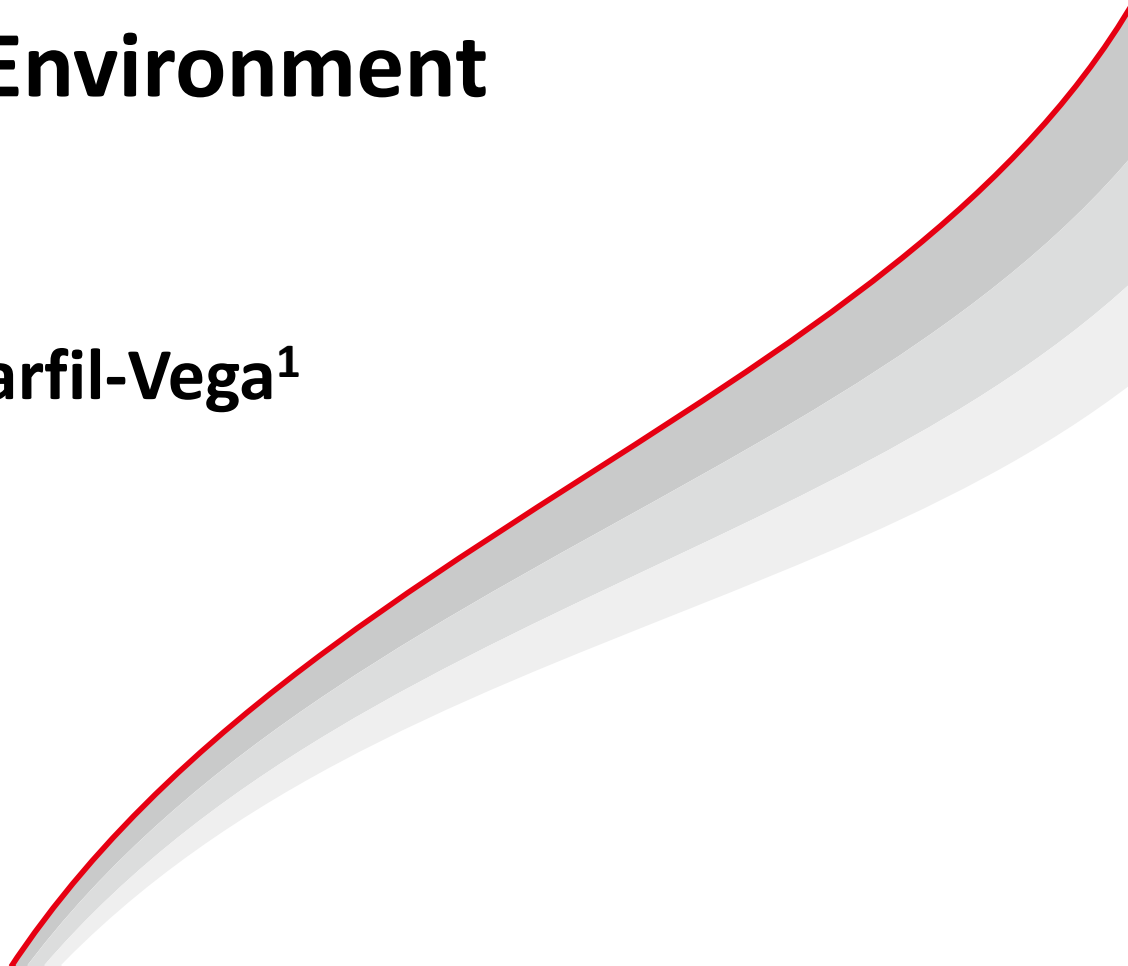


Multi-Approach Data Processing Workflow to Help Closing the Mass Balance of PFAS in the Environment

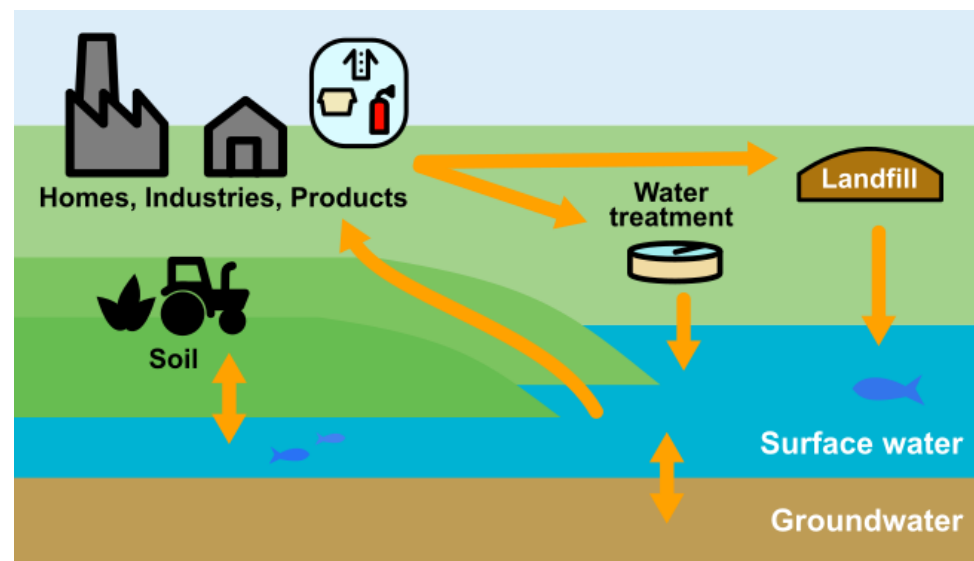
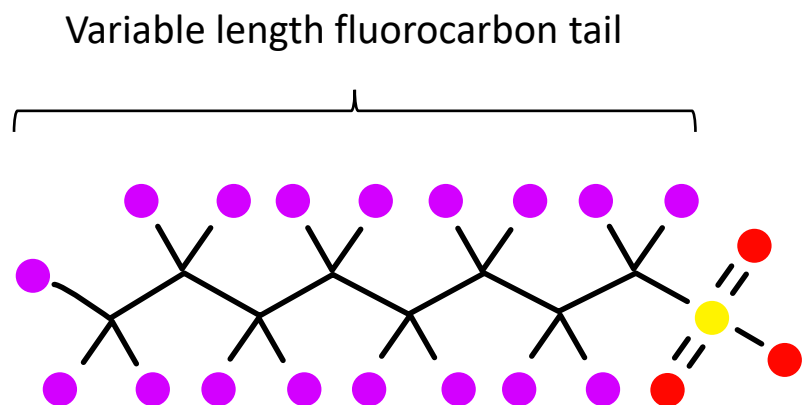
O. Shrestha¹, J. Dahl¹, T. Matsubara¹, R. Marfil-Vega¹

Shimadzu Scientific Instruments



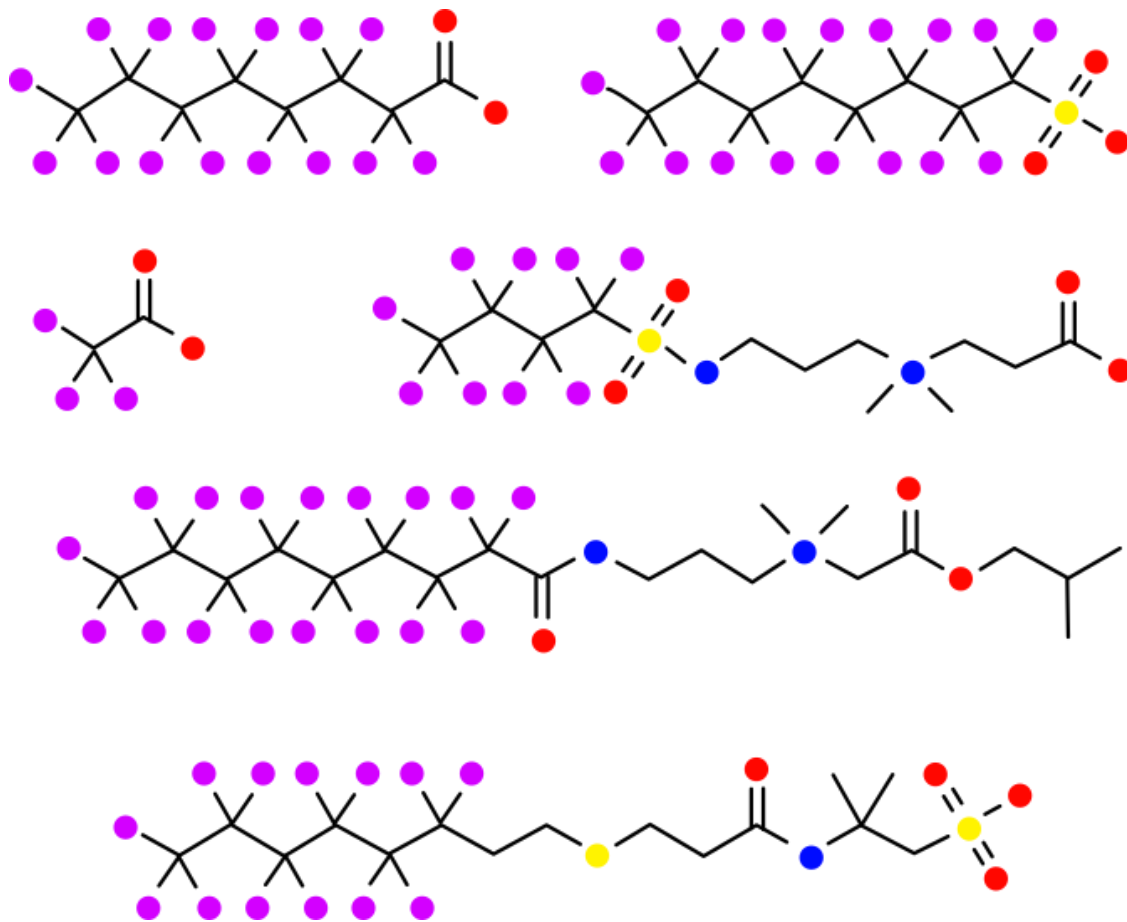
PFAS: A Global Issue

Fluorocarbons with possible health impact and environmental dispersal



PFAS are used in many consumer products and have slow environmental degradation, so they can disperse widely and bioaccumulate. They might have negative health effects.

PFAS – a Large and Diverse Group of Fluorocarbons



Large number of compounds (thousands) with different head groups, chain lengths, and branching make targeted detection difficult.

The possible PFAS are not all known in advance. In targeted analysis, rerun of the sample is required to measure additional targets.

Targeted vs Non-Targeted Analysis

Targeted

Target list known in advance

Excellent selectivity and sensitivity

Rapid

Easy data processing

Non-targeted

Can detect unknowns

Accurate mass gives confidence

Expand target list without reruns

DDA/DIA for MS2 spectra

Targeted vs Non-Targeted Analysis

Targeted

Target list known in advance

Excellent selectivity and sensitivity

Rapid

Easy data processing

Rerun sample to expand target list

Cannot detect unknowns



Non-targeted

Can detect unknowns

Accurate mass gives confidence

Expand target list without reruns

DDA/DIA for MS2 spectra

Data processing requires specialist

Generally higher detection limits



NIST Interlaboratory Study

Dear Researcher,

We are contacting you today to invite you to participate in our upcoming Per- and Polyfluoroalkyl Substances Non-Targeted Analysis (PFAS-NTA) interlaboratory study. The objective of this interlaboratory study is to evaluate the use of the new PFAS Mass Spectral Database developed by researchers at NIST and understand the measurement variability of multiple laboratories' NTA workflows. The study is **free** for laboratories to participate, although participation will be limited to the first 50 laboratories to apply.

Study Overview

There will be three test solutions of varying complexity, presented as methanolic extracts, that are intended to be directly analyzed (or diluted if needed) by each participant's preferred NTA workflow (general composition of the samples will be included in the shipment). The laboratories will be encouraged to use the new PFAS Mass Spectral Database as part of their identification workflow, either through using the mass spectral data in their own computational tools or the data analysis tools available alongside the database. The scope of the interlaboratory study will be limited to only those PFAS contained in the NIST List of Possible Per- and Polyfluoroalkyl Substances (<https://data.nist.gov/od/id/mds2-2387>). Additional PFAS may be present, but not included in the NIST suspect list. These additional PFAS are not of interest for this interlaboratory study.

Method information and results will be submitted via a Microsoft Excel workbook (*attached*). NIST will compile the results from all participating laboratories and distribute this information via a preliminary report, where all participating laboratories will be anonymized with participant codes (individual laboratories will know their participant code).

The benefit to participants is two-fold: 1) the ability for laboratories to access the new PFAS Mass Spectral Database with **hands-on assistance** in the application of the database and data tools for your lab, and 2) enable laboratories to understand their own NTA workflow performance in comparison to other laboratories.

PFAS Mass Spectral Database

Whether or not you are interested in participating in the interlaboratory study, we do encourage you to look at the new PFAS Mass Spectral Database that has been developed by researchers at NIST. To access the database toolkit, you can go to: <https://github.com/usnistgov/dimspec>

The user guide for accessing the information and utilizing the database and its data analysis tools are available at: <https://pages.nist.gov/dimspec/docs>

PFAS-NTA Interlaboratory Timeline

Participant sign-up deadline: February 29, 2024
Samples shipped to participants: March 31, 2024
Participants return results: June 30, 2024
Preliminary report by NIST: July 31, 2024

Still interested?

