Message

From: Washington, John [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=FDC3E8CE9F1D45C4894881FF420CA104-WASHINGTON, JOHN]
Sent: 12/11/2019 6:52:17 PM
To: Frithsen, Jeff [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=e3743bd6f3c345baaae407c1d6f78e92-FRITHSEN, JEFF]; Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
CC: Watkins, Tim [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=4cbd1c572f584fd7b0a3b5945f118558-Watkins, Tim]; Medina-Vera, Myriam [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=b081a1f48a044b4c9d1ebc4992c54dee-Medina-Vera, Myriam]; Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]; McCord, James [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=McCord, James]
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Hi Jeff,

New Jersey requested that ORD analyze samples primarily to investigate legacy PFAS including C9, C11 and C13 perfluorocarboxylates, but NJ also was interested in information we might generate with nontargeted analyses. Water was analyzed in RTP and soil/vegetation was analyzed in Athens.

Using nontargeted analysis techniques, Athens and RTP identified this chemical independently in our NJ samples. As we were refining our knowledge of the structure using our nontargeted data, Mark remembered an article, describing new compounds reported to be in use by industry, in which this chemical was identified as "Solvay's product." The source for this information was an article in EFSA (European Food Safety Authority) journal describing an EFSA safety assessment of the compound, with the compound and request for assessment being submitted by "Solvay Solexis."

So, we did not know to look for this compound, instead discovering it using nontargeted analyses. Then, as we elucidated specifics of the structure, we realized it was the chemical described as in use in peer-reviewed literature (see below).

Please let me know if this does not help.

Thanks,
John

Literature:

Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint

Fluorinated alternatives to long-chain perfluoroalkyl carboxylic acids (PFCAs), perfluoroalkane sulfonic acids (PFSAs) and their potential precursors

Zhanyun Wang [a], Ian T. Cousins [b], Martin Scheringer [a,*], Konrad Hungerbühler [a]

efsa

European Food Safety Authority

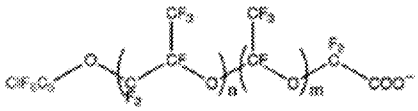
SCIENTIFIC OPINION

Scientific Opinion on the safety evaluation of the substance perfluoro acetic acid, α-substituted with the copolymer of perfluoro-1,2-propylene glycol and perfluoro-1,1-ethylene glycol, terminated with chlorohexafluoropropyloxy groups, CAS No. 329238-24-6 for use in food contact materials

EFSA Panel on food contact materials, enzymes, flavourings and processing aids (CEF)

European Food Safety Authority (EFSA), Parma, Italy

Solvay's product (CAS No. 329238-24-6)



Chemical structure: C3F6ClO-[CF2-CF(CF3)-O]n-[CF(CF3)-O]m-CF2COOH, where n ranges from 1 to 4 and m from 0 to 2.

dossier was submitted by the applicant, Solvay Solexis, Italy.

From: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Sent: Wednesday, December 11, 2019 12:55 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Watkins, Tim <Watkins.Tim@epa.gov>; Medina-Vera, Myriam <Medina-Vera.Myriam@epa.gov>; Washington, John <Washington.John@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; McCord, James <mccord.james@epa.gov>
Subject: Re: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Question. The Washington et always manuscript reads as if we didn't know about this Chem. The text below says that we have known sbouttthis chem since 2013. Please clarify.

Jeff

Sent from my iPhone

On Dec 11, 2019, at 9:47 AM, Strynar, Mark <Strynar.Mark@epa.gov> wrote:

Jeff,

Background:
Solvay formerly used a product called Surflon (mixture of PFNA, PFUnA and PFTriDA) as a polymer processing aid to make PVDF in West Deptford, NJ. They ceased the use of this product in 2010 due to the PFOA Stewardship Agreement.

In a presentation to the NJ DEP in September of 2013 they informed the NJ DEP about a new perfluoropolyether (PFPE) based Fluorosurfactant they were using but gave no CAS#.
<image001.jpg>
The CAS# we have was derived from a 2013 paper by Wang et al. Env. Intl that listed Solvay's product (**CAS No. 329238-24-6**). This is a unique chemical class as there is no one CAS to represent the chemicals included and are drawn as a Markush structure (from Wang paper below and attached). This is because the production of this product leads to a series of related congeners.
<image003.png>

Answer:
So to answer the questions asked below.

1)

2)

Ex. 5 Deliberative Process (DP)

3)

4)

I am glad to have any follow-up discussions and perhaps include someone for the NJ DEP to answer any questions OPPT may have.

Mark

From: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Sent: Wednesday, December 11, 2019 8:54 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Watkins, Tim <Watkins.Tim@epa.gov>
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Thanks Mark.

How was the meeting with NJ? Any concerns about the Washington et al. manuscript?

