# Expression® CMS:

Spettrometro di massa a singolo quadrupolo con sorgenti ESI e APCI

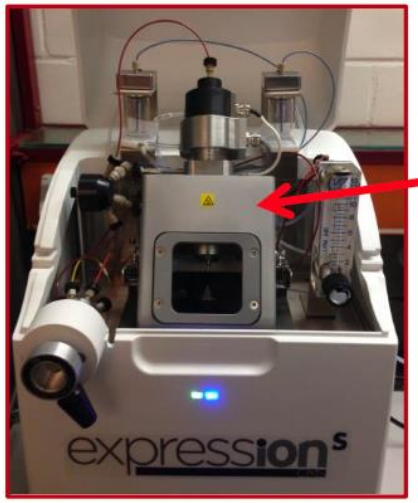
The expression CMS
*Compact - Fast - Easy*

VITALITY

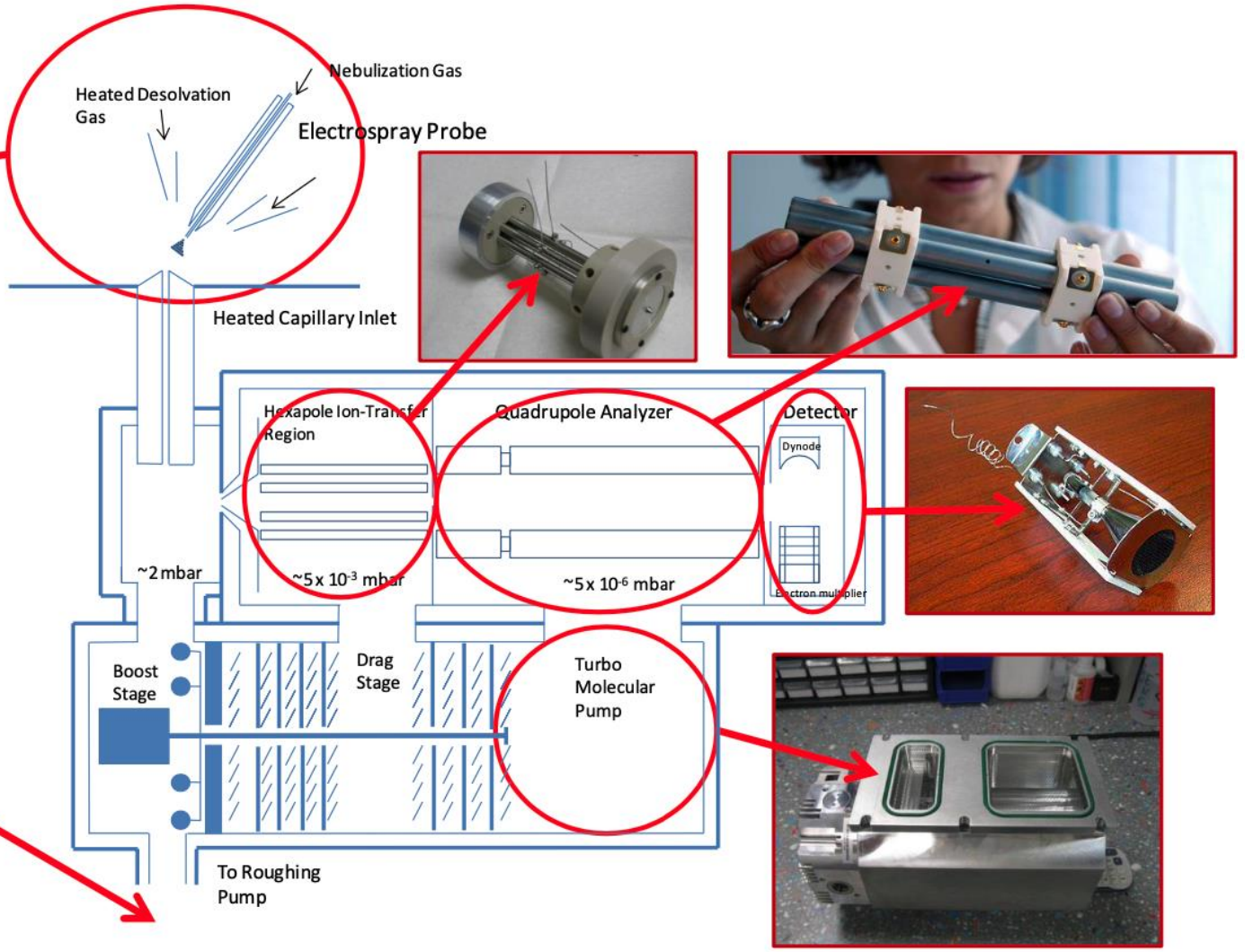
## Small and Compact Design



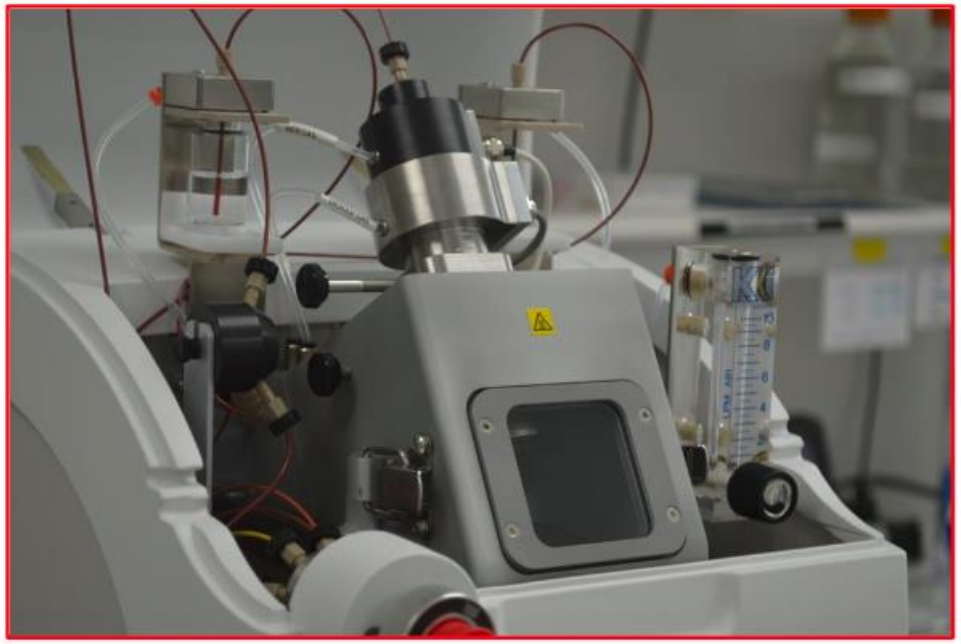
Cart-based portable




ESI, APCI & ASAP

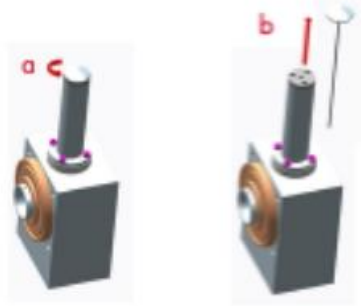



