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# Instrumentation & Principle of GCMS Technique

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## What is GC?

### The technique

GC stands for Gas Chromatography, an analytical technique which allows separation of organic compounds in a sample

### The instrument

The instrument used for gas chromatographic analysis is known as a gas chromatograph (also called GC)

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# ***Why we need GC***

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## The information

- By using GC we can perform:
  - Qualitative analysis
  - Quantitative analysis

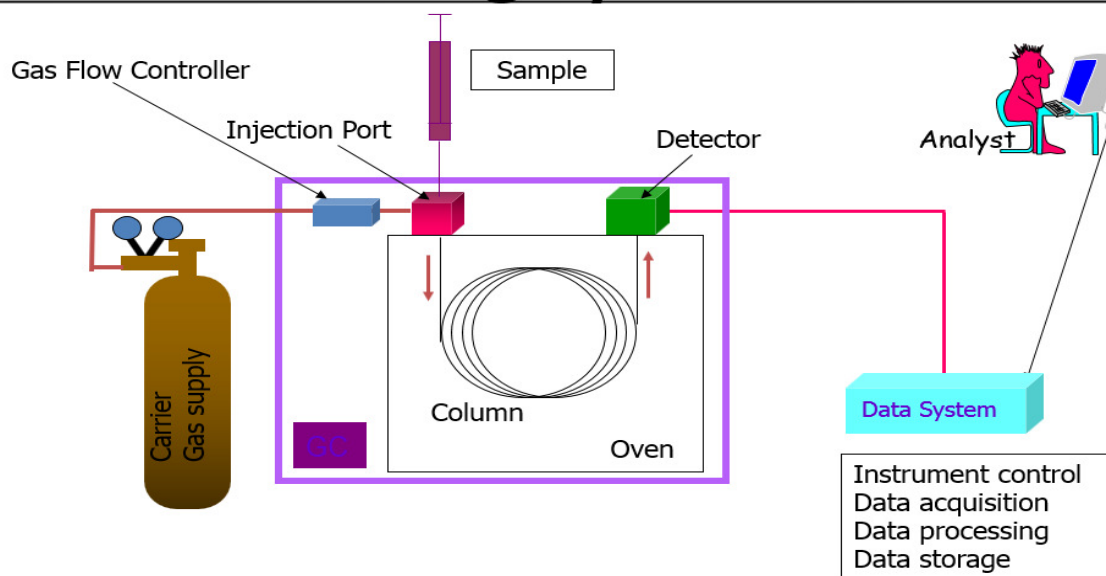
# ***Which Samples on GC***

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## Samples for GC

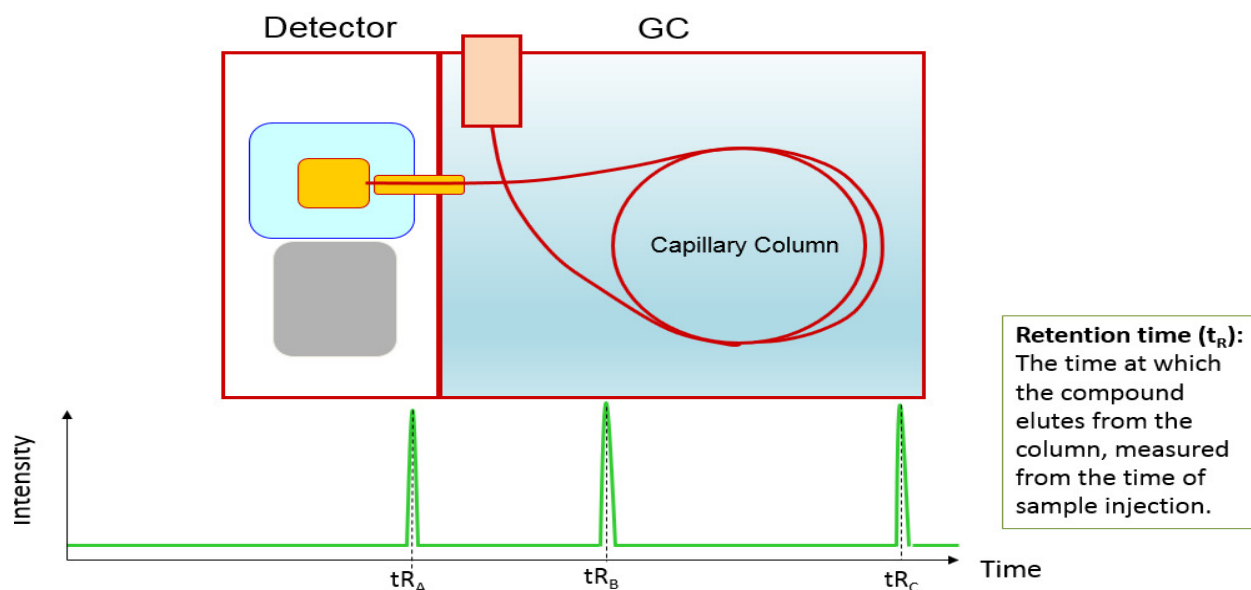
- Strictly speaking, samples for GC are organic compounds with
  - sufficient volatility (guideline: is in vapor form or can be turned to vapor at 400°C or less),
  - sufficient thermal stability (does not decompose on heating)
- In practice, some compounds which do not fulfill the criteria above can be made to fulfill the criteria by means of chemical reaction ('derivatization'), thus making it possible for these compounds to be analyzed by GC

