Asmund Rinnan

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	The physicochemical stability of oat-based drinks. Journal of Cereal Science, 2022, 104, 103422.	3.7	11
2	Processing Effects on Protein Structure and Physicochemical Properties. Foods, 2022, 11, 1607.	4.3	1
3	A multivariate perspective on the stability of oat-based drinks assessed by spectroscopy. Food Hydrocolloids, 2022, 131, 107831.	10.7	4
4	In-line fluorescence spectroscopy for quantification of low amount of active pharmaceutical ingredient. Journal of Pharmaceutical Sciences, 2022, , .	3.3	0
5	Detection of protein oxidation products by fluorescence spectroscopy and trilinear data decomposition: Proof of concept. Food Chemistry, 2022, 396, 133732.	8.2	1
6	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
7	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
8	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
9	Physiological Genetics Reformed: Bridging the Genome-to-Phenome Gap by Coherent Chemical Fingerprints – the Global Coordinator. Trends in Plant Science, 2021, 26, 324-337.	8.8	1
10	The physical stability of plant-based drinks and the analysis methods thereof. Food Hydrocolloids, 2021, 118, 106770.	10.7	26
11	Two Statistical Tools for Assessing Functionality and Protein Characteristics of Different Fava Bean (Vicia faba L.) Ingredients. Foods, 2021, 10, 2489.	4.3	7
12	Who is winning? A comparison of humans versus computers for calibration model building. Journal of Chemometrics, 2021, 35, e3378.	1.3	1
13	Survey on Methods for Investigating Protein Functionality and Related Molecular Characteristics. Foods, 2021, 10, 2848.	4.3	19
14	Study of Variability of Waste Wood Samples Collected in a Panel Board Industry. Frontiers in Chemistry, 2021, 9, 722090.	3.6	6
15	Advancing Therapeutic Protein Discovery and Development through Comprehensive Computational and Biophysical Characterization. Molecular Pharmaceutics, 2020, 17, 426-440.	4.6	25
16	Investigating challenges with scattering and inner filter effects in frontâ€face fluorescence by PARAFAC. Journal of Chemometrics, 2020, 34, e3286.	1.3	8
17	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
18	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

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19	Isothermal Chemical Denaturation: Data Analysis, Error Detection, and Correction by PARAFAC2. Analytical Chemistry, 2020, 92, 6958-6967.	6.5	6
20	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
21	Combined Markers to Assess Meat Intake—Human Metabolomic Studies of Discovery and Validation. Molecular Nutrition and Food Research, 2019, 63, e1900106.	3.3	34
22	Application of interpretable artificial neural networks to early monoclonal antibodies development. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 141, 81-89.	4.3	48
23	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
24	Quantifying crystalline \hat{l}_{\pm} -lactose monohydrate in amorphous lactose using terahertz time domain spectroscopy and near infrared spectroscopy. Vibrational Spectroscopy, 2019, 102, 39-46.	2.2	17
25	pH-induced structural forms of cyanidin and cyanidin 3-O-β-glucopyranoside. Dyes and Pigments, 2019, 165, 71-80.	3.7	13
26	Application of NIR imaging to the study of expanded snacks containing amaranth, quinoa and kañiwa. LWT - Food Science and Technology, 2019, 102, 8-14.	5.2	14
27	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
28	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
29	Seasonal sensitivity of Gammarus pulex towards the pyrethroid cypermethrin. Chemosphere, 2018, 200, 632-640.	8.2	16
30	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
31	Interaction mechanisms between polycyclic aromatic hydrocarbons (PAHs) and organic soil washing agents. Environmental Science and Pollution Research, 2018, 25, 299-311.	5.3	9
32	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
33	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
34	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
35	Recent chemometrics advances for foodomics. TrAC - Trends in Analytical Chemistry, 2017, 96, 42-51.	11.4	80
36	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

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37	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
38	The Shining Future of near Infrared Spectroscopy in Plant Phenomics, Crop Sorting and Biofuel Production. NIR News, 2016, 27, 20-23.	0.3	5
39	Large increases in Arctic biogenic volatile emissions are a direct effect of warming. Nature Geoscience, 2016, 9, 349-352.	12.9	83
40	Optimization and kinetic studies of photodegradation of Rhodamine B with immobilized Ag-, S-, and N-doped TiO ₂ under visible irradiation: using Box–Behnken designs (BBDs), multivariate curve resolution (MCR-ALS) and parallel factor (PARAFAC) analysis. Analytical Methods, 2016, 8, 4293-4299.	2.7	9
41	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
42	The effect of high pressure on the functional properties of pork myofibrillar proteins. Food Chemistry, 2016, 196, 1005-1015.	8.2	104
43	Confidence limits for contribution plots in multivariate statistical process control using bootstrap estimates. Analytica Chimica Acta, 2016, 908, 75-84.	5.4	7
44	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
45	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
46	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
47	Check-all-that-apply data analysed by Partial Least Squares regression. Food Quality and Preference, 2015, 42, 146-153.	4.6	11
48	Advanced and tailored applications of an efficient electrochemical approach assisted by AsLSSR–COW–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
49	Time Domain-NMR Combined with Chemometrics Analysis: An Alternative Tool for Monitoring Diesel Fuel Quality. Energy & Fuels, 2015, 29, 2299-2303.	5.1	14
50	Pre-processing in vibrational spectroscopy – when, why and how. Analytical Methods, 2014, 6, 7124-7129.	2.7	91
51	Recursive weighted partial least squares (rPLS): an efficient variable selection method using PLS. Journal of Chemometrics, 2014, 28, 439-447.	1.3	71
52	Untargeted Metabolomics as a Screening Tool for Estimating Compliance to a Dietary Pattern. Journal of Proteome Research, 2014, 13, 1405-1418.	3.7	121
53	Nucleic Acid Based Fluorescent Nanothermometers. ACS Nano, 2014, 8, 10372-10382.	14.6	68
54	Discovery of exposure markers in urine for Brassica-containing meals served with different protein sources by UPI C-oTOF-MS untargeted metabolomics. Metabolomics, 2013, 9, 984-997	3.0	41

