

Søren Balling Engelsen

List of Publications by Year in descending order

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Version: 2024-02-01

282
papers

15,473
citations

18479

62
h-index

24254

110
g-index

290
all docs

290
docs citations

290
times ranked

15435
citing authors

#	ARTICLE	IF	CITATIONS
1	Non-volatile molecular composition and discrimination of single grape white wines of Chardonnay, Riesling, Sauvignon Blanc and Silvaner using untargeted GC-MS analysis. Food Chemistry, 2022, 369, 130878.	8.2	10
2	Urinary and plasma metabolome of farm mink (<i>Neovison vison</i>) after an intervention with raw or cooked poultry offal: a ¹ H NMR investigation. Archives of Animal Nutrition, 2022, 76, 74-91.	1.8	0
3	Monitoring of the Rioja red wine production process by ¹ H- ¹³ C NMR spectroscopy. Journal of the Science of Food and Agriculture, 2022, 102, 3808-3816.	3.5	5
4	Human Blood Lipoprotein Predictions from ¹ H NMR Spectra: Protocol, Model Performances, and Cage of Covariance. Analytical Chemistry, 2022, 94, 628-636.	6.5	9
5	Effects of Water Stress, Defoliation and Crop Thinning on <i>Vitis vinifera</i> L. cv. Solaris: Part I: Plant Responses, Fruit Development and Fruit Quality. Metabolites, 2022, 12, 363.	2.9	6
6	Prediction of $\hat{1}$ -Lactalbumin and $\hat{2}$ -Lactoglobulin Composition of Aqueous Whey Solutions Using Fourier Transform Mid-Infrared Spectroscopy and Near-Infrared Spectroscopy. Applied Spectroscopy, 2021, 75, 718-727.	2.2	13
7	The effect of daily protein supplementation, with or without resistance training for 1 year, on muscle size, strength, and function in healthy older adults: A randomized controlled trial. American Journal of Clinical Nutrition, 2021, 113, 790-800.	4.7	33
8	Plasma Metabolomics to Evaluate Progression of Necrotising Enterocolitis in Preterm Pigs. Metabolites, 2021, 11, 283.	2.9	4
9	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
10	The plasma metabolome of Atlantic salmon as studied by ¹ H NMR spectroscopy using standard operating procedures: effect of aquaculture location and growth stage. Metabolomics, 2021, 17, 50.	3.0	9
11	Influence of Age, Sex, and Diet on the Human Fecal Metabolome Investigated by ¹ H NMR Spectroscopy. Journal of Proteome Research, 2021, 20, 3642-3653.	3.7	16
12	Cage of covariance in calibration modeling: Regressing multiple and strongly correlated response variables onto a low rank subspace of explanatory variables. Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104311.	3.5	17
13	Diagnosing indirect relationships in multivariate calibration models. Journal of Chemometrics, 2021, 35, e3366.	1.3	3
14	WHEY - The waste-stream that became more valuable than the food product. Trends in Food Science and Technology, 2021, 118, 230-241.	15.1	56
15	Staling of white wheat bread crumb and effect of maltogenic $\hat{1}$ -amylases. Part 3: Spatial evolution of bread staling with time by near infrared hyperspectral imaging. Food Chemistry, 2021, 353, 129478.	8.2	20
16	Chemometric Classification of Cocoa Bean Shells Based on Their Polyphenolic Profile Determined by RP-HPLC-PDA Analysis and Spectrophotometric Assays. Antioxidants, 2021, 10, 1533.	5.1	10
17	NIR Data Exploration and Regression by Chemometricsâ€”A Primer. , 2021, , 127-189.		4
18	On-Line Real-Time Monitoring of a Rapid Enzymatic Oil Degumming Process: A Feasibility Study Using Free-Run Near-Infrared Spectroscopy. Foods, 2021, 10, 2368.	4.3	3

