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	Multi-output chemometrics model for gasoline compounding. Fuel, 2022, 310, 122274.	3.4	4
2	Towards rational nanomaterial design by predicting drugâ€“nanoparticle system interaction vs. bacterial metabolic networks. Environmental Science: Nano, 2022, 9, 1391-1413.	2.2	5
3	Machine Learning Study of Metabolic NetworksvsChEMBL Data of Antibacterial Compounds. Molecular Pharmaceutics, 2022, 19, 2151-2163.	2.3	3
4	Synthesis, Pharmacological, and Biological Evaluation of 2-Furoyl-Based MIF-1 Peptidomimetics and the Development of a General-Purpose Model for Allosteric Modulators (ALLOPTML). ACS Chemical Neuroscience, 2021, 12, 203-215.	1.7	11
5	IFPTML mapping of nanoparticle antibacterial activity vs. pathogen metabolic networks. Nanoscale, 2021, 13, 1318-1330.	2.8	15
6	New Experimental and Computational Tools for Drug Discovery: Part - XI. Current Topics in Medicinal Chemistry, 2021, 21, 597-598.	1.0	0
7	New Experimental and Computational Tools for Drug Discovery. Part â€“ XII. Current Topics in Medicinal Chemistry, 2021, 21, 789-789.	1.0	1
8	Predicting Metabolic Reaction Networks with Perturbation-Theory Machine Learning (PTML) Models. Current Topics in Medicinal Chemistry, 2021, 21, 819-827.	1.0	10
9	Palladium-mediated synthesis and biological evaluation of C-10b substituted Dihydropyrrolo[1,2-b]isoquinolines as antileishmanial agents. European Journal of Medicinal Chemistry, 2021, 220, 113458.	2.6	11
10	Towards machine learning discovery of dual antibacterial drugâ€“nanoparticle systems. Nanoscale, 2021, 13, 17854-17870.	2.8	11
11	Prediction of Anti-Glioblastoma Drug-Decorated Nanoparticle Delivery Systems Using Molecular Descriptors and Machine Learning. International Journal of Molecular Sciences, 2021, 22, 11519.	1.8	5
12	MLb-LDLr. JACC Basic To Translational Science, 2021, 6, 815-827.	1.9	10
13	IFPTML Mapping of Drug Graphs with Protein and Chromosome Structural Networks vs. Pre-Clinical Assay Information for Discovery of Antimalarial Compounds. International Journal of Molecular Sciences, 2021, 22, 13066.	1.8	2
14	PTML Model of ChEMBL Compounds Assays for Vitamin Derivatives. ACS Combinatorial Science, 2020, 22, 129-141.	3.8	10
15	A Multi-Objective Approach for Anti-Osteosarcoma Cancer Agents Discovery through Drug Repurposing. Pharmaceuticals, 2020, 13, 409.	1.7	6
16	Predicting coated-nanoparticle drug release systems with perturbation-theory machine learning (PTML) models. Nanoscale, 2020, 12, 13471-13483.	2.8	27
17	Prediction of Antimalarial Drug-Decorated Nanoparticle Delivery Systems with Random Forest Models. Biology, 2020, 9, 198.	1.3	22
18	Web Server and R Library for the Calculation of Markov Chains Molecular Descriptors. Proceedings (mdpi), 2020, 54, 28.	0.2	0

