HYPHENATION OF SEPARATION METHODS AND MASS SPECTROMETRY

SEPARATION

↓

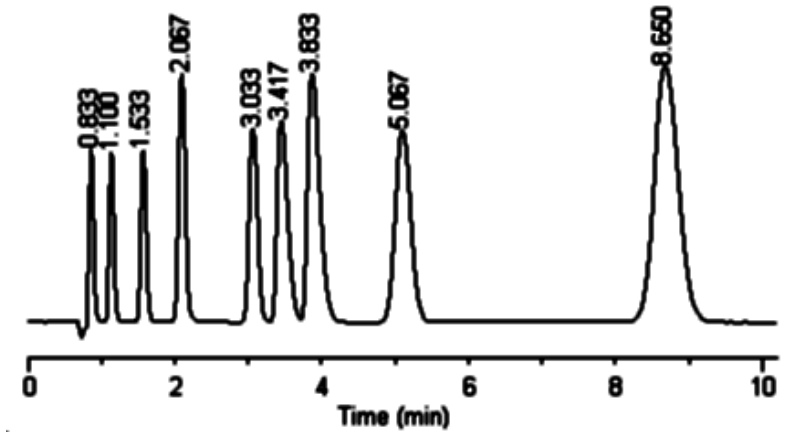
INTERFACE

↓

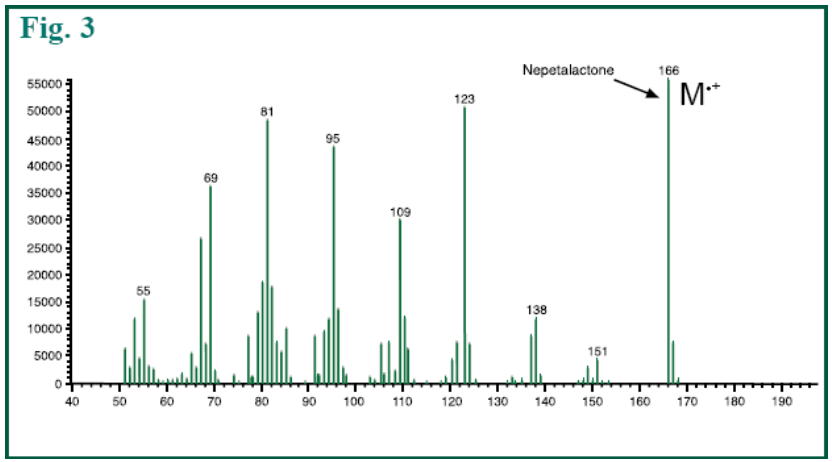
MS SPECTRUM

IDENTIFICATION

QUANTIFICATION



Heated capillary (GC)
Spray (LC, CZE, ITP)



IONIZATION AND MASS ANALYSIS

Ionization

Gas phase:

EI: M^+, fragmentation

– 70 eV (standard energy

– spectral library)

CI: M^+ ≈ PCI, M^- ≈ NCI;

ionization gas - methane

Liquid phase:

ESI; APCI; APPI

Adducts formation → **pseudomolecular ions**

$[M+H]^+$; $M+NH_4]^+$;

$[M-H]^-$; $M+Cl]^-$; $M+CH_3COO]^-$

$[M + zH]^{z+}$; $[M - zH]^{z-}$

Mass analysis (separation)

Quadrupole

(straight; spheric - trap)

