

# QTOF Small Molecule Application Update

**January 10, 2008**

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# Agenda

- **Goal – Share Best Practices, Updates Software/Hardware**
- **Training**
  - **R1904A 4 Day Customer Training Course (Jan 14<sup>th</sup> next one)**
  - **Recorded Webex's: Impurity Profiling, QTOF-(August, 2007)**
  - **QTOF User Sponsored Email Group (QTOF@googlegroups.com )**

## **Today's Topics:**

- **Upgrading TOF/QTOF to 4 GHz Acquisition Hardware (tuning)**
- **Answer Questions about Targeted MSMS, MFE and Excel 2003(7)**
- **Overview of MassHunter B.01.04 Quant**
- **Questions and Answer Period**



# New Parameters for 4GHz Electronics

- **Mid-Mirror (0.1V) Steps**

- **Slicer**

- **Bottom/Top Slits**

- **Ion Focus**

- **PMT (Max Now 1100)**

- **Amp Offset**

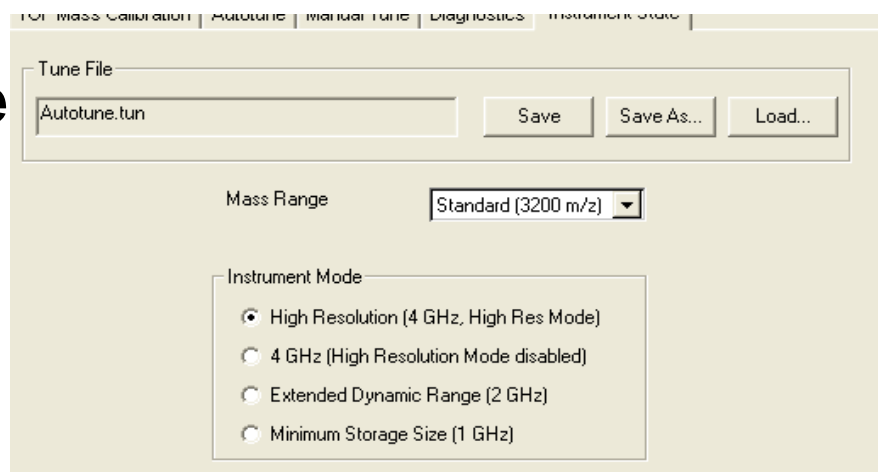
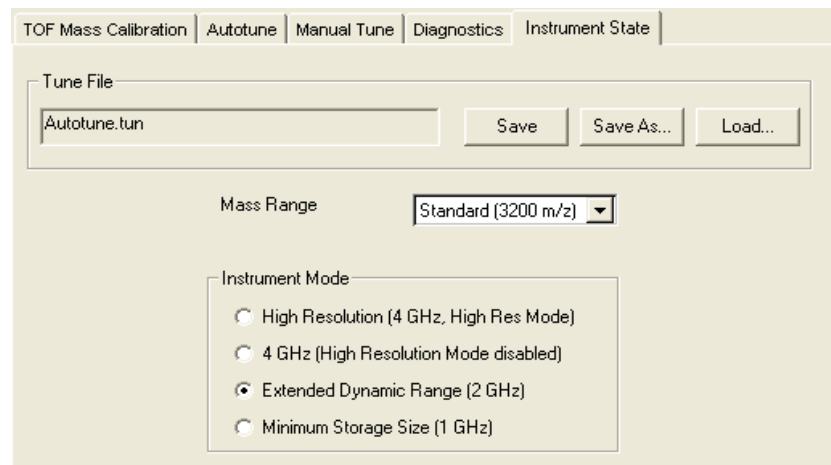
Pusher	1250	V	Mass Range	Min Range	100	m/z
Puller	-800	V		Max Range	3200	m/z
Puller Offset	34	V	Acquisition Rate/Time	Acquisition Rate	1	spectra/sec
Acc Focus	-1925	V		Acquisition Time	1000	msec/spectrum
Mirror Front	-6500	V		Transients/Spectrum	9652	
Mirror Mid	-1401.5	V		Length of Transients	199536	
Mirror Back	1650	V				

Oct2 DC	34.5	V	Horiz Q	29	V
			Vert Q	29.1	V
Ion Focus	-131	V	Top Slit	19	V
Slicer	-7.4	V	Bot Slit	19.1	V
TOF Energy Offset		0	V		

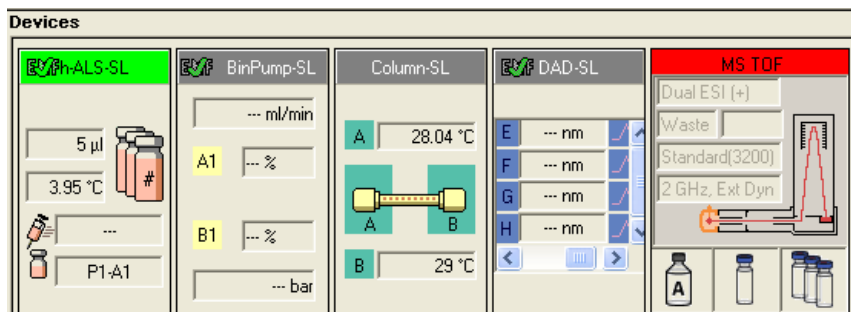
MCP	650	V
PMT	707	V
Amp Offset	39983	DAC

# AutoTuning G6220 and G6520 Systems

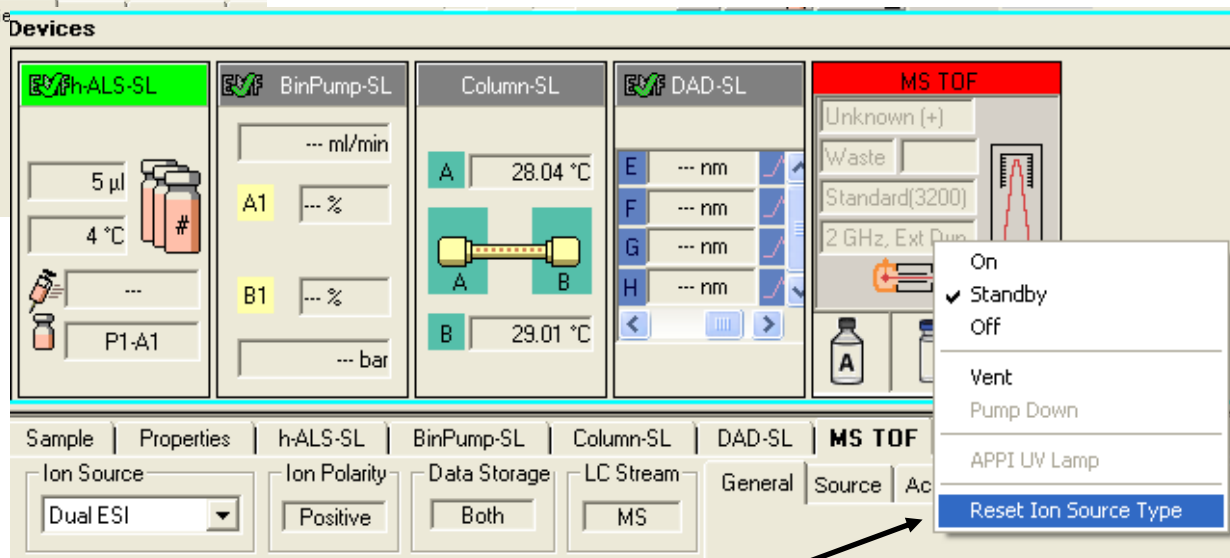
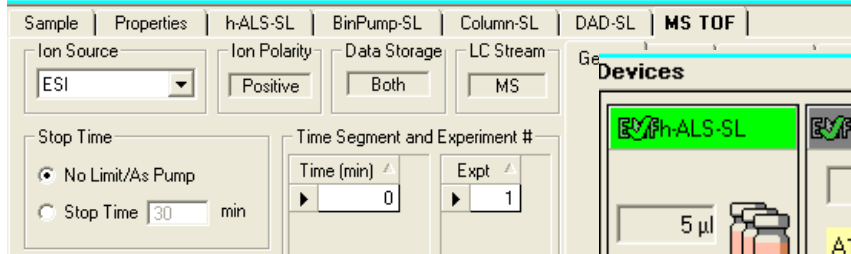
- **G6220/6520 Systems Utilize New Detection Electronics**
  - Changes to Voltage on Slits, Slicer, Lens, PMT
- **6210/6510 Parameters Not Compatible with 6220/6520**
- **Initial Autotune Must Be Done in all Modes and Polarities**
- **Prior to Loading B.01.03 Rename D:\MassHunter directory to D:\MassHunterold**



