Data Processing Using Thermo Freestyle Software with NIST MSMS Search for Compound Identifications

(*Alternative Less Efficient Approaches*)

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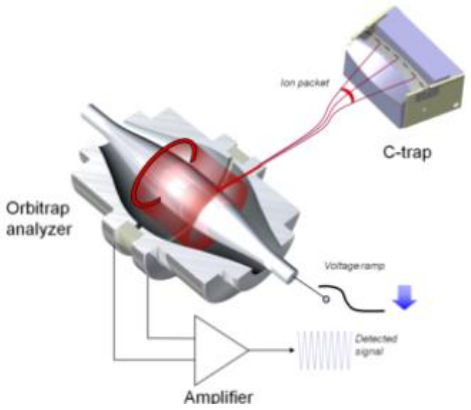
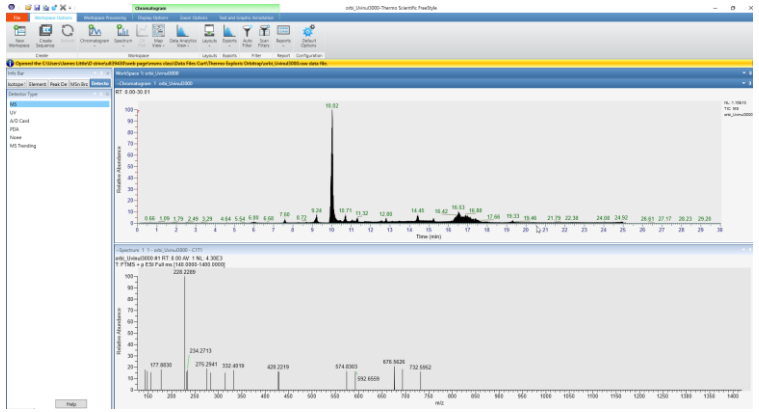
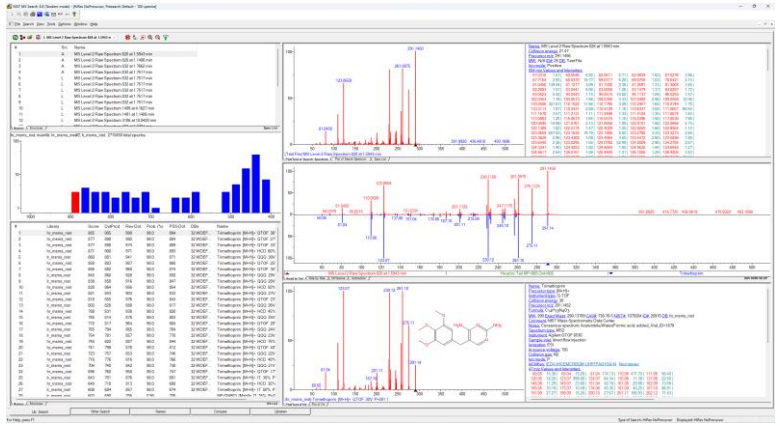
Thermo Orbitrap MSMS

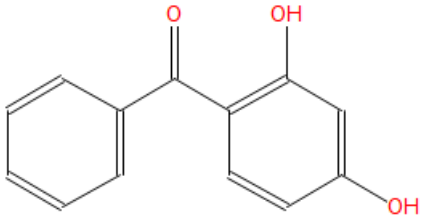


Thermo Freestyle



NIST MSMS Search





Uvinul 3000
MW 214
Thermo Orbitrap
LC-MS and Non-Targeted MSMS Analyses (Positive and Negative Modes)
with
Photo Array Detector (PDA) and UV-VIS Analyses

In My Opinion, Preferred Way of Processing Data
(*shared with me by colleague*)

- However, several other ways for processing data in Freestyle
- Some might think simpler, but after initially saving the layout in the “preferred approach,” really no advantage in my opinion to these simpler approaches

