MS Nose™ Atmospheric Pressure Chemical Ionisation Gas Phase Analyser (APcI-GPA)

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Introduction

The Micromass MS Nose™ ApcI-GPA is a new interface* for a mass spectrometer which has been designed for the analysis of volatile compounds. The low dead volume, inert sample introduction system, delivers the volatile compounds into the source where they are ionised at atmospheric pressure by a high voltage corona discharge. The ions are extracted from the atmospheric pressure region through a sampling orifice (sample cone) into an intermediate vacuum region and, from there, they are transported into the analyser region of the mass spectrometer where they are separated on the basis of their mass to charge ratio. APcI-GPA is a powerful tool enabling the analyst to monitor both the profile of compounds in the gas phase, and changes in that profile in real time.

Suitable for a range of applications, the system can be used to analyse volatile compounds from a wide variety of sources including human breath, perfumes, headspace autosamplers etc.

*European Patent #19937

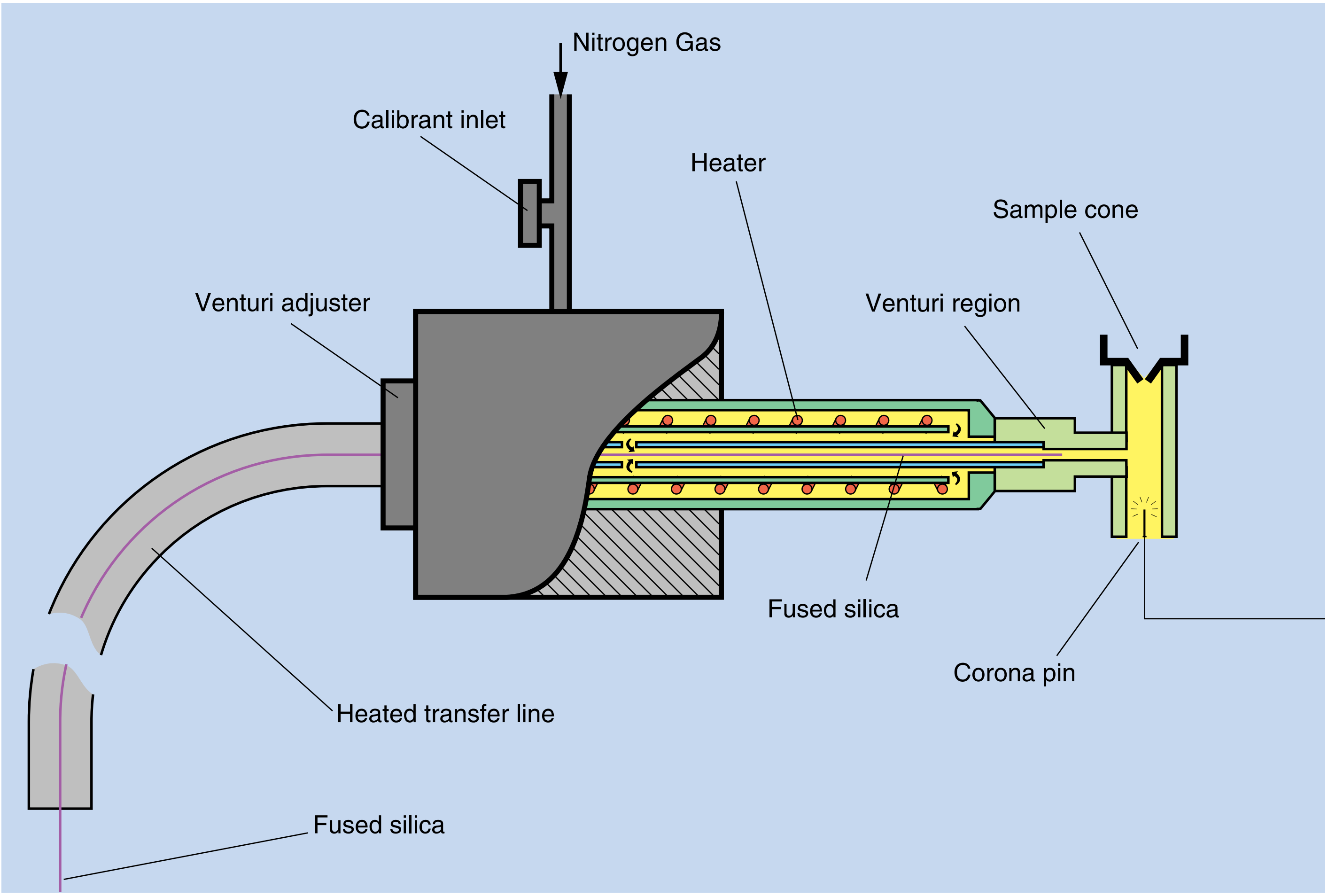

Figure 1: Schematic of the ApcI-GPA interface

Key Features:

- Temporal Resolution - The low dead volume of the interface coupled with the rapid response rates of mass spectrometers allows rapid changes in volatile concentration to be monitored.

- Sensitivity - APcI ionises a wide range of compounds (acids, alcohols, esters, ketones, pyrazines etc) which can typically be detected at 10ppbv in the gas phase.

- Simplicity - APcI is a soft ionisation technique giving minimal fragmentation. Compounds typically form the protonated molecule, $[M+H]^+$, simplifying ion profiles and making data interpretation easier

- Reduced sample preparation - With APcI-GPA, gas phase samples can be easily introduced without oxygen or moisture removal, minimising sample work-up.

- The Venturi - Changing the venturi region adapter sets the range of gas sampling flow rate available. The venturi adjustment alters the position of the silica in the venturi region allowing fine adjustment of the sampling rate.

- Flexibility - The APcI-GPA can be used to monitor both real-time temporal changes in volatile concentration and the volatile profile at a specific point in time.

- Transfer line - The flexible heated transfer line links the gas phase sample to the interface and the mass spectrometer.

- Quantitation - The absolute concentration of compounds in the gas phase can be determined by comparing the signal intensities of compounds in the sample with those of standards introduced via the calibration inlet.

- MS analysers - The APcI-GPA interface can be fitted to a wide variety of Micromass® mass spectrometers providing a range of detection modes. The interface may be used with quadrupole instruments, or it may use the enhanced sensitivity and mass accuracy of a time-of-flight instrument or the added specificity of an MS-MS instrument.

