Deep learning for MALDI-MSI: towards a common framework for transferable tissue diagnostics

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github.com/patmjen/maldi_dl

Summary

This work presents a deep learning pipeline for MALDI MSI analysis of human tissue samples, focusing on spectrum classification.

- We evaluate on three **MALDI datasets from different clinical sources**. Task: classify the spectra from different tissue types.
- Based on 3-fold cross validation, we report test accuracy, balanced accuracy and F1-score computed on a per-spectrum and per-tissue sample basis.
- **Without changing hyperparameters**, we achieve promising results on all datasets. Our pipeline is open source, see QR code. We hope it can serve as a starting point for future research.
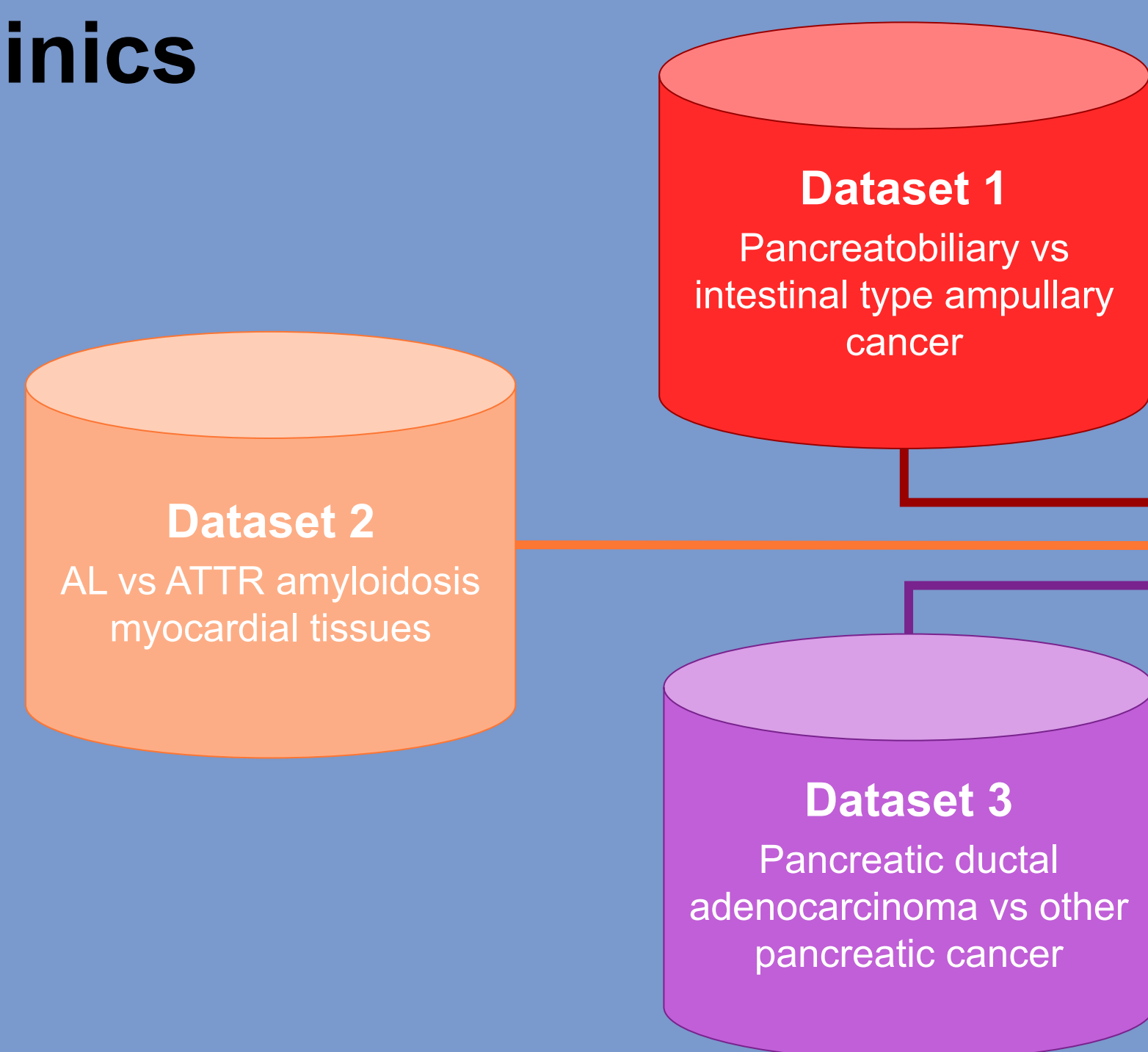
Datasets

