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Application Data Sheet

No.116

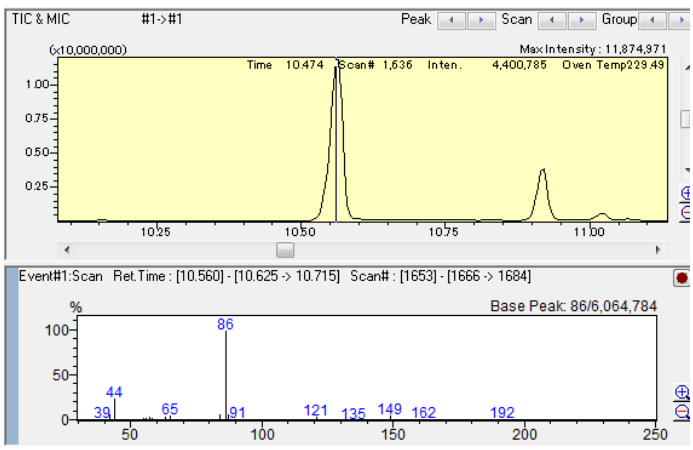
GC-MS
Gas Chromatograph Mass Spectrometer

Compound Identification Procedures Combined with Quick-CI

The Quick-CI function is enable easy and simple use of the EI and PCI (Positive ion chemical ionization) mode using an NCI ion source without venting the MS. PCI can be obtained as a simple method of confirming molecular weight by molecule protonation and the combination of EI and PCI is a powerful identification technique when a compound cannot be identified based on its EI mass spectrum alone. Also, since the selected ionization mode is saved in a method file, the user can switch between EI and PCI for consecutive analyses.
This Application Data Sheet presents a compound identification performed by combining the mass spectrum information obtained by the EI and the PCI using an NCI ion source.

Similarity Search Results Obtained Using Only EI

GC/MS with the EI can be used for compound identification since it produces many fragment ions, and a rich mass spectral library is available. However, the EI cannot detect molecular ions of some compounds such as those with functional groups that include amino groups, carbonyl groups, and carboxyl groups, and those with ether linkages. Therefore, performing a similarity search of a library will produce results that include compounds of similar structure and structural isomers. This makes it difficult to identify the target compound. In these cases, compounds can be identified easily by combining the information from the EI with molecular weight information obtained from protonated molecules by the PCI.
Fig.1 shows an example of a similarity search performed after the EI (Table 1) is used to measure a type of cathinone, which is a dangerous drug. Because the molecule ion is not detected and there is little mass spectral pattern to analyze, the similarity search shows other structurally similar cathinones and phenethylamines that have a similarity score close to the target molecule.



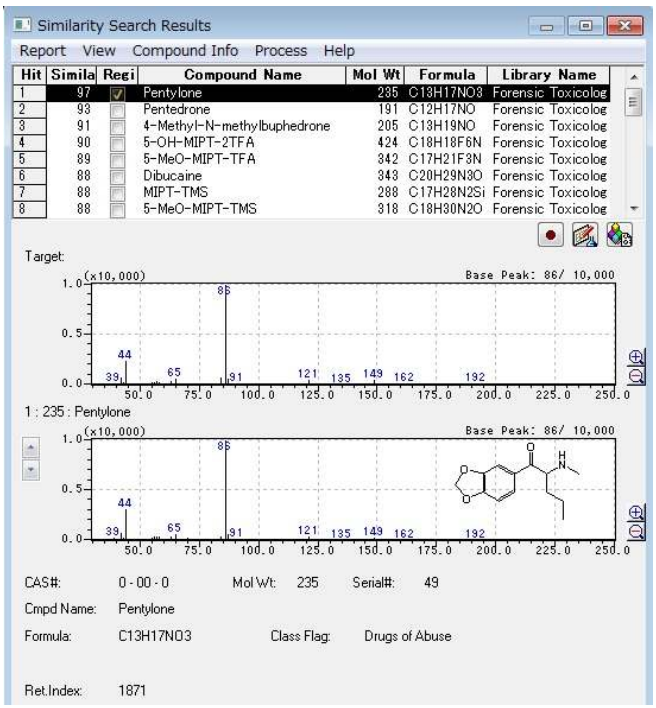


Fig. 1 Total Ion Current Chromatogram and Library Search Results for Pentylone Obtained Using the EI

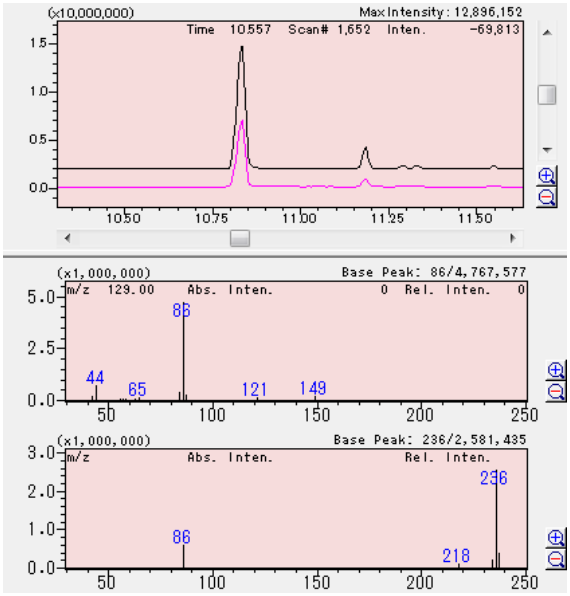
Table 1 Analytical Conditions

GC-MS:	GCMS-QP2020
Column:	Rxi®-5Sil MS (length: 30 m; 0.25 mm I.D.; df = 0.25 μm)
Glass Insert:	Splitless insert with wool (P/N: 221-48876-03)
[GC]	
Injection Unit Temp.:	260 °C
Column Oven Temp.:	60 °C (5 min) → (10 °C /min) → 320 °C (15 min)
Injection Mode:	Splitless
Carrier Gas Control:	Linear velocity (45.6 cm/sec)

