

Accurate Mass Library for PFAS Analysis in Environmental Samples and Workflow for Identification of Pollutants in Drinking Water Using GC/Q-TOF

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Abstract

Development of accurate mass libraries in environmental applications is key in expanding the scope of monitored compounds and allowing for target/suspect detection with high confidence. It also provides the opportunity to use a targeted data analysis approach that offers higher sensitivity and flexibility compared to nontarget screening.

This application note describes the development and use of an accurate mass personal compound database and library (PCDL) of per- and polyfluoroalkyl substances (PFAS) for the Agilent 7250 GC/Q-TOF and demonstrates how the PCDL can be applied in both target as well as nontarget screening approaches using environmental samples, such as drinking water extracts. This study also demonstrates the benefits of using the high-resolution accurate mass GC/Q-TOF in nontarget screening using NIST23 and third-party libraries for identifying a substantial number of other contaminants of industrial origin in drinking water.

Introduction

PFAS are emerging contaminants of increasing concern due to their environmental persistence, toxicity, and capability of bioaccumulation. There are currently thought to be over 6,000 PFAS that have been commercially produced¹, and recent studies have shown that many emerging PFAS detected in the environment can be volatile or semivolatile in nature²⁻⁴. Therefore, many analytical techniques are necessary for PFAS detection. Gas chromatography/mass spectrometry (GC/MS) is typically used for detecting volatile and semivolatile nonpolar PFAS compounds. In this study, the 7250 GC/Q-TOF system was used to take advantage of its high-resolution for detecting compounds with mass defects that are different from that of complex environmental matrixes.

To ensure the most sensitive and reliable detection of PFAS, an accurate mass library that includes over 150 electron ionization (EI) PFAS spectra and contains both retention times (RTs) and retention indices (RIs) was created.

The PFAS PCDL was further tested using both target and nontarget approaches when analyzing the drinking water extracts. In addition, to fully benefit from the GC/Q-TOF accurate mass capability combined with full-spectrum acquisition, enabling nontarget detection, NIST23 and the third-party library MassBank of North America (MassBank.us⁵) were also used to identify other contaminants in drinking water, with the false positives being effectively removed based on accurate mass information. Thus, many pollutants were identified in drinking water, including disinfection by-products (DBPs), industrial chemicals originated from personal care products, pharmaceuticals, as well as pesticide residues.

Experimental

Sample preparation

The drinking water samples were collected at two different locations in California, U.S. and represented two different water source categories: a small surface water (Weaverville) and a mixed surface and ground water (Irvine). Water samples (2.4 L) were extracted on a multimode solid phase extraction (SPE) using HLB, WAX, WCS, and Isoelut ENV sorbents, and eluted with 5% methyl tert-butyl ether (MTBE) in methanol (MeOH), dichloromethane (DCM), 0.5% NH₄OH in 1:1 ethyl acetate (EtAc):MeOH, and 1.7% formic acid in 1:1 EtAc:MeOH. The combined extracts were concentrated, solvent exchanged to EtAc, and diluted tenfold.

Table 1. Data acquisition parameters.

GC and MS Conditions	Agilent DB-5ms	Agilent DB-624
MS	Agilent 7250 GC/Q-TOF	
GC	Agilent 8890 GC	
Inlet	Agilent multimode inlet, Ultra Inert 4 mm liner, single taper with wool	
Inlet Temperature	70 °C for 0.01 min; 300 °C/min to 250 °C	
Injection Volume	1 µL	
Column	Agilent J&W DB-5ms Ultra Inert (UI), 30 m × 0.25 mm, 0.25 µm	Agilent DB-624 Ultra Inert, 30 m × 0.25 mm, 1.4 µm
Oven Temperature Program	35 °C for 2 min; 7 °C/min to 210 °C, 20 °C/min to 300 °C, 4 min hold	30 °C for 2 min; 3 °C/min to 75 °C, 2 °C/min to 110 °C, 10 °C/min to 210 °C, 20 °C/min to 240 °C, 2 min hold
Column Flow	1.2 mL/min constant flow	1 mL/min constant flow
Carrier Gas	Helium	
Transfer Line Temperature	250 °C	
Quadrupole Temperature	150 °C	
Source Temperature	200 °C	
Electron Energy	70 eV	
Emission Current	Variable by time segment, 0.01 to 5 µA	
Spectral Acquisition Rate	5 Hz	
Mass Range (Tune)	50 to 1,200 <i>m/z</i>	

Data acquisition and data processing

GC/MS analysis was performed using an Agilent 8890 GC coupled to an Agilent 7250 GC/Q-TOF using the data acquisition parameters described in Table 1. PFAS accurate mass spectra of GC-amenable compounds were acquired from individual PFAS standards.

The chromatographic deconvolution and library search were performed in Agilent MassHunter Unknowns Analysis software, version 11.1. Accurate mass electron ionization (EI) fragments were converted to the theoretical *m/z* using Agilent MassHunter Qualitative Analysis software, version 10.0, and the spectra were exported into the accurate mass Agilent Personal Compound Database and Library (PCDL) Manager, version 8.0. The Agilent GC/Q-TOF Pesticide PCDL, PFAS PCDL, NIST23, as well as MassBank.us were used to perform initial compound identification. Prior to performing the library search with MassBank.us, the spectra, along with metadata information from this database, were exported in the PCDL format using Agilent ChemVista software, version 1.0, as described elsewhere.⁶⁻⁷ RIs and accurate mass information were used to confirm the compound identification. Statistical analysis was performed in Agilent Mass Profiler Professional (MPP), version 15.1.

Results and discussion

Accurate mass library for PFAS

To create an accurate mass GC/MS PCDL, spectra were collected for over 100 volatile and semivolatile PFAS compounds. Accurate mass fragment ions were

automatically annotated with formulas based on accurate mass information and isotope ratios using MassHunter Qualitative Analysis software (Figure 1). The fragment formula annotations were verified, corrected when necessary, and automatically converted to the theoretical m/z .

