Message

From: Detlef Knappe [knappe@ncsu.edu]
Sent: 4/6/2017 1:51:07 PM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
CC: Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: Re: PFECA structures

Thank you, Mark. With the Orbitrap in MSn mode, will you be able to tease out which one is correct? Also, should we try a different column on the UPLC?

I am at the ACS meeting in San Francisco this week. A few interesting PFAS talks at the PFAS session. Lots of focus on AFFF.

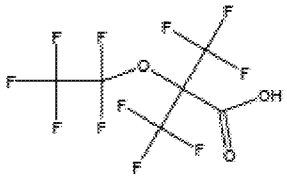
Detlef

On 4/6/17 5:51 AM, Strynar, Mark wrote:

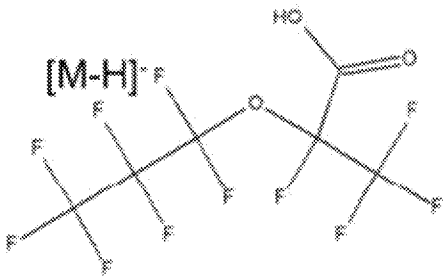
> Detlef,
> Here are the structures I have found using Chemspider and EPA Chemistry dashboard for the C3 through C7 (based on formulas) perfluoro ethers in the GenX series. I tried to include ONLY the reasonable ones for LC-ESI- mode.
> Mark
> **From:** Detlef Knappe [mailto:knappe@ncsu.edu]
> **Sent:** Tuesday, April 04, 2017 8:35 PM
> **To:** Strynar, Mark <Strynar.Mark@epa.gov>
> **Subject:** RE: PFECA structures
> Thank you, Mark. Can you let me know whether there are other structures that might not be right in figure S5?
> Detlef
> On Apr 4, 2017 12:20 PM, "Strynar, Mark" <Strynar.Mark@epa.gov> wrote:
>
> > Detlef,
> >
> > In figure S5 I think the structure is not correct from the 2015 SI. These were the suspected structures and we did not QTOFMS data at the time. If these were both correct we could tell them apart with MS/MS as they would likely cleave at the ether oxygen. The top would give a C2F5O (135) transition and the bottom a C3F7O (153) transition for the daughter assuming the O migrates with the fragment. If not we would get a C2F5 (119) and a C3F7 (169) transition respectively.
> >
> > I think they are both GenX and the lower structure is correct.
> >
> > Mark
> >
> > **From:** Detlef Knappe [mailto:knappe@ncsu.edu]
> > **Sent:** Tuesday, April 04, 2017 3:03 PM
> > **To:** Strynar, Mark <Strynar.Mark@epa.gov>
> > **Subject:** PFECA structures

Mark,

I am struggling with PFECA structures. In your 2015 paper, your homologous series (Figure S5) shows



Can we distinguish the above compound from GenX, which looks like this (same overall formula)



Detlef

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