We apply baseline removal, normalization, and downsampling to 0.2-0.3 Da bins. **No peak picking or other reduction was applied**.
Dataset 1: Pancreatobiliary vs. intestinal types of ampullary cancer. (2 classes, 14 tissue samples, 171241 spectra, TU Dresden).
Dataset 2: Myocardial tissues with ATTR vs. AL amyloidosis. (2 classes, 69 tissue samples, 141864 spectra, Charité Berlin).
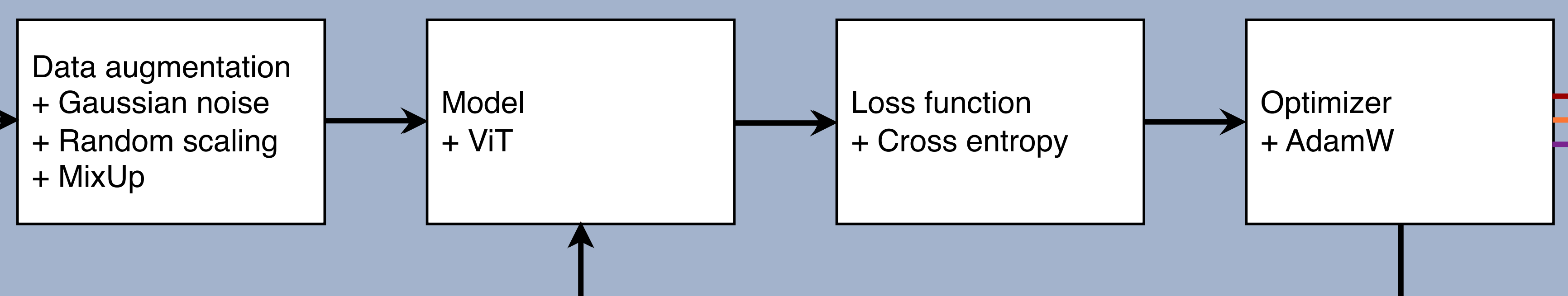**Dataset 3:** Ovarian clear cell carcinoma (OCC), borderline tumors (BOT), high-grade serous ovarian cancer (HGSC) and low-grade serous ovarian cancer (LGSC). (4 classes, 105 tissue samples, 23004 spectra, Charité Berlin).

Different datasets from different clinics

Dataset 1 — Pancreatobiliary vs intestinal type ampullary cancer
Dataset 2 — AL vs ATTR amyloidosis myocardial tissues
Dataset 3 — Pancreatic ductal adenocarcinoma vs other pancreatic cancer

Same deep learning pipeline

A 1D Visual Transformer (ViT) is trained using cross-entropy loss and the AdamW optimizer, with Gaussian noise, intensity scaling, and mixup as data augmentation (see below). For all tests, **we keep all training hyperparameters unchanged.**

Data augmentation + Gaussian noise + Random scaling + MixUp → Model + ViT → Loss function + Cross entropy → Optimizer + AdamW

Dataset 1 test set results

	Acc.		B. Acc.		F1-score	
	Spectra	Sample	Spectra	Sample	Spectra	Sample
Split I	0.92	0.67	0.92	0.67	0.92	0.67
Split II	0.72	0.67	0.83	0.75	0.81	0.67
Split III	0.72	0.80	0.81	0.83	0.74	0.80
Mean	0.79	0.71	0.85	0.75	0.82	0.71

