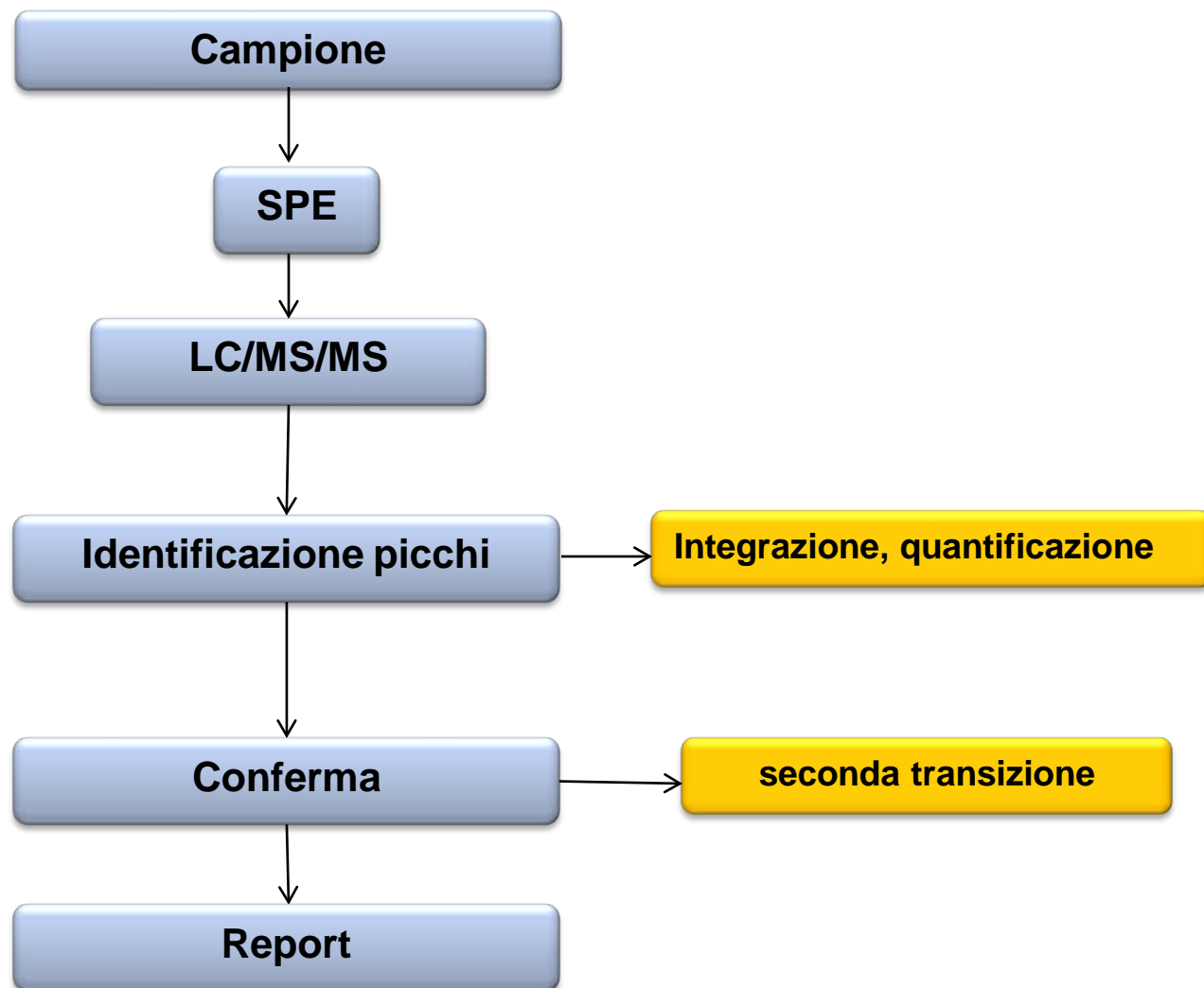




Orbitrap e Q-Orbitrap

Dr Igor Fochi
LSMS Product Specialist
Small Molecules
Palermo, 17/05/2013

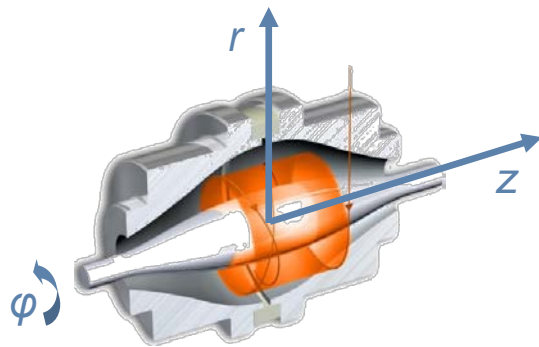
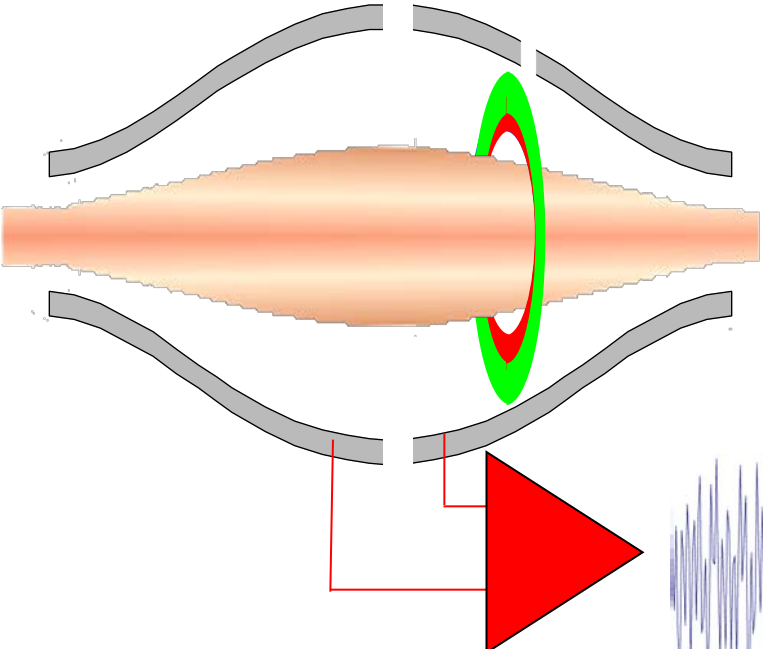
Analisi MS Quadrupolare



Caratteristiche:

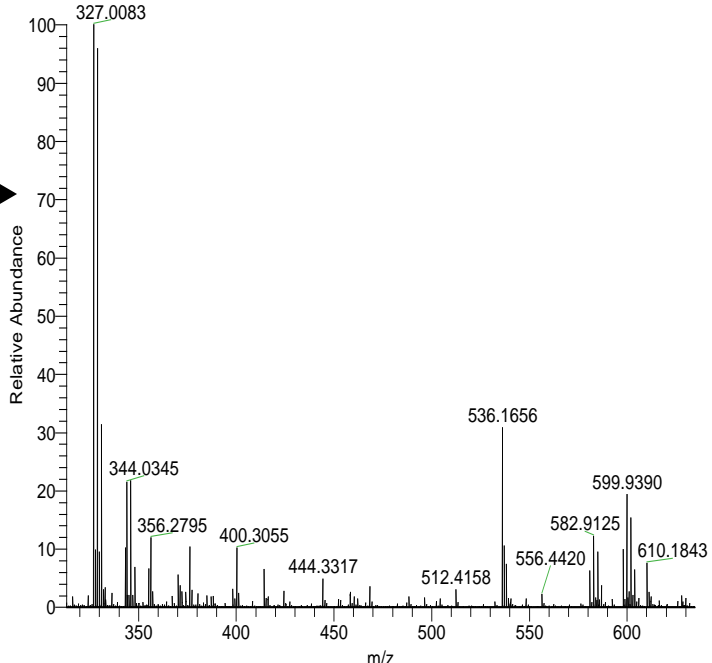
- Doppia transizione a bassa risoluzione
- Limite di 400-500 transizioni
- **Analiti predeterminati**

