Validation metrics:

The classification performance measures used in our study are listed below:

Parameter	Evaluation focus	Definition
Accuracy_i	Effectiveness of a classifier for i-th class	$\frac{\mathbf{TP_i + TN_i}}{\mathbf{TP_i + TN_i + FN_i + FP_i}}$
Sensitivity_i $/\text{Recall}_i$	Effectiveness of a classifier to identify positive labels for i-th class	$\frac{\mathbf{TP_i}}{\mathbf{TP_i + FN_i}}$
Specificity_i	Effectiveness of a classifier to identify negative labels for i-th class	$\frac{\mathbf{TN_i}}{\mathbf{TN_i + FP_i}}$
Precision_i	Class agreement of the data labels with the positive labels for i-th class	$\frac{\mathbf{TP_i}}{\mathbf{TP_i + FP_i}}$
$\text{F1} - \text{Score}_i$	Relations between positive labels and those given by a classifier for i-th class	$\frac{\mathbf{2 \times Precision_i \times Sensitivity_i}}{\mathbf{Precision_i + Sensitivity_i}}$
Accuracy_m	The average per-class effectiveness of a classifier	$\frac{\sum_{\mathbf{i=1}}^{\mathbf{l}}(\frac{\mathbf{TP_i + TN_i}}{\mathbf{TP_i + FN_i + FP_i}})}{\mathbf{l}}$
Sensitivity_m $/\text{Recall}_m$	Effectiveness of a classifier to identify class labels if calculated from sums of per-category decisions	$\frac{\sum_{\mathbf{i=1}}^{\mathbf{l}} \mathbf{TP_i}}{\sum_{\mathbf{i=1}}^{\mathbf{l}}(\mathbf{TP_i + FN_i})}$
Specificity_m	The average per class effectiveness of a classifier to identify negative labels	$\frac{\sum_{\mathbf{i=1}}^{\mathbf{l}} \mathbf{TN_i}}{\sum_{\mathbf{i=1}}^{\mathbf{l}}(\mathbf{TN_i + FP_i})}$
Precision_m	Agreement of the data class labels with those of a classifiers if calculated from sums of per-category decisions	$\frac{\sum_{\mathbf{i=1}}^{\mathbf{l}} \mathbf{TP_i}}{\sum_{\mathbf{i=1}}^{\mathbf{l}}(\mathbf{TP_i + FP_i})}$

$\mathrm{F1-Score_m}$	Relations between data's positive labels and those given by a classifier based on a per-class average	$\boldsymbol{\frac{2 \times Precision_m \times Sensitivity_m}{Precision_m + Sensitivity_m}}$

l is the number of categories. True positive (TP_i): Spectral data belong to the i-th category which is correctly identified; false positive (FP_i): Spectral data which do not belong to the i-th category, incorrectly identified; true negative (TN_i): Spectral data which do not belong to the i-th category, correctly identified; false negative (FN_i): Spectral data belong to the i-th category, incorrectly identified.