Legend: Pancreatobiliary, Intestinal
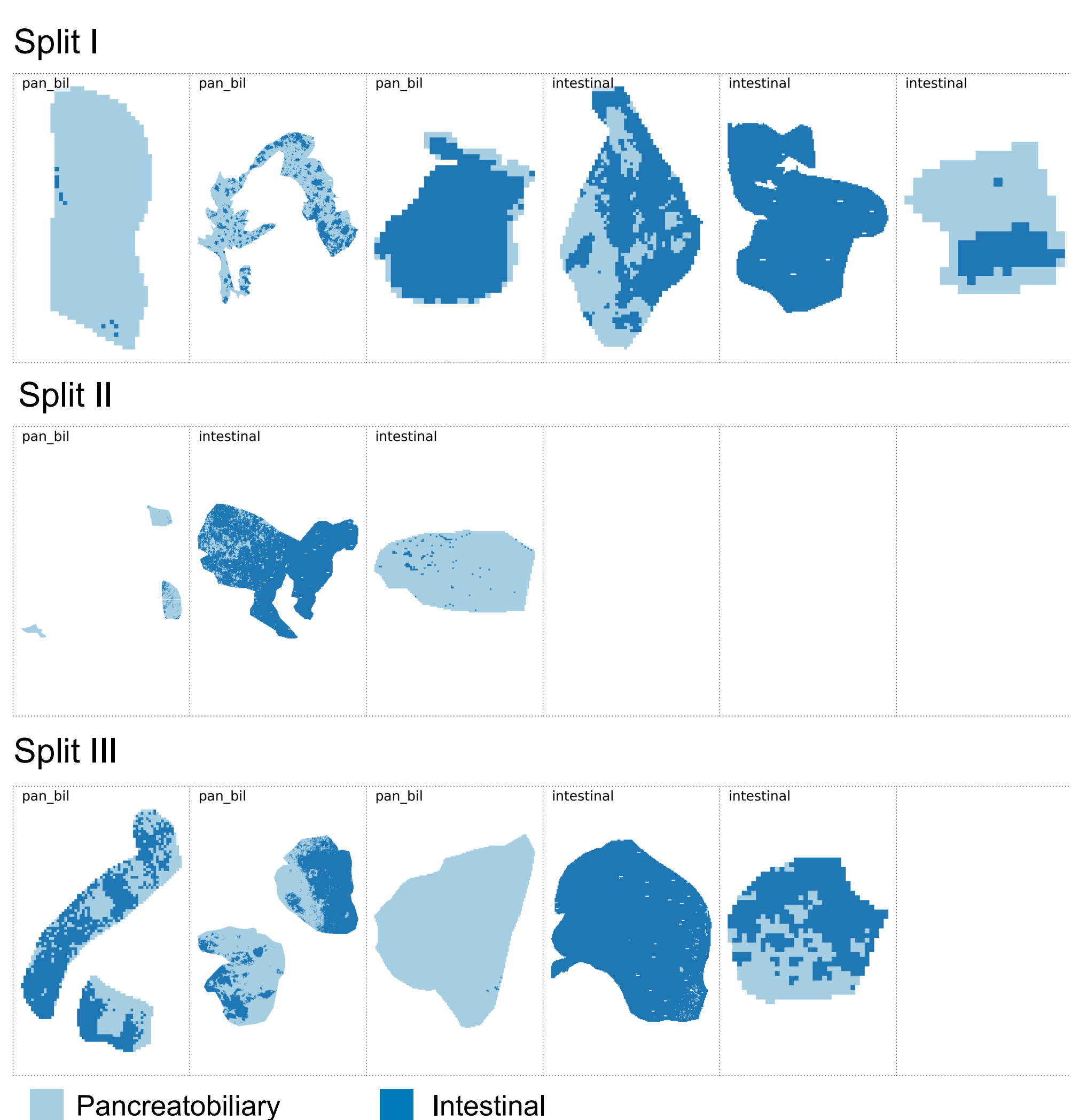
Dataset 2 test set results

	Acc.		B. Acc.		F1-score	
	Spectra	Sample	Spectra	Sample	Spectra	Sample
Split I	0.78	0.78	0.77	0.74	0.77	0.77
Split II	0.70	0.64	0.71	0.65	0.70	0.63
Split III	0.73	0.75	0.72	0.73	0.72	0.74
Mean	0.74	0.72	0.73	0.71	0.73	0.71

