# AccuTOF-GCv Series

## Group-type Analysis of Crude Oil by Using GC/FI-TOFMS 1

### *Determination of average molecular weights*

### Introduction

Field Desorption (FD) and Field Ionization (FI) are both techniques that ionize analytes by electron tunneling from the analyte molecules to a solid surface (emitter) in a high electric field. In the case of FD, the sample is applied directly onto the emitter and heated by applying an electric current through the emitter for desorption and ionization. In the case of FI, vaporized analyte molecules are introduced into the proximity of the emitter.

Both FI and FD are soft ionization methods that generally yield intact molecular ions and, in most cases, produce very few fragment ions. Generally, these two techniques are used to ionize analytes that are easy to fragment and do not generally produce molecular ions during electron ionization (EI), such as hydrocarbons in crude oil.

For complex mixtures such as crude oils or synthetic polymers, molar mass distributions and average molecular weights are important chemical properties. By analyzing an FI mass spectrum that mostly consists of molecular ions, even for complex hydrocarbon mixtures, and using a group-type analysis software, one can obtain the molar mass distributions and average molecular weights for the various hydrocarbon types (e.g., paraffin, naphthene, olefin, aromatics) present in the sample mixture.

In this work, we analyzed a crude oil sample by using the JMS-T100GC "AccuTOF-GC" GC/FI method and then processed the resulting data using a group-type analysis software package.

### Method

| Sample | Crude Oil |
|---|---|
| | (Refer to Fig. 1 for Sample Preparation) |

#### GC conditions

| | |
|---|---|
| GC: | Agilent 6890N |
| Column: | DB-5ms |
| | 30 m x 0.25 mm I.D., 0.25 μm |
| Oven: | 50°C→15°C/min→280°C |
| | (5 min) |
| Injection port: | 280 °C, Split (1:200) |
| Injection volume: | 1.0 μl |
| Career gas: | He（1mL/min, constant flow mode） |

#### MS conditions

| | |
|---|---|
| MS: | JMS-T100GC "AccuTOF GC" |
| Ionization: | FI+ (Cathode voltage: -10 kV, Emitter current: 0 mA) |
| Mass range: | *m/z* 35 - 500 |
| Acquisition rate: | 0.3 s/spectrum |

| Software | Polymerix™ (Sierra Analytics, Inc.) |
|---|---|



*Fig. 1 Sample preparation flow*

* Specify α and γ end groups and repeating unit.

* Perform group-type analysis.

* Results such as $M_n$, $M_w$, $M_z$, and poly-dispersity for each series are displayed.

