eurofins | Environment Testing

ANALYTICAL REPORT

PREPARED FOR

Attn: Roger Brewer
Hawaii Department of Health
919 Ala Moana Blvd
Room 206
Honolulu, Hawaii 96814

Generated 7/18/2023 2:31:52 PM

JOB DESCRIPTION

Red Hill AFFF

JOB NUMBER

320-99812-3

Eurofins Sacramento
880 Riverside Parkway
West Sacramento CA 95605

See page two for job notes and contact information.

my EOL

Eurofins Sacramento

Job Notes

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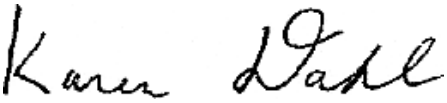
The test results in this report relate only to the samples as received by the laboratory and will meet all requirements of the methodology, with any exceptions noted. This report shall not be reproduced except in full, without the express written approval of the laboratory. All questions should be directed to the Eurofins Environment Testing Northern California, LLC Project Manager.

Authorization



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7/18/2023 2:31:52 PM

Authorized for release by
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(916)374-4384

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July 17, 2023

Hawaii Department of Health
919 Ala Moana Blvd
Room 206
Honolulu, HI 96814

Attn: Roger Brewer

RE: PFAS by NTA Results for Sample RH-AFFF; Eurofins Job 320-99812-3

Dear Mr. Brewer,

Enclosed are the Non-Target Analysis (NTA) results for potential PFAS parameters in the single sample submitted to Eurofins in Job 320-99812-3 with client ID 'RH-AFFFF. Analysis was requested via LC-QTOF MS (liquid chromatography quadrupole time-of-flight mass spectrometry) for identification of potential PFAS analytes not determined in the routine targeted analyses that are typically applied to tissue samples. The NTA determination inherently incurs an increased level of uncertainty and certified reference standards are not used to confirm reported results.

There were several non-target analytes that were identified as potential PFAS parameters in this sample; **6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate** and **6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium** were present in greatest apparent abundance.

Sample Preparation

1 mL of sample RH-AFFF was diluted 1000X in water due to the potential for high concentrations of both target and non-target analytes, as well as the empirically observed characteristics of the sample (foaming). A 150 uL aliquot of the aqueous dilution was adjusted to a final volume of 300 uL with methanol and the resulting extract was analyzed by LC-QTOF MS.

Analysis

The sample extract was introduced into the LC system utilizing an optimized gradient to enhance the identification of early eluting compounds. The gradient ramps slowly over a period of 20 minutes where the compounds are separated on a 3x50mm Phenomenex Gemini C18 analytical column using 20mM ammonium acetate in water and methanol as mobile phases. The SCIEX X500r quadrupole time-of-flight mass spectrometer (QTOF MS) was set to run in sequential Electrospray Ionization (ESI) techniques in both positive and negative polarities utilizing the same gradient and mobile phases.

Results

Data were processed with SCIEX MarkerView deconvolution software. This software extracts the raw chromatograms across a defined mass range from 0-1500 amu and examines peaks of interest utilizing exact mass and MS/MS fragmentation. The peaks are compared to comprehensive fluorinated compound libraries where the software algorithm assigns possible matches to each peak, or feature. The observed features were then evaluated by a Eurofins analyst to confirm ample signal-to-noise as well as confirming the compound fit to the library match. The reported results include only peaks with a signal-to-noise greater than 10:1 and an absolute intensity greater than 1000 counts.

One limitation the software cannot account for are multiple isomers of the same compound. While the skeletal backbone and molecular formula will be the same, the match might represent a structural isomer of the identified compound.

Please find the results for both positive SWATH and negative SWATH analyses in the attached Tables.

Please do not hesitate to let us know if there are any questions.

