

Thermo Scientific Portable Analytical Instruments for identification

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14.04.2020

ACM2

- **Antaris II FT-NIR**

Integrated sphere

Fiber Optic

Transmission module

Spectral Range – 12000 – 3800 cm^{-1}

Resolution – 4 cm^{-1}



- **Nicolet iS20 FT-IR**

- 0.4 cm⁻¹ resolution standard
- Signal/Noise 50,000:1
- DTGS standard
 - MCT-A optional
- External IR beam port
 - Microscope, AEM
- Mid/Near-IR range fixed B/S (KE)
 - Extended range XT-KBr option
- OMNIC Software Integrates:
 - Atmospheric suppression
 - QCheck™ QA/QC Verify Function
 - System Performance Verification



ACM2 Thermo Scientific Portable Analytical Instruments

Formerly Ahura Scientific, Inc.
& Polychromix Inc.



MICROPHAZIR



TruScan RM



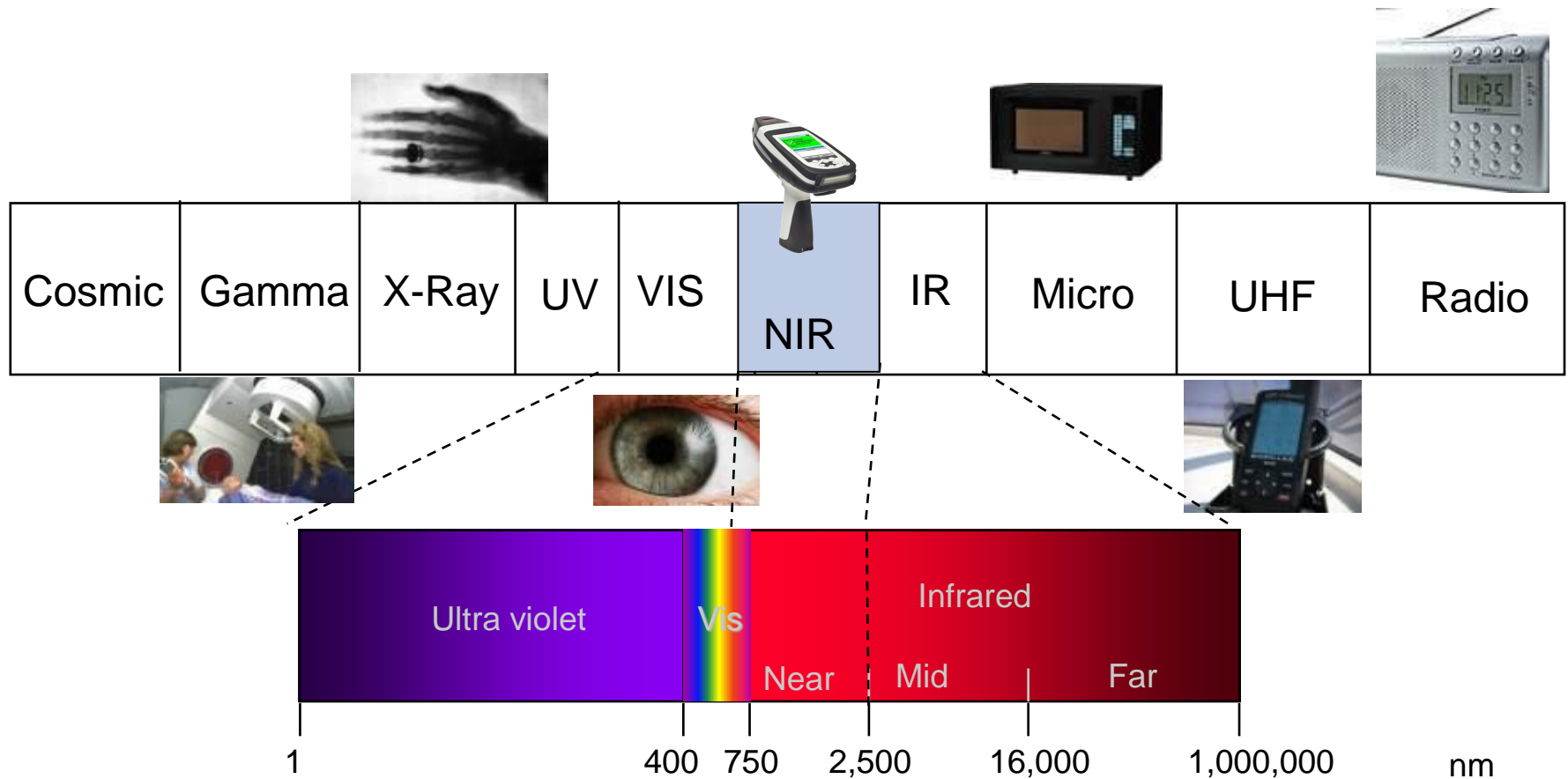
IonicX

Leading field-deployed analytical instruments
for human health and public safety, delivering lab-
accurate analysis at the point of need

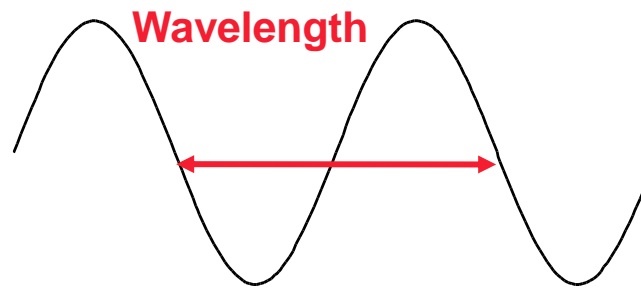
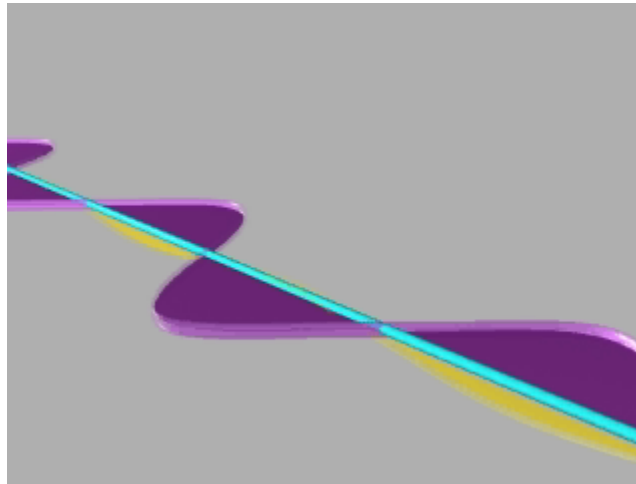


NIR Spectroscopy

ACM2 What is Near Infrared ?



ACM2 Electromagnetic Spectrum of Energy



Electromagnetic energy or energy of a photon of light is:

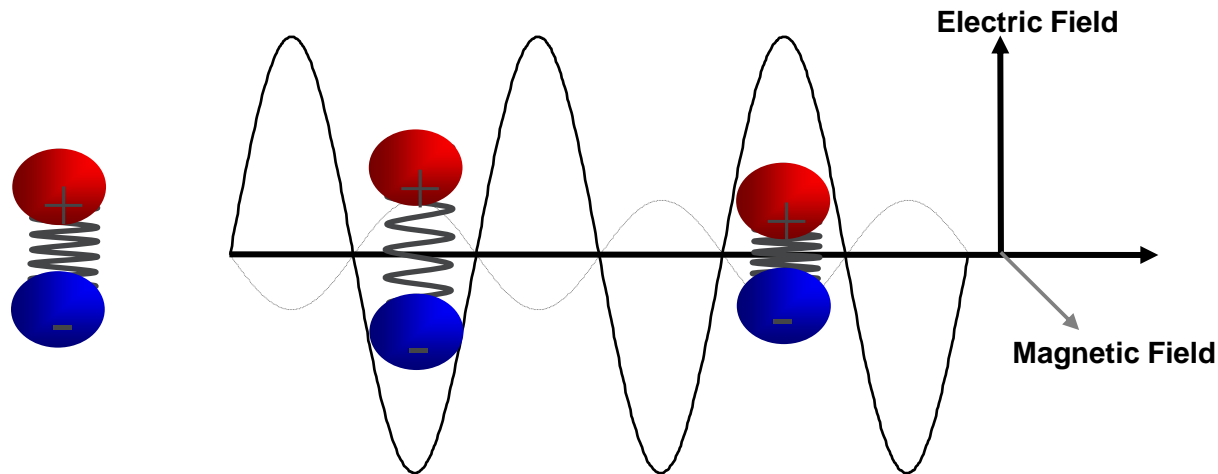
$$E = h \nu = hc/\lambda$$

h = Planck's constant, c = speed of light, ν = frequency, λ =wavelength

- Frequency (ν) is the number of peaks per second
- Wavelength (λ) is the distance between two peaks

ACM2 Interaction of IR Light and Matter

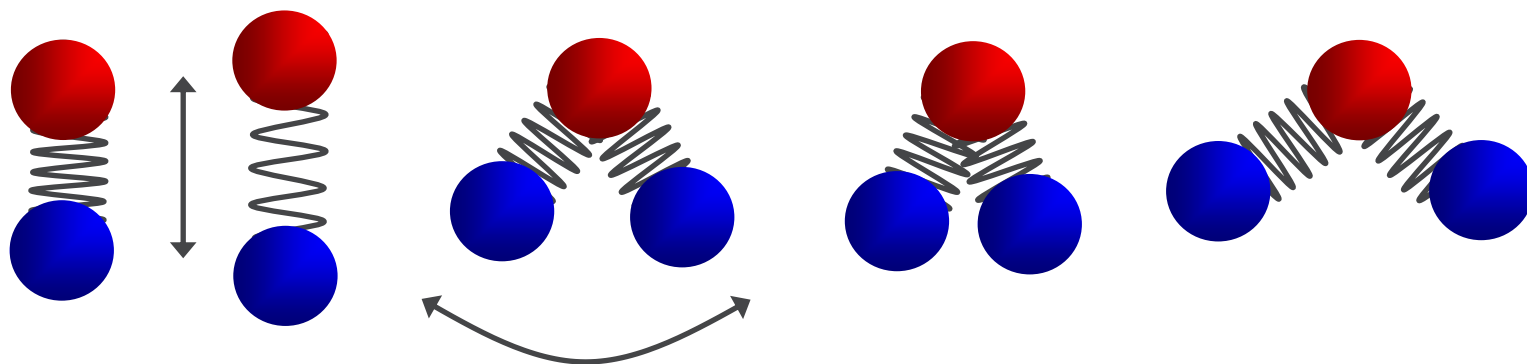
- Charged Balls and Electromagnetic Wave
 - Atoms interact with electric field of EM wave, stretching or compressing bond.



- ◆ Resonance at frequency (wavelength) that matches molecular characteristics.
- ◆ Light intensity decreased from increase in molecular vibrations.

ACM2 Interaction of IR Light and Matter

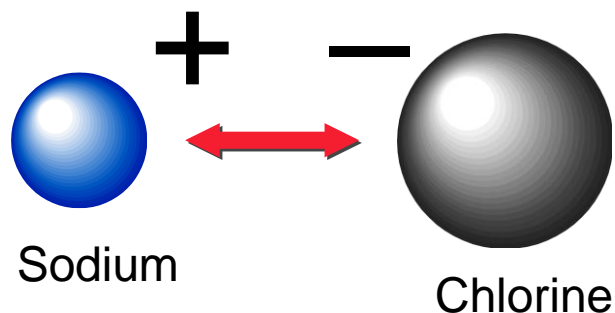
- Simple Model: Vibrating Balls and Springs
 - Mass of balls and strength of spring(s) will determine a resonant vibrational frequency.



