Detecting Toxins on Cannabis Leaves with Portable Miniature Mass Spectrometer

How can cannabis dispensaries ensure they are providing a safe product to its clientele?

© August 2018, BaySpec, Inc. Nam Lai and Brad Sohnlein

As more than 30 states have legalized medical marijuana, there is an ever-growing need for analytical services from the cannabis industry. Strict regulations are placed upon the farmers and distributors of the cannabis industry to ensure a quality, unadulterated product. Such laws require laboratory tests which may take a minimum of two weeks to process. The use of pesticides and herbicides during cannabis cultivation is of paramount concern to government bodies and consumers.

One such black-listed compound is piperonyl butoxide (PBO). Although having no pesticidal activity, PBO is used as a synergist in many formulations enhancing the potency of the pesticide. The E.P.A. has identified PBO as a Class C pesticide indicating its potential as a carcinogen.

In addition to the concern over pesticide use, many fear that other toxins such as fungicides and herbicides might be present. One such fungicide, myclobutanil, is known to be a reproductive or developmental toxin. Such cannabis products that have been tested positive for myclobutanil have prompted immediate recall and eradication. This herbicide is used in the formulation of popular fungicide product Eagle 20. Used properly on produce (i.e. grapes, apples, spinach), the fungicide poses no risk to humans. However, in the case that myclobutanil is heated, the compound is converted into hydrogen cyanide (classified as a schedule 3 substance by the Chemical Weapons Convention). This chemical reaction poses an extreme risk to cannabis users, because heat is required to activate the psychoactive compound Tetrahydrocannabinol (THC, MW: 314.47 g/mol).

Another popular herbicide used, paraquat, is a pulmonary toxin linked to increased risk of developing Parkinson’s disease. This herbicide has been in use since the 1950’s and largely outlawed by the European Union in 2007 and the United States since 2012. The herbicide is known for its toxicity to (but not limited to) the liver, kidneys, heart, and lungs. Evidence has shown paraquat to be deadly if ingested.

Mass spectrometry in connection with different separation techniques currently represents the main analytical approach for determination of residual pesticides in the Food & Agriculture industry. Traditionally, samples need to be collected and sent 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 spectrometer usually requires laborious sample pre-treatment, which does not allow for immediate in-situ sample determination.

Presented in this application note are data from a thermal desorption electrospray ionization (TD-ESI) or atmospheric pressure chemical ionization (APCI) source coupled to a portable mass spectrometer for toxin screening of cannabis leaves.

Figure 1. Molecular structures of (a) Piperonyl Butoxide (MW: 338.44 g/mol), (b) myclobutanil (MW: 288.78 g/mol), and (c) paraquat (MW: 225.16 g/mol; 187.16 g/mol when dissociated in aqueous solution).

Figure 2. BaySpec’s Portability™ Mass Spectrometer mounted with TD-ESI ambient ionization source.
Bayspec’s Portability™ mass spectrometer is less than 10 kg, highly portable, and battery-operated. Its linear ion trap mass analyzer can perform fast in-field detection of analytes, including residual toxins, by direct sampling of the surfaces of fresh food and plant products without any sample pre-treatment. In this study, BaySpec’s sampling probe was used to directly swab the surface of cannabis leaves and inserted into the TD-ESI or APCI sample inlet system for real-time analysis. Four different samples were studied:

- Fresh cannabis leaves
- Fresh cannabis leaves sprayed with PBO
- Fresh cannabis leaves sprayed with myclobutanil
- Fresh cannabis leaves sprayed with paraquat

All sprayed samples were air-dried prior to screening. No sample preparation was done to test the leaves. Both TD-ESI and APCI ionization methods tested positive for THC and toxins where applicable. See Figure 3 for recorded spectra.

Due to short analysis times (1-5 seconds per sample), this 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 toxins at parts per billion levels. The TD-ESI ion source with Portability™ miniature mass spectrometer is available from BaySpec. This system 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 turn-key system is user-friendly, does not require excessive training, and can be operated by persons with no previous mass spectrometry experiences.

Figure 3. Mass spectrum of a fresh cannabis leaf (a) and those after treatment with PBO (b), myclobutanil (c), and paraquat (d).