Δ M ≈ 0,1 – 1

TOF - time of flight

Δ M ≈ 0,001

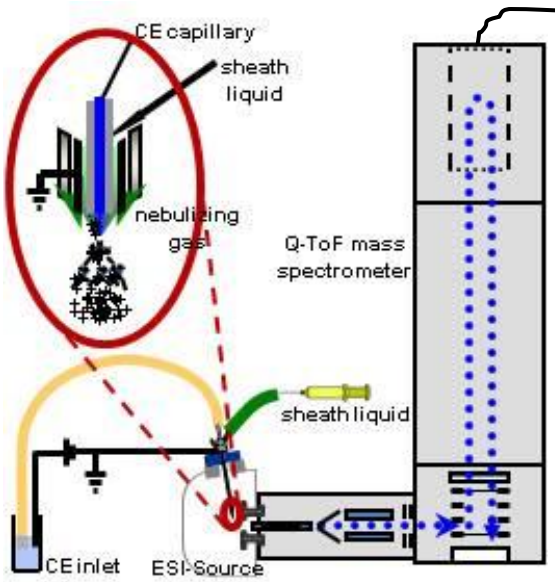
Orbitrap

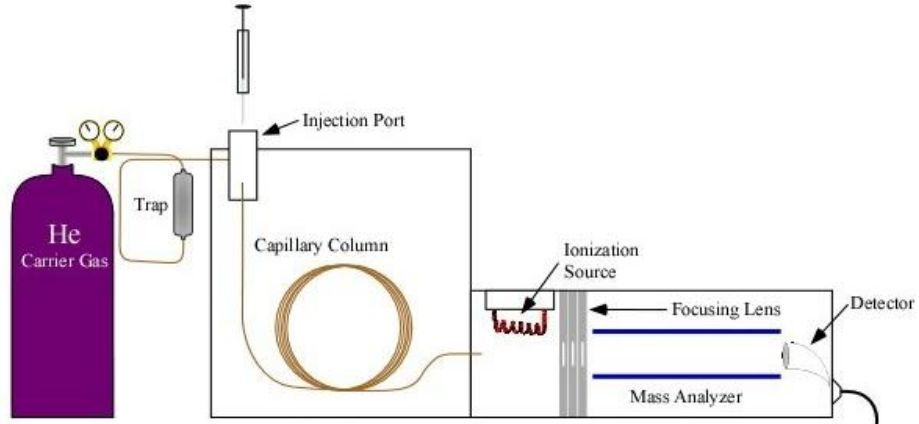
Δ M ≈ 0,0001

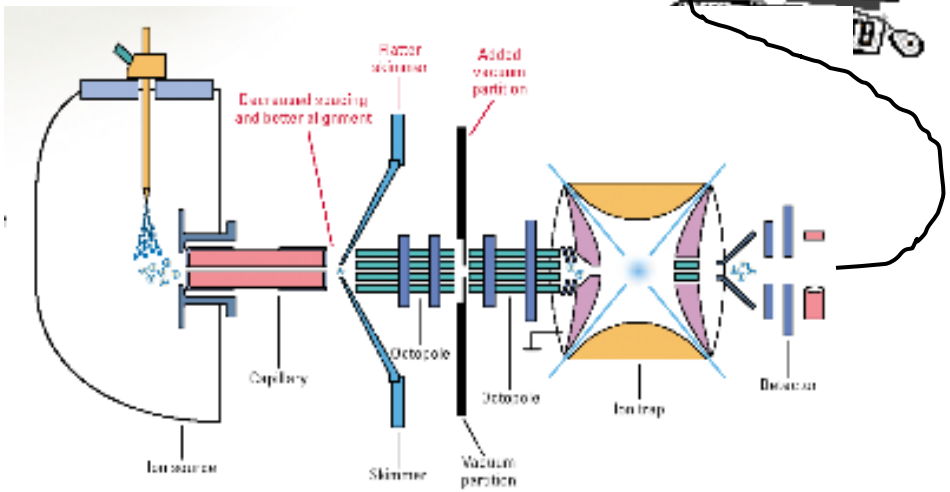
Multistage MS – fragmentation

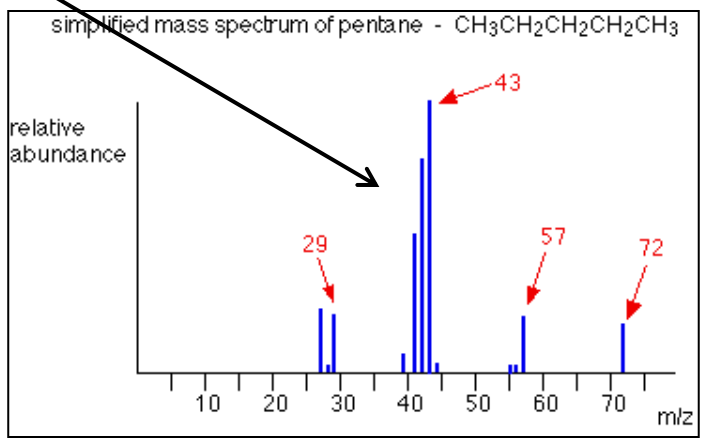
Combination: ion mobility + MS

HYPHENATION OF SEPARATION METHODS AND MASS SPECTROMETRY

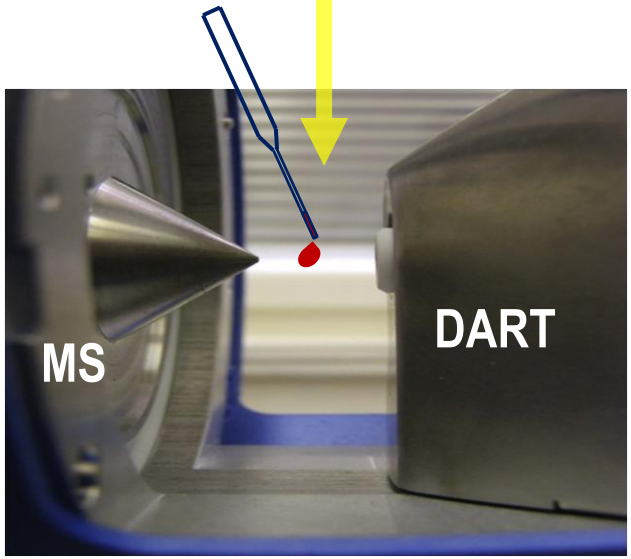


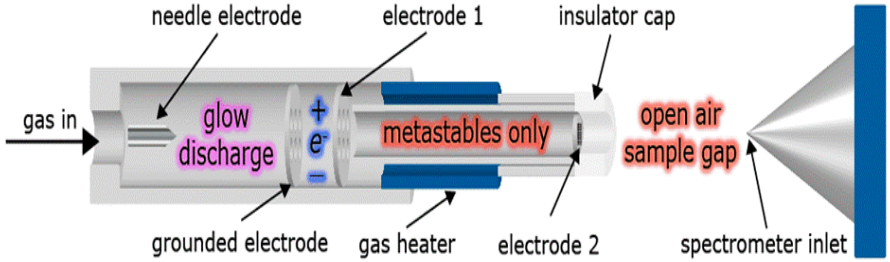


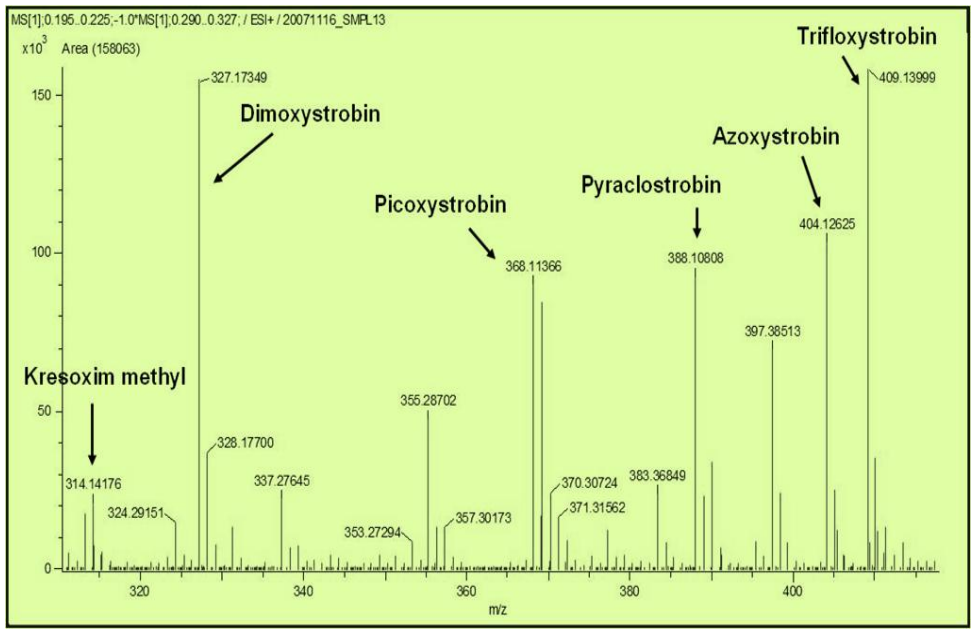




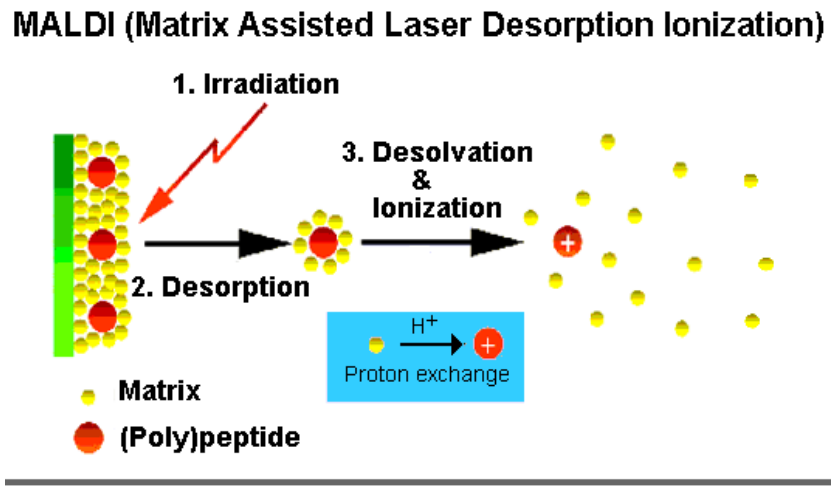
DIRECT MASS SPECTROMETRY – DART/MS

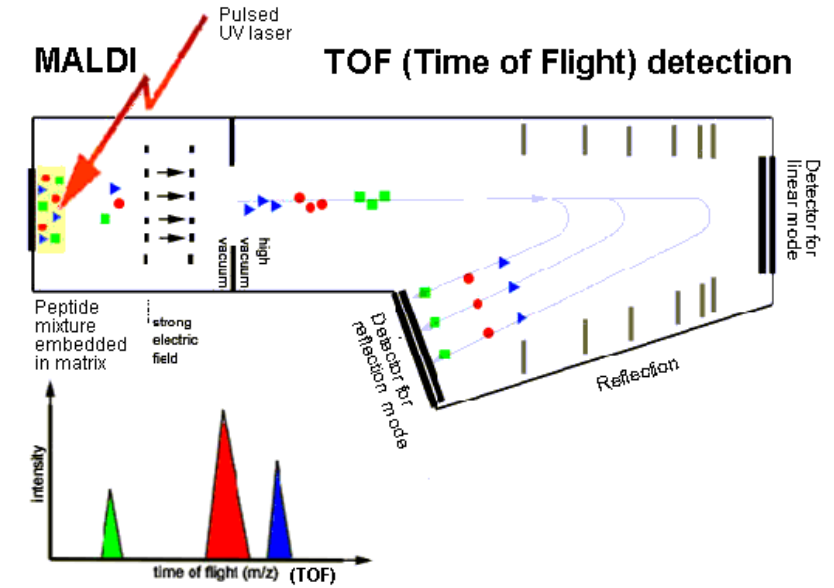






DIRECT MASS SPECTROMETRY – MALDI/TOF



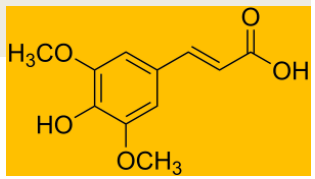


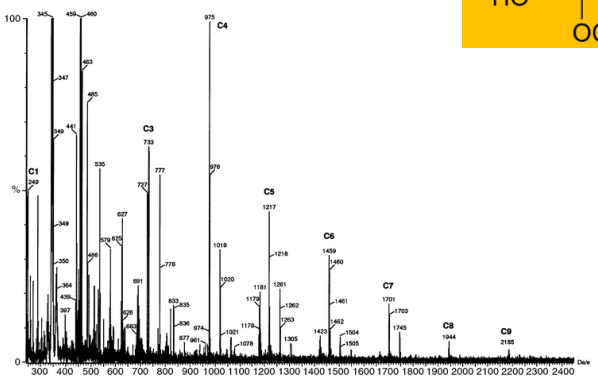
Suitable matrices - absorb radiation of used laser

UV: N_2 laser - 337 nm; Nd:YAG laser 355 nm