Legend: AL_Control, ATTR
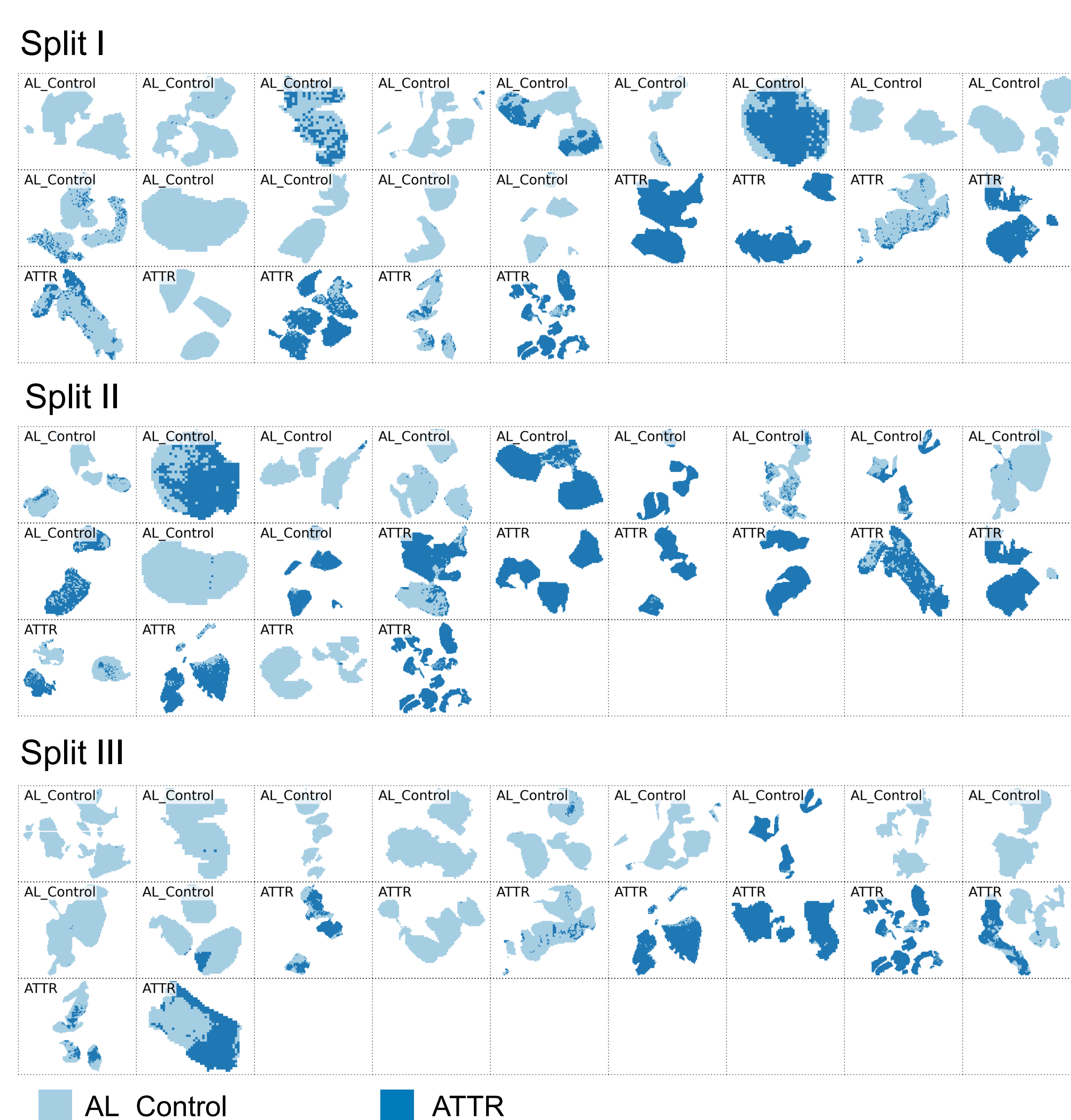
Dataset 3 test set results

	Acc.		B. Acc.		F1-score	
	Spectra	Sample	Spectra	Sample	Spectra	Sample
Split I	0.63	0.70	0.64	0.72	0.64	0.70
Split II	0.66	0.69	0.68	0.69	0.66	0.68
Split III	0.71	0.76	0.71	0.79	0.71	0.76
Mean	0.67	0.72	0.68	0.73	0.67	0.71

Legend: OCC, BOT, LGSC, HGSC

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