Gas Chromatograph coupled to triple quadrupole Mass Spectrometer

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GAS CHROMATOGRAPH

1.1 Brand **ThermoFisher Scientific** Model **Trace GC Ultra (TriPlus™ Autosampler)**

Technical specifications

- TriPlus™ Autosampler enables the sample introduction into two independent injection ports and it is available in two different configurations:
  - > For injections of liquid samples: up to 150 vials.
  - > For headspace sampling: the system consists of an incubation oven (40-150°C) with a built-in shaker which speeds up phase equilibration time. Sequential injection for sample enrichment. Up to 54 headspace vials.
- Injector allows different injection techniques: Split/splitless, headspace and large volume injection.
- Oven with capacity for placing two columns:
  - > Linear heating rate: between 0.1 and 120°C/min.
  - > Oven temperature range: from near ambient to 450°C.

Technique description

Gas chromatography (GC) is an analytical technique for separating and analyzing volatile and semivolatile compounds (relatively low molecular weight analytes) which are thermally stable.

Generally, the analysis involves the injection of the sample solution into the GC inlet where it is vaporized and swept onto the chromatographic column by the gas carrier (usually helium). The compounds are separated due to differences in their partitioning behaviour between the mobile phase and the column's stationary phase. Since temperature influences the volatility of the analytes, the column is placed in a thermostatically controlled oven. According to the column selected, the separation can be carried out by boiling point, polarity, size, etc. The mixture becomes separated, and as a result, individual compounds reach the detector with different retention times.

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MASS SPECTROMETER - TRIPLE QUADRUPOLE
Electron Capture Detector (ECD) - Flame Ionization Detector (FID)

1.2

Brand
ThermoFisher Scientific

Model
TSQ Quantum

Technical specifications

- Mass range up to *m/z* 3000.
- Scan speed up to 5000 u/s (300 SRM transitions per run).
- Ion production methods: electron ionisation (EI) and chemical ionisation (CI).
- Dwell time lower than 3 msec.
- Dynamic range higher than 10^6.
- Resolution of 1 or 0.7 Da.
- Hot splitless injection of 1 µL of a 100 fg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a minimum signal-to-noise ratio of 500:1 for the transition of *m/z* 272 to the product ion of *m/z* 241 when operated in Selected Reaction Monitoring mode (SRM).

Technique description

Mass spectrometry is a common technique which combines a high sensitivity with the unique property of being able to determine the molecular composition.

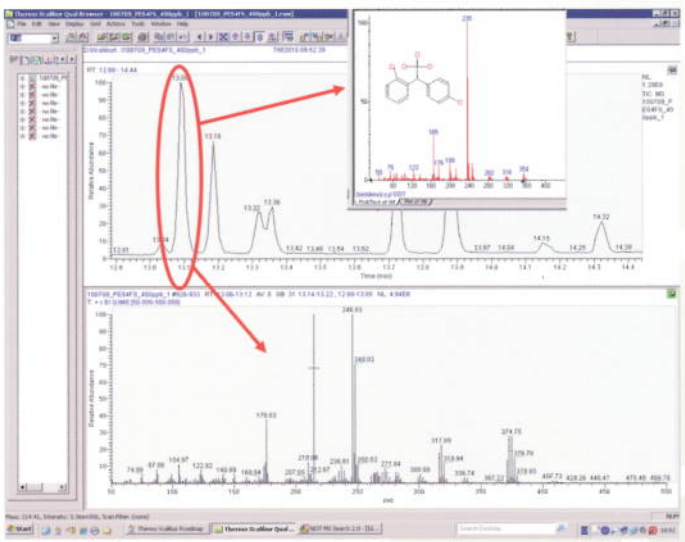
Mass spectrometry is based on the ionization and fragmentation of molecules in the ion source (high-energy electron bombardment) and the separation of the ions generated on a basis of their mass/charge ratio using an analyzer unit. Ions are detected by a dynode electron multiplier. The fragmentation pattern measured is characteristic for each molecule, making identification possible.

Applications

> Coupling gas chromatography and mass spectrometry, identification and quantification of volatile and semi-volatile organic compounds in complex mixtures can be obtained. Commonly this technique is used in the following applications: pollutants (polycyclic aromatic hydrocarbons, pesticides, alkylphenols, etc.) in drinking and wastewater, industrial by-products for quality control, food safety, toxicological and clinical research, etc.

> Structural determination of unknown organic compounds by matching their spectra with reference library and by spectral interpretation obtained empirically.

> *For detecting compounds containing electronegative elements such as halogens, ECD is recommended. In the case of universal detection of organic compounds at high concentration level, FID provides a good response.*



Pesticide chromatogram with the corresponding mass spectra