NIST recruited labs for non-targeted interlaboratory study of PFAS in three unknown samples

Blind study samples

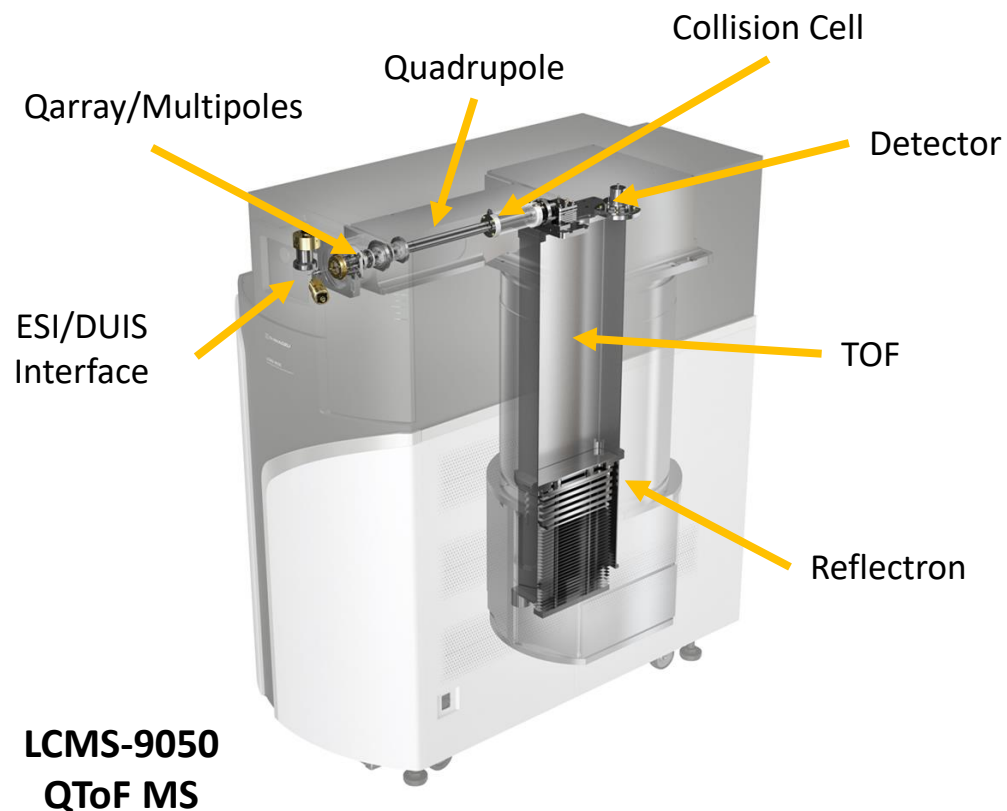
Sample A: analytical standards for PFAS

Sample B: mixture of two different AFFF commercial formulations diluted in methanol

Sample C: a methanolic extract of an AFFF-impacted soil



QToF Method for Non-Target PFAS Analysis

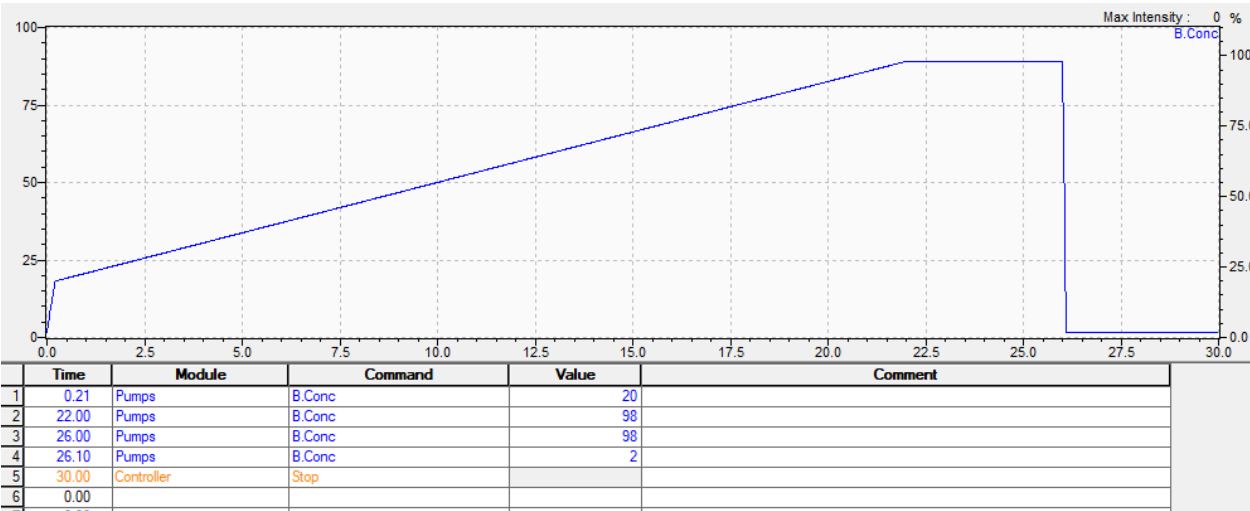


Method Conditions for Extended gradient for non-target PFAS

Modified from standard 1633 method, lengthened for capturing full range of suspects

DDA for MS2 spectrum comparison

QToF Method for Non-Target PFAS Analysis



Mode: Binary gradient

Total Flow: 0.4000 mL/min

Pump B Conc.: 2.0 %

Pump B Curv: 0

Configured Pumps

Pump A: LC-30AD

Pump B: LC-30AD

Pump C:

Pump D:

Pressure Limits (Pump A, B)

Maximum: 10000 psi

Minimum: 0 psi

Positive and Negative ESI runs

Main-Interface : DUIS

Ionization Mode : ESI

Nebulizing Gas Flow : 2.0 L/min

☒ Heating Gas Flow : 15.0 L/min

☒ Interface Temperature : 250 degC

☒ Desolvation Temperature : 444 degC

Sub-Interface

Interface Voltage (+) : 4.50 kV

Interface Voltage (-) : -3.50 kV

☐ Nebulizing Gas Flow : 1.0 L/min

Ion Guide

☒ Drying Gas Flow : 5.0 L/min

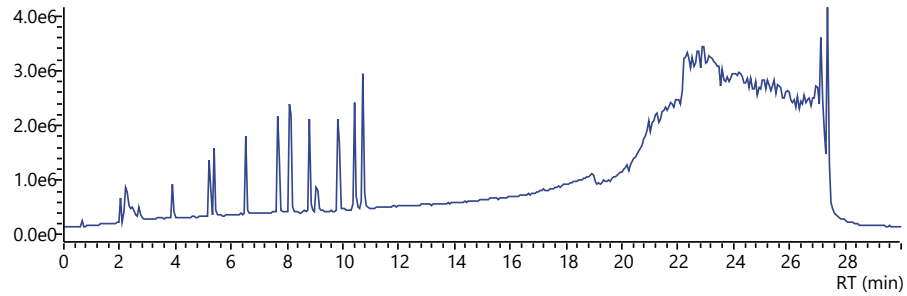
DL Temperature : 200 degC

Heat Block Temperature : 300 degC

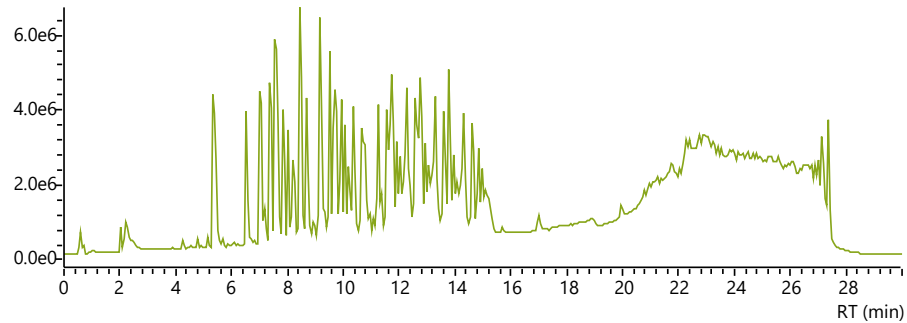
Event#	+/-	Type	Start (min)	End (min)	Precursor Ion	Product Ion	TOF Start m/z	TOF End m/z	Com	CE	CE Sp	ID	Event Time(s)	Pulser Inj. Times	Save Profile	Q1 Resolution	Threshold	Interface Voltage(kV)	Corona Voltage
1	-	MS	0.000	30.000			200.0000	1000.0000					0.300	594	☒		High	-1.00	

Scan range based on the suspect list. About 95% of suspects are between 200 and 1000 m/z.

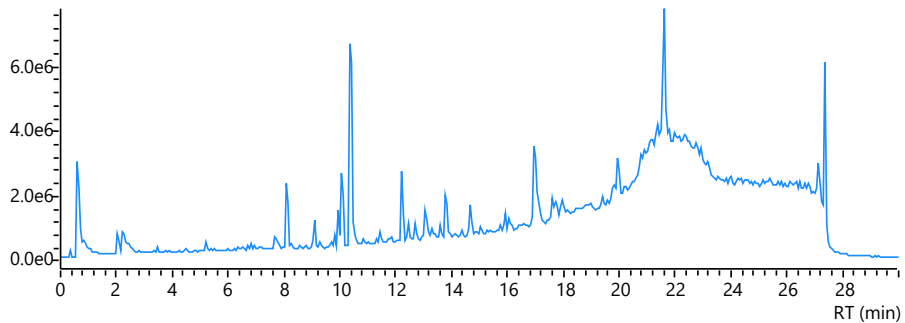
TIC Chromatographic View of the Samples



Sample A (-)

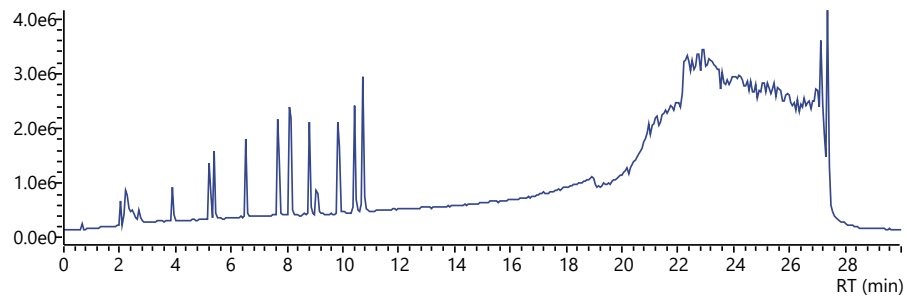


Sample B (-)

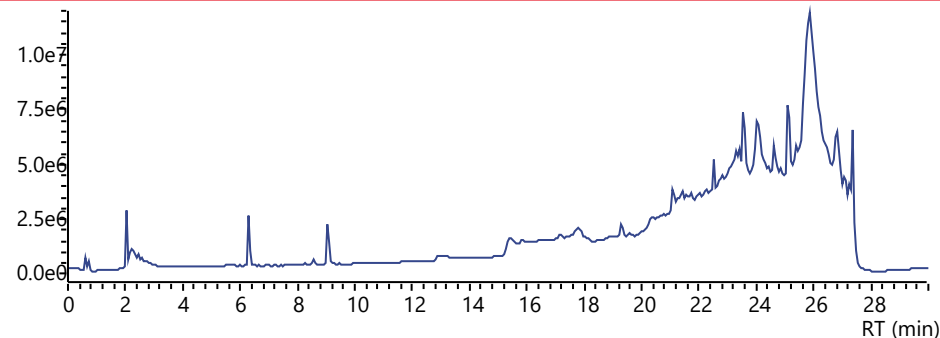


Sample C (-)

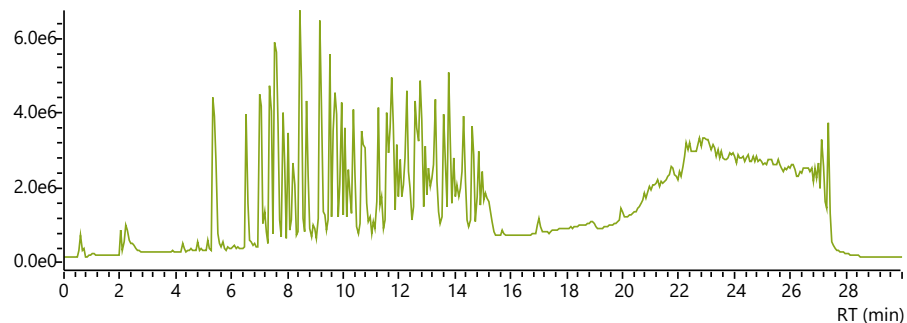
TIC Chromatographic View of the Samples



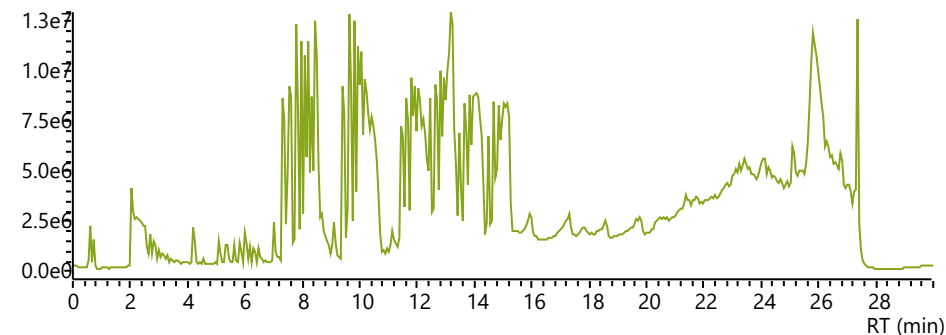
Sample A (-)



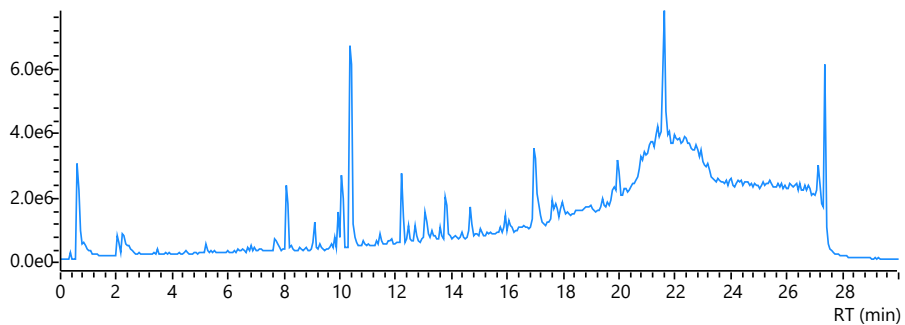
Sample A (+)



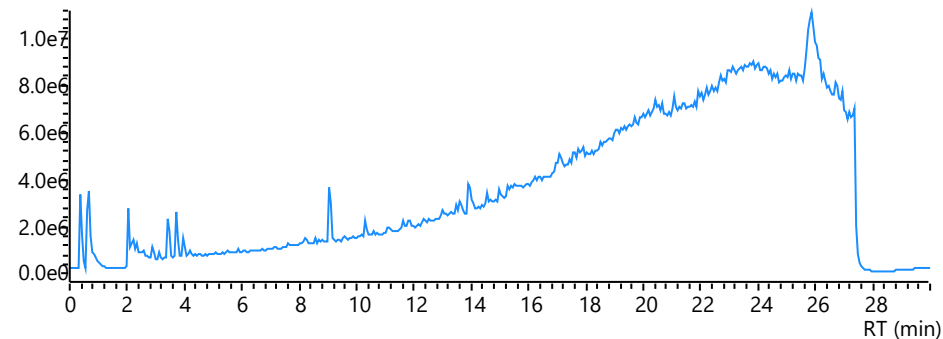
Sample B (-)



