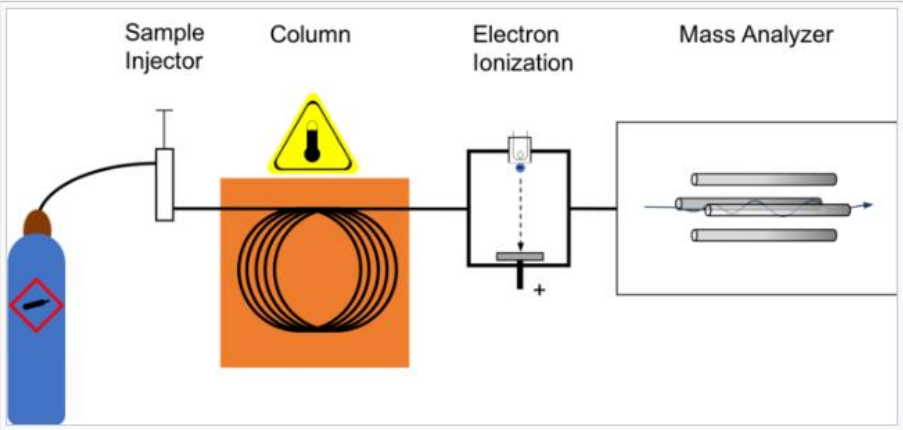
Free NIST GC-MS Software Lab for Universities:
Part 10: AMDIS Difficulties and Ways to Overcome Them



[Resource Link to 8 Files GCMS Analysis Files]

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38 years Eastman Chemical Company
7 years Mass Spec Interpretation Services
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Link to GCMS Schematic Above

Link to University Logos

Topics in This Video and Associated Handout

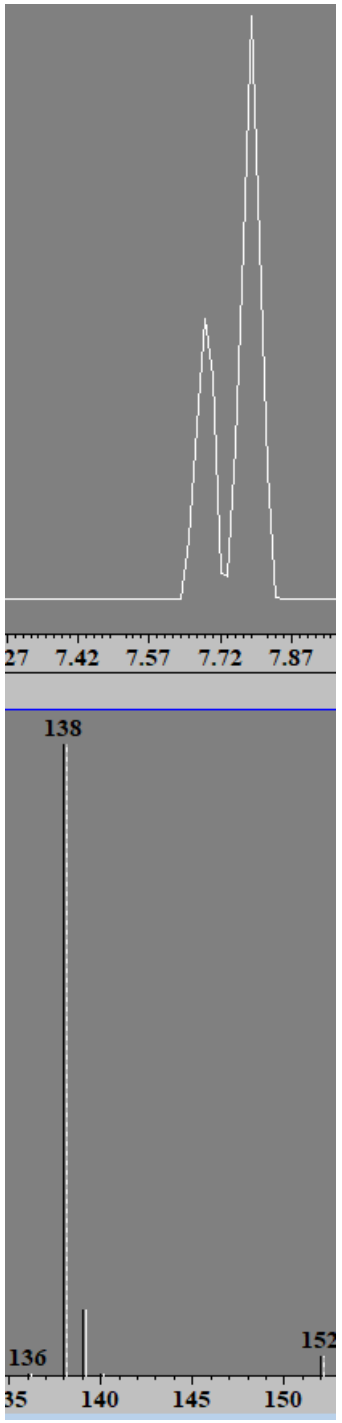
-Real world files ***sometimes*** cause problems with AMDIS
-Handling “Uncertain” Peaks in AMDIS
-Overcoming ”Over-Marked” chromatographic peaks
-Some additional files to demonstrate these AMDIS restrictions
-Types of files processed by AMDIS
-Other test files discussed
-Quantitative GCMS Laboratory at University of North Dakota Website