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19	Human Fecal Metabolome Reflects Differences in Body Mass Index, Physical Fitness, and Blood Lipoproteins in Healthy Older Adults. <i>Metabolites</i> , 2021, 11, 717.	2.9	7
20	Structurally different mixed linkage Î²-glucan supplements differentially increase secondary bile acid excretion in hypercholesterolaemic rat faeces. <i>Food and Function</i> , 2020, 11, 514-523.	4.6	9
21	An NMR Metabolomics Approach to Investigate Factors Affecting the Yoghurt Fermentation Process and Quality. <i>Metabolites</i> , 2020, 10, 293.	2.9	23
22	First-principles identification of C-methyl-scylo-inositol (mytilitol) â€” A new species-specific metabolite indicator of geographic origin for marine bivalve molluscs (<i>Mytilus</i> and <i>Ruditapes</i> spp.). <i>Food Chemistry</i> , 2020, 328, 126959.	8.2	7
23	Human Faecal ¹ H NMR Metabolomics: Evaluation of Solvent and Sample Processing on Coverage and Reproducibility of Signature Metabolites. <i>Analytical Chemistry</i> , 2020, 92, 9546-9555.	6.5	22
24	In Vitro Bioaccessibility and Functional Properties of Phenolic Compounds from Enriched Beverages Based on Cocoa Bean Shell. <i>Foods</i> , 2020, 9, 715.	4.3	25
25	Signature Mapping (SigMa): An efficient approach for processing complex human urine ¹ H NMR metabolomics data. <i>Analytica Chimica Acta</i> , 2020, 1108, 142-151.	5.4	53
26	Physical fitness in community-dwelling older adults is linked to dietary intake, gut microbiota, and metabolomic signatures. <i>Aging Cell</i> , 2020, 19, e13105.	6.7	41
27	Cocoa Bean Shellâ€”A By-Product with Nutritional Properties and Biofunctional Potential. <i>Nutrients</i> , 2020, 12, 1123.	4.1	90
28	Three different Fourierâ€”transform midâ€”infrared sampling techniques to characterize bioâ€”organic samples. <i>Journal of Environmental Quality</i> , 2020, 49, 1310-1321.	2.0	6
29	Human urine ¹ H NMR metabolomics reveals alterations of protein and carbohydrate metabolism when comparing habitual Average Danish diet vs. healthy New Nordic diet. <i>Nutrition</i> , 2020, 79-80, 110867.	2.4	11
30	IDDF2020-ABS-0174â€”...Onset of hypertriglyceridemia in relation to dietary intake, gut microbiome and metabolomics signatures among home dwelling elderly. , 2020, , .		2
31	Biomarkers of Individual Foods, and Separation of Diets Using Untargeted LCâ€”MSâ€”based Plasma Metabolomics in a Randomized Controlled Trial. <i>Molecular Nutrition and Food Research</i> , 2019, 63, e1800215.	3.3	34
32	Investigation of Variations in the Human Urine Metabolome amongst European Populations: An Exploratory Search for Biomarkers of People at Riskâ€”ofâ€”Poverty. <i>Molecular Nutrition and Food Research</i> , 2019, 63, e1800216.	3.3	10
33	Ancient Danish Apple Cultivarsâ€”A Comprehensive Metabolite and Sensory Profiling of Apple Juices. <i>Metabolites</i> , 2019, 9, 139.	2.9	14
34	Lipid oxidation degree of pork meat during frozen storage investigated by near-infrared hyperspectral imaging: Effect of ice crystal growth and distribution. <i>Journal of Food Engineering</i> , 2019, 263, 311-319.	5.2	50
35	A Dietary Mixture of Oxysterols Induces In Vitro Intestinal Inflammation through TLR2/4 Activation: The Protective Effect of Cocoa Bean Shells. <i>Antioxidants</i> , 2019, 8, 151.	5.1	24
36	A comparative study of mango solar drying methods by visible and near-infrared spectroscopy coupled with ANOVA-simultaneous component analysis (ASCA). <i>LWT - Food Science and Technology</i> , 2019, 112, 108214.	5.2	23