Disassembling and reassembling of sources and inlet capillary doable without difficulties and without venting the system (automatic capillary sealing valve).



Electrospray Ionization (ESI) Source Housing

Front and back





Direct analysis probe (ASAP)


TLC/CMS –
mass analysis of TLC spots


Detector for (U)HPLC


Compound identification
by direct injection

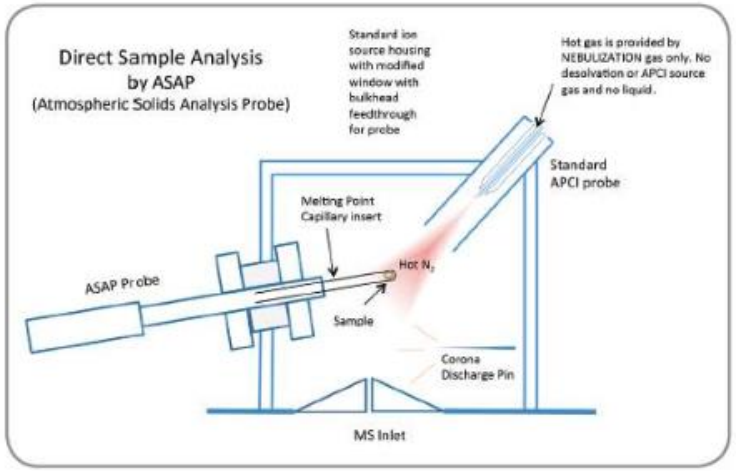
High performance compact mass spec
designed especially for chemists


