Method Name: 140415 Urine Bariatric Study Negative Sample FBI.m

Method Path: C:\MassHunter\Methods\B.06.00\140415 Urine Bariatric Study Negative Sample FBI.m

## **Chromatogram**

## Integrate (MS)

Integrator Selection Agile

## **MS ChemStation Integration settings**

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00
Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	1
0: Shoulders Mode	OFF
0: Baseline Now	False

## MS Universal integrator settings

Shoulder detection	<u>OFF</u>
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

#### MS Chromatogram peak filter settings

Peak area (%) >=	1.000
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

(unknown) ions

## **MS System Suitability**

Enable system suitability calculations False

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## **Integration Results settings**

Clear previous peak spectra	True
Highlight all peaks	False

## Integrate (MS/MS)

## MS/MS Integrator selection

Integrator Selection MS/MS

## MS/MS ChemStation Integration settings

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00
Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	_11
0: Shoulders Mode	OFF
0: Baseline Now	False

## MS/MS Universal integrator settings

Shoulder detection	OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

## MS/MS Chromatogram peak filter settings

Peak area (%) >=	1.000
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## **MS System Suitability**

Enable system suitability calculations False

## **Integration Results settings**

Clear previous peak spectra True



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Highlight all peaks False

## **Smooth**

## **Chromatogram smoothing settings**

Smoothing function:	Gaussian
Function width:	15
Gaussian width:	5.000

## Exclude Mass(es)

## Exclude mass(es) settings

Exclude masses: False

## Calculate Signal-to-Noise

# Signal to noise settings

Automatically compute when chi	omatograms False	
are integrated		
Signal definition:	Height	
Noise definition:	Peak-to-Peak	
Desired length:	1.000	
Minimum length:	0.100	
Start time:	0.000	_
End time:	10.000	
Noise region width:	0.250	

## **Define Chromatograms**

## ChromatogramDefinitions

1-Type:	Base Peak
1-Integrate when extracted	False
1-MS level:	MS
1-Scans:	All Single Stage Scan Types
1-Polarity:	Both
1-Do cycle sum	True
1-Ionization:	Unspecified
1-Single Mz expansion mode:	Symmetric (m/z)



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1-Single m/z width:	0.5000	
Exclude mass(es) settings		
Exclude masses:	False	
Exciduc masses.	1 4150	

## **Adjust Delay Time**

Device delay settings	
MS1 use delay	False

## **Extraction Data Format**

#### **Data storage options**

Extraction Mode	Centroid when available, otherwise Profile
Chrom Extraction Mode	Centroid when available, otherwise Profile

## **Spectrum**

## Extract (MS)

# Manual spectrum extraction settings

MS background source: None	
----------------------------	--

## MS Peak spectrum extraction settings

Average scans above (%):	10
TOF saturation limit (%):	10.0
Restrict saturation m/z range:	False
MS background source:	None
Also evaluate with no background	False
Never return an empty spectrum	True
Tof saturation mz range option	In the m/z ranges used in the chromatogram

## MS TOF peak finder settings



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Detect Maximum Spike Width	2
Detect Required Valley	0.70

## MS spectrum peak filter settings

Limit to the largest:	100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## Charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	1
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	True
charged	

# Extract (MS/MS)

# MS/MS Peak spectrum extraction settings

Average scans above (%):	10
TOF saturation limit (%):	10.0
Restrict saturation m/z range:	False
MS/MS background source:	None
Also evaluate with no background	False
Never return an empty spectrum	True
Tof saturation mz range option	In the m/z ranges used in the chromatogram

#### MS/MS TOF peak finder settings

Detect Maximum Spike Width	2	
Detect Required Valley	0.70	

## MS/MS spectrum peak filter settings

Limit to the largest:	100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## MS/MS Charge state assignement settings



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Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	2
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	False
charged	

## **Deconvolute: Resolved Isotope**

## MS TOF peak finder settings

Detect Maximum Spike Width	2
Detect Required Valley	0.70

## **Resolved Isotope Deconvolution peak filter settings**

Peak height (counts) >=	100
Peak height (%) >=	0.100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## **Resolved Isotope Deconvolution ion species settings**

