



Developing a Consensus Test Method for Measuring Volatile Organic Compounds (VOCs) in Water utilizing Headspace Analysis with Gas Chromatography and Mass Spectrometry (Headspace GC/MS)

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Headspace Cold Trap sampling introduction for the extraction of VOCs in water is an alternative to the use of a Purge and Trap aqueous extraction system.

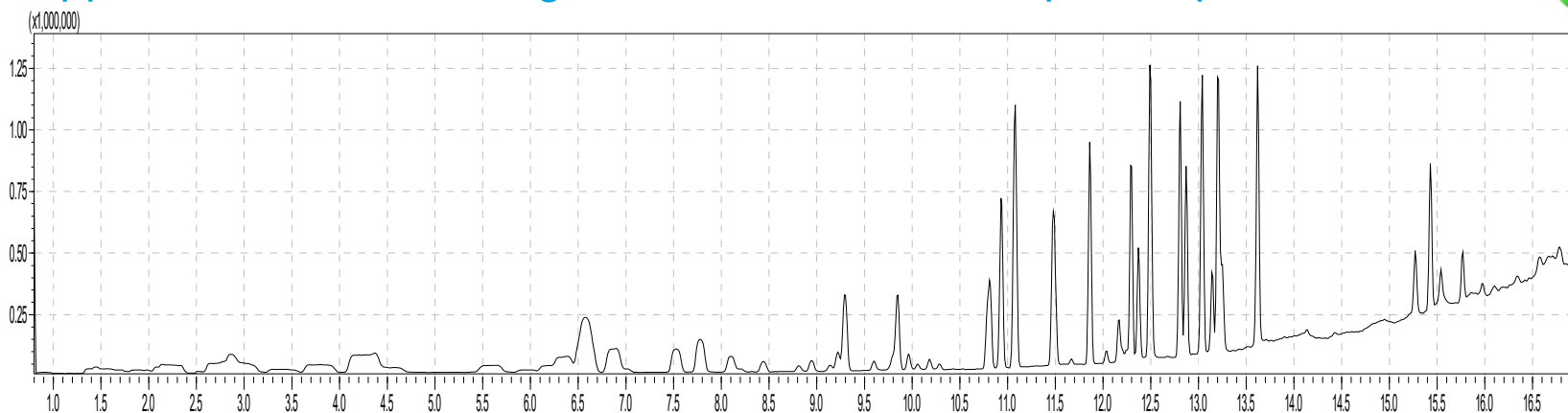


Headspace Equipment Sample Introduction Configuration Options.

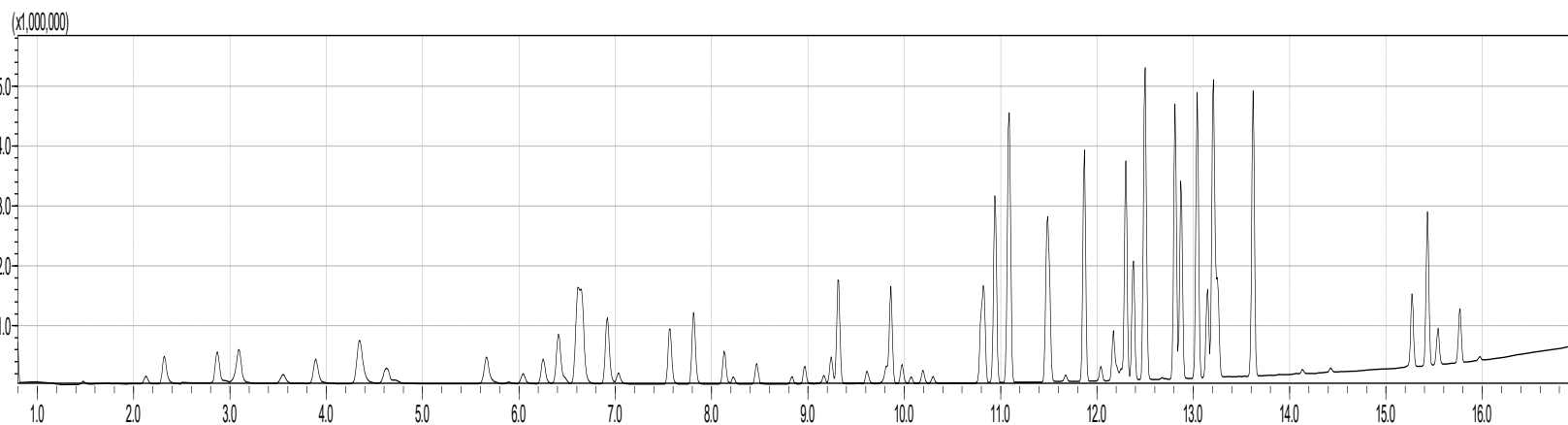
- **Sample Loop** - A Fixed volume of sample headspace introduced directly to GCMS system.
- **Cold Trap** - A portion of the sample headspace is concentrated on to the trap, and then is introduced to the GCMS system.



40 ppb Total Ion Chromatogram Standard with Sample Loop Introduction



40 ppb Total Ion Chromatogram Standard with Sample Cold Trap Introduction





Cold Trap Advantages over Loop

- Allows for lower detection limits in a similar range to a purge and trap system.
- Allows for sharper analyte peak separation.