Cart-based LC/MS


Coupled to Flow Reactors,
Hydrogenation & Batch Chemistry


Online Flash/CMS –
mass directed fraction collection


Purification by SFC or Prep-LC




## Atmospheric Solids Analysis Probe

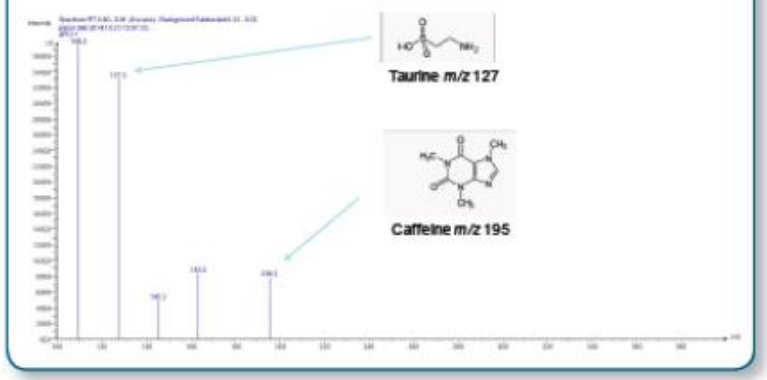
- No sample preparation
- No chromatography
- Data in < 1 minute

The closed end of a glass capillary is dipped into the sample of interest or scraped on a solid surface, and then placed into the CMS for analysis.

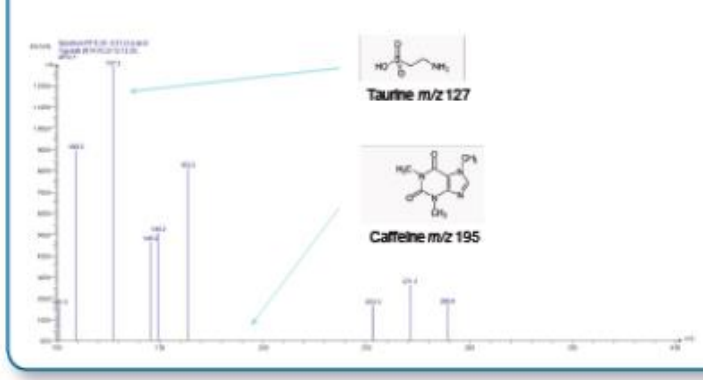
Ideal for:
- Reaction monitoring
- Compound ID
- Food safety
- Natural products

