



Faculty of Pharmaceutical Sciences

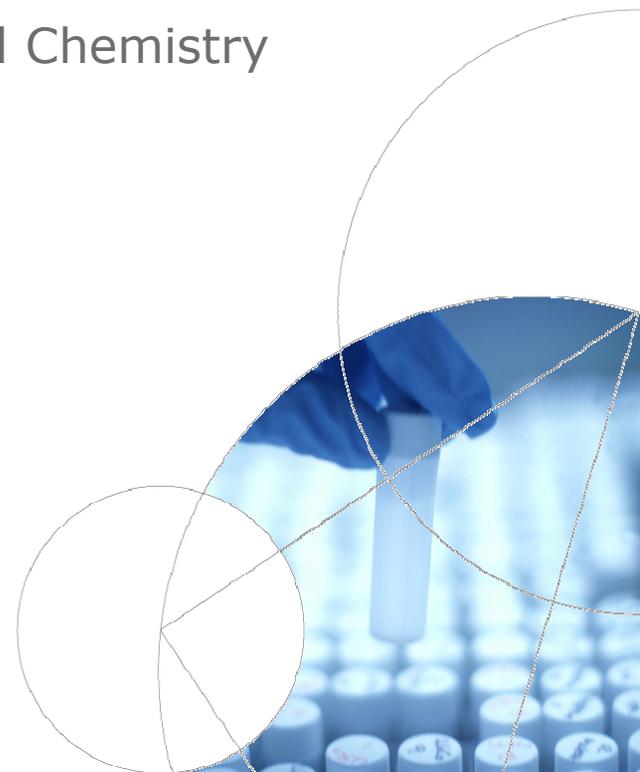


# Hot Cell MIMS:

## Direct analysis of semi-VOCs liberated from practically any type of solid sample

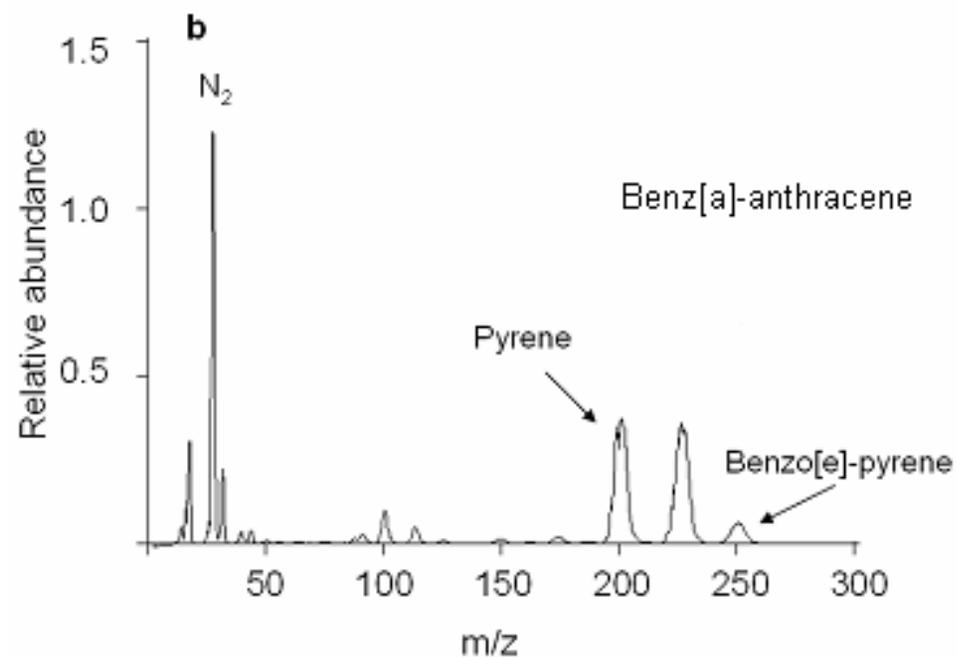
Frants R. Lauritsen

Department of Pharmaceutics and Analytical Chemistry



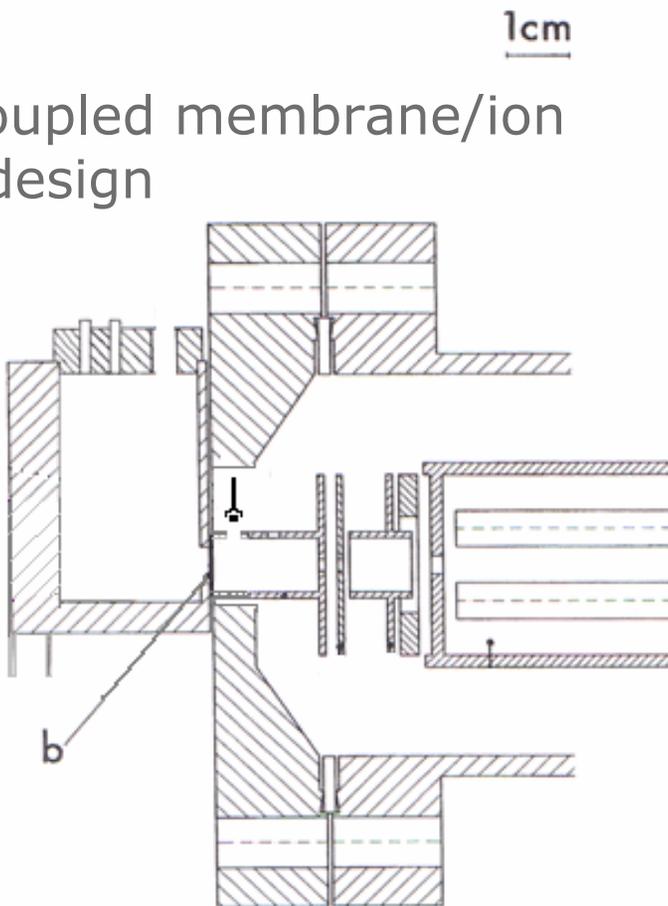
# HEMS - 2007

PAH analysis directly from soil