2023.07.06_SWATH_POS_005.wiff2 - 98812-1

Data File	2023.07.06_SWATH_POS_005.wiff2	**Result Table**	2023.07.06_NTA_SWATH_POS
Acquisition Date	7/6/2023 2:45:45 PM	**Algorithm Used**	MQ4
Acquisition Method	N/A	**Instrument Name**	X500 QTOF
Project	PFAS_A11	**Processing Method**	SWATH_PFAS_Pos_803_List.qmethod

Summary

#	Analyte Peak Name	Mass Error Confidence	Fragment Mass Error Confidence	RT Confidence	Isotope Confidence	Library Confidence	Formula Confidence	Ion Ratio Confidence	Sample Name
76	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	✓	●	●	▲	✓	●	●	98812-1
314	Class 19 (Cn+8H15O2SN2F2n+1) 523.07194	✓	●	●	✓	●	●	●	98812-1
506	6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium	✓	●	●	✓	●	●	●	98812-1
513	6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium	✓	●	●	✓	●	●	●	98812-1

#	Analyte Peak Name	Sample Type	Component Name	Area	Calculated Concentration	Formula	Precursor Mass	Found At Mass
76	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	Unknown	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	6.380e+06	<2 points	C15H18O4S2NF13	588.054	588.0535
314	Class 19 (Cn+8H15O2SN2F2n+1) 523.07194	Unknown	Class 19 (Cn+8H15O2SN2F2n+1) 523.07194	1.215e+06	<2 points	C14H15O2SN2F13	523.072	523.0719
506	6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium	Unknown	6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium	5.516e+06	<2 points	C14H18OSNF13	496.097	496.0975
513	6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium	Unknown	6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium	5.242e+05	<2 points	C14H18O2SNF13	512.092	512.0920

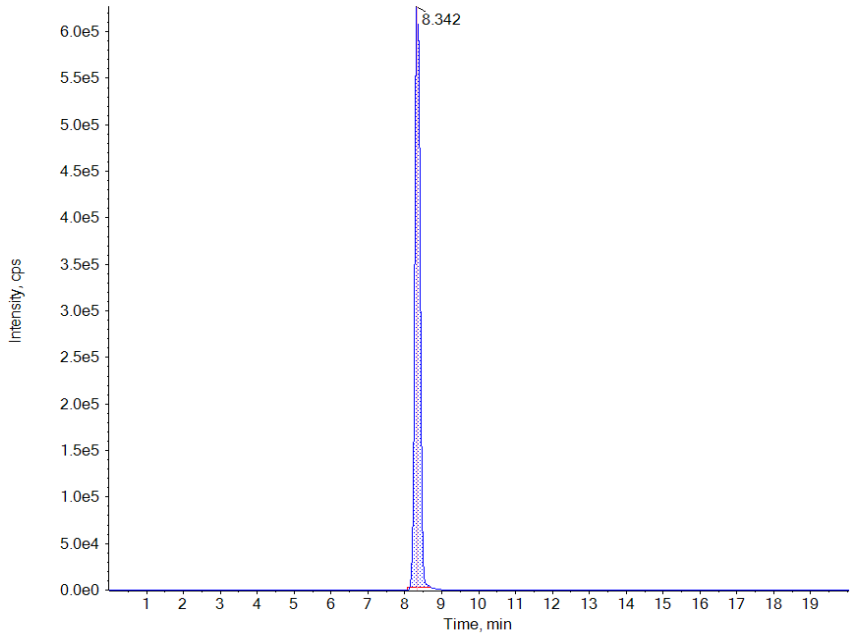
#	Analyte Peak Name	Mass Error (ppm)	Library Hit	Library Score	Isotope Ratio Difference
76	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	-1.3	6:2 FOThPA-MePS (6:2 tridecafluorooctyl thiapropanoamido-methylpropyl sulfonate) (neg,pos) Smart Confirmation	100.0	14.5
314	Class 19 (Cn+8H15O2SN2F2n+1) 523.07194	0.0	No Match	0.0	0.4
506	6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium	0.1	No Match	0.0	1.8
513	6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium	-0.7	No Match	0.0	4.8

End of Table

6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate (Mass/FragMass/RT/Isotope/Library/Formula/Ion Ratio)

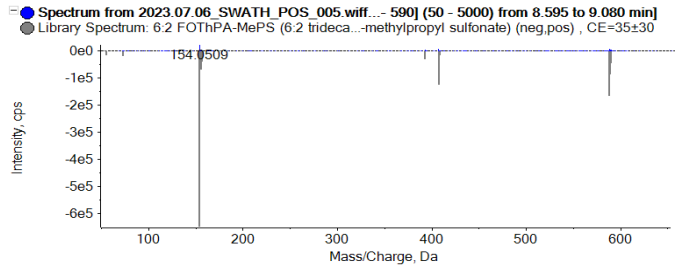
Retention Time: 8.34 minutes
Precursor m/z : 588.0542
Fit (%) 100.0% **RFit (%)** 100.0%