# … in food and drug analysis.

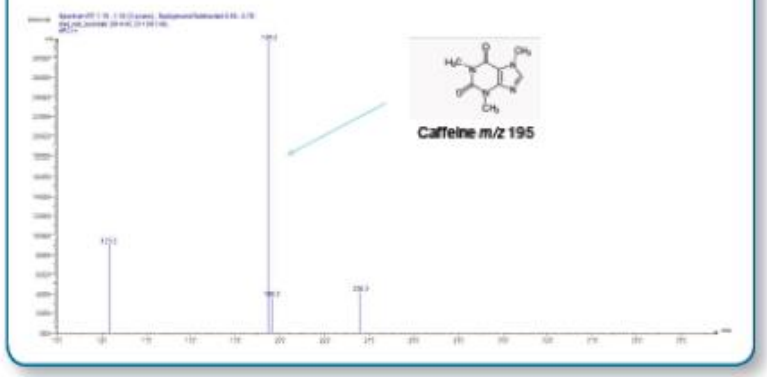
## COLA



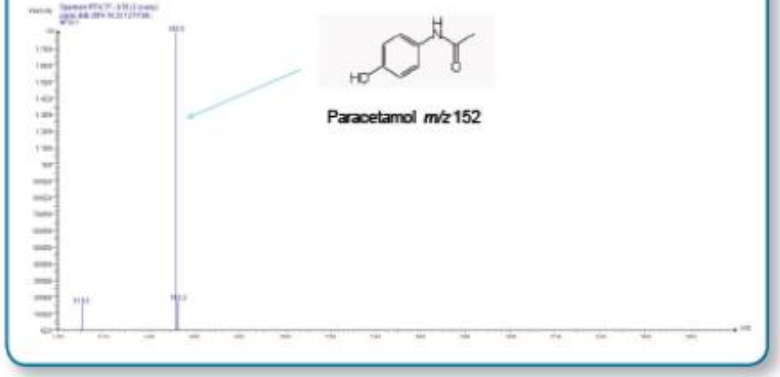

## CAFFEINE-FREE LEMONADE




## ENERGY DRINK




## PARACETAMOL TABLET



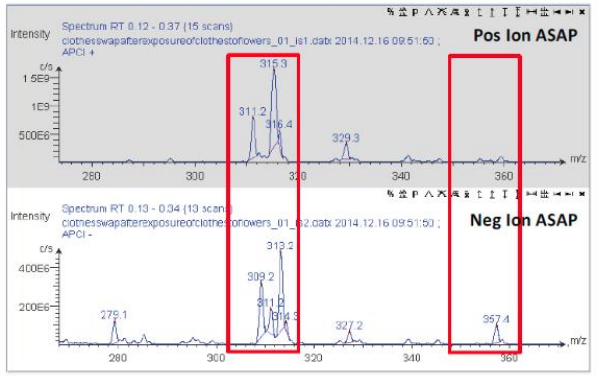

Finanziato dall'Unione europea
NextGenerationEU

Ministero dell'Università e della Ricerca

Italiadomani
PIANO NAZIONALE DI RIPRESA E RESILIENZA

## … for detecting traces of cannabis compounds.

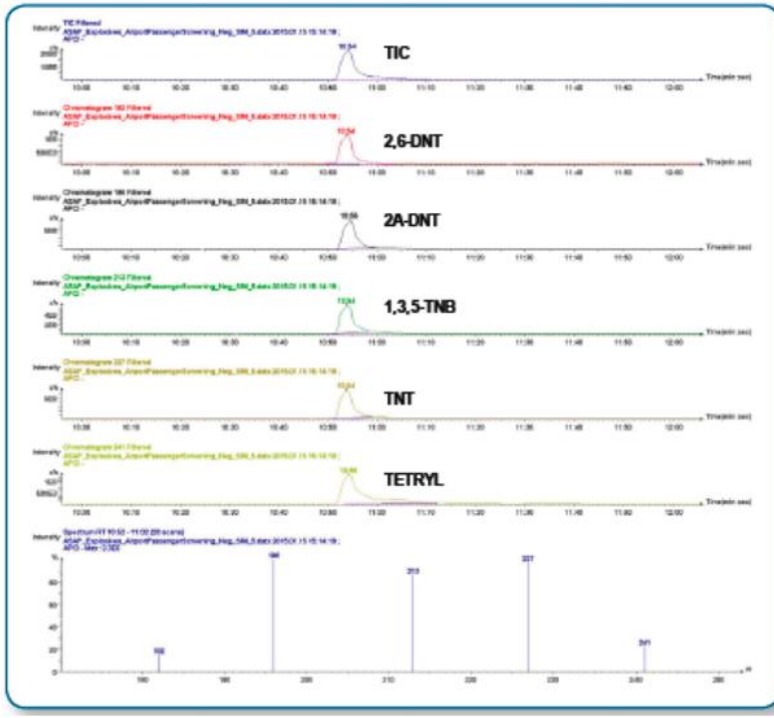
To simulate Cannabis contact with clothing fabric material as it would occur when handling raw material, a pinch of the sample was rolled over a shirt sleeve and sleeve the sampled with the ASAP probe by moving the glass capillary over the cotton material in a criss-cross movement.




MS data showing both positive ionization (top trace) and negative ionization (bottom trace) of the ASAP clothes swipe. The intense m/z signals at 311.2/309.1 and 315.2/313.2 correspond to the respective (M+H)+ and (M-H)- for Cannabinol (CBN) and THC/CBD, respectively, with the deprotonated molecule ion observed at m/z 357.2 for THC-acid/CBD-acid.

