OSAC RESEARCH NEEDS ASSESSMENT FORM

Title of research need: Objective comparisons of highly-dimensional spectral data

Keyword(s): forensic science, interpretation, spectroscopy, exclusionary differences

Submitting subcommittee(s): Trace Materials **Date Approved:** 02/24/2021

(If SAC review identifies additional subcommittees, add them to the box above.)

Background Information:

1. Does this research need address a gap(s) in a current or planned standard? (ex.: Field identification system for on scene opioid detection and confirmation)

Current standard documents ASTM E1610-18 Std Guide for Forensic Paint Analysis and Comparison, ASTM E2937-18 Std Guide for Using Infrared Spectroscopy in Forensic Paint Examinations, ASTM E2808-19 Std Guide for Microspectrophotometry in Forensic Paint Analysis , and Std Guide for Using Micro X-ray Fluorescence (µ-XRF) in Forensic Polymer Examinations address the questions related to the criteria to conduct comparative examinations. However, all these documents do not offer comprehensive guidance on how to objectively evaluate spectral similarities and slight dissimilarities.

2. Are you aware of any ongoing research that may address this research need that has not yet been published (e.g., research presented in conference proceedings, studies that you or a colleague have participated in but have yet to be published)?

Not at this time.

3. Key bibliographic references relating to this research need: (ex.: Toll, L., Standifer, K. M., Massotte, D., eds. (2019). Current Topics in Opioid Research. Lausanne: Frontiers Media SA. doi: 10.3389/978-2-88963-180-3)

Ausdemore M. A., Neumann C., Saunders C. P., Armstrong D., Muehlethaler C. Two-stage approach for the inference of the source of high-dimensional and complex chemical data in forensic science. *Journal of Chemometrics*, 2020, e3247.

Lavine B., Almirall J., Muehlethaler C., Neumann C., Workman Jr, J. Criteria for comparing infrared spectra–A review of the forensic and analytical chemistry literature. *Forensic Chemistry* 2020; *18*, 100224.

Muehlethaler C., Massonnet G., Hicks, T. Evaluation of infrared spectra analyses using a likelihood ratio approach: A practical example of spray paint examination. *Science & Justice* 2016, *56*(2), 61-72.

4. Review the annual operational/research needs published by the National Institute of Justice (NIJ) at https://nij.ojp.gov/topics/articles/forensic-science-research-and-development-technology-working-group-operational#latest? Is your research need identified by NIJ?

Not at this time.

5. In what ways would the research results improve current laboratory capabilities?

Comparisons between replicate spectra imply the evaluation of the overlap intra-source variation between compared spectral data sets. Most often, these evaluations include consideration of detailed spectral features. Currently available statistical, chemometric or probabilistic approaches have yet to demonstrate the ability to successfully detect small spectral differences. These approaches will be very beneficial to the trace evidence examiner in evaluating objectively a large number of spectral data during comparative examinations using different spectroscopy methods. Examples of relevant spectroscopic methods are infrared spectroscopy, microspectrophotometry, x-ray fluorescence spectrometry, or Raman spectroscopy.

6. In what ways would the research results improve understanding of the scientific basis for the subcommittee(s)?

Research studies in this area will bring objective and numerical information regarding how to assess and define the concepts of "exclusionary difference" or "(in)distinguishability" recently added in most standard documents on the basis of spectral data collected in specific case scenarios.

7. In what ways would the research results improve services to the criminal justice system?

Research studies in these areas are projected to add reliability and objectivity during comparison processes as well as time-effectiveness in the management of large quantities of highly dimensional data typically collected by means of spectroscopic methods.

8. Status assessment (I, II, III, or IV): I

	Major gap in current knowledge	Minor gap in current knowledge
No or limited current research is being conducted	I	III
Existing current research is being conducted	II	IV

This research need has been identified by one or more subcommittees of OSAC and is being provided as an informational resource to the community.