

Humbert González-Díaz

List of Publications by Year in descending order

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Version: 2024-02-01

283
papers

8,932
citations

36691

53
h-index

84171

75
g-index

291
all docs

291
docs citations

291
times ranked

3894
citing authors

#	ARTICLE	IF	CITATIONS
1	Multi-output chemometrics model for gasoline compounding. <i>Fuel</i> , 2022, 310, 122274.	3.4	4
2	Towards rational nanomaterial design by predicting drug–nanoparticle system interaction vs. bacterial metabolic networks. <i>Environmental Science: Nano</i> , 2022, 9, 1391-1413.	2.2	5
3	Machine Learning Study of Metabolic Networks vs. ChEMBL Data of Antibacterial Compounds. <i>Molecular Pharmaceutics</i> , 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). <i>ACS Chemical Neuroscience</i> , 2021, 12, 203-215.	1.7	11
5	IFPTML mapping of nanoparticle antibacterial activity vs. pathogen metabolic networks. <i>Nanoscale</i> , 2021, 13, 1318-1330.	2.8	15
6	New Experimental and Computational Tools for Drug Discovery: Part - XI. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 597-598.	1.0	0
7	New Experimental and Computational Tools for Drug Discovery. Part XII. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 789-789.	1.0	1
8	Predicting Metabolic Reaction Networks with Perturbation-Theory Machine Learning (PTML) Models. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>European Journal of Medicinal Chemistry</i> , 2021, 220, 113458.	2.6	11
10	Towards machine learning discovery of dual antibacterial drug–nanoparticle systems. <i>Nanoscale</i> , 2021, 13, 17854-17870.	2.8	11
11	Prediction of Anti-Glioblastoma Drug-Decorated Nanoparticle Delivery Systems Using Molecular Descriptors and Machine Learning. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11519.	1.8	5
12	MLb-LDLr. <i>JACC Basic To Translational Science</i> , 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. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13066.	1.8	2
14	PTML Model of ChEMBL Compounds Assays for Vitamin Derivatives. <i>ACS Combinatorial Science</i> , 2020, 22, 129-141.	3.8	10
15	A Multi-Objective Approach for Anti-Osteosarcoma Cancer Agents Discovery through Drug Repurposing. <i>Pharmaceutics</i> , 2020, 13, 409.	1.7	6
16	Predicting coated-nanoparticle drug release systems with perturbation-theory machine learning (PTML) models. <i>Nanoscale</i> , 2020, 12, 13471-13483.	2.8	27
17	Prediction of Antimalarial Drug-Decorated Nanoparticle Delivery Systems with Random Forest Models. <i>Biology</i> , 2020, 9, 198.	1.3	22
18	Web Server and R Library for the Calculation of Markov Chains Molecular Descriptors. <i>Proceedings (mdpi)</i> , 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 Drug-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 " 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 [³⁵ S]GTP ^γ S 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 " 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. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2538-2544.	2.5	73
38	Engineering faster transglycosidases and their acceptor specificity. <i>Green Chemistry</i> , 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). <i>Chemical Research in Toxicology</i> , 2019, 32, 566-577.	1.7	4
40	Modeling Antibacterial Activity with Machine Learning and Fusion of Chemical Structure Information with Microorganism Metabolic Networks. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1109-1120.	2.5	39
41	Designing nanoparticle release systems for drug-vitamin cancer co-therapy with multiplicative perturbation-theory machine learning (PTML) models. <i>Nanoscale</i> , 2019, 11, 21811-21823.	2.8	27
42	Complex Networks and Machine Learning: From Molecular to Social Sciences. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 4493.	1.3	5
43	MitoTarget Modeling Using ANN-Classification Models Based on Fractal SEM Nano-Descriptors: Carbon Nanotubes as Mitochondrial FOF1-ATPase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 86-97.	2.5	11
44	Chromosome Gene Orientation Inversion Networks (GOINs) of Plasmodium Proteome. <i>Journal of Proteome Research</i> , 2018, 17, 1258-1268.	1.8	11
45	Gene prioritization, communality analysis, networking and metabolic integrated pathway to better understand breast cancer pathogenesis. <i>Scientific Reports</i> , 2018, 8, 16679.	1.6	29
46	PTML Combinatorial Model of ChEMBL Compounds Assays for Multiple Types of Cancer. <i>ACS Combinatorial Science</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 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 Prolyl-leucyl-glycinamide Peptidomimetics. <i>ACS Chemical Neuroscience</i> , 2018, 9, 2572-2587.	1.7	38
49	Net-Net Auto Machine Learning (AutoML) Prediction of Complex Ecosystems. <i>Scientific Reports</i> , 2018, 8, 12340.	1.6	9
50	Perturbation Theory-Machine Learning Study of Zeolite Materials Desilication. <i>Journal of Chemical Information and Modeling</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 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 Fe ²⁺ -overload. <i>Carbon</i> , 2017, 115, 312-330.	5.4	11
53	Experimental-Computational Study of Carbon Nanotube Effects on Mitochondrial Respiration: In Silico Nano-QSPR Machine Learning Models Based on New Raman Spectra Transform with Markov-Shannon Entropy Invariants. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1029-1044.	2.5	32
54	A study of the Immune Epitope Database for some fungi species using network topological indices. <i>Molecular Diversity</i> , 2017, 21, 713-718.	2.1	7