Jeff

Jeffrey B. Frithsen, Ph.D.
National Program Director
Chemical Safety for Sustainability Research Program
Office of Research and Development (8101R)
202-564-3512 (office phone)
Ex. 6 Personal Privacy (PP) (cell phone)

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Wednesday, December 11, 2019 8:53 AM
To: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Cc: Watkins, Tim <Watkins.Tim@epa.gov>
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Hi Jeff,

Glad to do so. Let me read through and get a response to you as soon as I can. We just returned from our NJ trip last night. Catching up today so far.

Mark

From: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Sent: Wednesday, December 11, 2019 7:41 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Watkins, Tim <Watkins.Tim@epa.gov>
Subject: FW: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Mark:

Might you able to help with crafting a more complete answer to Tala's concerns related to NTA? Thanks.

Jeff

Jeffrey B. Frithsen, Ph.D.
National Program Director
Chemical Safety for Sustainability Research Program
Office of Research and Development (8101R)
202-564-3512 (office phone)
410-336-8535 (cell phone)

From: Frithsen, Jeff
Sent: Wednesday, December 11, 2019 7:34 AM
To: Henry, Tala <Henry.Tala@epa.gov>; Stedeford, Todd <Stedeford.Todd@epa.gov>
Cc: Morris, Jeff <Morris.Jeff@epa.gov>; Joe Tietge (Tietge.Joe@epa.gov) <Tietge.Joe@epa.gov>
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Tala:

I'll look into how we might be able more systematically provide a list of chemical names and CASRNs for future manuscripts. Regarding non-targeted analysis, I believe you are correct that generally there is generally not standards to verify identify of the analytes. But that is only a partial answer. I will get you a more complete answer.

Jeff

Jeffrey B. Frithsen, Ph.D.
National Program Director
Chemical Safety for Sustainability Research Program
Office of Research and Development (8101R)
202-564-3512 (office phone)
410-336-8535 (cell phone)

From: Henry, Tala <Henry.Tala@epa.gov>
Sent: Monday, December 9, 2019 3:17 PM
To: Stedeford, Todd <Stedeford.Todd@epa.gov>; Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Cc: Morris, Jeff <Morris.Jeff@epa.gov>
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Jeff F.
When things like this come out, OPPT often gets press and sometimes congressional questions.

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Thanks
Tala

Tala R. Henry, Ph.D.
Deputy Director
Office of Pollution Prevention and Toxics
U.S. Environmental Protection Agency

T: 202-564-2959
E: henry.tala@epa.gov

From: Stedeford, Todd <Stedeford.Todd@epa.gov>
Sent: Monday, December 09, 2019 3:01 PM
To: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Cc: Henry, Tala <Henry.Tala@epa.gov>; Morris, Jeff <Morris.Jeff@epa.gov>
Subject: RE: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

Hi Jeff,

Ex. 5 Deliberative Process (DP)

Todd

From: Frithsen, Jeff <Frithsen.Jeff@epa.gov>
Sent: Sunday, November 24, 2019 10:49 AM

To: Morris, Jeff <Morris.Jeff@epa.gov>; Henry, Tala <Henry.Tala@epa.gov>; Stedeford, Todd <Stedeford.Todd@epa.gov>; Pensak, Mindy <Pensak.Mindy@epa.gov>
Cc: Tietge, Joe <Tietge.Joe@epa.gov>; Fleming, Megan <Fleming.Megan@epa.gov>; Gillespie, Andrew <Gillespie.Andrew@epa.gov>; LaVay, Maggie <LaVay.Maggie@epa.gov>
Subject: ORD Advanced Notification: Manuscript: Washington et al., Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey

ORD is providing for advanced notification a recently developed manuscript. The manuscript is Washington et al., ***Nontargeted mas-spectral discovery of novel PFAS & their use to fingerprint legacy PFAS in New Jersey.***

This advanced notification is being provided to OCSPP-OPPT and Region 2.

The goal of this advanced notification is to ensure there are no policy statements contained within the product or factual errors regarding programs and to avoid surprises of published data relevant to the activities of our program and regional partners.

We ask for your comments by COB Monday, December 9.

Please provide any comments you might have and let me know should you have any questions. Thanks in advance!

Jeff

Jeffrey B. Frithsen, Ph.D.
National Program Director
Chemical Safety for Sustainability Research Program
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202-564-3512 (office phone)
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From: "Gillespie, Andrew" <Gillespie.Andrew@epa.gov>
Date: November 15, 2019 at 9:02:39 AM EST
To: "Rodan, Bruce" <rodan.bruce@epa.gov>
Cc: "Fleming, Megan" <Fleming.Megan@epa.gov>
Subject: ADVANCED NOTIFICATION - novel PFAS, fingerprinting, transport, New Jersey

(resending revised manuscript following comments from Bruce)...

Hello Bruce – here is another PFAS manuscript from CEMM for advanced notification, using some of our recently generated data from New Jersey to identify some new PFAS congeners in soil samples as well as using those data for fingerprinting likely sources. Given the novel nature of the PFAS and their presence in soil, I suggest sharing with OCSPP and OLEM for advanced notification. We made OCSPP aware of the novel PFAS findings last year, when we first generated the data, so this should not be a surprise.

