FUNDAMENTALS OF GC/MS ANALYSIS

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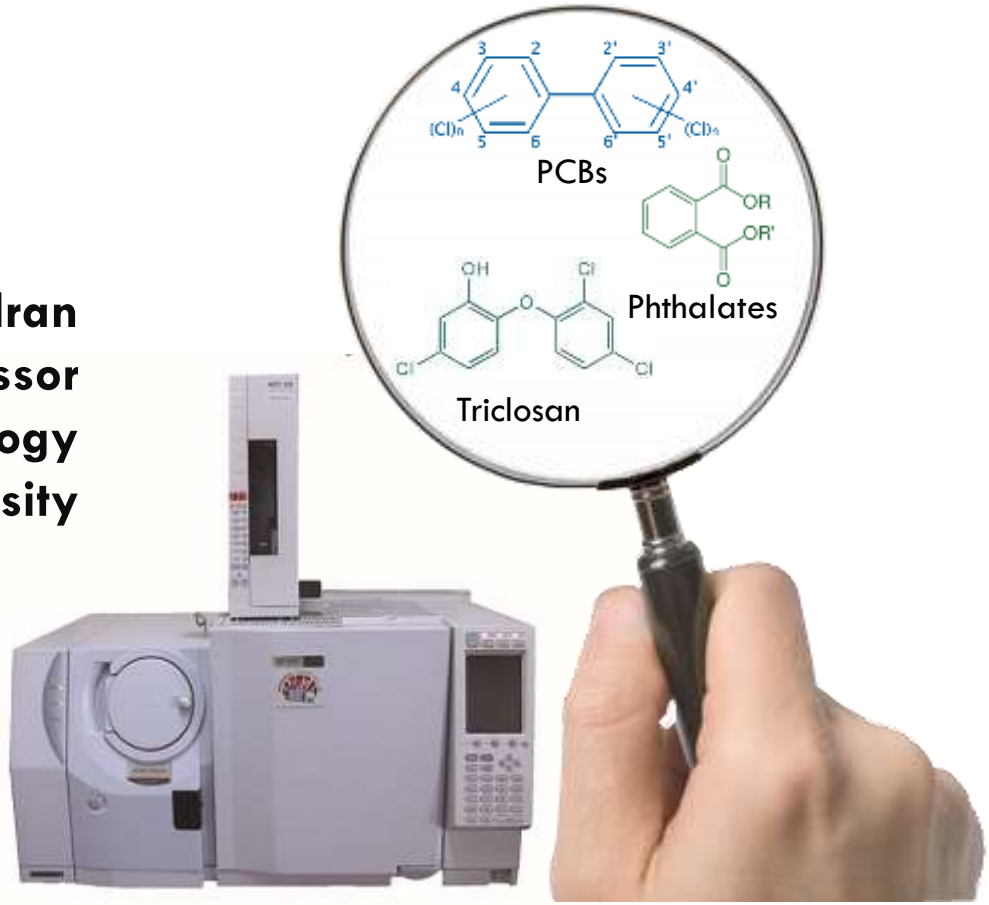


PURPOSE OF GC/MS ANALYSIS

Qualitative analysis

- What components ?
- What compounds ?