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37	Assessment of volatile fingerprint by HS-SPME/GC-qMS and E-nose for the classification of cocoa bean shells using chemometrics. <i>Food Research International</i> , 2019, 123, 684-696.	6.2	52
38	Staling of white wheat bread crumb and effect of maltogenic α -amylases. Part 2: Monitoring the staling process by using near infrared spectroscopy and chemometrics. <i>Food Chemistry</i> , 2019, 297, 124946.	8.2	16
39	Quantifying crystalline α -lactose monohydrate in amorphous lactose using terahertz time domain spectroscopy and near infrared spectroscopy. <i>Vibrational Spectroscopy</i> , 2019, 102, 39-46.	2.2	17
40	Authentication of cocoa bean shells by near- and mid-infrared spectroscopy and inductively coupled plasma-optical emission spectroscopy. <i>Food Chemistry</i> , 2019, 292, 47-57.	8.2	31
41	Repeatability and reproducibility of lipoprotein particle profile measurements in plasma samples by ultracentrifugation. <i>Clinical Chemistry and Laboratory Medicine</i> , 2019, 58, 103-115.	2.3	6
42	The foodome of bivalve molluscs: From hedonic eating to healthy diet. <i>Journal of Food Composition and Analysis</i> , 2018, 69, 13-19.	3.9	13
43	Pulsed Electric Field Assisted Extraction of Bioactive Compounds from Cocoa Bean Shell and Coffee Silverskin. <i>Food and Bioprocess Technology</i> , 2018, 11, 818-835.	4.7	103
44	Simultaneous classification of multiple classes in NMR metabolomics and vibrational spectroscopy using interval-based classification methods: iECVA vs iPLS-DA. <i>Analytica Chimica Acta</i> , 2018, 1021, 20-27.	5.4	6
45	Consumption of regular-fat vs reduced-fat cheese reveals gender-specific changes in LDL particle size - a randomized controlled trial. <i>Nutrition and Metabolism</i> , 2018, 15, 61.	3.0	11
46	Cool-Climate Red Wines' Chemical Composition and Comparison of Two Protocols for ^1H -NMR Analysis. <i>Molecules</i> , 2018, 23, 160.	3.8	15
47	Chemometric Analysis of NMR Spectra. , 2018, , 1649-1668.		3
48	Biogenic amines: a key freshness parameter of animal protein products in the coming circular economy. <i>Current Opinion in Food Science</i> , 2018, 22, 167-173.	8.0	12
49	Quantitative Analysis of Time Domain NMR Relaxation Data. , 2018, , 1669-1686.		0
50	Gum Arabic authentication and mixture quantification by near infrared spectroscopy. <i>Food Control</i> , 2017, 78, 144-149.	5.5	20
51	Predicting the ethanol potential of wheat straw using near-infrared spectroscopy and chemometrics: The challenge of inherently intercorrelated response functions. <i>Analytica Chimica Acta</i> , 2017, 962, 15-23.	5.4	12
52	SERS detection of the biomarker hydrogen cyanide from <i>Pseudomonas aeruginosa</i> cultures isolated from cystic fibrosis patients. <i>Scientific Reports</i> , 2017, 7, 45264.	3.3	26
53	Quinoa seed coats as an expanding and sustainable source of bioactive compounds: An investigation of genotypic diversity in saponin profiles. <i>Industrial Crops and Products</i> , 2017, 104, 156-163.	5.2	48
54	Monitoring the staling of wheat bread using 2D MIR-NIR correlation spectroscopy. <i>Journal of Cereal Science</i> , 2017, 75, 92-99.	3.7	32