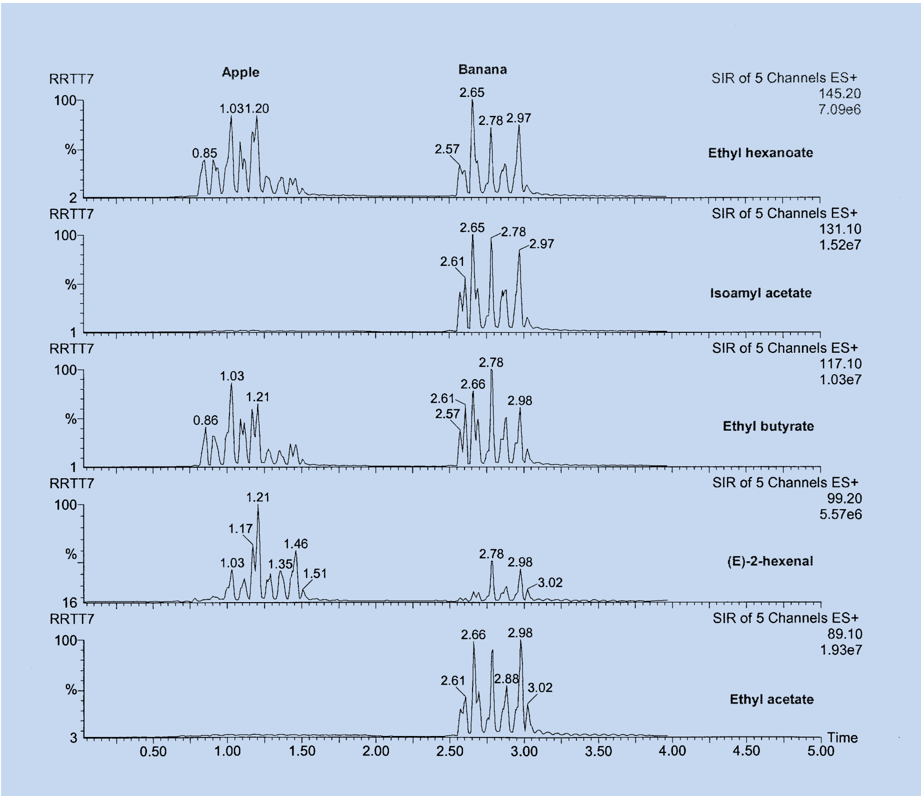

Figure 2: The temporal profiles of ethyl hexanoate (m/z 145), isoamyl acetate (m/z 131), ethyl butyrate (m/z 117), (E)-2-hexenal (m/z 99) and ethyl acetate (m/z 89) in the breath of an individual eating apples and bananas. The ethyl hexanoate and ethyl butyrate were present in the apple before consumption and were released earlier than the (E)-2-hexenal which was generated by enzymes during eating, causing a lag. Isoamyl acetate and ethyl acetate are characteristic compounds which are present in the banana but not in the apple.

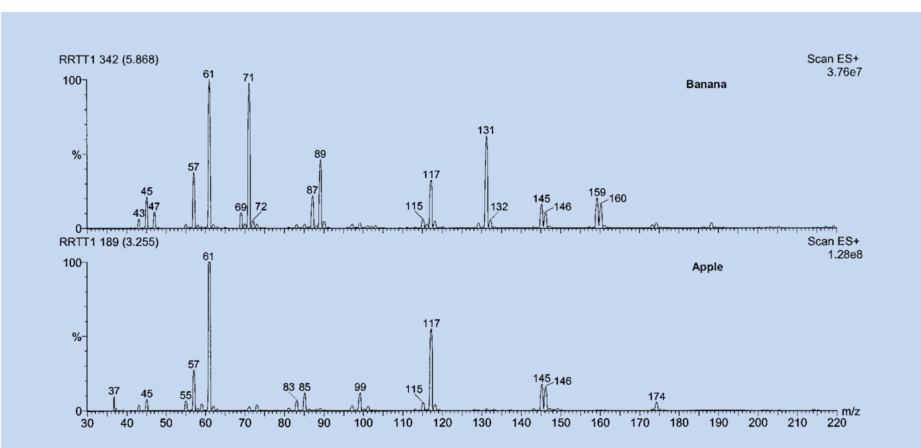

Figure 3: The aroma-ion profile of the headspace above a crushed apple and banana. The major ions (m/z 89, 117, 131, 145, 159) correspond to the masses of esters typical components of fruit aromas.

Example Application: The Aroma of Food

The aroma compounds present in foodstuffs are key characteristic components of quality. Their release during eating and their transport to the nose affect our perception of food and the delivery of the correct aroma profile to the consumer is of major importance to the food industry. The compounds present in exhaled breath are present at low concentrations and can change rapidly, even over the course of a single exhalation. The APcI-GPA, with its high sensitivity and rapid response rates, has been used to follow the concentration of aroma compounds in the exhaled breath of people eating a range of foods.

The examples shown here are for the analysis of apples and bananas. APCI-GPA can be used for rapid sample aroma profiling - samples can simply be eaten and, whilst chewing, the consumer breathes in and out through an adapter through which the aroma compounds present in the breath can monitored in real time. Figure 2 shows the intensity and rate of release of different compounds. Differences in flavour of the two fruits are due to the different compounds which are released during eating. For example, bananas contain isoamyl acetate (m/z 131) and ethyl acetate (m/z 89) which are not present in apples. Also, eating apples produces more (E)-2-hexenal (m/z 99) than bananas. The (E)-2-hexenal is produced by the action of enzymes released from the fruit when it is macerated, or chewed, which accounts for the profile for (E)-2-hexenal starting at a later retention time than the other compounds in the breath. The volatile compounds in the fruit can also be monitored by simply monitoring the headspace (Figure 3) for a few seconds to produce an aroma-ion profile.

For manufactured foodstuffs the effect of product formulation is often important (effect of fat content etc), yet this can be difficult to study in vitro. Measuring the aroma profile in the breath of individuals eating the food may show these differences in formulation and can be used in the development of processed foods.

Relevant Publications

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Journal of Food Science submitted May 98
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APPLICATION NOTE No. AN 301/ICA VERSION 1

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