MassHunter for AgilentNext GenerationGC/MS & GC/MS/MSData 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 El Libraries







Delivering Data to MassHunter Data Analysis

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











5975T LTM SQ

5975E SQ 7820 GC

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 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



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



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MassHunter WorkStation Qualitative Analysis





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 MassHunter Qualitative Analys	is B.04.00 - mh_testm
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Identify Compounds

Compound Automation Step

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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

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



Using NIST library matching from Qual

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Library Editor & Available Libraries

File Edit Tools Help

Compound ID

10

13

Max. # of panes: 1

29.0

20,00

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



Agilent provides over 15 El 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

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Compound Automation Steps	Integrate and Extract Peak Spectra Generate Analysis Report
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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.

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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.

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	0	Sample-1	Sample		11/11/2006 11:50 AM	1.0																
		Sample-2	Sample		11/1./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		11/11/2005 11:59 AM	1.0		2.105	2590	74.97		13.1551	13.1551		25.3	65.10		2.089	1284	29.8	129.91	
			Quantit	otion	Managara(a)											П	_					

🕑 Quantitation Message(s

0

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.

 V
 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.

Accuracy

132.7

115.0

109.4

107.0

104.6

111.2

99.6

Amp Results

3.3187

5.7493

13.6808

26.7561

5.2293

27.8039

4.8977

14.2183

124,4844

Final Conc.

BT

2.141

2.140

2.134

2.022

2.101

2.142

2.135

2.143

2.105





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.



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.



