

## Sub-ppt detection of 1,2,3-Trichloropropane in water with Ion Trap GC/MS/MS

ENVIRONMENTAL



### Agilent GC/MS/MS Technology Advantage



The well documented adverse health effects, particularly its carcinogenicity, prompted the monitoring of 1,2,3-trichloropropane (TCP) in water in California. While there is no current Maximum Contaminant Level (MCL) for TCP, several regulatory agencies have released guidelines:

California Department of Public Health  
Notification level = 0.005  $\mu\text{g/L}$   
Public Health Goal (PHG) = 0.0007  $\mu\text{g/L}$

Unregulated Contaminant Monitoring Rule (UCMR 3 administered by US EPA)  
Proposed Minimum Reportable Level (MRL) = 0.03  $\mu\text{g/L}$

American Water Works Association (AWWA)  
Recommended MRL = 0.005  $\mu\text{g/L}$ ; based upon 1/10 of Health Reference Level (HRL).

TCP is widely used as paint and varnish remover, as a cleaning and degreasing agent, and is a byproduct of pesticide and other chemical manufacturing processes. Due to the common occurrence and the high health risk associated with TCP, US wide TCP monitoring will start in 2013 as part of the proposed UCMR 3 list.

TCP is commonly measured by EPA methods 504.1, 551.1, 524.2, and 524.3, but these methods allow a much higher MDL level than the 0.005  $\mu\text{g/L}$  requested in California and recommended by the AWWA. To achieve reliable detection at 5 ppt MRL level, the Agilent 7890/240 GC/MS system was used in EI/MS/MS mode. The concentration was carried out by the Stratum Purge and Trap and Archon autosampler. 1,2-dibromo-3-chloropropane (DBCP) was also included in the GC/MS/MS measurements.

0.005  $\mu\text{g/L}$  0.005 ppb 5 ng/L 5 ppt

The concentrations units are used interchangeably to express trace level concentrations.

### Key Benefits

- The Agilent 240/7890 GC/MS/MS system enables sub-ppt detection of 1,2,3-Trichloropropane in drinking water satisfying the California Public Health Goal level
- High sensitivity and reliable quantitation was achieved by employing EI/MS/MS detection and optimized Purge and Trap and GC conditions
- The selectivity, simplicity and affordability of an Agilent 240 Ion Trap GC/MS makes it an excellent tool for trace detection in environmental and other samples

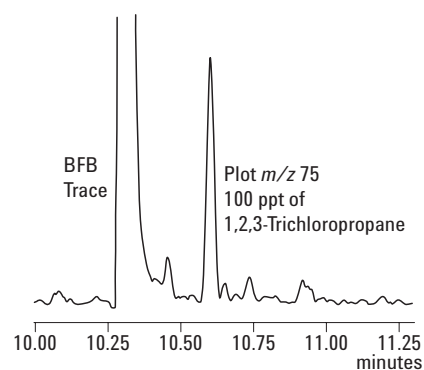


Figure 1. TCP is traditionally measured in full scan as outlined in EPA methods 524.2 and 524.3. Above is the quant ion plot of  $m/z$  75 for TCP at 100 ppt measured during a 524.3 analysis. The proposed new MRL level is much lower at 5 ppt.



Internal standard 1,2,3-trichloropropane-d5 (TCP-d5) was used at 25 ppt concentration level and calibration was performed for both TCP and DBCP in the range of 1 to 25 ppt.

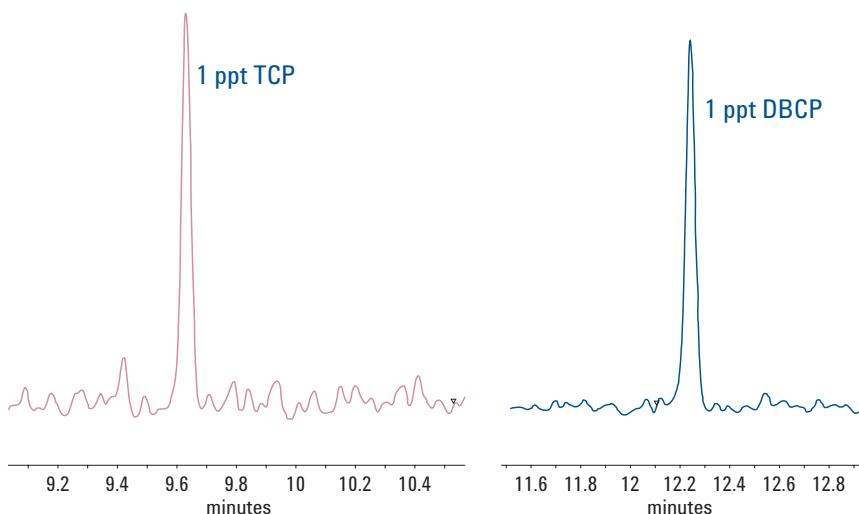


Figure 2. 1 ppt of TCP (product ion plot m/z 39) and 1 ppt DBCP (product ion plot m/z 45) from EI/MS/MS measurement. 1 ppt represents the lowest calibration level and was used for the MDL studies

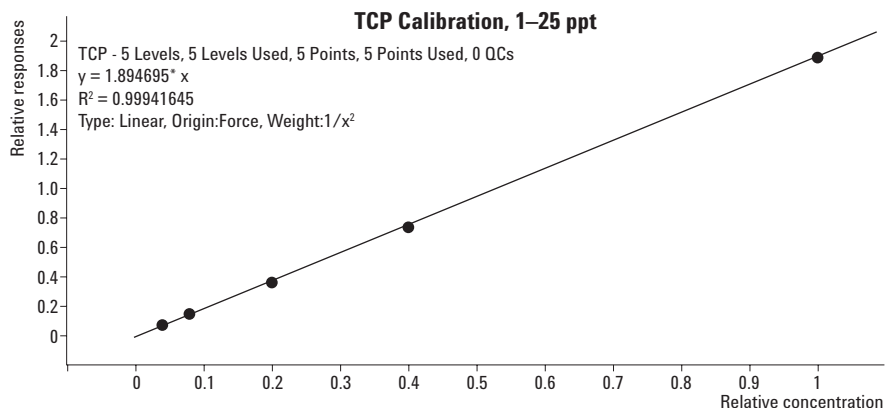


Figure 3. Calibration ranging from 1–25 ppt was performed for both analytes. The correlation coefficient for TCP was 0.999 and for DBCP was 0.989. These values represent the linearity of both the sample concentration process and the instrument response.

The MDL-LOQ-LOD levels were statistically determined by 9-replicate injections of 1ppt level water samples, using the 99% confidence level.

| Analyte | Rt minutes | Average conc. ppt | Concentration %RSD | MDL ppt | LOQ ppt | LOD ppt |
|---------|------------|-------------------|--------------------|---------|---------|---------|
| TCP     | 9.64       | 1.0299            | 2.5                | 0.0818  | 0.2604  | 0.0781  |
| DBCP    | 12.29      | 1.0112            | 2.3                | 0.0738  | 0.2347  | 0.0704  |

MDL values of less than 0.1 ppt were obtained for both analytes. MS/MS MDLs are 300–500 fold lower than the ones obtained by full scan 524 series methods and seven times lower than the Public Health Goal of 0.7 ppt.

A sensitive, precise and accurate method is presented for the ultra low level detection of 1,2,3-trichloropropane and 1,2-dibromo-3-chloropropane in water. The optimized concentrator and GC conditions along with the selectivity of MS/MS allowed sub-ppt detection levels for both TCP and DBCP.

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Published in USA, July 10, 2012  
5990-9526EN



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