# Analysis of metabolic profile data using batch-learning self-organizing map

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## Objectives

Kohonen's Self-Organizing Map (SOM) is an unsupervised neural network algorithm which has successfully been used to analyze very large data files in various fields, such as process monitoring and visualization, exploratory data analysis, and simulation of brain-like feature maps. The original SOM algorithm requires long time for calculation, and could have different clustering results in its topology depending on the order of data input. Recently, the original SOM had been improved to a batch-learning SOM (BL-SOM). The initial weight vectors are set by principal component analysis and the learning process is designed to be independent of the order of input of vectors, and hence the result is reproducible. BL-SOM can be done in a laboratory using a personal computer because the algorithm does not require high CPU (central processing unit) power. However, only a few examples of BL-SOM analysis of metabolome data have been performed yet. In our present study, BL-SOM was conducted to analyze the fold change database in the amounts of metabolites obtained by time-course sampling in *Arabidopsis thaliana* cells after salt stress treatment.

## Materials and Methods

### 1. Plant material

*Arabidopsis* T87 cells were obtained from the RIKEN Bio Resource Center (Tsukuba, Japan). The T87 cells were grown in modified liquid LS medium (30 ml) in a 100 ml flask under continuous light exposure at a photosynthetic photon flux density (PPFD) of 55 µmol $m^{-2}s^{-1}$ at 23 °C.

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## 2. Salt-stress treatment and metabolites analyses

The cells were grown for 3 d first and then treated with 100 mM NaCl. The cells were sampled for analysis after 0.5, 1, 2, 4, 12, 24, 48, and 72 h. Control cells were harvested by filtration, immediately ground in liquid nitrogen and stored at -80°C prior to analysis. Extraction, separation, identification, and measurement of metabolites by LC/MS/MS, LC/MS and GC/MS analysis were performed according to the procedures previously reported by our group (Kim *et al.*, 2005)

## Results and Discussion

The batch-learning self-organizing map (BL-SOM) for metabolome informatics making the learning process and resulting map independent of the order of data input was successfully used in analyzing and organizing metabolome data of *Arabidopsis thaliana* cell culture under salt stress condition. A 6 × 4 matrix showed the metabolites level patterns at different time periods. There is a negative correlation between the levels of amino acids and metabolites related to glycolysis metabolism as response to the salt stress. BL-SOM could be an excellent tool for clustering and visualizing high dimensional complex metabolome data in a single map.

## Reference

Kim JK, Harada K, Bamba T, Fukusaki E, Kobayashi A. (2005) Stable isotope dilution-based accurate comparative quantification of nitrogen-containing metabolites in *Arabidopsis thaliana* T87 cells using *in vivo* $^{15}$N-isotope enrichment. *Biosci. Biotech. Biochem.* 69: 1331-1340.