Ramon Garcia-Domenech

List of Publications by Year
in descending order

69 papers	1,899 citations	318942 23 h-index	299063 42 g-index
69 all docs	69 docs citations	69 times ranked	1628 citing authors

#	Article	IF	Citations
1	How Molecular Topology Can Help in Amyotrophic Lateral Sclerosis (ALS) Drug Development: A Revolutionary Paradigm for a Merciless Disease. Pharmaceuticals, 2022, 15, 94.	1.7	2
2	What place does molecular topology have in todayâ€™s drug discovery?. Expert Opinion on Drug Discovery, 2020, 15, 1133-1144.	2.5	18
3	Molecular Topology QSAR Strategy for Crop Protection: New Natural Fungicides with Chitin Inhibitory Activity. ACS Omega, 2020, 5, 16358-16365.	1.6	4
4	DesMol2, an Effective Tool for the Construction of Molecular Libraries and Its Application to QSAR Using Molecular Topology. Molecules, 2019, 24, 736.	1.7	3
5	Molecular topology and QSAR multi-target analysis to boost the in silico research for fungicides in agricultural chemistry. Molecular Diversity, 2019, 23, 371-379.	2.1	7
6	Alzheimer: A Decade of Drug Design. Why Molecular Topology can be an Extra Edge?. Current Neuropharmacology, 2018, 16, 849-864.	1.4	7
7	Molecular topology: A new strategy for antimicrobial resistance control. European Journal of Medicinal Chemistry, 2017, 137, 233-246.	2.6	11
8	Molecular topology: a strategy to identify novel compounds against ulcerative colitis. Molecular Diversity, 2017, 21, 219-234.	2.1	5
9	Molecular Topology as a Powerful Tool for Searching for New Repellents and Novel Drugs against Diseases Transmitted by Mosquitoes. , 2017, , 107-138.		1
10	Biodegradability Prediction of Fragrant Molecules by Molecular Topology. ACS Sustainable Chemistry and Engineering, 2016, 4, 4224-4231.	3.2	17
11	Predicting antiprotozoal activity of benzyl phenyl ether diamine derivatives through QSAR multi-target and molecular topology. Molecular Diversity, 2015, 19, 357-366.	2.1	12
12	Latest advances in molecular topology applications for drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 945-957.	2.5	34
13	Novel Cancer Chemotherapy Hits by Molecular Topology: Dual Akt and Beta-Catenin Inhibitors. PLoS ONE, 2015, 10, e0124244.	1.1	14
14	In silicoAntibacterial Activity Modeling Based on the TOMOCOMD-CARDD Approach. Journal of the Brazilian Chemical Society, 2015, , .	0.6	16
15	Antiprotozoan lead discovery by aligning dry and wet screening: Prediction, synthesis, and biological assay of novel quinoxalinones. Bioorganic and Medicinal Chemistry, 2014, 22, 1568-1585.	1.4	11
16	The Prediction of Human Intestinal Absorption Based on the Molecular Structure. Current Drug Metabolism, 2014, 15, 380-388.	0.7	4
17	QSAR Multi-Target in Drug Discovery: A Review. Current Computer-Aided Drug Design, 2014, 10, 129-136.	0.8	27
18	Novel potential agents for ulcerative colitis by molecular topology: suppression of IL-6 production in Caco-2 and RAW 264.7 cell lines. Molecular Diversity, 2013, 17, 573-593.	2.1	20

