Analysis of Volatile Organic Compounds in Human Breath by FAIMS/MS

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Overview

- Direct detection of VOCs in exhaled breath by MS and standalone FAIMS
- Comparing the performance of APCI-MS, ESI-MS, and FAIMS for breath analysis

Instrumentation and Methods

Data were collected on 3 instrumental setups: (A) Thermo Scientific LTQ XL Mass spectrometer using corona discharge atmospheric pressure chemical ionization (APCI), and a standalone micromachined FAIMS chip (flat plate linear Portable Gas Analyzer) using PSI ionization. The breathing apparatus was an Inteum Inc. mouthpiece with a one-way check valve. For MS, the apparatus fitted into a home-made ceramic-plate faceplate on the front of the fume-hood isolation chamber. For FAIMS, the apparatus was held orthogonal to, and a few centimeters above, the gas inlet.

APCI-MS Settings:
- Sheath Gas Flow Rate = 20 µl/min
- Auxiliary Gas Flow Rate = 10 µl/min
- Capillary Current = 250 µA
- Capillary Temperature = 350 °C
- APCI ion source corona current

FAIMS Settings:
- Analytical Field = 145 V
- Length of cell = 300 µm
- Methyl cellulose ion source corona current

Standards Analysis

- Blank of 95% Ethanol was used as a background. For all standards, 1 µl was injected on the ion source.

Breath Analysis

- Breath sample was pulled through a 1/4 in.-diameter glass tube from an adult subject. The sample was pulled through the FAIMS cell at a rate of 140 L/min

Results and Discussion

Direct Standard Analysis

- Figure 1: APCI-MS and FAIMS chromatogram, and a 3D plot of dispersion voltage vs. base line of air background.
- Figure 2: 3D plots of Dispersion Voltage (DV) vs. Base Line of Air Background.

Alternatives

- Figure 3: APCI-MS chromatogram, and a 3D plot of dispersion voltage vs. base line of air background.
- Figure 4: 3D plots of Dispersion Voltage (DV) vs. Base Line of Air Background.

Future Directions

- Figure 5: APCI-MS chromatogram, and spectra collected by spraying (D) 3D plots of dispersion voltage vs. base line of air background.
- Figure 6: 3D plots of dispersion voltage vs. base line of air background.

Conclusions

- Standalone FAIMS can detect VOC in breath (Fig. 2).
- Distinction possible between different compounds (Fig. 3).
- Separation/distinction possible between compounds in a single mixture (Fig. 4).
- APCI-MS and standalone FAIMS provide the capability for detection of VOCs in breath (Figs. 5, 6).
- Both can perform this breath analysis in real time.
- Distinction possible between different compounds.
- MS-MS also performed and capable of VOC detection and breath analysis in real-time, results very similar to APCI-MS so not shown.

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References