# Gas Chromatograph



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## GC Separation



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# GC Sample Injection Devices

- Samples that is introduced into the GC injector must be in the form of liquid or gas – and not solid
- Sample is most commonly injected in liquid form by using liquid microsyringe
- Gas injection using gas-tight syringe or gas sampling valve is commonly used in certain applications
- For solid samples, the sample must be pre-treated to convert it into liquid or gas form
  - Chemical means (e.g. dissolve sample in solvent)
  - Heating/incubation of sample (e.g. headspace extraction)
  - Thermal decomposition (e.g. pyrolysis)

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## Types of Sampler



AOC 20i + s



AOC 6000



HS - 20



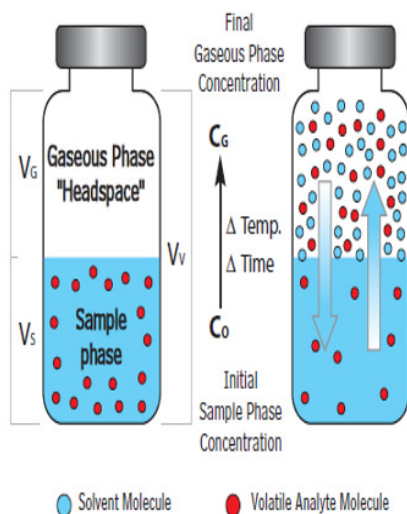
PY - 3030



TD - 30

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# Headspace (HS) Injection

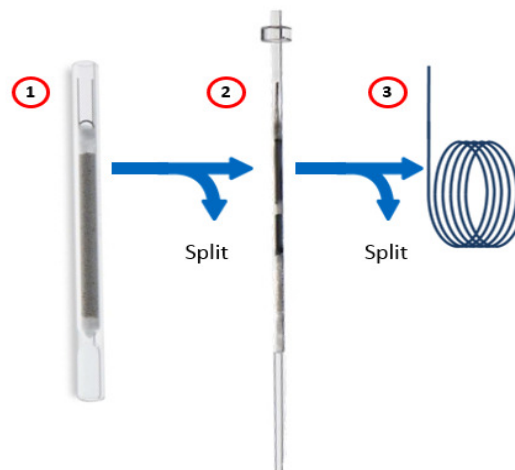


The sample Phase contains the compound of interest and is usually in the form of liquid or solid in combination with dilution solvent or matrix modifier.

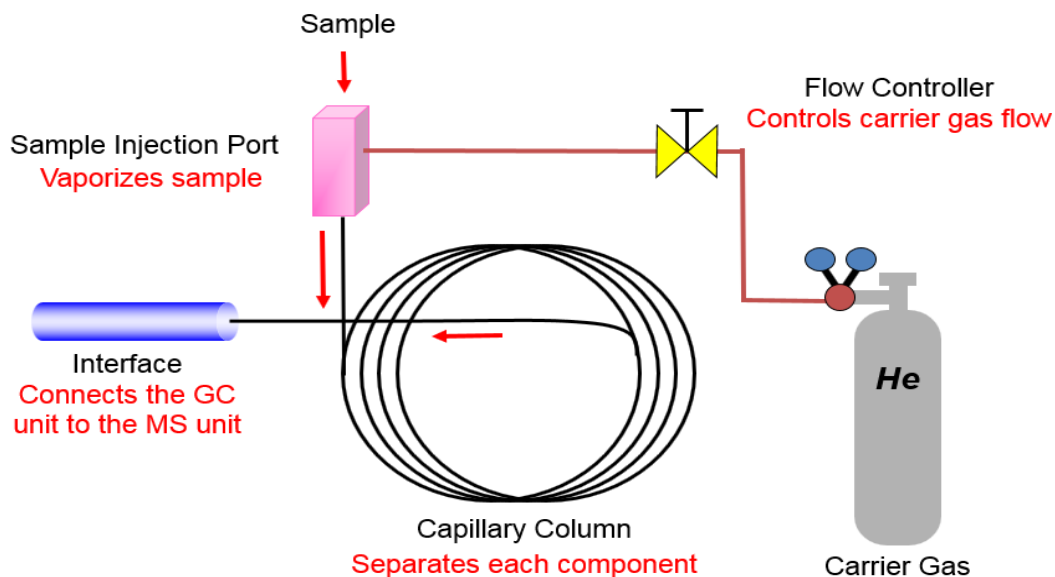
Once the sample phase is introduced in to the vial and the vial is sealed with septa and cap, Volatile components diffuse in to the gas phase called as "HEADSPACE", until the equilibrium state has been reached .

