FTIR Libraries for Drug Checking

Purpose and Scope

FTIR spectral libraries are digital tools used in the process of analysing drug samples to identify the substances that are present. There are several libraries available for free or at-cost, and most require regular updates to keep up with as new substances are added. The purpose of this document is to summarize the FTIR spectral libraries most commonly used by drug checking services in British Columbia (BC), and to outline procedures for how to apply these libraries in community-based drug checking.

Description of Libraries

FTIR libraries consist of reference spectra of numerous drugs that typically originate from laboratory standards, or street samples that have met inclusion criteria for a library. This includes verification by more sensitive methods such as gas chromatography-mass spectrometry (GCMS), and/or nuclear magnetic resonance (NMR). When performing a drug check, a sample is compared to reference spectra to determine which substances are identifiable. For the purposes of community-based drug checking with FTIRs, BCCSU has divided libraries into categories of primary and supplementary libraries to aid with the order of which they should be applied during an analysis.

Primary Libraries

The primary libraries (BCCSU, SWGDRG, TICTAC) have had long-standing usage among drug checking services in BC, and have been shown to produce reliable identification of substances. While the libraries may overlap in regards to the drugs they contain, the BCCSU libraries are

highly relevant to drug checking in the BC context as they are regularly updated with samples originating from community partnered sites. The larger libraries (SWGDRG, TICTAC) also include many spectra the BCCSU libraries do not. All drug checking services operating FTIRs in BC are required to use the primary libraries.

Supplementary Libraries

The supplementary libraries consist of the Bruker pharmaceutical libraries (Vol. 1-4), and two open-access libraries (ENFSI and Kykeon). The pharmaceutical libraries are expansive, and primarily contain validated spectra of substances found in regulated pharmaceutical drugs. However, they are not recommended as a primary library as the large volume of entries and duplicate entries will slow down OPUS. During the analysis process, it is also more difficult to search through the large number of suggested entries to determine a match. Entries which include mixtures of substances can also make it harder to identify the specific substance of interest. While the pharmaceutical libraries are especially useful when the sample is expected to be a pharmaceutical drug, they also include other substances not contained within the primary libraries (e.g., caffeine citrate, 1,4 BDO), so it is good practice to attempt subtractions with them whenever there appears to be unidentified components leftover from subtractive analysis with the primary libraries.

The two supplementary open-access libraries (Kykeon, ENFSI) may be of help after using the primary and pharmaceutical libraries if there still appears to be unidentified components. However, both libraries have only recently begun to be used by drug checking services in BC, and little is known about the samples' origins or how spectra are selected for inclusion. Similar to the pharmaceutical libraries, the ENFSI library contains a large volume of entries, including many duplicates, which can slow down the analysis process. Currently, the Kykeon library contains entries for novel psychoactive substances as well as other substances that are of growing concern in the unregulated drug supply (e.g. medetomidine/dexmedetomidine), that are not yet contained in other libraries.

Please see the tables at the end of this document for a more detailed summary of each library.

Procedures

Outlined below are the steps to follow when performing a drug check in cases where the primary libraries are not sufficient identify all detectable components in a sample. Applying the libraries in the sequence described will help to ensure that the approach to analyzing a drug sample and the subsequent results are as consistent as possible between technicians.

1. **Begin the drug check with the primary libraries:**
   1.1. Turn on the BCCSU, SWGDRG, and TICTAC libraries within OPUS' search function.
   1.2. Begin your analysis by subtracting suggested components that you can confidently identify.
   1.3. Attempt limit searches if there are residual peaks that cannot be identified through subtractions.
   1.4. If you did not identify any substances through subtractions, or there are residual peaks left over after your initial subtractions, proceed with next steps if you have access to supplementary libraries.
   1.5. If you do not have access to any supplementary libraries, proceed to **step 4**.

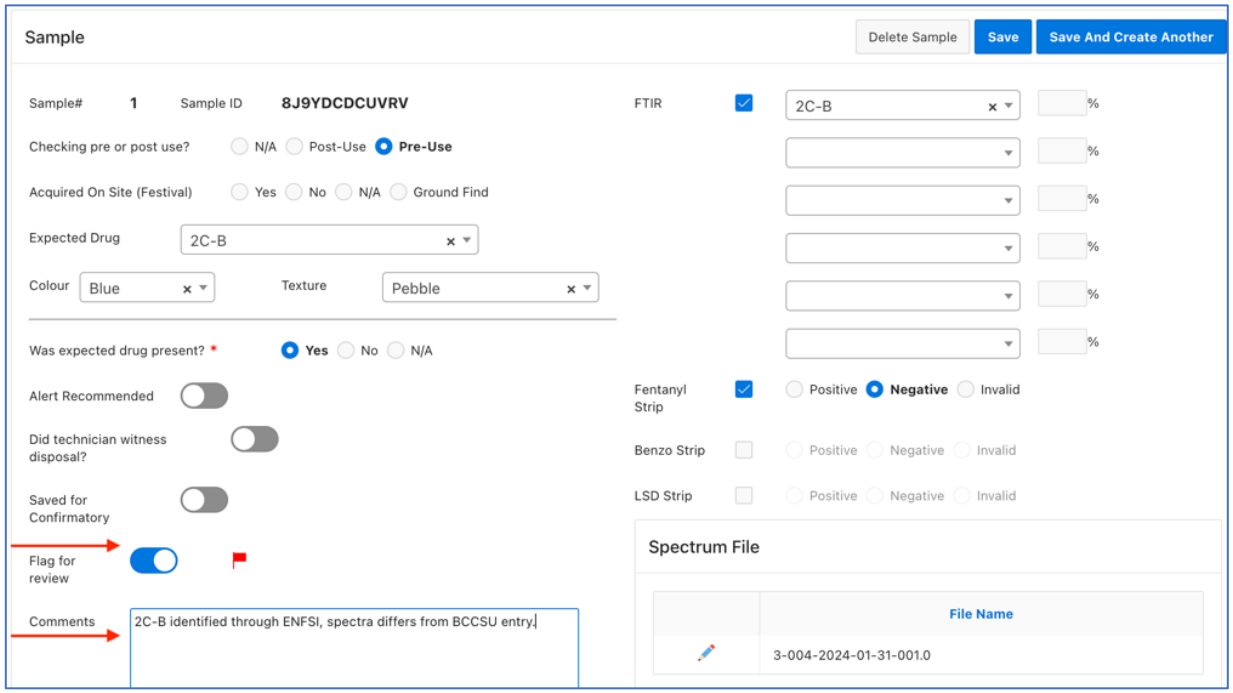
2. **Turn on supplementary libraries: Pharmaceutical libraries**
   2.1. Enable the Bruker pharmaceutical libraries within the search function alongside the primary libraries. Note that these libraries should not be turned on at the beginning of your analysis as the large volume of spectra will slow down OPUS.
   2.2. Continue with subtractions if OPUS suggests substances you can confidently identify.
   2.3. Attempt limit searches for residual peaks not yet identified through subtractions.
   2.4. If you did not identify any substances through subtractions, or there are residual peaks left over after your initial subtractions, turn off the pharmaceutical libraries and proceed with next steps if you have access to the other supplementary libraries.
   2.5. If you do not have any supplementary libraries, proceed to **step 4**.

