# MassHunter for Agilent GC/MS & GC/MS/MS

Next Generation
Data Analysis Software

Presented by :
Terry Harper
GC/MS Product Specialist

# Outline of Topics

**Topic 1: Introduction to MassHunter**

**Topic 2: Data Acquisition / Conversion**

**Topic 3: Qualitative Analysis**

**Topic 4: Quantitative Analysis**

**Topic 5: Reporting**

**Q & A**

My Goal : Spark an interest in using MassHunter Data Analysis in your lab!

# MassHunter – A Software Suite

**MassHunter software is modular:**

- **Different modules that focus on these specific tasks:**
  - ✓ **Acquisition (Instrument Specific)**
  - ✓ **Quantitative Analysis (Quant)**
  - ✓ **Qualitative Analysis (Qual)**

- **A common reporting engine that uses different templates which are based on the specific reporting that is required.**

- **Suite of accessory applications which aid in specific tasks:**
  - ✓ **Unknown Analysis: batch versions of deconvolution and library searching**
  - ✓ **Library editor**
  - ✓ **Method development assistants**
  - ✓ **Data Translators**

# MassHunter Data Analysis Software

**MassHunter's main *data analysis* modules have different functions:**

## Quantitative (Quant):

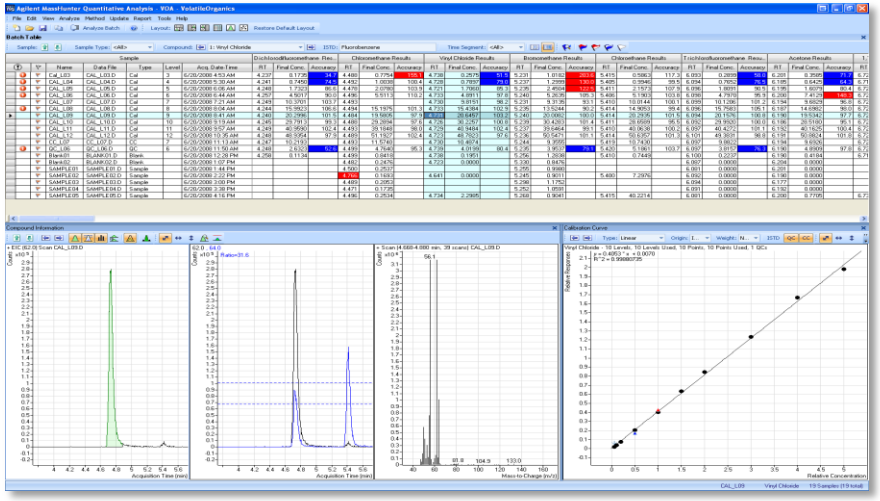
**(Target Analysis - Quantitation)**

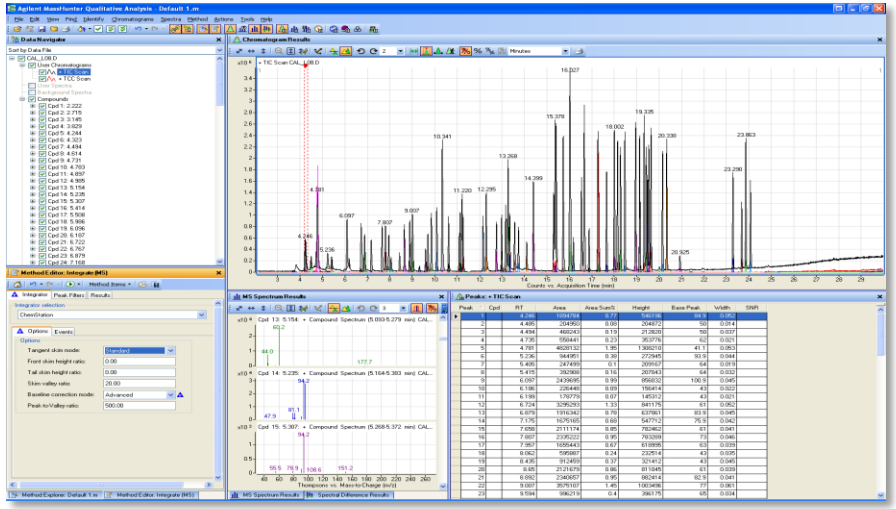
- **Review Batch results**
- **Visualize quality outliers**
- **Powerful quantitation engine**
- **Flexible result and report presentation**

## Qualitative (Qual):

**(Discovery of non-target compounds or features, & Method Development)**

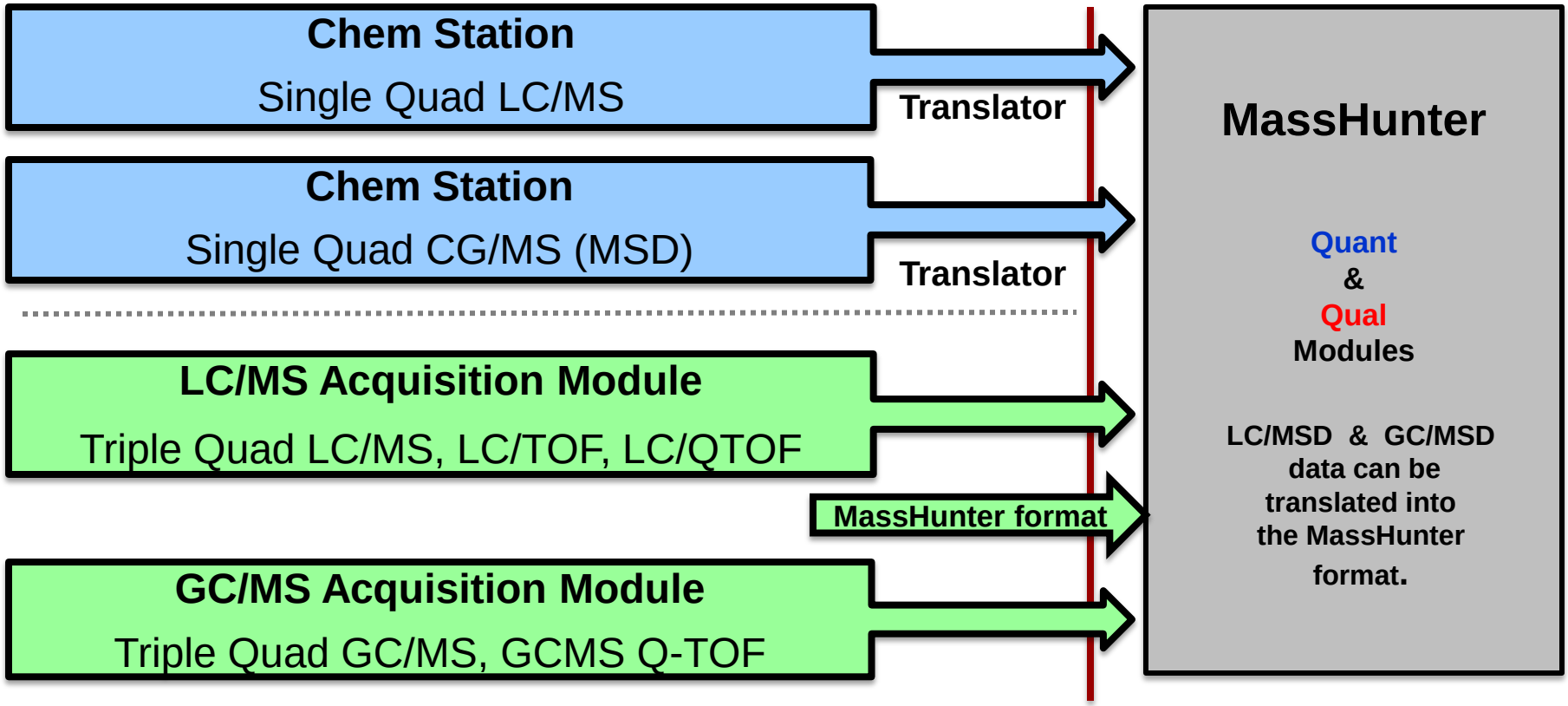
- **Finds compounds**
- **Identifies compounds**
- **Uses chromatogram and spectra extraction tools, i.e. deconvolution**
- **Searches EI Libraries**





# Delivering Data to MassHunter Data Analysis

**Quantitative (Quant) and Qualitative (Qual) analysis modules can process data from any Agilent MassHunter software system.**



**5975E SQ**
7820 GC

**5975C SQ**
7890 GC

**5975T LTM SQ**

# Agilent GC/MS

# Deploying MassHunter Software

# Agilent GC/MS/MS

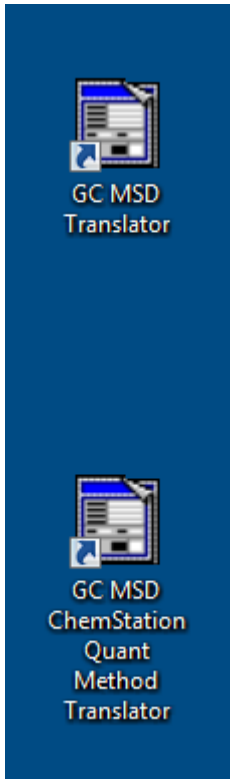
**220 IT**
7890 GC

**240 IT**
7890 GC

**7000 TQ**
**7890 GC**

**7200 Q-TOF**

# GCMS Translator – GC MSD

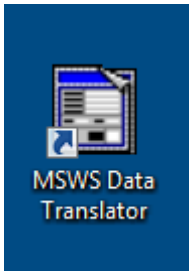



GC MSD Translator converts GCMS data files to MassHunter format.

a) single file translation
b) Multiple file translation
c) Automation with E.02.00 through macros

GC MSD ChemStation Quant Method Translator converts MSD Chemstation quant database to MassHunter quant format.

# GCMS Translator – Ion Trap




MSWS Data Translator coverts MS Workstation data files to MassHunter format.

a) single file translation
b) Multiple file translation
c) Automation with through command file


MSWS Quant Method Translator

GC/MS Translator for the MS Workstation
Quick Start

1
Translate an MS Workstation Quant Method into a MassHunter Method

Methods that were created by the MS Workstation can be automatically converted for use in MassHunter Quantitative Data Analysis using the GC/MS Translator software. Quantitation methods that were running successfully in the MS Workstation frequently convert and validate with no errors in MassHunter Quantitative Analysis. When validation issues are found, they are automatically identified and are correctable using the MassHunter Quantitative Analysis software.

# GCMS Translator – AIA / netCDF


GC AIA Translator converts AIA format MSD files to MassHunter format

GC/MS Translator is included with GC/MS MassHunter bundles: G7010AA, G7011AA, G6844AA, G6849AA, G6841AA *and* G6846AA

GCMS Translator is free!