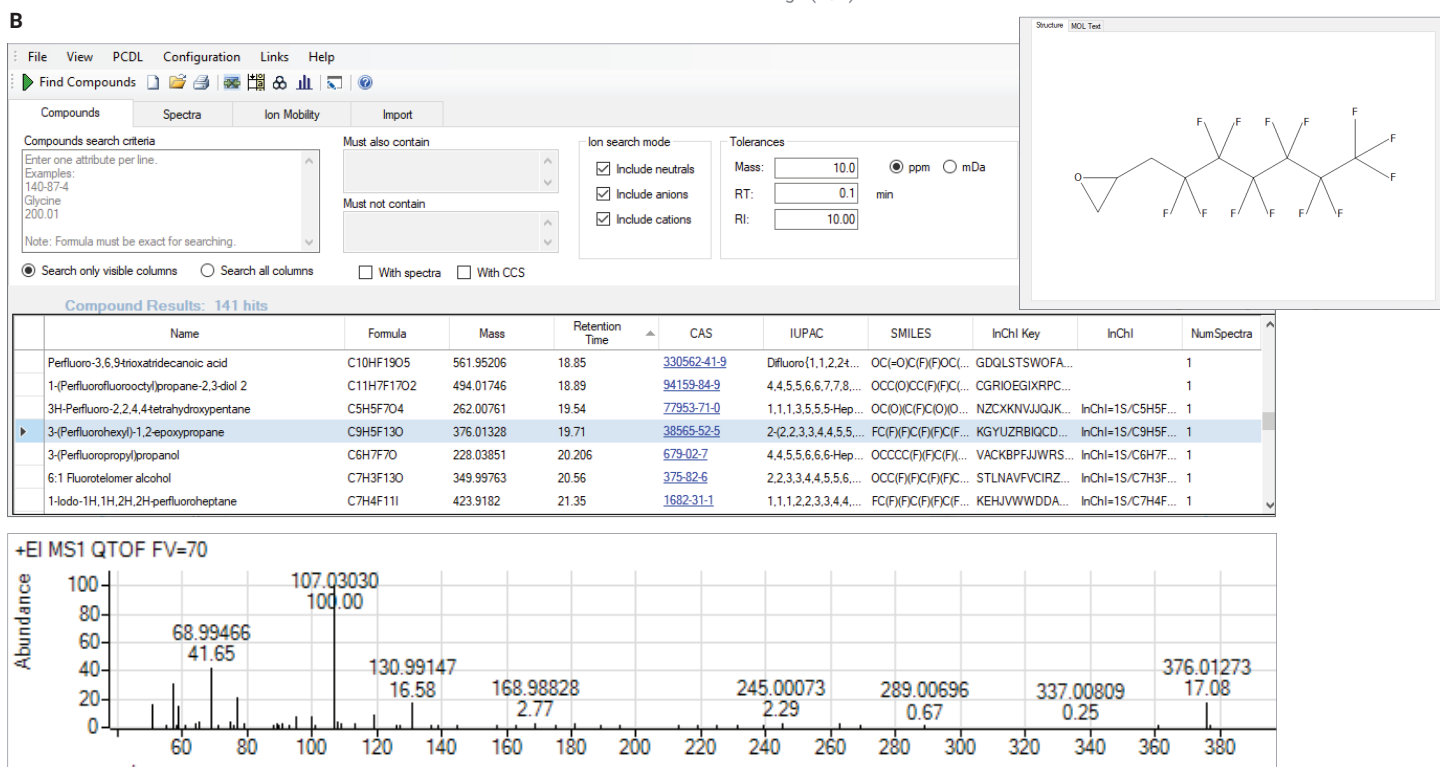
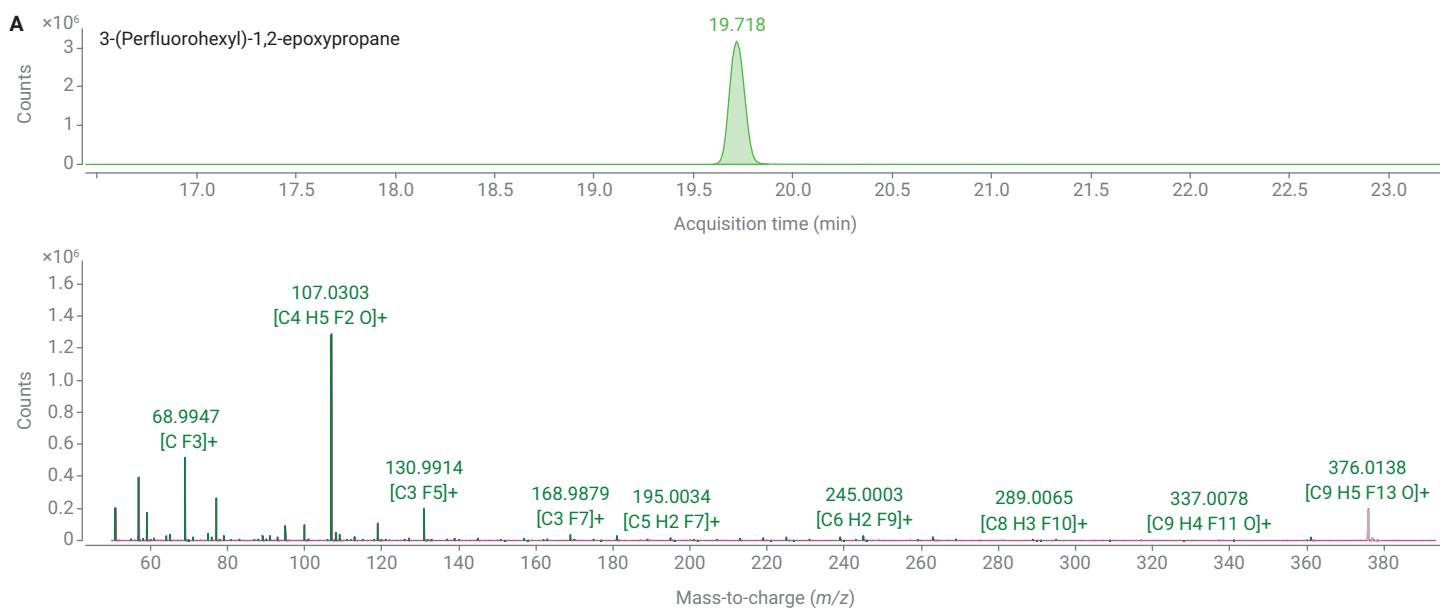


Figure 1. (A) Extracted ion chromatogram (EIC) of the molecular ion and fragment formula annotation of spectrum for one of the PFAS compounds in Agilent MassHunter Qualitative Analysis software. (B) The PFAS PCDL contains EI spectra as well as the metadata, including molecular structure and database identifiers.

The PFAS compound classes include perfluoroalkyl iodides (PFAIs), fluorotelomer iodides (FTIs), fluorotelomer alcohols (FTOHs), fluorotelomer olefins (FTOs), fluorotelomer acrylates (FTACs), fluorotelomer methacrylates (FTMACs), fluorotelomer carboxylic acids (FTCA), fluorotelomer unsaturated carboxylic acids (FTUCA), perfluoroalkane sulfonamides (FASA), and more (Figure 2).

To acquire spectra for the PFAS PCDL, the mid-polar DB-624 GC column (30 m × 0.25 mm, 1.4 μm) was used to ensure the best retention and separation of the challenging volatile PFAS. In addition to the RTs, RIs for the mid-polar column phase were also calculated for all compounds. Inclusion of RIs provides the flexibility of the GC method when using the PFAS PCDL as soon as GC column phase stays the same.

The remaining metadata, including compound structures and database identifiers, were added using PCDL Manager.

Compound overlap of the volatile and semivolatile PFAS classes between the accurate mass PFAS PCDL and NIST23 library is shown in Table 2.

