Non-Destructive Prediction of Metabolites Using Hyperspectral Imaging

Background/Objective

• Sustainable biomass production requires accurate, scalable drought monitoring. While traditional metabolite profiling is destructive, hyperspectral imaging (HSI) in the visible—near infrared (VNIR) and shortwave infrared (SWIR) ranges offers a high-throughput, non-destructive approach, its use for metabolite prediction remains limited.

Approach

- Apply VNIR+SWIR hyperspectral imaging and untargeted metabolomics to eight *Populus* genotypes and compared HSI metabolite profile predictions to metabolomics results.
- Use least absolute shrinkage and selection operator (LASSO) regression to identify spectral predictors of metabolite concentrations.

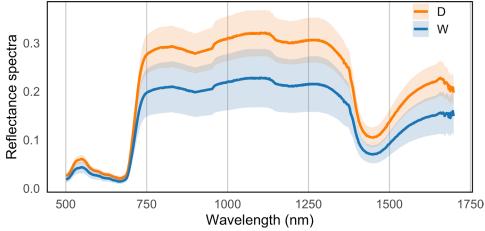
Results

- HSI captured clear drought-induced spectral shifts in poplar leaves.
- LASSO regression identified strong spectral–metabolite associations, with 15 metabolites predicted at adjusted $R^2 > 0.5$.
- VNIR best predicted amino acids and phenolics, while SWIR captured carbohydrates, organic acids, and terpenes.
- Several metabolites showed consistent spectral correlations under both drought and control, highlighting their potential as stable biomarkers.

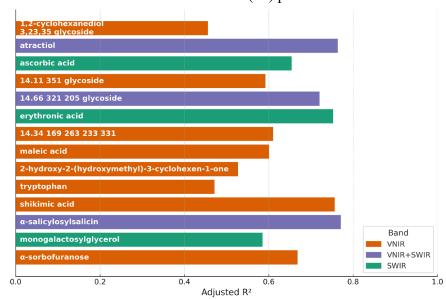
Significance/Impacts

- Demonstrated that HSI can non-destructively predict metabolite profiles in poplar and possibly other bioenergy crops.
- Established spectral biomarkers of drought stress, enabling real-time monitoring of plant physiological responses.
- Provided a scalable tool to bridge metabolomics and field phenotyping, accelerating breeding of drought-resilient poplar.

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Drought (D) plants show higher VNIR+SWIR reflectance than well watered (W) plants



Robust metabolite prediction from VNIR, VNIR+SWIR, SWIR