Text of fact sheet is below.

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Please let me know if there are any questions, and thank you for your assistance.

Best regards, Andy

Transmittal Summary Document
ORD Manuscript Review

1. Manuscript Title:

Use of Nontargeted PFAS to Develop a Legacy PFAS Fingerprint in New Jersey

Authors: John W. Washington1*, Charlita G. Rosal1, James P. McCord2, Mark J. Strynar2, Andrew B. Lindstrom2, Erica L. Bergman3, Sandra M. Goodrow3, Haile K. Tadesse2, Andrew N. Pilant2, Benjamin J. Washington4, Mary J. Davis1, Brittany G. Stuart5, Thomas M. Jenkins6

Affiliations: 1USEPA, Office Research and Development, Athens, GA.
2USEPA, Office Research and Development, Research Triangle Park, NC.
3NJDEP, Division of Science and Research, Trenton, NJ.
4USEPA, Office Research and Development, Washington, DC.
5USEPA, Office of Research and Development, Cincinnati, OH.
6Senior Environmental Employment Program (USEPA/ORD), Athens, GA.

1. Background/Overview:

New Jersey Department of Environmental Protection (NJDEP) requested ORD's assistance to investigate legacy PFAS distribution in NJ, including two potential PFAS sources. NJDEP collected soil, vegetation and water samples from transects and from across much of the state, delivering soil/veg samples to Athens and water to RTP.

In this manuscript, we report on soil PFAS in New Jersey, not US water. In soil, we identified ten new PFAS compounds, chlor-perfluoro-polyether-carboxylates (ClPFPECAs), using nontargeted analyses and semiquantitated the concentrations of these compounds. We contoured these ClPFPECA values on a map, forming a pattern focusing on one of the potential sources identified by NJDEP.

We used the ClPFPECA data, and PFAS reaction stoichiometry, to develop a fingerprint of legacy PFAS. When this legacy fingerprint was contoured on a map, it formed a pattern focusing on both potential

sources identified by NJDEP.

1. Relevancy to program office/regional research needs/priorities:
The data and information reported here suggest that fingerprinting of PFAS may be possible in certain situations to support risk managers in identifying sources of specific PFAS.

1. Name(s) of program/regional office coauthors or reviewer(s) of earlier drafts, if any
No program or regional coauthors or reviewers. Staff from NJ DEP are included as coauthors. Draft manuscript has been shared for awareness with R2 POC for the NJ collaboration.

1. Major observations and results:
Collectively, our results: (i) identify ten novel PFAS, ClPFPECAs, not previously detected in the environment, including congeners with no previous reports, so far as we know; (ii) suggest many ClPFPECA congeners have bioconcentration potential on the order of or greater than PFOA and PFOS; (iii) document the widespread distribution of ClPFPECAs over much of densely populated New Jersey; (iv) indicate the source of these ClPFPECAs in New Jersey dominantly are from Solvay; (v) were used to fingerprint historical sources of legacy long-chain PFCAs C11 and C13 being from Solvay, and C10 and C12 from the Chemours facility; and (vi) document discernable signals of these legacy PFCAs across an expansive breadth of south Jersey persisting today.

1. Potential implications of the findings:
These data and information: (i) are of interest to NJDEP staff; (ii) suggest a potential exposure of a large population to PFAS; and (iii) also suggest a potential for bioaccumulation.

1. Findings advancing existing scientific knowledge:
Advances in scientific knowledge include: (i) identification/elucidation of ten new PFAS congeners, potentially with isomers, in the environment; (ii) development of methods to detect these compounds on conventional LC/MS/MS; (iii) document sorting of PFAS in atmospheric plumes by molecular mass, perhaps for the first time; (iv) document considerable atmospheric transport distances of PFAS having very low vapor pressures (i.e., chemically non-gaseous PFAS), contrary to expectations of many chemists (e.g., me); (v) reporting of semiquantitative concentrations of nontargeted analytes for the first time in the peer-reviewed literature so far as I know (I had reported semi-quantitated values for targeted compounds in the past but not nontargeted); (vi) perhaps reports one of the first fingerprints of legacy compounds in a complex contaminant setting – there's lots of literature noise about fingerprinting, but I have seen no real-world examples that aren't isolated sites in generally pristine surroundings or unique compounds.

1. Publication information (journal, book) and estimated timelines: Optimistically, I hope to have this thru clearance by the end of November. When clearance is complete, I plan to submit to the journal Science. Realistically, I understand the strong chance of rejection by Science at which time I would rewrite for format and submit to ES&T.

Andrew J. R. Gillespie, Ph. D.
Associate Director, US EPA/ORD/CEMM
ORD Executive Lead for PFAS R&D

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<Wang et al., 2013.pdf>