General Single Ion Calibration

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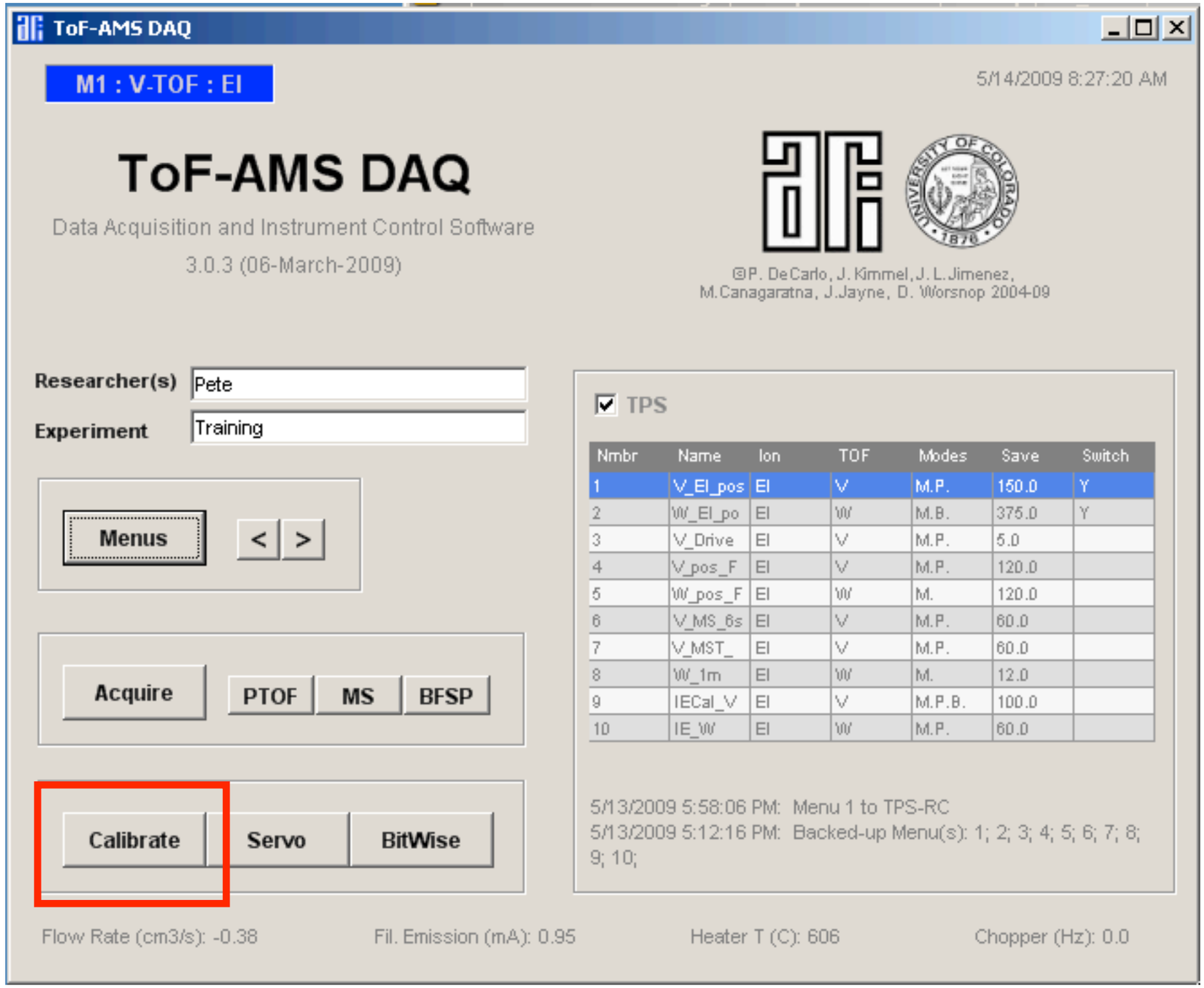
Purpose of SI calibration

- Measure the instrument response of a single ion.
- Necessary for understanding of error in instrument (counting statistics)
- Calculation of AB and IE
- The value is important, but cancels out in the calculation of mass.

