

Detection of residual pesticides on fruits and vegetables using Portability™ miniature mass spectrometer

Mass spectrometry can be now deployed for onsite pesticide screening in real time

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Pesticides are used in a variety of different ways during the production of food. Ranging from preventing crop damage by insects, rodents and molds during growth to prolonging storage of food after harvest. Because of the frequent usage, the residual pesticides are often found in many agricultural products and their monitoring and control is an important step in achieving and maintaining overall food safety in the modern society.

Mass spectrometry in connection with different separation techniques currently represents the main analytical approach for determination of residual pesticides in food. Traditionally, samples need to be collected and send to a laboratory for analysis using techniques such as GC-MS or HPLC-MS, which are costly and time-consuming. In addition, the conventional mass spectrometry usually requires laborious sample pretreatment, which does not allow for immediate in-situ sample determination. Presented here is an application of Thermal Desorption ElectroSpray Ionization (TD-ESI) for pesticide screening coupled to a portable mass spectrometer.

TD-ESI is a mass spectrometry technique from the family of ambient ionization methods that utilizes very simple probing of different surfaces with no or limited sample pretreatment while it is still noted for its selective and sensitive detection capabilities. In TD-ESI a solid surface or a liquid sample is touched by a simple metallic probe that absorbs the analyte. The probe is then inserted into a heated tube and the desorbed analyte is carried by gas flow into an orthogonally mounted electrospray. The electrospray plume extracts the analyte and further ionization and ion introduction follows the conventional electrospray mechanism.

Bayspec's Portability™ mass spectrometer is less than 10kg highly portable and battery operated linear ion trap mass spectrometer with atmospheric pressure inlet (API). When TD-ESI is combined with Portability™ then it is possible to perform fast in-field detection of analytes including residual pesticides, directly of the surfaces of fresh food products without any sample pre-treatment. Fast pesticide screening by Portability™ mass

spectrometer can immediately disclose fake organic food products as well as to discover elevated levels of residual pesticides.

TD-ESI-MS was used to rapidly screen residual pesticides on the surfaces of different fruits and vegetables. Direct sampling probe was used to introduce analytes from surfaces of unprocessed samples. Due to short analysis times (1-5s a sample), the technique allows for fast screening for applications in food and environmental safety. MS (as well as MS/MS) analyses can be performed on surface-residual pesticides at ppm and sub-ppm levels. The miniaturized TD-ESI ion source compatible with Portability™ is available from BaySpec. This ion source mounts on the Portability™ front inlet and does not require any additional support, external power or gases. The simple intuitive software interface is operated by touch screen and makes the instrument extremely easy to control. The external TD-ESI source is fully integrated into the main software environment and the hyphenated system is thus very user-friendly, does not require excessive training and can be operated by persons with no previous mass spectrometry experiences.

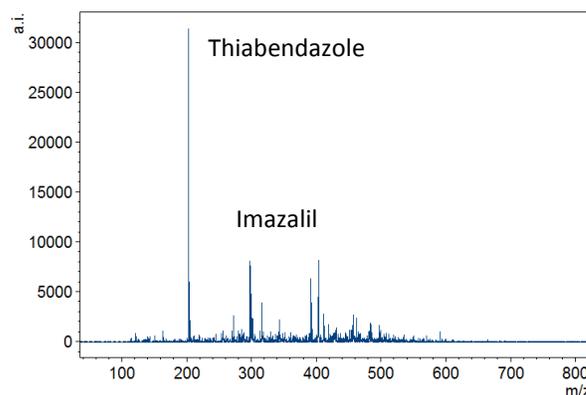


Figure 1. TD-ESI mass spectrum obtained by Portability from examined lemon. Imazalil $m/z = 297$; Thiabendazol $m/z = 202$

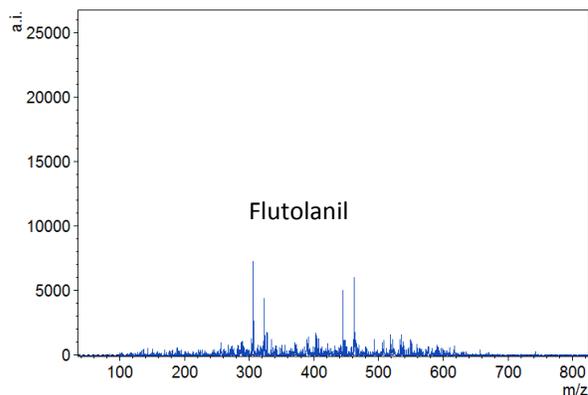


Figure 2. TD-ESI mass spectrum obtained by Portability from examined green apple. Flutolanil $m/z = 324$