Uncertain Peaks in AMDIS

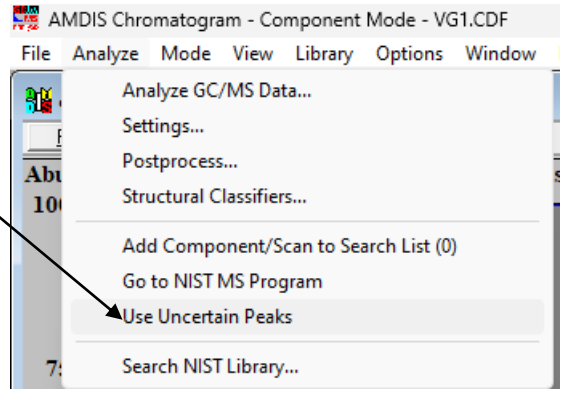
- The definition of uncertain peaks is defined as found in the AMDIS manual below:

Uncertain peaks are those ions in a mass spectrum that AMDIS finds impossible to assign to a specific component due to the uncertain deconvolution of the mass spectral data. For display information about uncertain peaks, see **3.3.4 Mass Spectral Display**.

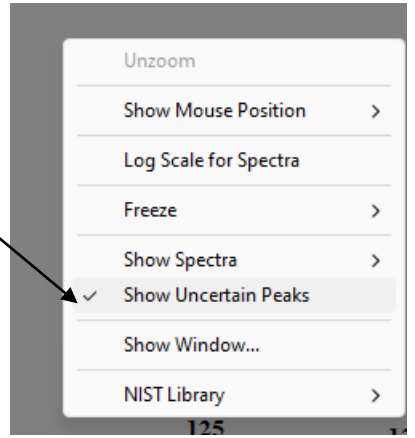
- They are shown as white dashed lines in the spectrum
- They will not be sent to the NIST library search unless certain settings are changed
- Sometimes data files will have uncertain peaks, but they really should be part of the spectrum
- I placed an example file in the set of file in the zipped folder
- m/z 138 is really part of the spectrum for the peak at 7.683 minutes shown to the right
- To send to the library search, one must Use Uncertain Peaks by choosing the option in the window to the left below
- Also must "Right Click" in spectrum window and check Show Uncertain Peaks in window to the right below
- If Show Uncertain Peaks is not selected, the uncertain peak will be shown in black NOT a dashed white line!
- In general, I just use the default as Use Uncertain Peaks and Show Uncertain peaks, can always turn off if I decide not part of spectrum!



