## Marina Cocchi

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Subject classification obtained by cluster analysis and principal component analysis applied to flow cytometric data. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2007, 71A, 334-344.	1.5	97
2	Automated evaluation of food colour by means of multivariate image analysis coupled to a wavelet-based classification algorithm. Analytica Chimica Acta, 2004, 515, 3-13.	5.4	95
3	Classification of bread wheat flours in different quality categories by a wavelet-based feature selection/classification algorithm on NIR spectra. Analytica Chimica Acta, 2005, 544, 100-107.	5.4	90
4	Simultaneous determination of sugars and organic acids in aged vinegars and chemometric data analysis. Talanta, 2006, 69, 1166-1175.	5.5	89
5	Assessing feature relevance in NPLS models by VIP. Chemometrics and Intelligent Laboratory Systems, 2013, 129, 76-86.	3.5	84
6	Determination of Carboxylic Acids in Vinegars and in Aceto Balsamico Tradizionale di Modena by HPLC and GC Methods. Journal of Agricultural and Food Chemistry, 2002, 50, 5255-5261.	5.2	82
7	Durum wheat adulteration detection by NIR spectroscopy multivariate calibration. Talanta, 2006, 68, 1505-1511.	5.5	75
8	Amino Acids Characterization by GRID and Multivariate Data Analysis. QSAR and Combinatorial Science, 1993, 12, 1-8.	1.2	69
9	Application of N-PLS to gas chromatographic and sensory data of traditional balsamic vinegars of modena. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 54-65.	3.5	68
10	Geographical traceability based on 87Sr/86Sr indicator: A first approach for PDO Lambrusco wines from Modena. Food Chemistry, 2013, 141, 2779-2787.	8.2	65
11	Chemometric Methods for Classification and Feature Selection. Comprehensive Analytical Chemistry, 2018, , 265-299.	1.3	63
12	Development of Quantitative Structureâ^'Property Relationships Using Calculated Descriptors for the Prediction of the Physicochemical Properties (nD, i, bp, Îμ, η) of a Series of Organic Solvents. Journal of Chemical Information and Computer Sciences, 1999, 39, 1190-1203.	2.8	61
13	Data fusion approaches in spectroscopic characterization and classification of PDO wine vinegars. Talanta, 2019, 198, 560-572.	5.5	61
14	A mid level data fusion strategy for the Varietal Classification of Lambrusco PDO wines. Chemometrics and Intelligent Laboratory Systems, 2014, 137, 181-189.	3.5	60
15	An analytical approach to Sr isotope ratio determination in Lambrusco wines for geographical traceability purposes. Food Chemistry, 2015, 173, 557-563.	8.2	60
16	Application of a wavelet-based algorithm on HS-SPME/GC signals for the classification of balsamic vinegars. Chemometrics and Intelligent Laboratory Systems, 2004, 71, 129-140.	3.5	57
17	WPTER: wavelet packet transform for efficient pattern recognition of signals. Chemometrics and Intelligent Laboratory Systems, 2001, 57, 97-119.	3.5	55
18	Multicomponent analysis of electrochemical signals in the wavelet domain. Talanta, 2003, 59, 735-749.	5.5	49

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19	A classification tool for N-way array based on SIMCA methodology. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 73-85.	3.5	49
20	Classification of Cereal Flours by Chemometric Analysis of MIR Spectra. Journal of Agricultural and Food Chemistry, 2004, 52, 1062-1067.	5.2	45
21	Analysis of sensory data of Aceto Balsamico Tradizionale di Modena (ABTM) of different ageing by application of PARAFAC models. Food Quality and Preference, 2006, 17, 419-428.	4.6	45
22	Determination of phenolic compounds and authentication of PDO Lambrusco wines by HPLC-DAD and chemometric techniques. Analytica Chimica Acta, 2013, 761, 34-45.	5.4	44
23	Different feature selection strategies in the wavelet domain applied to NIR-based quality classification models of bread wheat flours. Chemometrics and Intelligent Laboratory Systems, 2009, 99, 91-100.	3.5	42
24	Characterization and discrimination of different aged â€~Aceto Balsamico Tradizionale di Modena' products by head space mass spectrometry and chemometrics. Analytica Chimica Acta, 2007, 589, 96-104.	5.4	41