La_LI3 [Uchorotonicomer. x10 4 [85:0 Assa-Str3] 0.5- 0.5- 3.5 4 4.5 5	CAL_LUA [Dichrocofficione x104-850Area-6641 1-87.0Area-15589 0	LAL_LUS [Dicrosoftacione x10 4 [85:0 Assa-124123 2.87:0 Assa-3645 0	LAL_LUS [Dichorodinations. v10 4] 85.0 Area-124739 2- 0 35 4 45 5	LA07 [Dicrocoditioner. x10 5 [650 Asea-668267 1- 870 Asea-111324 0- 35 4 45 5	CAL_LUS [0:chrocotilactore s105 85:0 Ares-1003759 1 1 35 4 45 5	LAL_LUS [Dicrocoditionne x10 5 65:0 Asse-14/23491 2- 0 35 4 45 5	CAL_L 10 [Dichorodinations. 105 85.0 Area-2] 85561 25- 0 35 4 45 5	x10 * 850 Assa-3(0301 0.5-87.0 Assa-3(0301 0.5-35 4 45 5	CAL_L12 [0cmoonacome s105 850 Area-3945000 05 87.0 Area-183513 0 3.5 4 45 5
Cal_L03 [Chloromethane] ×10 1 500 Alexa-26630 4 520 Alexa-1 545 0 4 45 5	CAL_L04 [Chloronethane] x10 4 - 50.0 Area-3 (561 0.5 52.0 Area-10272 0 4 45 5	C4L_L05(Chloomethare) ×10 * 500 Alaa-68234 1 520 Alaa-82244 0 4 4/5 5	CAL_L05 [Chloromethane] 10 4 50.0 Area-115385 2-52.0 Area-3 410 0-4 45 5	CAL_L07 (Chloromethane) ×10 5 500 Asea-327263 0.5 52.0 Asea-1199393 0 A A A A A A A A A A A A A A A A A A A	CAL_U8 [Chloronethane] 10.5 [90.0 Area-590345 0.5 [0.5 Area-14484 0.5] 4 45 5	C4_L09[Chloomefrare] ×10 5 500 Assa-787084 1 520 Assa-787084 0 A.A.A.A.A.A.A.A.A.A.A.A.A.A.A.A.A.A.A.	CAL_L10 [Chloromethane] ±10.5 50.0 Area-1160408 2 - 52.0 Area-345552 0 - A. A. A. 4 45 5	CAL_L11 [Chloromethane] ×10 ⁵ 500 Aven-1407238 2 520 Aven-544703 0 <u>A A A</u> 4 4/5 5	CAL_L12 [Chloomethane] s105 - 50.0 Ama-2235588 52.0 Ama-2235588 2 0 4 4 5 5
Cal_L03 [/instChloride] x10 7 520 Assa-2335 540 Assa-4221 25 1 4 4 5 5 55	CAL_LOH (Vry/Chloride) x10.4 (62:0 Area-4754 0.5 (61:0 Area-1778 0.4 (45:5 5:5	C44_L05[Virgl Chloride] ×10 * 62.0 Avea-66767 1 0 4 4.5 5 5/5	CAL_L06 [VirstChoide] 10.4 62.0 Area-142287 2- 64.0 Area-3719 0 4 45 5 55	CAL_LO7 (Vegl Chloode) ×10 5 620 Axea - 454834 0.5 0 4 4 5 5 55	CAL_L08 [Virs/Chloride] s10.5 - 62.0 Area-762725 1 - 64.0 Area-762725 1 - 64.0 Area-762725 4 - 4.5 - 5 - 5.5	C44_L09[Virgl Chloride] x10 5 520 Assa-1641505 1 64 0 Assa-36053 4 4 5 5 55	CAL_L10 [virst Choids] s10.5 - 62.0 Area-1837089 2- 0 4 4 5 5 5 55	CAL_L11 [Virgl Chloride] ×10 ⁵ 62:0 Axes-2234323 2 0 4 4:5 5 5:5	CAL_L12 [Viryl Charide] s105 [52:0 Area-2804877 25 0 4 45 5 55
Cal_L03 (Bromomethane) ×10 3 94 0 Assa-7 75 2 950 Assa-7 10 2 4 5 5 55 6	CAL_L04 [Bronomethane] x103-[94.0 Area-14852 5- 95.0 Area-1730 25- 0 Area-1730 45-5-55-6	C4_L05(Bonomethare) ×10 + 94.0 Assa-49443 1 - 96.0 Assa-49643 0	CAL_L05 [Brononethane] 10.4.34.0 Area-80640 1.95.0 Area-70551 0.