Positive ions:	+H
Negative ions:	-H

## **Resolved Isotope Deconvolution charge state assignment settings**

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	2
Limit assigned charge states to a maximum	True
of:	
Isotope model	Peptides
Treat ions with unassigned charge as singly-	True
The state of the s	iiue

## **Extraction Data Format**

## **Data storage options**

Extraction Mode	Centroid when available, otherwise Profile
Chrom Extraction Mode	Centroid when available, otherwise Profile



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# **General**

# **File Open Actions**

File open actions

## File Save Options

## **File Save Options**

Save Complete Results	False
-----------------------	-------

## **Reports**

# **Analysis Report**

# Analysis report settings

Show user chromatograms	True
With peak tables	True
With signal to noise results	False
Show user spectra	True
Show library spectrum	False
Show difference spectrum	False
With peak tables	True
Show compound chromatograms	True
With peak tables	False
Show compound spectra	True
With peak tables	True

# **Compound Report**



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## **Compound report settings**

Show compound table	True
Sort compound table in increasing order:	True
Show user chromatogram(s)	False
Show compound chromatogram(s)	True
Overlay compound chromatogram(s)	False
Show MS spectrum	True
Show library spectrum	False
Show difference spectrum	False
Show MS peak table	True
Show predicted isotope match table	False
Show MS spectrum (zoomed in on special	True
peaks)	
Overlay predicted isotope distribution	True
Show MS/MS spectrum	True
Show MS/MS peak table	True
Left zoom limit	30.0
Right zoom limit	30.0
Sort compound table by	Retention Time
Exclude details for unidentified compounds	False

# **Common Reporting Options**

# Report templates

Report Template(s): -Template Folder	C:\Mass Hunter\Report Templates\Qual\B.06.00\en-US\Letter
Analysis report template :	Analysis Report
Compound report template :	Compound Report
Qualitative method report template :	Qualitative Method Report
Acquisition method report template :	Acg Method Report

# **Common report settings**

Page orientation	Portrait
Chromatogram peaks	True
Max Chrom Peaks	10
Mass spectrum peaks	True
Max Spectrum Peaks	10
Hide empty columns in tables	True
Show sample information	True
User chromatograms	False
Compound chromatograms	False
MS spectra	False
MS/MS spectra	False
Deconvoluted spectra	False
UV spectra	False

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# **Find Compounds**

## Find by Auto MS/MS

Eind	compounds	Auto	MC/MC	cottings
rına	combounds	Auto	M2/M2	settinas

Retention time window:	0.250
Positive MS/MS TIC threshold:	1000
Negative MS/MS TIC threshold:	1000
Mass match tolerance:	0.0500
Limit to the largest compounds:	False
Omit persistent background compounds >	5
Extract ECC:	True
Extract EIC:	True
EIC single m/z expansion:	75.000
Extract MS:	True
Extract MS:	False
Except when the TIC >	100000.0
Filter results by fragments	False
Single m/z expansion:	Symmetric (m/z)
Extract separate MS/MS spectrum per	True
collision energy	

## Exclude mass(es) settings

Exclude masses: False

# Find compounds results settings

Delete previous compounds	True
Highlight all compounds	False

## Find by Targeted MS/MS

# MS/MS Integrator selection

Integrator Selection MS/MS

## MS/MS ChemStation Integration settings

l angent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00

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Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	1
0: Shoulders Mode	OFF
0: Baseline Now	False

## Targeted MS/MS processing settings

Maximum chromatogram peak width	0.25
Limit to the largest compounds:	False
Extract MS/MS chromatogram	True
Extract MS/MS spectrum	True
Extract MS spectrum	False
Extract separate MS/MS spectrum per	True
collision energy	
Generate library spectra	False

## MS/MS Universal integrator settings

Shoulder detection	OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

## Targeted MS/MS chromatogram peak filter settings

Peak area (%) >=	5.000
Limit to largest:	10
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## MS/MS Peak spectrum extraction settings

Average scans above (%):	10
TOF saturation limit (%):	10.0
Restrict saturation m/z range:	False
MS/MS background source:	None
Also evaluate with no background	False
Never return an empty spectrum	True
Tof saturation mz range option	In the m/z ranges used in the chromatogram