Sample B (+)



Sample C (-)



Sample C (+)

Data Processing Workflow

Three different, complementary workflows used, results combined and quality controlled

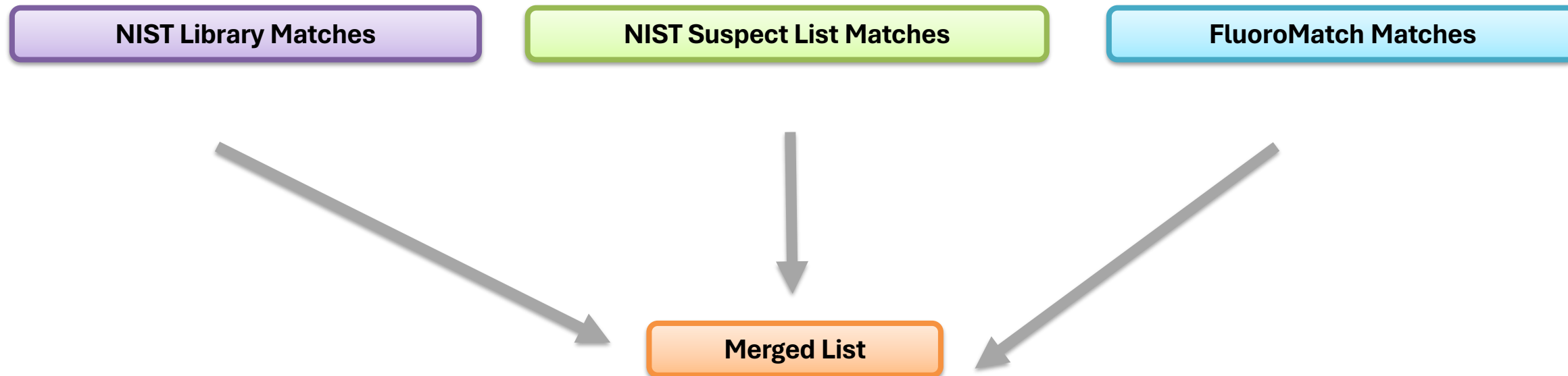
NIST Library Matches

NIST Suspect List Matches

FluoroMatch Matches

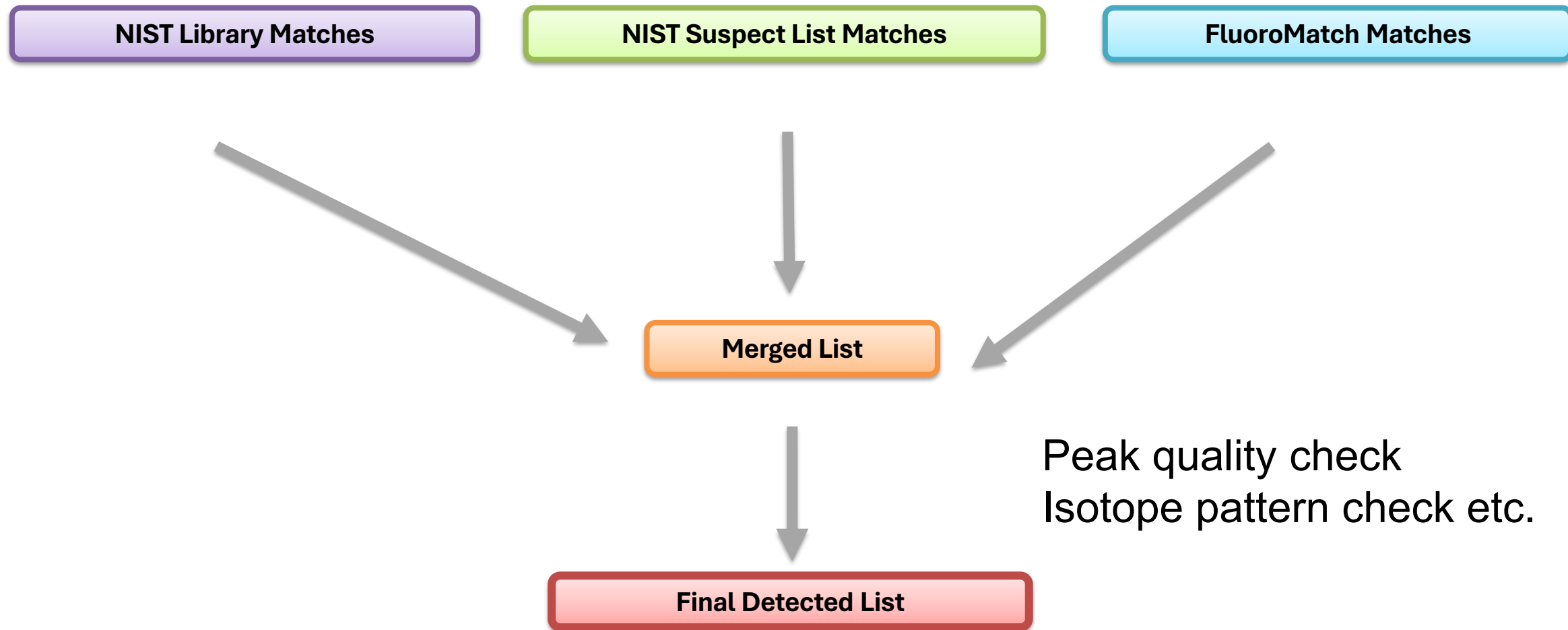
Data Processing Workflow

Three different, complementary workflows used, results combined and quality controlled



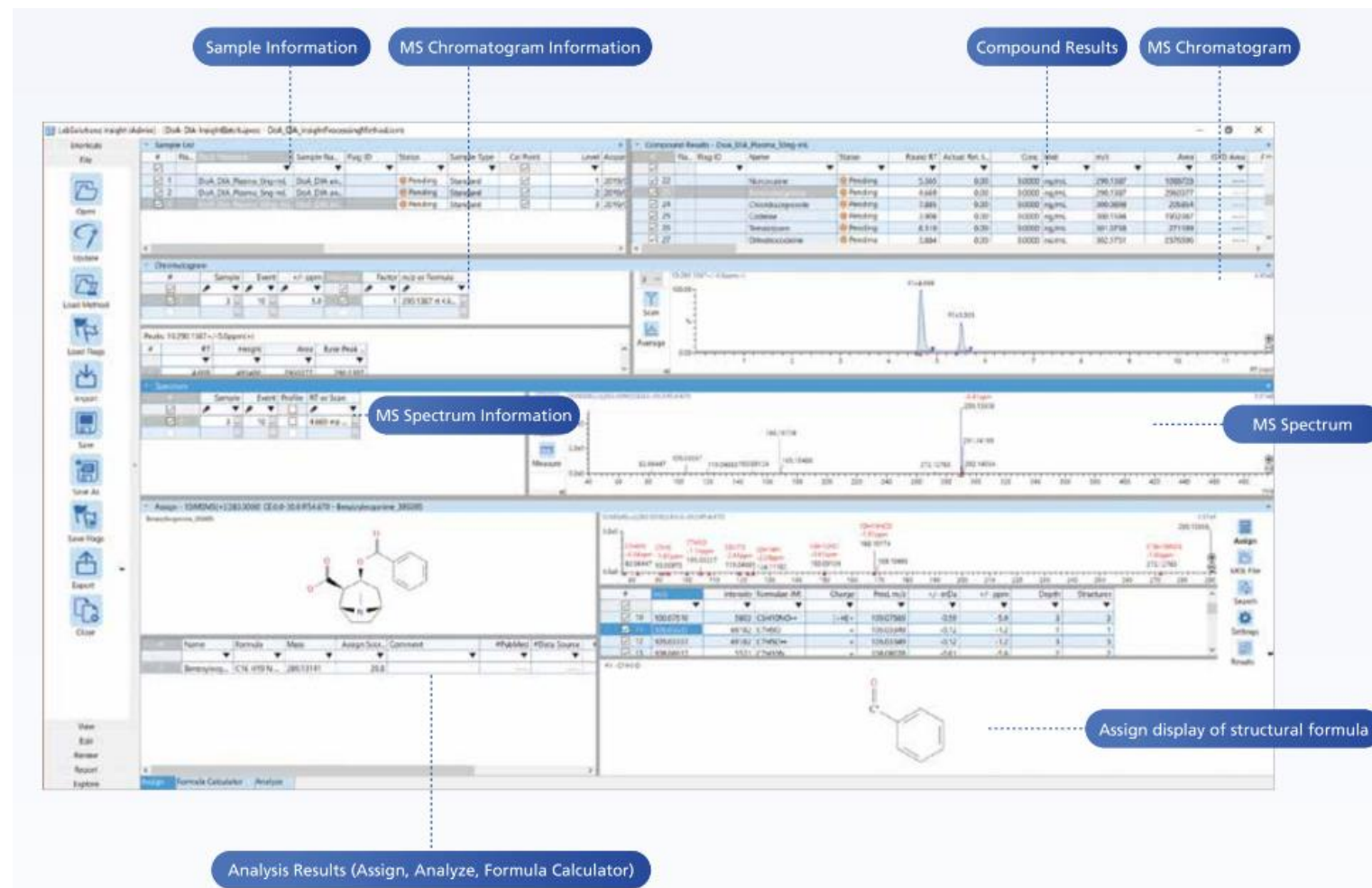
Data Processing Workflow

Three different, complementary workflows used, results combined and quality controlled



LabSolutions Insight Explore

- Shimadzu's commercial software for quantitative and qualitative analysis by QToF.
- Features library searching, elucidation of compound structure and sample composition.



NIST MS2 Spectrum Library Matching

NIST Library Matches

We converted the NIST library from the original form (SQLite DB) into Insight-readable form (.mlb)

Detected peaks with MS2 (DDA) spectra were searched against the library

NIST PFAS library conversion



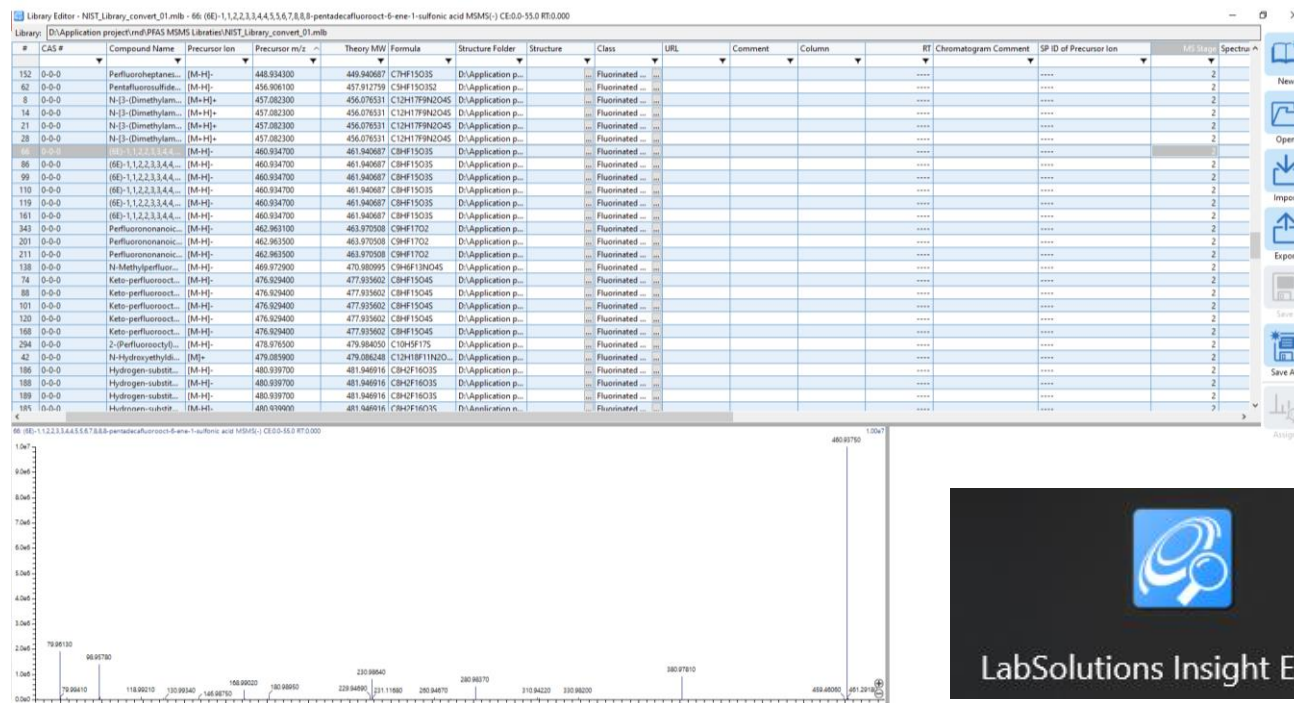
SQLite DB



Conversion criteria



.mlb



NIST Suspect List

NIST Suspect List Matches

Analyze - 240627_Setup_02_37_NIST-C-1X_Pos_036 - 1314 components found

Sample: 1

MS Event: ☐ MS/MS 1

Thresholds

Spectral Intensity: 1000

Response: Medium

User Defined Response: 100000

Analyze

Predict

Group

Spectrum

Chromatogram

#	m/z	RT	Response
592	485.05601	9.058	2720695
291	396.80118	3.719	634879
183	388.25372	2.434	560745
267	679.51112	3.442	543821
795	230.09601	11.823	535163
601	486.05906	9.053	525504
773	295.12270	11.581	513196
638	204.08046	9.527	491452
1027	313.14307	14.523	469068
74	297.99093	0.797	468937
687	671.08615	10.318	391706
978	399.25015	13.915	380721
541	471.04036	8.214	377327

