

Davide Ballabio

List of Publications by Year in descending order

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Version: 2024-02-01

103
papers

5,615
citations

117453

34
h-index

82410

72
g-index

104
all docs

104
docs citations

104
times ranked

5926
citing authors

#	ARTICLE	IF	CITATIONS
1	Classification tools in chemistry. Part 1: linear models. PLS-DA. <i>Analytical Methods</i> , 2013, 5, 3790.	1.3	893
2	Comments on the Definition of the Q^2 Parameter for QSAR Validation. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1669-1678.	2.5	483
3	Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. <i>Molecules</i> , 2012, 17, 4791-4810.	1.7	370
4	Evaluation of model predictive ability by external validation techniques. <i>Journal of Chemometrics</i> , 2010, 24, 194-201.	0.7	290
5	Multivariate comparison of classification performance measures. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 174, 33-44.	1.8	195
6	Quantitative Structure-Activity Relationship Models for Ready Biodegradability of Chemicals. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 867-878.	2.5	160
7	Geographical origin and authentication of extra virgin olive oils by an electronic nose in combination with artificial neural networks. <i>Analytica Chimica Acta</i> , 2006, 567, 202-210.	2.6	149
8	A MATLAB toolbox for Principal Component Analysis and unsupervised exploration of data structure. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 149, 1-9.	1.8	149
9	Evaluation of different storage conditions of extra virgin olive oils with an innovative recognition tool built by means of electronic nose and electronic tongue. <i>Food Chemistry</i> , 2007, 101, 485-491.	4.2	140
10	Particle size, chemical composition, seasons of the year and urban, rural or remote site origins as determinants of biological effects of particulate matter on pulmonary cells. <i>Environmental Pollution</i> , 2013, 176, 215-227.	3.7	125
11	Prediction of Italian red wine sensorial descriptors from electronic nose, electronic tongue and spectrophotometric measurements by means of Genetic Algorithm regression models. <i>Food Chemistry</i> , 2007, 100, 211-218.	4.2	120
12	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020, 128, 27002.	2.8	120
13	A MATLAB toolbox for Self Organizing Maps and supervised neural network learning strategies. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 118, 24-32.	1.8	113
14	The Kohonen and CP-ANN toolbox: A collection of MATLAB modules for Self Organizing Maps and Counterpropagation Artificial Neural Networks. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2009, 98, 115-122.	1.8	111
15	Monitoring of alcoholic fermentation using near infrared and mid infrared spectroscopies combined with electronic nose and electronic tongue. <i>Analytica Chimica Acta</i> , 2011, 697, 67-74.	2.6	95
16	Amperometric electronic tongue for food analysis. <i>Mikrochimica Acta</i> , 2008, 163, 11-21.	2.5	85
17	Beware of Unreliable Q^2 ! A Comparative Study of Regression Metrics for Predictivity Assessment of QSAR Models. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1905-1913.	2.5	84
18	Genetic Algorithms for architecture optimisation of Counter-Propagation Artificial Neural Networks. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2011, 105, 56-64.	1.8	66

