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High throughput dietary supplement quality control and pharmacovigilance

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Global consumption of nutraceutical, herbal medicines and supplements has increased substantially and recent reports of adulteration demonstrate the need for an increase in extensive pharmacovigilance to ensure product safety and quality. Weight-loss products are particularly likely to contain undeclared ingredients or adulterants; often stimulants with unknown toxicodynamics. Development of high throughput methods to assist in the regulation of such products is essential for consumer safety. Over 100 herbal medicines, weight-loss supplements and other nutraceutical commercially purchased have been analyzed using a DSA ion source on the Perkin Elmer AxION TOF-MS. All products have indications for use concerning the GI tract, weight-loss, to support diet and/or metabolism. The DSA-TOF-MS technique offers advantages of minimum sample preparation, rapid analysis and 5 ppm mass accuracy. Over 1600 compounds were screened in a matter of minutes using this method. The Solo software package allowed isotopic patterns to be used to identify possible adulterants and other undeclared ingredients. Coghlan et al., (2015) found ~50% of the products screened contained an undeclared pharmaceutical. Data from the DSA-TOF showed that, in fact, over 80% of the same products were adulterated or contaminated. For example, sample one was previously thought to contain brucine, strychnine, dexamethasone and ephedrine. Using the DSA-TOF, 18 new contaminants have been detected, including several potential steroids. With further data analysis in R, fine isotopic patterns were matched for greater confidence in adulterant identification. Combination of established metabolomic data analysis tools with the mass spectrometric profile generated by the DSA-TOF allowed prompt characterization of the metabolite profile. This will allow for batch comparisons and assessment of product quality and variation. This rapid, untargeted approach to pharmacovigilance integrates well with other methods such as DNA tagging, ICP-MS and targeted LC-MS/MS to give a complete view of a product's quality and safety.

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