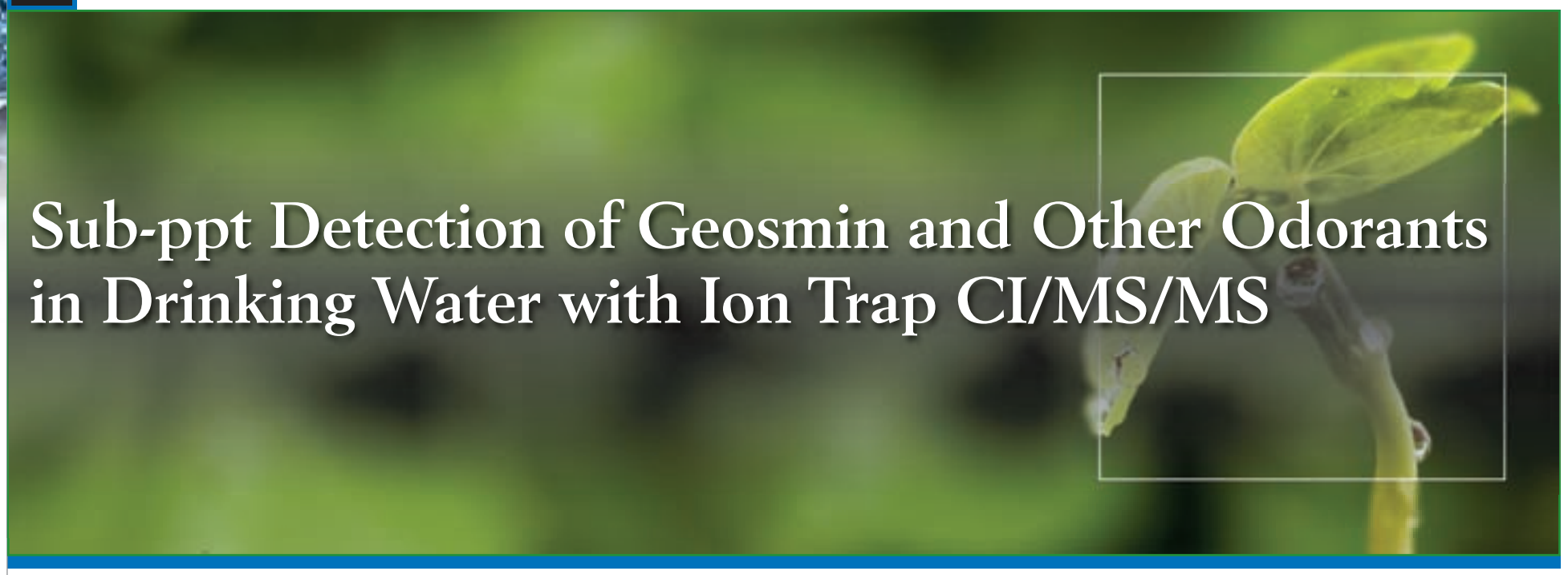

Sub-ppt Detection of Geosmin and Other Odorants in Drinking Water with Ion Trap CI/MS/MS

Agilent GC/MS/MS Technology Advantage

The quality and safety of drinking water is a health and environmental concern of a global scale. Municipalities are monitoring many harmful organic, inorganic, and microbiological contaminants. Most of these contaminants are not detectable by human sensory function. However, a type of contaminants, called odorants, is often detected, resulting in an alarming number of complaints to water agencies. The high number of reports is due to the very low human olfactory threshold for these contaminants, in the low ppt (ng/L) range. The two most common odorants, causing musty, earthy flavors, are geosmin and 2-methylisoborneol (MIB). They are ubiquitous in the environment, produced by a number of microorganisms, and released when these microbes die. 2-isobutyl-3-methoxypyrazine (IBMP) and 2-isopropyl-3-methoxypyrazine (IPMP) also were reported as contributors to the unpleasant odor of water, with similar origins as geosmin and MIB. While trichloroanisol (TCA) is more commonly measured in alcoholic beverages, it also may be present in water; therefore, it was included in the measurements. Trichloroanisole-d5 was added as an internal standard.

The Agilent 7890A GC with an Agilent 240 Ion Trap MS was used for the measurements. The GC was equipped with a split/splitless inlet and CombiPal autosampler with Solid Phase Micro Extraction (SPME) option. The 240 was configured in internal ionization mode, and methanol was used as CI reagent. SPME is a simple and convenient way to concentrate the contaminants using the CombiPal autosampler and the spit/splitless (or MMI) inlet of the 7890 GC, allowing fully automated sample enrichment.

The 240 GC/MS/MS delivered a simple, yet sensitive and reliable detection of the odorants at sub-ppt level in water. The low detection levels along with excellent linearity and precision were afforded by the selectivity, sensitivity and simplicity of chemical ionization and MS/MS detection of the 240 MS. The analysis can be extended to measure these analytes, particularly TCA in alcoholic beverages.

Key Benefits

- The Agilent 7890/240 Ion Trap GC/MS/MS offers exceptional CI sensitivity, comparable to EI sensitivity in internal mode.
- CI made simple and convenient with the use of gas and/or liquid reagents and automatic switching between EI/CI even in the same run.
- CI/MS/MS benefits from the most suitable precursor (high *m/z*, high intensity) ion and offers outstanding selectivity and sensitivity.
- Reliable qualitative and quantitative results obtained at sub ppt level concentration of the ordorants.