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19	Perturbation-Theory Machine Learning (PTML) Multilabel Model of the ChEMBL Dataset of Preclinical Assays for Antisarcoma Compounds. ACS Omega, 2020, 5, 27211-27220.	1.6	4
20	PTML Model for Selection of Nanoparticles, Anticancer Drugs, and Vitamins in the Design of Drugâ€“Vitamin Nanoparticle Release Systems for Cancer Cotherapy. Molecular Pharmaceutics, 2020, 17, 2612-2627.	2.3	12
21	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
22	Gene Prioritization through Consensus Strategy, Enrichment Methodologies Analysis, and Networking for Osteosarcoma Pathogenesis. International Journal of Molecular Sciences, 2020, 21, 1053.	1.8	13
23	Net-Net AutoML Selection of Artificial Neural Network Topology for Brain Connectome Prediction. Applied Sciences (Switzerland), 2020, 10, 1308.	1.3	2
24	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
25	PTML Multi-Label Algorithms: Models, Software, and Applications. Current Topics in Medicinal Chemistry, 2020, 20, 2326-2337.	1.0	8
26	New Experimental and Computational Tools for Drug Discovery. Part - IX. Current Topics in Medicinal Chemistry, 2020, 20, 711-712.	1.0	0
27	MCDCalc: Markov Chain Molecular Descriptors Calculator for Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2020, 20, 305-317.	1.0	4
28	New Experimental and Computational Tools for Drug Discovery - Part-VIII. Current Topics in Medicinal Chemistry, 2020, 20, 277-279.	1.0	0
29	New Experimental and Computational Tools for Drug Discovery. From Old Way to New Series â€“ Part-X. Current Topics in Medicinal Chemistry, 2020, 20, 2279-2280.	1.0	0
30	Perturbation Theory Machine Learning Modeling of Immunotoxicity for Drugs Targeting Inflammatory Cytokines and Study of the Antimicrobial G1 Using Cytometric Bead Arrays. Chemical Research in Toxicology, 2019, 32, 1811-1823.	1.7	9
31	New Experimental and Computational Tools for Drug Discovery. - Part-VII. Current Topics in Medicinal Chemistry, 2019, 19, 898-899.	1.0	0
32	Big Data Challenges Targeting Proteins in GPCR Signaling Pathways; Combining PTML-ChEMBL Models and [35S]GTPÎ³S Binding Assays. ACS Chemical Neuroscience, 2019, 10, 4476-4491.	1.7	21
33	Multioutput Perturbation-Theory Machine Learning (PTML) Model of ChEMBL Data for Antiretroviral Compounds. Molecular Pharmaceutics, 2019, 16, 4200-4212.	2.3	24
34	New Experimental and Computational Tools for Drug Discovery: Medicinal Chemistry, Molecular Docking, and Machine Learning - Part-VI. Current Topics in Medicinal Chemistry, 2019, 18, 2325-2326.	1.0	3
35	New Experimental and Computational Tools for Drug Discovery: Medicinal Chemistry, Personalized Medicine, Ethical & Legal Issues â€“ Part-V. Current Topics in Medicinal Chemistry, 2019, 18, 2141-2142.	1.0	0
36	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. Journal of Proteome Research, 2019, 18, 2735-2746.	1.8	29

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37	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
38	Engineering faster transglycosidases and their acceptor specificity. Green Chemistry, 2019, 21, 2823-2836.	4.6	15
39	Computational MitoTarget Scanning Based on Topological Vacancies of Single-Walled Carbon Nanotubes with the Human Mitochondrial Voltage-Dependent Anion Channel (hVDAC1). Chemical Research in Toxicology, 2019, 32, 566-577.	1.7	4
40	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
41	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
42	Complex Networks and Machine Learning: From Molecular to Social Sciences. Applied Sciences (Switzerland), 2019, 9, 4493.	1.3	5
43	MitoTarget Modeling Using ANN-Classification Models Based on Fractal SEM Nano-Descriptors: Carbon Nanotubes as Mitochondrial F0F1-ATPase Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 86-97.	2.5	11
44	Chromosome Gene Orientation Inversion Networks (GOINs) of Plasmodium Proteome. Journal of Proteome Research, 2018, 17, 1258-1268.	1.8	11
45	Gene prioritization, communality analysis, networking and metabolic integrated pathway to better understand breast cancer pathogenesis. Scientific Reports, 2018, 8, 16679.	1.6	29
46	PTML Combinatorial Model of ChEMBL Compounds Assays for Multiple Types of Cancer. ACS Combinatorial Science, 2018, 20, 621-632.	3.8	36
47	New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Metabolomics, Pharmacokinetics, and Medicinal Chemistry. Part - IV. Current Topics in Medicinal Chemistry, 2018, 18, 881-882.	1.0	1
48	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
49	Net-Net Auto Machine Learning (AutoML) Prediction of Complex Ecosystems. Scientific Reports, 2018, 8, 12340.	1.6	9
50	Perturbation Theoryâ€“Machine Learning Study of Zeolite Materials Desilication. Journal of Chemical Information and Modeling, 2018, 58, 2414-2419.	2.5	19
51	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
52	QSPR/QSAR-based Perturbation Theory approach and mechanistic electrochemical assays on carbon nanotubes with optimal properties against mitochondrial Fenton reaction experimentally induced by Fe2+-overload. Carbon, 2017, 115, 312-330.	5.4	11
53	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
54	A study of the Immune Epitope Database for some fungi species using network topological indices. Molecular Diversity, 2017, 21, 713-718.	2.1	7

