

## Usefulness of NCI Mass Spectral Library

In recent years, the effects of environmental pollutants on human beings is becoming a serious problem. In particular, endocrine disruptors affect human beings even in extremely small quantities. Therefore they need to be analyzed in extremely low concentrations.

The negative chemical ionization (NCI) is one of the ionization methods for GC/MS and is characterized by superior selectivity and sensitivity. For compounds with high electron affinity, NCI can increase sensitivity by 10 - 100 times compared to the commonly used the electron ionization method. In addition, target substances can be selectively ionized, reducing the effects of interfering components. Thanks to these advantages, NCI is increasingly adopted in various fields for the quantitation of trace substances.

NCI mass spectra are comparatively simple with smaller numbers of fragment ions, and had been thought to vary depending on the analytical conditions. Thus, its identification capability had not been highly evaluated. Accordingly there has been no mass spectral database for the NCI method.

However, we have proved that NCI mass spectral database (library) can be used for qualification as a result of examining the dependency of NCI mass spectra on analytical conditions. This Application News presents the details of the investigation.

### ■ Influence of Reagent Gas Pressure

In order to investigate the influence of reagent gas pressure on mass spectra, NCI mass spectra were measured using methane as the reagent gas, with the cylinder secondary pressure at 200kPa and 350kPa.

The result proved that the pressure of the reagent gas has no effect on the NCI mass spectra. Fig. 1 shows measurement examples.

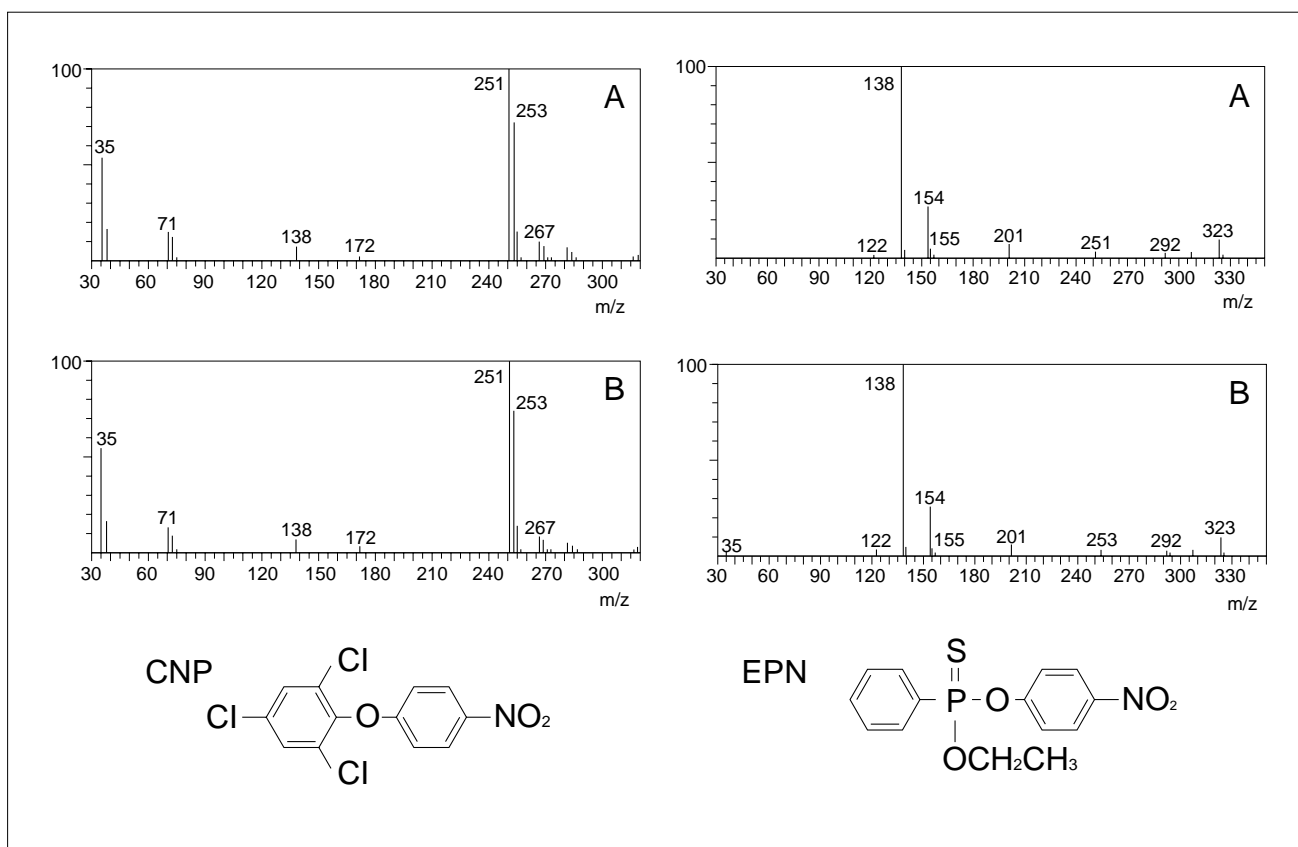


Fig.1 Influence of reagent gas pressure(Pressure A:200kPa,B:350kPa)

## ■ Influence of Temperature

In order to investigate the influence of temperature on mass spectra, NCI mass spectra were measured with interface temperatures at 250°C, 280°C and 320°C. As the temperature increased, the intensity of fragment ions increased and the relative intensity of molecular and quasi-molecular ions decreased. Fig. 2 shows measurement examples. The changes in relative intensity did not significantly affect the library search results.

