Florbela Pereira

List of Publications by Year in descending order

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38 papers	935 citations	471061 17 h-index	454577 30 g-index
39 all docs	39 docs citations	39 times ranked	1628 citing authors

#	Article	IF	Citations
1	Dereplication: racing to speed up the natural products discovery process. Natural Product Reports, 2015, 32, 779-810.	5.2	210
2	Machine Learning Methods to Predict Density Functional Theory B3LYP Energies of HOMO and LUMO Orbitals. Journal of Chemical Information and Modeling, 2017, 57, 11-21.	2.5	129
3	Computational Methodologies in the Exploration of Marine Natural Product Leads. Marine Drugs, 2018, 16, 236.	2.2	70
4	Have marine natural product drug discovery efforts been productive and how can we improve their efficiency?. Expert Opinion on Drug Discovery, 2019, 14, 717-722.	2.5	55
5	Antifouling Napyradiomycins from Marine-Derived Actinomycetes Streptomyces aculeolatus. Marine Drugs, 2020, 18, 63.	2.2	39
6	Machine learning for the prediction of molecular dipole moments obtained by density functional theory. Journal of Cheminformatics, 2018, 10, 43.	2.8	34
7	The Madeira Archipelago As a Significant Source of Marine-Derived Actinomycete Diversity with Anticancer and Antimicrobial Potential. Frontiers in Microbiology, 2016, 7, 1594.	1.5	32
8	Intraâ€clade metabolomic profiling of MAR4 Streptomyces from the Macaronesia Atlantic region reveals a source of antiâ€biofilm metabolites. Environmental Microbiology, 2019, 21, 1099-1112.	1.8	31
9	In Silico HCT116 Human Colon Cancer Cell-Based Models En Route to the Discovery of Lead-Like Anticancer Drugs. Biomolecules, 2018, 8, 56.	1.8	29
10	A Chemoinformatics Approach to the Discovery of Lead-Like Molecules from Marine and Microbial Sources En Route to Antitumor and Antibiotic Drugs. Marine Drugs, 2014, 12, 757-778.	2.2	28
11	A Computer-Driven Approach to Discover Natural Product Leads for Methicillin-Resistant Staphylococcus aureus Infection Therapy. Marine Drugs, 2019, 17, 16.	2.2	27
12	Triterpenes fromAcacia Dealbata. Natural Product Research, 1996, 8, 97-103.	0.4	26
13	A Computer-Aided Drug Design Approach to Predict Marine Drug-Like Leads for SARS-CoV-2 Main Protease Inhibition. Marine Drugs, 2020, 18, 633.	2.2	25
14	Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students. Journal of Chemical Education, 2013, 90, 1028-1031.	1.1	23
15	QSAR-Assisted Virtual Screening of Lead-Like Molecules from Marine and Microbial Natural Sources for Antitumor and Antibiotic Drug Discovery. Molecules, 2015, 20, 4848-4873.	1.7	22
16	Estimation of Mayr Electrophilicity with a Quantitative Structureâ€“Property Relationship Approach Using Empirical and DFT Descriptors. Journal of Organic Chemistry, 2011, 76, 9312-9319.	1.7	21
17	MOLinsight: A Web Portal for the Processing of Molecular Structures by Blind Students. Journal of Chemical Education, 2011, 88, 361-362.	1.1	20
18	Interactions of Omeprazole and Precursors withbeta-Cyclodextrin Host Molecules. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2003, 47, 47-52.	1.6	12

#	Article	IF	Citations
19	Encapsulation of sodium nimesulide and precursors in Î²-cyclodextrin. Organic and Biomolecular Chemistry, 2003, 1, 873-878.	1.5	11
20	NavMol 2.0 â€“ A Molecular Structure Navigator/Editor for Blind and Visually Impaired Users. European Journal of Organic Chemistry, 2013, 2013, 1415-1419.	1.2	10
21	Polypharmacology of Aconitum and Delphinium sp. Diterpene Alka loids: Antiarrhythmic, Analgesic and Anti-Inflammatory Effects. Mini-Reviews in Organic Chemistry, 2017, 14, .	0.6	10
22	Machine learning prediction of UVâ€“Vis spectra features of organic compounds related to photoreactive potential. Scientific Reports, 2021, 11, 23720.	1.6	10
23	A Ligandâ€Based Approach to the Discovery of Leadâ€Like Potassium Channel K_V1.3 Inhibitors. ChemistrySelect, 2018, 3, 1352-1364.	0.7	8
24	Machine learning methods to predict the crystallization propensity of small organic molecules. CrystEngComm, 2020, 22, 2817-2826.	1.3	8
25	A computer-aided drug design approach to discover tumour suppressor p53 protein activators for colorectal cancer therapy. Bioorganic and Medicinal Chemistry, 2022, 53, 116530.	1.4	8
26	Predicting Antifouling Activity and Acetylcholinesterase Inhibition of Marine-Derived Compounds Using a Computer-Aided Drug Design Approach. Marine Drugs, 2022, 20, 129.	2.2	8
27	Investigating theÂstructure-activity relationship ofÂmarineÂpolycyclicÂbatzelladineÂalkaloids asÂpromisingÂinhibitors for SARS-CoV-2ÂmainÂproteaseÂ(Mpro). Computers in Biology and Medicine, 2022, 147, 105738.	3.9	7
28	Prediction of the anomeric configuration, type of linkage, and residues in disaccharides from 1D 13C NMR data. Carbohydrate Research, 2011, 346, 960-972.	1.1	6
29	Machine Learning Methods to Predict the Terrestrial and Marine Origin of Natural Products. Molecular Informatics, 2021, 40, e2060034.	1.4	6
30	1D 13C-NMR Data as Molecular Descriptors in Spectra â€” Structure Relationship Analysis of Oligosaccharides. Molecules, 2012, 17, 3818-3833.	1.7	3
31	NavMol 3.0: enabling the representation of metabolic reactions by blind users. Bioinformatics, 2018, 34, 120-121.	1.8	3
32	Exploration of Quantitative Structureï£¿Reactivity Relationships for the Estimation of Mayr Nucleophilicity. Helvetica Chimica Acta, 2015, 98, 863-879.	1.0	2
33	A computational approach in the discovery of lead-like compounds for anticancer drugs. Frontiers in Marine Science, 0, 3, .	1.2	1
34	Correction to Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students. Journal of Chemical Education, 2013, 90, 1567-1567.	1.1	0
35	A QSAR approach for virtual screening of lead-like molecules en route to antitumor and antibiotic drugs from marine and microbial natural products. Frontiers in Marine Science, 0, 1, .	1.2	0
36	Marine actinomycetes from Madeira Archipelago preliminary taxonomic studies. Frontiers in Marine Science, 0, 1, .	1.2	0

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37	Phylogenetic and chemical diversity of MAR4 streptomycete lineage. Frontiers in Marine Science, 0, 1, .	1.2	0
38	Molecular Networking to target the isolation of novel isoprenoids derivatives from marine-derived actinomycetes. Frontiers in Marine Science, 0, 5, .	1.2	0