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4	C4L_L07 (Bonomethane) ×10 * 94.0 Assa-247845 2.5- 5 5.5 6	CAL_L08 [8romonethane] s10.5 - 94.0 Arcsi-382358 0.5 - 95.0 Arcsi-382358 0.5 - 95.0 Arcsi-38245 0 - 45.5 5.5 6	C4L_L09[Bonomethane] ×10 5 94 0 Assa-614781 1 - 96 0 Assa-614782	CAL_L10 [Brononethane] 10.5 [34.0 Area-396080 1 [36.0 Area-3][3137 0 [45.5 5.5 6]	CAL_L11 [Bonomethane] ×10 5 94.0 Assa-1260779 2- 96.0 Assa-1845337 0 4.5 5 5.5 6	CAL_L12 [Bronomethane] s10.5 [94.0 Anna-1943745 25 [96.0 Anna-1943745 26 [0 Anna-1943745 24 [96.0 Anna-1943745 25 [96.0 Anna-1943745 26 [96.0 Anna-1943745 27 [96.0 Anna-1943745 28 [96.0 Anna-1943745 29 [96.0 Anna-1943745 29 [96.0 Anna-1943745 20 [96.0 Anna-1945745 20 [96.0 Anna-194575 20 [96.0 Anna-194575575 20 [96.0 Anna-19575575 20 [96.0 Anna-1
Cal_L03 [Chloroethane] x10 7 64.0 Aasa-1 883 2 5 66.0 Aasa-6 73 0 44 6 Aasa-6 73 0 5 5 6	CAL_L04 [Chicrosthane] x10 3 [64 0 Area-20306 25 0 Area-0 37 0 5 55 6	C44_L05[Chicosefuses] ×10 * 64.0 Also=47081 0.5 0 5 5.5 6	CAL_U x10.4 64.0.An 570 1.65.0.An 405 0 5 15 6	41_L0 10 * 164228712 78431 2.5- 5 55 6	U costhana) Area-392307 Areas-183553 A S5 6	x10 3 Axes-5) 1 Axes-5) 0 5 0 5 5/5	10 [Chlorosthane] 64 0 Arba-762913 66 9 Arba-762913 150 4 Arba-21150 1 A A A 5 5 5 6	CAL_L11 [Chlosefhane] ×10.5 [64.0 Also=1104703 2 - 66.6 Also=389496 0	CAL_L12 [Chlorosthane] s105 - 640 Area-1 435279 2 - 650 Area-1 4745 0 - 7 - 5 - 55 - 6
Cal_L03 (Trichlorofluorometh x10 * 101.0 Asso-6404 1 103.0 Asso-6493 105.0 Asso-6493 0 105.0 Asso-6493 55 6 65 7	CAL_L04 [Trichloroflucomet. s104 101.0 Areas 498488 103.0 Areas 4740 105.0 Areas 4770 55 6 65 7	CAL_L05 [Tichlordhuromet. ×10 + 101:0 Aces+ 169272 100:0 Aces+ 13316 0 105:0 Aces+ 13316 0 55:5 6 6:5 7	CAL_L06 (Trichloroflucromet. x10.4 101.0 Area+249608 5-103.0 Area+259608 105.0 Area+2559 0 55.6 6.5 7	CAL_L07 [Tichkrofuzonet ×10 5 101.0 Asso-\$20961 103.0 Asso-\$2595 105.0 Asso-\$2595 105.0 Asso-\$2004 0 55 6 65 7	CAL_L09 [Trichloroflucromet. s10.5 101.0 Area+1336974 2 103.0 Area+1336974 0 103.0 Area+134565 0 55 6 65 7	CAL_L09 [Tichknolucronet. ×10 ⁵] 101.0 Ases- 103.0 Ases- 103.0 Ases- 105.0 Ases- 105.0 Ases- 175.2 0 55 6 65 7	CAL_L10 [Trichloroflucromet. s10.5 101.0 Area+2751219 5-103.0 Area+2751219 105.0 Area+27559 0 55.6 6.5 7	CAL_L11 [Tichlordhuoronet. ×10 f 101.0 Auso-3825064 0.5 105.0 Auso-465324 0.5 55 6 65 7	CAL_L12 [Trichlorofluoromet. s10.6] 101.0 Areas 572913 103.0 Areas 242582 0.5 105.0 Areas 21055 0 55.6 6.5 7
Cal_L03 Acetone] x10 + 430 Asea-24233 0.5- 0	CAL_L04 (Acetone) #10 4 43.0 Area+20338 0.5 58.1 Area+1 012 0 Aceto Area+1 012 0 Aceto Area+1 012 0 Aceto Area+1 012	C4L_L05 (Acetone) x10 + 430 Aces+53513 1.581 Aces+12014 0	CAL_L06 [Acetone] +10 +4 20 Ares+126374 2- 51 Ares+2 973 0 55 6 65 7	C44_L07(Acetone) ×10.4 43.0 Asea-262284 5-58.1 Asea-66285 0 55 6 65 7	CAL_L08 [Acetone] s10.5 43.0 Ares+415493 0.5 5 0 55 6 65 7	C44_L09 (Acetone) x10 * 43.0 Asea+568940 1 - 58.1 Asea+14052 0 - 55 6 6.5 7	CAL_L10 [Acetone] s10.5 42.0 Ares+986418 1. 58.1 Ares+285274 0. 55.6 6.5.7	CHL_L11 [Acetore] ×10.5 43.0 Asea+1256530 2_581 Asea+38536 055 6 65 7	C4L_L12 (Acetone) s10.5 43.0 Area+1632894 2 93.1 Area+1632894 2 0 55.6 6.5 7
