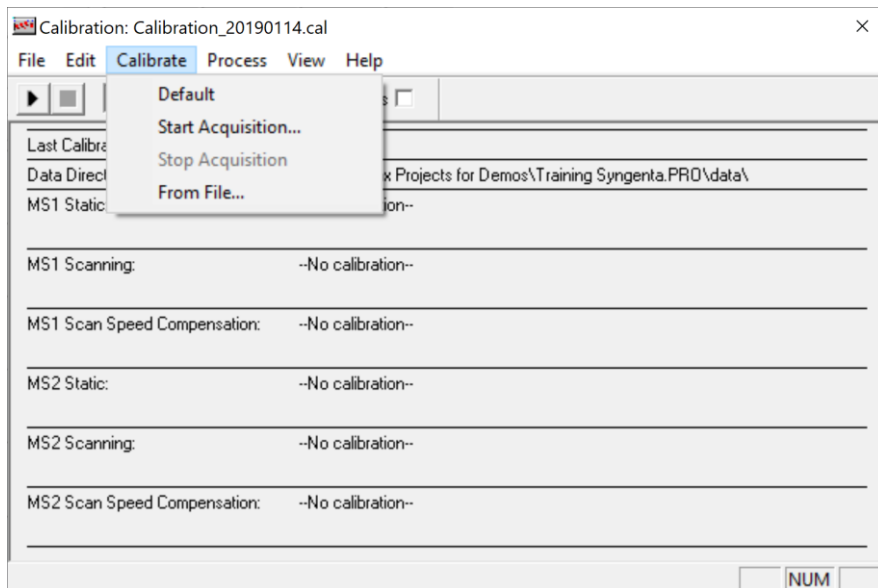


# How to correct the IntelliStart calibration to match reference peak m/z 74.10 on the Xevo TQ-XS

## Calibrate from File:

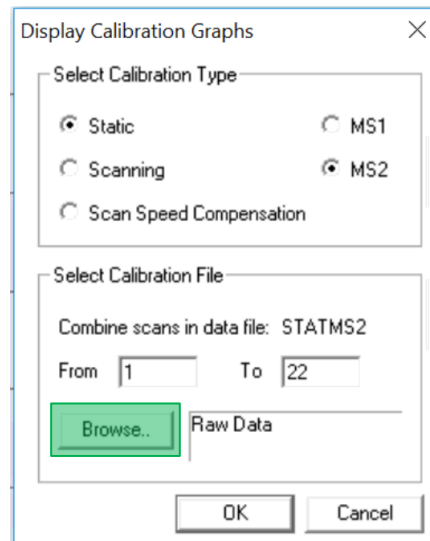
- From the MS Tune Page, Select «Default» from the «Calibration» menu in order to remove the current calibration. «No Calibration» should be displayed as below:
- Select «From File» from the «Calibration» menu.



# Calibration Modes and Data File Names

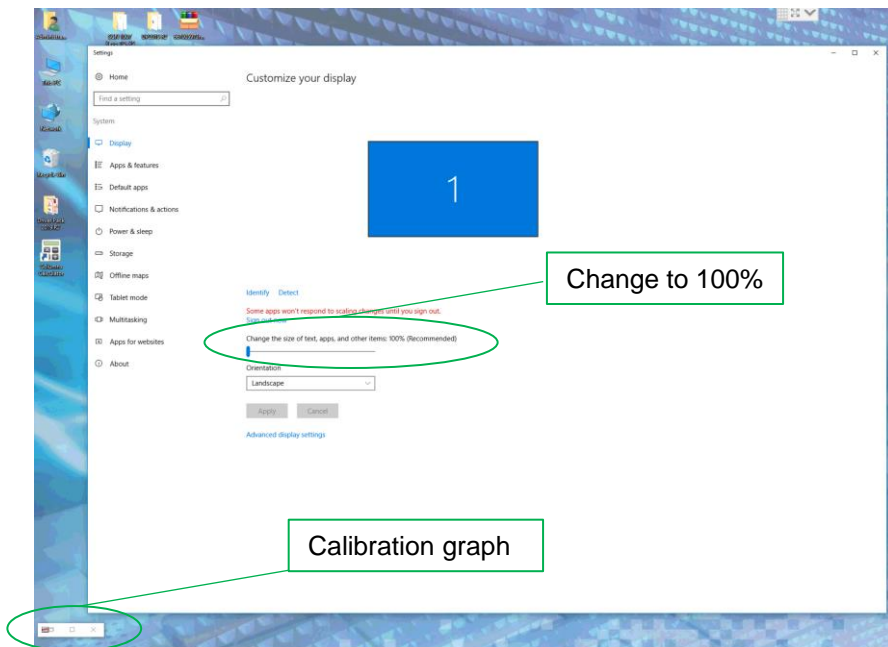
- Each calibration needs to be verified according to the table below.
- For each calibration, «Browse» to the correct raw file which is in: C:MassLynx > IntelliStart.pro > Data. You can find the right Data File Name in the table below:
- Once the right raw file for a specific calibration is selected, click «OK».

