Ãsmund Rinnan

List of Publications by Year
in descending order

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Version: 2024-02-01

81	4,419	159585 30	106344 65
papers	citations	h-index	g-index

85	85	85	5619
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Review of the most common pre-processing techniques for near-infrared spectra. TrAC - Trends in Analytical Chemistry, 2009, 28, 1201-1222.	11.4	1,894
2	Effects of species-specific leaf characteristics and reduced water availability on fine particle capture efficiency of trees. Environmental Pollution, 2013, 183, 64-70.	7.5	127
3	Application of near infrared reflectance (NIR) and fluorescence spectroscopy to analysis of microbiological and chemical properties of arctic soil. Soil Biology and Biochemistry, 2007, 39, 1664-1673.	8.8	124
4	Untargeted Metabolomics as a Screening Tool for Estimating Compliance to a Dietary Pattern. Journal of Proteome Research, 2014, 13, 1405-1418.	3.7	121
5	The effect of high pressure on the functional properties of pork myofibrillar proteins. Food Chemistry, 2016, 196, 1005-1015.	8.2	104
6	Stabilizing the PARAFAC decomposition of fluorescence spectra by insertion of zeros outside the data area. Chemometrics and Intelligent Laboratory Systems, 2004, 71, 97-106.	3.5	92
7	Pre-processing in vibrational spectroscopy â€“ when, why and how. Analytical Methods, 2014, 6, 7124-7129.	2.7	91
8	Large increases in Arctic biogenic volatile emissions are a direct effect of warming. Nature Geoscience, 2016, 9, 349-352.	12.9	83
9	Handling of first-order Rayleigh scatter in PARAFAC modelling of fluorescence excitationâ€“emission data. Chemometrics and Intelligent Laboratory Systems, 2005, 76, 91-99.	3.5	80
10	Recent chemometrics advances for foodomics. TrAC - Trends in Analytical Chemistry, 2017, 96, 42-51.	11.4	80
11	Doubled volatile organic compound emissions from subarctic tundra under simulated climate warming. New Phytologist, 2010, 187, 199-208.	7.3	78
12	First order Rayleigh scatter as a separate component in the decomposition of fluorescence landscapes. Analytica Chimica Acta, 2005, 537, 349-358.	5.4	73
13	Recursive weighted partial least squares (rPLS): an efficient variable selection method using PLS. Journal of Chemometrics, 2014, 28, 439-447.	1.3	71
14	Nucleic Acid Based Fluorescent Nanothermometers. ACS Nano, 2014, 8, 10372-10382.	14.6	68
15	Bootstrap based confidence limits in principal component analysis â€” A case study. Chemometrics and Intelligent Laboratory Systems, 2013, 120, 97-105.	3.5	64
16	Variations in the polyphenol content of seeds of field grown Amaranthus genotypes. Food Chemistry, 2011, 129, 131-138.	8.2	57
17	Tracking hydrophobicity state, aggregation behaviour and structural modifications of pork proteins under the influence of assorted heat treatments. Food Research International, 2017, 101, 266-273.	6.2	57
18	The shift in plant species composition in a subarctic mountain birch forest floor due to climate change would modify the biogenic volatile organic compound emission profile. Plant and Soil, 2012, 352, 199-215.	3.7	55

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19	Multi-way prediction in the presence of uncalibrated interferents. Journal of Chemometrics, 2007, 21, 76-86.	1.3	53
20	The potential of laser-induced breakdown spectroscopy for industrial at-line monitoring of calcium content in comminuted poultry meat. Food Control, 2016, 64, 226-233.	5.5	49
21	Application of interpretable artificial neural networks to early monoclonal antibodies development. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 141, 81-89.	4.3	48
22	The Use of Near-Infrared (NIR) Spectroscopy and Principal Component Analysis (PCA) To Discriminate Bark and Wood of the Most Common Species of the Pellet Sector. Energy & Fuels, 2017, 31, 2814-2821.	5.1	42
23	Discovery of exposure markers in urine for Brassica-containing meals served with different protein sources by UPLC-qTOF-MS untargeted metabolomics. Metabolomics, 2013, 9, 984-997.	3.0	41
24	Near infrared spectroscopy for the discrimination between different residues of the wood processing industry in the pellet sector. Fuel, 2018, 217, 650-655.	6.4	37
25	Few long-term effects of simulated climate change on volatile organic compound emissions and leaf chemistry of three subarctic dwarf shrubs. Environmental and Experimental Botany, 2011, 72, 377-386.	4.2	36
26	Emission of non-methane volatile organic compounds (VOCs) from boreal peatland microcosmsâ€"effects of ozone exposure. Atmospheric Environment, 2005, 39, 921-930.	4.1	34
27	Data Pre-processing. , 2009, , 29-50.		34
28	Combined Markers to Assess Meat Intakeâ€"Human Metabolomic Studies of Discovery and Validation. Molecular Nutrition and Food Research, 2019, 63, e1900106.	3.3	34
29	Determination of weight percent gain in solid wood modified with in situ cured furfuryl alcohol by near-infrared reflectance spectroscopy. Chemometrics and Intelligent Laboratory Systems, 2008, 92, 125-130.	3.5	33
30	Exploring genomes for glycosyltransferases. Molecular BioSystems, 2010, 6, 1773.	2.9	32
31	Effect of Gel Firmness at Cutting Time, pH, and Temperature on Rennet Coagulation and Syneresis: An in situ ¹H NMR Relaxation Study. Journal of Agricultural and Food Chemistry, 2010, 58, 513-519.	5.2	32
32	Advanced and tailored applications of an efficient electrochemical approach assisted by AsLSSRâ€"COWâ€"rPLS and finding ways to cope with challenges arising from the nature of voltammetric data. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 437-446.	3.5	31
33	Prediction of gross calorific value and ash content of woodchip samples by means of FT-NIR spectroscopy. Fuel Processing Technology, 2018, 169, 77-83.	7.2	31
34	Standard error of prediction for multilinear PLS. Chemometrics and Intelligent Laboratory Systems, 2005, 75, 69-76.	3.5	29
35	The physical stability of plant-based drinks and the analysis methods thereof. Food Hydrocolloids, 2021, 118, 106770.	10.7	26
36	Non-Methane Biogenic Volatile Organic Compound Emissions from a Subarctic Peatland Under Enhanced UV-B Radiation. Ecosystems, 2010, 13, 860-873.	3.4	25