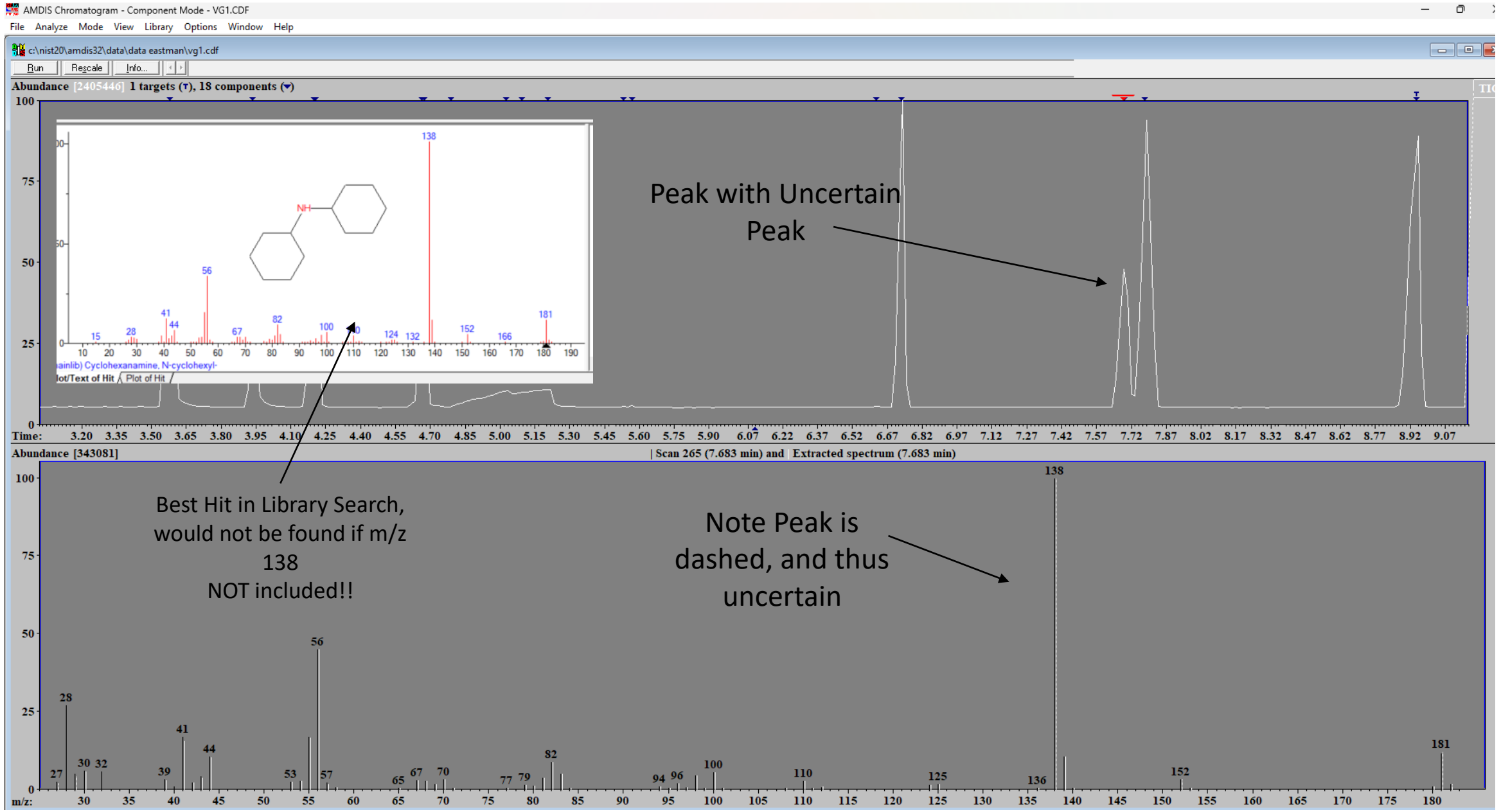
Select this option to send uncertain peaks to library search



Must check this to see Uncertain Peaks as white lines, if not they will be black



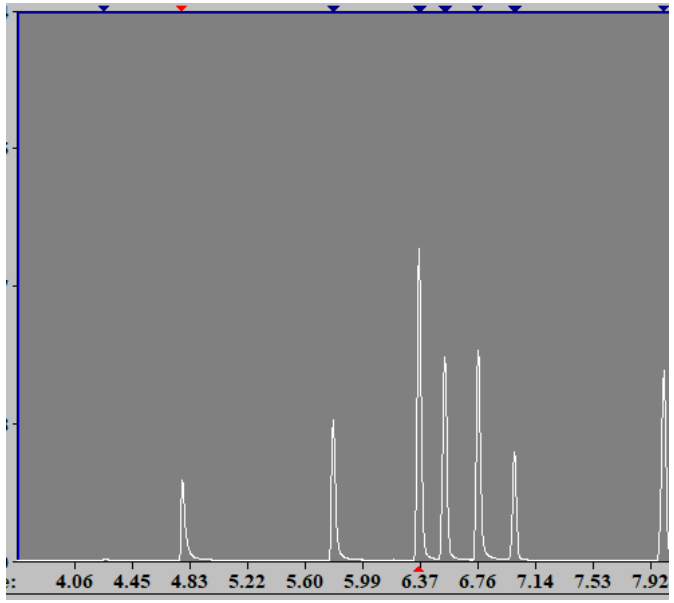
File with Uncertain Peak Which Is Part of Spectrum and Needs to Be Included