Cal_L03 [1.1-0ichloroethene] x10 7 61 0 Assa-29987 5 56 0 Assa-1 796 38 0 Assa-7 746 1.1.1 6 6 5 7 75	CAL_L04 [1.1-0ichlarosthene] #10.4 [61.0 Area-45770 1.950 Area-2779 0.930 Area-1275 0.955 7 75	C4L_L05(1.1.0ichloroetherne) x10 + 61.0 Axea-682733 2 + 96.0 Axea-54032 98.0 Axea-54032 0 + 66.5 + 7 - 7.5	CAL_L06 [1.1 Dichlorosthens] x10 4 [61.0 Ares] 122381 2 95.0 Ares] 7 193 0 33.0 Ares] 1633 6 6/5 7 7/5	C44_L07[11:Dichlosofhere] ×10 5 61:D Assa-480673 1 56:D Assa-280673 0.5 38:D Assa-18:151 0 6 6:5 7 7:5	CAL_L08 [1.1-Dichlorosthens] s10.5 [61.0 Area-788663 1 35.0 Area-4 2492 33.0 Area-2 7486 6 6.5 7 75	C4L_L09[1.10ichlosoethene] x10 ⁵ 51.0 Assa-1679101 2- 56.0 Assa-6 4952 0	CAL_L10 [1.1 Dichlorosthene] s10.5 61.0 Area-1602546 2 95.0 Area-3 2814 0 93.0 Area-60.231 6 6.5 7 7.5	C44_L11(1.1-Dichloroethene) x10 ⁵ (61.0 Axes-2231290 96.0 Axes-1 95746 0 <u>6 6.5 7 7.5</u>	C4L_L12 [1.1-0ichlaroethene] s10 6 - 61:0 Area-3127786 05 - 96:0 Area-1 624834 0 - 98:0 Area-1 624834 0 - 6 - 65 - 7 - 75
Cal_L03 (Réuryl Alcohol) x10 + 580 Asea-3261 430 Asea-3313 0	CAL_L04 (19ugl Alcohol) x10 4 - 5910 Area=10250 0.5 - 410 Area=2344 0	C4L_L05(19.04) Alcohol x10 + 59.04xes=21109 1.43.04xes=21109 0.43.04xes=3136 0.45.775	CAL_LOS \=Bugi Alcohol] 10.4 593.0 ares-38712 2- 43.0 ares-8455 0 6 6.5 7 7/5	C4L_L07 (H8utyl Alcohol) ×10 + 550 Azos=65582 5 + 430 Azos=14462 0	CAL_L08 (HBurgl Alcohol) x10.5 [53.0 Aress-7289 0.5 41.0 Aress-7289 0.5 6 6.5 7 7.5	C44_L09(H8u6)(Alcohol) x10 ⁵ 1, 430 Asses-225517 1, 430 Asses-32234 0 6 6:5 7 7:5	CAL_L10 +Eurgl Alcohol] µ10 ⁻⁵ [53:0 Arros-543031 1 41:0 Arros-56484 6 6:5 7 7:5	C44_L11() 8 upl Alcohol ×10 ⁵ 158.0 Area-555038 2 43.0 Area-578275 0 4 6 5 7 7.5	CAL_L12 [+84/gl(Alcohol] s10.7 93.0 Arcsa-737250 41.0 Arcsa-177155 0 40.0 Arcsa-17715 0 6 65 7 7/5
Cal_L03 (Methylene Chloride) x10 3 450 Asses 19851 2 860 Asses 19230 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	CAL_L04 [Methylene Chloside] x10 4 43 0 Ares-27216 0.5 86 0 Ares-2 315 0 4 4 43 0 Ares-2 315 0 4 4 4 4 5 4 5 5 7 75	C4L_L05 (Metrylene Chiode) x10 + 43.0 Ases-59356 1 - 96.0 Ases-39675 0	CAL_L06 [Methylere Chloride] x10 4 [43.0 Area-8]734 2-96.0 Area-6[070 0	C44_L07 [Methylene Chloride] ×10 5 450 Ases=3[2151 0.5 86.0 Ases=165824 0 46 5 5 7 75	CAL_L08 [Methylene Chloride] x105 43.0 Area-433111 1 - 86.0 Area-317310 0	C4L_L09 [Methylene Chloride] x10 5 430 Asea-672345 1 06.0 Asea-672345	CAL_L10 [Methylere Chloide] 105 43.0 Area-1007239 2-86.0 Area-616235 0 	C4L_L11 [Hefsylene Chloride] x10 ⁵ 49.0 Asea-1403893 2 00.0 Asea-9 6473 0 4.0 5 7 75	CAL_L12 [Methylene Chloide] +105 49.0 Area-1980522 86.0 Area-1 26400 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

