High-throughput DeepPRM-Stellar proteomics coupled with machine learning enables precise quantification of atherosclerosis-stroke progression biomarkers and risk prediction

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‡:This study is dedicated to the memory of Professor Pengyuan Yang (1949-2021)

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Figure S1

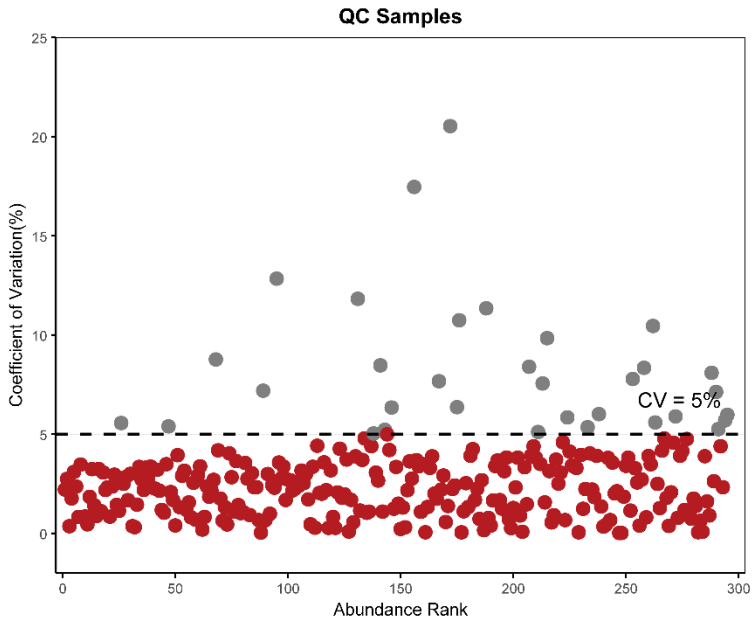


Figure S1. Quality control assessment of peptide measurements in PRM assays. Scatter plot showing coefficient of variation (CV) versus abundance rank for all QC sample measurements (n = 3 technical replicates per peptide). Each point represents an individual peptide measurement, with red points indicating high reproducibility (CV < 5%) and gray points showing greater variability (CV ≥ 5%). The dashed line at CV = 5% marks the acceptable variation threshold, with 90% of measurements demonstrating high reproducibility (red points clustered below the threshold line). The stable CV distribution across the full abundance range (0-300) confirms consistent instrument performance.

