

The focus of this report is to present and describe, to date, the non-targeted screening of per- and polyfluorinated alkyl substances (PFAS) in finished water collected on a weekly basis from the Sweeney Water Treatment Facility to NC Department of Environmental Quality. The sampling commenced on November 11, 2017 and this report describes data through May 16, 2018. The major findings include detection of several unreported PFAS compounds in finished waters by high resolution mass spectrometry. Several metrics were used to aid in generating and confirming the molecular formulas. These included the following; constraining elemental numbers, LEWIS check, isotope pattern filtering, fluorine to carbon ratio check and finally multidimensional mass spectrometry. Using this approach generated previously unreported PFAS compounds with neutral molecular formulas of $C_4F_8O_4H_2S_1$ and $C_{13}F_{24}O_6H_1Cl_1$. A chemical abstract search of $C_4F_8O_4H_2S_1$ yielded two possibilities with CAS numbers of 801209-99-4 and 905363-44-2. These are constitutional isomers and based upon fragmentation with multidimensional mass spectrometry, both of these compounds are present in the finished water. A similar chemical abstract search of $C_{13}F_{24}O_6H_1Cl_1$ produced a compound with a CAS number of 814917-77-6. Fragmentation of the compound by MS/MS produced fragments consistent with the structure. To summarize, three previously unreported PFAS compounds have been detected in finished waters collected at Sweeney Water Treatment Facility. Until authentic standards can be purchased or synthesized, any proposed structures are tentative as well as we cannot provide any quantitative information. These compounds have been detected in all samples collected and analyzed to date with the overall trend of decreasing peak areas. The level of these compounds has stayed above instrumental background as defined by a signal to noise ratio of three thus discernable from instrument background. Given the reported capture of all waste generated at the

Fayetteville Works facility, this suggests there may be other non-point source inputs (e.g. sediment release, atmospheric deposition) into the Cape Fear River.

Previously published sample processing and QA/QC procedures were followed throughout the study (Nakayama et al., 2010; Strynar et al., 2015). Briefly, water samples from finished drinking water were collected in methanol rinsed 500 mL HDPE bottles. For each sampling week, a travel blank was included that consisted of high purity water from a Millipore Sigma Milli-Q Reference system that has been shown to be PFAS free. The MQ water was poured into a separate cleaned 500 mL bottle when the last sample was collected and processed as a sample. In addition to travel blanks, routine method blanks were analyzed. All samples were analyzed on an Agilent 1290 LC coupled to a Bruker Micro-TOFQ II high resolution mass spectrometer with ionization by negative ESI.