

# Metabolomics - based machine learning method for the discovery and characterization of biomarkers implicated in Non-Alcoholic Fatty Liver Disease (NAFLD)

Ambrin Farizah Babu<sup>1</sup>, Sara Leal Siliceo<sup>2</sup>, Howell Leung<sup>2</sup>, Emmanouil Nychas<sup>2</sup>, Gianni Panagiotou<sup>2</sup>, Kati Hanhineva<sup>1</sup>

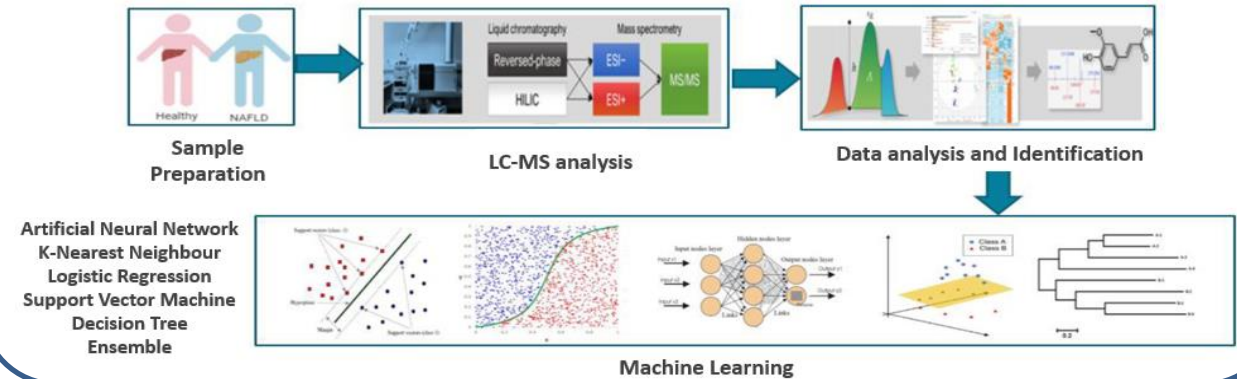
<sup>1</sup> Institute of Public Health and Clinical Nutrition, University of Eastern Finland, Kuopio, Finland

<sup>2</sup> Leibniz Institute for Natural Product Research and Infection Biology – Hans Knöll Institute (HKI), Systems Biology and Bioinformatics, Jena, Germany

## Introduction

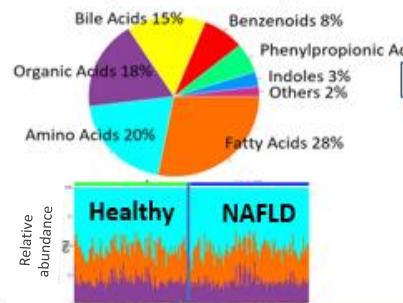
- Nonalcoholic fatty liver disease (NAFLD) is the **most common** chronic liver disease worldwide.
- However, the **diagnostic approaches** for NAFLD detection is **challenging** due to the limited availability of non-invasive biomarkers.
- **Metabolomics coupled to machine learning** can pave way to identify diagnostic biomarkers, understand disease mechanisms, and evaluate the treatment of various diseases.

## Methodology

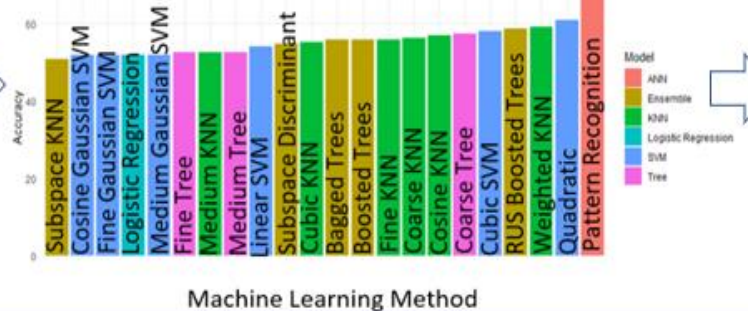


## Results and discussion

### Metabolite classes and composition of healthy and NAFLD subjects



### Application of metabolomics data on machine learning platforms (ANN – highest accuracy)



### ANN Confusion Matrix (71.5% Accuracy)

		All Confusion Matrix		
		0	1	
Output Class	0	58 32.4%	23 12.8%	71.6%
	1	28 15.6%	70 39.1%	71.4%
		67.4%	75.3%	71.5%
		32.6%	24.7%	28.5%
		Target Class		

- Of the 123 measured metabolites, 32 were identified as optimal to discriminate between NAFLD and control.
- ANN pattern recognition model has the highest accuracy in correctly classifying the subjects with and without NAFLD.
- The study demonstrates the potential of ANN for NAFLD metabolomics data classification in realistic situations