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55	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
56	Experimental study and Random Forest prediction model of microbiome cell surface hydrophobicity. Expert Systems With Applications, 2017, 72, 306-316.	4.4	22
57	Editorial: New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Part-II. Current Topics in Medicinal Chemistry, 2017, 17, 2901-2902.	1.0	0
58	Editorial: New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Part-1. Current Topics in Medicinal Chemistry, 2017, 17, .	1.0	0
59	Carbon Nanotubesâ€™ Effect on Mitochondrial Oxygen Flux Dynamics: Polarography Experimental Study and Machine Learning Models using Star Graph Trace Invariants of Raman Spectra. Nanomaterials, 2017, 7, 386.	1.9	14
60	Experimental Study and ANN Dual-Time Scale Perturbation Model of Electrokinetic Properties of Microbiota. Frontiers in Microbiology, 2017, 8, 1216.	1.5	3
61	Editorial: Improving Neuropharmacology using Big Data, Machine Learning and Computational Algorithms. Current Neuropharmacology, 2017, 15, 1058-1061.	1.4	22
62	Decrypting Strong and Weak Single-Walled Carbon Nanotubes Interactions with Mitochondrial Voltage-Dependent Anion Channels Using Molecular Docking and Perturbation Theory. Scientific Reports, 2017, 7, 13271.	1.6	22
63	Multi-Target Mining of Alzheimer Disease Proteome with Hanschâ€™s QSBR-Perturbation Theory and Experimental-Theoretic Study of New Thiophene Isosters of Rasagiline. Current Drug Targets, 2017, 18, 511-521.	1.0	18
64	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 1). Current Pharmaceutical Design, 2016, 22, 5041-5042.	0.9	22
65	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 2). Current Pharmaceutical Design, 2016, 22, 5177-5178.	0.9	22
66	Data Analysis in Chemistry and Bio-Medical Sciences. International Journal of Molecular Sciences, 2016, 17, 2105.	1.8	3
67	Chiral BrÃ¸nsted Acidâ€Catalyzed Enantioselective Î±â€Amidoalkylation Reactions: A Joint Experimental and Predictive Study. ChemistryOpen, 2016, 5, 540-549.	0.9	21
68	Gastrointestinal Spatiotemporal mRNA Expression of Ghrelin vs Growth Hormone Receptor and New Growth Yield Machine Learning Model Based on Perturbation Theory. Scientific Reports, 2016, 6, 30174.	1.6	9
69	QSPR-Perturbation Models for the Prediction of B-Epitopes from Immune Epitope Database: A Potentially Valuable Route for Predicting â€œIn Silicoâ€•New Optimal Peptide Sequences and/or Boundary Conditions for Vaccine Development. International Journal of Peptide Research and Therapeutics, 2016, 22, 445-450.	0.9	9
70	Perturbation theory model of reactivity and enantioselectivity of palladium-catalyzed Heckâ€“Heck cascade reactions. RSC Advances, 2016, 6, 38602-38610.	1.7	21
71	Predicting the binding properties of single walled carbon nanotubes (SWCNT) with an ADP/ATP mitochondrial carrier using molecular docking, chemoinformatics, and nano-QSBR perturbation theory. RSC Advances, 2016, 6, 58680-58693.	1.7	12
72	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