- 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.

📅 Agilent MassHunter Quant	titative Analysis - DrugsOfAbuse - MRM met	hod	
File Edit View Analyze Method	d Update Report Tools Help		
🗄 🛅 🗁 🛃 🖬 🖓 💭 Analyze	Batch 🛛 🔞 🧎 Layout: 🔜 🔢 🔛 🔝 🚺	Restore Default Layout	
Method Tasks 🗙	Method Table		
New / Open Method	Level Name Prefix: # of Lev	rels: 10 Create Levels	Time Segment: 👾 <all> 👻 🖒 Compound: 📾 CO> 👻 🐨 Reset Table View</all>
Method Setup Tasks	Sample		
Compound Setup	Name Data File	Type Level	Acq. Method File Acq. Date-Time
nt Retention Time Setup			
😥 ISTD Setup	Quantifier		
🚀 Concentration Setup	Name TS	Scan Type	
🛣 Qualifier Setup	Jocan Jocan		
🚀 Calibration Curve Setup	📑 New Method from Acc	uired MRM Data	
📝 Globals Setup			
Save / Exit	New Method from Acc	quired Scan Data	
🥁 Validate	New Method from Acc	uired Scan Data with Libr	rary Search
💼 Save			
Save As	New Method using Ma	🗖 📅 Agilent MassHunter Quanti	itative Analysis - [New Method]
🔀 Exit		File Edit View Analyze Method	d Update Report Tools Help
Manual Setup Tasks		🗄 🖆 🛃 📭 💭 🖓 Analyze	Batch 😧 Layout: 📅 🔀 📆 🛗 🖾 🧭 Restore Default Layout
<u>R</u> New Compound		Method Tasks X	Method Table
🕂 New Qualifier		New / Upen Method	E Levels : 10 Create Levels : Time Segment: ← <al> ▼ ← Compound: ← ▼ ← Reset Table View</al>
🕺 New Calibration Level		Method Setup Tasks	Sample
🗙 Delete		K MRM Compound Setup	Name Data File Type Level Acq. Method File Acq. Date-Time
	0	Retention Time Setup	
		is rono setup	declaration (TS T) Collision Scan Tune D
		- Concentration Setup	Amp 136.2 > 91.4 5.0 MRM Target 2.020
		🚊 Quainer Setup	Qualifier
		Calibration Lurve Setup	Precursor Ion Product Ion Transition <u>Bel Bean</u> Uncertainty
		🔄 Globals Setup	136.2 119.4 136.2 > 119.4 28.0 20.0
		Save / Exit	Quantifier
		Validate	Name / TS Transition Collision Sean Type RT
		Save Save	
		Save As	Volaire Province Ion Production Transition Bal Base Uncertaintu
		🔀 Exit	141.1 124.4 141.1 > 124.4 27.9 20.0
		Manual Setup Tasks	Quantifier
		Outlier Setup Tasks	Name Z TS Transition Collision Scan Type RT
		Advanced Tasks	□ Cocaine 1 304.1 -> 182.0 5.0 MRM Target 2.449
			Qualitier