ACM2 Ionic Bonds vs. Covalent Bonds

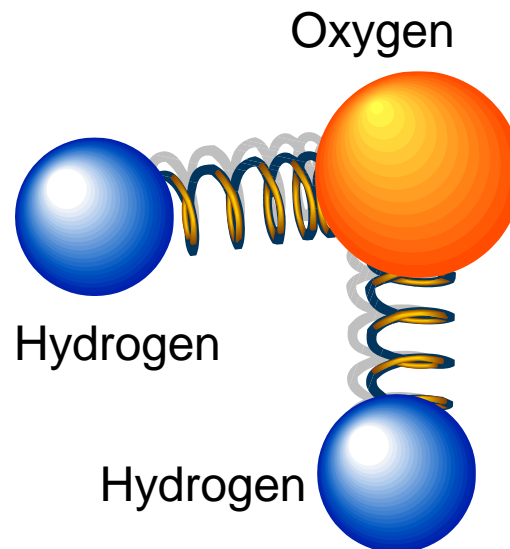
Ionic bonds

- Attraction of charges causes molecules to behave like magnets
- **Invisible to IR and Raman**



Covalent bonds

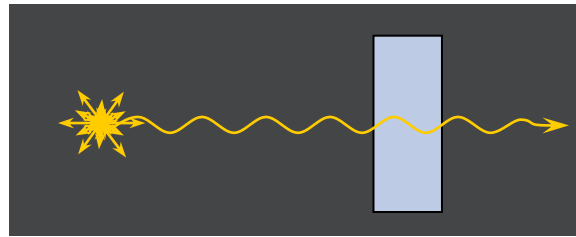
- Sharing of charges causes molecules to behave like a spring
- **Observable with IR and Raman**



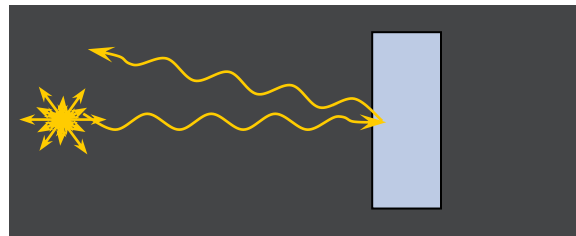
ACM2 The Interaction of Light in Optical Spectroscopy

Measurements with the microPHAZIR RX are possible both in reflectance and transmission modes. Typically reflectance is used.

Transmission



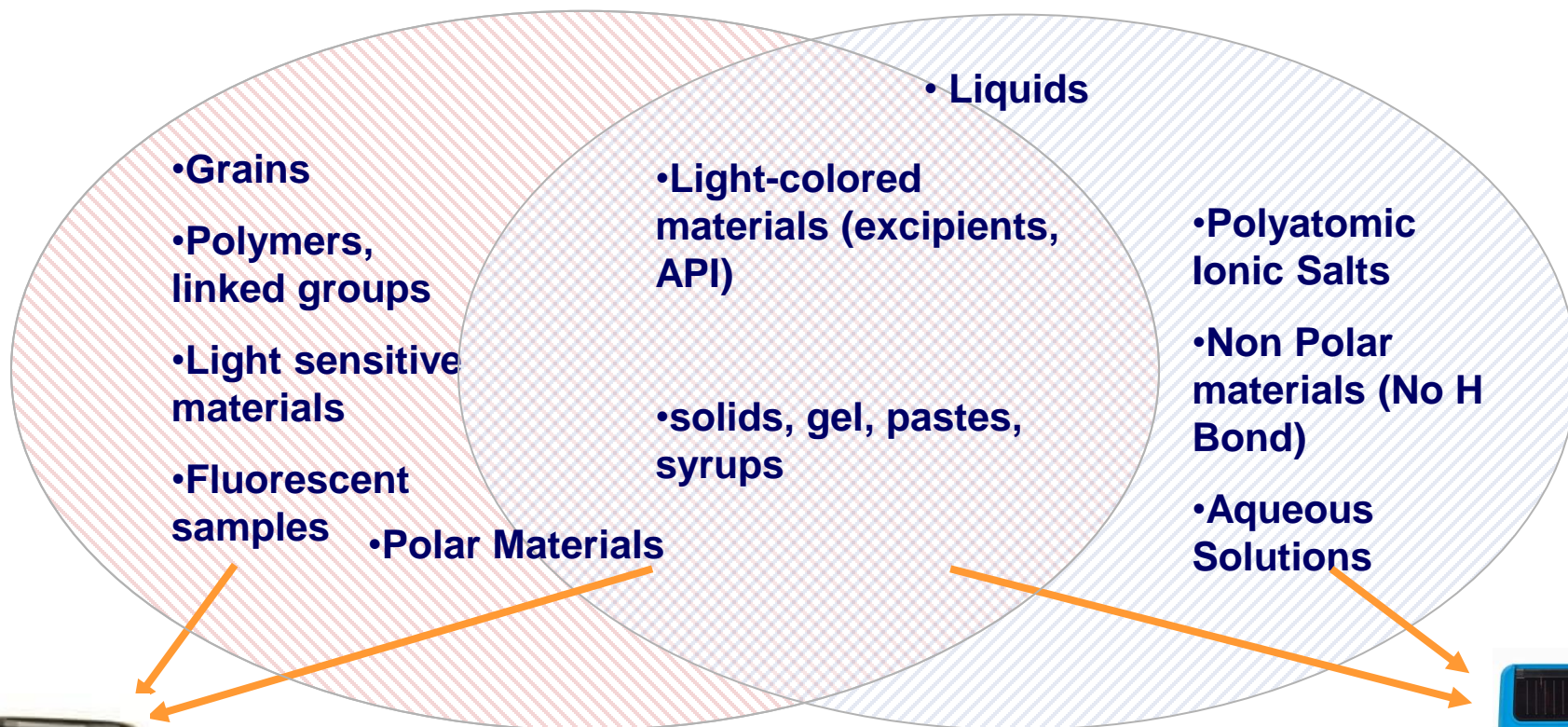
Reflectance



ACM2 NIR and Raman for RMID

NIR

Raman



•Out of scope: Gases, metals, ionic salts, chemicals without covalent bonds

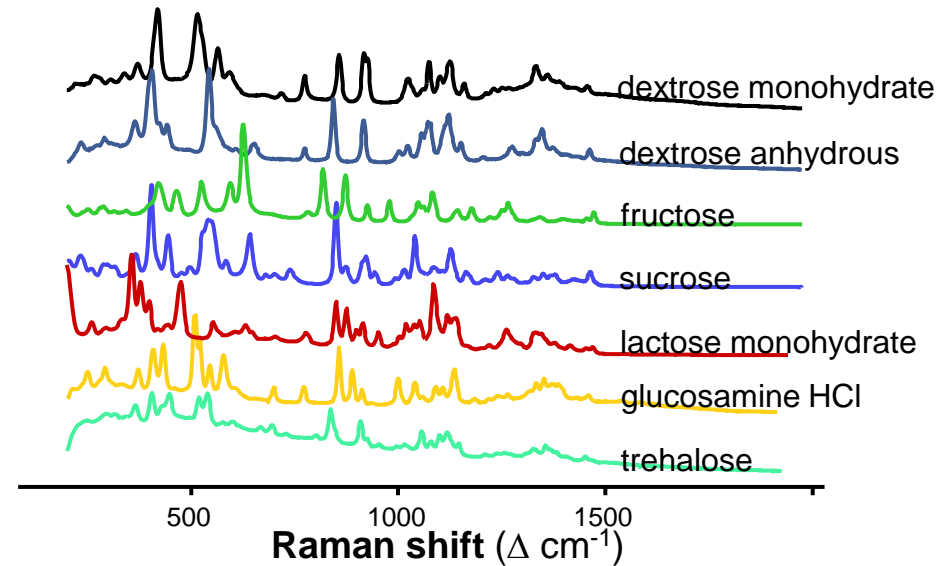
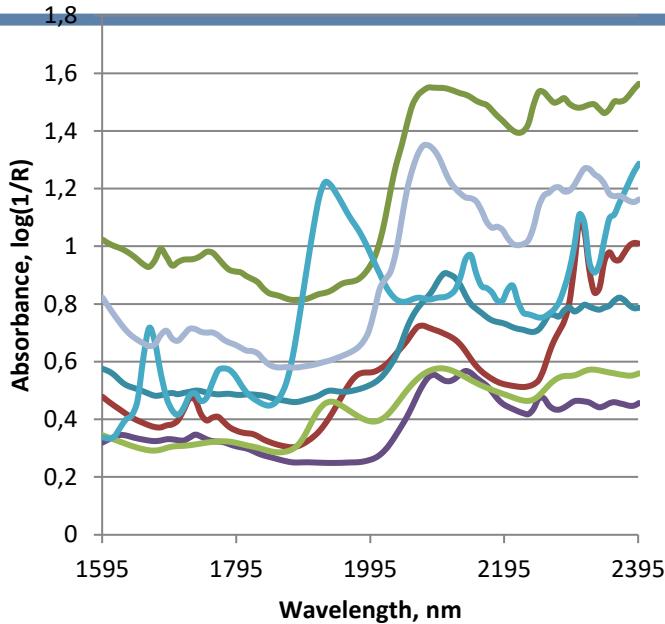
ACM2 NIR Applicability

90%

GREAT	API, organic solvents sugars, starches, polymers celluloses Most organic materials Packaging materials
DEPENDS	Some hydrates Some inorganic material in hydrated form
BAD	dark brown/black materials (low light return) water, highly dilute solutions HCl, HF (simple acids, poor selectivity) NaOH, KOH, MgOH, AlOH (poor selectivity)
N/A	metals & alloys, highly dilute solutions, ionic salts (NaCl, KCl, KI, HBr, KBr, etc.)

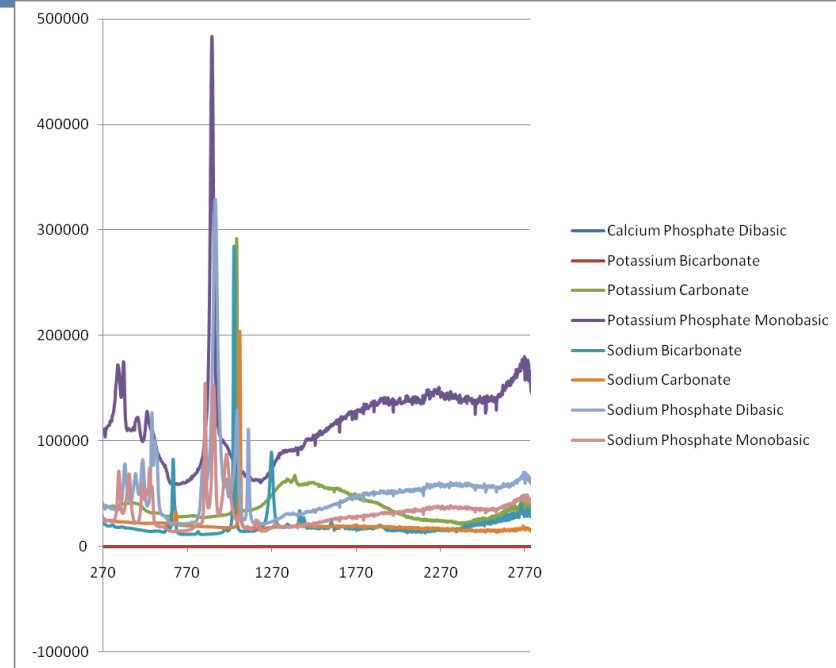
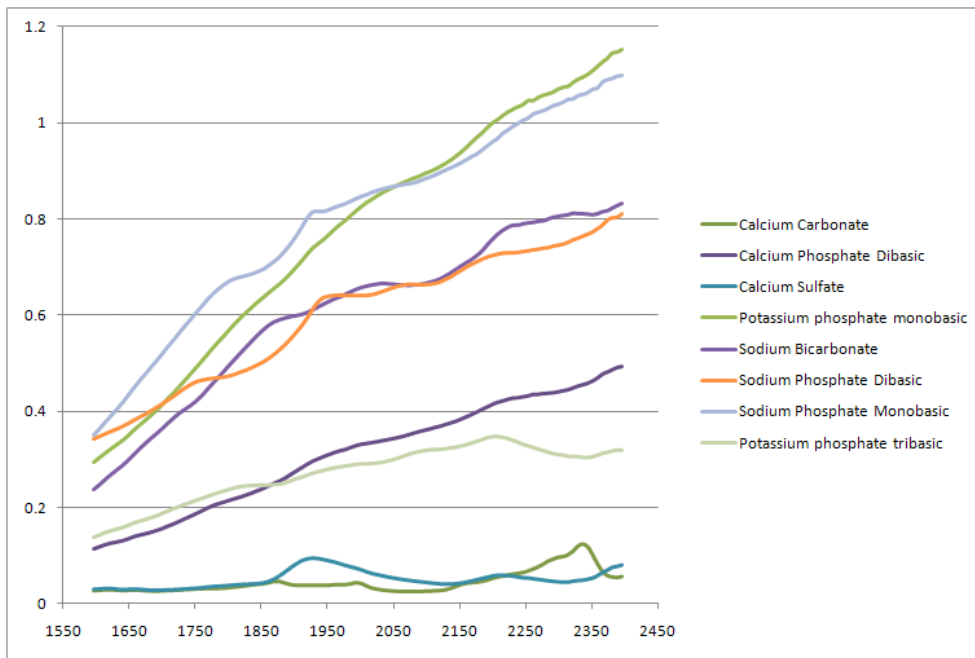
**Not appropriate for
FTIR, NIR or Raman**

