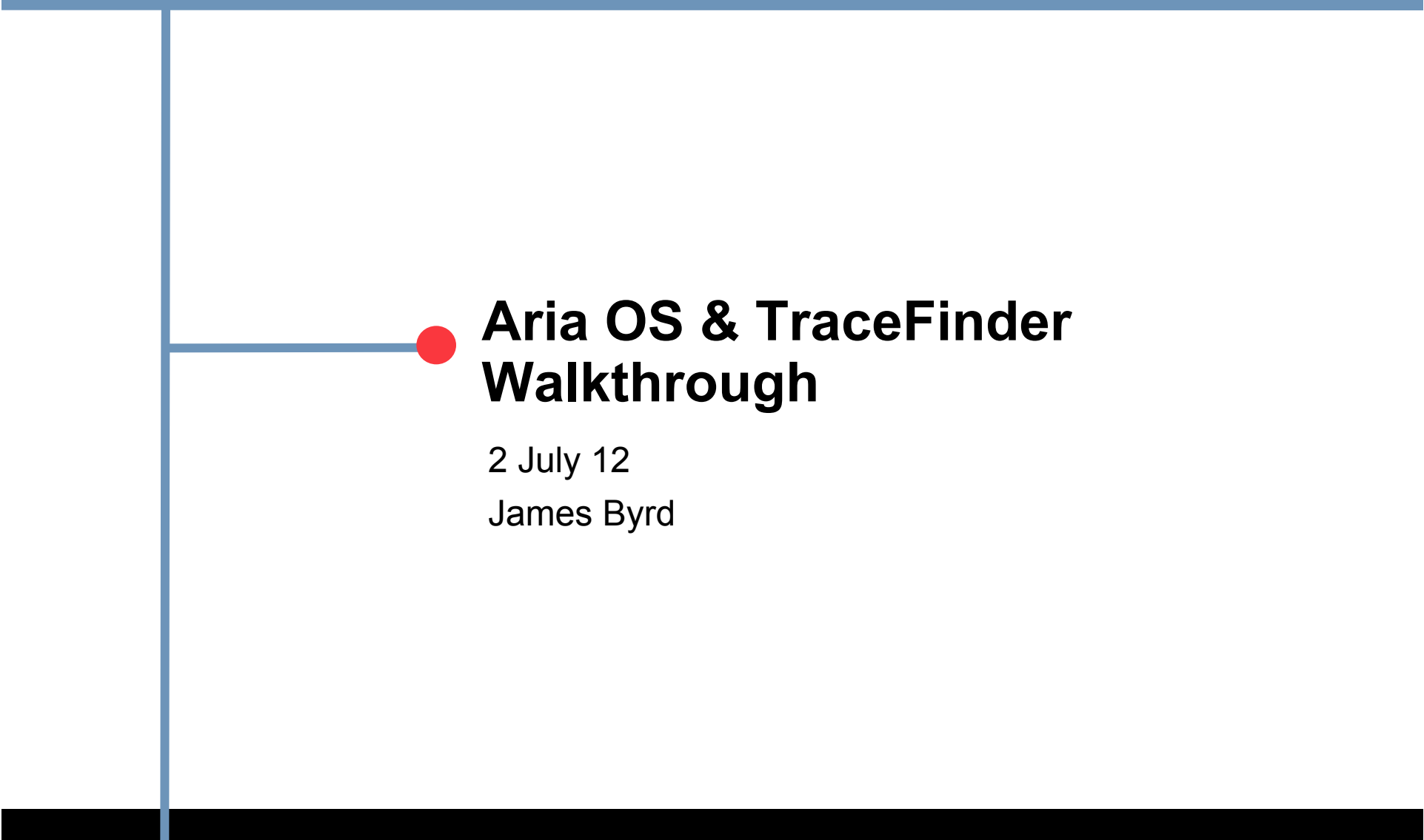




Aria OS & TraceFinder Walkthrough

2 July 12

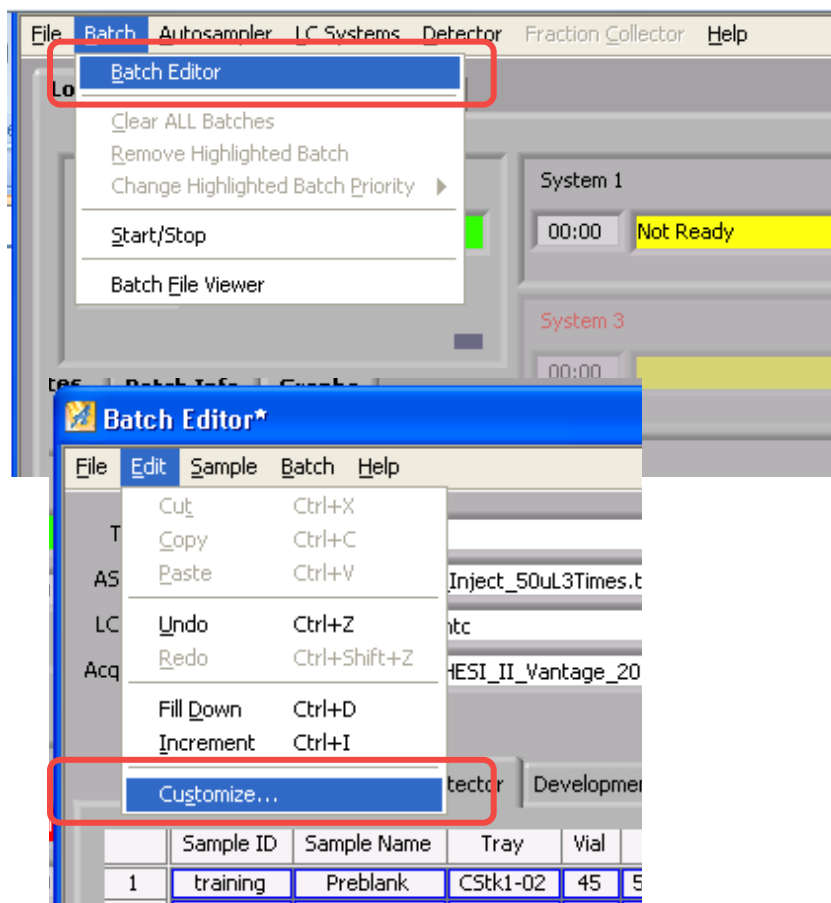
James Byrd

 The world leader in serving science

How to use this walkthrough

- The steps in this walkthrough will show you one way to use Aria OS and TraceFinder to acquire and process data
- Software components:
 - Aria OS 1.6.3f1– used for submitting samples for analysis
 - Xcalibur 2.2 sp1– runs the Mass Spec in the background
 - TraceFinder CT 2.0sp1– used for processing, after the run is complete
- The steps in this guide may be altered to suit your lab's needs

