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# Machine learning enabled breast cancer detection using salivary

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## Abstract

Metabolomics is one of omics technology enables comprehensive identification and quantification of hundreds of metabolites in various samples. This technology has been used for the biomarker exploratory to discriminate various metabolic diseases, such as diabetes, psychiatric diseases, chronic fatigue, and importantly, cancer. The biomarkers in a low-invasively available biofluid, e.g. blood, urine, and saliva, would contribute to the early detection and monitoring of these diseases. Here, we tried to discriminate breast cancer patients from healthy controls using non-invasively available saliva samples. Saliva samples were collected after 9 hours fasting and were immediately stored at −80 C. Salivary hydrophilic metabolites were quantified using capillary electrophoresis-time-of-flight mass spectrometry and liquid chromatography with triple quadrupole mass spectrometry. A multiple logistic regression (MLR) model and an alternative decision tree (ADTree)-based machine learning method were used to develop discrimination models. The generalization abilities of these mathematical models were validated using cross-validation and resampling methods. Unstimulated saliva samples were collected from 101 patients with invasive carcinoma of the breast (IC), 23 patients with ductal carcinoma in situ (DCIS), and 42 healthy controls (C). Among quantified 260 metabolites, spermine showed the highest area under the receiver operating characteristic curves [0.766; 95% confidence interval (CI) 0.671–0.840 to discriminate IC from C. The ADTree with an ensemble approach showed higher accuracy (0.912; 95% CI 0.838–0.961, P < 0.0001), which was more accurate than MLR model. These data with discrimination model would contribute to a non-invasive screening of breast cancers.

## Biography

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## Publications

1. Prediction of metabolite identity from accurate mass, migration time prediction and isotopic pattern information in CE□TOFMS data
2. Discrimination of oral squamous cell carcinoma from oral lichen planus by salivary metabolomics
3. Identification of modules and functional analysis in CRC subtypes by integrated bioinformatics analysis
4. Effect of oral functional training on immunological abilities of older people: a case control study

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