# INOVATIVNÍ IONTOVÉ ZDROJE

Jan Buček

# DART (Direct Analysis in Real Time)

DART (Direct Analysis in Real Time)

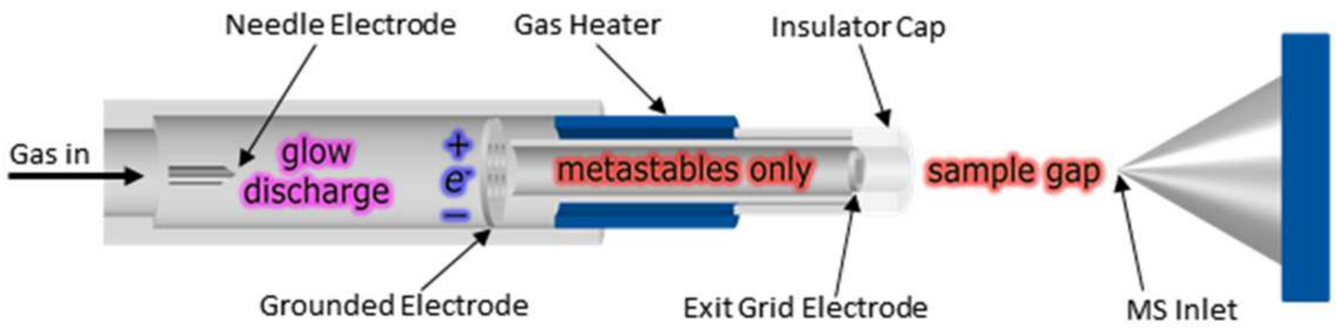
SESI (Secondary Electrospray Ionization)

DART (Direct Analysis in Real Time)

SESI (Secondary Electrospray Ionization)

SICRIT (Soft Ionization by Chemical Reaction in Transfer)

# DART (Direct Analysis in Real Time ) - Princip fungování



# DART SVP (Standard Voltage and Pressure) - Interface

# DART SVP (Standard Voltage and Pressure) - Interface



Multi DIP-it Holder

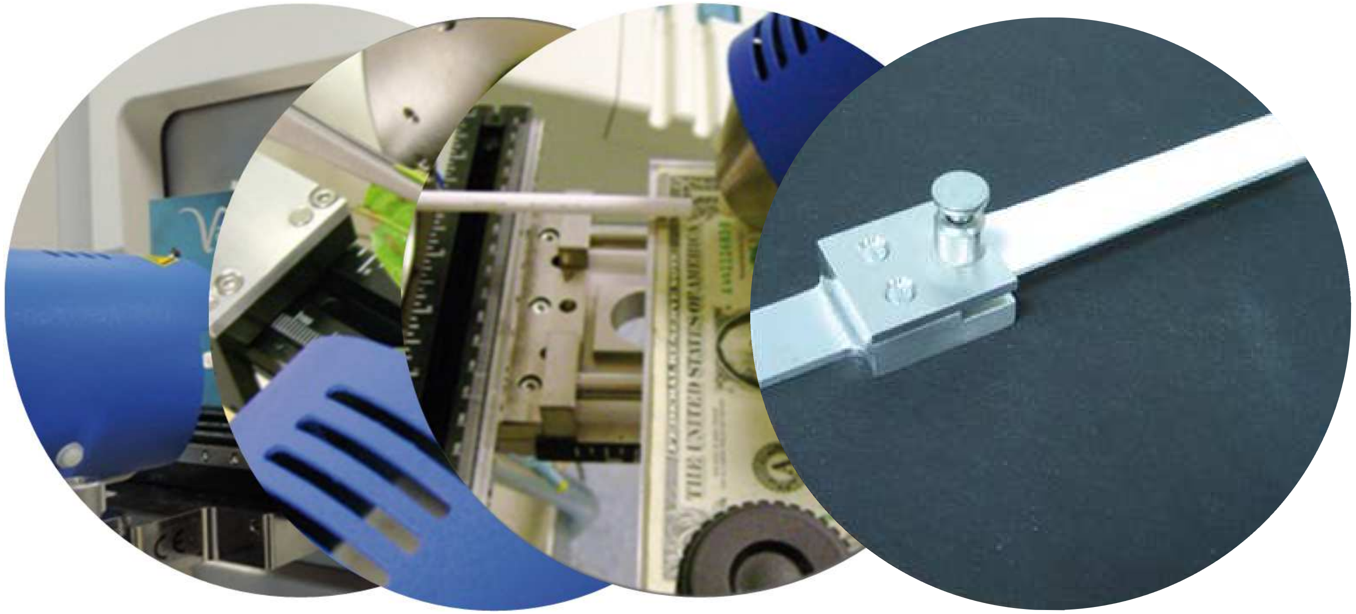
# DART SVP (Standard Voltage and Pressure) - Interface


Adjustable Tweezer Base

# DART SVP (Standard Voltage and Pressure) - Interface

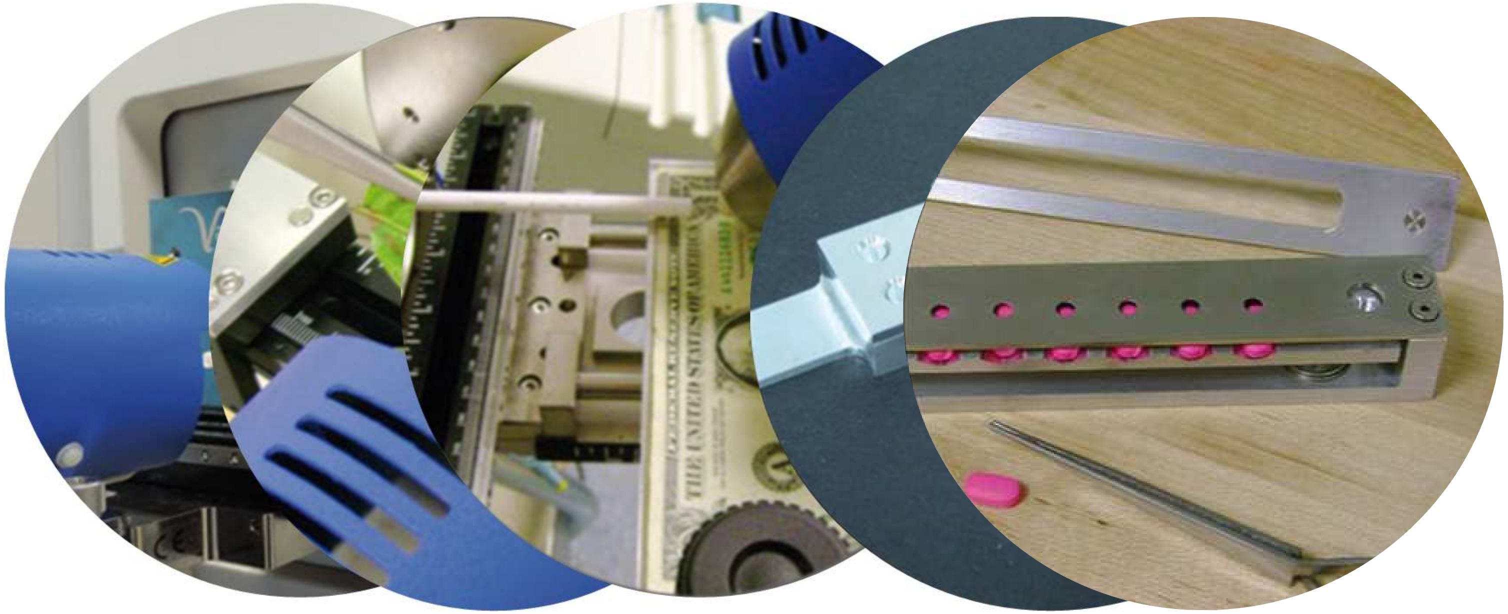

XY Scanner

# DART SVP (Standard Voltage and Pressure) - Interface

TLC Block

# DART SVP (Standard Voltage and Pressure) - Interface

Tablet Carrier

# DART SVP – Aplikace

Anal Bioanal Chem (2012) 403:2807–2812
DOI 10.1007/s00216-012-5853-6

TECHNICAL NOTE

## Evaluating a direct swabbing method for screening pesticides on fruit and vegetable surfaces using direct analysis in real time (DART) coupled to an Exactive benchtop orbitrap mass spectrometer

**Elizabeth Crawford · Brian Musselman**

Received: 16 December 2011 / Revised: 31 January 2012 / Accepted: 7 February 2012 / Published online: 25 February 2012


**Abstract** Rapid screening of pesticides present on the surfaces of fruits and vegetables has been facilitated by using a Direct Analysis in Real Time (DART®) open air surface desorption ionization source coupled to an Exactive® high-resolution accurate mass benchtop orbitrap mass spectrometer. The use of cotton and polyester cleaning swabs to collect and retain pesticides for subsequent open air desorption ionization is demonstrated by sampling the surface of various produce to which solutions of pesticides have been applied at levels 10 and 100 times below the tolerance levels established by the United States Environmental Protection Agency (US EPA). Samples analyzed include cherry tomatoes, oranges, peaches and carrots each chosen for their surface characteristics which include: smooth, pitted, fuzzy, and rough respectively. Results from the direct analysis of fungicides on store-bought oranges are also described. In all cases, the swabs were introduced directly into the heated ionizing gas of the DART source resulting in production of protonated pesticide molecules within seconds of sampling. Operation of the orbitrap mass spectrometer at 25,000 full-width half maximum resolution was sufficient to generate high-quality accurate mass data. Stable external mass calibration eliminated the need for addition of standards typically required for mass calibration, thus allowing multiple analyses to be completed without instrument recalibration.

Published in the special paper collection *Recent Advances in Food Analysis* with guest editors J. Hajslova, R. Krska, M. Nielen.

E. Crawford (✉) · B. Musselman
IonSense, Inc

**Keywords** Direct analysis in real time (DART) · Pesticide screening · High-resolution accurate mass (HRAM) · Benchtop orbitrap · Surface analysis

### Introduction

Direct analysis in real time ionization coupled with mass spectrometry (DART-MS) has been gaining momentum in the past few years in food quality and food safety, particularly in the application areas of authenticity [1–3], adulteration [4, 5], contamination [6–11], and food packaging [12, 13]. A review paper on the challenging applications in food quality and safety accomplished with the DART technique gives a perspective of where this technology has progressed to over the past 4 years [14]. The increase in concern with the quality of food has been growing with the demands of expanding global trade markets. The focus on development of faster and simpler analytical ionization techniques for mass spectrometric approaches has also flourished in the past 7 years where there is a need to always get the results faster, with lower analytical costs and minimized sample preparation steps [15–18]. In recent publications, the United States Food and Drug Administration (US FDA) scientists have developed a DART-based method utilizing high-resolution accurate mass detection to rapid screening of pesticides on the surfaces of fruits and vegetables with the objective of creating a simple protocol for testing that might be deployed at selected border points of entry. Using their experimental protocols pesticide screening per sample was completed in under 3 min per swab [6, 7]. The use of such a rapid method

# DART SVP – Aplikace

ionSense® Real-time science solutions

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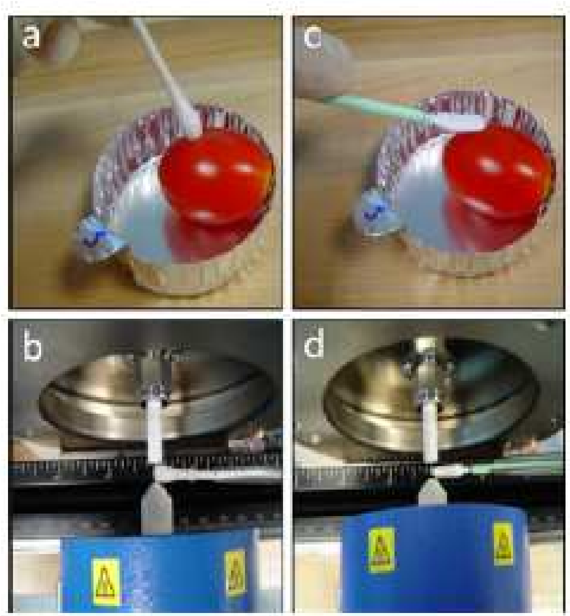
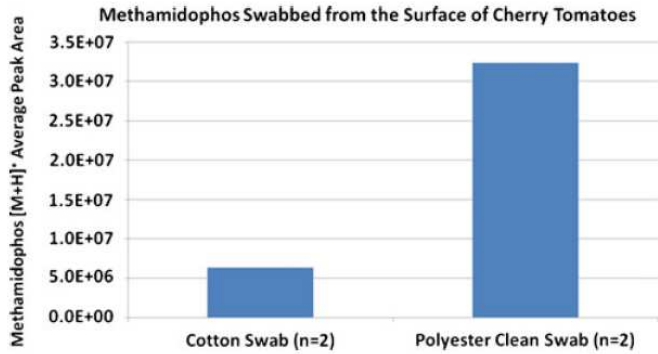