Sample List

#	Acquired Date	Data Filename	Sample Name	Sample ID
14	6/27/2024 6:40:...	240627_Setup_0...	Blank_Neg	Blank_Neg
13	6/27/2024 7:11:...	240627_Setup_0...	Blank_Neg	Blank_Neg
12	6/27/2024 7:41:...	240627_Setup_0...	NIST-A-1X_Neg	NIST-A-1X_Neg_01
11	6/27/2024 8:12:...	240627_Setup_0...	NIST-B-1X_Neg	NIST-B-1X_Neg_01
10	6/27/2024 8:43:...	240627_Setup_0...	NIST-C-1X_Neg	NIST-C-1X_Neg_01
9	6/27/2024 9:13:...	240627_Setup_0...	Blank_Neg	Blank_Neg
8	6/27/2024 9:44:...	240627_Setup_0...	NIST-A-1X_Neg	NIST-A-1X_Neg_02
7	6/27/2024 10:15:...	240627_Setup_0...	NIST-B-1X_Neg	NIST-B-1X_Neg_02
6	6/27/2024 10:45:...	240627_Setup_0...	NIST-C-1X_Neg	NIST-C-1X_Neg_02
5	6/27/2024 11:16:...	240627_Setup_0...	Blank_Neg	Blank_Neg
4	6/27/2024 11:46:...	240627_Setup_0...	NIST-A-1X_Neg	NIST-A-1X_Neg_03
3	6/28/2024 12:17:...	240627_Setup_0...	NIST-B-1X_Neg	NIST-B-1X_Neg_03
2	6/28/2024 12:48:...	240627_Setup_0...	NIST-C-1X_Neg	NIST-C-1X_Neg_03
1	6/28/2024 11:32:...	240627_Setup_0...	NIST-C-1X_Pos	NIST-C-1X_Pos_03

Analyze - DDA - 240627_Setup_02_28_NIST-B-1X_Pos_027 - 8325 components found - 8325 precursors

Sample: 1

MS Event: ☒ MS/MS 2-8

Thresholds

Spectral Intensity: 1000

Response: Medium

User Defined Response: 100000

Analyze

Predict

Group

Spectrum

Chromatogram

#	n/z	RT	Response
1976	29.07821	8.424	2616132
2011	29.07400	8.501	1645241
1769	12.32029	7.943	1641744
1832	56.34545	8.101	1585397
2687	84.37803	10.100	1455757
2582	96.32949	9.861	1379884
2736	28.40711	10.210	1365290
2478	32.26062	9.622	1356087
1873	71.08864	8.194	1354746
4353	96.41692	13.938	1347112
4381	40.44384	14.004	1346546
2764	72.43107	10.273	1344055
3569	56.43762	12.102	1343955

Sample List

#	Acquired Date	Data Filename	Sample Name	Sample ID
14	6/28/2024 4:53:...	240627_Setup_0...	Blank Pos	Blank Pos
13	6/28/2024 5:24:...	240627_Setup_0...	Blank Pos	Blank Pos
12	6/28/2024 5:54:...	240627_Setup_0...	Blank Pos	Blank Pos
11	6/28/2024 6:25:...	240627_Setup_0...	NIST-A-1X_Pos	NIST-A-1X_Pos_01
1	6/28/2024 6:56:...	240627_Setup_0...	NIST-B-1X_Pos	NIST-B-1X_Pos_01
10	6/28/2024 7:26:...	240627_Setup_0...	NIST-C-1X_Pos	NIST-C-1X_Pos_01
9	6/28/2024 7:57:...	240627_Setup_0...	Blank Pos	Blank Pos
8	6/28/2024 8:28:...	240627_Setup_0...	NIST-A-1X_Pos	NIST-A-1X_Pos_02
2	6/28/2024 8:58:...	240627_Setup_0...	NIST-B-1X_Pos	NIST-B-1X_Pos_02
7	6/28/2024 9:29:...	240627_Setup_0...	NIST-C-1X_Pos	NIST-C-1X_Pos_02
6	6/28/2024 10:00:...	240627_Setup_0...	Blank Pos	Blank Pos
5	6/28/2024 10:30:...	240627_Setup_0...	NIST-A-1X_Pos	NIST-A-1X_Pos_03
3	6/28/2024 11:01:...	240627_Setup_0...	NIST-B-1X_Pos	NIST-B-1X_Pos_03
4	6/28/2024 11:32:...	240627_Setup_0...	NIST-C-1X_Pos	NIST-C-1X_Pos_03

Insight Explore using Analyze function for peak picking, matched against NIST suspect list

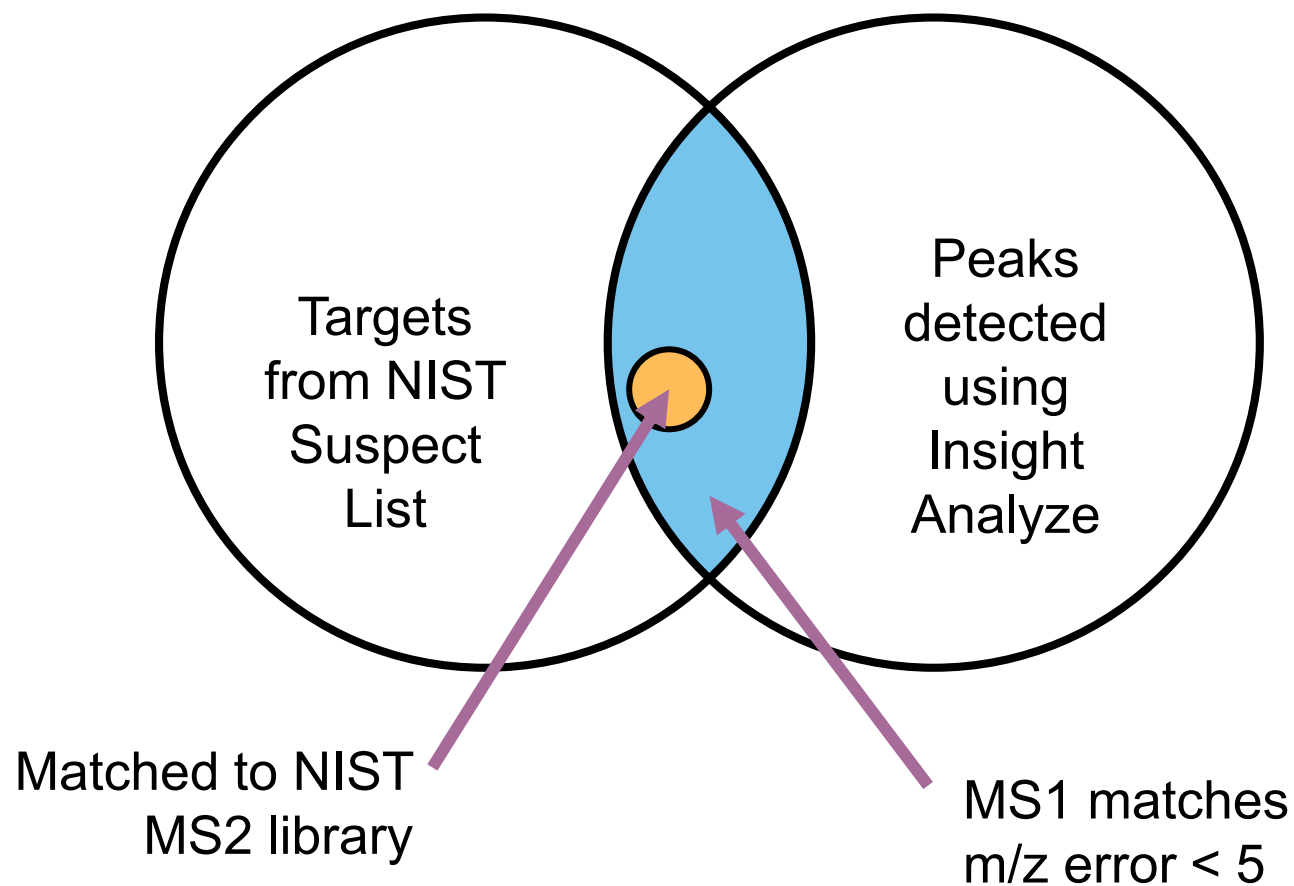
M+
M+H
M-H

NIST Suspect List Matches

NIST Suspect List Matches

Search these against MS2
DB from NIST to match a
few targets

Also search against known
common product ions and
neutral loss using custom
written C++ program



FluoroMatch Processing

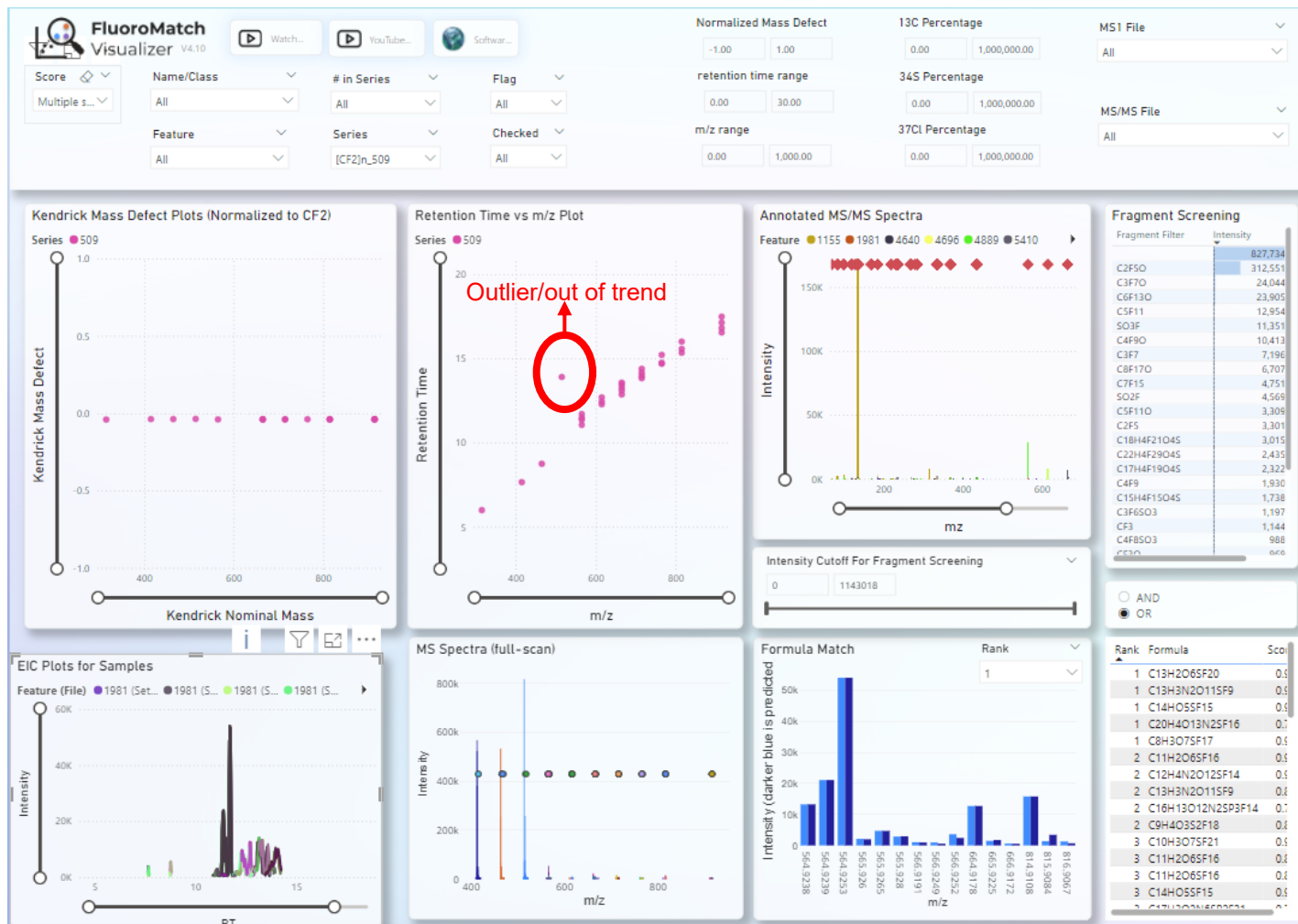
FluoroMatch Matches



- Negative mode DDA files were uploaded to FluoroMatch software.
- Internal library and Kendrick plots were used for identification.
- Results were visualized and further analyzed in Power BI.

FluoroMatch Processing

FluoroMatch Matches

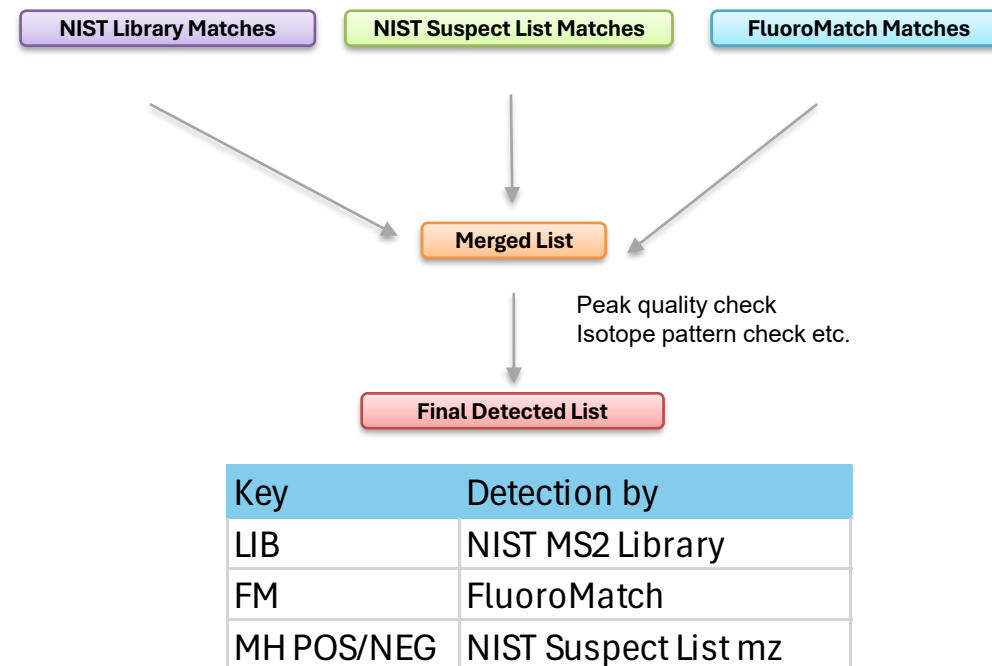


Each target was evaluated based on recommended scoring criteria. Identified matches were screened for outliers and false positives using Insight Explore.