* Mass spectral peaks are color coded based on the series to which they belong.
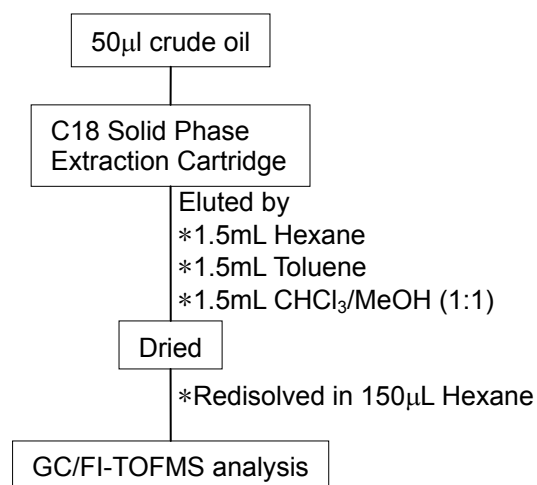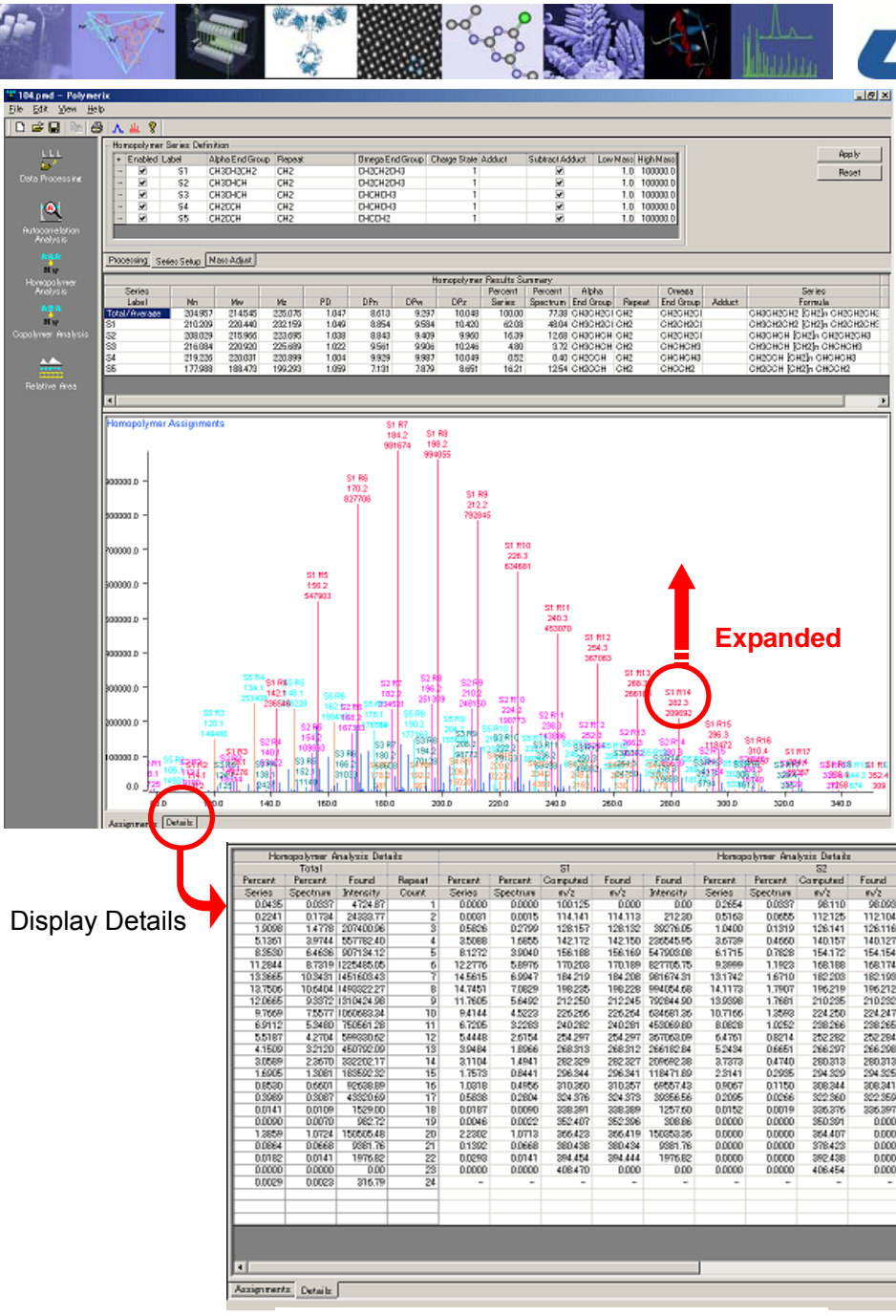
*Fig. 2 Group-type analysis results of crude oil*

**Results and Discussion**

All of the mass spectra acquired by the AccuTOF-GC during the retention time range of the sample were summed to form a single mass spectrum. Afterwards, this mass spectrum was directly read into the Polymerix™ software for processing. The output from the group-type analysis is shown in Fig. 2. Properties such as number average molecular weight ($M_n$), weight average molecular weight ($M_w$), z average molecular weight ($M_z$), and polydispersity (PD) were calculated for 5 hydrocarbon types with the degree of unsaturation from 0 to 4 and for the total/average of the 5 types.

**Conclusions**

Group-type analysis of complex hydrocarbon mixtures such as crude oil can be easily performed by using the GC/FI method on the AccuTOF-GC and the Polymerix™ group-type analysis software.