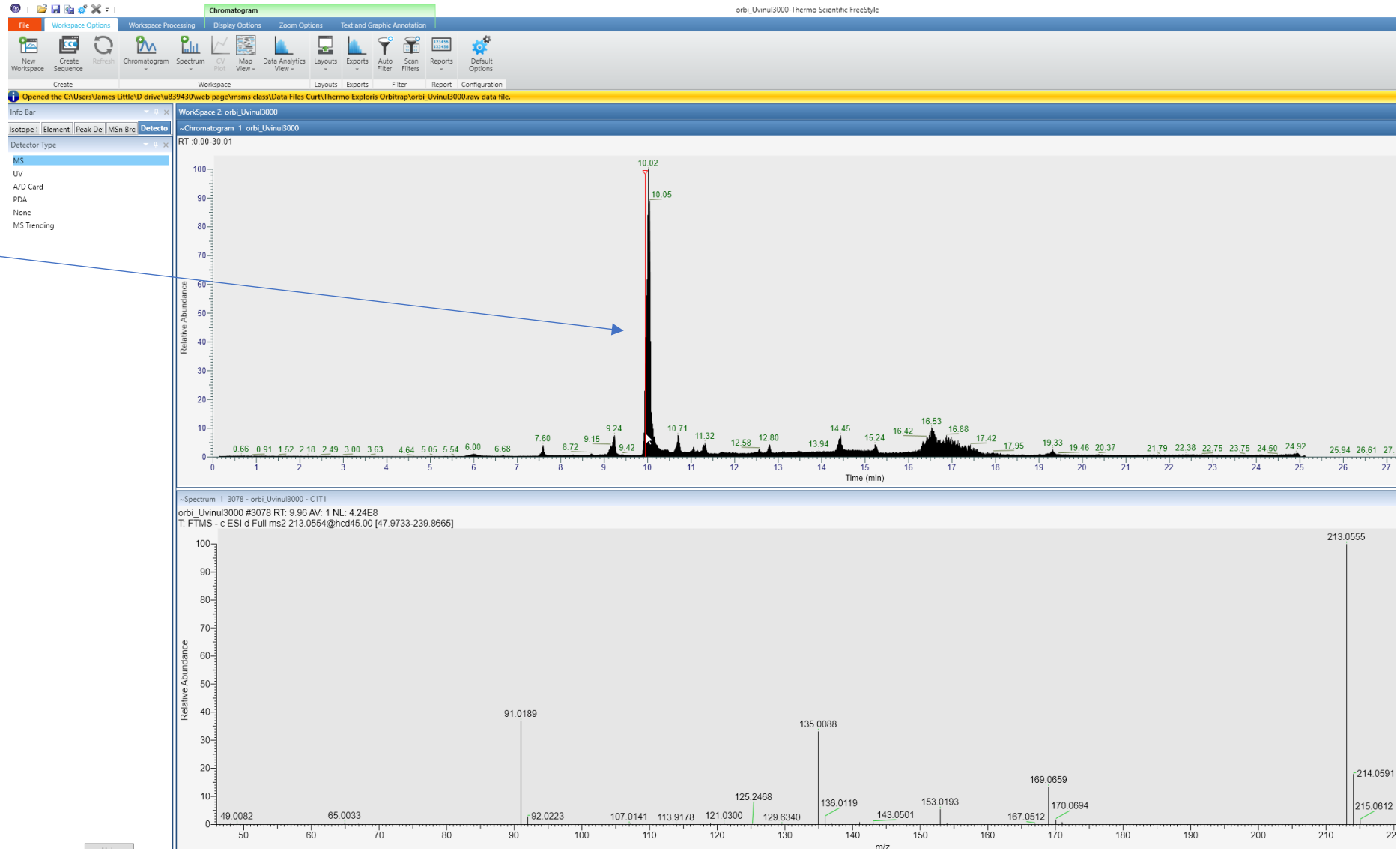
Windows Arrow Key Approach Using Total Ion Chromatogram, *NOT* Parsed into Separate Ones

After opening the file, the total ion chromatogram is displayed, just left click on the front of the peak, note red line showing the location of selected peak