## … for detecting traces of explosives


Explosives Residue Detected



Direct analysis probe (ASAP)

TLC/CMS –
mass analysis of TLC spots

Detector for (U)HPLC

Compound identification
by direct injection


High performance compact mass spec
designed especially for chemists

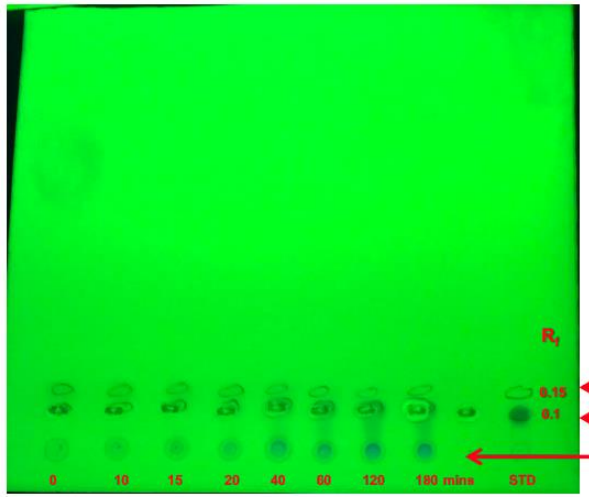
Cart-based LC/MS

Coupled to Flow Reactors,
Hydrogenation & Batch Chemistry

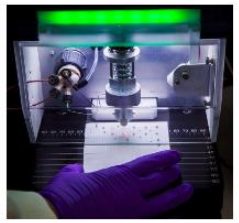
Online Flash/CMS –
mass directed fraction collection