[[MS]			
Interface Temp.:	280 °C		
Ion Source Temp.:	200 °C		
Measurement Mode:	Scan		
Scan Event Time:	0.3 sec		
EI		CI	
Scan Range:	*m/z* 40 – 600	Scan Range:	*m/z* 60 – 600
		Reagent Gas:	Isobutane (240 kPa)

Similarity Search Results Combined Molecular Weight Information

Fig. 2 shows the total ion current chromatogram (TICC) and mass spectra obtained after measuring pentylone by both the EI and the PCI using the Quick-CI function. The results obtained from the EI and the PCI can be used in tandem by utilizing a data comparison feature of GCMSsolution. The PCI mass spectrum shows that the protonated molecule is measured at *m/z* 236, which leads to an estimate that the molecular weight is 235. After the initial similarity search, search results can be narrowed down using the molecular weight data (Fig. 3). Inputting the estimated molecular weight before performing a similarity search of the EI mass spectrum reduces the number of results to that of just pentylone (Fig. 4).
When compound identification is difficult using only the mass spectrum obtained from the EI, combining the mass spectrum information from the EI with molecular weight information obtained from the PCI allows for easy compound identification.



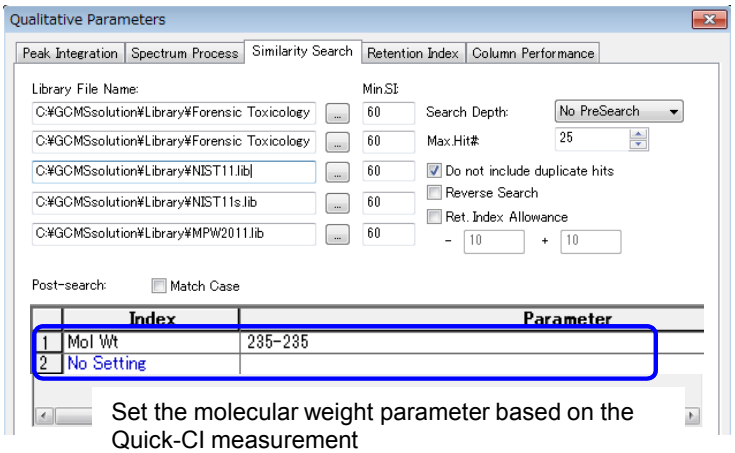
Black: TICC obtained by EI
Pink: TICC obtained by PCI

EI mass spectrum

PCI mass spectrum

A molecular weight of 235 can be estimated based on *m/z* 236 detected for the protonated molecular ion.

Fig. 2 TICC and Mass Spectra Obtained by the EI and PCI Using an NCI Ion Source



Set the molecular weight parameter based on the Quick-CI measurement

Fig. 3 Qualitative Analysis Parameter Window

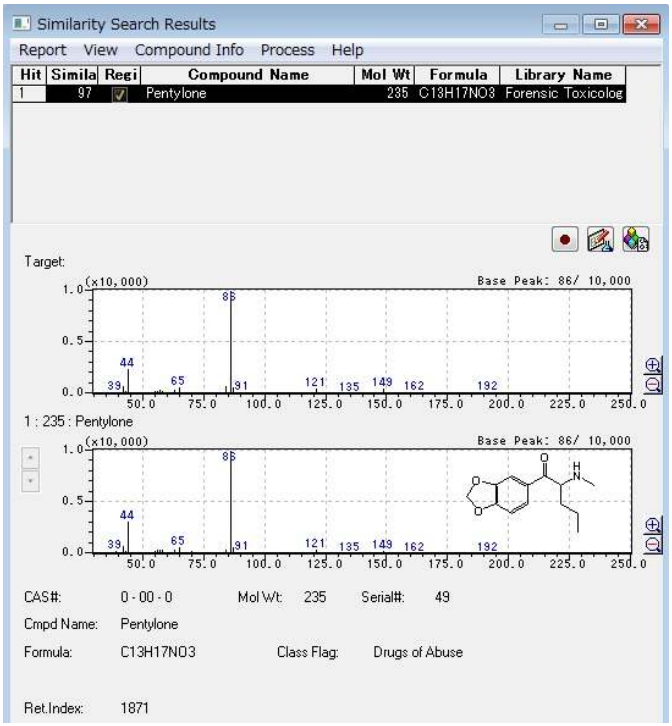


Fig. 4 Narrowing Down EI Mass Spectrum Similarity Search Results Using the Molecular Weight Information

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