Table 2. Compound overlap between the PFAS PCDL and NIST23 library.

	Percent Unique to PCDL	Total Number
All	53	158
PFCA	55	29
FTO	50	6
PFAI and FTI	17	6
FTCA and FTUCA	67	9
FTAC and FTMAC	25	8
FTOH	40	15
FASA	8	12

A significant number of the PFAS compounds (over 50%) were found to be present uniquely in the PFAS PCDL. In particular, the spectra of many per- and polyfluorinated carboxylic acids, fluorotelomer olefins, and fluorotelomer alcohols were found to be unique to the PCDL, thus highlighting the value of the accurate mass PFAS library in PFAS research.

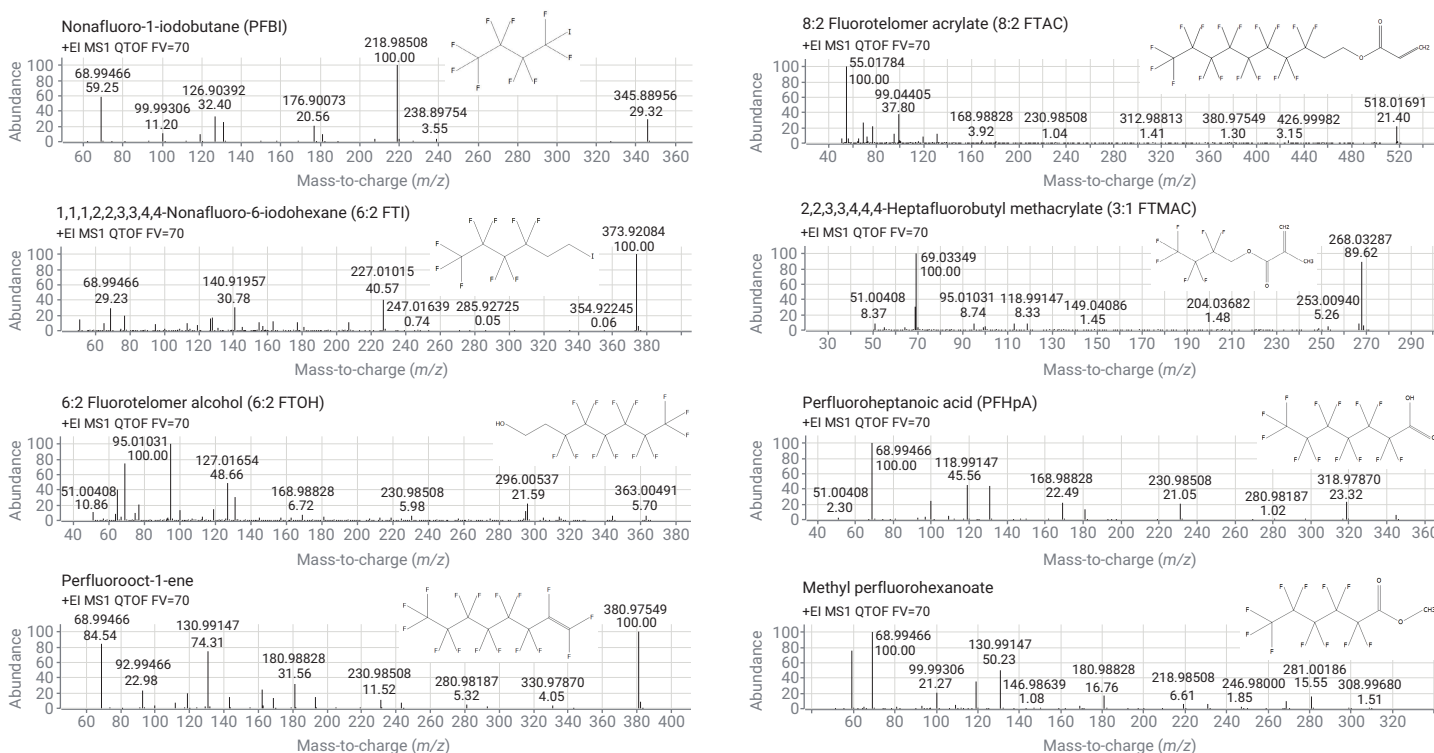


Figure 2. Examples of different PFAS compound classes from the PFAS PCDL.

PFAS in drinking water extracts

For PFAS detection, the extracts of drinking water were separated on a DB-624 column and analyzed using the 7250 GC/Q-TOF. To be able to detect early-eluting volatile PFAS, the emission current was set up by segment, as shown in Table 1, thus excluding the solvent peak from the detection.

Both target and nontarget approaches were evaluated using the PFAS PCDL. When performing the nontarget analysis, the chromatographic deconvolution was carried out in the

MassHunter Unknowns Analysis software using a SureMass algorithm, which is optimized for complex, high-resolution EI data. The PFAS PCDL then was used to search the deconvoluted spectra with RT matching. One of the PFAS—a transformation product of the perfluorocarboxylic acid—was identified in drinking water extract using this approach (Figure 3A). An additional benefit of nontarget screening is the use of multiple libraries (including libraries containing unit mass spectra) that can all be searched simultaneously.

