

## Abstract of Presentation

**Note: This paper should be typed in “Times New Roman” of 12pt.**

Name (Underline the family name)

Daisuke Shibata

Presentation Title(Should be no more than 20 words):

Metabolite databases for plant biotechnology

Abstract :

My lab has been working on metabolomics since 2003. One of the major drawbacks in metabolomics is that most of metabolites are not identifiable in a high-through-put, non-targeted manner. Thus, we introduced a liquid chromatography-coupled Fourier transform ion cyclotron resonance mass spectrometer (LC-FT-ICR-MS) and an orbitrap mass analyzer to analyze metabolites with a high mass accuracy of 0.5 ppm. Such ultra-high accuracy allows us to predict a molecular formula or possible formulas of a metabolite, and furthermore, the MS/MS fragmentation pattern of the metabolite provides a cue to speculate the chemical structure. We are challenging toward a comprehensive annotation of metabolites in various organisms, including diverse plant species, microorganisms and animals, which will provide a firm basis to the metabolome research. We analyzed several stages of tomato fruit by LC-FT-ICR-MS, and the whole chromatography datasets were processed manually to annotate metabolite peaks. Over 800 tomato metabolites including many novel ones were annotated (Iijima *et al.*, *Plant J.* 54, 949-962, 2008). As the annotation process was very time-consuming, we developed the pipeline PowerFT to treat MS data in a computational manner, where the whole processes of peak detection, isotope peak identification, formula prediction and web-information search were automated within 30 minutes. We also prepared another pipeline, PowerMatch, to compare the processed data sets on a graphical interface. To accommodate the metabolite datasets, we are now constructing the database "KOMICS" (Kazusa OMICS, <http://webs2.kazusa.or.jp/komics/>). To integrate quantitative datasets of transcripts and metabolites on metabolic maps, we also developed a graphical interface KaPPA-View (Tokimatsu *et al.*, *Plant Physiology* 138, 1289-1300, 2005, <http://kpv.kazusa.or.jp/kappa-view3/>). Our recent studies on metabolomics in Kazusa DNA Research Institute also will be summarized in my presentation.

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