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Rapid food analysis by ambient mass spectrometry

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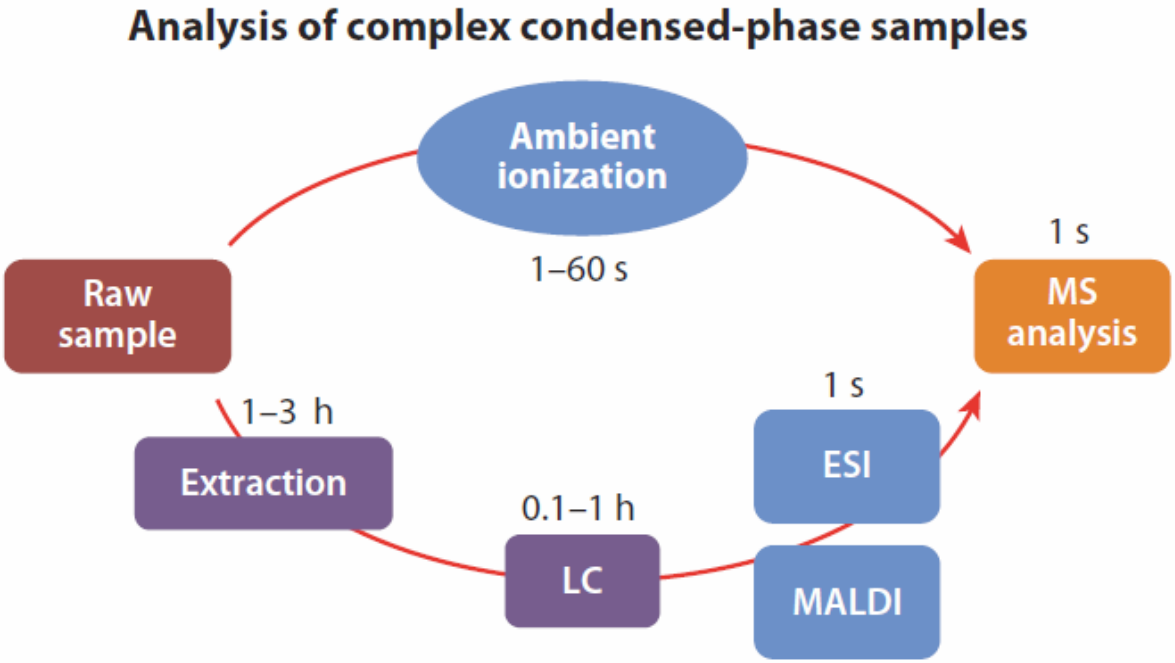
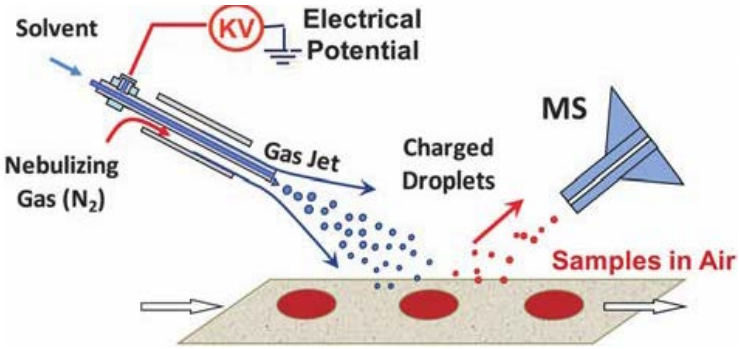
Outline:

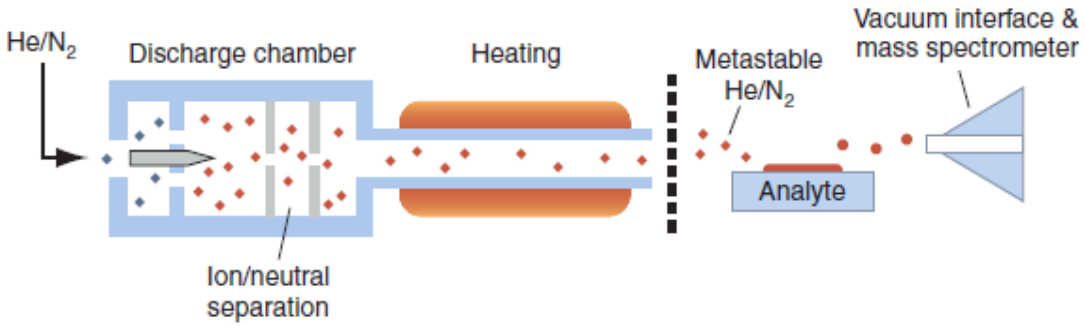
1. Introduction
2. Authentication analysis
3. Food packaging products analysis
4. Exposure pollution analysis
5. Disadvantages of AMS
6. Perspective

Introduction





DESI
(Desorption electrospay ionization)



DART
(Direct analysis in real time)

Advantage: needs few or no sample pretreatment & no LC separation

Annu. Rev. Phys. Chem. 2013.64:481-505.

Introduction

Food packaging products

(Environmental Hormone)

(semi-) Quantification

(targeted pollutant)

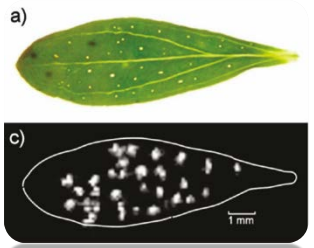
Fast & Simple;

High selectivity

AMS

Screening

(contaminant)

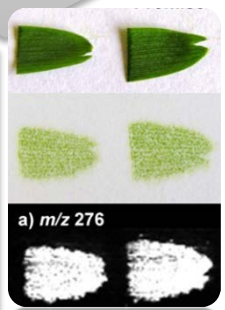


Authentication

(Marker compound)

Imaging

(biological source)

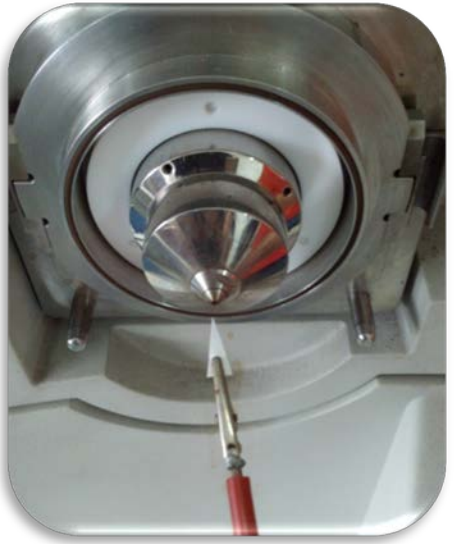


Anal. Chem. 2011, 83, 3256–3259
J. Mass. Spectrom. 2011, 1241–1246
J. of Anal. and Applied Pyrolysis 2012, 95, 134–137
J. Agric. Food Chem. 2010, 58, 4617–4625
J. Chromatogr. A 2012, 1259 ,179– 186
J. Am Soc Mass Spectrom 2009, 20, 2304–2311
Rapid Commun. Mass Spectrom. 2014, 28, 682–690