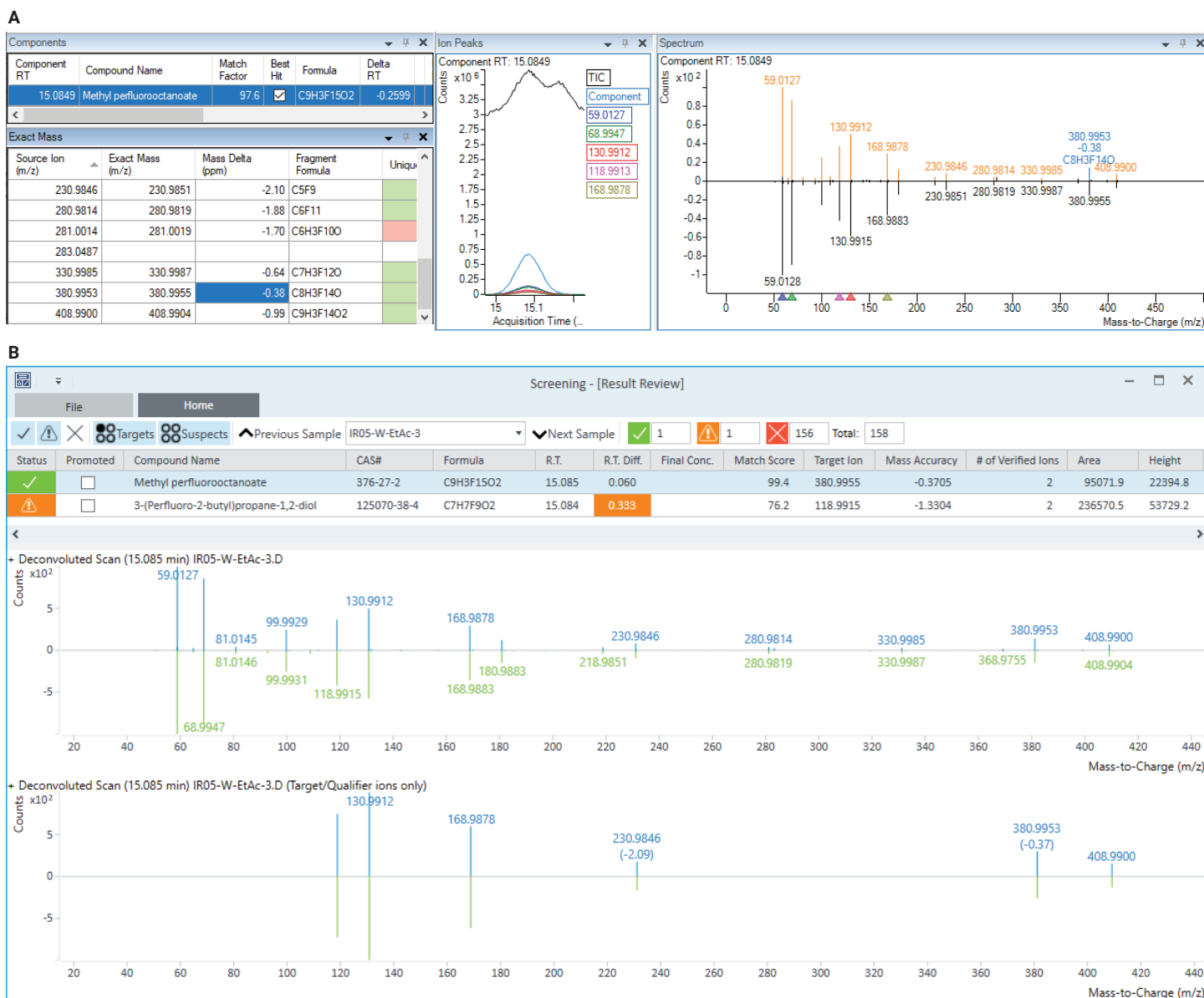


Figure 3. Example of PFAS (methyl perfluorooctanoate) identified in drinking water samples using PFAS PCDL in a nontarget approach using (A) Agilent MassHunter Unknowns Analysis software, and (B) a target GC/Q-TOF screening approach.

One of the advantages of the target approach based on the GC/Q-TOF Screener tool of the MassHunter Quantitative Analysis software (described in detail previously⁸) and PCDL is that all the parameters could be set up individually for every compound in the method. This approach allows for a substantial flexibility when performing the screening method optimization at the data processing level, enabling the highest degree of sensitivity and specificity. Another significant benefit of this approach is that it saves the time usually spent reviewing the results. The GC/Q-TOF Screener algorithm validates quantifier and qualifier ions based on outliers, and for most compounds, either confirms or rejects their presence automatically. Only a few compounds remain highlighted to indicate that a manual review might be necessary for confirmation of compound identity.

The same PFAS compound—methyl perfluorooctanoate—that was identified in drinking water extracts using a nontarget approach was also detected using the GC/Q-TOF Screener with library match scores (LMS) of > 99 (Figure 3B). It has previously been reported that perfluoroalkyl carboxylic acids can be converted to corresponding methyl esters in the presence of methanol⁹, thus plausibly explaining the presence of the methyl ester of PFOA in drinking water extracts.

Identification of other contaminants in drinking water samples

To screen for additional contaminants in drinking water samples in a nontarget manner, the GC/Q-TOF Pesticide PCDL, NIST23 library, and MassBank.us were used. The choice of the DB-5ms UI column enabled RI matching while searching the NIST23 library, thus enhancing the confidence in compound identification. The ExactMass tool in MassHunter Unknowns Analysis software was used to eliminate the false positives based on the accurate mass information and molecular formula of the hit. This is particularly practical when using unit mass libraries such as NIST23 (Figure 4A) and MassBank.us.

Over 100 contaminants were identified and confirmed using accurate mass information (Figure 4A and 4B, and Tables 3 and 4) from the sample without re-injection.

Among the identified contaminants, one of the significant groups was disinfection by-products, formed when chlorine and bromine interact with organic matter. These compounds included halomethanes and haloacetic acids, which are the most common disinfection by-products. Other prominent groups of contaminants included compounds originating from industrial processes (such as those used in cleaning products and manufacturing of plastics, dyes, and pharmaceuticals), PAHs and their derivatives, as well as pesticides.

Approximately 400 hits per sample with LMS > 70 were detected using MassBank.us, including over 20 contaminants—mostly DBPs and PAHs. Since this library does not contain RI information for most of the compounds, many hits could potentially be false positives. One such example is shown in Figure 5. The hit from MassBank.us was 1-bromooctane with a high LMS of 88.3 and an RI of 1,134, according to NIST23. This would make a difference of over 400 RI units between the hit and the compound in question, indicating that the ID is likely incorrect. The difference between the compound RI and the NIST23 hit was only 10 RI units (Figure 5B). Note that the hits from both NIST23 and MassBank.us perfectly match the accurate mass information displayed in the ExactMass tables (Figure 5).

