APPLICATION NOTE

Rapid Detection of Trace Levels of Deoxynivalenol in Wheat Flour by Portable Miniature Linear Ion Trap Mass Spectrometry

Battery-powered mass spectrometers can detect mycotoxins in the field in real time

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Deoxynivalenol (Cas:51481-10-8), also known as DON, is a trichothecene mycotoxin that is widely found in grains such as wheat, barley, and rice. The molecular structure of DON is provided in figure 1. DON is linked to two plant pathogens: Fusarium graminearum (wheat and corn), and Fusarium ear blight (corn only). DON inhibits the synthesis of DNA / RNA as well as protein synthesis at the ribosomal level, ultimately resulting in the loss of yield and contamination of seeds. An acute dose of DON can induce vomiting (emesis) in pigs, whereas at lower concentrations in the diet, it reduces growth and feed consumption (anorexia).[1] The U.S. FDA has established DON advisory levels to provide safe food and feed at concentrations of < 10 ppm to < 1 ppm depending on application.[2]

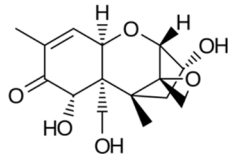

Figure 1. *The molecular structure of Deoxynivalenol, MW = 296.32 amu.*

Because DON is difficult to derivatize, this compound is typically analyzed via thin-layer chromatography (TLC) or high performance liquid chromatography (HPLC).[3] While TLC is simple, fast, and economical, this analytical technique does not provide high accuracy nor consistent results on a day-to-day basis. HPLC improves on accuracy and consistency but requires large quantities of costly solvents and produces large volumes of hazardous waste. Depending on sampling requirements and system performance, the annual maintenance costs for a standard HPLC instrument can run ~$10-20k per year.[4] Furthermore, although HPLC systems can be easy to use when properly configured, a trained professional is typically needed for troubleshooting, maintenance, and developing new methods.

Are there alternative analytical methods to consider? For simple detection and identification of DON, miniature linear ion trap mass spectrometry is a promising technique that is highly accurate, fast, and requires little maintenance.

Two samples were analyzed in a recent case study for an agricultural firm based in Canada. One sample contained 200 mg of wheat powder, while the other sample was 1 mg of the pure DON compound. Measurements were taken on a BaySpec Portability™ Mass Spectrometer (Figure 2) with both thermal desorption (TD) electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) methods. Samples were tested "dry" either by probing the surface of the sample vials or by spreading the powder onto a clean surface and swabbing. An enlarged image of the sampling probe with a small amount of wheat powder is shown in Figure 3.

Figure 2. *Portability™ Mass Spectrometer by BaySpec, Inc.*

Mass spectra were obtained by inserting the sample probe into the ionization port. Positive or negative ions were accelerated into the linear ion trap, and masses (m/z) were scanned from 70 – 650 amu's using the built-in graphical user interface. The Portability™ mass spectrometer provided a mass resolution of 0.5 – 1 amu and a sensitivity of < 1 ppm.

Figure 3. *Close-up of wheat powder on the inoculation loop of the Sample Probe*

Both ionization methods tested positive for the compound within both samples. Representative mass spectra are presented in Figure 4(a) – (c). Based on the intensity level of the parent ion peak at 397.3 amu, the concentration of DON in wheat is approximated as 5-10 ppm. Each mass spectrum was acquired and processed within a few seconds. As a result, the linear ion trap succeeded in quantifying DON to ppm levels and reduced

