ABSTRACT
Medicinal plant materials may contain pesticide residues and chemical contaminants which act as a major obstacle to the production of a wide array of herbal drugs which are marketed worldwide. Effective analytical methods are required for the screening and identification of these contaminants to ensure the quality of herbal products. High resolution mass spectrometry was employed for multi-class multi-residue screening in herbal products. The results obtained in this study confirm the potential of high resolution mass spectrometry for rapid and efficient multi-class multi-residue screening in herbal products.

INTRODUCTION
Botanical supplements or herbal remedies are one of the fastest growing markets worldwide. According to the WHO, more than 80% of the world's population relies on traditional medicine for their primary healthcare needs. The WHO and United Nations are actively promoting the use of herbal and natural products to overcome the global drug crises (1). The surge in the use of herbal medicines is mainly due to the growing awareness of their potential health benefits. The safety and efficacy of herbal products are often not known even in their traditional use. In the present study high resolution mass spectrometry was employed for multi-class multi-residue screening in herbal products. Analytical instruments like ion trap and quadrupole mass spectrometers are widely used in the identification of pesticides and mycotoxin residues such as ochratoxin A, fumonisin B1, Zearalenone, sterigmatocystin, aflatoxins, and fusarium toxins such as diacetoxyscirpenol and trichothecenes. GC/MS is the technique of choice for the detection of organic contaminant residues in herbal products.

MATERIALS AND METHODS
Sample Preparation:
Twelve commercially available Ashwagandha herbal products procured locally were used in this study. Two milligram of each sample was accurately weighed and were extracted using 2 ml of methanol. A volume of 100 mg of sample was accurately weighed and taken in a glass vial. Ten milliliters of methanol were added to this vial. The vial was sonicated for 10 minutes to remove any particulates. The supernatant was centrifuged at 11000 rpm for 10 minutes. The supernatant was decanted in a 10 ml glass vial and evaporated to dryness using a nitrogen evaporator. The sample was reconstituted with 100 μl of methanol. The solution was filtered through a 0.22 μm filter, before analysis.

Rapid High-Resolution Accurate Mass Multi-Class Multi-Residue Screening Method for Ashwagandha (Withania somnifera) Products
Results

Figure 1. Ashwagandha plant and products

Figure 2. Overlaid representative chromatograms in five replicates

Figure 3. Presence of common contaminant in herbal extracts

Figure 4. Identification of Betaxolol (Betalactam) using TOF-MS and TOF-MS/MS

Figure 5. Confirmation of Betaxolol using High resolution MS/MS data.

Figure 6. Formula/Pattern shows the elemental composition as C19H28O2

Figure 7. Theoretical fragments of Tingenone matching with the obtained TOF MS/MS with 100% matching

Figure 8. Confirmation of Betaxolol using High resolution MS/MS data.

For example, based on TOF-MS and MS/MS data, software calculates elemental formula as C19H28O2 for m/z 339.1884 in positive ionisation mode. Predicted formula was also cross-referenced against chemical database and identified the compound Tingenone. A full confirmation was done by matching theoretical fragments to obtained TOF-MS/MS of Tingenone.

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TRADEMARKS/LICENSING
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