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55	SERS spectroscopy for detection of hydrogen cyanide in breath from children colonised with <i>P. aeruginosa</i> . <i>Analytical Methods</i> , 2017, 9, 5757-5762.	2.7	5
56	Untargeted GC-MS Metabolomics Reveals Changes in the Metabolite Dynamics of Industrial Scale Batch Fermentations of <i>Streptococcus thermophilus</i> Broth. <i>Biotechnology Journal</i> , 2017, 12, 1700400.	3.5	10
57	Identification of weak and gender specific effects in a short 3 weeks intervention study using barley and oat mixed linkage β -glucan dietary supplements: a human fecal metabolome study by GC-MS. <i>Metabolomics</i> , 2017, 13, 108.	3.0	14
58	From metabolome to phenotype: GC-MS metabolomics of developing mutant barley seeds reveals effects of growth, temperature and genotype. <i>Scientific Reports</i> , 2017, 7, 8195.	3.3	25
59	Resveratrol in the foodomics era: 1:25,000. <i>Annals of the New York Academy of Sciences</i> , 2017, 1403, 48-58.	3.8	19
60	Antibiotic Treatment Preventing Necrotising Enterocolitis Alters Urinary and Plasma Metabolomes in Preterm Pigs. <i>Journal of Proteome Research</i> , 2017, 16, 3547-3557.	3.7	21
61	Quantification of lipoprotein profiles by nuclear magnetic resonance spectroscopy and multivariate data analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2017, 94, 210-219.	11.4	52
62	Long wavelength near-infrared transmission spectroscopy of barley seeds using a supercontinuum laser: Prediction of mixed-linkage beta-glucan content. <i>Analytica Chimica Acta</i> , 2017, 986, 101-108.	5.4	8
63	Toward Reliable Lipoprotein Particle Predictions from NMR Spectra of Human Blood: An Interlaboratory Ring Test. <i>Analytical Chemistry</i> , 2017, 89, 8004-8012.	6.5	46
64	The spatial composition of porcine adipose tissue investigated by multivariate curve resolution of near infrared spectra: Relationships between fat, the degree of unsaturation and water. <i>Journal of Near Infrared Spectroscopy</i> , 2017, 25, 45-53.	1.5	8
65	ICNIRS 2017, Copenhagen. <i>NIR News</i> , 2017, 28, 4-6.	0.3	2
66	The Effect of Season on the Metabolic Profile of the European Clam <i>Ruditapes decussatus</i> as Studied by $^1\text{H-NMR}$ Spectroscopy. <i>Metabolites</i> , 2017, 7, 36.	2.9	7
67	Spectroscopy for Process Analytical Technology (PAT)., 2017, , 188-197.		2
68	Vibrational Spectroscopy in Food Processing. , 2017, , 582-589.		4
69	Chemometric Analysis of NMR Spectra. , 2017, , 1-20.		6
70	Quantitative Analysis of Time Domain NMR Relaxation Data. , 2017, , 1-19.		2
71	The Shining Future of near Infrared Spectroscopy in Plant Phenomics, Crop Sorting and Biofuel Production. <i>NIR News</i> , 2016, 27, 20-23.	0.3	5
72	Screening for Triterpenoid Saponins in Plants Using Hyphenated Analytical Platforms. <i>Molecules</i> , 2016, 21, 1614.	3.8	31

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73	Development of an Optimized Protocol for NMR Metabolomics Studies of Human Colon Cancer Cell Lines and First Insight from Testing of the Protocol Using DNA G-Quadruplex Ligands as Novel Anti-Cancer Drugs. <i>Metabolites</i> , 2016, 6, 4.	2.9	21
74	A comprehensive and comparative GC-MS metabolomics study of non-volatiles in Tanzanian grown mango, pineapple, jackfruit, baobab and tamarind fruits. <i>Food Chemistry</i> , 2016, 213, 691-699.	8.2	56
75	Data on the changes of the mussels ^{x3} metabolic profile under different cold storage conditions. <i>Data in Brief</i> , 2016, 7, 951-957.	1.0	6
76	Metabolic responses of clams, <i>Ruditapes decussatus</i> and <i>Ruditapes philippinarum</i> , to short-term exposure to lead and zinc. <i>Marine Pollution Bulletin</i> , 2016, 107, 292-299.	5.0	11
77	New Nordic Diet versus Average Danish Diet: A Randomized Controlled Trial Revealed Healthy Long-Term Effects of the New Nordic Diet by GC-MS Blood Plasma Metabolomics. <i>Journal of Proteome Research</i> , 2016, 15, 1939-1954.	3.7	61
78	Near-Infrared Spectroscopy Using a Supercontinuum Laser: Application to Long Wavelength Transmission Spectra of Barley Endosperm and Oil. <i>Applied Spectroscopy</i> , 2016, 70, 1176-1185.	2.2	12
79	The use of rapid spectroscopic screening methods to detect adulteration of food raw materials and ingredients. <i>Current Opinion in Food Science</i> , 2016, 10, 45-51.	8.0	39
80	Metabolic changes of genetically engineered grapes (<i>Vitis vinifera</i> L.) studied by ¹ H-NMR, metabolite heatmaps and iPLS. <i>Metabolomics</i> , 2016, 12, 1.	3.0	6
81	Lepidopteran defence droplets - a composite physical and chemical weapon against potential predators. <i>Scientific Reports</i> , 2016, 6, 22407.	3.3	20
82	Counteracting Age-related Loss of Skeletal Muscle Mass: a clinical and ethnological trial on the role of protein supplementation and training load (CALM Intervention Study): study protocol for a randomized controlled trial. <i>Trials</i> , 2016, 17, 397.	1.6	36
83	Near Infrared Spectroscopy - A Unique Window of Opportunities. <i>NIR News</i> , 2016, 27, 14-17.	0.3	13
84	Identification and quantification of turkey meat adulteration in fresh, frozen-thawed and cooked minced beef by FT-NIR spectroscopy and chemometrics. <i>Meat Science</i> , 2016, 121, 175-181.	5.5	109
85	Real-time metabolomic analysis of lactic acid bacteria as monitored by in vitro NMR and chemometrics. <i>Metabolomics</i> , 2016, 12, 1.	3.0	22
86	GC-MS Metabolite Profiling of Extreme Southern Pinot noir Wines: Effects of Vintage, Barrel Maturation, and Fermentation Dominate over Vineyard Site and Clone Selection. <i>Journal of Agricultural and Food Chemistry</i> , 2016, 64, 2342-2351.	5.2	31
87	Staling of white wheat bread crumb and effect of maltogenic α -amylases. Part 1: Spatial distribution and kinetic modeling of hardness and resilience. <i>Food Chemistry</i> , 2016, 208, 318-325.	8.2	49
88	Metabolomics analysis of shucked mussels TM freshness. <i>Food Chemistry</i> , 2016, 205, 58-65.	8.2	45
89	Prediction of total fatty acid parameters and individual fatty acids in pork backfat using Raman spectroscopy and chemometrics: Understanding the cage of covariance between highly correlated fat parameters. <i>Meat Science</i> , 2016, 111, 18-26.	5.5	53
90	Fluorescence Spectroscopy in Process Analytical Technology (PAT): Simultaneous Quantification of Two Active Pharmaceutical Ingredients in a Tablet Formulation. <i>Applied Spectroscopy</i> , 2015, 69, 323-331.	2.2	10