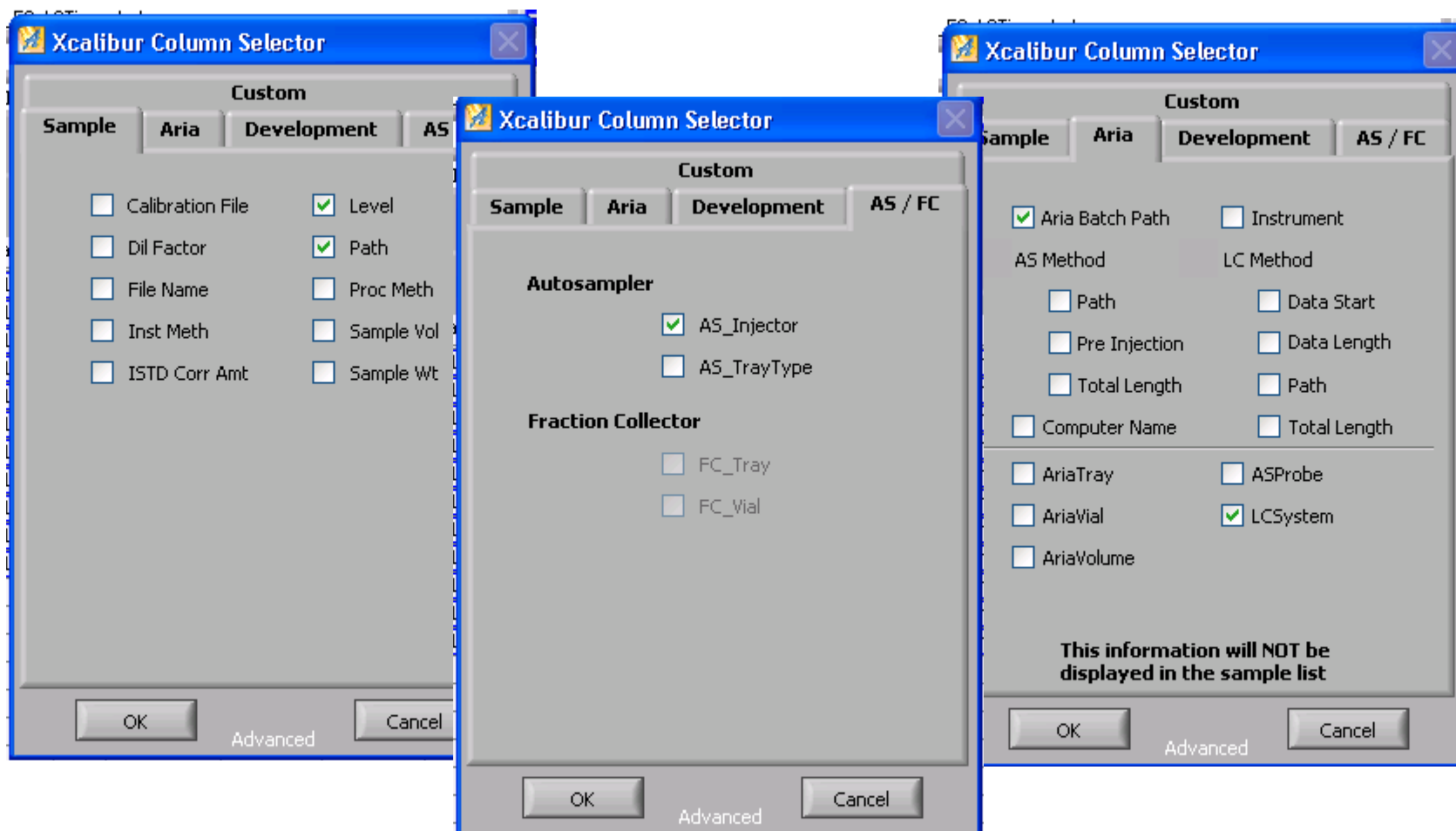
Creating a batch through Aria OS



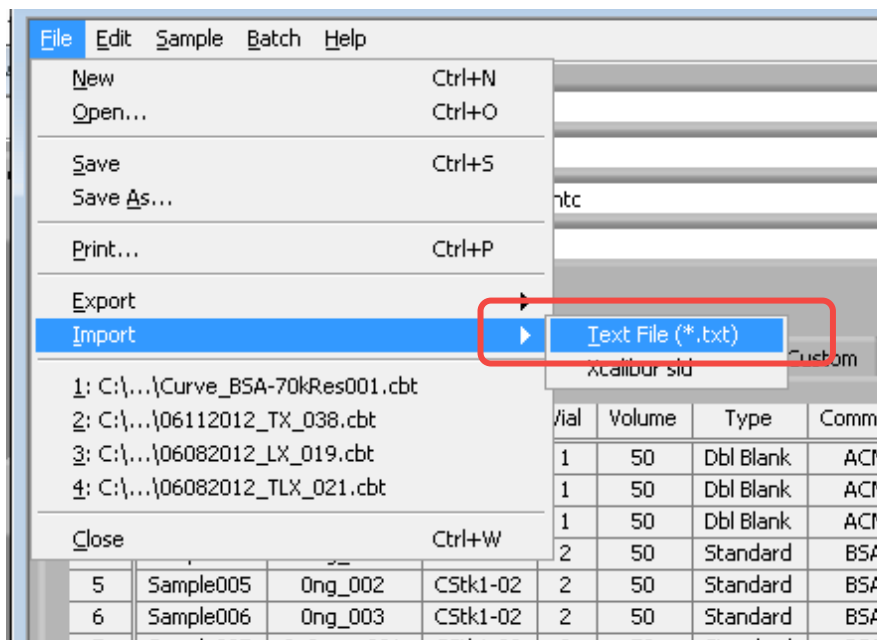
To configure columns

- Choose *Batch>Batch Editor>Customize*

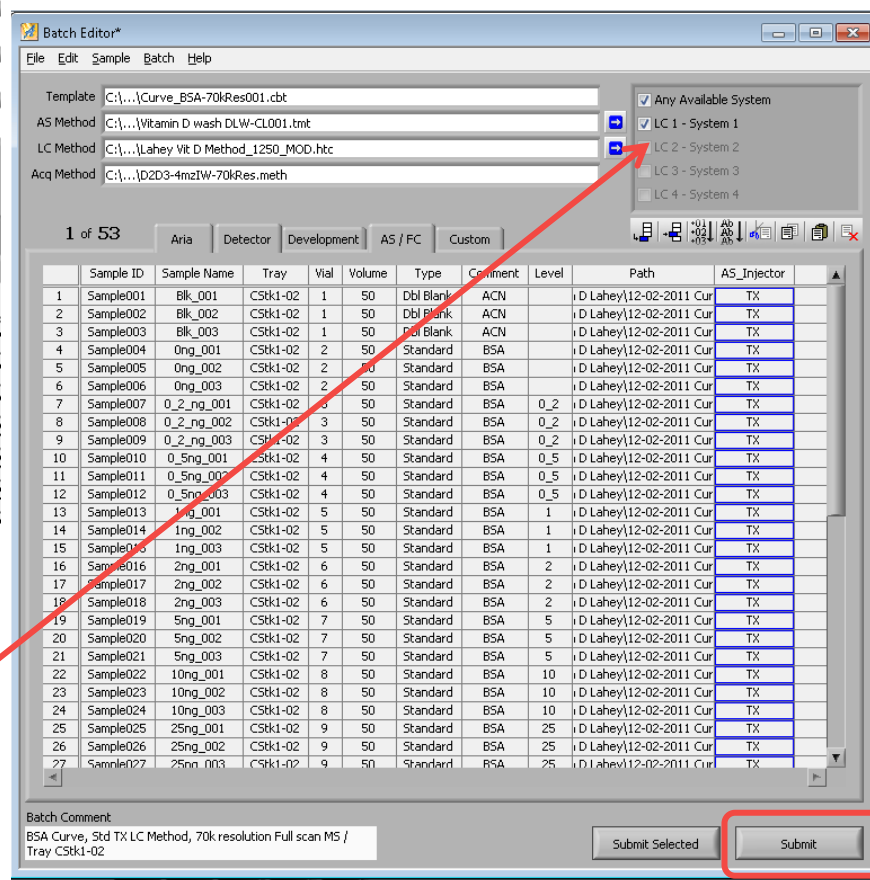
Recommended settings to configure columns



