Message

From: McCord, James [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=MCCORD, JAMES]
Sent: 6/28/2018 11:53:46 AM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]; Sivertsen, Scott [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=56a8b664924a40e18766f1c843eec111-Sivertsen, Scott]
CC: Zachary Hopkins [zrhopkin@ncsu.edu]
Subject: RE: test of HLB vs WAX in PFAS capture

I had to check with Zack to make sure I had the correct methods file. The table has the transitions he determined from infusion of the standards.

Compound	Precursor (m/z)	Fragment (m/z)	Cone (V)	Collision (V)
PFO3OA 1	311.1	84.9	22	20
PFO3OA 2	311.1	150.8	22	4
PFO4DDA	377.0	84.9	22	26
PFO5DoDA 1	442.99	94.7	10	33
PFO5DoDA 2	442.99	150.67	10	5
PFO5DoDA 3	442.99	216.83	10	5
PFESA BP1.1	442.98	96.75	35	31
PFESA BP1.2	442.98	130.5	35	25
PFESA BP1.3	442.98	146.8	35	25
PFESA BP2.1	462.87	212.9	35	36
PFESA BP2.2	462.87	262.93	35	28

As Mark mentioned, we observe isomers of the PFESA byproducts, and the BP1 seems to be quite finicky as a standard.
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James McCord

From: Strynar, Mark
Sent: Monday, June 25, 2018 3:44 PM
To: Sivertsen, Scott <Sivertsen.Scott@epa.gov>
Cc: McCord, James <mccord.james@epa.gov>; Zachary Hopkins <zrhopkin@ncsu.edu>
Subject: RE: test of HLB vs WAX in PFAS capture

Scott,

Sorry for slow reply I am away at the Gordon conference in NH.

The analytes we had trouble with were the low molecular weight PFECAs that decarboxylate and make it hard to find an M-H- peak. I think James or Zack can send you transitions.

I don't recall an issue with Nafion BP2 but I seem to recall BP1 gave us some issues. We use out LC-MS/MS and out TOFMS system as well as our Orbitrap Fusion for the analytes.

You should see PFESA 2 as 2 peaks we always do. We believe the PFESA1 converts to the PFESA2 as there is HF in the solution and think the HF gets added across the double bond.

Mark

From: Sivertsen, Scott
Sent: Friday, June 22, 2018 3:53 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: test of HLB vs WAX in PFAS capture

Hi Mark,

I recall a while ago that you said you were having problems finding transitions on your tandem instrument for at least one of the compounds you found and elucidated in the CFR.

What instrument are you using for this most recent work? We're having detection issues with our tandem quad (Waters Xevo TQ-S micro) and the selected transitions using the Chemours standards. In particular, PFO3OA, PFO4DA and PFESA 1 and 2 are troublesome. If you have transitions, they would be appreciated.

We are seeing two chromatographic peaks for PFESA 2. Also, PFESA 2 (contamination?) in the PFESA 1 standard. Is your experience similar?

Thanks,

Scott

From: Strynar, Mark
Sent: Wednesday, June 06, 2018 10:33 AM
To: Shoemaker, Jody <shoemaker.jody@epa.gov>; Sivertsen, Scott <Sivertsen.Scott@epa.gov>; Washington, John <Washington.John@epa.gov>
Subject: test of HLB vs WAX in PFAS capture

All,

I ran this experiment last week to check which analytes are captures when I stack HLB followed by WAX, and then Wax followed by HLB. See the attachments if you are interested. I did not quantitate, just check which cartridge captured the analyte when stacked.

A few things that differ from Method 537 was I processed 500 mL of nitric acid spiked and filtered surface water (in duplicate) and do not use Trizma. I also do not do the 7.5 mL (2X) water rinse of the HLB cartridge before methanol elution. The elution of the WAX SPE follows our usual procedures. I did not try to capture PFOSA as it comes out in the neutral wash, however I have done this before with WAX and know it is there.

In brief here is what we found.

HLB works very well from most of these analytes with a select set when the analytes pass through to some extent.

WAX works very well for all with small (<10%) breakthrough for PFMOAA.

As the Chemours effluent was very high in concentration for some PFAS based on our prior analysis, SPE capacity could be a partial contributor to break through.

Mark

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