# How To Reset Ion Source (No I-Button)

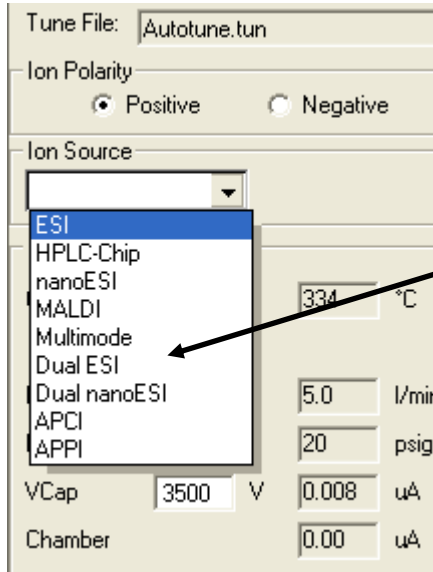


**No I-Button on Ion Source  
Unable to ID Ion Source Type**



**Right Click in MS TOF  
Select Reset Ion Source Type**

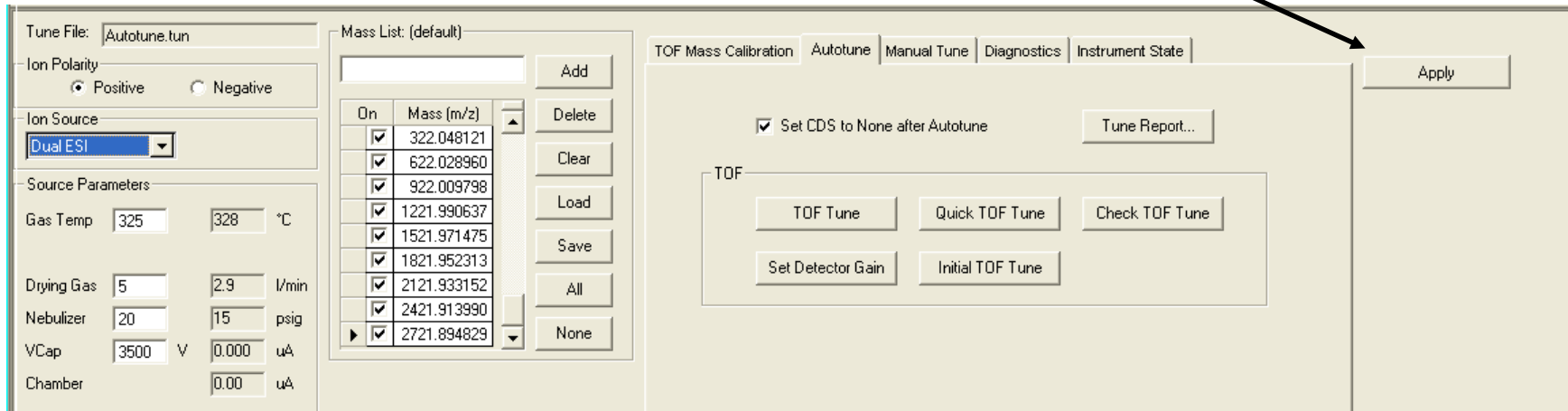
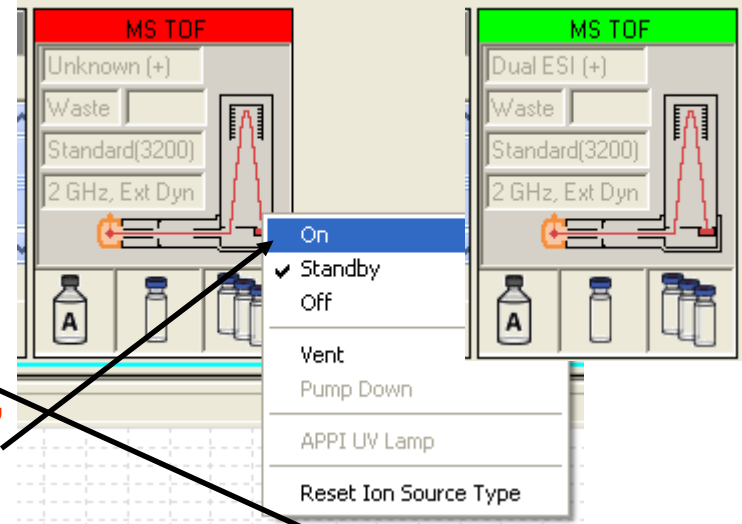
# How To Reset Ion Source (No I-Button)



In MS TOF Tab  
Select Ion Source  
"Dual ESI"

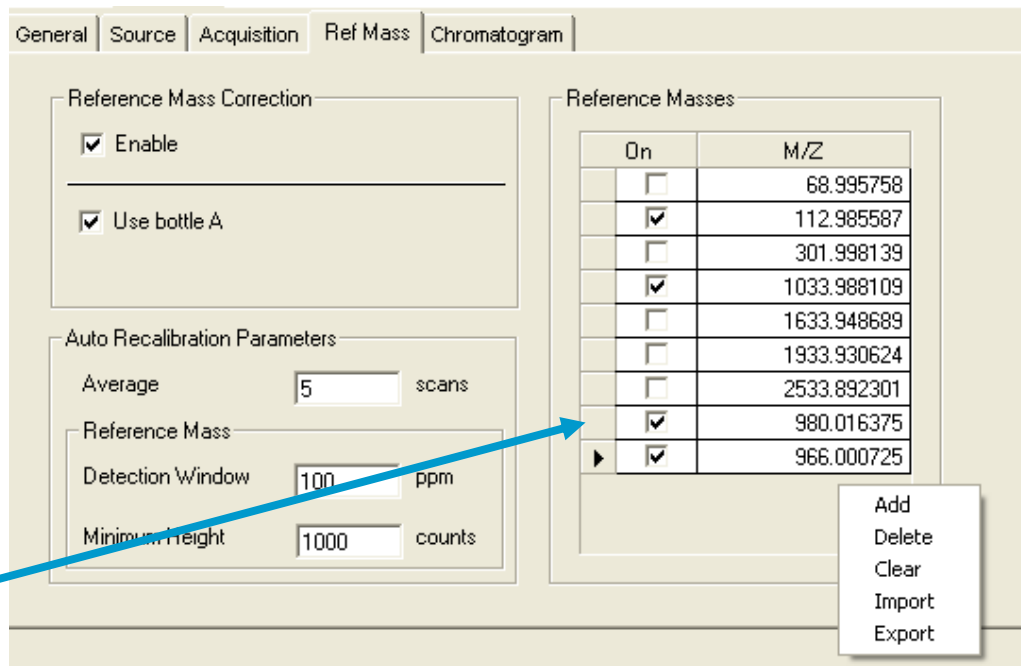
Select Apply

Right Click Select "On"



# Addition of Negative Ion Reference Ions

- From Acquisition
- MS TOF Tab
- General Tab
  - Ion Polarity – Negative
- Ref Mass Tab
  - Right Click “Add”
  - Input Mass 966.000725
  - Input Mass 980.016375



Reference Solution can also be introduced using a Binary or Isocratic with a 100:1 splitter designed by Agilent. Flow rate of LC set at between 0.5-1.0 mL/min and gives very stable flow.

# New Makeup Procedure for Reference Solution

2 mL of HP121 into 98 mL of 95/5 MeOH/Water

0.8 mL of HP921 into 99.2 mL of 95/5 MeOH/Water

Using a 500 mL volumetric flask, mix 25 mL of HP121 and 921 into 450 mL of 95/5 MeOH/Water with 0.2% Acetic Acid.

Better for Negative ion performance and also universal for use with MMI and APCI sources without changing reference solution.



# Determining Saturation Level of TOF

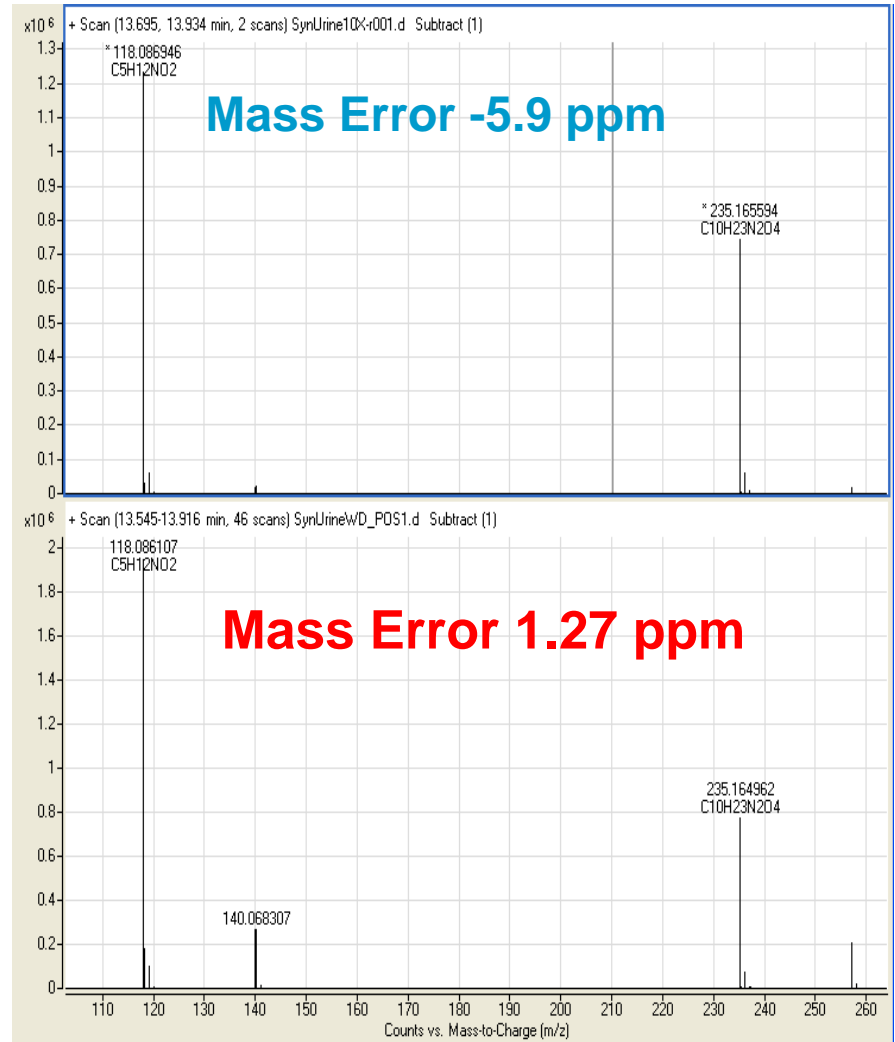
## High Resolution 4GHz Mode

1 Spectrum/s 10,000 transients\*255  
= 2.6 Million Counts

## Extended Dynamic Range 2GHz Mode

Ratio Low to High Gain  
Preamplifier is 12

1 Spectrum/s 10,000 transients\*255\*12  
= 30 Million Counts



# Saturation Correction in MassHunter QUAL

## Spectrum: Extract (MS)

Manual Extraction | Peak Spectrum Extraction (MS) | Peak Location | Peak

Spectra to include

At apex of peak

Average scans >  % of peak height

TOF spectra

Exclude if above  % of saturation

Anywhere

In m/z range(s)