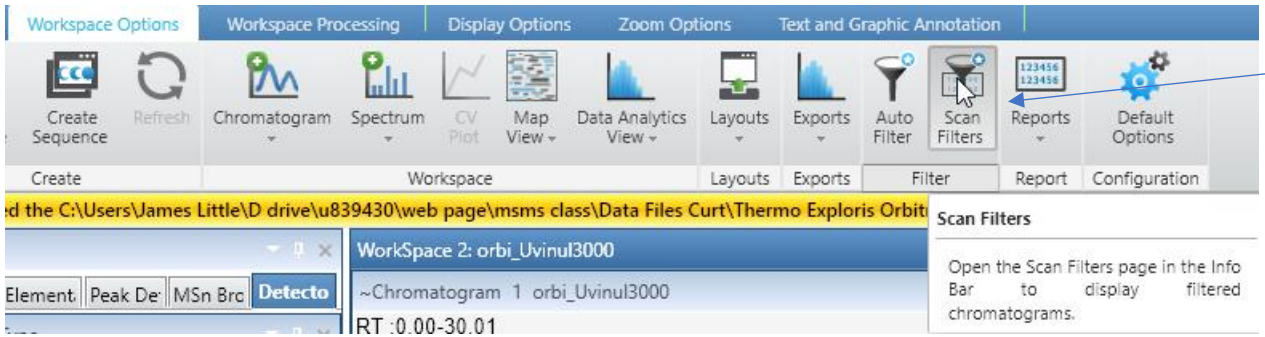
Then just “walk” through the peak using the left and right arrows on keyboard

The Header on the spectrum in bottom box will tell you the polarity and if a MS1 or MS2 peak is being displayed

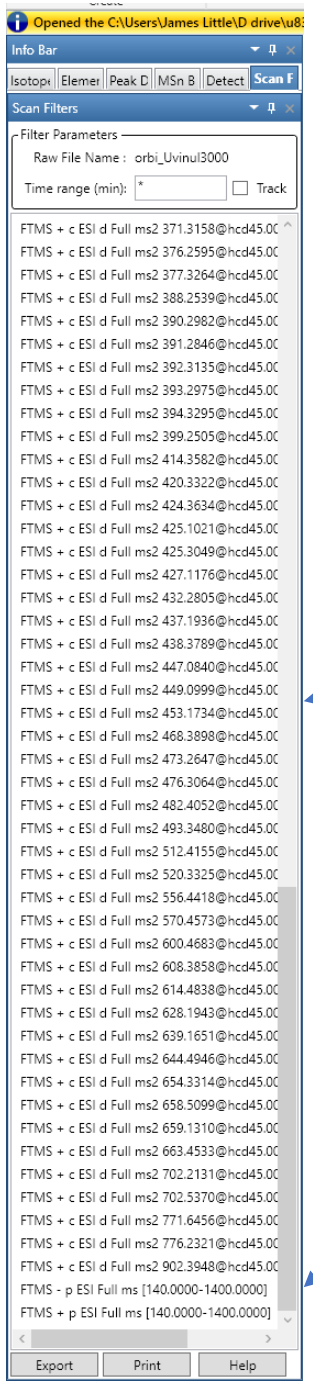
The MS2 spectrum of interest can be sent to NIST MS search



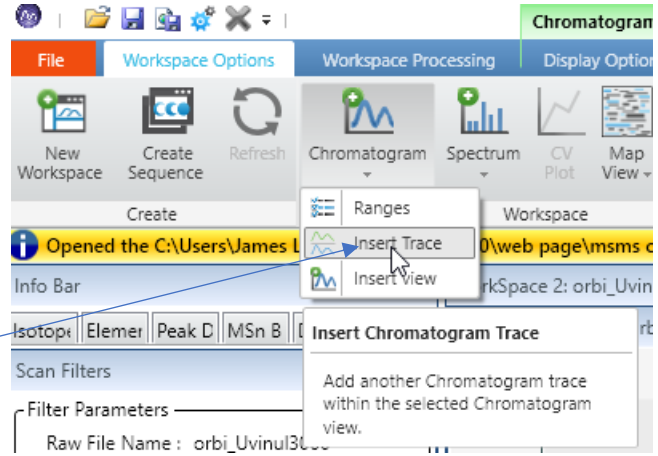
Manually Opening Windows



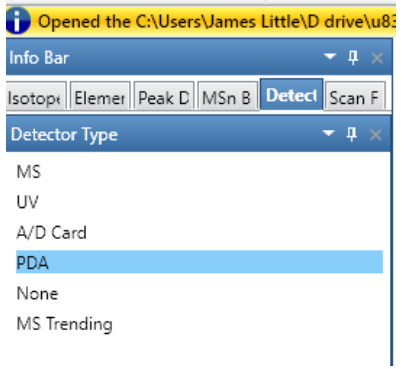
1) Click on the Scan Filters Icon in Workspace Processing Tab



2) That will open the list of ions, the positive and negative ion MS1 choices are at the ***bottom*** of the list



3) If you want to get another trace, for example, the PDA, click on Insert trace



4) The PDA or UV trace is found in the "Detector" Tab