



Fiveash Data Management, Inc.

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FDM Mixture Library FAQ

1: What are FDM Mixture Libraries?

They are collections of multicomponent spectra calculated from collections of neat compound spectra.

Since infrared absorbance spectra follow Beer's law, neat spectra can be used to calculate multicomponent spectra.

The table below shows part of a chemical name index from an FDM Mixture Library built with two components per spectrum and 10% concentration intervals. The concentrations vary over the range 10:90, 20:80, 30:70...90:10.

Capsaicin, 404-86-4:10% + Ibruprofen, 15687-27-1:90%
Capsaicin, 404-86-4:20% + Ibruprofen, 15687-27-1:80%
Capsaicin, 404-86-4:30% + Ibruprofen, 15687-27-1:70%
Capsaicin, 404-86-4:40% + Ibruprofen, 15687-27-1:60%
Capsaicin, 404-86-4:50% + Ibruprofen, 15687-27-1:50%
Capsaicin, 404-86-4:60% + Ibruprofen, 15687-27-1:40%
Capsaicin, 404-86-4:70% + Ibruprofen, 15687-27-1:30%
Capsaicin, 404-86-4:80% + Ibruprofen, 15687-27-1:20%
Capsaicin, 404-86-4:90% + Ibruprofen, 15687-27-1:10%

2: What are they used for?

FDM Mixture Libraries are used for mixture analysis using infrared spectra of unknown samples. Searching them provides suggestions of a mixture's components with **relative concentrations**.

3: When are they used?

We expect they will be used as a screening tool at the beginning of a complete mixture analysis process conducted by trained analytical chemists. If a search hitlist offers convincing suggestions, those suggestions could influence the choice of, for example, chromatographic methods and conditions.

4: How are they used?

FDM Mixture Libraries are formatted for use with most FTIR search programs. They are searched in exactly the same way as conventional neat spectra FTIR libraries. The better the hitlist score, the better the suggestion. A cluster of similar compounds with similar scores strengthens the suggestion.

5: What will they tell me?

Search results offer suggestions of the mixture components and their **relative concentrations**. They also offer an idea of what a mixture spectrum would look like in advance of any wet chemistry.

6: What advantages do they offer?

Running a new spectrum on an unknown sample is easy and suggestions of mixture components are available moments after starting a search.

Your FTIR instantly becomes even more useful since it can be used for rapid mixture analysis.

7: What's the chemometric basis for the FDM Mixture Libraries?

Searching mixture libraries is closely related to the widely used CLS (Classical Least Squares) method used for quantitative analysis. Instead of a calibration set, neat compound spectra from an FDM FTIR library are combined proportionately.

8: Does searching FDM Mixture Libraries have any advantages over CLS?

Yes. First, FTIR search programs are easy to use and widely available while CLS software requires (a) specialist software, (b) specialist knowledge and (c) a set of calibration spectra must first be built.

Second, for CLS to quantify a compound it has to be in the calibration. Mixture libraries can be built from hundreds of neat compound spectra so there is an inherent advantage in the number of compounds that can be recognized.

9: Can we get a custom FDM Mixture library?

Yes. We anticipate developing custom mixture libraries for a wide variety of customer defined applications. Please inquire with your requirements and specifications.

10: What are the advantages of custom FDM Mixture Libraries?

Many chemists may find it desirable to limit the range of compounds in the library. Others may find it useful to select a variety of very different compounds such as spectra taken from the FDM ATR Organics, the FDM ATR Inorganics and the FDM ATR Polymers.

11: Why are the results called suggestions?

The results are called suggestions because that is the most fitting description from an analytical perspective. The FDM Mixture Libraries provide only estimates of relative concentrations.

12: What about nonabsorbing mixture components?

As mentioned above, searching the FDM Mixture Libraries may provide relative concentrations. If a sample has just two components and both components have infrared spectra found in the mixture library then relative concentration and absolute concentration should be the same.

If even a few percent of nonabsorbing material, such as KBr, is blended in to the sample, the absolute concentration will obviously change but the spectrum will look much the same and the relative concentration of the component won't change.

13: How many components can be analyzed?

The first libraries are being built with two and three components per spectrum. Of course, depending on the sample, these may prove useful with samples with more components.

14: What if some mixture components are much lower in concentration compared to others?

Components in low (relative) concentration contribute minimally to a spectrum. Thus, we expect less success identifying them.

15: How does unknown spectrum quality effect mixture library searching?

Unknown spectrum quality is important when searching conventional neat compound spectral libraries or mixture libraries. Spectra should have clean baselines, detector cutoff artifacts removed, CO₂ peaks removed and, with condensed phase samples, water vapor peaks removed. Avoid searching over diamond ATR phonon bands.

16: What if peaks in real mixtures have shifted?

The best approach is to narrow the range of the spectral search to peaks that are not subject to shifts.

For instance, if your sample has lots of hydrogen bonding, search those peaks uninfluenced by hydrogen bonding.

17: How far can you go stating relative concentration?

If a mixture library has 10% concentration intervals (10%, 20%, 30%, ..) then the best achievable accuracy is +/- 5%.

18: What sample phases can be searched?

All phases (solids, liquids, gases) can be searched. Gases should be searched with a gas library.

19: Will my software search the FDM Mixture Libraries?

FDM provides FTIR libraries for use with most FTIR search programs. We will provide the FDM Mixture Libraries in many formats including, but not limited to, (alphabetically) ACD's UVIR Manager™, Bruker's OPUS™, Operant's Essential FTIR™, Perkin Elmer's Spectrum Search™, Shimadzu's IRsolution™, Thermo's OMNIC™ and Thermo's SpectralID™.