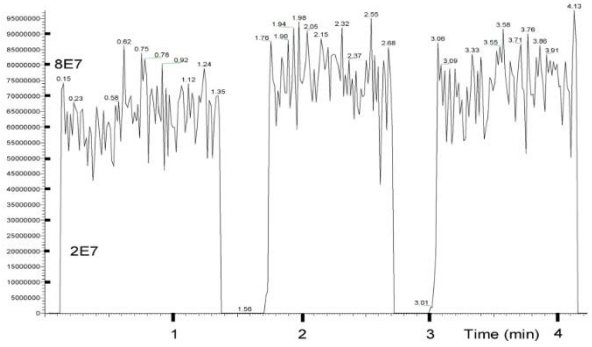
DESI, Direct spray

Fruit Spray

Leaf Spray

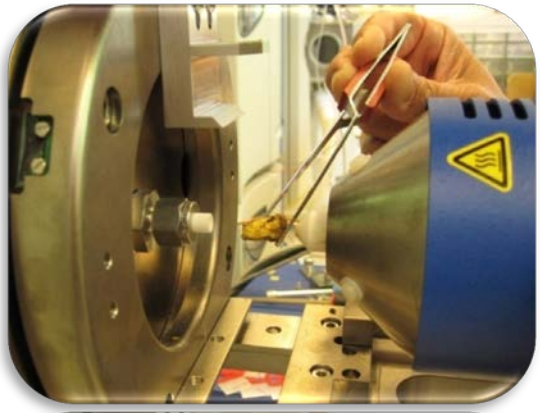


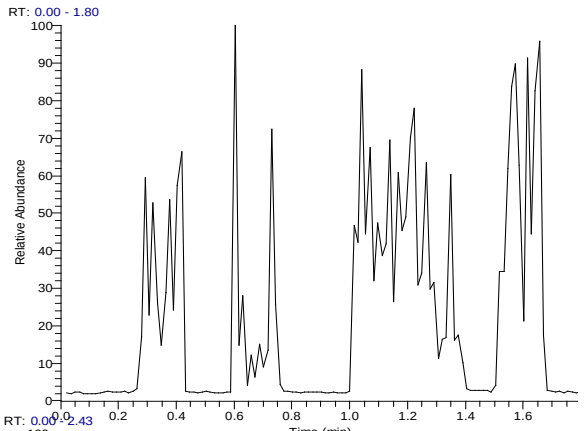
Paper Spray



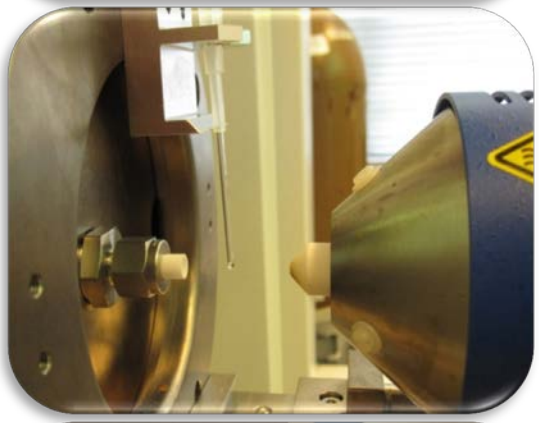
DART

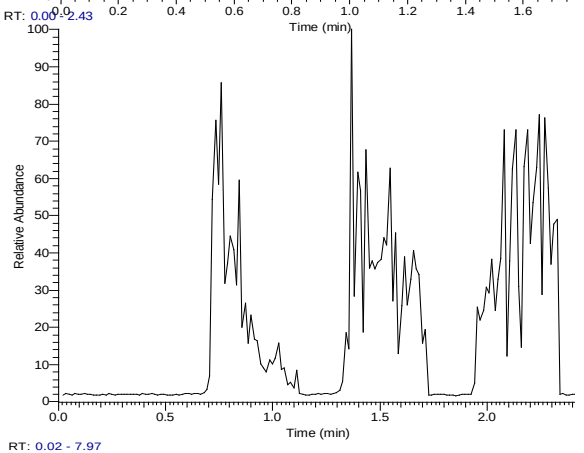
Solid Sample



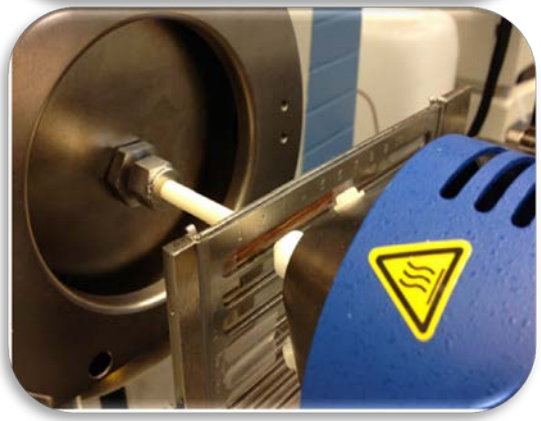


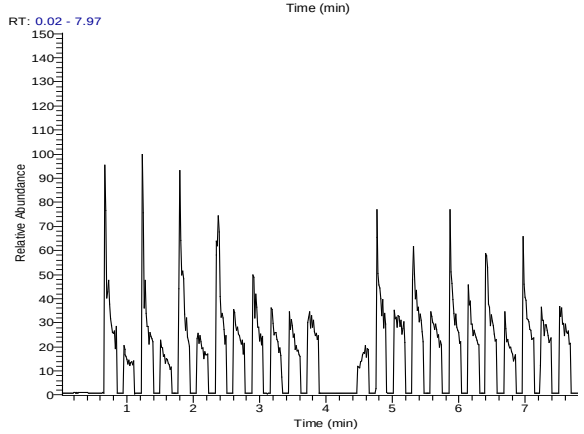
Liquid Sample





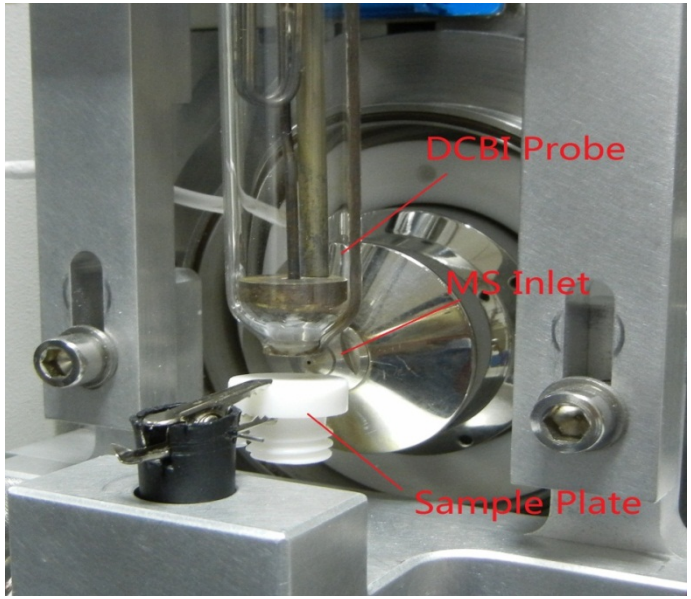
Automatic sampling

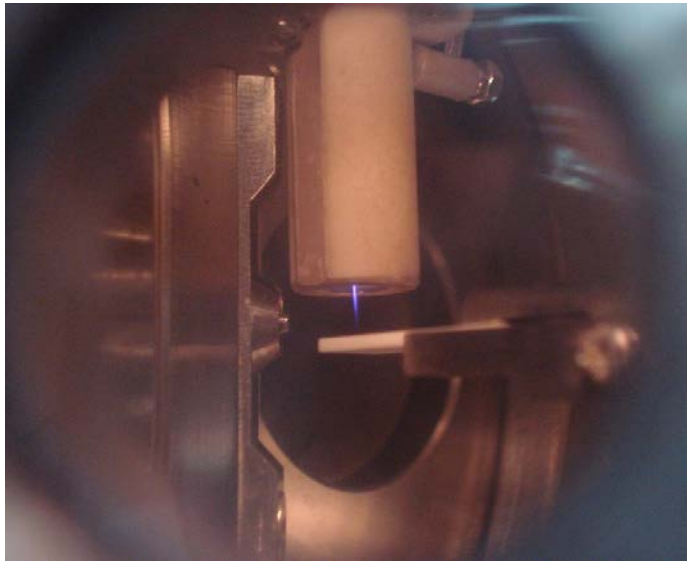




DCBI

(Desorption corona beam ionization)