Merging Detected Features

Merged List

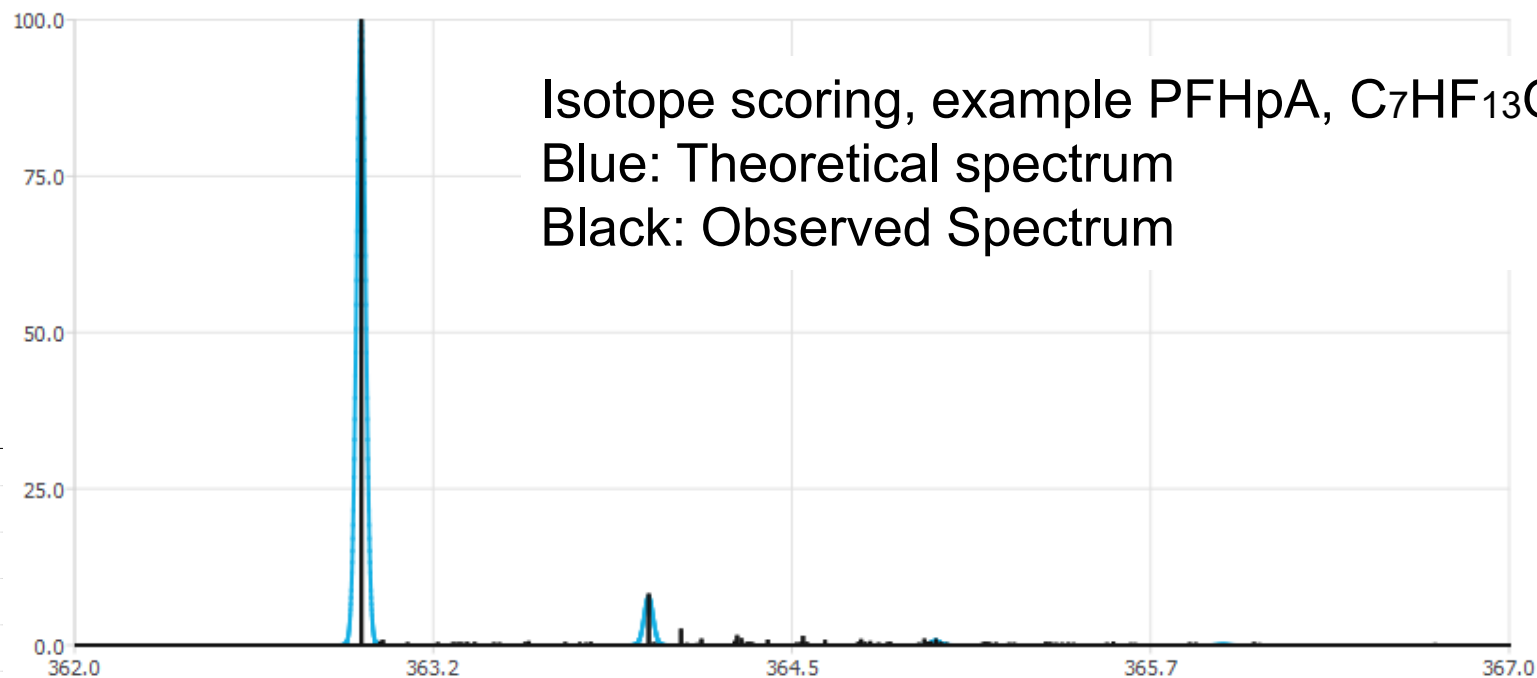
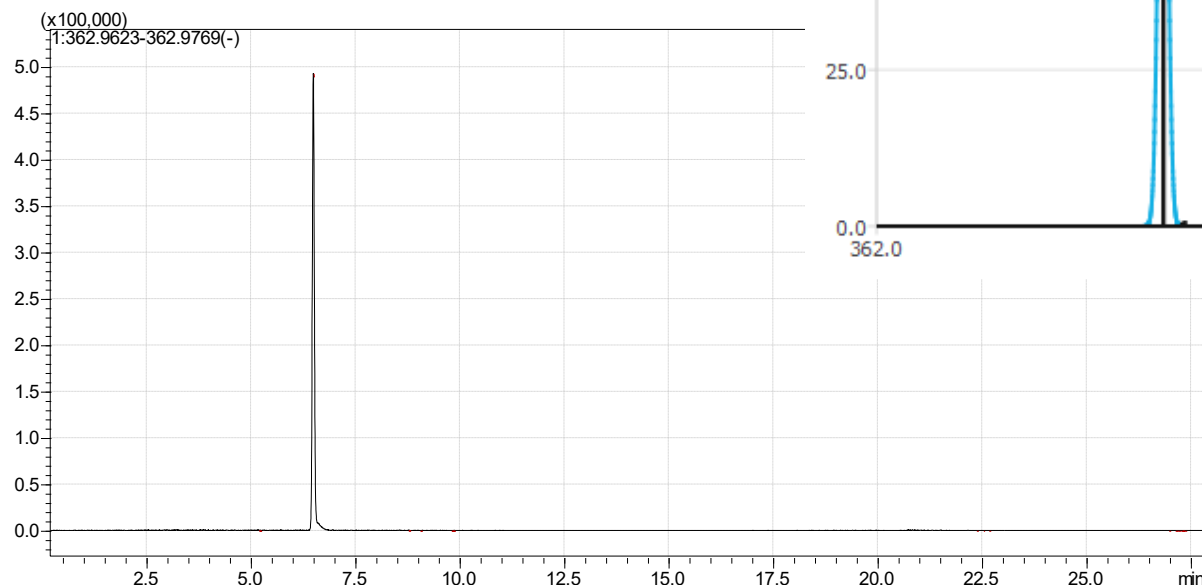
ID	INCHIKey	Files	Adduct	RT
51	SNGREZUHAYWORS-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	7.66133
52	ZWBAMYVPMDSJGQ-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	6.484
53	PXUULQAPEKKVAH-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	5.19533
58	QZHDEAJFRJCDMF-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	8.086
60	JGTNAGYHADQMCM-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	5.34978
71	CJZVOARZPASTAD-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2,	M-H	10.6688
163	VIONGDJUYAYOPU-UHFFFAOYSA-N	FMA1, FMA2, FMA3,	M-H	2.69233
166	AJMAYLFJZQYRHN-UHFFFAOYSA-N	FMA1, FMA2, FMA3,	M-H	5.195
182	INDOGKYZLAGEM-UHFFFAOYSA-N	FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	9.05633
200	PCIUEQPBYFRTEM-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	9.81378
201	UZUFPBIDKMEQEQ-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	8.76067
205	CXZGQIAOTKWDCB-UHFFFAOYSA-N	LIBA2, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	3.87743
225	TWDHAMRDYDLSPH-UHFFFAOYSA-N	FMA1, FMA2, FMA3,	M-H	6.48467
226	PUUPFOPNQLTVIU-OWOJBTEDSA-N	FMA1, FMA2, FMA3,	M-H	7.66333
227	IORHNHBOXCYSCM-UHFFFAOYSA-N	FMA1, FMA2, FMA3,	M-H	7.66067
235	BQOLVFQIEAAHQR-UHFFFAOYSA-N	FMA1, FMA2, FMA3,	M-H	10.373
333	YPJUNDFVDDCYIH-UHFFFAOYSA-N	LIBA1, LIBA2, LIBA3, FMA1, FMA2, FMA3, MHNEGA1, MHNEGA2, MHNEGA3,	M-H	2.69267
1001	WTVARZNOABXXMN-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	0.61433
1007	HGKNTSQKMGECCF-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	2.204
1011	ZQTIKDIHRRLSRV-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	3.87767
1013	UXPCZDYRRUONAJ-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	5.19433
1015	WXFBZGUXZMEPIR-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	5.19467
1021	JLMOIMFNFKVBGG-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	6.48267
1031	ADFQWOLUKYLWCE-OWOJBTEDSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	6.485
1033	UDLSJLBLOSNNHV-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	6.48267
1034	SKGBGOQHXBKAO-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	7.65967
1079	AWQSRASHARXGAH-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	7.65558
1087	IMFRQXJTPNCKAO-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	8.76233
1089	KBHBUUBXEQUIMV-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	8.76
1092	PCNHGPPSESDZSRB-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	8.76167
1098	FMEDKXCQTKWKE-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	9.80933
1103	IBDDYNPOMOFBDI-UHFFFAOYSA-N	MHNEGA1, MHNEGA2, MHNEGA3,	M-H	9.811



Features in the merged list were checked for peak quality, isotope score etc. to make the final list of detected features

Qualification of Features

Each match was qualified for isotope pattern, peak shape, RT in expected range etc.



Isotope scoring, example PFHpA, $C_7HF_{13}O_2$
Blue: Theoretical spectrum
Black: Observed Spectrum

Matches with poor peak or pattern quality were rejected. Peaks found in blanks were also rejected.

NIST Identification Criteria



Level 1a - Confirmed by reference standard

Level 1b - Indistinguishable from reference standard

Level 2a - Probable by library spectrum match

Level 2b - Probable by diagnostic fragmentation evidence

Level 2c - Probable by diagnostic homologue evidence

Level 3a - Positional isomer candidates

Level 3b - Fragmentation-based candidate

Level 3c - Circumstantial candidate based on fragmentation

Level 3d - Circumstantial candidate based on homologues

Level 4 - Unequivocal molecular formula

Level 5a - PFAS suspect screening exact mass match

Level 5b - Non-target PFAS exact mass of interest

Final Assignment Criteria

NIST Identification Criteria	Level 1a-5b
Multi platform match	NIST Library Match Suspect List Match FluoroMatch
Iso Score	>20
PPM error	<5
FlouroNatch Score	>C+
Number of Matching Neutral loss	>1

