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Food Analytics Conference 2026

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Abstracts

A Hybrid Physics-Based and Data-Driven Framework for Predicting Bread Quality Evolution During Baking Process

Aberham Hailu Feyissa

The development of formulations and the adoption of emerging baking technologies have increased the complexity of predicting bread quality. Key attributes such as texture, colour, moisture content, and volume are governed by strongly coupled heat and mass transfer phenomena, structural transformations, and reaction kinetics. Understanding and predicting these changes remain challenging due to the dynamic and interconnected nature of the baking process.

This work aims to develop an integrated framework that combines physics-based modelling, quality kinetics, and data-driven analytics to predict the evolution of key bread quality attributes during baking. A mechanistic model was developed to describe transient heat and moisture transfer within bread during baking. Kinetic models were used to characterise quality changes, including texture development, moisture loss, and crust colour formation. Experimental baking trials were conducted under varying processing conditions to measure temperature, moisture content, crumb firmness, specific volume, pore distribution, and colour attributes. The experimental data, together with model-derived process variables, were used to train predictive data-driven models for quality prediction. The integrated framework successfully linked transport phenomena and quality kinetics with the development of bread quality attributes. The combination of mechanistic and data-driven approaches enabled accurate prediction of texture, moisture content, colour development, and volume expansion under different baking conditions. The results also provided improved insight into the underlying mechanisms driving quality evolution during baking. While the pure first-principles approach offers explainability and exceptional data efficiency, it suffers from heavy computational bottlenecks when addressing complex phenomena in real time. Conversely, purely data-driven approaches (including machine learning) provide instant predictions but fail to extrapolate safely beyond their training data. The proposed hybrid framework supports the potential of combining physics-based modelling, kinetics, and data-driven analytics for digital food processing applications. Such an approach can support quality prediction, process optimisation, and intelligent control strategies, contributing to more consistent and sustainable bread production.

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Analytical Characterisation of Functional Mushroom Extracts with High Antimicrobial, Antioxidant and Neuroprotective Potential

Aleksandra Olejniczak

The demand for functional food ingredients has intensified the search for natural sources of bioactive compounds with scientifically verified biological properties. Edible mushrooms constitute an source of bioactive compounds whose composition varies considerably among species (Kozarski et al., 2015; Sharma et al., 2022). Although numerous studies have characterized individual mushroom species, comprehensive analytical comparisons of their bioactive profiles using standardized methodologies remain limited.

The aim of this study was to perform a comparative analytical assessment of selected edible mushroom extracts, with particular emphasis on Sparassis crispa, to evaluate the influence of extraction technique on their antioxidant, antimicrobial and neuroprotective properties. Extracts from Sparassis crispa, Boletus edulis, Imleria badia and Suillus luteus were prepared using ultrasound-assisted extraction (UAE) and supercritical carbon dioxide extraction (SFE-CO_2), enabling the comparison of two analytical extraction approaches for recovering bioactive compounds.

The analytical evaluation included determination of total phenolic content (TPC), total antioxidant capacity (TEAC), antimicrobial activity against selected indicator microorganisms, and inhibitory activity toward acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) (Tel-Çayan et al., 2012), as well as

spectroscopic measurements performed in the near-infrared (NIR) range 12 000 – 4 000 cm^{-1}) and additionally, the spectral data were interpreted through chemometric analysis using Unscrambler software (version 9.7; CAMO, Norway) (Mikola et al., 2020). The PCA model distinguishing prepared extracts according to extraction method (UAE/ SFE-CO_2) and it was characterized by high classification performance.

The obtained analytical data enabled a comprehensive comparison of the investigated mushroom species and extraction methods, providing insight into the relationship between extraction strategy and the functional characteristics of the resulting extracts.

The comparative analysis demonstrated substantial variability in the measured biological activities depending on both mushroom species and extraction technique, highlighting the importance of analytical methodology in the characterization of functional mushroom materials. Sparassis crispa exhibited a particularly promising analytical profile, characterized by high biological activity across several evaluated parameters, supporting its potential as a valuable ingredient for functional food and nutraceutical applications. NIR data combined with chemometrics allowed for effective discrimination of samples based on type extract and functional properties.

The study demonstrates how integrated analytical approaches combining quantitative determination of bioactive compounds with functional bioactivity assays can support the identification and characterization of promising mushroom-derived ingredients. The results contribute to the development of evidence-based strategies for evaluating functional mushrooms and emphasize the importance of selecting appropriate analytical methods for reliable assessment of their health-promoting potential.

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From Microstructure to Oxidative Stability: Analytical Characterization of Core-Shell Microcapsules for Bioactives Protection

Ana C. Mendes

The stabilization of oxidation-sensitive food bioactives remains a major challenge in the development of functional foods and fortified ingredients. This study presents the application of a range of advanced analytical techniques to investigate the structure-function relationships and oxidative stability of electrosprayed core-shell microcapsules

for the protection of highly oxidation-prone lipophilic compounds, including cod liver oil rich in omega-3 fatty acids1 and vitamin A palmitate2. Food-grade microcapsules with average diameter of about 2 to 3µm were produced by coaxial electrospraying using ethyl cellulose and bioactive compounds in the core and octenyl succinic anhydride (OSA)-modified starch as the shell material. A combination of scanning electron microscopy (SEM), confocal laser scanning microscopy (CLSM), Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR),

atomic force microscopy (AFM), and differential scanning calorimetry (DSC) was employed to characterize microcapsule morphology, microcapsules configuration, molecular interactions, crystallinity, mechanical properties, and oxidative stability. CLSM and Raman analyses confirmed the successful localization of bioactives within the microcapsule core and demonstrated the absence of the encapsulated bioactive on the particle surface for coaxial systems. FTIR revealed hydrophobic interactions and co-assembly phenomena between vitamin A palmitate and selected amino acids, providing mechanistic insight into their antioxidant protective effects. AFM measurements showed higher Young’s modulus of core-shell microcapsules compared with their monoaxial counterparts. Oxidative stability studies by DSC demonstrated substantial protection of encapsulated lipophilic bioactives. Core-shell encapsulation increased the oxidative stability of cod liver oil by up to 15-fold compared with the non-encapsulated oil. Furthermore, the incorporation of specific amino acids into vitamin A formulations significantly enhanced protection against oxidation, with histidine providing the most pronounced effect, resulting in more than a 200-fold increase in oxidative stability relative to non-encapsulated vitamin A palmitate. The enhancement of oxidative stability was mainly due to the hydrophobic interactions formed between vitamin A (except lysine) and amino acids, as confirmed by the FTIR analyses.

Collectively, the analytical characterization indicates that enhanced oxidative stability arises from the combined effects of physical barrier protection and molecular-level interactions. These findings demonstrate the potential of integrated analytical characterization in advancing the design and optimization of (micro)encapsulation systems for sensitive bioactives, supporting the development of food ingredients with improved oxidative stability, extended shelf life, and enhanced nutritional quality.

Acknowledgements This project has received funding from the BASF A/S.

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Adulteration of fruit juices and fruit juice concentrates with sugar syrups: Systematic investigations and identification of carbohydrate-based markers

Angelina Schneider

Adulteration of fruit juices and fruit juice concentrates with sugar syrups is financially attractive due to the high demand and natural variations in the raw materials and raw material shortages. With commonly used analytical methods, e.g. stable isotope analysis and the GC-FID method according to LOW [1], a detection of adulterations is difficult or not possible. In addition the limits of detection are rather high. This is derived from a lack of systematic investigations of different fruit matrices and sugar syrups but also methodological limits. For example, the structure of marker compounds used is yet unknown. Furthermore, the methods are only suitable for specific fruit matrix/foreign sugar combinations. In order to develop a HPLC-MS/MS multi method with marker compounds from the minor sugar fraction, for the unambiguous detection of adulteration with sugar syrups, different sugar syrups and fruit matrices were investigated systematically. To enable an investigation of the minor sugar profiles, a method for sample preparation, based on activated carbon [2,3], was developed. This approach allowed for a removal of the main sugars glucose, sucrose and fructose.

First, the minor sugar profiles of fruit juices and fruit juice concentrates from apple and orange were systematically investigated. In addition, different invert sugar syrups and starch syrups from different raw materials, which could be possibly used as cheap foreign sugars for adulteration, were analyzed with HPAEC-PAD/MS and compared. This allowed for the identification of compounds which could be used as markers for adulteration. Furthermore, the influence of various industrial processes, which are involved in the production of fruit juices and fruit juice concentrates, on the minor sugar profile of the respective products were investigated. In this context, particular attention was paid to heating, concentration and enzymatic processes. This approach yielded information on the potential formation of the identified marker compounds during the manufacturing process, which could lead to false-positive analytical results.