Compounds Evaluated

| | | | |
|--------------------------|----------------------------|----------------------------|-----------------------------|
| Dichlorodifluoromethane | Dibromofluoromethane (SUR) | 1,3-dichloropropane | tert-Butylbenzene |
| Chloromethane | Carbon Tetrachloride | 2-Hexanone | 1,3,5-Trimethylbenzene |
| Vinyl chloride | 1,1,1-trichloroethane | Dibromochloromethane | 1,2,4-Trimethylbenzene |
| Bromomethane | Pentafluorobenzene (IS) | 1,2-Dibromoethane | 1,3-Dichlorobenzene |
| Chloroethane | 1,1-dichloropropene | Chlorobenzene | p-Isopropyltoluene |
| Trichlorofluoromethane | Benzene | Chlorobenzene-d5 (IS) | 1,4-Dichlorobenzene-D4 (IS) |
| 1,1-dichloroethene | 1,2-Dichloroethane | Ethylbenzene | 1,4-Dichlorobenzene |
| Carbon disulfide | 1,4-difluorobenzene (SUR) | 1,1,1,2-Tetrachloroethane | n-Butyllbenzene |
| Acetone | Trichloroethene | m p-Xylene | sec-Butylbenzene |
| Methylene chloride | 1,2-Dichloropropane | o-Xylene | 1,2-Dichlorobenzene |
| Acrylonitrile | Dibromomethane | Bromoform | 1,2-Dibromo-3-chloropropane |
| trans-1,2-Dichloroethene | Bromodichloromethane | Styrene | 1,2,4-Trichlorobenzene |
| Vinyl Acetate | 2-chloroethylvinyl ether | Isopropylbenzene | Hexachlorobutadiene |
| n-Hexane | cis-1,3-dichloropropene | 4-Bromofluorobenzene (SUR) | Naphthalene |
| 1,1-dichloroethane | 4-methyl-2-pentanone | 1,1,2,2-Tetrachloroethane | 1,2,3-Trichlorobenzene |
| 2-Butanone | Toluene-D8 (SUR) | Bromobenzene | |
| 2,2-dichloropropane | Toluene | 1,2,3-Trichloropropane | |
| cis-1,2-Dichloroethene | trans-1,3-Dichloropropene | n-Propylbenzene | |
| Bromochloromethane | 1,1,2-trichloroethane | 2-Chlorotoluene | |
| Chloroform | Tetrachloroethene | 4-Chlorotoluene | |

Equipment and Consumables



Equipment:

- Shimadzu GC-2010 Plus/MS-QP2020
- Shimadzu HS-20 series equipped with cold trap

Consumables

- GC Column - RXI-624Sil MS 20 m x 0.18 x 1 um
- Headspace Trap – Carboxen[®] adsorbent /Carbosieve[®] adsorbent

Carboxen, Carbosieve and Carbopack are trademarks of Sigma-Aldrich Co.



Method Parameters



| Head space Parameter | | GC Parameters | | Mass Spec Parameters | |
|-------------------------------|------------|------------------|------------------------|---|-----|
| Collection mode loop/Trap: | Trap | Flow Control: | Linear velocity | Ion Source Temp: 200 °C | |
| Oven temperature: | 65 °C | Pressure: | 9.8 psi | Interface Temp: 230 °C | |
| Sample Line Temperature: | 75 °C | Total flow: | 5.5 mL/min | Solvent Cut Time: 0.8 min | |
| Transfer Line Temperature: | 120 °C | Column Flow: | 0.5 mL/min | Microscan width: 0 u | |
| Trap Cooling Temperature: | - 28 °C | Linear Velocity: | 31.1 cm/sec | Detector Voltage: 0 relative to tuning report | |
| Trap Desorb Temperature: | 250 °C | Split Ratio: | 1:10 | Scan Mode | SIM |
| Trap Equilibrium Temperature: | - 28 °C | Purge Flow: | 0 | | |
| Shaking Level: | 3 | Oven Ramp: | 35 °C hold 5 min | | |
| Multiinjection Count: | 1 | | 35 °C to 240 °C | | |
| | | | 15 °C/min hold 0.5 min | | |
| Pressurizing Gas Pressure: | 48 psi | Total Run Time: | 19.17 min | | |
| Dry Purge Gas Pressure: | 7.3 psi | | | | |
| Equilibrating Time: | 30 min | | | | |
| Pressurizing Time: | 2.00 min | | | | |
| Pressure Equilibration Time: | 0.10 min | | | | |
| Load Time: | 5.00 min | | | | |
| Load Equilibration Time: | 0.10 min | | | | |
| Dry Purge Time: | 0.50 min | | | | |
| Injection Time: | 6.00 min | | | | |
| Needle Flush Time: | 3.00 min | | | | |
| GC Cycle Time: | 30 minutes | | | | |