Final Assignment of Scores

Final Detected List

ID	INCHIKey		Files	Adduct	RT	Initial mz obs	Intensity	Theor	Insight formula (adduct corrected)	IsoScore	Found MZ	Corrected MZ	ppm err	Comment	Fluorimetry Scoring	All Keys	Number of common product ions	Common product ions	Number of NL	NL
51	SNGREZUHAYWORS-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	7.6613	412.9678	2139492	412.966426	C8HF15O2	71.34	412.968	412.96737	2.29	A	Level 2b	CAHRYLWSN	27	13,368.977419,11	6	177419,368.97
52	ZWBAMYVPMDSJGQ-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	6.484	362.970945	1769386	362.969619	C7HF13O2	72.06	362.971	362.97037	2.07	A	Level 2b	NEHOYPPKUM	17	17,318.979669,11	4	318.979669,
53	PXUULQAPEKVAH-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	5.1953	312.973711	1176032	312.972813	C6HF11O2	92.38	312.974	312.97337	1.78	A	Level 2b	XUULQAPEK	7	1,992815,268.983	2	268.983598,
58	QZHDEAFHJCDMF-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	8.086	398.937989	4549963	398.936605	C6HF13O3S	70.6	398.938	398.93737	1.92	A	Level 2b	ZHDEAFHJCD	35	9,949221,79.957	0	NA
60	JGTNAGYHADQMCM-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	5.3498	298.943922	2535585	298.942992	C4HF9O3S	75.38	298.944	298.94337	1.26	A	Level 2b	GWJUODILLO	35	1,168.989315,218	3	218.988347,
71	CJZVOARZPASTAD-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	10.669	514.902587	4903386	514.900667	C8HClF16O3S	50.67	514.903	514.90237	3.31	A-	Level 2b	CJZVOARZPAS	39	11,98.955841,129	0	NA
163	VIONGDJUYAYOPU-UHFFFAOYSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	2.6923	426.9675	6159	426.967905	C8H5F13O3S	24.72	426.967	426.96637	-3.60	B	Level 2c	VIONGDJUYAY	0	NA	0	NA
166	AJMAYLFJZQYRHN-UHFFFAOYSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	5.195	626.9554	10197	626.95513	C12H5F21O3S	68.84	626.955	626.95437	-1.21	B	Level 2c	AJMAYLFJZQY	0	NA	0	NA
182	INDOGKYZYLAGEM-UHFFFAOYSA-N	Level 2b - Probable by diagnostic fragmentation evidence	FMA1, F1A2, F	M-H	9.0563	483.043566	1424051	483.041738	1H13F13N2C	69.8	483.043	483.04237	1.31	A	Level 2b	OLNFCFQUIY	26	979226,118.9925	0	NA
200	PCIUEQPBVFRTM-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	9.8138	512.9613	2215343	512.960038	C10HF19O2	68.49	512.962	512.96137	2.60	A	Level 2b	ZUSAXRVION	38	17,118.993166,16	7	172181,468.97
201	UZUFPBIDKMEQE-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	8.7607	462.9645	2130724	462.963232	C9HF17O2	69.52	462.965	462.96437	2.46	A	Level 2b	ZUZFPBIDKME	24	17,118.992619,16	6	173140,418.97
205	CXZGQIAOTKWCDU-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	3.8774	262.976801	740682	262.976007	C5HF9O2	90.52	262.977	262.97637	1.38	C+	Level 3d	CXZGQIAOTKW	1	NA	1	NA
225	TWDHAMRDYDLSPH-UHFFFAOYSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	6.4847	274.9773	12891	274.97601	C6HF9O2	41.08	274.977	274.97637	1.31	B+	Level 2c	WDHAMRDY	0	NA	0	NA
226	PUUPFOPNQLTVIU-OWOJBTEDSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	7.6633	324.9744	15103	324.97281	C7HF11O2	60.11	324.974	324.97337	1.72	B+	Level 2c	PUUPFOPNQL	0	NA	0	NA
227	IORHNHBOXCYSCM-UHFFFAOYSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	7.6607	494.9713	15100	494.96946	C10H2F18O2	32.43	494.971	494.97037	1.84	B+	Level 2c	ORHNHBOXC	0	NA	0	NA
235	BQQLVFQIEAAHQ-R-UHFFFAOYSA-N	Level 2c - Probable by diagnostic homologue evidence	FMA1, F1A2, F	M-H	10.373	580.9346	9091	580.93325	C10H2F20O3S	39.89	580.935	580.93437	1.93	B+	Level 2c	BQQLVFQIEAA	0	NA	0	NA
333	YPJUNDVDDCYIH-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	2.6927	212.979389	476710	212.9792	C4HF7O2	95.5	212.98	212.97937	0.80	A	Level 2b	JDMCDWHX	3	168.989327,	3	168.989327,
1001	WTVARZNOABXMXN-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	0.6143	223.0206	38059	223.019922	C6H6F6O2	72.19	223.02	223.01937	-2.48	NA	FALSE	VTVARZNOAB	0	NA	0	NA
1007	HGKNTSQKMGCECF-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	2.204	249.027767	129835	249.026819	C7H5F7N2	52.87	249.027	249.02637	-1.80	NA	FALSE	HGKNTSQKMC	0	NA	0	NA
1011	ZQTIKDIHRRLSRV-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	3.8777	218.9869	650854	218.986177	C4HF9	90.92	218.987	218.98637	0.88	NA	FALSE	ZQTIKDIHRRLS	0	NA	0	NA
1013	UXPCZDYRRUONAJ-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	5.1943	374.974667	38205	374.974292	C10H5F9O3S	74.58	374.974	374.97337	-2.46	NA	FALSE	UXPCZDYRRU	10	12,268.982429,26	0	NA
1015	WXFBZGUXZMEPIR-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	5.1947	268.9839	911355	268.982984	C5HF11	90.4	268.984	268.98337	1.44	NA	FALSE	WXFBZGUXZM	3	118.991885,	0	NA
1021	JLMOIMFNFKVBGG-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	6.4827	424.971433	46058	424.970013	C8H3F13O5	65.48	424.971	424.97037	0.84	NA	FALSE	JLMOIMFNFKV	13	12,118.997576,16	0	NA
1031	ADFQWOLUKYLWCE-OWOJBTEDSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	6.485	296.978967	611440	296.977898	C6HF11O	71.74	296.979	296.97837	1.59	NA	FALSE	ADFQWOLUKY	15	1,992436,168.990	0	NA
1033	UDLSJLBLIOSNHV-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	6.4827	230.9869	47462	230.986177	C5HF9	86.98	230.987	230.98637	0.83	NA	FALSE	UDLSJLBLIOSH	0	NA	0	NA
1034	SKGBGOQHXBKAKO-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	7.6597	369.981267	96345	369.980106	C7H6F9NO4S	79.97	369.981	369.98037	0.71	NA	FALSE	SKGBGOQHXB	0	NA	0	NA
1079	AWQSRASHARXGAH-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	7.6556	280.983908	86267	280.982984	C6HF11	96.75	280.984	280.98337	1.37	NA	FALSE	AWQSRASHAP	0	NA	0	NA
1087	IMFRQJXTPNCKAO-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	8.7623	330.980967	113247	330.97979	C7HF13	69.49	330.981	330.98037	1.75	NA	FALSE	IMFRQJXTPNCK	0	NA	0	NA
1089	KBHBUUBXEQUIMV-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	8.76	418.9749	1068259	418.973403	C8HF17	71.35	418.975	418.97437	2.31	NA	FALSE	KBHBUUBXEQU	11	1,989337,218.986	0	NA
1092	PCNHGSPESDZSRB-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	8.7617	396.9729	1150531	396.971511	C8HF15O	71.35	396.973	396.97237	2.16	NA	FALSE	PCNHGSPESDC	19	17,180.989960,21	0	NA
1098	FMEDKXCQTKWGKE-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	9.8093	574.962167	44816	574.960432	C11H3F19O5	63.9	574.961	574.96037	-0.11	NA	FALSE	FMEDKXCQTK	14	14,168.991691,21	0	NA
1103	IBDDYNPOMOFBDI-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	9.811	380.9779	157932	380.976596	C8HF15	71.36	380.978	380.97737	2.03	NA	FALSE	IBDDYNPOMOF	10	13,118.992057,38	0	NA
1104	CUNIPPSHVAZKID-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	9.8113	468.9719	921562	468.970209	C9HF19	70.54	468.972	468.97137	2.48	NA	FALSE	CUNIPPSHVAZ	17	10,218.987011,26	0	NA
1111	AQGBOPDJGMMNAKJ-UHFFFAOYSA-N	Level 5a - PFAS suspect screening exact mass match	MHNEG-1, MI	M-H	0.6147	305.0242	42319	305.022957	C8H7F9O2	69.7	305.024	305.02337	1.36	NA	FALSE	AQGBOPDJGMM	0	NA	0	NA
1137	BSJCNKQSUXNNNN-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	6.4837	318.980967	1244182	318.97979	C6HF13	71.56	318.981	318.98037	1.82	NA	FALSE	BSJCNKQSUSU	7	1,992683,168.991	0	NA
1144	IBDDMESLXNZRNC-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	7.6613	474.9683	48607	474.96682	C9H3F15O5	70.36	474.968	474.96737	1.16	NA	FALSE	IBDDMESLXNZ	16	1,97585,168.9894	0	NA
1195	AJHOIKILYAOBA-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	8.565	499.0383	190719	499.036653	1H13F13N2C	65.92	499.038	499.03737	1.44	NA	FALSE	AJHOIKILYAO	17	17,168.989857,31	0	NA
1206	LQBYFRXNVGCFID-UHFFFAOYSA-N	Level 4 - Unequivocal molecular formula	MHNEG-1, MI	M-H	8.761	524.965667	44003	524.963626	C10H3F17O5	63.9	524.965	524.96437	1.42	NA	FALSE	LQBYFRXNVG	14	1,980980,168.992	0	NA
56	YFSUTJLHUFNCNZ-UHFFFAOYSA-N	Level 2a - Probable by library spectrum match	LIBA1, U3A2, I	M-H	10.372	498.931587	5165237	498.930218	C8HF17O3S	63.72	498.933	498.93211	3.79	A	Level 2b	YZNUCXUQH	62	55757,118.99228	0	NA

Submission of Results to NIST

	B	C	D	E	F	G	H
1		Back to General Instructions			Did you use MSMatch for compound identification?		
2			Measured				
3	uspect List I	Suspect List Preferred Name	recursor m>ention Time (mi	Ion State	Identification Confidence		
4	NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	499.07173	8.98 [M] ⁺	Level 2a - Probable by library spectrum match		
5	NISTPFA000	N-dimethyl ammonio propyl perfluoropropane sulfonate	407.08661	3.94 [M+H] ⁺	Level 2a - Probable by library spectrum match		
6	NISTPFA000						
7	NISTPFA000						
8	NISTPFA000						
9	NISTPFA000	Back to General Instructions			Did you use MSMatch for compound identification?		
10	NISTPFA000		Measured				
11	NISTPFA000	uspect List I	Suspect List Preferred Name	recursor m>ention Time (mi	Ion State	Identification Confidence	
12	NISTPFA000	4 NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	499.07173	8.98 [M] ⁺	Level 2a - Probable by library spectrum match	
13	NISTPFA000	5 NISTPFA000	N-dimethyl ammonio propyl perfluoropropane sulfonate	407.08661	3.94 [M+H] ⁺	Level 2a - Probable by library spectrum match	
14	NISTPFA000	6 NISTPFA000	3-(N-(3-(dimethylamino)propyl)-perfluoropentyl)sulfonate	507.08046	6.28 [M+H] ⁺	Level 2a - Probable by library spectrum match	
15	NISTPFA000	7 NISTPFA000	N,N,N-trimethyl-N-[(N?2-carboxyethyl)-3-perfluoroalkyl]ammonio propyl perfluoropropane sulfonate	571.09239	8.19 [M] ⁺	Level 2a - Probable by library spectrum match	
16	NISTPFA000	8 NISTPFA000	N-(3-(dimethylamino)propyl)-N-[(tridecafluorohexyl)sulfonamido]butane sulfonamide	557.07726	7.41 [M+H] ⁺	Level 2a - Probable by library spectrum match	
17	NISTPFA000	9 NISTPFA000	N-(3-(dimethylamino)propyl)-N-[(nonafluorobutyl)sulfonamido]butane sulfonamide	457.08357	5.1 [M+H] ⁺	Level 2a - Probable by library spectrum match	
18	NISTPFA000	10 NISTPFA000	Perfluoropentane sulfonamide amine	435.05911	7.65 [M+H] ⁺	Level 2a - Probable by library spectrum match	
19	NISTPFA000	11 NISTPFA000	Perfluorohexane sulfonamide amine	485.05612	9.05 [M+H] ⁺	Level 2a - Probable by library spectrum match	
20	NISTPFA000	12 NISTPFA000	Perfluorobutane sulfonamide amine	385.06239	6.07 [M+H] ⁺	Level 2a - Probable by library spectrum match	
21	NISTPFA000	13 NISTPFA000	N-carboxyethyl dimethyl ammonio propyl perfluoromethyl sulfonate	357.08962	2.88 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
22	NISTPFA000	14 NISTPFA000	N,N,N-trimethyl-N-[(N?2-carboxyethyl)-3-perfluoroalkyl]ammonio propyl perfluoropropane sulfonate	421.10221	3.8 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
23	NISTPFA000	15 NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	349.08116	3.98 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
24	NISTPFA000	16 NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	443.06778	4.97 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
25	NISTPFA000	17 NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	399.0781	5.39 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
26	NISTPFA000	18 NISTPFA000	N,N,N-trimethyl-N-[(N?2-carboxyethyl)-3-perfluoroalkyl]ammonio propyl perfluoropropane sulfonate	471.09329	5.81 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
27	NISTPFA000	19 NISTPFA000	4,2-Fluorotelomer sulfonamide propyl hydroxy dimethyl sulfonate	429.08861	5.99 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
28	NISTPFA000	20 NISTPFA000	N-(2-carboxyethyl)-3-(N-(2-carboxyethyl)-perfluoroalkyl)ammonio propyl perfluoropropane sulfonate	629.09337	5.99 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
29	NISTPFA000	21 NISTPFA000	N,N,N-trimethyl-N-[(N?2-carboxyethyl)-3-perfluoroalkyl]ammonio propyl perfluoropropane sulfonate	521.09595	6.11 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
30	NISTPFA000	22 NISTPFA000	8,2-Fluorotelomer sulfonamide betaine	671.08574	10.3 [M] ⁺	Level 2a - Probable by library spectrum match	
31	NISTPFA000	23 NISTPFA000	N-(3-perfluoroalkyl-N?2-methylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	413.03346	6.76 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
32	NISTPFA000	24 NISTPFA000	6,2-Fluorotelomer sulfonamide amine	513.08757	9.62 [M+H] ⁺	Level 2a - Probable by library spectrum match	
33	NISTPFA000	25 NISTPFA000	N-(3-perfluoroalkylsulfonamidopropan-1-yl)-N,N,N-trimethylammonio propyl perfluoropropane sulfonate	449.07438	6.79 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
34	NISTPFA000	26 NISTPFA000	6,2-Fluorotelomer thia hydroxy propyl trimethyl ammonio propyl perfluoropropane sulfonate	496.09738	10.02 [M] ⁺	Level 2a - Probable by library spectrum match	
35	NISTPFA000	27 NISTPFA000	6,2-Fluorotelomer sulfonamidopropyl trimethyl ammonio propyl perfluoropropane sulfonate	512.09217	7.72 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
36	NISTPFA000	28 NISTPFA000	N,N-dimethyl-N-2-hydroxyethyl-N-(3-perfluoroalkylsulfonamido)butane sulfonamide	629.07541	10.69 [M] ⁺	Level 2a - Probable by library spectrum match	
37	NISTPFA000	29 NISTPFA000	N,N-dimethyl-N-2-hydroxyethyl-N-(3-perfluoroalkylsulfonamido)butane sulfonamide	529.08049	8.47 [M] ⁺	Level 4 - Unequivocal molecular formula	
38	NISTPFA000	30 NISTPFA000	N-(2-Carboxyethyl)-N,N-dimethyl-N-[(methyl(perfluorooctyl)sulfonamido)propyl]ammonio propyl perfluoropropane sulfonate	593.1241	9.17 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
39	NISTPFA000	31 NISTPFA000	N-(2-carboxyethyl)-N,N-dimethyl-N-[(ethyl(perfluorooctyl)sulfonamido)propyl]ammonio propyl perfluoropropane sulfonate	585.10841	10 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
40	NISTPFA000	32 NISTPFA000	N,N,N-trimethyl-N-[(N?2-hydroxyethyl)-N-(2-hydroxy-3-sulfonamidopropyl)ammonio]propyl perfluoropropane sulfonate	967.06045	16.82 [M] ⁺	Level 5a - PFAS suspect screening exact mass match	
41	NISTPFA000	33 NISTPFA000	Undecafluorohexanoyl chloride	332.95204	0.62 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
42	NISTPFA000	34 NISTPFA000	4,2-Fluorotelomer sulfate;4,2-Fluorotelomer sulfate	344.98453	0.62 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
43	NISTPFA000	35 NISTPFA000	25,26,26,26,27,27,27-Heptafluorocholest-5-ene-3,7-diol	529.23201	2.61 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
44	NISTPFA000	36 NISTPFA000	N-dimethyl ammonio propyl perfluoroethane sulfonamide	285.06878	3.1 [M+H] ⁺	Level 4 - Unequivocal molecular formula	
45	NISTPFA000	37 NISTPFA000	N-dimethyl ammonio propyl perfluoropropane sulfonate	335.06571	4.5 [M+H] ⁺	Level 4 - Unequivocal molecular formula	
46	NISTPFA000	38 NISTPFA000	2-(N-Ethyl-N-(perfluorooctylsulfonamido)ethyl acrylate	626.0306	7.15 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
47	NISTPFA000	39 NISTPFA000	6,2-Fluorotelomer sulfonamidopropyl propanamide dimethyl ethyl sulfonate	604.0489	7.15 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
48	NISTPFA000	40 NISTPFA000	(2F)-2-(Acetoxyl)-3-(hexadecafluoropropyl)heptafluorooctanoate	555.29147	7.97 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
49	NISTPFA000	41 NISTPFA000	Octan-2-yl heptafluorobutanoate	327.1209	8.59 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		42 NISTPFA000	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptafluoro-10-isoocyl	490.01161	8.75 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		43 NISTPFA000	2-Fluoro-3-(4-fluoro-2-nitrobenzamido)-N-[(4-(1,1,2,3,3,4,4,5,5,6,6,7,7,8,8,8,9,9,10,10,10-Heptafluoro-2-methyl-2-((1H,1H,2H,2H-perfluoroalkyl)thio)propyl)ammonio]propyl]perfluoropropane sulfonate	594.10894	8.88 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		44 NISTPFA000	2-methyl-2-((1H,1H,2H,2H-perfluoroalkyl)thio)propyl	588.05393	9.07 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		45 NISTPFA000	1,1,1,2,2,3,3,4,4,11,11,12,12,13,13,14,14,14-Octadecafluorotetradecane	523.07169	9.92 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		46 NISTPFA000	4,2-Fluorotelomer sulfate;4,2-Fluorotelomer sulfate	344.9843	27.39 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	
		47 NISTPFA000	S-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptafluoro-2-methyl-2-((1H,1H,2H,2H-perfluoroalkyl)thio)propyl)ammonio propyl perfluoropropane sulfonate	523.00056	3.78 [M+H] ⁺	Level 5a - PFAS suspect screening exact mass match	