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73	Chemometric approach to fatty acid metabolism-distribution networks and methane production in ruminal microbiome. Chemometrics and Intelligent Laboratory Systems, 2016, 151, 1-8.	1.8	5
74	Experimental and chemometric studies of cell membrane permeability. Chemometrics and Intelligent Laboratory Systems, 2016, 154, 1-6.	1.8	8
75	Brain-inspired cheminformatics of drug-target brain interactome, synthesis, and assay of TVP1022 derivatives. Neuropharmacology, 2016, 103, 270-278.	2.0	59
76	Computational Modeling and Experimental Facts of Mixed Self- Assembly Systems. Current Pharmaceutical Design, 2016, 22, 5249-5256.	0.9	3
77	Experimental-Theoretic Approach to Drug-Lymphocyte Interactome Networks with Flow Cytometry and Spectral Moments Perturbation Theory. Current Pharmaceutical Design, 2016, 22, 5114-5119.	0.9	3
78	Multi-output Model with Box-Jenkins Operators of Quadratic Indices for Prediction of Malaria and Cancer Inhibitors Targeting Ubiquitin- Proteasome Pathway (UPP) Proteins. Current Protein and Peptide Science, 2016, 17, 220-227.	0.7	14
79	High-Order Perturbation Theory Models of Drug-Target Interactomes for Proteins Expressed on Networks of Hippocampus Brain Region of Alzheimer Disease Patients. , 2016, , 269-299.		0
80	ADMET-Multi-Output Cheminformatics Models for Drug Delivery, Interactomics, and Nanotoxicology. Current Drug Delivery, 2016, , .	0.8	0
81	Self-Assembled Binary Nanoscale Systems: Multioutput Model with LFER-Covariance Perturbation Theory and an Experimentalâ€“Computational Study of NaGDC-DDAB Micelles. Langmuir, 2015, 31, 12009-12018.	1.6	10
82	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
83	Mapping chemical structure-activity information of HAART-drug cocktails over complex networks of AIDS epidemiology and socioeconomic data of U.S. counties. BioSystems, 2015, 132-133, 20-34.	0.9	19
84	Experimental and computational studies of fatty acid distribution networks. Molecular BioSystems, 2015, 11, 2964-2977.	2.9	6
85	Mitoprotective activity of oxidized carbon nanotubes against mitochondrial swelling induced in multiple experimental conditions and predictions with new expected-value perturbation theory. RSC Advances, 2015, 5, 103229-103245.	1.7	10
86	Bio-AIMS Collection of Chemoinformatics Web Tools based on Molecular Graph Information and Artificial Intelligence Models. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 735-750.	0.6	5
87	Multiscale Mapping of AIDS in U.S. Countries vs Anti-HIV Drugs Activity with Complex Networks and Information Indices. Current Bioinformatics, 2015, 10, 639-657.	0.7	6
88	MI-NODES Multiscale Models of Metabolic Reactions, Brain Connectome, Ecological, Epidemic, World Trade, and Legal-Social Networks. Current Bioinformatics, 2015, 10, 692-713.	0.7	2
89	Multi-output Model with Box-Jenkins Operators of Quadratic Indices for Prediction of Malaria and Cancer Inhibitors Targeting Ubiquitin-Proteasome Pathway (UPP) proteins. Current Protein and Peptide Science, 2015, 16, 1-1.	0.7	2
90	MIANN Models of Networks of Biochemical Reactions, Ecosystems, and U.S. Supreme Court with Balaban-Markov Indices. Current Bioinformatics, 2015, 10, 658-671.	0.7	0

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91	Editorial (Thematic Issue: Multiscale Models in Cheminformatics, Complex Bio-Molecular Systems, and) Tj ETQq1 1 0.784314 rgBT /Over	0.7	0
92	Editorial (Thematic Issue: From Phytochemistry to Medicinal Chemistry: Isolation, Semisynthesis,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 7	1.0	2
93	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, From Molecular Mechanics, Dynamics,) Tj ETQq1 1 0.784314 rgBT /Overlo	0.7	1
94	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, Modeling Chemical Reactivity and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6	0.7	0
95	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
96	Editorial (Thematic Issue: Nanocarriers & Drug Delivery: Rational Design and Applications). Current Topics in Medicinal Chemistry, 2014, 14, 1095-1096.	1.0	3
97	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
98	Markov mean properties for cell death-related protein classification. Journal of Theoretical Biology, 2014, 349, 12-21.	0.8	13
99	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
100	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
101	A QSPR-like model for multilocus genotype networks of Fasciola hepatica in Northwest Spain. Journal of Theoretical Biology, 2014, 343, 16-24.	0.8	4
102	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
103	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
104	Mapping networks of anti-HIV drug cocktails vs. AIDS epidemiology in the US counties. Chemometrics and Intelligent Laboratory Systems, 2014, 138, 161-170.	1.8	8
105	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
106	Computational ecotoxicology: Simultaneous prediction of ecotoxic effects of nanoparticles under different experimental conditions. Environment International, 2014, 73, 288-294.	4.8	102
107	LECTINPred: web Server that Uses Complex Networks of Protein Structure for Prediction of Lectins with Potential Use as Cancer Biomarkers or in Parasite Vaccine Design. Molecular Informatics, 2014, 33, 276-285.	1.4	10
108	Galvez-Markov Network Transferability Indices: Review of Classic Theory and New Model for Perturbations in Metabolic Reactions. Current Drug Metabolism, 2014, 15, 557-564.	0.7	11

