Non-Target and Unknown Screening of Food Samples using High Resolution LC-MS/MS

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1. Open data files and select contaminated and suspect samples.
2. Define parameters to peak picking, formula finding, and library searching and start processing.
3. MasterView™ software will now automatically find peaks, compare signal intensity, and perform formula finding and library searching.
4. Review details of formula finding and MS/MS library searching. The logical OR of the spectral database in a MasterView™ search and MS/MS interpretations.
5. ChemSpider search results performed in MasterView™ software suggesting Boscalid being present in a tomato, the empirical formula of the compound is displayed in the structure view.

RESULTS

Data Analysis Workflow for Non-Targeted Screening for Pesticides

Figure 2. Tentative Identification based on ChemSpider Searching and MS/MS Interpretation

CONCLUSIONS

A novel approach of comparative non-target screening to identify unexpected and unknown chemicals in food by high resolution LC-MS/MS and peptide mass fingerprinting using a Quadrupole orthogonal TOF mass spectrometer with a chemical library of metabolites and pesticides, is being used under license. © 2015 AB Sciex.

REFERENCES

1. EU Commission Decision 98/340/EC
2. A. Schreiber et al.: 'Target and Non-Target Screening for Pesticide Residues in Food Samples using a Quadrupole orthogonal TOF mass spectrometer with a chemical library of metabolites and pesticides'.
3. A. Schreiber et al.: 'Target and Non-Target Screening for Pesticide Residues in Food Samples using a Quadrupole orthogonal TOF mass spectrometer with a chemical library of metabolites and pesticides'.

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