

Supplementary Tables and Figures

Table S1. Optimal hyperparameters of the SVM and RF models selected by grid search

Model	Modality	PCA dim.	Kernel	C	γ	Trees	Max depth	Min leaf
SVM	LIBS	50	linear	1	scale	–	–	–
SVM	Raman	30	linear	10	scale	–	–	–
SVM	Fusion	30/15	rbf	1	0.01	–	–	–
RF	LIBS	50	–	–	–	200	None	1
RF	Raman	50	–	–	–	200	20	2
RF	Fusion	30/15	–	–	–	200	20	2

Note: for the fusion models, the PCA dimensions are reported as LIBS branch / Raman branch. “None” means that no explicit depth limit was imposed.

Table S2. Architecture of the dual-stream 1D-CNN

Branch	Layer	Kernel size	Output channels	Stride	Output shape
LIBS / Raman (same topology)	AvgPool1d (pre-downsampling)	4	1	4	$1 \times (L/4)$
	Conv1d + BN + ReLU (stem)	7	32	2	$32 \times (L/8)$
	ResBlock (layer1)	3	64	2	$64 \times (L/16)$
	ResBlock (layer2)	3	128	2	$128 \times (L/32)$
	ResBlock (layer3)	3	256	2	$256 \times (L/64)$
	AdaptiveAvgPool1d	–	256	–	256×1
	Auxiliary FC head	–	6	–	6
Fusion	Concatenate	–	512	–	512
	FC(512→128) + ReLU + Dropout(0.4) + FC(128→6)	–	6	–	6

Note: L denotes the raw input length. Each residual block contains two Conv1d(kernel = 3)–BN–ReLU layers with an identity skip connection. The LIBS and Raman branches share the same topology but have independent parameters.

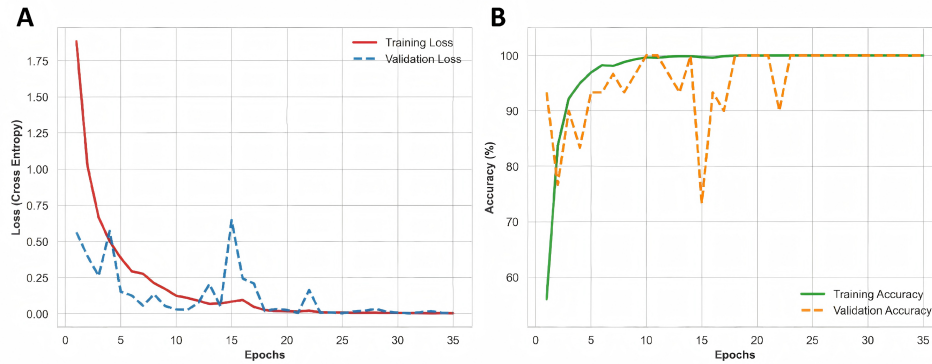


Figure S1. Training and validation curves of the fused dual-stream 1D-CNN. (A) Cross-entropy loss over training epochs for the training set (solid red) and validation set (dashed blue). (B) Classification accuracy (%) over training epochs for the training set (solid green) and validation set (dashed orange).

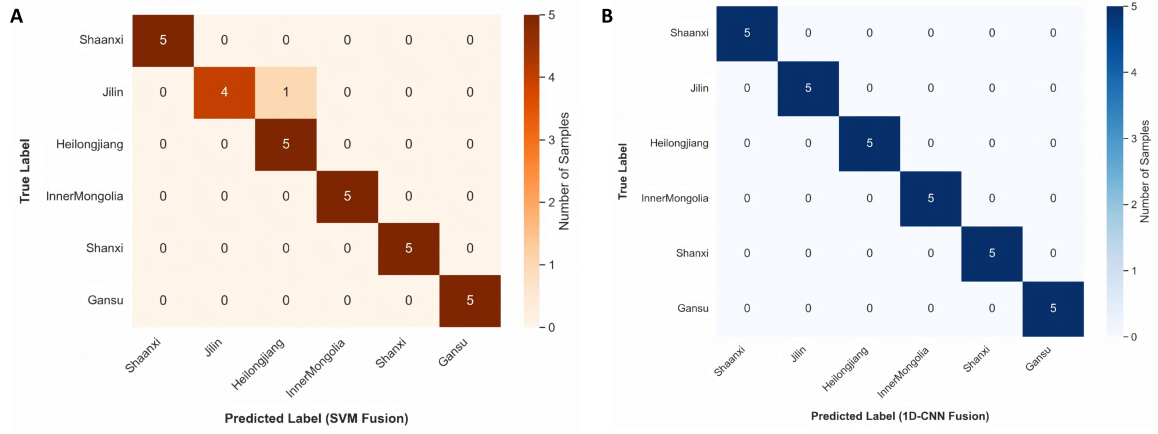


Figure S2. Representative confusion matrices on the external test set. (A) Confusion matrix of the fused SVM model (seed = 42). (B) Confusion matrix of the fused dual-stream 1D-CNN model (seed = 42).