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109	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
110	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
111	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
112	The RÃ¼ckerâ€“Markov invariants of complex Bio-Systems: Applications in Parasitology and Neuroinformatics. BioSystems, 2013, 111, 199-207.	0.9	12
113	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
114	Reversible Hypothalamic Dysfunction in Optic Nerve Germinoma. Journal of Craniofacial Surgery, 2013, 24, 468-469.	0.3	0
115	Editorial (Hot Topic: Bioinformatics and Quantitative Structure-Property Relationship (QSPR)) Tj ETQq1 1 0.784314 rgBT /Overlock 10	0.7	2
116	Editorial (Hot Topic : Computational Prediction of Drug-Target Interactions in Medicinal Chemistry). Current Topics in Medicinal Chemistry, 2013, 13, 1619-1621.	1.0	2
117	Synthetic Oxoisoaporphine Alkaloids: In Vitro, In Vivo and In Silico Assessment of Antileishmanial Activities. PLoS ONE, 2013, 8, e77560.	1.1	17
118	Legal issues for chem-bioinformatics models. Frontiers in Bioscience - Elite, 2013, E5, 361-374.	0.9	2
119	Patents of bio-active compounds based on computer-aided drug discovery techniques. Frontiers in Bioscience - Elite, 2013, E5, 399-407.	0.9	4
120	S2SNet: A Tool for Transforming Characters and Numeric Sequences into Star Network Topological Indices in Chemoinformatics, Bioinformatics, Biomedical, and Social-Legal Sciences. Current Bioinformatics, 2013, 8, 429-437.	0.7	17
121	MIANN Models in Medicinal, Physical and Organic Chemistry. Current Topics in Medicinal Chemistry, 2013, 13, 619-641.	1.0	25
122	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
123	Entropy Model for Multiplex Drug-Target Interaction Endpoints of Drug Immunotoxicity. Current Topics in Medicinal Chemistry, 2013, 13, 1636-1649.	1.0	32
124	Markov-Randic Indices for QSPR Re-Evaluation of Metabolic, Parasite- Host, Fasciolosis Spreading, Brain Cortex and Legal-Social Complex Networks. Current Bioinformatics, 2013, 8, 401-415.	0.7	5
125	Editorial [Hot Topic: QSAR/QSPR Models as Enabling Technologies for Drug & Targets Discovery in: Medicinal Chemistry, Microbiology-Parasitology, Neurosciences, Bioinformatics, Proteomics and Other Biomedical Sciences (Guest Editor: Humberto Gonzalez Diaz)]. Current Topics in Medicinal Chemistry, 2012, 12, 799-801.	1.0	9
126	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

