Message

From: Sun, Mei [msun8@uncc.edu]
Sent: 3/2/2017 10:48:10 PM
To: Detlef Knappe [knappe@ncsu.edu]
CC: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]; Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: Re: FW: Chemical Structures

Dear all

After a closer look at the structures, I found if we want to make the change, we will have to not only update the structure figure in SI, but also change the chemical names in both SI and the text.

In our published paper these two linear compounds are named as Perfluoro-3-methoxypropanoic acid (PFMOPrA) and Perfluoro-4-methoxybutanoic acid (PFMOBA). After making them branched, I think they should be named as Perfluoro-2-methoxypropanoic acid (PFMOPrA) and Perfluoro-3-ethoxypropanoic acid (PFEOPA) following the same rules. That would lead to changes in the text where the ether compounds are introduced for the first time, and all tables/figures/texts where the abbreviation PFMOBA is used.

I think that would cause enough trouble that a formal erratum is needed, and I'm not sure the gain would worth the trouble... Please let me know what you think.

Mei Sun

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On Thu, Mar 2, 2017 at 8:04 AM, Detlef Knappe <knappe@ncsu.edu> wrote:

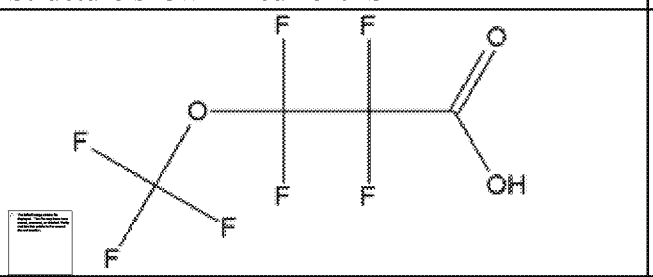
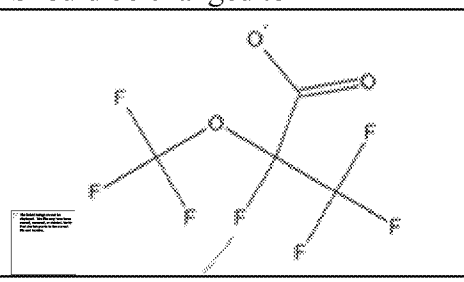
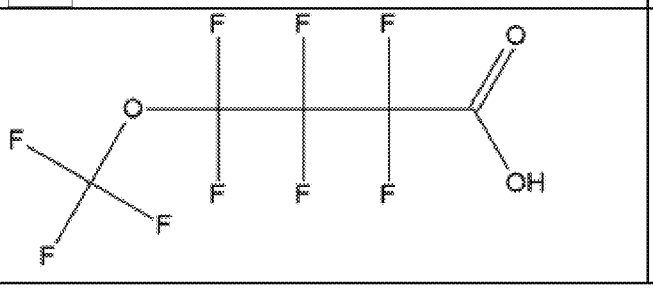
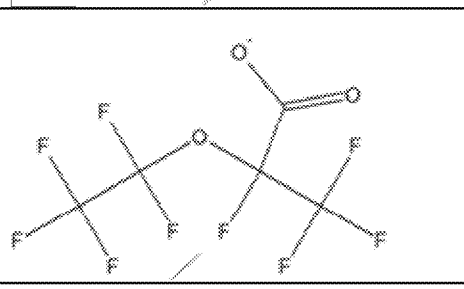
> Hi Mei,
>
> I made a few wording changes below. Also, it would be better to show the protonated forms, like we did in the original paper so that the molecular weights match the structures.
>
> Best,
>
> Detlef
>
> On 3/1/17 4:30 PM, Sun, Mei wrote:

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 am the corresponding author of the 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). The authors were recently contacted about two of the molecular structures we are showing in the supporting information of the paper. The suggestion was made that the two chemicals are more likely branched instead of linear as follows:

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

After a review of our high resolution mass spectrometry results, we concur that the branched structures are more likely.

I would like to know whether it is possible to update the SI of the above referenced paper. The revised SI with the two 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 I apologize for the inconvenience.

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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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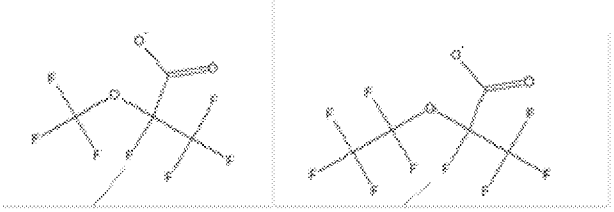
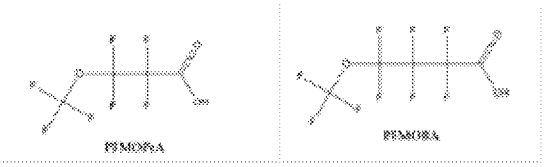
>
> On Tue, Feb 14, 2017 at 7:57 AM, Detlef Knappe <knappe@ncsu.edu> wrote:
>
> > I should have noticed that, too... Should we explore an erratum? Since it involves the SI, updating the SI may be possible even without an erratum.
> >
> > On 2/14/17 7:44 AM, Strynar, Mark wrote:
> >
> > > In our paper 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:p **Ex. 6 Personal Privacy (PP)**
> **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

Mei Sun,*,†,‡ Elisa Arevalo,‡ Mark Strynar,§ Andrew Lindstrom,§ Michael Richardson,∥ Ben Kearns,∥

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⊥Town of Pittsboro, Pittsboro, North Carolina 27312, United States

#Fayetteville Public Works Commission, Fayetteville, North Carolina 28301, United States

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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