ACM2 Example: Sucrose (sugar) and its analogs



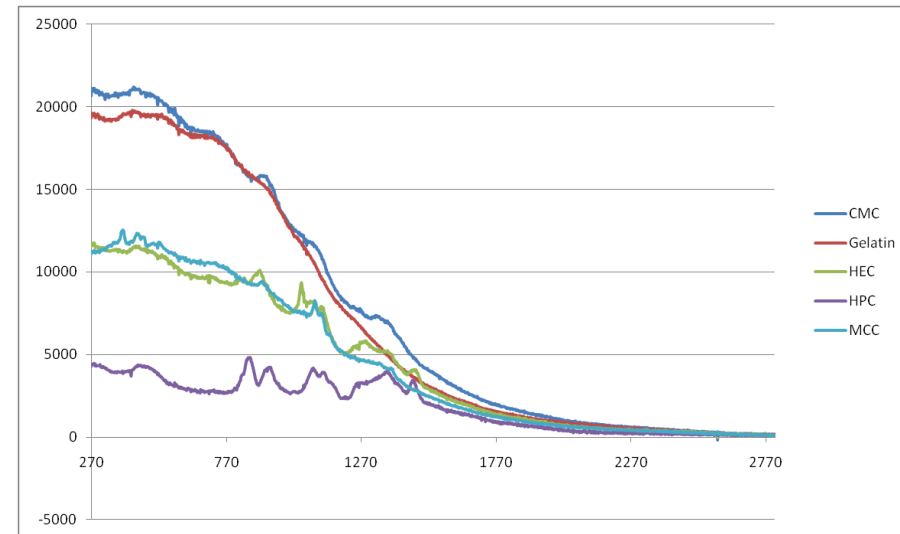
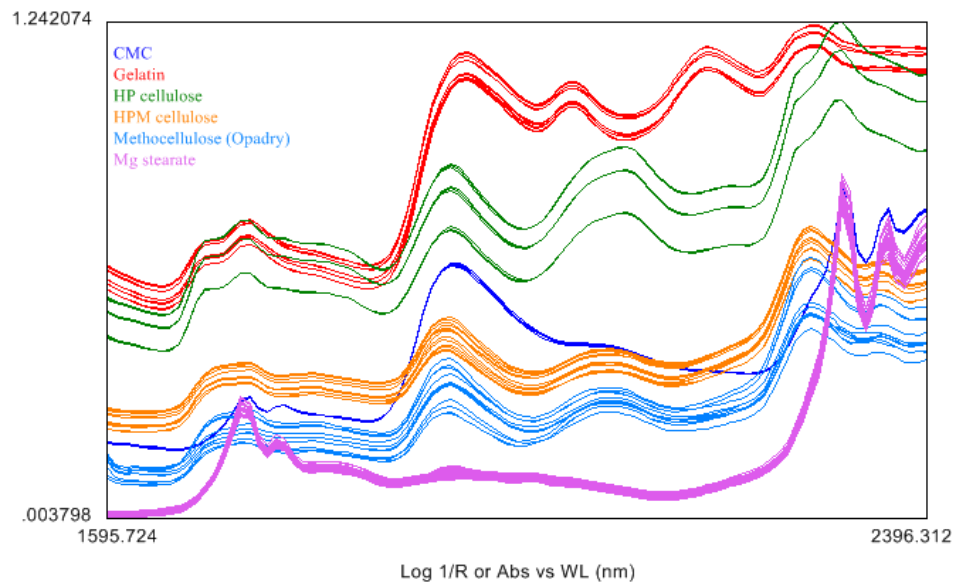
- Both spectra clearly differentiate different sugars
- Distinct peaks for the different types
- Classification is relatively straightforward
- Either method is appropriate

ACM2 Example: Polyatomic Inorganic salts



- Inorganic materials (e.g. no C-H_n bonds) and polyatomic salts show nor or extremely weak (if any) NIR features
 - Most common peak is due to un-bonded water
- Conversely, Raman has sharp features and salts are differentiable

ACM2 Example: Celluloses and starches



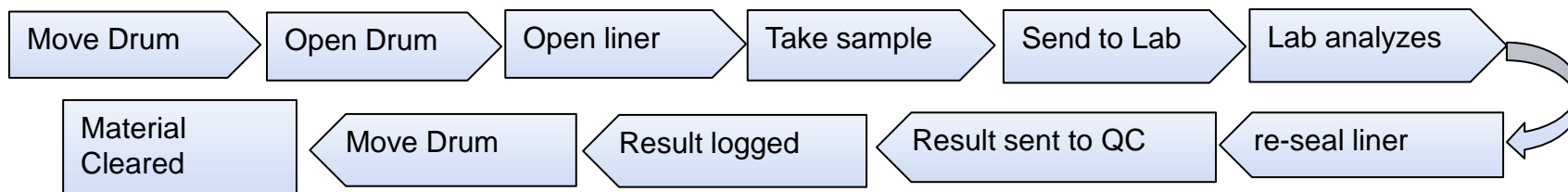
- Long chain connectivity weakens Raman signatures
- Fluorescence also an issue for certain materials
 - Broad peak, small signal peaks
- NIR shows enough peak variability to differentiate these materials

A decorative graphic consisting of a vertical blue line on the left side of the slide. A horizontal blue line extends from this vertical line to the left of the main title. A red dot is placed at the end of this horizontal line, and another red dot is placed at the bottom of the vertical line.

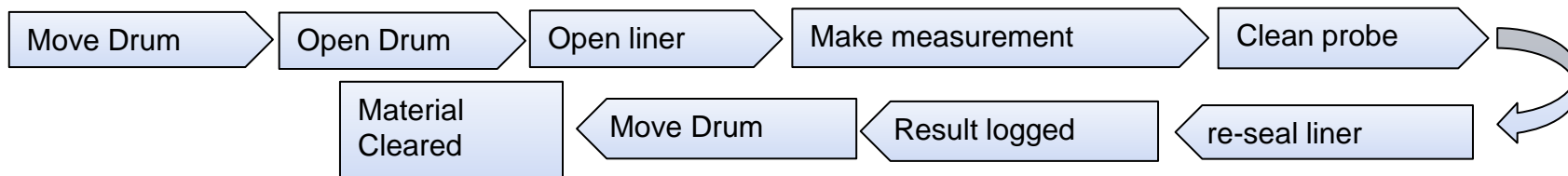
Operational Overview

ACM2 Pharmaceutical Raw Materials Testing: Methods

Traditional Laboratory Sample Analysis



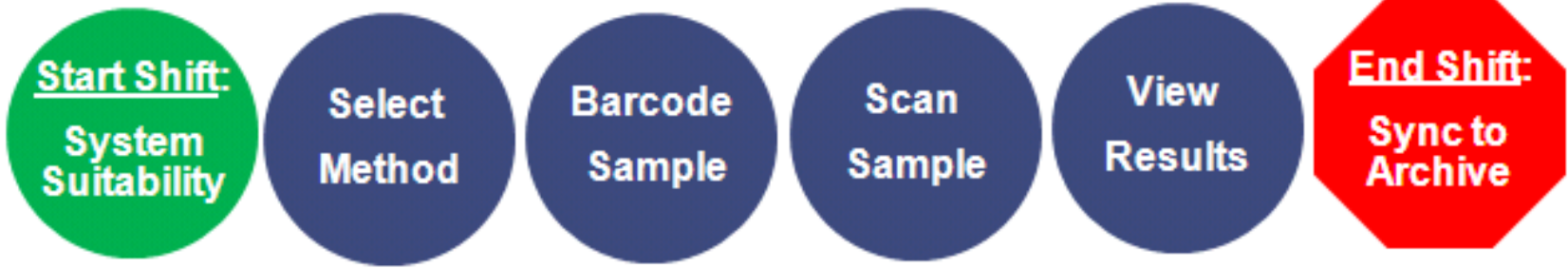
Analysis in "Clean room" by NIR, FT-IR with probes



On-spot analysis by Handheld NIR



ACM2 The microPHAZIR Rx workflow streamlines RMID



microPHAZIR RX reduces sample cycle times to seconds

ACM2 microPHAZIR Rx Attributes



- Portable
- Simple – Fast – Accurate
- Extremely Robust
- Operate in any environment

Direct Methods Transfer

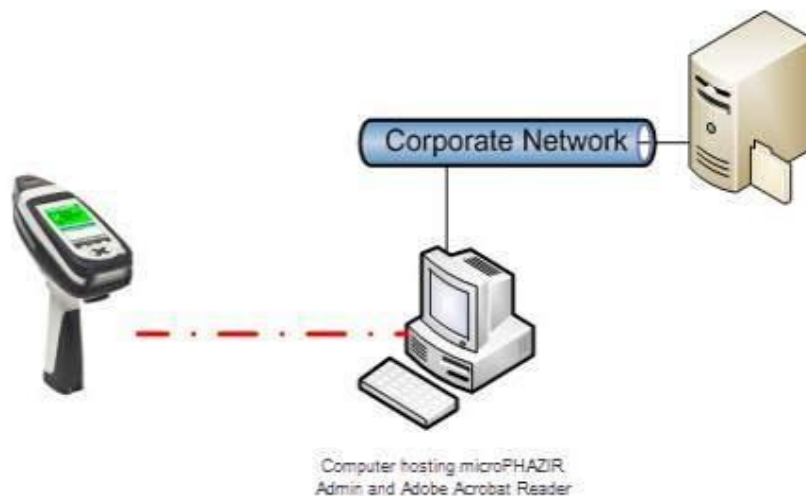
- Digitally tuned
- Highly repeatable CMOS MEMS Chips

Flexible

- Quantitative
- Qualitative
- Turnkey Applications

ACM2 Flexible Network Arrangements

- 2 network arrangements for fleet management, system configuration save, files transfer
 - Refer to User Guide and IT Memo for more detail.

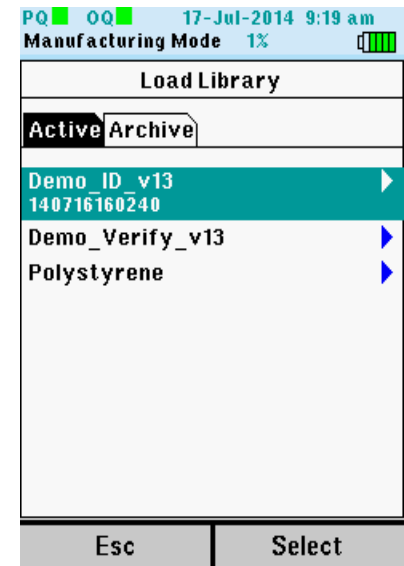
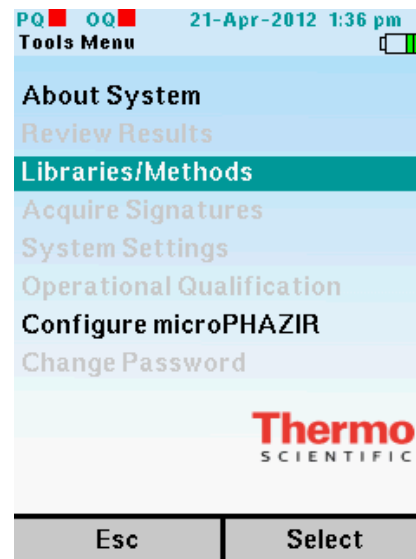
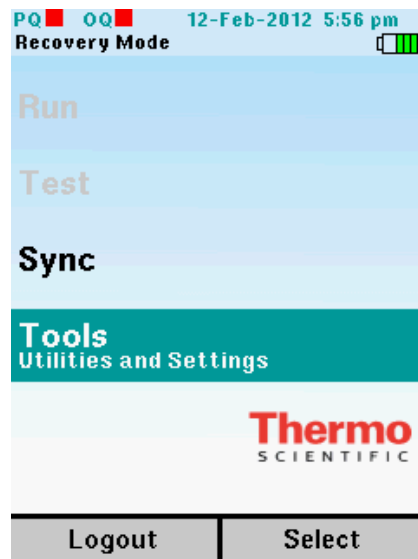
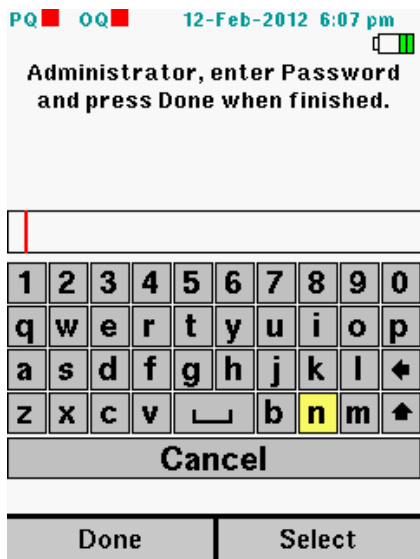


ACM2 microPHAZIR 4.0: Recovery Mode

Recovery mode is active anytime an instrument is upgraded, a Library is not selected or a software issue arises. This feature will allow a representative to provide assistance if an issue arises.