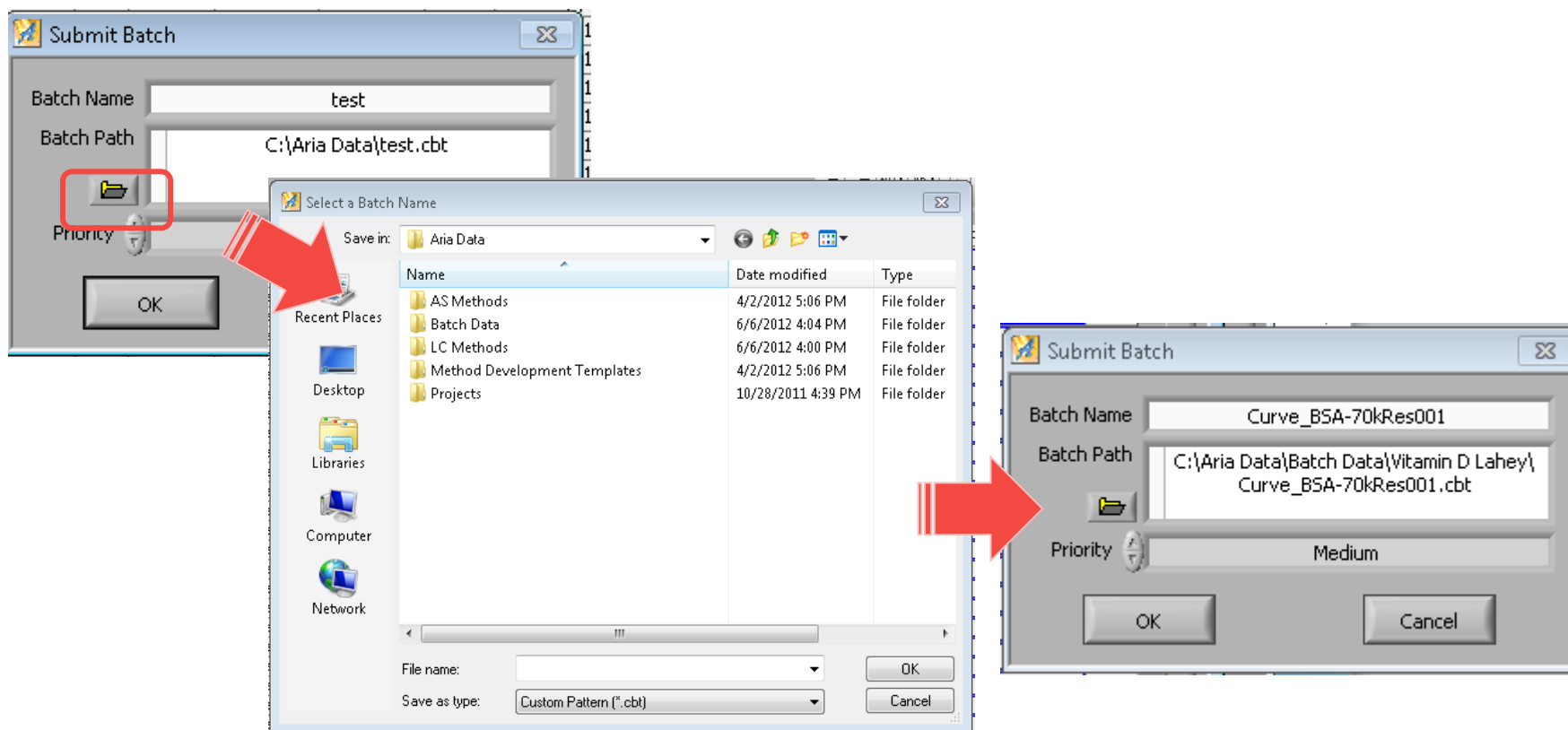
Create and submit a sample list



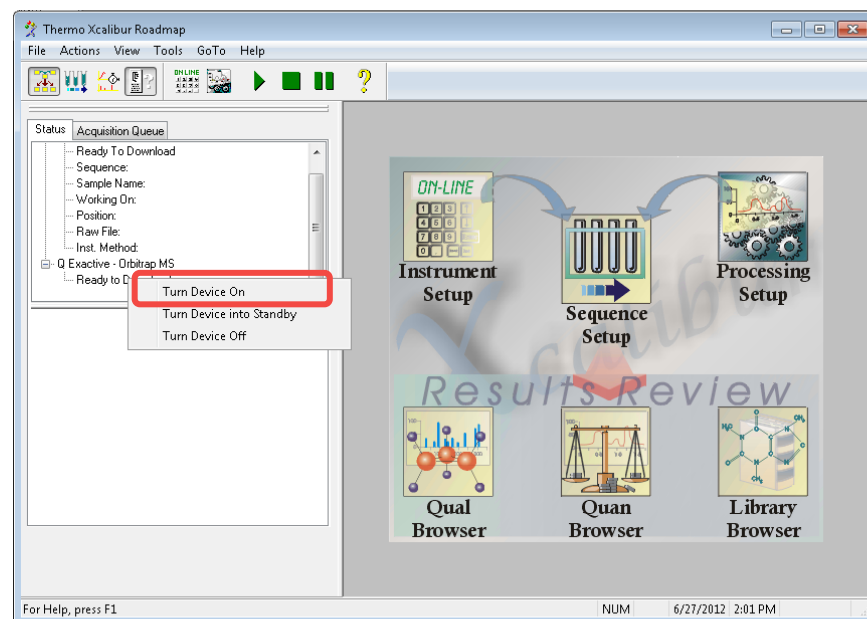
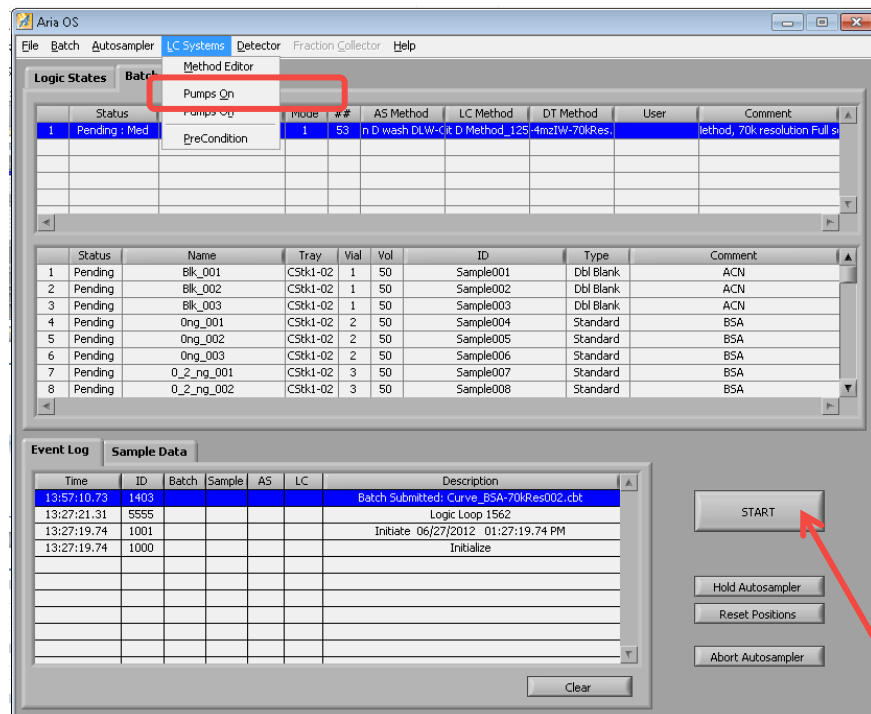
1. Type or import (File>Import>Text File) sample info
2. Choose the channels you want to use
3. Click Submit



Browse button to place & save the batch file



Turn on the pumps and the MS



- Then click Start

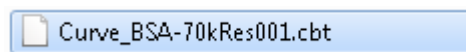
After the run...

- Several new files will be created
- Some of these files must be imported to TraceFinder for processing

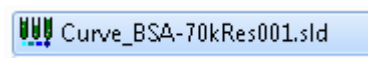


TraceFinder

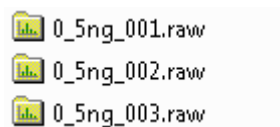
- Batch file



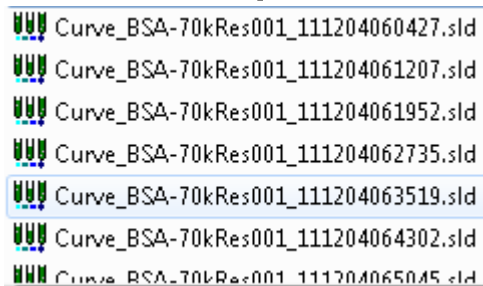
- Master Sequence file



- Raw files

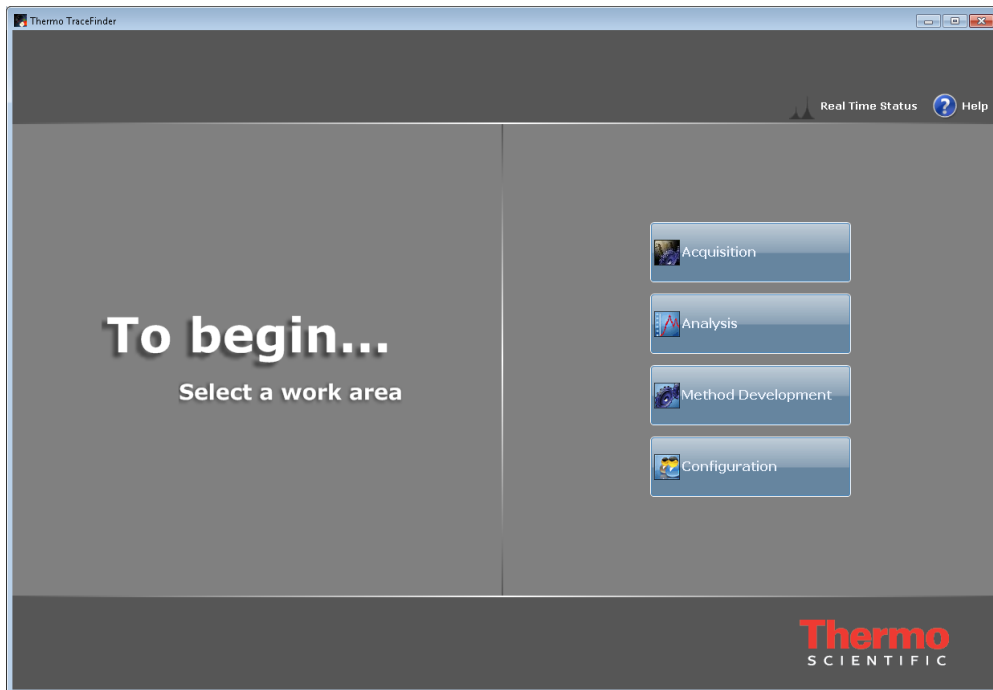
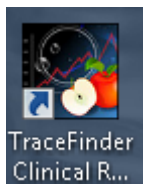


