KnowItAll Mass Spectrometry Training

Vendor Neutral Data Processing Solution for Spectral Analyses

WILEY

KnowItAll™

"Identification of Unresolved Components in GC-MS Peaks Using KnowItAll"

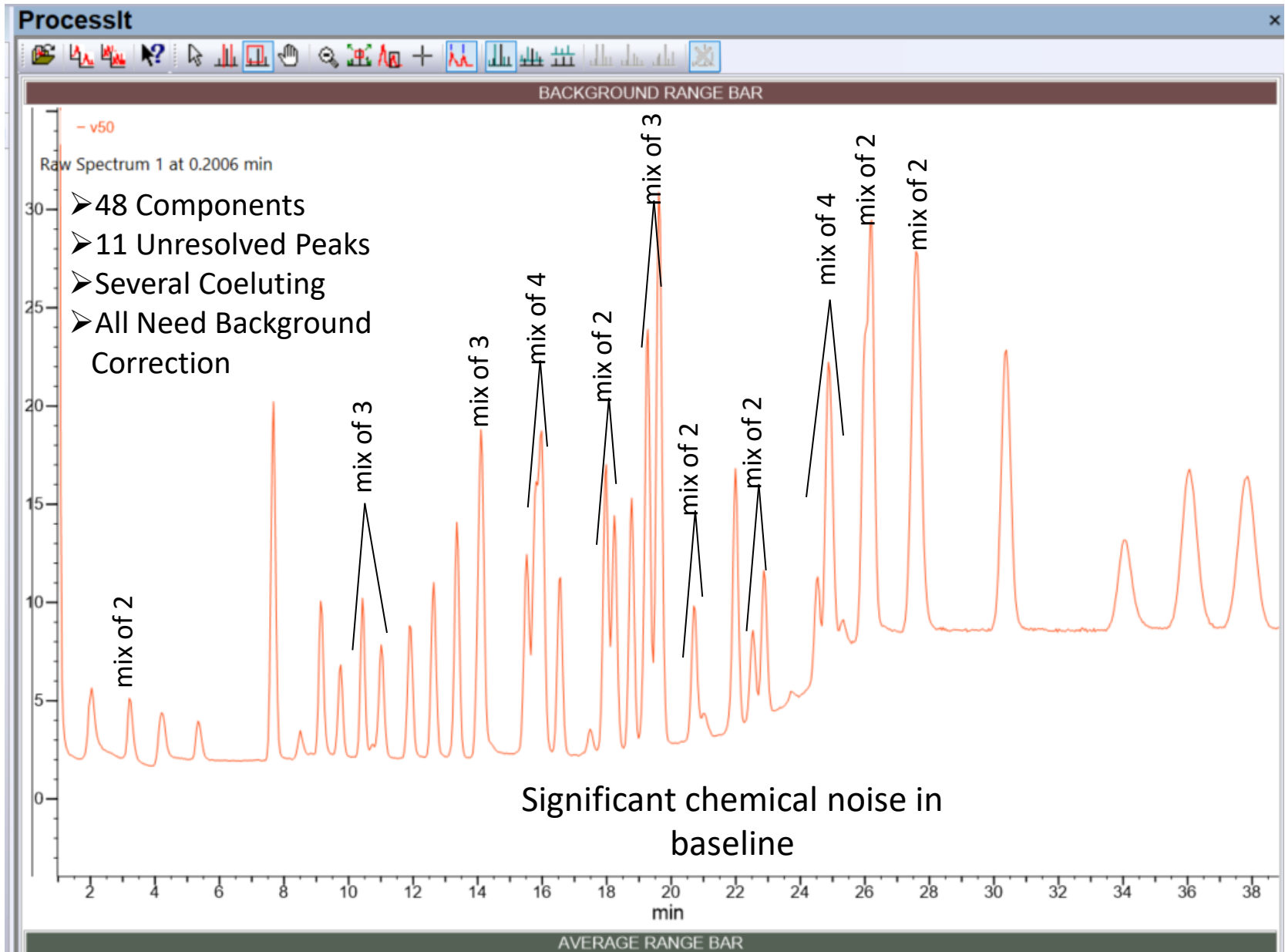James Little
Mass Spec Interpretation Services