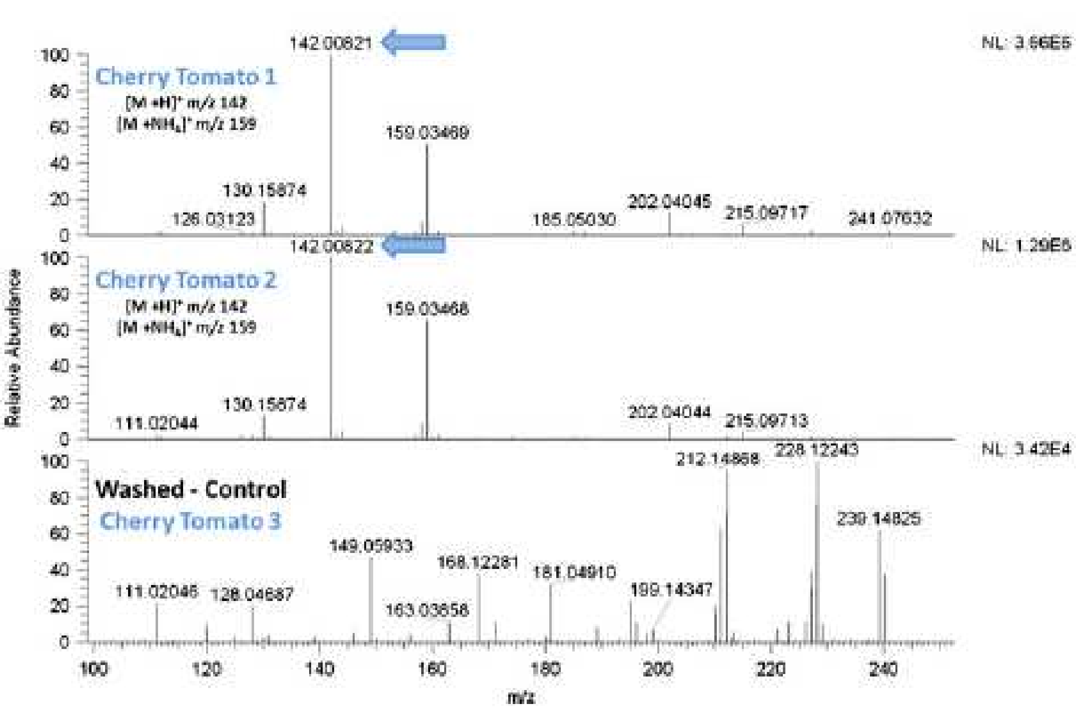



pragolab

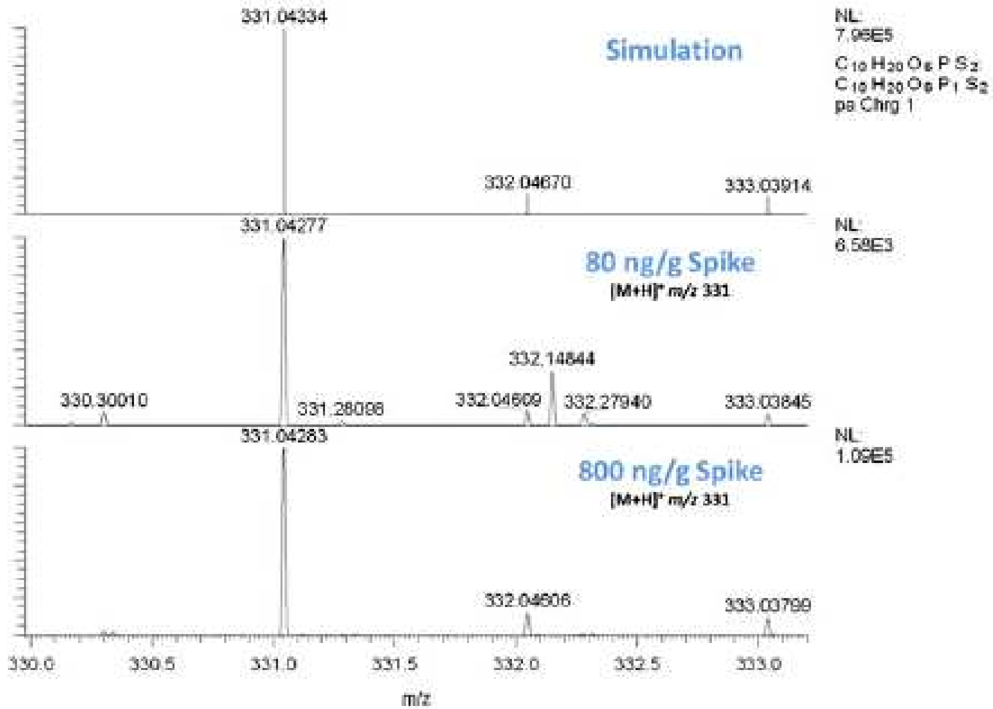
Thermo Fisher SCIENTIFIC

# DART SVP - Aplikace

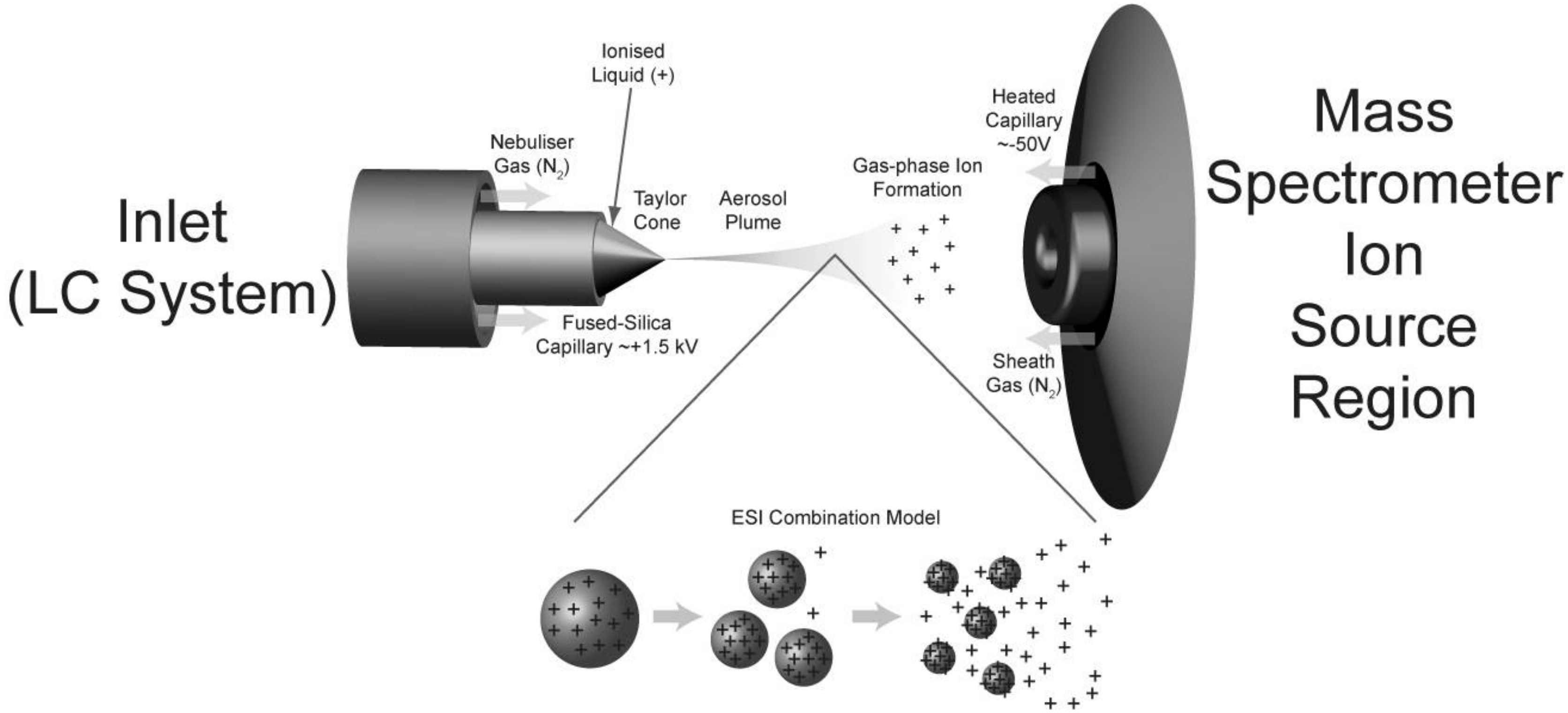
## Methamidophos spike 200 ppb



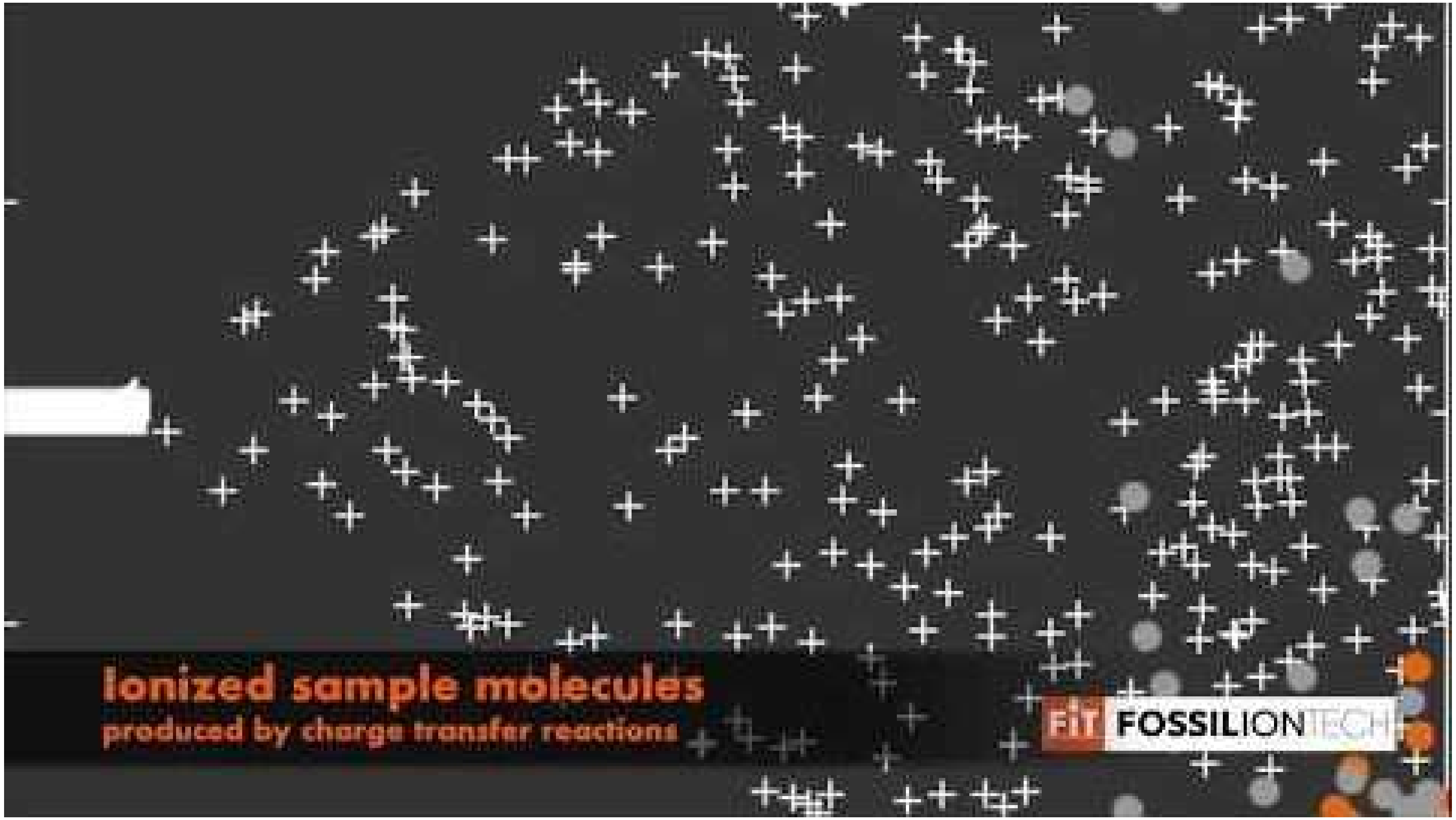

## Malathion spike 80 / 800 ppb



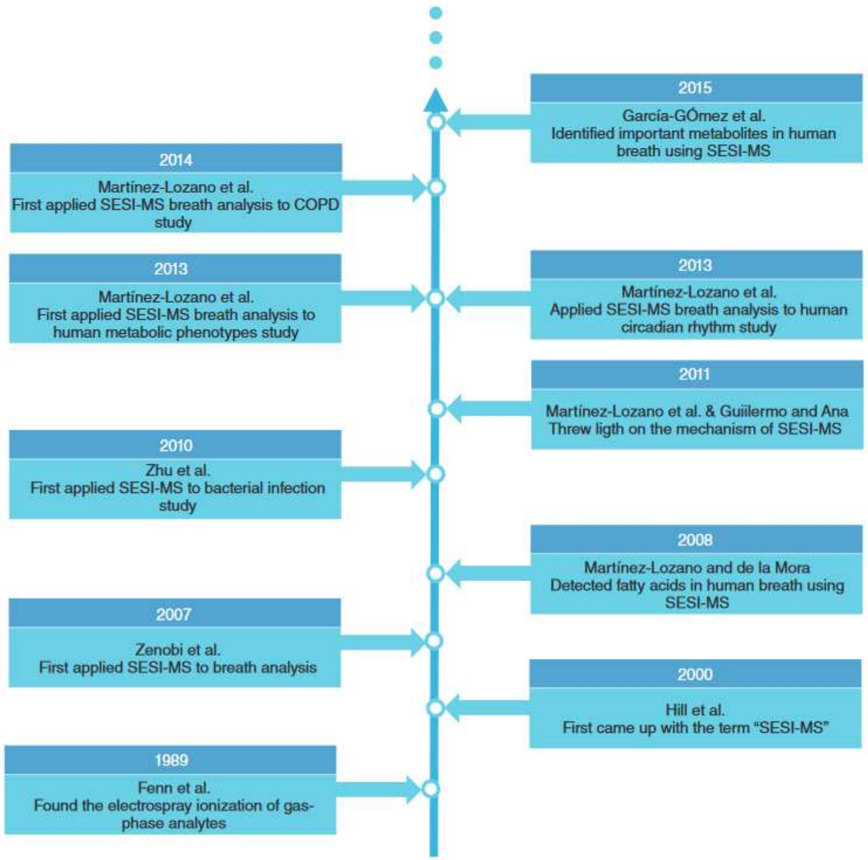
## ESI sv SESI


Inlet
(LC System)
Ionised
Liquid (+)
Nebuliser
Gas ($N_2$)
Taylor
Cone
Aerosol
Plume
Gas-phase Ion
Formation
Heated
Capillary