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Isoflavones Fingerprinting in Underutilized Legumes using FTIR Spectroscopy

Ankur Kumar

Soybeans contain the highest amount of isoflavones among crops. Aglycone isoflavones are known for their greater therapeutic effects than the β-glucosides form. The present study explores the use of black soybean (BS), an underutilized crop compared to yellow varieties. Although the oil yield is comparatively lower, the black seed coat of BS showed a significant amount of anthocyanins, thereby improving its overall polyphenolic profile, including isoflavones and anthocyanins. Colorimetric reaction-based methods are commonly used for the determination of total isoflavones, relying on complex formation and subsequent UV-Vis detection. These methods sometimes yield overestimates due to improper incubation and reagent quality. Another quantification method is based on HPLC and LC-MS separation, which requires extra pure solvents, reagents, and expensive instrumentation. Hence, the present work optimized a simple, rapid FTIR-based analytical method for quantifying isoflavones in black soybean. The method involves a simple acid-assisted aqueous-organic sample preparation and further quantification by FTIR. Three functional groups at 2835, 1640, and 1015 cm-1 wavenumber were identified for isoflavones quantification. These spectral peaks corresponded to the aldehyde groups, aromaticity and glucoside chain, assisting in isoflavones fingerprinting in the extracted samples. The isoflavones standard linearity was plotted in the range 0.5 to 5 µg/mL with a linear response. The results were further compared with the conventional methods.

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Stable Isotope Ratio Analysis as a Tool for Verifying the Authenticity of Austrian Wines

Ariana Rugova

This study investigates the application of stable isotope ratio analysis for the authentication of Austrian wines by examining the isotopic composition of key light elements, including carbon ($\delta^{13}C$), oxygen ($\delta^{18}O$) and hydrogen D/H. Wine samples representing different Austrian wine-growing regions and grape varieties were analyzed using isotope ratio mass spectrometry (IRMS), and the resulting isotopic signatures were compared with established reference databases. The findings demonstrate that stable isotope ratios effectively differentiate wines according to their geographical origin and can identify potential adulteration, such as dilution with water, addition of exogenous sugars. The study underscores the value of integrating stable isotope ratio analysis into routine quality control and regulatory frameworks for Austrian wines. By providing scientifically reliable evidence of origin and production authenticity, this approach strengthens traceability, supports the protection of protected designation of origin (PDO) products, and enhances consumer trust in the Austrian wine industry.

Keywords: $\delta^{13}C$, $\delta^{18}O$, D/H, Isotope ratio mass spectrometry, wine authenticity

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Headspace Analysis for Early Off-Flavour Detection in Beer

Artem Leonov

Trained sensory panels remain the gold standard for detecting off-flavours in beer, but their resource-intensive, low-throughput nature creates a need for analytical tools that can flag potential deviations early and complement human assessment. Untargeted headspace mass spectrometry, and PTR-MS in particular, offers a promising route to this goal, given its speed, sensitivity, and minimal sample preparation. Here, we present our ongoing work on predicting beer off-flavours directly from untargeted PTR-MS headspace data. Starting from a large set of raw spectral features, we explore statistical and heuristic approaches for feature selection, aimed at isolating the signal most relevant to specific off-flavours while filtering out day-to-day instrumental drift. On top of this reduced feature space, we evaluate a range of predictive modelling approaches suited to the small-sample, imbalanced nature of sensory-labelled data — including models that treat off-flavour severity as a continuous outcome and classification-based approaches for flagging problematic batches — together with complementary anomaly detection methods aimed at surfacing atypical samples independent of predefined labels. Particular attention is given to the more challenging cases: batches with a mild but detectable off-flavour that does not yet substantially lower the overall quality score, where early detection is most valuable but the signal is hardest to isolate. Our preliminary findings suggest that certain chemical signatures show promise as early indicators of specific off-flavours, while also highlighting the practical challenges of instrumental variability and limited labelled data in this setting. We discuss these early results as a step toward predictive tools that could complement sensory panels and support faster, more consistent quality control decisions in industrial brewing.

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Combining Microfluidics and FTIR Imaging to Resolve Fat Droplet Behaviour and Spreading at Air–Emulsion Interfaces

Dionysios D. Neofytos

Dairy foams and creams owe their stability to the way fat droplets adsorb and interact at the air–water interface, but the underlying chemical and compositional dynamics at this interface are difficult to resolve with conventional bulk techniques. (1,2) In our recent work we developed an in-situ platform combining microfluidics, confocal laser scanning microscopy (CLSM) and FTIR imaging to directly visualize and chemically map fat droplet adsorption, packing, and coalescence at controlled air–water interfaces and applied it to compare how emulsifier chemical structure governs these interfacial phenomena.

Oil-in-water emulsions were prepared by high-pressure homogenization using whey protein isolate (WPI) and Tween 20, 40, or 80, at three concentrations spanning coverage-limited, interface-saturated, and bulk-rich stabilization regimes. A microfluidic device was used to generate controlled, reproducible air–water interfaces and monitor fat droplet adsorption and coalescence in situ by CLSM. The same interfacial region was imaged by FTIR imaging within spatial resolution moving from the bulk emulsion toward the air interface, generating hyperspectral maps. Spectra were baseline-corrected, smoothed, and analyzed by k-means clustering and PCA to isolate spectral regions associated with water (H-O-H), carbonyl (C=O), and C-H stretching bands, from which droplet concentration, hydrogen-bonding, and acyl chain-order gradients (crystallization behavior) were derived, visualizing, for the first time, chemical transitions across the air–emulsion interface at μm scale. Complementary pendant drop tensiometry experiments were performed to relate the FTIR and microfluidics-based observations to interfacial tension dynamics.

Microfluidic assisted CLSM imaging showed pronounced, concentration-dependent droplet flocculation and coalescence at the interface for WPI, versus markedly less coalescence for Tweens, decreasing further with increasing alkyl chain length (Tween 80 < Tween 40 < Tween 20). FTIR hyperspectral imaging resolved a clear compositional gradient approaching the air interface: droplet (oil) concentration increased, hydrogen bonding weakened, and acyl chain order increased near the interface, indicating localized fat crystallization and structural reorganization distinct from the bulk emulsion. Overlaying the FTIR-derived chemical maps with the CLSM coalescence data, linked interfacial chain packing directly to the emulsifier-dependent stability differences, observed microscopically.

Coupling microfluidic interface generation with FTIR chemical imaging provides a label-free, spatially resolved method to probe interfacial composition and structure in situ, at a resolution inaccessible to bulk rheological or tensiometric methods. This platform offers a mechanistic tool for screening emulsifier chemistry and guiding clean-label reformulation of aerated dairy products such as whipped and aerosol creams.

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Fast, Reliable, and Transferable: Interlaboratory Validation of HPLC-ICP-MS for Methylmercury determination in Foods

Doaa Abouelenein

Mercury is a major food contaminant of concern, and its toxicity strongly depends on its chemical form. Among mercury species, methylmercury (MeHg) is the most toxic and readily absorbed, making mercury speciation analysis crucial for accurate assessment of dietary exposure. Reliable determination of MeHg is therefore essential for supporting food safety decisions [1]. However, most published methods for mercury speciation have only been validated within individual laboratories, leaving uncertainty about how well these methods perform when transferred to different analytical settings. This study addresses this gap by combining comprehensive in-house validation with an independent interlaboratory evaluation of a rapid HPLC-ICP-MS method for MeHg determination. The method, based on simple aqueous L-cysteine extraction and reversed-phase separation, enabled selective MeHg determination by achieving baseline separation from inorganic mercury within 3.2 min, ensuring reliable species-specific quantification while providing a faster alternative to conventional approaches and avoiding hazardous mobile-phase additives. In-house validation demonstrated excellent performance, with MeHg recoveries of 94–101% across certified reference materials, within-laboratory reproducibility ≤12.3%, and a quantification limit of 0.29 µg kg^{-1} in fresh seafood.

Transferability was assessed through an interlaboratory study involving nine European laboratories within the European Committee for Standardization (CEN), Technical Committee 275, Working Group 10 (CEN/TC 275/WG 10). Six diverse matrices from marine, terrestrial, and fungal sources were evaluated, including swordfish, dried tuna/bonito, white fish, shrimp, cricket flour (NRC KRIK-1), and porcini mushroom powder. For matrices containing MeHg levels between 0.06 and 2.0 mg kg^{-1}, the method showed excellent reproducibility across laboratories, with RSDR values of 11.7–19.8%, HorRat values below 1 (0.62–0.93), and no outliers among laboratories' results. Reliable performance was maintained despite variations in extraction conditions and column hardware, confirming method robustness, while reduced performance was observed only for porcini powder at the lowest tested concentration level. The method was applied to 54 Danish market foods, revealing distinct MeHg patterns across sample types. MeHg dominated in fish and crustaceans (≈85–94%), while lower contributions were observed in other matrices, highlighting the importance of direct MeHg determination. Overall, the combined in-house validation, interlaboratory evaluation, and market application demonstrate a rapid, robust, and transferable method for MeHg determination, suitable for standardisation and routine food safety monitoring. Its short analysis time and avoidance of hazardous reagents make it well suited for adoption across laboratories.