1. Log into instrument as an Administrator (factory password is **default**)
2. If Recovery Mode is active, Go to **Tools > Libraries / Methods** and select the **Demo_Verify** default Library or any other active library

NOTE: If an instrument was upgrade, perform a new **Calibrate Reference** after the upgrade is complete, go to **Tools > Configure microPHAZIR > Calibrate Reference** utilizing the white reference

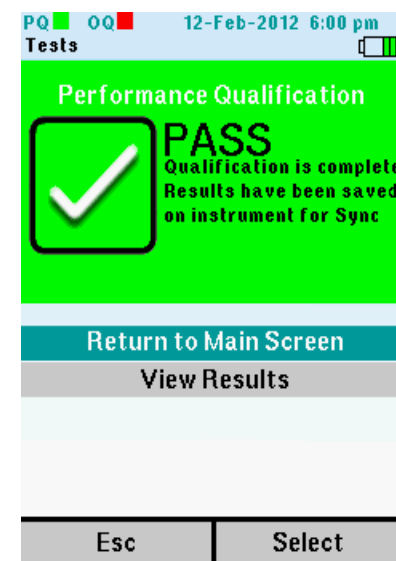
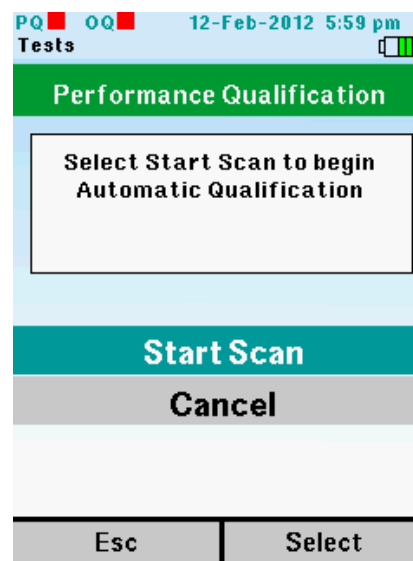
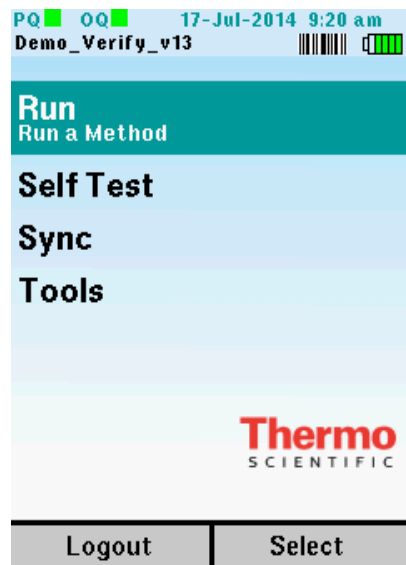


ACM2 microPHAZIR 4.0: Self Test

Self Test is the instrument performance qualification (PQ). No external references are required.

1. Select **Self Test** from Main Menu
2. Select **Start Scan** to begin Performance Qualification
3. Select **Esc** to return to Main Menu

NOTE: PQ and OQ files default location is C:\Thermo\Data\ARCHIVE\DDMMYY\Reports



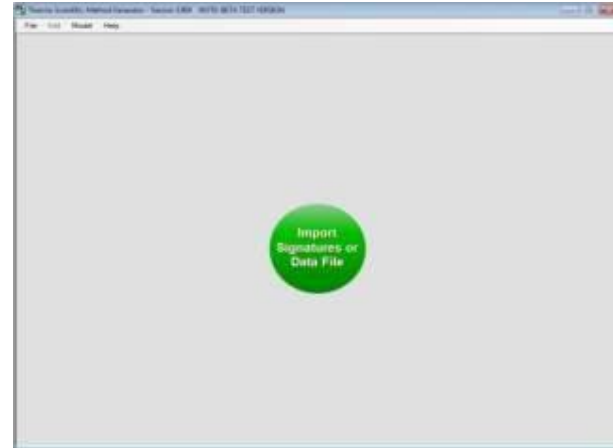
ACM2 microPHAZIR RX Method Building Process: overview

1



Acquire reference data

2



Create Library

3



Add library

ACM2 Organize your samples

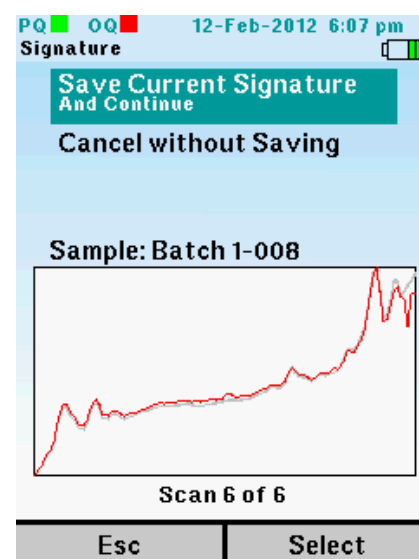
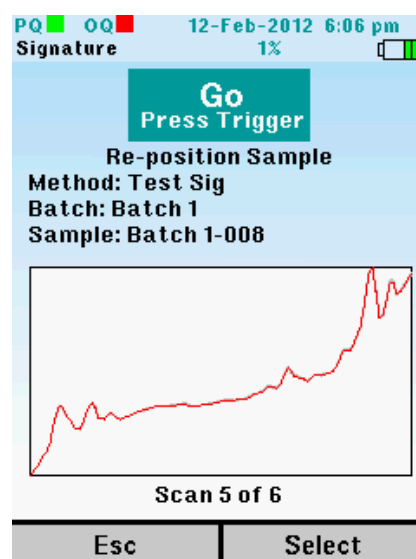
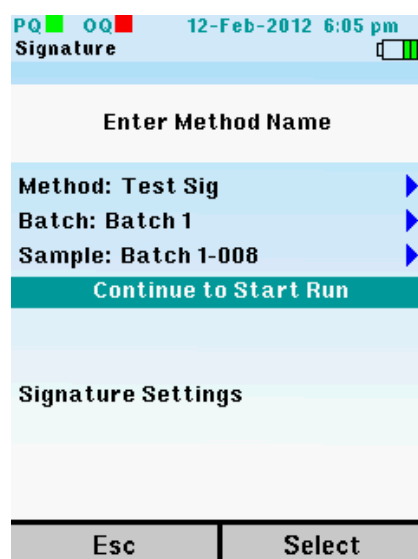
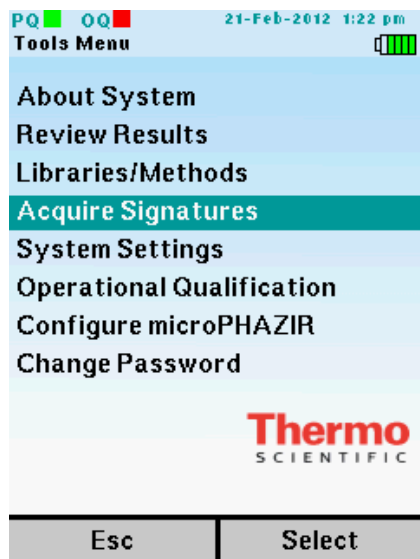
We recommend:

- Minimum 5 Lots of material for each sample
- Use plastic bags or glass vials
 - 4 mil plastic bags work well
 - Use flat bottom glass vials



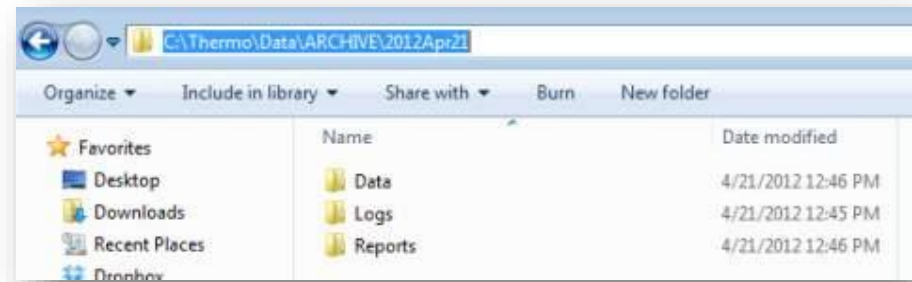
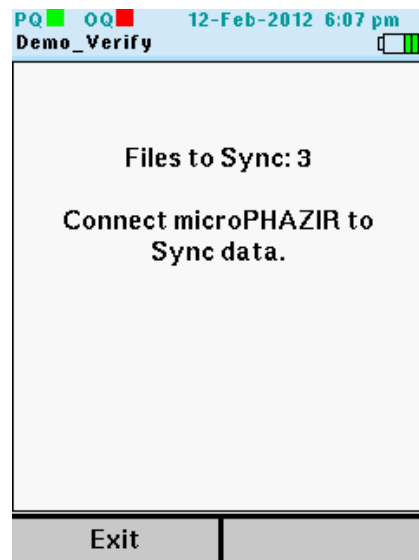
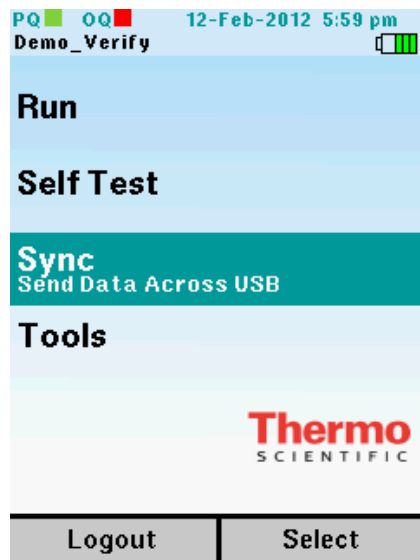
ACM2 microPHAZIR 4.0: Signatures

1. Select the **Tools** menu
2. Scroll down to **Acquire Signatures**
3. Enter a **Method** name or scan sample barcode (Batch and Sample information can be entered but not required)
4. Select **Continue to Start Run**
5. Place sample on nose and press the trigger to begin signature collections
Note: Each method (sample) requires at least 3 scans to ensure proper method development
6. Select **Save Current Signature**
Note: Signatures will transfer during Sync
7. Press **Esc** to exit Signature collection



ACM2 microPHAZIR 4.0: Sync Data

1. Select **Sync** from Main Menu
2. Connect microPHAZIR to computer via USB
3. Data is copied to C:\Thermo\Data\ARCHIVE\2012MMMDD (where MMM=Month 1st 3 letters, DD=Day 2 digit of the demo e.g. 2012Dec10)



ACM2 microPHAZIR 4.0: Building a Method

Signatures must be collected before the following steps can be executed

1. Select the **Sync** and connect microPHAZIR to computer to transfer previously acquired Signature files to computer

Note: Signature files are saved to the Thermo/Data/ARCHIVE/Data location by default

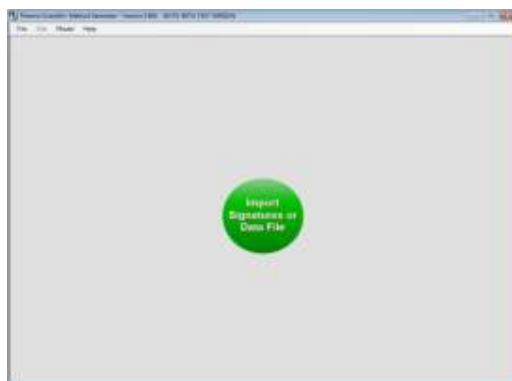
2. Launch Method Generator 

3. If easy mode is active, select the Green button, or Go to File > Open Data file in Advance mode

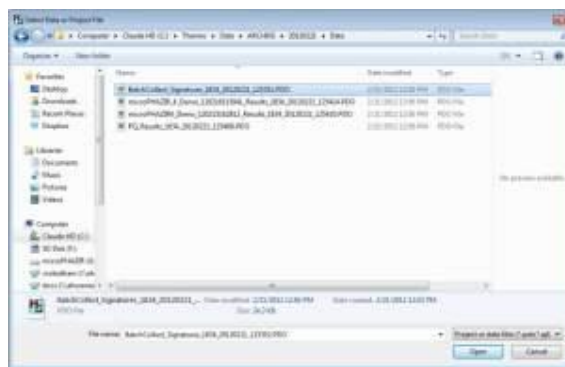
Note: Easy mode will create a Verify method (Pass/Fail), Advanced mode allows you to create Identify and PLS methods

4. Select the Signatures file (e.g. Signatures-9999-20120415-100557.PDO)
5. Method Generator will automatically create a new application library
6. Name the new method

Note: New Libraries/Methods are C:\Thermo\Data\Method Generator\Applications with a .pps extension