Please give me contact information to recieve a copy

# Outline of Topics

Topic 1: Introduction to MassHunter

Topic 2: Data Acquisition / Conversion

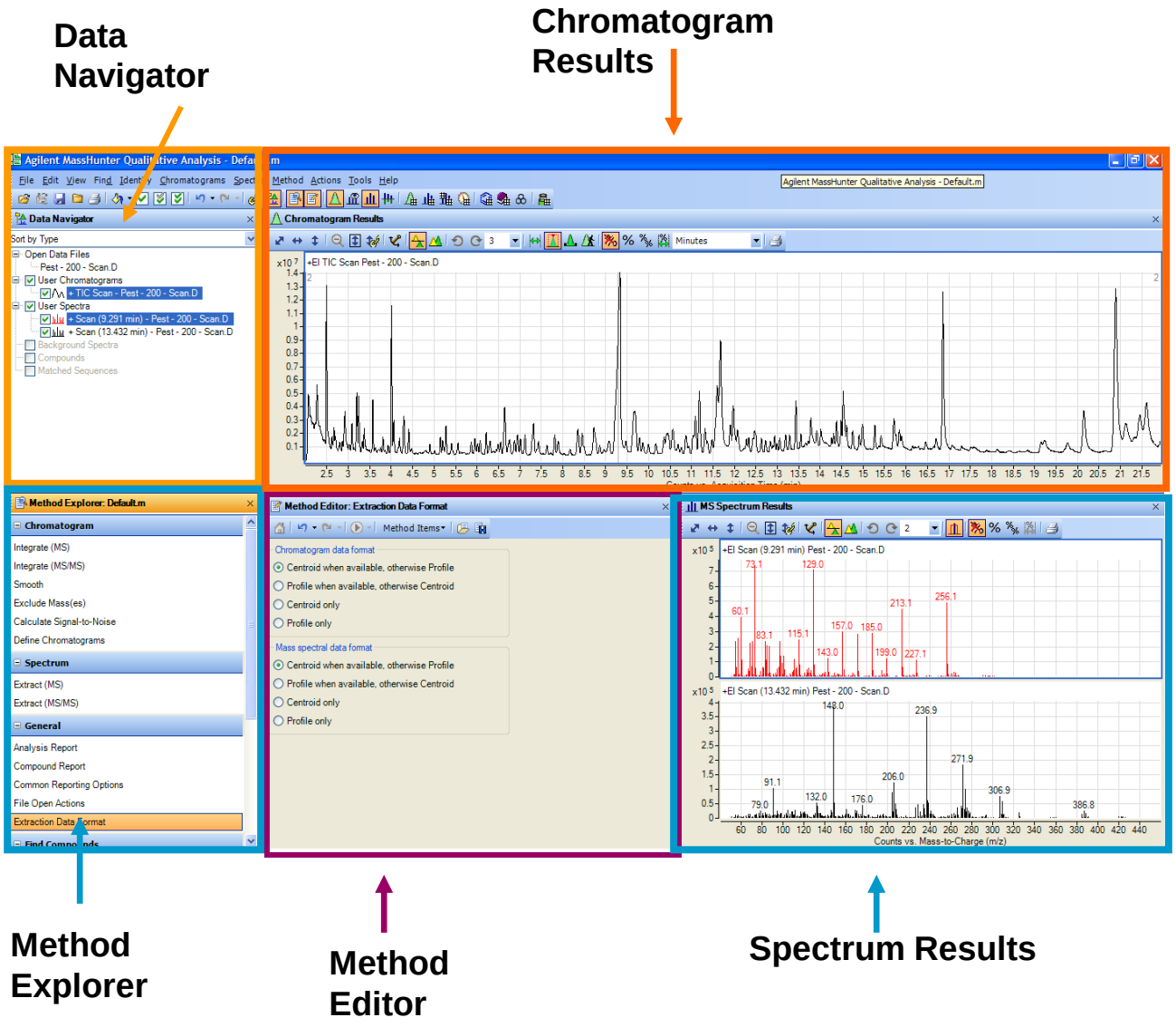
**Topic 3: Qualitative Analysis**

Topic 4: Quantitative Analysis

Topic 5: Reporting

Q & A

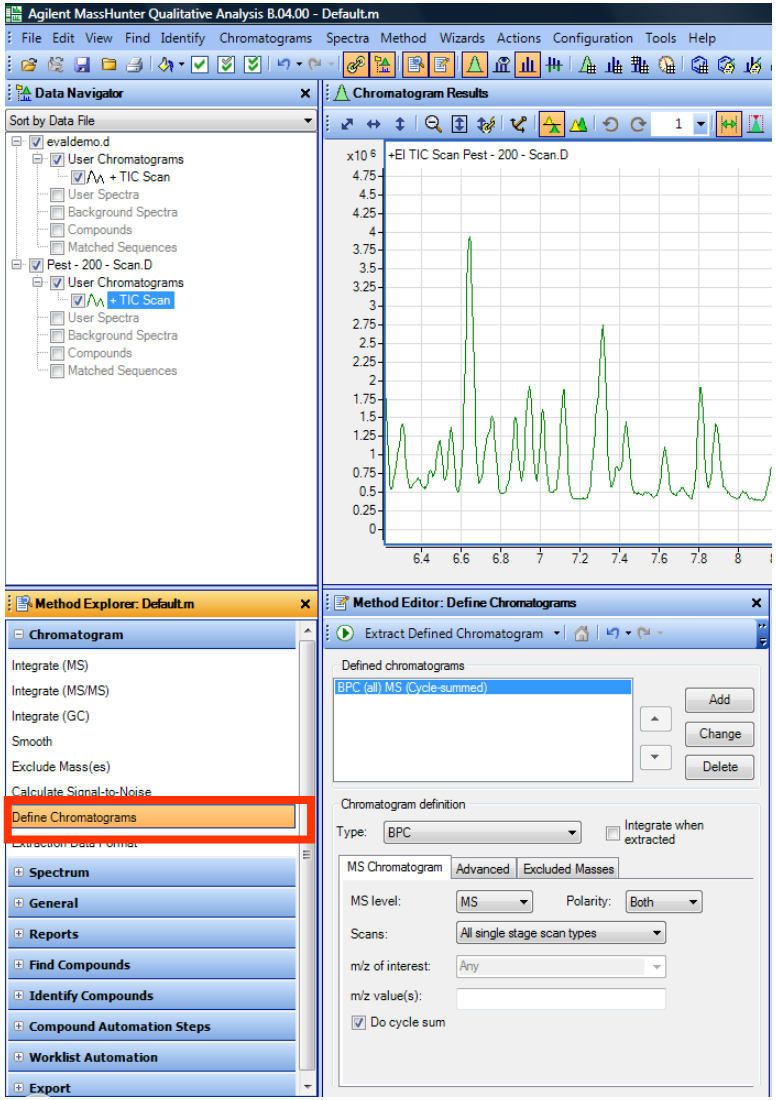
# MassHunter WorkStation Qualitative Analysis






Agilent Technologies

# Extract Chromatograms




- Extract multiple signal types to create Chromatograms
- Definition of signals can be stored in the method and used with automation

**Types of Chromatograms**

**TIC – Total Ion Chromatogram**

**BPC – Base Peak Chromatogram**

**EIC – Extracted Ion Chromatogram**

**SIM – Selected Ion Monitor**

**MRM – Multiple Reaction Monitor-QQQ**

**pNLC - Precursor Neutral Loss Chromatogram**

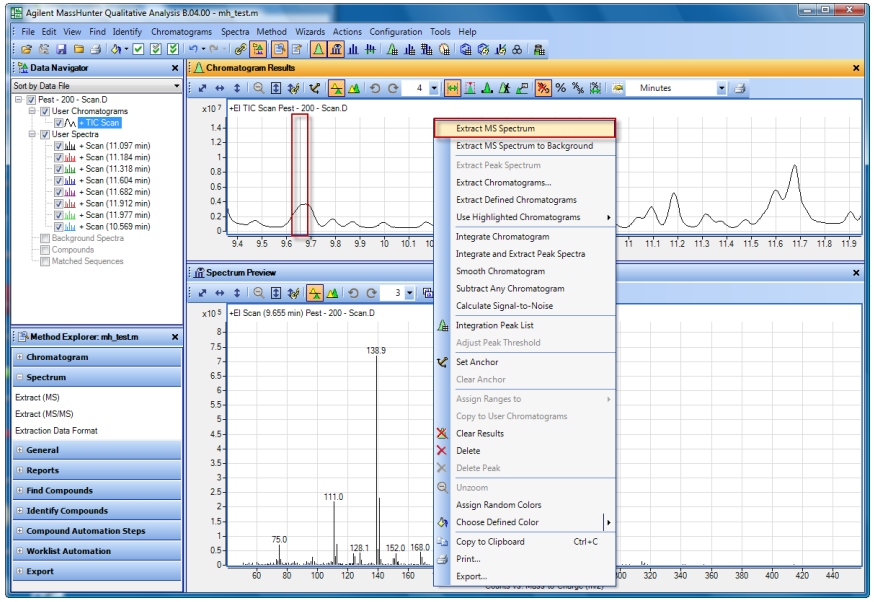
**Other Chromatograms – DAD, VWD, ADC, GC**

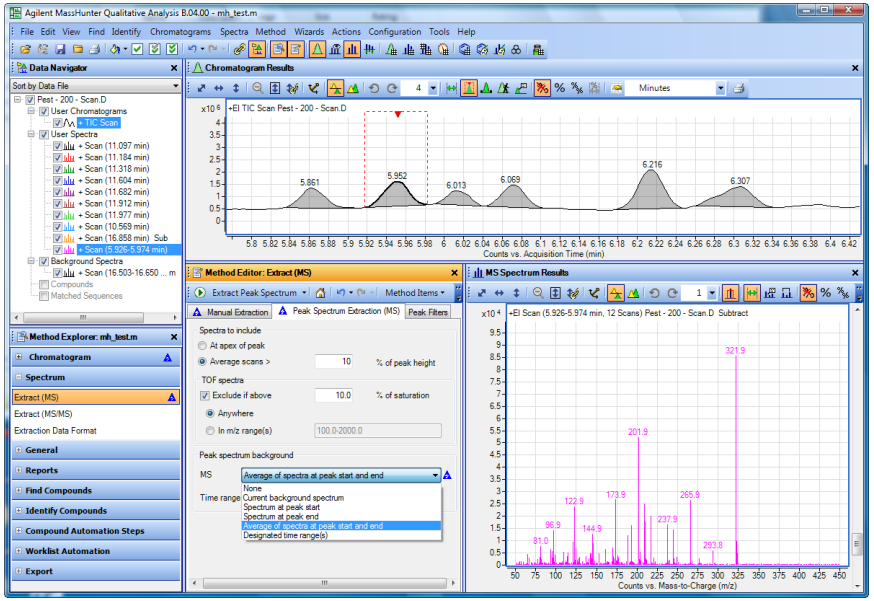
**Instrument Curve - %Comp., Temps, etc.**

# Extract Spectra

- Manual selection or based on integrated peaks

- Background subtraction based on defined regions or peak definition



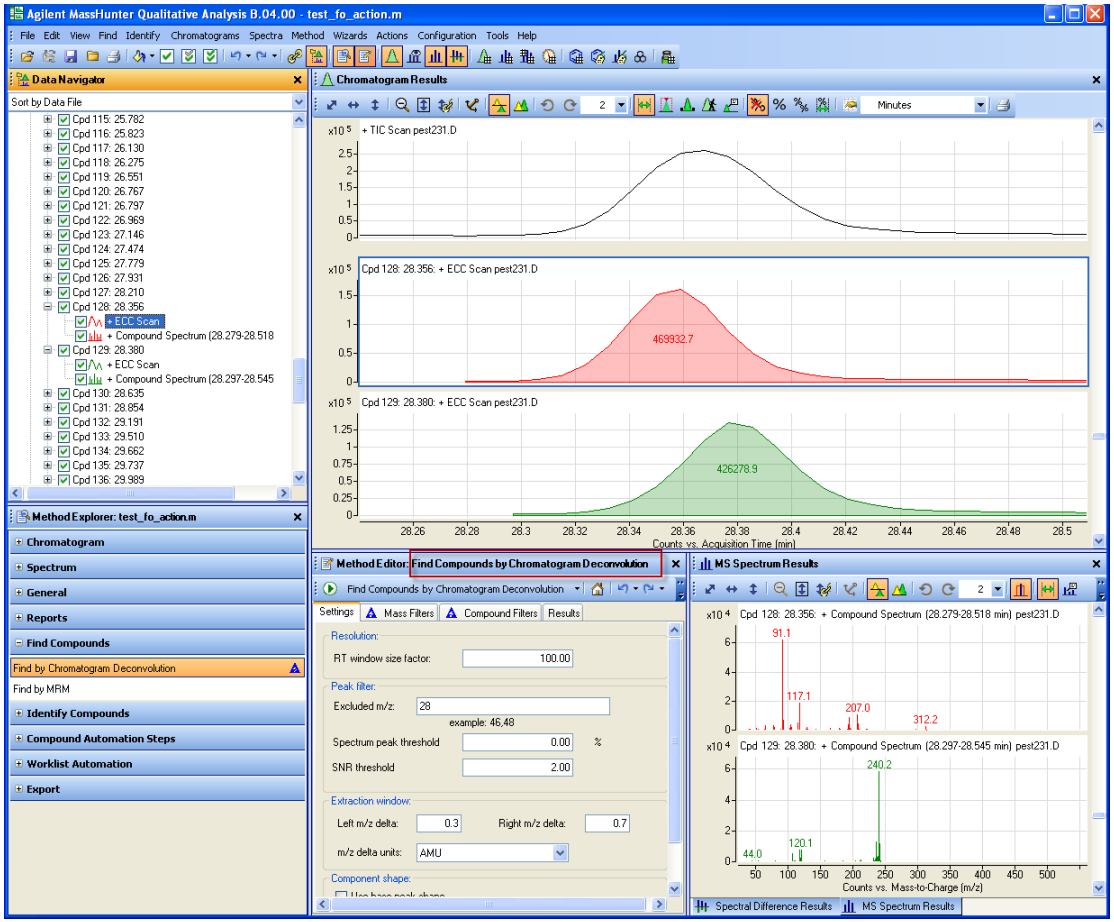



Agilent Technologies

# Find Compound by Chromatogram Deconvolution

- Agilent deconvolution algorithm similar to AMDIS but not equivalent

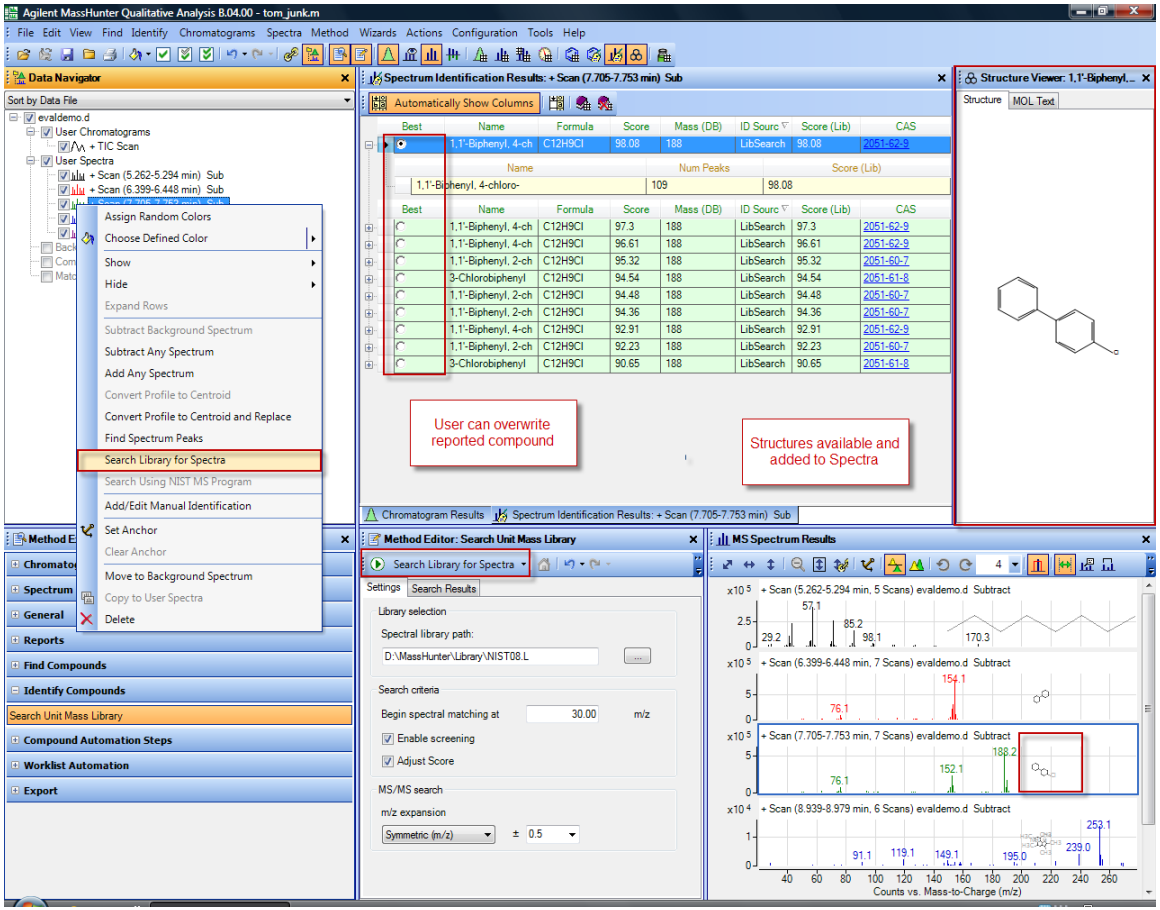
- Creates Compounds with chromatographic and spectral components






Agilent Technologies

# Identify Compounds with Library Search

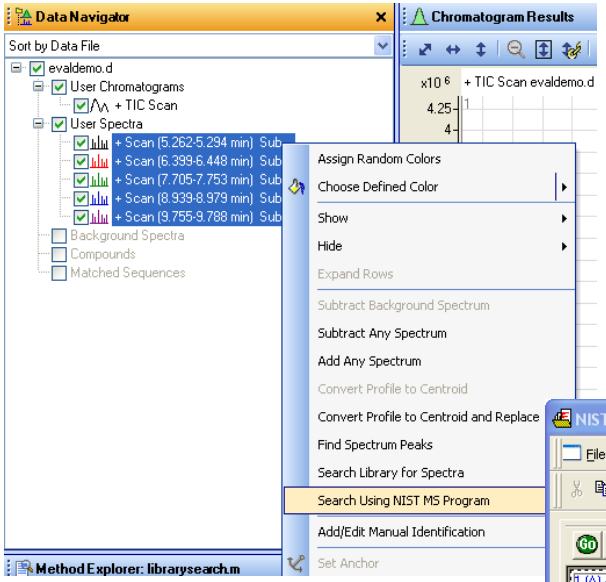



- Library search User Spectra or Compounds.
- Library search parameters are part of a method.
- May use Retention Time or Retention Index in seach