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37	Selection of representative calibration sample sets for near-infrared reflectance spectroscopy to predict nitrogen concentration in grasses. Chemometrics and Intelligent Laboratory Systems, 2012, 111, 59-65.	3.5	25
38	Advancing Therapeutic Protein Discovery and Development through Comprehensive Computational and Biophysical Characterization. Molecular Pharmaceutics, 2020, 17, 426-440.	4.6	25
39	Effect of vegetation removal and water table drawdown on the non-methane biogenic volatile organic compound emissions in boreal peatland microcosms. Atmospheric Environment, 2010, 44, 4432-4439.	4.1	21
40	Fast, cross cultivar determination of total carotenoids in intact carrot tissue by Raman spectroscopy and Partial Least Squares calibration. Food Chemistry, 2016, 204, 7-13.	8.2	20
41	Survey on Methods for Investigating Protein Functionality and Related Molecular Characteristics. Foods, 2021, 10, 2848.	4.3	19
42	Small-Angle X-ray Scattering Data in Combination with RosettaDock Improves the Docking Energy Landscape. Journal of Chemical Information and Modeling, 2017, 57, 2463-2475.	5.4	17
43	Quantifying crystalline Î±-lactose monohydrate in amorphous lactose using terahertz time domain spectroscopy and near infrared spectroscopy. Vibrational Spectroscopy, 2019, 102, 39-46.	2.2	17
44	Evaluation of chemometric approaches for polymorphs quantification in tablets using near-infrared hyperspectral images. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 134, 20-28.	4.3	17
45	Seasonal sensitivity of Gammarus pulex towards the pyrethroid cypermethrin. Chemosphere, 2018, 200, 632-640.	8.2	16
46	The effect of heat treatment on the front-face fluorescence spectrum of tryptophan in skim milk. Journal of Food Composition and Analysis, 2020, 92, 103569.	3.9	16
47	Identifying the fingerprint of permanganate oxidizable carbon as a measure of labile soil organic carbon using Fourier transform midâ€infrared photoacoustic spectroscopy. European Journal of Soil Science, 2021, 72, 1831-1841.	3.9	15
48	Time Domain-NMR Combined with Chemometrics Analysis: An Alternative Tool for Monitoring Diesel Fuel Quality. Energy & Fuels, 2015, 29, 2299-2303.	5.1	14
49	Application of NIR imaging to the study of expanded snacks containing amaranth, quinoa and kaÃ±iwa. LWT - Food Science and Technology, 2019, 102, 8-14.	5.2	14
50	pH-induced structural forms of cyanidin and cyanidin 3-O-Î²-glucopyranoside. Dyes and Pigments, 2019, 165, 71-80.	3.7	13
51	Predicting the ethanol potential of wheat straw using near-infrared spectroscopy and chemometrics: The challenge of inherently intercorrelated response functions. Analytica Chimica Acta, 2017, 962, 15-23.	5.4	12
52	Check-all-that-apply data analysed by Partial Least Squares regression. Food Quality and Preference, 2015, 42, 146-153.	4.6	11
53	The physicochemical stability of oat-based drinks. Journal of Cereal Science, 2022, 104, 103422.	3.7	11
54	Interval-Based Chemometric Methods in NMR Foodomics. Data Handling in Science and Technology, 2013, 28, 449-486.	3.1	10

