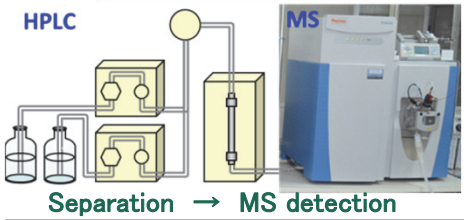
# Specification of differential compounds and exhaustive analysis by LC/MS multivariate statistical technique

The multivariate analysis of the chromatogram is known as the efficient and exact root-cause-analysis technique of unusual products. The differential compounds between samples can be specified by statistical analysis of the enormous organic compounds detected by LC/MS.

## LC/MS multivariate analysis flow

LC/MS data acquisition (>n=3)

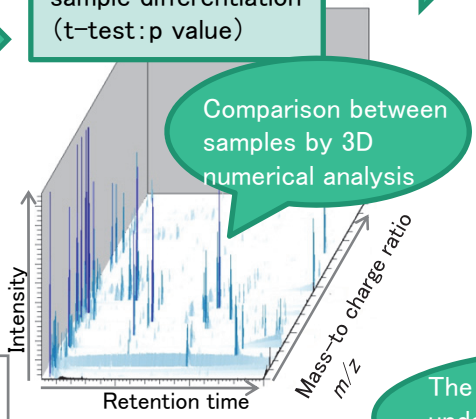



Separation → MS detection

Separating components by column retention, and acquiring data(m/z, peak intensity) for every retention time.

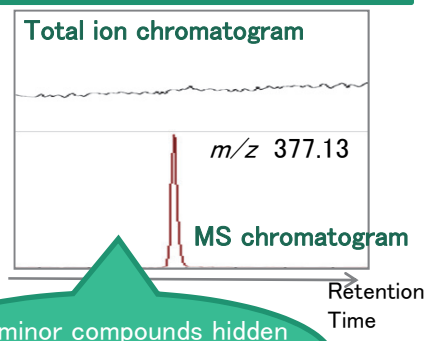
Statistical analysis of sample differentiation (t-test : p value)

Comparison between samples by 3D numerical analysis




LC/MS 3D-Map (RT, *m/z*, Intensity)

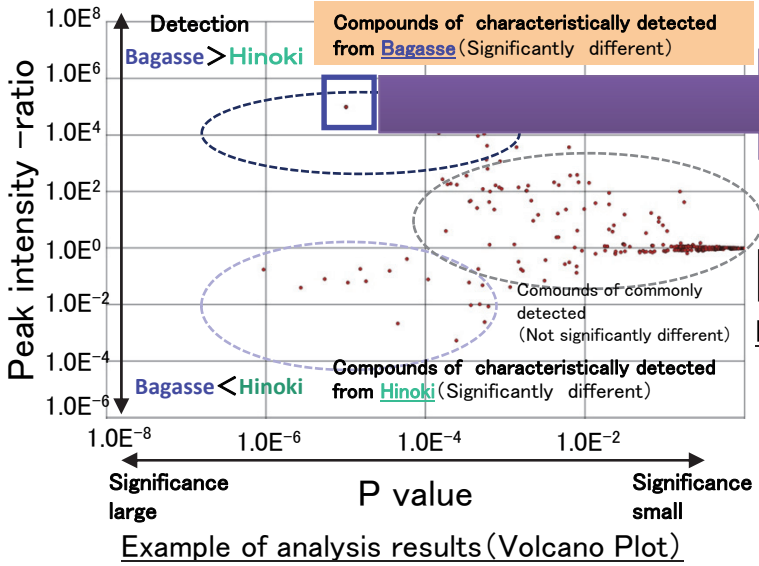
Variable analysis (specification of differential compounds, Principal component analysis)




The minor compounds hidden under the TIC baseline are not overlooked !

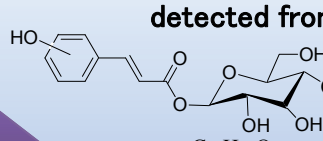
## Application examples (Biomass sample : differential organic analysis of lignin acid-hydrolysate)

### Data e.g.1 Selection of differential compounds




Example of analysis results (Volcano Plot)

**Compounds of characteristically detected from Bagasse※**




※The residual substance behind sugarcane juice

(Examples of estimated structure)

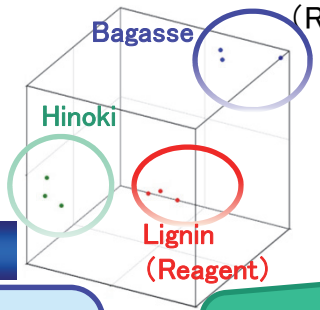
$C_{15}H_{18}O_8$

Exact Mass: 326.10

Conducting MS chromatogram analysis, coumaric acid glycoside was detected in ***Bagasse*** only.

### Data e.g..2 classification of multiple samples

Principal component (PCA) 3D score plot (RT, *m/z*, peak intensity)




Degree of similarity between samples can be classified and visualized.

### Other possible examples using the multivariate analysis

- Searching for characteristically detected compounds(degradation index) from unusual products
- Increasing/decreasing components according to treatments (variability analysis)
- Minor compounds comparison between samples.
- Classification of multiple samples and extraction of characteristic compounds

**Also undiscovered compounds in conventional manual analysis can be analyzed statistically and exhaustively!**

Bagasse samples were provided from Mitsui Sugar Co.Ltd.