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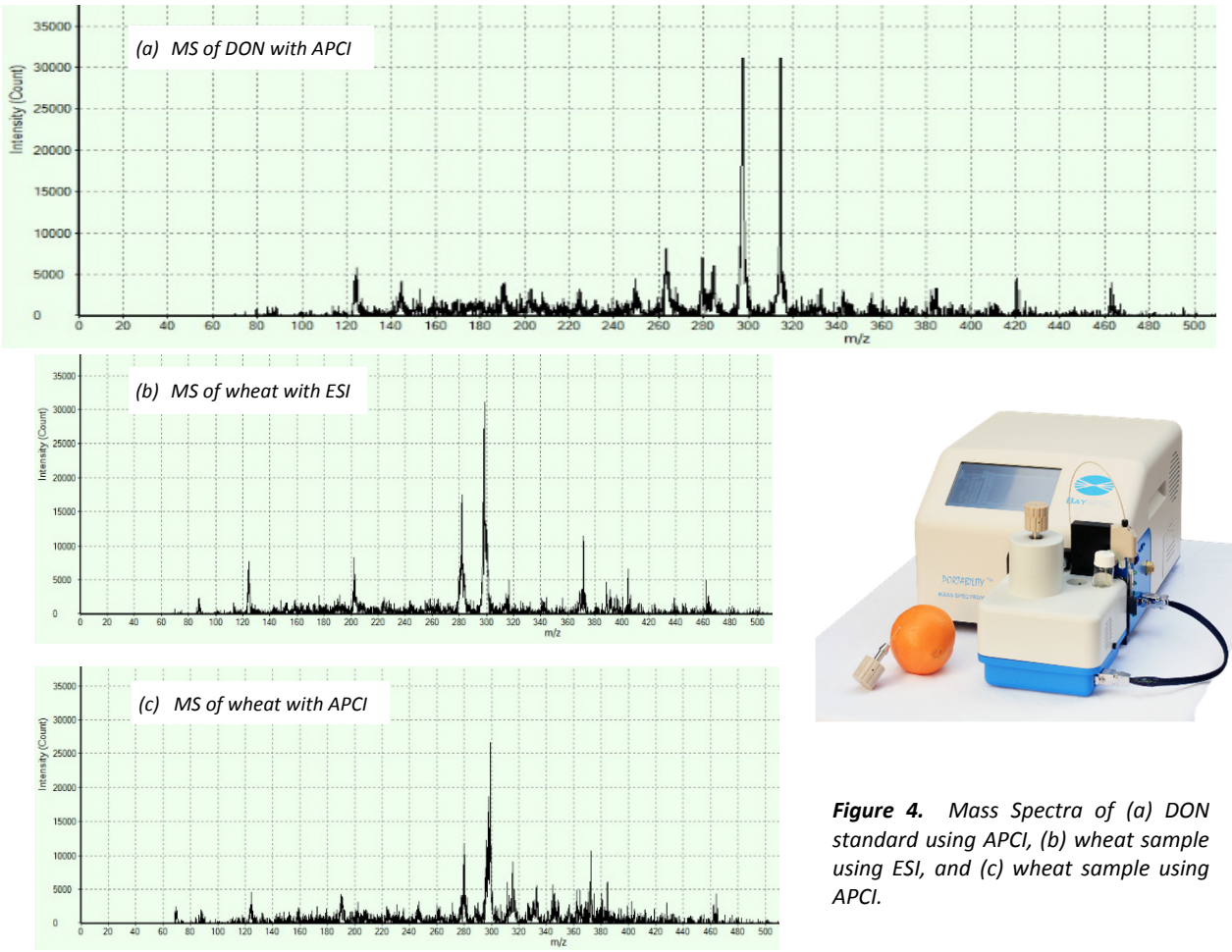

Figure 4. *Mass Spectra of (a) DON standard using APCI, (b) wheat sample using ESI, and (c) wheat sample using APCI.*

the acquisition time from >10 minutes (e.g. from HPLC) to < 5 seconds, a decrease by over two orders of magnitude. Such time and cost savings is relevant to quality control and regulation within Food & Agriculture, Pharmaceuticals, and Defense & Security markets.

BaySpec, Inc., founded in 1999 with 100% manufacturing in the USA (San Jose, California), is a vertically integrated spectral sensing company. BaySpec brings the lab to the sample by designing and manufacturing advanced spectral instruments with an emphasis on light weight and low power consumption. Our miniature UV-VIS-NIR-SWIR spectrometers, Raman analyzers, hyperspectral imagers, portable mass spectrometers, and OEM spectral engines and components have been deployed in a wide range of markets throughout the globe to provide solutions at the sample in real-time.

References:

1. Rotter, B.A., et al., J. Toxicol. Environ. Health, **48**, 1-34 (1996).
2. NDSU Extension Service, September 2005 Issue, http://www.southdakotaagriculturallaboratories.com/uploads/1/3/5/2/13521518/don_vomitoxin_in_wheat.pdf
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