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

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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, δ -gluconic, δ -lactone, and xanthine predicted potential antioxidant, antihypertensive, and antidiabetic bioactivities, supporting their relevance in functional food development. © 2026 Elsevier Ltd.

Author keywords

Buffalo milk; Cold storage; LC–MS/MS; Metabolomic; Yoghurt

Indexed keywords

MeSH

Animals; Buffaloes; Fermentation; Food Storage; Metabolomics; Milk; Molecular Docking Simulation; Tandem Mass Spectrometry; Yoghurt

Engineering controlled terms

Bioactivity; Biomolecules; Fermentation; Food storage; Metabolites; Nucleic acids

EMTREE drug terms

3 phenyllactic acid; alkaloid derivative; aromatic compound; atrolactic acid; carbohydrate; carboxylic acid; carboxylic acid derivative; cycloprolylthreonine; formylmethionine; glibenclamide; heterocyclic compound; lactone; nicotinic acid; nucleic acid; proline derivative; purine; raffinose; succinic acid; threonine; tryptophan; unclassified drug; xanthine; yoghurt; yoghurt

Engineering uncontrolled terms

3-phenyllactic acid; Bioactives; Biochemical changes; Buffalo milk; LC-MS-MS; Lc.ms/ms; Metabolomics; Milk yoghurt; Time-resolved; Yogurt

EMTREE medical terms

amino acid metabolism; antidiabetic activity; antihypertensive activity; antioxidant activity; Article; biological activity; buffalo milk; controlled study; cryopreservation; fermentation; functional food; liquid chromatography-mass spectrometry; metabolite; metabolomics; molecular docking; purine metabolism; storage temperature; animal; buffalo; chemistry; fermentation; food storage; metabolism; metabolomics; microbiology; milk; tandem mass spectrometry

Engineering main heading

Cold storage

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atrolactic acid	515-30-0
formylmethionine	4289-98-9
glibenclamide	10238-21-8
lactone	1338-03-0

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Funding details

Details about financial support for research, including funding sources and grant numbers as provided in academic publications.

Funding sponsor	Funding number	Acronym
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