Peak spectrum background

MS

Spectra to include

At apex of peak

Average scans >  % of peak height

TOF spectra

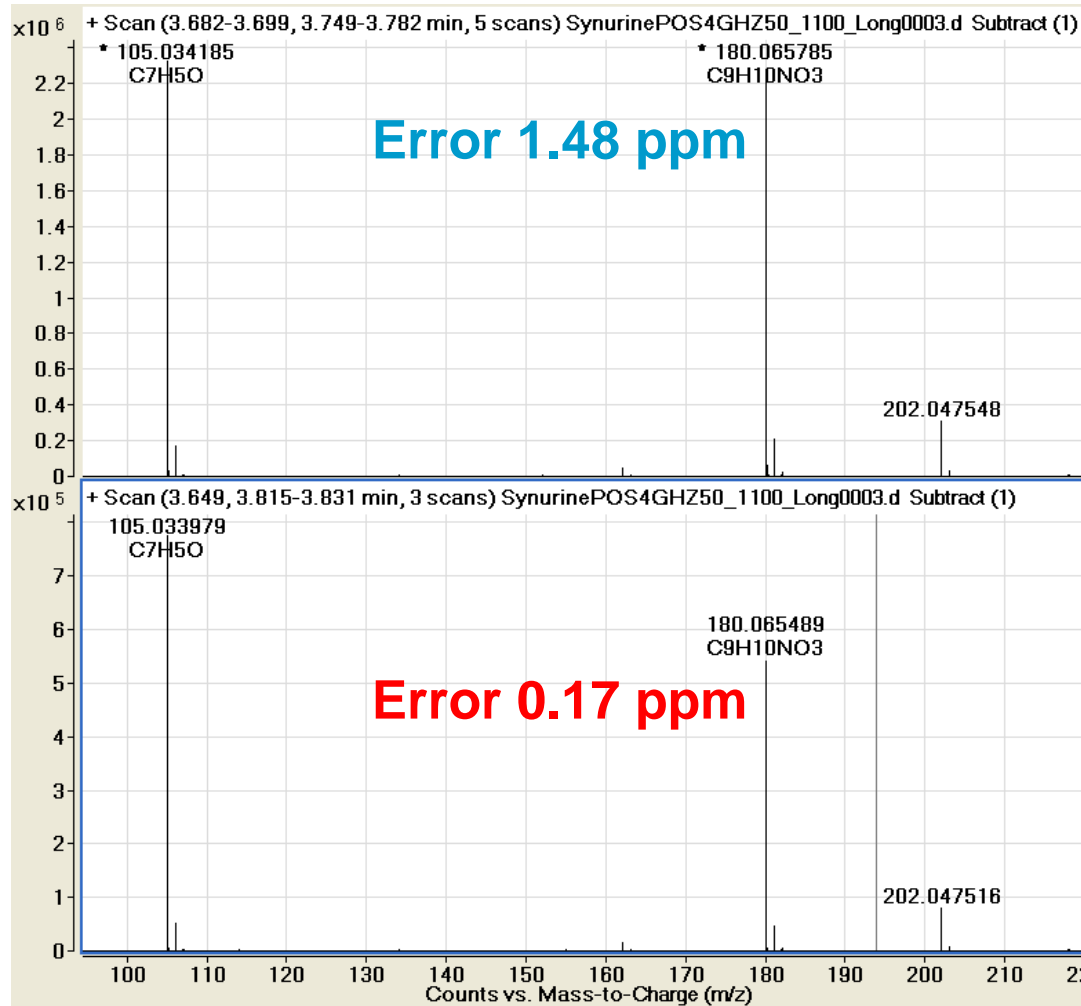
Exclude if above  % of saturation

Anywhere

In m/z range(s)

Peak spectrum background

MS



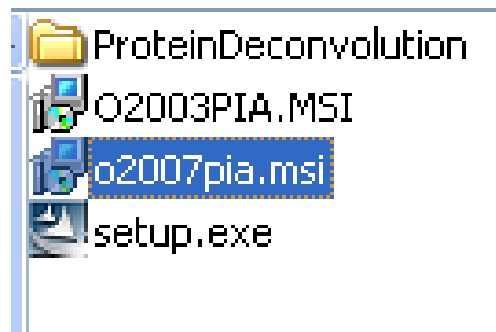
**We Listen..**  
**Your Submitted Questions Answered Here...**

# Question - Answers

1. Does MassHunter B.01.03 Qual and B.01.04 Quant Support Newer Versions of Excel (from 2003)?

**The New Version of MassHunter Software now Supports both Microsoft Excel 2003 and 2007.**

If upgrading either MassHunter or Excel Software make sure to apply the o2007pia.msi file after installation.



# MassHunter Qual B.01.03

## MS/MS Data Analysis Questions

- 1) How to generate empirical formulas from MSMS spectra
- 2) How to use find compounds by AutoMSMS
- 3) How to use find compounds by Targeted MSMS
- 4) How to get empirical formula of peaks from MSMS spectra without using find compound MSMS feature
- 5) How to generate simple Compound and Analysis Reports



# How to Generate Empirical Formula Information from Auto MS/MS Data Files? (Part 1)

**Set Parameters for Find Compounds by AutoMSMS**

**Set Retention Time to Match Chromatographic Peak Width**

Method Editor: Find Compounds by Auto MS/MS

Processing Excluded Masses Results

Compound identification

Retention time window: 0.250 min

Positive MS/MS TIC threshold: 1000

Negative MS/MS TIC threshold: 1000

Mass match tolerance: 0.050000 m/z

Limit to the largest 50 compounds

Persistent background compounds

Compounds with same precursor m/z occurring at different times:

Remove if there are more than 5

Except when the TIC exceeds 100000.0

**Check Extract MS and MS/MS**

Processing Excluded Masses Results

Previous results

Delete previous compounds

New results

Highlight first compound

Highlight all compounds

Chromatograms and spectra

Extract EIC

Extract ECC

Single m/z expansion: 75.000 ppm

Extract MS

Extract MS/MS

Subtract: None

**Execute Command from Menu**

Find Identify Chromatograms Spectra Meth

Find Compounds by Auto MS/MS

Find Compounds by Targeted MS/MS

# How to Generate Empirical Formula Information from Auto MS/MS Data Files? (Part 2)

Compound List							
Name	Show/Hide	File	RT	Height	Mass	MFG Formula	MFG Diff (ppm)
Compound 1	<input checked="" type="checkbox"/>	Synurine10xautom	0.418	6566			
Compound 2	<input checked="" type="checkbox"/>	Synurine10xautom	0.495	99922			
Compound 3	<input checked="" type="checkbox"/>	Synurine10xautom	0.504	8428			
Compound 4	<input checked="" type="checkbox"/>	Synurine10xautom	0.505	138591			
Compound 5	<input checked="" type="checkbox"/>	Synurine10xautom	0.514	39616			
Compound 6	<input checked="" type="checkbox"/>	Synurine10xautom	0.538	25018			
Compound 7	<input checked="" type="checkbox"/>	Synurine10xautom	0.544	7138			
Compound 8	<input checked="" type="checkbox"/>	Synurine10xautom	0.567	11664			
Compound 9	<input checked="" type="checkbox"/>	Synurine10xautom	0.575	8059			

Allowed Species | Limits | Charge State

Charge carrier to be assumed if not known

Positive ions:  Negative ions:

Allowed electron state:

Elements and limits

Element	Minimum	Maximum
▶ C	2	80
H	0	120
O	0	30
N	0	30
S	0	5
Cl	0	3
Si	0	1
P	0	1

+

Allowed Species | Limits | Charge State

Limits on input masses

Maximum neutral mass for which formulas should be calculated:

Limits on results

Minimum overall score

Maximum MS mass error

Require DBE from  to

Maximum number of hits

Advanced: expected data variation

MS mass:  mDa +  ppm

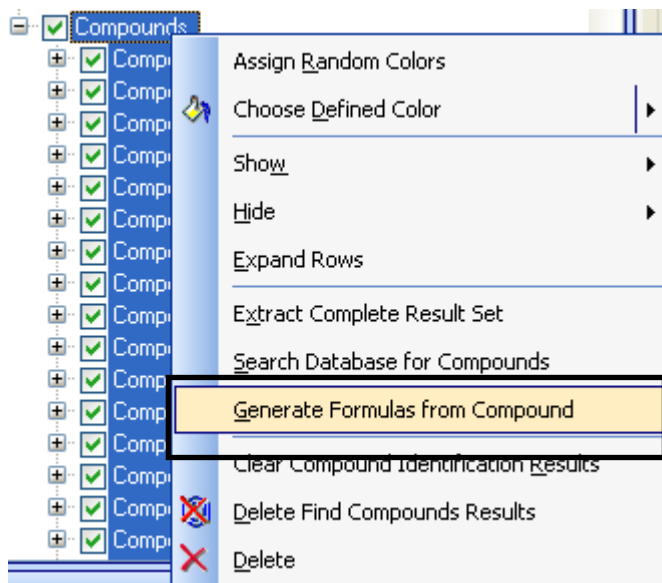
MS isotope abundance:  %

MS/MS mass:  mDa +  ppm

Generate Formulas  
Set Elements and  
Limits

# How to Generate Formulas from Compounds

## From Method Explorer



## From Compound Table

A screenshot of the 'Compound List' window showing a table of compounds. A context menu is open over the first row, with the option 'Generate Formulas from Compound' highlighted. The table contains the following data:

Name	Show/Hide	File	RT	Height
Compound 1	<input checked="" type="checkbox"/>	Synurine10xautom	0.418	6566
	<input type="checkbox"/>		0.495	99922
	<input type="checkbox"/>		0.504	8428
	<input type="checkbox"/>		0.505	138591
	<input type="checkbox"/>		0.514	39616
	<input type="checkbox"/>		0.538	25018
	<input type="checkbox"/>		0.544	7138
	<input type="checkbox"/>		0.567	11664
	<input type="checkbox"/>		0.575	8059
	<input type="checkbox"/>		0.607	8562
	<input type="checkbox"/>		0.662	12953



# How to Generate Empirical Formula Information from Auto MS/MS Data Files? (Part 3)

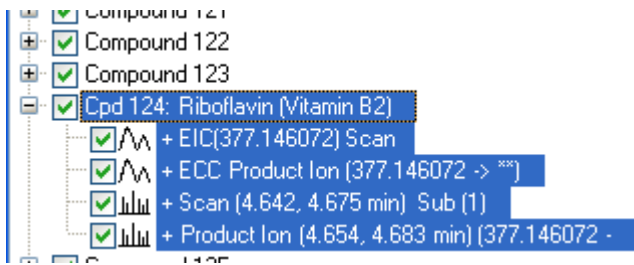
Name	Show/Hide	File	RT	Height	Mass	MFG Formula	MFG Diff (ppm)
Compound 1	<input checked="" type="checkbox"/>	Synurine10xautom	0.418	6566	146.105447	C6H14N2O2	0.55
Compound 2	<input checked="" type="checkbox"/>	Synurine10xautom	0.495	99922		<none>	
Compound 3	<input checked="" type="checkbox"/>	Synurine10xautom	0.504	8428	119.058125	C4H9NO3	1
Compound 4	<input checked="" type="checkbox"/>	Synurine10xautom	0.505	138591	117.079213	C5H11NO2	-2
Compound 5	<input checked="" type="checkbox"/>	Synurine10xautom	0.514	39616	161.105043	C7H15NO3	0.93
Compound 6	<input checked="" type="checkbox"/>	Synurine10xautom	0.538	25018	131.069372	C4H9N3O2	0.8
Compound 7	<input checked="" type="checkbox"/>	Synurine10xautom	0.544	7138		<none>	
Compound 8	<input checked="" type="checkbox"/>	Synurine10xautom	0.567	11664	115.063353	C5H9NO2	-0.21
Compound 9	<input checked="" type="checkbox"/>	Synurine10xautom	0.575	8059	279.095487	C10H17NO8	-0.25

## MS Formula Results Table

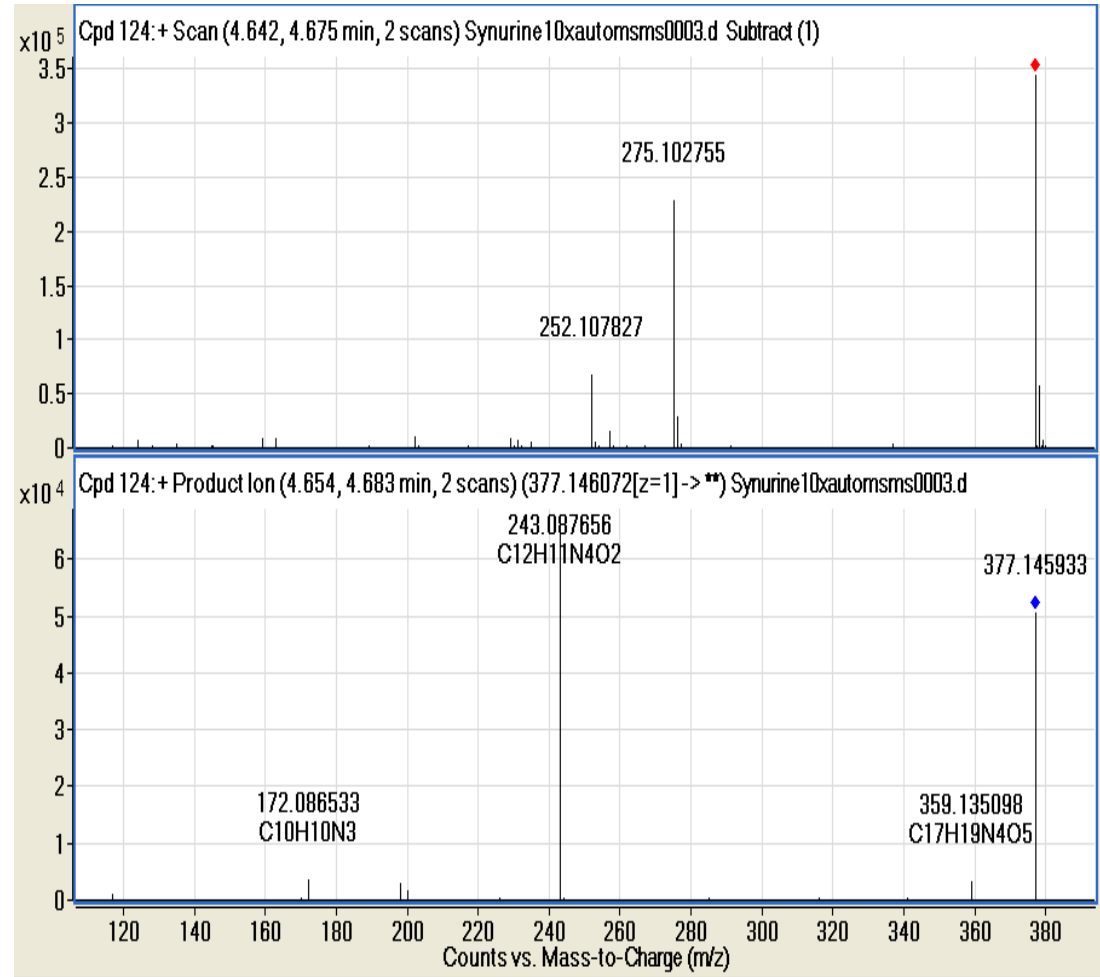
m/z	Ion	Formula	Abundance	Coverage			MS/MS			
377.146449	[M+H] <sup>+</sup>	C17H21N4O6	343544.9							
Best	Formula (M)	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Coverage	MS Score	MS/MS Score	DBE
<input checked="" type="checkbox"/>	C17H20N4O6	100		376.139172	376.138284	-2.36	100	92.32	100	10
Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Difference (ppm)					
1	100	100	377.146449	377.145561	-2.35					
2	17.25	20.32	378.149377	378.148506	-2.3					
3	2.11	3.19	379.151912	379.1508	-2.93					
Best	Formula (M)	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Coverage	MS Score	MS/MS Score	DBE
<input type="checkbox"/>	C15H25N2O7P	97.06		376.139172	376.139938	2.03	100	100	89.6	5
<input type="checkbox"/>	C12H17N12OP	95.23		376.139172	376.13859	-1.55	100	90.5	97.15	11
<input type="checkbox"/>	C18H16N8O2	87.93		376.139172	376.139622	1.19	100	81.18	99.99	15
<input type="checkbox"/>	C16H21N6O3P	82.04		376.139172	376.141275	5.59	100	75.87	99.82	10

# Empirical Formulas Auto MS/MS Data Files(Part 4)

Highlight Compound from Navigator Window to Display both MS and MS/MS Spectra



Select MSMS Formula Details from Menu to View Empirical Formulas for MSMS Peaks



# MSMS Formula Details Table: Vitamin B2 Example

MS/MS Formula Details: Cpd 124: Riboflavin (Vitamin B2) C17H20N4O6								
m/z	Calc m/z	Formula	Abund%	Abund	Difference (ppm)	Loss Mass	Loss Formula	
359.135098	359.134996	C17H19N4O5	4.56	3317	-0.28	18.010565	H2O	
243.087656	243.087652	C12H11N4O2	90.48	65796	-0.01	134.057909	C5H10O4	
243.087656	243.086315	C11H15O6	90.48	65796	-5.52	134.059246	C6H6N4	
172.086533	172.086924	C10H10N3	4.96	3609	2.27	205.058637	C7H11NO6	

Mass Loss and Elemental Composition is Based on Elemental Composition Determined for Precursor Ion (M+H)+ or (M-H)-.

Loss Mass and Loss Formula show Composition of Neutral Losses.

