OPUS 9.0 for Drug Checking Feedback Report

Project Overview

During the OPUS 9.0 Beta testing a group of 10 drug checking FTIR technicians with varying experience levels tested features currently under development by Bruker with drug checking in mind. Technician's feedback was tracked through note logs, surveys, interviews, and focus groups. The data was merged to find key themes technicians felt were important to share. Below is a summary of these themes that were presented back to Bruker on 3/19/24.

Software Component Overview

The primary enhancement in OPUS 9.0 is the development of a new feature, the Autonomous Component Identifier (AID). AID is an expansion upon a current feature called Mixture Analysis. As with the traditional Mixture Analysis and Spectrum Search features, AID uses a specific correlation algorithm to compare the submitted spectrum against library reference spectra. Each correlation algorithm associated with these different spectral search methods are similar but allow for minor differences in comparing the sample spectrum against the reference spectra.

Key Definitions List
- OPUS
    - Bruker software utilized for analyzing scans and identifying substances present in a sample recorded via FTIR.
- Autonomous Component Identifier (AID)
    - Autonomous version of Mixture Analysis OPUS feature where ten composite spectra are generated for each amount of components (1-8) with differences in substances identified and HIT qualities listed for each composite. Ability to slightly customize results, export to OPUS for further analysis, and to create a report based on 1 or more composite results.
- Composite Spectra
    - A spectrum is generated by the software after weighing library references to combine the spectra that best match the recorded sample mixture spectrum. The weight for each sample indicates the impact of each substance on the composite spectrum. The HIT quality represents how well the composite spectrum matches the sample spectrum.
- Custom Report Feature

o   Generate a report based on the composite that the user determines to best match the sample spectrum. Once chosen, the user selects the composite(s) they wish to create a report for as well as customization options for features to report on (header, spectra to display, plots, metrics, etc).

Feedback Provided to Bruker	
Theme	**Recommendations**
Composite Spectra reporting more than 5 components could be misleading for new technicians	• Add an option to select the number of desired components within a sample spectrum with the max limit being 5 • Create a similar limit or hide hits with greater than 5 components by default with an option to toggle them on as needed
The Custom Result feature was useful and appreciated	• Add an option to change the weights/percents of a substance in a custom composite spectrum • Include an auto-adjust option (all results will adjust accordingly after a single change) and a fully manual option • Customization would improve detection of commonly missed substances (xylazine, caffeine, acetaminophen) but depend on the technician's knowledge and ability to identify these substances
Autonomous Component Identifier (AID) was user friendly and intuitive	• Having basic OPUS features accessible in the AID popout (i.e. Shift Curve, Scale All Spectra, etc.) • Improvements to algorithm based on street drug samples for more accurate representation of identified substances and their quantifications
Reporting Feature	• Remove component weights, HIT number, and percentages, or ability to toggle on/off • Add brief descriptions of substances or ability to add custom notes by the technician • Provide an error message when technician attempts to create report but forgot to select the composite mixture analysis they wish to report on • Improve naming/clarity of features for generating reports
Technology Issues	• The OPUS 9.0 Beta could not be calibrated with either the Mobile IR or the ALPHA, therefore could not be used to collect with new scans. This may be addressed when the next version of OPUS is released but otherwise not solved with the beta software. • For the BETA to be downloaded, 7- Zip was required. Some versions of Windows 10 have this natively, most of the Bruker supplied