# Hot cell MIMS: Optimized design

Close coupled membrane/ion source design

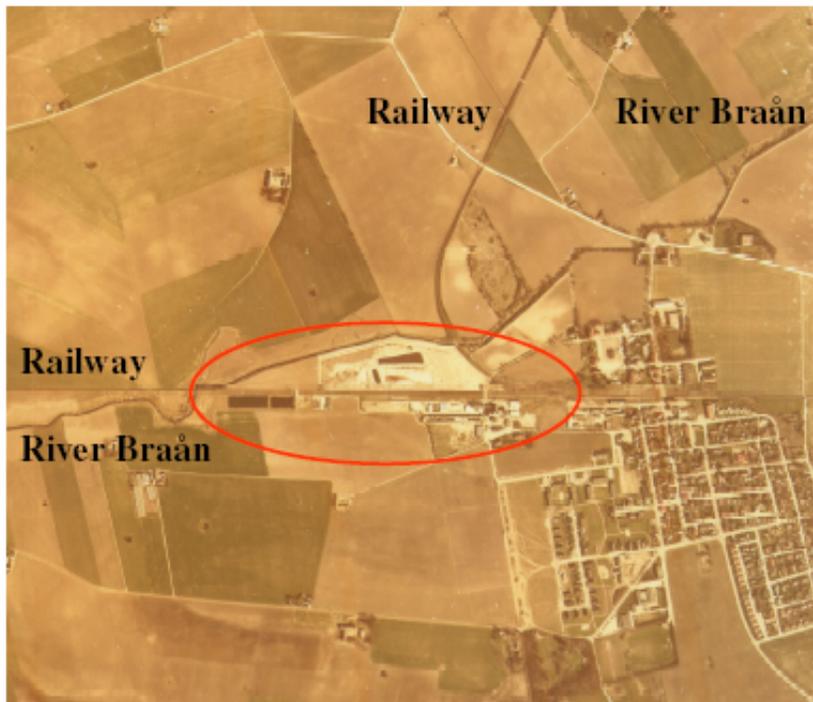


A hot cell design



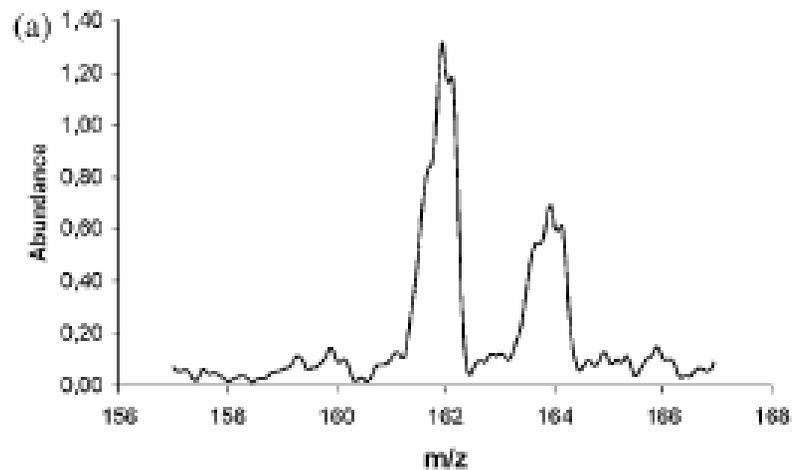
# On-site analysis of contaminants

## Aerial photo 1978 over BT Kemi site

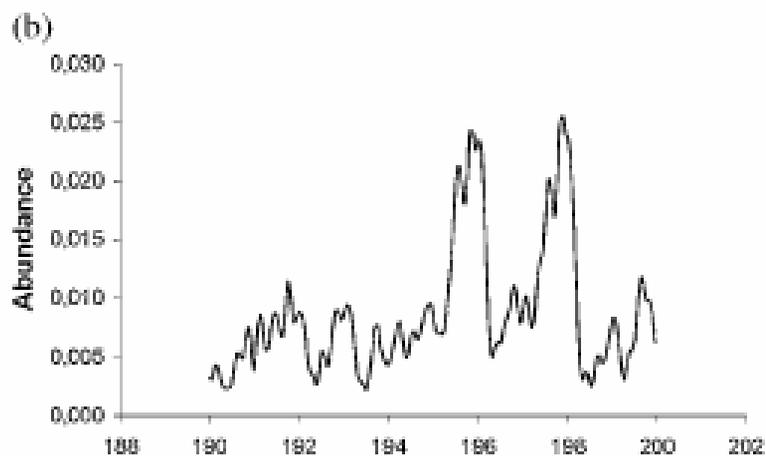
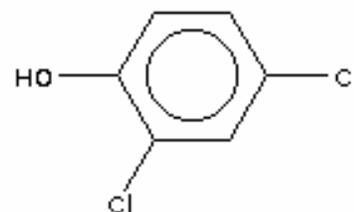


Waste sampling. Half masks was needed because of the odour.