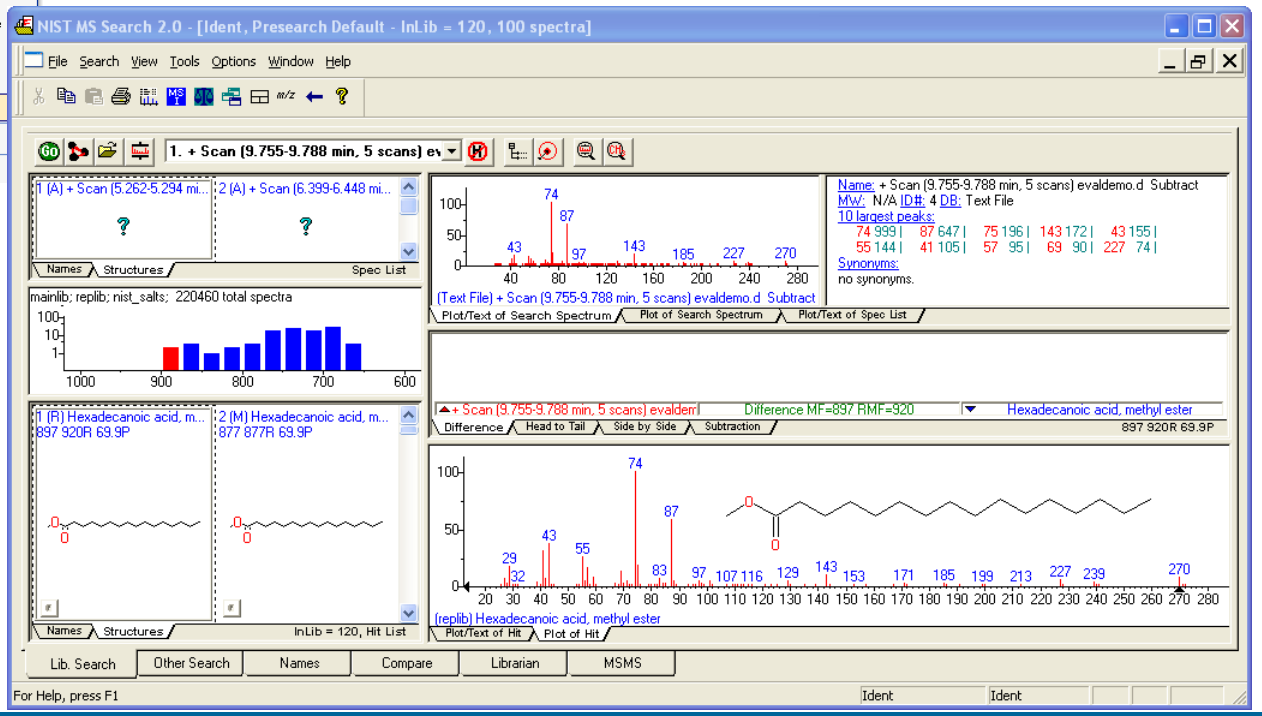


Agilent Technologies

# Using NIST library matching from Qual




- Export spectra to NIST
- Requires NIST (not included in Qual)
- Information does not flow back to Qual / MassHunter reports

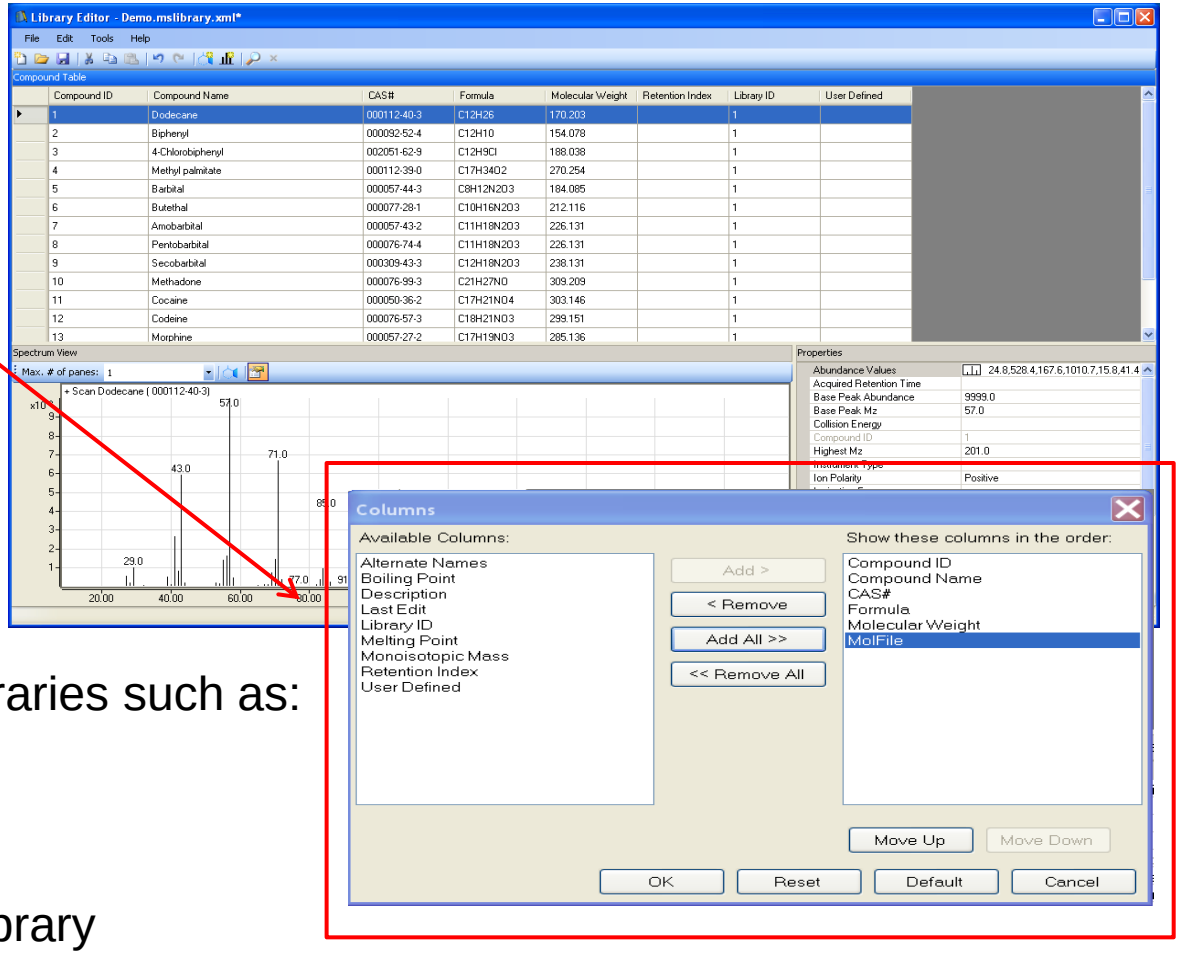





Agilent Technologies

# Library Editor & Available Libraries

A dedicated application, the *Library Editor*, is used to create, edit, and modify user libraries.


Agilent provides over 15 EI Libraries such as:

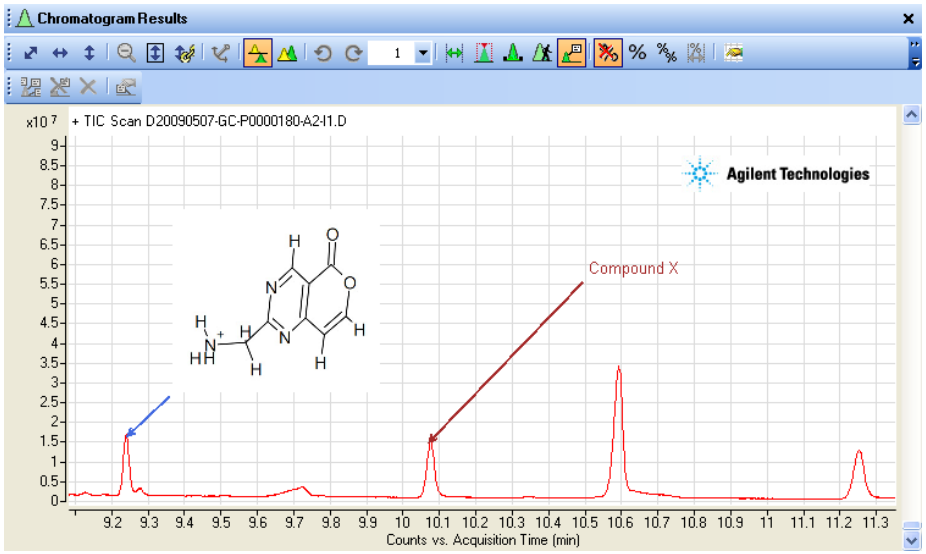
- ✓ NIST08
- ✓ Wiley8th+NIST08
- ✓ Fiehn Metabolite Library
- ✓ Japanese Pesticide list

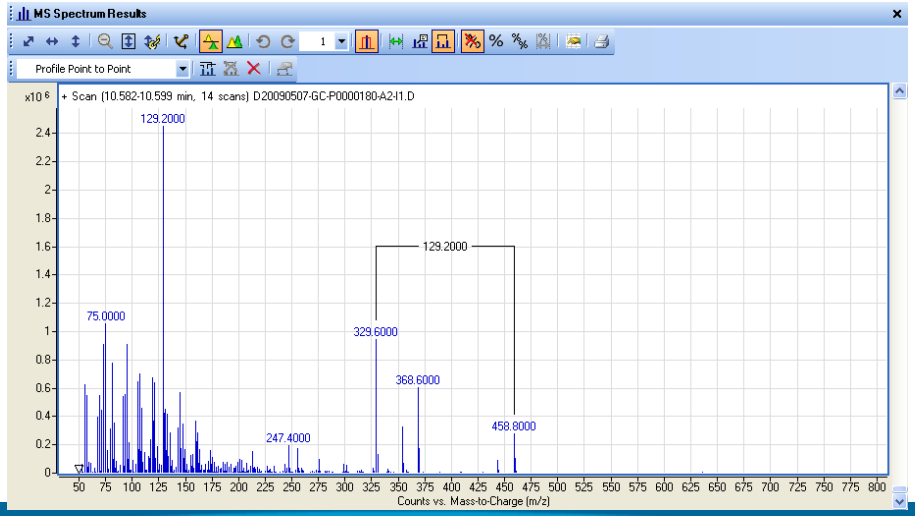
# Annotate and Document

Annotate chromatograms and spectra using text, graphics (.jpg) and chemical structures (.mol)

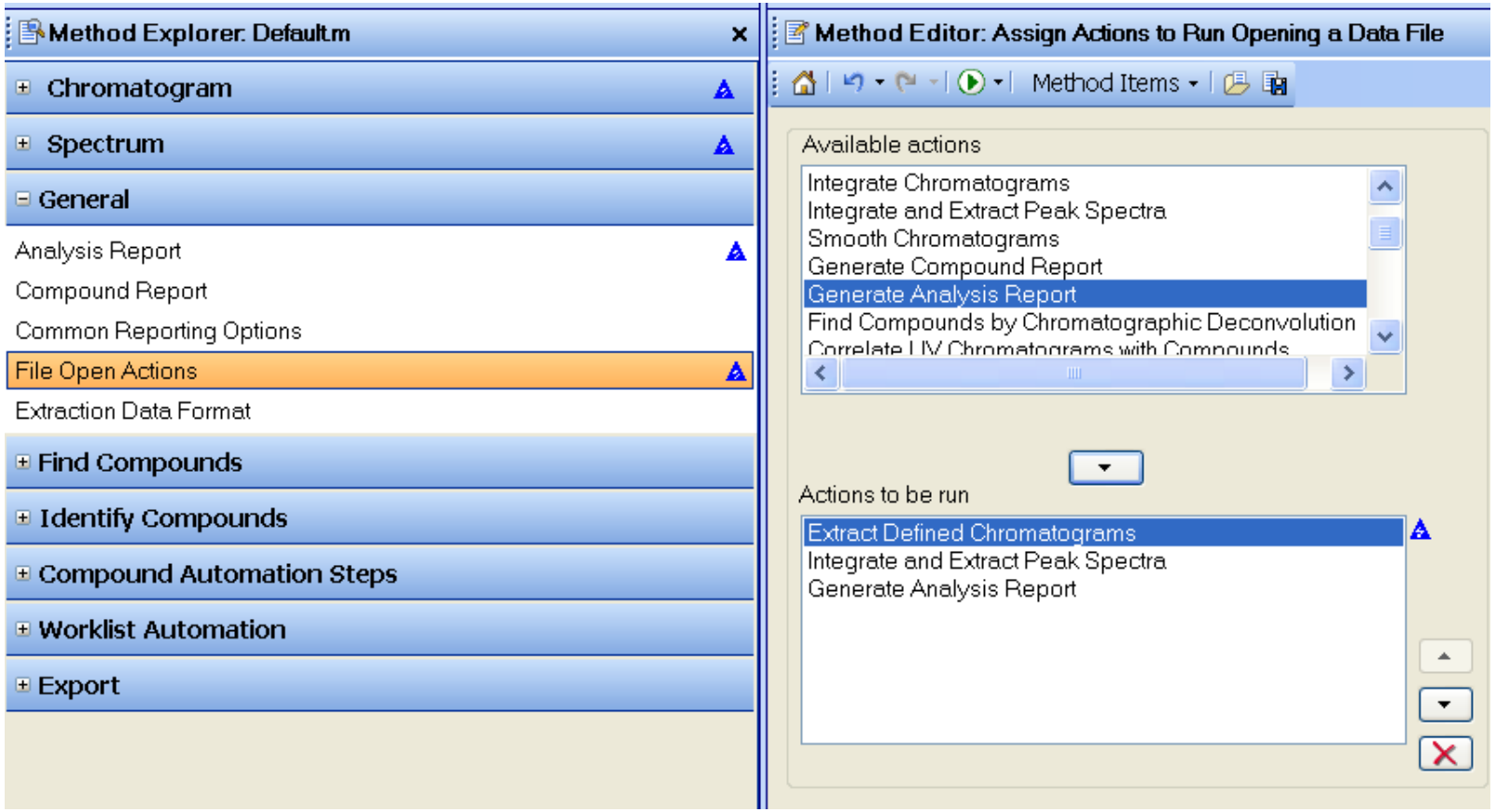
Mass Caliper to document fragmentation and losses

