Davide Ballabio

List of Publications by Year
in descending order

103	5,615	117625	82547
papers	citations	34 h-index	72 g-index

104	104	104	5926
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predicting molecular activity on nuclear receptors by multitask neural networks. Journal of Chemometrics, 2022, 36, e3325.	1.3	13
2	Evaluation of the predictivity of Acute Oral Toxicity (AOT) structure-activity relationship models. Regulatory Toxicology and Pharmacology, 2022, 129, 105109.	2.7	8
3	Expanding Antineoplastic Drugs Surface Monitoring Profiles: Enhancing of Zwitterionic Hydrophilic Interaction Methods. Separations, 2022, 9, 34.	2.4	1
4	NMR spectroscopy and chemometric models to detect a specific non-porcine ruminant contaminant in pharmaceutical heparin. Journal of Pharmaceutical and Biomedical Analysis, 2022, 214, 114724.	2.8	9
5	ChemTastesDB: A curated database of molecular tastants. Food Chemistry Molecular Sciences, 2022, 4, 100090.	2.1	10
6	Application of DNA mini-barcoding and infrared spectroscopy for the authentication of the Italian product â€œbottargaâ€• LWT - Food Science and Technology, 2021, 139, 110603.	5.2	9
7	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
8	A MATLAB toolbox for multivariate regression coupled with variable selection. Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104313.	3.5	22
9	Parsimonious Optimization of Multitask Neural Network Hyperparameters. Molecules, 2021, 26, 7254.	3.8	10
10	Chemometrics for QSAR Modeling. , 2020, , 599-634.		6
11	Analyzing 3D hyperspectral TOF-SIMS depth profile data using self-organizing map-relational perspective mapping. Biointerphases, 2020, 15, 061004.	1.6	10
12	Traceability of soybeans produced in Argentina based on their trace element profiles. Journal of Chemometrics, 2020, 34, e3252.	1.3	5
13	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A polypharmacology case study. Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104001.	3.5	2
14	ToF-SIMS and Machine Learning for Single-Pixel Molecular Discrimination of an Acrylate Polymer Microarray. Analytical Chemistry, 2020, 92, 6587-6597.	6.5	23
15	Self-Organizing Map and Relational Perspective Mapping for the Accurate Visualization of High-Dimensional Hyperspectral Data. Analytical Chemistry, 2020, 92, 10450-10459.	6.5	32
16	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
17	Consensus versus Individual QSARs in Classification: Comparison on a Large-Scale Case Study. Journal of Chemical Information and Modeling, 2020, 60, 1215-1223.	5.4	26
18	Geographical identification of Chianti red wine based on ICP-MS element composition. Food Chemistry, 2020, 315, 126248.	8.2	37

