“Ion mobility mass spectrometry: a new high-potential device for new life science ways” UHPLC–MS/MS system 6500 QTRAP© *Plus*

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SAPIENZA
UNIVERSITÀ DI ROMA

UHPLC–MS/MS system
6500 QTRAP© *Plus*

- **Hybrid Triple Quadrupole Linear Ion Trap**
- **SelexION® technology (*Ion Mobility*)**
- **Improved Ion source for high sensitivity (*sub pg/mL detection*)**
- **Fast polarity switching (5 ms)**
- **State-of-the-art software for data analysis**

➢ **3 DIMENSIONS OF SEPARATION: UHPLC+IM+MS**

Dipartimenti partecipanti alla proposta

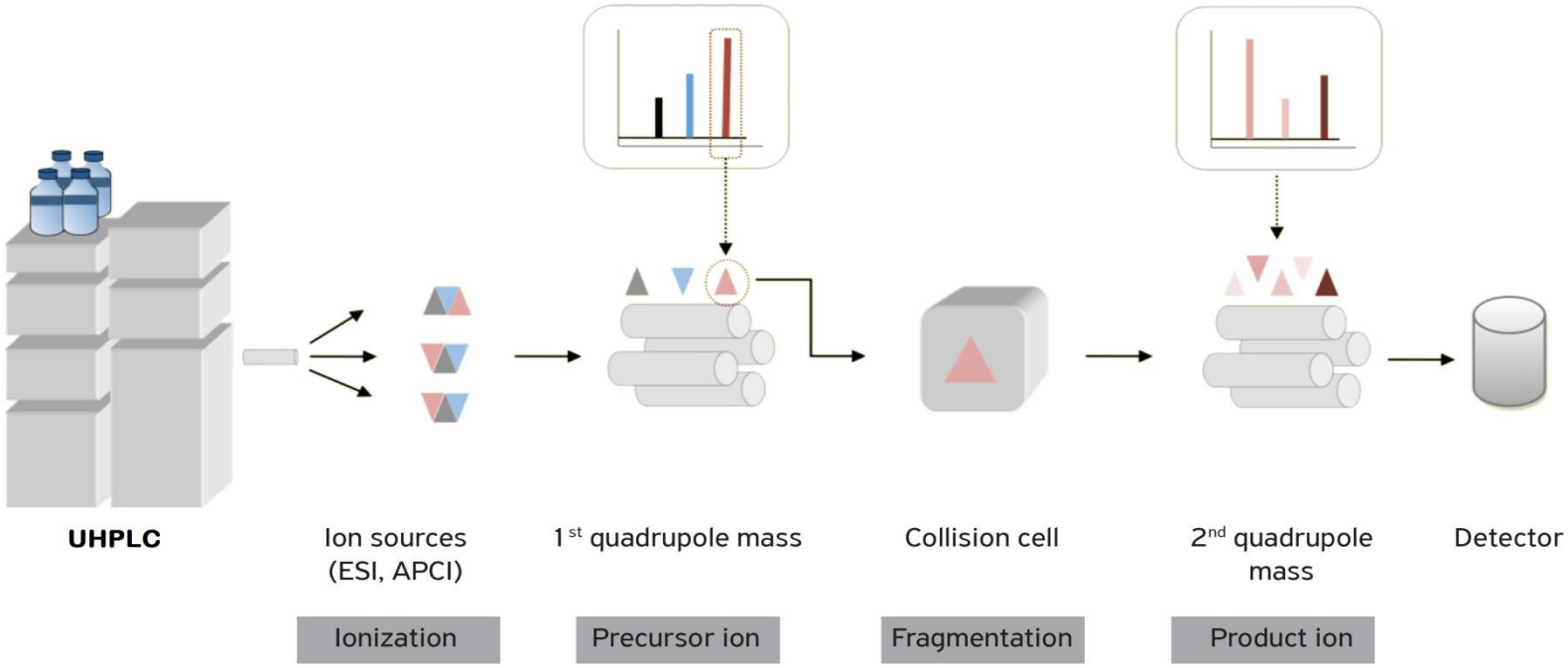
- CHIMICA
- BIOLOGIA AMBIENTALE
- CHIRURGIA GENERALE E SPECIALISTICA "PARIDE STEFANINI
- PEDIATRIA E NEUROPSICHIATRIA INFANTILE
- ORGANI DI SENSO
- SANITA' PUBBLICA E MALATTIE INFETTIVE
- SCIENZE MEDICO-CHIRURGICHE E DI MEDICINA TRASLAZIONALE
- SCIENZE ODONTOSTOMATOLOGICHE E MAXILLO-FACCIALI