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Comparative Chemical Characterization of Fermented Pomegranate Beverages produced from Fresh Fruit and Commercial Juice

Eka Mazumder

Pomegranate (Punica granatum L.) has gained increasing attention as a promising raw material for functional beverages due to its high levels of phenolic compounds, flavonoids, essential minerals, and distinctive aroma constituents. However, limited information is available comparing fermented beverages produced from fresh pomegranate fruit and commercially available pomegranate juice. This study investigated the effect of raw material on the physicochemical properties, bioactive composition, elemental profile, alcohol content, and volatile aroma of fermented pomegranate beverages. Two beverages were produced under identical laboratory conditions using fresh pomegranate fruit or commercial pomegranate juice as the fermentation substrate. Both formulations were fermented with Saccharomyces cerevisiae for 12 days. Physicochemical characteristics were evaluated by pH measurement, spectrophotometric determination of color intensity and tone, Folin–Ciocalteu assay for total phenolic content (TPC), aluminum chloride colorimetric assay for total flavonoid content (TFC), inductively coupled plasma optical emission spectrometry (ICP-OES) for elemental analysis, and gas chromatography–mass spectrometry (GC–MS) for ethanol, methanol, and volatile compound analysis. Both beverages exhibited identical pH values (3.75), indicating stable acidity regardless of the raw material. Color intensity (2.95–2.96) and tone (2.71–2.72) showed minimal variation, demonstrating good preservation of anthocyanin-derived pigments during fermentation. The fresh fruit beverage contained slightly higher total phenolic content (99.6 mg GAE/100 mL), whereas the juice-based beverage showed marginally higher total flavonoid content (15.1 mg CE/100 mL). Potassium was the predominant mineral, followed by calcium and magnesium, while trace elements remained within nutritionally relevant concentrations. Fermentation yielded approximately 8.6% (v/v) ethanol in both samples, whereas methanol remained below 0.01% (v/v), meeting international safety recommendations. GC–MS identified 22 volatile compounds, with fruity, sweet, creamy, roasted, and caramel-like aroma compounds predominating in both beverages. The findings demonstrate that both fresh pomegranate fruit and commercial pomegranate juice are suitable substrates for producing high-quality fermented beverages with comparable physicochemical characteristics, bioactive composition, elemental profile, and aroma. These results support the potential application of either raw material in the development of functional fermented pomegranate beverages

Keywords Alcoholic beverage, Fermentation, Pomegranate, Wine, Bioactive compounds, Yeast

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Development and Validation of a Quantitative Multi-Mycotoxin LC-MS/MS Method for Novel Foods and Plant-Based Alternatives

Hellen Sørensen

Increased interest in novel foods and plant-based alternatives has created a need for sensitive analytical methods validated for these matrices to ensure safety of consumption. As agricultural commodities are susceptible to toxigenic fungal contamination, the occurrence of mycotoxins presents a potential safety concern for novel foods and plant-based alternatives. This study aims to develop and validate a liquid chromatography-tandem mass spectrometry (LC-MS/MS) based method for simultaneous quantification of multiple mycotoxins in various novel food and plant-based matrices. The method targets 18 mycotoxins, both regulated and emerging, from multiple toxin classes including aflatoxins, trichothecenes, fumonisins, zearalenone, ochratoxin A, sterigmatocystin, citrinin, and enniatins. Four matrices, tiger nuts (Cyperus esculentus L.), a fermented soy-based product, a plant-based beverage and a plant-based meat alternative, were selected from the Danish market to represent popular novel foods and plant-based alternatives with diverse matrix compositions. Chromatographic separation is performed by RP-UPLC on an Acquity UPLC HSS T3 column using a water/methanol gradient buffered with ammonium formate and formic acid. Detection is performed using an Agilent 6495D Triple Quadrupole LC/MS system with dynamic multiple-reaction monitoring (dMRM), with a total method run time of 15 minutes.

Sample preparation is being optimised for the selected matrices, with different extraction and clean-up approaches being evaluated, to obtain adequate recovery of the target mycotoxins while minimising matrix effects. Method validation is being conducted in accordance with the performance criteria described in the Commission Implementing Regulation (EU) 2023/2782.

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Molecular diversity among commercial pea protein isolates and its implications for shear-induced structure formation

Jason Daniel Foley

Introduction Plant proteins (PPs) are widely used in plant-based meat analogue production, yet commercial isolates or concentrates intended for similar applications often display divergent behavior during shear-based structuring. While such variability is well recognized in practice, the underlying molecular diversity of commercial PP and its relevance to shear-induced structure formation remain insufficiently resolved, contributing to a continued reliance on empirical ingredient screening. This study aimed to systematically characterize the molecular diversity among commercial pea protein isolates (PPIs) and explore how this diversity relates to structuring behavior under controlled shear cell processing conditions. Methods Fifteen commercial PPIs were characterized at the powder level using complementary vibrational spectroscopy, proton mobility, and functional measurements capturing protein conformation, water association, and interfacial functionality. These data were integrated using multivariate analysis to map molecular variation across the commercial ingredient space. Structuring behavior was assessed for each isolate using a Couette-type shear cell under a controlled factorial design varying temperature and dry matter content, with spectroscopic, textural, and anisotropic properties used to describe product structure. Results The PPIs exhibited molecular heterogeneity, reflected in differences in protein secondary structure, water-binding characteristics, and functional attributes. Multivariate analysis resolved structured variation across isolates, indicating that commercial PPIs occupy a broad and non-uniform molecular descriptor space. Shear cell processing produced isolate-dependent differences in texture and structural anisotropy, highlighting pronounced variability in structuring behavior within the commercial ingredient set. The correspondence between powder-level molecular patterns and shear-induced structural outcomes was explored across the design space. Conclusions Commercial PPIs exhibit molecular diversity extending beyond conventional compositional and functional descriptors. Mapping diversity alongside shear-induced structuring behavior provides a structured basis

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Rapid prediction of antioxidant properties in Clausena harmandiana herbal tea using UV-Visible spectroscopy and chemometric models

Jordi Cruz Sanchez

Objective: Clausena harmandiana is a traditional Thai medicinal herb known for its high content of carbazole alkaloids and coumarins, showing strong potential as a functional herbal tea. While traditional assays such as the Folin-Ciocalteu, DPPH, and ABTS methods are widely used to measure total polyphenolic content (TPC) and antioxidant activity, they are often time-consuming and require toxic chemical reagents. The objective of this study was to develop a rapid, green, and efficient analytical approach to predict these parameters using UV-Visible spectroscopy coupled with chemometric and machine learning algorithms. Methodology: Aqueous extracts (tea) from the leaves of C. harmandiana were prepared and analyzed using traditional spectrophotometric assays for TPC, ABTS, and DPPH radical scavenging activities. Simultaneously, UV-Visible spectra of the tea samples were acquired. To correlate the spectral data with the reference chemical values, we applied and compared three predictive modeling algorithms: Partial Least Squares (PLS) regression, Support Vector Machine (SVM), and Artificial Neural Networks (ANN). Model performance was evaluated based on the root mean square errors of calibration (RMSEC), cross-validation (RMSECV), and prediction (RMSEP), along with their respective coefficients of determination (R2). Results: LC-MS/MS analysis confirmed that the C. harmandiana leaf tea contains multiple bioactive constituents, including phenolic acids, flavonoids, and mangiferin, which contribute to its strong, concentration-dependent antioxidant capacity. Our modeling results indicated that different algorithms excelled at predicting different parameters. Specifically, the SVM model demonstrated superior predictive performance for antioxidant activities, achieving lower prediction errors for both the DPPH (RMSEP = 3.85) and ABTS (RMSEP = 2.78) assays compared to PLS and ANN. Conversely, the PLS algorithm achieved the highest accuracy in predicting TPC, yielding an R2 of 0.92 and an RMSEP of 2.51. The ANN models also exhibited high calibration accuracy but showed higher cross-validation errors. Conclusions: Clausena harmandiana leaf tea is a promising functional beverage rich in health-promoting antioxidants. This study successfully demonstrates that combining simple UV-Visible spectroscopy with targeted chemometric and machine learning techniques, such as SVM for radical scavenging assays and PLS for phenolic content, offers a robust, rapid, and environmentally friendly alternative to conventional chemical testing for the quality control of herbal teas.

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Valorization of brewers' spent grain through enzymatic hydrolysis: effects of pretreatment on hydrolysate composition and properties

Josipa Matic

Brewers’ spent grain (BSG), the major byproduct of the brewing industry, is a protein- and fiber-rich biomass with considerable potential for valorization into food, feed, and biobased ingredients (Lynch et al., 2016; Mussatto, 2014). Enzymatic protein hydrolysis has been widely investigated as a strategy for BSG valorization, often following prior protein extraction in alkaline conditions (Bazsefidpar et al., 2024; Celus et al., 2009). Direct hydrolysis of whole BSG biomass has received much less attention (Connolly et al., 2019; Treimo et al., 2008). Previous studies have demonstrated that pretreatment can improve access to proteins embedded within the lignocellulosic matrix of BSG (Castilla-Archilla et al., 2023). However, knowledge of how different pretreatment strategies affect subsequent protein hydrolysis and the composition of BSG hydrolysates remains fragmented, making direct comparisons between studies difficult. Furthermore, some treatments may introduce non-native constituents, such as inorganic salts, that affect hydrolysate quality and increase downstream purification requirements, but also complicate analytical characterization. These factors are not always considered when comparing the outcomes of different hydrolysis and pretreatment studies. The objective of this study was to evaluate the impact of alkaline, pulsed electric field (PEF), and enzymatic pretreatments on the hydrolysis of BSG, and to improve understanding of how these treatments influence hydrolysate composition. Following the pretreatments, BSG was subjected to Alcalase hydrolysis, and hydrolysates were characterized for their protein content, and by size-exclusion chromatography (SEC) and 1H NMR spectroscopy. In addition, time-resolved sampling during hydrolysis enabled monitoring of molecular-weight changes throughout the process by SEC.