~-50V
Fused-Silica
Capillary ~+1.5 kV
Sheath
Gas ($N_2$)
Mass
Spectrometer
Ion
Source
Region
ESI Combination Model

# SESI – Princip fungování

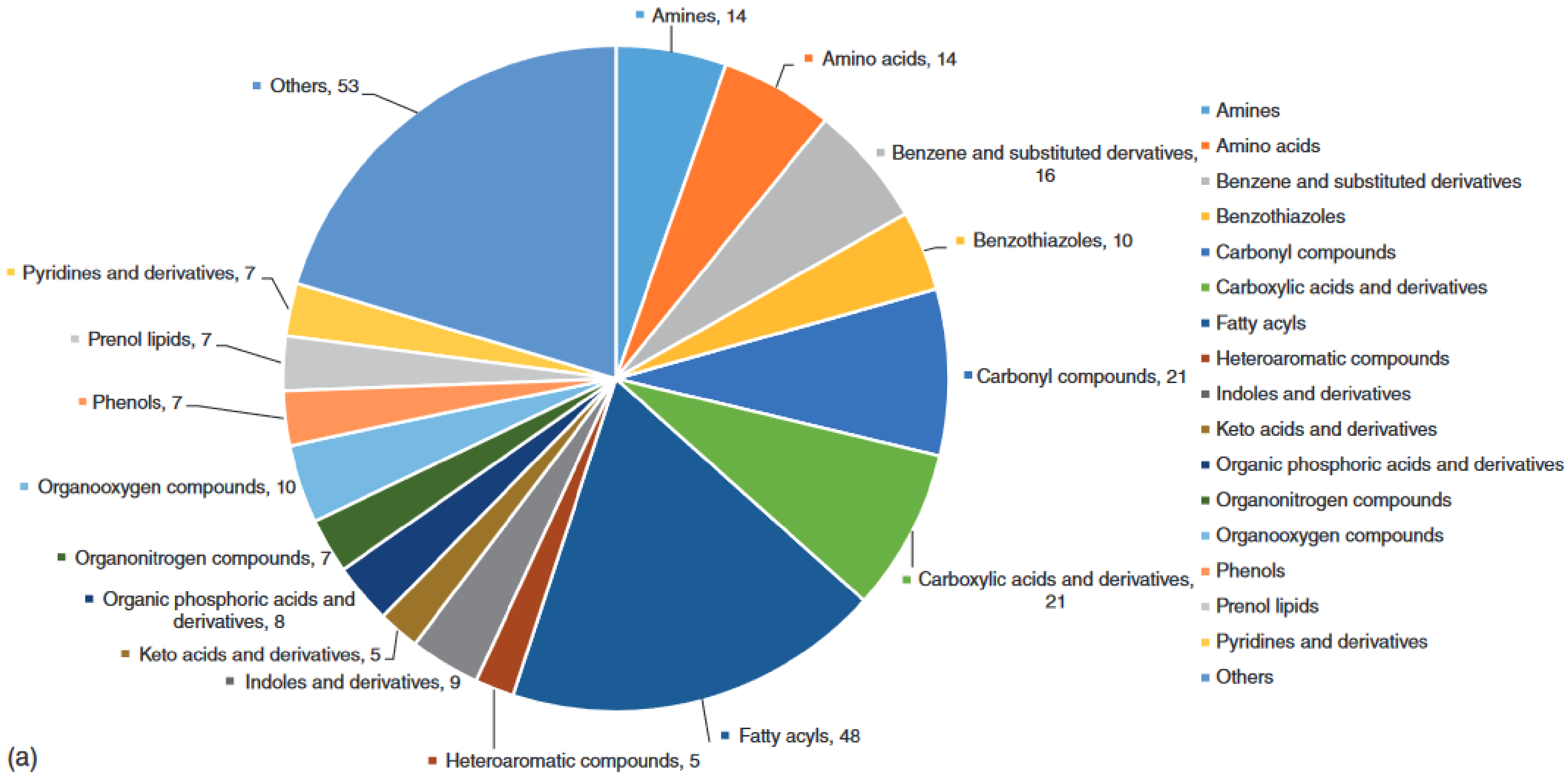


# SESI – Historie



# SESI – Analytická variabilita

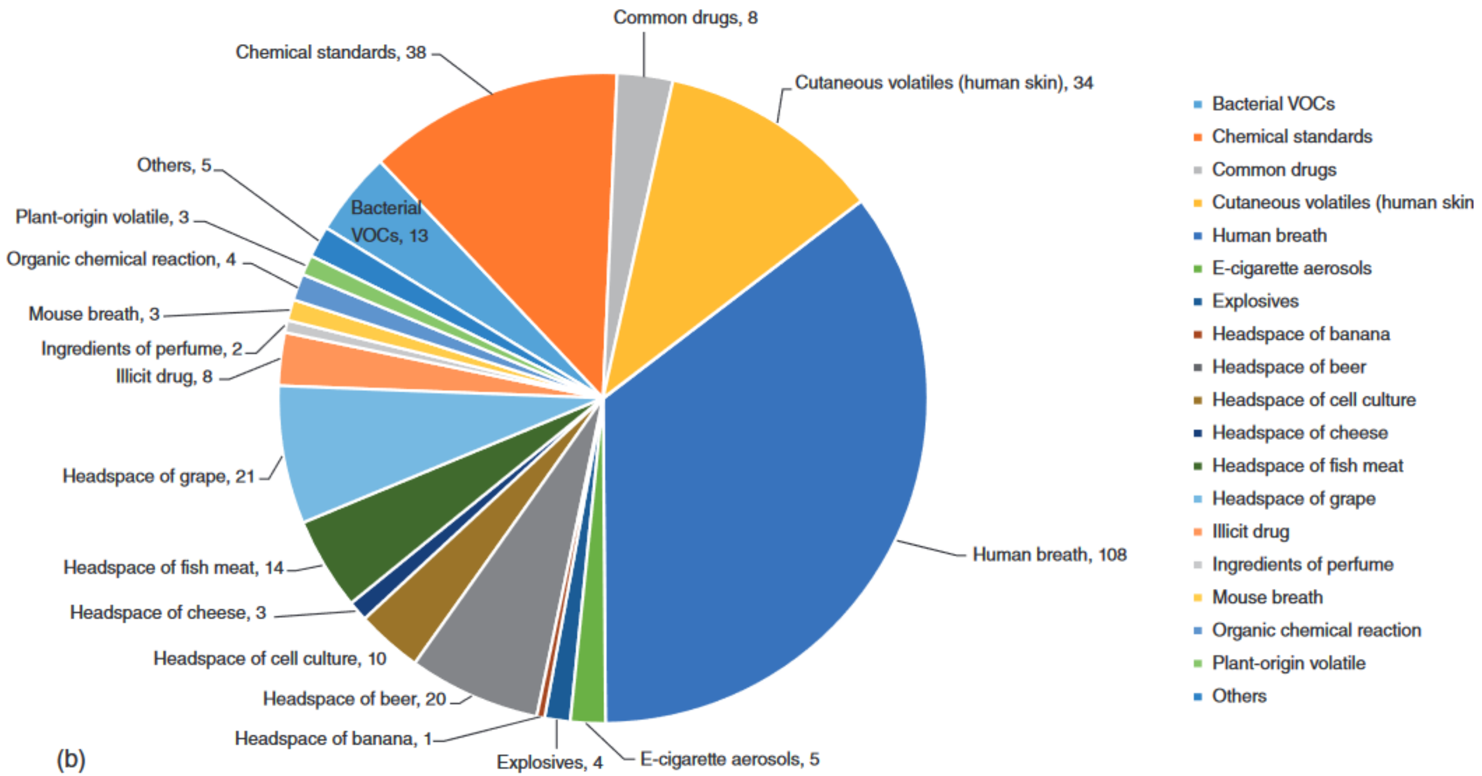
FIT FOSSILIONTECH




(a)

# SESI – Analytická variabilita

FIT FOSSILIONTECH



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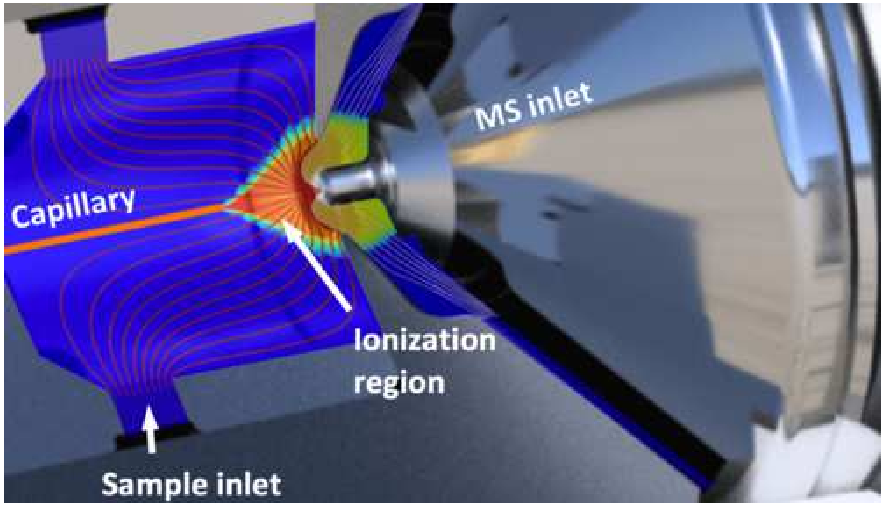
# SESI - Interface