How to Do SI calibration

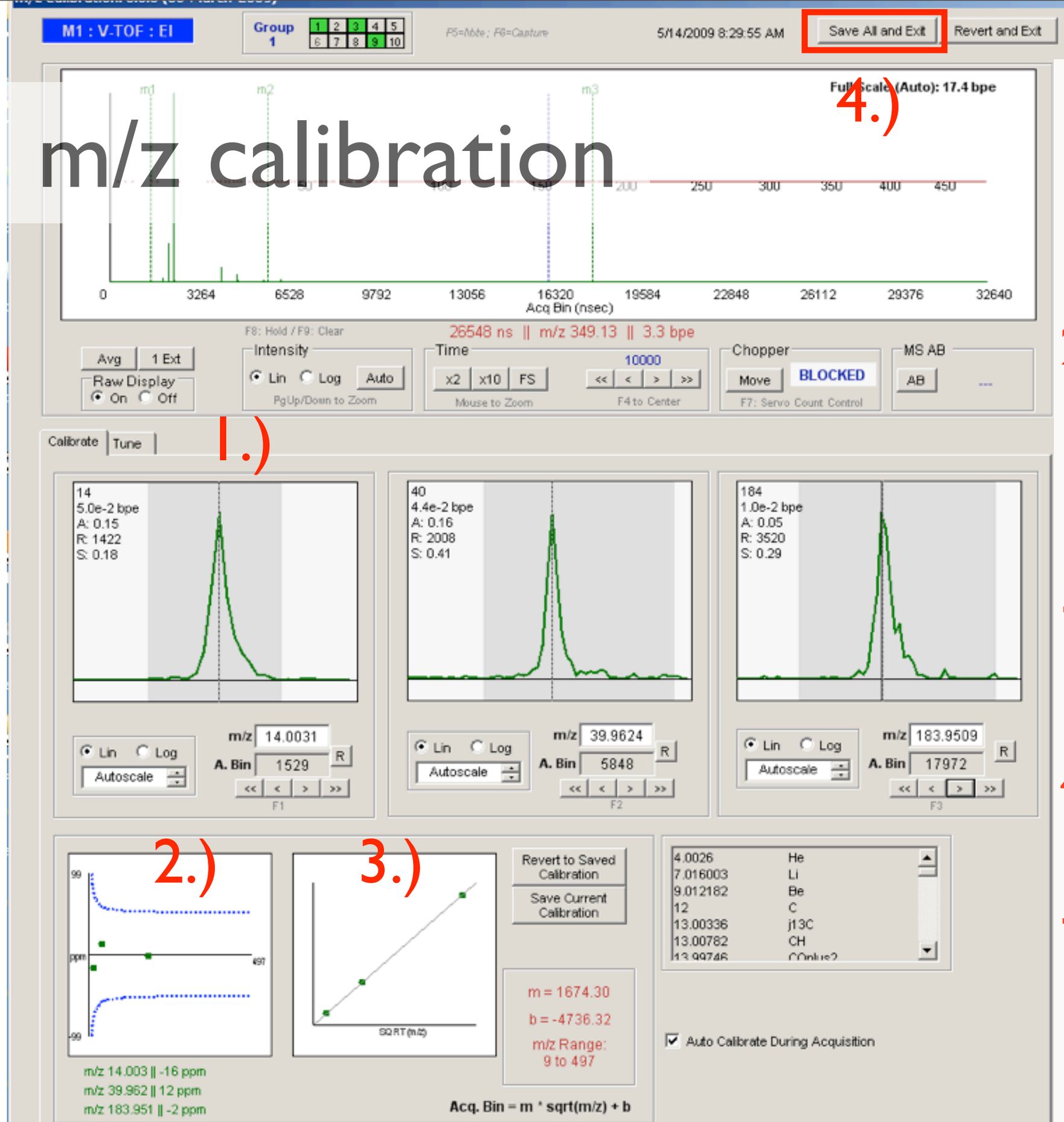
- m/z calibration
- baseline / threshold calibration
- check for saturation
- look at SI values
- thresholding (advanced diagnostics)
- m/z ratio - in particular 40/28
- if on a HR-ToF-AMS do it for BOTH modes

m/z calibration



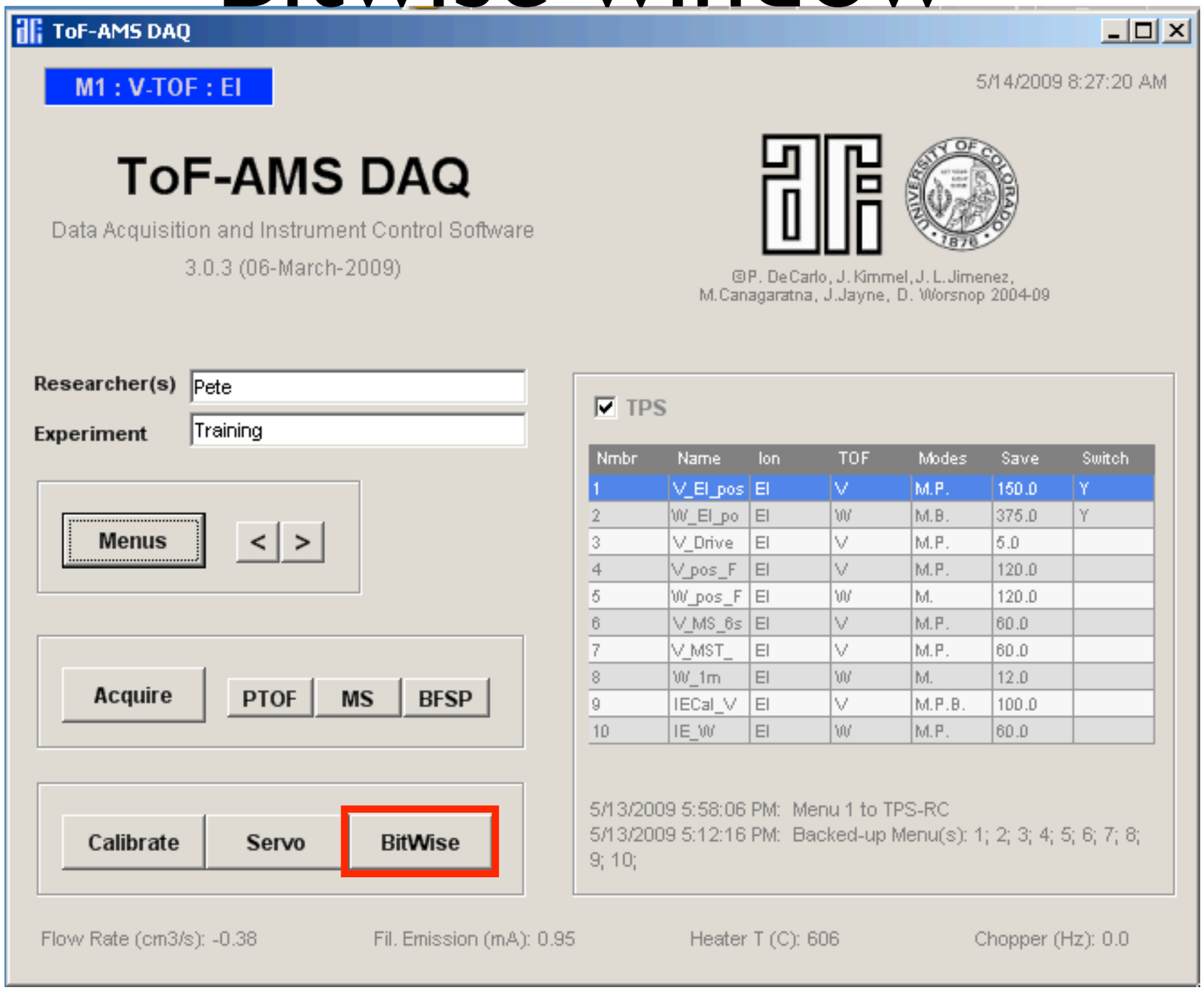
- the m/z calibration window is also where you can tune the instrument