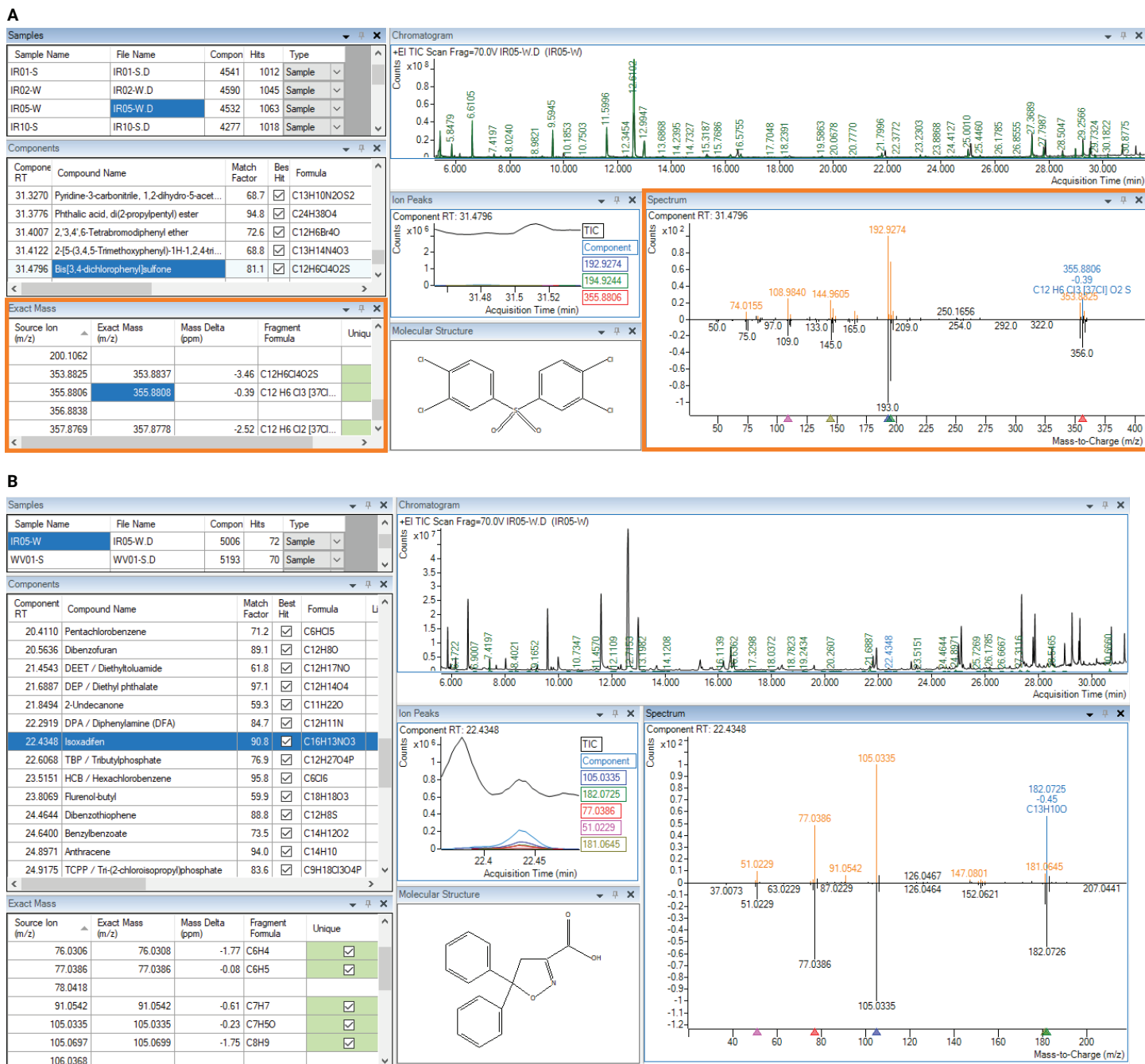


Figure 4. Examples of the contaminants identified in drinking water extracts using (A) NIST23 and (B) Agilent GC/Q-TOF Pesticide PCDL. The ExactMass tool (outlined in orange) helped to provide additional confirmation of unit mass library hits based on accurate mass. Compound ions are highlighted in the mirror plot when m/z corresponds to the library hit formula.

Table 3. Contaminants identified in drinking water using the NIST23 library with LMS > 75. *The cases where delta RI was calculated considering predicted RIs rather than experimental (experimental not available) are denoted by an asterisk. Some of the prominent disinfection by-products are highlighted in red.

RT	Compound Name	Match Score	Formula	RI Difference
4.79	Bromodichloromethane	95.4	CHBrCl ₂	-56
4.81	Chloral	78.8	C ₂ HCl ₃ O	-9
4.91	Dichloroacetonitrile	86.4	C ₂ HCl ₂ N	-76
4.95	Chloromethylmethyl sulfide	94	C ₂ H ₅ ClS	-59*
5.11	Dimethyl disulfide	98.4	C ₂ H ₆ S ₂	-35
5.35	Methyldiallylamine	85.7	C ₇ H ₁₃ N	-50*
5.47	Bromoacetonitrile	82.8	C ₂ H ₂ BrN	1
5.95	Dibromochloromethane	95.5	CHBr ₂ Cl	-25
6.01	Tetrachloroethylene	96.5	C ₂ Cl ₄	-12
6.04	1,1-Dimethyl-3-chloropropanol	88.4	C ₃ H ₇ ClO	7
6.34	Bromoacetone	87.8	C ₂ HBrClN	-3
6.59	Dichloroacetic acid methyl ester	89.2	C ₃ H ₄ Cl ₂ O ₂	-7*
7.67	Tribromomethane	98.2	CHBr ₃	-10
8.24	Methyl bromo(chloro)acetate	77.4	C ₃ H ₄ BrClO ₂	-3
8.31	Dibromoacetonitrile	86.6	C ₂ HBr ₂ N	-15
10.63	2,2-Dichloroacetamide	83.5	C ₂ H ₂ Cl ₂ NO	-4*
10.73	1,2-Dichlorobenzene	98.5	C ₆ H ₄ Cl ₂	9
14.12	Naphthalene	81.9	C ₁₀ H ₈	-4
15.45	Caprolactam	89.6	C ₆ H ₁₁ NO	3
16.43	2-Methylnaphthalene	89.3	C ₁₁ H ₁₀	-1
16.64	Phthalic anhydride	92.5	C ₈ H ₄ O ₃	5
16.98	Benzamide	82.8	C ₇ H ₇ NO	18
18.05	Biphenyl	83.2	C ₁₂ H ₁₀	-1
18.18	Benzeneacetamide	84.3	C ₉ H ₉ NO	13
19.27	Dimethyl phthalate	75.1	C ₁₀ H ₁₀ O ₄	8
19.96	Acenaphthene	91.2	C ₁₂ H ₁₀	-4
20.18	4-Methylbiphenyl	79.4	C ₁₃ H ₁₂	-4
20.28	2,4-Di-tert-butylphenol	90.2	C ₁₄ H ₂₂ O	10
20.56	Dibenzofuran	92.4	C ₁₂ H ₈ O	-5
21.23	1-Bromododecane	75.7	C ₁₂ H ₂₅ Br	-10
21.45	Diethyltoluamide (DEET)	78.1	C ₁₂ H ₁₇ NO	10
21.69	Diethyl phthalate	96	C ₁₂ H ₁₄ O ₄	8
21.71	Fluorene	75.3	C ₁₃ H ₁₀	-4
22.01	2-(Methylmercapto)benzothiazole	77.8	C ₈ H ₇ NS ₂	2
22.43	Benzophenone	94.8	C ₁₃ H ₁₀ O	4
22.60	Tributyl phosphate	93	C ₁₂ H ₂₇ O ₄ P	7
23.51	Hexachlorobenzene	97.2	C ₆ Cl ₆	9