Results



Calibration levels and Curve Fit

| | std 1 | std 2 | std 3 | std 4 | std 5 | std 6 | std 7 | std 8 | std 9 | std 10 | std 11 | Curve | R2 or RF(% RSD) |
|--|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|-----------|-----------------|
| | * 0.5 ppb | * 1 ppb | * 1.5 ppb | * 2(ppb) | * 5 ppb | * 7 ppb | * 10 ppb | * 15 ppb | * 20 ppb | * 30 ppb | * 40 ppb | Fit | |
| | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | | |
| Dichlorodifluoromethane | 0.53 | 1.04 | 1.55 | 2.06 | 4.75 | 6.24 | | | | | | Mean RF | 6.44 |
| Chloromethane | 0.45 | 1.25 | 1.59 | 2.18 | 5.27 | 6.78 | 9.42 | 15.4 | | | | Quadratic | 0.99 |
| Vinyl chloride | | 1.16 | 1.65 | 2.10 | 5.00 | 6.31 | 8.51 | | | | | Quadratic | 0.99 |
| Bromomethane | 0.46 | 1.03 | 1.65 | 2.47 | 5.18 | 6.66 | 9.14 | 14.1 | 17.7 | | | Mean RF | 11.3 |
| Chloroethane | 0.49 | 1.05 | 1.59 | 2.05 | 5.31 | 7.15 | 9.94 | 14.5 | 20.2 | 28.0 | 36.1 | Mean RF | 5.16 |
| Trichlorofluoromethane | 0.48 | 1.01 | 1.55 | 2.01 | 5.22 | 7.19 | 10.0 | 14.9 | 20.5 | 29 | 37.5 | Mean RF | 3.42 |
| 1,1-dichloroethene | 0.58 | 1.09 | 1.59 | 2.02 | 5.04 | 6.86 | 9.56 | 14.2 | 19.5 | 27.6 | 36.1 | Mean RF | 7.69 |
| Carbon disulfide | 0.60 | 1.09 | 1.60 | 2.04 | 4.99 | 6.78 | 9.45 | 14.1 | 19.3 | 27.3 | 36.0 | Mean RF | 8.94 |
| Acetone | 0.41 | 1.15 | 1.56 | 1.80 | 4.83 | 6.95 | 10.1 | 15.7 | 21.0 | 29.6 | 39.5 | Linear | 0.99 |
| Methylene chloride | 0.61 | 1.07 | 1.6 | 2.08 | 5.03 | 6.73 | 9.61 | 14.3 | 18.8 | 26.7 | 36.0 | Mean RF | 9.38 |
| Acrylonitrile | 0.51 | 0.98 | 1.44 | 1.88 | 4.68 | 7.66 | 8.54 | 15.6 | 22.3 | 32.8 | 39.0 | Mean RF | 8.06 |
| trans-1,2-Dichloroethene | 0.57 | 1.07 | 1.58 | 2.02 | 4.98 | 6.9 | 9.41 | 14.5 | 19.7 | 27.6 | 37.3 | Mean RF | 6.52 |
| Vinyl Acetate | 0.49 | 1.12 | 1.36 | 2.11 | 4.80 | 6.36 | | | | | | Mean RF | 8.49 |
| n-Hexane | | | 1.63 | 1.95 | 4.91 | 6.83 | 9.6 | 14.5 | 20.8 | 30.2 | 40.4 | Mean RF | 4.12 |
| 1,1-dichloroethane | 0.42 | 0.95 | 1.49 | 1.97 | 5.31 | 7.20 | 10.2 | 15.5 | 21.1 | 30.2 | 40.9 | Mean RF | 6.03 |
| 2-Butanone | 0.62 | 1.17 | 1.61 | 1.96 | 4.94 | 6.31 | 9.07 | 13.9 | 18.8 | 27.0 | 38.6 | Mean RF | 11.7 |
| 2,2-dichloropropane | 0.54 | 1.21 | 1.61 | 2.16 | 5.17 | 6.83 | 9.39 | 13.9 | 18.2 | 26.2 | 36.3 | Mean RF | 10.3 |
| cis-1,2-Dichloroethene | 0.53 | 1.05 | 1.55 | 2.00 | 4.98 | 6.81 | 9.65 | 14.7 | 19.9 | 28.7 | 39.4 | Mean RF | 3.51 |
| Bromochloromethane | 0.56 | 1.06 | 1.59 | 2.01 | 5.08 | 6.76 | 9.67 | 14.6 | 19.4 | 27.8 | 37.9 | Mean RF | 5.80 |
| Chloroform | 0.47 | 1.01 | 1.54 | 2.02 | 5.08 | 6.99 | 9.81 | 15.1 | 20.6 | 29.6 | 40.3 | Mean RF | 2.70 |
| Dibromofluoromethane (SUR) 30 ppb | 31.5 | 31.5 | 30.0 | 31.2 | 30.5 | 29.8 | 27.9 | 30.9 | 29.0 | 29.5 | 29.8 | Mean RF | 3.80 |
| Carbon Tetrachloride | 0.62 | 1.05 | 1.49 | 2.02 | 5.08 | 7.00 | 9.69 | 14.8 | 20.4 | 29.7 | 40.1 | Linear | 0.99 |

*Calibration level concentrations with the exception of internal standards, surrogates, and m p-Xylene ** concentrations double since results are m-xylene and p-xylene combined.

