Chemical Ionization Meets MS/MS Simplicity

The Thermo Scientific TSQ 8000 triple quadrupole GC-MS/MS is built with simplicity as a top priority. Whether you are managing retention times, starting from the beginning with a completely new analysis, transferring a method from a single quadrupole GC-MS, or porting a known MRM method from another instrument, the TSQ™ 8000 GC-MS/MS, through its integrated software tools, ensures the fastest route to high performance results, routinely.

This simplicity allows you to take advantage of the benefits of MS/MS especially when you require more flexibility from your system. Chemical ionization (CI) is an example; sometimes you need a different way of addressing the unique chemistries facing you in a particular application. This less frequently used technique can lead users to feel a little uncertainty in set-up and method development of CI methods. With the TSQ 8000 GC-MS, the uncertainty can be removed; as the system takes care of the critical aspect of method development and set-up, allowing you to proceed with sample analysis.

Where Can CI be Applied in GC-MS/MS?

Generally, the best chance of high sensitivity in MS/MS occurs when the precursor ion can be selected from a single high mass ion which carries a significant amount of the ion current. Electron impact Ionization (EI), although universal, is a high energy process that, in a lot of cases, leads to extensive source fragmentation in less stable compounds. This moves us away for the ideal situation for MS/MS. Since chemical ionization is a softer form of ionization, it offers an opportunity to generate more abundant high mass ions.

CI can also offer a higher degree of selectivity or sensitivity in the source ionization process too, especially with negative chemical ionization (NCI), favoring electronegative compounds such as halogenated species.

Examples for routine analysis using positive chemical ionization (PCI) include applications with target compounds such as phthalates and nitrosamines (US EPA Method 521). PCI is also applied to compound elucidation taking advantage of pseudo molecular ion formation and subsequent MS/MS structural characterization. The obtained data can help screen and confirm any compound candidates obtained through EI spectra and library searching. This is especially useful in conjunction with a direct sample probe, which enables the user to place a sample directly into the source for immediate identification of chemical reaction products.

Applications reported using NCI sometimes include organochloro pesticides (especially pyrethroids), some persistent organic pollutant (POPs) applications like short chain chloropariffins, toxaphenes, and brominated compounds such as polybrominated diphenyl ethers (PBDEs).

