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Summary

MACHINE LEARNING-DRIVEN MULTIMODAL RAMAN SPECTROSCOPY AND METABOLOMICS SIGNATURES IDENTIFY NON-INVASIVE BIOMARKERS OF INTESTINAL BARRIER INTEGRITY AND CLINICAL OUTCOMES IN INFLAMMATORY BOWEL DISEASE

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Machine learning integration of Raman spectroscopy and metabolomics accurately predicts intestinal barrier impairment and 12-month major adverse outcomes in IBD using non-invasive plasma biomarkers.

KEY POINTS

- In 70 IBD patients (42 Crohn's disease, 28 ulcerative colitis), multimodal integration of plasma Raman spectroscopy, tissue Raman spectroscopy, and untargeted metabolomics predicted major adverse outcomes at 12 months with 74% accuracy and AUC 0.84.
- Multimodal integration outperformed single modalities for predicting epithelial barrier impairment (accuracy 77%, AUC 0.84) and vascular barrier impairment (accuracy 76%, AUC 0.80) as assessed by probe-based confocal laser endomicroscopy and endocytoscopy.
- Barrier impairment was observed in 19/42 patients (45%) by endocytoscopy and 27/36 (75%) by probe-based confocal laser endomicroscopy, while major adverse outcomes occurred in 31/70 (44.3%) patients.
- Pathway enrichment analysis identified arginine and proline metabolism linked to epithelial barrier dysfunction in ulcerative colitis (pFDR 0.008), and tryptophan, citrate cycle, and glutamate metabolism linked to vascular barrier dysfunction in Crohn's disease (pFDR 0.03).
- Multimodal machine learning integration enables disease-specific barrier endotype stratification and prediction of clinical trajectories, supporting precision management strategies in IBD.

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