Press green icon to import signatures



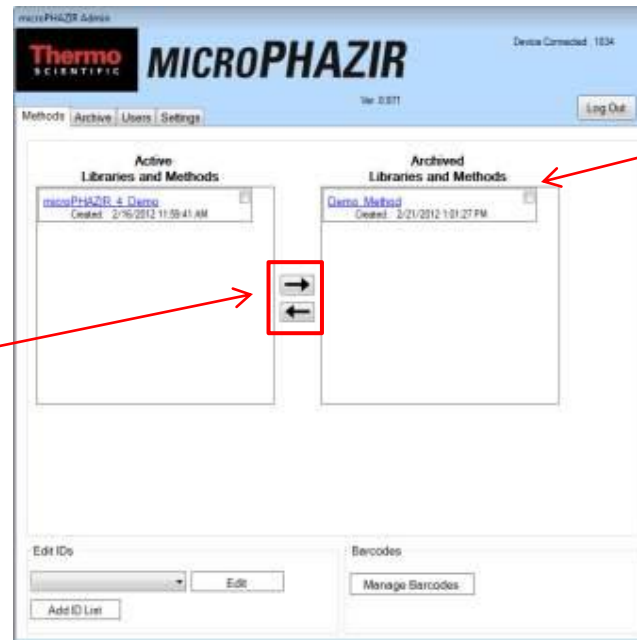
Import a signatures file from
C:\Thermo\Data\Method Generator\Applications



ACM2 microPHAZIR 4.0: Adding New Methods/Libraries

1. Disconnect the microPHAZIR from the computer
NOTE: Make sure the new Library or application .pss file is copied to C:\Thermo\Data\Method Generator\Applications folder
2. Select the **Tools** menu on the microPHAZIR
3. Scroll down to **Configure microPHAZIR**
4. Select **Configure with Libraries**
5. Connect microPHAZIR to computer via USB cable to launch microPHAZIR Admin
6. Select a Library or Method from the Archived side and then use the arrows to move file(s) to microPHAZIR
7. Log Out and disconnect from USB

Use arrows to add or remove files from microPHAZIR



Select file(s) located on PC

Select file(s) located on PC
NOTE: The default PC Archived Libraries and Method location is C:\Thermo\Data\Method Generator\Applications . Place all Libraries, Applications, and Methods in this location to view them in microPHAZIR admin.

ACM2 microPHAZIR 4.0: Run a Method

1. Select **Run** or scan a barcode to start a method/sample collection

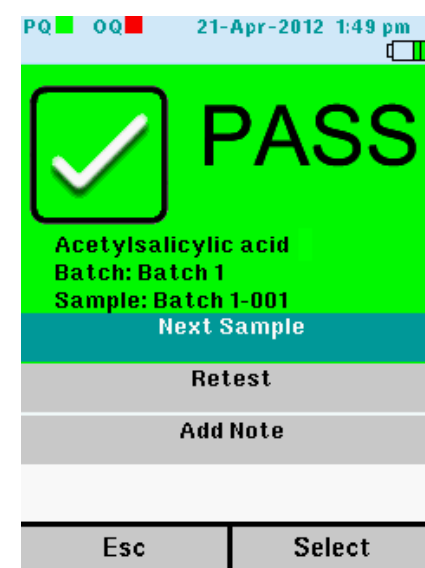
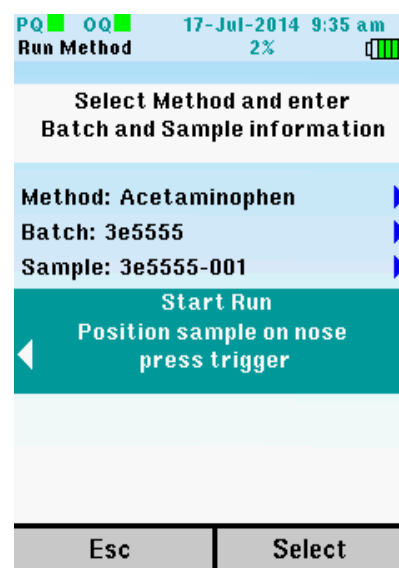
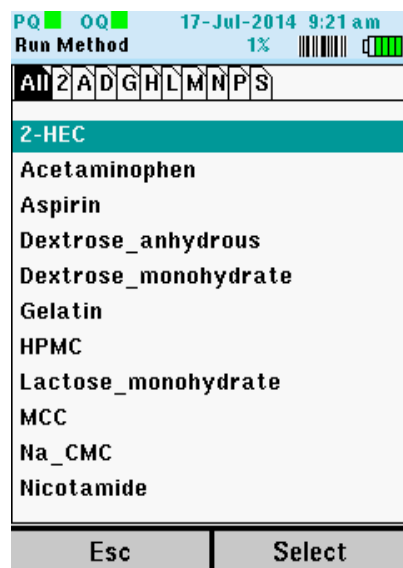
NOTE: Methods can be activated directly from the Run menu by scanning a barcode. The barcode icon (|||||) indicates the barcode reader is active when trigger is pressed

2. Press **Select softkey** to chose a Method

3. Enter Batch or Sample information if available

4. Position sample on nose and select **Start Run** to begin sample collection

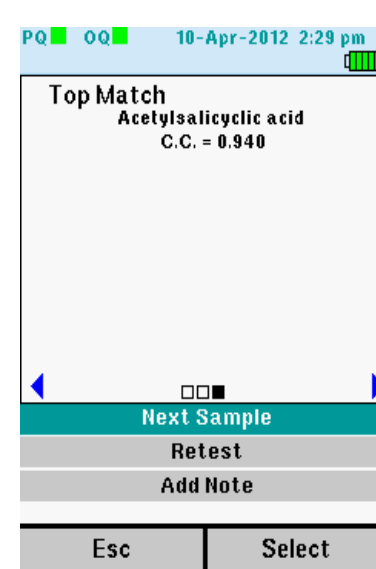
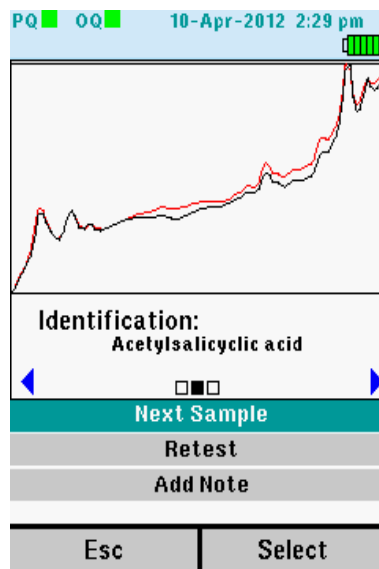
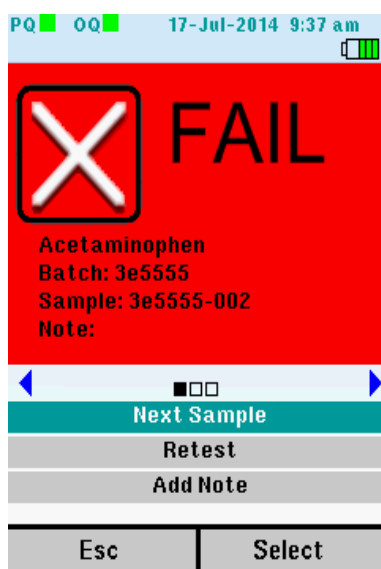
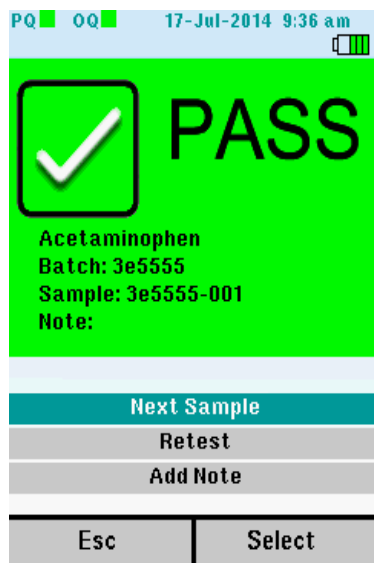
Note: To scan a new background, press the right arrow softkey when Start Run is highlighted



ACM2 microPHAZIR 4.0: Discovery Result

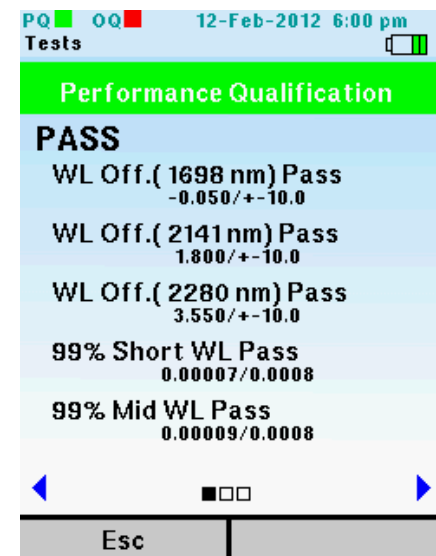
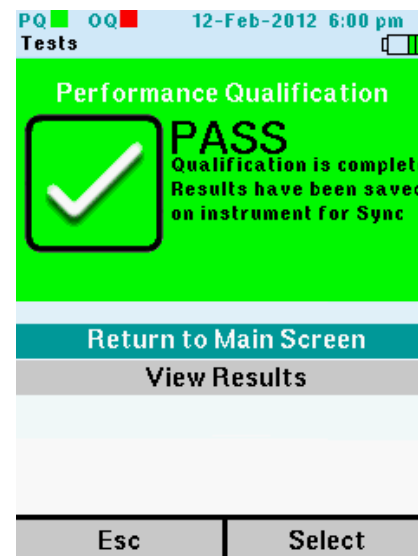
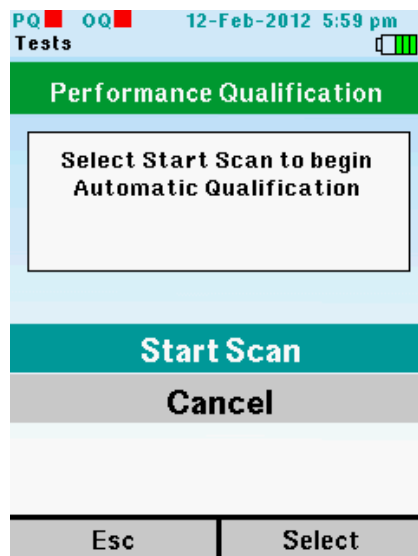
If the selected method (sample) matches library method then a PASS result is displayed. If a method fails, a FAIL result is displayed and discover mode is automatically activated. The results of the discover search can be viewed.

1. To view the discover library search result, press the **Right softkey**
2. To view the top match press the **Right softkey** again
3. Select Next Sample or Retest to continue scanning methods or Esc softkey to return to Main Menu
4. These results are stored with the run and will appear on the reports



ACM2 microPHAZIR 4.0: Performance Qualification

1. Select **Self Test** from Main Menu
2. Select **Start Scan** to begin Performance Qualification
3. Select **View Results** to see performance details
Note: Use left and right arrow buttons to view all test results
4. Sync to view Qualification report



ACM2 microPHAZIR Admin: Archive, Logo and Export settings

1. Choose a local PC folder or mapped network drive folder to Archive all Data, Reports and Logs
2. Change report logo
3. Select 'Export Configuration' settings for deployment to other microPHAZIR instruments

The screenshot displays the Thermo Scientific microPHAZIR Admin V4.2 web interface. The top navigation bar includes 'Methods', 'Cal Files', 'Data', 'Users', 'Settings', and 'Support'. The 'Settings' tab is active, showing the following configuration options:

- Archive Destination:** A text field contains 'C:\Thermo\Data\ARCHIVE\'. Below it are 'Browse...' and 'Default' buttons. Example text above the field reads: 'Example: "C:\Thermo\Data\" or a mapped network drive'.
- File Formats:** Two sub-sections are visible: 'Reports' and 'Data'. Under 'Reports', 'PDF' and 'PNG' are checked. Under 'Data', 'TXT' and 'PDO (microPHAZIR internal format)' are checked.
- Report Logo:** A preview of the Thermo Scientific logo is shown. A 'Browse...' button is located below the preview.
- Export Configuration:** A section with several unchecked checkboxes: 'Libraries/Methods (includes ID lists)', 'Barcodes', 'Archive Settings', 'Users', and 'System Settings (includes security and OQ PQ)'. An 'Export' button is positioned below these options.
- Import Configuration:** A section with an 'Import' button.

Additional interface elements include a 'Logout' button in the top right corner and system information: 'Device Connected: MP1834', 'FW Version: 4.2 15219', 'Device Type: RX', and 'Admin Version: 4.2.15232'.