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127	Immunotoxicity, Flow Cytometry, and Chemoinformatics: Review, Bibliometric Analysis, and New QSAR Model of Drug Effects Over Macrophages. Current Topics in Medicinal Chemistry, 2012, 12, 1815-1833.	1.0	2
128	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	13
129	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
130	New Markov-Autocorrelation Indices for Re-evaluation of Links in Chemical and Biological Complex Networks used in Metabolomics, Parasitology, Neurosciences, and Epidemiology. Journal of Chemical Information and Modeling, 2012, 52, 3331-3340.	2.5	18
131	LIBP-Pred: web server for lipid binding proteins using structural network parameters; PDB mining of human cancer biomarkers and drug targets in parasites and bacteria. Molecular BioSystems, 2012, 8, 851.	2.9	19
132	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
133	Generalized String Pseudo-Folding Lattices in Bioinformatics: State-of-Art Review, New Model for Enzyme Sub-Classes, and Study of ESTs on Trichinella spiralis. Current Bioinformatics, 2012, 7, 7-34.	0.7	1
134	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
135	Immunotoxicity, Flow Cytometry, and Chemoinformatics: Review, Bibliometric Analysis, and New QSAR Model of Drug Effects Over Macrophages. Current Topics in Medicinal Chemistry, 2012, 12, 1815-1833.	1.0	6
136	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
137	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
138	Editorial[Hot Topic:Applications of Topological Indices and Complex Networks in Bioinformatics(Guest Editor: Humberto Gonzalez-Diaz)]. Current Bioinformatics, 2011, 6, 1-2.	0.7	7
139	Editorial {Hot topic: QSPR Models for Computer-Aided Drug Design in Microbiology, Parasitology, and Pharmacology (Guest Editor: Humberto Gonzalez-Diaz)]. Current Computer-Aided Drug Design, 2011, 7, 228-230.	0.8	0
140	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
141	MISS-Prot: web server for self/non-self discrimination of protein residue networks in parasites; theory and experiments in Fasciola peptides and Anisakis allergens. Molecular BioSystems, 2011, 7, 1938.	2.9	20
142	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
143	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
144	Entropy multi-target QSAR model for prediction of antiviral drug complex networks. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 227-233.	1.8	32

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145	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
146	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
147	Definition of Markov-Harary Invariants and Review of Classic Topological Indices and Databases in Biology, Parasitology, Technology,and Social-Legal Networks. Current Bioinformatics, 2011, 6, 94-121.	0.7	17
148	From Chemical Graphs in Computer-Aided Drug Design to General Markov-Galvez Indices of Drug-Target, Proteome, Drug-Parasitic Disease, Technological, and Social-Legal Networks. Current Computer-Aided Drug Design, 2011, 7, 315-337.	0.8	10
149	Review of Computer-Aided Models for Predicting Collagen Stability. Current Computer-Aided Drug Design, 2011, 7, 287-303.	0.8	2
150	Network Topological Indices from Chem-Bioinformatics to Legal Sciences and back. Current Bioinformatics, 2011, 6, 53-70.	0.7	14
151	Markov Entropy Centrality: Chemical, Biological, Crime, and Legislative Networks. , 2011, , 199-258.		5
152	Editorial [Hot topic: Network Topological Indices, Drug Metabolism, and Distribution (Guest Editor:) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.7	42
153	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
154	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
155	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
156	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
157	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
158	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
159	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
160	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
161	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
162	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

#	Article	IF	Citations
163	Protein Graphs in Cancer Prediction. , 2010, , 125-140.		1
164	Study of Parasitic Infections, Cancer, and other Diseases with Mass-Spectrometry and Quantitative Proteome-Disease Relationships. Current Proteomics, 2009, 6, 246-261.	0.1	18
165	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
166	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
167	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
168	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
169	Study of peptide fingerprints of parasite proteins and drugâ€“DNA interactions with Markov-Mean-Energy invariants of biopolymer molecular-dynamic lattice networks. Polymer, 2009, 50, 3857-3870.	1.8	1
170	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
171	Generalized lattice graphs for 2D-visualization of biological information. Journal of Theoretical Biology, 2009, 261, 136-147.	0.8	41
172	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
173	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
174	Multi-target spectral moment: QSAR for antifungal drugs vs. different fungi species. European Journal of Medicinal Chemistry, 2009, 44, 4051-4056.	2.6	53
175	Scoring function for DNAâ€“drug docking of anticancer and antiparasitic compounds based on spectral moments of 2D lattice graphs for molecular dynamics trajectories. European Journal of Medicinal Chemistry, 2009, 44, 4461-4469.	2.6	21
176	QSAR and complex network study of the chiral HMGR inhibitor structural diversity. Bioorganic and Medicinal Chemistry, 2009, 17, 165-175.	1.4	24
177	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
178	Multi-target spectral moment: QSAR for antiviral drugs vs. different viral species. Analytica Chimica Acta, 2009, 651, 159-164.	2.6	32
179	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
180	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