# Thermal Decomposition(TD)

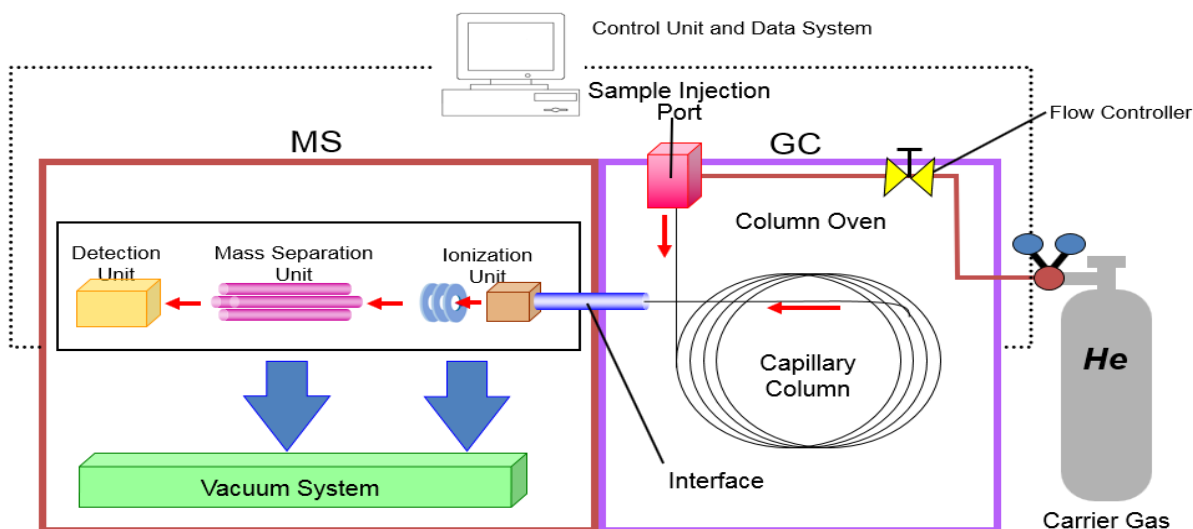
1. Sample adsorbed in TD tube is thermally desorbed.
2. Extracted constituents are concentrated in the cold focusing trap, which sharpens the peaks.
3. Target analytes are introduced into GC column by backflush technique.