3. **Turn on supplementary libraries: ENFSI/Kykeon**
   3.1. Ensure the pharmaceutical libraries are off, and enable the other supplementary libraries alongside the primary libraries within the search function.
   3.2. Note that because of the large volume of spectra in the ENFSI library, you may choose to select only the Kykeon library first before turning on the ENFSI library if still needed.

3.3. Continue with subtractions if OPUS suggests substances you can confidently identify.
3.4. Attempt limit searches for residual peaks not yet identified through subtractions.
3.5. Proceed to step 4.

4. Record results in DCBC

4.1. Log results in DCBC in the order which you identified components.
4.2. If there residual peaks left over after your initial subtractions, log as “uncertain match”
4.3. If no substances were identified through subtractions, log this as “no library match”.
4.4. Leave a comment in DCBC if a substance was detected with a supplementary library that has a differing spectra in the primary libraries. This will help us monitor the accuracy of these libraries as it relates to the BC drug supply. For example, there are differing spectra for 2C-B across primary and supplementary libraries. See image below for an example.



Example of logging results in DCBC when spectra differ between primary and supplementary libraries

Summary of Libraries

PRIMARY LIBRARIES	
BCCSU FTIR-ATR Library of Drugs and Common Adulterants	FTIR spectra library of drugs, cuts, and common adulterants found in BC. Most spectra originate from samples checked by community partners, and others are derived from laboratory standards. As part of the library inclusion criteria, all samples have been externally and independently validated using either qNMR and/or GCMS analysis. Cost: None, open-access creative commons license Updated: Every six months or as needed Number of spectra: 100+
BCCSU FTIR-ATR Library of Tryptamine Analogues and other NPS	FTIR spectra library of tryptamine analogues and other novel psychoactive substances (NPS). All spectra in this library originate from drug samples checked by community partners in BC. As part of the library inclusion criteria, all samples have been externally and independently validated using either qNMR and/or GCMS analysis. Cost: None, open-access creative commons license Updated: Every six months or as needed Number of spectra: 20+
Scientific Working Group for the Analysis of Seized Drugs Library (SWGDRG)	Spectra for the SWGDRUG library is compiled through the U.S. Drug Enforcement Administration's Special Testing and Research Laboratory using structurally confirmed reference materials. Cost: None Updated: No set schedule (last updated May 2024) Number of spectra: 800+
TICTAC Spectral Library for Drugs and New Psychoactive Substances (TICTAC)	Spectra library provided by Communications, Ltd (St. George's University of London, England) aimed to assist criminal justice and health sectors. This library has significant overlap with the SWGDRUG library but there remain some things not accounted for by SWGDRUG. The BCCSU recommends purchasing TICTAC if funds are available. Cost: $5,486.30 (Bruker offers 20% discount for Canadian harm reduction services) Updated: Advertised as once per year, may be less often Cost: $2,813.70 (may provide additional discount within Canada) Number of spectra: 600+

SUPPLEMENTARY LIBRARIES	
Bruker ATR-FTIR Pharmaceuticals Libraries (Vol. 1-4)	Contains many pharmaceutical drug spectra not present in other libraries. There are many duplicate entries, and the large size of the library makes analysis slow. Cost: $3600 with instrument ($7000 after) Updated: Never Number of spectra: 10,000+
Kykeon Analytics Library	Kykeon Analytics is a harm reduction initiative in Spain that provides an open-access spectra library. Most spectra for this library originate from community samples, and a few are derived from laboratory standards. Note that while all samples are confirmed via LC-MS and NMR, some include substances not detected by these methods (e.g. sugar alcohols). Cost: None, open-access creative commons license Updated: Every 4-6 months Number of spectra: 270+
European Network of Forensic Science Institutes Library (ENFSI)	Spectra for this library originate from the ENFSI Drugs Working Group. It is a large library, with many duplicate entries. Cost: None Updated 1-2 times per year Number of spectra: 3500+

Additional Resources

- Standard Operating Procedures: Installing FTIR Libraries for Drug Checking
- BCCSU DCBC Manual
- BCCSU Drug Checking Technician Manual

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