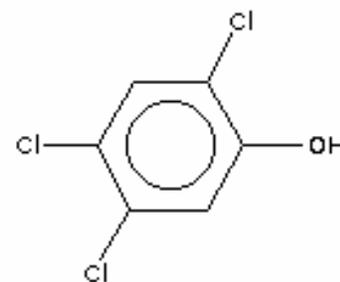
# Mass spectra of contaminated soil



2,4-dichlorophenol

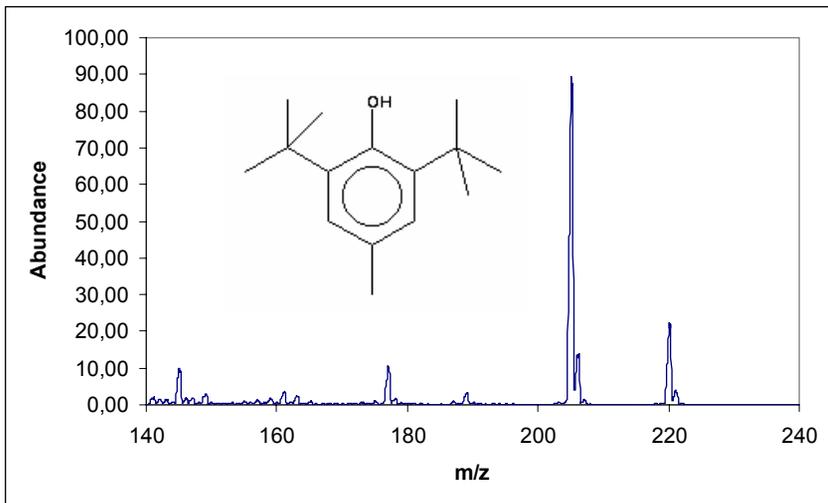


2,4,5-trichlorophenol

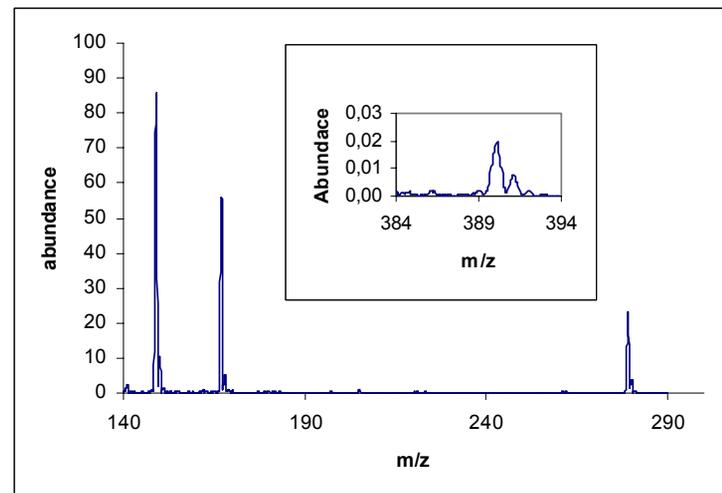


# Direct analysis of plastic materials

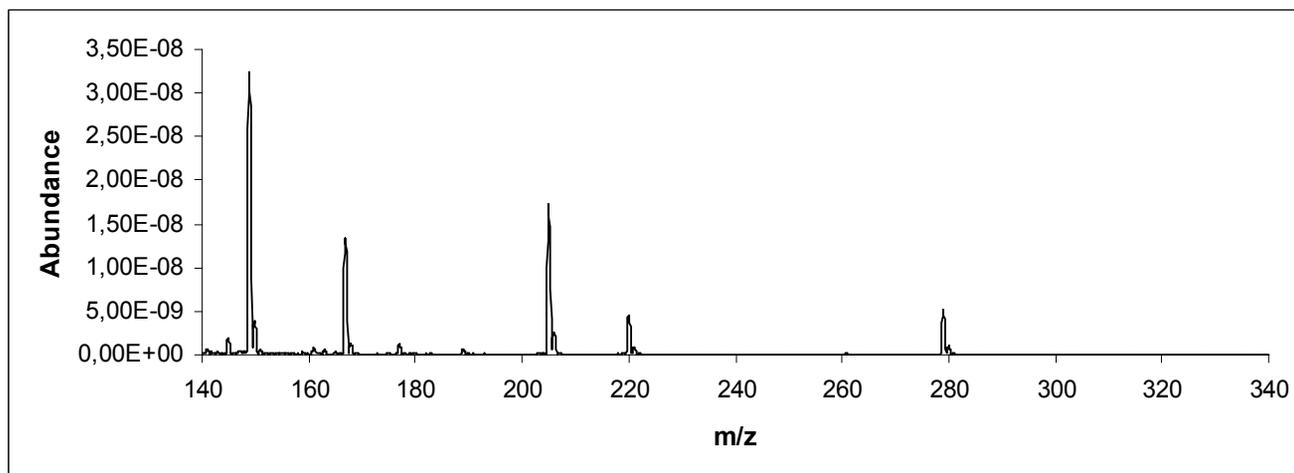