Note: Abundance Values < 100 counts may give higher mass errors

**Colored Peaks Indicate the Presence of Multiple Compositions/Mass**

# How to Generate Empirical Formula Information from Targeted MS/MS Data Files? (Part 1)

## Integration Parameters

Integrator Processing Cpd TIC Peak Filters Peak Spectrum Results

Integrator selection

MS/MS Integrator  General Integrator

Detector

Point sampling:  Start threshold:

Smoothing Stop threshold:

Filtering:  Peak location:

Baseline allocation

Baseline reset >

If either edge <  %

## Chromatographic Peak Width

Integrator Processing Cpd TIC Peak Filters Peak Spectrum Results

Compound identification

Maximum chromatogram peak width  min

Limit to the largest compounds:  compounds

Integrator Processing Cpd TIC Peak Filters Peak Spectrum Results

Filter on

Peak height  Peak area

Height filters

Absolute height > =  counts

Relative height > =  % of largest peak

Area filters

Absolute area > =  counts

Relative area > =  % of largest peak

Maximum number of peaks

Limit (by height) to the largest

Integrator Processing Cpd TIC Peak Filters Peak Spectrum Results

Spectra to include

At apex of peak

Average scans >  % of peak height

TOF spectra

Exclude if above  % of saturation

Anywhere

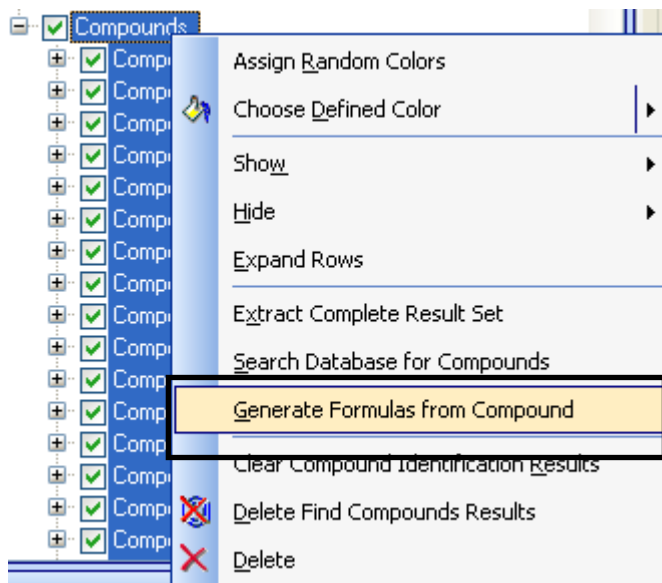
In m/z range(s)

Peak spectrum background

MS/MS

# How to Generate Formulas from Compounds

## From Method Explorer



## From Compound Table

A screenshot of the 'Compound List' window showing a table of compounds. A context menu is open over the first row, with 'Generate Formulas from Compound' highlighted. The table has columns for Name, Show/Hide, File, RT, and Height.

Name	Show/Hide	File	RT	Height
Compound 1	<input checked="" type="checkbox"/>	Synurine10xautom	0.418	6566
	<input type="checkbox"/>		0.495	99922
	<input type="checkbox"/>		0.504	8428
	<input type="checkbox"/>		0.505	138591
	<input type="checkbox"/>		0.514	39616
	<input type="checkbox"/>		0.538	25018
	<input type="checkbox"/>		0.544	7138
	<input type="checkbox"/>		0.567	11664
	<input type="checkbox"/>		0.575	8059
	<input type="checkbox"/>		0.607	8562
	<input type="checkbox"/>		0.662	12953

# How to Generate Empirical Formula Information from Targeted MS/MS Data Files? (Part 2)

## Compound Table Addition of Columns

**Columns**

Available Columns:

- Fit
- Group
- Hits (DB)
- HMP
- Ions
- KEGG
- m/z
- Max Z
- MFG Diff (mDa)
- MFG Mass
- Min Z
- Modified
- Notes
- Polarity
- RT (DB)
- RT Diff
- Saturated
- Shared (DB)
- Start
- Std Dev
- Tgt Diff (mDa)
- Tgt Diff (ppm)
- Tgt Formula
- Tgt Mass
- Unique (DB)
- Vol

Show these columns:

- DB Diff (ppm)
- DB Formula
- DB Mass
- File
- Height
- Mass
- MFG Diff (ppm)
- MFG Formula
- Name
- RT
- Show/Hide

Buttons: Add ->, <- Remove, Add All ->>, <<- Remove All

Buttons: OK, Cancel

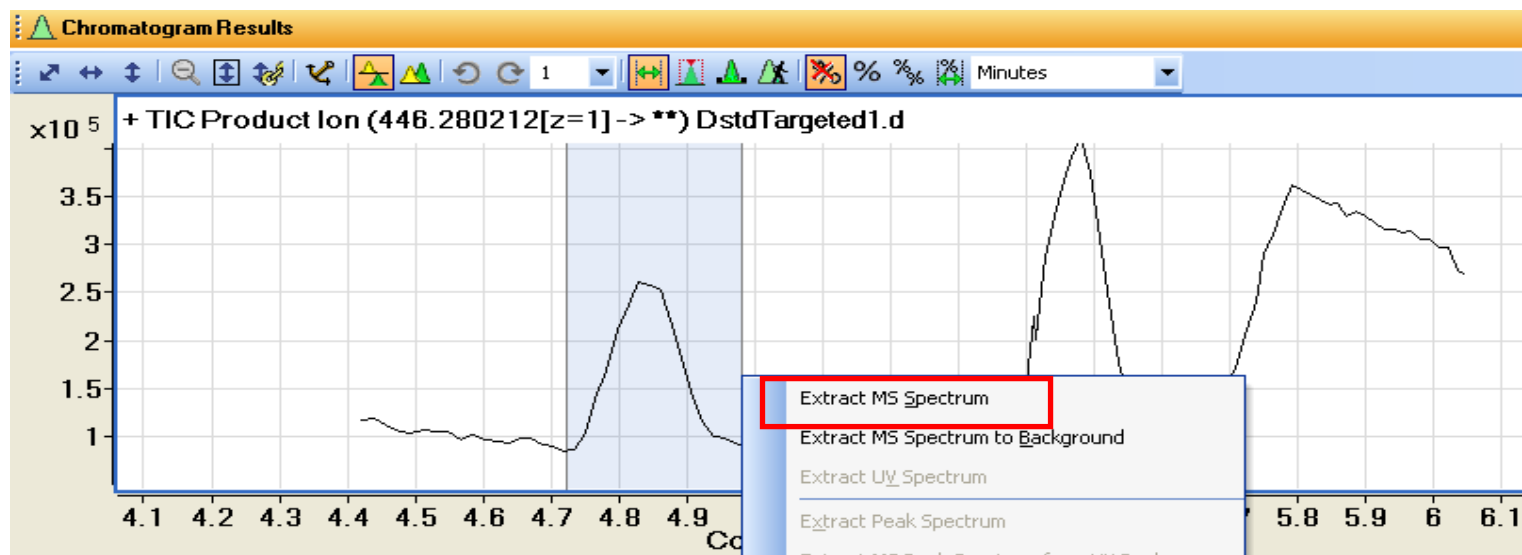
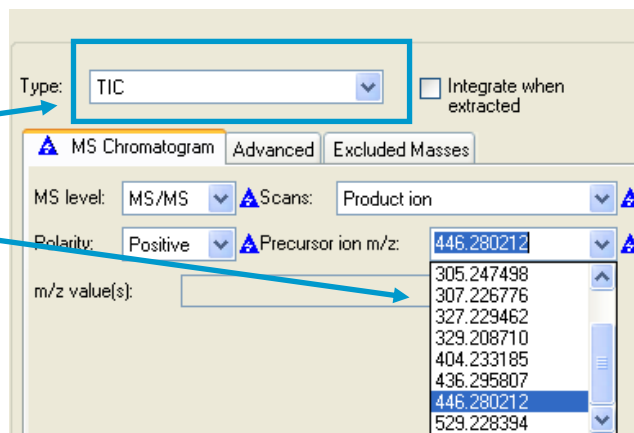
Name	Show/Hide	File	RT	Height	Mass	MFG Formula	MFG Diff (ppm)
Compound 12	<input checked="" type="checkbox"/>	DstdTargeted1.d	8.389	34029	304.239169	C20H32O2	3.49
Compound 10	<input checked="" type="checkbox"/>	DstdTargeted1.d	6.881	31363	306.219793	C19H30O3	-0.97
Compound 8	<input checked="" type="checkbox"/>	DstdTargeted1.d	6.766	122855	328.203239	C21H28O3	1.85
Compound 2	<input checked="" type="checkbox"/>	DstdTargeted1.d	4.378	401617	403.226098	C25H29N3O2	-0.3
Compound 1	<input checked="" type="checkbox"/>	DstdTargeted1.d	3.719	275963	403.226274	C25H29N3O2	-0.74
Compound 3	<input checked="" type="checkbox"/>	DstdTargeted1.d	4.428	1539143	435.286335	C27H37N3O2	5.15
Compound 5	<input checked="" type="checkbox"/>	DstdTargeted1.d	5.664	1325404	435.289034	C27H37N3O2	-1.05
Compound 6	<input checked="" type="checkbox"/>	DstdTargeted1.d	5.797	218196	445.269159	C22H39NO8	-3.57
Compound 4	<input checked="" type="checkbox"/>	DstdTargeted1.d	5.479	294005	445.272811	C28H35N3O2	0.26

