Broadband, Fully Automated Identification of Drugs Using a Field Deployable DART-ITMS

Berk Oktem , Alexander Misharin, Konstantin Novoselov and Vladimir M. Doroshenko

MassTech Inc,, Columbia, MD

A field deployable ion trap mass spectrometer (ITMS) coupled with a Direct Analysis in Real Time (DART) ion source capable of broadband MS/MS to do multi-target monitoring is discussed. The presentation discusses how identification of the targeted compounds is done by using on board libraries with little or no user intervention. On board libraries are composed of both user generated library as well as commercially available MS/MS library. For forensics applications, it can be used for conclusive analysis of controlled substances and explosives by using tandem mass spectrometry. Same technique can be used to differentiate closely related compounds.

 An ITMS with a 3D ion trap ruggedized and optimized for field use is equipped with a DART source that is also optimized for field use. Using nitrogen as the supply gas, the expected mass spectra and tandem mass spectra were obtained for all drugs tested. This method did not require sample preparation. Tablets as well as native plant material could be used to introduce samples.

Broadband MS/MS analysis, i.e. isolating multiple parent ions simultaneously and fragmenting them, increases the number of targets being monitored as well as throughput.

Fully automated identification is accomplished by a combination of two libraries: a user generated library which was built with 25 compounds as well as a commercially available library that has about 42,000 ions. If the compound is available in user library, it was readily identifiable when used in conjunction with 2 or more fragments. If not, then the commercial library is used, with additional steps taken for increasing confidence as fragment ions may originate from several similar compounds.