MassHunter Data Analysis on Single Quad - An Introduction

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Agilent Technologies
Agilent GC/MS
Deploying MassHunter Software
Agilent GC/MS/MS
MassHunter GC/MSD Rollout Plan

Feb 2013:
- Add GC/MSD systems
  - 5975 & 5977 Series GC/MSD
  - 7890B & 7820A
  - 7697A HSS
- Continue MassHunter GC/MS and GC support
  - 7000 Series Triple Quad GC/MS
  - 7200 Series Q-TOF GC/MS
- MH DrugQuant
- GC and GC/MSD Data Analysis with MassHunter OR MSD ChemStation modes

Late 2013:
- Expand Compatibility
  - 5973 Network
  - 6890 Network & 6850 GC
- MH EnviroQuant
Delivering Data to MassHunter Data Analysis

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

Chem Station
Single Quad LC/MS

Chem Station
5975 and Earlier Single Quad CG/MS (MSD)

LC/MS Acquisition Module
Triple Quad LC/MS, LC/TOF, LC/QTOF

GC/MS Acquisition Module
5975 and 5977A MSD, Triple Quad GC/MS, GCMS Q-TOF

MassHunter

Quant & Qual Modules

LC/MSD & GC/MSD data can be translated into the MassHunter format.
Migrate Data to MassHunter Format

- GC MSD Translator
- MSWS Data Translator
- GC AIA Translator

Data

MassHunter Quant

MassHunter Unknowns Analysis

ChemStation (.D)

WorkStation (.SMS)

Generic (.CDF)
Migrate Quantitative Methods to MassHunter Format

ChemStation (QDB.MTH)

WorkStation (.mth)

MassHunter Quant
MassHunter Benefits

Unified Software for Agilent Instruments

• Cross Instrument Training
  – Reduce long term training costs
  – Flexible Staffing and Scheduling
• Lab Expansion and Diversification
  – GC/MSD & LC/TOF … same software
  – Grow you market presence or expand your product offering.
• Modern software technologies using Industry Standards
  – i.e. data exchange via XML
  – MS Excel Reporting
  – Microsoft Scripting in “Visual Studio C#” etc.
• Productivity And Quality Enhancement
  – Quant: Batch-at-a-Glance, Compounds-at-a-Glance, Quality Metric Checking with outlier flags, parameterless integration, Quant method building tools (Create method from …)
  – Qual: Integrated deconvolution, flexible data layout and display,
MassHunter GC/MS Acquisition With ChemStation Data Analysis

MSD ChemStation remains supported software for MSD

ChemStation will have service packs and patches but no significant enhancements are planned

Migration to MassHunter will be driven by user preference, product benefits and users timeframe
MassHunter GC/MS Acquisition for GC/MSD

Unified GC/MS Acquisition and MassHunter Data Analysis; with MSD ChemStation workflow for GC/MSD

Familiar GC/MS Acquisition

Simplified MSD Method Editor

Comprehensive EMF (Including MS)

New GC Driver with Integrated Calculators

Agilent Technologies
GC/MSD Software

Both DA Applications preinstalled, Customer’s Choice! G1701FA
<table>
<thead>
<tr>
<th>MSD ChemStation</th>
<th>MassHunter</th>
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<tbody>
<tr>
<td><strong>Established</strong> Agilent GC/MSD User</td>
<td><strong>New to Agilent or GC/MSD</strong></td>
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<tr>
<td>– Adding instrument to <strong>routine</strong> production</td>
<td>– Competitive situation.</td>
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<tr>
<td>– <strong>Established</strong> workflows</td>
<td>– Looking for <strong>modern software</strong></td>
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<tr>
<td>– Macros, Macros, Macros</td>
<td><strong>Superior Quantitation</strong></td>
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<tr>
<td><strong>DRS</strong> or Screener DB</td>
<td><strong>21CFR11</strong> &amp; Other Regulated Labs</td>
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<tr>
<td><strong>EnviroQuant</strong> User</td>
<td><strong>Multi disciplinary</strong> MS lab</td>
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<tr>
<td>– Uses the US EPA workflow, especially reports and QA/QC criteria.</td>
<td>– Have Agilent Triple Quad or (Q-)TOF</td>
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<td>– <strong>MassHunter EnviroQuant</strong> targeted for late 2013</td>
<td>– LC/MS, ICP-MS, &amp; GC/MS</td>
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<td></td>
<td>– MS and MS/MS</td>
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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:
  