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55	PTML Model for Proteome Mining of B-Cell Epitopes and Theoretical Experimental Study of Bm86 Protein Sequences from Colima, Mexico. <i>Journal of Proteome Research</i> , 2017, 16, 4093-4103.	1.8	41
56	Experimental study and Random Forest prediction model of microbiome cell surface hydrophobicity. <i>Expert Systems With Applications</i> , 2017, 72, 306-316.	4.4	22
57	Editorial: New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Part-II. <i>Current Topics in Medicinal Chemistry</i> , 2017, 17, 2901-2902.	1.0	0
58	Editorial: New Experimental and Computational Tools for Drug Discovery: From Chemistry to Biology. Part-1. <i>Current Topics in Medicinal Chemistry</i> , 2017, 17, .	1.0	0
59	Carbon Nanotubes™ Effect on Mitochondrial Oxygen Flux Dynamics: Polarography Experimental Study and Machine Learning Models using Star Graph Trace Invariants of Raman Spectra. <i>Nanomaterials</i> , 2017, 7, 386.	1.9	14
60	Experimental Study and ANN Dual-Time Scale Perturbation Model of Electrokinetic Properties of Microbiota. <i>Frontiers in Microbiology</i> , 2017, 8, 1216.	1.5	3
61	Editorial: Improving Neuropharmacology using Big Data, Machine Learning and Computational Algorithms. <i>Current Neuropharmacology</i> , 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. <i>Scientific Reports</i> , 2017, 7, 13271.	1.6	22
63	Multi-Target Mining of Alzheimer Disease Proteome with Hansch™s QSBR-Perturbation Theory and Experimental-Theoretic Study of New Thiophene Isosters of Rasagiline. <i>Current Drug Targets</i> , 2017, 18, 511-521.	1.0	18
64	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 1). <i>Current Pharmaceutical Design</i> , 2016, 22, 5041-5042.	0.9	22
65	Editorial (Thematic Issue: Chemoinformatics Models for Pharmaceutical Design, Part 2). <i>Current Pharmaceutical Design</i> , 2016, 22, 5177-5178.	0.9	22
66	Data Analysis in Chemistry and Bio-Medical Sciences. <i>International Journal of Molecular Sciences</i> , 2016, 17, 2105.	1.8	3
67	Chiral Brønsted Acid-Catalyzed Enantioselective β -Amidoalkylation Reactions: A Joint Experimental and Predictive Study. <i>ChemistryOpen</i> , 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. <i>Scientific Reports</i> , 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 α -Syn Silico-New Optimal Peptide Sequences and/or Boundary Conditions for Vaccine Development. <i>International Journal of Peptide Research and Therapeutics</i> , 2016, 22, 445-450.	0.9	9
70	Perturbation theory model of reactivity and enantioselectivity of palladium-catalyzed Heck Heck cascade reactions. <i>RSC Advances</i> , 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. <i>RSC Advances</i> , 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. <i>British Journal of Health Psychology</i> , 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. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 151, 1-8.	1.8	5
74	Experimental and chemometric studies of cell membrane permeability. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 154, 1-6.	1.8	8
75	Brain-inspired cheminformatics of drug-target brain interactome, synthesis, and assay of TVP1022 derivatives. <i>Neuropharmacology</i> , 2016, 103, 270-278.	2.0	59
76	Computational Modeling and Experimental Facts of Mixed Self-Assembly Systems. <i>Current Pharmaceutical Design</i> , 2016, 22, 5249-5256.	0.9	3
77	Experimental-Theoretic Approach to Drug-Lymphocyte Interactome Networks with Flow Cytometry and Spectral Moments Perturbation Theory. <i>Current Pharmaceutical Design</i> , 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. <i>Current Protein and Peptide Science</i> , 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. <i>Current Drug Delivery</i> , 2016, , .	0.8	0
81	Self-Assembled Binary Nanoscale Systems: Multioutput Model with LFER-Covariance Perturbation Theory and an Experimental-Computational Study of NaGDC-DDAB Micelles. <i>Langmuir</i> , 2015, 31, 12009-12018.	1.6	10
82	Multi-output model with Box-Jenkins operators of linear indices to predict multi-target inhibitors of ubiquitin-proteasome pathway. <i>Molecular Diversity</i> , 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. <i>BioSystems</i> , 2015, 132-133, 20-34.	0.9	19
84	Experimental and computational studies of fatty acid distribution networks. <i>Molecular BioSystems</i> , 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. <i>RSC Advances</i> , 2015, 5, 103229-103245.	1.7	10