- Extra Sequence files



Importing to TraceFinder

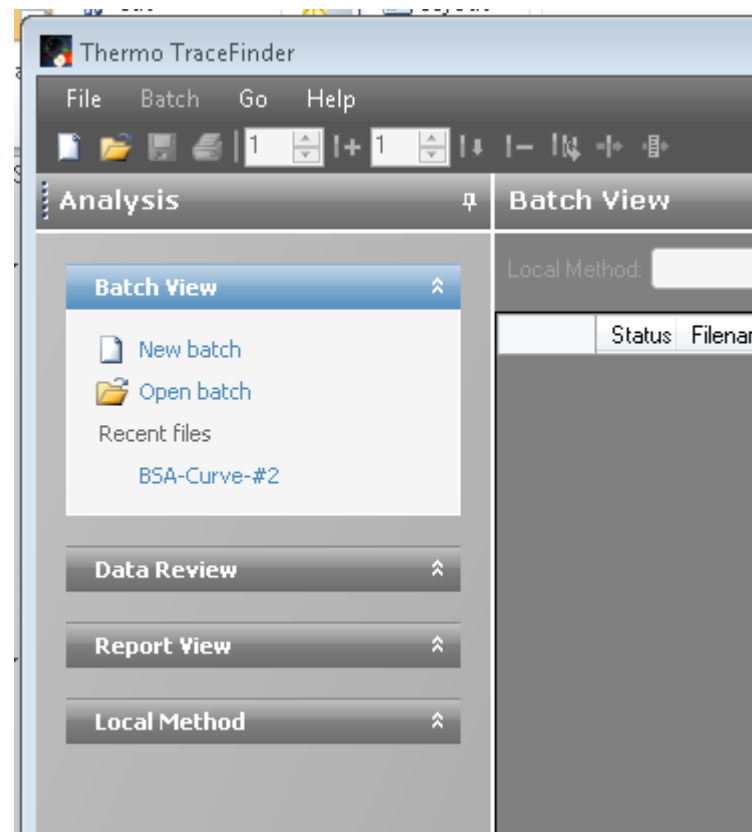
- Open “TraceFinder for Clinical Research”



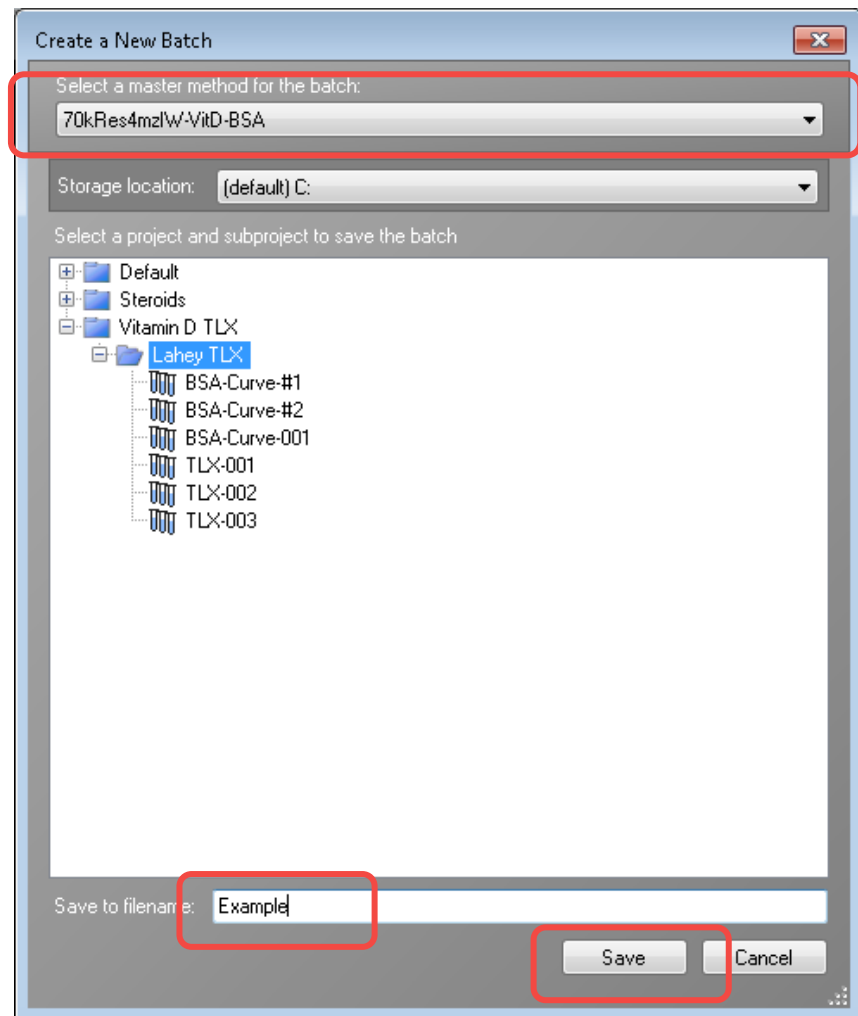
- Click *Analysis*

Create a blank batch

- In *Analysis* tab
 - Open *Batch View* sub-tab
 - Click *New Batch*



- Select a Master Method
 - (See TraceFinder help for assistance creating a master method)
- Select a location and name for the batch



A blank batch is created

The screenshot displays the Thermo TraceFinder software interface. The main window is titled "Batch View - Example". The "Local Method" is set to "70kRes4mzIW-ViD-BSA". The "Instrument" is "Thermo Scientific Instrument" and the "User" is "AMER\usfra-lab".

The "Batch View" table shows a single sample:

	Status	Filename	Sample type	Level	Sample ID	Sample name	Comment	Vial position	Injection volume	Dilution
1		Unknown1	Specimen						50.0	1.0

The "Automated Batch Reports" section shows a list of reports:

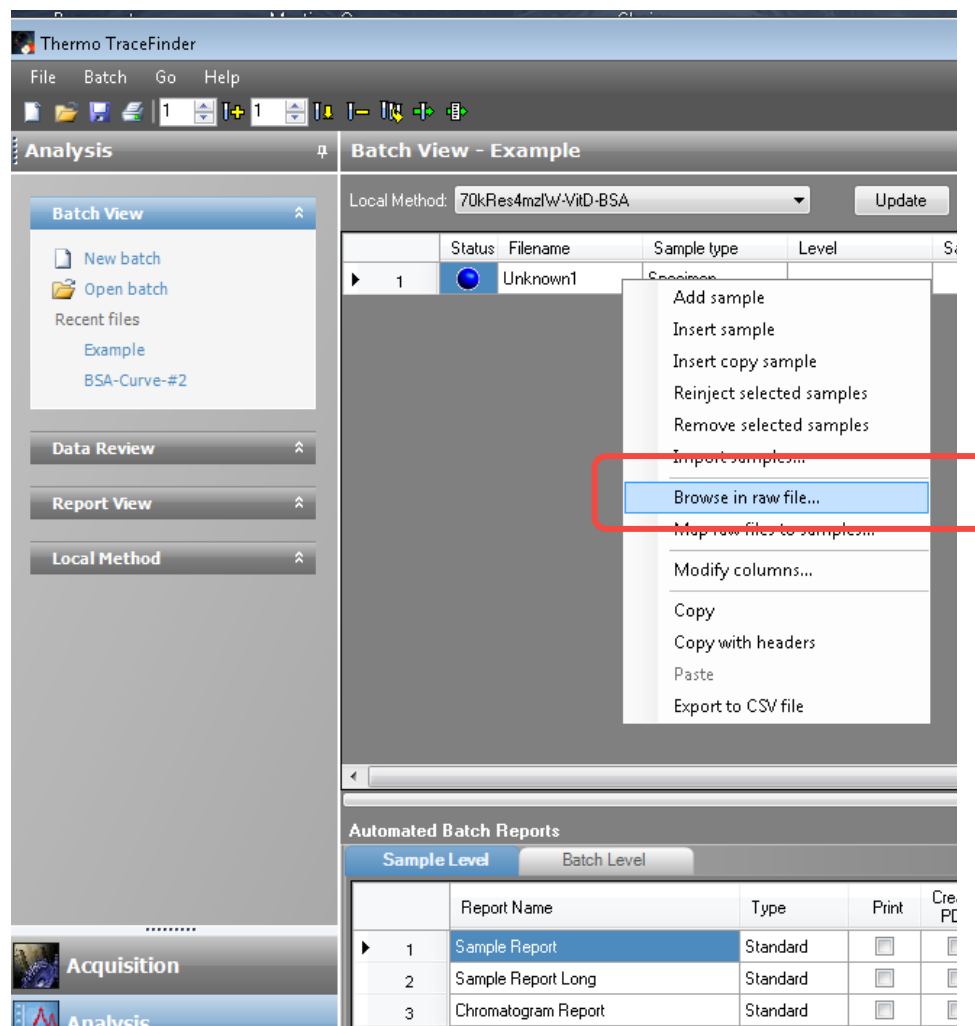
	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
1	Sample Report	Standard	☐	☐	☐	☐
2	Sample Report Long	Standard	☐	☐	☐	☐
3	Chromatogram Report	Standard	☐	☐	☐	☐
4	Confirmation Report	Standard	☐	☐	☐	☐
5	High Density Internal Standard Report	Standard	☐	☐	☐	☐
6	High Density Internal Standard Report ...	Standard	☐	☐	☐	☐
7	High Density Sample Report 1	Standard	☐	☐	☐	☐
8	High Density Sample Report 1 Long	Standard	☐	☐	☐	☐
9	High Density Sample Report 2	Standard	☐	☐	☐	☐
10	High Density Sample Report 2 Long	Standard	☐	☐	☐	☐