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19	Chemical profiling and multivariate data fusion methods for the identification of the botanical origin of honey. <i>Food Chemistry</i> , 2018, 266, 79-89.	4.2	66
20	Defining a novel k-nearest neighbours approach to assess the applicability domain of a QSAR model for reliable predictions. <i>Journal of Cheminformatics</i> , 2013, 5, 27.	2.8	65
21	CATMoS: Collaborative Acute Toxicity Modeling Suite. <i>Environmental Health Perspectives</i> , 2021, 129, 47013.	2.8	63
22	Locally centred Mahalanobis distance: A new distance measure with salient features towards outlier detection. <i>Analytica Chimica Acta</i> , 2013, 787, 1-9.	2.6	60
23	A novel variable reduction method adapted from space-filling designs. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 136, 147-154.	1.8	60
24	Prediction of Acute Aquatic Toxicity toward <i>Daphnia Magna</i> by using the GA-k-NN Method. <i>ATLA Alternatives To Laboratory Animals</i> , 2014, 42, 31-41.	0.7	59
25	Classification of GC-MS measurements of wines by combining data dimension reduction and variable selection techniques. <i>Journal of Chemometrics</i> , 2008, 22, 457-463.	0.7	58
26	Multiblock variance partitioning: A new approach for comparing variation in multiple data blocks. <i>Analytica Chimica Acta</i> , 2008, 615, 18-29.	2.6	56
27	A traceability study on the Moscato wine chain. <i>Food Chemistry</i> , 2013, 138, 1914-1922.	4.2	55
28	Multivariate Classification for Qualitative Analysis. , 2009, , 83-104.		50
29	A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (<i>Pimephales promelas</i>). <i>SAR and QSAR in Environmental Research</i> , 2015, 26, 217-243.	1.0	50
30	Interactions between oral burn, meat flavor and texture in chili spiced pork patties evaluated by time-intensity. <i>Food Quality and Preference</i> , 2007, 18, 909-919.	2.3	49
31	A QSTR-Based Expert System to Predict Sweetness of Molecules. <i>Frontiers in Chemistry</i> , 2017, 5, 53.	1.8	41
32	CAIMAN (Classification And Influence Matrix Analysis): A new approach to the classification based on leverage-scaled functions. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007, 87, 3-17.	1.8	39
33	Multi-method Approach to Trace the Geographical Origin of Alpine Milk: a Case Study of Tyrol Region. <i>Food Analytical Methods</i> , 2016, 9, 1262-1273.	1.3	38
34	Geographical identification of Chianti red wine based on ICP-MS element composition. <i>Food Chemistry</i> , 2020, 315, 126248.	4.2	37
35	Towards Global QSAR Model Building for Acute Toxicity: Munro Database Case Study. <i>International Journal of Molecular Sciences</i> , 2014, 15, 18162-18174.	1.8	36
36	Machine Learning Consensus To Predict the Binding to the Androgen Receptor within the CoMPARA Project. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1839-1848.	2.5	36

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37	Development of models for predicting toxicity from sediment chemistry by partial least squares-discriminant analysis and counter-propagation artificial neural networks. <i>Environmental Pollution</i> , 2010, 158, 607-614.	3.7	32
38	N3 and BNN: Two New Similarity Based Classification Methods in Comparison with Other Classifiers. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2365-2374.	2.5	32
39	Self-Organizing Map and Relational Perspective Mapping for the Accurate Visualization of High-Dimensional Hyperspectral Data. <i>Analytical Chemistry</i> , 2020, 92, 10450-10459.	3.2	32
40	On the Misleading Use of for QSAR Model Comparison. <i>Molecular Informatics</i> , 2019, 38, e1800029.	1.4	31
41	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. <i>Molecular Informatics</i> , 2019, 38, e1800124.	1.4	30
42	On the application of chemometrics for the study of acoustic-mechanical properties of crispy bakery products. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007, 86, 52-59.	1.8	28
43	Molecular Descriptors for Structure-Activity Applications: A Hands-On Approach. <i>Methods in Molecular Biology</i> , 2018, 1800, 3-53.	0.4	28
44	Geographical classification of wine and olive oil by means of classification and influence matrix analysis (CAIMAN). <i>Analytica Chimica Acta</i> , 2006, 570, 249-258.	2.6	27
45	A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 157, 50-57.	1.8	27
46	Quantitative structure-activity relationships to predict sweet and non-sweet tastes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	27
47	Consensus versus Individual QSARs in Classification: Comparison on a Large-Scale Case Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1215-1223.	2.5	26
48	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications. <i>Analytica Chimica Acta</i> , 2009, 648, 45-51.	2.6	25
49	Classification of ancient Etruscan ceramics using statistical multivariate analysis of data. <i>Applied Physics A: Materials Science and Processing</i> , 2004, 79, 299-307.	1.1	24
50	Assessing the Validity of QSARs for Ready Biodegradability of Chemicals: An Applicability Domain Perspective. <i>Current Computer-Aided Drug Design</i> , 2014, 10, 137-147.	0.8	24
51	Characterization of the traditional Cypriot spirit Zivania by means of Counterpropagation Artificial Neural Networks. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007, 87, 52-58.	1.8	23
52	ToF-SIMS and Machine Learning for Single-Pixel Molecular Discrimination of an Acrylate Polymer Microarray. <i>Analytical Chemistry</i> , 2020, 92, 6587-6597.	3.2	23
53	A chemometric approach based on a novel similarity/diversity measure for the characterisation and selection of electronic nose sensors. <i>Analytica Chimica Acta</i> , 2006, 578, 170-177.	2.6	22
54	Relationships between apple texture and rheological parameters by means of multivariate analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 111, 28-33.	1.8	22

