# Dataset Folder:

C:\MSIQuickView\_code

# Saving Parameters and Settings:

Current setup includes saving details to 2 xml files and a mat file struct.

1. nic\_instrument\_settings.xml
2. nic\_saved\_parameters.xml
3. Saved\_Parameters.mat

Plan is to load Saved\_Parameters.mat file into MATLAB memory and pre-fill the appropriate input boxes.

# Save ion images

Changes:

1. Ion Images saved without extra borders.
   1. Select all the images to save and hit save, this should start saving the images one by one. The change you will notice here is that images will start popping up and closing by itself after saving. Enter the aspect ratio values; else there will be an error.

# Draw ROI on ion image

1. ROI selection is applied to all files in the excel spreadsheet, individual ion images are saved with the ROI selection. The filename will have ‘\_MASK’. Previously I was using Josh’s spectrometry toolkit output text file to generate the ROI values. I have moved away from that approach and am now generating my own matrix txt file. For generating this matrix file, save all the images first, this is the step that outputs the matrix txt file. Then go through the normal process 🡪 select “BOX” or “FREEHAND” option from the drop-down box to determine how you will draw on the ion image 🡪click “Register Image” 🡪 “NO” to draw ROI on Optical Image 🡪 Ion image opens up, draw on it, enter excel spreadsheet info 🡪 the rest is automated (saving images, spreadsheets etc) 🡪 you will get a message box “Files have been saved” when the process is complete.

# IT Times:

07/30/15 – Replaced Josh’s matrix method. Now the matrix is generated from MSI QuickView. The logic is that: the matrix is generated only for the m/z range values loaded from the spreadsheet. Column1 is the lower limit for the m/z range and columns 2:end are the intensity values. The ROI estimations are based on this matrix. The idea now is to multiply each pixel with the IT times, determine the invalid IT times or maxed IT times (logic is to look for really high and static values, 500, 1000, etc), determine the average intensity and standard deviations while discarding the invalid IT times, mark the invalid IT times on the ROI images. Save csv files for with and without the multiplication with IT timestamps.

When you select the ROI on the ion image, it will look for the excel files containing the ionization times (created using the previous Header\_Files\_Info GUI)….If the files are present, it will use those excel sheets to generate the ionization times etc for the ROI drawn. Two excel sheets will be generated in the “Images” folder within the dataset…Option will be displayed like before to provide a new name for the excel file and the sheet…The sheet will contain the same values that were present in the last version, but a new sheet will be added named “Matrix\_ROI” that will contain the ROI values….Top 6 rows contain the line no, scan no, IT: ionization time, ST: time for each scan, RT: retention time (time stamp), TIC: Total Ion Current…First column contains the m/z values starting with the 7th row…..

### How is IT times obtained? What softwares are needed? How to do it directly from the software?

### Functions

#### check\_IT\_times\_folder

%% Function to check the existence of IT Times within a dataset folder and generate if not present

% Requirements:

% Extract\_Xcal\_Header\_Info.exe has to be present in the C drive for

% windows, not set up currently for Linux

#### IT\_times = get\_max\_IT\_time

%% Function to get the max IT time (ERROR IT Time) from a folder containing xls files of IT times for all scans and all lines

% Input: folder containing the IT files (xls)

% Output: IT\_timess, for e.g., 500

#### IT\_mask\_image = create\_IT\_mask(IT\_times, pathname, ll)

%% function to create a mask of IT time points to display in MSI QuickView

% It is basically an image of 0s and 1s, where 1s represent bad IT times.

% Function has 2 parts: (1) to get the max number of scans from all lines

% (2) to create an IT mask image

% Inputs are :::

% 1) pathname: directory of the raw files

% 2) IT\_times: max IT\_time, e.g., 500

% 3) ll: list of raw filenames {cell}

% Outputs are:

% 1) IT\_mask\_image: the IT\_mask image of 0s and 1s

%% Architecture

% 1) get the max number of scans from all lines in the dataset

% 2) create an empty mask and append for each IT header file (for each

% line)

#### display\_average\_ROI\_with\_std

%% Function to usew the ROI pixels drawn by the user to generate the mean value and standard deviation of the pixels within the ROI.

% Inputs:

% roi\_pts: ROI x and y pixel values

% IT\_mask: IT\_mask to multiply with the ROI and discard those values

% ion\_image: sum\_of\_intensities image or ion image

% Output

% mean: mean intensity value from the ROI

% std: standard deviation of the intensity values within the ROI

%% Architecture

% 1) from ion\_image, get all intensity values within ROI

% 2) from the binary IT\_mask, get all the values within the ROI

% 3) Multiply 1\*2 and remove 0 values to discard the bad IT time pixels from

% the mean calculation

% 4) get mean and std value

# Structure:

To display in the excel spreadsheet:

4 columns - (1,2) mass list, (3) average normalized intensities x IT, (4) and standard deviations

## “intensity\_fake\_matrix”:

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Max Number of scans | Intensity Values (scan 1) | Intensity Values (scan 2) | Intensity Values (scan 3) | Intensity Values (scan 4) | Intensity Values (scan 5) | Intensity Values (scan 6) | … | Intensity Values (scan n-1) | Intensity Values (scan n) |
| 1 |  |  |  |  |  |  |  |  |  |
| 2 |  |  |  |  |  |  |  |  |  |
| … |  |  |  |  |  |  |  |  |  |
| 12 (point\_count max) |  |  |  |  |  |  |  |  |  |

Temp:

prev\_sum\_of\_intensities\_number 4634

6134

3841