Authentication

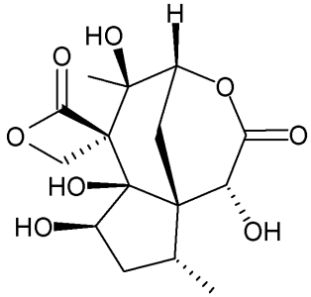
DART-HRMS / Fruit Spray-HRMS --- Star anise

Illicium anisatum

Illicium verum

Japanese star anise

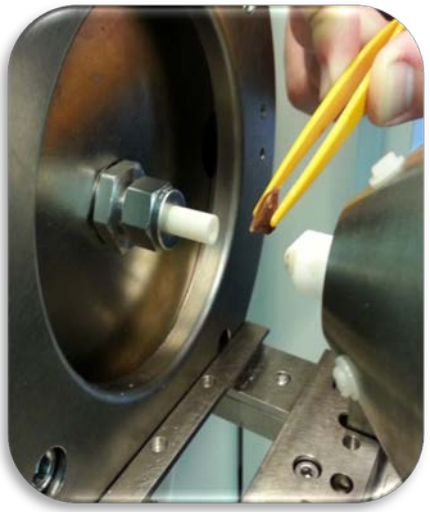
Chinese star anise



Anisatin

In 2001 in Holland poisoning by Chinese star anise tea contaminated with Japanese star anise: epilepsy, hallucinations, heart problems, nausea.

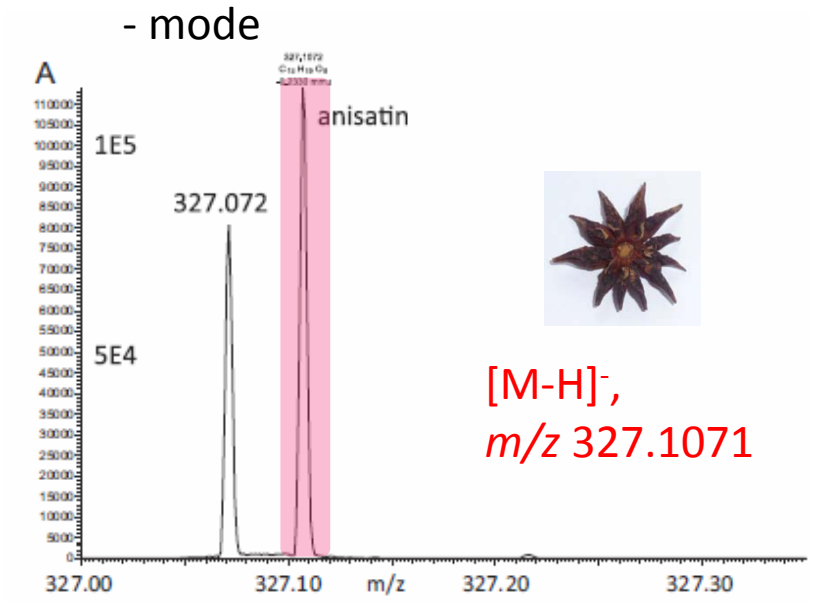
Neurotoxin: anisatin



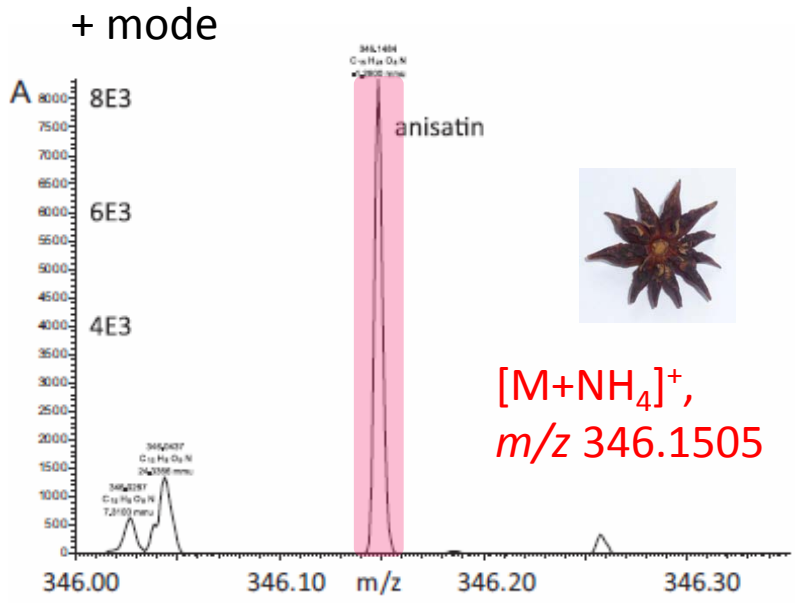
J. Chromatogr. A 2012, 1259 ,179– 186
J. Chromatogr. A 2013, 1317, 246– 253