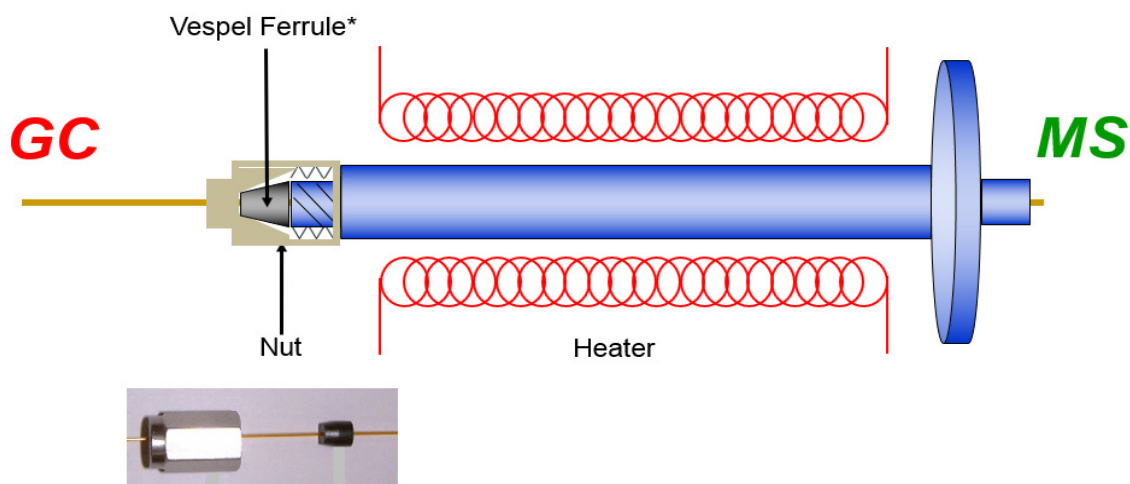
# GC Unit



# GC-MS Schematic Diagram

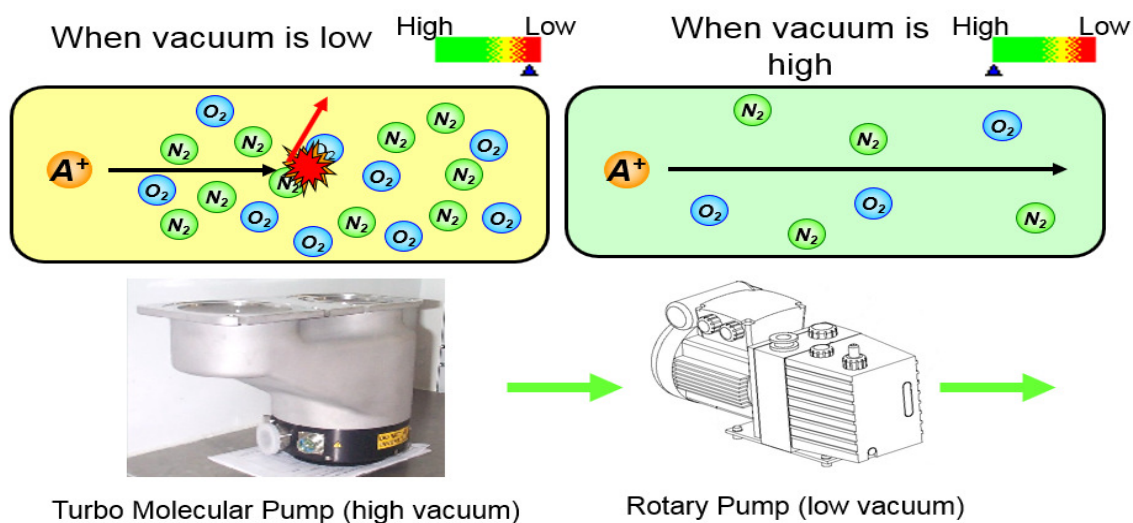


# GC-MS Interface

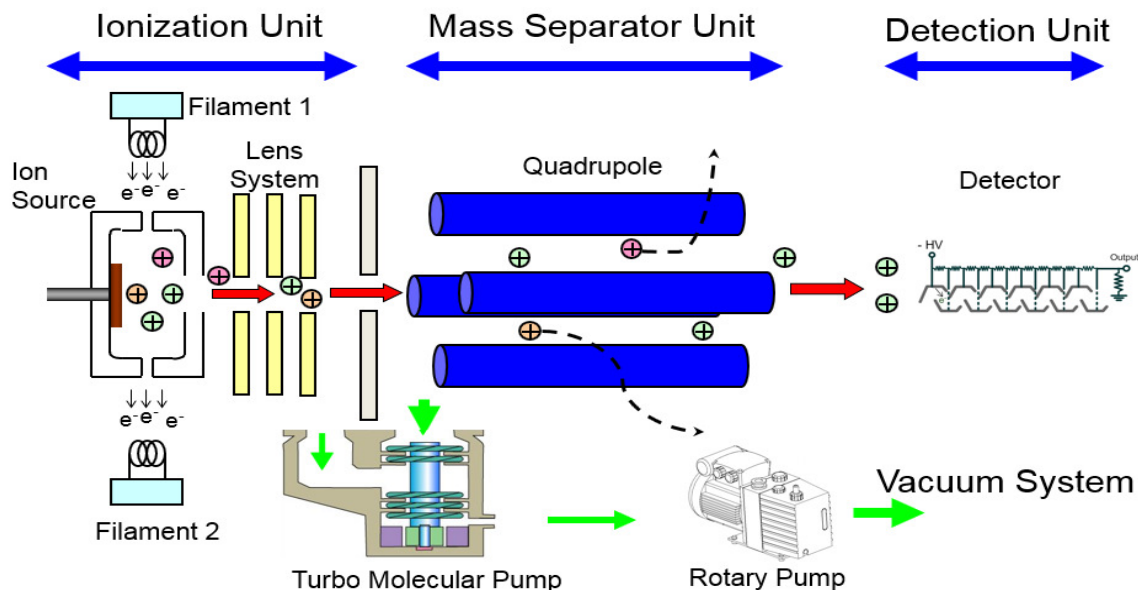


\* The Vespel ferrule is used as a vacuum seal.