Orbitrap Technology: Makarov A. "Anal. Chem. 2000, 72, 1156-1162"



Electrostatic potential distribution

2057_2_new #505-731 RT: 8.53-12.16 AV: 227 NL: 5.16E5
 T: FTMS {1,1} + p ESI Full lock ms [120.00-650.00]



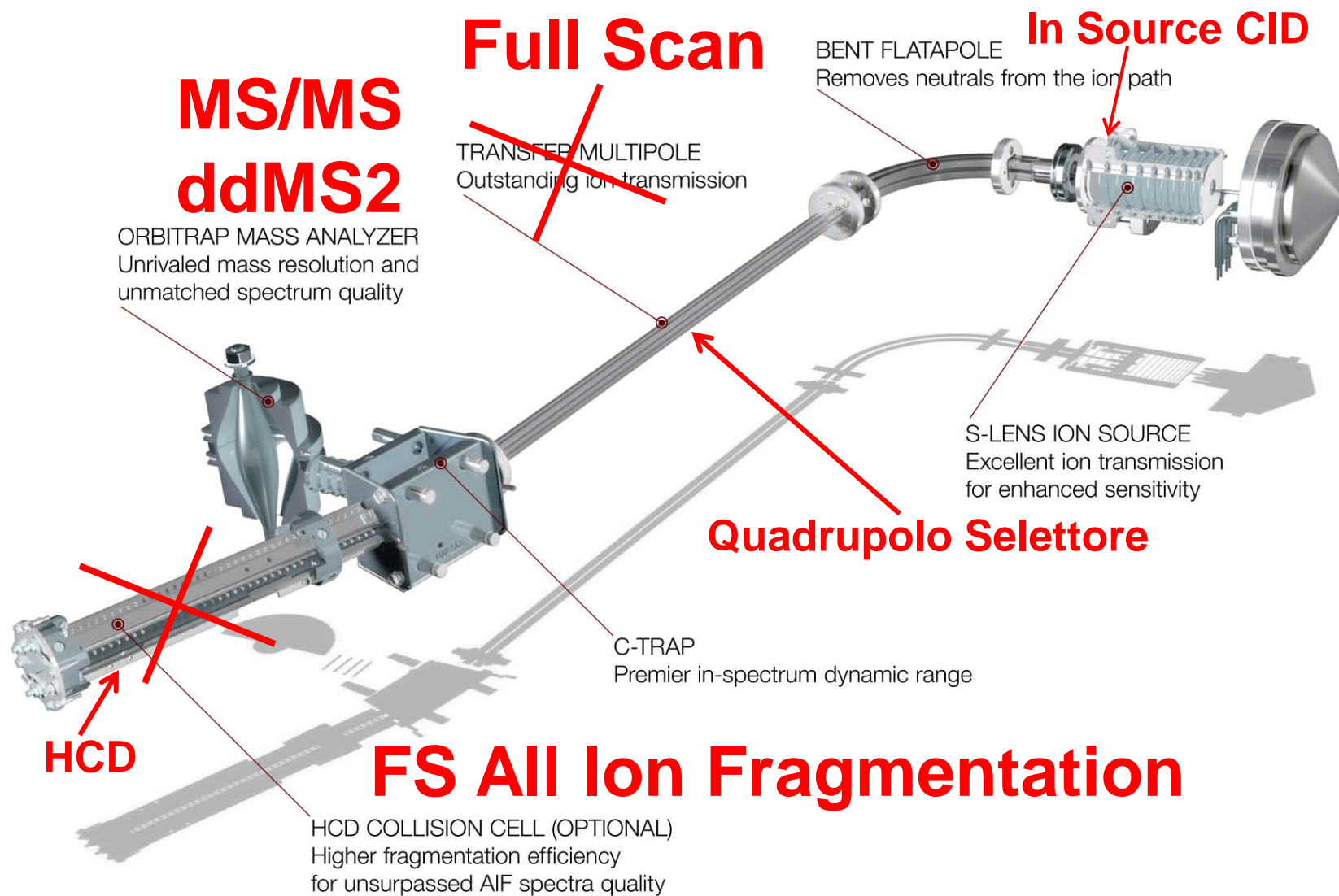
FT



Baron, Joseph Fourier

$$\omega_z = \sqrt{\frac{k}{m/q}}$$

Exactive Plus / Q Exactive