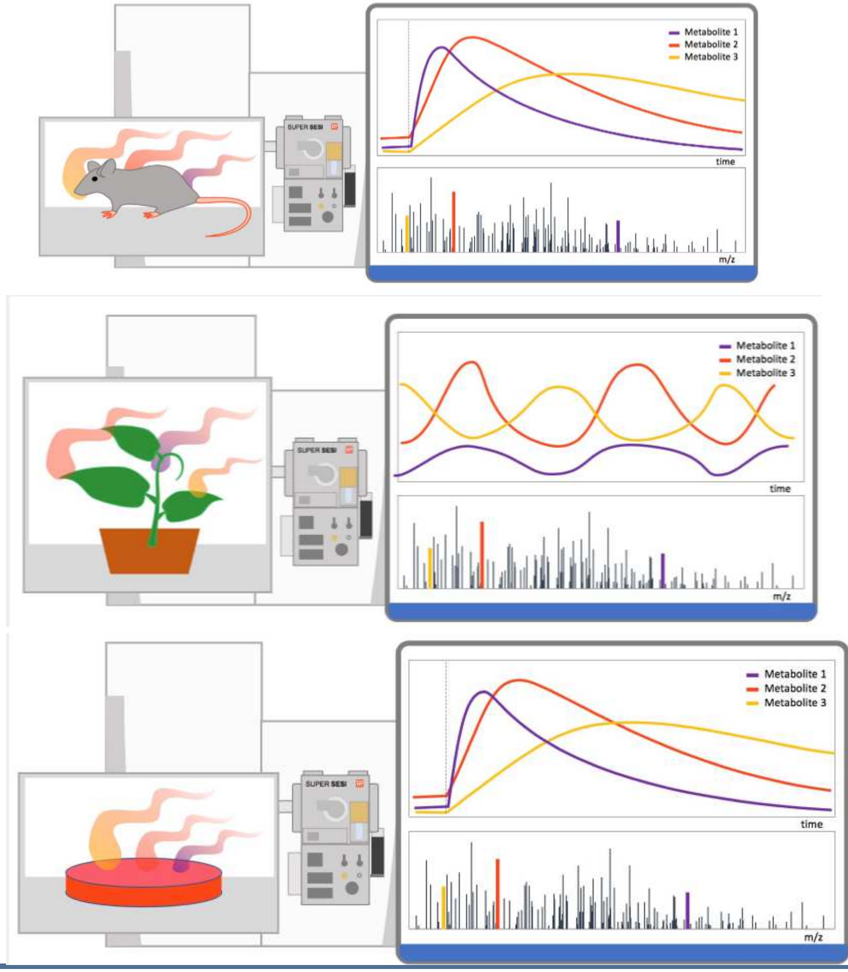



Analýza dechu

# SESI - Interface


Metabolomické profilování

# SESI - Interface


Metabolomické profilování

# SESI – Aplikace

Respiration

Clinical Investigations

Respiration 2014;87:301–310
DOI: 10.1159/000357785

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Published online: February 19, 2014

## Breath Analysis in Real Time by Mass Spectrometry in Chronic Obstructive Pulmonary Disease

Pablo Martinez-Lozano Sinues[a] Lukas Meier[a] Christian Berchtold[a] Mark Ivanov[d] Noriane Sievi[b] Giovanni Camen[b] Malcolm Kohler[b, c] Renato Zenobi[a]

[a]Department of Chemistry and Applied Biosciences, ETH Zurich, [b]Pulmonary Division, University Hospital Zurich, and [c]Zurich Center for Integrative Human Physiology, University of Zurich, Zurich, Switzerland; [d]Institute for Energy Problems of Chemical Physics, Russian Academy of Science, Moscow, Russian Federation

**Key Words**
Breath test · Chronic obstructive pulmonary disease · Exhaled biomarkers

**Abstract**
***Background:*** It has been suggested that exhaled breath contains relevant information on health status. ***Objectives:*** We hypothesized that a novel mass spectrometry (MS) technique to analyze breath in real time could be useful to differentiate breathprints from chronic obstructive pulmonary disease (COPD) patients and controls (smokers and nonsmokers). ***Methods:*** We studied 61 participants including 25 COPD patients [Global Initiative for Obstructive Lung Disease (GOLD) stages I–IV], 25 nonsmoking controls and 11 smoking controls. We analyzed their breath by MS in real time. Raw mass spectra were then processed and statistically analyzed. ***Results:*** A panel of discriminating mass-spectral features was identified for COPD (all stages; n = 25) versus healthy nonsmokers (n = 25), COPD (all stages; n = 25) versus healthy smokers (n = 11) and mild COPD (GOLD stages I/II; n = 13) versus severe COPD (GOLD stages III/IV; n = 12). A blind classification (i.e. leave-one-out cross validation) resulted in 96% sensitivity and 72.7% specificity (COPD vs. smoking controls), 88% sensitivity and 92% specificity (COPD vs. nonsmoking controls) and 92.3% sensitivity and 83.3% specificity (GOLD I/II vs. GOLD III/IV). Acetone and indole were identified as two of the discriminating exhaled molecules. ***Conclusions:*** We conclude that real-time MS may be a useful technique to analyze and characterize the metabolome of exhaled breath. The acquisition of breathprints in a rapid manner may be valuable to support COPD diagnosis and to gain insight into the disease. 

### Introduction

Chronic obstructive pulmonary disease (COPD) is a complex illness, which is sometimes difficult to properly diagnose and for which many fundamental questions remain unanswered [1]. There is a clear need to increase our knowledge of the COPD phenotype for the ultimate purpose of improving diagnostics [2].

Taking samples from the lung itself (e.g. induced sputum) to perform analytical measurements can be difficult, and for this reason the analysis of exhaled breath is eliciting considerable interest as it offers the unique advantage

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0025–7931/14/0874–0301$39.50/0

Renato Zenobi
ETH Zurich
Department of Chemistry and Applied Biosciences
CH–8093 Zurich (Switzerland)
E-Mail zenobi@org.chem.ethz.ch

# SESI – Aplikace

FIT FOSSILIONTECH

Respiration

Clin

Respi
DOI: 1

## Breath Analysis in R
## Spectrometry in Ch
## Pulmonary Disease

Pablo Martinez-Lozano Sinues[a] Luka
Mark Ivanov[d] Noriane Sievi[b] Giova
Renato Zenobi[a]

[a]Department of Chemistry and Applied Biosciences, E
and [c]Zurich Center for Integrative Human Physiology,
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ly analyzed. ***Results:*** A panel of discriminating r
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n = 13) versus severe COPD (GOLD stages III/I
blind classification (i.e. leave-one-out cross va
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0025–7931/14/0874–0301$39.50/0

| m/z | COPD subjects | Nonsmoking controls |
|---|---|---|
| 79 | 63 (49–77) | 102 (65–138) |
| 102.1 | 134 (111–156) | 191 (160–221) |
| 118.0 | 120 (60–180) | 217 (134–300) |
| 143.1 | 931 (684–1,179) | 1,218 (1,025–1,411) |
| 157.1 | 664 (531–798) | 844 (744–945) |
| 158.1 | 557 (459–656) | 723 (632–814) |
| 160.1 | 214 (164–263) | 335 (262–409) |
| 174.1 | 338 (264–413) | 391 (344–438) |
| 180.1 | 541 (180–901) | 623 (300–946) |
| 185.1 | 493 (426–560) | 580 (526–635) |
| 185.9 | 62 (53–72) | 77 (70–84) |
| 186.2 | 496 (381–610) | 956 (654–1,258) |
| 188.1 | 284 (232–337) | 357 (309–406) |
| 190.1 | 301 (242–360) | 393 (335–451) |
| 202.2 | 268 (229–308) | 416 (302–529) |
| 227.1 | 722 (548–896) | 509 (379–639) |
| 240.2 | 152 (130–174) | 216 (173–259) |
| 245.2 | 228 (200–256) | 193 (152–233) |
| 247.2 | 386 (313–458) | 320 (222–418) |
| 258.1 | 161 (138–184) | 203 (174–232) |
| 265.1 | 129 (86–171) | 114 (111–118) |
| 268.2 | 95 (80–110) | 119 (102–136) |
| 271 | 110 (88–131) | 78 (71–86) |
| 271.3 | 912 (682–1,141) | 614 (433–796) |
| 277.1 | 160 (108–212) | 107 (88–125) |
| 287.3 | 218 (147–288) | 125 (102–148) |
| 327 | 419 (364–473) | 484 (439–528) |
| 328 | 54 (50–59) | 62 (57–66) |
| 329 | 416 (361–471) | 477 (433–520) |
| 329.3 | 111 (80–141) | 77 (48–106) |
| 330 | 60 (55–64) | 67 (63–71) |
| 331 | 148 (131–164) | 165 (152–179) |
| 332.2 | 71 (63–79) | 95 (84–106) |
| 344.1 | 270 (218–321) | 362 (316–408) |
| 345 | 58 (54–63) | 67 (61–73) |
| 346 | 256 (205–307) | 359 (312–406) |
| 348.1 | 103 (84–121) | 134 (118–149) |

The signal intensity values listed are means (95% confidence interval) in units of counts.



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# SESI – Aplikace

FIT FOSSILIONTECH

Clin
Respiration
Respi
DOI: 1

**Breath Analysis in F**
**Spectrometry in Ch**
**Pulmonary Disease**

Pablo Martinez-Lozano Sinues[a] Luka
Mark Ivanov[d] Noriane Sievi[b] Giova
Renato Zenobi[a]

[a]Department of Chemistry and Applied Biosciences, E
and [c]Zurich Center for Integrative Human Physiology,
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| m/z |
|---|
| 79 |
| 102.1 |
| 118.0 |
| 143.1 |
| 157.1 |
| 158.1 |
| 160.1 |
| 174.1 |
| 180.1 |
| 185.1 |
| 185.9 |
| 186.2 |
| 188.1 |
| 190.1 |
| 202.2 |
| 227.1 |
| 240.2 |
| 245.2 |
| 247.2 |
| 258.1 |
| 265.1 |
| 268.2 |
| 271 |
| 271.3 |
| 277.1 |
| 287.3 |
| 327 |
| 328 |
| 329 |
| 329.3 |
| 330 |
| 331 |
| 332.2 |
| 344.1 |
| 345 |
| 346 |
| 348.1 |

The signa
interval) in u

| m/z | COPD subjects | Smoking controls | m/z | COPD subjects | Smoking controls |
|---|---|---|---|---|---|
| 59 | 2,155 (1,644–2,666) | 1,042 (752–1,332) | 235.2 | 1,173 (949–1,397) | 747 (173–1,321) |
| 60.1 | 168 (136–200) | 95 (78–111) | 236.2 | 287 (218–355) | 209 (70–348) |
| 98 | 38 (27–50) | 74 (36–112) | 239.2 | 168 (142–194) | 131 (109–153) |
| 122 | 85 (70–99) | 133 (105–160) | 241.2 | 141 (123–158) | 112 (79–145) |
| 123.1 | 220 (98–342) | 746 (219–1,274) | 244.2 | 578 (461–695) | 621 (–96 to 1,338) |
| 124.1 | 86 (59–113) | 191 (110–272) | 247.2 | 386 (313–458) | 287 (128–446) |
| 126 | 71 (40–102) | 223 (81–365) | 249.2 | 279 (196–362) | 189 (161–216) |
| 146 | 132 (78–187) | 335 (128–543) | 251.2 | 186 (167–206) | 150 (129–172) |
| 150 | 111 (81–141) | 241 (112–370) | 253.1 | 138 (99–178) | 106 (90–122) |
| 155.1 | 1,280 (617–1,943) | 468 (260–677) | 255.1 | 258 (–17 to 532) | 98 (89–107) |
| 160.1 | 235 (164–306) | 433 (252–614) | 256.2 | 164 (78–250) | 96 (69–122) |
| 172.1 | 553 (411–695) | 288 (102–475) | 257.2 | 253 (–11 to 518) | 84 (42–126) |
| 182 | 68 (41–95) | 186 (62–309) | 258.1 | 161 (138–184) | 121 (85–157) |
| 189.1 | 195 (154–237) | 132 (102–162) | 267.2 | 172 (152–192) | 129 (95–163) |
| 191.1 | 366 (323–408) | 271 (210–333) | 269.2 | 104 (92–117) | 76 (61–92) |
| 194.1 | 105 (75–136) | 181 (103–259) | 271.3 | 912 (682–1,141) | 357 (30–684) |
| 195.2 | 1,856 (1,448–2,265) | 1,065 (475–1,655) | 272.3 | 265 (212–318) | 146 (64–227) |
| 198.1 | 167 (144–191) | 115 (91–139) | 273.2 | 96 (81–111) | 66 (48–84) |
| 199.1 | 435 (374–497) | 282 (173–391) | 276.2 | 131 (102–160) | 246 (–121 to 612) |
| 201.1 | 345 (284–407) | 228 (179–278) | 279.2 | 1,536 (1,310–1,762) | 1,111 (839–1,384) |
| 203.1 | 417 (326–509) | 235 (118–352) | 285.2 | 338 (53–623) | 100 (57–143) |
| 204.1 | 361 (302–421) | 241 (132–351) | 288.3 | 474 (363–586) | 309 (69–550) |
| 205.2 | 553 (158–948) | 237 (137–338) | 288.9 | 34 (28–39) | 68 (43–93) |
| 207.1 | 1,159 (924–1,394) | 981 (19–1,943) | 289.3 | 150 (121–179) | 101 (43–159) |
| 208.2 | 508 (394–621) | 390 (35–745) | 298.9 | 50 (40–60) | 74 (51–97) |
| 211.2 | 342 (288–395) | 229 (166–293) | 299.3 | 258 (136–381) | 74 (48–101) |
| 213.1 | 299 (244–354) | 214 (166–263) | 316.3 | 194 (100–289) | 68 (32–103) |
| 214 | 156 (132–181) | 106 (70–142) | 317.3 | 82 (59–105) | 49 (37–62) |
| 214.1 | 232 (195–270) | 165 (123–208) | 319.1 | 43 (34–53) | 55 (42–68) |
| 215.1 | 272 (236–308) | 166 (111–221) | 323.1 | 37 (30–44) | 48 (36–59) |
| 218.1 | 294 (243–345) | 216 (135–298) | 325.1 | 36 (28–45) | 60 (38–82) |
| 222.2 | 224 (181–266) | 275 (–49 to 599) | 329.3 | 111 (80–141) | 45 (10–80) |
| 223.1 | 1,390 (1,109–1,670) | 954 (833–1,075) | 330.3 | 65 (52–79) | 34 (18–50) |
| 224.1 | 317 (250–384) | 242 (210–273) | | | |
| 227.1 | 722 (548–896) | 538 (–29 to 1,105) | | | |
| 228.2 | 215 (181–250) | 186 (36–335) | | | |

The signal intensity values are listed as means (95% confidence interval) in units of counts.