Figure S2

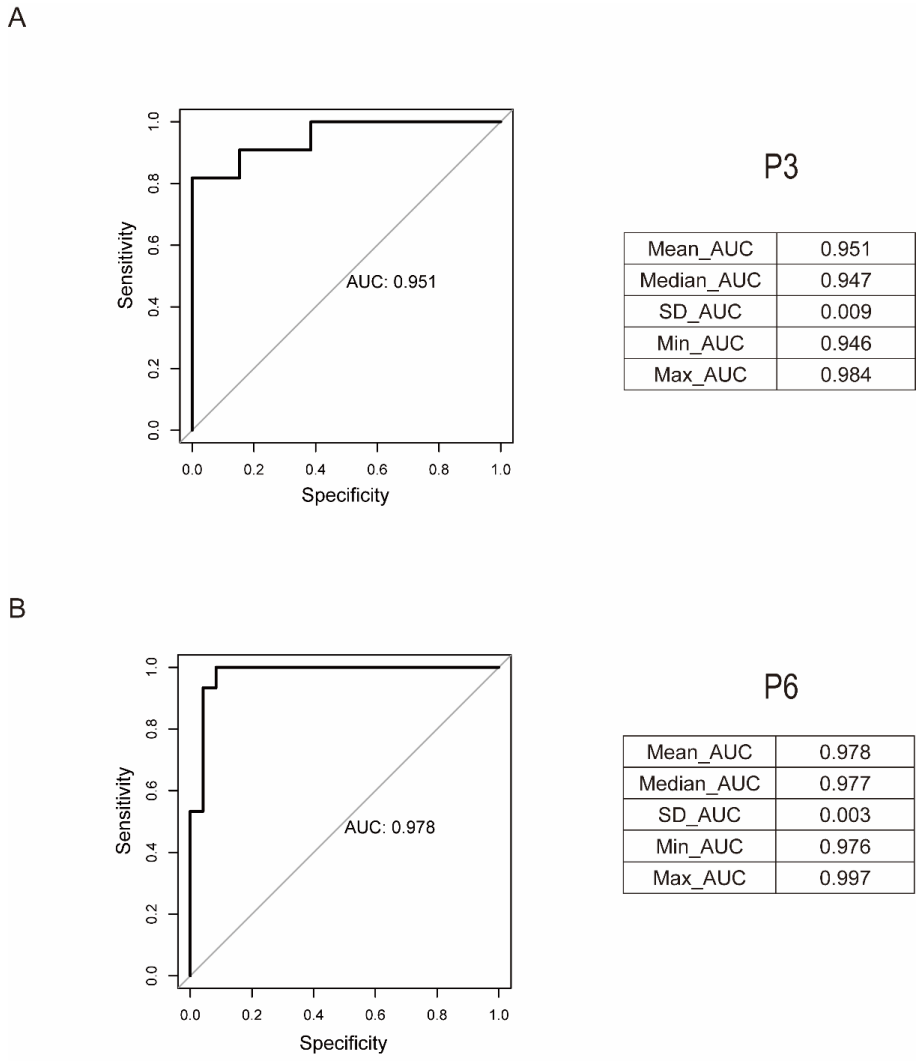


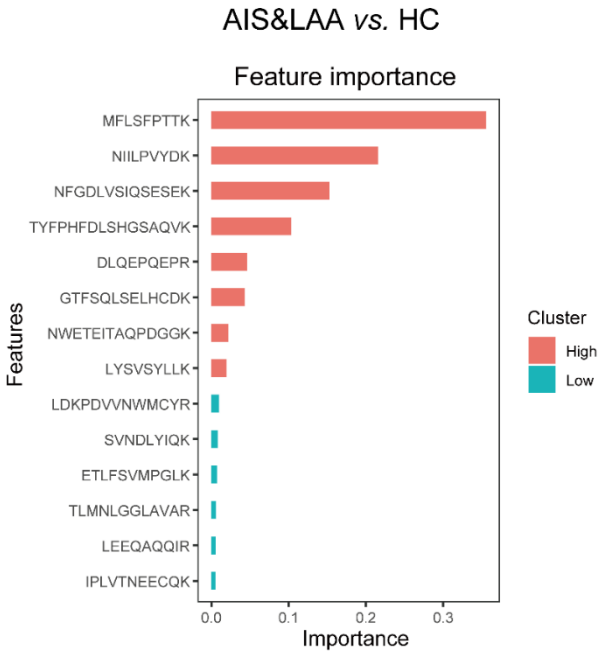
Figure S2. Model performance evaluation using Leave-One-Out Cross-Validation (LOOCV).

A). ROC curve for AIS vs LAA classification (*n* = 24). The black solid line shows the model performance (AUC = 0.951), with the diagonal representing random guessing (AUC = 0.5). The right-side table summarizes AUC statistics from LOOCV iterations: Mean_AUC = 0.951, Median_AUC = 0.947, SD_AUC = 0.009, Min_AUC = 0.946, Max_AUC = 0.984.

B). ROC curve for AIS&LAA vs HC classification (*n* = 39, AUC = 0.978). The table lists LOOCV results: Mean_AUC = 0.978, Median_AUC = 0.977, SD_AUC = 0.003, Min_AUC = 0.976, Max_AUC = 0.997. All models were trained using XGBoost .

Figure S3

A



B

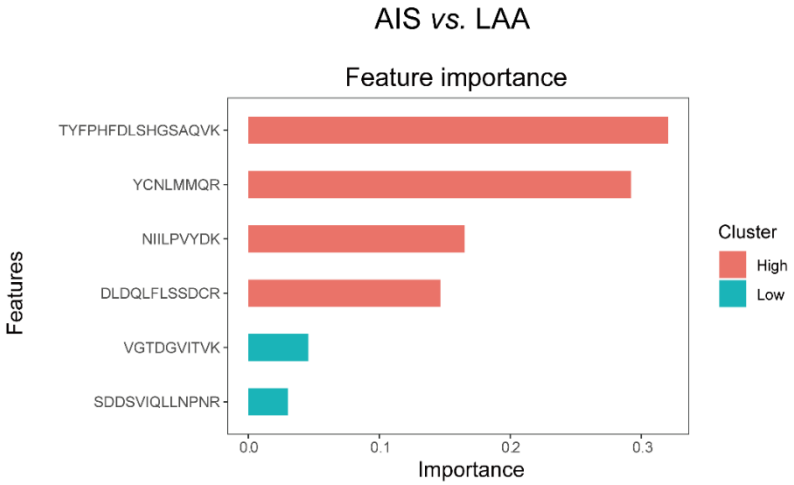


Figure S3. Feature importance analysis of candidate biomarkers.

A). Feature importance ranking for distinguishing AIS&LAA from healthy controls (HC). Proteins are sorted by their Cover-based importance scores from XGBoost.

B). Feature importance ranking for distinguishing AIS from LAA subtypes. In both panels, features are color-coded by their relative importance (red: high; blue-green: low).