The "Compound Active Status" section shows a list of compounds:

	Compound	Active
1	d6-25-OH Vitamin D3 FullMS 389...	☒
2	25-OH Vitamin D3 MS2 383.330	☒
3	25-OH Vitamin D3 Full MS 383.330	☒
4	25-OH Vitamin D2 Full MS 395.330	☒
5	25-OH Vitamin D2 MS2 395.330	☒

The left sidebar shows the "Analysis" menu with options: "Batch View", "Data Review", "Report View", and "Local Method". The bottom status bar indicates "Ready" and "User: AMER\usfra-lab".

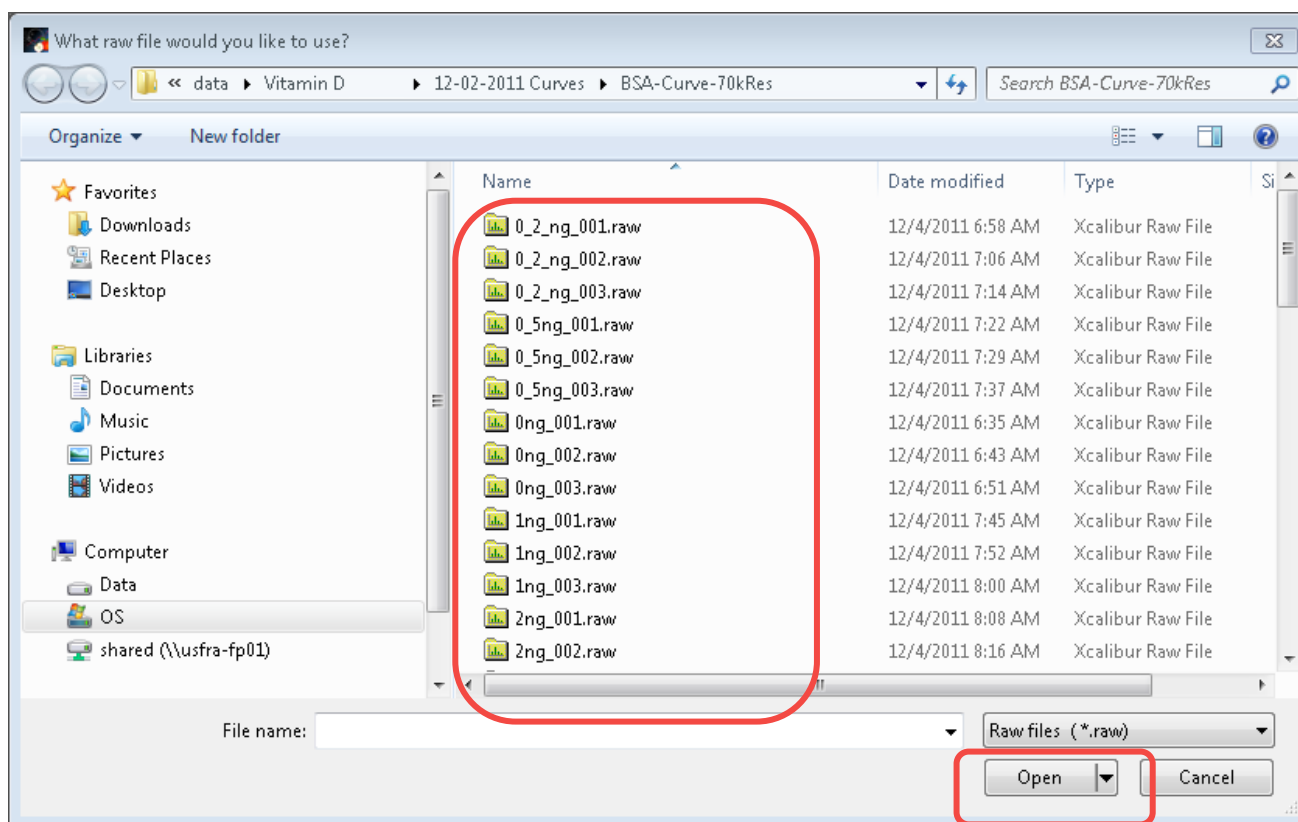
“Browse in” the raw files



- Right click and select *Browse in raw file...*
- This “Browse in” tool will copy the raw files into TraceFinder for processing

Select all the raw files

- Use shift-click to select all raw files
- Click open



TraceFinder Batch now contains samples

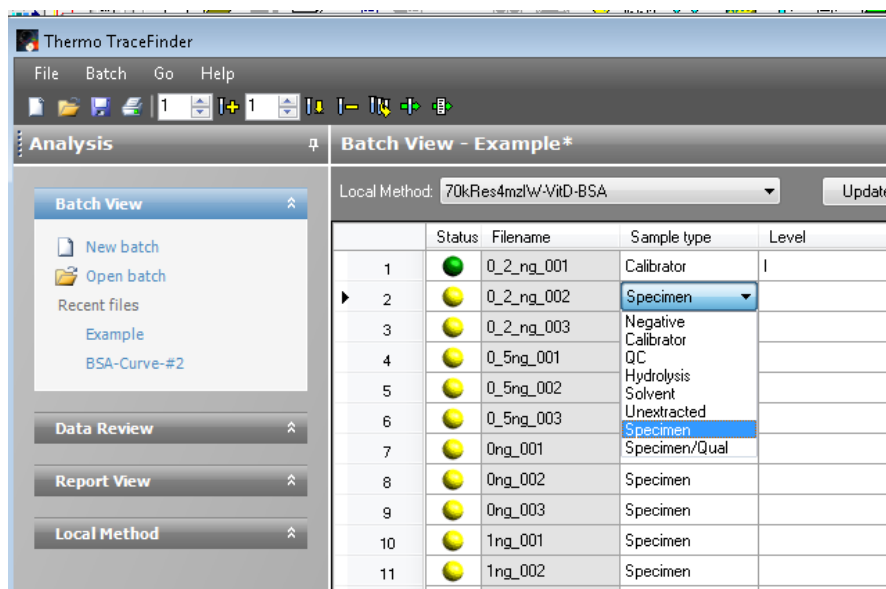
The screenshot displays the Thermo TraceFinder software interface. The main window is titled 'Batch View - Example*'. It features a menu bar (File, Batch, Go, Help) and a toolbar. The left sidebar contains navigation options: 'Batch View' (selected), 'Data Review', 'Report View', and 'Local Method'. The 'Batch View' section shows a list of samples with columns: Status, Filename, Sample type, Level, Sample ID, Sample name, Comment, and Vial position. A 'Please wait' dialog box is overlaid on the sample list, indicating 'Inserting rawfile into batch: P-0ng_002.raw'. The bottom right corner shows the 'Compound Active Status' table and the user 'User: AMER\usfra-lab'.