Quantitative analysis

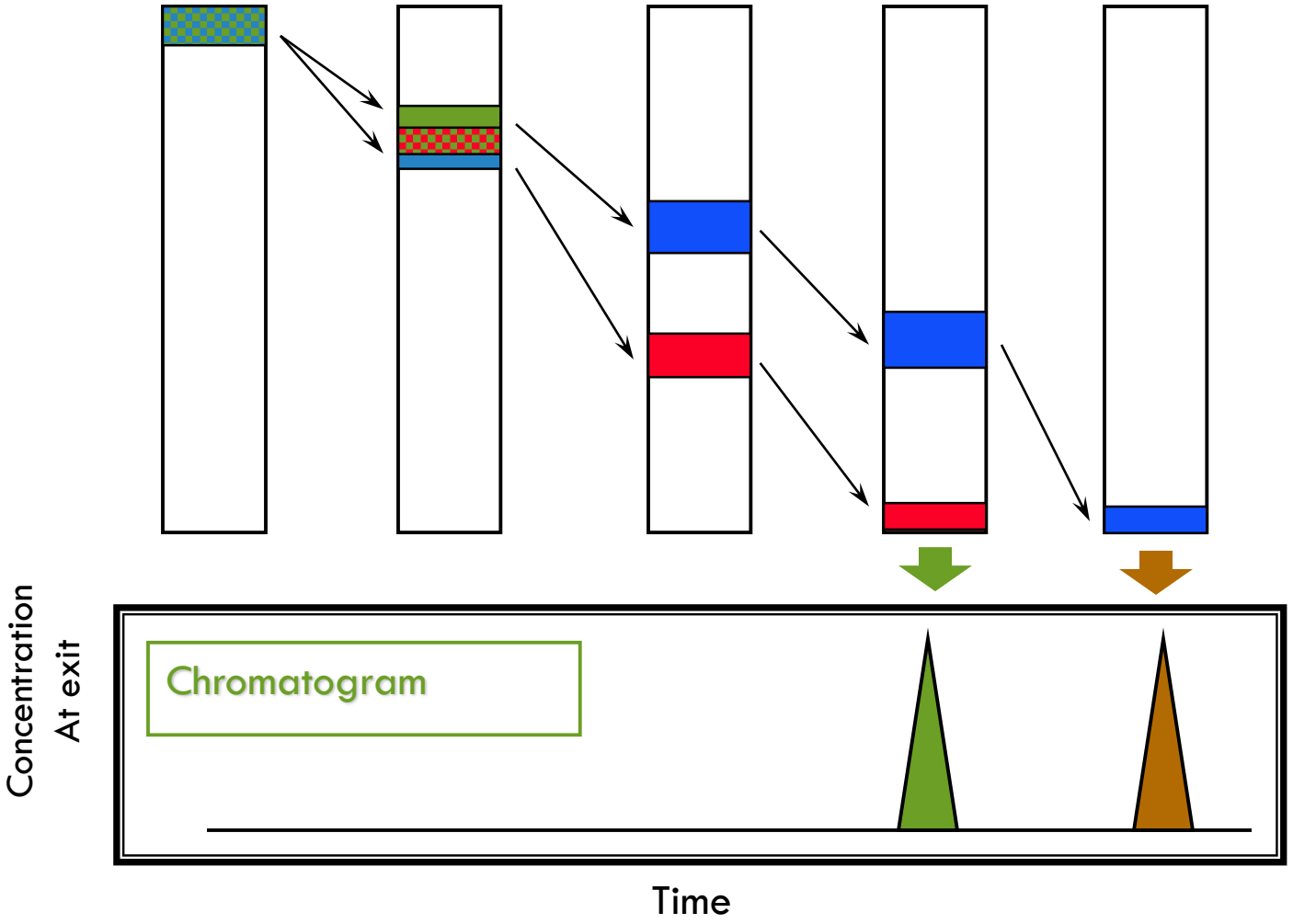
- How much of the component ?
- What an amount of the component ?