Vacuum tube of rubber



Soft PVC tube

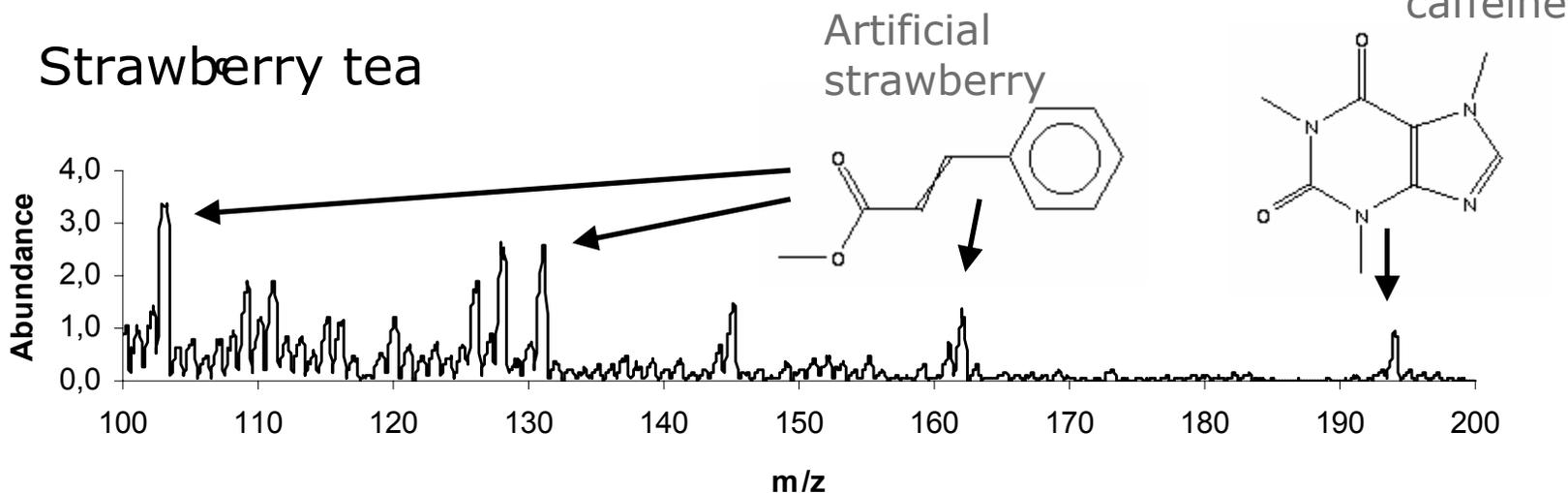


Plastic bag for medical infusion at hospitals

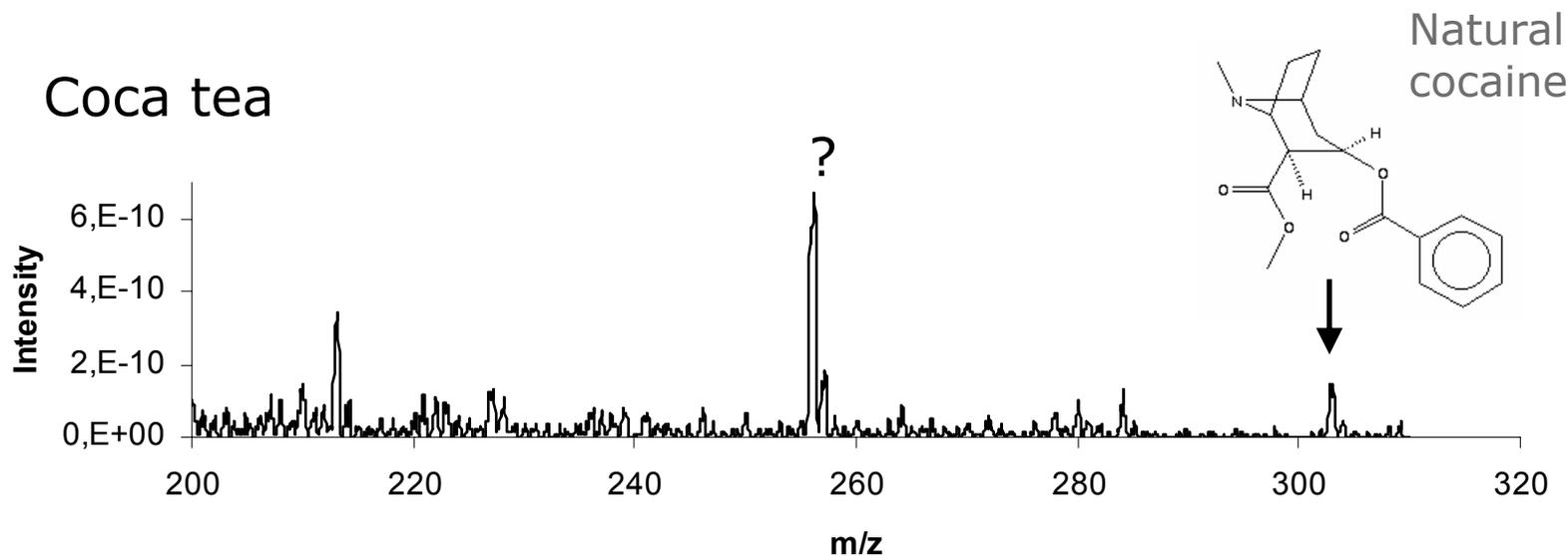


# Analysis of plant materials

## Strawberry tea

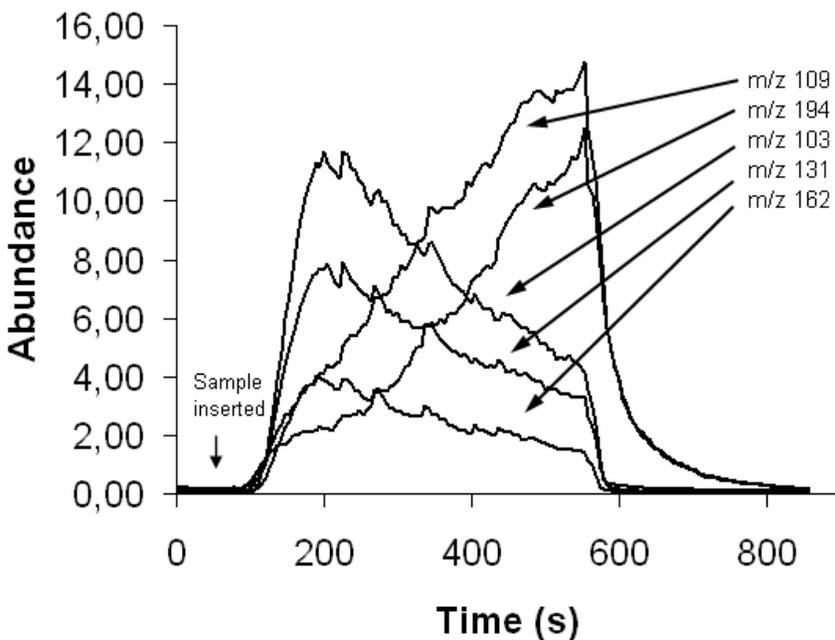