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55	A MATLAB toolbox for multivariate regression coupled with variable selection. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 213, 104313.	1.8	22
56	A chemometric approach to the environmental problem of predicting toxicity in contaminated sediments. <i>Journal of Chemometrics</i> , 2010, 24, 379-386.	0.7	21
57	Screening oil spills by mid-IR spectroscopy and supervised pattern recognition techniques. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 114, 132-142.	1.8	20
58	K-CM: A new artificial neural network. Application to supervised pattern recognition. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 138, 110-119.	1.8	20
59	Recent Advances in High-Level Fusion Methods to Classify Multiple Analytical Chemical Data. <i>Data Handling in Science and Technology</i> , 2019, 31, 129-155.	3.1	19
60	Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards <i>Daphnia magna</i> . <i>SAR and QSAR in Environmental Research</i> , 2014, 25, 1013-1036.	1.0	18
61	Classification of multiway analytical data based on MOLMAP approach. <i>Analytica Chimica Acta</i> , 2007, 605, 134-146.	2.6	17
62	Effects of supervised Self Organising Maps parameters on classification performance. <i>Analytica Chimica Acta</i> , 2013, 765, 45-53.	2.6	17
63	Capsaicinoids in Chili Habanero by Flow Injection with Coulometric Array Detection. <i>Electroanalysis</i> , 2019, 31, 844-850.	1.5	17
64	NURA: A curated dataset of nuclear receptor modulators. <i>Toxicology and Applied Pharmacology</i> , 2020, 407, 115244.	1.3	17
65	Chemometric analysis of gas chromatography with flame ionisation detection chromatograms: A novel method for classification of petroleum products. <i>Journal of Chromatography A</i> , 2012, 1238, 121-127.	1.8	15
66	Qualitative consensus of QSAR ready biodegradability predictions. <i>Toxicological and Environmental Chemistry</i> , 0, , 1-24.	0.6	14
67	Characterization of DNA Primary Sequences by a New Similarity/Diversity Measure Based on the Partial Ordering. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1905-1911.	2.5	13
68	Self Organizing Maps for Analysis of Polycyclic Aromatic Hydrocarbons 3-Way Data from Spilled Oils. <i>Analytical Chemistry</i> , 2010, 82, 4264-4271.	3.2	13
69	Structural alerts for the identification of bioaccumulative compounds. <i>Integrated Environmental Assessment and Management</i> , 2019, 15, 19-28.	1.6	13
70	Predicting molecular activity on nuclear receptors by multitask neural networks. <i>Journal of Chemometrics</i> , 2022, 36, e3325.	0.7	13
71	Impact of medium-distance pollution sources in a Galician suburban site (NW Iberian peninsula). <i>Science of the Total Environment</i> , 2015, 512-513, 114-124.	3.9	11
72	Valorization of Side-Streams from a SSF Biorefinery Plant: Wheat Straw Lignin Purification Study. <i>BioResources</i> , 2016, 12, .	0.5	11

