

P35 THE CRITICAL COMPARISON OF GC-HRMS AND DART-HRMS POTENTIAL FOR THE WHISKY AUTHENTICATION

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In the recent years, the interest in alcoholic beverages has been rapidly growing. However, some of the specifically high value spirits such as Scotch whisky may become a subject of fraud. While adulteration of whisky is relatively easy to perform, the detection is a great challenge for chemical laboratories. In general, the adulteration of whisky may occur in several ways, e.g. mixing it with ethanol originated from a raw spirit or even synthetic ethanol, adding certain ingredients with flavouring properties. Alternatively, a cheaper whisky may be bottled and sold as a more expensive whisky. Several methods have been used for whisky authentication such as UV/VIS spectroscopy, near red spectroscopy, capillary electrophoresis or gas chromatography coupled to mass spectrometry (MS). In our previous study, we analyzed a large set of whisky samples using solid phase microextraction (SPME) with GC coupled to high resolution mass spectrometry (HRMS). The results showed some low molecular phenolic compounds might be important markers for some whisky group. In following experiments realized within present study, we decided to extract phenolic compounds using ethylacetate and eliminate abundant whisky components not responsible for group classification such as water and alcohols. The preconcentrated ethylacetate extracts were directly injected in GC-HRMS. For a rapid screen of phenolic fraction also an ambient ionization technique DART (Direct Analysis in Real Time) coupled to HRMS was employed. A unique set of samples analysed in this study consisted of Scotch blended whiskies (n=77) and Scotch single malt whiskies (n=71) was obtained from The Scotch Whisky Research Institute. For single malt whiskies information on maturation cask (cask used for the bourbon or sherry production), production area (Speyside, Islay, Highland, Lowland), technological production (peated, non-peated) and ageing period (8-21 years) were available. To assess variability among different whisky groups according to the technological production process, production area, maturation cask and aging period, chemometric tools such as principle component analysis (PCA), partial least square regression (PLS-DA) and orthogonal PLS were used for the processing of generated data. The potential of both GC-HRMS and DART-HRMS for whisky authentication will be discussed in a detail.

Keywords: whisky, authenticity, adulteration, DART-HRMS, GC-HRMS

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