| Mode                    | MS  | Data File Name |
|-------------------------|-----|----------------|
| Static                  | MS1 | STATMS1.raw    |
| Scanning                | MS1 | SCNMS1.raw     |
| Scan Speed Compensation | MS1 | FASTMS1.raw    |
| Static                  | MS2 | STATMS2.raw    |
| Scanning                | MS2 | SCNMS2.raw     |
| Scan Speed Compensation | MS2 | FASTMS2.raw    |



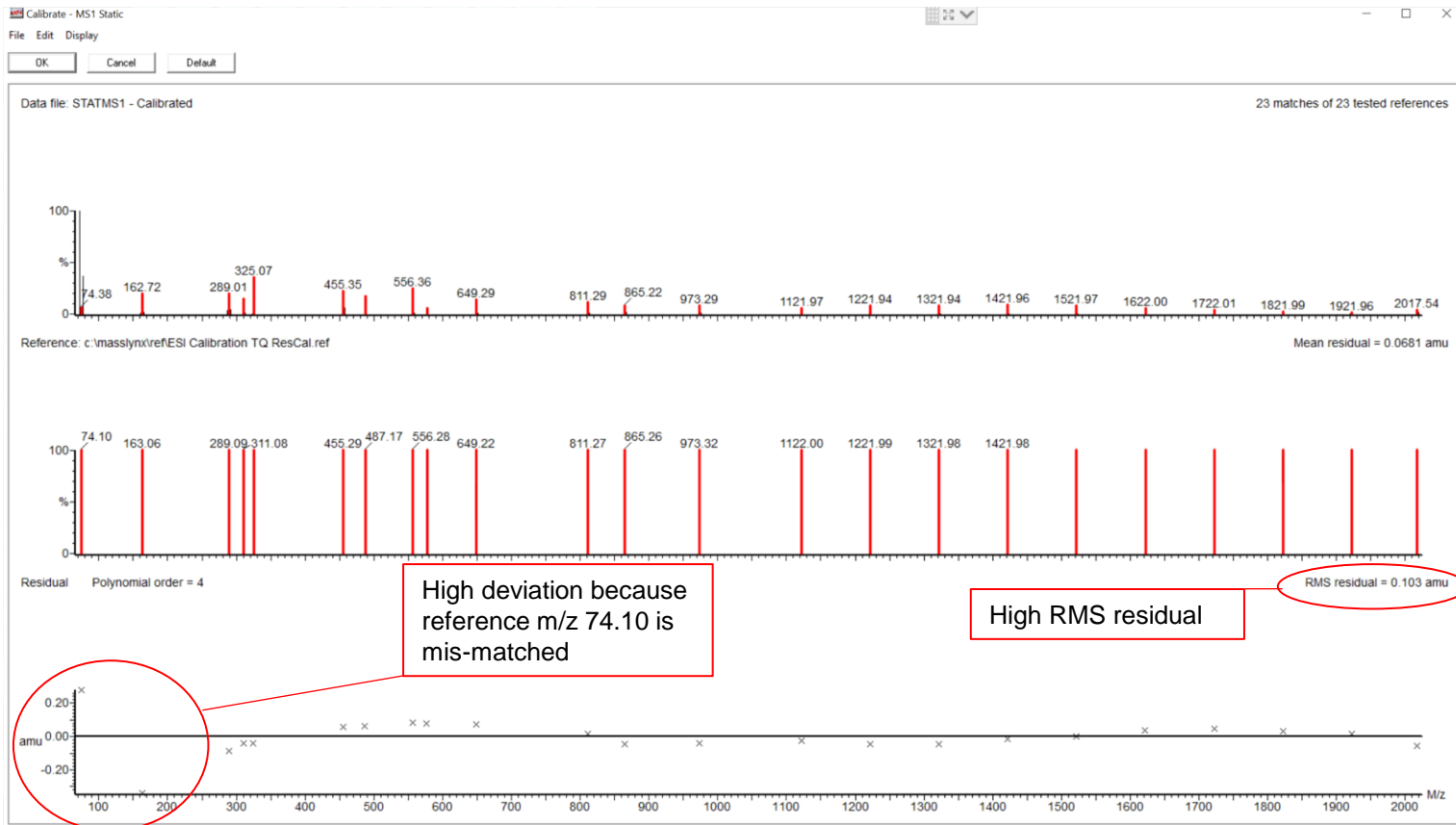
# If you do not see the Calibration graph on screen

