Jorge GÃ¡lvez

List of Publications by Year
in descending order

65	1,796	377584 21	312153 41
papers	citations	h-index	g-index

68	68	68	2191
all docs	docs citations	times ranked	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	COVID-19 and the Importance of Being Prepared: A Multidisciplinary Strategy for the Discovery of Antivirals to Combat Pandemics. Biomedicines, 2022, 10, 1342.	1.4	2
3	Macrolides May Prevent Severe Acute Respiratory Syndrome Coronavirus 2 Entry into Cells: A Quantitative Structure Activity Relationship Study and Experimental Validation. Journal of Chemical Information and Modeling, 2021, 61, 2016-2025.	2.5	13
4	Computational analysis of macrolides as SARS-CoV-2 main protease inhibitors: a pattern recognition study based on molecular topology and validated by molecular docking. New Journal of Chemistry, 2021, 45, 8654-8675.	1.4	2
5	Chitin Deacetylase, a Novel Target for the Design of Agricultural Fungicides. Journal of Fungi (Basel,) Tj ETQq1 1 0.784314 rgBT /Overlo	1.5	10
6	Identification of New Templates for the Synthesis of BEA, BEC, and ISV Zeolites Using Molecular Topology and Monte Carlo Techniques. Journal of Chemical Information and Modeling, 2020, 60, 2819-2829.	2.5	5
7	What place does molecular topology have in todayâ€™s drug discovery?. Expert Opinion on Drug Discovery, 2020, 15, 1133-1144.	2.5	18
8	Molecular Topology QSAR Strategy for Crop Protection: New Natural Fungicides with Chitin Inhibitory Activity. ACS Omega, 2020, 5, 16358-16365.	1.6	4
9	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
10	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
11	Alzheimer: A Decade of Drug Design. Why Molecular Topology can be an Extra Edge?. Current Neuropharmacology, 2018, 16, 849-864.	1.4	7
12	Molecular topology: A new strategy for antimicrobial resistance control. European Journal of Medicinal Chemistry, 2017, 137, 233-246.	2.6	11
13	Molecular topology: a strategy to identify novel compounds against ulcerative colitis. Molecular Diversity, 2017, 21, 219-234.	2.1	5
14	Molecular Topology as a Powerful Tool for Searching for New Repellents and Novel Drugs against Diseases Transmitted by Mosquitoes. , 2017, , 107-138.		1
15	Biodegradability Prediction of Fragrant Molecules by Molecular Topology. ACS Sustainable Chemistry and Engineering, 2016, 4, 4224-4231.	3.2	17
16	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
17	Latest advances in molecular topology applications for drug discovery. Expert Opinion on Drug Discovery, 2015, 10, 945-957.	2.5	34
18	Computer-guided drug repurposing: Identification of trypanocidal activity of clofazimine, benidipine and saquinavir. European Journal of Medicinal Chemistry, 2015, 93, 338-348.	2.6	63

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19	Novel Cancer Chemotherapy Hits by Molecular Topology: Dual Akt and Beta-Catenin Inhibitors. PLoS ONE, 2015, 10, e0124244.	1.1	14
20	Molecular Topology Applied to the Discovery of 1-Benzyl-2-(3-fluorophenyl)-4-hydroxy-3-(3-phenylpropanoyl)-2H-pyrrole-5-one as a Non-Ligand-Binding-Pocket Antiandrogen. Journal of Chemical Information and Modeling, 2014, 54, 2953-2966.	2.5	11
21	Molecular Topology as Novel Strategy for Discovery of Drugs with AÎ² Lowering and Anti-Aggregation Dual Activities for Alzheimerâ€™s Disease. PLoS ONE, 2014, 9, e92750.	1.1	12
22	QSAR Multi-Target in Drug Discovery: A Review. Current Computer-Aided Drug Design, 2014, 10, 129-136.	0.8	27
23	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
24	Molecular topology â€“ dissimilar similarities. Drug Discovery Today: Technologies, 2013, 10, e475-e481.	4.0	10
25	QSAR methods for the discovery of new inflammatory bowel disease drugs. Expert Opinion on Drug Discovery, 2013, 8, 933-949.	2.5	8
26	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
27	Predicting Dyspnea Inducers by Molecular Topology. Journal of Chemistry, 2013, 2013, 1-11.	0.9	2
28	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
29	Molecular topology as a novel approach for drug discovery. Expert Opinion on Drug Discovery, 2012, 7, 133-153.	2.5	18
30	Synthesis, biological evaluation and chemometric analysis of indazole derivatives. 1,2-Disubstituted 5-nitroindazolinones, new prototypes of antichagasic drug. European Journal of Medicinal Chemistry, 2012, 58, 214-227.	2.6	45
31	Modeling Drug-Induced Anorexia by Molecular Topology. Journal of Chemical Information and Modeling, 2012, 52, 1337-1344.	2.5	9
32	Introduction to Molecular Topology: Basic Concepts and Application to Drug Design. Current Computer-Aided Drug Design, 2012, 8, 196-223.	0.8	15
33	A Graph-Theoretical Approach to Calculate Vibrational Energies of Atomic and Subatomic Systems. Open Journal of Physical Chemistry, 2012, 02, 204-211.	0.1	4
34	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
35	Chemistry Explained by Topology: An Alternative Approach. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 279-283.	0.6	7
36	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