Exp RT: 0.00 minutes
Analyte Name:
6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate

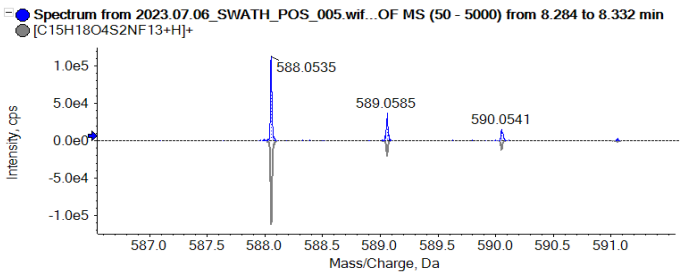


Collision Energy = 35 ± 15 eV

Acquired / Library MSMS



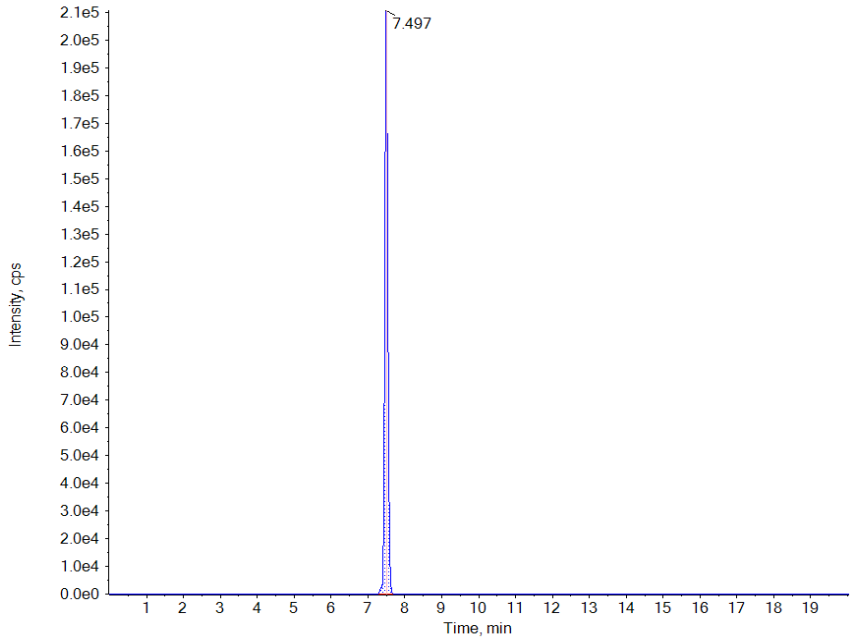
Acquired / Theoretical MS



Class 19 (Cn+8H15O2SN2F2n+1) 523.07194 (Mass/FragMass/RT/Isotope/Library/Formula/Ion Ratio)

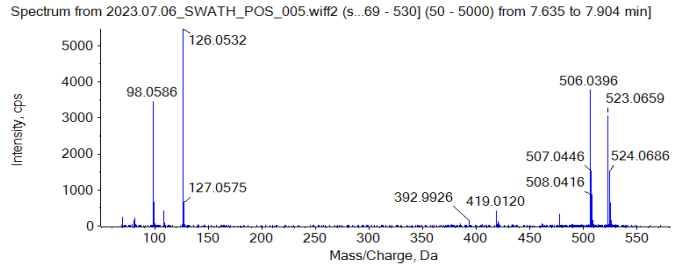
Retention Time: 7.50 minutes
Precursor m/z : 523.0719
Fit (%) N/A **RFit (%)** N/A