Authentication

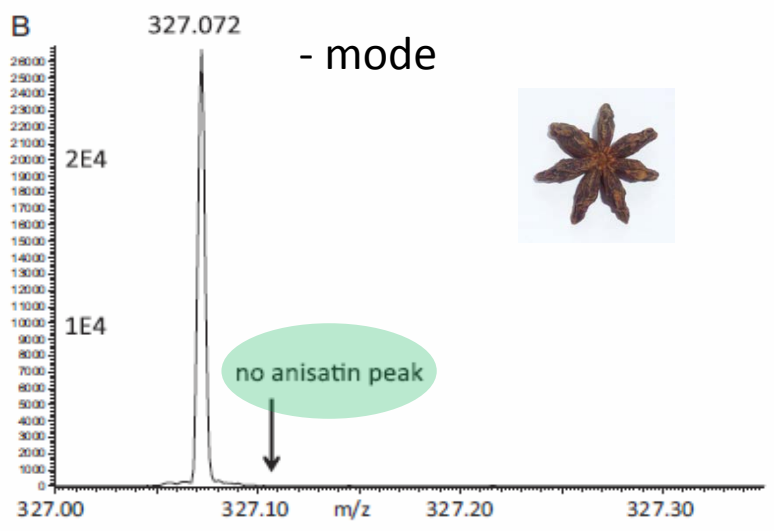
DART-HRMS

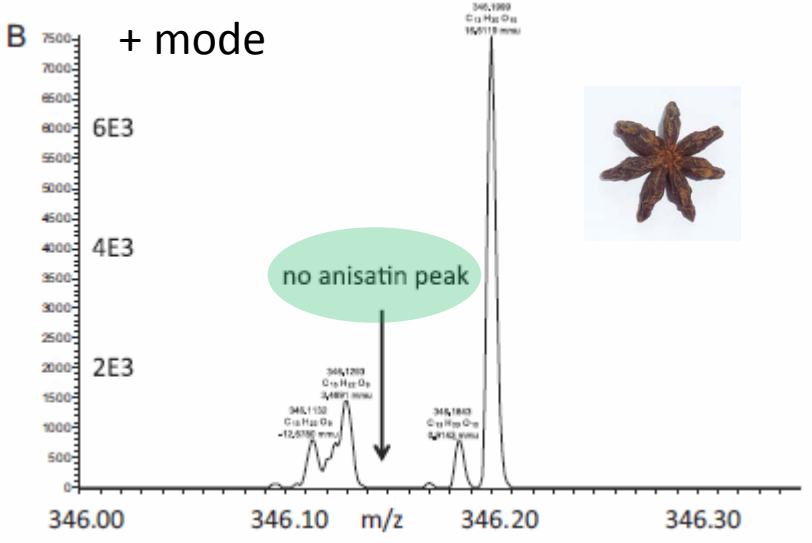


$[M-H]^-$, *m/z* 327.1071



$[M+NH_4]^+$, *m/z* 346.1505

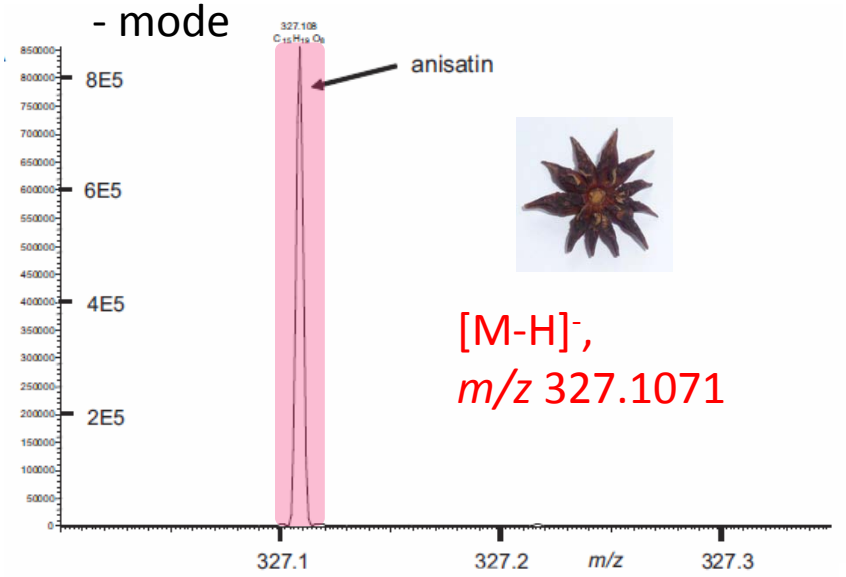


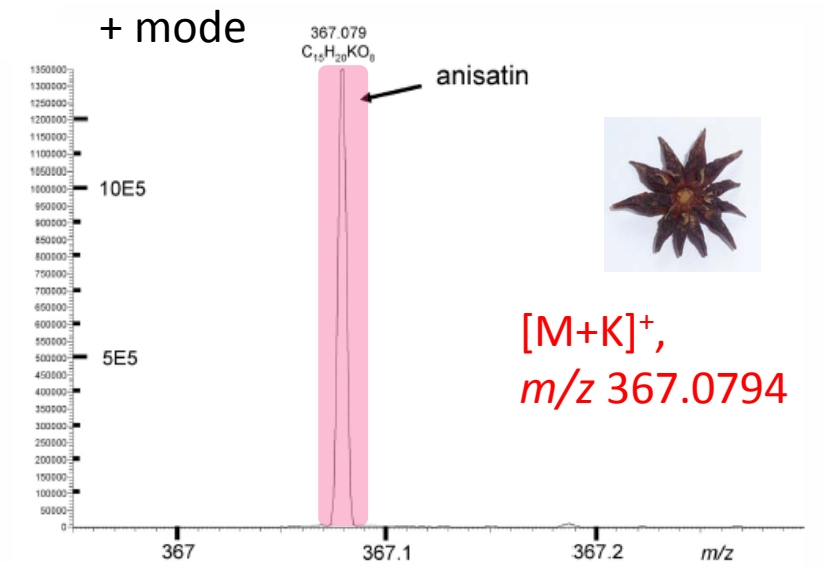


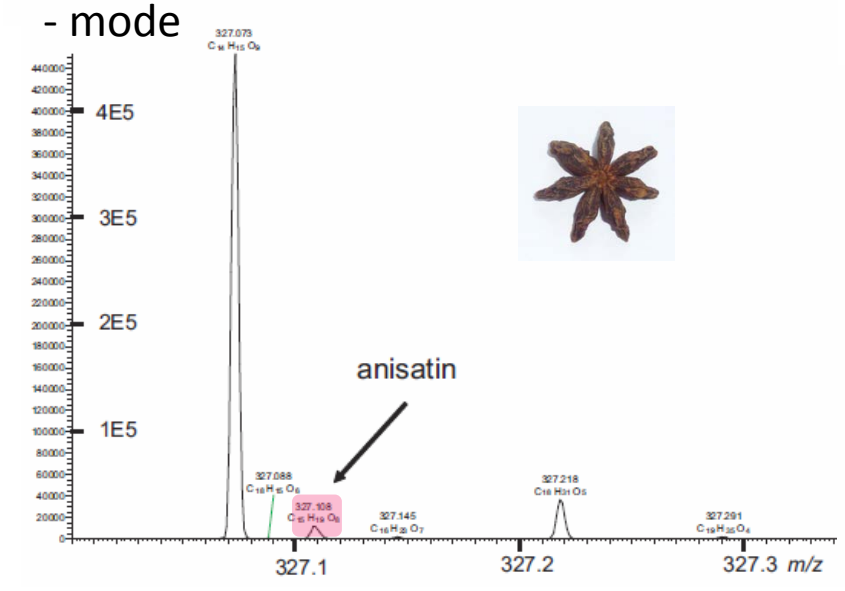
HR-MS necessary ! In both samples is $C_{14}H_{15}O_9$, *m/z* 327.07212 present (- mode)