Export or copy & paste graphics into presentations



# Automation - File Open Actions & Post Acquisition Worklist Processing



# Outline of Topics

Topic 1: Introduction to MassHunter

Topic 2: Data Acquisition / Conversion

Topic 3: Qualitative Analysis

**Topic 4: Quantitative Analysis**

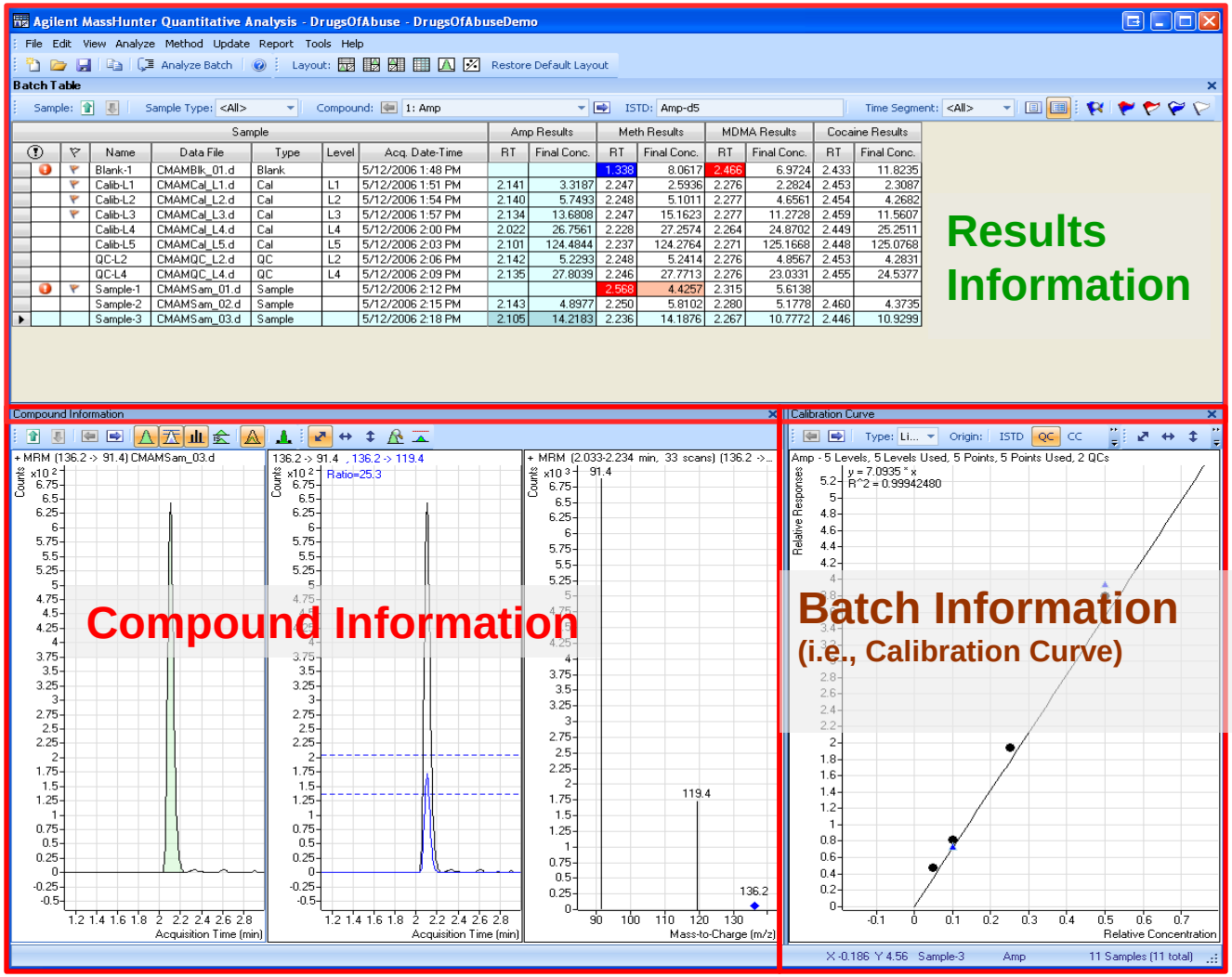
Topic 5: Reporting

Q & A

# Quantitative Analysis Screen

**The Quant Batch screen looks like this.**

- **Results Information** for the batch can be displayed. Visual guides highlight specific data that fall outside specific, predefined conditions.
- **Compound Information** displays graphical representation of the peak, qualifier information, spectral information, and the ISTD. Visual guides help identify associated data problems.
- **Batch Information** provides easy visualization and customization of relevant desired data.



# Batch Screen – Sample & Results Information

**In Results Information, the Quantitation Message is a human-readable string that contains a list of error messages that result from a compound's quantitation.**

Sample: | Sample Type: <All> | Compound: 1: Amp | ISTD: Amp-d5 | Time Segment: <All>

Compound Group: <All>

| Sample | | | | | | | Amp Met... | Amp Results | | | | | | | Qualifier (136.2 -... | | | Amp-d5 (IS... | | Qualifier (141.1 -... | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Name | Type | Level | Acq. Date-Time | Dil. | Exp. Conc. | RT | Resp. | S/N | MI | Calc. Conc. | Final Conc. | Accuracy | Ratio | S/N | MI | RT | Resp. | Ratio | S/N | MI |
| ! | | Blank-1 | Blank | | 11/11/2006 11:05 AM | 1.0 | | | | | | | | | | | | | | | | |
| | | Calib-L1 | Cal | L1 | 11/11/2006 11:10 AM | 1.0 | 2.5000 | 2.141 | 658 | 49.10 | | 2.1151 | 2.1151 | 84.6 | 24.3 | 45.47 | | 2.129 | 1397 | 25.9 | Infinity | |
| | ▼ | Calib-L2 | Cal | L2 | 11/11/2006 11:15 AM | 1.0 | 5.0000 | 2.140 | 1059 | 42.25 | | 4.5770 | 4.5770 | 91.5 | 33.5 | Infinity | | 2.128 | 1298 | 25.9 | 48.46 | |
| | | Calib-L3 | Cal | L3 | 11/11/2006 11:20 AM | 1.0 | 12.5000 | 2.134 | 2673 | 107.28 | | 12.6107 | 12.6107 | 100.9 | 29.7 | 146.48 | | 2.121 | 1377 | 26.3 | 46.09 | |
| | | Calib-L4 | Cal | L4 | 11/11/2006 11:25 AM | 1.0 | 25.0000 | 2.022 | 4952 | 20.26 | | 25.8545 | 25.8545 | 103.4 | 29.1 | 49.40 | | 1.990 | 1304 | 28.8 | 21.54 | |
| | | Calib-L5 | Cal | L5 | 11/11/2006 11:30 AM | 1.0 | 125.0000 | 2.101 | 18605 | 47.90 | | 124.8426 | 124.8426 | 99.9 | 27.0 | 39.22 | | 2.076 | 1053 | 26.4 | Infinity | |
| | | QC-L2 | QC | L2 | 11/11/2006 11:35 AM | 1.0 | 5.0000 | 2.142 | 1006 | 81.00 | | 4.0502 | 4.0502 | 81.0 | 27.7 | 34.47 | | 2.131 | 1356 | 31.1 | 42.99 | |
| | | QC-L4 | QC | L4 | 11/11/2006 11:40 AM | 1.0 | 25.0000 | 2.135 | 4716 | 91.48 | | 26.9159 | 26.9159 | 107.7 | 25.[illegible] | 60.79 | | 2.121 | 1196 | 31.1 | 91.84 | |
| ! | | Sample-1 | Sample | | 11/11/2006 11:50 AM | 1.0 | | | | | | | | | | | | | | | | |
| | | Sample-2 | Sample | | 11/11/2006 11:55 AM | 1.0 | | 2.143 | 1004 | 80.65 | | 3.7144 | 3.7144 | | 30.9 | 70.54 | | 2.130 | 1445 | 25.7 | 29.89 | |
| | | Sample-3 | Sample | | 11/11/2006 11:59 AM | 1.0 | | 2.105 | 2590 | 74.97 | | 13.1551 | 13.1551 | | 25.3 | 65.40 | | 2.089 | 1284 | 29.8 | 129.91 | |

**Quantitation Message(s)**

Amp-d5: Integrator did not find any peaks
Amp-d5: Qualifier M/Z = 124.4: Qualifier peak not found or does not match quantitation criteria
Cocaine-d3: Integrator did not find any peaks
Cocaine-d3: Qualifier M/Z = 85.0: Qualifier peak not found or does not match quantitation criteria
Meth-d5: Qualifier M/Z = 121.4: Integrator did not find any peaks

**These icons filter outliers in the display.**

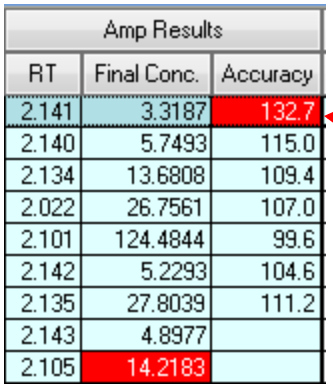
**Outlier(s)** **Blue = low / Red = high**

Amp: Qualifier ratio = 33.5 is outside the allowed range [21.2, 31.8]

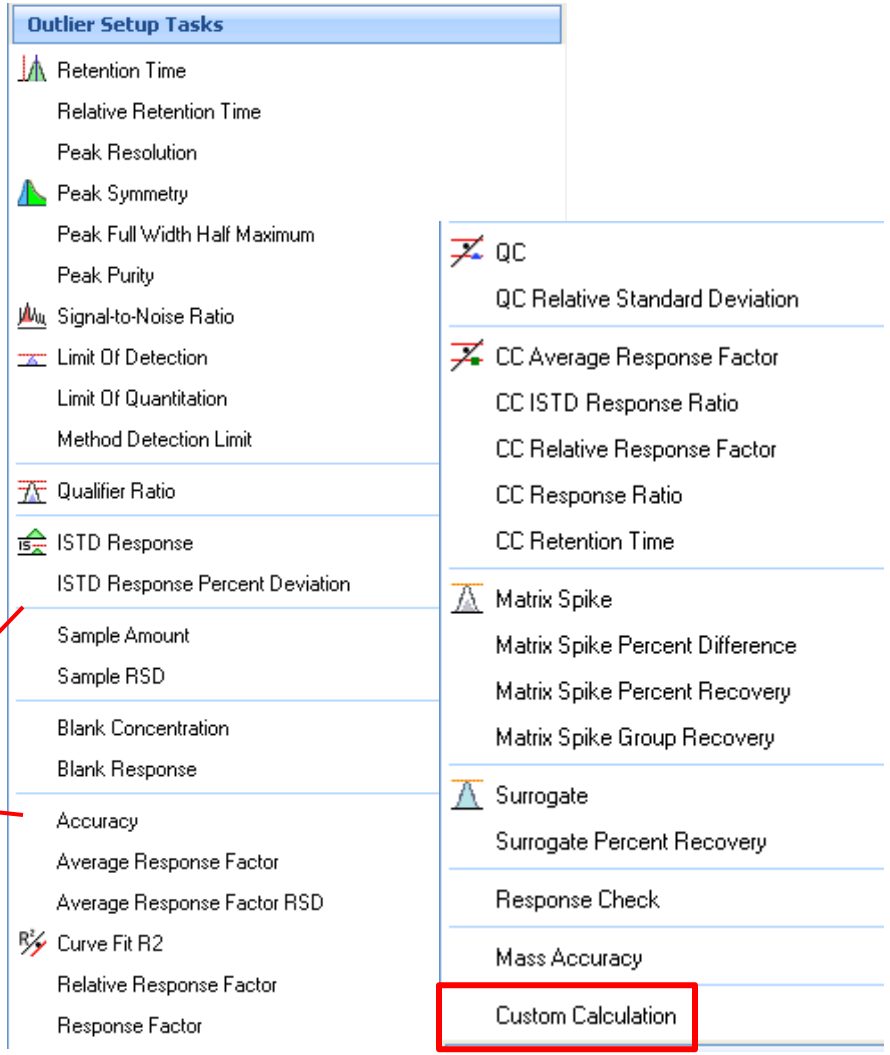
**"Outliers" define and specify results of known problem samples/substances that fall outside predefined conditions.**

# Results Information: Outlier Options

- **39 quality checks can be specified to highlight outliers in results.**
- **Can set high and low limits.**
- **User defined quality check can be added to predefined calculations.**

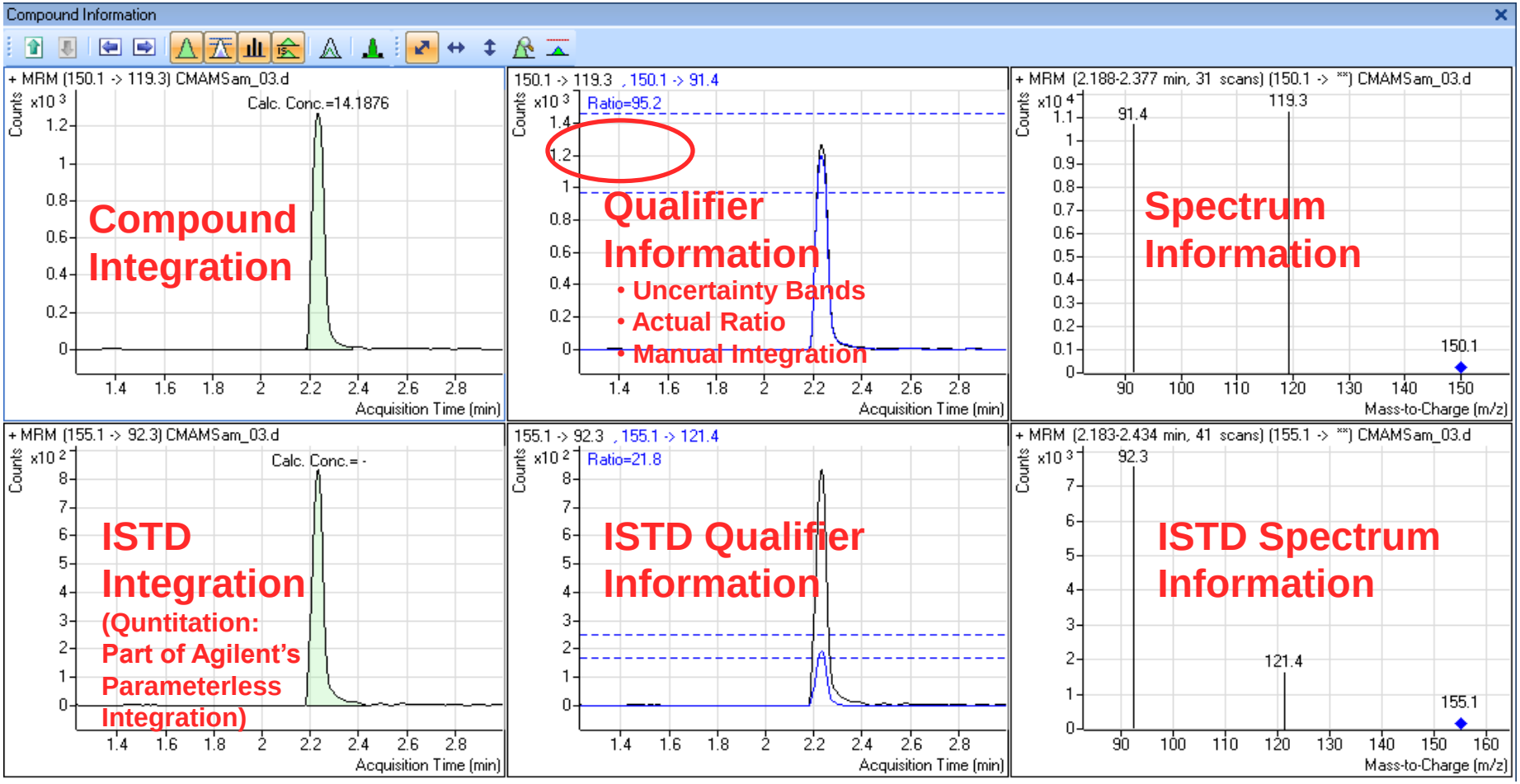


| Amp Results | | |
|---|---|---|
| RT | Final Conc. | Accuracy |
| 2.141 | 3.3187 | 132.7 |
| 2.140 | 5.7493 | 115.0 |
| 2.134 | 13.6808 | 109.4 |
| 2.022 | 26.7561 | 107.0 |
| 2.101 | 124.4844 | 99.6 |
| 2.142 | 5.2293 | 104.6 |
| 2.135 | 27.8039 | 111.2 |
| 2.143 | 4.8977 | |
| 2.105 | 14.2183 | |