# Find compounds results settings

Delete previous compounds	True
Highlight all compounds	False

# **Find by Molecular Feature**

MFF	processing	and ion	snecies	settings
1.11	pi ocessiiiq	and ion	<b>SPECIES</b>	<b>Jettiiig</b>

= processing and for openes se	
Retention time range:	0.35 - 19
Restrict m/z range:	False
Use peaks with height >=	500
Positive ions:	_
Modifier	+H
Modifier	+Na
Negative ions:	_
Modifier	<u>-H</u>
Modifier	+Cl
Salt dominated positive ions:	False
Include representative raw spectrum for	False
each compound	
Assume unidentified ions are radical ions	False
Target data type	Small molecules (chromatographic)
Neutral Species Definitions	
Include representative raw spectrum for	False
each compound	
Extract ECC	False
Extract MFE spectrum	False
Typical RT peak width	False
min	0.200
Smoothing	True
times peak width	0.200
Smoothing	True
length	50.000
Remove spikes	False
max spike width	0.250
Smooth peaks	True
times peak width	1.000
Remove wide peaks	False
min peak width	10.000
Display only the largest	False
Extract MS/MS Spectrum	False
Average MSMSSpectrum per CE	False
Single m\z Expansion mode	Asymmetric (m/z)
Tolerance	20.00
Tolerance	0.05
Tolerance Unit	ppm
Deisotope MS/MS spectrum	True

# **Charge state assignment settings**

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	1
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	True
charged	



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#### **MFE** result filters

Peak height (counts) >=	2000
Restrict retention times:	False
Restrict charge states:	False
Restrict to neutral losses:	False
Filter mass list	False
Quality score	50.00

## Mass defect filter settings

Filter results on mass defects	False

#### MS/MS spectrum peak filter settings

Limit to the largest:	100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## MFE result options

Delete previous compounds	True
Highlight all compounds	True

## MFE database location

Database Path	C:\Mass Hunter\PCDL\default.csv

## Find by MRM

## MS/MS Integrator selection

Integrator Selection	MS/MS
·	·

## MS/MS ChemStation Integration settings

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00
Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5

0: Height Reject	1	
0: Shoulders Mode	OFF	
0: Baseline Now	False	

## MS/MS Universal integrator settings

Shoulder detection	OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

## Targeted MS/MS chromatogram peak filter settings

Peak area (%) >=	5.000
Limit to largest:	10
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## MS/MS Peak spectrum extraction settings

Average scans above (%):	10
TOF saturation limit (%):	10.0
Restrict saturation m/z range:	False
MS/MS background source:	None
Also evaluate with no background	False
Never return an empty spectrum	True
Tof saturation mz range option	In the m/z ranges used in the chromatogram

## Find compounds results settings

Delete previous compounds	True
Highlight all compounds	False

## **MRM Settings**

Extract MRM chromatogram	True
Extract MRM spectrum	True
Group transitions by compound name	True
Detect most abundant peak by peak area	True

## Signal to noise settings

Automatically compute when chromatograms False	
are integrated	
Signal definition:	Height
Noise definition:	Peak-to-Peak
Desired length:	1.000

Minimum length:	0.100
Start time:	0.000
End time:	10.000
Noise region width:	0.250

## **Find by Integration**

# Find by Integration Integrator selection

## Find by Integration ChemStation integrator settings

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00
Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	1
0: Shoulders Mode	OFF
0: Baseline Now	False

## Find by Integration Universal integrator settings

Shoulder detection	OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

## Find by Integration Chromatogram peak filter settings

Peak area (%) >=	1.000
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## **Chromatogram extraction options**

Identify individual peaks in spectrum	True
Maximum number of peaks to identify (per	5
spectrum)	
Search a database for each peak	False
Generate formula for each peak	False



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Chromatogram used to find mass spectra	Total Ion
Get Signal A from	DAD
Signal Device Name	<u>_</u>
Signal Ordinal Number	1
Exclude mass(es) settings	
Exclude masses:	<u>False</u>
Device delay settings	
MS1 use delay	False
MC Book an advance automation and	
MS Peak spectrum extraction setti Average scans above (%):	ngs 10
	10.0
TOF saturation limit (%):	— <del></del>
Restrict saturation m/z range:	False
	NI
MS background source:	None
Also evaluate with no background	False

# Charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	1
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	True
charged	

#### Find compounds results settings

rina compounds results settings		
Delete previous compounds	True	
Highlight all compounds	False	

# **Find Compounds by Formula**

## Find by Formula - Options

**Find Compounds by Formula options** 



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Formula source to confirm	Compound exchange file (.CEF):
Use Absolute Mass Tolerance	False
Retention Time Tolerance	0.500
Single Mz expansion mode:	Symmetric (ppm)
Expected retention time	2.00
Search Fields	Mass, Retention Time
Relative Mass Tolerance	20.00
Single ppm width:	35.0
Cef Path	C:\Mass Hunter\Data\131003 Characterize QC Bariatric
	Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg
	Mode.cef
Automatically increase for isomeric	True
compounds	
Do not match if score is	True
Reject score threshold	60.00
Do not match if the (unobserved) second	True
ion's abundance is expected to be	
Reject second ion threshold	300.00
Prefer profile for raw spectra, if available	True
Clip extracted raw spectra	True
Extracted spectrum expansion mode	Symmetric (m/z)
Asymmetric low width	5.0000
Asymmetric high width	10.0000
Single width	5.0000
Extract MS/MS spectrum	False
Average MS/MS spectrum for all CE's	False
Precursor tolerance	20.00
Precursor tolerance	0.05
Tolerance unit	ppm
Deisotope MS/MS spectrum	True
Include structure	False
Warn if score is	True
Warn if the (unobserved) second ion's	True
abundance is expected to be	
Warn score threshold	75.00
Warn single ion threshold	50.00
Smooth EIC before integration	False

# **Database location settings**

Database Path C:\Mass Hunter\PCDL\default.csv

# **Probable Pos Species settings**

Positive ions:	
Modifier	+H
Modifier	+Na
Positive Neutral Loss:	
Positive Charge State Range	1-1
Positive Dimer	False
Positive Trimer	False

## **Probable Neg Species settings**



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Negative ions:	
Modifier	<u>-Н</u>
Modifier	+Cl
Negative Neutral Loss:	
Negative Charge State Range	1-1
Negative Dimer	False
Negative Trimer	False

## **Identification Scoring**

MS mass coeff (m Da)	2.0
MS mass coeff (ppm)	5.6
MS/MS mass coeff (MDa)	5.0
MS/MS mass coeff (ppm)	7.5
MS isosope abundance	7.5
Retention time:	0.250
Isotope abundance score	60.00
Mass score	100.00
Isotope spacing score	50.00
Retention time score	100.00
MS/MS score weight	50.00

## Find compounds results settings

Delete previous compounds	True
Highlight all compounds	False

## Find by Formula All Ions settings

LOW energy channel spectra with	LOW energy channel spectra
Confirm with fragment ions	False
Coelution score	90
Spectral library if spectrum available,	True
otherwise use average fragment spectrum	
Number of most abundant ions from spectral	5
library	
Number of most abundant ions from average	7
fragment spectrum	
RT difference	0.10
S/N ratio	True
SNRatio	5.00
Minimum number of qualified fragments	True
Num Of Confirmed Fragments	1
Minimum percent of qualified fragments	75

## Find by Formula - Chromatograms

## Find Compounds by Formula options

Formula source to confirm	Compound exchange file (.CEF):