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73	Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. <i>Journal of Cheminformatics</i> , 2016, 8, 49.	2.8	10
74	Analyzing 3D hyperspectral TOF-SIMS depth profile data using self-organizing map-relational perspective mapping. <i>Biointerphases</i> , 2020, 15, 061004.	0.6	10
75	Parsimonious Optimization of Multitask Neural Network Hyperparameters. <i>Molecules</i> , 2021, 26, 7254.	1.7	10
76	ChemTastesDB: A curated database of molecular tastants. <i>Food Chemistry Molecular Sciences</i> , 2022, 4, 100090.	0.9	10
77	Oblique rotation of factors: a novel pattern recognition strategy to classify fluorescence excitation-emission matrices of human blood plasma for early diagnosis of colorectal cancer. <i>Molecular BioSystems</i> , 2016, 12, 1963-1975.	2.9	9
78	Nonlinear classification of commercial Mexican tequilas. <i>Journal of Chemometrics</i> , 2017, 31, e2939.	0.7	9
79	Application of DNA mini-barcoding and infrared spectroscopy for the authentication of the Italian product "bottarga". <i>LWT - Food Science and Technology</i> , 2021, 139, 110603.	2.5	9
80	NMR spectroscopy and chemometric models to detect a specific non-porcine ruminant contaminant in pharmaceutical heparin. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2022, 214, 114724.	1.4	9
81	Evaluation of the predictivity of Acute Oral Toxicity (AOT) structure-activity relationship models. <i>Regulatory Toxicology and Pharmacology</i> , 2022, 129, 105109.	1.3	8
82	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. <i>Analytica Chimica Acta</i> , 2009, 648, 52-59.	2.6	7
83	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 3. Variable selection in classification. <i>Analytica Chimica Acta</i> , 2010, 657, 116-122.	2.6	7
84	QSPR STUDY OF RHEOLOGICAL AND MECHANICAL PROPERTIES OF CHLOROPRENE RUBBER ACCELERATORS. <i>Rubber Chemistry and Technology</i> , 2014, 87, 219-238.	0.6	7
85	Classification-based QSAR Models for the Prediction of the Bioactivity of ACE-inhibitor Peptides. <i>Protein and Peptide Letters</i> , 2018, 25, 1015-1023.	0.4	7
86	Chapter 9 The DART (Decision Analysis by Ranking Techniques) Software. <i>Data Handling in Science and Technology</i> , 2008, , 193-207.	3.1	6
87	Oxygen Consumption in South African Sauvignon Blanc Wines: Role of Glutathione, Sulphur Dioxide and Certain Phenolics. <i>South African Journal of Enology and Viticulture</i> , 2016, 34, .	0.8	6
88	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 191, 129-137.	1.8	6
89	Chemometrics for QSAR Modeling. , 2020, , 599-634.		6
90	Chapter 5 Similarity/Diversity Measure for Sequential Data Based on Hasse Matrices. <i>Data Handling in Science and Technology</i> , 2008, , 111-138.	3.1	5

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91	Traceability of soybeans produced in Argentina based on their trace element profiles. Journal of Chemometrics, 2020, 34, e3252.	0.7	5
92	Diabetes mellitus type 2: Exploratory data analysis based on clinical reading. Open Chemistry, 2020, 18, 1041-1053.	1.0	5
93	Dairy cream response in instrumental texture evaluation processed by multivariate analysis. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 258-263.	1.8	3
94	The use of diagnostic ratios, biomarkers and 3-way Kohonen neural networks to monitor the temporal evolution of oil spills. Marine Pollution Bulletin, 2015, 96, 313-320.	2.3	3
95	Principal Component Analysis to interpret changes in chromatic parameters on paint dosimeters exposed long-term to urban air. Chemometrics and Intelligent Laboratory Systems, 2017, 167, 113-122.	1.8	3
96	Plasma Proteome Profiles of Stable CAD Patients Stratified According to Total Apo B Levels. Proteomics - Clinical Applications, 2019, 13, e1800023.	0.8	3
97	Chapter 8 Multi-Criteria Decision-Making Methods. Data Handling in Science and Technology, 2008, 27, 169-191.	3.1	2
98	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A polypharmacology case study. Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104001.	1.8	2
99	Applications of Self-Organizing Maps to Address Environmental Studies. , 2010, , 331-352.		2
100	Comparing roadsoils pollution patterns extracted by MOLMAP and classical three-way decomposition methods. Analytica Chimica Acta, 2010, 677, 64-71.	2.6	1
101	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activity-rich structural regions. Journal of Chemometrics, 2018, 32, e2994.	0.7	1
102	Expanding Antineoplastic Drugs Surface Monitoring Profiles: Enhancing of Zwitterionic Hydrophilic Interaction Methods. Separations, 2022, 9, 34.	1.1	1
103	Geographical Characterization of Olive Oil by Means of Multivariate Classification. , 2010, , 129-137.		0