The results demonstrated molecular-weight reduction and increased solubilization during hydrolysis across all treatments. The effect of the specific pretreatment was observed in protein recovery and in hydrolysate composition. The study contributes to a better understanding of how pretreatment influences the conversion of BSG into protein-rich hydrolysates and evaluates different routes for valorization of this abundant brewing side stream.

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NIR spectroscopy and chemometrics approach for coffee adulteration detection

Katarzyna Pawlak-Lemańska

The adulteration of roasted coffee is a common and diversified application. It affects the quality of the coffee beans due to the addition of certain substances including coffee husk and stems, maize, barley, wheat, soybean, chicory etc. (Toci et al., 2016; Chen et al. 2023) The aim of the study was to examine and develop the models for detection of different kinds of adulterations in coffee beans. The test material consisted of different coffee varieties: Arabica (Coffea arabica) and Robusta (Coffea canephora) coffee beans sourced from Cameroon and Brazil. Chicory root (CY) and cascara (CR) were selected as adulterants and milled before used. Mixtures of ground coffee (labelled A and R separately) were prepared with the selected adulterants at concentrations (v/v %) ranging from 0 to 35%, in 2.5% increments (for each model there was prepared 16 test samples in duplicate).

The spectral data of the prepared mixtures were recorded in the NIR range (12 500–4 000 cm^{-1}) in diffuse reflectance mode using a Bruker MPA spectrometer (Bruker, Ettlingen, Germany) equipped with OPUS 7.2 software. For each sample 5 measurements were taken. To optimize the models, the spectra range was limited (8 800 – 4 000 cm-1) and the spectra were pre-processed using methods: smoothing and standard normal variate (SNV). Principal Component Analysis (PCA) was performed on the NIR spectra to identify interrelationships between the samples. Partial Least Squares (PLS) analysis was then applied to extract new latent variables, providing an approach to model the covariance structure between the NIR spectra and concentration of the adulterants. After selecting the optimal number of latent variables, the resulting models were used to verify by test sample sets. Multivariate data analysis was conducted using The Unscrambler version 9.7 (Camo, Norway). The PCA model distinguishing coffees according to coffee

variety (Robusta/Arabica) and type of adulteration (CY/CR) was characterized by high classification performance. The models based on NIR spectra for prediction of CY content showed good classification performance with errors at the level of 1.4% and 1.8% for prediction for Arabica and Robusta separately, and 1,6% for prediction model for mixed Arabica and Robusta. The NIR models for CR adulterant showed classification performance with errors 1.7 and 2.3% for prediction separately for Arabica and Robusta. Overall, these findings highlight and prove the potential of NIR spectroscopy as rapid, robust, and non-destructive tools for screening adulterations in coffee beans in logistic chain.

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Rapid determination of sugar content in commercial coconut water using near infrared spectroscopy and chemometrics

Katarzyna Włodarska

Coconut water is a natural beverage valued for its high content of minerals and low fat content, easily absorbed sugars, and diversity of other bioactive compounds. The concentrations of individual compounds in this product vary significantly throughout the maturation process of coconut fruit (Kumar et al. 2021). Global consumption of coconut water is growing rapidly, transforming the market into a multi-billion-dollar industry (IMARC Report, 2026).

The aim of this study was to assess the feasibility of Fourier-transform near infrared (FT-NIR) spectroscopy combined with chemometrics for the determination of sugars in commercially available coconut water. Organic and non-organic coconut waters from different manufacturers located in the Philippines, Sri Lanka, Thailand and Vietnam were analyzed. The samples originated from coconuts of different maturity stages, although the maturity stage was not specified for all products. FT-NIR spectra were measured in transmittance and transflectance modes. Sugar compounds were determined by high-performance liquid chromatography (HPLC) with an evaporative light scattering detector (ELSD). Fructose, glucose, sucrose, and sorbitol were quantified using the external standard method. Partial least squares (PLS) regression was applied to develop calibration models. For model development, all samples were divided into training and test sets using the Kennard-Stone algorithm. Various spectral preprocessing methods were tested to optimize model performance.

The analyzed coconut water samples exhibited considerable variation in sugar concentrations. Predictive models with good performance were developed for all analyzed parameters, namely fructose, glucose, sucrose, sorbitol, and total sugars. Similar results were obtained for spectra recorded in both transmittance and transflectance measurement techniques. These findings demonstrate that FT-NIR spectroscopy combined with chemometrics can serve as a valuable alternative to HPLC for the determination of sugars in coconut water. Although HPLC remains the reference technique owing to its superior sensitivity and analytical precision, FT-NIR spectroscopy offers several advantages, including rapid analysis, non-destructive measurements, the absence of chemical reagents, and reduced negative environmental impact. Therefore, FT-NIR spectroscopy represents a promising green analytical approach for the routine screening and quality control of coconut water.

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Beyond total phenolics: Individual phenolic compounds in Nannochloropsis oceanica and their response to food-grade side-stream nitrogen

Konstantina Rapti

Nannochloropsis oceanica is a promising microalgal species for sustainable food production due to its favourable protein and lipid composition, including the nutritionally relevant omega-3 fatty acid eicosapentaenoic acid (EPA). Recent studies have shown that food-grade industrial side streams can partially replace conventional nutrients during cultivation without negatively affecting biomass composition, protein quality, or EPA content [1]. Phenolic compounds constitute another chemical group occurring in microalgae, but their characterization in Nannochloropsis sp. remains limited and heterogeneous. Their analysis has frequently relied on total phenolic content determined by the Folin–Ciocalteu assay, although these measurements can be affected by interference from pigments and other reducing compounds present in algal matrices [2]. Identification and quantification of individual phenolic compounds in N. oceanica have not been reported. Consequently, this study aims to detect, identify and quantify individual phenolic compounds in N. oceanica and investigate how their abundance varies with cultivation conditions using an industrial side stream as an alternative nitrogen source. N. oceanica was cultivated for 144 h in triplicate 250-mL vessels at 23 °C under 350 µmol·m−2· s−1 continuous white-light illumination and continuous sparging (50 mL· min−1) with a 1% CO2 gas mixture in 3.0% artificial seawater medium. Three iso-nitrogenous conditions were investigated, with 0%, 50% or 100% of medium nitrogen supplied by food-grade industrial process water, while maintaining a total nitrogen concentration of 112 mg $N{\cdot}L^{-1}$. Thus, total nitrogen was maintained across treatments, while the nitrogen source and associated nutrient composition differed. At the end of cultivation, biomass from cultures with sufficient growth was harvested by centrifugation, washed with 0.05 M ammonium formate, and freeze-dried. Freeze-dried biomass was mechanically disrupted using ceramic beads and extracted with methanol containing 0.1% formic acid. Fifteen target phenolic compounds were analyzed by UHPLC coupled to an ISQ EC single-quadrupole mass spectrometer with electrospray ionization operated in negative-ion selected-ion monitoring mode. Compound identification was based on agreement with authentic reference standards in retention time and monitored m/z, with procedural blanks used to exclude background signals. In this study, four targeted phenolic compounds have been identified in conventionally cultivated biomass: gallic acid, protocatechuic acid, p-hydroxybenzoic acid and chlorogenic acid. Quantification of the identified compounds, optimization of the analytical workflow, and analysis of biomass cultivated with different side-stream nitrogen substitution are ongoing. The completed study will establish a compound-specific phenolic profile of N. oceanica and determine whether the phenolic composition is affected by the nitrogen source and associated cultivation conditions.

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Succinylation of Rapeseed Proteins: Synthesis, Structural, and Functional Characterisation

Laoise Murray

Rapeseed protein isolate (RPI) is an underutilised byproduct of rapeseed oil production with potential for use as an alternative plant protein ingredient in food applications. However, its utilisation is currently limited by poor functional properties. This study investigated the effect of increasing succinylation on the functional and structural properties of RPI and identified the specific amino acids and protein residues modified. Low and moderate succinylation of RPI resulted in improved overall solubility, gel-forming ability (least gelation concentration 5% (w/v)), thermal stability, and water holding capacity (maximum value 92.88 ± 1.60%). In contrast, RPI no longer formed gels at the highest level of succinylation, while solubility and thermal stability decreased. Mass photometry, intrinsic fluorescence spectroscopy, and DSF structural analyses revealed alterations in tertiary structure and partial unfolding as succinylation degree increased, as well as dissociation of the cruciferin hexameric assembly at the highest level of succinylation. LC-MS/MS and amino acid analysis identified lysine as the primary residue modified during succinylation, with serine, threonine, and tyrosine also succinylated to a lesser extent. Furthermore, LC-MS/MS enabled the identification of the precise localisation of modification sites on cruciferin and napin chains, revealing that the number of modified sites on cruciferin increased progressively with succinylation degree, whereas napin modification remained relatively constant. These findings improve the understanding of the relationship between the functional and structural properties of RPI and the extent and location of succinylation of the protein, allowing the modification level to be precisely tuned to optimise the functionality of RPI for food applications.