Handouts for Videos:
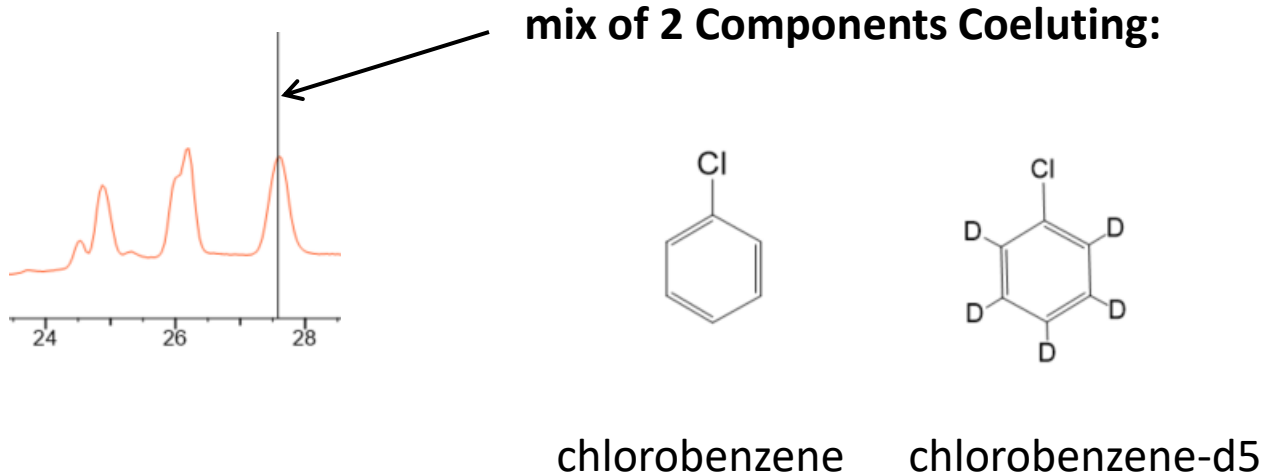Website: Little Mass Spec and Sailing
https://littlemsandsailing.wordpress.com

NOTE: Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

Sept 9, 2022

Demo File V50.CDF, Many Unresolved Peaks

ProcessIt

BACKGROUND RANGE BAR

− v50

Raw Spectrum 1 at 0.2006 min

➤ 48 Components
➤ 11 Unresolved Peaks
➤ Several Coeluting
➤ All Need Background Correction

mix of 2
mix of 3
mix of 3
mix of 4
mix of 2
mix of 3
mix of 2
mix of 2
mix of 4
mix of 2
mix of 2

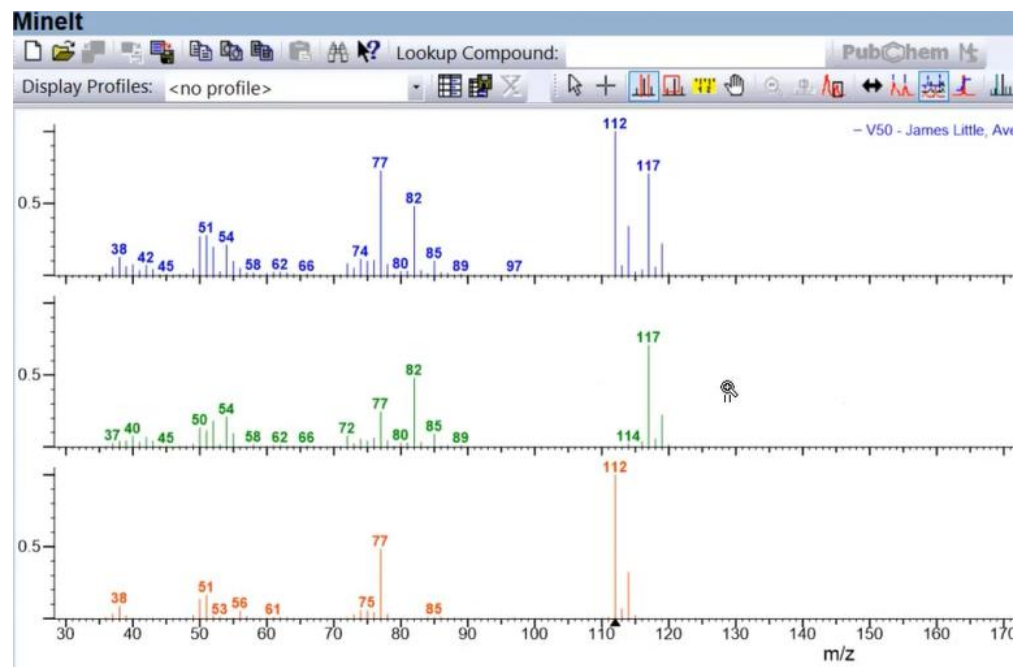Significant chemical noise in baseline

min

AVERAGE RANGE BAR

Techniques for Unresolved Peaks for Components in GC-MS Analyses

➤ProcessIt using leading or trailing edge of peak with background subtraction

➤Mix directly searched with standard similarity search using subtraction view

➤"2 mixture", "3 mixture" approaches unique to Wiley, very effective for IR because no chromatographic separation