Target:
Organic compounds

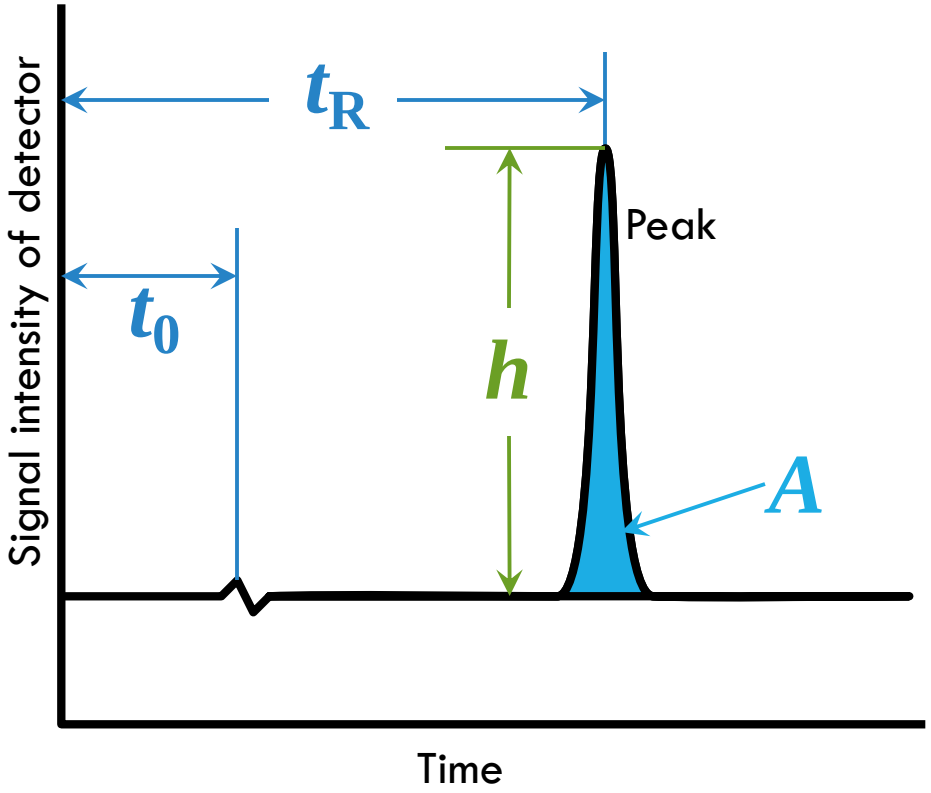
CHROMATOGRAPHY
•CHROMATOGRAPH
•CHROMATOGRAM

Chromatography	: Analytical method
Chromatograph	: Instrument
Chromatogram	: Obtained “picture”
Chromatographer	: Analyst

COLUMN-CHROMATOGRAPHY: SEPARATING PROCESS AND CHROMATOGRAM



CHROMATOGRAM



t_R : Retention Time

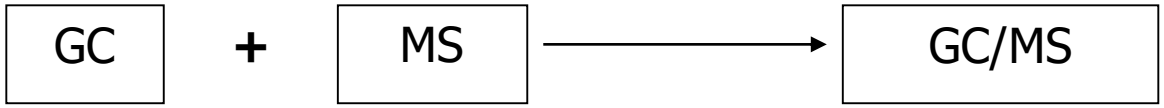
t_0 : Dead Time of Column

A : Peak Area

h : Peak Height

WHAT IS GC/MS ?

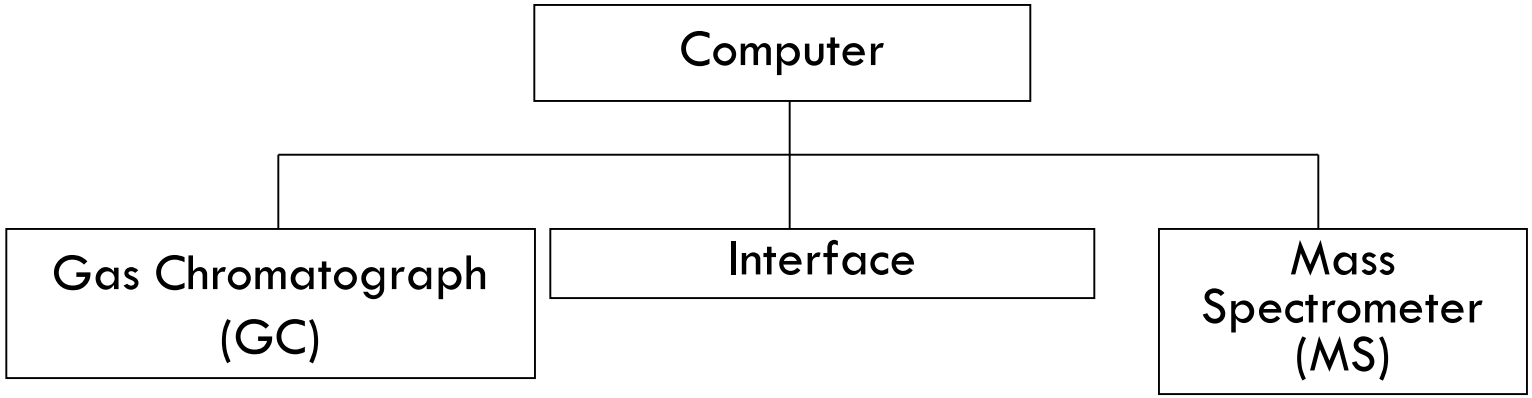
Composite instrument made up of GC and MS