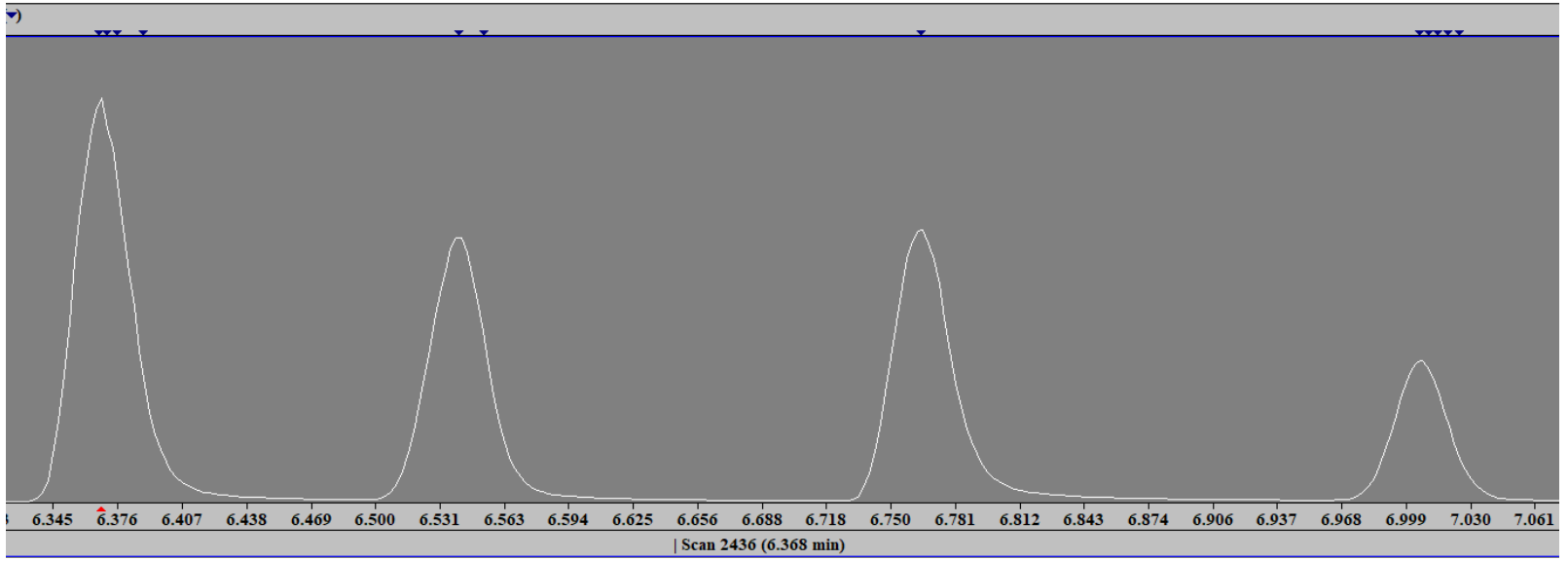


Sometimes Almost Impossible to Get AMDIS Not to Mark the Same Peak Several Times!

- This overmarking peaks can be aggravating
- I included a file ADAM_339.D to illustrate the problem
- Always have to deconvolute
- But then instead of clicking on the triangles, just click within the spectrum to get a spectrum with no background for big peaks
- Little peaks might require manual subtraction as defined in the Part 4: Processing GCMS Data with AMDIS video
- Sometimes adjusting the deconvolution settings and S/N filter as shown in Part 4: Processing GCMS Data with AMDIS video can help somewhat

Sometimes Almost Impossible to Get AMDIS Not to Mark the Same Peak Several Times!