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19	NURA: A curated dataset of nuclear receptor modulators. Toxicology and Applied Pharmacology, 2020, 407, 115244.	2.8	17
20	Diabetes mellitus type 2: Exploratory data analysis based on clinical reading. Open Chemistry, 2020, 18, 1041-1053.	1.9	5
21	On the Misleading Use of for QSAR Model Comparison. Molecular Informatics, 2019, 38, e1800029.	2.5	31
22	Structural alerts for the identification of bioaccumulative compounds. Integrated Environmental Assessment and Management, 2019, 15, 19-28.	2.9	13
23	Plasma Proteome Profiles of Stable CAD Patients Stratified According to Total Apo Câ€III Levels. Proteomics - Clinical Applications, 2019, 13, e1800023.	1.6	3
24	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making. Chemometrics and Intelligent Laboratory Systems, 2019, 191, 129-137.	3.5	6
25	Machine Learning Consensus To Predict the Binding to the Androgen Receptor within the CoMPARA Project. Journal of Chemical Information and Modeling, 2019, 59, 1839-1848.	5.4	36
26	Recent Advances in High-Level Fusion Methods to Classify Multiple Analytical Chemical Data. Data Handling in Science and Technology, 2019, 31, 129-155.	3.1	19
27	Capsaicinoids in Chili Habanero by Flow Injection with Coulometric Array Detection. Electroanalysis, 2019, 31, 844-850.	2.9	17
28	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. Molecular Informatics, 2019, 38, e1800124.	2.5	30
29	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activityâ€rich structural regions. Journal of Chemometrics, 2018, 32, e2994.	1.3	1
30	Multivariate comparison of classification performance measures. Chemometrics and Intelligent Laboratory Systems, 2018, 174, 33-44.	3.5	195
31	Chemical profiling and multivariate data fusion methods for the identification of the botanical origin of honey. Food Chemistry, 2018, 266, 79-89.	8.2	66
32	Molecular Descriptors for Structureâ€“Activity Applications: A Hands-On Approach. Methods in Molecular Biology, 2018, 1800, 3-53.	0.9	28
33	Classification-based QSAR Models for the Prediction of the Bioactivity of ACE-inhibitor Peptides. Protein and Peptide Letters, 2018, 25, 1015-1023.	0.9	7
34	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.	3.5	3
35	Nonlinear classification of commercial Mexican tequilas. Journal of Chemometrics, 2017, 31, e2939.	1.3	9
36	A QSTR-Based Expert System to Predict Sweetness of Molecules. Frontiers in Chemistry, 2017, 5, 53.	3.6	41

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37	Valorization of Side-Streams from a SSF Biorefinery Plant: Wheat Straw Lignin Purification Study. BioResources, 2016, 12, .	1.0	11
38	Oxygen Consumption in South African Sauvignon Blanc Wines: Role of Glutathione, Sulphur Dioxide and Certain Phenolics. South African Journal of Enology and Viticulture, 2016, 34, .	0.4	6
39	Oblique rotation of factors: a novel pattern recognition strategy to classify fluorescence excitationâ€“emission matrices of human blood plasma for early diagnosis of colorectal cancer. Molecular BioSystems, 2016, 12, 1963-1975.	2.9	9
40	Beware of Unreliable Q²! A Comparative Study of Regression Metrics for Predictivity Assessment of QSAR Models. Journal of Chemical Information and Modeling, 2016, 56, 1905-1913.	5.4	84
41	Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. Journal of Cheminformatics, 2016, 8, 49.	6.1	10
42	A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. Chemometrics and Intelligent Laboratory Systems, 2016, 157, 50-57.	3.5	27
43	Quantitative structureâ€“activity relationships to predict sweet and non-sweet tastes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	27
44	Multi-method Approach to Trace the Geographical Origin of Alpine Milk: a Case Study of Tyrol Region. Food Analytical Methods, 2016, 9, 1262-1273.	2.6	38
45	Impact of medium-distance pollution sources in a Galician suburban site (NW Iberian peninsula). Science of the Total Environment, 2015, 512-513, 114-124.	8.0	11
46	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.	5.0	3
47	A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (Pimephales promelas). SAR and QSAR in Environmental Research, 2015, 26, 217-243.	2.2	50
48	N3 and BNN: Two New Similarity Based Classification Methods in Comparison with Other Classifiers. Journal of Chemical Information and Modeling, 2015, 55, 2365-2374.	5.4	32
49	A MATLAB toolbox for Principal Component Analysis and unsupervised exploration of data structure. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 1-9.	3.5	149
50	Prediction of Acute Aquatic Toxicity toward Daphnia Magna by using the GA-kNN Method. ATLA Alternatives To Laboratory Animals, 2014, 42, 31-41.	1.0	59
51	Towards Global QSAR Model Building for Acute Toxicity: Munro Database Case Study. International Journal of Molecular Sciences, 2014, 15, 18162-18174.	4.1	36
52	QSPR STUDY OF RHEOLOGICAL AND MECHANICAL PROPERTIES OF CHLOROPRENE RUBBER ACCELERATORS. Rubber Chemistry and Technology, 2014, 87, 219-238.	1.2	7
53	Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards Daphnia magna. SAR and QSAR in Environmental Research, 2014, 25, 1013-1036.	2.2	18
54	K-CM: A new artificial neural network. Application to supervised pattern recognition. Chemometrics and Intelligent Laboratory Systems, 2014, 138, 110-119.	3.5	20