Calibration levels and Curve Fit



| | std 1 | std 2 | std 3 | std 4 | std 5 | std 6 | std 7 | std 8 | std 9 | std 10 | std 11 | Curve | R2 or RF(% RSD) |
|---|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|---------|-----------------|
| | * 0.5 ppb | * 1 ppb | * 1.5 ppb | * 2(ppb | * 5 ppb | * 7 ppb | * 10 ppb | * 15 ppb | * 20 ppb | * 30 ppb | * 40 ppb | Fit | |
| | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | | |
| 1,1,1-trichloroethane | 0.47 | 0.99 | 1.53 | 1.98 | 5.13 | 7.06 | 9.85 | 15.0 | 20.8 | 29.9 | 40.5 | Mean RF | 2.80 |
| Pentafluorobenzene (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | |
| 1,1-dichloropropene | 0.63 | 1.11 | 1.64 | 2.07 | 5.02 | 6.89 | 9.61 | 14.6 | 20.6 | | | Linear | 0.99 |
| Benzene | 0.60 | 1.10 | 1.60 | 2.00 | 4.87 | 6.55 | 9.27 | 14.1 | 19.4 | 28.0 | 38.7 | Mean RF | 8.56 |
| 1,2-Dichloroethane | 0.47 | 1.03 | 1.51 | 2.04 | 5.18 | 6.94 | 10.0 | 15.2 | 20.4 | 28.8 | 39.1 | Mean RF | 3.00 |
| 1,4-difluorobenzene (SUR) 30 ppb | 30.7 | 30.6 | 30.6 | 30.8 | 30.5 | 30.1 | 30.4 | 30.1 | 29.6 | 29.3 | 29.4 | Mean RF | 2.68 |
| Trichloroethene | 0.59 | 1.05 | 1.62 | 1.93 | 4.85 | 6.65 | 10.5 | 13.4 | 19.9 | 27.7 | 38.0 | Mean RF | 8.34 |
| 1,2-Dichloropropane | 0.5 | 1.01 | 1.54 | 2 | 5.11 | 6.90 | 9.79 | 15.0 | 20.4 | 29.0 | 40.0 | Mean RF | 1.82 |
| Dibromomethane | 0.53 | 1.08 | 1.57 | 2.04 | 5.07 | 6.76 | 9.73 | 14.6 | 19.7 | 28.1 | 38.1 | Mean RF | 4.56 |
| Bromodichloromethane | 0.47 | 1.00 | 1.52 | 1.99 | 5.13 | 6.88 | 9.86 | 15.1 | 20.6 | 29.8 | 40.9 | Mean RF | 2.50 |
| 2-chloroethylvinyl ether | 0.43 | 0.95 | 1.51 | 1.93 | 5.39 | 7.30 | 11.0 | 16.4 | | | | Mean RF | 8.06 |
| cis-1,3-dichloropropene | 0.45 | 0.97 | 1.48 | 1.94 | 5.03 | 6.85 | 9.92 | 15.3 | 21.0 | 31.2 | 44.1 | Mean RF | 5.42 |
| 4-methyl-2-pentanone | 0.44 | 0.91 | 1.38 | 1.86 | 4.93 | 6.8 | 9.56 | 15.4 | 21.9 | 34.1 | 47.1 | Mean RF | 9.81 |
| Toluene-D8 (SUR) 10 ppb | 9.85 | 9.91 | 9.92 | 9.92 | 9.93 | 10.0 | 10.0 | 10.1 | 10.2 | 10.2 | 10.1 | Mean RF | 0.99 |
| Toluene | 0.54 | 1.06 | 1.59 | 1.94 | 4.99 | 6.94 | 9.75 | 15.2 | | | | Linear | 0.99 |
| trans-1,3-Dichloropropene | 0.44 | 0.95 | 1.45 | 1.92 | 5.04 | 7.00 | 9.87 | 15.3 | 21.3 | 31.5 | 44.0 | Mean RF | 5.97 |
| 1,1,2-trichloroethane | 0.54 | 1.07 | 1.59 | 2.00 | 4.96 | 6.78 | 9.5 | 14.4 | 19.9 | 28.5 | 38.9 | Mean RF | 4.93 |
| Tetrachloroethene | 0.57 | 1.06 | 1.52 | 1.90 | 4.69 | 6.60 | 9.13 | 14.1 | 20.5 | 30.7 | 42.3 | Mean RF | 6.84 |
| 1,3-dichloropropane | 0.44 | 0.99 | 1.45 | 1.96 | 5.01 | 6.95 | 9.85 | 15.3 | 21.4 | 31.0 | 43.0 | Mean RF | 5.21 |
| 2-Hexanone | 0.49 | 0.92 | 1.28 | 1.85 | 4.78 | 6.64 | 9.48 | 14.8 | 21.7 | 35.1 | 49.1 | Mean RF | 11.4 |
| Dibromochloromethane | 0.46 | 1.02 | 1.51 | 1.95 | 4.97 | 6.91 | 9.72 | 15.1 | 21.0 | 30.6 | 41.8 | Mean RF | 3.67 |
| 1,2-Dibromoethane | 0.47 | 0.99 | 1.51 | 1.97 | 5.07 | 6.95 | 9.77 | 15.2 | 20.9 | 30.4 | 41.3 | Mean RF | 2.97 |
| Chlorobenzene | 0.65 | 1.16 | 1.64 | 2.05 | 5.01 | 6.79 | 9.49 | 14.7 | 20.6 | | | Linear | 0.99 |
| Chlorobenzene-d5 (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | |
| Ethylbenzene | 0.48 | 0.94 | 1.39 | 1.80 | 4.74 | 6.75 | 9.6 | 15.3 | 22.1 | 33.5 | 46.5 | Mean RF | 8.82 |
| 1,1,1,2-Tetrachloroethane | 0.51 | 1.08 | 1.61 | 2.04 | 5.09 | 6.96 | 9.43 | 14.4 | 20.0 | 28.4 | 38.1 | Mean RF | 4.78 |
| m p-Xylene ** | 0.98 | 1.95 | 2.95 | 3.88 | 10.13 | 14.3 | 19.8 | 30.5 | 42.4 | 59.9 | 79.2 | Mean RF | 2.61 |

*Calibration level concentrations with the exception of internal standards, surrogates, and m p-Xylene ** concentrations double since results are m-xylene and p-xylene combined.