Number of detected features

Sample	Pos	Neg	Total
A	9	40	49
B	44	57	101
C	29	105	134

NIST Interlaboratory Study Results

Sample A – PFAS standards

Compound Name	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS002640 - Perfluoroheptanoic acid	2a	2b	2a	2c	1a	1a	1a	1a	1a	2b	3d	1a	1a	1a	1a	2a		1a	1a	1a	1a	2b	1a	1a	2a	1a	1a	1a	96%
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	3d	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	3b	2a	1a	1a	1a	96%
NISTPFAS002635 - Perfluorononoic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002643 - Perfluorohexanoic acid	2a	2c	2a	2c	1a		1a	1a	1a	2b	3d	1a	1a	1a	1a	4	1a	1a	1a	1a	1a	2c	1a		2a	1a	1a	1a	93%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1a	1a	2b	2a	1a	1a	1a	1a		2b	1a	1a	1a	1a	3b	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a		2a	1a	1a	1a	89%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	2b	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a		1a	1a	1a	1a	3b	2a	1a	1a	1a	89%
NISTPFAS000878 - Perfluorohexane sulfomido amine			2a	3c	1a	4	2b	3c	2a	2b	2b	4	4	2b	3b		2b	2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	85%
NISTPFAS002632 - Perfluorodecanoic acid	2a		2a	2c		1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	85%
NISTPFAS003238 - Chloro-perfluorooctane sulfote	2a		2a	3b	1b		2c	3c	2a		2b	1a	2a	1b	2a	2a	2b			2a	1a	2c	1b	3d	2a	2a	2a	1a	81%
NISTPFAS002646 - Perfluoropentanoic acid			2a	2c	1a		1a	1a	1a	2b	3d	1a	1a	1a	1a			1a	1a	1a	1a	3b	1a		2a	1a	1a	1a	78%
NISTPFAS002649 - Perfluorobutanoic acid	2a		2a	2c	1a		1a	1a	2a		2a	1a	1a	1a	1a			1a	1a	1a	1a	4			2a	1a	1a	1a	74%
NISTPFAS000852 - Perfluorohexane sulfomido amine oxide		2c	4	2b		2c			4				1a		4				3a		3c	3b					1a	1a	41%
NISTPFAS002560 - Perfluorohexanesulfomide			2b		1b		2b		1a	2b	2a			1a				1a	1b						2a			1a	37%
NISTPFAS003794 - 5:3 Fluorotelomer betaine			2a								3c								1a	2a		4			2a		2a	1a	26%
NISTPFAS004053 - Dihydrogen-substituted fluoro triether tridecanoic acid			4			4			2c		4	4												3d			4	2c	26%
NISTPFAS004634 - Dihydrogen-substituted fluoro triether undecanoic acid			4			4			2c		4	4		5a														2c	22%
NISTPFAS002338 - 1H-Perfluoronone			4												5b		2b					2a		3d				2a	19%
NISTPFAS002342 - 8H-Perfluorooctane			4			4									5b							2a		3d				2a	19%
NISTPFAS002350 - 1,1,1,2,2,3,3,4,4,5,5-Undecafluoropentane			4												5b		2c					2c		3d				2c	19%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

NIST Interlaboratory Study Results

Sample A – PFAS standards

Compound Name	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS002640 - Perfluoroheptanoic acid	2a	2b	2a	2c	1a	1a	1a	1a	1a	2b	3d	1a	1a	1a	1a	2a		1a	1a	1a	1a	2b	1a	1a	2a	1a	1a	1a	96%
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	3d	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	3b	2a	1a	1a	1a	96%
NISTPFAS002635 - Perfluorononoic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002643 - Perfluorohexanoic acid	2a	2c	2a	2c	1a		1a	1a	1a	2b	3d	1a	1a	1a	1a	4	1a	1a	1a	1a	1a	2c	1a		2a	1a	1a	1a	93%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1a	1a	2b	2a	1a	1a	1a	1a		2b	1a	1a	1a	1a	3b	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a		2a	1a	1a	1a	89%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	2b	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a		1a	1a	1a	1a	3b	2a	1a	1a	1a	89%
NISTPFAS000878 - Perfluorohexane sulfonamide			2a	3c	1a	4	2b	3c	2a	2b	2b	4	4	2b	3b		2b	2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	85%
NISTPFAS002632 - Perfluorodecanoic acid	2a		2a	2c		1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	85%
NISTPFAS003238 - Chloro-perfluorooctane sulfonate	2a		2a	3b	1b		2c	3c	2a		2b	1a	2a	1b	2a	2a	2b			2a	1a	2c	1b	3d	2a	2a	2a	1a	81%
NISTPFAS002646 - Perfluoropentanoic acid			2a	2c	1a		1a	1a	1a	2b	3d	1a	1a	1a	1a			1a	1a	1a	1a	3b	1a		2a	1a	1a	1a	78%
NISTPFAS002649 - Perfluorobutanoic acid	2a		2a	2c	1a		1a	1a	2a		2a	1a	1a	1a	1a			1a	1a	1a	1a	4			2a	1a	1a	1a	74%
NISTPFAS000852 - Perfluorohexane sulfonamide oxide		2c	4	2b		2c			4				1a		4				3a		3c	3b					1a	1a	41%
NISTPFAS002560 - Perfluorohexanesulfonamide			2b		1b		2b		1a	2b	2a			1a				1a	1b						2a			1a	37%
NISTPFAS003794 - 5:3 Fluorotelomer betaine			2a								3c								1a	2a		4			2a		2a	1a	26%
NISTPFAS004053 - Dihydrogen-substituted fluoro triether tridecanoic acid			4			4			2c		4	4												3d			4	2c	26%
NISTPFAS004634 - Dihydrogen-substituted fluoro triether undecanoic acid			4			4			2c		4	4		5a														2c	22%
NISTPFAS002338 - 1H-Perfluoronone			4												5b		2b					2a		3d				2a	19%
NISTPFAS002342 - 8H-Perfluorooctane			4			4									5b							2a		3d				2a	19%
NISTPFAS002350 - 1,1,1,2,2,3,3,4,4,5,5-Undecafluoropentane			4												5b		2c					2c		3d				2c	19%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

NIST Interlaboratory Study Results

Sample B – AFFF extract

Compound Name	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	2b	2a	2c	1a	1a	1a	1b	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	96%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a		1a	1a	1a	1a	1a	2a	1a	1a	1a	89%
NISTPFAS003044 - Perfluoropentanesulfonic acid	2a	2b	2a	2c	1a	4	1a	5a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a		1a	5a	2a		1a	1a	85%
NISTPFAS003052 - 6:2 Fluorotelomer sulfonic acid	2a		2a	2c	1a	1a	1a		1a	2b	2a	4	1a		1a	2a	2b	1a		1a	1a	1a	1a	1a	2a	1a	1a	1a	85%
NISTPFAS000878 - Perfluorohexane sulfomido amine		2c	2a	2b	2a		2b	3c	2c	2b	2b	4	4	2b	2a			2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	81%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b		1a	1a	1a	1a			1a	1a	1a	1a		1a	1a	2a	1a	1a	1a	81%
NISTPFAS003285 - 6:2 Fluorotelomer thia propionoamido dimethyl ethyl sulfote	2a	2b	2a	3b		2a		2a	2a	2b	2b	4		2a	2a		2b		2b	2a	2a		4	3d	2a	2a	2a	2a	78%
NISTPFAS000880 - Perfluorobutane sulfomido amine		2c	2a	2b	3d		2c		2c	2c	5b	4	4	2a	3c			2c		2a	2a		3d	5a	2b		2a	2a	70%
NISTPFAS002643 - Perfluorohexanoic acid	2a	2c	2b	2b	1a		1a	1b	1a	2b	3d	4	1a		1a			3d	1a	1a	1a				2a		1a	1a	70%
NISTPFAS000879 - Perfluoropentane sulfomido amine		2c	2a	2c	3c	4	2b		2b	2c	2b			2a	2c			2c		2a	2a	4	3d		2b		2a	2a	67%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2c	2a	2c	1a		1a			2b	2a	1a	1a	1a	1a			3d	1a	1a	1a				2a		1a	1a	67%
NISTPFAS003042 - Perfluoroheptanesulfonic acid		3d	2a	2b	1a	4	1a		1a	2b	2a	1a			2a			1a	1a	1a	1a	3a	1a		2a			1a	67%
NISTPFAS003492 - Perfluoropropane sulfote	4	3b	3d	2b	2c		2b		1a	2b	3b		2a			4		1a	1a	2a	1a		1a		2a		1a	1a	67%
NISTPFAS003407 - 6:2 Fluorotelomer sulfinyl propamido dimethyl ethyl sulfote			2a			2b			2a	2b	2b		2b		2a		2b		2b	3c	2a	2a		5a	2a		2b	2a	56%
NISTPFAS003430 - 3-(N-(3-(dimethylamino)propyl)- perfluoropentylsulfomido)propanoic acid	4	2c	2a	2c		2b			2a	3d			2c		4			2c		2a	2a	4		5a			2a	2a	56%
NISTPFAS003455 - N-Dimethyl ammonio propyl perfluoropropane sulfomide		2c	3d	2b	3c		2b		2a	2c	2b		4		2c	4					3d			5a	2b		2b	2a	56%
NISTPFAS000881 - 6:2 Fluorotelomer sulfomide amine			2a	2b					2b		2b	4	3c		2a				2b	2a	2a	4		5a	2a		2b	2a	52%
NISTPFAS004390 - 6:2 Fluorotelomer thia ammoniohydroxypropyl ethanoic acid			5a			2b			3a			4	4	5a	4		2b		3a	3c	4	3a		5a			3b	2b	52%
NISTPFAS000861 - N-[3-(Dimethylamino)propyl]-N- [(tridecafluorohexyl)sulfonyl]-beta-alanine	2a	2c	2a	2c					3b	2c		4						2c	3b		2a	4		5a			2a	2a	48%
NISTPFAS000862 - N-[3-(Dimethylamino)propyl]-N- [(nofluorobutyl)sulfonyl]-beta-alanine	4	2c	2a	2c		4			3a	2c	2b							2c			2a	4					2a	2a	44%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

NIST Interlaboratory Study Results

Sample B – AFFF extract

Compound Name	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	2b	2a	2c	1a	1a	1a	1b	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	96%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	2c	2a	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a		1a	1a	1a	1a	1a	2a	1a	1a	1a	89%
NISTPFAS003044 - Perfluoropentanesulfonic acid	2a	2b	2a	2c	1a	4	1a	5a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a		1a	5a	2a		1a	1a	85%
NISTPFAS003052 - 6:2 Fluorotelomer sulfonic acid	2a		2a	2c	1a	1a	1a		1a	2b	2a	4	1a		1a	2a	2b	1a		1a	1a	1a	1a	1a	2a	1a	1a	1a	85%
NISTPFAS000878 - Perfluorohexane sulfomido amine		2c	2a	2b	2a		2b	3c	2c	2b	2b	4	4	2b	2a			2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	81%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b		1a	1a	1a	1a			1a	1a	1a	1a		1a	1a	2a	1a	1a	1a	81%
NISTPFAS003285 - 6:2 Fluorotelomer thia propionoamido dimethyl ethyl sulfote	2a	2b	2a	3b		2a		2a	2a	2b	2b	4		2a	2a		2b		2b	2a	2a		4	3d	2a	2a	2a	2a	78%
NISTPFAS000880 - Perfluorobutane sulfomido amine		2c	2a	2b	3d		2c		2c	2c	5b	4	4	2a	3c			2c		2a	2a		3d	5a	2b		2a	2a	70%
NISTPFAS002643 - Perfluorohexanoic acid	2a	2c	2b	2b	1a		1a	1b	1a	2b	3d	4	1a		1a			3d	1a	1a	1a				2a		1a	1a	70%
NISTPFAS000879 - Perfluoropentane sulfomido amine		2c	2a	2c	3c	4	2b		2b	2c	2b			2a	2c			2c		2a	2a	4	3d		2b		2a	2a	67%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2c	2a	2c	1a		1a			2b	2a	1a	1a	1a	1a			3d	1a	1a	1a				2a		1a	1a	67%
NISTPFAS003042 - Perfluoroheptanesulfonic acid		3d	2a	2b	1a	4	1a		1a	2b	2a	1a			2a			1a	1a	1a	1a	3a	1a		2a			1a	67%
NISTPFAS003492 - Perfluoropropane sulfote	4	3b	3d	2b	2c		2b		1a	2b	3b		2a			4		1a	1a	2a	1a		1a		2a		1a	1a	67%
NISTPFAS003407 - 6:2 Fluorotelomer sulfinyl propamido dimethyl ethyl sulfote			2a			2b			2a	2b	2b		2b		2a		2b		2b	3c	2a	2a		5a	2a		2b	2a	56%
NISTPFAS003430 - 3-(N-(3-(dimethylamino)propyl)- perfluoropentylsulfomido)propanoic acid	4	2c	2a	2c		2b			2a	3d			2c		4			2c		2a	2a	4		5a			2a	2a	56%
NISTPFAS003455 - N-Dimethyl ammonio propyl perfluoropropane sulfomide		2c	3d	2b	3c		2b		2a	2c	2b		4		2c	4					3d			5a	2b		2b	2a	56%
NISTPFAS000881 - 6:2 Fluorotelomer sulfomide amine			2a	2b					2b		2b	4	3c		2a				2b	2a	2a	4		5a	2a		2b	2a	52%
NISTPFAS004390 - 6:2 Fluorotelomer thia ammoniohydroxypropyl ethanoic acid			5a			2b			3a			4	4	5a	4		2b		3a	3c	4	3a		5a			3b	2b	52%
NISTPFAS000861 - N-[3-(Dimethylamino)propyl]-N- [(tridecafluorohexyl)sulfonyl]-beta-alanine	2a	2c	2a	2c					3b	2c		4						2c	3b		2a	4		5a			2a	2a	48%
NISTPFAS000862 - N-[3-(Dimethylamino)propyl]-N- [(nofluorobutyl)sulfonyl]-beta-alanine	4	2c	2a	2c		4			3a	2c	2b							2c			2a	4					2a	2a	44%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

