Message

From: Sun, Mei [msun8@uncc.edu]
Sent: 3/1/2017 9:30:21 PM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
CC: Detlef Knappe [knappe@ncsu.edu]; Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: Re: FW: Chemical Structures

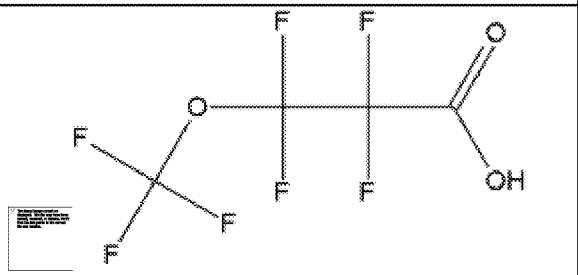
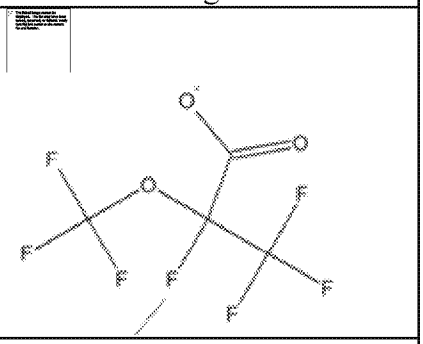
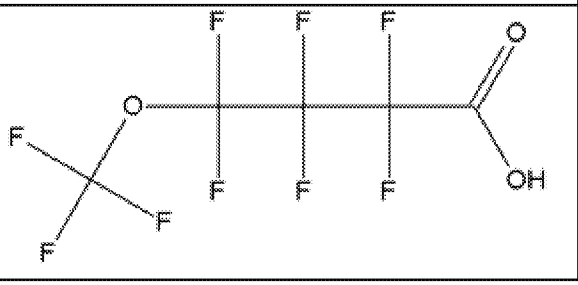
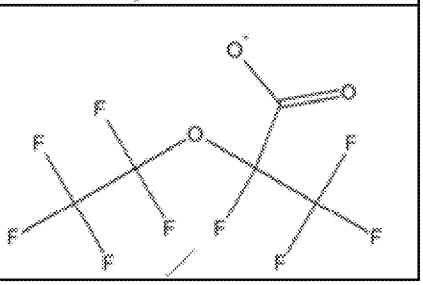
Mark and Andy

I drafted an email to the editor for updating the structures in SI. Please see if you think it's appropriate. For this draft I coped the structure in Mark's paper, but before I send it to the editor I will redraw them with the same software I used for other compounds to make the appearance more uniformed.

Dear Dr. Arnold

I'm requesting an update of the Supporting Information document for our paper "Legacy and Emerging Perfluoroalkyl Substances Are Important Drinking Water Contaminants in the Cape Fear River Watershed of North Carolina" published in Env. Sci. & Tech. Letters 2016 3 (12) 415 (DOI: 10.1021/acs.estlett.6b00398).

In Figure S1 of this paper, we showed the chemical structures of seven emerging perfluoroalkyl substances. After a more careful comparison with the LCMS results, we decided two of the compounds are more possibly branched instead of linear as shown in the paper SI. Here is the comparison of the structures:

Chemical	Structure shown in current IS	Should be changed to
PFMOPrA		
PFMOBA		

The revised SI with the chemical structures updated is in the attachment. Since we do not need to change anything in the paper itself but only the SI, could we just replace the SI document without a formal erratum? Thank you very much and sorry for the inconvenience.

Mei Sun

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On Tue, Feb 14, 2017 at 11:48 AM, Strynar, Mark <Strynar.Mark@epa.gov> wrote:

If it is easy to change the SI lets do it. If it is not, it is really not a big deal. Plus we have not standard to confirm which is correct. Could be both. Paul Resnick seems to think the branched isomers are more likely.

Mark

From: Sun, Mei [mailto:msun8@uncc.edu]
Sent: Tuesday, February 14, 2017 10:10 AM
To: Detlef Knappe <knappe@ncsu.edu>
Cc: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>

Subject: Re: FW: Chemical Structures

Sorry for the mistake... if updating the SI is not too much trouble, I'd say let's try it.

Mei Sun

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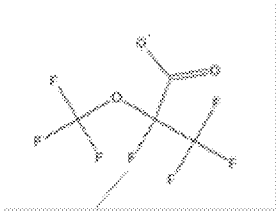
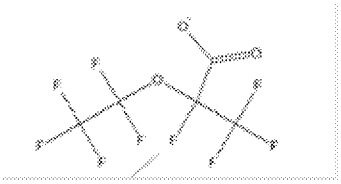
On Tue, Feb 14, 2017 at 7:57 AM, Detlef Knappe <knappe@ncsu.edu> wrote:

I should have noticed that, too... Should we explore an erratum? Since it involves the SI, updating the SI may be possible even without an erratum.

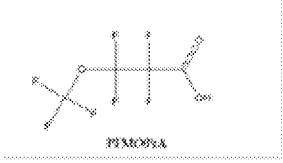
On 2/14/17 7:44 AM, Strynar, Mark wrote:

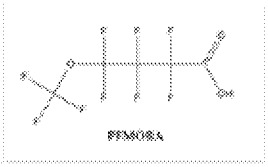
In our paper Strynar et al., 2015 we proposed these structures as below: (Figure S7). These are the ones Paul suggests are more likely.





In Sun et al., 2016 we showed them different (Figure S1).





I should have noted this in the SI.

The QTOF can distinguish between the two as the likely breaking point is at the ether oxygen. We would get different fragments for the PFMOBA, not the PFMOPrA.

Mark

From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Monday, February 13, 2017 8:13 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; msun8@uncc.edu
Subject: Re: FW: Chemical Structures

Interesting... But Synquest does make the non-branched compounds we are showing (see first two compounds in the attached). Would QTOF work be able to distinguish between linear and branched?

On 2/13/17 7:22 AM, Strynar, Mark wrote:

> FYI,
>
> I will need to take a closer look at his comment later.
>
> Mark

From: Paul [mailto: Personal Matters / Ex. 6
Sent: Saturday, February 11, 2017 6:30 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: Chemical Structures

Mark:

Just finishing looking at Env. Sci. & Tech. Letters 2016 3 (12) 415 for use as a reference.

Legacy and Emerging Perfluoroalkyl Substances Are Important

Drinking Water Contaminants in the Cape Fear River Watershed of

North Carolina

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I believe that the structural assignments for PFMOBA [$CF_3OCF_2CF_2CF_2COOH$] and PFMOPrA [$CF_3OCF_2CF_2COOH$] are most likely incorrect.

More reasonably the correct structures are isomers $CF_3CF_2OCF(CF_3)COOH$ and $CF_3OCF(CF_3)COOH$ respectively. I doubt that the MS/MS could tell the isomers apart.

If you want to discuss this further please call me. (703) 567-6832.

Best regards,

Paul

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