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Spatial–Spectral Integrative 3D Convolutional Neural Network for MSI-Based Cancer Diagnosis

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Mass spectrometry imaging (MSI) is a label-free technique that directly maps spatial distributions of biomolecules. It enables objective detection of molecular heterogeneity and treatment-related changes that are difficult to discern by morphology alone.

However, MSI is inherently high dimensional, as each location contains a spectrum with thousands of *m/z* peaks, which makes data analysis difficult. To address this, linear regression tools as well as various deep learning models have been employed. These methods enable the reduction of irrelevant variables, extraction of informative features, and modeling of non-linear relationships that are otherwise difficult to capture with conventional statistical techniques. In this study, we employ a 3 dimensional convolutional neural network(3D CNN). Unlike many previously proposed approaches for MSI analysis, this architecture considers both spectral and spatial information directly from the input, providing an integrated framework for feature learning.

We analyzed breast tissues using Desorption Electrospray Ionization(DESI)-MSI with standardized preprocessing and trained a 3D CNN. The model achieved 95–97% cancer diagnostics accuracy at both patch and slide levels. Ablation experiments demonstrated that model relies on spectral-spectrum interaction features. Unlike previous studies, 3D CNN-based analysis confirmed that it relies on both on spectrum and spatial features and it can be used as a direct and objective strategy for cancer diagnosis. Moreover, the model identified discriminative patterns that can be serve as molecular signature, highlighting its potential not only for diagnosis but also for biomarker discovery.