RT	Compound Name	Match Score	Formula	RI Difference
24.19	9H-Fluoren-9-one	97.1	C ₁₃ H ₈ O	8
24.26	9H-Fluoren-9-ol	81.5	C ₁₃ H ₁₀ O	9*
24.90	Anthracene	94.4	C ₁₄ H ₁₀	0
24.91	Tris(2-chloroisopropyl)phosphate	82.2	C ₉ H ₁₈ Cl ₃ O ₄ P	27
25.02	Benzo[h]quinoline	88.2	C ₁₃ H ₉ N	-2
25.53	2,4-Diphenyl-4-methyl-2(E)-pentene	76.5	C ₁₈ H ₂₀	8
25.55	Benzo[f]quinoline	91.1	C ₁₃ H ₉ N	-1
25.73	Carbazole	76.8	C ₁₂ H ₉ N	-4
25.96	Di-sec-butyl phthalate	90.8	C ₁₆ H ₂₂ O ₄	-2
26.09	3,3-Diphenyl-2-propenenitrile	82.7	C ₁₅ H ₁₁ N	18*
26.27	3-Methyldibenzothiophene	80.8	C ₁₃ H ₁₀ S	-5
26.66	3-Methylphenanthrene	84	C ₁₅ H ₁₂	1
27.00	2-Methylantracene	88.5	C ₁₅ H ₁₂	-27
27.31	Dibutyl phthalate	92.4	C ₁₆ H ₂₂ O ₄	9
27.59	9,10-Anthracenedione	93.2	C ₁₄ H ₈ O ₂	-27
28.21	Octachlorostyrene	88.6	C ₈ Cl ₈	-7
28.36	Cyclic octaatomic sulfur	93.1	S ₈	-18
28.51	Drometrizole	82.3	C ₁₃ H ₁₁ N ₃ O	-5
28.53	Fluoranthene	97.8	C ₁₆ H ₁₀	-12
28.54	Phenindione	79	C ₁₆ H ₁₀	-28*
28.91	Dibenzothiophene sulfoxide	87.2	C ₁₂ H ₈ OS	-41*
28.94	Pyrene	89.3	C ₁₆ H ₁₀	-25
29.02	1-Azapyrene	78.4	C ₁₅ H ₉ N	2
29.34	Bisphenol A	84.1	C ₁₅ H ₁₆ O ₂	26*
29.37	2-Amino-9-fluorenone	83.3	C ₁₃ H ₉ NO	2*
29.69	Bis(4-chlorophenyl) sulfone	77	C ₁₂ H ₈ Cl ₂ O ₂ S	-1
29.87	2,2'-Methylene-bis-(4-methyl-6-t-butylphenol)	87.5	C ₂₃ H ₃₂ O ₂	2
30.79	Benzo[b]naphtho[1,2-d]thiophene	77.2	C ₁₆ H ₁₀ S	13
30.90	7H-Benz[de]anthracen-7-one	89.2	C ₁₇ H ₁₀ O	85
30.94	Benzo[b]naphtho[2,1-d]thiophene	81.3	C ₁₆ H ₁₀ S	-16
31.04	Phthalic acid, di(2-propylpentyl) ester	94.8	C ₂₄ H ₃₈ O ₄	-5
31.38	Bis[3,4-dichlorophenyl]sulfone	82.3	C ₁₂ H ₆ Cl ₄ O ₂ S	3*
31.48	Bumetrizole	78.6	C ₁₇ H ₁₈ ClN ₃ O	57
31.51	Benz(a)anthracene-7,12-dione	76.1	C ₁₈ H ₁₀ O ₂	-48*
31.82	Bis(2-ethylhexyl) isophthalate	84.7	C ₂₄ H ₃₈ O ₄	-35
32.37	Decachlorobiphenyl	94.3	C ₁₂ Cl ₁₀	-81

Table 4. Additional contaminants identified in drinking water using the Agilent GC/Q-TOF Pesticide PCDL.

RT	Compound Name	Match Factor	Formula
6.17	2-Picoline	96.7	C ₆ H ₇ N
6.90	Methanesulfonate-methyl	79.6	C ₂ H ₆ O ₃ S
8.17	PPD/p-Phenylenediamine	80.0	C ₆ H ₈ N ₂
8.40	o-Toluidine	82.3	C ₇ H ₉ N
8.93	Thanite	83.9	C ₁₃ H ₁₉ NO ₂ S
9.17	Benzaldehyde	98.5	C ₇ H ₆ O
9.52	Phenol	89.6	C ₆ H ₆ O
11.46	Acetophenone	94.3	C ₈ H ₈ O

RT	Compound Name	Match Factor	Formula
11.99	2,4,5-Trimethylaniline	82.7	C ₉ H ₁₃ N
12.90	2-Nitrophenol	77.1	C ₆ H ₅ NO ₂
22.29	DPA/Diphenylamine (DFA)	84.7	C ₁₂ H ₁₁ N
22.44	Isoxadifen	93.3	C ₁₆ H ₁₃ NO ₃
24.64	Benzylbenzoate	83.0	C ₁₄ H ₁₂ O ₂
25.96	DIBP/Diisobutyl phthalate	86.1	C ₁₆ H ₂₂ O ₄
27.00	1-Methylphenanthrene	85.3	C ₁₅ H ₁₂