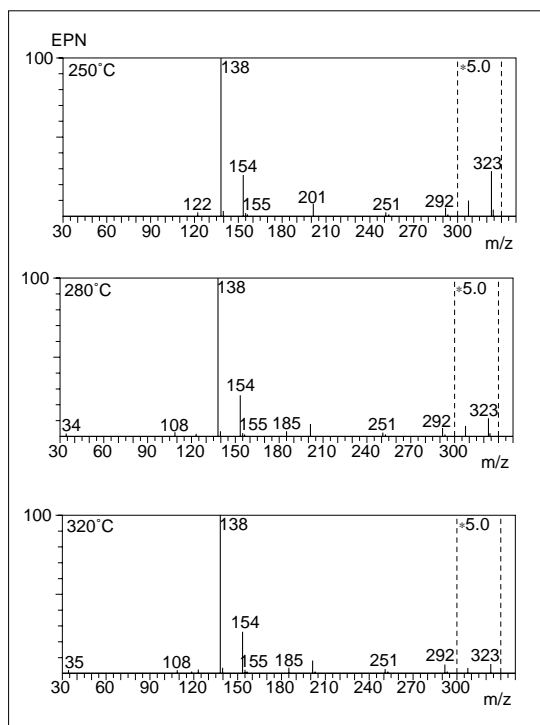


Fig 2 Influence of Temperature (Interface Temp.: 250, 280 and 320°C)

## ■ Conclusion

The NCI library is effective for qualification. Furthermore, the reliability is improved using the NCI and the EI.

## ■ Library Search

NCI library was created and library search was performed for independently obtained measurement data. Fig. 3 shows examples of search results. For most substances, the target substance appeared near the top of the search results, verifying that libraries are effective for NCI qualification.

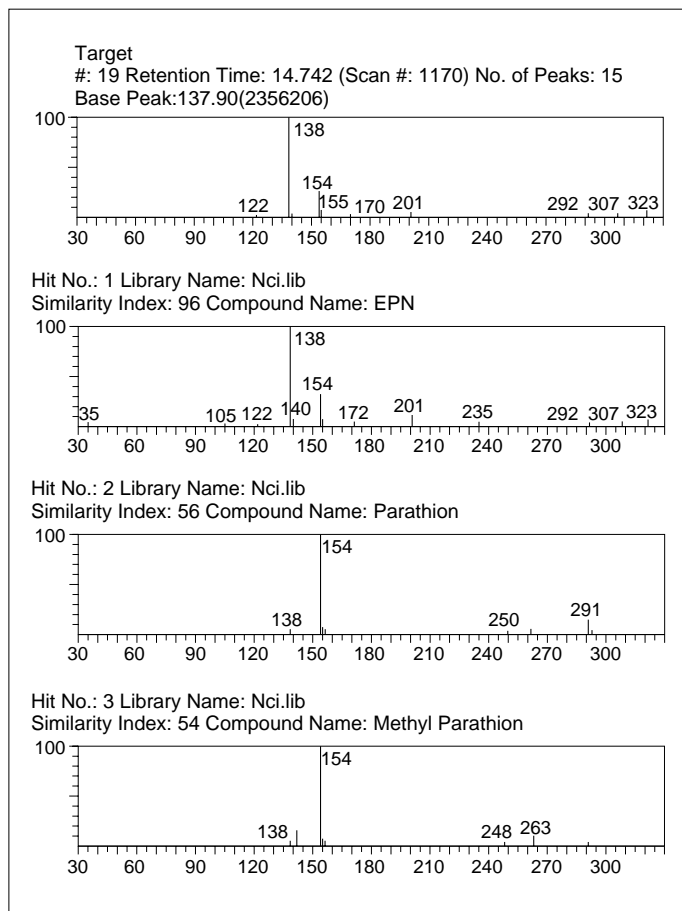


Fig 3 Library Search Results (EPN)

Injector Temp.

Table 1 Analytical conditions

|                   |  |
|-------------------|--|
| -GC-              |  |
| Column            | : DB-5 30m×0.25mm I.D. df=0.25μm (J&W)                 |
| Column Temp.      | : 60°C (2min)→30°C/min→<br>170°C→10°C/min→280°C (5min) |
| Injector Temp.    | : 250°C  |
| Carrier Gas       | : 100kPa   |
| Injection         | : Splitless (Sampling Time=2min)                       |
| -MS-              |  |
| Interface Temp.   | : 250, 280, 320°C                                      |
| Scan Range        | : m/z 30~400   |
| Ionization Method | : NCI  |
| Reagent Gas       | : CH <sub>4</sub> 200, 300, 350kPa                     |



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