JoÃ£o Aires de Sousa

List of Publications by Year
in descending order

67	2,597	186209	197736
papers	citations	28 h-index	49 g-index

76	76	76	3137
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	1.3	453
2	Prediction of1H NMR Chemical Shifts Using Neural Networks. Analytical Chemistry, 2002, 74, 80-90.	3.2	178
3	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
4	Design, synthesis and biological evaluation of novel isoniazid derivatives with potent antitubercular activity. European Journal of Medicinal Chemistry, 2014, 81, 119-138.	2.6	97
5	Random Forest Prediction of Mutagenicity from Empirical Physicochemical Descriptors. Journal of Chemical Information and Modeling, 2007, 47, 1-8.	2.5	88
6	Estimation of melting points of pyridinium bromide ionic liquids with decision trees and neural networks. Green Chemistry, 2005, 7, 20.	4.6	85
7	Computational Methodologies in the Exploration of Marine Natural Product Leads. Marine Drugs, 2018, 16, 236.	2.2	70
8	A new enantioselective synthesis of N-arylaziridines by phase-transfer catalysis. Tetrahedron Letters, 1996, 37, 3183-3186.	0.7	65
9	Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250.	2.5	65
10	Structure-Based Classification of Chemical Reactions without Assignment of Reaction Centers. Journal of Chemical Information and Modeling, 2005, 45, 1775-1783.	2.5	62
11	Prediction of ¹H NMR Coupling Constants with Associative Neural Networks Trained for Chemical Shifts. Journal of Chemical Information and Modeling, 2007, 47, 2089-2097.	2.5	60
12	New Description of Molecular Chirality and Its Application to the Prediction of the Preferred Enantiomer in Stereoselective Reactions. Journal of Chemical Information and Computer Sciences, 2001, 41, 369-375.	2.8	58
13	Structure-Based Predictions of1H NMR Chemical Shifts Using Feed-Forward Neural Networks. Journal of Chemical Information and Computer Sciences, 2004, 44, 940-945.	2.8	55
14	Asymmetric synthesis of N-aryl aziridines. Tetrahedron: Asymmetry, 2002, 12, 3349-3365.	1.8	53
15	A big data approach to the ultra-fast prediction of DFT-calculated bond energies. Journal of Cheminformatics, 2013, 5, 34.	2.8	51
16	Geographical classification of crude oils by Kohonen self-organizing maps. Analytica Chimica Acta, 2006, 556, 374-382.	2.6	50
17	Comparing the chemical spaces of metabolites and available chemicals: models of metabolite-likeness. Molecular Diversity, 2007, 11, 23-36.	2.1	50
18	Prediction of enantiomeric selectivity in chromatography. Journal of Molecular Graphics and Modelling, 2002, 20, 373-388.	1.3	48

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19	QSAR analysis of phenolic antioxidants using MOLMAP descriptors of local properties. Bioorganic and Medicinal Chemistry, 2006, 14, 1199-1206.	1.4	47
20	Synthesis and properties of new functionalized guanidinium based ionic liquids as non-toxic versatile organic materials. Tetrahedron, 2010, 66, 8785-8794.	1.0	45
21	Prediction of Enantiomeric Excess in a Combinatorial Library of Catalytic Enantioselective Reactions. ACS Combinatorial Science, 2005, 7, 298-301.	3.3	43
22	Prediction of enantioselectivity using chirality codes and Classification and Regression Trees. Analytica Chimica Acta, 2005, 544, 315-326.	2.6	41
23	Exploration of quantitative structureâ€“property relationships (QSPR) for the design of new guanidinium ionic liquids. Tetrahedron, 2008, 64, 2216-2224.	1.0	40
24	Chirality Codes and Molecular Structure. Journal of Chemical Information and Computer Sciences, 2004, 44, 831-836.	2.8	37
25	Genome-scale classification of metabolic reactions and assignment of EC numbers with self-organizing maps. Bioinformatics, 2008, 24, 2236-2244.	1.8	36
26	Genome-Scale Classification of Metabolic Reactions: A Chemoinformatics Approach. Angewandte Chemie - International Edition, 2006, 45, 2066-2069.	7.2	35
27	Machine learning for the prediction of molecular dipole moments obtained by density functional theory. Journal of Cheminformatics, 2018, 10, 43.	2.8	34
28	JATOON: Java tools for neural networks. Chemometrics and Intelligent Laboratory Systems, 2002, 61, 167-173.	1.8	32
29	Assignment of EC Numbers to Enzymatic Reactions with MOLMAP Reaction Descriptors and Random Forests. Journal of Chemical Information and Modeling, 2009, 49, 1839-1846.	2.5	28
30	The Impact of Available Experimental Data on the Prediction of1H NMR Chemical Shifts by Neural Networks. Journal of Chemical Information and Computer Sciences, 2004, 44, 946-949.	2.8	25
31	Physicochemical Stereodescriptors of Atomic Chiral Centers. Journal of Chemical Information and Modeling, 2006, 46, 2278-2287.	2.5	24
32	QSAR modeling of antitubercular activity of diverse organic compounds. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 69-74.	1.8	24
33	Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students. Journal of Chemical Education, 2013, 90, 1028-1031.	1.1	23
34	Automatic Assignment of Absolute Configuration from 1D NMR Data. Journal of Organic Chemistry, 2005, 70, 2120-2130.	1.7	22
35	Machine learning of chemical reactivity from databases of organic reactions. Journal of Computer-Aided Molecular Design, 2009, 23, 419-429.	1.3	21
36	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