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.

📅 Agilent MassHunter Quant	titative Analysis - [New Method													
File Edit View Analyze Method	d Update Report Tools Help													
🗄 🛅 🕞 📕 🖬 🕻 💭 Analyze	Batch 🛛 🕜 🕴 Layout: 🔜 🔛		🔼 📝 Restore Default Layo	ut										
Method Tasks 🗙	Method Table													
New / Open Method	Level Name Prefix:	#	of Levels: 10	Treate Levels Time Segm	nent: 🖛	<all></all>	·▼ ⇒ [(
Method Setup Tasks	Sample													
K MRM Compound Setup	Name Da	ita File	Туре	Level Acq. Metho	od File 🛛 🖌	koq. Date-Time								
🎢 Retention Time Setup	CMAMCal_L4.d CMAM	al_L4.d												
😥 ISTD Setup	Quantifier													
🚀 Concentration Setup	Name 🗠	TS	Transition Collision	Scan	L:	/pe	RT							
🛣 Qualifier Setup	E Amp	1 1	36.2 -> 91.4	5.0 MRM	2.020									
🚀 Calibration Curve Setup	Qualifier		I	1 1	_									
📝 Globals Setup	Precursor Ion 136.2	Produ	uct Ion Transition 119.4 136.2 -> 119.4	Rel. Resp. Uncertaint 28.0 2	ty 20.0									
Save / Exit	Quantifier													
瀫 Validate	Name 🛆	TS	Transition Collision	Scan	L:	/pe	RT							
💼 Save	Amp-d5	1 1	41.1 -> 93.4	5.0 MRM	ISTD		1.990							
Save As	Qualifier	Metho	d Table											
🔀 Exit	Precursor Ion 141.1	Le	vel Name Prefix:	# of	Levels:	10	Crea	ate Levels	Time Segment	: 🖛 <ali></ali>	-	🕨 📔 Compo	ound:	(
Manual Setup Tasks	Quantifier	Sa	ample		_									
Outlier Setup Tasks	Name 🛆	-		Data Dia		T		Laural		The Area Data Time	-			
Advanced Tasks	Cocaine		Name	Data File		туре		Level	Acq. Method F	rile Acq. Date-Lime				
	Qualifier)	Cal_L07.d	Cal_L07.d										
			Quantifier											
				Name	T	5 Scan	Туре	MZ	CAS#	Library Match Score	RT	Library RT	RI	Library RI
			Compound_1			1 Scan	Target	44.0			3.833			
			Dichlorodifluoro	methane		1 Scan	Target	84.9	75-71-8	95.6	4.249			
			Methane, chloro).		1 Scan	Target	50.0	74-87-3	89.3	4.493		\square	
			Cyclobutane, et	hyl-		1 Scan	Target	41.1	4806-61-5	69.3	4.790			
			Compound_6	-		1 Scan	Target	60.0			5.168			
	Methane, bromo-					1 Scan	Target	95.9	74-83-9	88.7	5.241		\square	
		ulfonic acid		1 Scan	Target	64.0	13881-91-9	50.2	5.410					
			Trichloromonoflu	uoromethane		1 Scan	Target	100.9	75-69-4	91.0	6.098		\square	
			Acetone			1 Scan	Target	43.0	67-64-1	81.9	6,194	í		