# How to Generate Empirical Formula Information from Targeted MS/MS Data Files? (Part 3)

MS/MS Formula Details: Compound 10 C19H30O3						
m/z	Formula	Abund%	Abund	Difference (ppm)	Loss Mass	Loss Formula
307.189525		2.28	112			
289.216192	C19H29O2	30.08	1478	0.05	18.010565	H2O
271.204698	C19H27O	15.88	780	3.48	36.021129	H4O2
253.193137		5.76	283			
233.154435	C15H21O2	1.46	72	-3.55	74.073165	C4H10O
229.194411	C17H25	7.36	362	2.91	78.031694	C2H6O3
213.16398	C16H21	2.33	115	-0.95	94.062994	C3H10O3
193.122526	C12H17O2	1.45	71	-1.14	114.104465	C7H14O
181.124194	C11H17O2	1.38	68	-10.42	126.104465	C8H14O
179.105897	C11H15O2	1.26	62	4.24	128.120115	C8H16O
175.1473	C13H19	2.7	133	4.72	132.078644	C6H12O3
161.135052	C12H17	1.27	63	-15.98	146.094294	C7H14O3
159.117185	C12H15	1.95	96	-2.25	148.109944	C7H16O3
153.090096	C9H13O2	1.41	69	5.95	154.135765	C10H18O
149.129874	C11H17	3.52	173	17.46	158.094294	C8H14O3
147.116877	C11H15	2	98	-0.34	160.109944	C8H16O3
145.098907	C11H13	1.26	62	15.64	162.125594	C8H18O3
139.074598	C8H11O2	1.37	67	5.45	168.151415	C11H20O
135.11775	C10H15	3.27	161	-6.83	172.109944	C9H16O3
133.099182	C10H13	1.95	96	14.99	174.125594	C9H18O3
123.117351	C9H15	1.37	67	-4.26	184.109944	C10H16O3
121.100613	C9H13	6.83	335	4.66	186.125594	C10H18O3
119.085301	C9H11	1.86	91	1.9	188.141245	C10H20O3

# How to Generate Empirical Formula Information from Extracted MS/MS Spectra

Generate TIC, BPC, or EIC for Specific Precursor Ion MS/MS Spectra





# Generate Empirical Formula Information from Extracted MS/MS Spectra

Highlight Each Peak, then Right Click and Select Generate Formulas from Spectrum Peaks

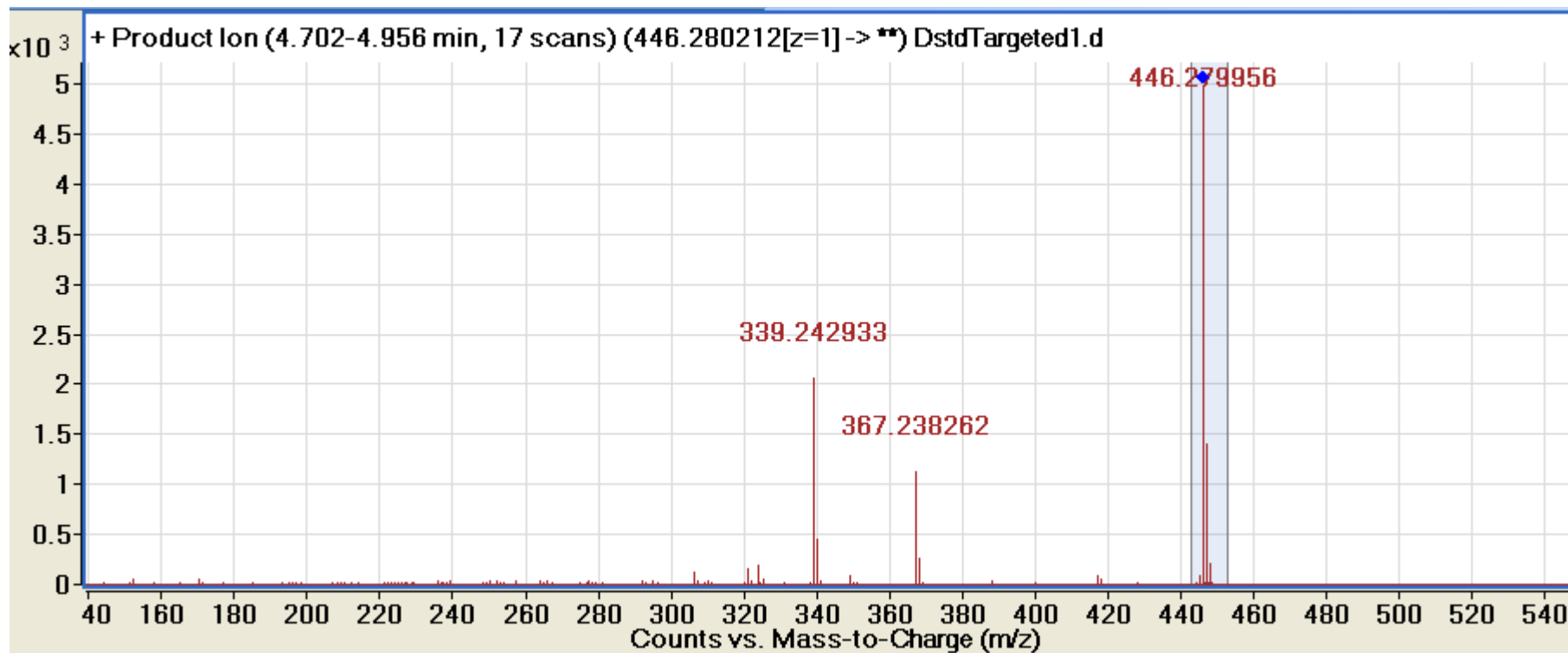
Search Database for Compounds

Search Database for Spectrum Peaks

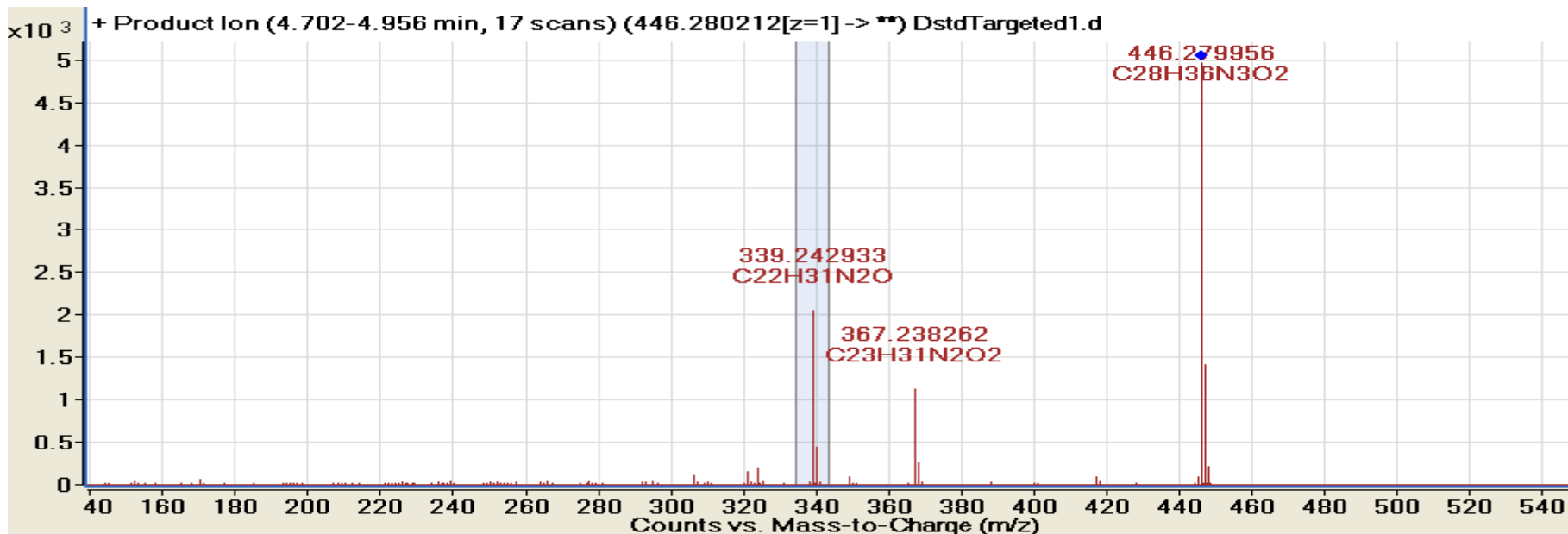
Generate Formulas from Compound

Generate Formulas from Spectrum Peaks

Deconvolute



# Generate Empirical Formula Information from Extracted MS/MS Spectra – Formula for each peak



m/z	Ion	Formula	Abundance							
339.242933	M <sup>+</sup>	C <sub>22</sub> H <sub>31</sub> N <sub>2</sub> O	2051.2							
Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	Difference (mDa)	DBE
<input checked="" type="checkbox"/>	C <sub>22</sub> H <sub>31</sub> N <sub>2</sub> O	C <sub>22</sub> H <sub>31</sub> N <sub>2</sub> O	100		339.243481	339.243639	0.46	0.46	0.16	8.5
m/z	Ion	Formula	Abundance							
367.238262	M <sup>+</sup>	C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub>	1126.8							
Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	Difference (mDa)	DBE
<input checked="" type="checkbox"/>	C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>23</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub>	100		367.238811	367.238553	-0.7	0.7	-0.26	9.5
m/z	Ion	Formula	Abundance							
446.279956	M <sup>+</sup>	C <sub>28</sub> H <sub>36</sub> N <sub>3</sub> O <sub>2</sub>	4967.8							
Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	Difference (mDa)	DBE
<input checked="" type="checkbox"/>	C <sub>28</sub> H <sub>36</sub> N <sub>3</sub> O <sub>2</sub>	C <sub>28</sub> H <sub>36</sub> N <sub>3</sub> O <sub>2</sub>	100		446.280505	446.280752	0.56	0.56	0.25	12.5