10Comparison of bootstrap and asymptotic confidence limits for control charts in batch MSPC9.6910Effects of speciesspecific leaf characteristics and reduced water availability on fine particle capture7.512711Bootstrap based confidence limits in principal component analysis AC Acase study. Chemometrics and0.60.412Bootstrap based confidence limits in principal component analysis AC Acase study. Chemometrics and0.60.413Messurement of Active Content In Eschalopram Tablets by a Near-Infrared Transmission Spectroscopy0.3714Bootstrap Lasend Confidence Inits in principal component analysis AC Acase study. Chemometrics and0.60.415Internol Lasend Content In Eschalopram Tablets by a Near-Infrared Transmission Spectroscopy0.3716Significance of the structure of data in partial least squares regression predictions involving both3.3516Significance of the structure of data in partial least squares regression predictions involving both3.3517Besel Change concentration in gasses. Chemometric and Intelligent Laboratory Systems, 2012, 111, 23, 733.518Francisco With modify the biogene volatile organic compound emission profile. Plant and Soll, 2012, 3.83.719Internol Lasend Change change on volatile organic compound emissions and leaf3.73.610Singerity of three salarity the biogene volatile organic compound emissions profile. Plant and Soll, 2012, 2.83.73.610Singerity of three salarity of three salarity of three salarity of three salarity of three salari	#	Article	IF	CITATIONS
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17 Bootstrap based confidence limits in principal component analysis & C A case study. Chemometrics and Laboratory Systems, 2013, 120, 97-105. 8.4 64 18 Measurement of Active Content in Escitalopram Tablets by a Near-Infrared Transmission Spectroscopy and Chemometric Methods in NMR Foodomics. Data Handling in Science and Technology, and and the student international data in partial least squares regression predictions involving both and the student international data in partial least squares regression predictions involving both in a species composition in a subarctic mountain birch forest floor due to climate of the structure of data in partial least squares regression predictions involving both international predict nitrogen concentration in gresses. Chemometrics, 2012, e18, 489-486. 1.0 60 Significance of the structure of data in partial least squares regression predictions involving both internation in gresses. Chemometrics, 2012, e18, 489-486. 1.0 2.6 61 Specific nitrogen concentration in gresses. Chemometrics and Intelligent Laboratory Systems, 2012, 111, 3.6 3.7 55 62 The shift in plant species composition in a subarctic mountain birch forest floor due to climate chemostry of the subarctic charaf shurbs. Environmental and Experimental Botany, 2011, 22, 377, 386. 4.2 3.6 63 Few long term effects of simulated climate change on volatile organic compound emissions and leaf chemistry of three subarctic Volatile Organic Compound Envisions from a Subarctic Paetaland Luder 3.8 2.7 64 Variations in the polyphenol cont	56	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
64Measurement of Active Content in Escitalopram Tablets by a Near-Infrared Transmission Spectroscopy Model that Encompasses Barch Variability. Journal of Pharmaceutical Sciences, 2013, 102, 1268-1280.3.3769Interval Based Chemometric Methods in NMR Foodomics. Data Handling in Science and Technology, 2013, 28, 449-486.1.060Significance of the structure of data in partial least squares regression predictions involving both natural and human experimental design. Journal of Chemometrics, 2012, 26, 487-495.1.3561Selection of representative calibration sample sets for near-infrared reflectance spectroscopy to \$9.45.3.52562Re-britt in plant species composition in a subarctic mountain bich forest floor due to climate of ange would modify the blogenic volatile organic compound emission profile. Plant and Soil, 2012, 21, 31- 35, 35, 199-215.3.63663Few long term effects of simulated climate change on volatile organic compound emissions and leaf britt of three subarctic dwarf shrubs. Environmental and Chermental Botany, 2011, 72, 377-366.4.23664Variations in the polyphenol content of seeds of field grown Amaranthus genotypes. Food Chemistry, 2011, 129, 131-138.3.42565Iffect of vegetation removal and water table drawdown on the non-methane blogenic volatile 412, 413.2.12.166Non-Methane Biogenic Volatile Organic compound emissions from a Subarctic Restand Under 429.7.37.867Iffect of vegetation removal and water table drawdown on the non-methane blogenic volatile 422, 4439.1.32.168Doubled volatile organic compound emissions fr	57	Bootstrap based confidence limits in principal component analysis — A case study. Chemometrics and Intelligent Laboratory Systems, 2013, 120, 97-105.	3.5	64