# Vacuum System

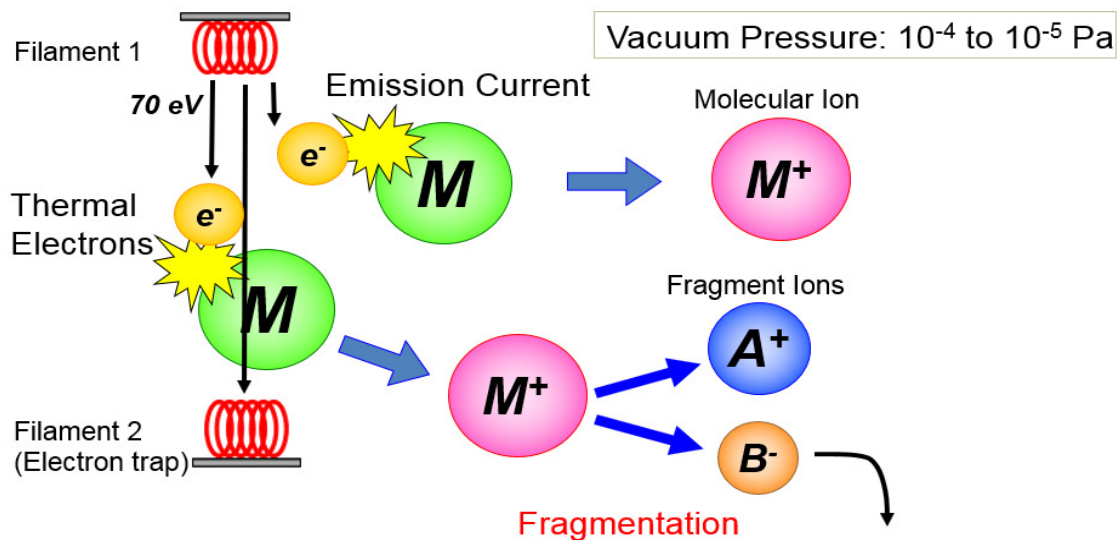


# GCMS Unit

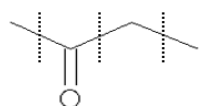


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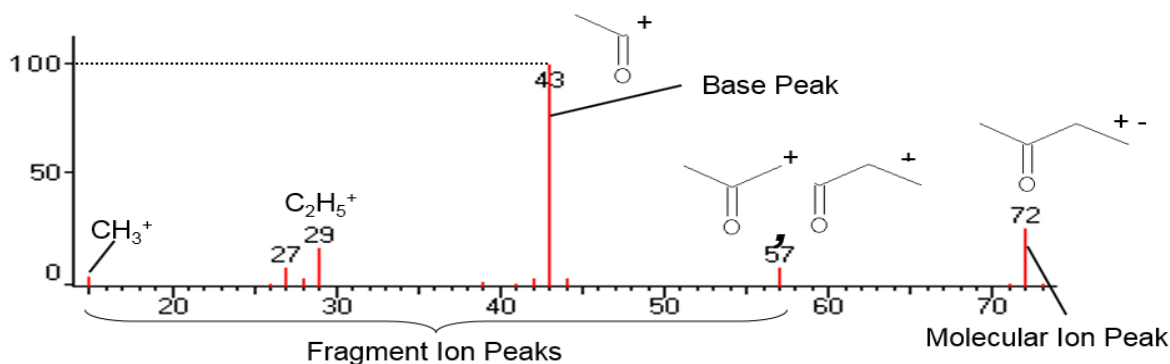
## Electron Ionization (EI)



# Fragmentation



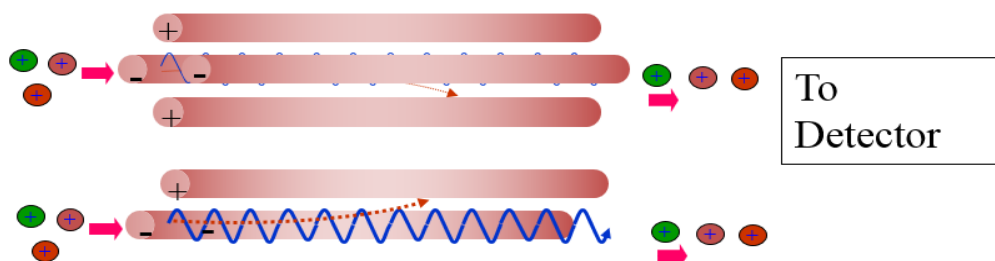
2-butanone ( $C_4H_8O$ , M.W.: 72)



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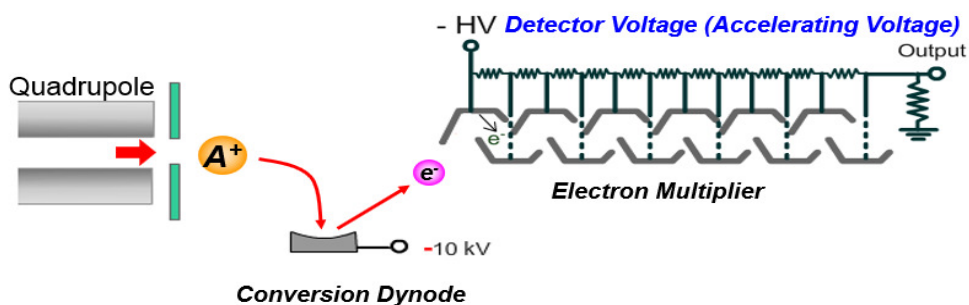
# Quadrupole MS System

- Voltages applied to four cylindrical quadrupole rods generate a quadrupole field in the center axis of the mass spectrometer
- Ions entering the field will oscillate; the oscillation characteristics depend on the mass-to-charge ratio of the ions and the voltage applied



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# Detection Unit

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## GC-MS Data Acquisition Mode

### SCAN MODE

#### Qualitative Analysis

- For identification of compounds by using mass spectrum
- For determination of SIM mode parameters

### SIM MODE

#### Quantitative Analysis

- Lower detection limits, because SIM sensitivity is tens to hundred times higher than that of SCAN mode
- MS set to measure only specified masses

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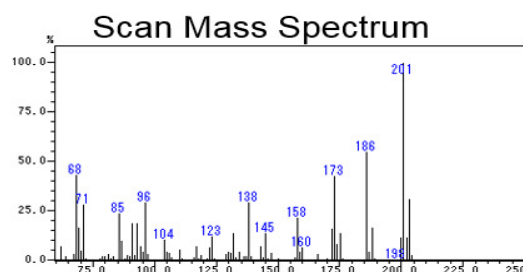
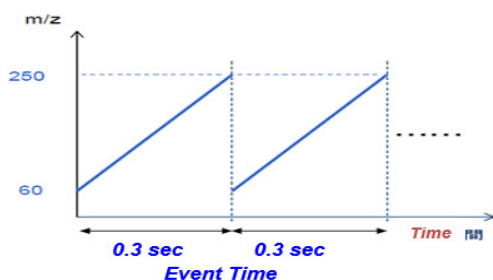
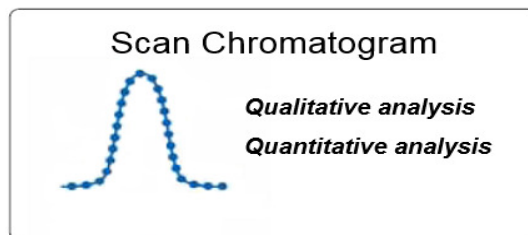
# Scan Mode

## Advantages

- Qualitative information from mass spectra
- Information about non-target components