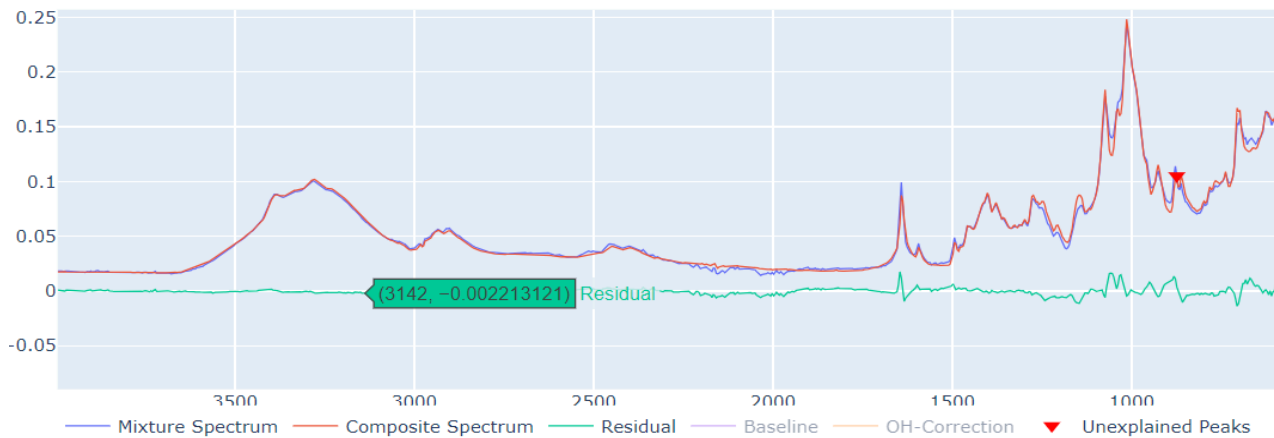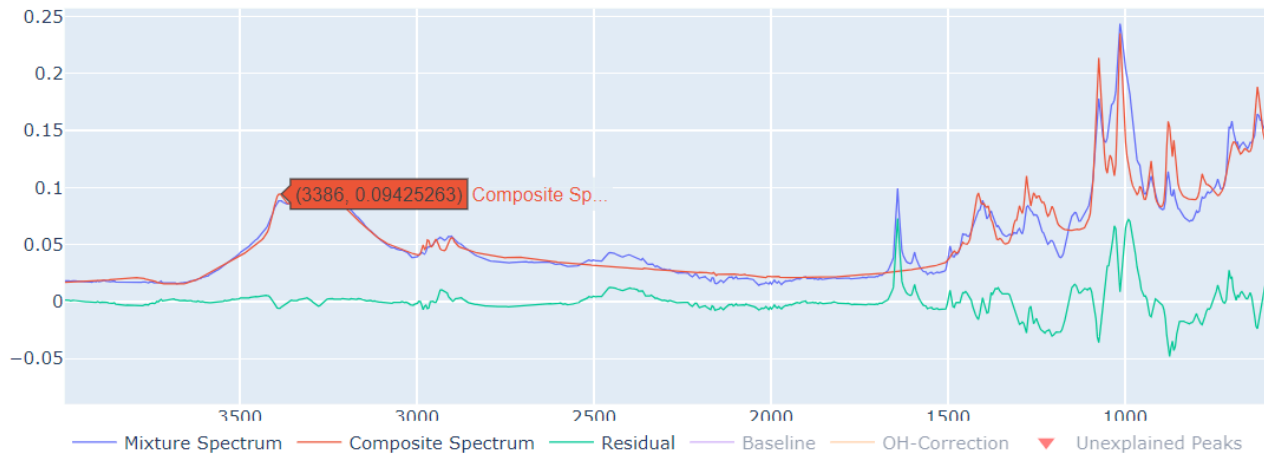|	
	laptops did not, and there was no mention of this requirement on instructions on how to unzip 7z. Zip Files ● For AID to function properly the app WebViewer 2 was required. We suggest Bruker to include this in the download instructions. ● User manual was not shared at the time of beta testing leading to much troubleshooting to be able to successfully install OPUS 9. ● Closing OPUS/AID should not leave certain parts of OPUS software running in the background. This prevented new OPUS windows from being opened and required manually closing OPUS in in the background app section of task manager
General OPUS Feedback	● When dragging and dropping a spectrum into a new window, keep the substance name instead of changing to "entry007" ● Ability to "freeze frame" when shifting curves/zooming in so toggling on or dropping in a new spectrum doesn't reset the display ● More accessible for color deficiency by adding new background color options, ability to alter thickness of spectra lines, ability to make dashed / dotted spectra lines ● Add a title or description to display window tabs

Impact

Updates to AID Since Providing Bruker with Feedback
- Custom Result Feature:
  - Developers have incorporated notes on the Custom Result Feature to allow the operator to customize the weights of substances that will auto-adjust to add up to 100% for a composite spectrum. There is an option to increase or decrease the weights in small increments (0.1%), similar to the preexisting Manual Subtraction feature in regular OPUS.
- Algorithm Improvements
  - In the real-world sample scans we asked the technicians to review as part of this beta testing, it was reported that AID struggled to detect low lying components such as xylazine. These scans were shared with developers so the algorithm could be improved to detect xylazine in a low concentration.
- Composite Spectra Reporting 6+ Components
  - Feedback was heard in where seeing results for mixture samples reporting 6 or more substances can be confusing and misleading. This note was taken under consideration and now limits the composite spectra provided immediately to be limited to 5 or fewer component spectra.

This project was overseen by Dr. Traci Green as the first in a series of projects collectively named Network 1. Network 1 is an initiative to improve existing and support the development of new drug checking technologies to improve the quality of drug checking programs in the US and beyond.

Appendix