m/z calibration



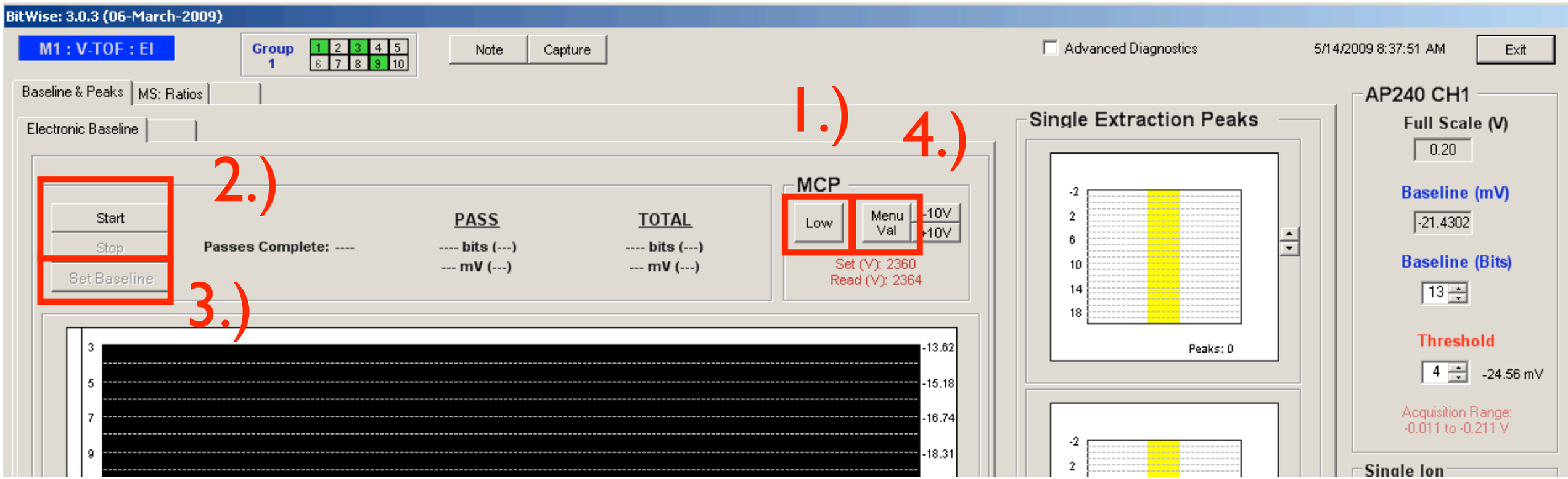
1. Line up the masses in the 3 boxes using the arrows
2. Check that the points fall in or close to the blue dotted lines
3. Check that the points fall on a line
4. If all is okay, press "save all and exit"
5. If the points are not on a line, then one of the masses is probably off.

