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## i) Introduction

Breath analysis is a non-invasive, repeatable method, applicable to all ages. It can be used as a diagnostic tool for measuring Volatile Organic Compounds (VOCs) that are present in exhaled breath.

Nowadays, this can be done in real-time with techniques that are capable of detecting VOCs in real time in trace level.

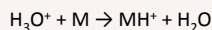
Proton Transfer Reaction Time of Flight Mass Spectrometry is such a technique, which, until recently, was mainly applied in atmospheric chemistry for the determination of VOCs in air.

This study focuses on whether drugs of abuse, such as alcohol, opioids, MDMA, cannabinoids, NPS etc. could be detected in VOCs exhaled in breath.

## ii) PTR-ToF-MS

Proton Transfer Reaction Time of Flight Mass Spectrometry is a soft ionisation technique introduced in the late 1990s. It is mainly used for the fast detection of VOCs in air. Owing to its high mass resolution and low detection limits (trace gas limits) it's been used lately for the detection of VOCs in breath.<sup>1,2</sup>

PRT-ToF-MS principle:



Ability of  $\text{H}_3\text{O}^+$  to react exothermically with VOCs and produce organic ions.<sup>3</sup>

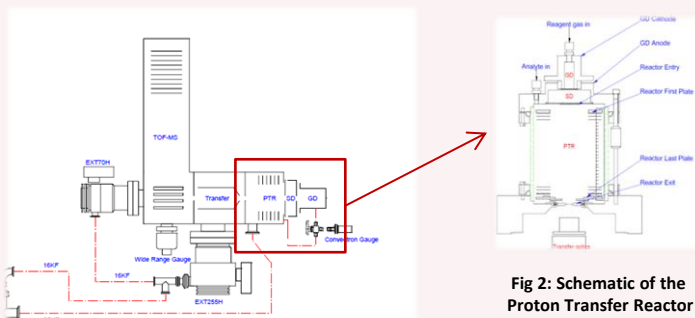


Fig 2: Schematic of the Proton Transfer Reactor

Fig 1: Schematic of PTR-ToF-MS

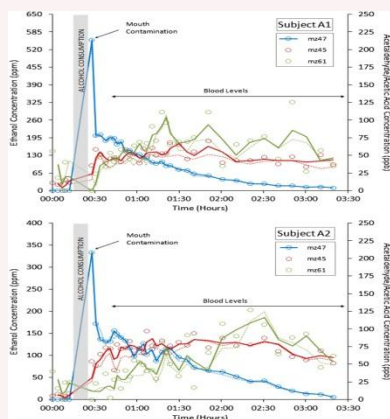


Fig 3: Breath profile of ethanol metabolism in two subjects<sup>4</sup>



Fig. 4: Real-time breath analysis

## iii) Background/gaps

Not much research has been done regarding breath analysis and drugs of abuse. The only widely known drug of abuse that has been tested a lot is alcohol.<sup>5</sup>

Only in the recent years, with breath analysis gaining ground in medical applications, have people been trying to find a way to introduce breath analysis to forensic science.

Since breath sampling is relatively straightforward and easy, using breath for testing drugs could overcome many problems faced until now, such as difficulties in sampling.<sup>5</sup>

## iv) Research Aim

- Can we detect drugs of abuse on breath?
- What kind of compounds can we detect?<sup>6</sup>
- Are there common compounds (biomarkers) for different classes of drugs of abuse?
- Can the metabolic pathway of drugs breakdown be detected in breath?
- Are there similarities between the metabolic pathway of illicit drugs? Are there similarities between the metabolic pathway of "legal highs"?

## References:

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The work leading to this invention has received funding from the European Union Seventh Framework Programme (FP7/2007-2013) under grant agreement no 607930

