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Mitigation of Fire Debris Compound Naming Error through Automation

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Abstract: The state-of-the-art for analyzing fire debris samples involves a highly-trained technician evaluating each GC-MS peak to assure correct naming. This process is time-consuming and potentially error prone. The best way to mitigate errors is to remove the opportunity to make the errors originally. We show results from a fully automated compound-identification package for GC-MS which accurately names chromatographic peaks to 0.1% response. The system names the broad array of hydrocarbons found in fire debris samples, such as toluene, trimethylbenzenes, alkanes, and naphthalenes; further it identifies a variety of common background compounds. The technique combines information from both the spectral match and the retention time to achieve consistent identifications. A visualization tool annotates the chromatogram with names of the compounds and displays associated Extracted Ion Chromatograms. Report generation gives full details of the location and size of each compound. As well as naming individual compounds, the method categorizes compounds into groups such as alkanes, alkenes, and aromatics, easing comparison to the ASTM E1618 standard. Using this objective method for analysis of fire debris samples significantly reduces the chance of error, saves time for the technician, and increases in-lab repeatability as well as improving reproducibility across laboratories.