➤Reverse search

➤Deconvolution (MS Expert Program)

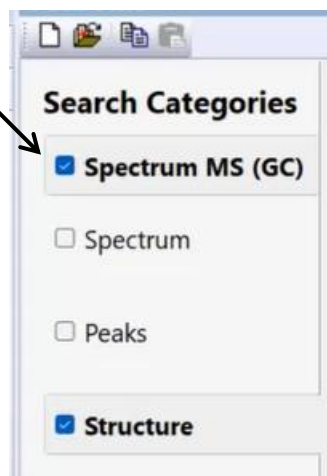**mix of 2 Components Coeluting:**

chlorobenzene   chlorobenzene-d5

Important Points in Performing a Search of the Difference Spectrum in MineIt

➢To obtain the difference spectrum sent to SearchIt for searching, user MUST use the subtraction view and NOT the butterfly view

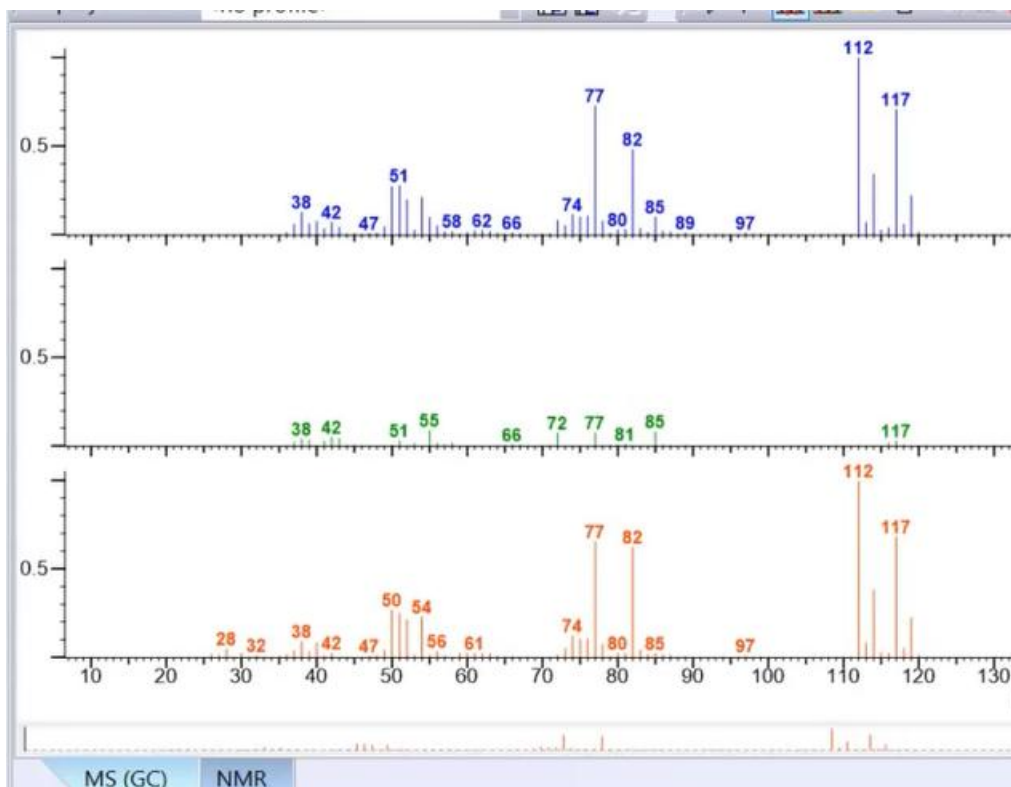➢When going back to the SearchIt view, user MUST deselect the Structure Box

MUST deselect this before searching, or search will fail!

How to Decide if 2 (Mixture) or 3 (Mixture) Search Should be Used

➢Look at the Difference Spectrum and the total mix spectrum for 2 (Mixture) search
➢If significant residual ions, repeat search with 3 (Mixture) search
➢Also, if the Hit Quality Index, HQI results significantly lower than 90% for 2 (Mixture) search
➢Repeat search with 3 (Mixture) search

Conclusions

Automated Approach:

➢ Start with MS Expert and do deconvolution, *very efficient* compared to manual ones
➢ If problems noted in the MS Expert result, use the manual approaches below:

Manual Approaches:

➢ Take spectrum on front or trailing edge in ProcessIt if possible
➢ If necessary, first choice try either "2 mixture" or "3 mixture" search function
➢ Next choice, regular similarity search using subtraction and searching difference spectrum or spectra
➢ Last choice would be reverse search using subtraction and searching difference spectrum

NOTE: Be sure to see other video on deconvolution using MS Expert and other Mass Spec KnowItAll training videos on my personal website