Exp RT: 13.33 minutes
Analyte Name:
Class 19 (Cn+8H15O2SN2F2n+1)
523.07194

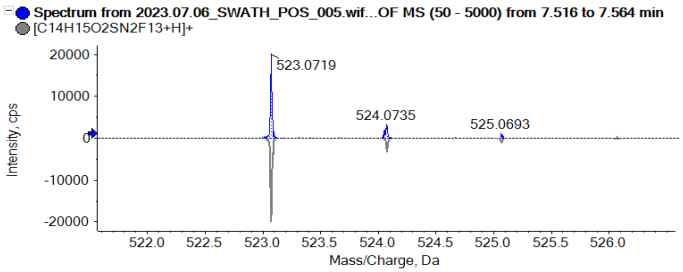


Collision Energy = 35 ± 15 eV

Acquired / Library MSMS



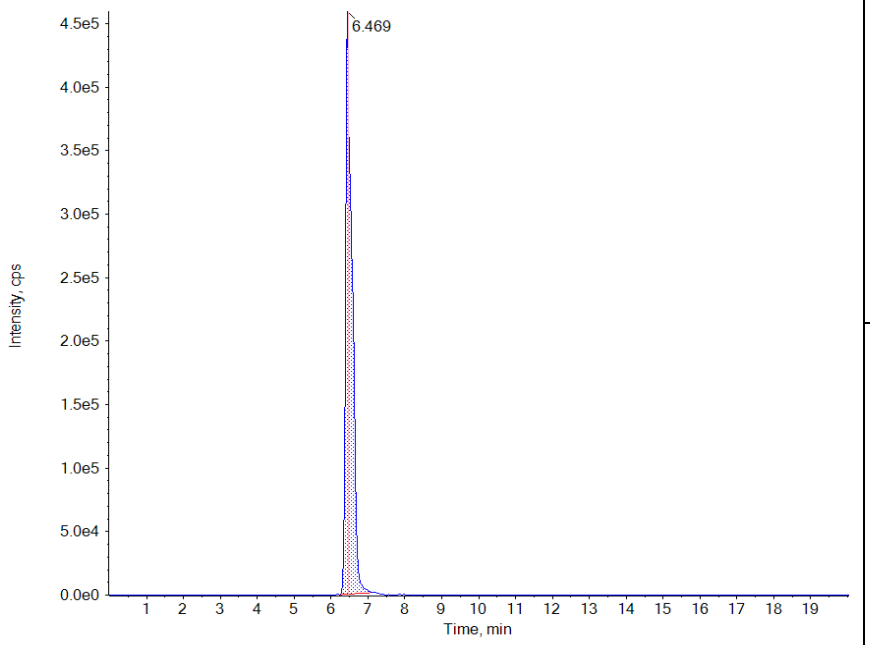
Acquired / Theoretical MS



6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium (Mass/FragMass/RT/Isotope/Library/Formula/Ion Ratio)

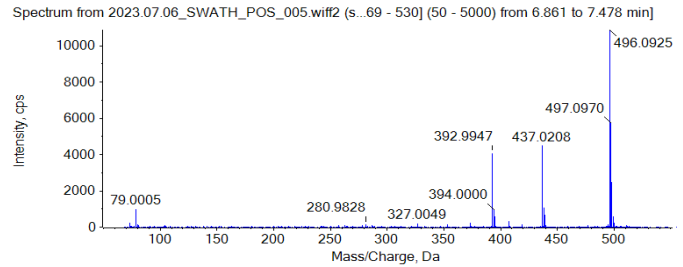
Retention Time: 6.47 minutes
Precursor m/z : 496.0974
Fit (%) N/A **RFit (%)** N/A

Exp RT: 8.28 minutes
Analyte Name:
6:2 fluorotelomer thia hydroxy propyl trimethyl ammonium