Status	Filename	Sample type	Level	Sample ID	Sample name	Comment	Vial position
1	0_2_ng_001	Specimen		Sample007	0_2_ng_001	BSA	3
2	0_2_ng_002	Specimen		Sample008	0_2_ng_002	BSA	3
3	0_2_ng_003	Specimen		Sample009	0_2_ng_003	BSA	3
4	0_5ng_001	Specimen		Sample010	0_5ng_001	BSA	4
5	0_5ng_002	Specimen		Sample011	0_5ng_002	BSA	4
6	0_5ng_003	Specimen		Sample012	0_5ng_003	BSA	4
7	0ng_001	Specimen		Sample004	0ng_001	BSA	2
8	0ng_002	Specimen		Sample005	0ng_002	BSA	2
9	0ng_003	Specimen		Sample006	0ng_003	BSA	2
10	1ng_001	Specimen		Sample013	1ng_001	BSA	5
11	1ng_002	Specimen		Sample014	1ng_002	BSA	5
12	1ng_003	Specimen		Sample015	1ng_003	BSA	5
13	2ng_001	Specimen		Sample016	2ng_001	BSA	6
14	2ng_002	Specimen		Sample017	2ng_002	BSA	6
				Sample018	2ng_003	BSA	6
				Sample019	5ng_001	BSA	7

Compound	Active
d6-25-OH Vitamin D3 FullMS 389.330	☒
25-OH Vitamin D3 MS2 383.330	☒
25-OH Vitamin D3 Full MS 383.330	☒
25-OH Vitamin D2 Full MS 395.330	☒
25-OH Vitamin D2 MS2 395.330	☒

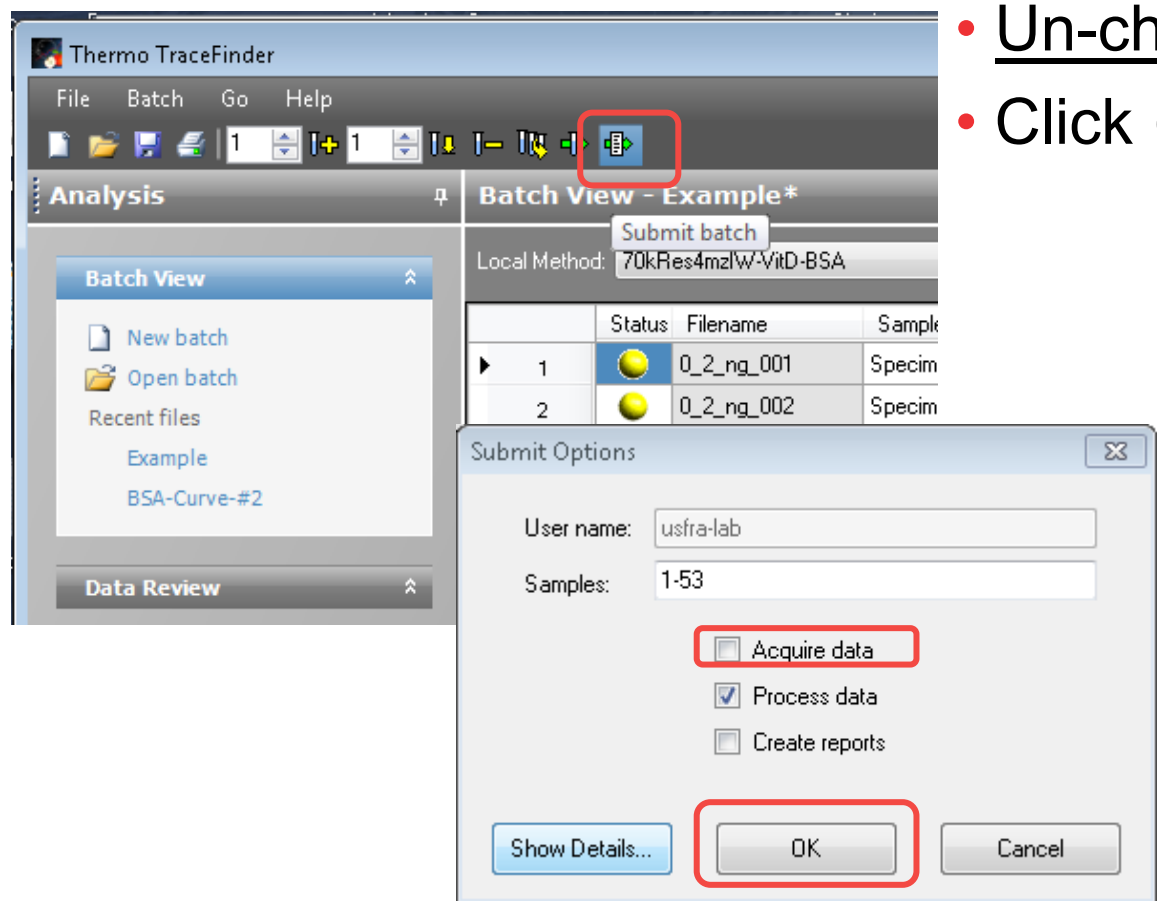
If needed, update the sample types and levels

- Click on the drop-down menus

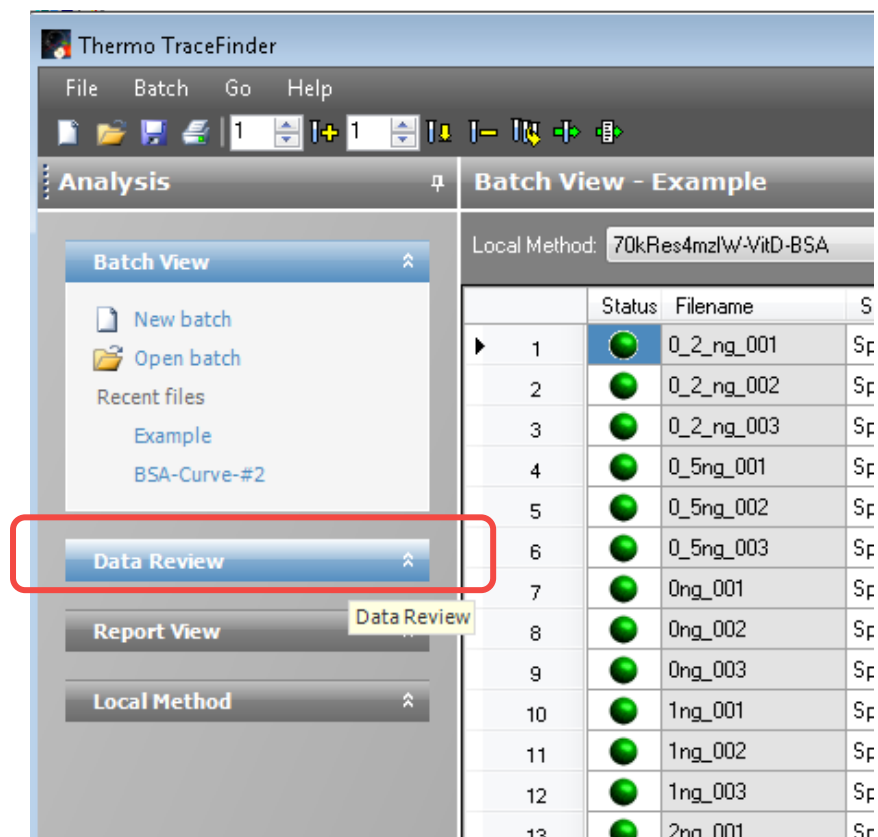


Process the batch

- Click *Submit batch* button
- Un-check *Acquire data*
- Click *OK*



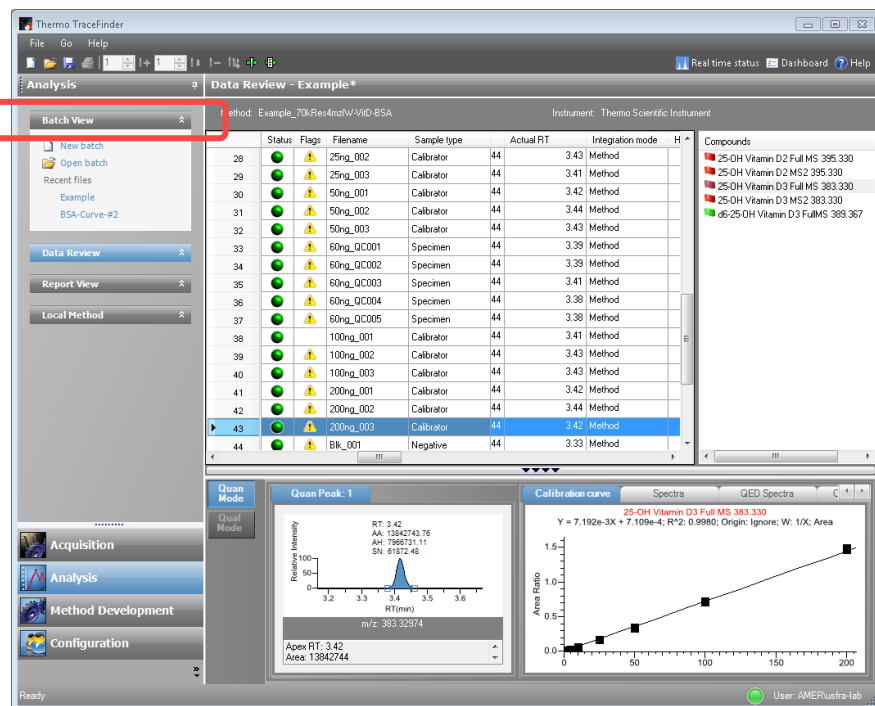
Reviewing the run



- Sample Status icons will all turn green
- Then click *Data Review*

Manual review

- You may want to click through each line to see the quality of the integration before accepting the run
- Click on any yellow flags to view details about the flag
- Save the batch, then go back to *Batch view* to generate reports



Generating reports (First option)

- Select the check box next to any reports you want to generate
- Click *Submit batch*
- Check *Create reports*

The screenshot displays the Thermo TraceFinder software interface. The main window shows a 'Batch View - Example*' with a table of samples. A 'Submit Options' dialog box is open in the foreground, and the 'Create reports' checkbox is selected. The 'Automated Batch Reports' section at the bottom shows a list of reports with checkboxes for selection.