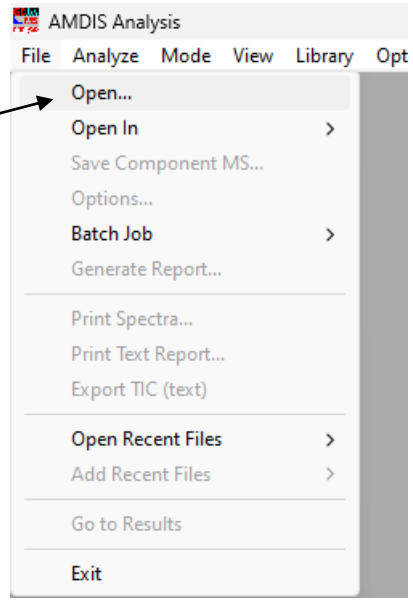


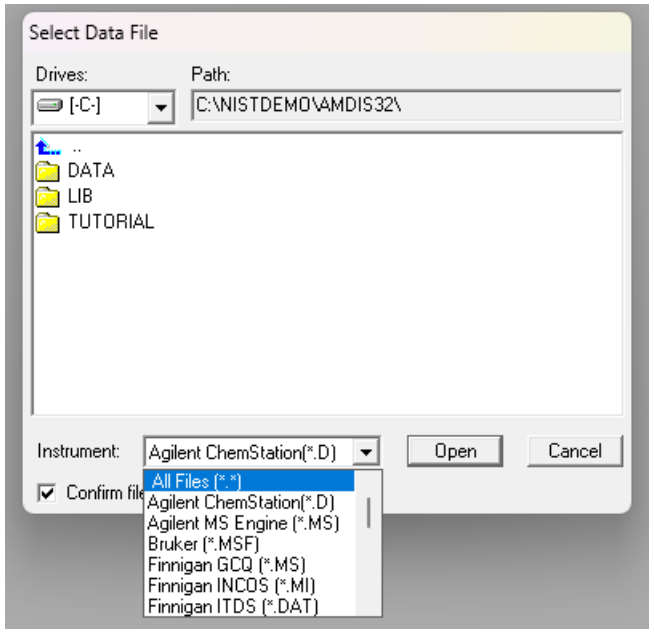


Other Types of Mass Spec Files Processed by AMDIS

- AMDIS can search a variety of file types
- We have mainly discussed file.D type files, where file is the file name
- These are Agilent GCMS files, and inside they always have a data.ms file
- Many manufacturers support netCDF file which is a common file format, it is seen at the top level, not in a folder
- Almost all mass spec processing software packages support this format
- Best just to select All to see which ones are present and can be opened by AMDIS
- Most times the files are stored in the DATA folder on the C drive, but NIST has put theirs in the TUTORIAL folder

To open a data file





Some Additional Files Included for Your Entertainment

- I included a few additional files
- Will need to have all the extra libraries installed to have a chance of identifying them
- Many will not be in any of these libraries
- But the majority would be found in the NIST and Wiley full scale versions of the library
- In many cases, some peaks can be a mixture of up to three components
- AMDIS can often deconvolute them and give good pure spectra to be sent to NIST search

Files

- ADAM_339.D, file demonstrating “over-marking” of deconvoluted peaks
- VG1.cdf, file showing importance of understanding “Uncertain Peaks”
- JEOL file Oban_14_EI_5.cdf, Analysis of SPME samples from Scotch Whiskey, Chip Cody
- 25CALNAA.D, File from University of North Dakota, Quantitation GCMS Lab
- Agilent_test_file.D, complext mixture of >120 components, chlorinated species, aromatics, etc.
- EXP1-5.D, some aromatics, be careful a few might have ”Uncertain” peaks!
- V50.cdf, a complex mixture of chlorinated species, aromatics, etc., will find peaks that are mixtures and require the ability of AMDIS to deconvolute.

Quantitation Laboratory from University of North Dakota

- Excellent GC-MS lab on Quantitation found at the following link
- I have included one of their files
- Good one for adding something to your personal MS library!

Link to Their Webpage

UNIVERSITY OF NORTH DAKOTA

College of Arts & Sciences

Chromatography and Mass Spectrometry

GC-MS Lab

Homework on Quantitation

Quantitation Laboratory from University of North Dakota *My Proposed Structures*
Compound 4 is the Internal Standard