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19	Molecular topology â€“ dissimilar similarities. Drug Discovery Today: Technologies, 2013, 10, e475-e481.	4.0	10
20	Selection of nutraceutical compounds as COX inhibitors by molecular topology. Medicinal Chemistry Research, 2013, 22, 3466-3477.	1.1	2
21	QSAR methods for the discovery of new inflammatory bowel disease drugs. Expert Opinion on Drug Discovery, 2013, 8, 933-949.	2.5	8
22	Advances in the molecular modeling and quantitative structureâ€“activity relationship-based design for antihistamines. Expert Opinion on Drug Discovery, 2013, 8, 305-317.	2.5	5
23	Predicting Dyspnea Inducers by Molecular Topology. Journal of Chemistry, 2013, 2013, 1-11.	0.9	2
24	Application of Molecular Topology to the Prediction of the Reaction Yield and Anticancer Activity of Imidazole and Guanidine Derivatives. International Journal of Chemoinformatics and Chemical Engineering, 2013, 3, 64-74.	0.1	0
25	Modeling Anti-Allergic Natural Compounds by Molecular Topology. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 628-635.	0.6	11
26	Molecular topology as a novel approach for drug discovery. Expert Opinion on Drug Discovery, 2012, 7, 133-153.	2.5	18
27	Modeling Drug-Induced Anorexia by Molecular Topology. Journal of Chemical Information and Modeling, 2012, 52, 1337-1344.	2.5	9
28	Retrained Classification of Tyrosinase Inhibitors and â€œIn Silicoâ€•Potency Estimation by Using Atom-Type Linear Indices. International Journal of Chemoinformatics and Chemical Engineering, 2012, 2, 42-144.	0.1	0
29	Introduction to Molecular Topology: Basic Concepts and Application to Drug Design. Current Computer-Aided Drug Design, 2012, 8, 196-223.	0.8	15
30	Modeling Natural Anti-Inflammatory Compounds by Molecular Topology. International Journal of Molecular Sciences, 2011, 12, 9481-9503.	1.8	35
31	Application of Molecular Topology for the Prediction of Reaction Yields and Anti-Inflammatory Activity of Heterocyclic Amidine Derivatives. International Journal of Molecular Sciences, 2011, 12, 1281-1292.	1.8	10
32	Search of QSAR Models for Predicting the Antiprotozoal Activity and Cytotoxicity In Vitro of a Group of Pentamidine Analogous Compounds. Letters in Drug Design and Discovery, 2011, 8, 172-180.	0.4	1
33	Discovery of novel anti-inflammatory drug-like compounds by aligning in silico and inÂvivo screening: The nitroindazolinone chemotype. European Journal of Medicinal Chemistry, 2011, 46, 5736-5753.	2.6	39
34	Topological virtual screening: a way to find new compounds active in ulcerative colitis by inhibiting NF-Î°B. Molecular Diversity, 2011, 15, 917-926.	2.1	44
35	Bondâ€extended stochastic and nonstochastic bilinear indices. I. QSPR/QSAR applications to the description of properties/activities of smallâ€medium size organic compounds. International Journal of Quantum Chemistry, 2011, 111, 8-34.	1.0	2
36	Bond-based linear indices of the non-stochastic and stochastic edge-adjacency matrix. 1. Theory and modeling of ChemPhys properties of organic molecules. Molecular Diversity, 2010, 14, 731-753.	2.1	15

