Ensuring High-quality Data from NOAA's GC-MS Perseus Instrument

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The NOAA Earth System Research Laboratory Global Monitoring Division collects routine air samples in programmable flask packages (PFPs) from sites across North America and stainless steel and glass flasks across the globe. These sites include atmospheric profiles in small aircraft, stationary locations at tall towers, baseline observatories, and cooperative fixed sites. Starting in 2015, a new gas chromatography-mass spectrometry (GC/MS) analytical system for Preconcentration of Environmentally Relevant Species (or PERSeus) has been making measurements of ~60 halocarbons, hydrocarbons, and sulfur-containing compounds from these PFPs and a subset of flask samples.

Over the past 18 months, more than 15,000 discrete air samples were measured on Perseus for this suite of analytes. Data quality assurance (QA) and quality control (QC) are a fundamental part of these data records. Part of the QA work is performed in the Perseus measurement lab with archive tanks analyzed every 3-5 days, quarterly tertiary and secondary comparisons, bi-annual gravimetric standards comparisons, and routine inter-comparisons among different measurement labs. QC is completed with software developed in GMD and at the Scripps Institution of Oceanography (SIO) to look at raw analysis files, time series plots, and instrument response sensitivities. These tools, and other plotting routines, help us identify sample collection problems and measurement problems (Fig. 1). This presentation will focus on our quality assurance and quality control strategies and findings.

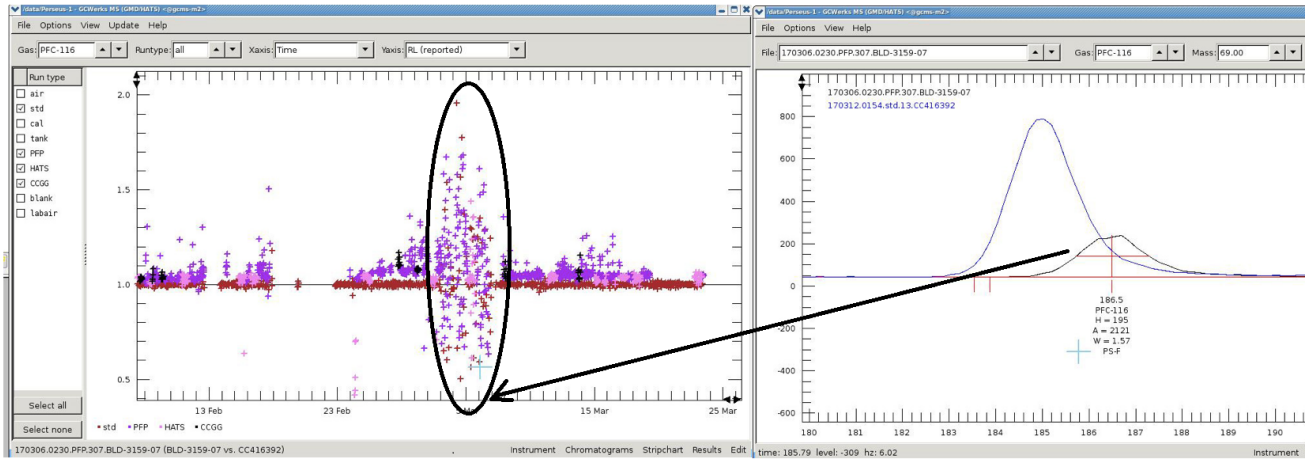

Figure 1. Perseus PFC-116 ratios of sample area/pressure to standard area/pressure are plotted in figure 1 as an analysis date time-series. Standard results are shown in red, PFP results are shown in purple. The results identified with the black circle were determined to have temperature problems during the first trapping phase. The figure to the right shows a PFC-116 chromatogram of detector response vs. retention time (sec) from a "bad" result during this time period (black) compared to a "good" (blue) chromatogram from a later time period.