25	Ranking brain areas encoding the perceived level of pain from fMRI data. NeuroImage, 2014, 90, 153-162.	4.2	40
26	Discrimination of Healthy and Neoplastic Human Colon Tissues by ex Vivo HR-MAS NMR Spectroscopy and Chemometric Analyses. Journal of Proteome Research, 2009, 8, 1859-1869.	3.7	39
27	Data Fusion Strategies in Food Analysis. Data Handling in Science and Technology, 2019, , 271-310.	3.1	36
28	Density and volumetric properties of ethane-1,2-diol+di-ethylen-glycol mixtures at different temperatures. Fluid Phase Equilibria, 2000, 172, 93-104.	2.5	34
29	Multivariate calibration of analytical signals by WILMA (wavelet interface to linear modelling) Tj ETQq1 1 0.7843	14 <sub>.rg</sub> BT /(	Overlock 10
30	Near Infrared Spectroscopy and multivariate analysis methods for monitoring flour performance in an industrial bread-making process. Analytica Chimica Acta, 2009, 642, 69-76.	5.4	33
31	Application of data fusion techniques to direct geographical traceability indicators. Analytica Chimica Acta, 2013, 769, 1-9.	5.4	32
32	Development of 87 Sr/ 86 Sr maps as targeted strategy to support wine quality. Food Chemistry, 2018, 255, 139-146.	8.2	30
33	Multicomponent analysis in the wavelet domain of highly overlapped electrochemical signals: Resolution of quaternary mixtures of chlorophenols using a peg-modified Sonogel–Carbon electrode. Chemometrics and Intelligent Laboratory Systems, 2008, 91, 110-120.	3.5	29
34	Theoretical versus empirical molecular descriptors in monosubstituted benzenes. Chemometrics and Intelligent Laboratory Systems, 1992, 14, 209-224.	3.5	28
35	Study of the monosaccharides and furfurals evolution during the preparation of cooked grape musts for Aceto Balsamico Tradizionale production. Journal of Food Engineering, 2007, 79, 1438-1444.	5.2	28
36	α1-Adrenoceptor subtype selectivity: Molecular modelling and theoretical quantitative structure—affinity relationships. Bioorganic and Medicinal Chemistry, 1997, 5, 809-816.	3.0	27

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37	A Chemometric Approach to the Comparison of Different Sample Treatments for Metals Determination by Atomic Absorption Spectroscopy in Aceto Balsamico Tradizionale di Modena. Journal of Agricultural and Food Chemistry, 2004, 52, 4047-4056.	5.2	27
38	Three-way principal component analysis of the volatile fraction by HS-SPME/GC of aceto balsamico tradizionale of modena. Talanta, 2008, 74, 547-554.	5.5	27
39	Optimization of a Dynamic Headspace – Thermal Desorption – Gas Chromatography/Mass Spectrometry procedure for the determination of furfurals in vinegars. Talanta, 2011, 85, 863-869.	5.5	27
40	Theoretical quantitative structure-activity relationship analysis of congeneric and non-congeneric α1-adrenoceptor antagonists: a chemometric study. Computational and Theoretical Chemistry, 1995, 331, 79-93.	1.5	26
41	Mitochondrial DNA Haplogroups and Highly Active Antiretroviral Therapy–Related Lipodystrophy. Clinical Infectious Diseases, 2008, 47, 962-968.	5.8	26
42	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. Computational Materials Science, 2010, 47, 739-751.	3.0	26
43	Evolution of 5-(hydroxymethyl)furfural and furfural in the production chain of the aged vinegar Aceto Balsamico Tradizionale di Modena. Food Chemistry, 2011, 124, 822-832.	8.2	23
44	A Quantum Chemical QSAR Analysis of Carbonic Anhydrase Inhibition by Heterocyclic Sulfonamides. Sulfonamide Carbonic Anhydrase Inhibitors: Quantum Chemical QSAR. QSAR and Combinatorial Science, 1987, 6, 51-53.	1.2	22
45	RP-HPLC and chemometrics for wheat flour protein characterisation in an industrial bread-making process monitoring context. Food Chemistry, 2013, 139, 553-562.	8.2	21
46	Conformational analysis, molecular modeling and quantitative structure-activity relationship studies of 2,4-diamino-6,7-dimethoxy-2-substituted quinazoline α1-adrenergic antagonists. Computational and Theoretical Chemistry, 1991, 251, 307-318.	1.5	20
47	Molecular modelling and quantitative structure- activity relationship analysis using theoretical descriptors of 1,4-benzodioxan (WB-4101) related compounds α1-adrenergic antagonists. Computational and Theoretical Chemistry, 1992, 276, 327-340.	1.5	20