Calibration levels and Curve Fit

| | std 1 | std 2 | std 3 | std 4 | std 5 | std 6 | std 7 | std 8 | std 9 | std 10 | std 11 | Curve | R2 or RF(% RSD) |
|---|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|---------|-----------------|
| | * 0.5 ppb | * 1 ppb | * 1.5 ppb | * 2(ppb) | * 5 ppb | * 7 ppb | * 10 ppb | * 15 ppb | * 20 ppb | * 30 ppb | * 40 ppb | Fit | |
| | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | calculated (ppb) | | |
| o-Xylene | 0.50 | 0.98 | 1.49 | 1.98 | 5.05 | 7.04 | 9.87 | 15.2 | 20.9 | 29.6 | 39.0 | Mean RF | 1.94 |
| Bromoform | 0.61 | 1.12 | 1.63 | 2.11 | 5.15 | 6.87 | 9.35 | 14.1 | 18.9 | 25.8 | 33.2 | Mean RF | 11.5 |
| Styrene | 0.48 | 0.96 | 1.44 | 1.89 | 5.11 | 7.20 | 10.2 | 15.8 | 21.5 | 30.2 | 39.5 | Mean RF | 4.24 |
| Isopropylbenzene | 0.47 | 0.93 | 1.43 | 1.86 | 5.14 | 7.29 | 10.1 | 15.7 | 22.0 | 30.9 | 40.1 | Mean RF | 5.76 |
| 4-Bromofluorobenzene (SUR) 10 ppb | 11.2 | 10.9 | 10.9 | 10.9 | 10.7 | 10.6 | 10.4 | 10.1 | 9.7 | 9.17 | 8.66 | Mean RF | 13.0 |
| 1,1,2,2-Tetrachloroethane | 0.43 | 1.22 | 1.51 | 2.22 | 5.39 | 7.20 | 7.6 | 16.5 | 19.9 | 30.1 | 39.9 | Linear | 0.99 |
| Bromobenzene | 0.65 | 1.17 | 1.68 | 2.09 | 5.00 | 6.78 | 9.19 | 13.8 | 18.2 | 25.1 | 32.6 | Mean RF | 14.7 |
| 1,2,3-Trichloropropane | 0.55 | 1.14 | 1.63 | 2.05 | 5.21 | 6.86 | 9.67 | 14.4 | 19.2 | 26.1 | 34.5 | Mean RF | 9.11 |
| 2-Chlorotoluene | 0.51 | 1.03 | 1.55 | 2.00 | 5.18 | 7.10 | 9.85 | 14.9 | 20.3 | 28.3 | 36.8 | Mean RF | 3.84 |
| 4-Chlorotoluene | 0.47 | 0.96 | 1.48 | 1.92 | 5.13 | 7.15 | 9.91 | 15.4 | 21.3 | 30.3 | 40.5 | Mean RF | 3.72 |
| tert-Butylbenzene | 0.44 | 0.91 | 1.4 | 1.83 | 5.11 | 7.27 | 10.1 | 15.7 | 22.3 | 32.1 | 42.3 | Mean RF | 7.68 |
| 1,3,5-Trimethylbenzene | 0.43 | 0.91 | 1.39 | 1.83 | 5.06 | 7.20 | 10.1 | 16.0 | 22.4 | 32.4 | 42.6 | Mean RF | 8.46 |
| 1,2,4-Trimethylbenzene | 0.46 | 0.92 | 1.43 | 1.89 | 5.21 | 7.36 | 10.2 | 15.7 | 21.7 | 30.5 | 39.5 | Mean RF | 5.56 |
| 1,3-Dichlorobenzene | 0.42 | 0.96 | 1.48 | 1.94 | 5.23 | 7.42 | 10.2 | 15.7 | 21.8 | 30.0 | 39.1 | Mean RF | 6.66 |
| p-Isopropyltoluene | 0.43 | 0.89 | 1.37 | 1.80 | 5.06 | 7.24 | 10.2 | 16.0 | 22.8 | 32.6 | 42.7 | Mean RF | 9.22 |
| 1,4-Dichlorobenzene-D4 (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | |
| 1,4-Dichlorobenzene | 0.55 | 1.1 | 1.57 | 2.03 | 5.05 | 6.88 | 9.57 | 14.5 | 19.6 | 27.6 | 36.8 | Mean RF | 6.34 |
| n-Butylbenzene | 0.47 | 0.91 | 1.37 | 1.77 | 4.96 | 7.13 | 9.94 | 15.5 | 22.4 | 33.0 | 43.8 | Mean RF | 8.22 |
| sec-Butylbenzene | 0.44 | 0.91 | 1.41 | 1.86 | 5.17 | 7.38 | 10.2 | 15.8 | 22.3 | 32.0 | 40.0 | Mean RF | 7.55 |
| 1,2-Dichlorobenzene | 0.57 | 1.04 | 1.51 | 1.91 | 4.82 | 6.66 | 9.48 | 14.6 | 20.5 | 29.7 | 40.6 | Mean RF | 5.65 |
| 1,2-Dibromo-3-chloropropane | 0.49 | 0.96 | 1.27 | 1.76 | 5.24 | 7.05 | 9.85 | 15.4 | 21.0 | 29.8 | 39.5 | Linear | 0.99 |
| 1,2,4-Trichlorobenzene | 0.61 | 1.15 | 1.60 | 2.00 | 4.90 | 6.68 | 9.27 | 14.1 | 19.3 | 27.0 | 36.0 | Mean RF | 10.5 |
| Hexachlorobutadiene | 0.54 | 1.07 | 1.60 | 1.98 | 5.02 | 6.96 | 9.36 | 14.2 | 20.1 | 29.0 | 37.8 | Mean RF | 5.10 |
| Naphthalene | 0.66 | 1.15 | 1.54 | 1.90 | 4.91 | 6.77 | 9.68 | 15.0 | 20.7 | 29.6 | 40.1 | Linear | 0.99 |
| 1,2,3-Trichlorobenzene | 0.60 | 1.13 | 1.61 | 2.01 | 4.93 | 6.78 | 9.42 | 14.1 | 19.4 | 26.9 | 35.5 | Mean RF | 9.78 |

* Calibration level concentrations with the exception of internal standards, surrogates, and m p-Xylene ** concentrations double since results are m-xylene and p-xylene combined.

