

Improving Rigor in Polycyclic Aromatic Source Fingerprinting

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Background/Objectives. Source identification of polycyclic aromatic hydrocarbons in environmental samples has advanced greatly in the last 20 years and continues to advance. There are two main tracks of advancement, analytical methodologies and data analysis approaches. Much has been published in this specific application of environmental forensics and many techniques are available. To realize potential benefits and avoid possible pitfalls of this array of approaches, great care is needed as one develops data and applies published diagnostic tools to data sets. This presentation will focus on recommended approaches, unadvisable short-cuts, and examples where errors can be made by applying published methods blindly.

Approach/Activities. Case studies will be used to illustrate three major themes: 1) caveats in the use of existing methods: PAH lists of analytes; PAH ratio analyses; inference of weathering of PAHs; multiple combined data sets without usability/normalization; 2) the needs for the use of multiple lines of evidence in data gathering for PAH forensics work, inclusive of historical reconstruction of operations and releases with multiple lines of chemical evidence – GC of samples to evaluate the overall boiling point distribution and the presence of the petroleum-associated UCM; use of quantitative analysis by GC/MS/SIM for parent and alkylated PAH analyses; use of quantitative analysis by GC/MS/SIM for geochemical petroleum biomarker (and other source related tracers); use of new/emerging techniques such as GCxGC/MS for confirmatory analyses; 3) the use of multiple data analyses methods related to these analytical tools to analyze data and derive a scientifically robust analysis of PAH sources in environmental media and mixtures therein.

Results/Lessons Learned. Case studies will illustrate the major points and the lessons learned, thus pointing the way to more rigorous work by environmental forensic practitioners in the future.