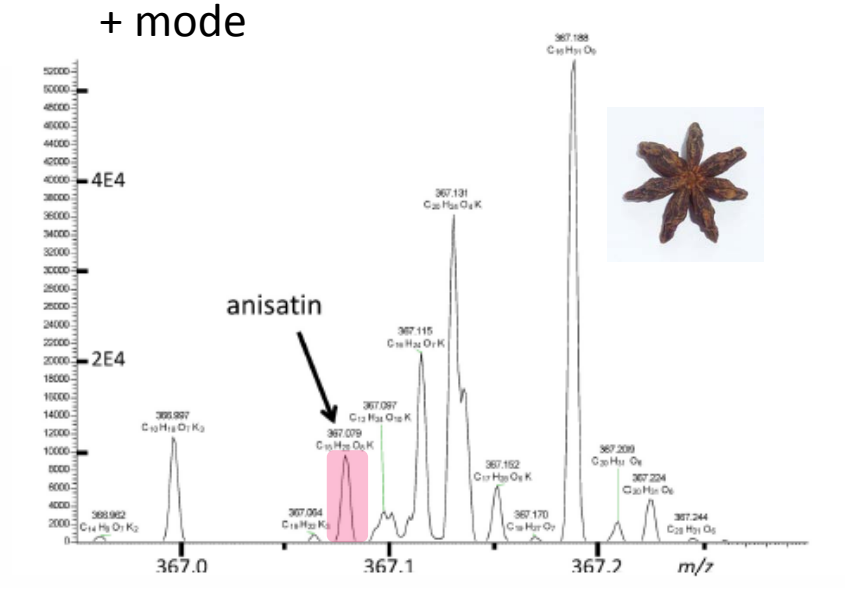
Authentication

Fruit spray-HRMS

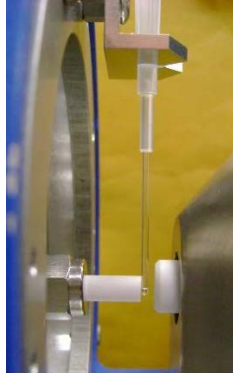


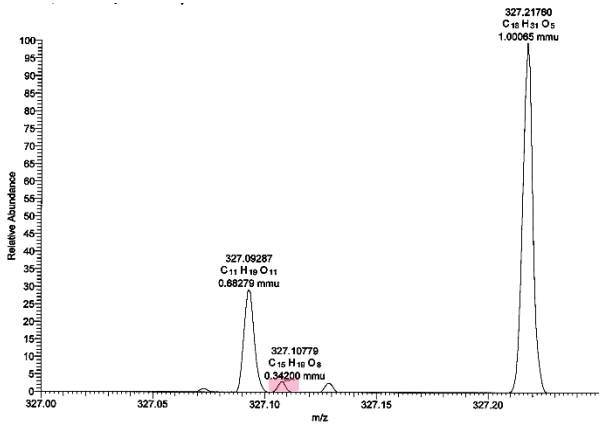




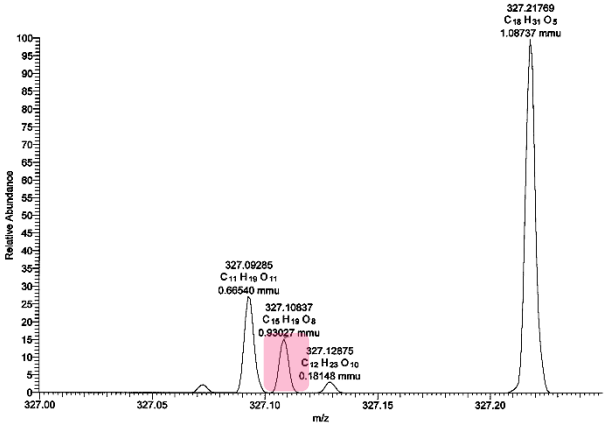


Semi-quantification

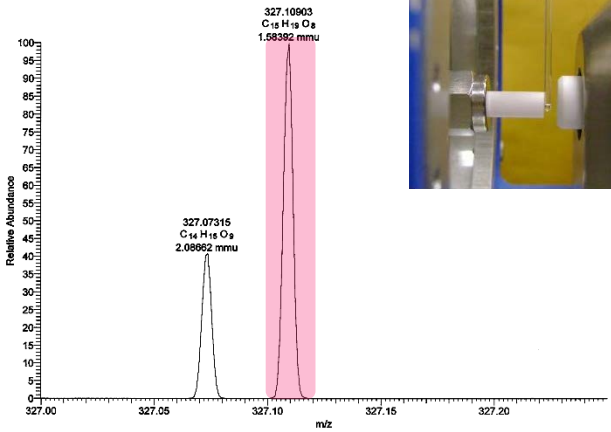




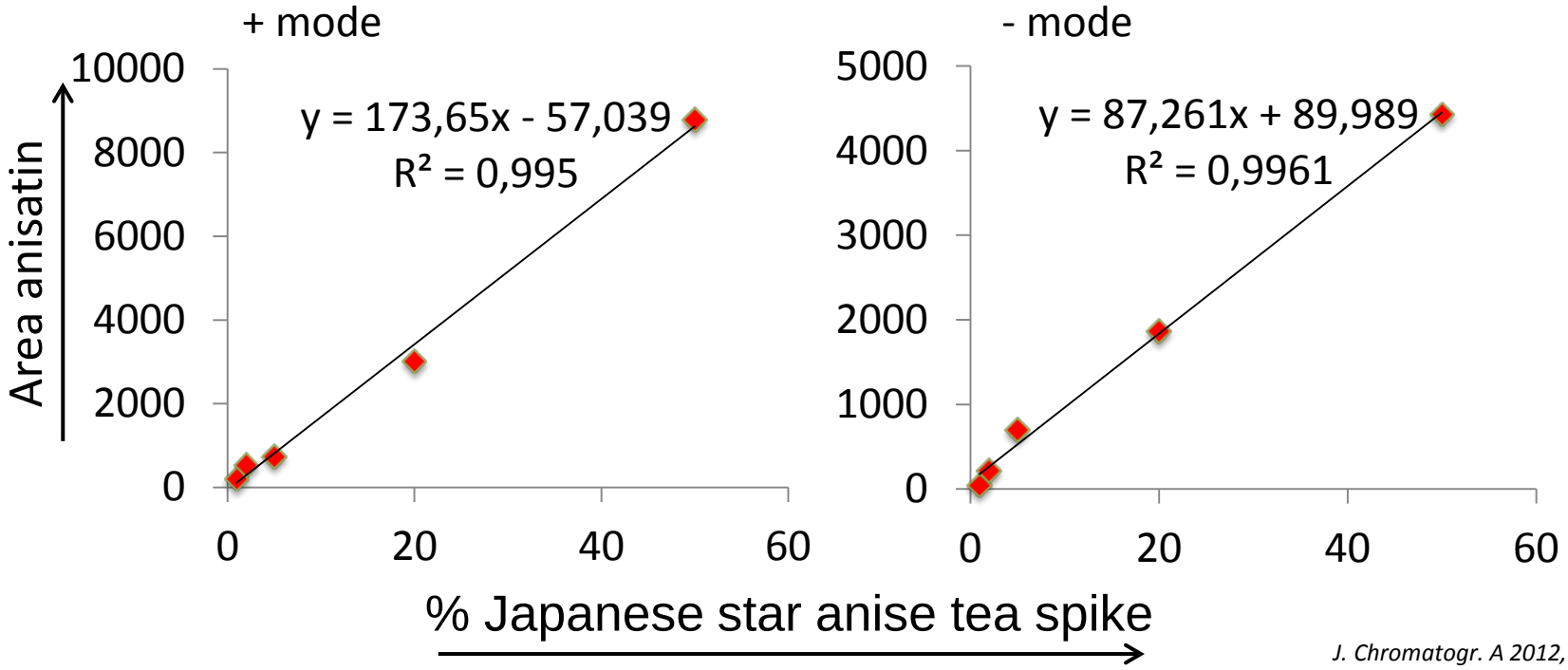
Chinese star anise tea



star anise tea spiked with 1% "Japanese star anise tea"



"Japanese star anise tea"



J. Chromatogr. A 2012, 1259 ,179– 186

Authentication

Comparison

Raw plant

- Grind dried plant
- Extract with hexane, filter
- Dry 30 min at 100 ºC
- Sonication 30 min in MeOH
- Centrifuge 10 min
- Evaporate 4 mL with N_2
- Redissolve in 3 mL water
- Centrifuge 5 min
- Apply to Extrelut, 10 min
- Elute with 12 mL MTBE
