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Machine Learning Based Urinary Metabolome Profiling to Differentiate Primary Glomerular Diseases

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Objectives : Glomerular diseases (GDs) comprise a biologically heterogeneous group of kidney disorders that frequently present with overlapping clinical manifestations, thereby limiting non-invasive subtype differentiation and reinforcing reliance on kidney biopsy. Although metabolomics provides an integrated view of disease-associated biological processes, its utility for subtype differentiation and molecular stratification across GDs remains insufficiently explored.
Methods : Urinary metabolomic profiling was conducted in biopsy-confirmed GDs (IgA nephropathy [IgAN], focal segmental glomerulosclerosis [FSGS], minimal change disease [MCD], membranous nephropathy [MN]) from a nationwide multicenter cohort across six tertiary hospitals in Korea, including a discovery set (n = 1,060) and an independent validation set (n = 550). Metabolites were quantified using an IVDr-based ^{1}H NMR platform. Machine learning–based feature selection identified an eight-metabolite panel for disease discrimination, which was externally validated in the independent cohort.
Results : Urinary metabolomic profiles differed across glomerular disease subtypes, providing additional metabolic characterization beyond conventional clinical factors. Machine learning–based feature selection yielded eight candidate metabolites for disease discrimination. The eight-metabolite panel achieved excellent discrimination between controls and GDs (area under the receiver operating characteristic curve [AUC] 0.983) and demonstrated strong subtype classification for IgAN (AUC 0.829), MN (0.842), and MCD (0.823), whereas performance was comparatively limited for FSGS (0.681). Overall multiclass performance was robust (macro-average AUC 0.831). Performance also remained stable when diabetic nephropathy was included as a disease control (macro-average AUC 0.850). Consistent performance was observed in the independent external validation cohort
Conclusions : Urinary metabolomic profiling identifies subtype-associated metabolic signatures across glomerular diseases. These findings suggest the potential of machine learning–derived metabolite panels as a complementary non-invasive approach to disease stratification.

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Figure. Receiver operating characteristic (ROC) curves of the Random Forest classifier in discovery cohort