No. di proponenti firmatari della proposta: 26

Facilities

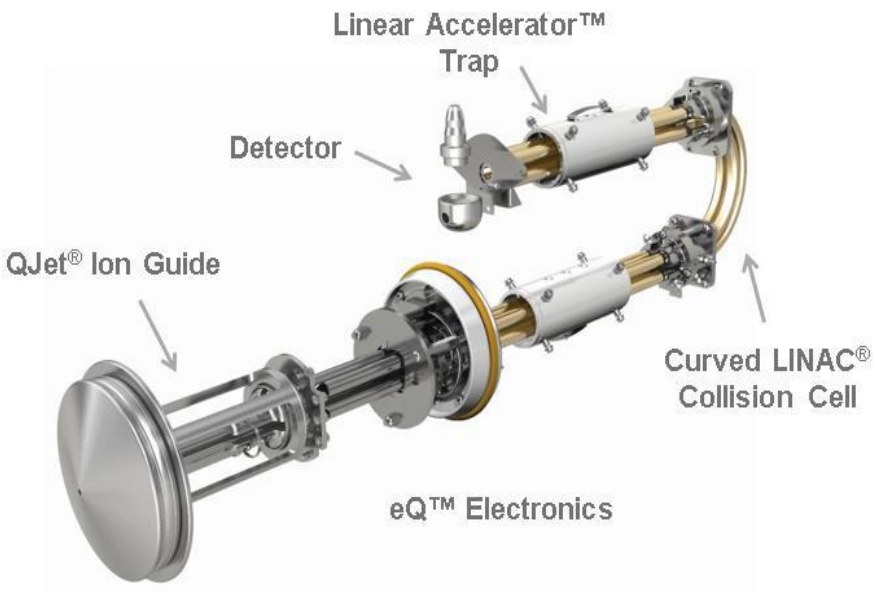
- The **Mass Spectrometry laboratory** headed by Prof. Curini is located on ground floor of the Department of Chemistry (Cannizzaro Building) – Room 063
- At present the laboratory is equipped with 3 LC–MS/MS systems in different hardware configurations that were acquired in the year 2000 not more usefull for actual research problems because the lower sensitivity and selectivity
- The new 6500 Qtrap system will be presumably available before the end of 2019 (??)

LC–MS/MS



- The technique combines the physical separation capabilities of liquid chromatography with the mass analysis capabilities of mass spectrometry
- Nowadays LC–MS has become one of the most widely used analytical technique
- Suitable for analysis of complex mixtures (**food, biological matrices, environmental and pharmaceutical samples etc.)**

Mass spectrometric features of the new system



A QTRAP is based on the conventional ion path of a QqQ mass spectrometer. However, the third quadrupole (Q3) can also be operated as a **Linear Ion Trap (LIT)**. The dual functionality of Q3 provides to the system complete functionality as a QqQ mass spectrometer, with great sensitivity for quantitative measurements, but with additional powerful scan functions.

The use of **MRM^3**, which consent a further fragmentation of the isolated fragments of the investigated analytes, can greatly improve method sensitivity.

Enhanced Resolution Scan allows for high resolution MS with peak widths of ~0.15–0.30 amu (FWHM); this is important for structural information, and database or library searches.

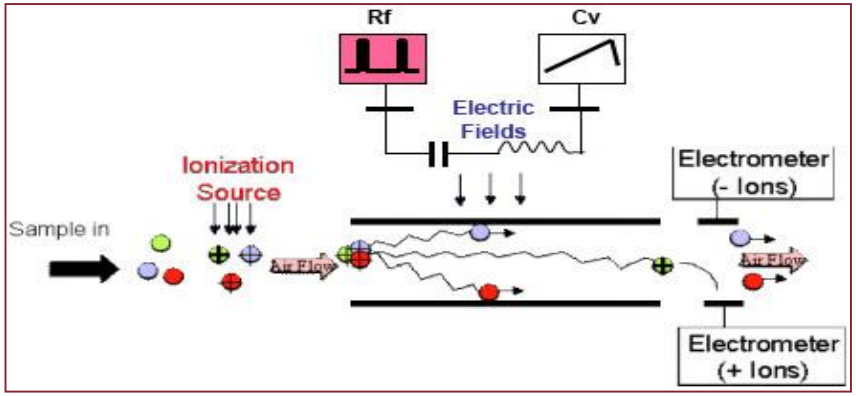
✓**QUANTITATIVE AND QUALITATIVE SCANS MODES**

SelexION®+ Technology
Differential Mobility Spectrometry (DMS)

➢ A NEW DIMENSION OF SELECTIVITY

An effective ion mobility separation tool for improving data quality in the quantitation and characterization of **challenging samples** requiring advanced analytical selectivity.