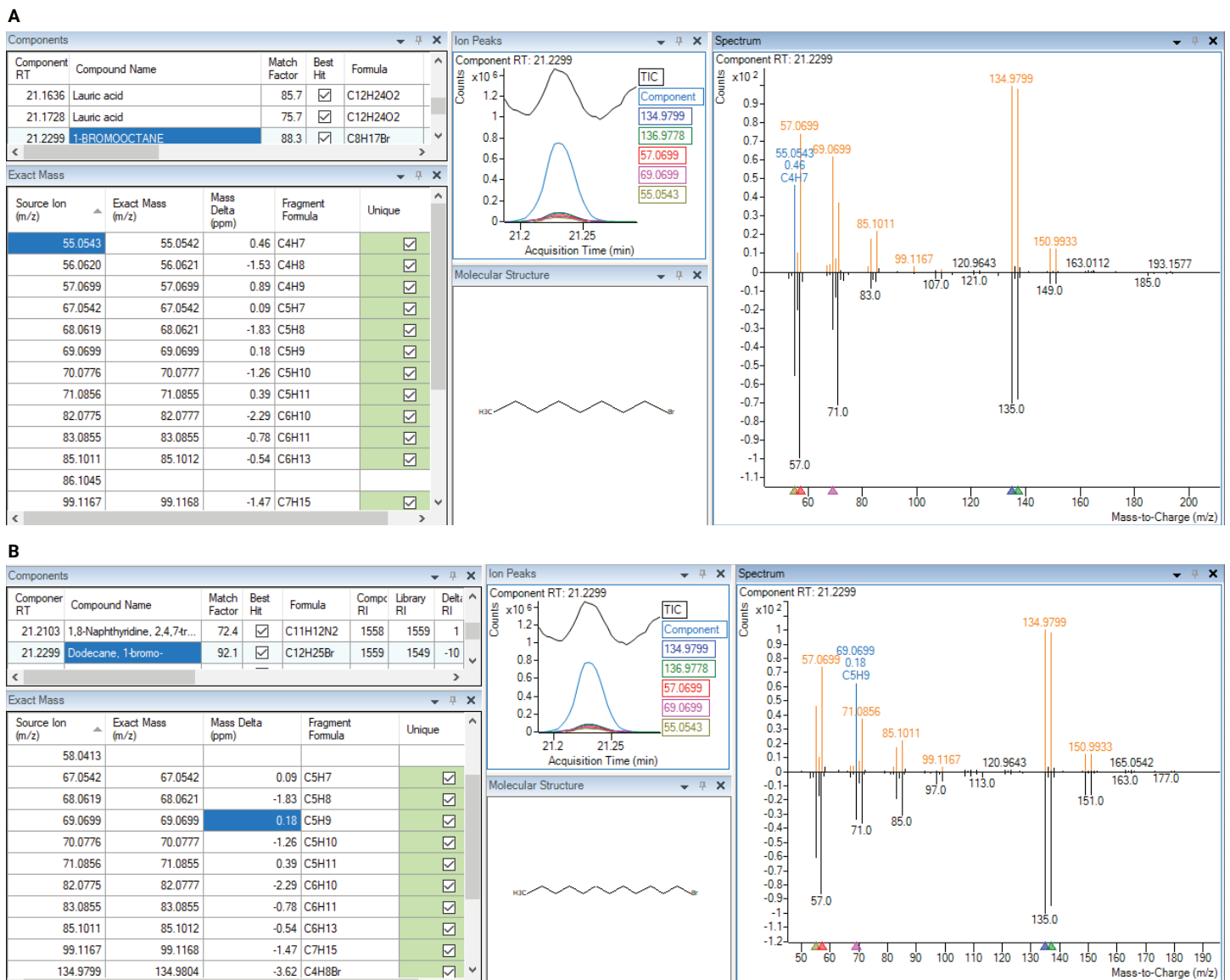


Figure 5. Compound misidentified by MassBank.us due to lack of the RI information. (A) MassBank.us hit. (B) NIST23 hit.

Additionally, an interesting case was observed for a compound with an RI of 1,858, whereby MassBank.us likely provided correct ID (with the LMS of 85.8) while NIST23 did not (Figure 6), proving the value of including third-party libraries in a compound identification workflow. The compound's most likely ID is thioxanthene, with a NIST23 experimental RI of 1,977, and an AI-predicted RI of 1,876. The experimental RI for this compound, used for the NIST23 library search, provided a significant RI delta of 124 RI units. However, the experimental RI for this compound was only based on one data point, and thus may not be accurate. The AI-predicted NIST23 RI generated a significantly smaller RI delta (18 RI units). Due to the large RI difference between the compound RI and the NIST23 experimental RI of thioxanthene, another NIST23 hit, 1-methyldibenzothiophene with the lower LMS of 81.1 was chosen (Figure 6B).

Among the contaminants with the highest response, which were identified in drinking water extracts using all three libraries, were mostly PAHs, DBPs, and phthalates (Figure 7). Individual samples of drinking water from the same group represented different households.

The contaminants in drinking water extracts were detected at a wide range of concentrations, estimated to be from low- and sub-ppb levels (for pesticides) to hundreds of ppb (in the case of PAHs), suggesting that an extended dynamic range might be desirable for this application.

Statistical analysis was performed in the MPP software, where the differences between Weaverville and Irvine water sources ($n = 5$ per group) were evaluated and displayed on a volcano plot (Figure 8). The volcano plot displays fold change versus statistical significance, and is used to quickly detect differences between the two groups. Compounds that were present in higher concentrations in Irvine water compared to Weaverville are colored in red and shown in the upper-right quadrant. Compounds that were found at higher concentrations in Weaverville water extracts compared to Irvine are colored in blue and displayed in the upper-left quadrant. Most contaminants occurred at higher levels in drinking water from Irvine (a more densely populated urban area) compared to Weaverville.

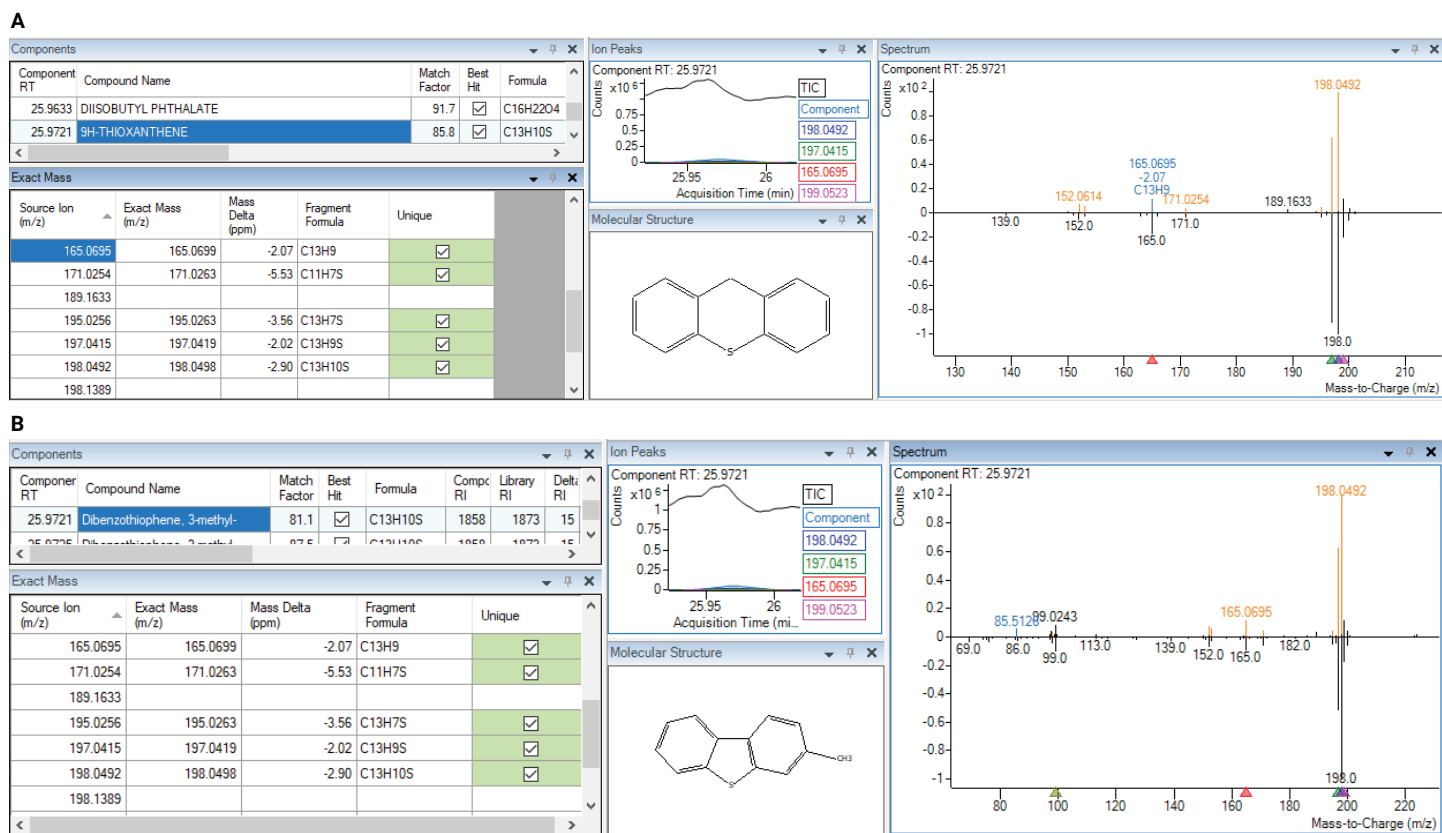


Figure 6. Compound likely misidentified by NIST23 due experimental RI information available for only one data point. (A) MassBank.us hit. (B) NIST23 hit.