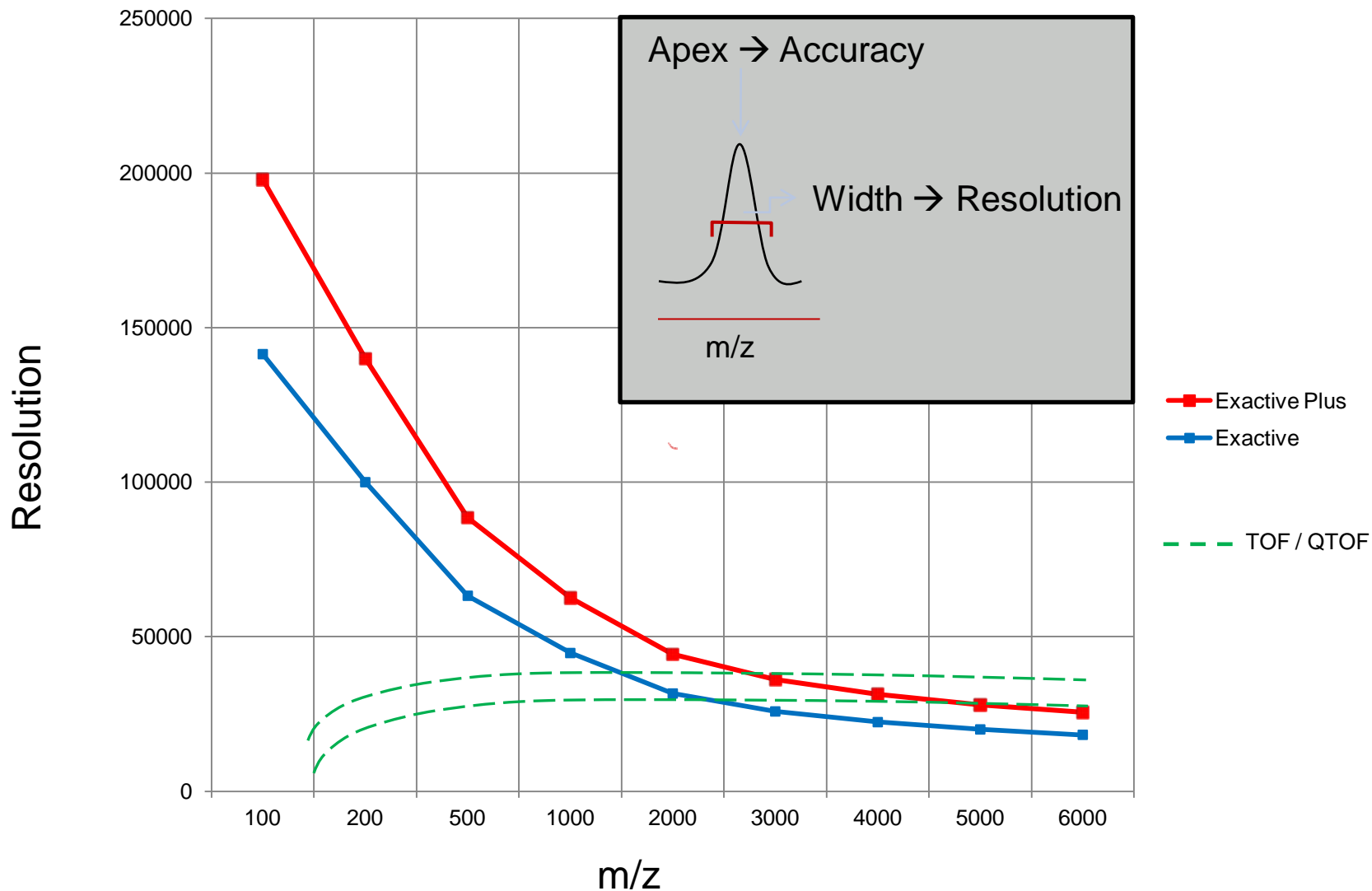


Exactive Plus™ - Q Exactive™

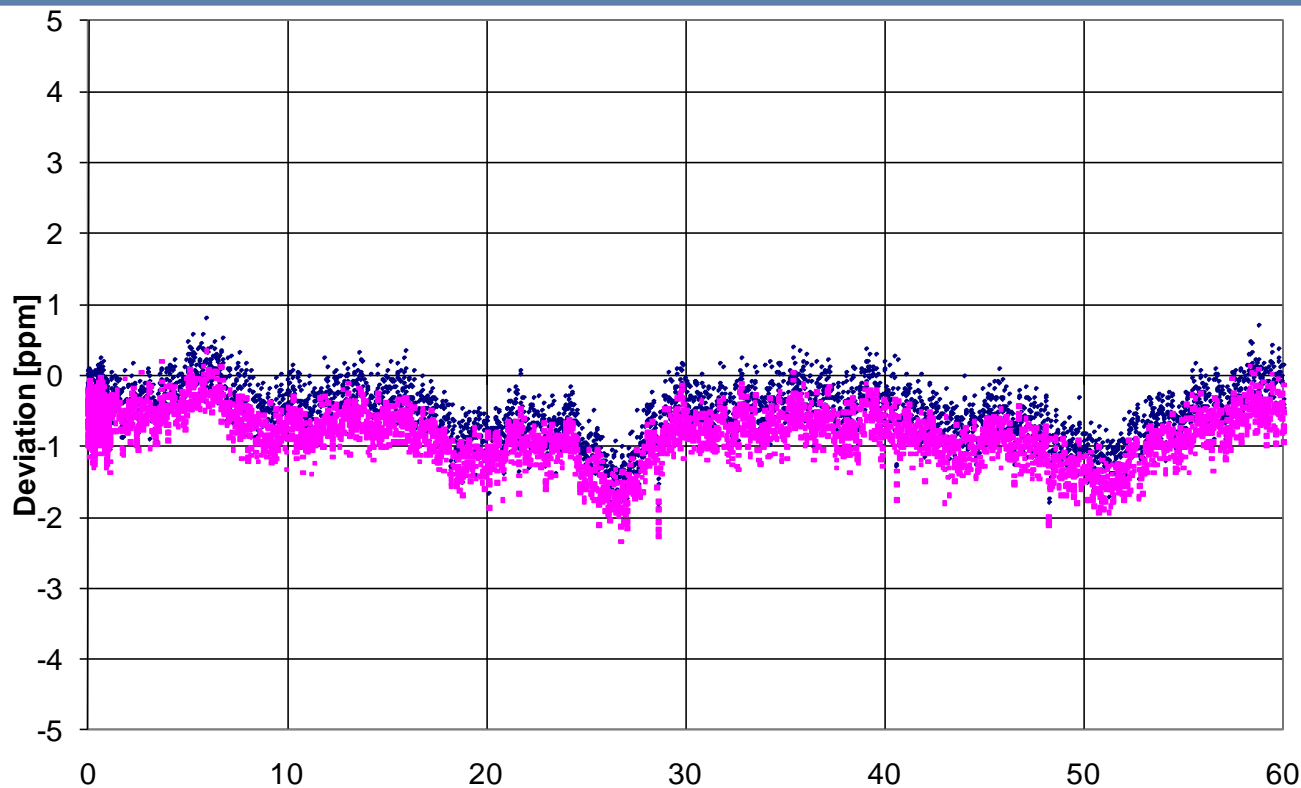


- Risoluzione: 140K a 200m/z
- Accuratezza misura m/z: <1ppm con lock mass; <3ppm con calibrazione esterna
- Velocità scansione: 1.5 Hz a risoluzione 140K
- Scan Range: Full Scan 50-6000 m/z; MS/MS 50-2500 m/z con isolamento del precursore da 0.4 Da