Bitwise window



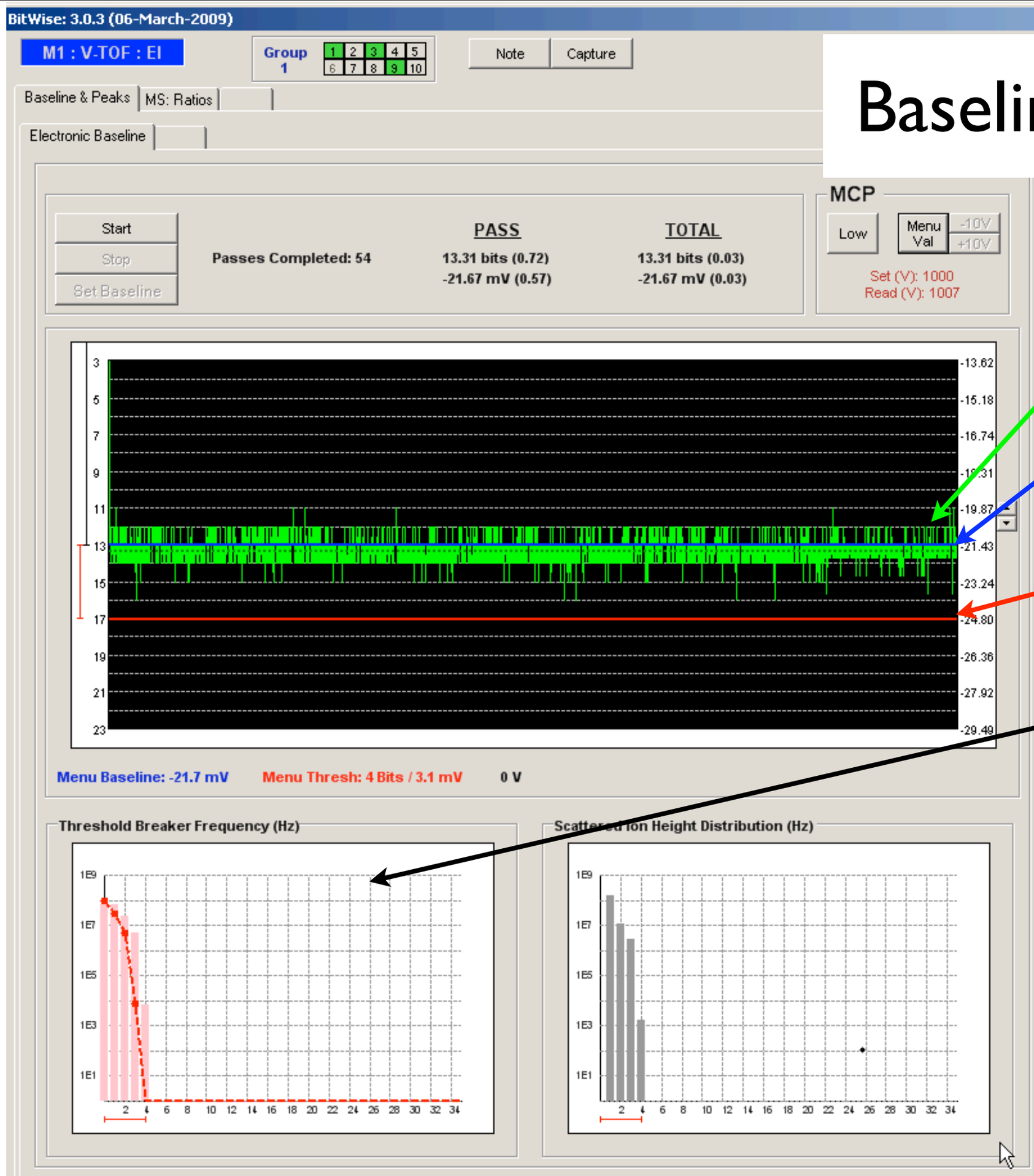
- The bitwise window is where one can check the baseline, thresholding, Saturation, and single ion

Baseline / Threshold



1. Set the MCP value to "Low" which = 1000 V (wait until value read value reaches 1000)
2. Press Start and wait for at least 30 passes to complete then press stop.
3. Inspect the baseline, if all appears okay, then press "Set Baseline"
4. Reset the MCP to the "Menu Val" wait for the Read value to reach the set value, and then wait for another minute or so.

Baseline Check Output



raw electronic baseline

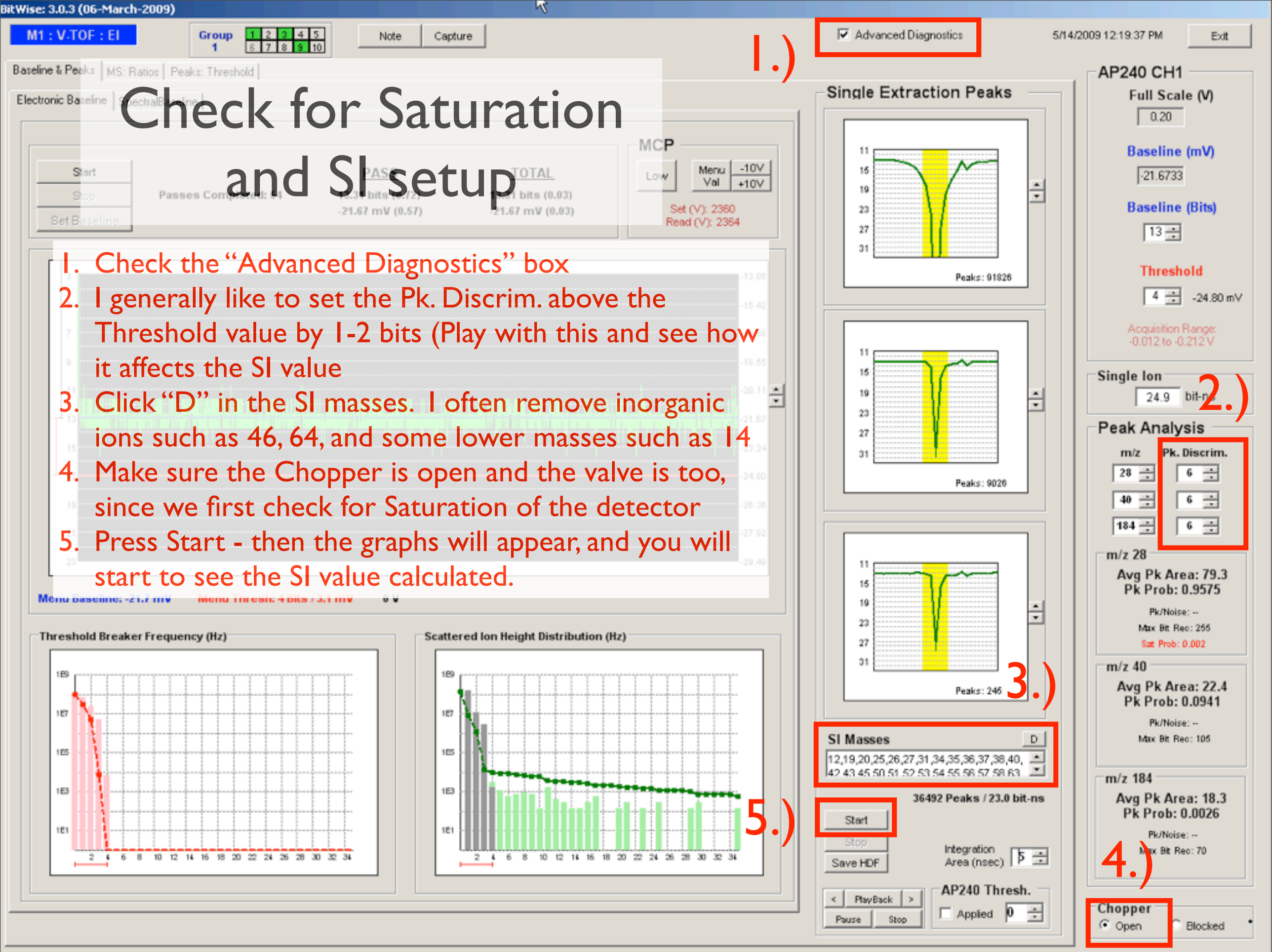
Set electronic baseline in ADC
Blue line should be in center of green trace

