JoÃ£o Aires de Sousa

List of Publications by Year
in descending order

67 papers	2,597 citations	186265 28 h-index	197818 49 g-index
76 all docs	76 docs citations	76 times ranked	3137 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.	2.9	453
2	Prediction of1H NMR Chemical Shifts Using Neural Networks. Analytical Chemistry, 2002, 74, 80-90.	6.5	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.	5.4	129
4	Design, synthesis and biological evaluation of novel isoniazid derivatives with potent antitubercular activity. European Journal of Medicinal Chemistry, 2014, 81, 119-138.	5.5	97
5	Random Forest Prediction of Mutagenicity from Empirical Physicochemical Descriptors. Journal of Chemical Information and Modeling, 2007, 47, 1-8.	5.4	88
6	Estimation of melting points of pyridinium bromide ionic liquids with decision trees and neural networks. Green Chemistry, 2005, 7, 20.	9.0	85
7	Computational Methodologies in the Exploration of Marine Natural Product Leads. Marine Drugs, 2018, 16, 236.	4.6	70
8	A new enantioselective synthesis of N-arylaziridines by phase-transfer catalysis. Tetrahedron Letters, 1996, 37, 3183-3186.	1.4	65
9	Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250.	5.4	65
10	Structure-Based Classification of Chemical Reactions without Assignment of Reaction Centers. Journal of Chemical Information and Modeling, 2005, 45, 1775-1783.	5.4	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.	5.4	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.	6.1	51
16	Geographical classification of crude oils by Kohonen self-organizing maps. Analytica Chimica Acta, 2006, 556, 374-382.	5.4	50
17	Comparing the chemical spaces of metabolites and available chemicals: models of metabolite-likeness. Molecular Diversity, 2007, 11, 23-36.	3.9	50
18	Prediction of enantiomeric selectivity in chromatography. Journal of Molecular Graphics and Modelling, 2002, 20, 373-388.	2.4	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.	3.0	47
20	Synthesis and properties of new functionalized guanidinium based ionic liquids as non-toxic versatile organic materials. Tetrahedron, 2010, 66, 8785-8794.	1.9	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.	5.4	41
23	Exploration of quantitative structureâ€“property relationships (QSPR) for the design of new guanidinium ionic liquids. Tetrahedron, 2008, 64, 2216-2224.	1.9	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.	4.1	36
26	Genome-Scale Classification of Metabolic Reactions: A Chemoinformatics Approach. Angewandte Chemie - International Edition, 2006, 45, 2066-2069.	13.8	35
27	Machine learning for the prediction of molecular dipole moments obtained by density functional theory. Journal of Cheminformatics, 2018, 10, 43.	6.1	34
28	JATOON: Java tools for neural networks. Chemometrics and Intelligent Laboratory Systems, 2002, 61, 167-173.	3.5	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.	5.4	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.	5.4	24
32	QSAR modeling of antitubercular activity of diverse organic compounds. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 69-74.	3.5	24
33	Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students. Journal of Chemical Education, 2013, 90, 1028-1031.	2.3	23
34	Automatic Assignment of Absolute Configuration from 1D NMR Data. Journal of Organic Chemistry, 2005, 70, 2120-2130.	3.2	22
35	Machine learning of chemical reactivity from databases of organic reactions. Journal of Computer-Aided Molecular Design, 2009, 23, 419-429.	2.9	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.	3.2	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.	3.8	20
38	MOLinsight: A Web Portal for the Processing of Molecular Structures by Blind Students. Journal of Chemical Education, 2011, 88, 361-362.	2.3	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.	5.4	20
40	A QSPR approach for the fast estimation of DFT/NBO partial atomic charges. Chemometrics and Intelligent Laboratory Systems, 2014, 134, 158-163.	3.5	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.	3.7	20
42	Representation of DNA sequences with virtual potentials and their processing by (SEQREP) Kohonen self-organizing maps. Bioinformatics, 2003, 19, 30-36.	4.1	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.	3.5	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.	3.5	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.	2.1	14
46	Neural networks to approach potential energy surfaces: Application to a molecular dynamics simulation. International Journal of Quantum Chemistry, 2007, 107, 2120-2132.	2.0	13
47	Structure-based predictions of 1H NMR chemical shifts of sesquiterpene lactones using neural networks. Tetrahedron Letters, 2004, 45, 6931-6935.	1.4	12
48	Machine Learning Estimation of Atom Condensed Fukui Functions. Molecular Informatics, 2016, 35, 62-69.	2.5	11
49	Approach to potential energy surfaces by neural networks. A review of recent work. International Journal of Quantum Chemistry, 2010, 110, 432-445.	2.0	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.	2.4	10
51	Machine learning prediction of UVâ€“Vis spectra features of organic compounds related to photoreactive potential. Scientific Reports, 2021, 11, 23720.	3.3	10
52	An Arduino-Based Talking Calorimeter for Inclusive Lab Activities. Journal of Chemical Education, 2020, 97, 1677-1681.	2.3	8
53	Linking Databases of Chemical Reactions to NMR Data:Â an Exploration of1H NMR-Based Reaction Classification. Analytical Chemistry, 2007, 79, 854-862.	6.5	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.	3.8	7

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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.	4.9	6
56	Classification of Chemical Reactions and Chemoinformatic Processing of Enzymatic Transformations. Methods in Molecular Biology, 2011, 672, 325-340.	0.9	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.	3.9	5
58	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	6.1	4
59	QSPR Modeling of Liquidâ€liquid Equilibria in Twoâ€phase Systems of Water and Ionic Liquid. Molecular Informatics, 2020, 39, e2000001.	2.5	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.	5.4	4
61	NavMol 3.0: enabling the representation of metabolic reactions by blind users. Bioinformatics, 2018, 34, 120-121.	4.1	3
62	Automatic NMR-Based Identification of Chemical Reaction Types in Mixtures of Co-Occurring Reactions. PLoS ONE, 2014, 9, e88499.	2.5	3
63	Automatic Perception of Chemical Similarities Between Metabolic Pathways. Molecular Informatics, 2012, 31, 135-144.	2.5	2
64	Comparing roadsoils pollution patterns extracted by MOLMAP and classical three-way decomposition methods. Analytica Chimica Acta, 2010, 677, 64-71.	5.4	1
65	Chirality Codes and Molecular Structure.. ChemInform, 2004, 35, no.	0.0	0
66	Prediction of mutagenicity based on empirical physicochemical descriptors. Toxicology Letters, 2009, 189, S7.	0.8	0
67	Correction to Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students. Journal of Chemical Education, 2013, 90, 1567-1567.	2.3	0