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91	Insight into the Functionality of Microbial Exopolysaccharides by NMR Spectroscopy and Molecular Modeling. <i>Frontiers in Microbiology</i> , 2015, 6, 1374.	3.5	13
92	Accurate determination of endpoint temperature of cooked meat after storage by Raman spectroscopy and chemometrics. <i>Food Control</i> , 2015, 52, 119-125.	5.5	38
93	Hurrah for the increasing longevity: feasible strategies to counteract age-related loss of skeletal muscle mass. <i>Scandinavian Journal of Medicine and Science in Sports</i> , 2015, 25, 1-2.	2.9	75
94	Trends in the application of chemometrics to foodomics studies. <i>Acta Alimentaria</i> , 2015, 44, 4-31.	0.7	59
95	Quantitative determination of mold growth and inhibition by multispectral imaging. <i>Food Control</i> , 2015, 55, 82-89.	5.5	15
96	Protein residual fouling identification on UF membranes using ATR-FT-IR and multivariate curve resolution. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 144, 39-47.	3.5	8
97	Forecasting individual breast cancer risk using plasma metabolomics and biocontours. <i>Metabolomics</i> , 2015, 11, 1376-1380.	3.0	54
98	Investigation of UF and MF Membrane Residual Fouling in Full-Scale Dairy Production Using FT-IR to Quantify Protein and Fat. <i>International Journal of Food Engineering</i> , 2015, 11, 1-15.	1.5	6
99	Simultaneous quantification of the boar-taint compounds skatole and androstenone by surface-enhanced Raman scattering (SERS) and multivariate data analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2015, 407, 7787-7795.	3.7	15
100	Characterization of Alginates by Nuclear Magnetic Resonance (NMR) and Vibrational Spectroscopy (IR). <i>Trends in Analytical Chemistry</i> , 2015, 60, 71-79.	11.4	74
101	Comprehensive and Comparative Metabolomic Profiling of Wheat, Barley, Oat and Rye Using Gas Chromatography-Mass Spectrometry and Advanced Chemometrics. <i>Foods</i> , 2014, 3, 569-585.	4.3	54
102	Quantification of individual fatty acids in bovine milk by infrared spectroscopy and chemometrics: Understanding predictions of highly collinear reference variables. <i>Journal of Dairy Science</i> , 2014, 97, 7940-7951.	3.4	71
103	POLYS 2.0: An open source software package for building three-dimensional structures of polysaccharides. <i>Biopolymers</i> , 2014, 101, 733-743.	2.4	38
104	Cereal β -glucan immune modulating activity depends on the polymer fine structure. <i>Food Research International</i> , 2014, 62, 829-836.	6.2	28
105	Moving from recipe-driven to measurement-based cleaning procedures: Monitoring the Cleaning-In-Place process of whey filtration units by ultraviolet spectroscopy and chemometrics. <i>Journal of Food Engineering</i> , 2014, 126, 82-88.	5.2	14
106	High-throughput cereal metabolomics: Current analytical technologies, challenges and perspectives. <i>Journal of Cereal Science</i> , 2014, 59, 393-418.	3.7	93
107	Raman spectroscopic study of effect of the cooking temperature and time on meat proteins. <i>Food Research International</i> , 2014, 66, 123-131.	6.2	55