Set Threshold value in ADC

This graph shows the electronic noise around the baseline. In general one does not want vertical bars exceeding your threshold value red line at bottom. One should *not* adjust the baseline to prevent this, as that can reduce the linearity of the ion measurement and compromise data quality. The next tests guide ones decision on the threshold value

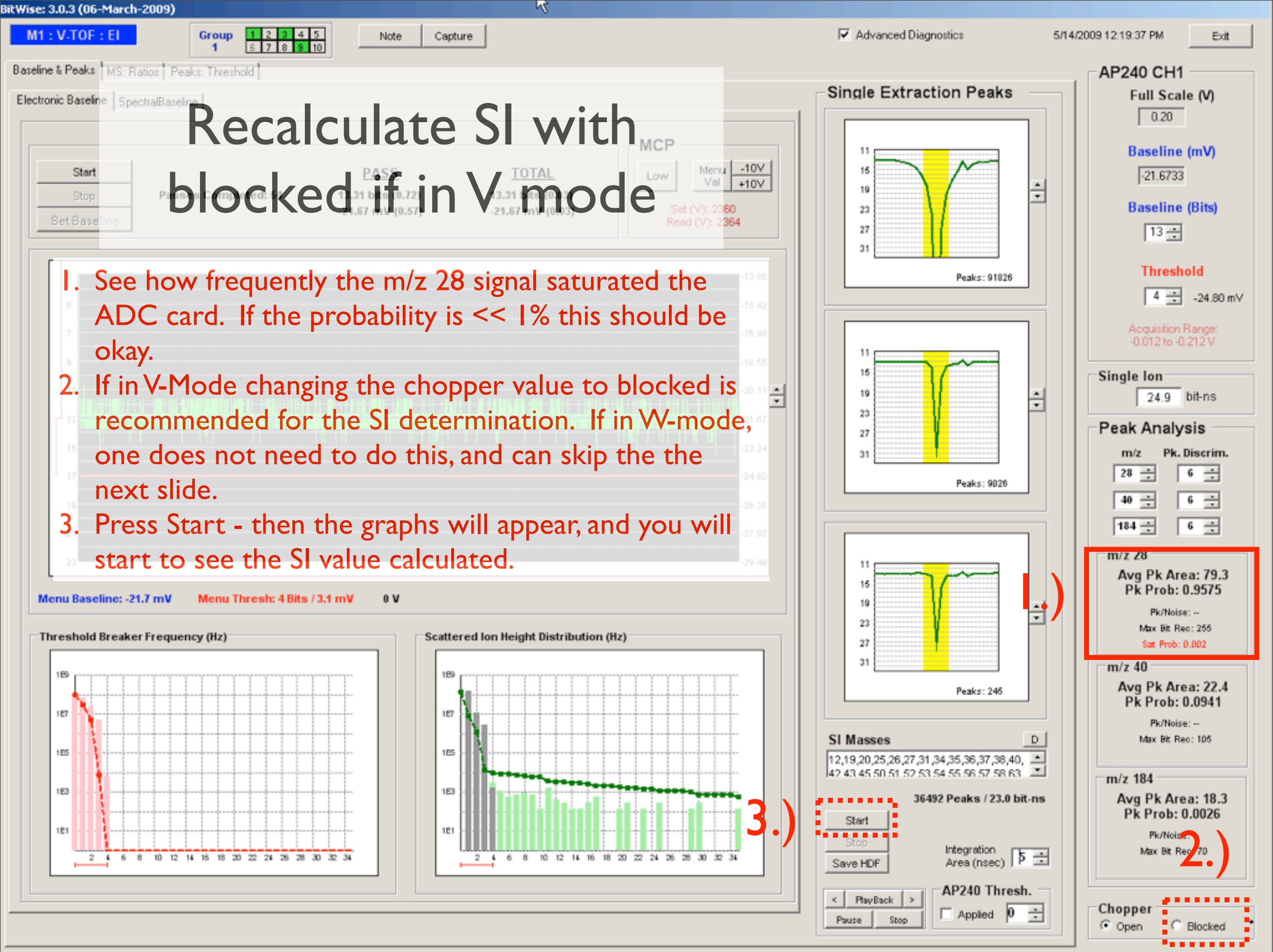
Check for Saturation and SI setup

1. Check the "Advanced Diagnostics" box
2. I generally like to set the Pk. Discrim. above the Threshold value by 1-2 bits (Play with this and see how it affects the SI value
3. Click "D" in the SI masses. I often remove inorganic ions such as 46, 64, and some lower masses such as 14
4. Make sure the Chopper is open and the valve is too, since we first check for Saturation of the detector
5. Press Start - then the graphs will appear, and you will start to see the SI value calculated.



