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Time-resolved metabolomics of Murrah buffalo milk yoghurt reveals fermentation- and storage-dependent metabolite dynamics with insights into bioactive potential

By

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Abstract

This study applied LC-MS/MS-based metabolomics to profile biochemical changes during fermentation and storage (raw, 0 h to 28 d). A total of 173 metabolites were annotated, with 172 showing significant differential expression (p-adjusted < 0.05), mainly organic acids, fatty acyls, alkaloids, nucleic acids, and carbohydrates. PLS-DA revealed distinct temporal clustering, driven by 88 key metabolites (VIP > 1). Early stages (0-48 h) showed increased levels of metabolites such as 3-phenyllactic acid and cyclo prolyl-threonine reflected active fermentation, while potential spoilage-related compounds like N-formylmethionine emerged after 7 days. Pathway enrichment indicated shifts in purine, nicotinate, and amino acid metabolism. Several metabolites, including succinic acid, threonine, phenylacetaldehyde, 3-phenyllactic acid, cyclo prolyl-threonine, and raffinose exhibited significant temporal changes and were associated with key biochemical processes during yoghurt maturation. Molecular docking of storage-related metabolites like cyclomethyl tryptophan, delta-gluconic, delta-lactone, and xanthine predicted potential antioxidant, antihypertensive, and antidiabetic bioactivities, supporting their relevance in functional food development.

Keywords

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Data availability statement

Data will be made available on request.

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