48	Kinematic viscosities of ternary mixtures containing ethane-1,2-diol, 2-methoxyethanol and water from â^10°C to 80°C. Fluid Phase Equilibria, 1999, 157, 317-342.	2.5	20
49	Application of infrared spectroscopy and multivariate quality-control methods in PVC manufacturing. Analytica Chimica Acta, 2005, 554, 207-217.	5.4	20
50	Classification Methods of Multiway Arrays as a Basic Tool for Food PDO Authentication. Comprehensive Analytical Chemistry, 2013, , 339-382.	1.3	20
51	Model calculations of chemical interactions. Part 3.—Rotational energy profiles in simple molecules: evaluation, additivity and role of bond–bond, bond–lone-pair and lone-pair–lone-pair interactions. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 249-258.	1.7	19
52	Preliminary Assessment of Parmigiano Reggiano Authenticity by Handheld Raman Spectroscopy. Foods, 2020, 9, 1563.	4.3	19
53	The heuristic-direct approach to quantitative structure-activity relationship analysis. Computational and Theoretical Chemistry, 1993, 285, 147-153.	1.5	18
54	Comparative molecular dynamics study of the seven-helix bundle arrangement of G-protein coupled receptors. Computational and Theoretical Chemistry, 1995, 333, 49-69.	1.5	18

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55	The Impact of Chemometrics on Food Traceability. Data Handling in Science and Technology, 2013, 28, 371-410.	3.1	18
56	The Ethane-1,2-diol + 2-methoxyethanol + 1,2-dimethoxyethane Ternary Solvent System: Density and Volume Properties at Different Temperatures. Physics and Chemistry of Liquids, 2001, 39, 481-498.	1.2	17
57	Near infrared spectroscopy and multivariate analysis to evaluate wheat flour doughs leavening and bread properties. Analytica Chimica Acta, 2013, 764, 17-23.	5.4	17
58	A Metabolomic Approach to Beer Characterization. Molecules, 2021, 26, 1472.	3.8	17
59	Molecular orbital study of the nitrogen basicity of prazosin analogues in relation to their α1-adrenoceptor binding affinity. Computational and Theoretical Chemistry, 1991, 233, 343-351.	1.5	16
60	Theoretical quantitative size and shape activity and selectivity analyses of 5-HT1A serotonin and α1-adrenergic receptor ligands. Computational and Theoretical Chemistry, 1994, 305, 101-110.	1.5	16
61	Viscosimetric properties and internal structure of N,N-dimethylformamide + 1,2-dimethoxyethane binary mixtures. Journal of Molecular Liquids, 2003, 102, 309-345.	4.9	15
62	Use of X-ray diffraction technique and chemometrics to aid soil sampling strategies in traceability studies. Talanta, 2012, 98, 178-184.	5.5	15
63	QSAR Analysis in 2,4-Diamino-6,7-dimethoxy Quinoline Derivatives – α1-Adrenoceptor Antagonists âÂ Using the Partial Least Squares (PLS) Method and Theoretical Molecular Descriptors. QSAR and Combinatorial Science, 1990, 9, 340-345.	̀" 1.2	14
64	Model calculations of chemical interactions. Part 2.—Intramolecular interactions and double-bond pyramidalization in polycyclic alkenes. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 783-787.	1.7	14
65	Theoretical quantitative structure-activity analysis and pharmacophore modelling of selective non-congeneric α1a-adrenergic antagonists. Computational and Theoretical Chemistry, 1993, 280, 283-290.	1.5	14
66	Computer Modeling of Size and Shape Descriptors of α1-Adrenergic Receptor Antagonists and Quantitative Structure–Affinity/Selectivity Relationships. Methods, 1998, 14, 239-254.	3.8	14
67	Chemical composition and characterisation of seeds from two varieties (pure and hybrid) of Aesculus hippocastanum. Food Chemistry, 2007, 104, 229-236.	8.2	14
68	The heuristic-direct approach to theoretical quantitative structure-activity relationship analysis of $\hat{l}\pm 1$ -adrenoceptor ligands. Computational and Theoretical Chemistry, 1994, 314, 265-276.	1.5	13
69	Soil sampling planning in traceability studies by means of Experimental Design approaches. Chemometrics and Intelligent Laboratory Systems, 2013, 124, 14-20.	3.5	13
70	Multivariate data analysis to assess dry powder inhalers performance from powder properties. Powder Technology, 2016, 301, 830-838.	4.2	13
71	Towards a routine application of vibrational spectroscopy to the detection of bone fragments in feedingstuffs: Use and validation of a NIR scanning microscopy method. Food Chemistry, 2010, 121, 826-831.	8.2	12