#	Article	IF	Citations
181	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
182	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
183	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
184	Natural/random protein classification models based on star network topological indices. Journal of Theoretical Biology, 2008, 254, 775-783.	0.8	39
185	Proteomics, networks and connectivity indices. Proteomics, 2008, 8, 750-778.	1.3	207
186	Quantitative structureâ€antibacterial activity relationship modeling using a combination of piecewise linear regressionâ€discriminant analysis (I): Quantum chemical, topographic, and topological descriptors. International Journal of Quantum Chemistry, 2008, 108, 1856-1871.	1.0	6
187	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
188	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
189	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
190	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
191	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
192	Quantitative Proteomeâ€“Property Relationships (QPPRs). Part 1: Finding biomarkers of organic drugs with mean Markov connectivity indices of spiral networks of blood mass spectra. Bioorganic and Medicinal Chemistry, 2008, 16, 9684-9693.	1.4	18
193	Multi-target QSPR assemble of a Complex Network for the distribution of chemicals to biphasic systems and biological tissues. Chemometrics and Intelligent Laboratory Systems, 2008, 94, 160-165.	1.8	13
194	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
195	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
196	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
197	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
198	Comparative Study of Topological Indices of Macro/Supramolecular RNA Complex Networks. Journal of Chemical Information and Modeling, 2008, 48, 2265-2277.	2.5	38

#	Article	IF	Citations
199	Editorial [Hot Topic: Quantitative studies on Structure-Activity and Structure-Property Relationships (QSAR/QSPR) (Guest Editor: Humberto Gonzalez-Diaz)]. Current Topics in Medicinal Chemistry, 2008, 8, 1554-1554.	1.0	13
200	Predicting Antimicrobial Drugs and Targets with the MARCH-INSIDE Approach. Current Topics in Medicinal Chemistry, 2008, 8, 1676-1690.	1.0	142
201	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
202	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
203	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
204	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
205	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
206	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
207	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
208	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
209	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
210	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
211	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
212	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
213	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
214	Unify QSAR approach to antimicrobials. Part 1: Predicting antifungal activity against different species. Bioorganic and Medicinal Chemistry, 2006, 14, 5973-5980.	1.4	69
215	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
216	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

#	Article	IF	Citations
217	QSAR study for mycobacterial promoters with low sequence homology. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 547-553.	1.0	35
218	Simple Stochastic Fingerprints Towards Mathematical Modeling in Biology and Medicine 2. Unifying Markov Model for Drugs Side Effects. Bulletin of Mathematical Biology, 2006, 68, 1527-1554.	0.9	9
219	Simple stochastic fingerprints towards mathematical modeling in biology and medicine. 3. ocular irritability classification model. Bulletin of Mathematical Biology, 2006, 68, 1555-1572.	0.9	14
220	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
221	Stochastic molecular descriptors for polymers. 3. Markov electrostatic moments as polymer 2D-folding descriptors: RNAâ€“QSAR for mycobacterial promoters. Polymer, 2005, 46, 6461-6473.	1.8	21
222	Predicting stability of Arc repressor mutants with protein stochastic moments. Bioorganic and Medicinal Chemistry, 2005, 13, 323-331.	1.4	52
223	Design, synthesis and photobiological properties of 3,4-cyclopentenepsoralens. Bioorganic and Medicinal Chemistry, 2005, 13, 809-817.	1.4	28
224	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
225	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
226	A topological substructural approach applied to the computational prediction of rodent carcinogenicity. Bioorganic and Medicinal Chemistry, 2005, 13, 2477-2488.	1.4	60
227	Proteins Markovian 3D-QSAR with spherically-truncated average electrostatic potentials. Bioorganic and Medicinal Chemistry, 2005, 13, 3641-3647.	1.4	38
228	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
229	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
230	Proteins QSAR with Markov average electrostatic potentials. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5088-5094.	1.0	36
231	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
232	Stochastic-based descriptors studying biopolymers biological properties: Extended MARCH-INSIDE methodology describing antibacterial activity of lactoferricin derivatives. Biopolymers, 2005, 77, 247-256.	1.2	18
233	Biopolymer stochastic moments. I. Modeling human rhinovirus cellular recognition with protein surface electrostatic moments. Biopolymers, 2005, 77, 296-303.	1.2	30
234	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

