Understanding a chemical composition of foods is vital to accurately predict the bioactivity of multicomponent drugs, nutraceuticals, and foods. However, no analytical approach has existed so far to predict the bioactivity of multicomponent systems easily due to the complex behaviors of multiple coexisting factors in foods.

The research groups of Associate Professor Yoshinori Fujimura herein represent a metabolic profiling (MP) strategy to evaluate the bioactivity in systems containing various small molecules. The authors utilized a high-throughput screening method, non-targeted analytical procedure to collect composition profiles of diverse bioactive herbal samples from 21 green tea extract (GTE) panels. This employed the matrix-assisted laser desorption ionization-mass spectrometry (MALDI-MS) technique, using 1,5-diaminonaphthalene (1,5-DAN) as the optical matrix for detecting GTE-derived components. Multivariate statistical analyses revealed the differences among the GTEs in their antioxidant activity, especially oxygen radical absorbance capacity (ORAC). This bioactivity-prediction model was reliable and designed to predict the ORAC of diverse GTEs from their compositional balance. This chemometric procedure allowed the evaluation of GTE bioactivity by gathering information of multicomponent rather than single-component.

This research confirmed that MALDI-MS-MP represents a promising strategy for screening the bioactivity-predictive multicomponent factors and selecting the effective bioactivity-predictive chemical combinations for crude multicomponent systems. This research achievement has been published on May 23, 2017 (UK local Time), in Scientific Reports. For more details, see “A Chemometrics-driven Strategy for the Bioactivity Evaluation of Complex Multicomponent Systems and the Effective Selection of Bioactivity-predictive Chemical Combinations.” (DOI: 10.1038/s41598-017-02499-1)

Fig. 1. Overview of New Bioactivity Evaluation Technique, MALDI-MS Metabolic Profiling