MDLs



| | MDL 1 | MDL 2 | MDL 3 | MDL 4 | MDL 5 | MDL 6 | MDL 7 | MDL 8 | MDL 9 | Mean | Mean Recovery | STDEV | RSD | MDL |
|--|---------|---------|---------|---------|---------|---------|---------|---------|---------|------|---------------|-------|------|-------|
| | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | ppb | % | | % | ppb |
| Dichlorodifluoromethane | 1.96 | 2.22 | 2.47 | 2.42 | 2.34 | 2.41 | 2.33 | 2.47 | 2.45 | 2.34 | 117 | 0.164 | 7.02 | 0.516 |
| Chloromethane | 1.85 | 2.00 | 3.45 | 2.19 | 1.91 | 2.16 | 1.84 | 2.10 | 1.89 | 2.15 | 108 | 0.503 | 23.4 | 1.581 |
| Vinyl chloride | 2.29 | 2.95 | 3.01 | 3.39 | 3.08 | 3.21 | 3.19 | 3.18 | 2.94 | 3.03 | 151 | 0.311 | 10.3 | 0.977 |
| Bromomethane | 2.20 | 2.02 | 2.36 | 2.52 | 2.34 | 2.37 | 2.24 | 2.29 | 2.27 | 2.29 | 115 | 0.137 | 5.99 | 0.431 |
| Chloroethane | 2.01 | 1.97 | 2.06 | 2.03 | 2.01 | 2.05 | 2.09 | 2.09 | 2.13 | 2.05 | 102 | 0.050 | 2.42 | 0.156 |
| Trichlorofluoromethane | 1.73 | 1.86 | 1.97 | 1.92 | 1.91 | 1.95 | 1.99 | 2.03 | 2.06 | 1.94 | 96.8 | 0.099 | 5.09 | 0.309 |
| 1,1-dichloroethene | 1.83 | 1.89 | 1.98 | 1.93 | 1.93 | 1.97 | 2.01 | 2.04 | 2.07 | 1.96 | 98.1 | 0.075 | 3.83 | 0.236 |
| Carbon disulfide | 1.88 | 1.89 | 1.97 | 1.92 | 1.89 | 1.92 | 1.97 | 1.98 | 2.02 | 1.94 | 96.9 | 0.049 | 2.53 | 0.154 |
| Acetone | 1.81 | 1.83 | 1.90 | 2.14 | 1.90 | 1.90 | 1.67 | 1.66 | 1.73 | 1.84 | 91.9 | 0.148 | 8.05 | 0.465 |
| Methylene chloride | 2.26 | 1.99 | 2.12 | 2.01 | 2.02 | 2.02 | 2.09 | 2.12 | 2.16 | 2.09 | 104 | 0.088 | 4.21 | 0.276 |
| Acrylonitrile | 1.95 | 2.27 | 2.43 | 2.35 | 2.31 | 2.30 | 2.38 | 2.40 | 2.42 | 2.31 | 116 | 0.147 | 6.35 | 0.461 |
| trans-1,2-Dichloroethene | 1.99 | 1.93 | 1.98 | 1.94 | 1.89 | 1.90 | 1.96 | 1.99 | 2.02 | 1.96 | 97.8 | 0.044 | 2.25 | 0.138 |
| Vinyl Acetate | 3.08 | 2.63 | 2.76 | 2.54 | 2.51 | 2.27 | 2.49 | 2.52 | 2.56 | 2.60 | 130 | 0.223 | 8.59 | 0.700 |
| n-Hexane | 1.49 | 1.60 | 1.66 | 1.61 | 1.59 | 1.61 | 1.64 | 1.65 | 1.67 | 1.61 | 80.7 | 0.054 | 3.35 | 0.170 |
| 1,1-dichloroethane | 2.26 | 2.02 | 2.09 | 2.01 | 1.98 | 2.06 | 2.04 | 2.05 | 2.09 | 2.07 | 103 | 0.081 | 3.92 | 0.254 |
| 2-Butanone | 2.31 | 1.93 | 2.03 | 1.91 | 1.86 | 1.80 | 1.87 | 1.95 | 1.98 | 1.96 | 98.0 | 0.148 | 7.55 | 0.464 |
| 2,2-dichloropropane | 3.51 | 3.01 | 3.02 | 2.91 | 2.81 | 2.63 | 2.79 | 2.67 | 2.64 | 2.89 | 144 | 0.276 | 9.57 | 0.868 |
| cis-1,2-Dichloroethene | 2.21 | 1.97 | 2.04 | 1.97 | 1.93 | 1.92 | 1.97 | 1.98 | 2.02 | 2.00 | 100 | 0.087 | 4.35 | 0.273 |
| Bromochloromethane | 2.35 | 2.00 | 2.07 | 2.01 | 2.03 | 1.97 | 2.07 | 2.05 | 1.98 | 2.06 | 103 | 0.115 | 5.59 | 0.361 |
| Chloroform | 2.30 | 2.08 | 2.16 | 2.10 | 2.06 | 2.08 | 2.13 | 2.13 | 2.17 | 2.13 | 107 | 0.072 | 3.40 | 0.228 |
| Dibromofluoromethane (SUR) 30 ppb | 35.7 | 30.5 | 30.6 | 30.8 | 31.0 | 29.8 | 30.4 | 30.6 | 30.9 | 31.1 | 104 | 1.73 | 5.56 | |
| Carbon Tetrachloride | 2.03 | 2.02 | 2.19 | 2.07 | 2.09 | 2.03 | 1.97 | 2.17 | 2.15 | 2.08 | 104 | 0.076 | 3.65 | 0.238 |
| 1,1,1-trichloroethane | 2.05 | 1.99 | 2.07 | 2.01 | 1.99 | 1.99 | 2.05 | 2.06 | 2.07 | 2.03 | 102 | 0.036 | 1.75 | 0.112 |
| Pentafluorobenzene (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | | | | |

*Calibration level concentrations with the exception of internal standards, surrogates, and m p-Xylene ** concentrations double since results are m-xylene and p-xylene combined.