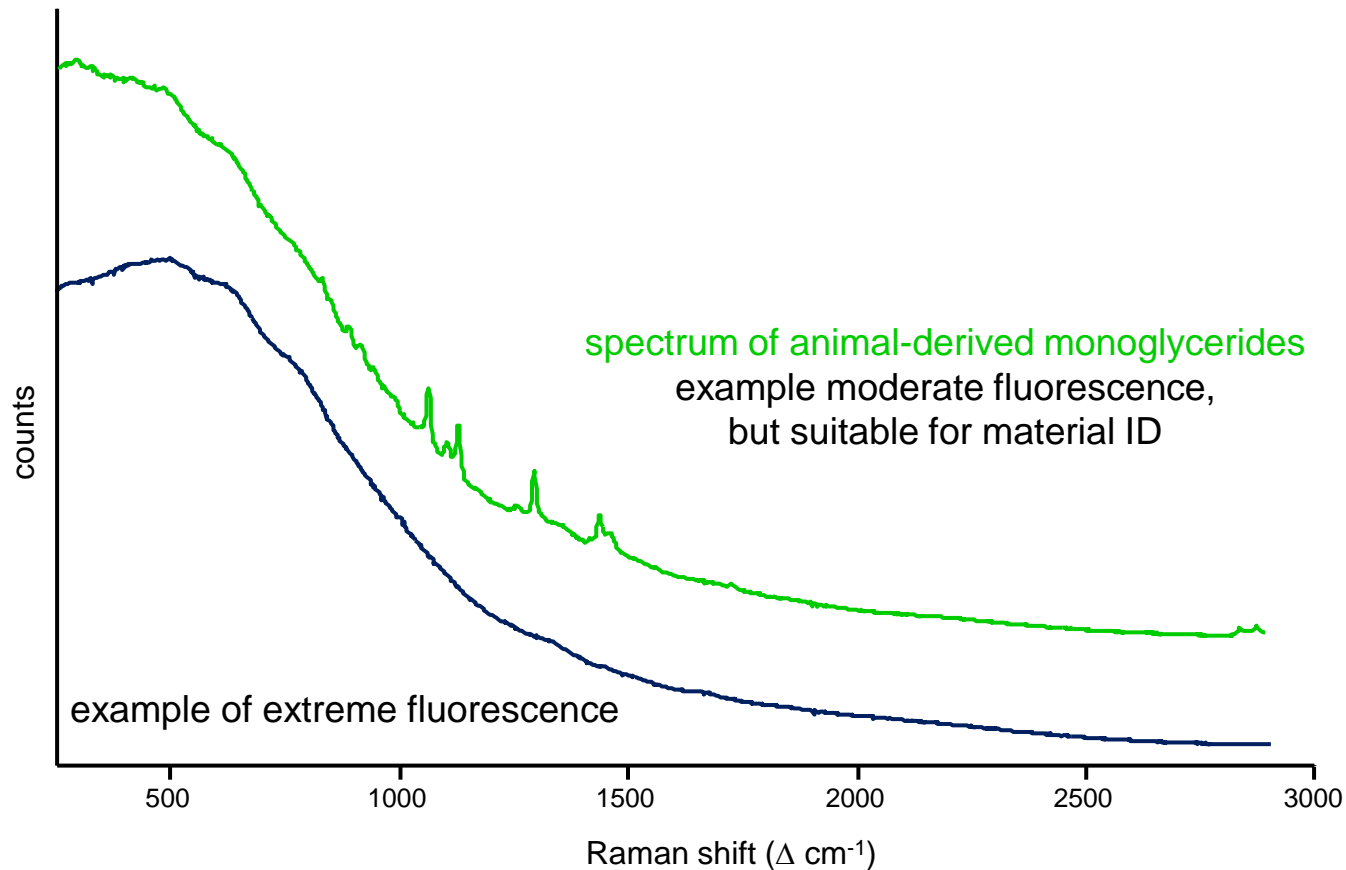


ThermoFisher
S C I E N T I F I C

TruScan RM

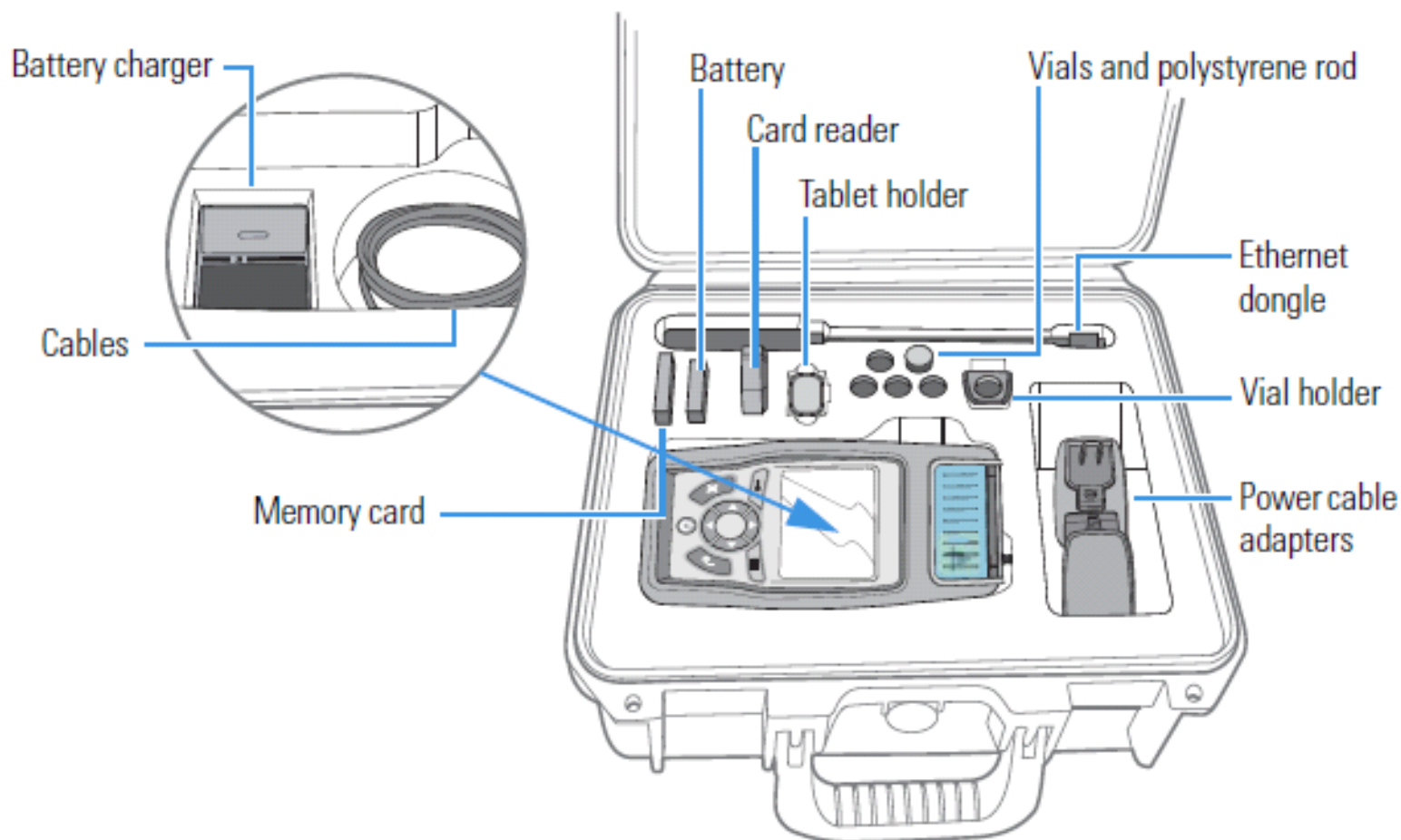
ACM2 Fluorescence

Fluorescence is an additional source of noise, and if present, will slow down the data acquisition



in extreme cases. fluorescence can prohibit data acquisition

ACM2 What is in the carrying Case?

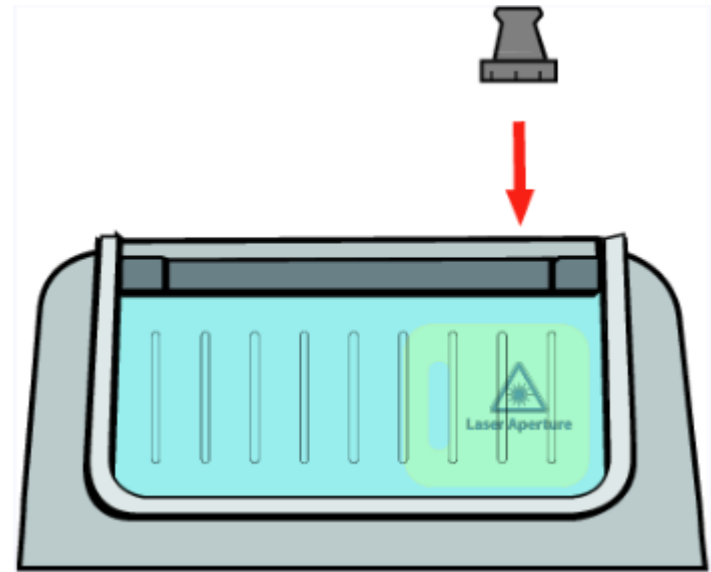
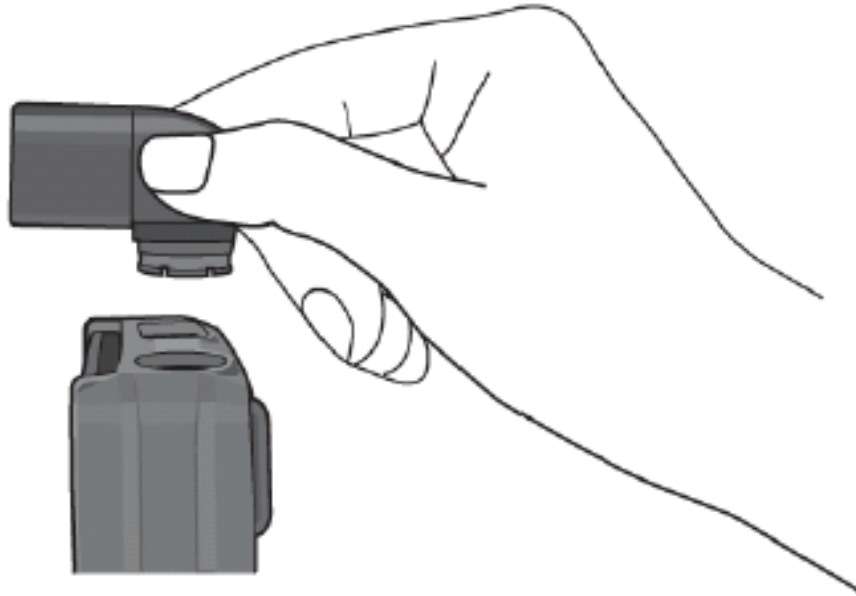


ACM2 TruScan RM



ACM2 Attaching the Accessories on the Laser Aperture

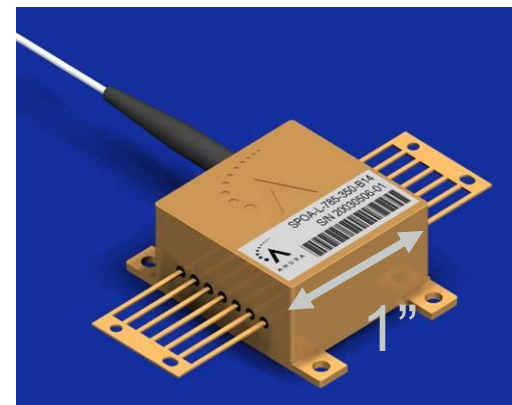
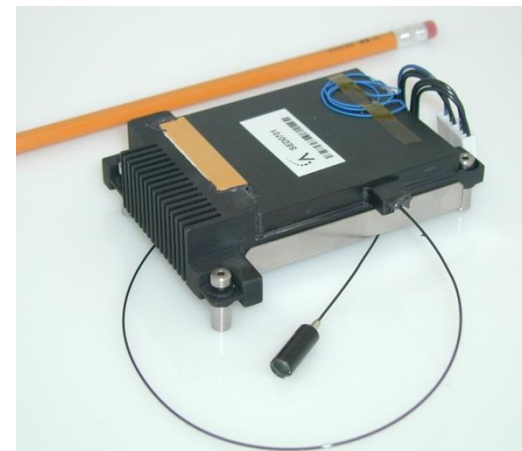
- All accessories for TruScan RM are snapped on type attachments



- Align the desired accessory with the laser aperture of the instrument and press the accessory until it is firmly seated
- Accessory should be aligned with the nose of the instrument and the laser aperture labels

ACM2 TruScan RM Analyzer Spectrometric Specifications

technique	Raman spectroscopy
spectral range	250 – 2875 Δ cm^{-1}
resolution	8-10.5 cm^{-1} max
excitation λ	785 +/- 0.5 nm
output power	250 mW +/- 25mW
laser linewidth	~3 cm^{-1} FWHM
exposure options	AUTO (12 ms minimum)
detector	2048 element silicon CCD, TE cooled
spectrometer	single-pass dispersive
probe working d	18 mm
spot size	2-2.5 mm
OS/SBC	Windows CE embedded; intel 400MHz
data analysis	in-house custom development
GUI/architecture	in-house custom development
display/output	integrated color LCD; CF card data export



ACM2 Fingerprint Enrollment

- User account must be set up for fingerprint login in WebAdmin
- Users must login into his/her account and go to Password

Tools - Menu 14:26 03-Dec-2010

About System
Change Password

Register Fingerprint 14:25 03-Dec-2010

To register fingerprint, press Start, then swipe finger 3 or more times over the fingerprint

Register Fingerprint 14:27 03-Dec-2010

Swipe finger 3 or more times.