Multiple Integrators / Compound Specific

Metho	d Table													-
E Le	vel Nam	e Prefix:	# 0	of Levels: 10		Create Levels	Time Segment: 🔸	⊨ <all></all>	🔻 🔿 🗌 Com	npound: 🔙	Amp	🔻 📑 🛛 Reset Table View		
S	ample													
	N	lame	Data File	Туре		Level	Acq. Method File	Acq. Date-Tim	e					
	Calib-I	L5	CMAMCal_L5.d	Cal	L	15	APCIautotune.m	5/12/2006 2:03						
	Quanti	tifier			1		_							
		Name	TS	Transition		Scan T.	Туре	BT 2 102	Int A sile	Int.	Parms.			
		usifier		30.2 7 31.4		110	aiget	2.102	Agile			l		
		Precursor	Ion Produ 136.2	ction 1 119.4 136.2	ransition -> 119.4	Rel. Resp. 26.1	Uncertainty 8 20.0	Int. Parms.						
	Quant	tifier	TC	Tanadian		C	Tura	DT		lut	Dema			
		mp-d5	1 1	1 ransition 41.1 -> 93.4	MBM	scan IS	TD	2.078	MS-MS (GC)	int.	rams.			
		ualifier			1							1		
		Precursor	Ion Produ	ction 1	ransition	Rel. Resp.	Uncertainty	Int. Parms.	_	Integ	ration		2 🞽	
			141.1	124.4 141.1	-> 124.4	26.	4 20.0			Inte	egrator Gener	ral Universal Peak Filter		
	Quanti	tifier								Ie	tearstor			
		Name	TS	Transition	9	Scan	Туре	BT	Int.		aile			
Ē		ocaine	1 3	04.1 -> 182.0	MBM	Ta	arget	2.449	Universal		gile			
Comp	ound Info	ormation								M	IS-MS IS-MS (GC)			-
2	+ ‡	<u>ــــ 🔬 ا</u>			1 🚖 🛓					G	eneral niversal			
+ MRI + MRI + MRI	M (136.2 03- 4- 3.5- 3- 2.5- 2- 1.5- 1.5- 0.5- 0.5- 0.5- 0.5- 0.5- 0.5- 0.5- 0	2-> 91.4) CM/ .2 1.4 -> 93.4) CM/	AMCal_L5.d RT N AMCal_L5.d RT=	=2.102 min, ami=Amp ea=19301	4 2.6 Acqui	2.8 3 isition Time (min)	136.2 > 91.4 , 136.2 2 2 2 3 2 5 2 1.5 1 0.5 0 1.2 1 141.1 > 93.4 , 141.1 2 2 1.5 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	> 119.4 	8 2 22	2.4	niversal		Apply to All	136.2 30 135 >to-Charge (m
Lx Lounts	0 2 2.5- 2-		RT= Nam An	2.076 min. e=Amp-d5 ea≠1048			≝ ×10 ² + Ratio=26.5 2 - 1.75 - 1.5 -					DK Reset Defa	ult Cancel Apply	



Overview of Unknowns Analysis



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





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	В	С	D	E F	Ī
1	DIR	J SUBDIR	FAST 🔽	ExcelTemplate	ExcelWorkbook PDF	
2	ESTD	Parts	FAST	QuantReport_ESTD_Summary_FAST_B_04_00.xltx	HyperLink to Workbook (.xlsx) HyperLink to Adobe Acrol	_
3	ESTD	Parts		QuantReport_ESTD_Summary_B_04_00.xltx	HyperLink to Workbook (.xlsx) HyperLink to Adobe Acrol	ī
4	ESTD	Parts	FAST	QuantReport_ESTD_Samples_FAST_B_04_00.xltx	Sample Sheet(s)	÷
5	ESTD	Parts		QuantReport_ESTD_Samples_B_04_00.xltx	Hy Bungle Brice (By	
6	ESTD	Results	FAST	QuantReport_ESTD_ResultsSummary_FAST_B_04_00.xltx	Hy Batch Info	
7	ESTD	Results		QuantReport_ESTD_ResultsSummary_B_04_00.xltx	H record batch identification information	
8	ESTD	Results	FAST	QuantReport_ESTD_ResultsQualifierRatios_FAST_B_04_00.xltx	H Analyze Info	
9	ESTD	Results		QuantReport_ESTD_ResultsQualifierRatios_B_04_00.xltx	Sample Chromatogram	
10	ESTD	Results	FAST	QuantReport_ESTD_ResultsComplete_FAST_B_04_00.xltx	H Include sample chromatogram graphic	
11	ESTD	Results		QuantReport_ESTD_ResultsComplete_B_04_00.xltx	Hy Quantitation Results	
12	ESTD	Results	FAST	QuantReport_ESTD_ResultsByCompound_FAST_B_04_00.xltx	H list results and concentration for compounds	
13	ESTD	Results		QuantReport_ESTD_ResultsByCompound_B_04_00.xltx	display compound graphics for each compound	
14	ESTD	NotDetected	FAST	QuantReport_ESTD_NotDetected_FAST_B_04_00.xltx	H	
15	ESTD	NotDetected		QuantReport_ESTD_NotDetected_B_04_00.xltx	H	
16	FSTD	Not Detected		QuantReport ESTD NotDetectedByCompound B 04 00 vity	H	