# SESI – Aplikace

FIT FOSSILIONTECH

Respiration

Clin

Respi

DOI: 1

**Breath Analysis in F**
**Spectrometry in Ch**
**Pulmonary Disease**

Pablo Martinez-Lozano Sinues[a] Luka
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**Key Words**
Breath test · Chronic obstructive pulmonary dis
Exhaled biomarkers

**Abstract**
***Background:*** It has been suggested that exl contains relevant information on health status We hypothesized that a novel mass spectromet nique to analyze breath in real time could be ferentiate breathprints from chronic obstructiv disease (COPD) patients and controls (smoke smokers). ***Methods:*** We studied 61 participants COPD patients [Global Initiative for Obstructi ease (GOLD) stages I–IV], 25 nonsmoking con smoking controls. We analyzed their breath b time. Raw mass spectra were then processed ar ly analyzed. ***Results:*** A panel of discriminating r features was identified for COPD (all stages; n healthy nonsmokers (n = 25), COPD (all stages; r healthy smokers (n = 11) and mild COPD (GOL n = 13) versus severe COPD (GOLD stages III/I blind classification (i.e. leave-one-out cross v sulted in 96% sensitivity and 72.7% specificit

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| m/z |
|---|
| 79 |
| 102.1 |
| 118.0 |
| 143.1 |
| 157.1 |
| 158.1 |
| 160.1 |
| 174.1 |
| 180.1 |
| 185.1 |
| 185.9 |
| 186.2 |
| 188.1 |
| 190.1 |
| 202.2 |
| 227.1 |
| 240.2 |
| 245.2 |
| 247.2 |
| 258.1 |
| 265.1 |
| 268.2 |
| 271 |
| 271.3 |
| 277.1 |
| 287.3 |
| 327 |
| 328 |
| 329 |
| 329.3 |
| 330 |
| 331 |
| 332.2 |
| 344.1 |
| 345 |
| 346 |
| 348.1 |

The signal
interval) in u

| m/z | COPD subjects | Smoking controls |
|---|---|---|
| 59 | 2,155 (1,644–2,666) | 1,042 (752–1,332) |
| 60.1 | 168 (136–200) | 95 (78–111) |
| 98 | 38 (27–50) | 74 (36–112) |
| 122 | 85 (70–99) | 133 (105–160) |
| 123.1 | 220 (98–342) | 746 (219–1,274) |
| 124.1 | 86 (59–113) | 191 (110–272) |
| 126 | 71 (40–102) | 223 (81–365) |
| 146 | 132 (78–187) | 335 (128–543) |
| 150 | 111 (81–141) | 241 (112–370) |
| 155.1 | 1,280 (617–1,943) | 468 (260–677) |
| 160.1 | 235 (164–306) | 433 (252–614) |
| 172.1 | 553 (411–695) | 288 (102–475) |
| 182 | 68 (41–95) | 186 (62–309) |
| 189.1 | 195 (154–237) | 132 (102–162) |
| 191.1 | 366 (323–408) | 271 (210–333) |
| 194.1 | 105 (75–136) | 181 (103–259) |
| 195.2 | 1,856 (1,448–2,265) | 1,065 (475–1,655) |
| 198.1 | 167 (144–191) | 115 (91–139) |
| 199.1 | 435 (374–497) | 282 (173–391) |
| 201.1 | 345 (284–407) | 228 (179–278) |
| 203.1 | 417 (326–509) | 235 (118–352) |
| 204.1 | 361 (302–421) | 241 (132–351) |
| 205.2 | 553 (158–948) | 237 (137–338) |
| 207.1 | 1,159 (924–1,394) | 981 (19–1,943) |
| 208.2 | 508 (394–621) | 390 (35–745) |
| 211.2 | 342 (288–395) | 229 (166–293) |
| 213.1 | 299 (244–354) | 214 (166–263) |
| 214 | 156 (132–181) | 106 (70–142) |
| 214.1 | 232 (195–270) | 165 (123–208) |
| 215.1 | 272 (236–308) | 166 (111–221) |
| 218.1 | 294 (243–345) | 216 (135–298) |
| 222.2 | 224 (181–266) | 275 (–49 to 599) |
| 223.1 | 1,390 (1,109–1,670) | 954 (833–1,075) |
| 224.1 | 317 (250–384) | 242 (210–273) |
| 227.1 | 722 (548–896) | 538 (–29 to 1,105) |
| 228.2 | 215 (181–250) | 186 (36–335) |

| m/z | COPD subjects | Smoking controls |
|---|---|---|
| 235.2 | 1,173 (949–1,397) | 747 (173–1,321) |
| 236.2 | 287 (218–355) | 209 (70–348) |
| 239.2 | 168 (142–194) | 131 (109–153) |
| 241.2 | 141 (123–158) | 112 (79–145) |
| 244.2 | 578 (461–695) | 621 (–96 to 1,338) |
| 247.2 | 386 (313–458) | 287 (128–446) |
| 249.2 | 279 (196–362) | 189 (161–216) |
| 251.2 | 186 (167–206) | 150 (129–172) |
| 253.1 | 138 (99–178) | 106 (90–122) |
| 255.1 | 258 (–17 to 532) | |
| 256.2 | 164 (78–250) | |
| 257.2 | 253 (–11 to 518) | |
| 258.1 | 161 (138–184) | |
| 267.2 | 172 (152–192) | |
| 269.2 | 104 (92–117) | |
| 271.3 | 912 (682–1,141) | |
| 272.3 | 265 (212–318) | |
| 273.2 | 96 (81–111) | |
| 276.2 | 131 (102–160) | |
| 279.2 | 1,536 (1,310–1,762 | |
| 285.2 | 338 (53–623) | |
| 288.3 | 474 (363–586) | |
| 288.9 | 34 (28–39) | |
| 289.3 | 150 (121–179) | |
| 298.9 | 50 (40–60) | |
| 299.3 | 258 (136–381) | |
| 316.3 | 194 (100–289) | |
| 317.3 | 82 (59–105) | [illegible] |
| 319.1 | 43 (34–53) | 55 (42–68) |
| 323.1 | 37 (30–44) | 48 (36–59) |
| 325.1 | 36 (28–45) | 60 (38–82) |
| 329.3 | 111 (80–141) | 45 (10–80) |
| 330.3 | 65 (52–79) | 34 (18–50) |

The signal intensity values are listed as means (95% confidence interval) in units of counts.

| m/z | GOLD I/II | GOLD III/IV |
|---|---|---|
| 165 | 277 (210–344) | 210 (178–242) |
| 286.3 | 70 (56–84) | 228 (6–451) |
| 302.3 | 63 (46–80) | 358 (21–695) |
| 308.2 | 53 (17–90) | 55 (41–70) |

The signal intensity values listed are means (95% confidence interval) in units of counts.



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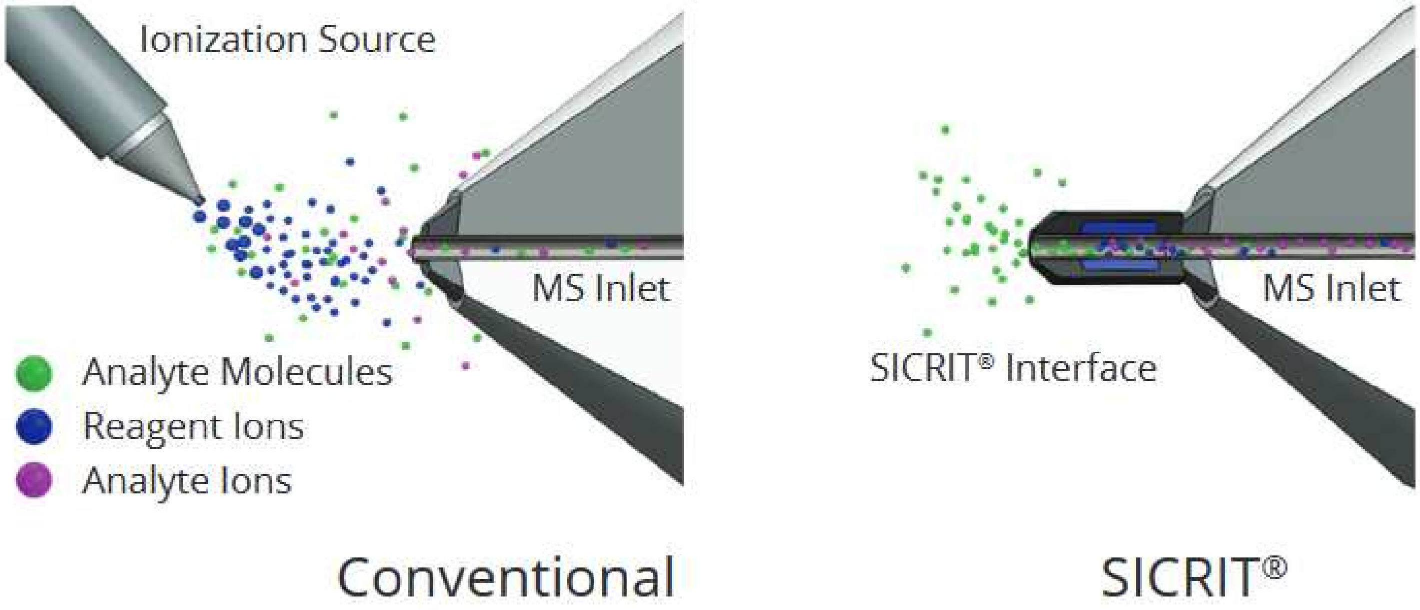
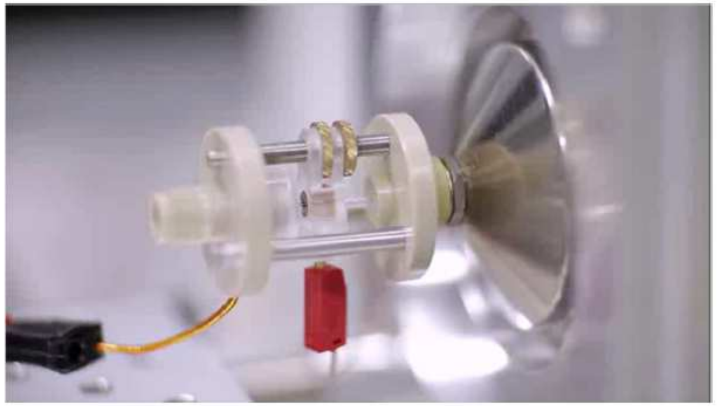
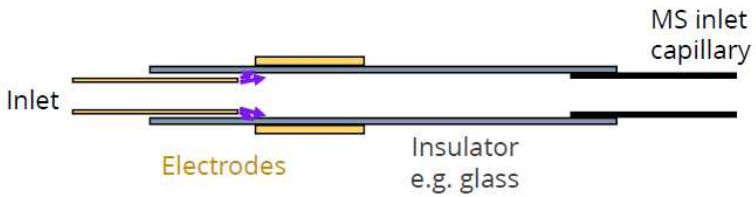
# SICRIT® (Soft Ionization by Chemical Reaction in Transfer)



# SICRIT ® (Soft Ionization by Chemical Reaction in Transfer)

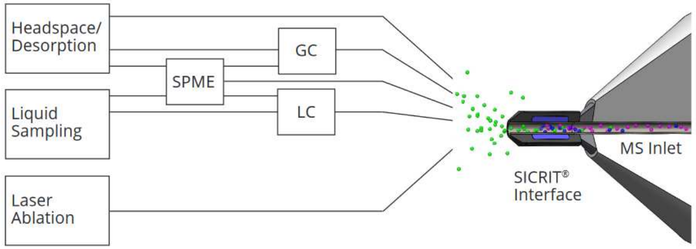




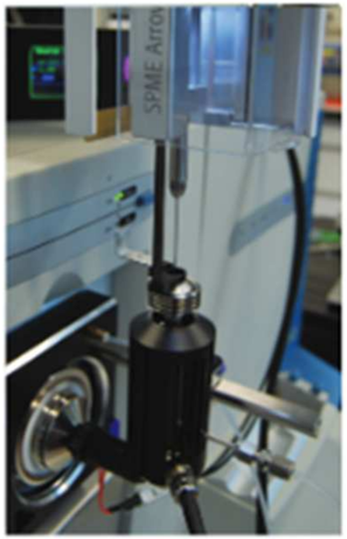


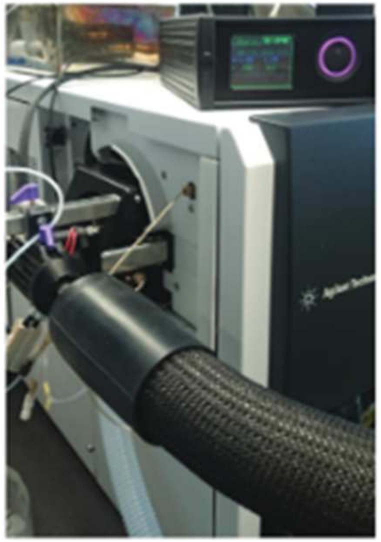
SICRIT® GC/SPME Module, Ion Source and Control Unit