Tools - Menu 14:27 03-Dec-2010

About System TruScan RM v2.0.0

Fingerprint registration is complete.

Press any key to continue.

Main Menu

Authentication Method

Self Test/PQ

Data Transfer

Settings/Tools



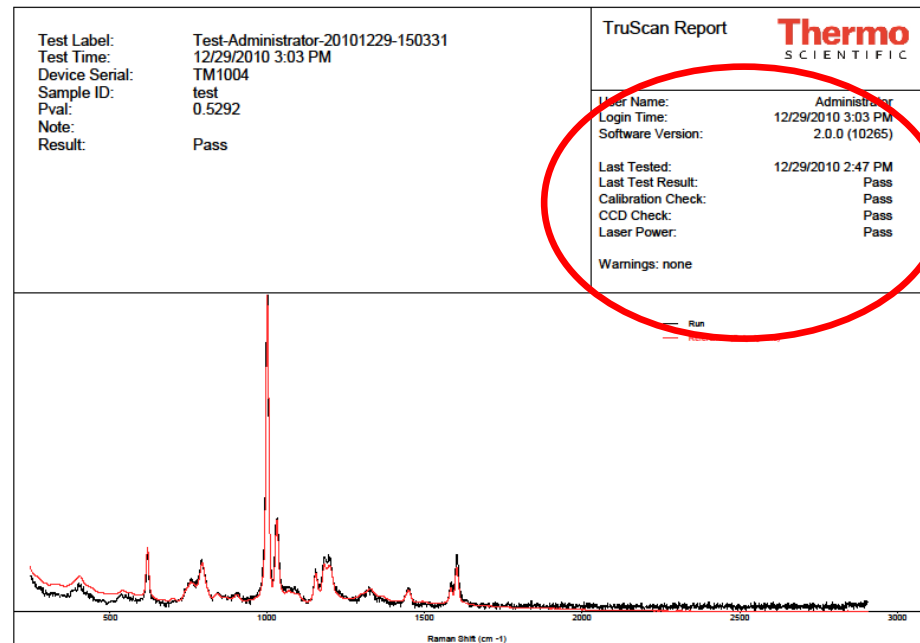
ACM2 Routine System Suitability Testing

- Flexibility for Routine Testing with five ASTM E 1840 standards :
 - Acetaminophen
 - Benzotrile
 - Cyclohexane
 - Polystyrene
 - Toluene
- ASTM Standards easily source from suppliers like Sigma-Aldrich®
- Certificate of Analysis (CoA) of ASTM Standards supplied in the user manual
- Standards can be changed in the WebAdmin Interface

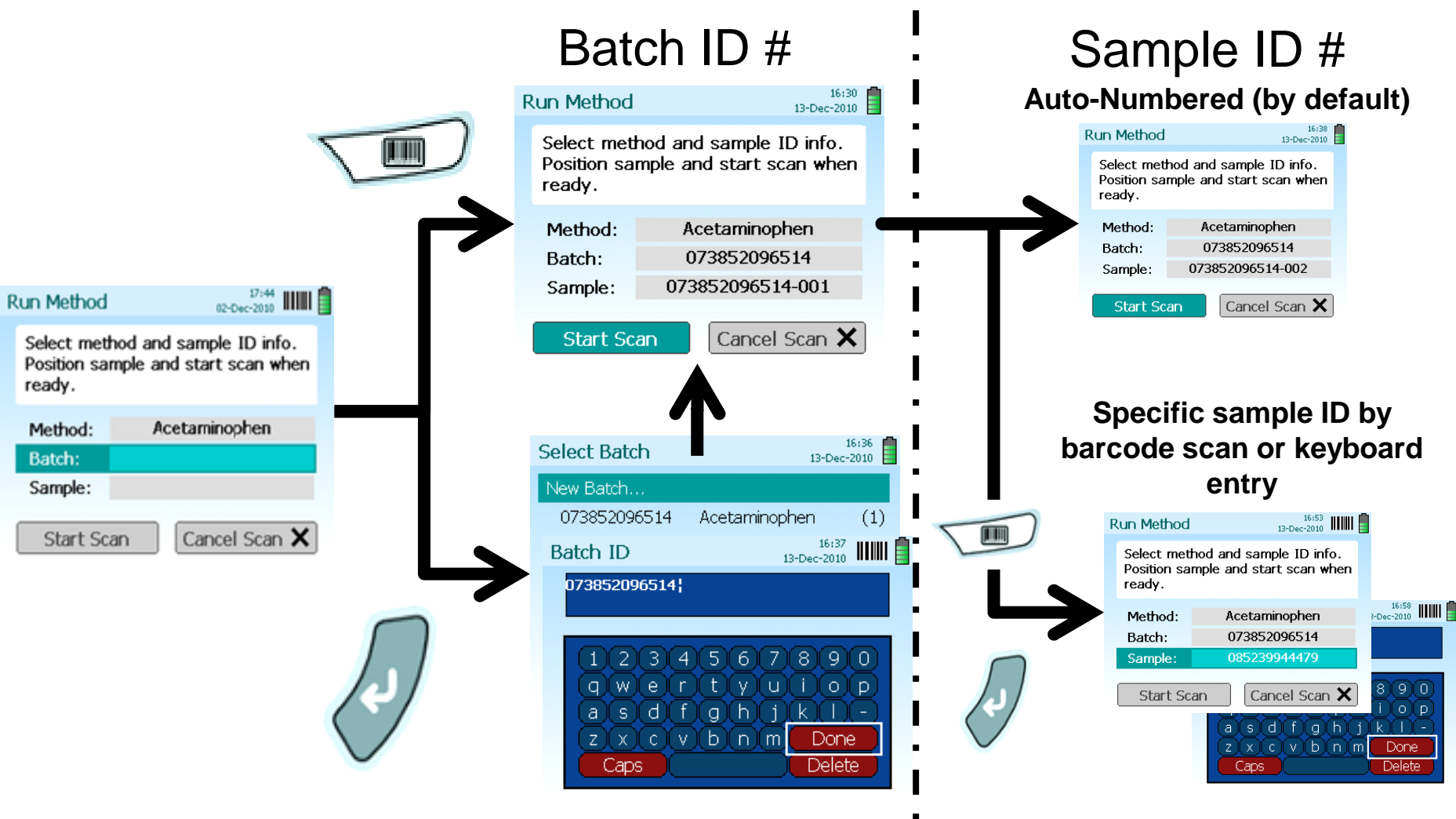
ACM2 Self Suitability Test Function

- Fast daily check of instrument's proper working order
- Can use Polystyrene, Acetaminophen, Toluene, Cyclohexane, or Benzonitrile (selected in WebAdmin)
- System self-suitability results found on every report

The screenshot shows the ACM2 self-test interface. At the top, it says "Test - Position Sample" with a timestamp of 14:46 on 29-Dec-2010. Below this is a blue bar labeled "Self Test". The main instruction is "Attach vial holder and insert test standard:". A "Scanning" window is overlaid, showing "Scan in progress..." and a warning: "Hold unit still, at arm's length away from eyes, for safety!". Below the scanning window, a green bar displays a checkmark and the word "Pass", with a "test" label and a "T" icon. A "Note:" field is empty. At the bottom, there are two buttons: "Repeat Test" and "Main Menu".




ACM2 Batch Runs: Run identified by Batch # and Sample ID



Scans results with common Method and Batch ID # will be summarized in a single batch report

ACM2 Next, Re-Test Functions

Run-Administrator-20101... 17:06 13-Dec-2010

 **Pass**
Acetaminophen
Batch: 073852096514
Sample: 073852096514-005


Note:

Run Method 17:06 13-Dec-2010

Select method and sample ID info.
Position sample and start scan when ready.

Method:
Batch:
Sample:

Run-Administrator-20101... 17:07 13-Dec-2010

 **Fail**
Acetaminophen
Batch: 073852096514
Sample: 073852096514-006

Note:

Run Method 17:07 13-Dec-2010

Select method and sample ID info.
Position sample and start scan when ready.

Method:
Batch:
Sample:

Tools Menu

System info

Review runs and Discover

Methods Library

Signatures Library

Signatures (References) acquisition

Settings (Network, Date)

Remote Certification

Password change



Thermo
SCIENTIFIC

TRUSCAN RM

Tools - Menu

14:56

08-Apr-2012



About System TruScan RM v2.5.0

Review Results

Methods

Signatures

Acquire Signature

System Settings

Instrument Certification

Change Password





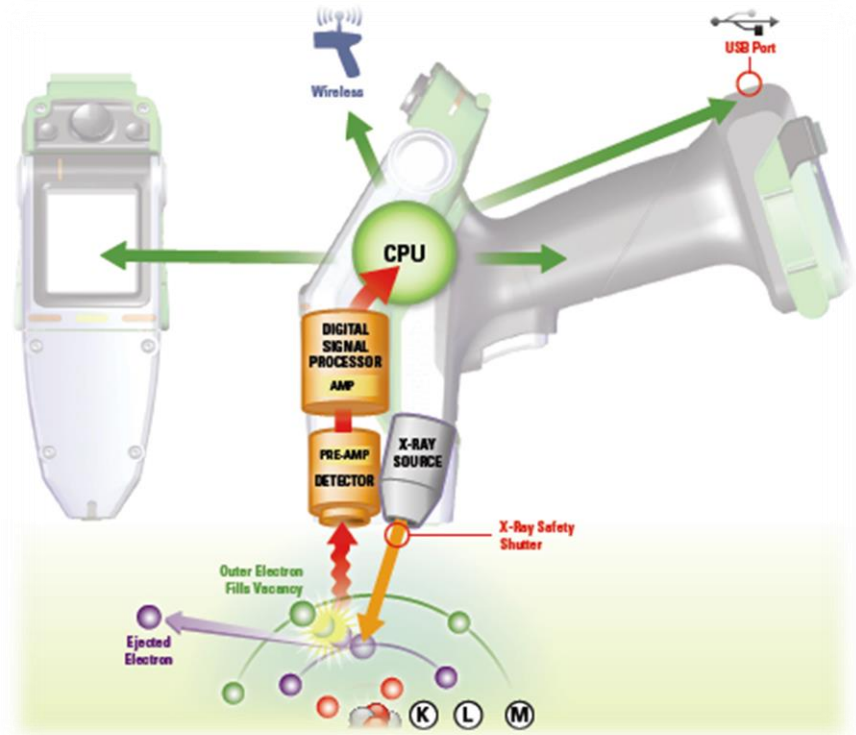
Raise the Bar

ThermoFisher
SCIENTIFIC

Portable Verification of Ionic Salts: Thermo Scientific IonicX

ACM2 XRF Technology

- X-ray tube emits radiation that strikes a sample's surface, exciting the sample.
- An electron is dislodged from each of the sample's atoms, emitting a characteristic x-ray fluorescence (photons).
- The emitted photons produce an electric signal in the detector; each sample molecule possesses unique spectral peaks.
- The resulting signal spectrum is processed in the central processor unit (CPU) and the elemental composition is calculated.



ACM2 IonicX Algorithm Selectivity

	NaCl	KCl	MgCl ₂	CaCl ₂	NaOH
NaCl	Green	Red	Red	Red	Red
KCl	Red	Green	Red	Red	Red
MgCl ₂	Red	Red	Green	Red	Red
CaCl ₂	Red	Red	Red	Green	Red
NaOH	Red	Red	Red	Red	Green

- The algorithm is currently built for **NaCl, KCl, MgCl₂, CaCl₂, and NaOH**

- ❑ The algorithm produces a correlation value (C-Val) between sample being tested (left column) and stored sample spectrum (top rows).
- ❑ This 'selectivity' test is to test against 'nearest neighbors' or chemicals that are similar in makeup to the target to ensure no false positives.