The Agilent 240 Ion Trap MS connected to the Agilent 7890A GC

The odorants are small polar molecules and produce extensive fragmentation during EI ionization. Performing chemical ionization with methanol as reagent not only reduces background and enhances selectivity but also delivers a high intensity, high *m/z* precursor ion for the MS/MS process, leading to additional sensitivity increase. Switching between EI and CI is convenient; software controlled, and can be automatically changed even during a chromatographic run.

Water samples from commercially available bottled water and tap water from two different municipalities were analyzed. The bottled water had only trace level of MIB, while the municipality samples had low ppt concentration of geosmin and MIB. One of the municipality samples also had trace levels of the other odorants.

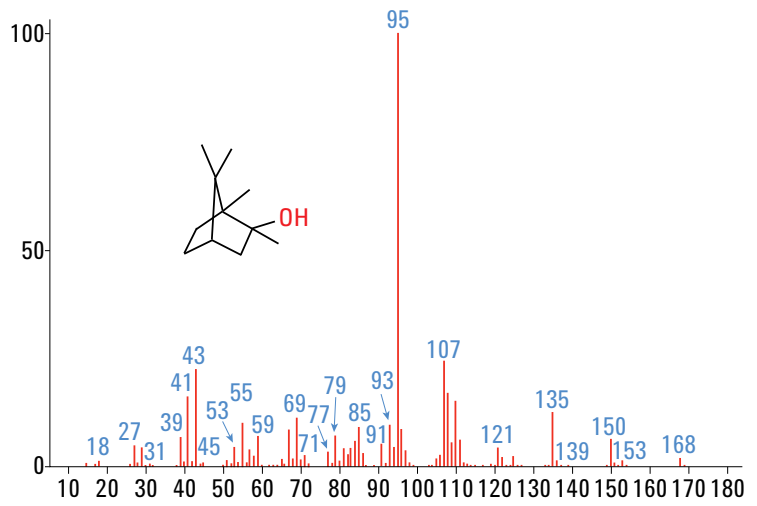

Figure 1. The highly fragmented EI-spectrum of 2-Methylisoborneol (MIB) does not offer a desirable precursor ion (MW 168).

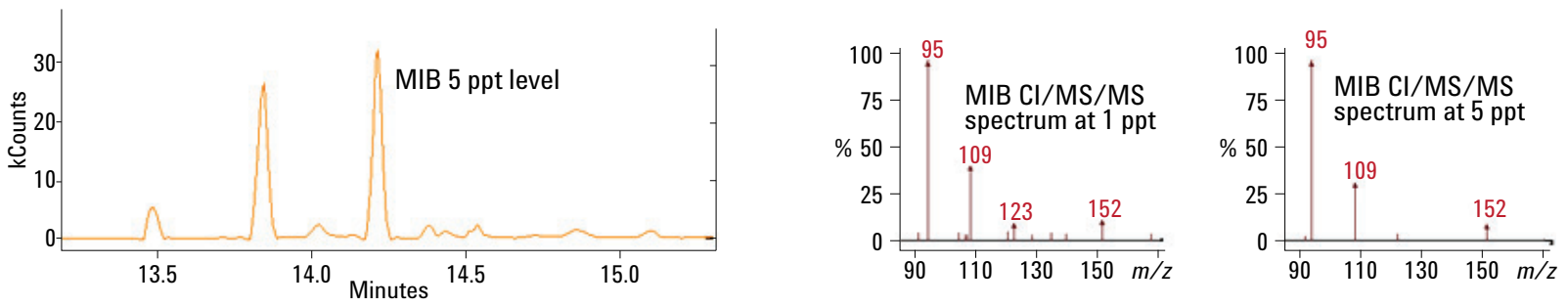

Figure 2. MIB CI/MS/MS chromatogram at 5 ng/L and spectra at 1 and 5 ng/L levels. The spectrum at 1 ng/L matches well the spectrum obtained at higher concentration. The selectivity of CI/MS/MS enhances detection to allow reliable identification and quantitation even at trace levels.

Table 1. Calibration, MDL, and Sample Results

Analyte	Correlation coefficient* 0.50–100 ng/L	MDL** (ng/L)	%RSD of replicate injections	Commercial bottled water ng/L	Municipality-I Water sample ng/L	Municipality-II Water sample ng/L
IPMP	0.9994	0.067	3.6	nd	nd	0.431
IBMP	0.9988	0.069	4.0	nd	nd	0.389
2-Methylisoborneol	0.9944	0.096	5.7	0.442	2.961	1.678
Trichloroanisol	0.9950	0.052	2.6	nd	nd	0.676
Geosmin	0.9970	0.056	3.0	nd	2.054	3.259

*Calibration for all analytes was performed in the 0.5–100 ppt range resulting excellent linearity with R^2 from 0.9944 to 0.9994. These values represent the combined linearity of the concentration process and the GC/MS/MS analysis. Reliable quantitation was established at 0.5 ng/L concentration for all analytes. This level is lower than the human olfactory threshold.

**MDLs, all below 0.1 ng/L were determined statistically by eight replicate injections of 0.5 ng/L standards, using 99% confidence level.

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