# SICRIT ® - Interface

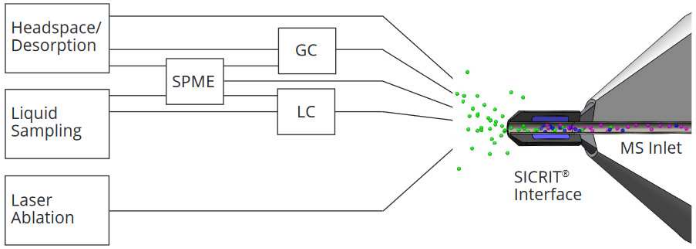


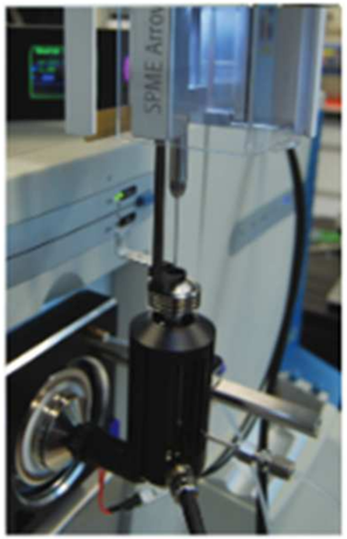

Desorpce

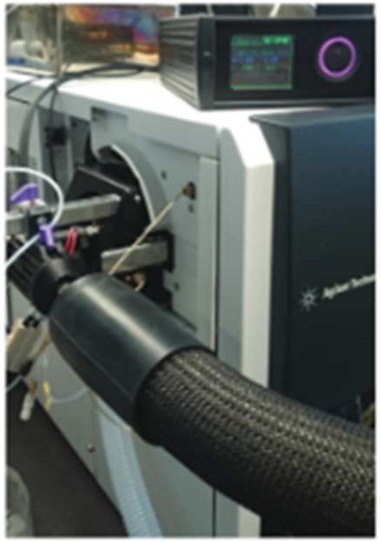


# SICRIT ® - Interface

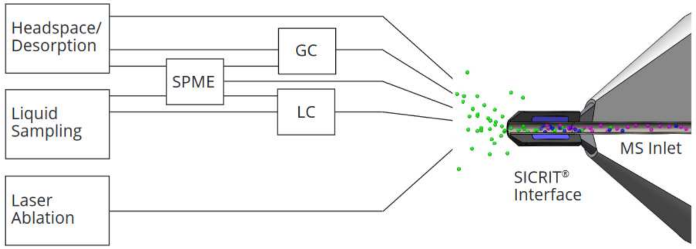


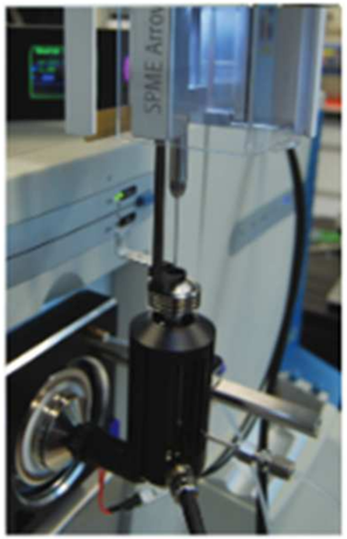



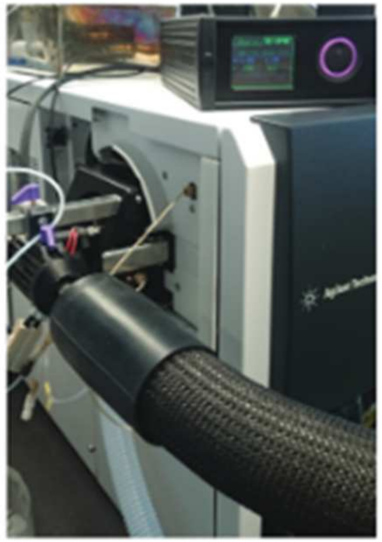


Direct SPME

# SICRIT ® - Interface

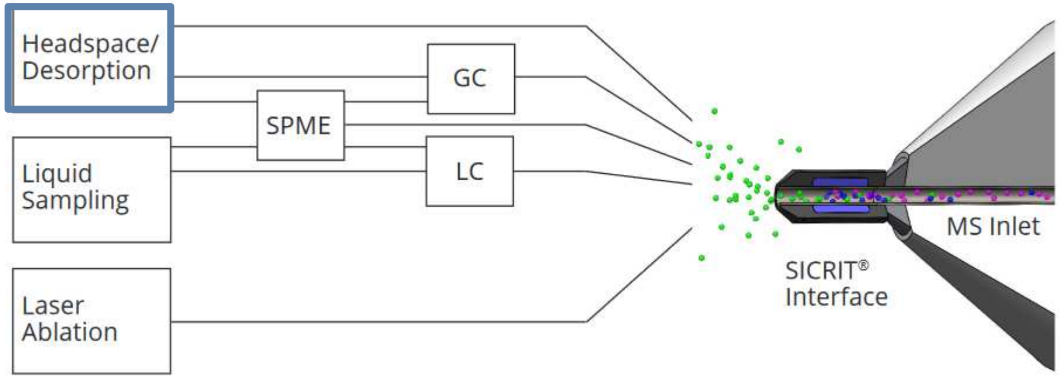




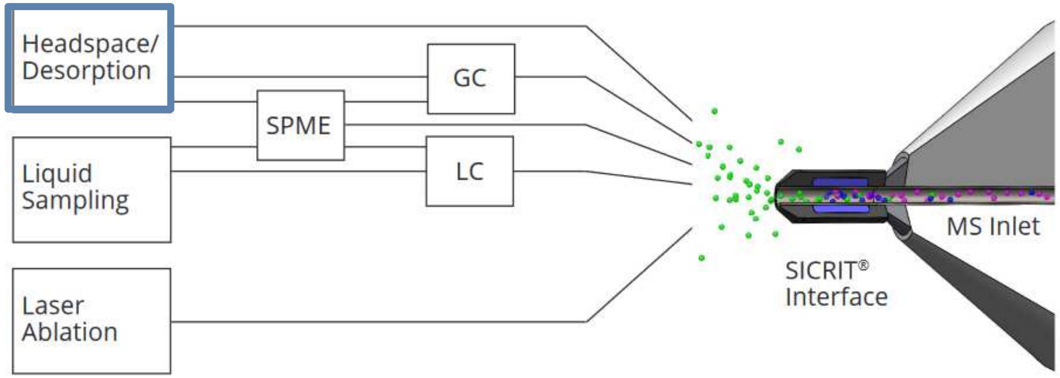
GC-MS

# SICRIT ® - Aplikace / Desorpce



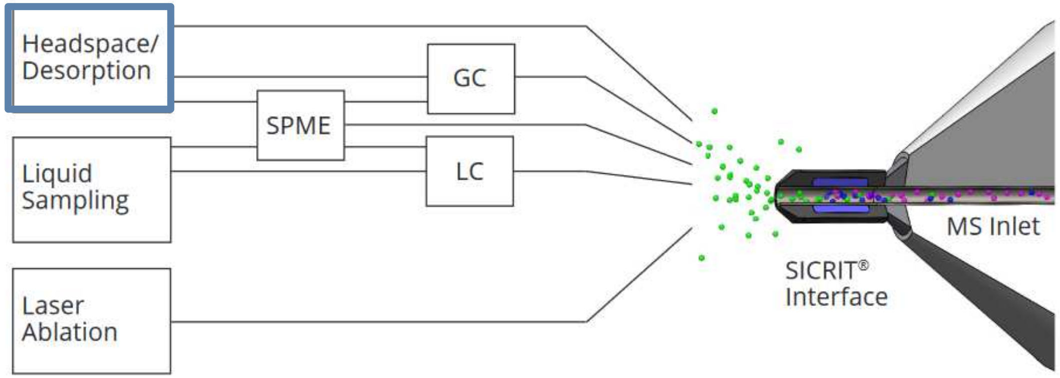

Heated (100°C) support gas
Thermo LTQ Orbitrap MS

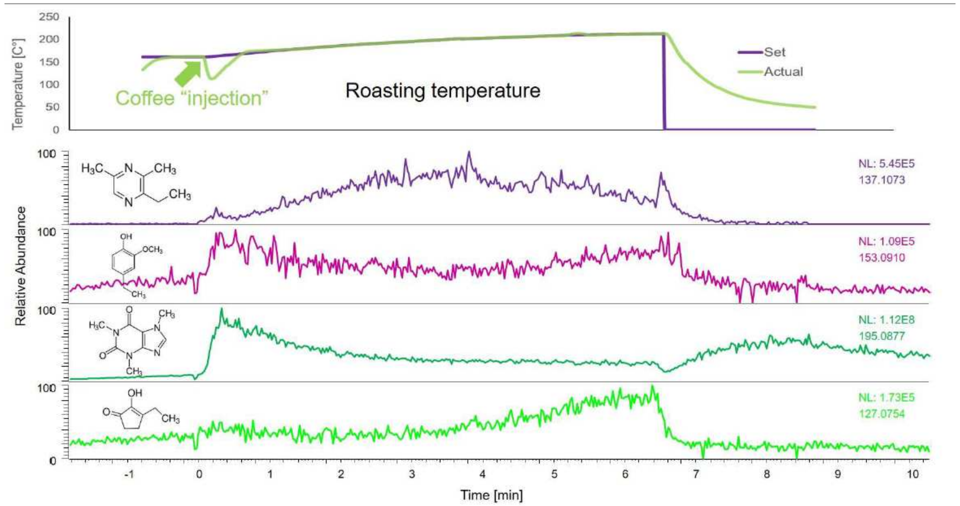
# SICRIT ® - Aplikace / Desorpce



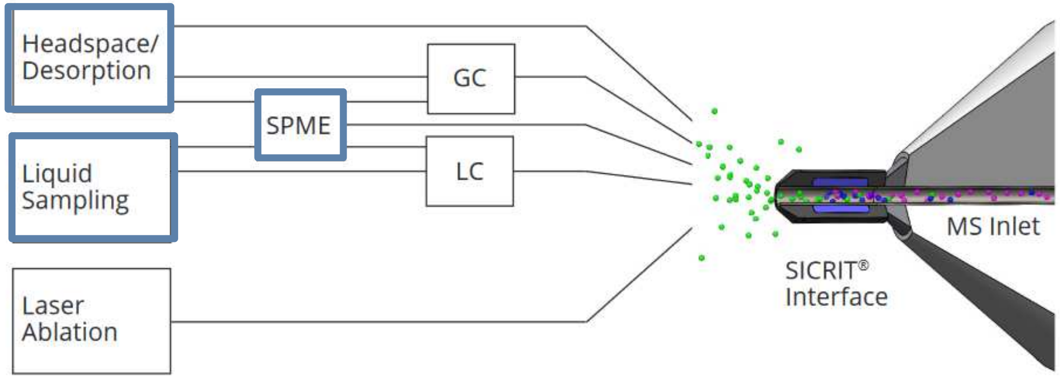

| Flavour compound (excerpt) | Sum formula | M+H (calc) | M+H (meas) | Dev (mmu) |
|---|---|---|---|---|
| 2-ethyl-3,5-dimethylpyrazine | C8H12N2 | 137,1073 | 137,1077 | 0,37 |
| 2,3-diethyl-5-methylpyrazine | C9H14N2 | 151,1230 | 151,1235 | 0,53 |
| (E)-beta-damascenone | C13H18O | 191,1430 | 191,1437 | 0,66 |
| Guaiacol | C7H8O2 | 125,0597 | 125,0603 | 0,59 |
| 4-vinylguaiacol | C9H10O2 | 151,0754 | 151,0760 | 0,64 |
| 4-ethylguaiacol | C9H12O2 | 153,0910 | 153,0915 | 0,49 |
| vanilin | C8H8O3 | 153,0546 | 153,0551 | 0,48 |
| 5-ethyl-3-hydroxy-4-methyl-2(5H)-furanone | C7H10O3 | 143,0703 | 143,0707 | 0,43 |
| 2-isobutyl-3-methoxypyrazine | C9H14N2O | 167,1179 | 167,1184 | 0,51 |
| propionic acid | C3H6O2 | 75,0441 | 75,0456 | 1,51 |
| cresol | C7H8O | 109,0648 | 109,0652 | 0,41 |
| trigonelline | C7H7NO2 | 138,0550 | 138,0554 | 0,42 |
| caffeine | C8H10N4O2 | 195,0877 | 195,0882 | 0,56 |
| 6-methyl-3-pyridinol | C6H7NO | 110,0600 | 110,0604 | 0,35 |
| 3-hydroxypyridine | C5H5NO | 96,0444 | 96,0446 | 0,20 |
| 2-methylpyrazine | C5H6N2 | 95,0604 | 95,0606 | 0,27 |
| 1-methylpyrrole | C5H7N | 82,0651 | 82,0651 | 0,00 |
| 2,5-dimethyl-4-hydroxy-3(2H)-furanone | C6H8O3 | 129,0546 | 129,0550 | 0,40 |
| furfural | C5H4O2 | 97,0284 | 97,0286 | 0,21 |
| 2-acetylfuran | C6H6O2 | 111,0441 | 111,0444 | 0,35 |
| 5-hydroxymethylfurfural | C6H6O3 | 127,0390 | 127,0394 | 0,41 |
| 4,4-dimethyl-2-cyclopenten-1-one | C7H10O | 111,0804 | 111,0808 | 0,34 |
| 2,3-dimethyl-2-cyclopenten-1-one | C7H10O | 111,0804 | 111,0808 | 0,34 |
| 2-hydroxy-3-methyl-2-cyclopenten-1-one | C6H8O2 | 113,0597 | 113,0601 | 0,35 |
| 3-ethyl-2-hydroxy-2-cyclopenten-1-one | C7H10O2 | 127,0754 | 127,0758 | 0,39 |
| phenol | C6H6O | 95,0491 | 95,0494 | 0,22 |

