Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 8/31/2018 1:38:47 PM
To: Risen, Amy J [Amy.Risen@ncdenr.gov]
CC: McCord, James [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=McCord, James]
Subject: RE: [External] RE: PFAS compounds list
Attachments: structural isomers PFECAs Strynar.pptx

Amy,

An additional confusion is structural isomers exist. PFECA-F or PFMOPrA and PMPA may all refer to the same chemical if the structure is not defined correctly. They will both result in a loss of a CO2 which is the primary ion most would monitor for with MS/MS (229-185) in addition the secondary ion could be in common (229-85) which is the CF3O left at the tail of both. For the PFECA-A or PFMOBA and PEPA the primary transition would still be the loss of a CO2 (279-235) however they would have different secondary transitions (279-85) vs (279-135). We have reason to believe both isomeric forms could be present is water.

Structural isomers have the same formula but are simply put together differently. Likely what is being seen in the water is PMPA and PEPA. See the attached PPT file. In these two examples the molecular weight of the first two is the same and the second two are the same. The fragments you get when one does MS/MS MAY be in common for these analytes BUT also can give different fragments.

I will call as this may be confusing.

Mark

From: Risen, Amy J [mailto:Amy.Risen@ncdenr.gov]
Sent: Thursday, August 30, 2018 1:29 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: McCord, James <mccord.james@epa.gov>
Subject: RE: [External] RE: PFAS compounds list

Hi Mark,

Naming certainly is a challenge!

So, we are finding high concentrations of some of the compounds you mentioned. PFECA-F is the name Chemours is using for PFMOPrA and this compound is showing up at up to 3,000 ng/L in one of the private wells near the facility. PFECA-A refers here to PFMOBA, which is also in wells up to ~1,000 ng/L in some cases.

Would James be a good person to follow up with for additional questions about naming consistency and which chemicals EPA has detected in association with the site?

Thanks and best regards,
Amy

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From: Strynar, Mark [mailto:Strynar.Mark@epa.gov]
Sent: Thursday, August 30, 2018 8:48 AM
To: Risen, Amy J <Amy.Risen@ncdenr.gov>
Cc: McCord, James <mccord.james@epa.gov>
Subject: [External] RE: PFAS compounds list

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Amy,

It's hard for me to go through all of these to confirm they are correct right now. However what you have for PEPA is NOT correct. Here is the correct structure and CAS. It seems another chemical in the dashboard also goes by the name PEPA and has the CAS you show below.

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID60896486

The second one I see is for the chemical you have called TAFN4. We call this PFO5DoDA as I recall. The IUPAC name and CAS are correct. I have no idea about the shorthand name. The line just above it is correct???

https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID50723994

I don't this the ones called PFECA-F, PFECA-A or PFECA-G need to be here. They were used as surrogate chemicals before we could get standards. I think they should be removed unless there is a good reason to keep them.

Everything else seems reasonable but I have not checked all of them.

Mark

From: Risen, Amy J [mailto:Amy.Risen@ncdenr.gov]
Sent: Wednesday, August 29, 2018 4:53 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFAS compounds list

Hi Mark,

I hope all is well with you.

Could you take a look at the list of PFAS chemicals below and let me know if there are any that we are missing? I'm looking for chemicals that have been detected in association with the Chemours facility in air/soil/water. I realize that our list has some chemicals that are not detected at meaningful levels, but are just part of our list of analytes for our lab. At this point we are looking for any additional analytes that have been detected for Chemours, and for which we are not currently considering for analysis.

