MassHunter for Agilent GC/MS & GC/MS/MS Next Generation Data Analysis Software

Presented by:
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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’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
Quantitative (Quant) and Qualitative (Qual) analysis modules can process data from any Agilent MassHunter software system.
Agilent GC/MS
Deploying MassHunter Software
Agilent GC/MS/MS
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 converts 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

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 receive a copy
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Q & A
MassHunter WorkStation Qualitative Analysis

Data Navigator

Chromatogram Results

Method Explorer

Method Editor

Spectrum Results

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
Find Compound by Chromatogram Deconvolution

- Agilent deconvolution algorithm similar to AMDIS but not equivalent
- Creates Compounds with chromatographic and spectral components
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 search.

User can overwrite reported compound.
Structures available and added to Spectra.
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
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

- Chromatogram
- Spectrum
- General
  - Analysis Report
  - Compound Report
  - Common Reporting Options
  - File Open Actions
    - Extraction Data Format
  - Find Compounds
  - Identify Compounds
  - Compound Automation Steps
  - Worklist Automation
  - Export

Available actions:
- Integrate Chromatograms
- Integrate and Extract Peak Spectra
- Smooth Chromatograms
- Generate Compound Report
- Generate Analysis Report
- Find Compounds by Chromatographic Deconvolution
- Correlate UV Chromatograms with Compounds

Actions to be run:
- Extract Defined Chromatograms
- Integrate and Extract Peak Spectra
- Generate Analysis Report
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Q & A
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.
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.

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

- Compound Integration
- ISTD Integration (Quantitation: Part of Agilent’s Parameterless Integration)
- Qualifier Information:
  - Uncertainty Bands
  - Actual Ratio
  - Manual Integration
- ISTD Qualifier Information
- ISTD Spectrum Information

Agilent Technologies
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

Calculates all possible calibration curve combinations.

<table>
<thead>
<tr>
<th>Type</th>
<th>Origin</th>
<th>Weight</th>
<th># of Disabled Points</th>
<th>R2</th>
<th>Standard Error</th>
<th>Max % Residual</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>Ignore</td>
<td>None</td>
<td>3</td>
<td>1.000000</td>
<td>0.0</td>
<td>0.0</td>
<td>y = 0.1403*x + 0.1746</td>
</tr>
<tr>
<td>Linear</td>
<td>Ignore</td>
<td>1/x</td>
<td>3</td>
<td>1.000000</td>
<td>0.0</td>
<td>0.0</td>
<td>y = 0.1478*x + 0.1200</td>
</tr>
<tr>
<td>Linear</td>
<td>Ignore</td>
<td>1/x^2</td>
<td>3</td>
<td>1.000000</td>
<td>0.0</td>
<td>0.0</td>
<td>y = 0.1379*x + 0.000000</td>
</tr>
<tr>
<td>Linear</td>
<td>Ignore</td>
<td>1/y</td>
<td>3</td>
<td>1.000000</td>
<td>0.0</td>
<td>0.0</td>
<td>y = 0.1478*x + 0.1200</td>
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</tr>
<tr>
<td>Linear</td>
<td>Include</td>
<td>1/x</td>
<td>3</td>
<td>1.000000</td>
<td>0.0</td>
<td>0.0</td>
<td>y = 0.1478*x + 0.1200</td>
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</tr>
</tbody>
</table>
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 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 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
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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
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

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.
MassHunter Workstation
Increase your productivity significantly

Questions?

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