To: Oshima, Kevin[Oshima.Kevin@epa.gov]; Buckley, Timothy[Buckley.Timothy@epa.gov]
Cc: Strynar, Mark[Strynar.Mark@epa.gov]; McCord, James[mccord.james@epa.gov]; Schumacher, Brian[Schumacher.Brian@epa.gov]
From: Medina-Vera, Myriam[/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=B081A1F48A044B4C9D1EBC4992C54DEE-MEDINA-VERA, MYRIAM]
Sent: Tue 7/10/2018 6:14:19 PM (UTC)
Subject: Heads-up Clearance package- Non-targeted screening based identification of per- and polyfluorinated contaminants in the Cape Fear River

Final McCord_Strynar Cape Fear paper.pdf
Lang_363 Review comments_McCord_Strynar Cape Fear.pdf
McCord_CapeFearCompoundDiscovery - QAForm_Signed.pdf
McCord_CapeFearCompoundDiscovery - STICS.PDF
McCord_CapeFearCompoundDiscovery - Supplemental Information.docx
McCord_CapeFearCompoundDiscovery_363 Review Form - JRL.PDF
McCord_CapeFearCompoundDiscovery_363 Review Form - SRN.PDF
McCord_Strynar_SDMP_20180510.docx
NERL Fact Sheet McCord_Strynar_Cape Fear Compound Discovery.docx
Newton_363 Review Comments_McCord_Strynar Cape Fear paper .pdf
Supplemental Table 1_All Chemical Features.xlsx
Supplemental Table 2_Assigned Chemical Species.xlsx
Supplemental Table 3_Profinder Settings.xlsx
TOC_Figure.png

Kevin, Tim:

Attached are the files that will be send to Leeann to enter into STICS. This is a heads-up. The questions are: who will give the heads up to NC DEQ and R4?
Mark Strynar (Fed) and James McCord (ORISE) are the contacts for any additional questions.

- **Product type, subtype:** Journal Article, Peer Reviewed
- **Product title:** Non-targeted screening based identification of per- and polyfluorinated contaminants in the Cape Fear River by high resolution mass spectrometry
- **Author(s):** James McCord, Mark Strynar (all authors have EPA e-mail addresses).
- **Initiator:** Leeann Mosley ,ORD/NERL/EMMD
- **ORD Tracking Number:**
- **Product Description / Abstract:** Ongoing chemical development in response to the regulation of historical perfluorinated compounds has resulted in a proliferation of novel per- and polyfluorinated species. A lack of publicly available information on these compounds necessitates an untargeted approach to screening and monitoring. Herein we apply a non-targeted screening approach to the Cape Fear River of North Carolina, a fluorochemically impacted watershed. The presence of previously described perfluorinated ether acids and carboxylic acids was confirmed, and a further 22 novel fluorinated species were identified, including acid species containing multiple acidic sites, species containing a single hydrogenation, and unreported perfluorinated ether acids. Roughly half of these novel compounds could be assigned a unique chemical structure based on high resolution MS/MS fragmentation, while the remainder could only be assigned a chemical class. Compounds identified by an initial non-targeted screen were monitored over repeated sampling to track longitudinal trends during source control activities by the state Department of Environmental Quality. Monitored compounds demonstrated a decrease in abundance over the monitored period. Hierarchical clustering of the time trend data was used to associate non-targeted species with each other and to identify underlying chemical sources. The resulting six clusters were loosely associated based on chemical class.
- **Tracking and Planning**
  - **Task ID:** SSWR 6.02B

- Task: Novel monitoring technologies for occurrence, exposure and effect for individual and groups of contaminants

- **Product Category:** High Visibility/ Requires Advance Notification
- **QA form attached in STICS?:** Yes
- **QAPP Reference:** QAPP #: D-EMMD-PHCB-006-QAPP-01: "Non Targeted Analyses (NTA) and Suspect Screening of Chemicals in Environmental and Biological Samples in the Analytical Laboratories"

- **Journal Name:** Environmental Science and Technology

- **Keywords:** PFAS, non-targeted, mass defect

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