Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 10/7/2020 1:03:31 PM
To: Leung, Lam-Wing H [LAM.H.LEUNG-1@chemours.com]
CC: McCord, James [mccord.james@epa.gov]
Subject: RE: ?RE: ?RE: ?RE: Linear & Branched Isomers

Hi Lam,

I don't have time until at least Tuesday of next week. If 30 minutes is enough we could chat in a window working around our obligations. I have not done anything on my end toward answering these questions for ourselves.

Mark

From: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Sent: Tuesday, October 06, 2020 3:51 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: McCord, James <mccord.james@epa.gov>
Subject: RE: ?RE: ?RE: ?RE: Linear & Branched Isomers

Mark,

We received his from DEQ late last week and perhaps we can discuss more sometime this week if you and/or James are available. Please let me know. Thanks.

Lam

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Wednesday, September 30, 2020 10:18 AM
To: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Cc: McCord, James <mccord.james@epa.gov>
Subject: ?RE: ?RE: ?RE: Linear & Branched Isomers

External email. Confirm links and attachments before opening.

Hi Lam,

Glad to chat but I would be very concerned about monitoring for either the branched or the linear forms of either of the PFECAs below using only one MRM. It is quite possible the decarboxylation and the ether fragmentation are different between the two isomeric forms and could be seen by ion ratio comparisons. Both are possible even if one is preferred. I would always prefer two ions for the MRMs rather than one even if the case is made one is seen. If MS conditions change that could change.

As I think I have all of these standards I will see if I can do some work on this.

Mark

From: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Sent: Tuesday, September 29, 2020 4:34 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: ?RE: ?RE: Linear & Branched Isomers

Mark,

Thanks for the info. However, our external testing labs now have established (not validated yet) a method that includes both isomers (along with many other PFAS analytes) using the 2 different MRMs and they reported that "**repeated analysis of PMPA/PEPA (only) standards, as well as PFECA F/A (only) standards under these conditions, and once again concluded that there is almost no spectral crossover or overlap between branched and linear isomers".** I somewhat agree with your points regarding potential overlap when it comes to the PMPA and PFMOPrA but at the concentrations we are looking at (1-100sppt), there can be easily separated based on MRMs.

My key point of the message is that GEL lab (hence DEQ) has been reporting the results as from linear isomers using the "incorrect" MRMs as they should be the branched isomers all along.

Perhaps we can discuss more over the phone regarding this. Thanks.

Best,
Lam

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Tuesday, September 29, 2020 1:05 PM
To: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Subject: ?RE: ?RE: Linear & Branched Isomers

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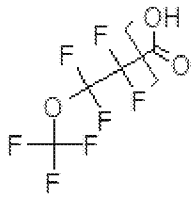
Lam,

Sorry for the slow response I was in the lab getting things functional the last 2 days. Here is something I sent to Amy in the past on this topic in response to a GEL labs report. In short the decarboxylation transition for both PMPA and PEPA is not unique. You can get that transition from both the branched and the linear. For PMPA both transitions are in common so they cant be told apart from only MS experiments. I suggest chromatography as a way to tell apart. For PEPA there is a unique transition (279-135) however the other transition (279-235) is shared if decarboxylation occurs.

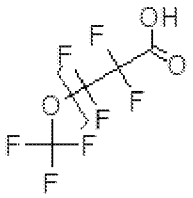
Mark

Amy
Based on MS/MS experiments alone these are not able to be distinguished from one another. Can be both based on transition 229-185 (loss of CO2) and 229-85 being in common to both. Only chromatography could tell these apart in LC-MS/MS or NMR.

PFMOPrA
[M-H]-: 228.9

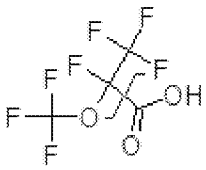


C_3F_7O
184.9

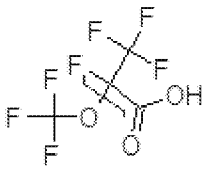


CF_3O
84.9

PMPA
[M-H]-: 228.9



C_3F_7O
184.9

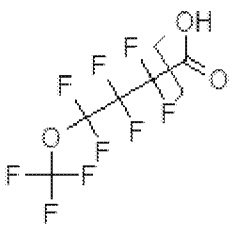


CF_3O
84.9

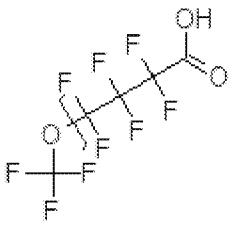
>> PFMOPrA/PMPA
>> 377-73-1 CAS provided by Chemours?
>> (could also be 13140-29-9)
>> 229/185

For these two isomers this transition 279-135 can ONLY come from the PEPA (CAS 267239-61-2) and NOT the PFMOBA CAS 863090-89-5). If the unique transition of 249-85 were used it would be ONLY for the PFMOBA and NOT the PEPA.
>> PFMOBA/PEPA
>> 863090-89-5 provided by Chemours?
>> (new MS-MS observations suggest primarily 267239-61-2)
>> 279/135

PFMOBA
[M-H]-: 278.9

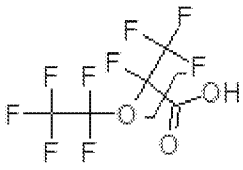


C_4F_9O
234.9

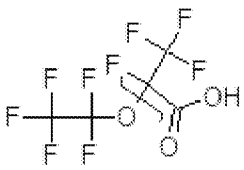


CF_3O
84.9

PEPA
[M-H]-: 278.9



C_4F_9O
234.9



C_2F_5O
134.9

From: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Sent: Tuesday, September 29, 2020 11:05 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: FW: ?RE: Linear & Branched Isomers

Hi Mark,

Just to follow up, any comments?

Thanks,
Lam

From: Leung, Lam-Wing H
Sent: Monday, September 28, 2020 1:54 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: ?RE: Linear & Branched Isomers

Yes, the MRMs they listed are for the branched isomers but they are reporting them as linear isomers in their reports.

- a mass transition of 229→185, which is the mass transition for PMPA (branched), and calling the result PFMOPrA (for which the mass transition should be 229→85).

- a mass transition of 279→235, which is the mass transition for PEPA (branched), and calling the result PFMOBA (for which the mass transition should be 279→85).

Method 533 used these MRMs for the linear isomers and our studies indicate that for branched isomers, there does not seem to have any responses at ppt levels from the branched isomers for these MRMs (i.e. you can essentially separate the isomers using their corresponding MRMs).

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Monday, September 28, 2020 1:48 PM
To: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Subject: ?RE: Linear & Branched Isomers

External email. Confirm links and attachments before opening.

Hi Lam. Which analytes are we discussing on page 72? Is it PFMOPrA and PFMOBA? 229- 185 and 270-235 respectively?

Mark

From: Leung, Lam-Wing H <LAM.H.LEUNG-1@chemours.com>
Sent: Monday, September 28, 2020 1:12 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: Linear & Branched Isomers

Hi Mark,

This is coming up again from DEQ. So can you please take a look at this GEL method and specifically how they report the linear/branched isomers? Basically, they are using the "wrong" MRMs (pg.72) for the reporting. I had a very difficult time convincing DEQ otherwise as they have been reporting all the results as the linear isomers. Can we discuss this and I might need your help in "convincing" them and/or GEL in this as well? Please let me know.

Best Regards,
Lam

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