Thanks!
Amy

Chemours PFAS Shorthand	DEQ PFAS Shorthand	Chemical Name	CASN	Chemical Formula	Carbon-chain length
HFPO-DA	PFPrOPrA, "GenX"	2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-propanoic acid)	13252-13-6	C6HF11O3	6
PFMOAA		Perfluoro- 2-methoxyacetic acid	674-13-5	C3HF5O3	3
PMPA		Perfluoro-2-methoxypropanoic acid	13140-29-9	C4HF7O3	4
PFO2HXA		Perfluoro(3,5-dioxahexanoic) acid	39492-88-1	C4HF7O4	4
PFECA-F	PFMOPrA	Perfluoro-3-methoxypropanoic acid	377-73-1	C4HF7O3	4
PFECA-A	PFMOBA	Perfluoro-4-methoxybutanoic acid	863090-89-5	C5HF9O3	5
PFO3OA		Perfluoro(3,5,7-trioxaoctanoic) acid	39492-89-2	C5HF9O5	5
PFO4DA		Perfluoro(3,5,7,9-tetraoxadecanoic) acid	39492-90-5	C6HF11O6	6
PFESA-BP1	Nafion BP #1	Nafion Byproduct 1	66796-30-3; 29311-67-9	C7HF13O5S	7
PFESA-BP2	Nafion BP #2	Nafion Byproduct 2	749836-20-2	C7H2F14O5S	7
PFECA-G		Hexanoic acid, 2,2,3,3,4,4,5,5,6,6-decafluoro-6-(trifluoromethoxy)-; Butanoic acid, 2,2,3,3,4,4-hexafluoro-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethoxy]-	174767-10-3; 801212-59-9	C7HF13O3	7
PFO5DA		Perfluoro(3,5,7,9,11-pentadodecanoic) acid	39492-91-6	C7HF13O7	7
TAFN4		2,2,4,4,6,6,8,8,10,10,12,12,12-tridecafluoro-3,5,7,9,11-pentaoxadodecanoic acid	39492-91-6	C7HF13O7	7
PEPA		Acetamide, 2-[2,6-difluoro-4-[[2-[(phenylsulfonyl)amino]ethyl]thio] phenoxy]-	141286-78-4	C16H16F2N2O4S2	16
4:2 FTS		4:2-fluorotelemersulfonate	757124-72-4	C6H5F9O3S	6
6:2 FTS		6:2-fluorotelemersulfonate	27619-97-2	C8H5F13O3S	8
8:2 FTS		8:2-fluorotelemersulfonate	39108-34-4	C10H5F17O3S	10
10:2 FTS		10:2-fluorotelemersulfonate	120226-60-0	C12H5F21O3S	12
PFOSA		Perfluorooctanesulfonamide	754-91-6	C8H2F17NO2S	8
NMePFOSA		N-methyl-perfluoro- octane-1-sulfonamide	31506-32-8	C9H4F17NO2S	9

NEtPFOSA	N-ethylperfluoro- octane-1-sulfonamide	4151-50-2	C10H6F17NO2S	10
NMeFOSAA	N-methyl perfluoro- octane-sulfon-amidoacetic acid	2355-31-9	C11H6F17NO4S	11
NMePFOSAE	N-methylperfluoro- octane-sulfon-amidoethanol	24448-09-7	C11H8F17MO3S	11
NEtFOSAA	N-ethyl perfluoro- octane-sulfon-amidoacetic acid	2991-50-6	C12H8F17NO4S	12
NEtPFOSAE	N-ethyl-N-perfluoro-octylsulfonylaminoethanol	1691-99-2	C12H10F17NO3S	12
PFBS	Perfluorobutanesulfonic acid	375-73-5	C4HF9O3S	4
PFBA	Perfluorobutanoic acid	375-22-4	C4HF7O2	4
PFPeS	Perfluoropentanesulfonic acid	2706-91-4	C5HF11O3S	5
PFPeA	Perfluoropentanoic acid	2706-90-3	C5HF9O2	5
PFHxS	Perfluorohexanesulfonic acid	355-46-4	C6HF13O3S	6
PFHxA	Perfluorohexanoic acid	307-24-4	C6HF11O2	6
PFHpS	Perfluoroheptanesulfonic acid	375-92-8	C7HF15O3S	7
PFHpA	Perfluoroheptanoic acid	375-85-9	C7HF13O2	7
PFOS	Perfluorooctanesulfonic acid	1763-23-1	C8HF17O3S	8
PFOA	Perfluorooctanoic acid	335-67-1	C8HF15O2	8
PFNS	Perfluorononanesulfonic acid	68259-12-1	C9HF19O3S	9
PFNA	Perfluorononanoic acid	375-95-1	C9HF17O2	9
PFDS	Perfluorodecanesulfonic acid	335-77-3	C10HF21O3S	10
PFDA	Perfluorodecanoic acid	335-76-2	C10HF19O2	10
PFUdA	Perfluoroundecanoic acid	2058-94-8	C11HF21O2	11
PFDoS	Perfluorododecanesulfonic acid	79780-39-5	C12HF25O3S	12
PFDoA	Perfluorododecanoic acid	307-55-1	C12HF23O2	12
PFTeDA	Perfluorotetradecanoic acid	376-06-7	C14HF27O2	14
PFTrDA	Perfluorotridecanoic acid	72629-94-8	C13HF25O2	13
PFHxDA	Perfluorohexadecanoic acid	67905-19-5	C16HF31O2	16
PFODA	Perfluorooctadecanoic acid	16517-11-6	C18HF35O2	18

Amy Risen, PhD
Toxicologist, Division of Waste Management
North Carolina Department of Environmental Quality
(919) 707-8223 (Office)
Amy.Risen@ncdenr.gov

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