# How to Generate Analysis Reports

The image displays the 'Print Analysis Report' dialog box in the Agilent software. The background shows the 'Method Editor: Analysis Report' window with the following settings:

- User chromatograms:**  Show user chromatograms,  With peak tables,  With signal to noise results
- User spectra:**  Show user spectra,  With peak tables
- Compounds:**  Show compound chromatograms,  With peak tables,  Show compound spectra,  With peak tables

The 'Print Analysis Report' dialog box contains the following options:

- List of open data files:** Synurine10xautomsms0003.d
- Report contents:**  All results,  Separate report per data file,  Only highlighted results
- Print report:**  Print report, Printer name: <Default>,  Print preview
- Save report:**  Save report to file,  Inside data file's reports subdirectory,  At specified directory: E:\MassHunterData\reports,  If report file already exists:  Overwrite existing report,  Auto-generate new report file name

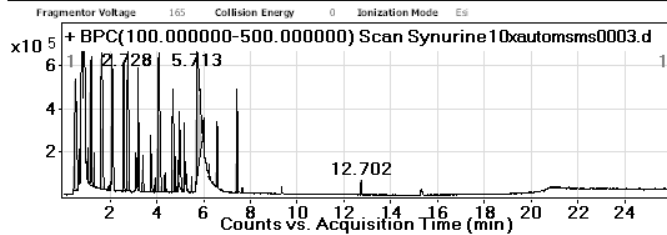
Buttons: OK, Cancel

# Example Analysis Report

## Chromatograms, MS Spectra, Compounds

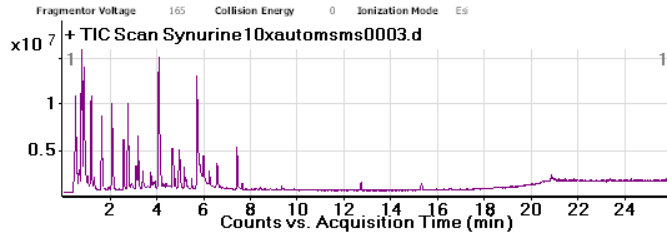
### Qualitative Analysis Report

**Data Filename:** Synurine10xautomsm003.d  
**Sample Name:** Uline  
**Sample Type:** Sample  
**Instrument Name:** Instrument 1  
**Acq Method:** PPCI  
**DAMethod:** PPCI  
**Position:** P1-F8  
**User Name:** Training  
**IRM Calibration Status:** Success  
**Comment:**



Integration Peak List

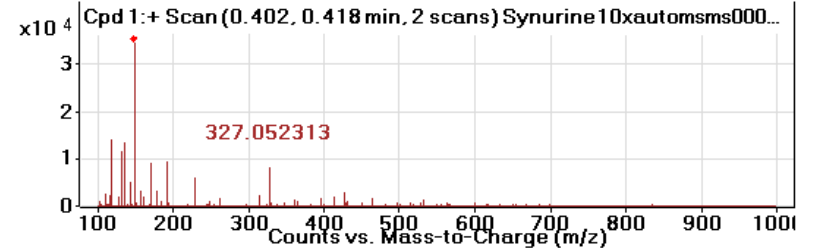
Peak	Start	RT	End	Height	Area	Area%
1	0.402	0.479	0.589	515216	2856537	52.69
4	1.101	1.150	1.218	592696	1878044	34.64
6	1.563	1.602	1.751	627983	1738993	32.07
7	2.010	2.050	2.105	593569	1744319	32.17
8	2.505	2.560	2.617	596118	1006717	18.57
9	2.632	2.728	2.790	638155	1111172	20.49
11	3.132	3.172	3.243	553792	825141	15.22
15	3.990	4.041	4.187	641507	2666713	49.19
23	5.638	5.713	5.939	618349	5421754	100
26	7.346	7.389	7.453	476935	735713	13.57



User Spectra

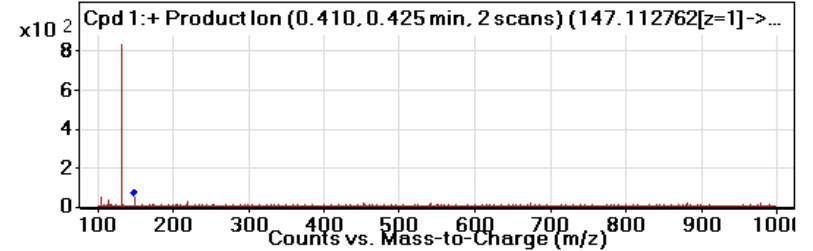
Fragmentor Voltage: 165 Collision Energy: 0 Ionization Mode: ESI

### Qualitative Analysis Report



Peak List

m/z	z	Abund.	Name	Formula	Ion	Score (DB)	Hits (DB)
116.070886	1	14272					
130.086043	1	11480					
133.097294	1	13721					
141.958133	1	5268					
147.112724	1	35930	Lysine	C6H15N2O2	(M+H)+	97.24	2
148.115074	1	2017					
169.094241	1	9178					
191.076238	1	9417					
226.951616	1	5988					
327.052313	1	8254					

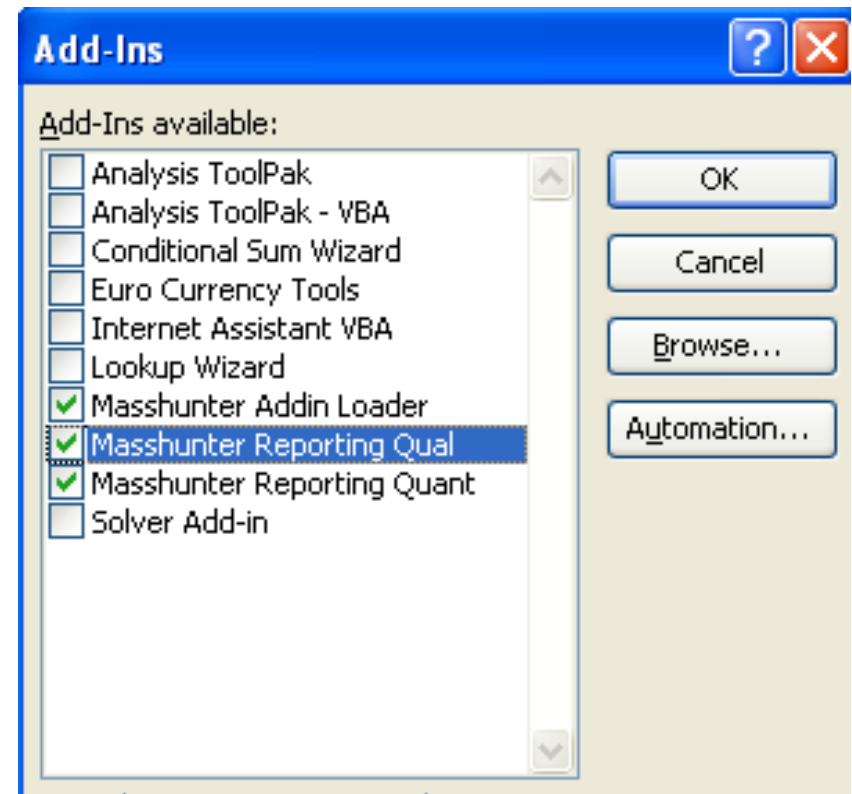
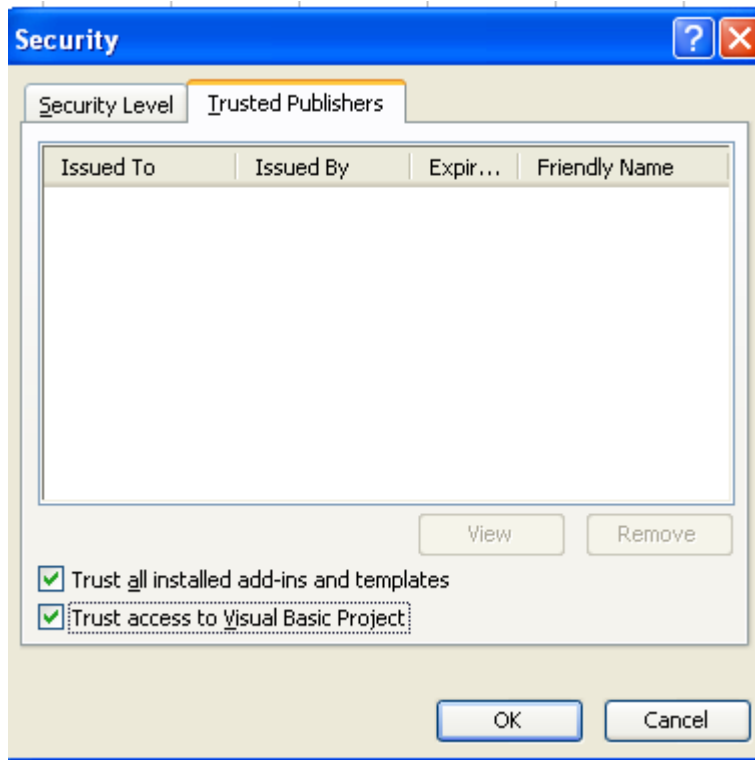