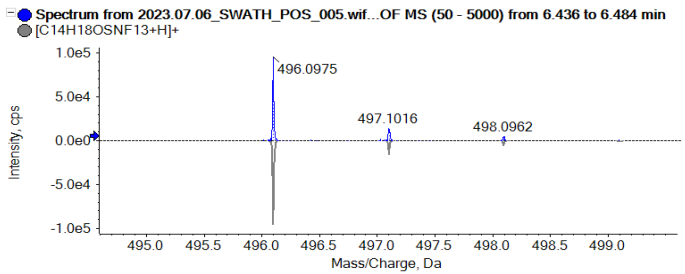


Collision Energy = 35 ± 15 eV

Acquired / Library MSMS



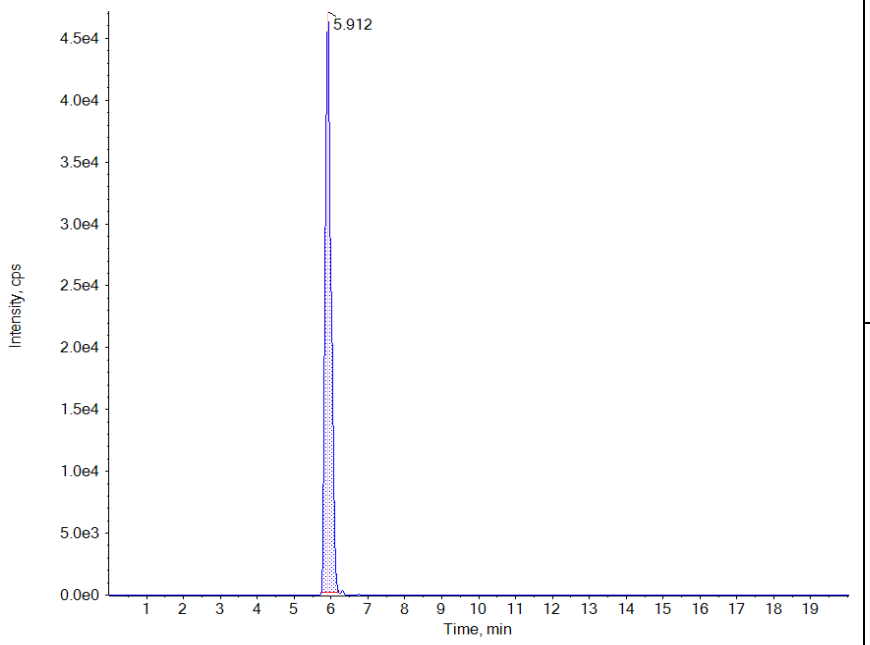
Acquired / Theoretical MS



6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium (Mass/FragMass/RT/Isotope/Library/Formula/Ion Ratio)

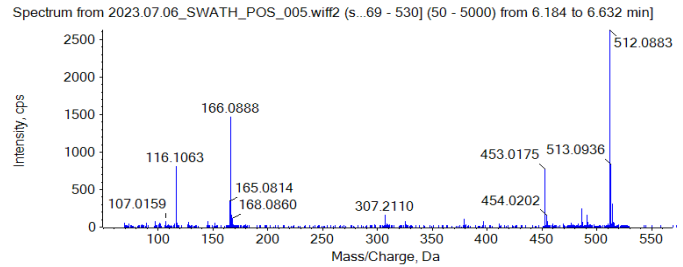
Retention Time: 5.91 minutes
Precursor m/z : 512.0923
Fit (%) N/A **RFit (%)** N/A

Exp RT: 11.98 minutes
Analyte Name:
6:2 fluorotelomer sulfinyl hydroxypropyl trimethyl ammonium

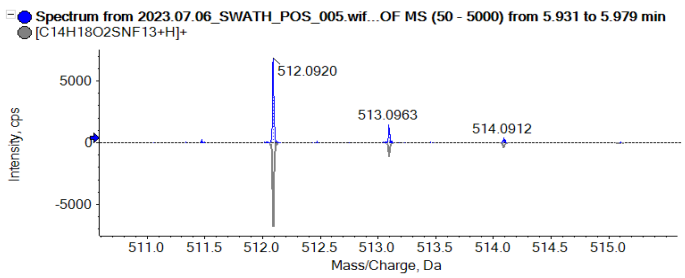


Collision Energy = 35 ± 15 eV

Acquired / Library MSMS



Acquired / Theoretical MS



2023.07.06_SWATH_NEG_005.wiff2 - 98812-1

Data File	2023.07.06_SWATH_NEG_005.wiff2	**Result Table**	2023.07.06_NTA_SWATH_NEG
Acquisition Date	7/6/2023 12:59:21 PM	**Algorithm Used**	MQ4
Acquisition Method	N/A	**Instrument Name**	X500 QTOF
Project	PFAS_A11	**Processing Method**	SWATH_PFAS_Neg_1659_ListV2.qmethod

Summary

#	Analyte Peak Name	Mass Error Confidence	Fragment Mass Error Confidence	RT Confidence	Isotope Confidence	Library Confidence	Formula Confidence	Ion Ratio Confidence	Sample Name
308	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	✓	●	●	▲	✓	●	●	98812-1

#	Analyte Peak Name	Sample Type	Component Name	Area	Calculated Concentration	Formula	Precursor Mass	Found At Mass	Mass Error (ppm)	Library Hit
308	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	Unknown	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	1.075e+07	<2 points	C15H18O4S2NF13	586.040	586.0402	0.8	6:2 FOThPA-MePS (6:2 tridecafluorooctyl thiapropanoamido-methylpropyl sulfonate) (neg,pos) Smart Confirmation