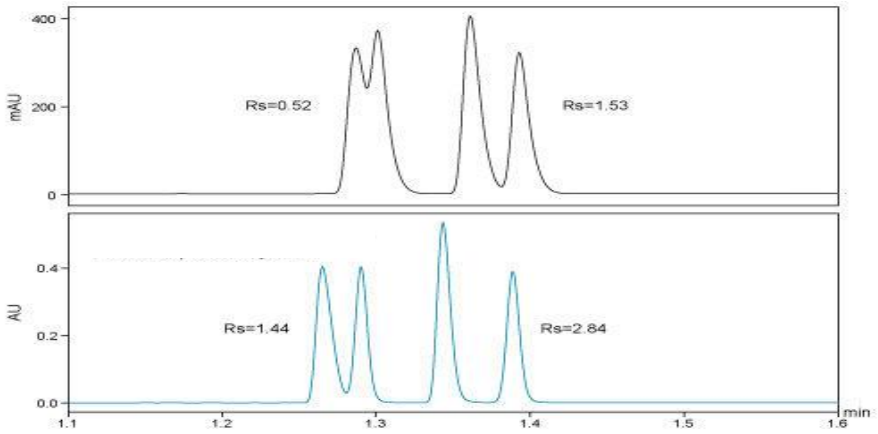
Well-suited for any application requiring the separation of isobaric species, **isolation of challenging co-eluting analytes and reduction of high background noise**.



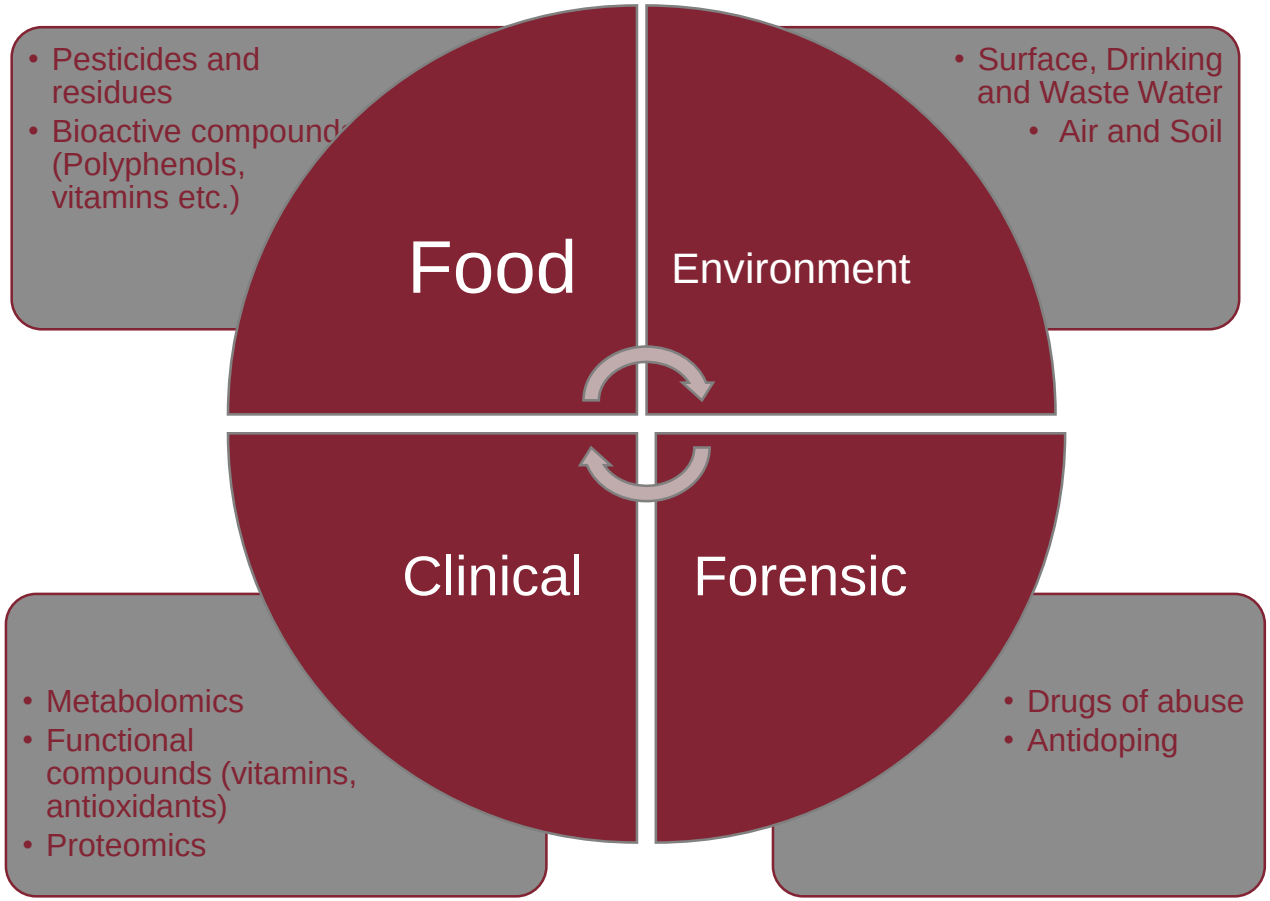
*DMS identifies and detects chemicals based on a chemical species **ion mobility,** which depends of ion dimension (geometry) and charge**,** in low and high electric fields. The DMS device can be used as a filter (**improved selectivity**) or in scan mode (**improved characterization**)*