Peak List

m/z	Abund.	Formula
102.091125	51	C5H12NO
130.085641	836	C6H12NO2
130.108475	51	
147.110984	43	



# Microsoft Excel Error



# How to Generate Compound Reports

**Method Editor: Compound Report**

Method Items

**Compound table**

Show compound table

Sort by: Retention time

Sort order: Group number, Compound number, Retention time, Hit count

**Chromatograms**

Show user chromatogram(s)

Show compound chromatogram(s)

**MS Spectrum**

Show MS spectrum  Show MS peak table

Show predicted isotope match table

Show MS spectrum (zoomed in on special peaks)

Zoom padding: - 30.0 + 30.0 m/z

Overlay predicted isotope distribution

**MS/MS Spectrum**

Show MS/MS spectrum  Show MS/MS peak table

List of open data files:

- Synurine10xautomsms0001.d
- Synurine10xautomsms0003.d

**Report contents**

All results  Separate report per data file

Only highlighted results

**Print report**

Print report

Printer name: <Default>

Print preview

**Save report**

Save report to file

Inside data file's reports subdirectory

At specified directory:

E:\MassHunterData\reports

If report file already exists:

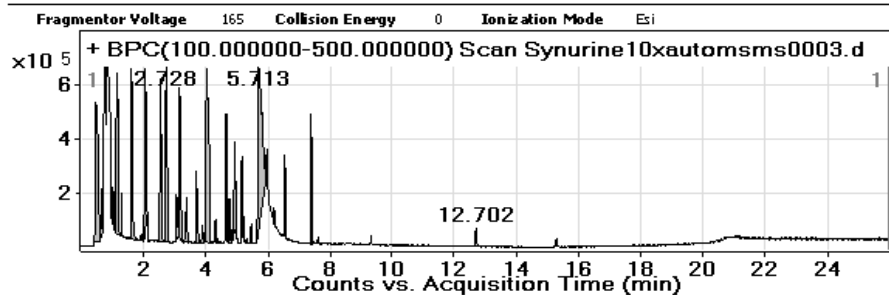
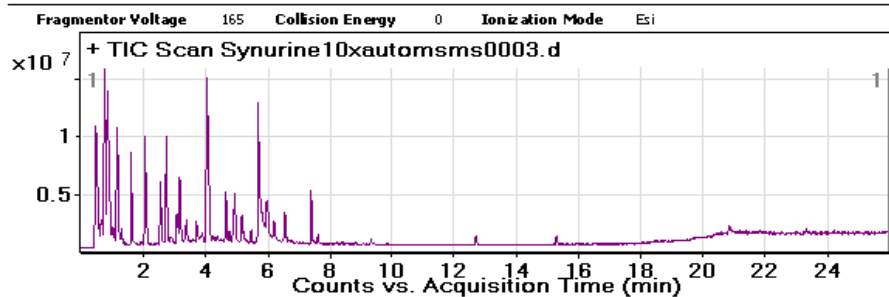
Overwrite existing report

Auto-generate new report file name

## Qualitative Compound Report

<b>Data Filename</b>	Synurine10xautomsms0003.d	<b>Sample Name</b>	Urine
<b>Sample Type</b>	Sample	<b>Position</b>	P1-F8
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	Training
<b>Acq Method</b>		<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	PPCP.m	<b>Comment</b>	

### User Chromatograms



### Compound Table

Name	RT	Mass	Abund.	MFG Formula	MFG Diff (ppm)	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 1: Lysine	0.4	146.105447		C6H14N2O2	0.55	C6H14N2O2	0.55	2
Cpd 3: Homoserine	0.5	119.058125	78720	C4H9NO3	1	C4H9NO3	1	4

# Example Compound Report

## Chromatograms, MS Spectra, Compounds

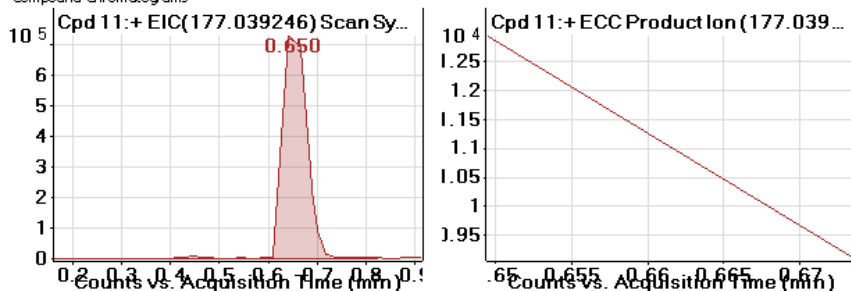
Compound Table

Name	RT	Mass	MFG Formula	MFG Diff (ppm)	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 11: Ascorbic acid (Vitamin C)	0.7	176.031927	C6H8O6	0.91	C6H8O6	0.91	2

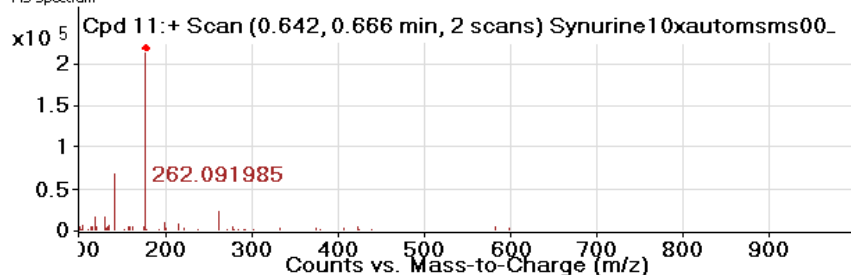
Compounds

Name	m/z	RT	Algorithm	Mass
Cpd 11: Ascorbic acid (Vitamin C)	177.039204	0.662	Auto MS/MS	176.031927

Compound Chromatograms



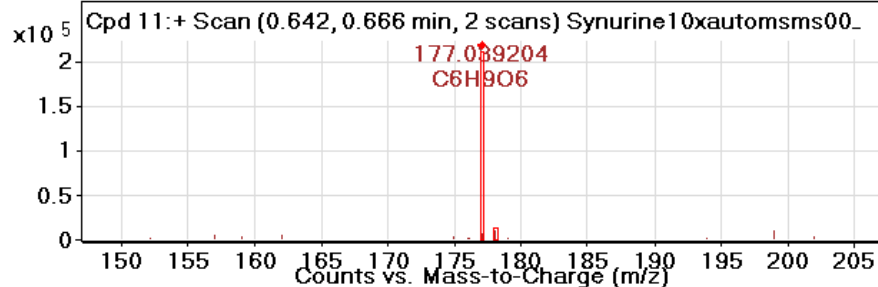
MS Spectrum



MS Spectrum Peak List

m/z	z	Abund.	Formula	Ion	Diff(ppm)
118.086409	1	16531			
129.018046	1	16234			
141.018168	1	68795			
177.039204	1	214526	C6H9O6	(M+H)+	0.91

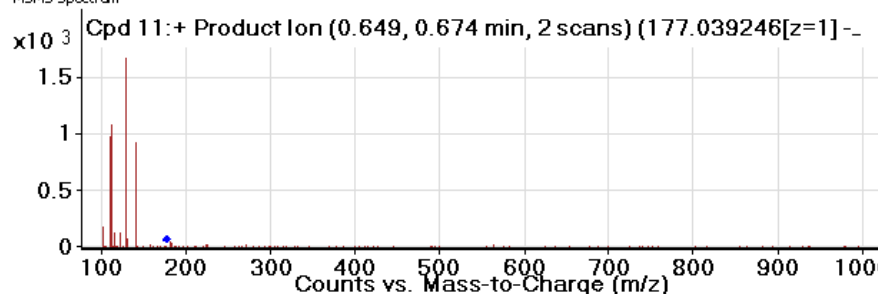
ms zoomed spectrum



Predicted Isotope match table

Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Diff (ppm)
1	100	100	177.039204	177.039364	0.91
2	5.03	6.82	178.042423	178.042792	2.08

MSMS Spectrum



MSMS Spectrum Peak List

m/z	Abund.	Formula	Diff (ppm)
101.02363	190	C4H5O3	-3.07
111.008103	1000	C5H3O3	-3.9
113.023211	1111	C5H5O3	0.97
113.070715	144		
115.039679	128	C5H7O3	-6.16
123.006015	137		
129.018046	1678	C5H5O4	1.46
141.017402	929	C6H5O4	5.9

--- End Of Report ---





# Mass Hunter Quant B.01.04



# MassHunter Quantitative Analysis B.01.04

Provides enhancements for the QQQ, plus support for TOF/Q-TOF including dual mode data and use of MFE to Find Compounds in Samples

- **Support of Excel 2007**
- **Overlay all MRM chromatograms from one sample**
- **Support compound grouping**
- **Honor manual integrations on reprocessing of batch**
- **Add report templates which report “not detected”**
- **Significantly faster processing and browsing**
- **Support TOF/QTOF**
  - better quant method creation from full scan MS and MS/MS data
  - TOF/Q-TOF shows applicable mass precision, scan types, menu choices
  - support dual mode data (profile AND centroid)

# Future Webex (Feb and March)

- **Overview of New MassHunter Profiler Software**
- **Overview of Metlin Personal Database Software**
  - Applications for Metabolomics, Metabolite ID
  - Applications for Small Molecule Analysis
- **MassHunter B.01.04 Quantitation MS and MS/MS Modes**

# Questions and Answers