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37	MT103 inhibits tumor growth with minimal toxicity in murine model of lung carcinoma via induction of apoptosis. Investigational New Drugs, 2011, 29, 846-852.	1.2	13
38	Application of Molecular Topology to the Prediction of Water Quality Indices of Alkylphenol Pollutants. International Journal of Chemoinformatics and Chemical Engineering, 2011, 1, 1-11.	0.1	0
39	Application of molecular topology to the prediction of mosquito repellents of a group of terpenoid compounds. Molecular Diversity, 2010, 14, 321-329.	2.1	17
40	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
41	On the Contribution of Molecular Topology to Drug Design and Discovery. Current Computer-Aided Drug Design, 2010, 6, 252-268.	0.8	16
42	A review on molecular topology: applying graph theory to drug discovery and design. Die Naturwissenschaften, 2009, 96, 749-761.	0.6	29
43	A novel quinoline, MT477: suppresses cell signaling through Ras molecular pathway, inhibits PKC activity, and demonstrates in vivo anti-tumor activity against human carcinoma cell lines. Investigational New Drugs, 2008, 26, 223-232.	1.2	45
44	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
45	Some New Trends in Chemical Graph Theory. Chemical Reviews, 2008, 108, 1127-1169.	23.0	214
46	New Active Drugs against Liver Stages of Plasmodium Predicted by Molecular Topology. Antimicrobial Agents and Chemotherapy, 2008, 52, 1215-1220.	1.4	56
47	Improving the local vertex invariants in alkane graphs through a standard molecular orbital approach. Chemical Physics Letters, 2007, 449, 249-254.	1.2	4
48	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
49	Computational Methods in Developing Quantitative Structure-Activity Relationships (QSAR): A Review. Combinatorial Chemistry and High Throughput Screening, 2006, 9, 213-228.	0.6	324
50	Identification of new antimalarial drugs by linear discriminant analysis and topological virtual screening. Journal of Antimicrobial Chemotherapy, 2006, 57, 489-497.	1.3	88
51	In vitro activity of linezolid, clarithromycin and moxifloxacin against clinical isolates of Mycobacterium kansasii. Journal of Antimicrobial Chemotherapy, 2005, 55, 950-953.	1.3	47
52	Search of Chemical Scaffolds for Novel Antituberculosis Agents. Journal of Biomolecular Screening, 2005, 10, 206-214.	2.6	46
53	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
54	Getting new bronchodilator compounds from molecular topology. European Journal of Pharmaceutical Sciences, 2004, 22, 271-277.	1.9	11

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55	Getting new bronchodilator compounds from molecular topology. European Journal of Pharmaceutical Sciences, 2004, 22, 271-271.	1.9	1
56	Prediction of Molecular Volume and Surface of Alkanes by Molecular Topology.. ChemInform, 2003, 34, no.	0.1	0
57	Prediction of Molecular Volume and Surface of Alkanes by Molecular Topology. Journal of Chemical Information and Computer Sciences, 2003, 43, 1231-1239.	2.8	19
58	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
59	General topological patterns of known drugs. Journal of Molecular Graphics and Modelling, 2001, 20, 84-94.	1.3	30
60	Molecular topology: a useful tool for the search of new antibacterials. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2033-2036.	1.0	35
61	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
62	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
63	Virtual Combinatorial Syntheses and Computational Screening of New Potential Anti-Herpes Compounds. Journal of Medicinal Chemistry, 1999, 42, 3308-3314.	2.9	116
64	New antifungals selected by molecular topology. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 2577-2582.	1.0	30
65	Application of Molecular Topology to the Prediction of Water Quality Indices of Alkylphenol Pollutants. , 0, , 1-10.		0