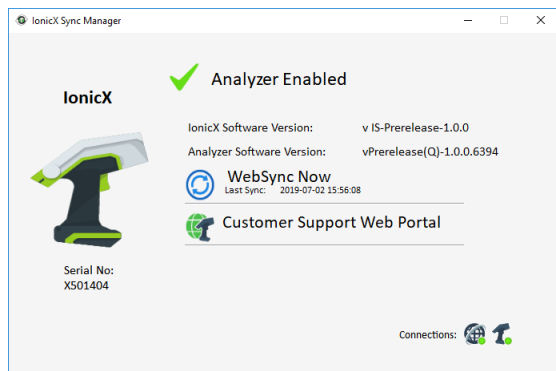
ACM2 Customer Benefits



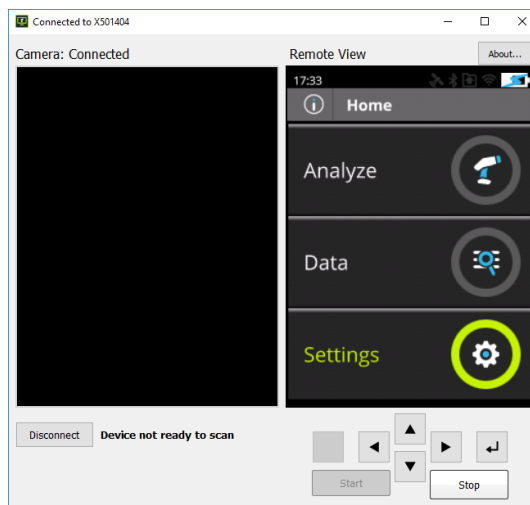
- ❑ Reduction in time associated with conventional laboratory testing
 - ❑ No transportation period, reduced test time, no quarantine period
- ❑ Reduction in associated cost
 - ❑ No additional chemical components necessary
- ❑ Complete accuracy in ionic salt verification
- ❑ Substantially reduced footprint, total portability

ACM2 IonicX Software Overview

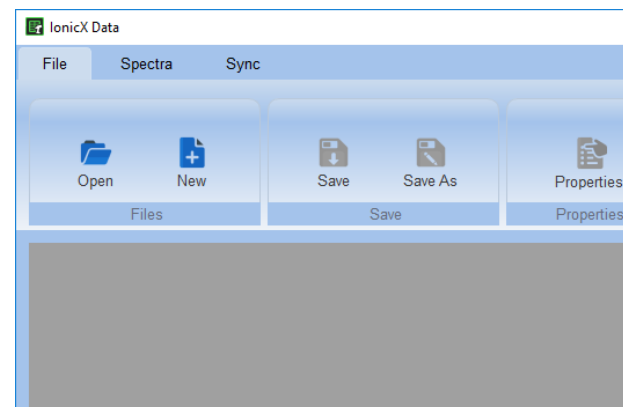
IonicX Sync
Manager



IonicX
Remote



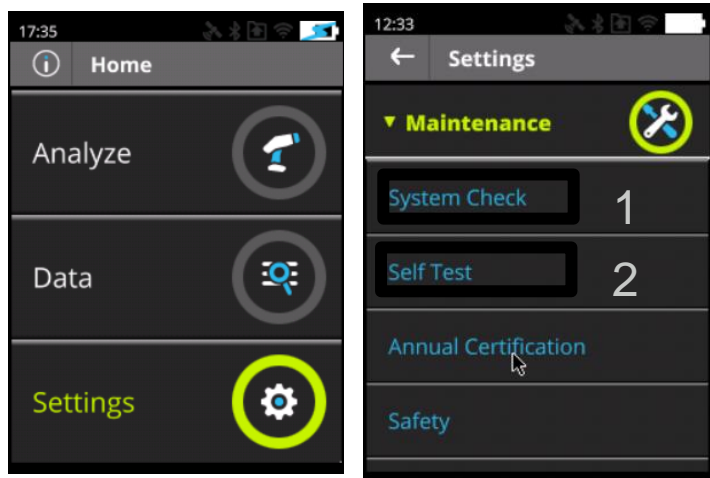
IonicX Data



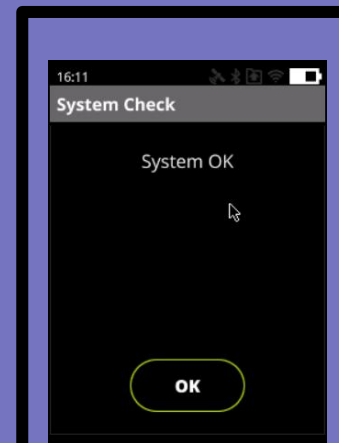
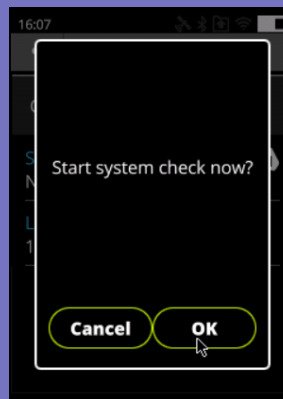
These three applications make up Thermo Scientific IonicX Software Suite

ACM2 System Check/Self-Test

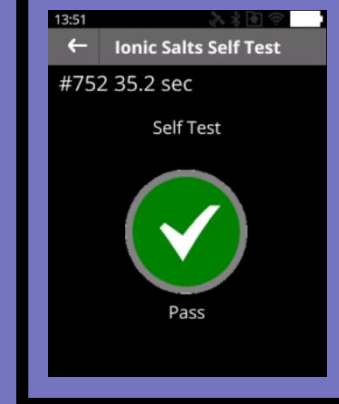
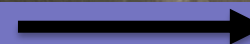
- Settings → Maintenance
- Recommended to be Run Daily
- Run System Check **then** Self Test
- 10.0% KCl fused bead from XRF Scientific



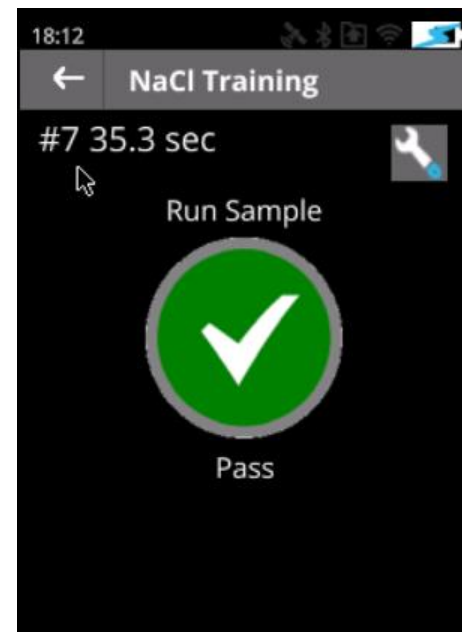
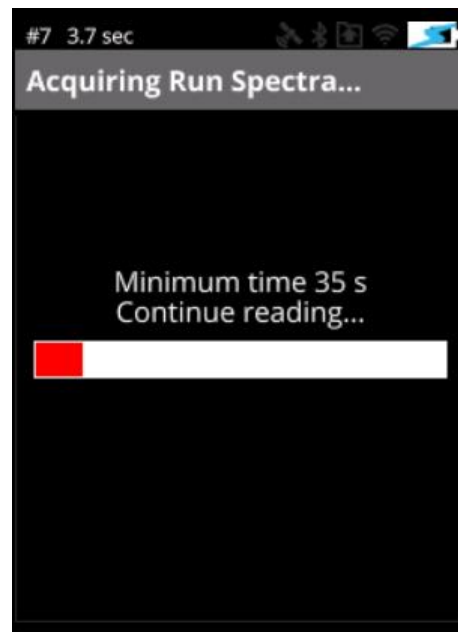
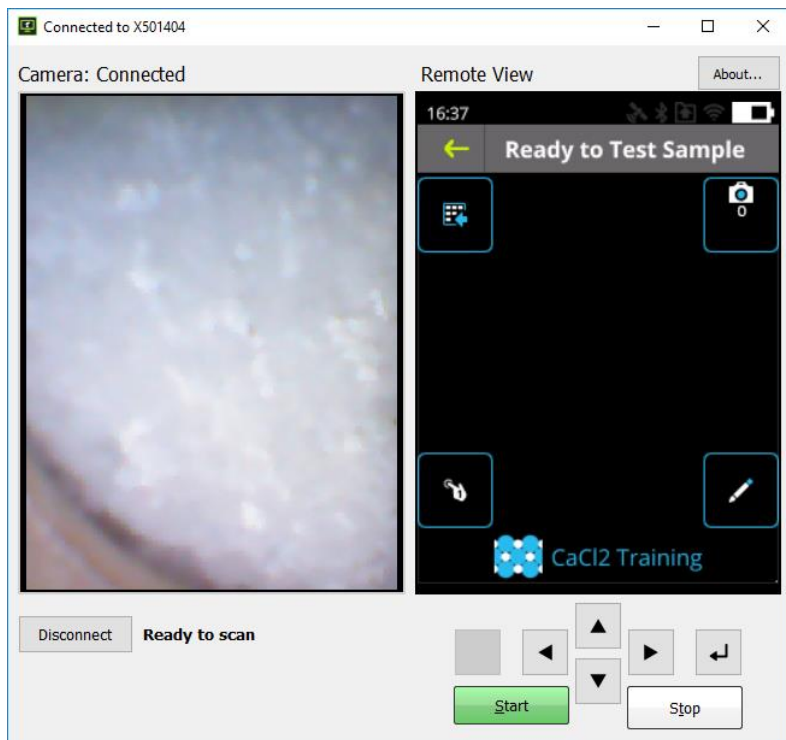
1



2

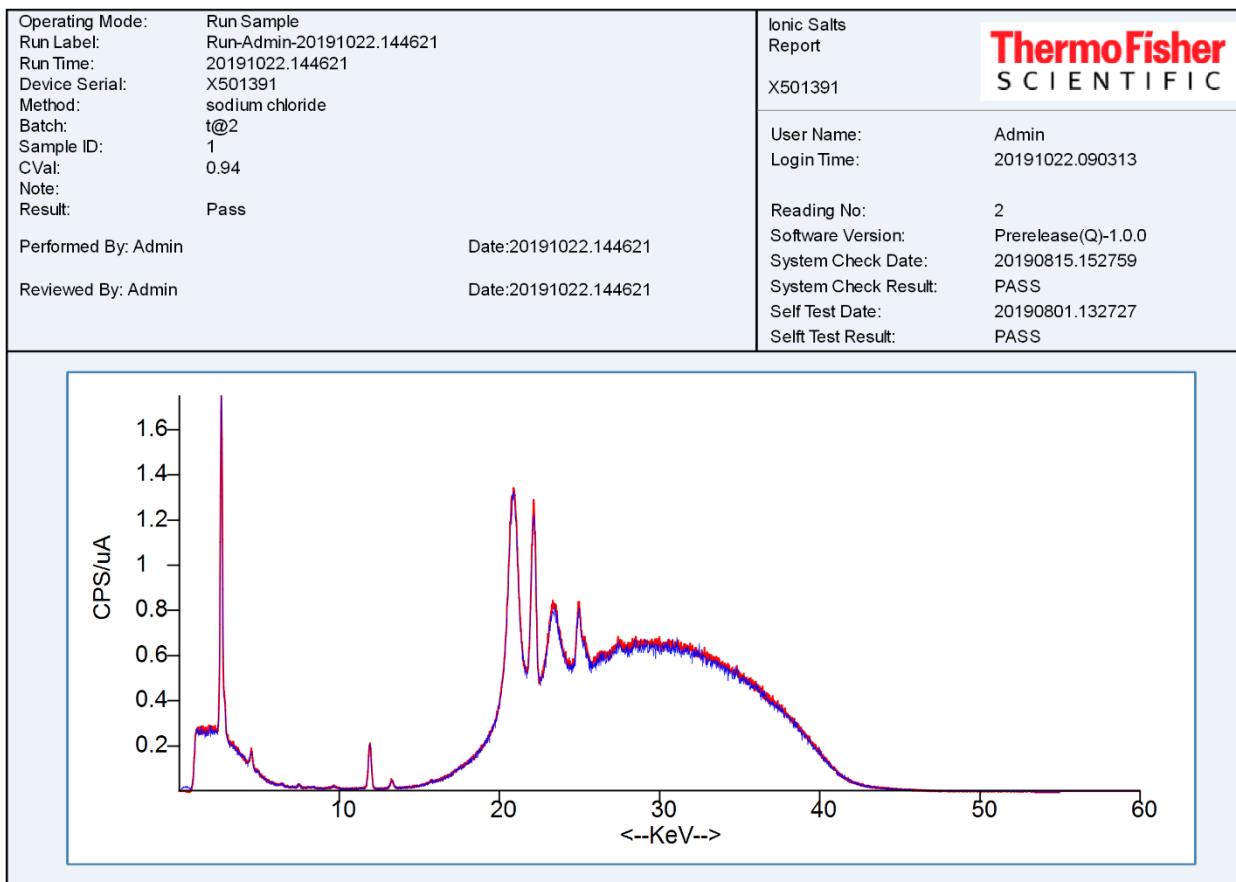


ACM2 Running Samples



All runs are 35 seconds: 5 seconds for the light filter and 30 for the main filter.

ACM2 Run_report (.pdf, .txt and .png files)-Pass Report





Ques