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From Biodiversity to Biosolutions: Robotics-Assisted Discovery of Fungal Enzymes for Off-Flavor Degradation

Lise Friis Christensen

The transition towards more sustainable food systems relies on improved utilization of protein-rich side-streams from agricultural processing. Potato protein recovered from industrial starch production is an attractive food ingredient due to its high nutritional value and favorable functional properties. However, its broader use is limited by off-flavors, including the bitter tasting glycoalkaloids α-chaconine and α-solanine.

Microbial degradation of potato glycoalkaloids has previously been reported, suggesting that microorganisms represent a potential source of biological solutions for improving potato-derived ingredients. Several filamentous fungi associated with potato have evolved mechanisms to tolerate and transform glycoalkaloids as part of their adaptation to the host environment. While initial glycoalkaloid transformation steps have been described, the downstream processes involved in complete degradation remain largely unexplored.

The challenge is therefore not only to identify fungi capable of transforming glycoalkaloids, but to efficiently discover the enzymes underlying these activities across large and diverse fungal strain collections. In this study, we investigate a diverse panel of filamentous fungi for glycoalkaloid-degrading activity through a robotics-assisted high-throughput screening platform for standardized assessment and comparison of glycoalkaloid-transforming activities. The platform combines automated cultivation, analytical assessment of glycoalkaloid conversion, and systematic data generation to enable efficient identification of fungal enzyme candidates for off-flavor degradation.

Using glycoalkaloid degradation as a model system, this work explores how automation and high-throughput analytics can facilitate the systematic investigation of fungal biodiversity for food applications. More broadly, the project aims to develop scalable workflows for translating microbial diversity into candidate enzymes and biosolutions for the food industry.

This study is part of the REFINES project that is funded by Plant2Food (https://projects.au.dk/plant2food/funded-projects/refines).

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Development and Validation of an Analytical Method for Determination of Nitrosamines in Processed Meat Products Using QuEChERS based Extraction and analysis with Gas Chromatography-Tandem Mass Spectrometry (GC-MS/MS)

Manisha Dhanshetty

Nitrites, nitrates, and their salts such as sodium and potassium nitrate and nitrite which are classified as permitted food additives are commonly incorporated into processed meat products to enhance colour and flavour, extend shelf life, and reduce microbial contamination including the growth prevention of Clostridium botulinum. Regulatory authorities, such as European Union, establish and enforce limits on the use of sodium and potassium nitrates and nitrites in cured meat products [Regulation (EC) 1333/2008]. However, one of the major concerns regarding nitrites is their contribution to the formation of nitrosamines during the processing of meat products. These compounds are typically formed through the reaction of secondary amines with nitrosating agents such as nitrite, particularly under acidic conditions or during high-temperature processing. These N-nitrosamines are of significant concern in food safety due to their well-documented carcinogenic and mutagenic properties. Many nitrosamines, including include full name (NDMA), have been classified as probable human carcinogens by regulatory agencies. Considering these significant global food safety concerns, this project aims to reduce nitrate and nitrite levels, as well as nitrosamines, in meat and processed products. on the chemical analysis of nitrosamines. This study presents an optimised sample preparation workflow including the extraction of processed meat samples using a QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) based solid-phase extraction protocol and analysis using gas chromatography–tandem mass spectrometry (GC-MS/MS). The method was validated in a range of meat matrices, including bacon, meat rasher and salami. The optimized sample preparation involved extracting meat samples with acetonitrile, followed by QuEChERS salts ($MgSO_4$ and sodium acetate) and a freezing step at −20 °C to remove co-extractives. The extract was then cleaned using dispersive solid-phase extraction, evaporated, and directly analyzed by GC–MS/MS. This approach effectively reduced matrix interferences. Nitrosamines were analysed by GC–MS/MS within a runtime of 15 min. The optimal analytical approach was validated for three product categories in terms of linearity, matrix effects, accuracy, and precision. The limit of quantification (LOQ) was 0.01 mg/kg. The recoveries at LOQ and higher levels ranged between 70% and 120%, with precision-RSDs of < 20%. Overall, the developed method provided a robust, reliable, and high-throughput analytical tool for the determination of nitrosamines in this complex food matrices- meat. This methodology can be effectively applied for routine-surveillance and regulatory monitoring to ensure the safety, quality of food products, as well as to support risk assessment studies related to dietary-exposure to nitrosamines.

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From Fragmented Experiments to AI-Ready Knowledge: Building the Data Foundation for AI4Food

Mansi Goel

Artificial intelligence is increasingly presented as a route to faster discovery and innovation in food science. Its relevance is compelling: AI can connect composition, structure, processing, sensory response, functionality, and consumer acceptance; reveal patterns across experiments; identify research gaps; generate hypotheses; and support prediction of costly or time-consuming endpoints1. These capabilities could accelerate the development of nutritious, sustainable, and desirable foods at a time when global food systems face environmental, health, and efficiency challenges. Yet the promise of AI4Food rests on a neglected prerequisite: whether results from different laboratories, instruments, and studies can be brought together on a common footing, and whether the origin and quality of each result can be traced2. Food research data are fragmented across instruments, spreadsheets, laboratory systems, publications, and individual projects. Two laboratories reporting the same compound in the same food may define the sample differently, use different units and different compound identifiers; the analytical results cannot safely be pooled, and no one can tell which measurement is the better one. Scientific articles preserve conclusions but rarely record complete experiments in a form a computer can read. When a project or doctoral study ends, much of its context, metadata, and knowledge becomes difficult to find, interpret, or reuse3. Consequently, large language models cannot reliably transform the available information into trustworthy, reusable evidence. AI readiness is therefore primarily a data-management challenge before it becomes a modelling challenge. AI4Food addresses this by building a shared way of recording food experiments in which the sample, what was done to it, what was measured, how, with which instrument and with what quality checks all stay attached to the result. It has three parts: capture at source, so context is recorded as the work happens rather than reconstructed afterwards4; a common vocabulary, so that "red wine", "resveratrol" and "mg/L" mean the same thing in every dataset5; and preserved links, so any published number can be traced back to the sample and method behind it6. The vocabulary layer reuses established international resources for foods, chemicals, food processes and analytical measurements7-10, adding new concepts only where a concrete use case shows existing ones cannot represent the structural, biological, functional, sensory or consumer properties food science requires11. The result is a searchable network of research data supporting questions that span many studies and giving AI systems evidence they can cite and a scientist can check12. Traceability makes verification possible; it does not by itself make outputs

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From Protein Structure to Colloidal Functionality: A Multi-Analytical Study of Ultrasound-Extracted Black Chickpea Proteins

Marco Torre

The valorization of neglected legume landraces can diversify plant protein sources while preserving agrobiodiversity. This study evaluated the effects of ultrasound-assisted extraction (UAE) on the physicochemical, structural, and emulsifying properties of protein isolates from a neglected rough black chickpea (Cicer arietinum L.) landrace from Sicily (Italy), with particular emphasis on analytical approaches linking protein structure to colloidal functionality. Conventional alkaline extraction (STD) was compared with ultrasound treatments at 20 kHz, 80% amplitude for 5, 10, and 15 min. Protein yield, purity, amino acid and mineral composition, total phenolics, SDS-PAGE, DSC, FTIR spectroscopy, surface hydrophobicity, intrinsic fluorescence, dynamic light scattering (DLS), and emulsion characterization were employed. UAE increased protein extraction yield from 57.57% (STD) to 67.21–68.97%, while protein purity remained high (85.38–88.09%). The analytical characterization revealed substantial structural and colloidal modifications. Surface hydrophobicity increased from 352.85 to 494.62–534.13 a.u., indicating exposure of hydrophobic domains, while solubility decreased from 92.5% to approximately 75–78%. DLS showed an increase in hydrodynamic diameter from 62.74 nm for STD to 92.87 nm after the 10-min treatment, accompanied by more negative protein ζ-potential values (from –22.09 to –24.10 mV). FTIR and DSC further evidenced conformational rearrangements without extensive degradation of the major protein fractions. Nutritional characterization showed an increase in total essential amino acids from 223.57 to 295.35 mg/g protein, with lysine increasing from 23.25 to 41.92 mg/g. These analytical changes translated into improved interfacial performance. UAE-derived proteins generated smaller initial O/W emulsion droplets than STD proteins, while all formulations maintained physical stability over 10 days, with emulsion ζ-potential values shifting from approximately –25 to –30 mV and no evident coalescence or flocculation by CLSM. Rheological analysis showed a near-Newtonian response (n = 1.05–1.06) that was unaffected by extraction treatment, demonstrating that ultrasound improved interfacial stabilization without altering bulk flow behavior. Overall, the integration of spectroscopic, compositional, colloidal, microscopic, and rheological analyses demonstrated that UAE can selectively modulate black chickpea protein structure and functionality. The study highlights analytical characterization as a powerful tool for elucidating structure–function relationships and supporting the valorization of neglected chickpea proteins as sustainable functional ingredients for food colloidal systems.