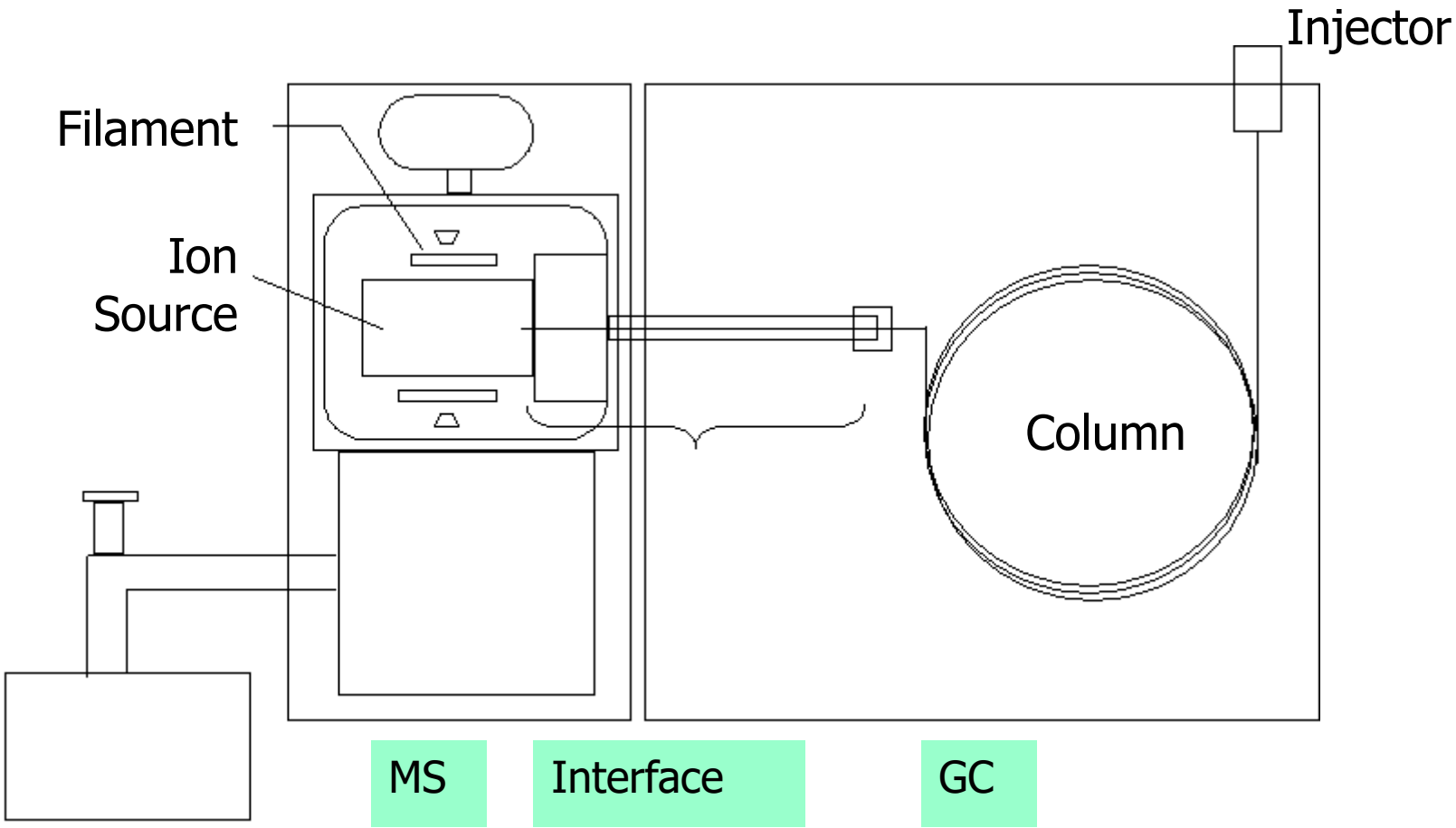
- GC is superior in separating of multi-components.
- GC is not good at identifying peak components.
- MS allows identification from mass spectrum.
- GC/MS is a composite instrument having the good points of GC and MS.
- SIM method of GC/MS allows accurate quantitation.