## Disadvantages

- Lower sensitivity than SIM mode



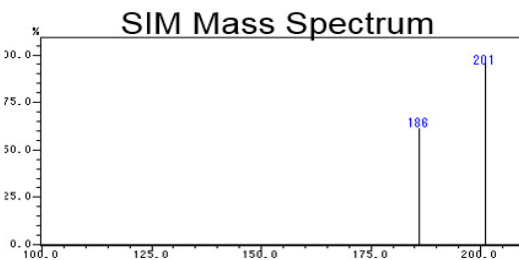
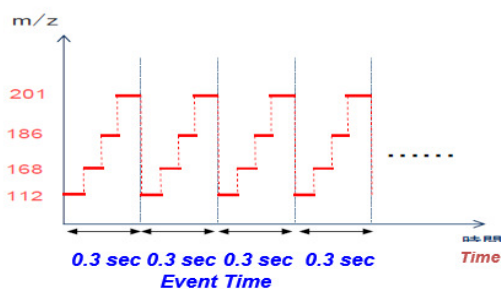
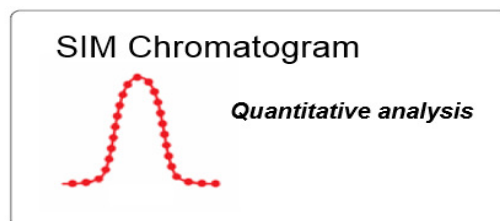
# SIM Mode