72	Prototropic molecular forms and theoretical descriptors in QSAR analysis. Computational and Theoretical Chemistry, 1995, 333, 1-17.	1.5	11

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73	Conformational analysis and theoretical quantitative size and shape-affinity relationships of N4-protonated N1-arylpiperazine 5-HT1A serotoninergic ligands. Computational and Theoretical Chemistry, 1997, 397, 129-145.	1.5	11
74	Use of the Supermolecule Approach to Derive Molecular Similarity Descriptors for QSAR Analysis. Journal of Molecular Modeling, 1998, 4, 113-131.	1.8	11
75	Density and Volume Properties of the 2-Methoxyethanol + 1,2-Dimethoxyethane + Water Ternary Solvent System at Various Temperatures. Physics and Chemistry of Liquids, 2001, 39, 151-168.	1.2	11
76	Model calculations of chemical interactions. Part 1.—Intramolecular interactions and rotational barriers. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 777-781.	1.7	10
77	Viscosity of (ethane-1,2-diol + 1,2-dimethoxyethane + water) at temperatures from 263.15 K to 353.15 K. Journal of Chemical Thermodynamics, 2002, 34, 593-611.	2.0	10
78	<i>N</i> â€way modeling for wavelet filter determination in multivariate image analysis. Journal of Chemometrics, 2015, 29, 379-388.	1.3	10
79	Fused adjacency matrices to enhance information extraction: The beer benchmark. Analytica Chimica Acta, 2019, 1061, 70-83.	5.4	10
80	Use of Multivariate Analysis of MIR Spectra to Study Bread Staling. Annali Di Chimica, 2005, 95, 657-666.	0.6	9
81	Multi-sensor data fusion and parallel factor analysis reveals kinetics of wood weathering. Talanta, 2021, 225, 122024.	5.5	9
82	Chemometric-assisted cocrystallization: supervised pattern recognition for predicting the formation of new functional cocrystals. Chemometrics and Intelligent Laboratory Systems, 2022, 226, 104580.	3.5	9
83	Title is missing!. Journal of Solution Chemistry, 2001, 30, 149-169.	1.2	8
84	Analytical Concentrations of Some Elements in Seeds and Crude Extracts from Aesculus hippocastanum, by ICP-OES Technique. Agronomy, 2021, 11, 47.	3.0	8
85	Studies of 13C n.m.r. substituent chemical shifts of disubstituted benzenes using multivariate data analysis. Journal of the Chemical Society Perkin Transactions II, 1989, , 1773.	0.9	7
86	Electronic and electrostatic aspects of carbonic anhydrase inhibition by sulphonamides. Computational and Theoretical Chemistry, 1992, 256, 217-229.	1.5	7
87	The ad hoc supermolecule approach to receptor ligand design. Computational and Theoretical Chemistry, 2000, 503, 1-16.	1.5	7
88	At-Line Monitoring of the Leavening Process in Industrial Bread Making by near Infrared Spectroscopy. Journal of Near Infrared Spectroscopy, 2008, 16, 223-231.	1.5	7
89	Investigation of the applicability of Zernike moments to the classification of SDS 2D-PAGE maps. Analytical and Bioanalytical Chemistry, 2011, 400, 1419-1431.	3.7	7
90	Exploring local spatial features in hyperspectral images. Journal of Chemometrics, 2020, 34, e3295.	1.3	7

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91	Fast GC E-Nose and Chemometrics for the Rapid Assessment of Basil Aroma. Chemosensors, 2022, 10, 105.	3.6	7
92	Study of the Dependence on Temperature and Composition of the Volumic Properties of Ethane-1,2-diol + 2-Methoxyethanol + 1,2-Dimethoxyethane + Water Solvent System and Graphical Representation in the Quaternary Domain. Journal of Solution Chemistry, 2006, 35, 139-159.	1.2	6
93	Changes in the Chemical Composition of Reduced Cooked Musts during the Heating Process. Journal of Agricultural and Food Chemistry, 2008, 56, 6397-6407.	5.2	6
94	Evaluation of the behaviour of fluorine-containing bioactive glasses: reactivity in a simulated body fluid solution assisted by multivariate data analysis. Journal of Materials Science: Materials in Medicine, 2012, 23, 639-648.	3.6	6
95	A metabolomic data fusion approach to support gliomas grading. NMR in Biomedicine, 2020, 33, e4234.	2.8	6
96	Quantitative structure-affinity/selectivity relationship analysis on three-dimensional models of the complexes between the ETA and ETB receptors and C-terminal endothelin hexapeptide antagonists. Computational and Theoretical Chemistry, 1995, 333, 243-248.	1.5	5
