BEYOND MEASURE

SCION INSTRUMENTS

Determination of 1,4-Dioxane in Water

Application Note

INTRODUCTION

1,4-Dioxane is a synthetic industrial chemical stabiliser used for many different purposes such as paint strippers, greases and waxes. Historically, 90% of all 1,4-Dioxane was used for the transport of chlorinated hydrocarbons in aluminium containers[1].

This highly soluble clear ether does not readily bind to soils therefore it can easily leach into groundwater resulting in contamination of drinking water. Contamination of water supplies is vast in the USA with dioxane levels ranging from 2 ppb to over 11,000 ppb being detected at 67 different sites1. Critically, over 34 of these different locations have been deemed a national priority for the release of the contaminant/hazardous substance into the drinking water supply[2]. Due to being resistant in nature, 1,4-Dioxane does not undergo natural bio-degradation processes.

The United States Environmental Protection Agency (US EPA) classified 1,4-Dioxane as a likely carcinogenic to humans with common side effects including irritation to eyes, nose and throat with longer effects being liver and kidney damage[1].

Federal screening levels and state health-based drinking water guidance values have been established however as of yet, no federal law has been determined. The

guideline range is from 0.25 ppb to 77 ppb, with the average contamination ranging between 3-6ppb[1].

EXPERIMENTAL

Instrumentation: Teledyne Tekmar Atomx XYZ Purge and Trap couple with a SCION Single Quad GC-MS

Software: SCION Mass Spectrometry Work Station

The analytical conditions of the GC-MS can be found in Table 1 whereas Figure 1 shows the instrumentation used.

1,4-Dioxane is a synthetic industrial chemical stabiliser used.

Table 1. Analytical Conditions of GC-MS

Conditions	
Injector	S/SL at 200˚C Split 50mL/min
Atomx Sample Temp	30˚C
Atomx Trap	#9
Sample Sweep Time	0.25 min
Purge Time	1 min
Desorb Time	1 min
Columns	30m x 0.25mm x 1.4µm (SCION624-MS)
Oven Conditions	40˚C Hold 2 Minutes 100˚C at 10˚C 200˚C at 30˚C Hold 4 minutes
Carrier	Helium 1mL/min
MS	SIM Method
Peak Identification	1,4- Dioxane: m/z 88

Table 2. Expected and actual values, peak area and levels associated with spiked calibrators.

Expected Value (ppb)	Actual Value (ppb)	Area	Recovery (%)	Level
0.30	0.292	57027	97	6
0.50	0.521	90774	104	5
1.0	1.217	152159	122	4
2.0	2.437	303620	122	3
3.0	3.120	332391	104	2
6.0	6.143	642293	102	1

Fig 1. Atomx XYZ Purge and Trap System with SCION 456 Single Quad MS

High purity water was gravimetrically spiked with low level concentrations of 1,4-Dioxane. Since standards were prepared with a concentration range of 0.3 ppb to 6 ppb, with the addition of fluorobenzene as an internal standard. Samples were prepared using the Atomx Sparge 5mL vessel with no heating unit installed on the purge and trap system.

Single Ion Monitoring (SIM) was used to identify m/z 88, the quantifier ion of 1,4-Dioxane.

RESULTS

The results shown in Table 2 were generated from the six analysed standards of 1,4-Dioxane. These values were used to form the calibration curve with an R^2 of 0.999 (Figure 2).

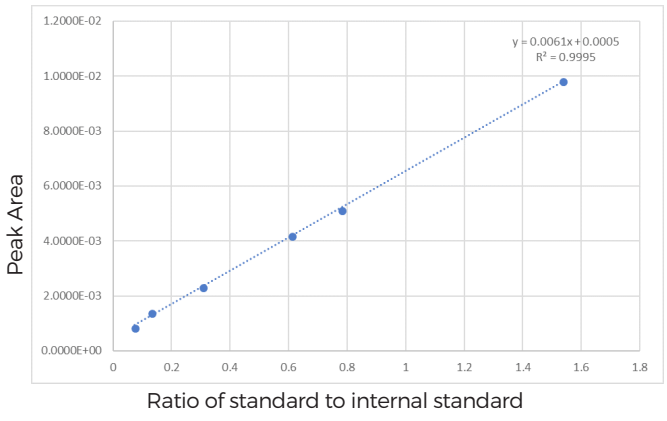
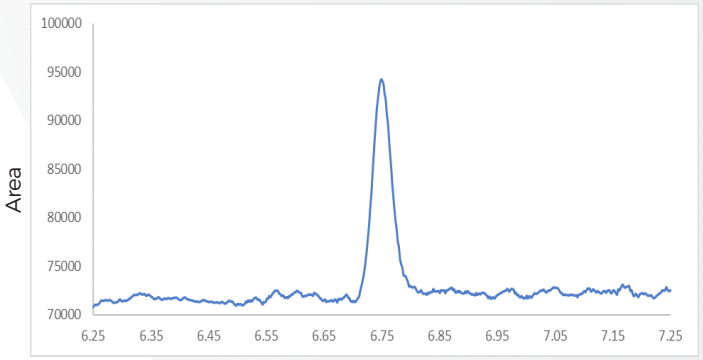


Fig 3. Chromatogram m/z 88 of 1,4 - Dioxane

Fluorobenzene, the internal standard used and 1,4-Dioxane have a retention time of 5.94 minutes and 6.75 minutes respectively, making this application time efficient. Figure 3 shows the extracted ion chromatogram of 1,4-Dioxane at 0.3 ppb using m/z 88.



Although the limit of detection (LOD) was not tested, the lowest standard of 0.3ppb yielded a S/N (RMS) of 11, this indicating that the LOD would be considerably lower.

DISCUSSION

Using a highly sensitive, automated SCION GC-MS (SQ) coupled with the Teledyne Tekmar Atomx XYZ Purge and Trap, it was possible to detect low level concentrations of 1,4-Dioxane in drinking water. The simple yet reliable method demonstrates excellent sensitivity with low detection limits of 0.3 ppb being easily quantified and distinguishable from the baseline. It is possible to increase the sensitivity of the system through the addition of a heating unit on the Atomx, which would also allow the LOD to be determined.

REFERENCES

[1] 1, 4-Dioxane Fact Sheet: Support Document". OPPT Chemical Fact Sheets. United States Environmental Protection Agency. November 2017

[2] United Stated Environmental Protection Agency. 2018. National Priorities List. [ONLINE] Available at: https://www.epa.gov/superfund/superfund-national-priorities-list-npl. [Accessed 29 May 2018].

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