IR: Er:YAG laser - 2940 nm

Typically: 2,5-dihydroxybenzoic acid or sinapic acid





DATA HANDLING AND INTERPRETATION

Parameter	Spectral information		Interpretation / Recognition
Ionization	Molecular ion	→	M
	Pseudomolecular ion	→	M
	Fragment ions	→	Molecular structure
Mass separation	Accurate mass	→	M; elementary composition
	Izotopic cluster of molecular ion	→	Charge size; izotopic representation
	Izotopic cluster of fragment ions	→	Molecular structure
Stored data	Full spectra	→	Target/non-target analysis; retrospective analysis
	Selected ions	→	Identification/quantification of known compounds
	MS^n transitions		

Expected benefits according to applied method

Hyphenation with the separation method

- RT + signal intensity
- Spectral information - identification → simplification of methods optimization (injection of mixed standard solutions) and data evaluation
- Acceleration of separation - MS can distinguish the compounds in the overlapped elution zones

Direct MS

- mixed spectrum → marker identification
- profiling → multivariate data analysis

APPLICATIONS

Practically universally applicable - from highly volatile substances to high-molecular biopolymers → organic chemistry, petrochemistry, pharmacy, food analysis

Routine analysis - speed, reliability, accuracy, identification, quantification → inspection activity, operational control

Targeted and non-targeted analysis - inspection activity, forensic analysis - retrospective data analysis

Scientific purposes - identification, quantification, profiling - spectral patterns, multivariate data analysis, metabolomic studies