#	Article	IF	Citations
235	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
236	Recognition of stable protein mutants with 3D stochastic average electrostatic potentials. FEBS Letters, 2005, 579, 4297-4301.	1.3	48
237	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
238	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
239	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
240	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
241	Designing Antibacterial Compounds Through a Topological Substructural Approach.. ChemInform, 2004, 35, no.	0.1	0
242	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
243	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
244	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
245	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
246	A TOPS-MODE approach to predict permeability coefficients. Polymer, 2004, 45, 2073-2079.	1.8	39
247	Stochastic molecular descriptors for polymers. 1. Modelling the properties of icosahedral viruses with 3D-Markovian negentropies. Polymer, 2004, 45, 3845-3853.	1.8	40
248	A topological sub-structural approach for predicting human intestinal absorption of drugs. European Journal of Medicinal Chemistry, 2004, 39, 905-916.	2.6	60
249	Markov entropy backbone electrostatic descriptors for predicting proteins biological activity. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4691-4695.	1.0	59
250	Designing Antibacterial Compounds through a Topological Substructural Approach. Journal of Chemical Information and Computer Sciences, 2004, 44, 515-521.	2.8	82
251	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
252	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

#	Article	IF	Citations
253	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
254	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
255	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
256	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
257	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
258	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
259	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
260	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
261	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
262	MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), 2017, 3rd edition.. , 0, , .		1
263	MOL2NET: FROM MOLECULES TO NETWORKS (PROC. BOOK), ISBN: 978-3-03842-820-6, 2019, Vol. 4, 2985 pp. . , 0, , .		1
264	USEDAT: USA-Europe Data Analysis Training Worldwide Program, 2019 ed.. , 0, , .		1
265	QSAR Study for Macromolecular RNA Folded Secondary Structures of Mycobacterial Promoters with Low Sequence Homology. , 0, , .		0
266	Design, Synthesis and Pharmacological Evaluation of New Coumarin Derivatives as Monoamine Oxidase A and B Inhibitors. , 0, , .		1
267	Computational model for multiplex assay of drug immunotoxicity in macrophage - study of the anti-microbial G1 using flow cytometry. , 0, , .		0
268	Using Bob-Jenkins Operators and Spectral Moments to Predict In-Out Perturbations in the Synthetic Pathways involving Assymetric Catalysis of Intra-molecular Carbolithiations. , 0, , .		0
269	Prediction of Neurological Enzyme Targets for Known and New Compounds with a Model using Galvez's Topological Indices. , 0, , .		0
270	Editorial: MOL2NET 2015, International Conference on Multidisciplinary Sciences.. , 0, , .		0

#	Article	IF	Citations
271	MOL2NET 2015 - 1st International Conference on Synergies of Experimental Groups of Molecular and Biomedical Sciences with Data, Networks, and Social Sciences Experts. Bilbao,5–15 Dec, 2015.. , 0, , .		0
272	Perturbation Theory Modeling of Intramolecular Carbolithiation Reactions. , 0, , .		0
273	Bio-AIMS Chemoinformatics Web tools for proteins. , 0, , .		0
274	QSRR Prediction of Parham reactions yield taking into consideration different reaction conditions. , 0, , .		0
275	Artificial Neural Network Schedulers for Food Webs. , 0, , .		0
276	SRI-08: The 8th Annual Undergraduate Summer Research Symposium of Saint Thomas University. , 0, , .		0
277	Editorial: MOL2NET 2016, International Conference Series on Multidisciplinary Sciences.. , 0, , .		0
278	FRAMA 1.0: Framework for Moving Average Operators Calculation in Data Analysis. , 0, , .		0
279	Notes Towards a Network Approach to Gene Orientation. , 0, , .		0
280	Prediction of RIFIN proteins with gene orientation network indices. , 0, , .		0
281	MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), 2016, 2nd edition.. , 0, , .		0
282	MOL2NET: FROM MOLECULES TO NETWORKS (PROC. BOOK), 2018, Vol. 1, 761 pp. . , 0, , .		0
283	PTML: Perturbation-Theory Machine Learning notes. , 0, , .		3