- Evaporate with N_2
- Dissolve in MeCN-water
- LC-ESI-MS/MS

About 90 min

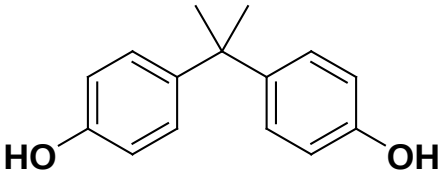
- An unambiguous distinction
- Within seconds
- Without any sample pretreatment

Hold one carpel of Star Anise analysed by DART-HRMS

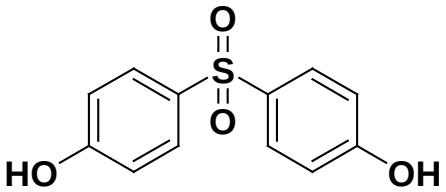
Data analysis

Food packaging products

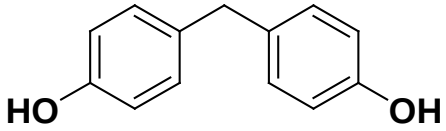
PS-MS --- Bisphenol A and Its Analogues



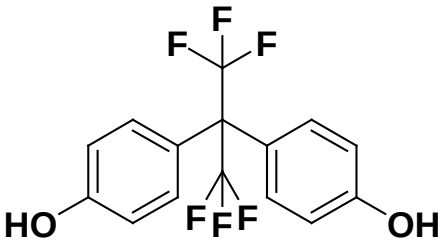
1. Bisphenol A



2. Bisphenol S



3. Bisphenol F

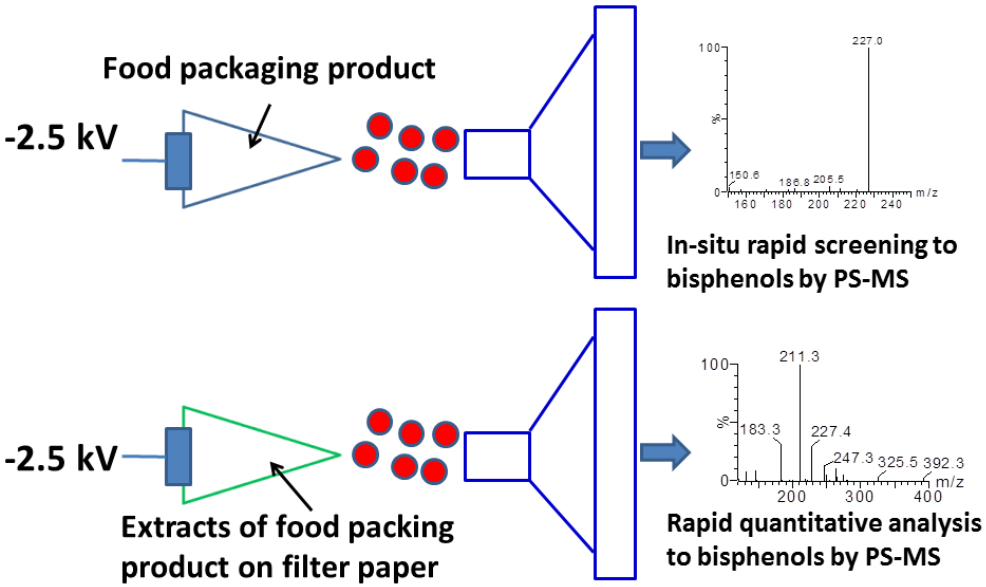


4. Bisphenol AF

- Used in plastic food packaging products, including baby bottles, drinking containers, and snack packaging
- Migrate into food
- Environmental Hormone , or Endocrine Disrupting Chemicals， EDCs