UHPLC system ExionLC™ AD

- Full UHPLC capabilities, pressures up to 18,850 PSI (1,300 bar)
- UHPLC overcomes traditional HPLC, allowing higher resolution in reduced time, by using columns with < 3 µm particles.



UHPLC–MS/MS Applications Overview



The common thread of the lines of research that will be carried out is the detection of analytes at very low concentration (ppb-ppt) in complex matrices, exploiting the selectivity of the new instrument.

Clinical applications

Biomarkers of oxidative stress in pre-term newborns

- Screening and dosage of oxidative damage biomarkers in non conventional biological matrices
  - *Isoprostanes, Isofuranes, Neuroprostanes, Neurofurans*

Liposoluble antioxidants in biological matrices

- Development of a method for the determination of the main antioxidants in non conventional matrices
  - *α-,β-,γ-,δ- tocopherol, α-,β-,γ-,δ- tocotrienol, all-trans-retinol, all-trans-lutheine, all-trans-zeaxanthine etc.*

P75 neurotrophic receptor (NTR) in Cancer Stem Cells and Circulating Tumor Cells

- Study and correlation of prosurvival molecules (p75NTR and p75CTF) and proapoptotic (p75ICD) in target tissues and fluids.

Clinical applications

Vitamin K (KV): vitamin K1 (phylloquinone) + vitamin K2 (menaquinones, from MK-4 to MK-13)

- Vitamin K is crucial in the fetal and neonatal period to ensure the child's correct neurological development but at the level of aging it plays a very important role in cognitive diseases as well as playing an important role in the appearance and development of *glaucoma* correlated with aging. KV deficiency has been observed in patients with Alzheimer's disease (AD) and related dementia. Numerous studies have shown an association between high KV dietary intake and cognitive abilities.

Forensic applications

Illicit drug testing

- Development of ultrasensitive methods for traditional drugs and NPS in conventional and non-conventional matrices

Metabolite Identification of NPS

- Identification of unknown metabolites of new psychoactive substances

Explosives analysis

- Development of methods for the determination of explosives, gunshot residues and stabilizers in different matrices

Food and environment applications

Residues analysis in food

- Development of ultrasensitive methods for pesticides and residues in food

Wastewater analysis

- Development of ultrasensitive methods for the determination of contaminants such as pharmaceuticals, illicit drugs, pesticides etc in wastewater
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Biologically active compounds in food

- Determination of carotenoids, antioxidants, polyphenols in food products

Access to the analytical services and costs

- The new analytical instrumentation will be available to the Sapienza Community and for third parties in accordance with a specific regulation.
- Information for reservation and costs will be provided in the Scientific Labs website of the Department of Chemistry (www.chem.uniroma1.it/strutture/laboratori-scientifici)

Third Parties

- € 150-180 for sample (target analysis)
- > € 180 for untarget analysis (to be agreed, based on the complexity of the analytical problem)

Sapienza Community

- € 50-80 for sample (target analysis)
- To be agreed for untarget analysis based on the complexity of the analytical problem

CONTACTS

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