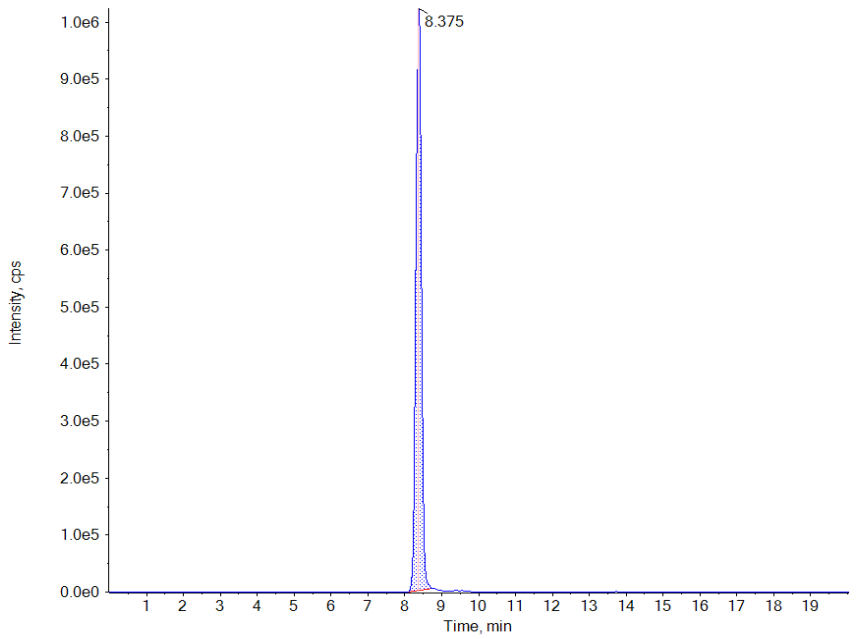
#	Analyte Peak Name	Library Score	Isotope Ratio Difference
308	6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate	100.0	20.0

End of Table

6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate (Mass/FragMass/RT/Isotope/Library/Formula/Ion Ratio)

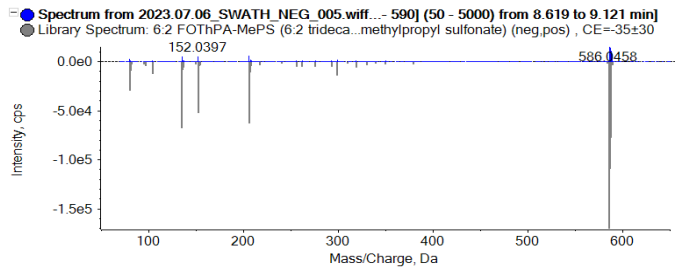
Retention Time: 8.38 minutes
Precursor m/z : 586.0397
Fit (%) 100.0% **RFit (%)** 95.3%

Exp RT: 10.23 minutes
Analyte Name:
6:2 fluorotelomer thia propanoamido dimethyl ethyl sulfonate

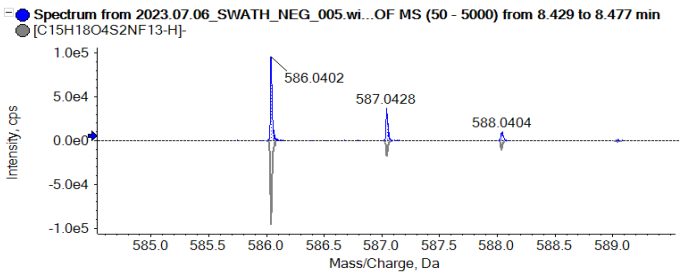


Collision Energy = 35 ± 15 eV

Acquired / Library MSMS



Acquired / Theoretical MS



Sample Summary

Client: Hawaii Department of Health
Project/Site: Red Hill AFFF

Job ID: 320-99812-3

Lab Sample ID	Client Sample ID	Matrix	Collected	Received
320-99812-1	RH-AFFF	Water	04/28/23 12:00	05/03/23 10:00

Eurofins Sacramento
880 Riverside Parkway
West Sacramento, CA 95605-1500
phone 916.373.5600 fax 303.467.7248

Chain of Custody Record

eurofins | Environment Testing America

Regulatory Program: ☐ DW ☐ NPDES ☐ RCRA ☐ Other:

Eurofins Environment Testing Northern California, LLC

Client Contact	Project Manager: Roger Brewer	INVOICE & Lab Report CC:	Date:	COC No:
Roger Brewer HDOH	Email: roger.brewer@doh.hawaii.gov	Eric Jensen, Tetra Tech, Inc. eric.jensen@tetratech.com 808.441.4784		_____ of _____ COCs
2385 Waimano Home Rd, Ste 100	Tel/Fax: 808-586-4229	Lab Contact:	Carrier:	TALS Project #:
Honolulu, HI 96872	Analysis Turnaround Time			Sampler:
(808) 586-4229 Phone	☐ CALENDAR DAYS ☑ WORKING DAYS			For Lab Use Only:
	TAT if different from Below ____30_____			Walk-in Client:
Project Name: Red Hill AFFF	☐ 2 weeks			Lab Sampling:
Site: Red Hill, HI	☐ 1 week			Job / SDG No.:
Project ID: **103S864023110.02**	☐ 2 days			
	☑ 1 day			

Sample Identification	Sample Date	Sample Time	Sample Type (C=Comp, G=Grab)	Matrix	# of Cont.	Filtered Sample (Y / N)	Perform MS / MSD (Y / N)	Metjod 537/TOP Assay- Pre-Analysis, Oxidation & Post-Analysis	ELLE SOP Adsorbable Organic Fluorine	Sample Specific Notes:
RH-AFFF			G	Liquid	2	N		X	X	Concentrated AFFF Product (SDS Attached)

320-99812 Chain of Custody

Preservation Used: 1

Possible Hazard Identification:
Are any samples from a listed EPA Hazardous Waste? Please List any EPA Waste Codes for the sample in the Comments Section if the lab is to dispose of the sample.

☑ Non-Hazard ☐ Flammable ☐ Skin Irritant ☐ Poison B ☐ Unknown

Sample Disposal (A fee may be assessed if samples are retained longer than 1 month)

☐ Return to Client ☑ Disposal by Lab ☐ Archive for_____ Months

Special Instructions/QC Requirements & Comments:
This is a sample of undiluted, Ansulite AFFF Concentrate. High PFAS concentrations anticipated.
Reports to : DOH (Roger Brewer) roger.brewer@doh.hawaii.gov and Tetra Tech (Eric Jensen) eric.jensen@tetratech.com
Invoices to: Tetra Tech (Eric Jensen) eric.jensen@tetratech.com

Custody Seals Intact: ☐ Yes ☐ No | Custody Seal No.: | Cooler Temp. (°C): Obs'd:_____ Corr'd:_____ Therm ID No.:_____

Relinquished by: Roger B	Company: HI DOH	Date/Time: 5/2/23 12:00 pm	Received by:	Company:	Date/Time: 5/3/23 1000
Relinquished by:	Company:	Date/Time:	Received by:	Company:	Date/Time:
Relinquished by:	Company:	Date/Time:	Received in Laboratory by:	Company:	Date/Time:

7/18/2023

Login Sample Receipt Checklist

Client: Hawaii Department of Health

Job Number: 320-99812-3

Login Number: 99812
List Number: 1
Creator: Pratali, Sandra A

List Source: Eurofins Sacramento

Question	Answer	Comment
Radioactivity wasn't checked or is </= background as measured by a survey meter.	True	
The cooler's custody seal, if present, is intact.	N/A	
Sample custody seals, if present, are intact.	N/A	
The cooler or samples do not appear to have been compromised or tampered with.	True	
Samples were received on ice.	False	Thermal preservation not required.
Cooler Temperature is acceptable.	True	
Cooler Temperature is recorded.	True	
COC is present.	True	
COC is filled out in ink and legible.	True	
COC is filled out with all pertinent information.	True	
Is the Field Sampler's name present on COC?	False	
There are no discrepancies between the containers received and the COC.	True	
Samples are received within Holding Time (excluding tests with immediate HTs)	True	
Sample containers have legible labels.	True	
Containers are not broken or leaking.	True	
Sample collection date/times are provided.	True	
Appropriate sample containers are used.	True	
Sample bottles are completely filled.	True	
Sample Preservation Verified.	N/A	
There is sufficient vol. for all requested analyses, incl. any requested MS/MSDs	True	
Containers requiring zero headspace have no headspace or bubble is <6mm (1/4").	True	
Multiphasic samples are not present.	True	
Samples do not require splitting or compositing.	True	
Residual Chlorine Checked.	N/A	