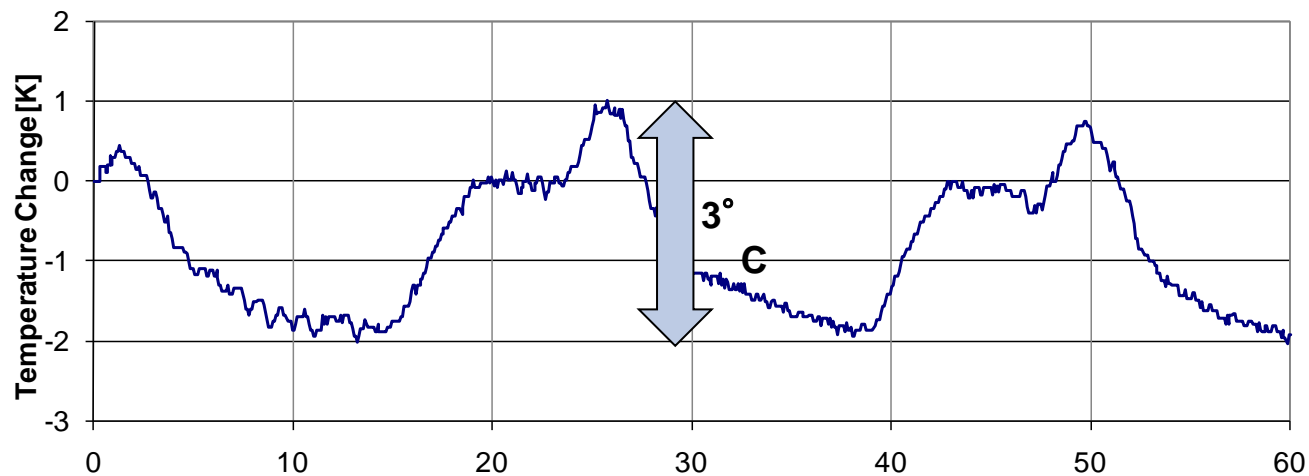
Risoluzione (FWHM) vs m/z



Accuratezza di Massa a lungo termine in calibrazione esterna



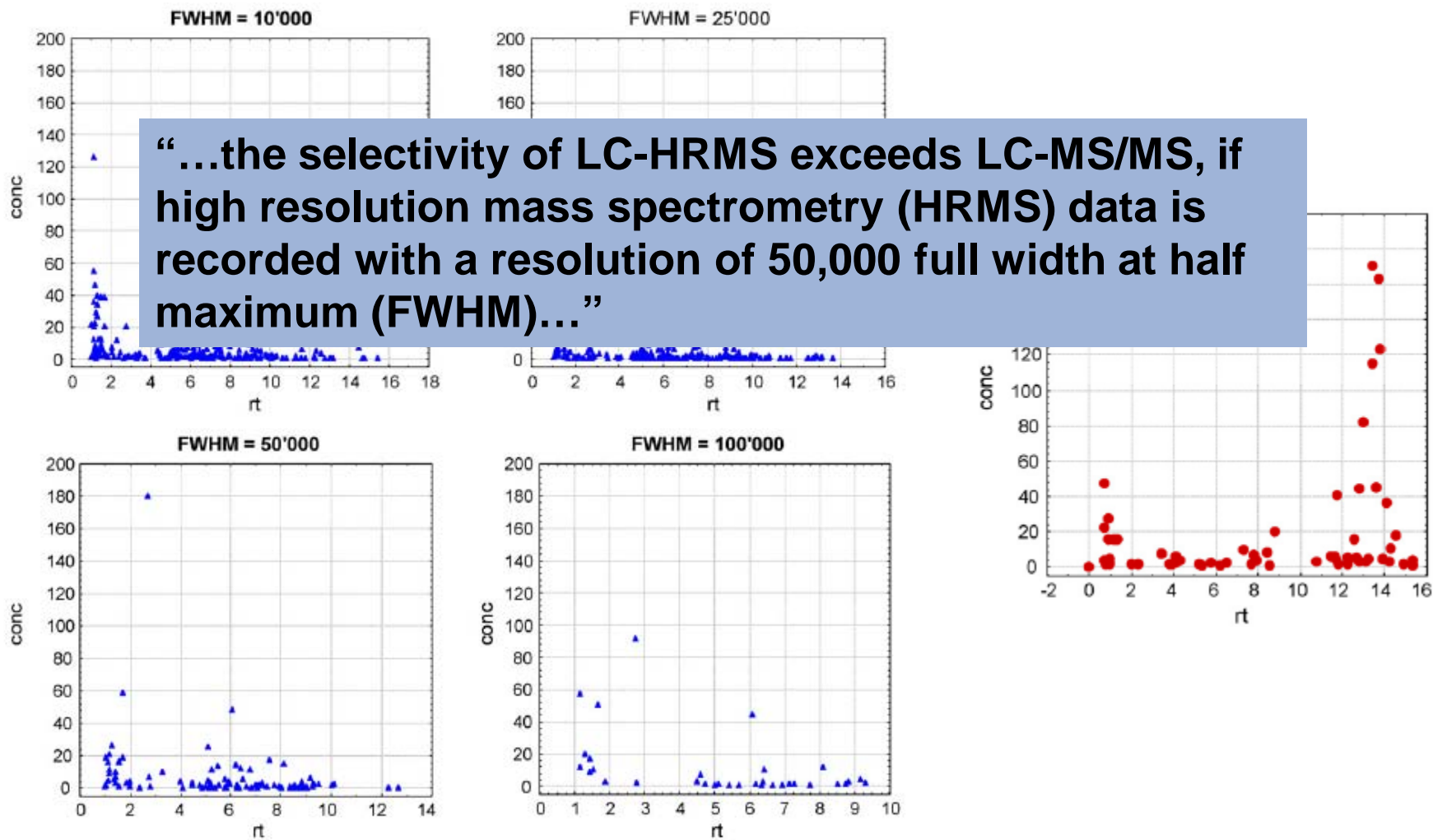
Time [h]



Time [h]

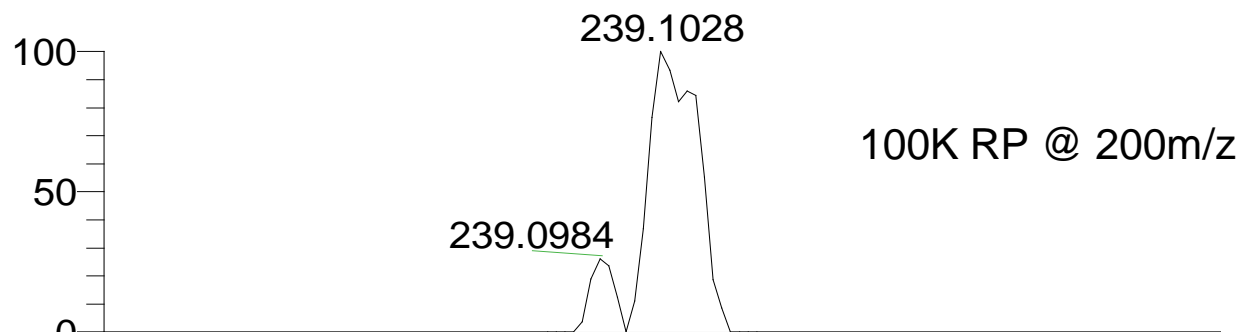
- Realistic conditions of an average lab
- Temperature variations up to 3°C peak-to-peak, up to 1°C/hour

Selettività: HRMS vs QqQ

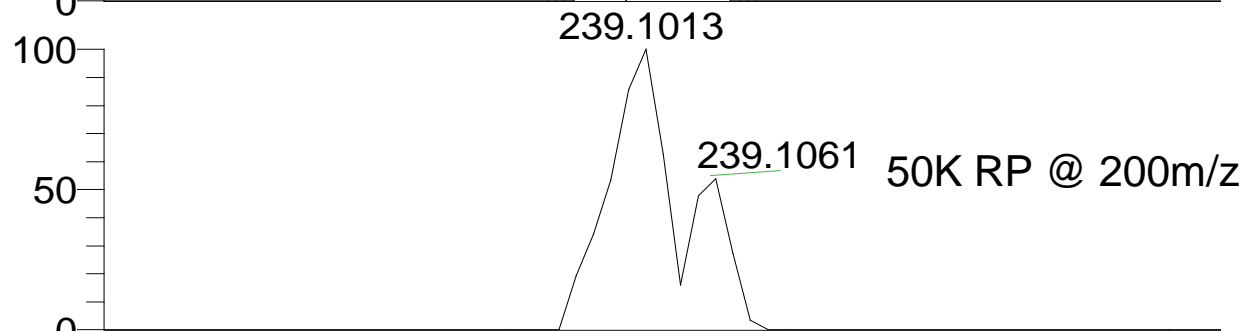


Kaufmann et al: *Anal. Chim. Acta* 673, (2010) 60-72

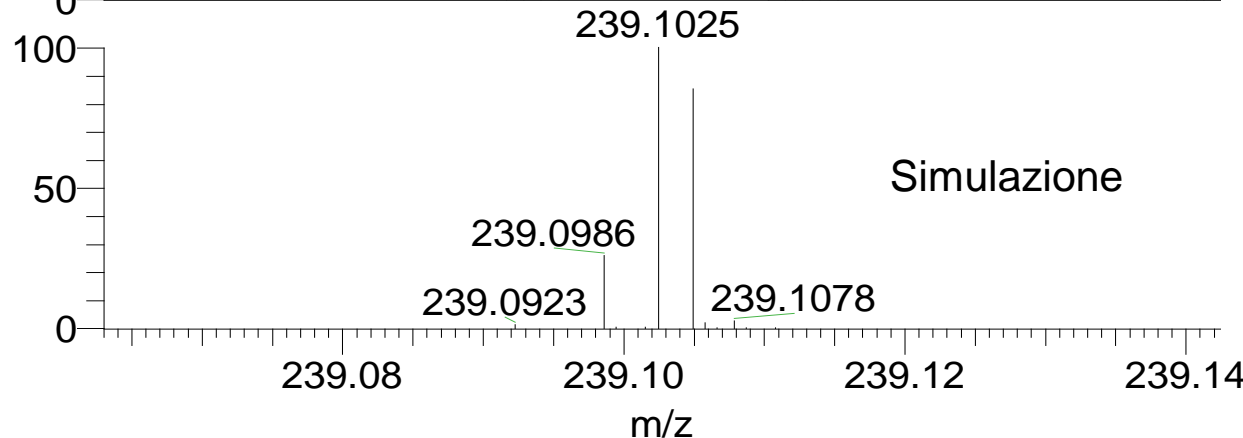
Formulato veterinario di Carbazochrome 1%. “secondo multipletto del pattern isotopico”



NL:
1.51E3
20ppm_pos100k_01#106 RT:
1.59 AV: 1 T: FTMS {1,1} + p
ESI Full lock ms
[100.00-800.00]