## Coca tea

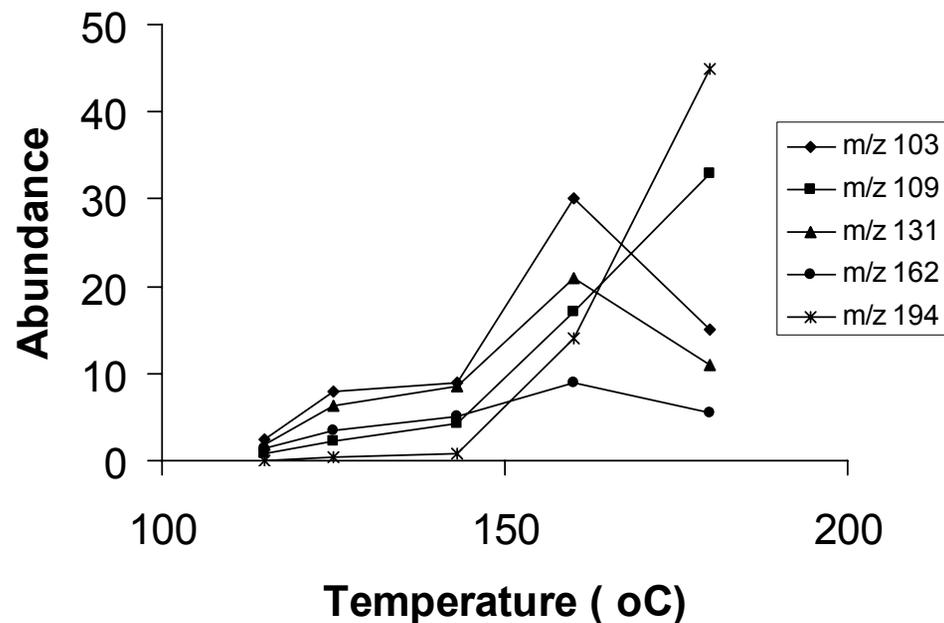


# Selectivity in hot cell MIMS without MS/MS

## Dynamics



## Cell temperature



Sample: Strawberry tea

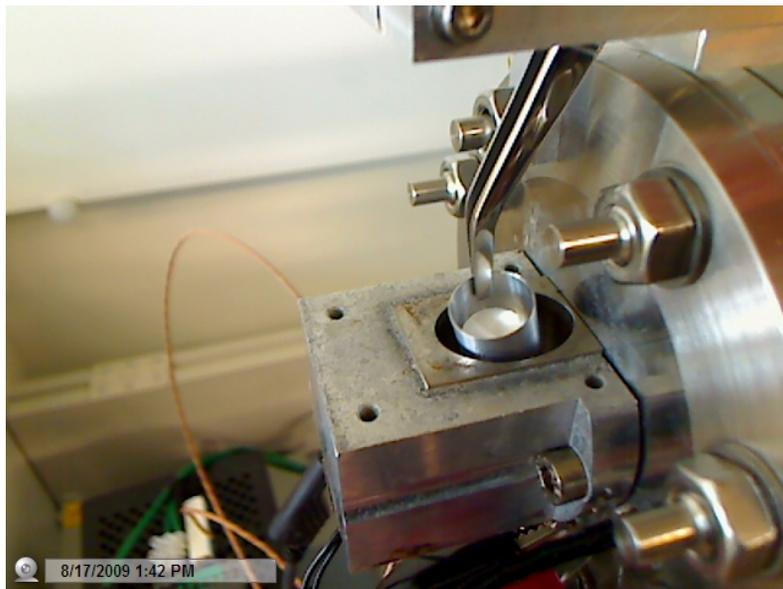
Caffeine (m/z 109 and 194)

