterial promoter sequences recognition with 2D-RNA entropies. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 20-26.	1.8	30
116	Gene prioritization, communality analysis, networking and metabolic integrated pathway to better understand breast cancer pathogenesis. Scientific Reports, 2018, 8, 16679.	1.6	29
117	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. Journal of Proteome Research, 2019, 18, 2735-2746.	1.8	29
118	Prediction of breast cancer proteins involved in immunotherapy, metastasis, and RNA-binding using molecular descriptors and artificial neural networks. Scientific Reports, 2020, 10, 8515.	1.6	29
119	Design, synthesis and photobiological properties of 3,4-cyclopentenepsoralens. Bioorganic and Medicinal Chemistry, 2005, 13, 809-817.	1.4	28
120	3D QSAR Markov model for drug-induced eosinophiliaâ€"theoretical prediction and preliminary experimental assay of the antimicrobial drug G1. Bioorganic and Medicinal Chemistry, 2005, 13, 1523-1530.	1.4	28
121	Stochastic molecular descriptors for polymers. 4. Study of complex mixtures with topological indices of mass spectra spiral and star networks: The blood proteome case. Polymer, 2008, 49, 5575-5587.	1.8	27
122	Designing nanoparticle release systems for drugâ€“vitamin cancer co-therapy with multiplicative perturbation-theory machine learning (PTML) models. Nanoscale, 2019, 11, 21811-21823.	2.8	27
123	Predicting coated-nanoparticle drug release systems with perturbation-theory machine learning (PTML) models. Nanoscale, 2020, 12, 13471-13483.	2.8	27
124	Unified drugâ€“target interaction thermodynamic Markov model using stochastic entropies to predict multiple drugs side effects. European Journal of Medicinal Chemistry, 2005, 40, 1030-1041.	2.6	26
125	QSAR Models for Proteins of Parasitic Organisms, Plants and Human Guests: Theory, Applications, Legal Protection, Taxes, and Regulatory Issues. Current Proteomics, 2009, 6, 214-227.	0.1	26
126	NaÃ¯ve Bayes QSDR classification based on spiral-graph Shannon entropies for protein biomarkers in human colon cancer. Molecular BioSystems, 2012, 8, 1716.	2.9	26

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127	Matrix Trace Operators: From Spectral Moments of Molecular Graphs and Complex Networks to Perturbations in Synthetic Reactions, Micelle Nanoparticles, and Drug ADME Processes. Current Drug Metabolism, 2014, 15, 470-488.	0.7	26
128	Stochastic entropy QSAR for the in silico discovery of anticancer compounds: Prediction, synthesis, and in vitro assay of new purine carbanucleosides. Bioorganic and Medicinal Chemistry, 2006, 14, 1095-1107.	1.4	25
129	On the applicability of QSAR for recognition of miRNA bioorganic structures at early stages of organism and cell development: Embryo and stem cells. Bioorganic and Medicinal Chemistry, 2007, 15, 2544-2550.	1.4	25
130	Prediction of Multi-Target Networks of Neuroprotective Compounds with Entropy Indices and Synthesis, Assay, and Theoretical Study of New Asymmetric 1,2-Rasagiline Carbamates. International Journal of Molecular Sciences, 2014, 15, 17035-17064.	1.8	25
131	Multi-output model with Boxâ€"Jenkins operators of linear indices to predict multi-target inhibitors of ubiquitinâ€"proteasome pathway. Molecular Diversity, 2015, 19, 347-356.	2.1	25
132	MIANN Models in Medicinal, Physical and Organic Chemistry. Current Topics in Medicinal Chemistry, 2013, 13, 619-641.	1.0	25
133	QSAR study of anticoccidial activity for diverse chemical compounds: Prediction and experimental assay of trans-2-(2-nitrovinyl)furan. Bioorganic and Medicinal Chemistry, 2007, 15, 962-968.	1.4	24
134	QSAR and complex network study of the chiral HMGR inhibitor structural diversity. Bioorganic and Medicinal Chemistry, 2009, 17, 165-175.	1.4	24
135	Plasmod-PPI: A web-server predicting complex biopolymer targets in plasmodium with entropy measures of proteinâ€"protein interactions. Polymer, 2010, 51, 264-273.	1.8	24
136	Model for Vaccine Design by Prediction of B-Epitopes of IEDB Given Perturbations in Peptide Sequence, In Vivo Process, Experimental Techniques, and Source or Host Organisms. Journal of Immunology Research, 2014, 2014, 1-15.	0.9	24
137	Multioutput Perturbation-Theory Machine Learning (PTML) Model of ChEMBL Data for Antiretroviral Compounds. Molecular Pharmaceutics, 2019, 16, 4200-4212.	2.3	24
138	QSPR and Flow Cytometry Analysis (QSPR-FCA): Review and New Findings on Parallel Study of Multiple Interactions of Chemical Compounds with Immune Cellular and Molecular Targets. Current Drug Metabolism, 2014, 15, 414-428.	0.7	24
139	3D MI-DRAGON: New Model for the Reconstruction of US FDA Drug- Target Network and Theoretical-Experimental Studies of Inhibitors of Rasagiline Derivatives for AChE. Current Topics in Medicinal Chemistry, 2012, 12, 1843-1865.	1.0	23
140	QSAR for RNases and theoreticâ€"experimental study of molecular diversity on peptide mass fingerprints of a new Leishmania infantum protein. Molecular Diversity, 2010, 14, 349-369.	2.1	22
141	Modeling Complex Metabolic Reactions, Ecological Systems, and Financial and Legal Networks with MIANN Models Based on Markov-Wiener Node Descriptors. Journal of Chemical Information and Modeling, 2014, 54, 16-29.	2.5	22
142	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 1). Current Pharmaceutical Design, 2016, 22, 5041-5042.	0.9	22
143	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 2). Current Pharmaceutical Design, 2016, 22, 5177-5178.	0.9	22
144	Experimental study and Random Forest prediction model of microbiome cell surface hydrophobicity. Expert Systems With Applications, 2017, 72, 306-316.	4.4	22

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145	Editorial: Improving Neuropharmacology using Big Data, Machine Learning and Computational Algorithms. Current Neuropharmacology, 2017, 15, 1058-1061.	1.4	22
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