86	Bio-AIMS Collection of Cheminformatics Web Tools based on Molecular Graph Information and Artificial Intelligence Models. <i>Combinatorial Chemistry and High Throughput Screening</i> , 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. <i>Current Bioinformatics</i> , 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. <i>Current Bioinformatics</i> , 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. <i>Current Protein and Peptide Science</i> , 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. <i>Current Bioinformatics</i> , 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	1,0	2
93	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, From Molecular Mechanics, Dynamics,) Tj ETQq1 1 0,784314 rgBT /Over	0,7	1
94	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, Modeling Chemical Reactivity and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	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 " 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. <i>Current Drug Metabolism</i> , 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. <i>Current Drug Metabolism</i> , 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. <i>ACS Chemical Neuroscience</i> , 2013, 4, 1393-1403.	1.7	50
112	The Rá¼ckerâ€“Markov invariants of complex Bio-Systems: Applications in Parasitology and Neuroinformatics. <i>BioSystems</i> , 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. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 1870-1879.	1.4	48
114	Reversible Hypothalamic Dysfunction in Optic Nerve Germinoma. <i>Journal of Craniofacial Surgery</i> , 2013, 24, 468-469.	0.3	0
115	Editorial (Hot Topic: Bioinformatics and Quantitative Structure-Property Relationship (QSPR)) <i>Tj ETQq1 1 0.784314rgBT /Overlock 10 T</i>	0.7	2
116	Editorial (Hot Topic : Computational Prediction of Drug-Target Interactions in Medicinal Chemistry). <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 1619-1621.	1.0	2
117	Synthetic Oxoisoaporphine Alkaloids: In Vitro, In Vivo and In Silico Assessment of Antileishmanial Activities. <i>PLoS ONE</i> , 2013, 8, e77560.	1.1	17
118	Legal issues for chem-bioinformatics models. <i>Frontiers in Bioscience - Elite</i> , 2013, E5, 361-374.	0.9	2
119	Patents of bio-active compounds based on computer-aided drug discovery techniques. <i>Frontiers in Bioscience - Elite</i> , 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. <i>Current Bioinformatics</i> , 2013, 8, 429-437.	0.7	17
121	MIANN Models in Medicinal, Physical and Organic Chemistry. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 1713-1741.	1.0	83
123	Entropy Model for Multiplex Drug-Target Interaction Endpoints of Drug Immunotoxicity. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Bioinformatics</i> , 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)]. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Bioorganic and Medicinal Chemistry</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 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. <i>Molecular BioSystems</i> , 2012, 8, 851.	2.9	19
132	Naïve Bayes QSDR classification based on spiral-graph Shannon entropies for protein biomarkers in human colon cancer. <i>Molecular BioSystems</i> , 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 <i>Trichinella spiralis</i> . <i>Current Bioinformatics</i> , 2012, 7, 7-34.	0.7	1
134	New Markov-Shannon Entropy models to assess connectivity quality in complex networks: From molecular to cellular pathway, Parasite-Host, Neural, Industry, and Legal-Social networks. <i>Journal of Theoretical Biology</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 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. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 1843-1865.	1.0	23
137	MIIND-BEST: Web Server for Drugs and Target Discovery; Design, Synthesis, and Assay of MAO-B Inhibitors and Theoretical-Experimental Study of G3PDH Protein from <i>Trichomonas gallinae</i> . <i>Journal of Proteome Research</i> , 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)]. <i>Current Bioinformatics</i> , 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)}. <i>Current Computer-Aided Drug Design</i> , 2011, 7, 228-230.	0.8	0
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