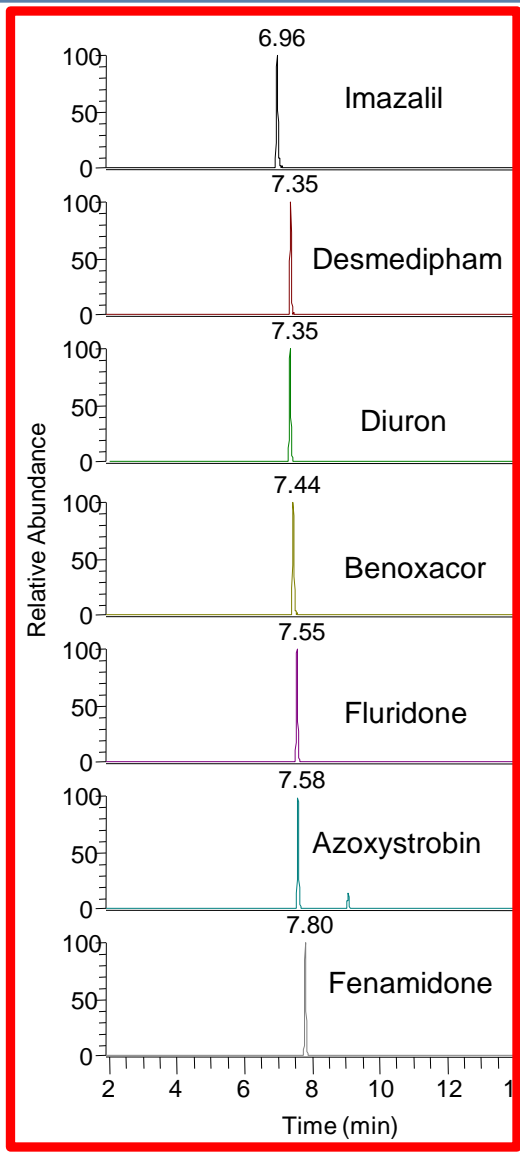


NL:
4.21E2
20ppm_sw50k_02#127-132
RT: 1.58-1.64 AV: 6 T: FTMS
{1,1} + p ESI Full lock ms
[100.00-800.00]



NL:
5.41E3
 $C_{10}H_{13}N_4O_3$:
 $C_{10}H_{13}N_4O_3$
pa Chrg 1

MS/HRMS Target



NL: 1.98E7
 m/z= 297.0541-297.0571 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

NL: 4.67E6
 m/z= 301.1163-301.1193 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

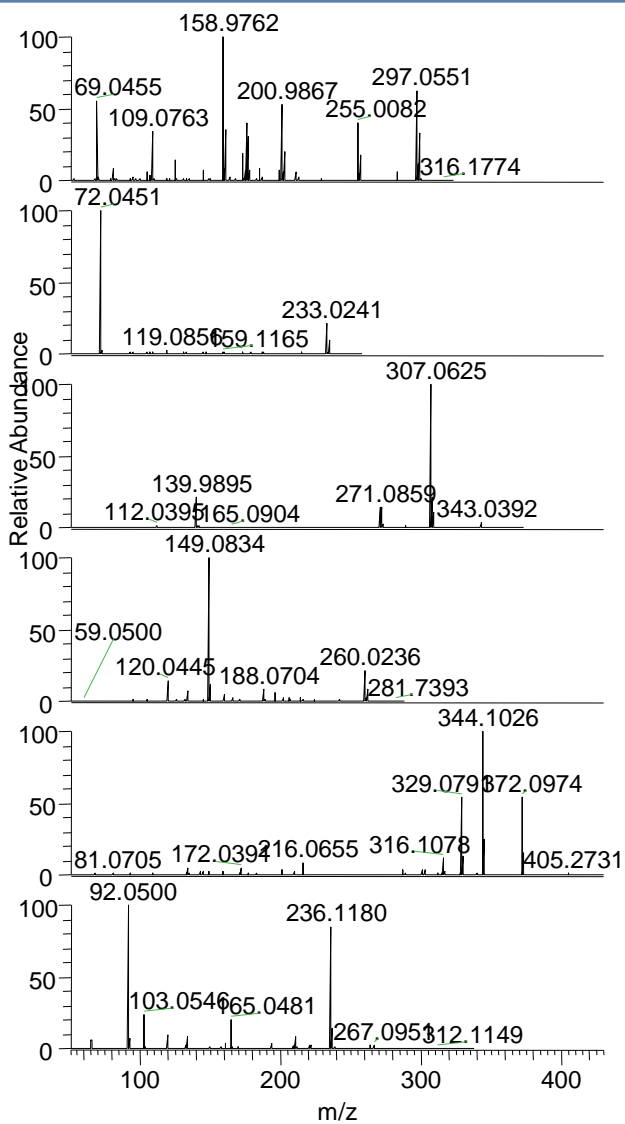
NL: 8.97E7
 m/z= 233.0231-233.0255 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

NL: 1.15E7
 m/z= 260.0226-260.0252 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

NL: 2.21E7
 m/z= 330.1084-330.1118 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

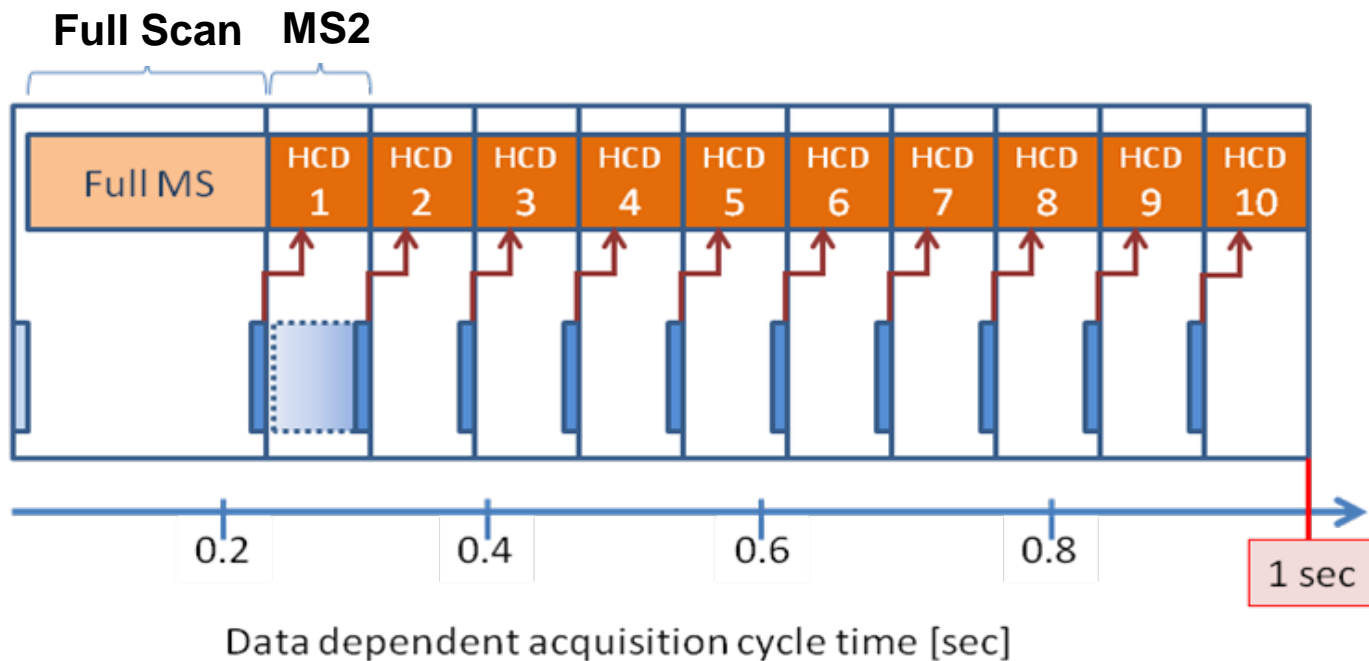
NL: 1.42E7
 m/z= 404.1221-404.1261 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

NL: 4.23E7
 m/z= 312.1149-312.1181 F: FTMS
 + p ESI Full ms [50.00-750.00]
 MS 4xloq_02