# Batch Screen - Compound Information

**Compound information displays all relevant information in one view.**



# Batch Screen – Calibration Curve

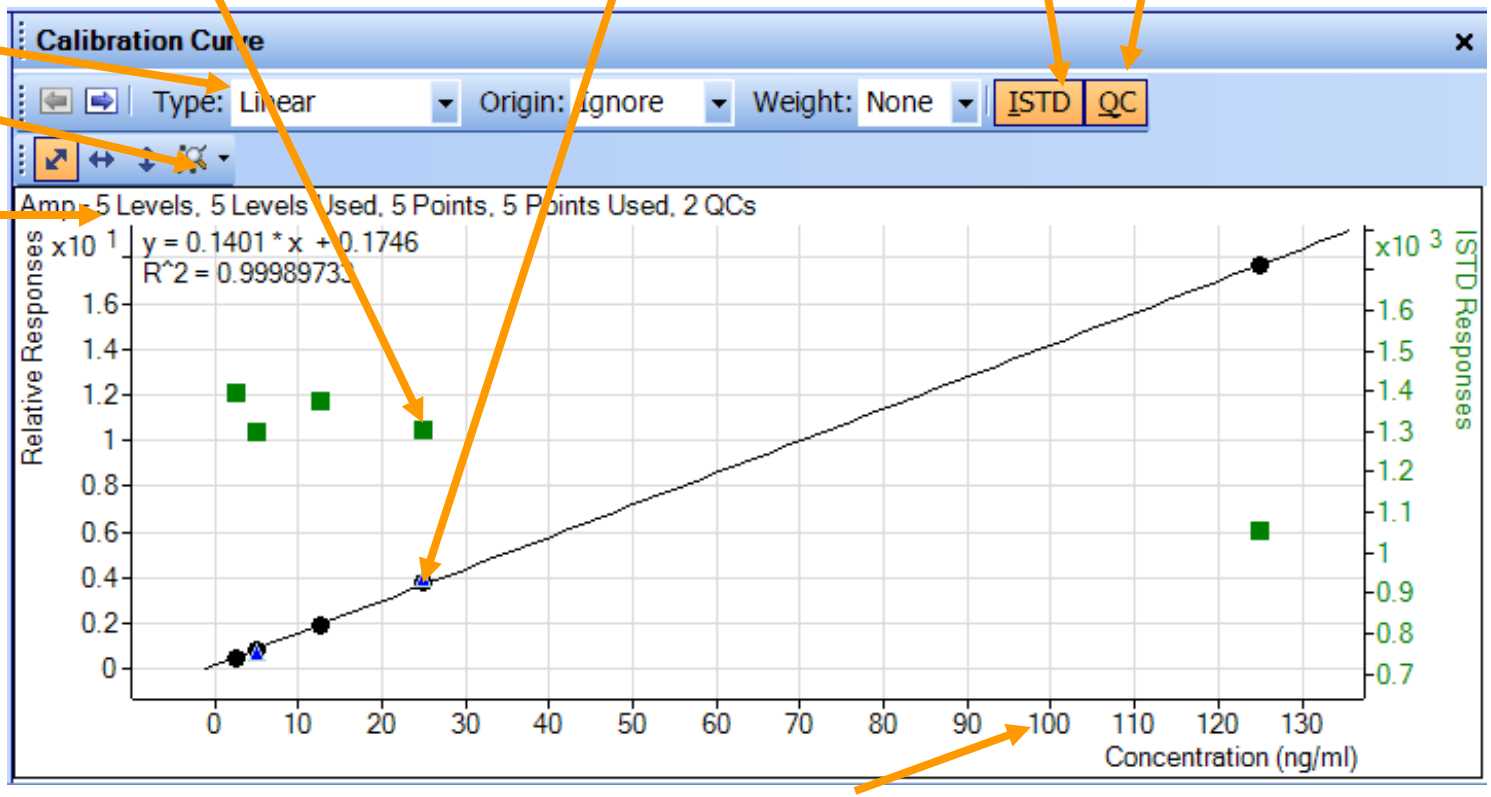
**An example of Batch Information is this view of the Calibration Curve. The Curve fit can be changed and data can be updated instantaneously.**

**View ISTD responses or display QC samples - click either the ISD or QC button.**

**Change Curve Fit**

**Zoom in/out button (right click/drag)**

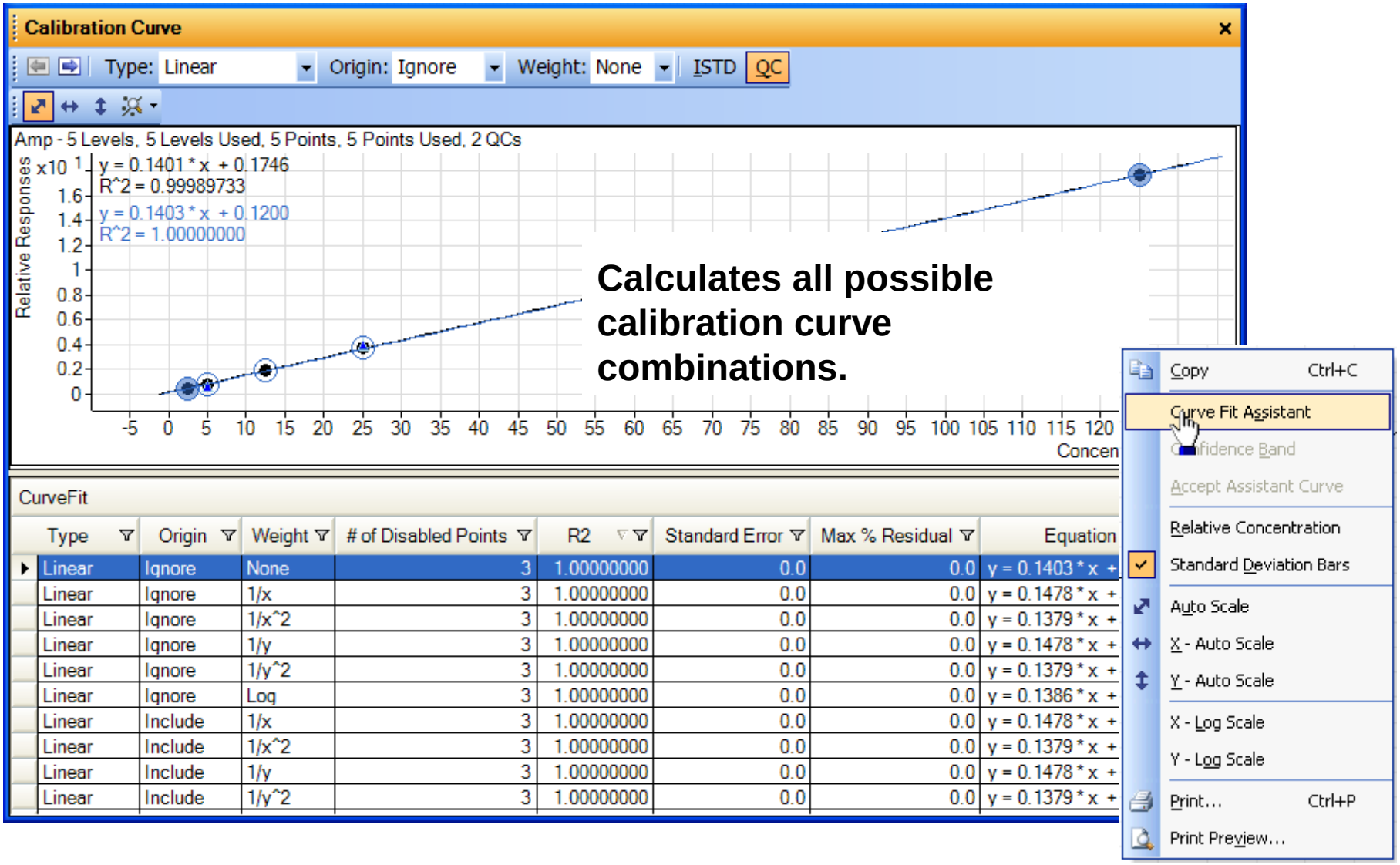
**$R^2$.**




**After editing the calibration curve, you must reanalyze the batch.**

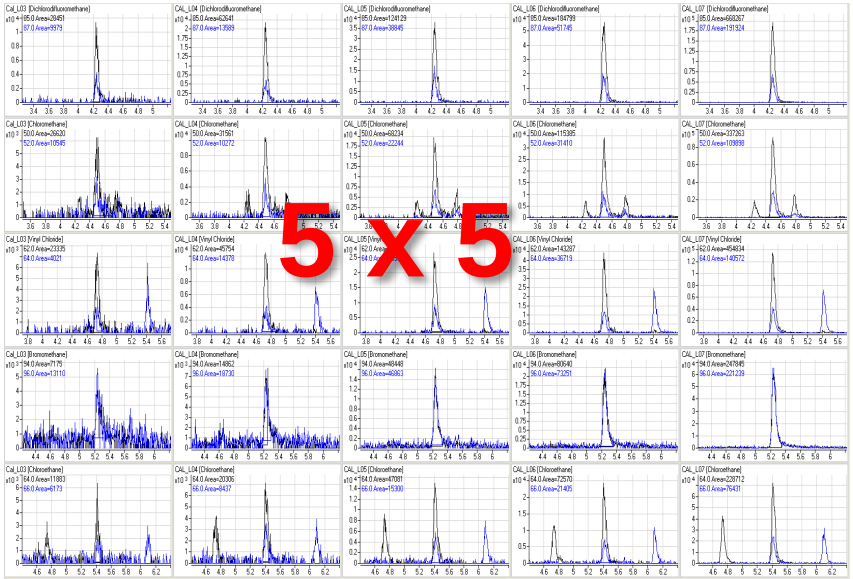
**Concentration can be set as relative (to ISTD) or actual.**

# Batch Screen - Curve Fit Assistant



# Compounds-at-a-Glance

**Compounds-at-a-Glance allows you to view multiple traces of compounds at a single glance.**

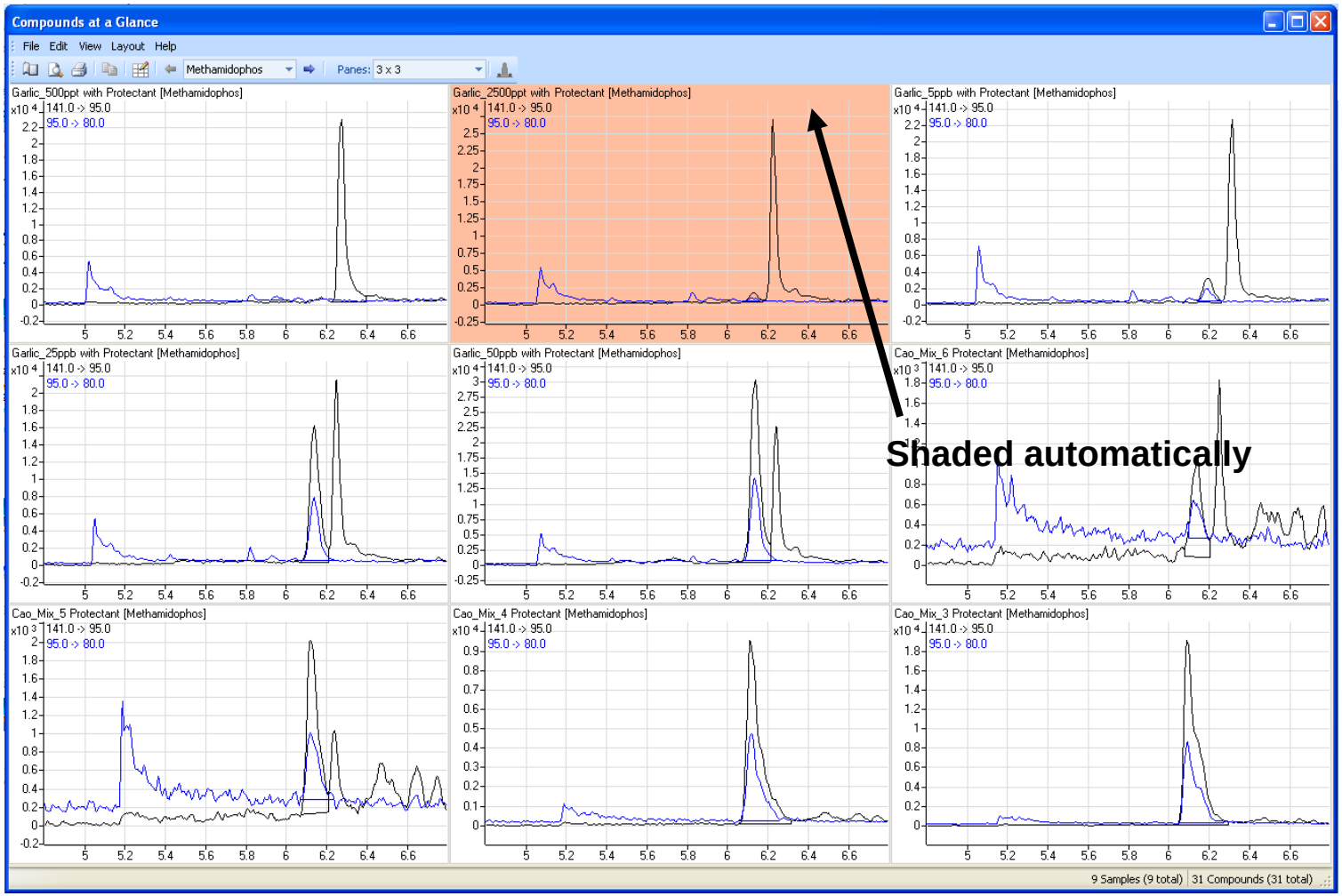




- View up to 10 x 10 chromatograms
- Overlay Target with ISTD
- Overlay Quantifier with Qualifiers
- View chromatograms across 100 samples