Methylcinnamic acid (m/z 103, 131 and 162)

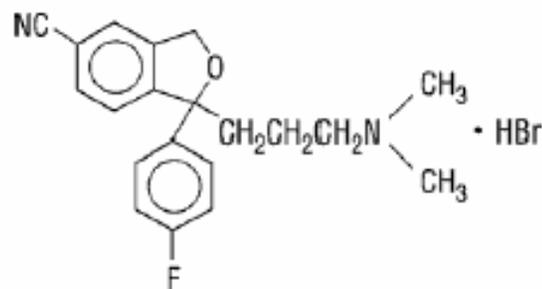


# Direct analysis of tablets

Sample cell and sample vial for direct analysis of tablets



Citalopramhydrobromide (40 mg)



MW: 405

## Tablet content (fillers):

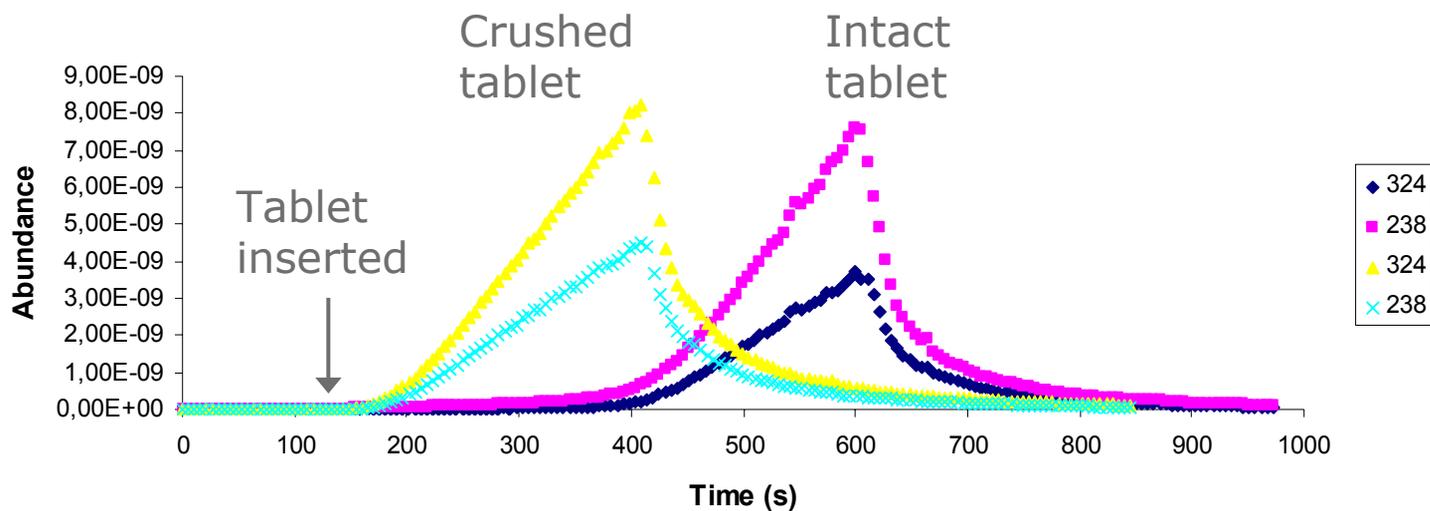
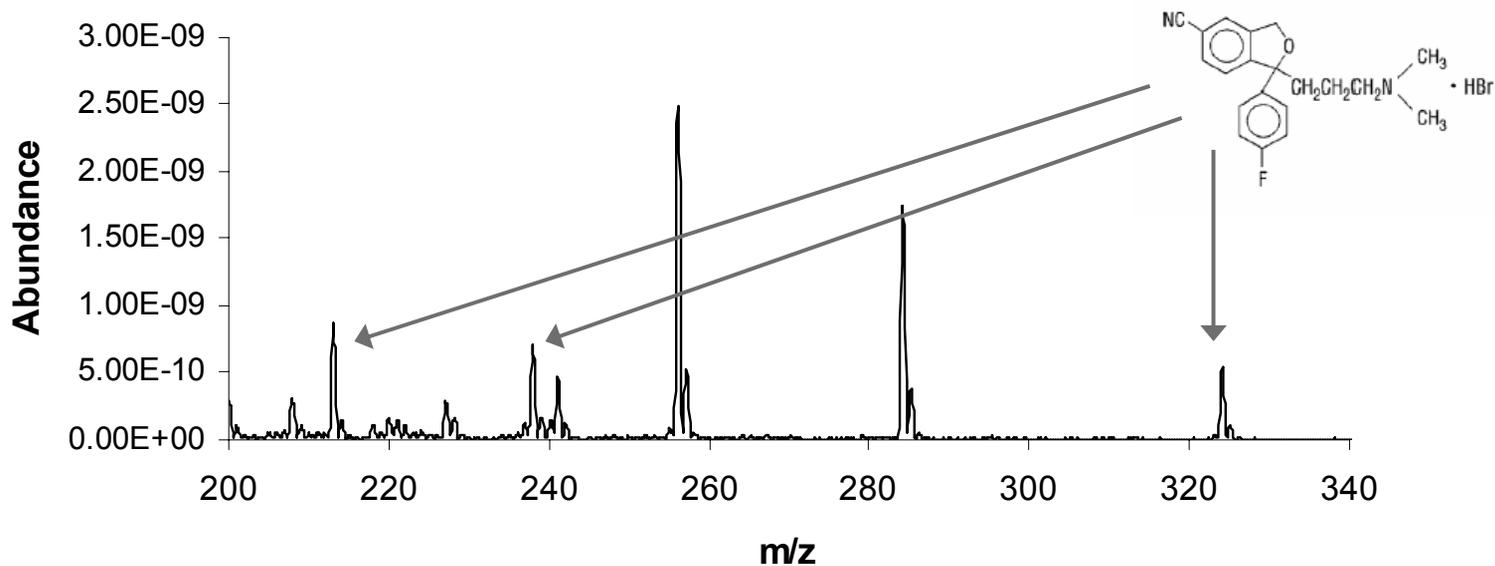
Cellulose, glycerol, corn starch, lactose monohydrate, magnesium stearate, copolyvidone, sodium cross carmellose.