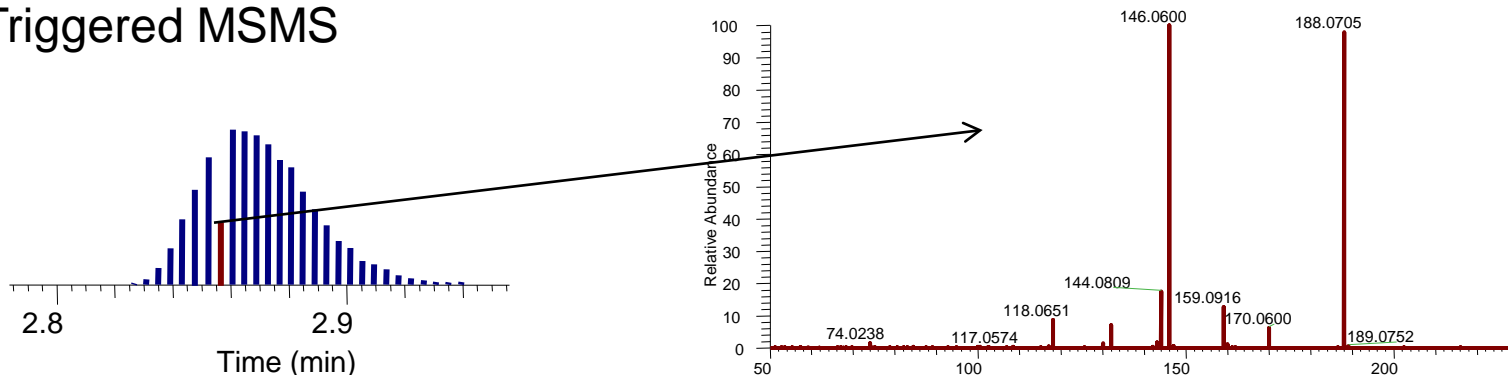


Data Dependent MS/MS

1 full scan @ 70K res
+ 10 MS/MS @ 17.5K



Apex Triggered MSMS



ddMS2 con polarit  alternata: metaboliti ranitidina (fegato di ratto)

LC/MS Chromatogram

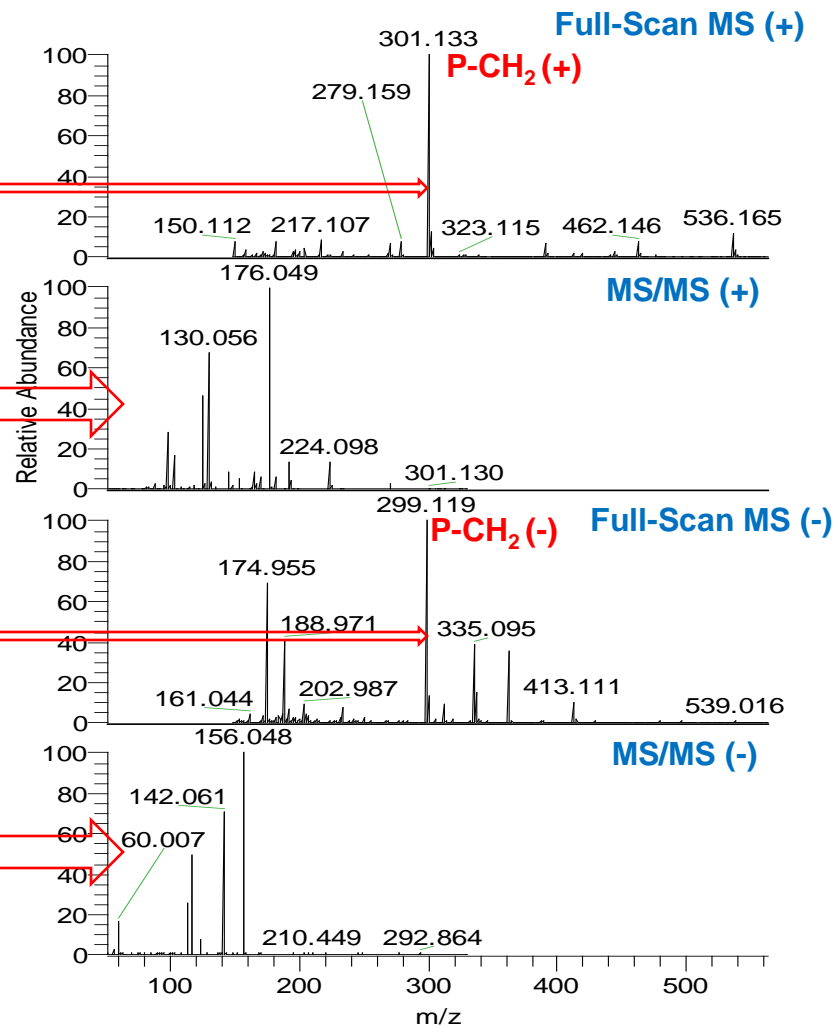
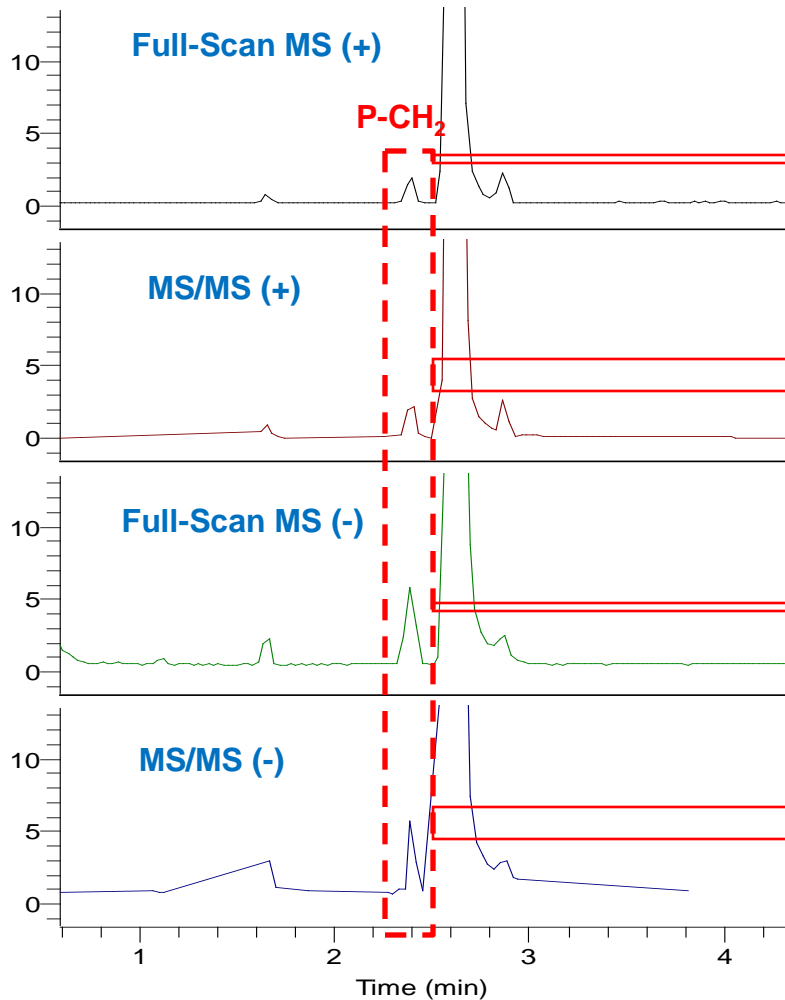
HR-MS Spectra