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109	Recursive weighted partial least squares (rPLS): an efficient variable selection method using PLS. <i>Journal of Chemometrics</i> , 2014, 28, 439-447.	1.3	71
110	Measurement of Boar Taint in Porcine Fat Using a High-Throughput Gas Chromatography–Mass Spectrometry Protocol. <i>Journal of Agricultural and Food Chemistry</i> , 2014, 62, 9420-9427.	5.2	15
111	New insights from a β -glucan human intervention study using NMR metabolomics. <i>Food Research International</i> , 2014, 63, 210-217.	6.2	10
112	Cleaning up NMR spectra with reference deconvolution for improving multivariate analysis of complex mixture spectra. <i>Journal of Chemometrics</i> , 2014, 28, 656-662.	1.3	21
113	In honor of Rasmus Bro for being awarded with the 10th Herman Wold medal in gold. <i>Journal of Chemometrics</i> , 2014, 28, 606-607.	1.3	0
114	Process Analytical Technology in the food industry. <i>Trends in Food Science and Technology</i> , 2013, 31, 27-35.	15.1	90
115	The use of trimethylsilyl cyanide derivatization for robust and broad-spectrum high-throughput gas chromatography–mass spectrometry based metabolomics. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 9193-9205.	3.7	56
116	^1H NMR-based metabolomics approach in a rat model of acute liver injury and regeneration induced by CCl_4 administration. <i>Toxicology</i> , 2013, 303, 115-124.	4.2	61
117	Molecular structure of large-scale extracted β -glucan from barley and oat: Identification of a significantly changed block structure in a high β -glucan barley mutant. <i>Food Chemistry</i> , 2013, 136, 130-138.	8.2	55
118	Investigating Depth Profiles from Porcine Adipose Tissue by HR MAS NMR Spectroscopy. <i>Special Publication - Royal Society of Chemistry</i> , 2013, , 81-89.	0.0	1
119	Measurement of Active Content in Escitalopram Tablets by a Near-Infrared Transmission Spectroscopy Model that Encompasses Batch Variability. <i>Journal of Pharmaceutical Sciences</i> , 2013, 102, 1268-1280.	3.3	7
120	A primer to nutritional metabolomics by NMR spectroscopy and chemometrics. <i>Food Research International</i> , 2013, 54, 1131-1145.	6.2	82
121	Flaxseed dietary fibers suppress postprandial lipemia and appetite sensation in young men. <i>Nutrition, Metabolism and Cardiovascular Diseases</i> , 2013, 23, 136-143.	2.6	67
122	A NMR metabolomics study of the ripening process of the Fiore Sardo cheese produced with autochthonous adjunct cultures. <i>Food Chemistry</i> , 2013, 141, 2137-2147.	8.2	79
123	Extracted Oat and Barley β -Glucans Do Not Affect Cholesterol Metabolism in Young Healthy Adults. <i>Journal of Nutrition</i> , 2013, 143, 1579-1585.	2.9	32
124	Interval-Based Chemometric Methods in NMR Foodomics. <i>Data Handling in Science and Technology</i> , 2013, 28, 449-486.	3.1	10
125	Three-Dimensional Images of Porcine Carcass Fat Quality Using Spatially Resolved near Infrared Spectroscopy. <i>NIR News</i> , 2013, 24, 9-11.	0.3	4
126	An On-Line Near-Infrared (NIR) Transmission Method for Determining Depth Profiles of Fatty Acid Composition and Iodine Value in Porcine Adipose Fat Tissue. <i>Applied Spectroscopy</i> , 2012, 66, 218-226.	2.2	34