Purification by SFC or Prep-LC

## TLC separation of a Suzuki reaction mixture




The developed TLC plate with Suzuki reaction mixture under UV 254nm



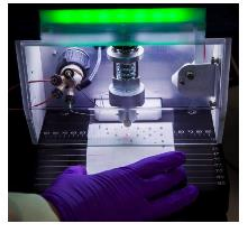
### Synthesis of 4-aminobiphenyl

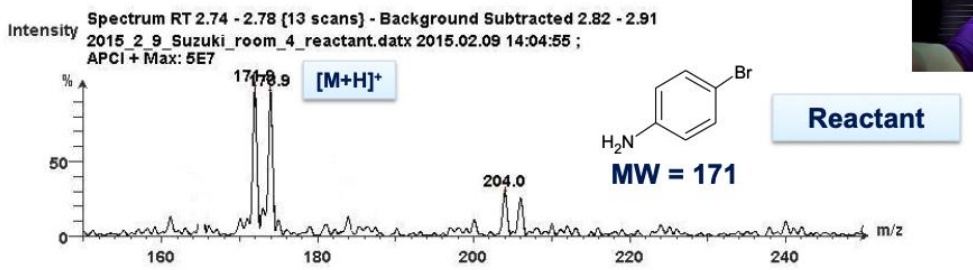

**Reactant:** 4-bromoaniline; rf= 0.15

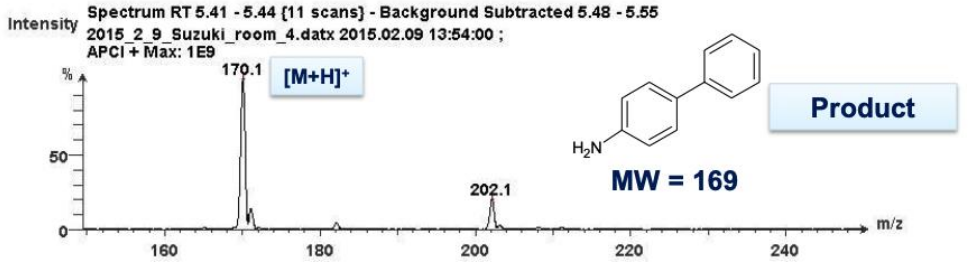
**Product:** 4-aminobiphenyl; rf = 0.10

**Origin:** Spotting of Reaction Mixture

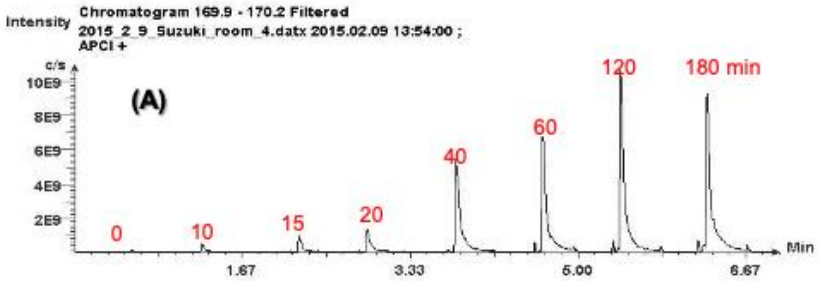
## Suzuki Reaction Reactant/Product Mass Spectra