NIST Interlaboratory Study Results

Sample C – Soil extract

Compound me	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	2b	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	96%
NISTPFAS002560 - Perfluorohexanesulfonide	2a	3d	2a	2b	2a	2b	2b	2a	1a	2b	2a	1a		1a	2c	2a	1a	1a	1a	1a	1a	2b	1a	5a	2a		1a	1a	93%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	3d	2b	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002559 - Perfluorooctanesulfonide	2a	2c	2a	2b	1a	1a	1a	1b	1a	2b	2a	1a	1a		1a			1a	1a	1a	1a	2c	1a	1a	2a	1a	1a	1a	89%
NISTPFAS003042 - Perfluoroheptanesulfonic acid	2a	2b	2a	2b	1a	1a	1a		1a	2b	2a	1a	1a		1a		1a	1a	1a	1a	1a	1a	1a	1a	2a	2a	1a	1a	89%
NISTPFAS003044 - Perfluoropentanesulfonic acid	2a	2b	2a	2b	1a	3d	1a	5a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	3a	1a	3b	2a		1a	1a	89%
NISTPFAS000878 - Perfluorohexane sulfonido amine		3d	2a	2c	2a	4	2b	3c	2a	2b	2b	4	2a	2b	2a			2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	85%
NISTPFAS002630 - Perfluoroundecanoic acid	2a	2b	2a	2b	1a	2b	1a	1b	1a	2b	3d	1a	1a	1a	1a			1a	1a	1a	1a			1a	2a	1a	1a	1a	85%
NISTPFAS002632 - Perfluorodecanoic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a		1a	2a	1a	1a	1a	85%
NISTPFAS002643 - Perfluorohexanoic acid	2a	3d	2a	2c	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a	4	1a	1a	1a	1a	1a		1a		2a		1a	1a	85%
NISTPFAS003039 - Perfluorodecanesulfonic acid	2a	3d	2a	2b	1a	1a	1a		1a	3d	2a	1a	1a	1a	1a			1a	1a	1a	1a	2c	1a		2a	1a	1a	1a	85%
NISTPFAS003040 - Perfluorononesulfonic acid	2a	3d	2a	2b	1a		1a		1a	2b	2a	1a	1a	1a	1a		2b	1a	1a	1a	1a	3b	1a		2a	2b	1a	1a	85%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a		1a	1a	2a	2a	1a	1a	85%
NISTPFAS003085 - Pentafluorosulfide perfluorooctane sulfate	2a	2b	2a			2b	2b	2a	2a	2b	2b	4	2a	2b	2a		2b	2c	2b	2b	2a	2a	4		2b	2a	2a	2a	85%
NISTPFAS003086 - Pentafluorosulfide perfluoronone sulfate		2b	2b			4	2b	2b	2a	2b	2b	4	2b	3b	4	2a		2c	2b	2b	2b	2a	4	5a	2b	2a	2c	2a	85%
NISTPFAS000009 - Perfluorobutylsulfonide	2a	2c	2a	2c	2a	3d	2b		1a	2c	2a		1a		3b			1a	1a	1a	1a	3a	1a	3d	2a	2a	1a	1a	81%
NISTPFAS000708 - N-Ethyl-N-((tridecafluorohexyl)sulfonyl)glycine	2a	2c	2b	2b	4	4		5b		3d	2b	4	4	2b	3b		2b	2c	3c	2c		4	4		5a	5a	4	2a	81%
NISTPFAS002629 - Perfluorododecanoic acid	2a	2c	2a	2b	1a	1a	1a		1a	3d	3d	1a	1a	1a	1a			3d	1a	1a	1a	3d		3b	2a	2a		1a	81%
NISTPFAS003038 - Perfluorododecanesulfonic acid		3d	2b	2b	1a	1a	1a		2b	2b	2b	1a	1a	2a	2a			1a	1a	2c	1a	1a	1a	5a	2a		1a	1a	81%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2b	2a	2c	1a		1a	1a		2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a		2a		1a	1a	78%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

NIST Interlaboratory Study Results

Sample C – Soil extract

Compound me	DIM001	DIM002	DIM003	DIM004	DIM005	DIM006	DIM011	DIM014	DIM017	DIM018	DIM020	DIM021	DIM023	DIM027	DIM029	DIM032	DIM033	DIM035	DIM037	DIM038	DIM040	DIM043	DIM044	DIM045	DIM047	DIM048	DIM049	Maximum	Reporting
NISTPFAS003043 - Perfluorohexanesulfonic acid	2a	2b	2a	2b	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a	2a		1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	96%
NISTPFAS002560 - Perfluorohexanesulfonide	2a	3d	2a	2b	2a	2b	2b	2a	1a	2b	2a	1a		1a	2c	2a	1a	1a	1a	1a	1a	2b	1a	5a	2a		1a	1a	93%
NISTPFAS003041 - Perfluorooctanesulfonic acid	2a	3d	2b	2c	1a	1a	1a	1a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a	1a	2a	1a	1a	1a	93%
NISTPFAS002559 - Perfluorooctanesulfonide	2a	2c	2a	2b	1a	1a	1a	1b	1a	2b	2a	1a	1a		1a			1a	1a	1a	1a	2c	1a	1a	2a	1a	1a	1a	89%
NISTPFAS003042 - Perfluoroheptanesulfonic acid	2a	2b	2a	2b	1a	1a	1a		1a	2b	2a	1a	1a		1a		1a	1a	1a	1a	1a	1a	1a	1a	2a	2a	1a	1a	89%
NISTPFAS003044 - Perfluoropentanesulfonic acid	2a	2b	2a	2b	1a	3d	1a	5a	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	3a	1a	3b	2a		1a	1a	89%
NISTPFAS000878 - Perfluorohexane sulfonido amine		3d	2a	2c	2a	4	2b	3c	2a	2b	2b	4	2a	2b	2a			2a	1a	2a	1a	2a	1a	5a	2b		1a	1a	85%
NISTPFAS002630 - Perfluoroundecanoic acid	2a	2b	2a	2b	1a	2b	1a	1b	1a	2b	3d	1a	1a	1a	1a			1a	1a	1a	1a			1a	2a	1a	1a	1a	85%
NISTPFAS002632 - Perfluorodecanoic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a		1a	2a	1a	1a	1a	85%
NISTPFAS002643 - Perfluorohexanoic acid	2a	3d	2a	2c	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a	4	1a	1a	1a	1a	1a		1a		2a		1a	1a	85%
NISTPFAS003039 - Perfluorodecanesulfonic acid	2a	3d	2a	2b	1a	1a	1a		1a	3d	2a	1a	1a	1a	1a			1a	1a	1a	1a	2c	1a		2a	1a	1a	1a	85%
NISTPFAS003040 - Perfluorononesulfonic acid	2a	3d	2a	2b	1a		1a		1a	2b	2a	1a	1a	1a	1a		2b	1a	1a	1a	1a	3b	1a		2a	2b	1a	1a	85%
NISTPFAS003045 - Perfluorobutanesulfonic acid	2a	2b	2a	2b	1a		1a	1b	1a	2b	2a	1a	1a	1a	1a			1a	1a	1a	1a		1a	1a	2a	2a	1a	1a	85%
NISTPFAS003085 - Pentafluorosulfide perfluorooctane sulfate	2a	2b	2a			2b	2b	2a	2a	2b	2b	4	2a	2b	2a		2b	2c	2b	2b	2a	2a	4		2b	2a	2a	2a	85%
NISTPFAS003086 - Pentafluorosulfide perfluoronone sulfate		2b	2b			4	2b	2b	2a	2b	2b	4	2b	3b	4	2a		2c	2b	2b	2b	2a	4	5a	2b	2a	2c	2a	85%
NISTPFAS000009 - Perfluorobutylsulfonide	2a	2c	2a	2c	2a	3d	2b		1a	2c	2a		1a		3b			1a	1a	1a	1a	3a	1a	3d	2a	2a	1a	1a	81%
NISTPFAS000708 - N-Ethyl-N-((tridecafluorohexyl)sulfonyl)glycine	2a	2c	2b	2b	4	4		5b		3d	2b	4	4	2b	3b		2b	2c	3c	2c		4	4		5a	5a	4	2a	81%
NISTPFAS002629 - Perfluorododecanoic acid	2a	2c	2a	2b	1a	1a	1a		1a	3d	3d	1a	1a	1a	1a			3d	1a	1a	1a	3d		3b	2a	2a		1a	81%
NISTPFAS003038 - Perfluorododecanesulfonic acid		3d	2b	2b	1a	1a	1a		2b	2b	2b	1a	1a	2a	2a			1a	1a	2c	1a	1a	1a	5a	2a		1a	1a	81%
NISTPFAS002637 - Perfluorooctanoic acid	2a	2b	2a	2c	1a		1a	1a		2b	2a	1a	1a	1a	1a			1a	1a	1a	1a	1a	1a		2a		1a	1a	78%

NIST Internal Report 8544 Per- and Polyfluoroalkyl Substances –Non-Targeted Analysis Interlaboratory Study Final Report, Benjamin J. Place et al. 2024
(<https://doi.org/10.6028/NIST.IR.8544>)

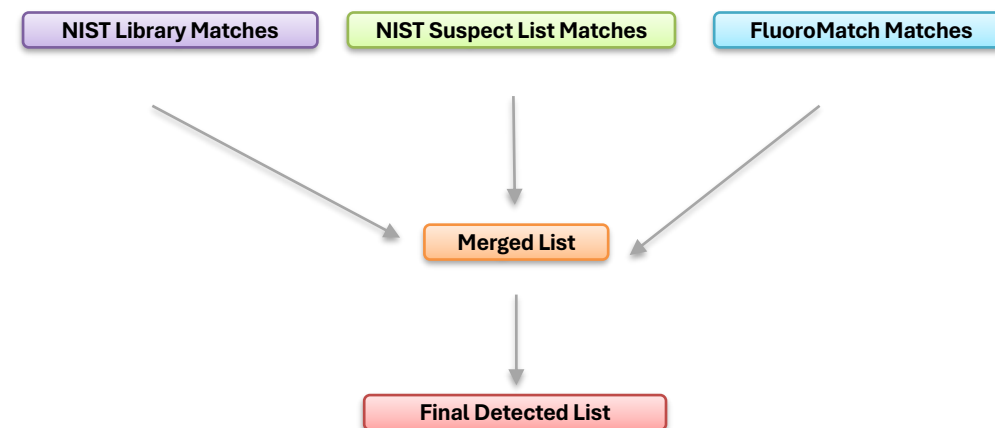
Identification Result

Sample	Positive Match	Negative Match	Total
A	9	40	49
B	44	57	101
C	29	105	134

- Our laboratory [DIM003] was the only one which successfully reported 100% of the analytes in all three tables.
- Our three-pronged approach gave comprehensive identifications without excess false positives.

Conclusion

- We developed a non-target screening method for PFAS
- Participated in the NIST interlaboratory study
- Method uses three complementary approaches
- Merging of matches and quality checking
- Assignment of identification confidence level
- Favorable results in interlaboratory study



Acknowledgements



Jeffrey Dahl

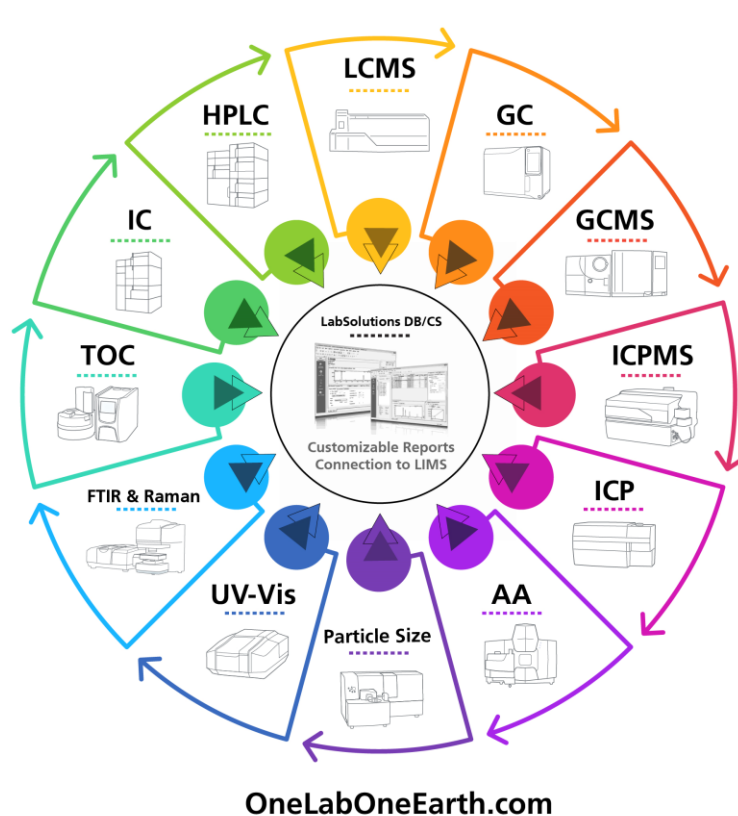


Toshiya Matsubara



Ruth Marfil-Vega

HPLC	Carbamate Diquat Glyphosate
IC	Anions Chromium VI Ammonia
TOC	Nitrogen Organic Carbon Phosphorous
FTIR & Raman	Microplastics
UV-Vis	Chlorine UV254 Others
Particle Size	Solids



LCMS	Cyanotoxins PFAS Pesticides Emerging Contaminants Unknowns (QTOF)
GC	HAAs Herbicides Pesticides
GCMS	Phenols Other Organics PCBs
GCMS	1,4-dioxane Dioxins & Furans Nitrosamines Other Organics Microplastics
ICPMS	Semivolatiles Taste & Odor Volatiles THMs
ICPMS	Metals
ICP	Metals
AA	Metals

For any questions, contact:
Ruth Marfil-Vega
rmmarfilvega@shimadzu.com

Om Shrestha
okshrestha@shimadzu.com

Jeff Dahl, PhD
jhdahl@shimadzu.com

Connect with us:

X - [@shimadzussi](#)

Instagram - [@shimadzussi](#)

LinkedIn - [/company/shimadzu-scientific-instruments/](#)

YouTube - [@ShimadzuScientificInstruments](#)

For more information, visit:
www.OneLabOneEarth.com