rantidine_70k_p_n_top3_inclu

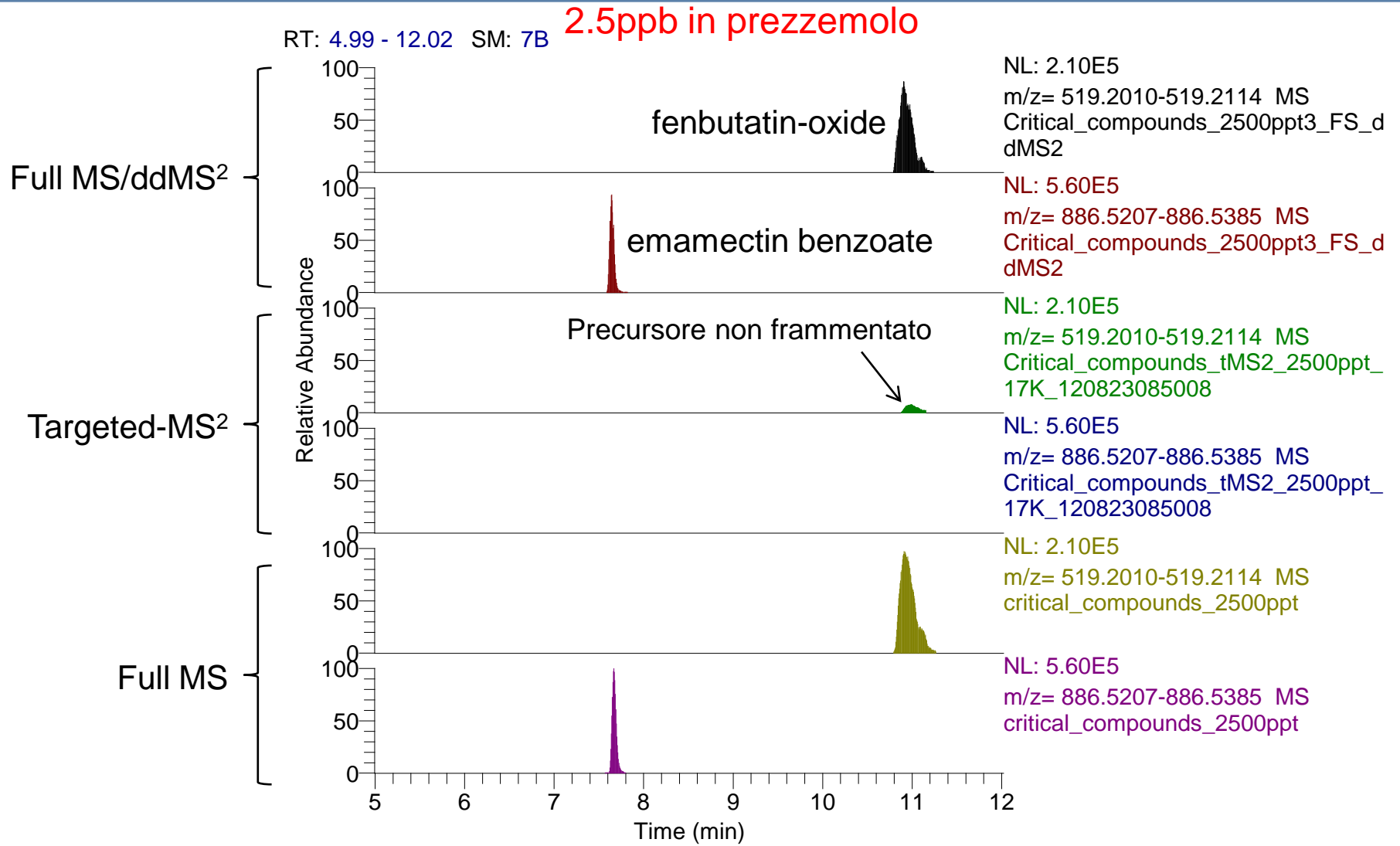
5/10/2011 2:58:42 PM

Ranitidine

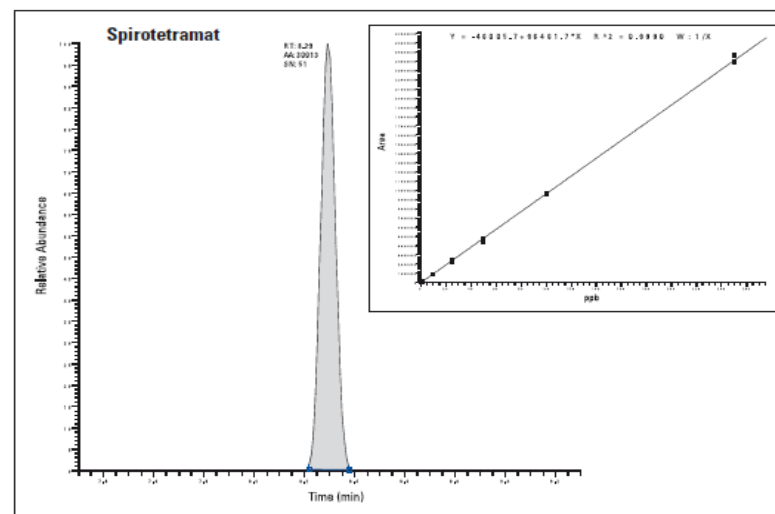
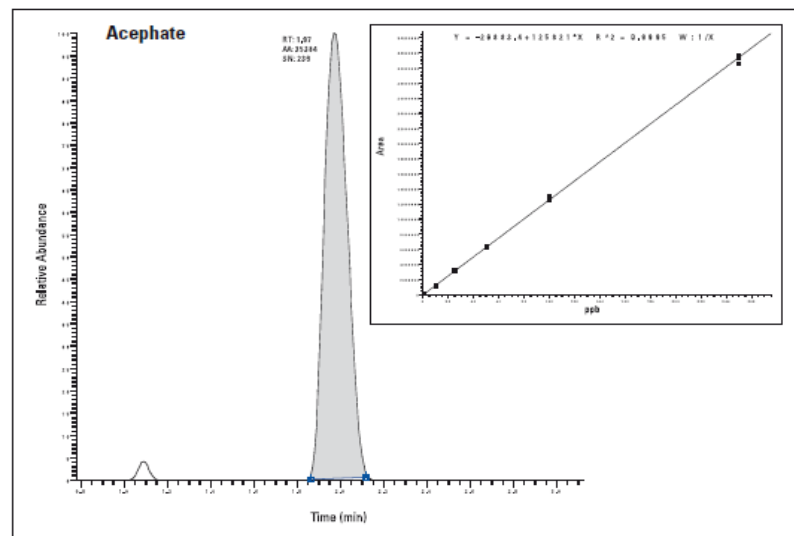
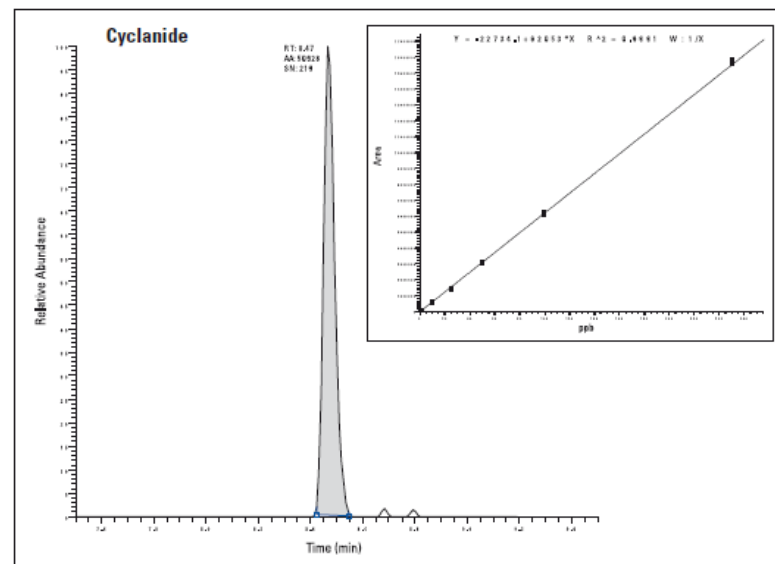
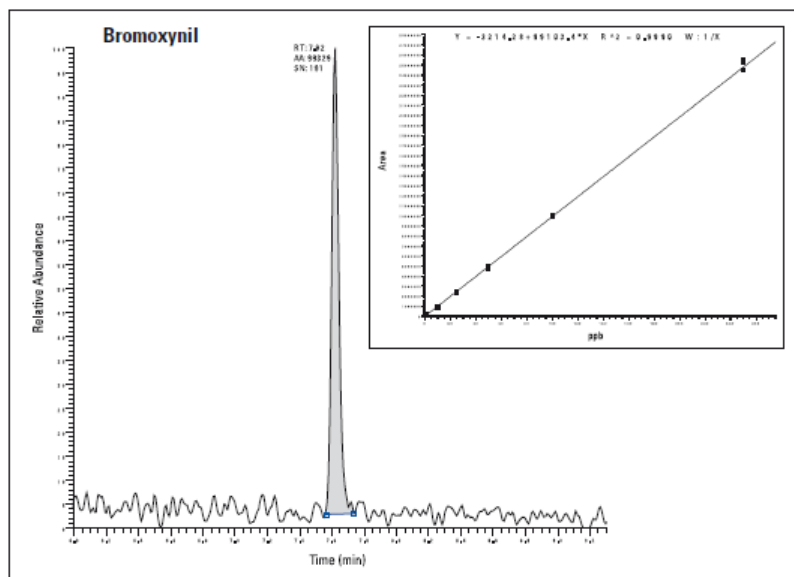
RT: 0.58 - 4.31