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Design of experiments, agricultural statistics and chemometrics in food quality and authenticity research

Maria Tarapoulouzi

The transition toward sustainable and data-driven agri-food systems requires robust experimental and analytical approaches capable of addressing the complexity of agricultural production. This presentation explores the integration of Design of Experiments (DoE), agricultural statistics, spectroscopy, and chemometrics for the optimization of production practices and the assessment of food quality and authenticity. Spectroscopic techniques, including NIR, FTIR, Raman spectroscopy, and hyperspectral imaging, are coupled with chemometric methods such as principal component analysis (PCA), partial least squares regression/discriminant analysis (PLS/PLS-DA), and artificial neural networks (ANNs). A representative case study on avocado cultivation demonstrates the application of DoE and agricultural statistics to identify key agronomic factors affecting quality-related attributes. In parallel, emerging portable, handheld, and miniaturised sensing technologies, including lab-on-a-chip platforms, are explored for rapid and potentially in-field analysis, as well as for applications in ready-to-eat foods, such as acrylamide detection in fried potatoes. Our integrated approach demonstrates how DoE and chemometrics can transform agricultural experimentation from empirical trial-and-error approaches toward systematic, predictive, and data-driven optimization, supporting improved food quality, authenticity assessment, resource efficiency, and sustainable agri-food production.

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Mapping Global Whole-Systems Adaptive Sustainability Strategies in Agri-Food Supply Chains: A Systematic Mapping Review

Megan Crockard

Agri-food sustainability faces a critical "implementation gap" where high-level policy fails to translate into effective, on-the-ground action. This gap is driven by a fragmented research landscape focusing on isolated supply chain segments rather than viewing the system as an interconnected whole.

To address these systemic failures, this PhD research applies a Whole Systems Approach (WSA) to develop an industry-backed conceptual sustainability toolkit. This specific phase executes a unique Systematic Mapping Review (SMR) to synthesise the global distribution and scope of data regarding whole-systems adaptive sustainability strategies across agri-food supply chains.

Registered on the Open Science Framework (DOI: 10.17605/OSF.IO/B2MAV), this study transfers traditional systematic mapping protocols from environmental and health sciences directly into agri-food supply chain management. Following PRISMA 2020 guidelines, the search strategy uses the Context, Intervention, Mechanism, and Outcome (CIMO) framework to map data across all food system actors. The search captures peer-reviewed academic literature across four core databases (Web of Science, Scopus, Embase, Science Direct) and grey literature from institutional repositories (FAO AGRIS, CGIAR, World Bank OKR, IFPRI eBrary) published between 2015 and 2026. Screening is managed via a dual-blind protocol in Rayyan.ai.

The systematic search produced a diverse dataset of 1,120 records, capturing 548 peer-reviewed academic papers and 572 grey literature reports managed in Zotero. Initial screening reveals that while sustainability is widely discussed, most research lacks concrete interventions, offering theoretical recommendations instead. To address this, the ongoing full-text thematic analysis is specifically targeting the remaining evidence base to isolate and extract documented, successful interventions. This process will map metadata on viable multi-stakeholder partnerships, collaborative risk-sharing, and measurable environmental, economic, or social outcomes.

By bridging academic databases with institutional repositories, this SMR establishes a comprehensive evidence base capturing real-world policy and industry discussions. A novel aspect of this research is the direct translation of this dataset into an interactive Evidence Gap Map (EGM) matrix. This highly visual tool crosses sustainability interventions against multi-dimensional outcomes, exposing over-researched clusters and critical knowledge voids.

These mapped global insights will facilitate targeted stakeholder engagement within the Northern Irish dairy industry to co-design the localised toolkit. Although initially focused on this regional case study, the final conceptual toolkit is intended to serve as a transferable methodological blueprint with the potential to be scaled and replicated across international agri-food supply chains facing similar implementation challenges.

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Tyrosinase-Mediated Cross-Linking of Rapeseed Proteins

Nora Jahn

Rapeseed proteins are promising sustainable food ingredients because they are a by-product of rapeseed oil production. However, due to limited techno-functional properties as well as undesirable flavor and color characteristics, they are currently used primarily as animal feed. Enzymatic cross-linking represents a promising strategy to modify protein functionality and improve their suitability for human food applications. Tyrosinase catalyzes the oxidation of tyrosine residues to reactive quinone intermediates, which may promote protein aggregation and cross-link formation.

To evaluate the cross-linking potential of tyrosinase towards rapeseed proteins, reaction conditions were first optimized and subsequently applied to the major rapeseed storage proteins cruciferin and napin, a mixture of both proteins, and a commercially available rapeseed protein isolate. Protein modifications were assessed using sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE), fluorescence

measurements, and liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis. SDS-PAGE analysis of tyrosinase-treated samples revealed increased smearing and decreased intensities of several protein bands compared with untreated controls, whereas only a few bands showed increased intensity following treatment. No distinct new high-molecular-weight bands were detected. Fluorescence measurements targeting tyrosine residues revealed lower fluorescence intensities in all tyrosinase-treated samples than in untreated controls, suggesting modification of tyrosine residues during enzymatic treatment. In contrast, no pronounced increase in dityrosine-related fluorescence was detected, except in napin samples. Untargeted LC-MS/MS peptide analysis confirmed the presence of several tyrosine modifications in enzyme-treated samples. However, the formation of intermolecular cross-links could not be confirmed. Together, these results indicate that tyrosinase treatment induces measurable changes in rapeseed proteins. However, the underlying mechanisms remain unclear and may involve protein modifications, intramolecular cross-linking and changes in protein solubility. Further work will focus on the development of data-processing workflows for the identification and localization of potential cross-links in rapeseed proteins.

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Development and analytical evaluation of thermally processed model precision-fermentation broth for casein production

Norbert Raak

Precision fermentation (PF) is an emerging technology to produce food proteins, but its commercial scalability is challenged by low product yields and complex downstream processing requirements, often leading to high costs. Specifically, systematic investigation of downstream processing remains limited, majorly due to the restricted availability of representative PF fermentation broths. This study therefore developed a model PF broth and applied a complementary analytical workflow to evaluate thermal cell disruption and the resulting protein and DNA characteristics.

Bacillus subtilis was selected as a model production organism and caseins as model food proteins, reflecting their importance in dairy-based foods. The model broth was subjected to heating at 90 °C under acidic and near-neutral pH conditions. UV–visible spectroscopy and bicinchoninic acid (BCA) analysis monitored bacterial lysis and protein release. Casein solubility was assessed following thermal treatment, while inductively coupled plasma (ICP) analysis was used to investigate the potential contribution of mineral components to casein behavior. SDS-PAGE characterized the protein profile, and DNA analysis assessed intact DNA following treatment.

Heating at 90 °C effectively promoted bacterial lysis, with the kinetics strongly dependent on pH. Under acidic conditions, no further increase in lysis was observed after approximately 30 min, indicating that a plateau had been reached. In contrast, near-neutral conditions required approximately 70 min to reach maximum lysis, corresponding to a 2.3-fold longer treatment time. Despite differences in bacterial lysis kinetics, casein solubility remained comparable under the two pH conditions. ICP analysis indicated the presence of calcium, which may contribute to the observed behavior of caseins during processing. SDS-PAGE showed that the bacterial protein fraction was predominantly composed of proteases, while the protein profile showed no substantial evidence of thermal denaturation at 90 °C. No intact DNA was detected following heat treatment, potentially due to thermal fragmentation.

Overall, the complementary analytical workflow provided insight into cell lysis, protein solubility, protein composition and DNA integrity during thermal processing of a model PF broth. The results support thermal treatment as a promising downstream processing strategy for casein production, particularly under acidic conditions where effective cell disruption was achieved in a shorter treatment time. More broadly, the model system provides a practical platform for analytical evaluation and optimization of downstream processing where representative PF broths are not readily available. The approach may support future assessment of processing-related quality and safety characteristics of precision-fermented food proteins.

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Proactive Bacterial Load Detection for Dairy QA: A process optimization tool

Pablo Bondia

Dairy quality assurance today is reactive: without real-time information on bacterial load, processors act blind, forced to shut down and clean processing lines every ~6 hours purely as a safety precaution rather than in response to actual contamination data. Traditional lab-based bacterial testing takes days, offering no help in the moment. Wren Bioscience, a Danish deeptech spinout from DTU Bioengineering, replaces this blind precaution with real bacterial insight: a proprietary sample-preparation protocol paired with a lateral flow biosensor and digital reader detects bacterial load directly in milk in minutes. This turns bacterial testing into a process optimization tool; dairies can extend run times based on actual bacterial data instead of fixed schedules, fine-tune CIP cycles, and catch contamination early, cutting the food waste driven by late detection and unnecessary precautionary shutdowns. By making bacterial insight fast and actionable, Wren shifts dairy QA from reactive compliance to proactive, data-driven process control.