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55	A novel variable reduction method adapted from space-filling designs. Chemometrics and Intelligent Laboratory Systems, 2014, 136, 147-154.	3.5	60
56	Assessing the Validity of QSARs for Ready Biodegradability of Chemicals: An Applicability Domain Perspective. Current Computer-Aided Drug Design, 2014, 10, 137-147.	1.2	24
57	Classification tools in chemistry. Part 1: linear models. PLS-DA. Analytical Methods, 2013, 5, 3790.	2.7	893
58	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. Environmental Pollution, 2013, 176, 215-227.	7.5	125
59	Effects of supervised Self Organising Maps parameters on classification performance. Analytica Chimica Acta, 2013, 765, 45-53.	5.4	17
60	A traceability study on the Moscato wine chain. Food Chemistry, 2013, 138, 1914-1922.	8.2	55
61	Locally centred Mahalanobis distance: A new distance measure with salient features towards outlier detection. Analytica Chimica Acta, 2013, 787, 1-9.	5.4	60
62	Quantitative Structureâ€“Activity Relationship Models for Ready Biodegradability of Chemicals. Journal of Chemical Information and Modeling, 2013, 53, 867-878.	5.4	160
63	Defining a novel k-nearest neighbours approach to assess the applicability domain of a QSAR model for reliable predictions. Journal of Cheminformatics, 2013, 5, 27.	6.1	65
64	Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. Molecules, 2012, 17, 4791-4810.	3.8	370
65	A MATLAB toolbox for Self Organizing Maps and supervised neural network learning strategies. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 24-32.	3.5	113
66	Relationships between apple texture and rheological parameters by means of multivariate analysis. Chemometrics and Intelligent Laboratory Systems, 2012, 111, 28-33.	3.5	22
67	Screening oil spills by mid-IR spectroscopy and supervised pattern recognition techniques. Chemometrics and Intelligent Laboratory Systems, 2012, 114, 132-142.	3.5	20
68	Chemometric analysis of gas chromatography with flame ionisation detection chromatograms: A novel method for classification of petroleum products. Journal of Chromatography A, 2012, 1238, 121-127.	3.7	15
69	Genetic Algorithms for architecture optimisation of Counter-Propagation Artificial Neural Networks. Chemometrics and Intelligent Laboratory Systems, 2011, 105, 56-64.	3.5	66
70	Monitoring of alcoholic fermentation using near infrared and mid infrared spectroscopies combined with electronic nose and electronic tongue. Analytica Chimica Acta, 2011, 697, 67-74.	5.4	95
71	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 3. Variable selection in classification. Analytica Chimica Acta, 2010, 657, 116-122.	5.4	7
72	Development of models for predicting toxicity from sediment chemistry by partial least squares-discriminant analysis and counter-propagation artificial neural networks. Environmental Pollution, 2010, 158, 607-614.	7.5	32