# SICRIT ® - Aplikace / Desorpce

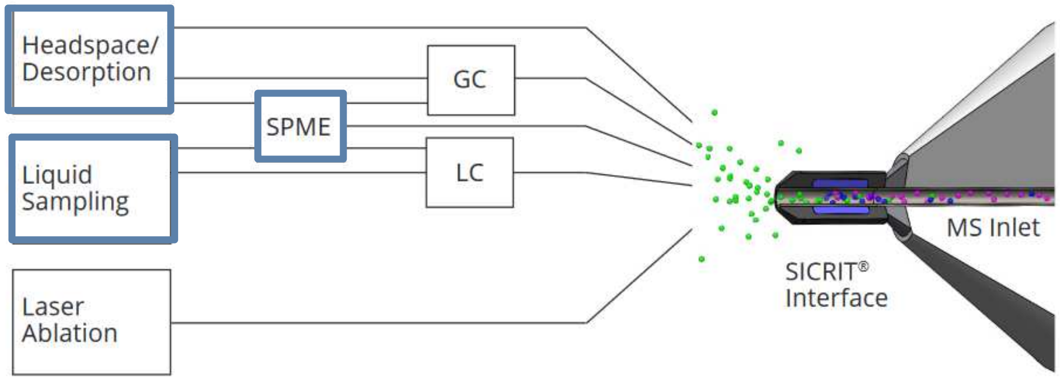


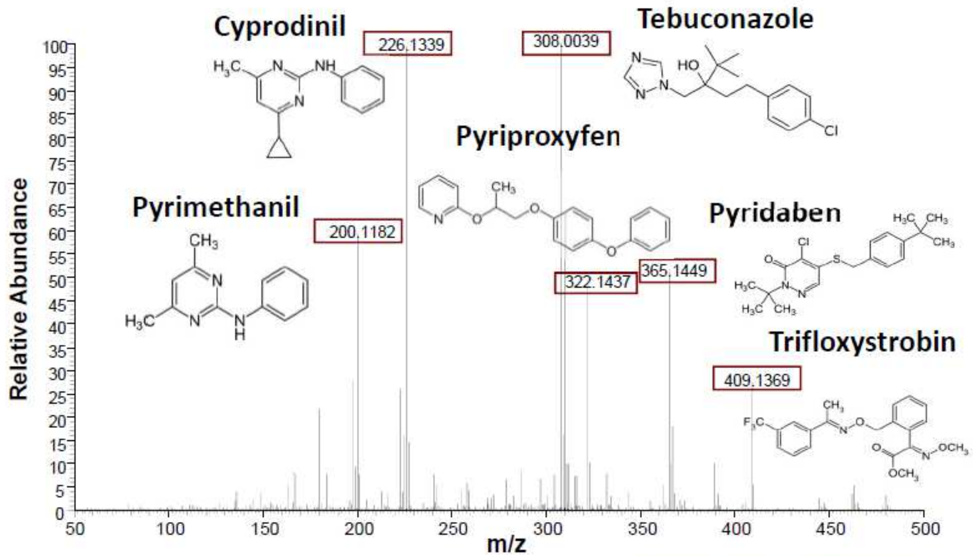



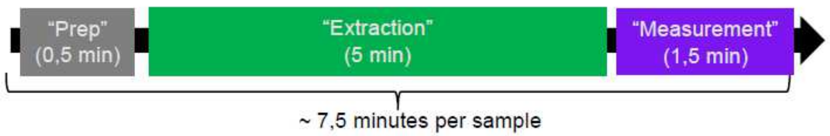
# SICRIT ® - Aplikace / Direct SPME




# SICRIT ® - Aplikace / Direct SPME

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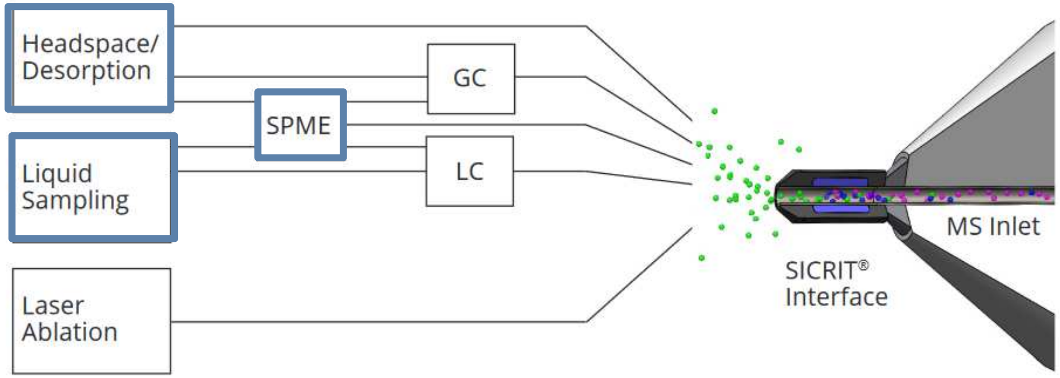


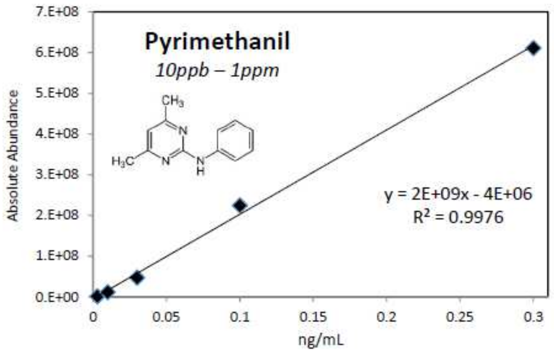


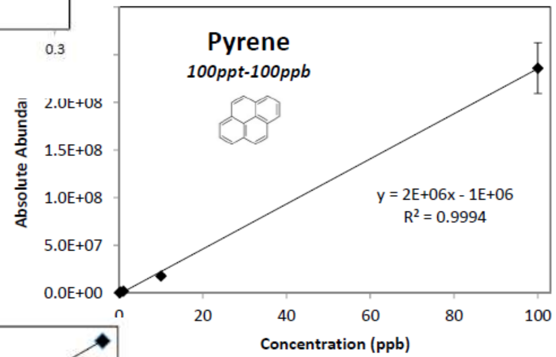


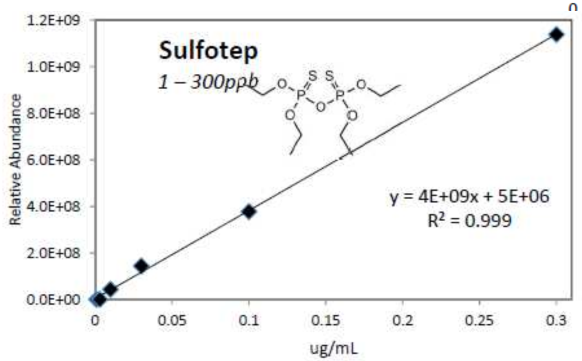

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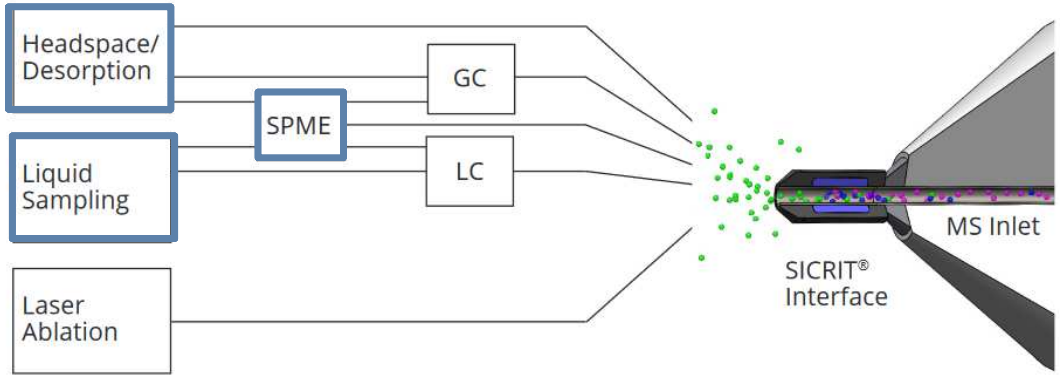
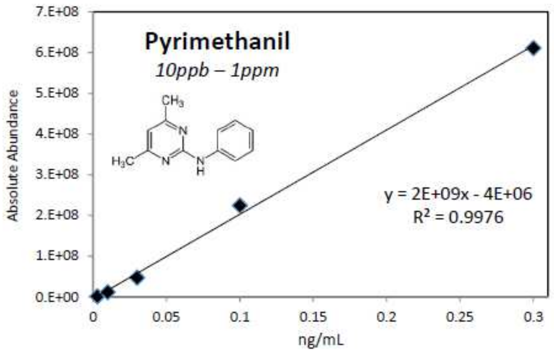
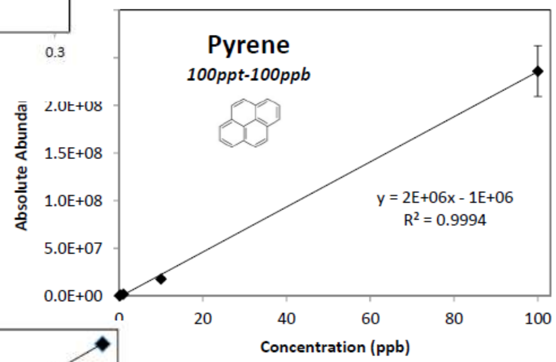
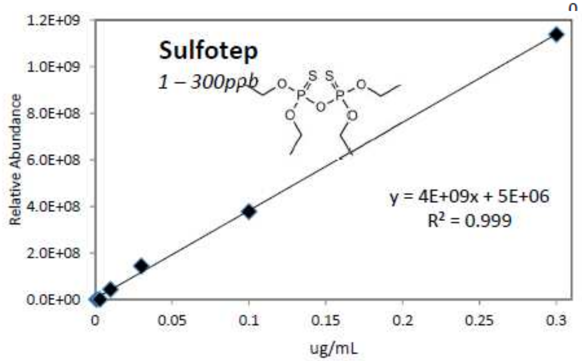
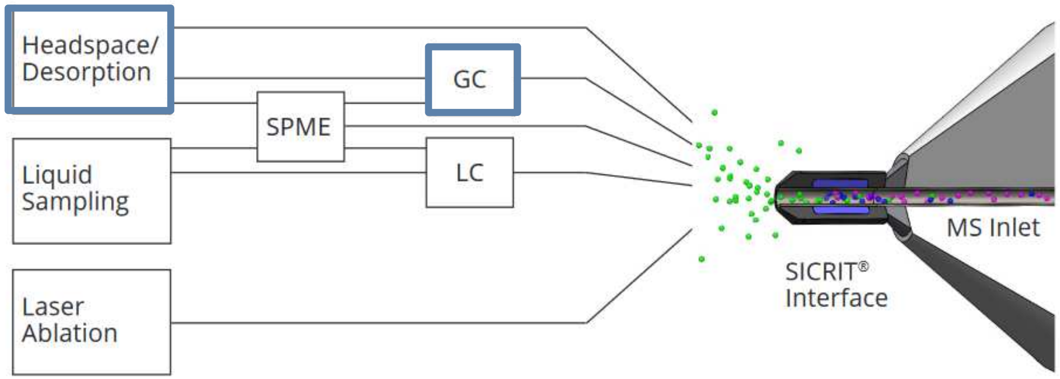