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37	Mapping Potential Energy Surfaces by Neural Networks: The ethanol/Au(111) interface. Journal of Electroanalytical Chemistry, 2008, 624, 109-120.	1.9	20
38	MOLinsight: A Web Portal for the Processing of Molecular Structures by Blind Students. Journal of Chemical Education, 2011, 88, 361-362.	1.1	20
39	Models for Identification of Erroneous Atom-to-Atom Mapping of Reactions Performed by Automated Algorithms. Journal of Chemical Information and Modeling, 2012, 52, 3116-3122.	2.5	20
40	A QSPR approach for the fast estimation of DFT/NBO partial atomic charges. Chemometrics and Intelligent Laboratory Systems, 2014, 134, 158-163.	1.8	20
41	Theoretical and experimental studies of aryl-bithiophene based push-pull Ï€-conjugated heterocyclic systems bearing cyanoacetic or rhodanine-3-acetic acid acceptors for SHG nonlinear optical applications. Dyes and Pigments, 2018, 149, 566-573.	2.0	20
42	Representation of DNA sequences with virtual potentials and their processing by (SEQREP) Kohonen self-organizing maps. Bioinformatics, 2003, 19, 30-36.	1.8	15
43	Geographical classification of weathered crude oil samples with unsupervised self-organizing maps and a consensus criterion. Chemometrics and Intelligent Laboratory Systems, 2010, 101, 43-55.	1.8	15
44	Combining Kohonen neural networks and variable selection by classification trees to cluster road soil samples. Chemometrics and Intelligent Laboratory Systems, 2010, 102, 20-34.	1.8	15
45	Multivariate statistical approaches for wine classification based on low molecular weight phenolic compounds. Australian Journal of Grape and Wine Research, 2012, 18, 138-146.	1.0	14
46	Neural networks to approach potential energy surfaces: Application to a molecular dynamics simulation. International Journal of Quantum Chemistry, 2007, 107, 2120-2132.	1.0	13
47	Structure-based predictions of 1H NMR chemical shifts of sesquiterpene lactones using neural networks. Tetrahedron Letters, 2004, 45, 6931-6935.	0.7	12
48	Machine Learning Estimation of Atom Condensed Fukui Functions. Molecular Informatics, 2016, 35, 62-69.	1.4	11
49	Approach to potential energy surfaces by neural networks. A review of recent work. International Journal of Quantum Chemistry, 2010, 110, 432-445.	1.0	10
50	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
51	Machine learning prediction of UVâ€“Vis spectra features of organic compounds related to photoreactive potential. Scientific Reports, 2021, 11, 23720.	1.6	10
52	An Arduino-Based Talking Calorimeter for Inclusive Lab Activities. Journal of Chemical Education, 2020, 97, 1677-1681.	1.1	8
53	Linking Databases of Chemical Reactions to NMR Data:Â an Exploration of1H NMR-Based Reaction Classification. Analytical Chemistry, 2007, 79, 854-862.	3.2	7
54	Synthesis of Pyridazine Derivatives by Suzuki-Miyaura Cross-Coupling Reaction and Evaluation of Their Optical and Electronic Properties through Experimental and Theoretical Studies. Molecules, 2018, 23, 3014.	1.7	7

#	Article	IF	Citations
55	Exploration of automatic learning to establish relationships between the molecular structure of chiral ionic liquids and the specific optical rotation. Journal of Molecular Liquids, 2018, 254, 231-240.	2.3	6
56	Classification of Chemical Reactions and Chemoinformatic Processing of Enzymatic Transformations. Methods in Molecular Biology, 2011, 672, 325-340.	0.4	5
57	Machine learning to predict the specific optical rotations of chiral fluorinated molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 223, 117289.	2.0	5
58	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	2.8	4
59	QSPR Modeling of Liquidâ€Liquid Equilibria in Twoâ€phase Systems of Water and Ionic Liquid. Molecular Informatics, 2020, 39, e2000001.	1.4	4
60	Machine Learning Classification of One-Chiral-Center Organic Molecules According to Optical Rotation. Journal of Chemical Information and Modeling, 2021, 61, 67-75.	2.5	4
61	NavMol 3.0: enabling the representation of metabolic reactions by blind users. Bioinformatics, 2018, 34, 120-121.	1.8	3
62	Automatic NMR-Based Identification of Chemical Reaction Types in Mixtures of Co-Occurring Reactions. PLoS ONE, 2014, 9, e88499.	1.1	3
63	Automatic Perception of Chemical Similarities Between Metabolic Pathways. Molecular Informatics, 2012, 31, 135-144.	1.4	2
64	Comparing roadsoils pollution patterns extracted by MOLMAP and classical three-way decomposition methods. Analytica Chimica Acta, 2010, 677, 64-71.	2.6	1
65	Chirality Codes and Molecular Structure.. ChemInform, 2004, 35, no.	0.1	0
66	Prediction of mutagenicity based on empirical physicochemical descriptors. Toxicology Letters, 2009, 189, S7.	0.4	0
67	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