Analytical Chemistry's role in the development of reduced risk* products

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* Reduced-risk product statements are based on the weight of evidence and assume a complete switch from cigarette smoking. These products are not risk-free and are addictive.

Introduction

As the landscape of tobacco products evolves towards harm reduction, there's a growing need for robust analytical methodologies to evaluate tobacco and nicotine products that provide alternatives to traditional cigarettes. This poster gives examples of the application of spectroscopic and chromatographic analytical techniques to support these evaluations.

Screening

Spectroscopy

Spectroscopic techniques are often rapid, non-destructive and can be applied for qualitative or quantitative analysis.

Near Infrared (NIR)

NIR is used for quick analysis of PG, VG, nicotine and water present in E-liquids.

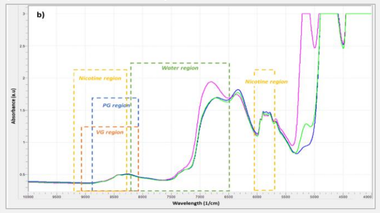

Figure 1: NIR spectrum showing absorbance bands characteristic to the main constituents of e-liquids [1]

Ultraviolet/Visible (UV/Vis)

UV/Vis spectra shows broad absorbance peaks, useful for qualitative analysis. UV/Vis is used for the determination of total alkaloids (such as nicotine) in tobacco extracts.

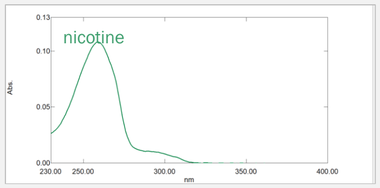

Figure 2: UV spectra showing a nicotine absorbance peak

Fourier Transform Infrared (FTIR)

FTIR analysis details the functional groups present in the sample, FTIR is useful when determining the composition of the aerosol produced by reduced risk products.

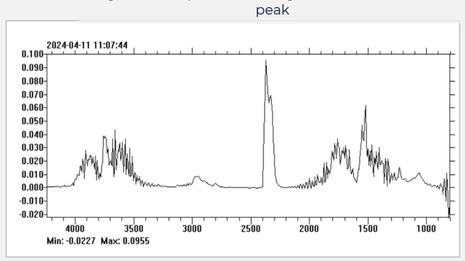

Figure 3: FTIR spectrum acquired from the aerosol of a THP product

Targeted

Gas Chromatography

Liquid Chromatography

Chromatography is a separation technique. Gas chromatography (GC) is best suited when analytes are non-polar, small, volatile molecules while liquid chromatography (LC) when analytes have high boiling points.

Increasing sensitivity

Flame Ionization Detector (FID)

GC coupled with an FID is useful for analytes that are easily separated from the sample matrix, for example analysis of nicotine and flavorings in modern oral pouches.

MS

MS is useful for identification of analytes that have similar retention times or that co-elute with unwanted molecules.

MS/MS

Mass Spectrometry (MS) involves the production, separation and identification of ions based on their m/z ratio.

Ultraviolet (UV)

LC coupled with an UV detector is useful for analytes that are easily separated from the sample matrix, for example analysis of nicotine in e-liquids.

MS/MS

MS/MS involves the production, separation and identification of fragments produced by a second mass spectrometer after ions have undergone the initial ionization and detection.

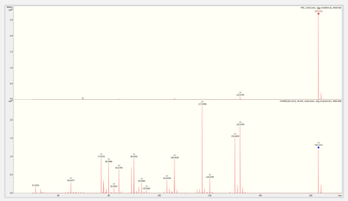

Figure 4: Nicotine mass spectrum

Non-targeted

Gas Chromatography

Liquid Chromatography

Increasing resolution

GC MS

GC×GC TOFMS

Time of flight (TOF) MS involves subjecting the ions produced to an accelerating voltage. The detector then measures the velocity of the ion which corresponds to the m/z.

GC×GC involves two consecutive separations, using two distinct columns connected via a modulator. This allows identification / visualisation of coeluting compounds.

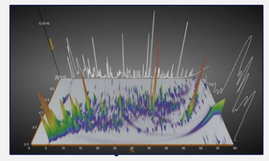

Figure 6: A 3D chromatogram acquired using GC×GC TOFMS

GC×GC HRMS

TOF-HRMS

High resolution MS (HRMS) can detect small differences in the mass of the ions.

timsTOF

Trapped Ion Mobility Spectrometry (TIMS) adds an additional degree of separation, which is dependent on the 3D shape of the ions.

Figure 5: Graphic of timsTOF Pro technology [2]

Orbitrap LC-MS

The Orbitrap is an accurate mass analyser that separates ions based on the frequency at which they oscillate around the central electrode and between the outer electrodes.

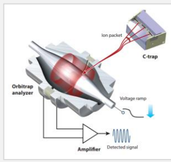

Figure 7: Cross section of the C-trap ion accumulation device and the Orbitrap mass analyser with an example of an ion trajectory. [3]

Conclusion

The application of these analytical techniques facilitates a thorough understanding of the studied products' chemical composition, aiding in regulatory assessments and product development. By comparing the profiles of traditional cigarettes with emerging alternative products, researchers and product developers can conduct toxicological assessments and support formulation of evidence-based approaches to promote tobacco harm reduction strategies.

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