	GC	MS	GC/MS
Separation	**Very Good**	**Normal**	**Very Good**
Identification	**Not Good**	**Very Good**	**Very Good**
Quantitation	**Very Good**	**Good**	**Very Good**

STRUCTURE OF GC/MS



SCHEMATIC DIAGRAM OF GC/MS



MASS SPECTROMETER

- Ionization Part

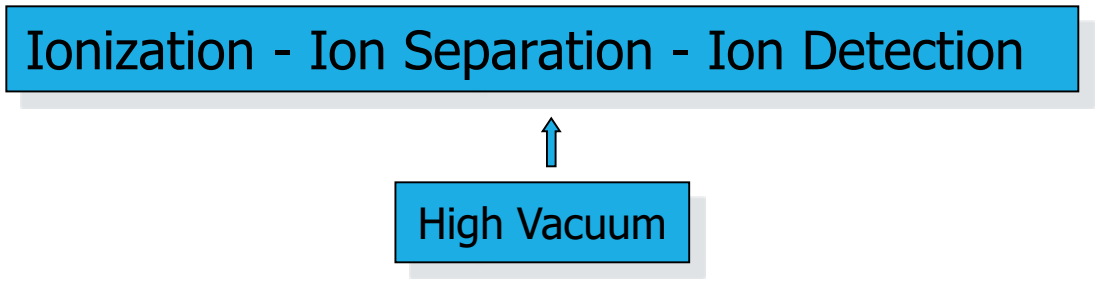
  Ionizes sample molecules in vacuum

- Mass Separation part

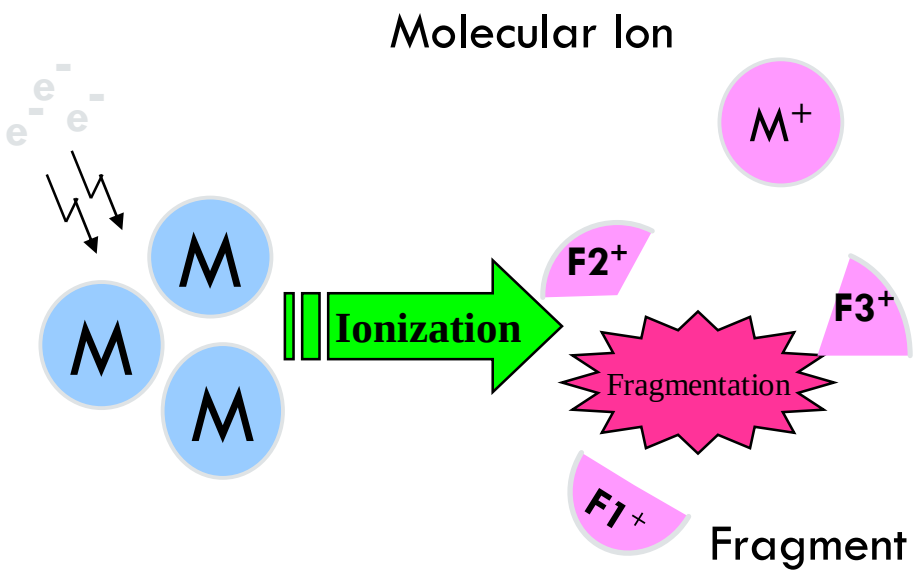
  Separates ions according to their masses

- Ion Detection Part

  Detects ions



IONIZATION WITH EI (ELECTRON IONIZATION)