# SICRIT ® - Aplikace / GC-MS

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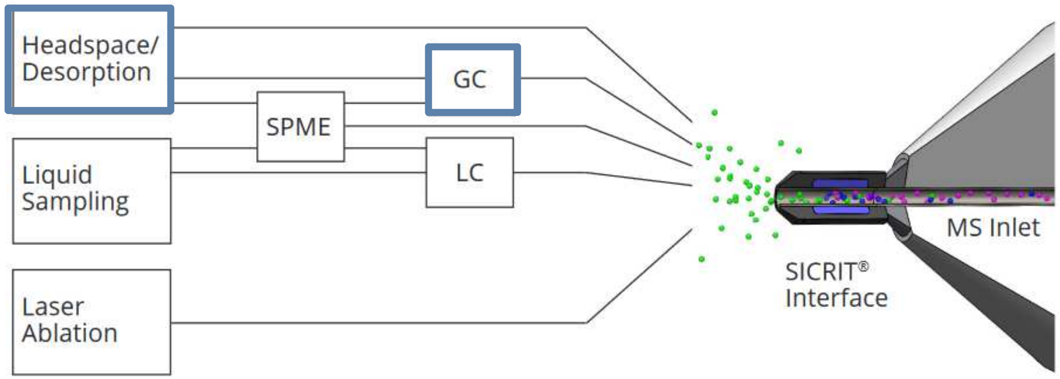
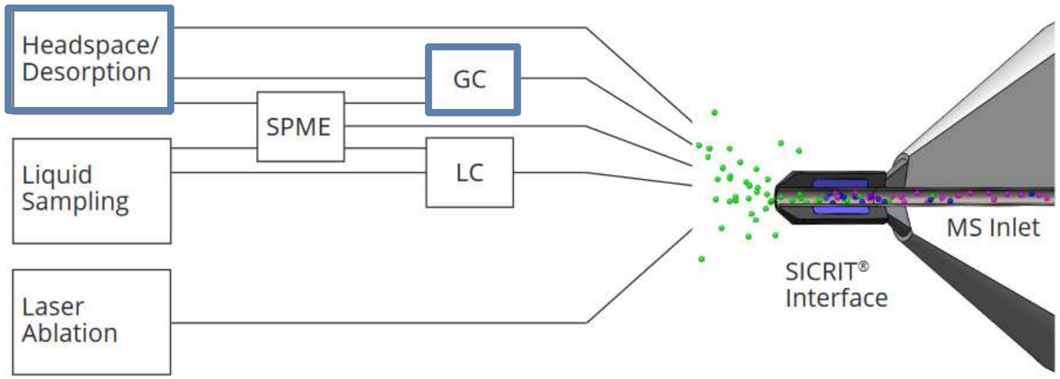


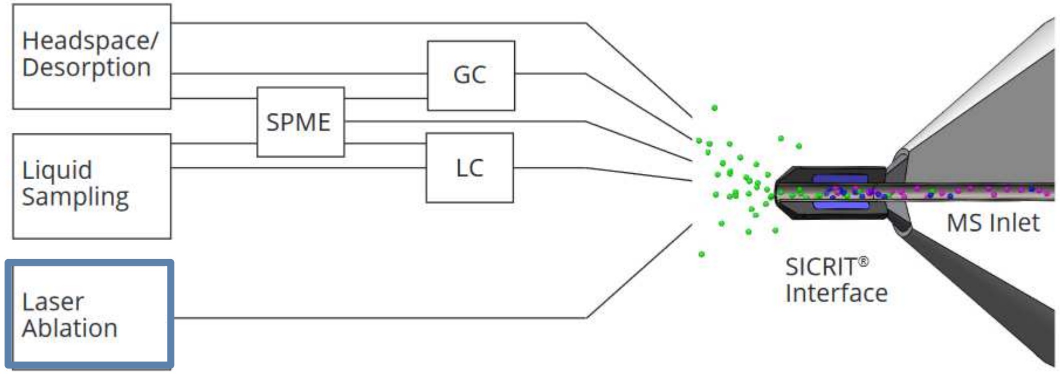

- 2,4-isobutylester
- 3-decen-2-one
- Acetamiprid
- Atrazine
- Azoxystrobin
- Beflubutamid
- Chlorpyrifos
- Chlorpyrifos-methyl
- Deltamethrin
- Demeton-S-methyl
- Dichlobenil
- Dieldrin
- DMSA
- EPN
- Genite
- Hexaconazole
- Methamidhopos
- Myclobutanil
- Omethoate
- Primiphos-ethyl
- Primiphos-methyl
- Pyrazpohos
- Quinalphos
- Simeconazole
- Triadimefone
- Vinclozolin
- Dichlorvos
- Difufenican
- Flurprimidol

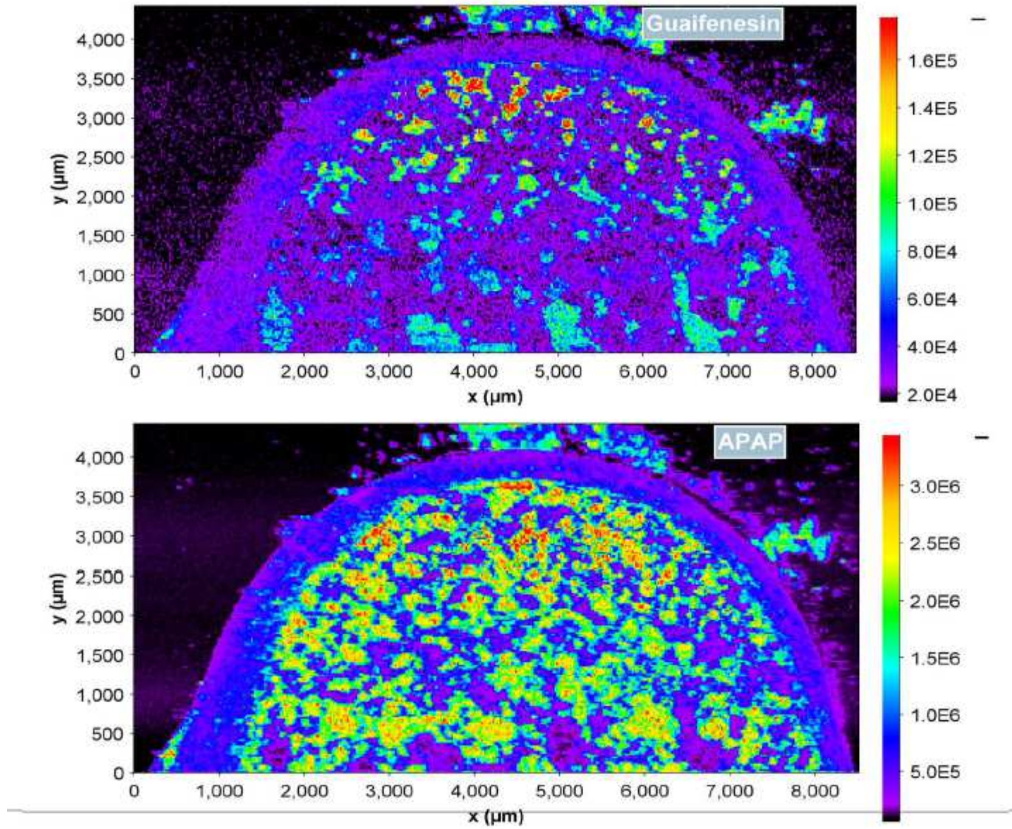
# SICRIT ® - Aplikace / GC-MS



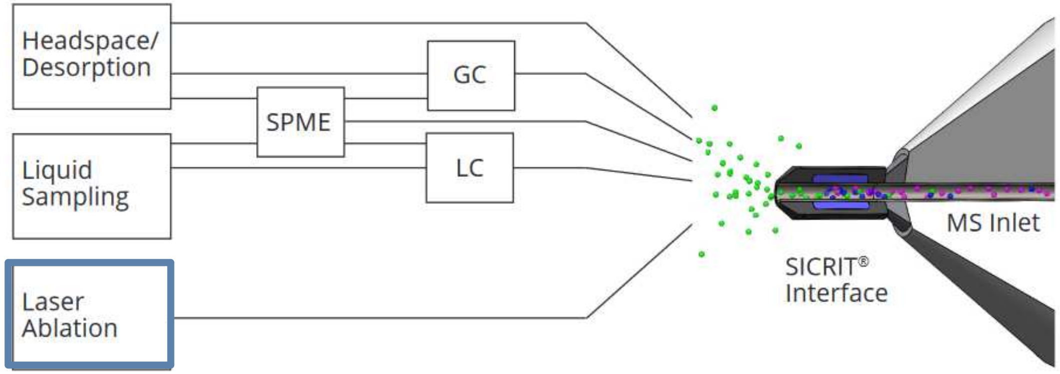

| S/N hodnoty | | |
|---|---|---|
| **Analyt** | **SICRIT-GC-MS** | **APGC-MS** |
| 2,4-D-isobutylester 1 | 5 | 5.9 |
| 3-decen-2-one 1 | 188.4 | - |
| Acetamiprid 1 | 314.5 | 2.9 |
| Atrazine 1 | 482.3 | 19.6 |
| Azoxystrobin 1 | 455.2 | 97.5 |
| Beflubutamid 1 | 2874.6 | 2.2 |
| Chlorpyrifos 1 | 719.5 | 9.5 |
| Chlorpyrifos-methyl 1 | 352.7 | 53.1 |
| Cypermethrin(sum) 1 | 205.6 | 41.9 |
| DDE-PP 1 | 25.9 | 43.4 |
| Deltamethrin 1 | 112.2 | 21.7 |
| Demeton-S-methyl 1 | 66.5 | 9.9 |
| Dichlobenil 1 | 46.3 | 28.9 |
| Dichlorvos 1 | 89.3 | 163.8 |
| Dieldrin 1 | 508.7 | 9.5 |
| Diflufenican 1 | 825.7 | 242.9 |
| DMSA 1 | 761.7 | 19.4 |
| EPN 1 | 422.2 | 32.9 |
| Flurprimidol 1 | 283.7 | 308.5 |
| Genite 1 | 16.8 | 48.1 |
| Hexaconazole 1 | 65.6 | 12.8 |
| Methamidophos 1 | 146.7 | 3558 |
| Myclobutanil 1 | 391.6 | 111.2 |
| Omethoate 1 | 703.1 | 31.2 |
| Pirimiphos-ethyl 1 | 570.2 | 16.5 |
| Pirimiphos-methyl 1 | 332.3 | 94.7 |
| Pyrazophos 1 | 729.8 | 66.9 |
| Quinalphos 1 | 172 | 12983.6 |
| Simeconazole 1 | 129.4 | 22361.8 |
| Triadimefon 1 | 257.1 | 7.9 |
| Vinclozolin 1 | 2.4 | 1.4 |

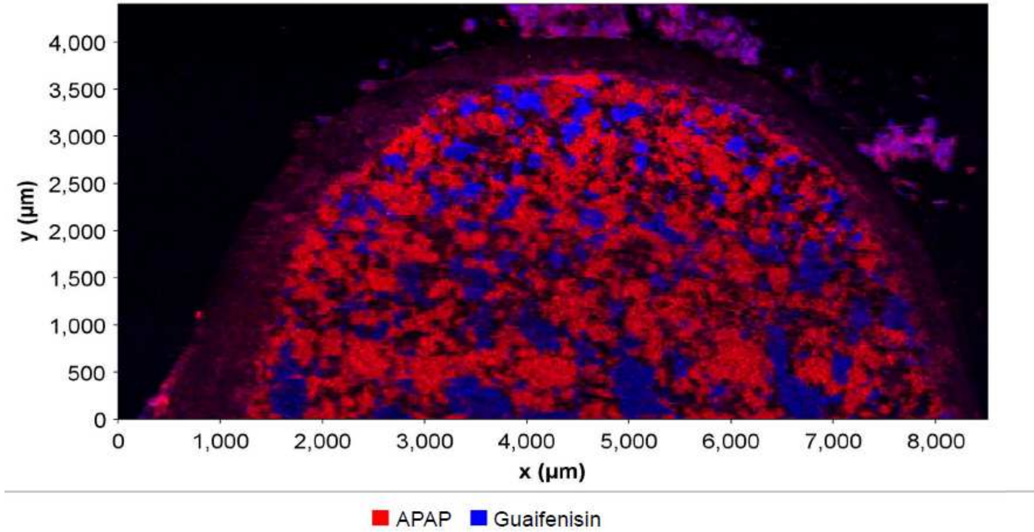
# SICRIT ® - Aplikace / Laserová ablace



# SICRIT ® - Aplikace / Laserová ablace



Děkuji za pozornost

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bucek@pragolab.cz



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