Batch View - Example*

Status	Filename	Sample type	Level	Sample ID	Sample name	Comment	Vial position
1	0_2_ng_001	Calibrator	I	Sample007	0_2_ng_001	BSA	3
2	0_2_ng_002	Calibrator	I	Sample008	0_2_ng_002	BSA	3
3	0_2_ng_003	Calibrator	I	Sample009	0_2_ng_003	BSA	3
4	0_5ng_001	Calibrator	II	Sample010	0_5ng_001	BSA	4
5	0_5ng_002	Calibrator	II	Sample011	0_5ng_002	BSA	4
6	0_5ng_003	Calibrator	II	Sample012	0_5ng_003	BSA	4
7	0ng_001	Negative		Sample004	0ng_001	BSA	2
8	0ng_002	Negative		Sample005	0ng_002	BSA	2
9	0ng_003	Negative		Sample006	0ng_003	BSA	2
10	1ng_001	Calibrator	III	Sample013	1ng_001	BSA	5
11	1ng_002	Calibrator	III	Sample014	1ng_002	BSA	5
12	1ng_003	Calibrator	III	Sample015	1ng_003	BSA	5
13	2ng_001	Calibrator	IV	Sample016	2ng_001	BSA	6
14	2ng_002	Calibrator	IV	Sample017	2ng_002	BSA	6
15	2ng_003	Calibrator	IV	Sample018	2ng_003	BSA	6
16	5ng_001	Calibrator	V	Sample019	5ng_001	BSA	7

Submit Options

User name: usfra-lab

Samples: 1-53

☐ Acquire data

☐ Process data

☒ Create reports

Show Details... OK Cancel

Automated Batch Reports

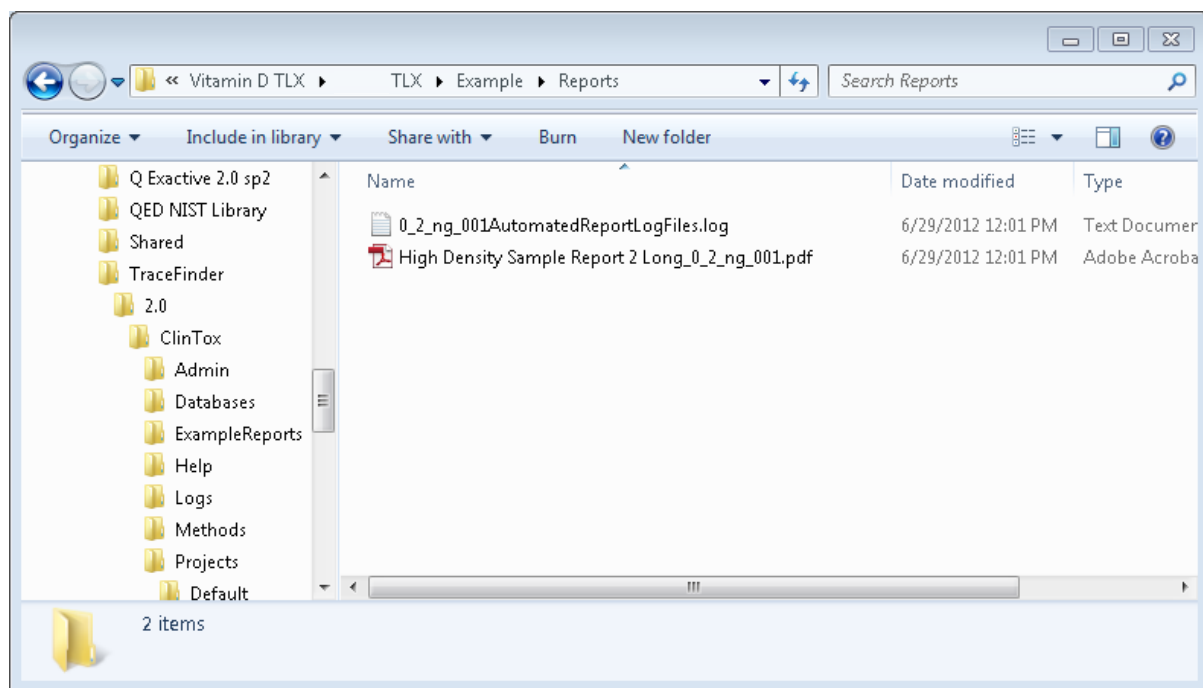
Report Name	Type	Create PDF
10 High Density Sample Report 2 Long	Standard	☒
11 High Density Sample Report 3	Standard	☐
12 High Density Sample Report 3 Long	Standard	☐
13 Internal Standard Summary Report	Standard	☐
14 Ion Ratio Failure Report	Standard	☐
15 Manual Integration Report	Standard	☐
16 Negative Report	Standard	☐
17 Qualitative Peak Report	Standard	☐

Compound Active Status

Compound	Active
1 d5-25-OH Vitamin D3 Full MS 389...	☒
2 25-OH Vitamin D3 MS2 383.330	☒
3 25-OH Vitamin D3 Full MS 383.330	☒
4 25-OH Vitamin D2 Full MS 395.330	☒
5 25-OH Vitamin D2 MS2 395.330	☒

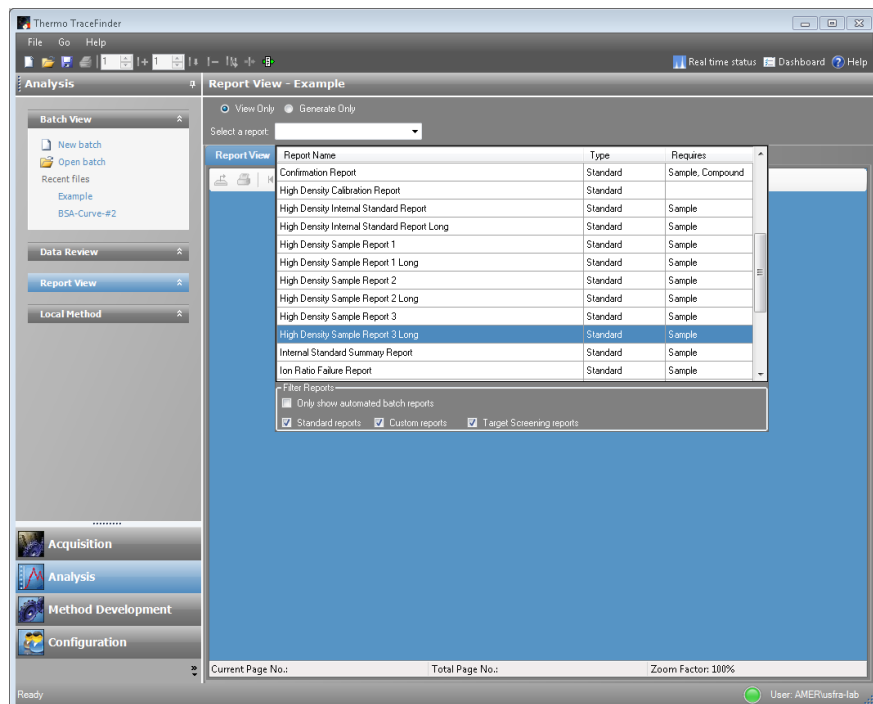
Report location

- Reports will be generated within the *reports* folder of the TraceFinder batch
- E.g. C:\Thermo\TraceFinder\2.0\ClinTox\Projects\Vitamin D TLX\TLX\Example\Reports



