Contemporary and temporal investigation of per- and polyfluorinated compounds in Cape Fear river, North Carolina surface water samples.

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Recent regulatory pressure has altered the chemistry of per- and polyfluorinated compounds being manufactured and used in industrial and consumer applications. Many manufacturers have been moving toward the production of shorter chain per- and polyfluorinated compounds. A series of polyfluorinated compounds that contain central ether oxygens have been recently documented in the peer reviewed literature to be present in the Cape Fear river, NC in both surface and drinking water samples. Non-targeted analysis of water samples using high resolution mass spectrometry (HRMS) LC/MSD TOF was used in the past to identify novel polyfluorinated compounds. Contemporary samples were collected recently to: 1) confirm the presence of previously identified chemicals 2) investigate novel chemicals present 3) analyze via TOFMS and QTOFMS for platform cross validation 4) retroactively investigate samples from over 5 years past. Contemporary TOFMS/QTOFMS analysis revealed the presence of a series of polyfluorinated ether sulfonic acids that were previously undescribed. Precursor compounds were selected from a list of molecular features (accurate mass, retention time, abundance) that were unknown. QTOFMS data dependent analysis (DDA) was performed on select precursors to generate fragmentation spectra. One advantage of HRMS and proper data banking is retrospective investigation of past samples. This presentation will focus on TOF/QTOF based analytical approaches used to identify novel chemicals species and temporal occurrence of detected compounds.