1. Overview
The purpose of this study is to screen and identify pesticide chemicals in green tea. Compounds from green tea were extracted with QuEChERS method and analysed with MS/MS using a LC-TOF-MS.

2. Introduction
With population growth and the development of agriculture and food industries, food safety is becoming a greater concern in recent years. The increasingly stricter regulations of residual food contaminants require faster and more accurate analytic techniques. For this purpose, targeted screening by simultaneous MRM measurements using a high quadrupole mass spectrometer is the most common strategy. Data acquisition using a high-resolution and accurate mass spectrometer (HRMS), such as a Time-Of-Flight, is also carried out coupled with MRM-based analysis for the purpose of guaranteeing the robustness and reliability of screening. In addition, HRMS also provides a different advantage from MRM measurement because a compound which was not included as a target when acquiring data can be processed later without rescoping data.

3. Methods
Compounds in green tea samples were extracted with QuEChERS extraction after gridding with copperr wire (Figure 2). The resulted analyte-free samples were collected and purified by a fully automated solid phase extraction system (STQ-9030; Shimadzu Corporation, Kyoto, Japan) coupled with conventional flow liquid chromatography (Nexera X2; Shimadzu). LC separation was performed using a Raptor Biphenyl (2.1 mm × 100 mm, RESTEK) with gradient of 2 mmol/L ammonium formate + 0.002% formic acid in water and 2 mmol/L ammonium formate + 0.002% formic acid in methanol. Assignments with MS/MS spectra and predicted fragments from a molecular structure are performed using a third-party software, AGILENT Workstation (Agilent, Toronto, Canada).

4. Results

4-1. Analysis conditions for pesticides
We prepared a mixed standard sample of 157 pesticide compounds frequently used in local tea agriculture. The theoretical m/z of each chemical was calculated and listed up. Mass chromatogram was confirmed by a mass error tolerance of ±10ppm. The retention time of each chemical was recorded by injection of standard sample by using the following instrument parameters.

**HRMS (Nexera X2)**
- Acquitation Mode: Multiple Reaction Monitoring
- Sample: 10 min
- Mobile Phase A: 2 mmol/L ammonium formate + 0.002% formic acid - Water
- Mobile Phase B: 2 mmol/L ammonium formate + 0.002% formic acid - Methanol
- Injection Volume: 10 μL
- Gradient Program: 2 min (0–10%) → 1 min (10–20%) → 1 min (20–30%) → 1 min (30–100%) → 1 min (100–100%)
- Flow Rate: 0.6 mL/min
- Column Temperature: 35°C
- Nebulizing gas: 35 L/min
- Carrier gas flow: 10 L/min
- Drying Gas Flow: 15 L/min
- Ionization: ESI positive
- Gas Flow: 10 L/min
- Heating Gas Flow: 10 L/min
- Collision Energy: 35°C
- D.I. Temperature: 150°C
- H.I. Temperature: 350°C
- TOF range: m/z 50–1,000
- Event Time: 0.4 s (Pulser: ≤ 754)
- m/z: 50–2,000
- Mass accuracy: 1 ppm
- Maximum acquisition rate: 100 Hz
- High-resolution and accurate mass spectrometer

Figure 2: Sample preparation of pesticides in green tea

Figure 4: Screening result of pesticide residues in green tea

Figure 5: Example of formula prediction (LabSolutions Insight Explore)

5. Conclusions
According to the official guideline of CODEX, and Japanese Ministry of Health, residual concentrations quantified here is far below the criteria defined for them. Thus, our results indicate that LCMS-9030 system successfully achieves robust and reliable residue screening in foods by coexistence with both high-sensitivity quantitation and qualification with high mass accuracy.