## Advantages

- Higher sensitivity than SCAN mode

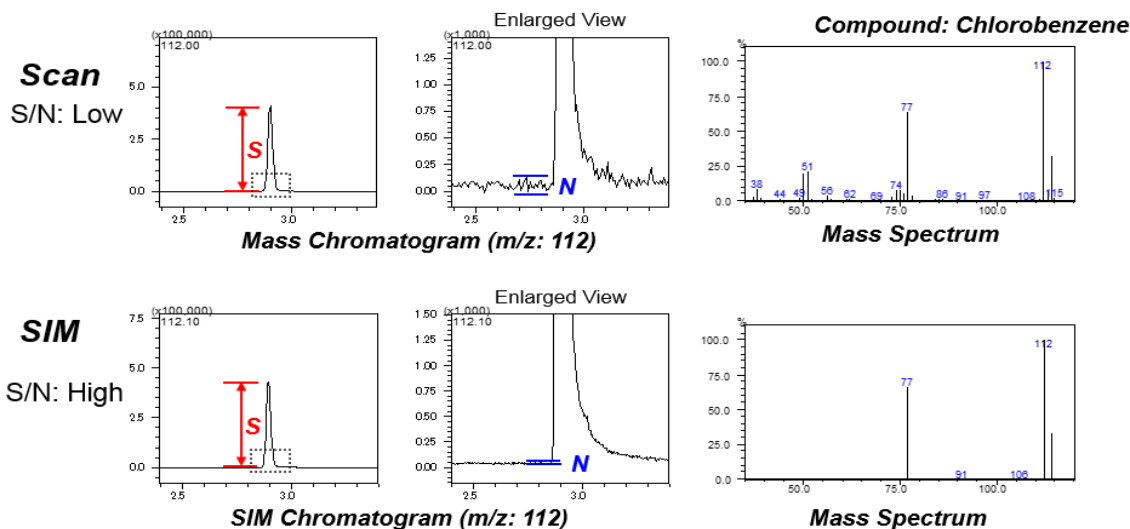
## Disadvantages

- Complete mass spectra not obtained
- Only information about target components



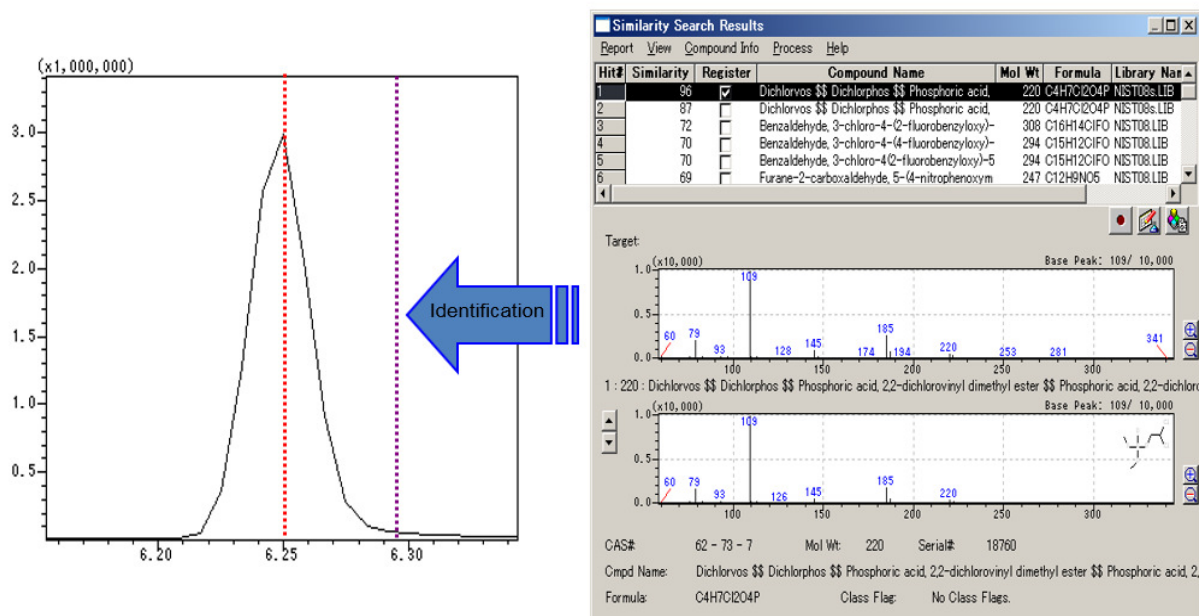
**Library search not possible**

# Comparison of Scan and SIM



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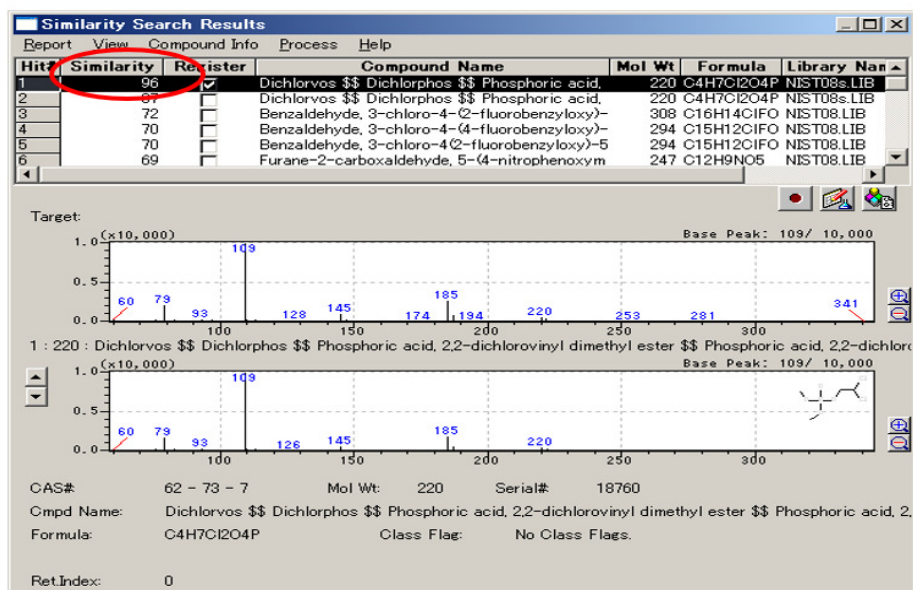
# Searching Libraries



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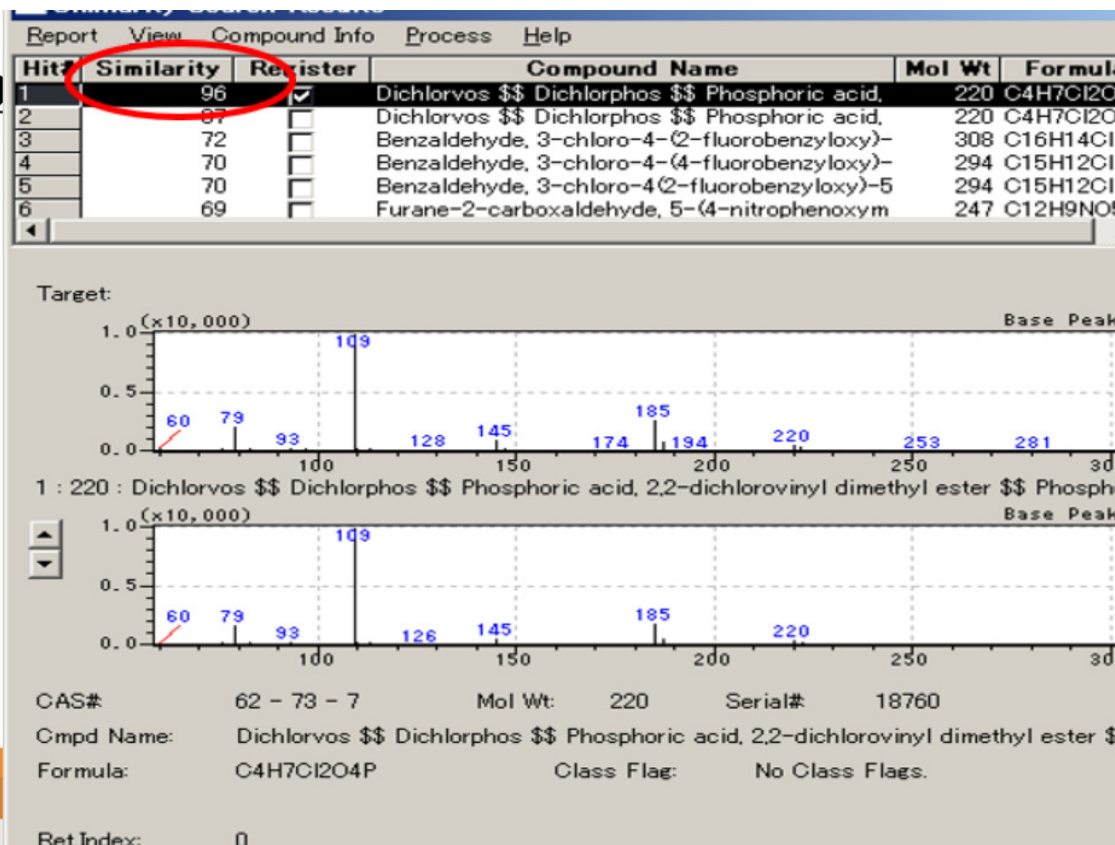
# Library Search Results