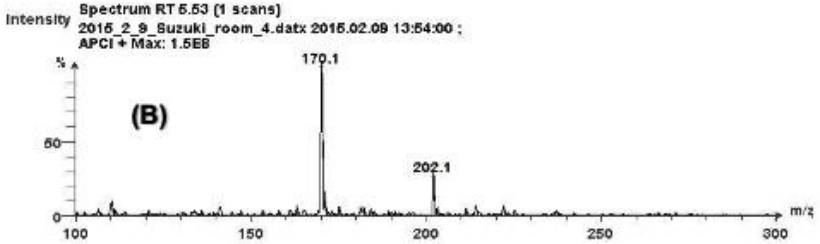


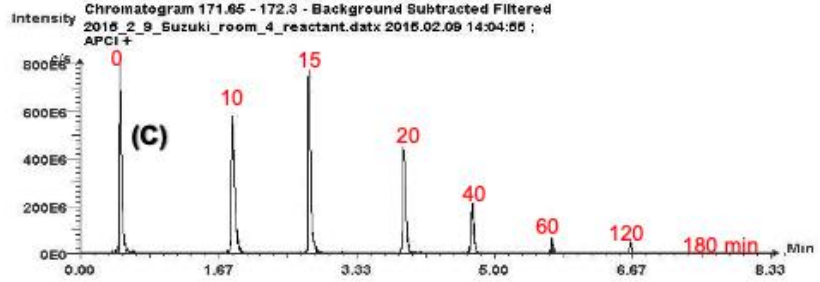
**Appearance of product**



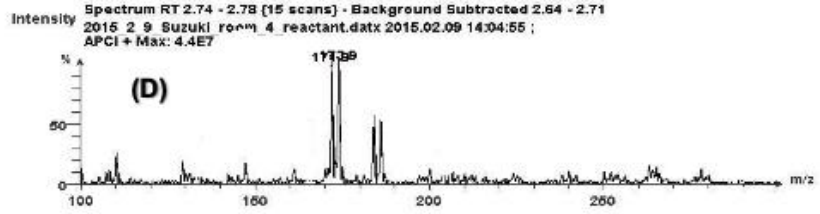

**Mass spectrum of product**



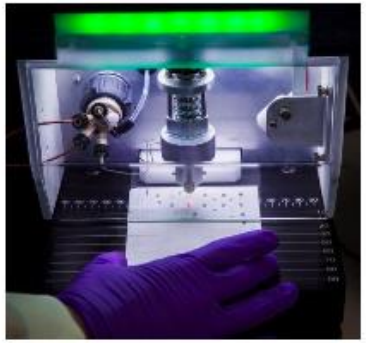

**Disappearance of reactant**



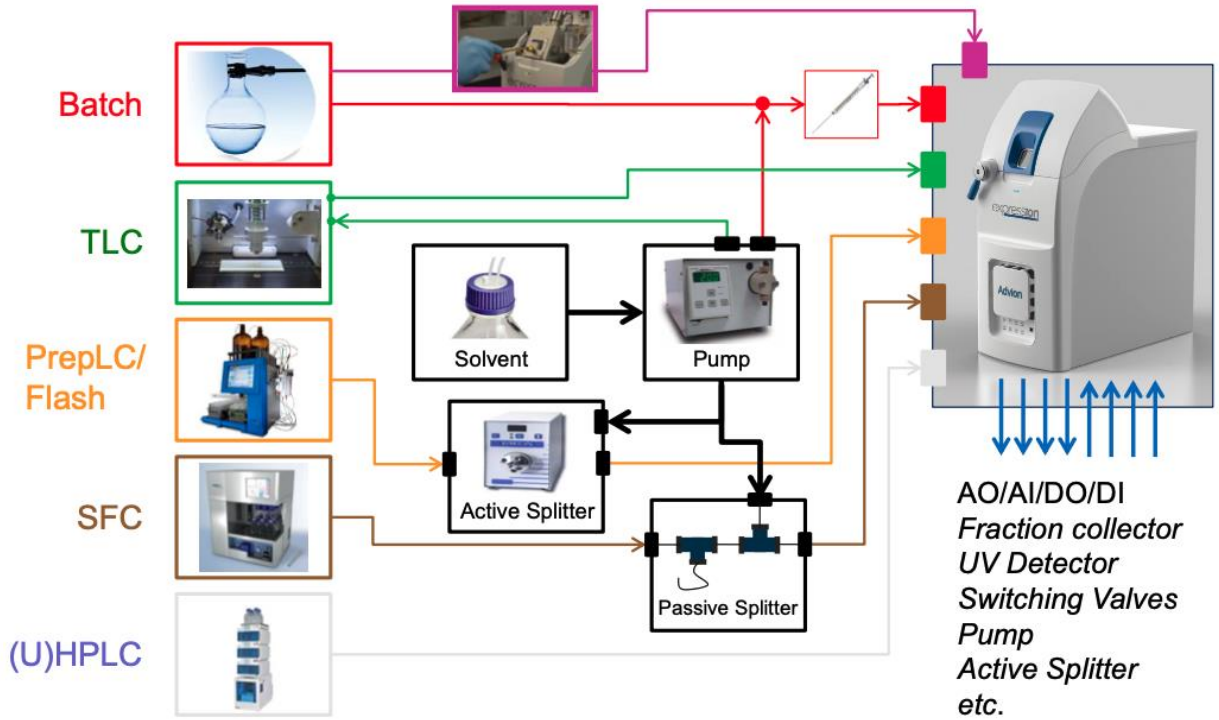

**Mass spectrum of reactant**




**Suzuki Reaction monitored by mass spectrometry**



- Ion Source: ESI, APCI & ASAP
- Polarity: Positive & negative ion switching in single analysis
- Flow rate: ESI: 10 µl/min to 1 mL/min
  APCI: 10 µl/min to 2 mL/min
- Mass Range: expression S up to m/z 1,200
  expression L up to m/z 2,000
- Scan Speed: 10,000 *m/z* units/sec
- Sensitivity: 10 pg Reserpine (FIA – 5 µl injection at 100 µl/min) 100:1 S/N (RMS) with SIM of m/z 609.3
- Resolution: 0.5-0.7 *m/z* units (FWHM) at 1000 *m/z* units $sec^{-1}$ over entire acquisition range
- Accuracy: 0.1 m/z units over entire acquisition range



Q: WHY DID YOU INCORPORATE THE EXPRESSION® CMS INTO YOUR LABORATORY?

A: The expression® CMS allows us to efficiently analyze the mass of newly formed compounds in (almost) real time. We particularly value that the instrument allows us to monitor the reaction progress of crude mixtures. Separated on a TLC, products and potential side products can be identified, which results in an optimized and faster down-stream-processing, e.g. column chromatography, and only desired products are isolated on a preparative scale. Furthermore, the ASAP mode is very helpful and extremely fast, when looking for expected product masses, e.g. in the fractions of preparative HPLC separations – just dip it in and measure the MS... it takes 30 seconds per fraction. The possibility to easily switch between the ionization modes ESI and APCI as well to measure MS spectra in positive and negative mode in parallel is very helpful for a fast and reliable analysis.


Wennemers Research Group
ETH, Laboratory of Organic Chemistry, Zurich, Switzerland

Q: WHO WOULD YOU RECOMMEND TO PURCHASE THE EXPRESSION® CMS?

A: We recommend the expression® CMS in combination with the TLC-Reader Plate Express™ to any group working in the field of synthetic organic chemistry. The reliable and fast identification of molecules is extremely helpful to monitor reactions, to identify the desired products and potential side products, and to simplify downstream processing.

**Grazie per l'attenzione**