97	A Study of the Dielectric Behaviour and the Liquid Structure of a Ternary Solvent System. Annali Di Chimica, 2004, 94, 165-176.	0.6	5
98	Characterization of Basil Volatile Fraction and Study of Its Agronomic Variation by ASCA. Molecules, 2021, 26, 3842.	3.8	5
99	Fusing NIR and Process Sensors Data for Polymer Production Monitoring. Frontiers in Chemistry, 2021, 9, 748723.	3.6	5
100	A theoretical study of conformation-electronic structure relationships in benzensulfonamide inhibitors of the carbonic anhydrase enzyme. Computational and Theoretical Chemistry, 1989, 183, 393-401.	1,5	4
101	Determination of Metal Concentration in Fat Supplements for Swine Nutrition by Atomic Absorption Spectroscopy. Journal of AOAC INTERNATIONAL, 2005, 88, 393-398.	1.5	4
102	Wheat flour formulation by mixture design and multivariate study of its technological properties. Journal of Chemometrics, 2010, 24, 523-533.	1.3	4
103	Seeds of Horse Chestnut (Aesculus hippocastanum L.) and Their Possible Utilization for Human Consumption. , 2011, , 653-661.		4
104	GENOCOP algorithm and hierarchical grid transformation for image warping of two dimensional gel eletrophoretic maps. Molecular BioSystems, 2012, 8, 975.	2.9	4
105	Coupling 2Dâ€wavelet decomposition and multivariate image analysis (2D WTâ€MIA). Journal of Chemometrics, 2018, 32, e2970.	1.3	4
106	A New Protocol of Computer-Assisted Image Analysis Highlights the Presence of Hemocytes in the Regenerating Cephalic Tentacles of Adult Pomacea canaliculata. International Journal of Molecular Sciences, 2021, 22, 5023.	4.1	4
107	Ceramic polyaniline-carbon composite obtained by ultrasound-assisted sol–gel route: Electrochemical performance towards environmental pollutants. Journal of Electroanalytical Chemistry, 2022, 905, 115971.	3.8	4
108	Multiresolution Analysis and Chemometrics for Pattern Enhancement and Resolution in Spectral Signals and Images. Data Handling in Science and Technology, 2016, , 409-451.	3.1	3

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109	Temperature and composition dependence of the refractive indices of the 2-chloroethanol + 2-methoxyethanol binary mixtures. Annali Di Chimica, 2002, 92, 187-201.	0.6	3
110	A Multiblock Approach to Fuse Process and Near-Infrared Sensors for On-Line Prediction of Polymer Properties. Sensors, 2022, 22, 1436.	3.8	3
111	Theoretical conformational analysis, electronic structure and molecular modelling studies in dihydropteroate synthase in hibition by multisubstituted s. Computational and Theoretical Chemistry, 1991, 233, 293-300.	1.5	2
112	Correlation and multivariate analyses of spectroscopic and dihydropteroate synthase inhibitory activity data in 4-aminoaryl (multisubstituted aryl) sulfones. Structural Chemistry, 1992, 3, 129-137.	2.0	2
113	Computational Insights into ADAMTS4, ADAMTS5 and MMP13 Inhibitor Selectivity. Molecular Informatics, 2012, 31, 421-430.	2.5	2
114	Correlation and multivariate analyses of the spectroscopic data in 4′-substituted 4-nitrodiphenylsulfones. Structural Chemistry, 1991, 2, 47-55.	2.0	1
115	A molecular dynamics simulation of sequence-directed recognition peptides interacting with bigendothelin. Computational and Theoretical Chemistry, 1993, 286, 95-108.	1.5	1
116	Monitoring Flour Performance in Bread Making. , 2011, , 15-25.		1
117	Modeling the Binding Affinity of p38α MAP Kinase Inhibitors by Partial Least Squares Regression. Chemical Biology and Drug Design, 2012, 80, 455-470.	3.2	1
118	A novel proposal to investigate the interplay between the spatial and spectral domains in near-infrared spectral imaging data by means of Image Decomposition, Encoding and Localization (IDEL). Analytica Chimica Acta, 2022, 1191, 339285.	5.4	1
119	Beta-functionalised polythiophenes as microelectrode modifiers in low conductive media. Annali Di Chimica, 2002, 92, 177-85.	0.6	1
120	Multi Way Classification. , 2020, , 701-721.		0
121	Determination of metal concentration in fat supplements for swine nutrition by atomic absorption spectroscopy. Journal of AOAC INTERNATIONAL, 2005, 88, 393-8.	1.5	0