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

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3	Batch Info													
4	Batch Data	Path												_
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Excel XML Source Window

- Reporting uses XML mapping to import results into templates
- ¥ C10 fx • В С D F F G A XML Source ▼ × 1 Batch Info XML maps in this workbook: Batch Data Path 2 QuantitationDataSet_Map Y 3 Analysis Time Analyst Name 4 Report Time Reporter Name 😑 🧑 ns1:TargetCompound ^ 5 Last Calib Update Batch State 付 ns1:BatchID 付 ns1:SampleID 6 付 ns1:CompoundID 7 CMD:Repeat CompoundID Ins1:AccuracyLimitMultiplierLOQ 8 CMD:SheetBreak Compound Ins1:AccuracyMaximumPercentDeviation CompoundID CompoundName ▼ GraphicCalibr ▼ RetentionTime ▼ 9 SampleID Ins1:AreaCorrectionFactor 10 Ins1:AreaCorrectionMZ 11 Ins1:AverageRelativeRetentionTime 💌 Compound 🔽 🔽 Data File Type 12 CompoundID PeakID SampleID Name Ins1:AverageResponseFactor 13 Ins1:BlankResponseOffset 14 Ins1:CASNumber 15 Ins1:CCISTDResponseRatioLimitHigh SampleName
 SampleType 💌 Graphiceal 💌 romatogram 16 SampleID CompoundID CompoundType Ins1:CCISTDResponseRatioLimitLow 17 Ins1:CCResponseRatioLimitHigh 18 Ins1:CCResponseRatioLimitLow 19 CMD:EndRepeat CompoundID Ins1:CollisionEnergy 20 Ins1:CompoundGroup 21 ns1:CompoundName 22 Ins1:CompoundType < 23 To map repeating elements, drag the elements from the tree onto 24 the worksheet where you want the data headings to appear. 25 26 To import XML data, right click an XML mapped cell, point to XML, and then click Import. 27 28 Options 🔻 XML Maps... 29 Verify Map for Export... 30 31 ⑦ Tips for mapping XML Options Design-Compound <u>وم</u>
- Drag and drop to add data to existing reports



MassHunter Reporting User Information (CBT)



Reporting User Information Welcome to Agilent MassHunter Reporting User Information **Quick Access** 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 **Reporting Training** MassHunter reporting in one location. MassHunter Reporting Training **Familiarization Guide** 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 **Reporting Help - Quant** unique learning style. The MassHunter Reporting Training provides: Written topics that summarize procedures Reporting Help - Qual · Demo movies to show you how to use the software Software reviews that allow you to interact with the programs No-fail guizzes with instant feedback List of Demo Movies 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 o 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: o 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.



Agilent MassHunter

MassHunter Workstation Increase your productivity significantly





Questions?

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