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37	Application of molecular topology for the prediction of the reaction times and yields under solvent-free conditions. Green Chemistry, 2010, 12, 1056.	4.6	27
38	Application of Molecular Topology to the Search of Novel NSAIDs: Experimental Validation of Activity. Letters in Drug Design and Discovery, 2010, 7, 438-445.	0.4	14
39	On the Contribution of Molecular Topology to Drug Design and Discovery. Current Computer-Aided Drug Design, 2010, 6, 252-268.	0.8	16
40	Novel 2D TOMOCOMD-CARDD molecular descriptors: atom-based stochastic and non-stochastic bilinear indices and their QSPR applications. Journal of Mathematical Chemistry, 2008, 44, 650-673.	0.7	20
41	Bond-based linear indices in QSAR: computational discovery of novel anti-trichomonal compounds. Journal of Computer-Aided Molecular Design, 2008, 22, 523-540.	1.3	31
42	Estimation of ADME Properties in Drug Discovery: Predicting Caco-2 Cell Permeability Using Atom-Based Stochastic and Non-stochastic Linear Indices. Journal of Pharmaceutical Sciences, 2008, 97, 1946-1976.	1.6	72
43	Applying pattern recognition methods plus quantum and physicoâ€chemical molecular descriptors to analyze the anabolic activity of structurally diverse steroids. Journal of Computational Chemistry, 2008, 29, 317-333.	1.5	19
44	Bondâ€based 3Dâ€chiral linear indices: Theory and QSAR applications to central chirality codification. Journal of Computational Chemistry, 2008, 29, 2500-2512.	1.5	26
45	Application of molecular topology to the prediction of the antimalarial activity of a group of uracil-based acyclic and deoxyuridine compounds. International Journal of Pharmaceutics, 2008, 363, 78-84.	2.6	17
46	Some New Trends in Chemical Graph Theory. Chemical Reviews, 2008, 108, 1127-1169.	23.0	214
47	New Active Drugs against Liver Stages of Plasmodium Predicted by Molecular Topology. Antimicrobial Agents and Chemotherapy, 2008, 52, 1215-1220.	1.4	56
48	Prediction of acute toxicity of organophosphorus pesticides using topological indices. SAR and QSAR in Environmental Research, 2007, 18, 745-755.	1.0	18
49	Improving the local vertex invariants in alkane graphs through a standard molecular orbital approach. Chemical Physics Letters, 2007, 449, 249-254.	1.2	4
50	Application of a Mathematical Topological Pattern of Antihistaminic Activity for the Selection of New Drug Candidates and Pharmacology Assays. Journal of Medicinal Chemistry, 2006, 49, 3667-3673.	2.9	23
51	Identification of new antimalarial drugs by linear discriminant analysis and topological virtual screening. Journal of Antimicrobial Chemotherapy, 2006, 57, 489-497.	1.3	88
52	Application of molecular topology to the prediction of potency and selection of novel insecticides active against malaria vectors. Computational and Theoretical Chemistry, 2005, 727, 107-113.	1.5	4
53	Search of Chemical Scaffolds for Novel Antituberculosis Agents. Journal of Biomolecular Screening, 2005, 10, 206-214.	2.6	46
54	New Potential Antihistaminic Compounds. Virtual Combinatorial Chemistry, Computational Screening, Real Synthesis, and Pharmacological Evaluation. Journal of Medicinal Chemistry, 2005, 48, 1260-1264.	2.9	24

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55	Getting new bronchodilator compounds from molecular topology. European Journal of Pharmaceutical Sciences, 2004, 22, 271-277.	1.9	11
56	Structural invariants for the prediction of relative toxicities of polychloro dibenzo-p-dioxins and dibenzofurans. Molecular Diversity, 2004, 8, 331-342.	2.1	4
57	New agents active against Mycobacterium avium complex selected by molecular topology: a virtual screening method. Journal of Antimicrobial Chemotherapy, 2003, 53, 65-73.	1.3	67
58	Search of a Topological Pattern to Evaluate Toxicity of Heterogeneous Compounds. SAR and QSAR in Environmental Research, 2001, 12, 237-254.	1.0	18
59	Indices of differences of path lengths: novel topological descriptors derived from electronic interferences in graphs. Journal of Computer-Aided Molecular Design, 2000, 14, 679-687.	1.3	5
60	Anti- Toxoplasma Activities of 24 Quinolones and Fluoroquinolones In Vitro: Prediction of Activity by Molecular Topology and Virtual Computational Techniques. Antimicrobial Agents and Chemotherapy, 2000, 44, 2771-2776.	1.4	58
61	Molecular Search of New Active Drugs AgainstToxoplasma Gondii. SAR and QSAR in Environmental Research, 1999, 10, 47-60.	1.0	50
62	Virtual Combinatorial Syntheses and Computational Screening of New Potential Anti-Herpes Compounds. Journal of Medicinal Chemistry, 1999, 42, 3308-3314.	2.9	116
63	Designing sedative/hypnotic compounds from a novel substructural graph-theoretical approach. Journal of Computer-Aided Molecular Design, 1998, 12, 583-595.	1.3	109
64	New bronchodilators selected by molecular topology. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 477-482.	1.0	54
65	New antifungals selected by molecular topology. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 2577-2582.	1.0	30
66	New cytostatic agents obtained by molecular topology. Bioorganic and Medicinal Chemistry Letters, 1996, 6, 2301-2306.	1.0	31
67	Topological Approach to Drug Design. Journal of Chemical Information and Computer Sciences, 1995, 35, 272-284.	2.8	182
68	Spectrophotometric Determination of Hydralazine with 2-Hydroxy-1-naphthaldehyde in Pharmaceuticals. Journal of Pharmaceutical Sciences, 1991, 80, 690-692.	1.6	6
69	Application of Molecular Topology to the Prediction of Water Quality Indices of Alkylphenol Pollutants. , 0, , 1-10.		0