## Surface coating:

Macrogol 6000 (polyethylene glycol), hypromellose, titanium dioxide

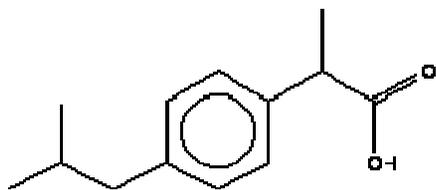


# Citalopram tablets

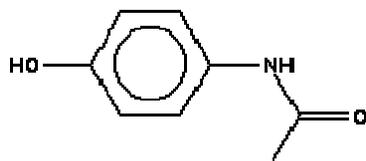


# Tested tablets/powder commonly used in suicidal attempts

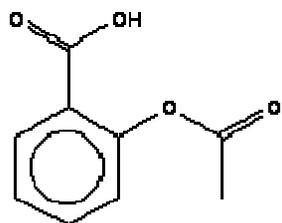
## Pain killers



**Ibuprofen**

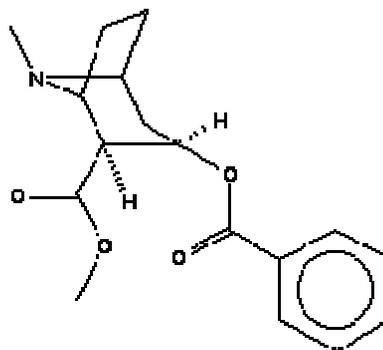


**Paracetamol**

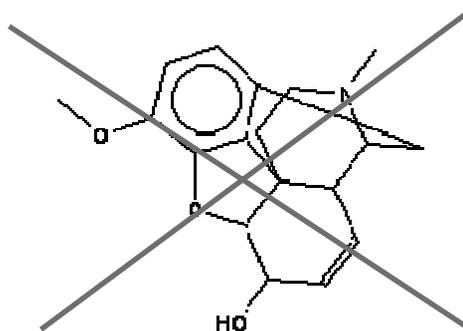


**Acetyl salicylic acid**

## Narcotics

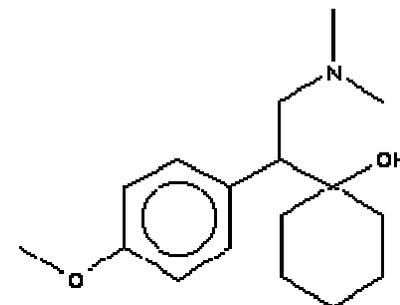


**Cocaine**

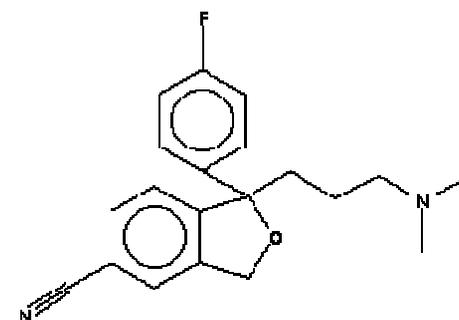


**Codeine phosphate**

## Anti depressives



**Venlafaxine**

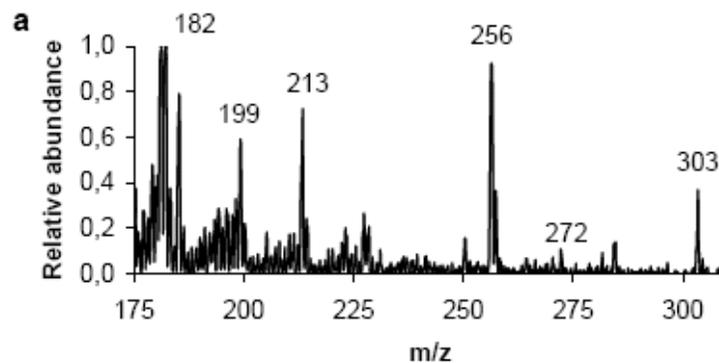


**Citalopram**

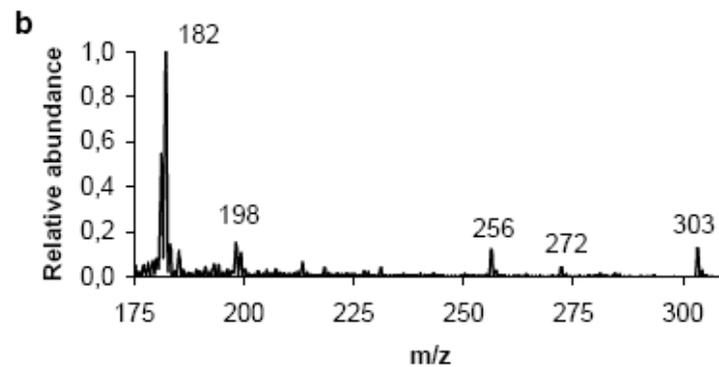


# Quantitative analysis

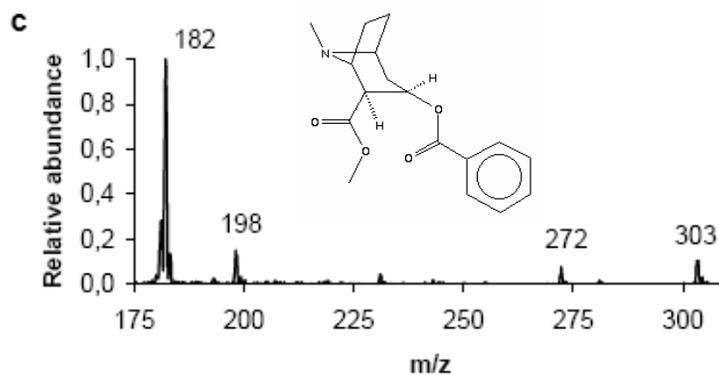
Coca plant



**Direct analysis of leaves**

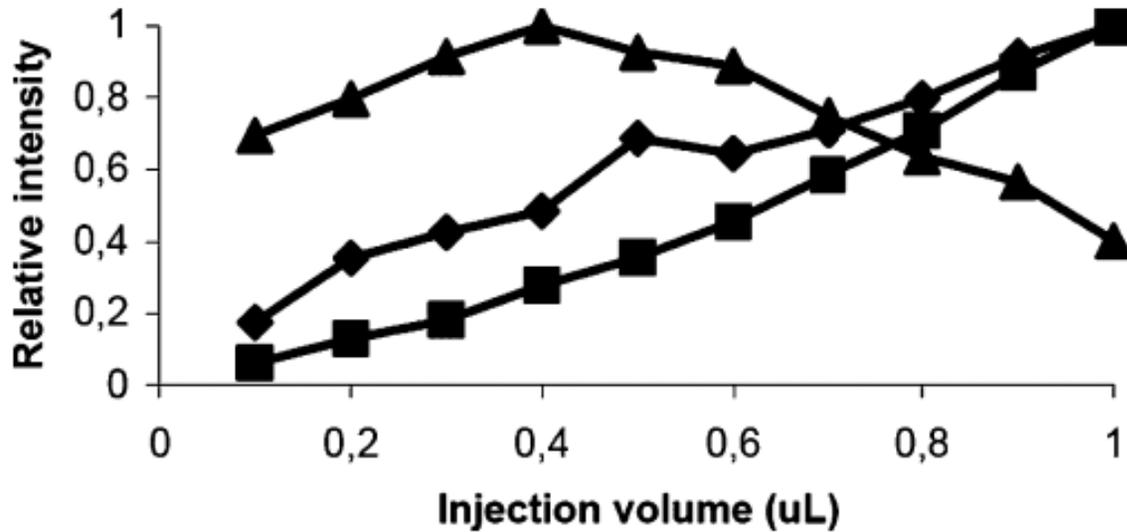


**Micro extract in methanol**



**Cocaine standard**

# Choosing a solvent



**Figure 4.** Recorded peak height from BHT as a function of sample volume.  $\blacklozenge$  BHT dissolved in toluene,  $\blacksquare$  BHT dissolved in methanol, and  $\blacktriangle$  BHT dissolved in water. For easy comparison between the solvents each solvent series was normalized to 1 for the maximum recorded peak height.



# Conclusion

With **Hot cell MIMS** it has become possible to analyse almost any solid material for its potential liberation of large hydrophobic chemicals directly and without any treatment of the sample.

Test examples:

Plastizisers and stabilisers in plastic materials

Active ingredients in plant materials

Pharmaceuticals from tablets

Contaminated soil

**Hot cell MIMS** is fully compatible with field portable mass spectrometers



# Special thanks to:

**Katrine Nielsen**

**Anders Jensen**

**Claus H. Nielsen**

**Dr. Hua Chen**

**Prof. Zhining Xia**

**Prof. Bo Svensmark**

**Mikrolab Aarhus A/S**

## **Funding**

The Danish Natural Science Council

The Danish CarlsbergFonden