  - Compliance tools (Acquisition & Quant)
  - Unknown Analysis
  - Batch processing of deconvolution and library searching
    - Library editor
    - Method development assistants
    - Data Translators
MassHunter Acquisition

Familiar Look & Feel
New Sequence Table

User Customization of Sequence Fields
Configure for MassHunter or MSD ChemStation Automation
Consolidated GC/MSD Method Editor:

- Tune Selection and Preview
- Consolidated Detector Settings
- New Timed Events
Scan Method Editor

Tune Selection and Preview

Consolidated Detector Settings

Scan Table
SIM Method Editor

- **Tune Selection and Preview**
- **Consolidated Detector Settings**
- **SIM Ion Table**
- **SIM Table**

![Image of SIM Method Editor interface with highlights on different sections]
SIM/Scan

Tune Selection and Preview

Consolidated Detector Settings

Scan Table

SIM Table
MassHunter Data Analysis Software

MassHunters 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 El Libraries
Chromatogram Display

Comprehensive Display Options

• Display multiple Chromatograms, from one or many data files.

• Extract multiple signal types, i.e. TIC, EIC, FID, Instrument curves, etc.

• Annotate peaks or chromatograms with text or images

Definition of chromatograms can be stored in the method and used with automation.
Spectra

- Flexible Spectral Display and Identification

- Extract Spectra via:
  - Manual spectra selection
  - integrated peaks
  - Find-by tools, i.e. Deconvolution

- Identify Spectra from Library Searching
  - Multiple Libraries (*.L)
  - Link to NIST MS Search

- Background subtraction based on defined regions or peak definition
Find Compound by Chromatogram Deconvolution

- Integrated Agilent deconvolution
  - Creates Compounds with chromatographic and spectral components
Annotate and Document

- Annotate chromatograms and spectra using graphics (*.jpg), text, and chemical structures (.mol)
- Use Mass Caliper to document fragmentation and losses in spectrum
- Export or use copy & paste to add graphics or results into presentations and documents
Automation - File Open Actions & Post Acquisition Worklist Processing

- Automate common file open actions in manual review
- Standardize review processes
- Automate common actions, i.e. extract EIC.
- Define Qualitative methodology for sequence computation.
- No user interaction required.
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 contains a list of error messages that result from a compound's quantitation.

These icons filter outliers in the display.

“Outliers” define and specify results of known problem samples/substances that fall outside predefined conditions.
Results Information: Outlier Options

More than 40 quality checks can be specified to highlight outliers in results.

• Set high and low limits.

Custom Calculations can be added for User defined quality checks.
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
- Spectrum Information
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.  

Concentration can be set as relative (to ISTD) or actual.
Batch Screen - Curve Fit Assistant

Calculates all possible calibration curve combinations.
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
Compound Specific Integration Choice: Including parameterless integration
Microsoft Excel Based MassHunter Reporting

- Over 100 shipping report templates
- Templates define report formatting

- Customization using standard Excel features (function, formatting, code)
- Reports can be altered for desired information & appearance
- Computer Based Training for report customization by users
- Some customization available through Agilent
- Excel 2010 supported

- MassHunter application exports data in XML and graphics files for easy integration with third party software, i.e. LIMS.
MassHunter Quant Templates

Wide array of templates for different applications and uses

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

Application reports for LIMS output, compliance, Drug Analysis & EnviroQuant

Report Index:

• Summary of report template
Excel XML Source Window

• Reporting uses XML mapping to import results into templates
• Drag and drop to add data to existing reports
Agilent’s New SMA: Summary

• **Satisfies customer needs …**
  – Lower price
  – Increase value – new SMA includes updates **and upgrades**
  – Upgrades are included – completely eliminates confusion regarding updates and upgrades
  – Customers are automatically notified of all updates/upgrades

**Improved experience**

– Proactive notification to the customers when new software is available
– License management, notifications, and software download (or media request) through a single contact point (SubscribeNet)
– Customers can review software changes and apply software updates at any time when additional features add value to their work