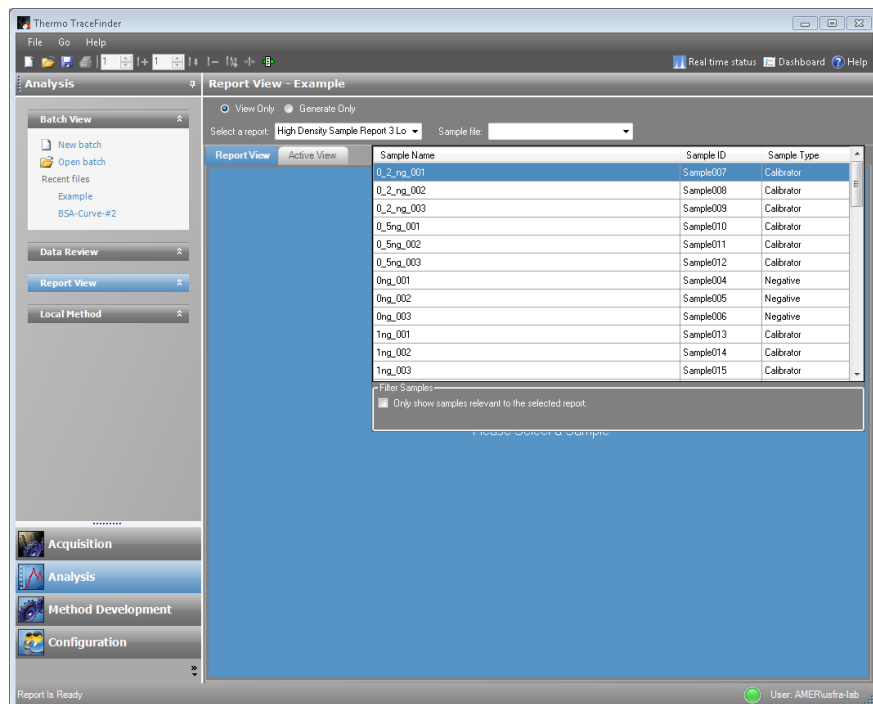
Generating reports (second option)

- You can also generate reports through the *Report view*
- First choose a report style



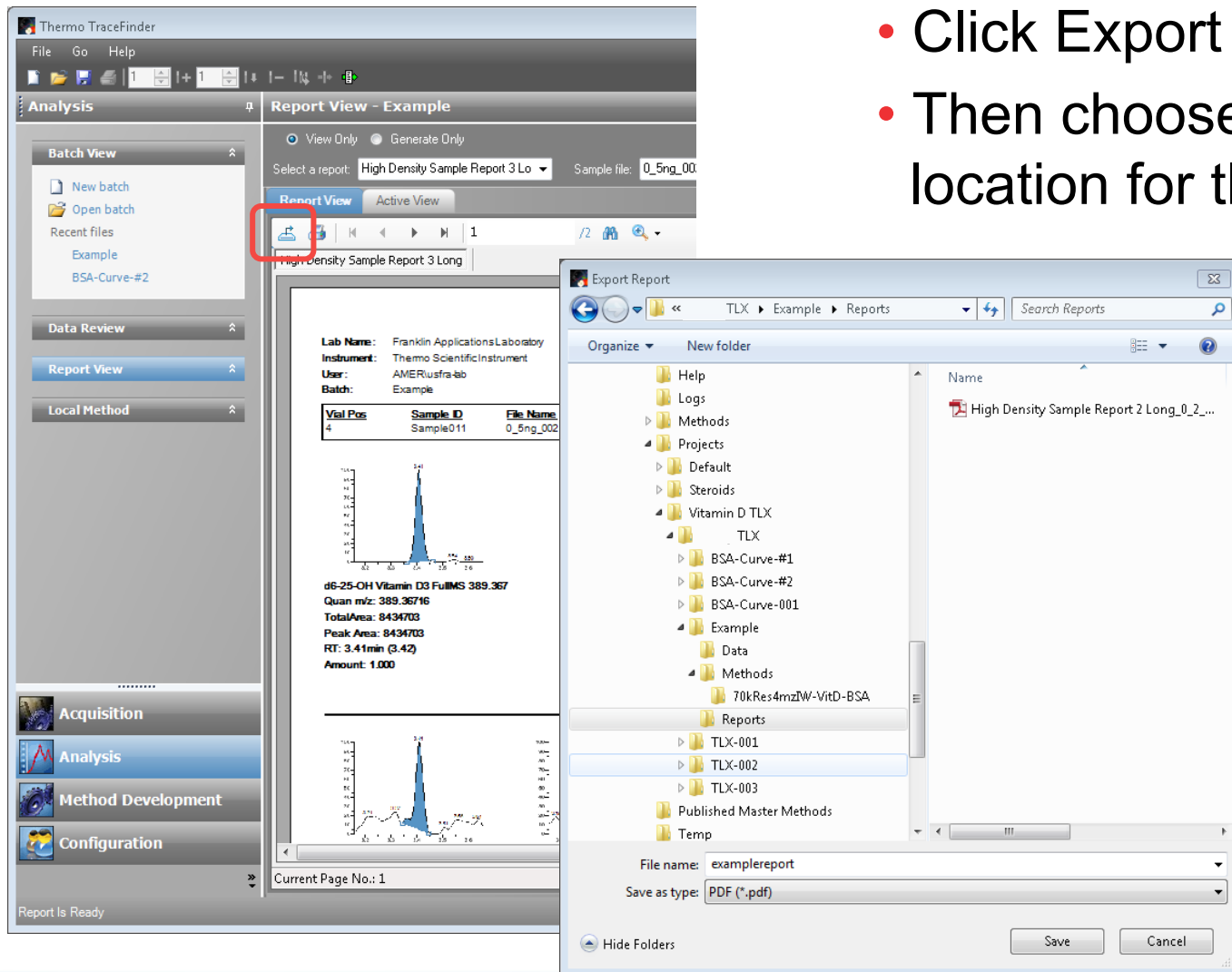
Generating reports, continued

- Next, choose the sample that you want to report



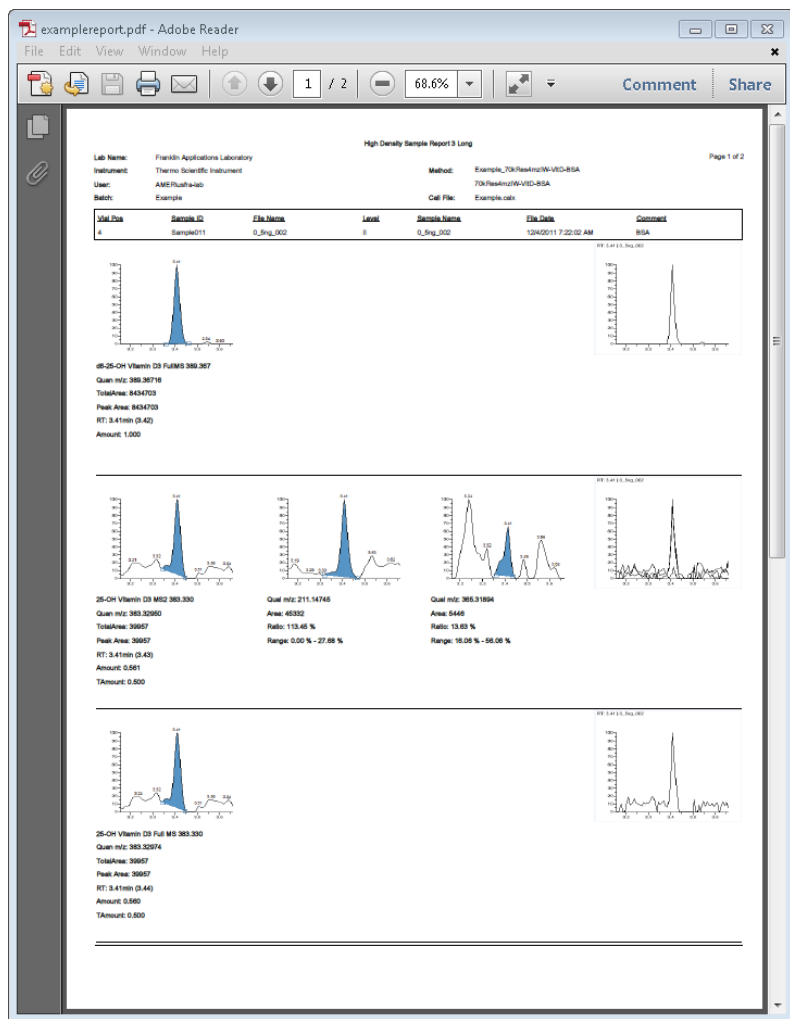
Generating reports, continued

- Click Export or print
- Then choose a name and location for the report



Final product

- Report is generated as a pdf or hard copy



Addendum

- For more tips and tricks,
 - Check out our blog,
MyTraceFinder.com