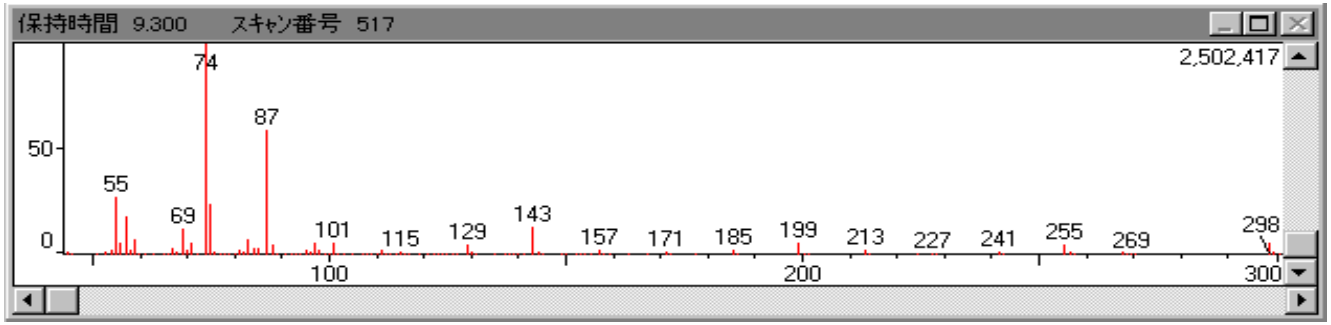
Thermal electrons emitted from filament hit gaseous molecules.

The molecules are ionized.

Molecular weight is deduced from molecular ion

Chemical structure is deduced from fragment ions.

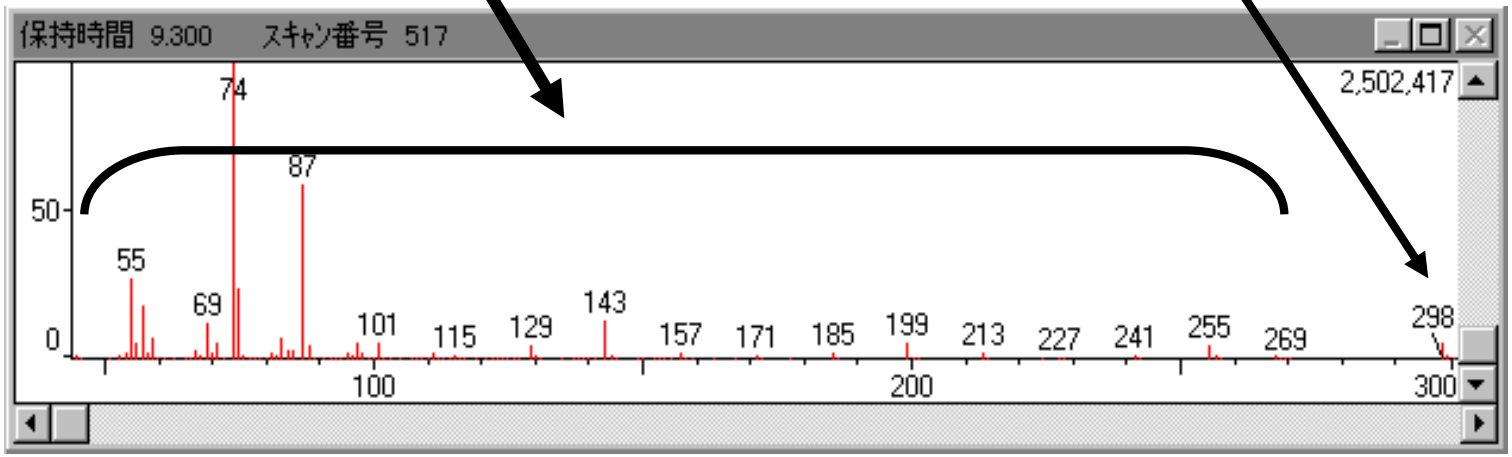
Qualitative and quantitative analyses are available.



MASS SPECTRUM

Fragment Ions (chemical structure)

Molecular Ion (molecular weight)



DATA ACQUISITION MODE OF GC/MS

- SCAN

Acquires mass spectra in sequence at constant intervals (eg 0.5 sec) .
All acquired mass spectra are stored in PC.
Investigation of data on PC (TIC, mass spectrum, MC etc.).
Qualitative analysis / Quantitative analysis.

- SIM

Detection of specific masses.

Quantitative analysis.

MASS SPECTRUM

(2) Isotope ion peak (estimation of element)）

(3) Fragment ion peak (determination of chemical structure)

(1) Molecular ion peak (determination of molecular weight)