Message

From: Detlef Knappe [knappe@ncsu.edu]
Sent: 4/5/2017 12:35:11 AM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
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.

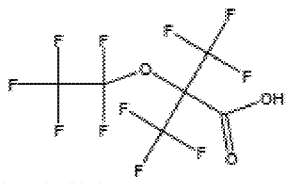
I think they are both GenX and the lower structure is correct.

Mark

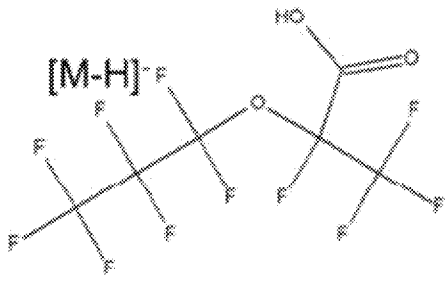
From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Tuesday, April 04, 2017 3:03 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFECA structures

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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Detlef Knappe
Professor
319-E Mann Hall
Department of Civil, Construction, and Environmental Engineering
North Carolina State University
Campus Box 7908
Raleigh, NC 27695-7908

Phone: 919-515-8791
Fax: 919-515-7908
E-mail: knappe@ncsu.edu
Web page: http://knappelab.wordpress.ncsu.edu/