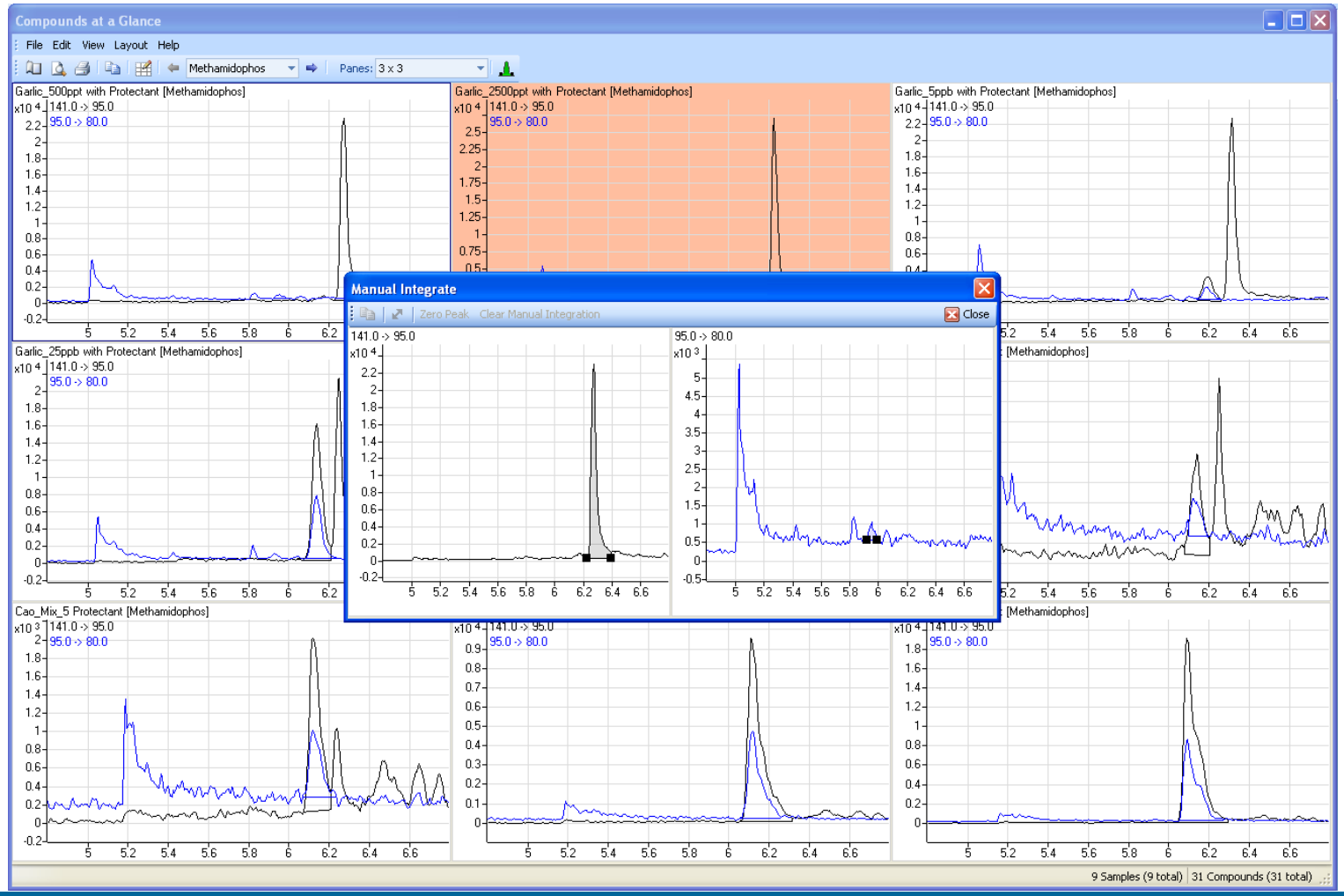
# Compounds-at-a-Glance

**You can view compound outliers at-a-glance too.**



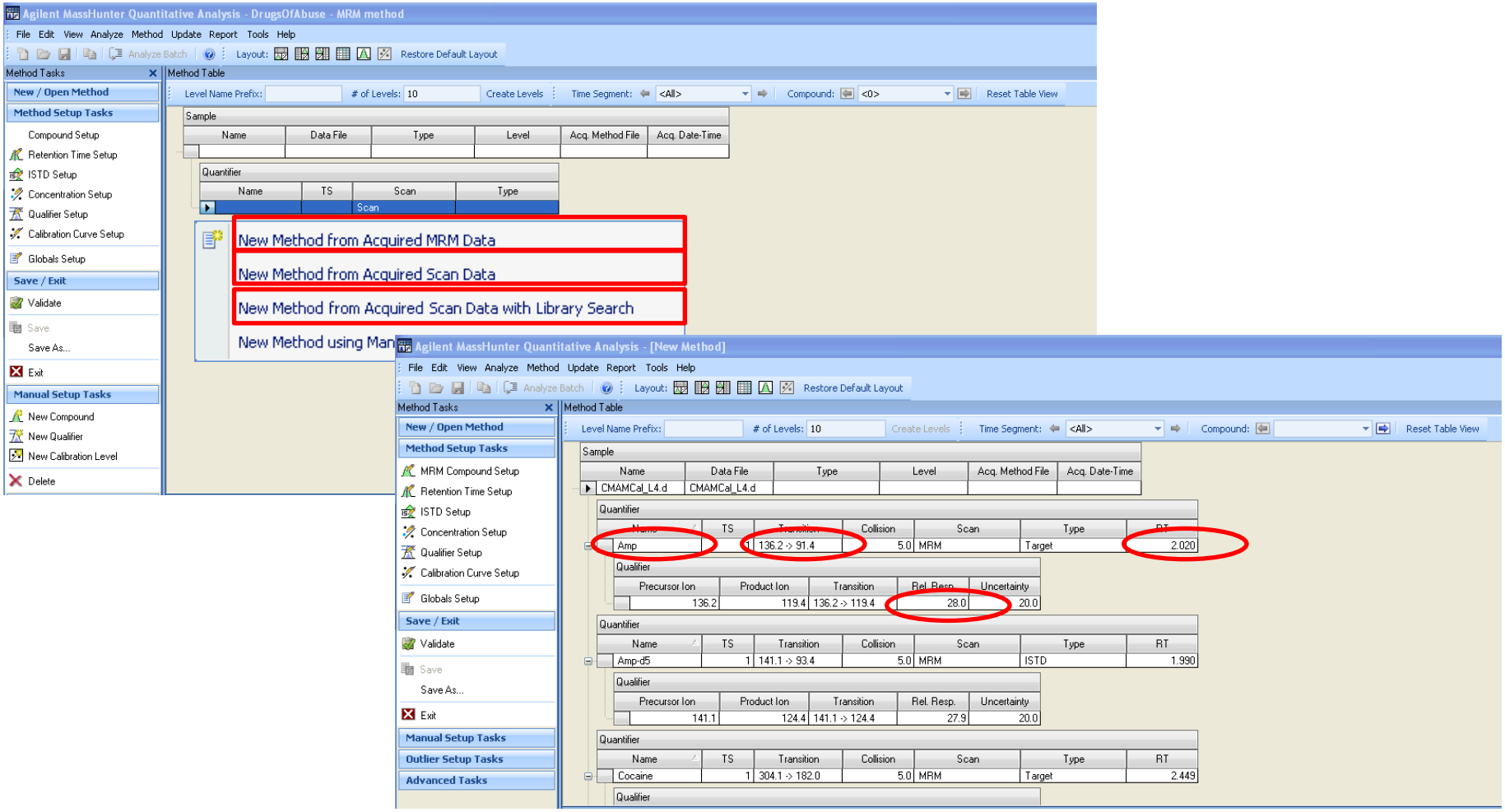
# Compounds-at-a-Glance

**You can view the manual integration of compounds at a glance too.**



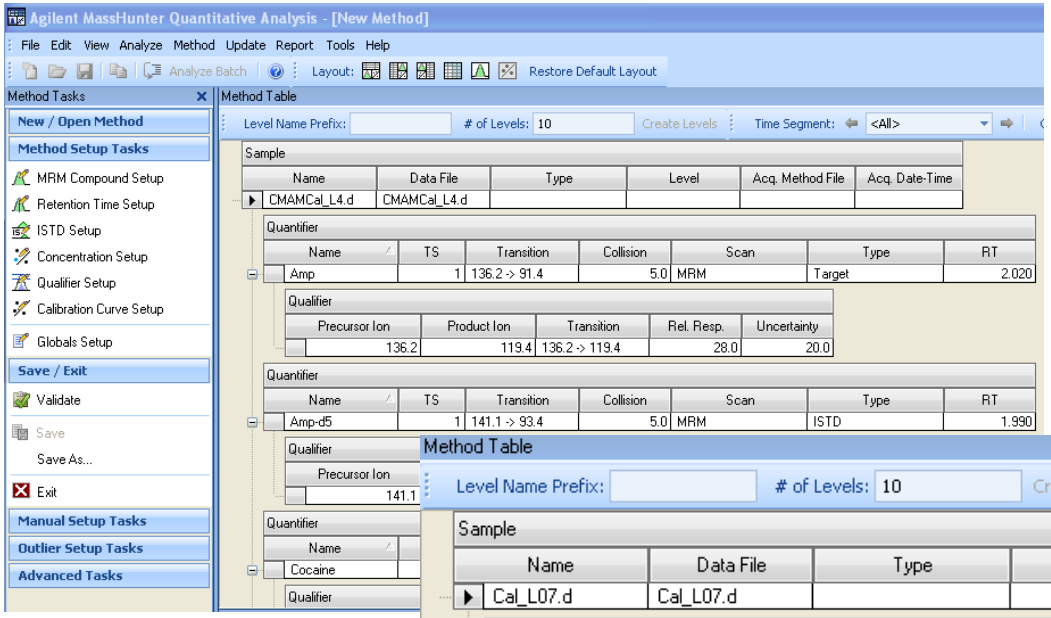
# Quantitation Method Creation

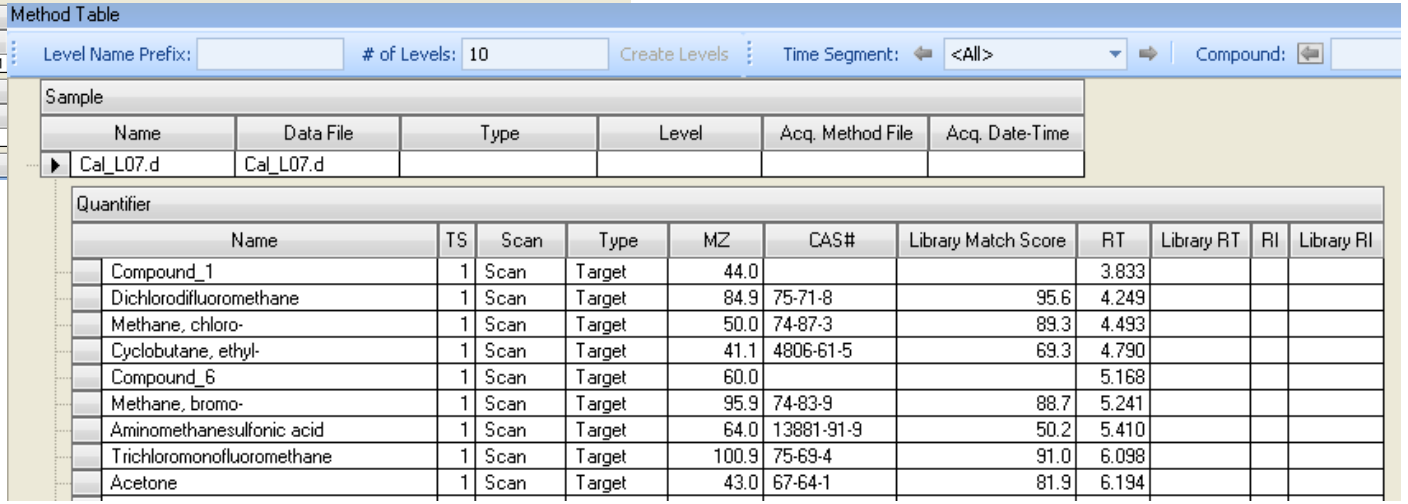
Easy way to create a target method from acquired data (MRM, SIM or Scan).
Using information from a data file, MassHunter Quant can create a target compound list - generating Compound Name, Retention Time, Quant and Qual ions, and ratios automatically.



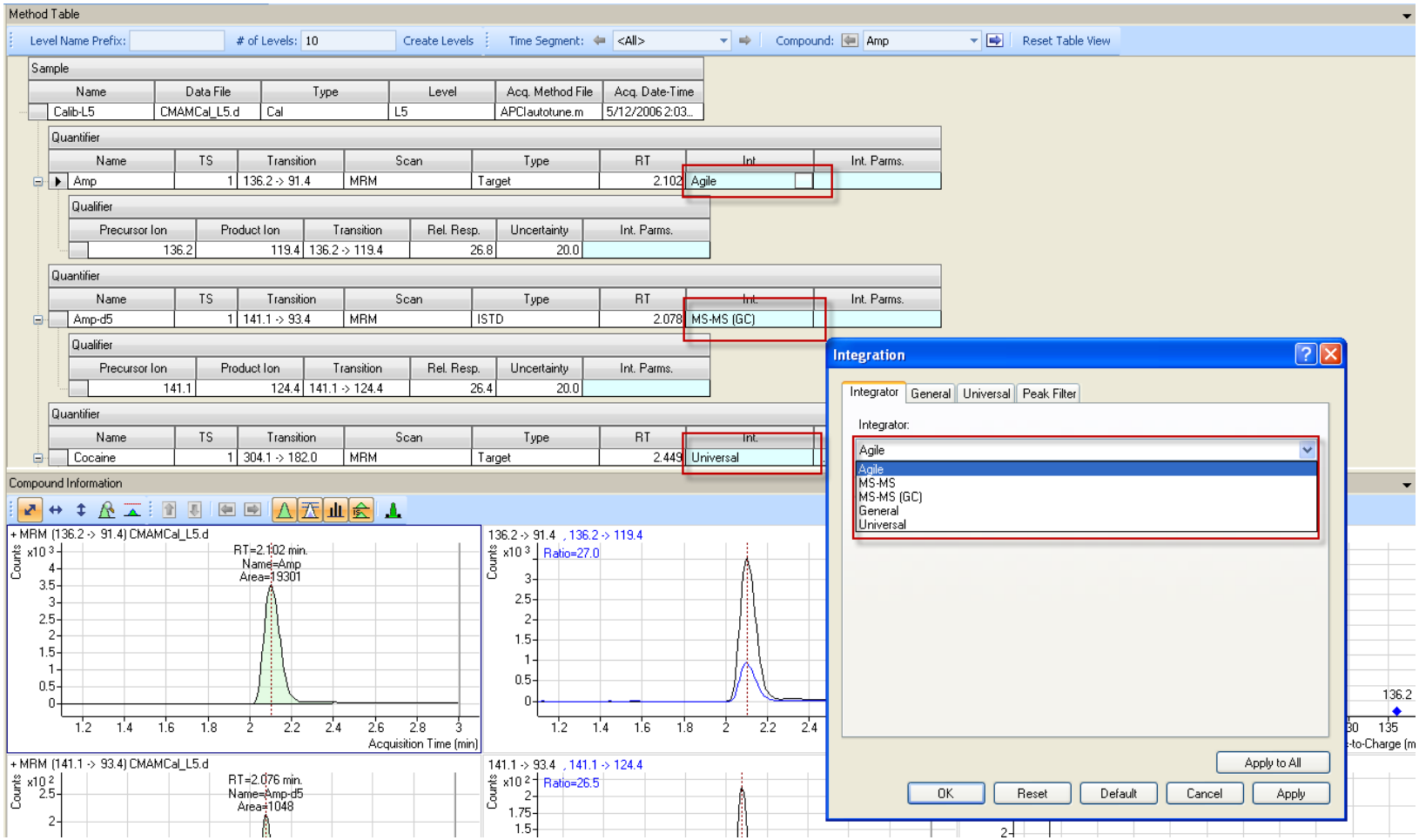
# Automatic Compound Detection – Scan Data

Automatic compound detection works with both MRM and Scan data.
For scan data, Library information can be used to add compound name and CAS#;
The Quant and Qual ions and ratios are taken from the data file information.