Compatibilità frammentazione con analisi retrospettiva



Analisi Quantitativa Pesticidi in matrice – HR Full Scan



UltiMate 3000 x2 Dual-Systems

L'unico vero sistema Dual LC

Unique dual-gradient pump: two ternary pumps in one housing

Solvent Rack with 6-channel degasser

Autosampler with optional thermostating

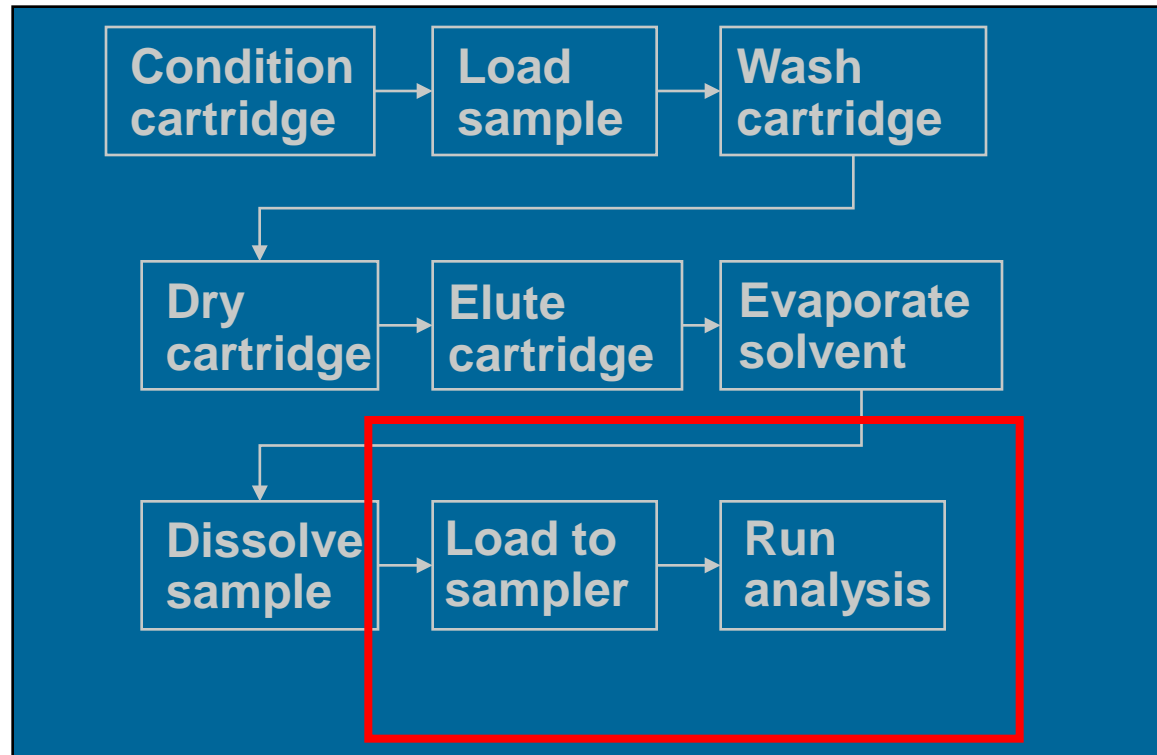
Unique column compartment with up to two switching valves

Variable wavelength or photodiode array detector



Preparazione dei campioni

Workflow



SPE convenzionale (12 campioni)

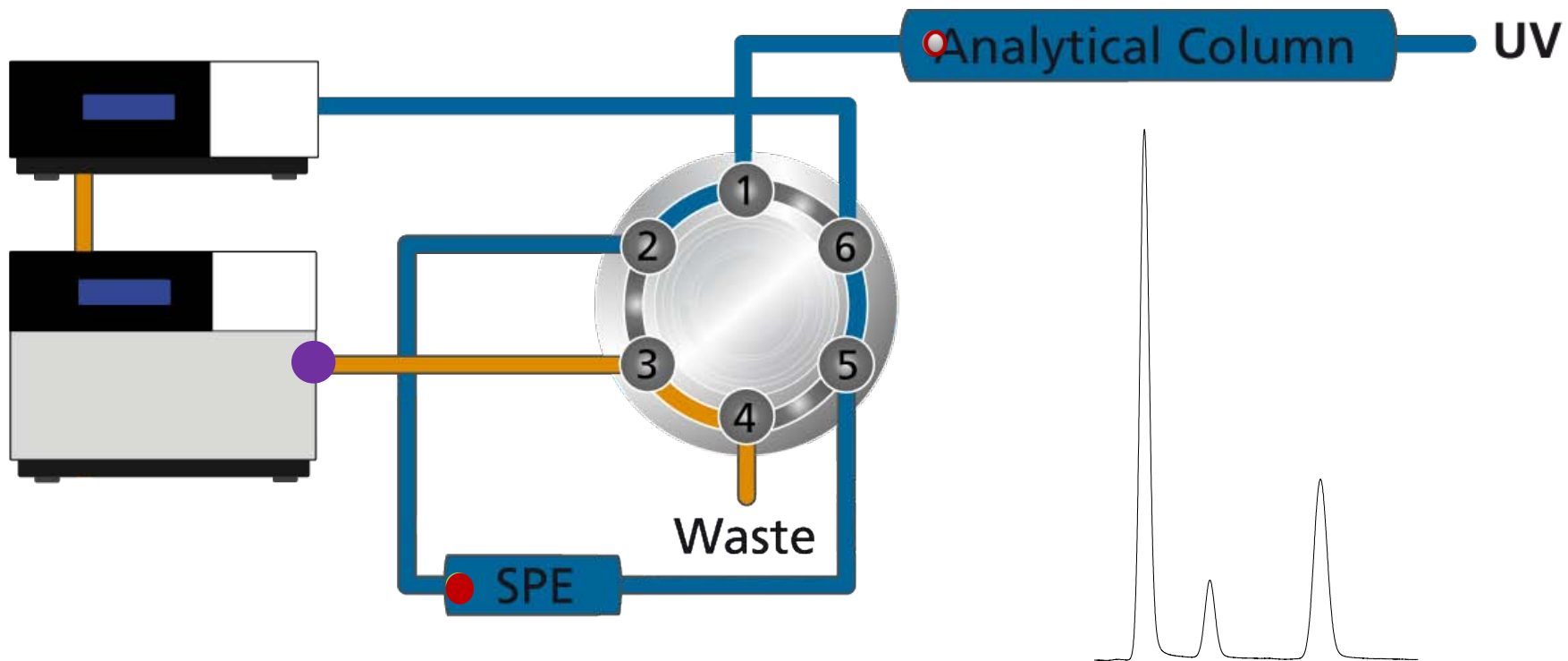
- 240 minuti lavoro manuale
- 480 minuti tempo totale

on-line SPE-LC automatica

- 24 minuti lavoro manuale (risparmio del **90 %**)
- 320 minuti tempo totale (risparmio del **33%**)

Online SPE LC

1. Caricamento del campione ed estrazione
2. Trasferimento analiti
3. Separazione HPLC e condizionamento colonna SPE



GRAZIE PER L'ATTENZIONE



www.thermo.com/ms

igor.fochi@thermofisher.com