MDLs



| | MDL 1 | MDL 2 | MDL 3 | MDL 4 | MDL 5 | MDL 6 | MDL 7 | MDL 8 | MDL 9 | Mean | Mean Recovery | STDEV | RSD | MDL |
|---|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|---------------|--------------|-------------|--------------|
| | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | ppb | % | | % | ppb |
| 1,1-dichloropropene | 2.11 | 2.14 | 2.21 | 2.14 | 2.08 | 2.09 | 2.12 | 2.12 | 2.16 | 2.13 | 107 | 0.039 | 1.83 | 0.123 |
| Benzene | 2.17 | 2.00 | 2.04 | 1.99 | 1.93 | 1.96 | 2.01 | 2.02 | 2.05 | 2.02 | 101 | 0.068 | 3.36 | 0.213 |
| 1,2-Dichloroethane | 2.44 | 2.00 | 2.10 | 2.06 | 1.99 | 1.98 | 2.05 | 2.08 | 2.13 | 2.09 | 105 | 0.140 | 6.69 | 0.440 |
| 1,4-difluorobenzene (SUR) 30 ppb | 33.3 | 30.5 | 30.2 | 30.3 | 30.5 | 30.1 | 30.1 | 30.3 | 30.2 | 30.6 | 102 | 1.02 | 3.32 | |
| Trichloroethene | 2.00 | 1.98 | 1.95 | 1.89 | 1.86 | 1.93 | 1.97 | 1.97 | 2.00 | 1.95 | 97.5 | 0.048 | 2.49 | 0.152 |
| 1,2-Dichloropropane | 2.30 | 2.03 | 2.04 | 2.01 | 1.97 | 2.00 | 2.01 | 2.04 | 2.07 | 2.05 | 103 | 0.097 | 4.74 | 0.305 |
| Dibromomethane | 2.36 | 1.98 | 2.03 | 2.03 | 1.97 | 1.94 | 2.02 | 2.05 | 2.04 | 2.05 | 102 | 0.123 | 6.01 | 0.386 |
| Bromodichloromethane | 2.41 | 2.13 | 2.14 | 2.11 | 2.04 | 2.07 | 2.12 | 2.11 | 2.14 | 2.14 | 107 | 0.106 | 4.96 | 0.333 |
| 2-chloroethylvinyl ether | 2.96 | 2.15 | 2.20 | 1.92 | 2.27 | 2.05 | 2.14 | 2.09 | 1.93 | 2.19 | 110 | 0.311 | 14.2 | 0.976 |
| cis-1,3-dichloropropene | 2.63 | 2.24 | 2.25 | 2.18 | 2.13 | 2.11 | 2.18 | 2.18 | 2.18 | 2.23 | 112 | 0.156 | 7.00 | 0.490 |
| 4-methyl-2-pentanone | 2.10 | 1.97 | 2.02 | 1.84 | 1.90 | 1.84 | 1.91 | 1.91 | 1.88 | 1.93 | 96.5 | 0.086 | 4.45 | 0.270 |
| Toluene-D8 (SUR) 10 ppb | 9.39 | 9.78 | 9.81 | 9.82 | 9.82 | 9.8 | 9.74 | 9.83 | 9.81 | 9.76 | 32.5 | 0.140 | 1.43 | |
| Toluene | 1.65 | 1.78 | 1.86 | 1.85 | 1.76 | 1.81 | 1.86 | 1.87 | 1.86 | 1.81 | 90.6 | 0.072 | 3.99 | 0.227 |
| trans-1,3-Dichloropropene | 2.35 | 2.22 | 2.29 | 2.24 | 2.18 | 2.16 | 2.19 | 2.15 | 2.19 | 2.22 | 111 | 0.065 | 2.94 | 0.205 |
| 1,1,2-trichloroethane | 2.1 | 1.97 | 2.04 | 2.02 | 1.93 | 1.94 | 2.02 | 1.97 | 2.08 | 2.01 | 100 | 0.060 | 2.98 | 0.188 |
| Tetrachloroethene | 1.69 | 1.93 | 1.99 | 1.95 | 1.91 | 1.95 | 1.97 | 2.00 | 1.98 | 1.93 | 96.5 | 0.094 | 4.89 | 0.297 |
| 1,3-dichloropropane | 2.12 | 2 | 2.06 | 2.03 | 1.95 | 1.99 | 2.01 | 2.00 | 2.05 | 2.02 | 101 | 0.049 | 2.42 | 0.154 |
| 2-Hexanone | 2.16 | 2.03 | 1.96 | 1.81 | 1.99 | 1.75 | 1.91 | 1.89 | 1.82 | 1.92 | 96.2 | 0.127 | 6.57 | 0.397 |
| Dibromochloromethane | 2.12 | 1.98 | 2.09 | 2.01 | 1.97 | 2.05 | 2.03 | 2.07 | 2.08 | 2.04 | 102 | 0.051 | 2.50 | 0.160 |
| 1,2-Dibromoethane | 2.08 | 2.00 | 1.99 | 1.91 | 1.95 | 1.96 | 2.01 | 2.00 | 1.98 | 1.99 | 99.3 | 0.047 | 2.36 | 0.147 |
| Chlorobenzene | 2.09 | 2.1 | 2.19 | 2.14 | 2.08 | 2.12 | 2.13 | 2.13 | 2.16 | 2.13 | 106 | 0.035 | 1.63 | 0.109 |
| Chlorobenzene-d5 (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | | | | |
| Ethylbenzene | 1.67 | 1.8 | 1.89 | 1.82 | 1.79 | 1.84 | 1.86 | 1.87 | 1.88 | 1.82 | 91.2 | 0.068 | 3.71 | 0.212 |
| 1,1,1,2-Tetrachloroethane | 2.09 | 2.13 | 2.17 | 2.12 | 2.07 | 2.1 | 2.18 | 2.14 | 2.21 | 2.13 | 107 | 0.046 | 2.14 | 0.143 |
| m p-Xylene ** | 3.61 | 3.97 | 4.07 | 3.93 | 3.89 | 3.95 | 4.10 | 4.03 | 4.07 | 3.96 | 98.9 | 0.149 | 3.76 | 0.467 |

* Calibration level concentrations with the exception of internal standards, surrogates, and m p-Xylene ** concentrations double since results are m xylene and p-xylene combined.