101Interval-Based Chemometric Methods in NMR Foodomics. Data Handling in Science and Technology, 2013, 28, 449-486.3.110102Significance of the structure of data in partial least squares regression predictions involving both ratural and human experimental design, Journal of Chemometrics, 2012, 26, 487-495.1.35103Selection of representative calibration sample sets for near-infrared reflectance spectroscopy to system, 2012, 111, 	58	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
60Significance of the structure of data in partial least squares regression predictions involving both natural and human experimental design. Journal of Chemometrics, 2012, 26, 487-495.1.3561Selection of representative calibration sample sets for near-infrared reflectance spectroscopy to predict nitrogen concentration in grasses. Chemometrics and Intelligent Laboratory Systems, 2012, 111.8.52662The 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 Soli, 2012, 	59	Interval-Based Chemometric Methods in NMR Foodomics. Data Handling in Science and Technology, 2013, 28, 449-486.	3.1	10
61Selection of representative calibration sample sets for near-infrared reflectance spectroscopy to predict nitrogen concentration in grasses. Chemometrics and Intelligent Laboratory Systems, 2012, 111, a.53.52562The 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, 3.73.75563Few long-term effects of simulated climate change on volatile organic compound emissions and leaf for the subarctic dwarf shrubs. Environmental and Experimental Botany, 2011, 72, 377-386.4.23664Variations in the polyphenol content of seeds of field grown Amaranthus genotypes. Food Chemistry. 2011, 129, 131-138.8.25765Non-Methane Biogenic Volatile Organic Compound Emissions from a Subarctic Peatland Under thanke Radiation. Ecosystems, 2010, 15, 860-873.8.42566How 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, 17-22.2.9967Effect of vegetation removal and water table drawdown on the non-methane biogenic volatile 4432-4439.1.12168Doubled volatile organic compound emissions from subarctic tundra under simulated climate warming. New Phytologist, 2010, 187, 199-208.7.83270Effect of Cel Firmness at Cutting Time, pH, and Temperature on Rennet Coagulation and Syneresis: An 31-3519.5.23271Data Pre-processing ., 2009, .29-50.34	60	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
62The 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, 199-215.3.75563Few long term effects of simulated climate change on volatile organic compound emissions and leaf 2011, 129, 131-138.4.23664Variations in the polyphenol content of seeds of field grown Amaranthus genotypes. Food Chemistry, 2011, 129, 131-138.8.26765Non-Methane Biogenic Volatile Organic Compound Emissions from a Subarctic Peatland Under Enhanced UV-B Radiation. Ecosystems, 2010, 13, 860-873.8.42566How 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, 17-22.9967Effect of vegetation removal and water table drawdown on the non-methane biogenic volatile organic compound emissions from subarctic tundra under simulated climate organic compound emissions from subarctic tundra under simulated climate organic compound emissions from subarctic tundra under simulated climate franced UV-B Radiation Structurg Time, PH, and Temperature on Rennet Coagulation and Syneresis: An in situ (sup) 1 (sup) H NMR Relaxition Study. Journal of Agricultural and Food Chemistry, 2010, 58, 133-519.9.23271Data Pre-processing., 2009, 29-50.34	61	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
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69Exploring genomes for glycosyltransferases. Molecular BioSystems, 2010, 6, 1773.2.93270Effect of Gel Firmness at Cutting Time, pH, and Temperature on Rennet Coagulation and Syneresis: An in situ ^{15.23271Data Pre-processing. , 2009, , 29-50.34}	68	Doubled volatile organic compound emissions from subarctic tundra under simulated climate warming. New Phytologist, 2010, 187, 199-208.	7.3	78
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	71	Data Pre-processing. , 2009, , 29-50.		34

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73	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
74	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
75	Multi-way prediction in the presence of uncalibrated interferents. Journal of Chemometrics, 2007, 21, 76-86.	1.3	53
76	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
77	First order Rayleigh scatter as a separate component in the decomposition of fluorescence landscapes. Analytica Chimica Acta, 2005, 537, 349-358.	5.4	73
78	Standard error of prediction for multilinear PLS. Chemometrics and Intelligent Laboratory Systems, 2005, 75, 69-76.	3.5	29
79	Handling of first-order Rayleigh scatter in PARAFAC modelling of fluorescence excitation–emission data. Chemometrics and Intelligent Laboratory Systems, 2005, 76, 91-99.	3.5	80
80	Emission of non-methane volatile organic compounds (VOCs) from boreal peatland microcosms—effects of ozone exposure. Atmospheric Environment, 2005, 39, 921-930.	4.1	34
81	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