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127	Investigations of La Rioja Terroir for Wine Production Using ¹ H NMR Metabolomics. Journal of Agricultural and Food Chemistry, 2012, 60, 3452-3461.	5.2	121
128	Plant metabolomics: Resolution and quantification of elusive peaks in liquid chromatography-mass spectrometry profiles of complex plant extracts using multi-way decomposition methods. Journal of Chromatography A, 2012, 1266, 84-94.	3.7	51
129	Assessment of the Effect of High or Low Protein Diet on the Human Urine Metabolome as Measured by NMR. Nutrients, 2012, 4, 112-131.	4.1	74
130	Depth profiling of porcine adipose tissue by Raman spectroscopy. Journal of Raman Spectroscopy, 2012, 43, 482-489.	2.5	55
131	Assessment of dietary exposure related to dietary GI and fibre intake in a nutritional metabolomic study of human urine. Genes and Nutrition, 2012, 7, 281-293.	2.5	41
132	Real-time modeling of milk coagulation using in-line near infrared spectroscopy. Journal of Food Engineering, 2012, 108, 345-352.	5.2	41
133	LC-MS metabolomics top-down approach reveals new exposure and effect biomarkers of apple and apple-pectin intake. Metabolomics, 2012, 8, 64-73.	3.0	51
134	Residue Specific Hydration of Primary Cell Wall Potato Pectin Identified by Solid-State ¹³ C Single-Pulse MAS and CP/MAS NMR Spectroscopy. Biomacromolecules, 2011, 12, 1844-1850.	5.4	59
135	Characterization of marama bean (Tylosema esculentum) by comparative spectroscopy: NMR, FT-Raman, FT-IR and NIR. Food Research International, 2011, 44, 373-384.	6.2	38
136	Metabolomics as a Powerful Tool for Molecular Quality Assessment of the Fish Sparus aurata. Nutrients, 2011, 3, 212-227.	4.1	60
137	Lipid composition and deposition during grain filling in intact barley (Hordeum vulgare) mutant grains as studied by 1H HR MAS NMR. Journal of Cereal Science, 2011, 54, 442-449.	3.7	16
138	icoshift: An effective tool for the alignment of chromatographic data. Journal of Chromatography A, 2011, 1218, 7832-7840.	3.7	203
139	Standardization of factors that influence human urine metabolomics. Metabolomics, 2011, 7, 71-83.	3.0	64
140	Characterisation of the arabinose-rich carbohydrate composition of immature and mature marama beans (Tylosema esculentum). Phytochemistry, 2011, 72, 1466-1472.	2.9	20
141	Exploratory Study of Potato Cultivar Differences in Sensory and Hedonistic Applicability Tests. Potato Research, 2011, 54, 13-28.	2.7	6
142	First Principles Insight into the Î±-Glucan Structures of Starch: Their Synthesis, Conformation, and Hydration. Chemical Reviews, 2010, 110, 2049-2080.	47.7	92
143	A combined nuclear magnetic resonance and molecular dynamics study of the two structural motifs for mixed-linkage Î²-glucans: methyl Î²-cellobioside and methyl Î²-laminarabioside. Carbohydrate Research, 2010, 345, 474-486.	2.3	22
144	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

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145	NMR and interval PLS as reliable methods for determination of cholesterol in rodent lipoprotein fractions. <i>Metabolomics</i> , 2010, 6, 129-136.	3.0	25
146	Prediction of the degradability and ash content of wheat straw from different cultivars using near infrared spectroscopy. <i>Industrial Crops and Products</i> , 2010, 31, 321-326.	5.2	46
147	A physicochemical theory on the applicability of soft mathematical modelsâ€™ experimentally interpreted. <i>Journal of Chemometrics</i> , 2010, 24, 481-495.	1.3	34
148	icoshift: A versatile tool for the rapid alignment of 1D NMR spectra. <i>Journal of Magnetic Resonance</i> , 2010, 202, 190-202.	2.1	696
149	Metabolic profiling and aquaculture differentiation of gilthead sea bream by 1H NMR metabonomics. <i>Food Chemistry</i> , 2010, 120, 907-914.	8.2	61
150	Mathematical chromatography solves the cocktail party effect in mixtures using 2D spectra and PARAFAC. <i>TrAC - Trends in Analytical Chemistry</i> , 2010, 29, 281-284.	11.4	32
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