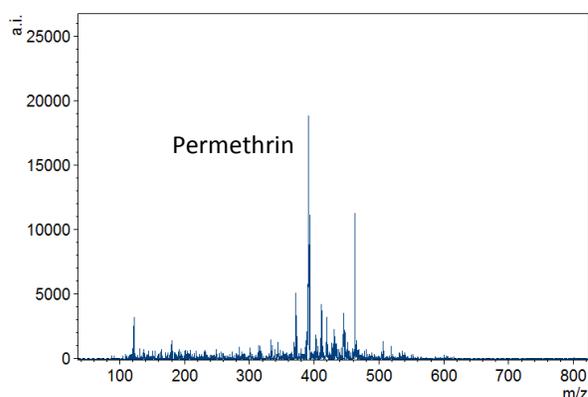


Figure 3. TD-ESI mass spectrum obtained by Portability from examined tomato. Permethrin $m/z = 392$

Portability™ Mass Spectrometer

The Portability™ linear ion trap mass spectrometer is one of BaySpec's newest portable instruments. Designed to bring the benefits of mass spectrometry chemical analysis to the field, the Portability™ can service a variety of bulk or trace detection applications. This instrument is small enough to be carried by one person and is controlled by a simple user friendly software.

The Portability™ is compatible with in-situ and direct analysis techniques. The front inlet allows direct connection with electrospray, thermal-desorption electrospray and atmospheric-pressure chemical ionization. This atmospheric pressure inlet (API) is compatible with direct injection through electrospray as well as with majority of ambient ionization techniques such as DESI or DART. The side port allows access to the internal electron ionization source; membrane inlet

or gas chromatograph can be coupled there. The Portability™ mass spectrometer can operate in positive and negative ion mode and can be made in multiple deployment configurations based on actual application needs.

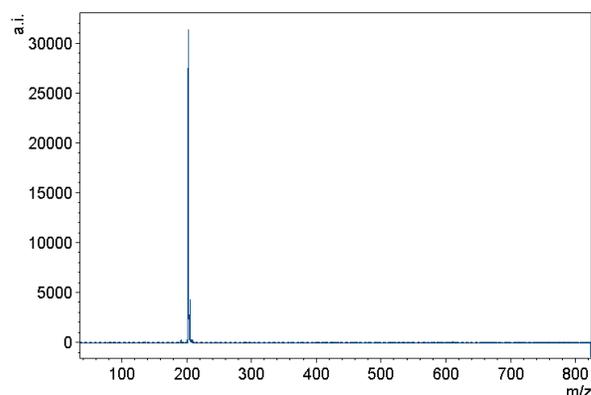


Figure 5. TD-ESI mass spectrum measured in Selected Ion Monitoring mode obtained by Portability directly from an orange surface. The only peak corresponds to pesticide thiobendazol at $m/z = 202$

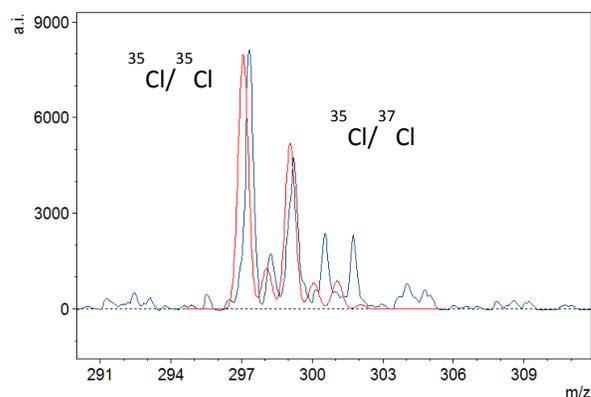


Figure 6. TD-ESI mass spectrum obtained by Portability from examined lemon. The zoomed spectrum shows chlorine isotopic distribution in ionized imazalil. Pesticide. Match with theoretical isotopic spectrum: Blue = experimental spectrum; Red = simulated spectrum

All fruits and vegetables were purchased from a local market in San Jose, CA and immediately analyzed by TD-ESI coupled to Portability™ mass spectrometer without any sample treatment.

REFERENCE:

Shiea C et al.: Rapid Commun. Mass Spectrom. 2015, 29, 163-170.