Recalculate SI with blocked if in V mode

1. See how frequently the m/z 28 signal saturated the ADC card. If the probability is << 1% this should be okay.
2. If in V-Mode changing the chopper value to blocked is recommended for the SI determination. If in W-mode, one does not need to do this, and can skip the the next slide.
3. Press Start - then the graphs will appear, and you will start to see the SI value calculated.



Reading the Values

1. Check the SI value from m/z 40 (if Pk Prob < 10%)
2. Check the SI value from the default list of masses
3. Enter one of the values into the SI box. IMPORTANT: be consistent with the whichever one you choose. With the newer versions of the software there is automatic monitoring which uses the default list.

BitWise: 3.0.3 (06-March-2009)

M1 : V-TOF : EI

Advanced Diagnostics

5/14/2009 12:45:11 PM

Exit

Start

Stop

Set Baseline

Passes Completed: 54

PASS: 13.31 bits (0.72), -21.67 mV (0.57)

TOTAL: 13.31 bits (0.03), -21.67 mV (0.03)

MCP: Low, Menu Val, -10V, +10V

Set (V): 2360

Read (V): 2364

Menu Baseline: -21.7 mV Menu Thresh: 4 Bits / 3.1 mV 0 V

Threshold Breaker Frequency (Hz)

Scattered Ion Height Distribution (Hz)

Single Extraction Peaks

Peaks: 90822

Peaks: 3328

Peaks: 483

SI Masses

12,19,20,25,26,27,31,34,35,36,37,38,40,42,43,45,50,51,52,53,54,55,56,57,58,63

20616 Peaks / 22.4 bit-ns

Start

Stop

Save HDF

Integration Area (nsec) 5

AP240 Thresh. Applied 0

AP240 CH1

Full Scale (V) 0.20

Baseline (mV) -21.6733

Baseline (Bits) 13

Threshold 4 -24.80 mV

Acquisition Range: -0.012 to -0.212 V

Single Ion 22.4 bit-ns

Peak Analysis

m/z	Pk. Discrim.
28	6
40	6
184	6

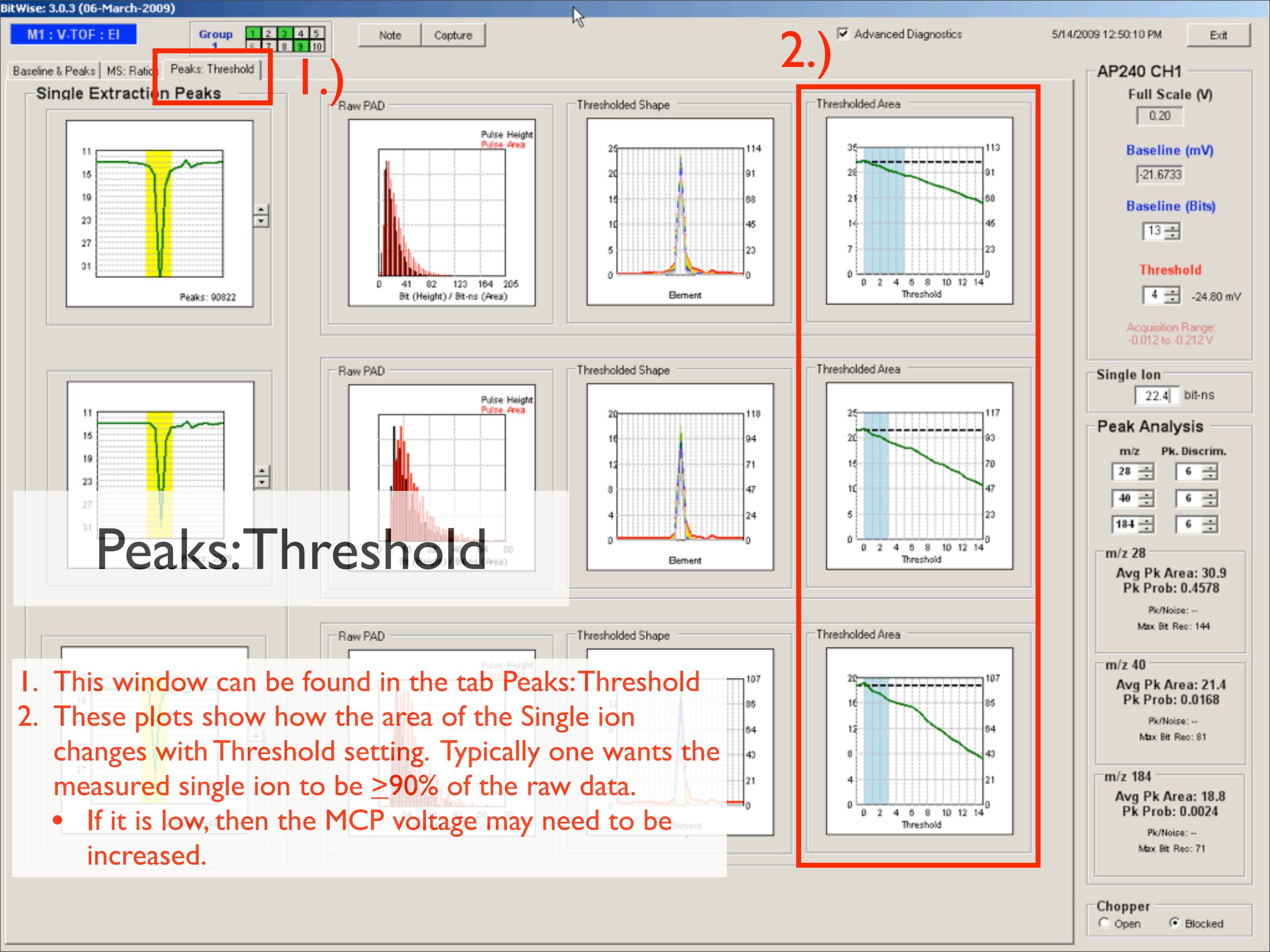
m/z 28: Avg Pk Area: 30.9, Pk Prob: 0.4578, Pk/Noise: --, Max Bit Rec: 144

