B181 Expert System for Characterization Using AMDIS Plus Excel® (Escape): Connecting Cultural Heritage Research to Trace Evidence Analysis by Pyrolysis-Gas Chromatography/Mass Spectrometry (Py-GC/MS)

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Learning Overview: After attending this presentation, attendees will be aware of the technology and expert database used by cultural heritage scientists.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing details about the automated system for evaluating complex Py-GC/MS data, resulting in a more detailed classification of paint-binding media.

Cultural heritage research shares several things in common with the field of trace evidence analysis. Both are interested in learning as much as possible about the major, minor, and trace components present in tiny samples originating from a diverse range of materials. Sample characterization typically involves Fourier-transform infrared spectrometry, Raman spectroscopy, scanning electron microscopy with energy-dispersive X-ray spectrometry, and polarized light microscopy. For in-depth compositional information about paints, coatings, adhesives, plastics, and a range of other organic materials used by artists—and to learn how the materials have changed over time—cultural heritage scientists routinely turn to Py-GC/MS. Microfurnace pyrolyzers possess many advantages over other pyrolyzer types, including an ambient temperature sample introduction area purged with helium, a deactivated quartz furnace tube, a reproducible pyrolysis event ensured by sample cups dropping into a pre-heated zone, and mounting the furnace directly onto the GC inlet to minimize problems of cold spots.

New practitioners of Py-GC/MS face a number of daunting challenges: locating relevant information scattered throughout disparate literature, selecting an optimum analytical method, recognizing material types that require derivatization, processing hundreds of GC peaks, accurate compound identification when mass spectral libraries are incomplete, recognizing characteristic patterns of marker compounds that relate to specific materials, proper characterizing material mixtures, and the need for data presentation that is meaningful to non-scientists. As interpretation of Py-GC/MS data requires considerable expertise, many potential users in both disciplines avoid learning the technique.

The Expert System for Characterization using Automated Mass spectral Deconvolution and Identification System (AMDIS) Plus Excel® (ESCAPE) was developed at the Getty Conservation Institute (GCI) as a two-step Py-GC/MS data processing tool to identify compositions of decorative lacquers, coatings, and paints. AMDIS (from the National Institute of Standards and Technology [NIST]) is used with a specialized 1,500 compound library to identify marker compounds in sample data. Specialized Excel® reports sort the AMDIS marker compound report by material type and provide users with expert knowledge needed for confirming the presence of materials in the sample. Expert knowledge in ESCAPE originates from interviews of Py-GC/MS experts in material characterization and from publications. Excel® reports present the analytical results in various ways—marker compound tables, diagnostic bar graphs, pie charts of composition, and correlation coefficient tables of marker compounds—to best convey the results to both practitioners and non-scientists. Shared databases of the final analytical results provide benefit to the entire cultural heritage community.

In order to evaluate the accuracy of ESCAPE and its applicability to forensic paint samples, Collaborative Testing Services (CTS) samples were tested at the GCI in a collaboration with trace evidence examiners from the Los Angeles County Sherriff's Department. The results were fully consistent with the known compositions, and compositional differences between Q and K specimens were clearly illustrated by bar graphs of key markers in the binding media. Additional studies of the diverse types of paints used in the creation of art—tube colors, house paints, industrial paints, and spray paints—illustrated best practices for clear presentation of compositional data for acrylic, vinyl, alkyd, epoxy, and urethane binding media.

ESCAPE could be considered as a common platform for sharing paint composition data between the forensic and cultural heritage research communities. It can be customized to meet the unique needs of the forensic community, especially in regard to developing meaningful formats for presenting analytical results in court. Interested researchers learn ESCAPE in workshops conducted by the GCI, so that researchers with Py-GC/MS instrumentation can immediately start applying ESCAPE in their work. For laboratories without a Py-GC/MS, ESCAPE provides justification for equipment purchase as the expert knowledge in the system overcomes the steep learning curve for new users. Collaboration with experts in toxicology, arson, tapes, and fibers can extend the utility of ESCAPE beyond paints and coatings. One desired outcome is the development of a shared paint composition database that would benefit the cultural heritage and forensic communities on both a national and an international level.

Py-GC/MS, Paint Analysis, Shared Database