- Right click on the desktop and select «Display Settings».
- Change the size of text, apps and other items to 100%
- You can find the calibration graph at the bottom left of the screen.
- Maximize the calibration graph.



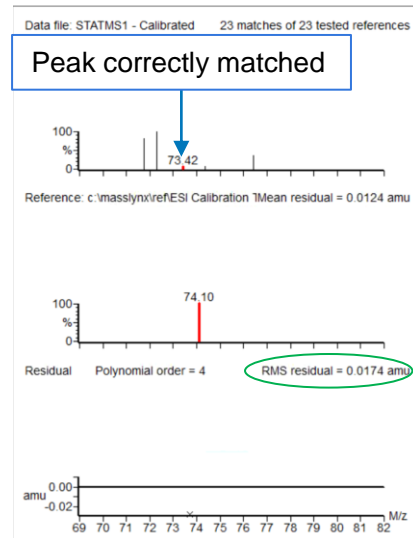
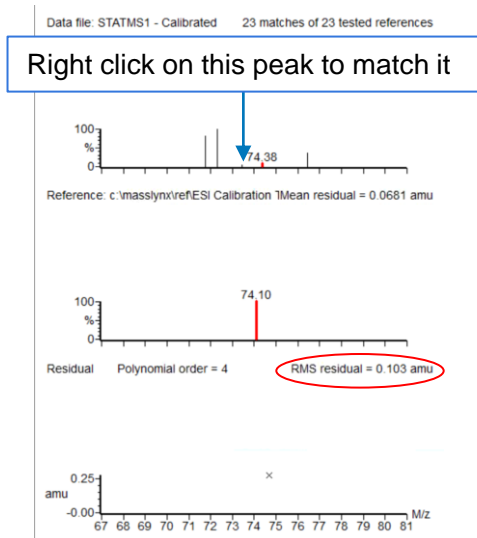
# Calibration plot

## Mis-matched peak for reference m/z 74.10



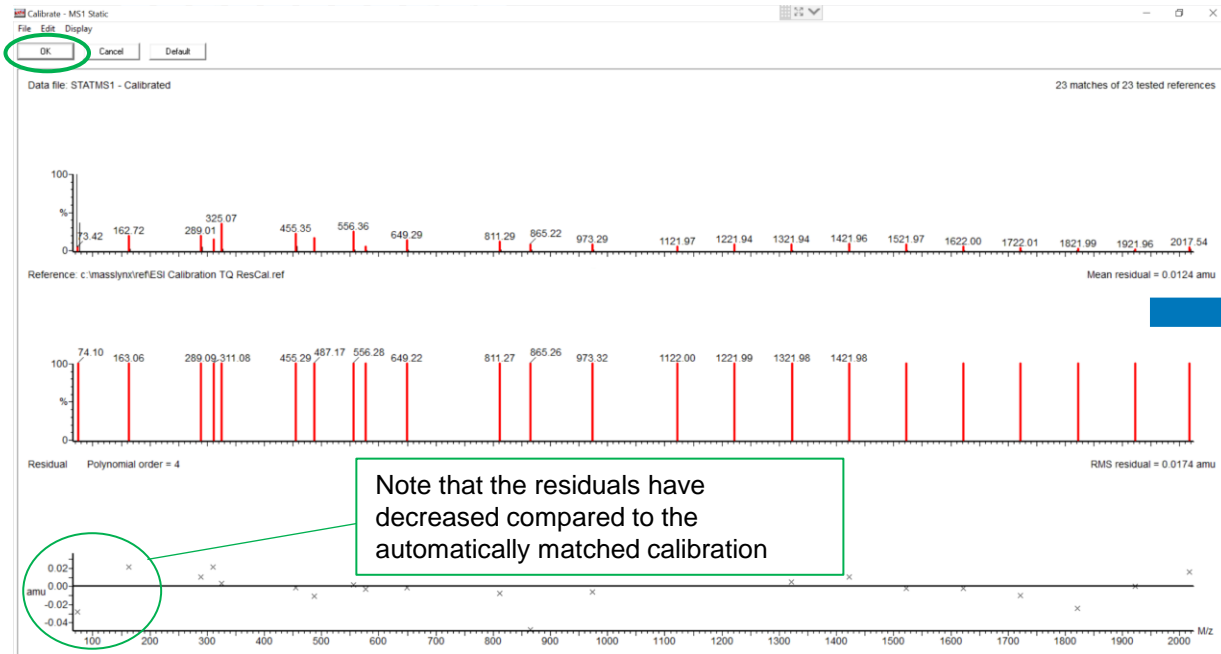
# How to match the correct peak for reference m/z 74.10