m/z 40: Avg Pk Area: 21.4, Pk Prob: 0.0168, Pk/Noise: --, Max Bit Rec: 81

m/z 184: Avg Pk Area: 18.8, Pk Prob: 0.0024, Pk/Noise: --, Max Bit Rec: 71

Chopper: Open, Blocked

1.) 2.) 3.)

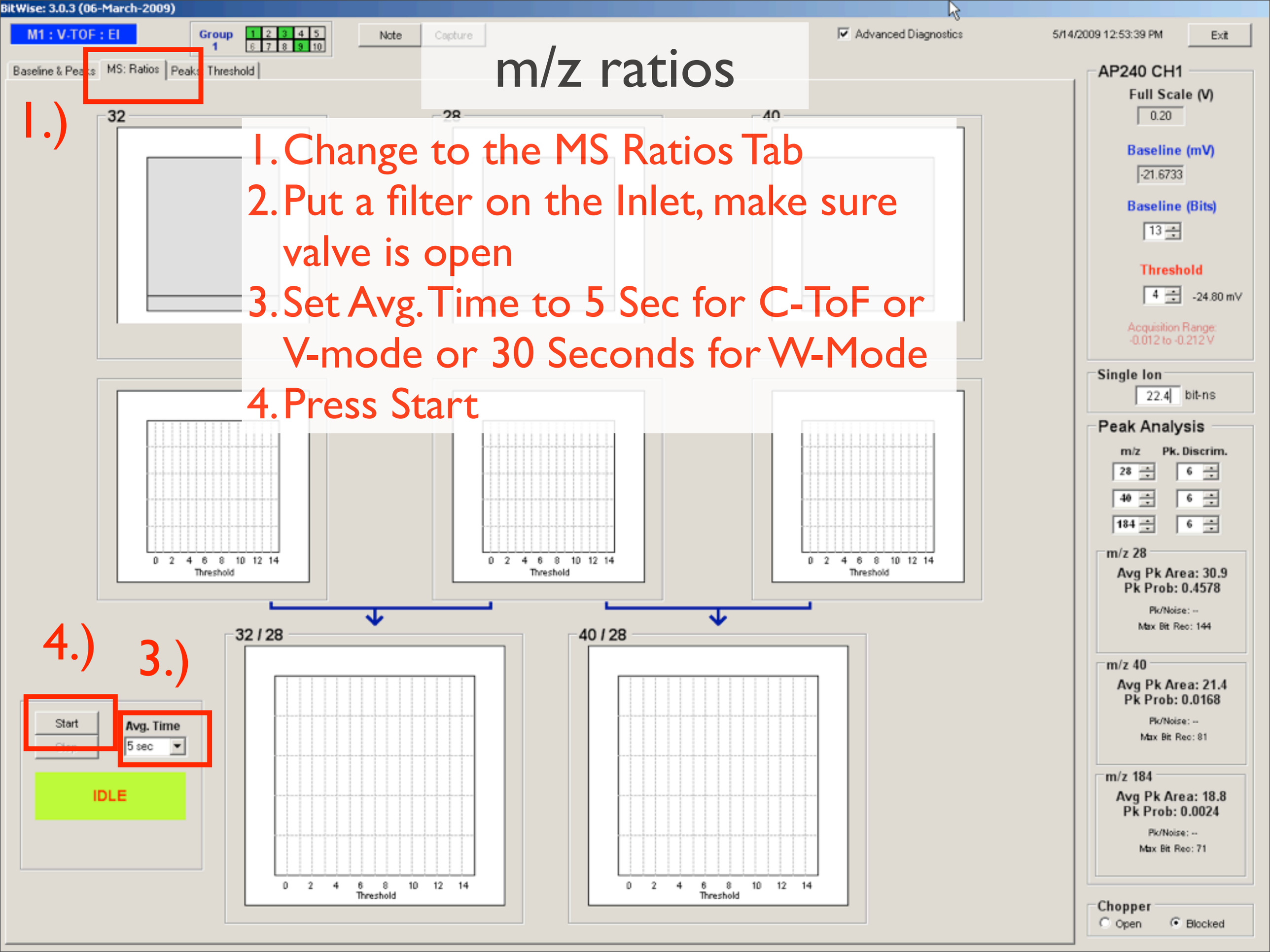


Peaks: Threshold

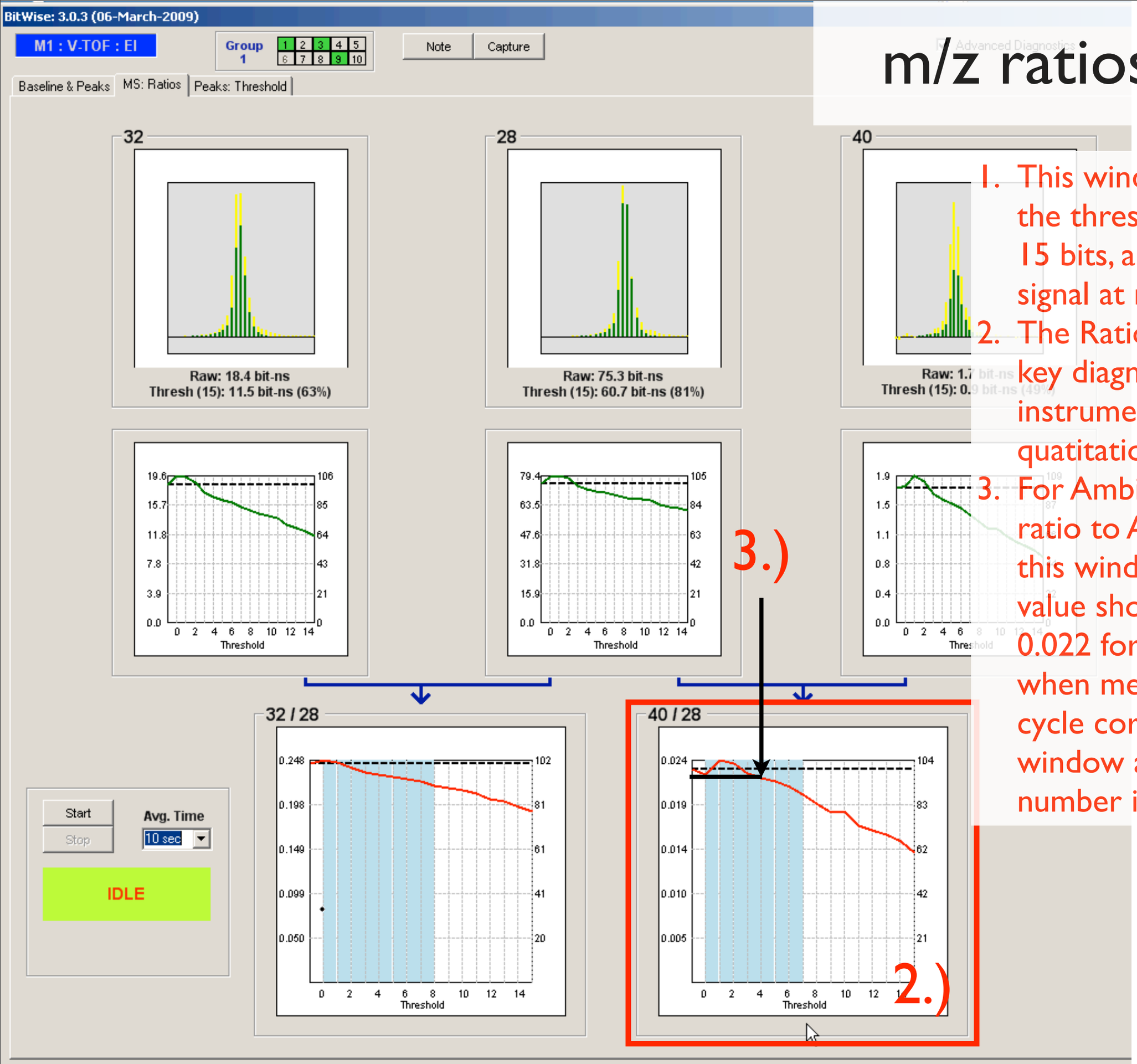
1. This window can be found in the tab Peaks: Threshold
2. These plots show how the area of the Single ion changes with Threshold setting. Typically one wants the measured single ion to be ≥90% of the raw data.
   - If it is low, then the MCP voltage may need to be increased.

m/z ratios

1.) Change to the MS Ratios Tab
2.) Put a filter on the Inlet, make sure valve is open
3.) Set Avg. Time to 5 Sec for C-ToF or V-mode or 30 Seconds for W-Mode
4.) Press Start



m/z ratios output



1. This window scan through the thresholds from raw to 15 bits, and calculates the signal at m/z 32, 28, and 40.
2. The Ratio of m/z 40/28 is a key diagnostic for the instrument performance and quatitation.
3. For Ambient air this is the ratio to Argon to N2 and in this window the absolute value should be around 0.022 for the threshold used when measuring (when duty cycle corrected in the DAQ window and in Sqrl the number is 0.018)

Baseline, SI, and Threshold

- Baseline set in instrument based on electronic noise with low V on MCP
- Saturation of m/z 28 checked to see if MCP too high (if too high reduce emission current or MCP)
- Single Ion value determined from m/z 40 or default ion list, and updated in text box
- Threshold parameters checked
- Check 40/28 ratio to make sure threshold value is appropriate for measurement