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55	Fluorescence Spectroscopy in Process Analytical Technology (PAT): Simultaneous Quantification of Two Active Pharmaceutical Ingredients in a Tablet Formulation. Applied Spectroscopy, 2015, 69, 323-331.	2.2	10
56	Non-Destructive Determination of Quality Traits of Cashew Apples (Anacardium Occidentale, L.) Using a Portable near Infrared Spectrophotometer. Journal of Near Infrared Spectroscopy, 2016, 24, 77-82.	1.5	10
57	How the energy evaluation method used in the geometry optimization step affect the quality of the subsequent QSAR/QSPR models. Journal of Computer-Aided Molecular Design, 2010, 24, 17-22.	2.9	9
58	Optimization and kinetic studies of photodegradation of Rhodamine B with immobilized Ag-, S-, and N-doped TiO₂ under visible irradiation: using Boxâ€“Behnken designs (BBDs), multivariate curve resolution (MCR-ALS) and parallel factor (PARAFAC) analysis. Analytical Methods, 2016, 8, 4293-4299.	2.7	9
59	Interaction mechanisms between polycyclic aromatic hydrocarbons (PAHs) and organic soil washing agents. Environmental Science and Pollution Research, 2018, 25, 299-311.	5.3	9
60	Study of the scattering effects on NIR data for the prediction of ash content using EMSC correction factors. Journal of Chemometrics, 2019, 33, e3111.	1.3	9
61	The anserine to carnosine ratio: an excellent discriminator between white and red meats consumed by free-living overweight participants of the PREVIEW study. European Journal of Nutrition, 2021, 60, 179-192.	3.9	9
62	Investigating challenges with scattering and inner filter effects in frontâ€face fluorescence by PARAFAC. Journal of Chemometrics, 2020, 34, e3286.	1.3	8
63	Measurement of Active Content in Escitalopram Tablets by a Near-Infrared Transmission Spectroscopy Model that Encompasses Batch Variability. Journal of Pharmaceutical Sciences, 2013, 102, 1268-1280.	3.3	7
64	Confidence limits for contribution plots in multivariate statistical process control using bootstrap estimates. Analytica Chimica Acta, 2016, 908, 75-84.	5.4	7
65	Two Statistical Tools for Assessing Functionality and Protein Characteristics of Different Fava Bean (Vicia faba L.) Ingredients. Foods, 2021, 10, 2489.	4.3	7
66	Simultaneous classification of multiple classes in NMR metabolomics and vibrational spectroscopy using interval-based classification methods: iECVA vs iPLS-DA. Analytica Chimica Acta, 2018, 1021, 20-27.	5.4	6
67	Novel non-linear curve fitting to resolve protein unfolding transitions in intrinsic fluorescence differential scanning fluorimetry. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 142, 506-517.	4.3	6
68	Long-term effects of elevated CO2, nighttime warming and drought on plant secondary metabolites in a temperate heath ecosystem. Annals of Botany, 2020, 125, 1065-1075.	2.9	6
69	Isothermal Chemical Denaturation: Data Analysis, Error Detection, and Correction by PARAFAC2. Analytical Chemistry, 2020, 92, 6958-6967.	6.5	6
70	Study of Variability of Waste Wood Samples Collected in a Panel Board Industry. Frontiers in Chemistry, 2021, 9, 722090.	3.6	6
71	Significance of the structure of data in partial least squares regression predictions involving both natural and human experimental design. Journal of Chemometrics, 2012, 26, 487-495.	1.3	5
72	Comparison of bootstrap and asymptotic confidence limits for control charts in batch MSPC strategies. Chemometrics and Intelligent Laboratory Systems, 2013, 127, 102-111.	3.5	5

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73	The Shining Future of near Infrared Spectroscopy in Plant Phenomics, Crop Sorting and Biofuel Production. NIR News, 2016, 27, 20-23.	0.3	5
74	A multivariate perspective on the stability of oat-based drinks assessed by spectroscopy. Food Hydrocolloids, 2022, 131, 107831.	10.7	4
75	New Advanced Glycation End Products Observed in Rat Urine by Untargeted Metabolomics after Feeding with Heatâ€Treated Skimmed Milk Powder. Molecular Nutrition and Food Research, 2021, 65, 2001049.	3.3	3
76	Calibration Transfer Methods. , 2009, , 105-118.		2
77	Physiological Genetics Reformed: Bridging the Genome-to-Phenome Gap by Coherent Chemical Fingerprints â€“ the Global Coordinator. Trends in Plant Science, 2021, 26, 324-337.	8.8	1
78	Who is winning? A comparison of humans versus computers for calibration model building. Journal of Chemometrics, 2021, 35, e3378.	1.3	1
79	Processing Effects on Protein Structure and Physicochemical Properties. Foods, 2022, 11, 1607.	4.3	1
80	Detection of protein oxidation products by fluorescence spectroscopy and trilinear data decomposition: Proof of concept. Food Chemistry, 2022, 396, 133732.	8.2	1
81	In-line fluorescence spectroscopy for quantification of low amount of active pharmaceutical ingredient. Journal of Pharmaceutical Sciences, 2022, , .	3.3	0