



*Liquid Chromatograph
Coupled to Mass
Spectrometer*

Ultra performance liquid chromatograph coupled to quadrupole ion trap

LIQUID CHROMATOGRAPH

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Brand
Waters

Model
Acquity

Technical specifications

- Comprehensive system components, including Sample Organizer, Column Manager and Heater/Cooler, Binary Solvent Manager and Sample Manager.
- The binary solvent manager uses two individual serial flow pumps to deliver a parallel binary gradient mixed under high pressure.
- Pump flow programmed from 10 μ L to 2 μ L/min.
- 15,000 psi pressure limit to take full advantage using columns with sub-2 μ m particles.
- XYZ autosampler with cooled Peltier system.
- Below 150 μ L death volume.

Technique description

Liquid chromatography (LC) is used to separate mixed compounds and is based on the analyte interaction with the stationary phase (chromatographic column).

The sample is injected across the stationary phase by pumping a liquid (mobile phase) at high pressure. The analytes are retained in the stationary phase depending on the chemical and/or physical interaction with the chromatographic column. The retention grade depends on the nature of the compound, stationary phase and mobile phase composition. The retention time is the time it takes for a particular analyte to pass through the system under set conditions and is a characteristic property of the analyte in a specific stationary and mobile phase.

Ultraperformance liquid chromatograph designed to operate at pressure up to 15.000 psi enables columns with particle size under 2 μ m. This fact increases the lineal speed of the analytes and reduces their diffusion in the column to improve both the chromatographic performance and resolution.

MASS SPECTROMETER

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Brand
ABSciex

Model
QTrap®5500

Technical specifications

- The Turbo V source with quick-change Esi and APci probes.
- m/z range from 5 to 1,250 amu.
- Scan rate up to 12,000 amu/s working with Q and up to 20,000 amu/s using QTrap.
- Dynamic range of 5 orders of magnitude.
- Sensitivity: injection of 50fg of Reserpine in column at 200µL/min enables S/N: 60(MRM); 500fg of Reserpine in column at 200µL/min enables S/N>500(EPI and MS³).

Technique description

Once the chromatographic separation has been carried out, the ions are obtained in gas phase in the ionization source. The most common atmospheric pressure ionization techniques in coupling with LC are electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCi).

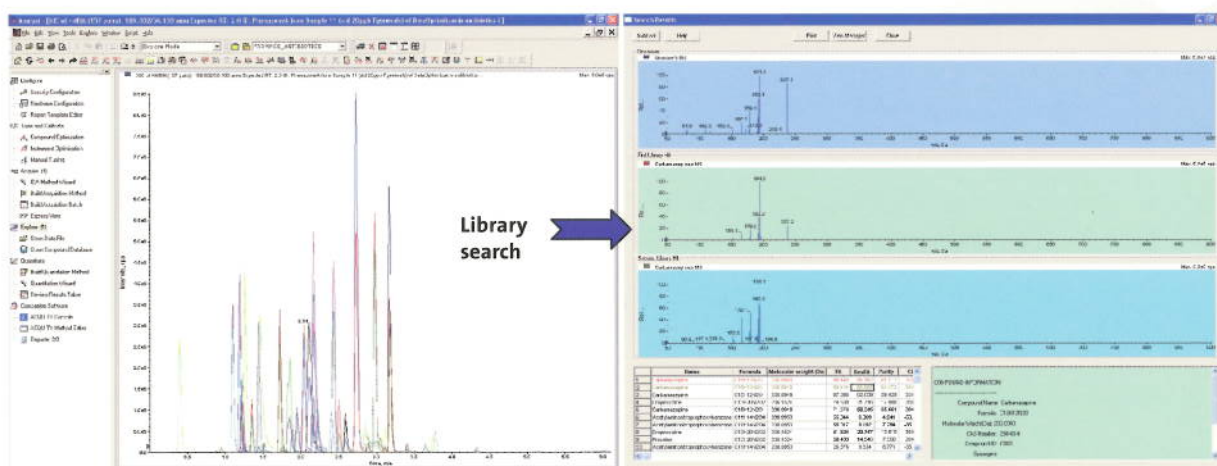
The generated ions are then transferred to the mass analyzer across an interface between the atmospheric pressure and vacuum zones. By means of the application of magnetic and electrical fields the formed ions are separated according to their ratio mass/charge and subsequently detected.

The graphical representation of the mass spectrum of the molecule is commonly known as a fingerprint of the molecule and allows its unequivocal identification.

The hybrid technology of QTrap5500 allows the ability to combine quadrupole scan functions with high sensitivity linear ion trap scans. The analyzer is composed of 3 quadrupoles: Q1 and Q3 are used as a mass filter; Q2 is a high collision pressure cell (LINAC) where the molecules and/or fragments from Q1 are fragmented to low mass fragments. Additionally Q3 could be used as a linear ion trap storing the formed ions obtaining an increase of sensitivity.

Applications

- > The determination of emerging contaminants in the environment is related to the capacity of analysis of the available equipment, especially in the field of mass spectrometry. The development of more sensitive and versatile instrumentation allows detection at the low levels found in the environment, and also provides the necessary tools to guarantee a precise identification, in accordance with the increasingly-strict criteria established by European directives.
- > The enhanced speed and sensitivity also provides a more efficient tool for identifying metabolites.
- > Identification of compounds by means of obtaining ion product spectra and the comparing it with in-house or commercial libraries.



TIC chromatogram, mass spectra and identification of pharmaceutical compounds through library.