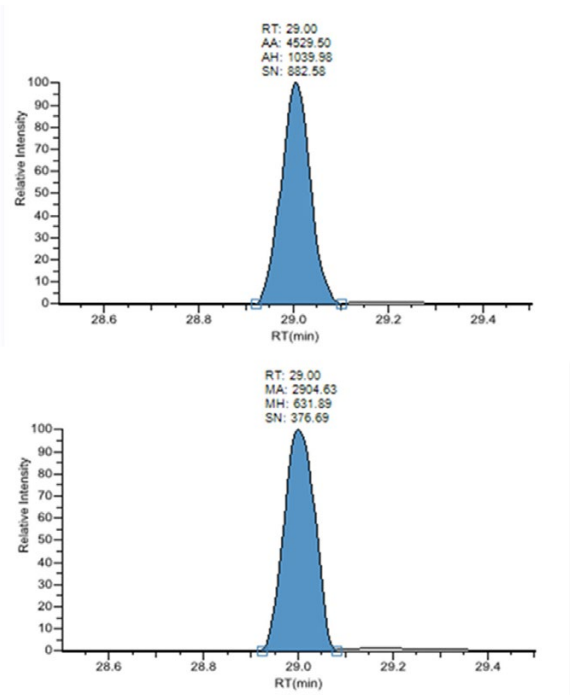

Figure 1. PBDE 209 at 2.5 ppb using NCI on the TSQ 8000 GC-MS System

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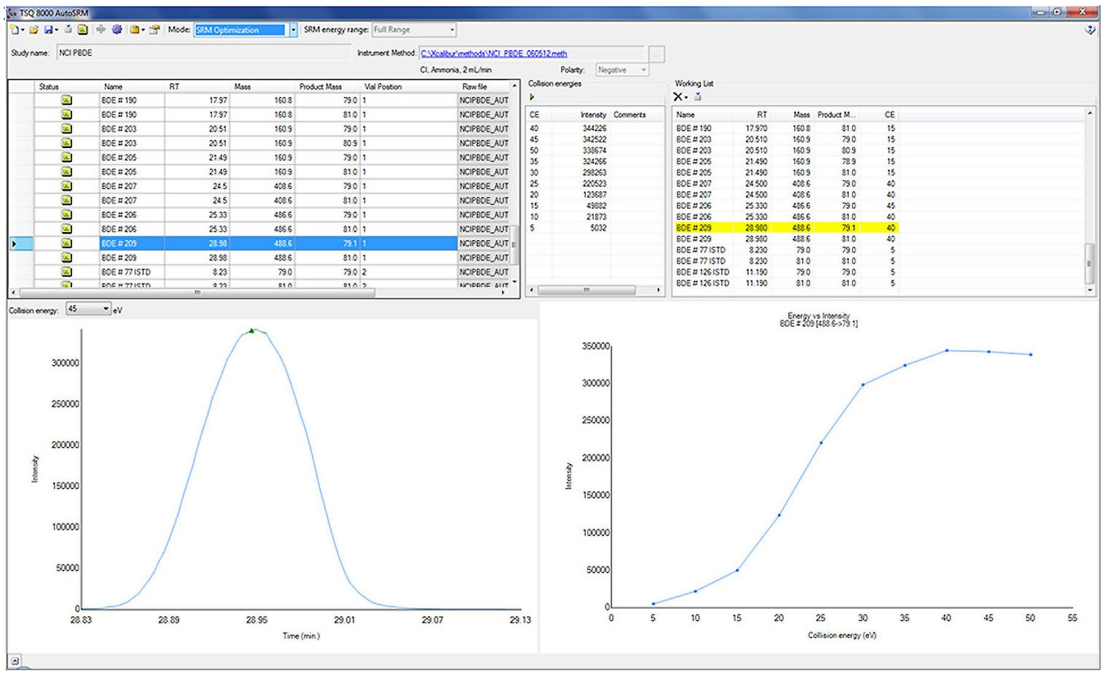

Figure 2. AutoSRM precursor ion selection PBDE

Examples of PBDE data acquired on the TSQ 8000 GC-MS are shown in Table 1 and Figure 1. Also of interest are applications that utilize halogenated derivatized reagents, such as the analysis of estrogenic compounds or tetrahydrocannabinol (THC) in hair.

Table 1. Quantitative performance for PBDEs using NCI SRM on the TSQ 8000 GC-MS System.

MDLs @ 99% Confidence Level n = 8				
PBDE #	Concentration Range Measured (pg/µL)	RSD	R^2 Value	MDL (pg/µL)
47	0.5–250	7%	0.9999	0.106
99	0.5–250	5%	0.9997	0.081
100	0.5–250	8%	0.9995	0.113
153	1-500	5%	0.9996	0.147
154	1-500	9%	0.9997	0.276

CI Method Development

Compared to EI, CI is not as widely used in GC-MS/MS. Consequently, there is not a significant amount of reference information available to help with the setting up of new methods. This technique has the potential to be an unfamiliar and laborious method development process for laboratories. It's especially complex for applications like this, which offers a compelling reason to use the TSQ 8000 GC-MS system.

How the TSQ 8000 GC-MS Can Assist CI Method Development

1. The stages of instrument set-up and method development are all manageable through smart software tools integrated into the workflows needed for both positive and negative mode CI.
2. The TSQ 8000 GC-MS automatically handles CI source tuning and optimization, and offers automated switching between two CI gases.
3. AutoSRM software walks you through the CI method development process to obtained fully optimized SRM transitions (see Figure 2).
4. The TSQ 8000 GC-MS method, linked with AutoSRM, can automatically import developed CI SRMs and optimize MS/MS acquisition for maximum sensitivity through timed-SRM.
5. Thermo Scientific TraceFinder Software methods can also import compound information, control sequences, and quantify target compounds
6. Sample probes, which enable sample placement directly into the source, allow for fast and easy compound characterization of solids or liquids in CI, further facilitated by MS/MS which is available on the TSQ 8000 GC-MS system.

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