



## ERGOT ALKALOIDS



Figure 1. Clavine alkaloids

What is being measured: Utilizing a global data dependent acquisition (DDA) approach, this method screens for ergot alkaloids in various plant and animal tissues. Ergot alkaloids are produced in the fungal species of the Ascomycota phylum upon prenylation of the amino acid tryptophan. This class of compounds comprise of clavines, ergoamides (lysergic acid derivatives), ergopeptines, and ergopeptams.

Ergot Alkaloids

How it is done: The samples are analyzed using liquid chromatograph coupled to an ultra-high resolution mass spectrometer. Putative IDs of compounds are generated through the matching of accurate mass (<2 ppm error) and fragmentation pattern with online, in silico, and in-house mass spectral libraries. Absolute quantitation is possible when the authentic standards are available. Relative quantitation is determined by normalization with ergotamine internal standard.



Dimethylallyltryptophan





Figure 3. Workflow for the mass spectrometer method approach for mass spectral data acquisition

**INSTRUMENTATION** 

<u>Thermo Orbitrap Fusion™ Tribrid™ Mass Spectrometer</u>

Primary applications

**Figure 4.** Relative abundance of ergot alkaloids

identified in ergot infected grass (MUAL data).

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## • Combines quadrupole, ion trap and Orbitrap mass analysis in Tribrid architecture

- Ultrahigh resolution up to 500,000 FWHM
- Sub ppm mass accuracy
- Multiple dissociation techniques—CID, HCD, ETD
- ID-X capability for small molecule identification
- Coupled to HESI and nano-ESI interfaces
- UltiMate 3000 RS UHPLC & UltiMate 3000 RSLCnano



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