J. Agric. Food Chem. 2017, 65, 4859−4865.

Food packaging products



Rapid in situ screening and simultaneous quantitative analysis (bisphenol A-d_{16} used as I.S.) by paper spray

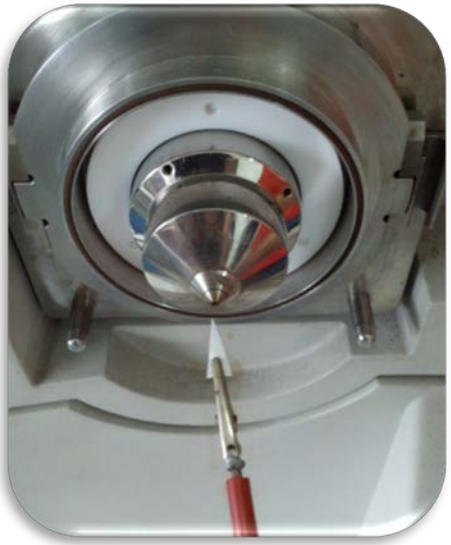


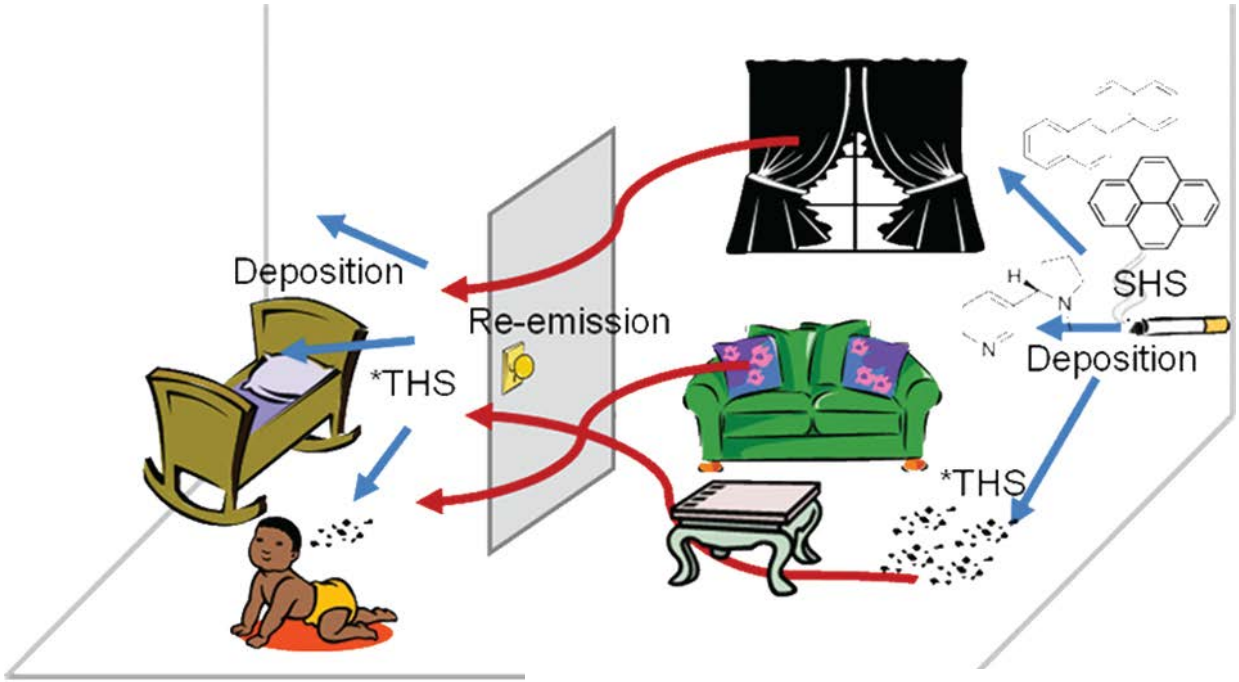
Table 1. Comparison Results between PS-MS and HPLC-MS/MS

	PS-MS (mg/kg) (n = 5)		HPLC-MS/MS (mg/kg) (n = 5)	
sample	1	2	1	2
paper cup	12.2 ± 0.7	nd[a]	11.8 ± 0.3	nd
baby bottle 1	nd	7.9 ± 0.3	nd	8.5 ± 0.2
baby bottle 2	34.6 ± 2.5	nd	36.2 ± 1.3	nd
food packaging paper	67.2 ± 5.7	nd	69.9 ± 2.4	nd
food packaging film	32.3 ± 1.7	nd	33.7 ± 0.9	nd

[a]Not detected.

Exposure pollution

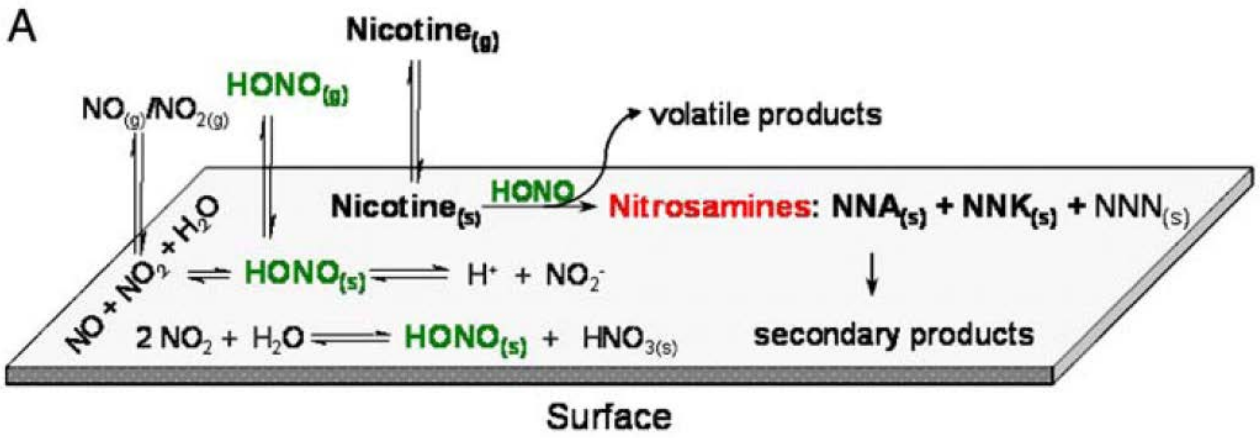
DCBI-MS/MS --- Third hand smoke (THS)