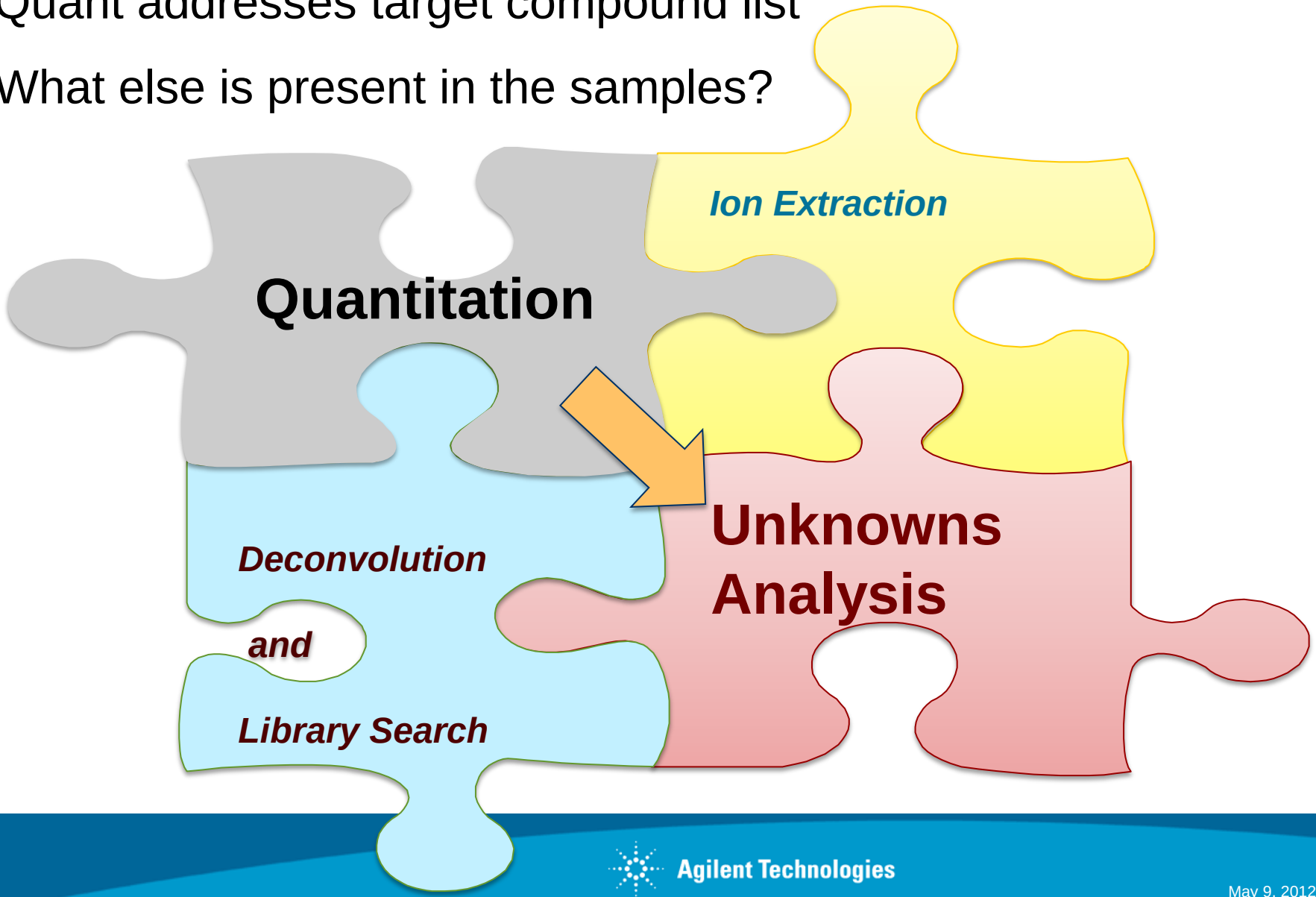
# Multiple Integrators / Compound Specific



# Overview of Unknowns Analysis

Quant addresses target compound list

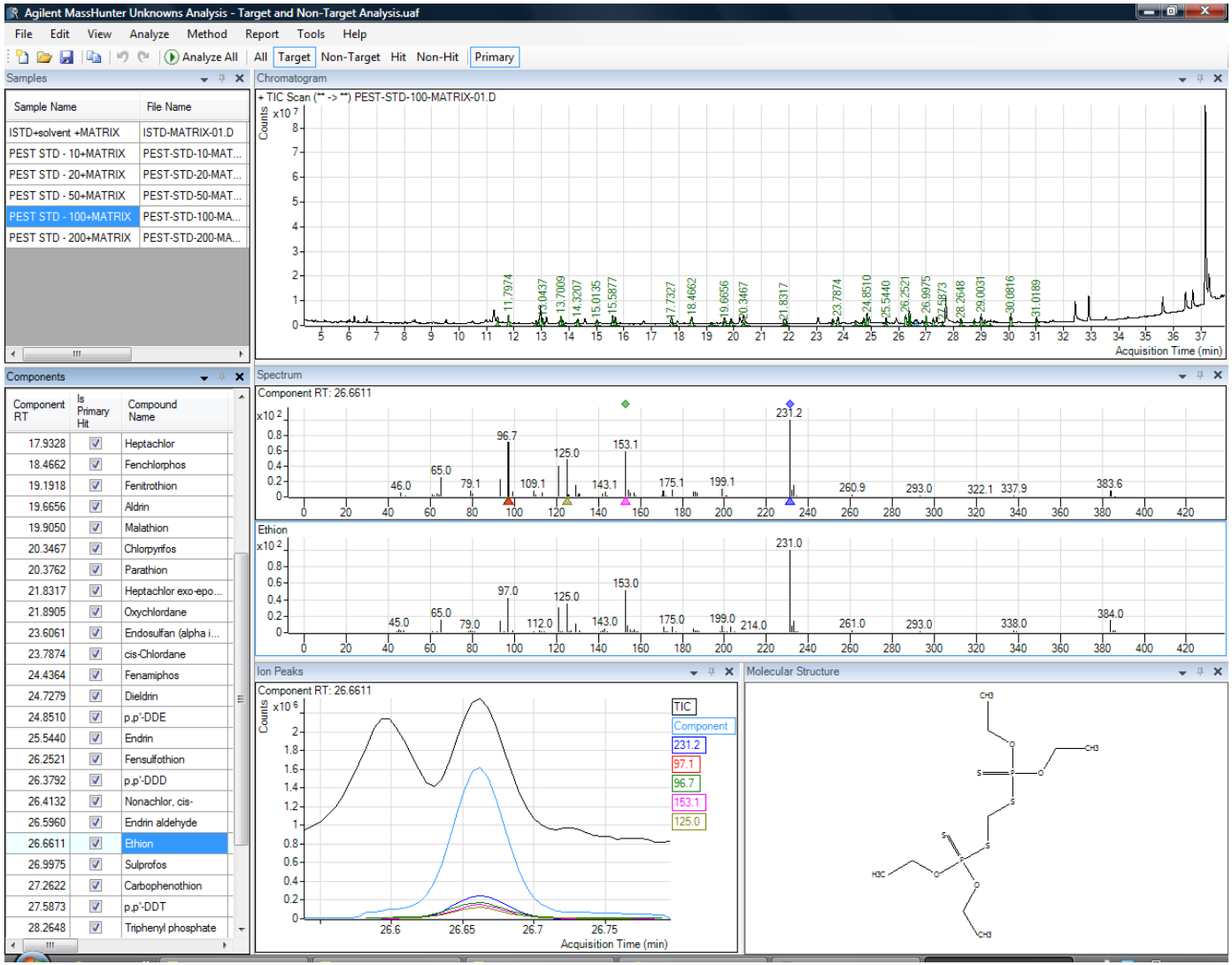
What else is present in the samples?

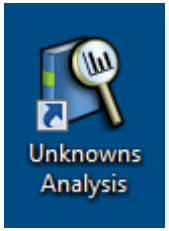


# Unknowns Analysis Workflow

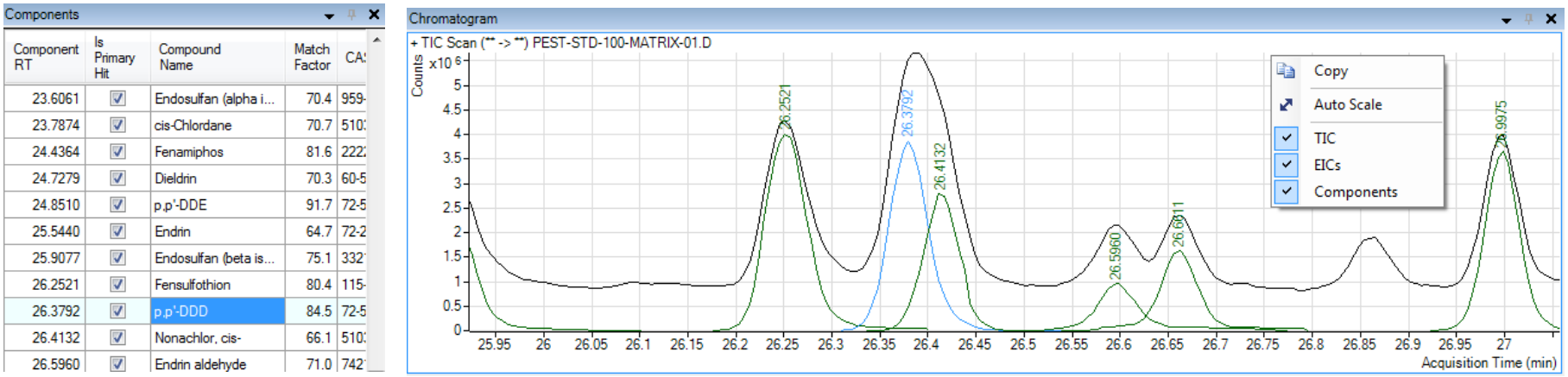
- Process batch of samples in Quantitative Analysis
- Run Unknowns Analysis
- Analyze
  - Perform **deconvolution** to create **components**
  - Perform **library matching** on components, assign compound ID
  - Link **components to Quant target** compounds from
  - Assign **estimated concentrations** to non target components
- Review data
  - View component and library spectra
  - View molecular structure vs. spectrum
  - View ion peak shapes vs. component peak shape vs. TIC
  - Edit components (change compound ID, delete)
  - Run queries for custom review
- Print Report

# Unknowns Analysis



# Chromatogram




Chromatogram displays selected component(s) in Blue

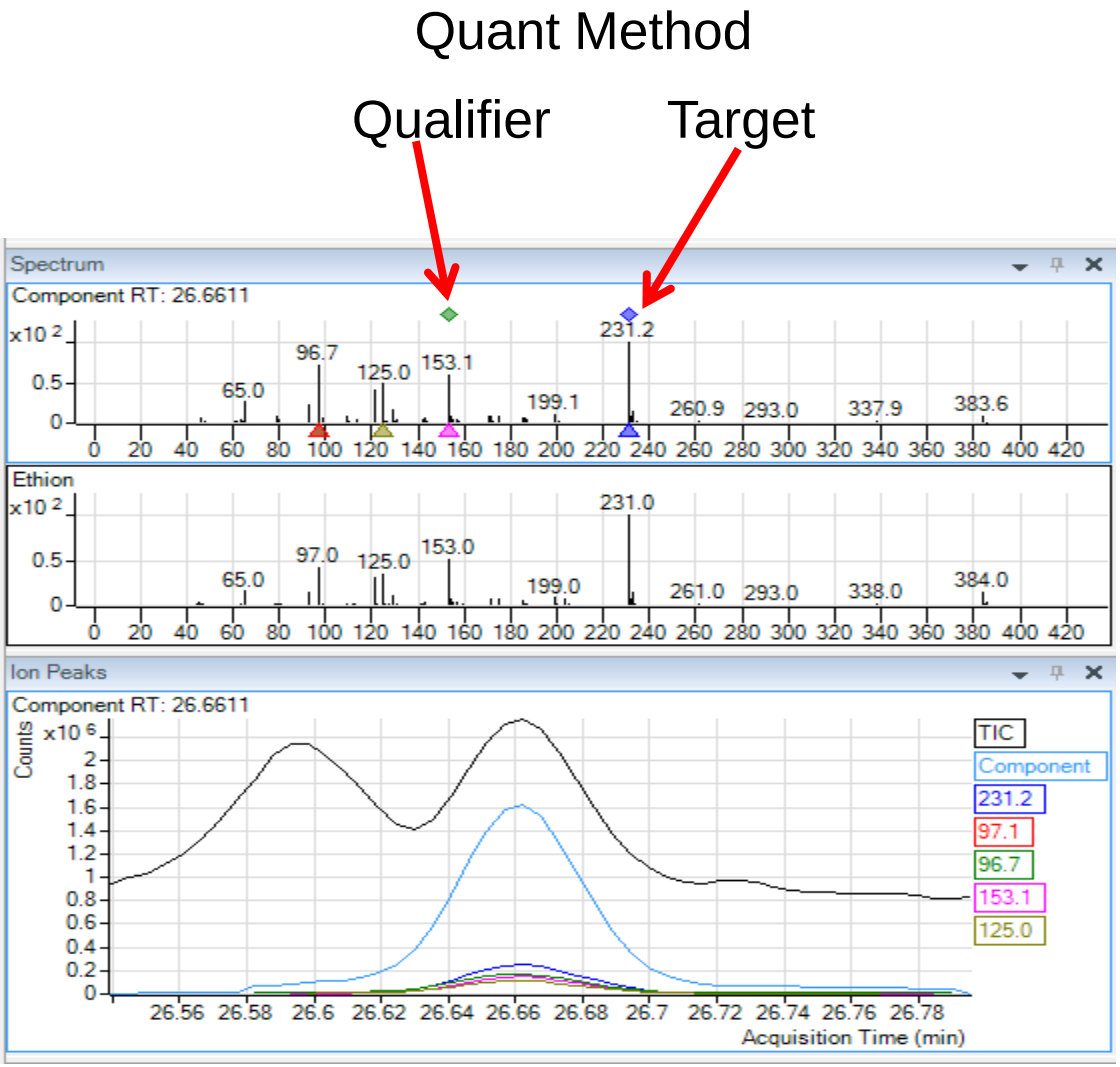
All non-selected ions (EIC) displayed in Green

TIC displayed in **Black**

Clicking in the Chromatogram display selects the nearest peak and selects it in Components table

# Spectrum & Ion Peaks

- Default number ions displayed in Ions Peaks is 5, limit is 10
- Click on ion in Spectrum to make it add / remove in Ion Peaks
- Click on label in Spectrum or Ion Peaks to remove






Agilent Technologies

# Outline of Topics

Topic 1: Introduction to MassHunter

Topic 2: Data Acquisition / Conversion

Topic 3: Qualitative Analysis

Topic 4: Quantitative Analysis

**Topic 5: Reporting**

Q & A

# MassHunter Excel Reporting

- Excel Based (Excel 2007 & 2010 supported)
- MassHunter application exports data in XML and graphics files
- Templates define report formatting
- Over 100 shipping report templates
- Reports can be altered for desired information & appearance
- Customization using Excel features (function, formatting, code)
- Computer Based Training for report customization by users
- Some customization available through Agilent

# Shipping Quant 5.0 Templates

90 Shipping Quant Templates - 14 “New” Templates added for B.05 release

English (Letter & A4), Chinese (A4), Japanese (A4)

Significant new templates for

- Compliance (1)
- DrugQuant (2)
- EnviroQuant (2)
- Unknowns Analysis (4)