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73	A chemometric approach to the environmental problem of predicting toxicity in contaminated sediments. Journal of Chemometrics, 2010, 24, 379-386.	1.3	21
74	Evaluation of model predictive ability by external validation techniques. Journal of Chemometrics, 2010, 24, 194-201.	1.3	290
75	Comparing roadsoils pollution patterns extracted by MOLMAP and classical three-way decomposition methods. Analytica Chimica Acta, 2010, 677, 64-71.	5.4	1
76	Geographical Characterization of Olive Oil by Means of Multivariate Classification. , 2010, , 129-137.		0
77	Self Organizing Maps for Analysis of Polycyclic Aromatic Hydrocarbons 3-Way Data from Spilled Oils. Analytical Chemistry, 2010, 82, 4264-4271.	6.5	13
78	Applications of Self-Organizing Maps to Address Environmental Studies. , 2010, , 331-352.		2
79	Dairy cream response in instrumental texture evaluation processed by multivariate analysis. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 258-263.	3.5	3
80	The Kohonen and CP-ANN toolbox: A collection of MATLAB modules for Self Organizing Maps and Counterpropagation Artificial Neural Networks. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 115-122.	3.5	111
81	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications. Analytica Chimica Acta, 2009, 648, 45-51.	5.4	25
82	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Analytica Chimica Acta, 2009, 648, 52-59.	5.4	7
83	Comments on the Definition of the Q² Parameter for QSAR Validation. Journal of Chemical Information and Modeling, 2009, 49, 1669-1678.	5.4	483
84	Multivariate Classification for Qualitative Analysis. , 2009, , 83-104.		50
85	Multiblock variance partitioning: A new approach for comparing variation in multiple data blocks. Analytica Chimica Acta, 2008, 615, 18-29.	5.4	56
86	Amperometric electronic tongue for food analysis. Mikrochimica Acta, 2008, 163, 11-21.	5.0	85
87	Classification of GCâ€“MS measurements of wines by combining data dimension reduction and variable selection techniques. Journal of Chemometrics, 2008, 22, 457-463.	1.3	58
88	Chapter 8 Multi-Criteria Decision-Making Methods. Data Handling in Science and Technology, 2008, 27, 169-191.	3.1	2
89	Chapter 9 The DART (Decision Analysis by Ranking Techniques) Software. Data Handling in Science and Technology, 2008, , 193-207.	3.1	6
90	Chapter 5 Similarity/Diversity Measure for Sequential Data Based on Hasse Matrices. Data Handling in Science and Technology, 2008, , 111-138.	3.1	5

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91	Interactions between oral burn, meat flavor and texture in chili spiced pork patties evaluated by time-intensity. Food Quality and Preference, 2007, 18, 909-919.	4.6	49
92	CAIMAN (Classification And Influence Matrix Analysis): A new approach to the classification based on leverage-scaled functions. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 3-17.	3.5	39
93	On the application of chemometrics for the study of acoustic-mechanical properties of crispy bakery products. Chemometrics and Intelligent Laboratory Systems, 2007, 86, 52-59.	3.5	28
94	Characterization of the traditional Cypriot spirit Zivania by means of Counterpropagation Artificial Neural Networks. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 52-58.	3.5	23
95	Classification of multiway analytical data based on MOLMAP approach. Analytica Chimica Acta, 2007, 605, 134-146.	5.4	17
96	Prediction of Italian red wine sensorial descriptors from electronic nose, electronic tongue and spectrophotometric measurements by means of Genetic Algorithm regression models. Food Chemistry, 2007, 100, 211-218.	8.2	120
97	Evaluation of different storage conditions of extra virgin olive oils with an innovative recognition tool built by means of electronic nose and electronic tongue. Food Chemistry, 2007, 101, 485-491.	8.2	140
98	Characterization of DNA Primary Sequences by a New Similarity/Diversity Measure Based on the Partial Ordering. Journal of Chemical Information and Modeling, 2006, 46, 1905-1911.	5.4	13
99	Geographical origin and authentication of extra virgin olive oils by an electronic nose in combination with artificial neural networks. Analytica Chimica Acta, 2006, 567, 202-210.	5.4	149
100	Geographical classification of wine and olive oil by means of classification and influence matrix analysis (CAIMAN). Analytica Chimica Acta, 2006, 570, 249-258.	5.4	27
101	A chemometric approach based on a novel similarity/diversity measure for the characterisation and selection of electronic nose sensors. Analytica Chimica Acta, 2006, 578, 170-177.	5.4	22
102	Classification of ancient Etruscan ceramics using statistical multivariate analysis of data. Applied Physics A: Materials Science and Processing, 2004, 79, 299-307.	2.3	24
103	Qualitative consensus of QSAR ready biodegradability predictions. Toxicological and Environmental Chemistry, 0, , 1-24.	1.2	14