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Common lactic-acid bacteria as natural detoxifiers of the zearalenone mycotoxin - HPLC and NIR spectroscopy study

Paulina Gluzińska

Zearalenone is a widely spread mycotoxin produced by several Fusarium species that poses a significant safety concern both during agricultural production and food processing. Due to high resistance to chemical and physical factors such as high temperature, mycotoxins pose many challenges to traditional food safety methods, thus proving the need to find alternatives (Ryu et al., 2003).

The aim of this study was to evaluate the detoxification efficiency of zearalenone using various strains of lactic acid bacteria under model conditions and to develop a rapid detection model. Thirty strains of lactic acid bacteria, both live and dead, were used in the experiment, incubated with a standard concentration of the mycotoxin, and compared with a control sample. The identification of ZEA by HPLC was carried out in accordance with own protocol. Subsequently the samples' spectral data was recorded in the NIR range (12 500–4 000 cm^{-1}) in transitions mode using a Bruker MPA spectrometer (Bruker, Ettlingen, Germany) equipped with OPUS 7.2 software. The optimisation of spectral data included pre-processing methods consisting of smoothing and standard normal variate (SNV). Principal Component Analysis (PCA) was performed on the NIR spectra to identify interrelationships between the samples. Multivariate data analysis was conducted using The Unscrambler version 9.7 (Camo, Norway).

The PCA modelling effectively distinguished samples according to cell viability and demonstrated high classification performance of bacteria when combined with the HPLC analysis. The study revealed the high performance of some LAB strains (approx. 70% reduction using L. reuteri), as well as several strains showing unexpectedly higher detoxification in the dead-cell state, suggesting that structural cell-wall components may dominate adsorption mechanisms (Zhang et al., 2019). Overall, these results highlight the potential of common lactic acid bacteria as natural zearalenone detoxifying agents and demonstrate the value of combining HPLC with rapid, nondestructive near-infrared (NIR) spectroscopy to monitor the detoxification process. This research was funded by The National Centre for Research and Development (NCBR), grant number FENG.01.01-IP.01-A0WG/25-00

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Influence of salt type and concentration on the physical stability of OSA-starch based vegan mayonnaise

Rasmus Mikkelsen

Mayonnaise is a high fat oil-in-water emulsion traditionally stabilized with egg yolk. With increasing demand for vegetarian and vegan alternatives, egg yolk can be substituted with octenyl succinic anhydride (OSA)-modified starch. However, starch-based mayonnaise can undergo structural changes during storage including aggregation, and gelation related to starch retrogradation. Some evidence suggests that salt content can affect starch retrogradation. The aim of the study was therefore to evaluate the influence on salt concentration and type on the physical and structural stability of vegan mayonnaise. NaCl was tested in concentrations between 0 and 3.0wt% while KCl, and CaCl2 were tested in 0.6wt%, 1.2wt% and 2.4wt% in 70% rapeseed oil mayonnaise stabilized with 0.6wt% OSA-modified potato starch. The samples were stored for three months, during which droplet size, zeta potential, cryo-SEM, rheology, and a simple smear test were performed. After 10 days, mayonnaise containing CaCl2 showed significantly larger oil droplets than the other emulsions together with large standard deviations suggesting reduced emulsion stability. This might be related to the presence of divalent Ca2+ ions promoting droplet aggregation or coalescence. The smallest droplet size was observed with 1.2wt% NaCl, however no clear relationship between salt concentration and droplet size was observed. Furthermore, substituting NaCl with KCl had no apparent effect on the droplet size. No visible phase separation or creaming was observed for any mayonnaise during storage, indicating generally high emulsion stability.

In contrast, large differences in overall structure were observed using the smear test. NaCl showed an inverse parabolic relationship with structural stability, where the best stability was observed with 1.2wt% NaCl. At lower concentrations starch retrogradation was associated with gel and aggregate formation, while concentrations above 1.2wt% resulted in grainy structure. For KCl and CaCl2 increasing salt concentration generally reduced aggregation although CaCl2 resulted in a thinner structure at higher concentration, possibly due to the cation hindering a starch network formation. The structural changes became more severe during storage.

Notably, the observed structural differences did not correlate with rheological measurements, and were not apparent in cryo-SEM images, potentially because the weak starch network was disrupted during sample preparation or measurement.

The results show that salt type and concentration strongly influence the structural stability of starch-based mayonnaise. Further, the results also indicate that the conventional measurements of emulsion stability can fail to capture important storage-induced structural changes. Therefore, new analytical methods that better correlate with the visual observations of starch-based mayonnaise are needed.

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Linking Physicochemical Indicators to Functional and Microbial Stability of Liquid Egg White during Cold Storage following Microwave–Ultrasound–Pectin Processing

Sadaqat Ali

Liquid egg white (LEW) is widely used in aerated food systems, yet maintaining its functional and microbial quality during refrigerated storage remains challenging. This study investigated an integrated analytical framework for monitoring physicochemical, functional, freshness, and microbiological changes in LEW following microwave (MW), ultrasound (US), and pectin-assisted processing during cold storage. Five treatment groups were evaluated: untreated LEW (EW), ultrasound-treated LEW at 600 W (U600), ultrasound–pectin-treated LEW (U600–P), microwave (300 W)–ultrasound (600 W)-treated LEW (M300–U600), and microwave–ultrasound–pectin-treated LEW (M300–U600–P). All samples were pasteurized at 57 °C for 3 min and stored at 4 °C for 35 days. Foaming capacity (FC) and stability (FS), ζ-potential, particle size, surface hydrophobicity, and total volatile basic nitrogen (TVB-N) were monitored at 7-day intervals. Microbial quality was assessed by total colony count (TCC), and Pearson correlation analysis was used to evaluate relationships among measured quality indices. All samples exhibited significant deterioration in functional and quality characteristics during storage; however, M300–U600–P consistently showed the greatest functional retention. FC of untreated LEW decreased from 137.7 ± 5.0% to 85.5 ± 2.93%, whereas M300–U600–P maintained significantly higher FC, decreasing from 253.33 ± 3.3% to 222.2 ± 6.93% after 35 days. Improved foaming performance was associated with enhanced electrostatic repulsion, controlled aggregation, and altered interfacial protein behavior, as reflected by ζ-potential, particle size, and surface hydrophobicity. Based on the regulatory TCC limit of 3×10^4 CFU/mL, untreated LEW exhibited an estimated shelf life of approximately 24 days, whereas M300–U600–P extended it to approximately 33 days. These findings demonstrate that integrating physicochemical, functional, freshness, and microbiological measurements provides a comprehensive approach for characterizing storage-induced quality deterioration in LEW. The identified analytical relationships may support quality monitoring and evaluation of emerging processing strategies for refrigerated liquid egg products.

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Microstructure of Bread: Effects of Formulation and Emerging Processing

Saroj Katwal

The microstructure of bread crumb is an important quality characteristic that directly influences the physical and textural properties. Therefore, to gain a deeper understanding of how formulation and processing conditions affect crumb development, the microstructure of crumb structure is necessary for a quantitative description of the structural changes during baking.

This work aims to investigate the microstructure (crumb pore structure) of bread produced under different formulation and processing conditions, with particular emphasis on the effects of chickpea flour substitution and emerging processing. To investigate the effect, Response Surface Methodology (Central Composite Design) was applied for the baking experiment. For analyzing the crumb structure, cross-sectional images of all bread samples were acquired using multispectral imaging (Video meter). Python was used for image processing, where the images were converted from RGB to greyscale and then into binary images, allowing segmentation between pore and solid regions of the crumb. A defined region of interest was selected for each sample, and individual pores were identified and quantified with image scale calibrated using a reference grid. The bread crumb structure was characterized based on porosity (φ), pore distribution, average pore diameter (d_av), and maximum pore diameter (d_max). Results indicated that formulation significantly affected the product of bread crumb structure as well as physical properties were significantly influenced by structural changes during the baking. Chickpea concentration effects were particularly important for the porosity and maximum pore diameter, and developed models showed good predictive performance for the porosity ($R^2 = 0.861$) and maximum pore diameter ($R^2 = 0.821$), Further, differences in crumb porosity were observed between emerging technology and conventional baking, indicating that baking method affected pore development. The image processing

provided a deeper insight into microstructure changes during baking, which can be used to better understand the relationship between formulation, processing conditions, and the structural quality of the final product.

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Effect of maturation time on industrial- and quality-related parameters of cooked and peeled Pandalus borealis prawns

Signe Vangsgaard

The industrial production of cooked and peeled (C&P) cold-water prawns (Pandalus borealis) requires a maturation step in which whole, raw prawns, either fresh or thawed, are immersed in a salt-based brine. This process promotes shell loosening and is essential for achieving high yield and peelability during the subsequent mechanical peeling of cooked prawns. In this study, the effect of maturation time (0-24 hours) on key industrial and quality-related parameters was investigated, including yield, mechanical peelability, physicochemical properties and color-quality assessed using a trained and validated hyperspectral imaging model developed for this purpose.