*Thirdhand Smoke

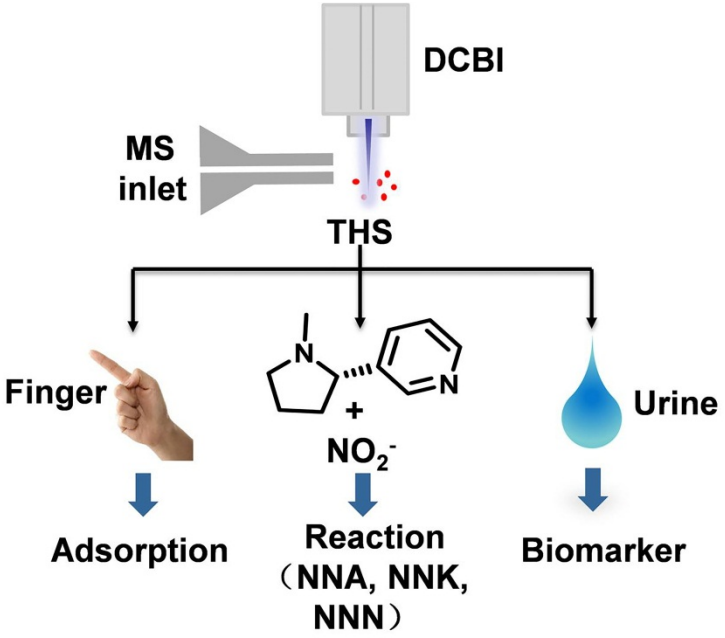
- Re-emission
- Remain
- Reaction, e.g with ambient nitrous acid (HONO)

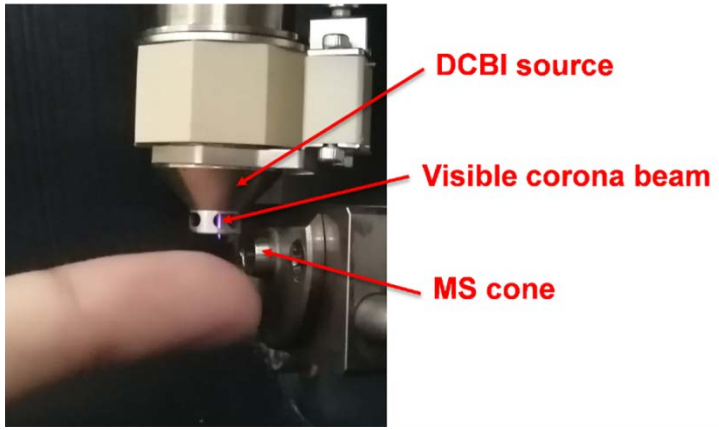
Formation of tobacco-specific nitrosamines (TSNAs).



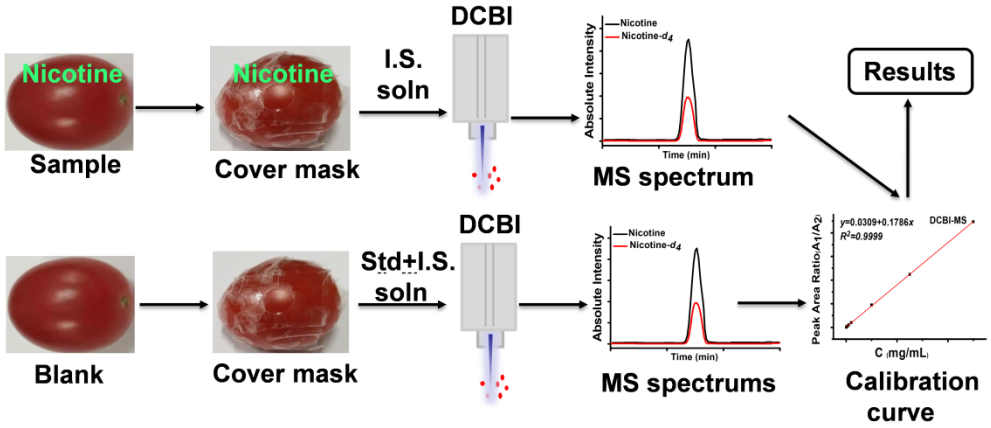
Environ. Sci. Technol. 2012, 46, 4174–4183

Exposure pollution



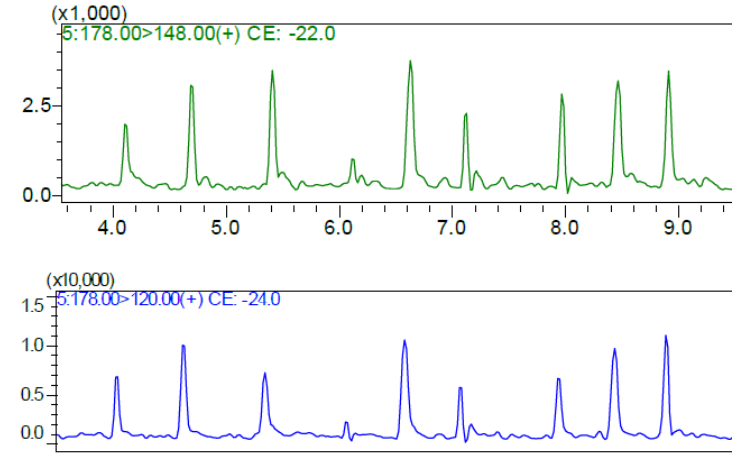


In-situ analysis on finger surface



Quantification analysis

NNN



In-situ monitoring TSNAs forming on the contaminated sausage surface

Disadvantages of AMS

- There is a certain amount of “noise” present in the spectrum.
- Accurate quantification is limited.
- Ionization suppression in complex matrix affects sensitivity.

Perspective

- Developing new sample pretreatment methods.
- Developing new ionization probes.
- Synthesizing Isotope internal standards and developing isotope-coded derivatization strategies.
- Developing portable mass separator for analysis in field.

Acknowledgement

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Professor Shouzhuo Yao
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