Mockup reports for both PDF and XLSX formats

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | DIR | SUBDIR | FAST | ExcelTemplate | ExcelWorkbook | PDF |
| 2 | ESTD | Parts | FAST | QuantReport_ESTD_Summary_FAST_B_04_00.xltx | HyperLink to Workbook (.xlsx) | HyperLink to Adobe Acrob |
| 3 | ESTD | Parts | | QuantReport_ESTD_Summary_B_04_00.xltx | HyperLink to Workbook (.xlsx) | HyperLink to Adobe Acrob |
| 4 | ESTD | Parts | FAST | QuantReport_ESTD_Samples_FAST_B_04_00.xltx | | |
| 5 | ESTD | Parts | | QuantReport_ESTD_Samples_B_04_00.xltx | | |
| 6 | ESTD | Results | FAST | QuantReport_ESTD_ResultsSummary_FAST_B_04_00.xltx | | |
| 7 | ESTD | Results | | QuantReport_ESTD_ResultsSummary_B_04_00.xltx | | |
| 8 | ESTD | Results | FAST | QuantReport_ESTD_ResultsQualifierRatios_FAST_B_04_00.xltx | | |
| 9 | ESTD | Results | | QuantReport_ESTD_ResultsQualifierRatios_B_04_00.xltx | | |
| 10 | ESTD | Results | FAST | QuantReport_ESTD_ResultsComplete_FAST_B_04_00.xltx | | |
| 11 | ESTD | Results | | QuantReport_ESTD_ResultsComplete_B_04_00.xltx | | |
| 12 | ESTD | Results | FAST | QuantReport_ESTD_ResultsByCompound_FAST_B_04_00.xltx | | |
| 13 | ESTD | Results | | QuantReport_ESTD_ResultsByCompound_B_04_00.xltx | | |
| 14 | ESTD | NotDetected | FAST | QuantReport_ESTD_NotDetected_FAST_B_04_00.xltx | | |
| 15 | ESTD | NotDetected | | QuantReport_ESTD_NotDetected_B_04_00.xltx | | |

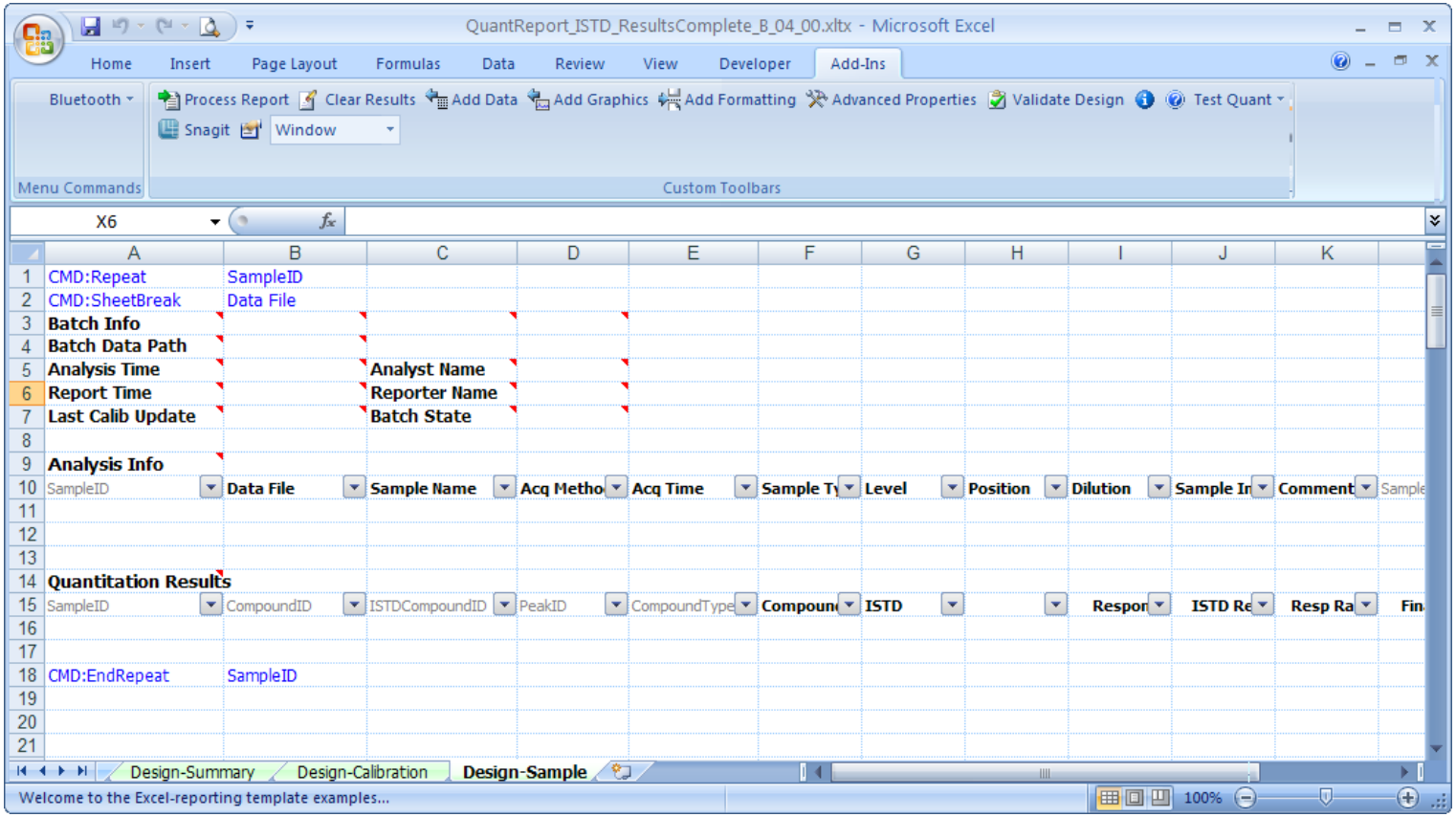
Sample Sheet(s)

Batch Info
record batch identification information
Analyze Info
show sample specific information
Sample Chromatogram
Include sample chromatogram graphic
Quantitation Results
list results and concentration for compounds
Compound Graphics
display compound graphics for each compound

# Report Template Design Worksheets

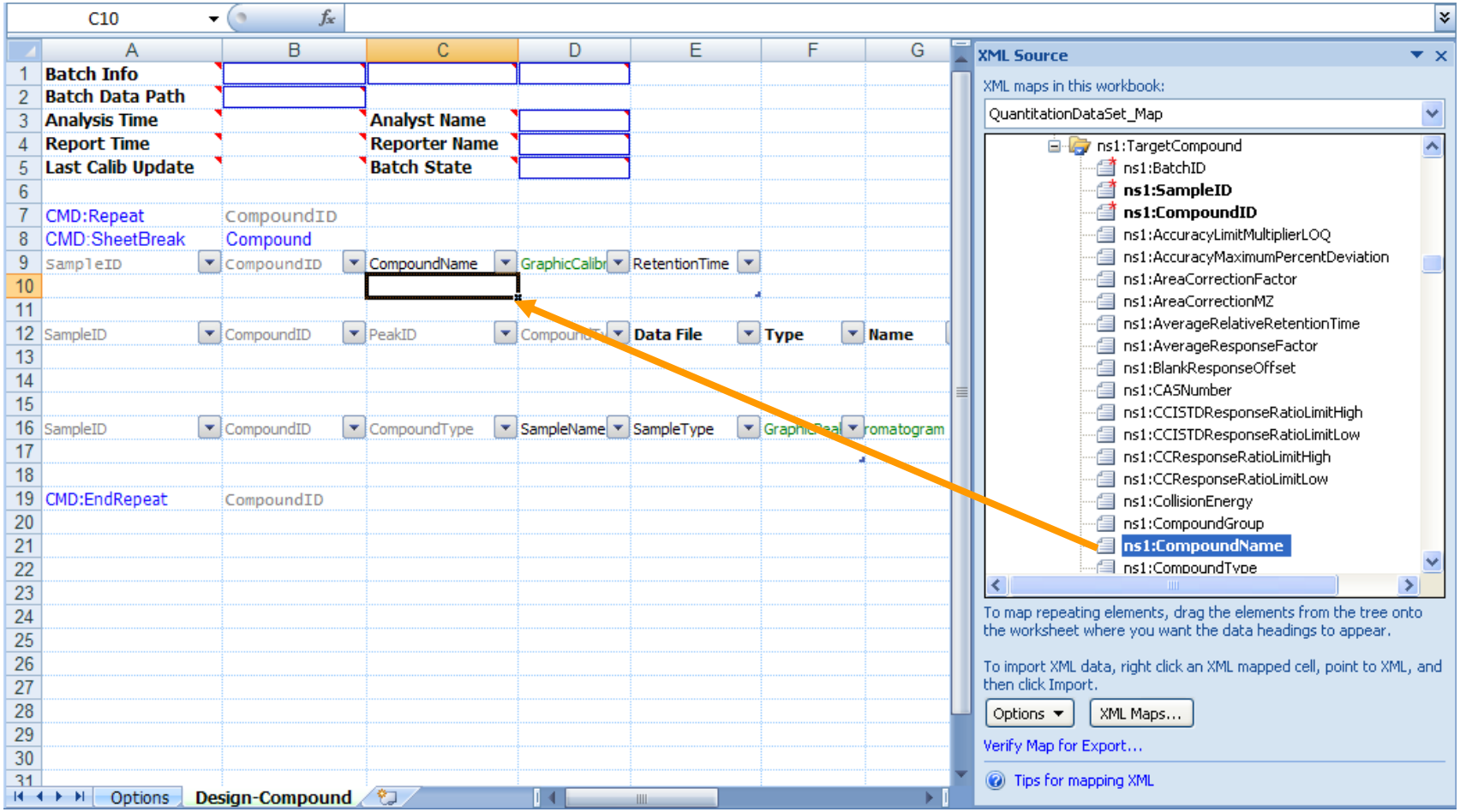
Customize the template by placing data and graphics in the desired locations

Templates may have multiple Design worksheets with different layouts



# Excel XML Source Window

- Reporting uses XML mapping to import results into templates
- Drag and drop to add data to existing reports



# MassHunter Reporting User Information (CBT)

Agilent Technologies

Agilent MassHunter
Reporting User Information

MassHunter Reporting
User Information

**Welcome to Agilent MassHunter Reporting User Information**

Whether you want to use preconfigured reports or customize templates for special applications, this collection brings together all the training for MassHunter reporting in one location.

**MassHunter Reporting Training**

Read it, see it, hear it, do it! This self-paced curriculum incorporates multiple formats, to reinforce concepts and to allow you to adapt the training to your unique learning style. The MassHunter Reporting Training provides:

- Written topics that summarize procedures
- Demo movies to show you how to use the software
- Software reviews that allow you to interact with the programs
- No-fail quizzes with instant feedback

In addition, this DVD includes:

- Comprehensive familiarization exercises that guide you through the software step-by-step – and provide tips along the way
- Extensive online Help for MassHunter Reporting
  - Quantitative
  - Qualitative
- A list of the demo movies, for quick access

**Where do I start?**

While you can customize your path through the training, we recommend the following:

1. Start with the MassHunter Reporting Training and follow the suggested order of topics.
2. Next, work through the Familiarization Guide to solidify your knowledge. Do all the familiarization exercises at once, or intersperse them with the Reporting Training, where the topics tell you when a familiarization exercise is available.
3. When you perform a task for the first time or forget how to do it later:
   - Consult the online Help for MassHunter Reporting, which you can access from this DVD or directly from the Add-Ins tab in Microsoft® Excel.
   - View the list of the demo movies to select one for a quick refresher.

**Quick Access**

Reporting Training

Familiarization Guide

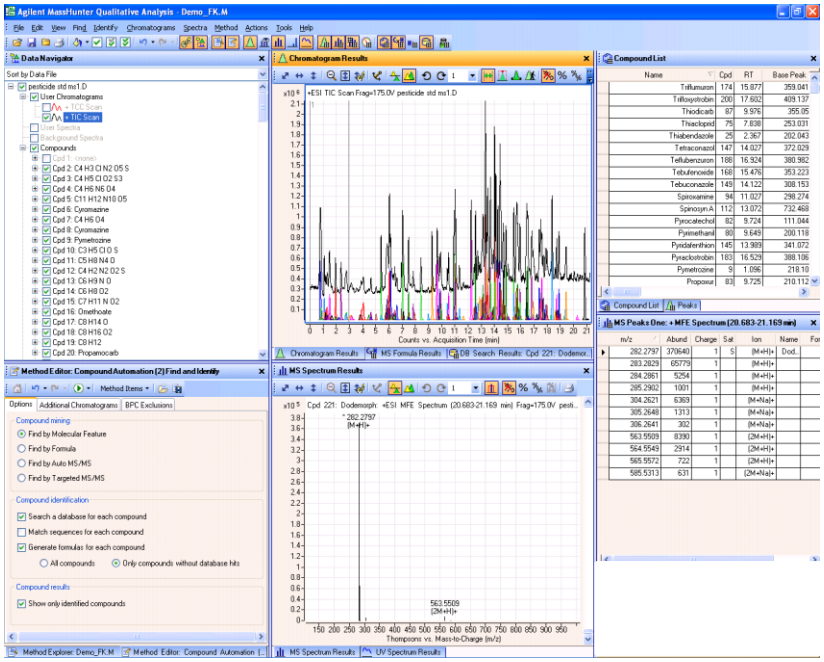
Reporting Help - Quant

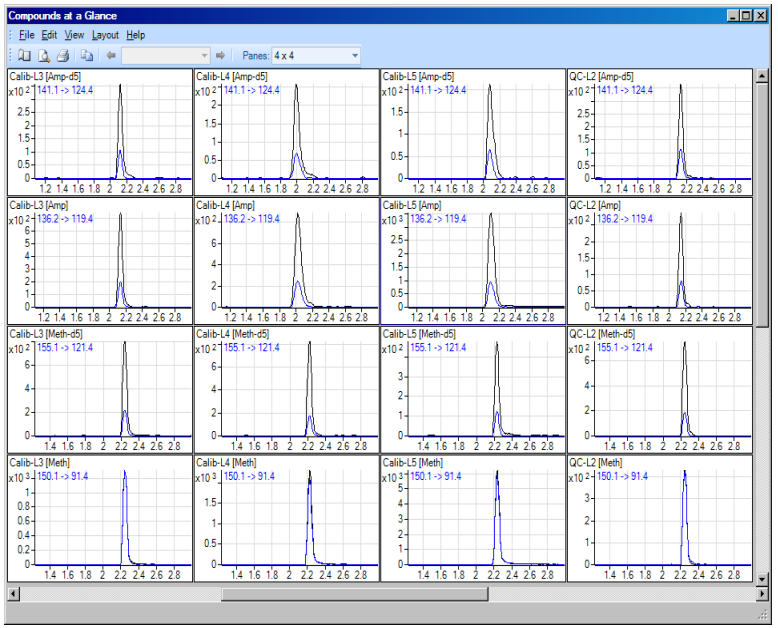
Reporting Help - Qual

List of Demo Movies

# MassHunter Workstation

## Increase your productivity significantly




# Questions?

Terry is available today for questions, software demos and problem solving.



Agilent Technologies