Maturation time had a highly significant effect on all measured parameters. Maturation periods shorter than 8 hours resulted in poor yield, mechanical peelability and color-quality. While neither yield nor color-quality changed significantly beyond 8 hours of maturation, peelability continued to improve throughout the entire 24-hour period. All physicochemical properties exhibited significant changes after 4 hours of maturation; however, pH was the only parameter that differed significantly across all tested maturation times. These findings demonstrate the successful application of a trained and validated hyperspectral imaging model for color-quality determination and highlight the critical role of maturation time in achieving optimal product quality in the industrial C&P prawn production.

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Targeted Phenolic Profiling of Australian Native Lemon Myrtle (Backhousia citriodora) and River Mint (Mentha australis) Following Microencapsulation: Insights into Compound-Specific Retention

Synne Hylen Røsten

Phenolic compounds are important bioactive constituents of botanical extracts but are susceptible to degradation during food processing. Australian native aromatic plants, including lemon myrtle (Backhousia citriodora, LM) and river mint (Mentha australis, RM), are promising sources as a phenolic-rich functional ingredient. Spray-drying microencapsulation offers a potential strategy to retain these compounds and develop stable functional powders. This study investigated the compound-specific encapsulation of phenolics in LM and RM extracts using maltodextrin and maltodextrin:gum Arabic carrier systems.

Extracts were spray dried using maltodextrin:gum Arabic ratios of 1:0, 3:1 and 1:1. Targeted multiple reaction monitoring (MRM) analysis was performed using a Waters ACQUITY™ I-Class UPLC coupled to a Xevo™ TQ-S micro triple-quadrupole mass spectrometer. A panel of 20 phenolic compounds was used to characterise the extracts and evaluate compound retention following encapsulation. Distinct phenolic profiles were observed between LM and RM, with p-coumaric acid, chrysin and myricetin not detected in either species, while catechin, epicatechin, hesperidin, sinapic acid and gentisic acid were not detected in RM. Gallic acid and rosmarinic acid were selected as representative biomarkers for LM and RM, respectively.

Gallic acid showed high encapsulation efficiency (EE) in LM, ranging from approximately 78–85%, with the maltodextrin-only formulation providing the highest EE. Rosmarinic acid exhibited higher EE overall (approximately 88–96%) in RM, with the 1:1 maltodextrin:gum Arabic formulation providing the highest EE. These results demonstrate compound- and formulation-specific differences in phenolic encapsulation and highlight the influence of carrier composition on the retention of individual phenolic compounds.

These findings demonstrate the value of targeted LC–MS/MS MRM for characterising phenolic profiles and evaluating compound-specific retention during microencapsulation. The results support the potential of lemon myrtle and river mint as Australian native sources of phenolic-rich functional ingredients and provide insight into the optimisation of carrier systems for preserving bioactive phenolic compounds during food processing.

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Hyperspectral imaging and chemometrics for monitoring formulation, processing, and homogeneity in hybrid sausages

Victor Cardoso

Hybrid sausages are emerging as sustainable alternatives that combine plant-based ingredients and meat, aiming to create more sustainable foods [1]. This approach also enables the upcycling of food by-products, whose fermentation can enhance nutrient availability as well as functional and gastronomic properties [2]. Fermenting brewer’s spent grains (fBSG), a major by-product of beer production, represents an attractive option to support the circular economy while increasing dietary fibre in hybrid products [2]. In early-stage product development, however, it is often challenging to understand nutrient and ingredient distribution, which directly affects sensory perception and consumer acceptance. In this context, hyperspectral imaging (HSI) in the near- infrared (NIR) region was used for comprehensive characterization across multiple stages of the production chain [3]. Raw ingredients, sausage batter, and sausages from six formulations with varying levels of meat and fBSG were analysed using a Specim FX17 line-scanner (900-1700 nm). Chemometric tools such as principal component analysis, ANOVA-simultaneous component analysis, and partial least square regression were employed to characterize raw ingredients, formulations and processes. A pixel-wise approach allowed us to obtain spatial distribution maps of ingredients and macronutrients, revealing regions of uneven distribution of fat, formulation homogeneity, microstructure, which was quantitatively assessed by grey-level co-occurrence matrix algorithm. Overall, the results demonstrate the potential of NIR-HSI as a rapid, non-destructive tool for multi-stage analysis and to guide the design of new hybrid meat products. As perspectives, alternative illumination sources, such as LED arrays and supercontinuum lasers, have been showing promising results to replace classical halogen lamps in food analysis using HSI.

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Machine Learning Models for Predicting Extent of Conversion in Food Extrusion

Yoganivas Balamurugan

A food extruder subjects raw materials to a combination of thermal and mechanical forces, leading to structural, chemical, and nutritional transformations. During extrusion, starch undergoes gelatinization and melting, proteins denature in response to thermal and mechanical stresses, and heat-sensitive vitamins are degraded. While these transformations have been studied individually, no comprehensive model currently exists to predict the extent of conversion across food matrices. To address this need, machine learning models were trained to predict the degree of transformation of diverse food compositions subjected to extrusion, using barrel temperature, residence time, shear stress, and substrate identity as input variables. A dataset compiled from the literature, comprising observations such as starch gelatinization/melting, protein denaturation, and vitamin degradation, was used to train and compare four machine learning approaches: multiple linear regression, polynomial regression, artificial neural networks, and random forests. Hyperparameters and polynomial degree were selected via 5-fold cross-validation. Model metrics such as RMSE, MAE, and R2 were used to evaluate the prediction performance of the models. Random forest achieved the best performance for predicting the extent of conversion in an extruder, followed by polynomial regression, the neural network, and multiple linear regression, which performed the weakest. This ranking was consistent with 5-fold cross-validation, indicating that the observed performance differences were driven by the models' ability to capture underlying relationships rather than by variability arising from a single train-test split. Machine learning successfully captured the non-linear effects of extrusion conditions on food transformation behavior, highlighting its potential as a predictive tool for quantifying extrusion conditions-induced conversions and supporting data-driven design and optimization of extrusion operation. This approach could facilitate the development of food product formulations and process conditions that minimize undesirable transformations, such as excessive protein denaturation and vitamin degradation.

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Mapping the Formulation Space of 1000 Plant-Based Powder Blends with NIR Spectroscopy

Ziyun Zhong

Plant-based food formulation increasingly relies on powdered ingredients from novel botanical sources and processing backgrounds to achieve targeted nutritional and functional properties. However, variability in composition and physicochemical characteristics makes these powder blends challenging to characterize. Near-infrared (NIR) spectroscopy provides a rapid and non-destructive approach for composition analysis, but robust calibration requires datasets that capture realistic formulation diversity, which remain scarce. This study introduces an NIR dataset of plant-based powder blends, designed to cover a broad and systematically varied formulation space, and to support model development for mixed powder systems.

This dataset contains 1000 unique powder blends. Each blend was prepared from one to three proteins, one starch, and one fibre. The protein sources came from eight suppliers, including three soy, three pea, and two faba bean proteins. The starch types were pea, corn, and potato starch, and the fibres were pea and oat fibre. Ingredient ratios were generated through stratified random sampling. Each blend was measured in triplicate by NIR diffuse reflectance spectroscopy across 350–2500 nm, yielding 3000 spectra. Six proximate targets were determined by reference methods: protein (N × 5.7), starch, dietary fibre, fat, moisture, and ash. PLSR was applied to predict the composition targets.

Descriptive analysis confirmed well-distributed compositional ranges, with protein ranging 9.6–74.8 wt% (mean ± SD: 44.5±19.1), starch 4.7–73.0 wt% (26.9±16.4), dietary fibre 1.8–42.7 wt% (12.1±8.0), fat 0.4–8.2 wt% (3.41±1.80), moisture 5.6–17.5 wt% (9.35±2.34), and ash 0.8–6.1 wt% (3.13±1.11). A strong negative protein–starch co-dependence ($r = -0.90$) reflected the formulation closure constraint. Within-replicate spectral variability was 10–50 times lower than between-blend variability, confirming negligible noise. Principal component analysis revealed that SNV correction was essential to distinguish

protein crop-source clusters. PLSR achieved high prediction accuracy for protein (R^2 = 0.997, RMSEP = 1.12 wt%), fat (R^2 = 0.995, RMSEP = 0.14 wt%), starch (R^2 = 0.992, RMSEP = 1.48 wt%), ash (R^2 = 0.990, RMSEP = 0.12 wt%), moisture (R^2 = 0.988, RMSEP = 0.27 wt%), and dietary fibre (R^2 = 0.979, RMSEP = 1.29 wt%).

In conclusion, this 1000-blend NIR dataset is among the largest and most systematically designed plant-protein NIR calibration sets reported to date. The consistently strong PLSR performance across all six proximate targets demonstrated that the dataset supports reliable multicomponent composition modelling. This dataset also provides a foundation for further developing transferable prediction models for plant-based food formulation.

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