- Zoom in the region of the peak at m/z 74.10 and match the correct peak as shown below:



# MS1 Static Calibration Plot with correctly matched peak for reference peak m/z 74.10

- Once the correct peak is matched, click “OK” to accept the calibration.
- Note that in the calibration window, MS1 Static is now calibrated.



MS1 static is now correctly calibrated

The 'Calibration: Default' window shows the following parameters:

|  |      |              |         |      |      |
|--|------|--------------|---------|------|------|
| File   | Edit | Calibrate    | Process | View | Help |
| ESI Calibration TC   |      | Use air refs |         |      |      |
| Last Calibrated: 19 Mar 21 09:14                                     |      |              |         |      |      |
| Data Directory: C:\Projects\Xevo TQ-XS\DR-0064_KL_BL_2021_PROD\data\ |      |              |         |      |      |
| MS1 Static: Mass 72 Da to 2020 Da                                    |      |              |         |      |      |
| High Mass Resolution=14.8 Low Mass Resolution=2.7 Ion Energy=-0.5    |      |              |         |      |      |
| MS1 Scanning: -No calibration-                                       |      |              |         |      |      |
| MS1 Scan Speed Compensation: -No calibration-                        |      |              |         |      |      |
| MS2 Static: -No calibration-   |      |              |         |      |      |
| MS2 Scanning: -No calibration-                                       |      |              |         |      |      |
| MS2 Scan Speed Compensation: -No calibration-                        |      |              |         |      |      |
| Ready  |      |              |         |      | NUM  |

Note that the residuals have decreased compared to the automatically matched calibration

# Proceed for the other calibrations

- Proceed with the other calibrations according to the table below.
- At the end, verify that all mode are calibrated as shown on the Calibration window **and save the calibration.**

| Mode                    | MS  | Data File Name |
|-------------------------|-----|----------------|
| Static                  | MS1 | STATMS1.raw    |
| Scanning                | MS1 | SCNMS1.raw     |
| Scan Speed Compensation | MS1 | FASTMS1.raw    |
| Static                  | MS2 | STATMS2.raw    |
| Scanning                | MS2 | SCNMS2.raw     |
| Scan Speed Compensation | MS2 | FASTMS2.raw    |

The screenshot shows the 'Calibration: Default' window with the following details:

- Menu: File Edit Calibrate Process View Help
- Buttons: Play, Stop, ESI Calibration TC (dropdown), Use air refs (checkbox)
- Last Calibrated: 19 Mar 21 09:33
- Data Directory: C:\Projects\Xevo TQ-XS\DR-0064\_KL\_BL\_2021.PRO\data\
- MS1 Static: Mass 72 Da to 2020 Da. High Mass Resolution=14.8 Low Mass Resolution=2.7 Ion Energy=-0.5
- MS1 Scanning: Mass 2 Da to 2048 Da. High Mass Resolution=14.8 Low Mass Resolution=2.7 Ion Energy=-0.5
- MS1 Scan Speed Compensation: Scan 100 to 2000 amu/sec. High Mass Resolution=14.8 Low Mass Resolution=2.7 Ion Energy=-0.5
- MS2 Static: Mass 72 Da to 2020 Da. High Mass Resolution=14.7 Low Mass Resolution=2.7 Ion Energy=0.6
- MS2 Scanning: Mass 2 Da to 2048 Da. High Mass Resolution=14.7 Low Mass Resolution=2.7 Ion Energy=0.6
- MS2 Scan Speed Compensation: Scan 100 to 10000 amu/sec. High Mass Resolution=14.7 Low Mass Resolution=2.7 Ion Energy=0.6
- Status: Ready NUM