Rapid Authentication of Flavors using DART-MS

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INTRODUCTION
Characterization of flavors in food and beverages is critical for consumer’s perception of aroma, taste, quality and branding. Maintaining consistent flavor requires quality control testing of raw materials and finished products to ensure product quality.

Analysis of flavor compounds is challenging and time consuming as it requires several lab based measurements. Based on the source of the flavor (e.g., natural versus synthetic), the flavor formulations can contain a few hundred compounds with varying solubility, volatility, concentrations and stabilities. A combination of gas chromatography (GC) and liquid chromatography (LC) based methods integrated with mass spectrometry (MS) detection are typically applied for identification and quantification of flavors.

This application demonstrates the utility of DART-MS technology (Direct Analysis in Real Time) for rapid, accurate and cost effective flavor characterization, to monitor product quality and reduce production costs.

METHOD
DART-QDa was applied to characterize volatile and semi-volatile flavors in commercially available whiskey, chewing gum and tobacco samples with different characteristic flavors. No sample preparation was performed prior to DART-MS.

Three different sampling techniques were used:
- Whiskey: Liquid sampling by spotting a Quickstrip card
- Chewing Gum: Solid sampling by holding a piece of gum in the path of the ionizing helium beam
- Tobacco: Aroma sampling by analyzing the volatiles in the headspace above the open moist snuff tobacco can

RESULTS AND DISCUSSIONS
- The nominal mass was used for tentative identifications of some of these ions for characterizing the flavor profiles.
- Unique whiskey profiles generated by the DART-QDa for four different brands of whiskeys. Some ions are common among a few of the samples (m/z 342, 198, 127, 97), but vary by relative intensity and ratio.
- The bourbon sample contains a significant peak at m/z 209, which may be attributed to sinapaldehyde, a breakdown product of lignin resulting from the wooden aging barrel. The Scotch blend, Canadian, and Irish whiskeys contain an ion at m/z of 145. This ion could be attributed to ethyl hexanoate, which imparts a fruity odor.
- For chewing gum samples, the peaks at m/z 159, 236 and 237 were common to all the samples and may be attributed to the gum matrix. The cinnamon mass profile shows the presence of its characteristic flavor ingredient, cinnamaldehyde (m/z 133).
- The mass profile of spearmint flavored gum shows the presence of characteristic flavor, carvone (m/z 150). Methyl salicylate (m/z 153) was also observed in both spearmint and original gum samples.
- In tobacco samples, the nicotine peak (m/z 163, protonated) is the base peak irrespective of the applied flavor. Ions with m/z 80, 86, 108, 132, 136, 276 and 325 were observed in all the tobacco samples and may be attributed to the tobacco matrix.
- Methyl salicylate (m/z 153, protonated) and Ethyl salicylate (m/z 167, protonated) are the characterizing flavors of wintergreen and straight flavored tobacco products, respectively. Mint tobacco sample are characterized by the presence of limonene (m/z 137) and menthone (m/z 155).

CONCLUSIONS: APPLICATION BENEFITS
- Direct analysis of volatile and semi-volatile compounds
- Little to no sample preparation
- Ease of use and no chromatography needed

Application Note: Real-Time Analysis of Flavors Using DART and the ACQUITY QDa Mass Detector (720000601EN)