Similarity



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Lib  
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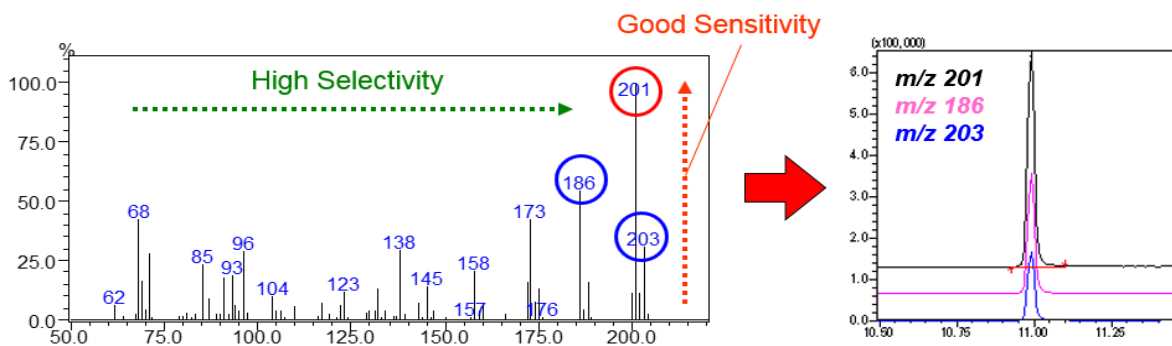
# Selection of Ions

**Target Ions** : Ions used for quantitation

**Confirmation Ions** : Ions used for identification

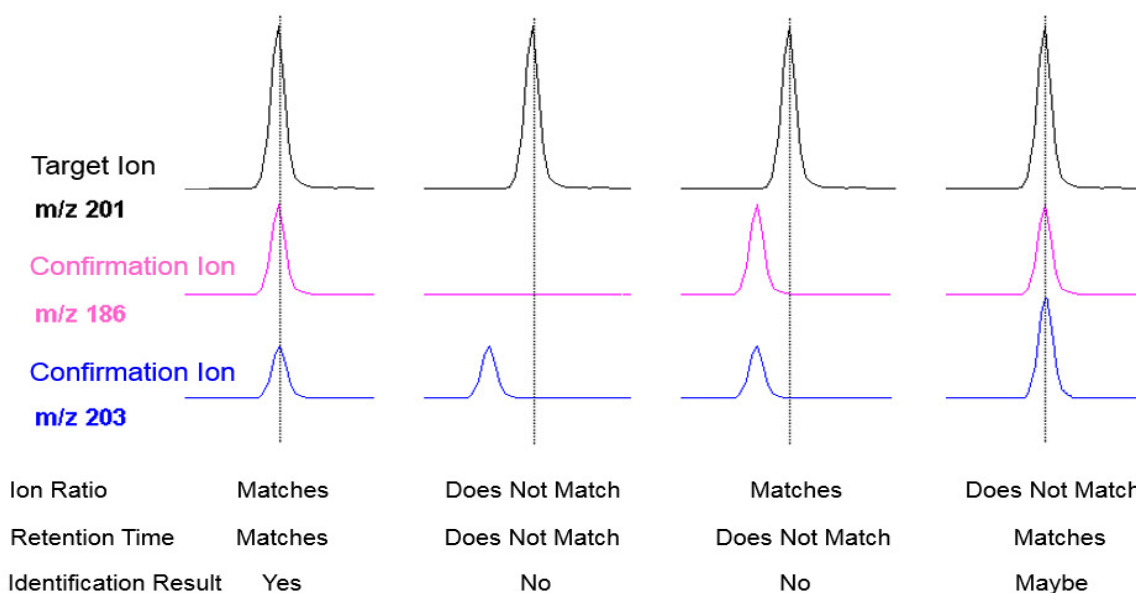
The key criteria for selecting ions are:

1. High intensity (good sensitivity)
2. Large mass (high selectivity: not prone to overlap with other substances)



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## Identification Method in GC-MS



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# Environmental Applications

- Environment segment can be roughly classified into 3 major sub-segments



**Water**

**Soil**

**Air**

- Let us understand more about each sub-segment

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# Environmental Applications

| <b>Segments</b> | <b>Sample Types</b>                       | <b>Key Applications</b>                |
|-----------------|-------------------------------------------|----------------------------------------|
| Water           | Drinking water – Tap & Packaged           | Pesticides , PAH,<br>PCB /Dioxin & VOC |
|                 | Environmental water – Ground, river & sea |                                        |
|                 | Waste water – Industrial & Domestic       |                                        |
| Soil            | Soil                                      | Pesticides / PCB &<br>VOC              |
|                 | Geological Samples                        |                                        |
|                 | Sludges / Sediments                       |                                        |
|                 | Industrial Waste                          |                                        |
| Air             | Air                                       | PCB & VOC                              |

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# Food Applications

| <b>Segments</b>        | <b>Sample Types</b>                                 | <b>Key Applications</b> |
|------------------------|-----------------------------------------------------|-------------------------|
| Contaminants           | Dairy, Agricultural, Marine products etc.           | Residual Pesticides     |
| Additives              | Food product, essential oil, Meat, soft drinks etc. | Flavour Compounds       |
| Processing / Packaging | Processed and Packed products                       | Off – Flavour           |

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**THANK YOU FOR YOUR ATTENTION!**



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