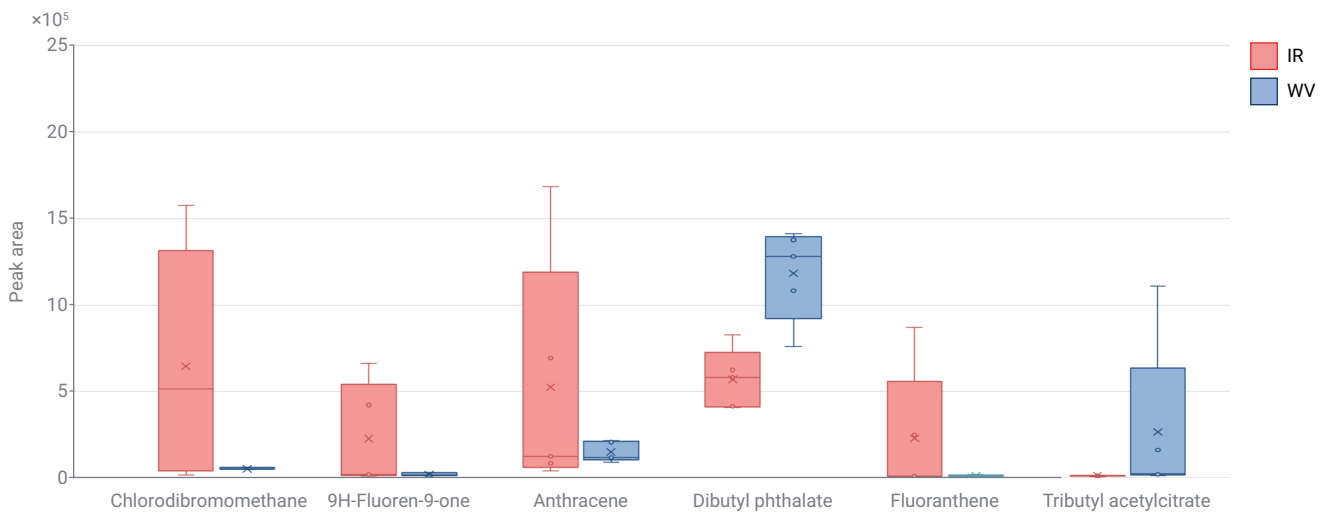


Figure 7. High-level contaminants identified in the drinking water of different households (n = 5 for each group) from Irvine (IR) and Weaverville (WV).

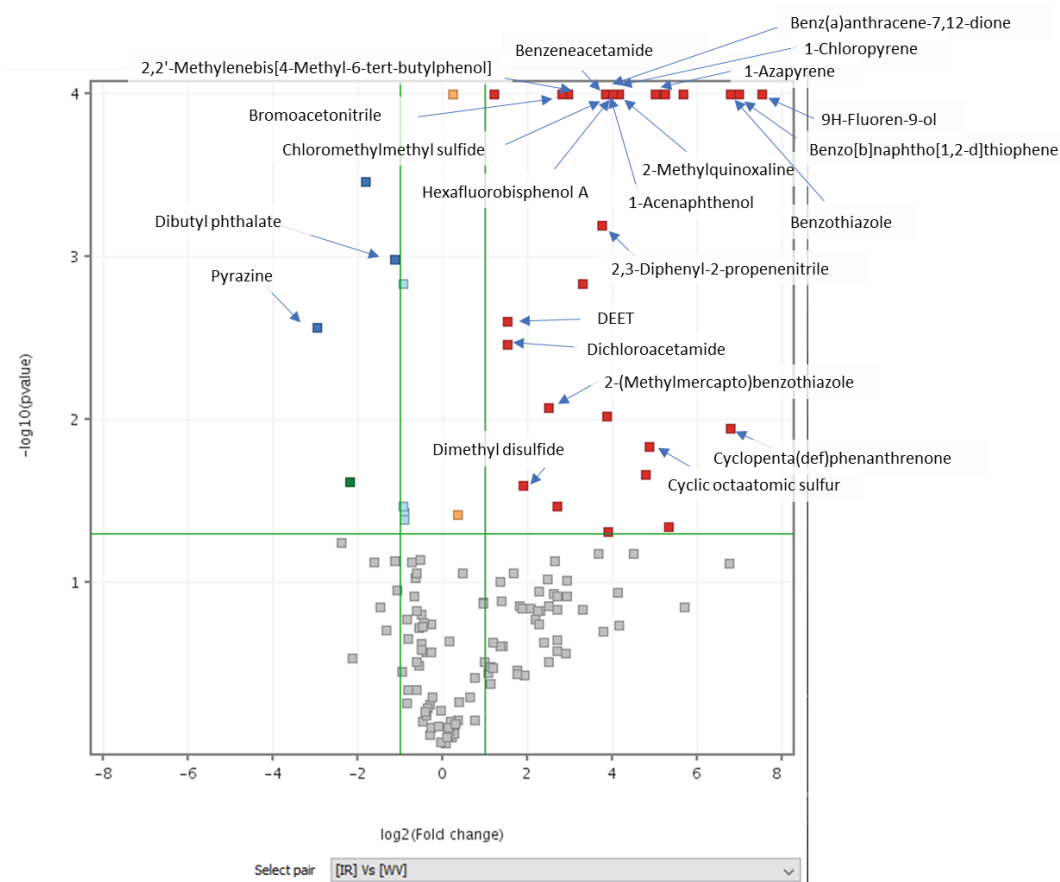


Figure 8. Comparison of water sourced in Irvine versus Weaverville on volcano plot, showing log₂ of fold change (FC) versus -log₁₀ of p-value.

Conclusion

Accurate mass libraries of environmental contaminants (such as PFAS) broaden the scope of suspects screened in environmental samples and increase confidence in the identification of pollutants. The accurate mass library described in this application note, containing over 150 PFAS EI spectra, including several emerging volatile PFAS, enabled identification of PFAS in drinking water samples using both nontarget and target workflows.

Additional contaminants were identified in drinking water from two different source categories, including disinfection by-products, PAHs, pesticides, and other industrial contaminants. Two drinking water sources were compared, and a higher number of contaminants were identified in the water extracts from Irvine compared to Weaverville.

Acknowledgement

The authors would like to thank the U.S. Environmental Protection Agency (EPA) for preparing the PFAS standards and providing them to Agilent Technologies through a material transfer agreement.

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Printed in the USA, December 5, 2023
5994-6966EN