MDLs



| | MDL 1 | MDL 2 | MDL 3 | MDL 4 | MDL 5 | MDL 6 | MDL 7 | MDL 8 | MDL 9 | Mean | Mean Recovery | STDEV | RSD | MDL |
|---|---------|---------|---------|---------|---------|---------|---------|---------|---------|------|---------------|-------|------|-------|
| | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | * 2 ppb | ppb | % | | % | ppb |
| o-Xylene | 1.91 | 2.02 | 2.06 | 2.02 | 1.97 | 1.99 | 2.05 | 2.07 | 2.13 | 2.02 | 101 | 0.064 | 3.14 | 0.200 |
| Bromoform | 2.37 | 2.23 | 2.31 | 2.21 | 2.17 | 2.26 | 2.29 | 2.24 | 2.3 | 2.26 | 113 | 0.060 | 2.65 | 0.188 |
| Styrene | 1.95 | 1.95 | 1.98 | 1.96 | 1.92 | 1.97 | 1.97 | 2.02 | 2.05 | 1.97 | 98.7 | 0.039 | 1.98 | 0.123 |
| Isopropylbenzene | 1.73 | 1.94 | 2.01 | 1.96 | 1.93 | 1.98 | 2.02 | 2.01 | 2.05 | 1.96 | 97.9 | 0.094 | 4.82 | 0.296 |
| 4-Bromofluorobenzene (SUR) 10 ppb | 11.1 | 10.9 | 10.8 | 10.9 | 10.9 | 10.8 | 10.9 | 10.8 | 10.8 | 10.9 | 36.3 | 0.082 | 0.75 | |
| 1,1,2,2-Tetrachloroethane | 2.63 | 2.35 | 2.52 | 2.44 | 2.39 | 2.24 | 2.42 | 2.38 | 2.41 | 2.42 | 121 | 0.109 | 4.49 | 0.341 |
| Bromobenzene | 2.09 | 2.13 | 2.16 | 2.13 | 2.03 | 2.11 | 2.17 | 2.15 | 2.17 | 2.13 | 106 | 0.045 | 2.13 | 0.142 |
| 1,2,3-Trichloropropane | 2.42 | 2.2 | 2.24 | 2.22 | 2.14 | 2.19 | 2.29 | 2.2 | 2.22 | 2.24 | 112 | 0.080 | 3.58 | 0.251 |
| 2-Chlorotoluene | 1.96 | 2.04 | 2.11 | 2.06 | 2.01 | 2.06 | 2.1 | 2.09 | 2.13 | 2.06 | 103 | 0.053 | 2.59 | 0.167 |
| 4-Chlorotoluene | 1.89 | 1.98 | 2.04 | 2 | 1.96 | 1.99 | 2.04 | 2.02 | 2.06 | 2.00 | 100 | 0.052 | 2.59 | 0.162 |
| tert-Butylbenzene | 1.65 | 1.9 | 1.98 | 1.92 | 1.89 | 1.94 | 1.98 | 1.97 | 1.99 | 1.91 | 95.7 | 0.105 | 5.51 | 0.331 |
| 1,3,5-Trimethylbenzene | 1.71 | 1.89 | 1.97 | 1.92 | 1.9 | 1.93 | 1.97 | 1.94 | 1.99 | 1.91 | 95.7 | 0.083 | 4.35 | 0.261 |
| 1,2,4-Trimethylbenzene | 1.81 | 1.96 | 2.04 | 1.98 | 1.94 | 1.97 | 2.02 | 2.01 | 2.04 | 1.97 | 98.7 | 0.071 | 3.60 | 0.223 |
| 1,3-Dichlorobenzene | 1.71 | 2.01 | 2.1 | 2.08 | 2.1 | 2.05 | 2.11 | 2.05 | 2.15 | 2.04 | 102 | 0.130 | 6.39 | 0.409 |
| p-Isopropyltoluene | 1.65 | 1.9 | 1.97 | 1.92 | 1.89 | 1.94 | 1.96 | 1.97 | 1.99 | 1.91 | 95.5 | 0.103 | 5.40 | 0.324 |
| 1,4-Dichlorobenzene-D4 (IS) 30 ppb | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | | | | | |
| 1,4-Dichlorobenzene | 2.04 | 2.08 | 2.14 | 2.11 | 2.05 | 2.08 | 2.14 | 2.12 | 2.16 | 2.10 | 105 | 0.042 | 2.00 | 0.132 |
| n-Butyllbenzene | 1.61 | 1.86 | 1.95 | 1.89 | 1.85 | 1.9 | 1.94 | 1.93 | 1.94 | 1.87 | 93.7 | 0.105 | 5.63 | 0.331 |
| sec-Butylbenzene | 1.66 | 1.94 | 2.02 | 1.97 | 1.93 | 1.99 | 2.02 | 2.03 | 2.04 | 1.96 | 97.8 | 0.118 | 6.01 | 0.369 |
| 1,2-Dichlorobenzene | 1.96 | 1.95 | 2.02 | 1.97 | 1.92 | 1.95 | 1.99 | 1.98 | 2.02 | 1.97 | 98.7 | 0.033 | 1.68 | 0.104 |
| 1,2-Dibromo-3-chloropropane | 2.10 | 1.83 | 1.87 | 1.89 | 1.84 | 1.99 | 1.77 | 1.84 | 1.79 | 1.88 | 94.0 | 0.104 | 5.53 | 0.327 |
| 1,2,4-Trichlorobenzene | 2.26 | 2.17 | 2.18 | 2.13 | 2.07 | 2.11 | 2.16 | 2.11 | 2.15 | 2.15 | 107 | 0.054 | 2.52 | 0.170 |
| Hexachlorobutadiene | 1.75 | 2.09 | 2.17 | 2.13 | 2.09 | 2.14 | 2.15 | 2.16 | 2.18 | 2.10 | 105 | 0.133 | 6.37 | 0.419 |
| Naphthalene | 2.60 | 2.14 | 2.03 | 1.97 | 1.91 | 1.89 | 1.97 | 1.96 | 1.99 | 2.05 | 103 | 0.218 | 10.6 | 0.685 |
| 1,2,3-Trichlorobenzene | 2.49 | 2.21 | 2.19 | 2.13 | 2.07 | 2.11 | 2.15 | 2.11 | 2.17 | 2.18 | 109 | 0.124 | 5.67 | 0.389 |

* Calibration level concentrations with the exception of internal standards, surrogates, and m,p-Xylene ** Concentrations double since results are m-xylene and p-xylene combined.



Conclusions

- A GCMS-HS trap system utilizing SIM and a higher temperature limit RXI-624Sil MS column is capable of allowing for the detection and identification of 75 volatile organic compounds within 17 minutes.
- Dynamic analytical ranges between 0.5 ppb to 40 ppb can be obtained for the majority of analytes.
- A precision of < 15 % RSD for the majority of analytes.

Path Forward



- Experiment with improving retention of early eluting compounds with a cold trap packed with Carboxen[®] adsorbent and Carbopack[™] adsorbent to improve retention of early eluting compounds.
- Analyze and spike samples with various matrixes.

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Questions?

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