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Retention Time Tolerance Single Mz expansion mode: Symmetric (ppm) Search Fields Mass, Retention Time 2.00 Search Fields Mass Tolerance 20.00 Single ppm width: 35.0 Cef Path C:\Mass Hunter\Data\131003 Characterize QC Bariatric Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef Automatically increase for isomeric True True Compounds Do not match if score is Reject score threshold Do not match if the (unobserved) second Ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Extracted spectrum expansion mode Symmetric low width Asymmetric low width Asymmetric high width S.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance 20.00 True  Union Section Section True  Prefer profile for raw spectra True  Extracted spectrum expansion mode Symmetric (m/z)  Symmetric low width S.0000  Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance 20.00 Tolerance unit ppm Deisotope MS/MS spectrum True  Warn if the (unobserved) second ion's True Warn if score is Warn score threshold Smooth EIC before integration False  Warn store threshold Smooth EIC before integration False	Use Absolute Mass Tolerance	False
Expected retention time  Search Fields  Relative Mass Tolerance  Single ppm width:  CF Path  C:\Mass Hunter\Data\131003 Characterize QC Bariatric  Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef  Automatically increase for isomeric  compounds  Do not match if score is  Reject score threshold  Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold  Clip extracted raw spectra  Extracted spectrum expansion mode  Asymmetric high width  Sou000  Single width  Sou000  Precursor tolerance  Precursor tolerance  Do not  Precursor tolerance  Do not  Precursor tolerance  Do not  Deisotope MS/MS spectrum  True  False  Warn if score is  True  True  True  True  True  False  Warn if the (unobserved) second ion's  True  True  True  True  True  True  False  Warn if the (unobserved) second ion's  True  True	Retention Time Tolerance	0.500
Search Fields         Mass, Retention Time           Relative Mass Tolerance         20.00           Single ppm width:         35.0           Cef Path         C:\Mass Hunter\Data\131003 Characterize QC Bariatric           Timepoints\140415 QC FBI for FBI of Samples Neg Mode.cef           Automatically increase for isomeric         True           compounds         True           Do not match if score is         True           Reject score threshold         60.00           Do not match if the (unobserved) second ion's abundance is expected to be         True           Reject second ion threshold         300.00           Prefer profile for raw spectra, if available         True           Clip extracted raw spectra is available         True           Clip extracted raw spectra is available         True           Asymmetric low width         5.0000           Asymmetric low width         5.0000           Asymmetric high width         10.0000           Single width         5.0000           Extract MS/MS spectrum         False           Precursor tolerance         20.00           Precursor tolerance         0.05           Tolerance unit         ppm           Deisotope MS/MS spectrum         True <t< td=""><td>Single Mz expansion mode:</td><td>Symmetric (ppm)</td></t<>	Single Mz expansion mode:	Symmetric (ppm)
Relative Mass Tolerance 20.00  Single ppm width: 35.0  Cef Path C:\Mass Hunter\Data\131003 Characterize QC Bariatric  Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef  Automatically increase for isomeric True  Compounds  Do not match if score is  Reject score threshold 60.00  Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold 300.00  Prefer profile for raw spectra, if available Clip extracted raw spectra  Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric low width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 20.00  Precursor tolerance ppm  Deisotope MS/MS spectrum True  Nam if score is True  Warn if the (unobserved) second ion's True  Warn single ion threshold 75.00  Warn single ion threshold 75.00  Time Sanda Automatically 131003 Characterize QC Bariatric  Time Oct. PBI 10103 Characterize QC Bariatric  Time Oct. PBI 10103 Characterize QC Bariatric  True  100000  10000  10000  10000  10000  10000  10000  10000  10000  100000  10000  10000  10000  10000  10000  10000  10000  10000  100000  1000	Expected retention time	2.00
Single ppm width:  Cef Path  C:\Mass Hunter\Data\131003 Characterize QC Bariatric  Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef  Automatically increase for isomeric  compounds  Do not match if score is  Reject score threshold  Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold  Prefer profile for raw spectra, if available  Clip extracted raw spectra  Extracted spectrum expansion mode  Symmetric (m/z)  Asymmetric low width  5.0000  Extract MS/MS spectrum  False  Average MS/MS spectrum  Precursor tolerance  Precursor tolerance  Donot  Donot match if the (unobserved) second  True  True  True  True  Extracted raw spectra  Symmetric (m/z)  Sound  Extract MS/MS spectrum  False  Average MS/MS spectrum  False  Average MS/MS spectrum  Precursor tolerance  Donot  Donot  True  Include structure  False  Warn if score is  True  Warn if the (unobserved) second ion's  True  Warn single ion threshold  Toue  True  Toue  True  T	Search Fields	Mass, Retention Time
C:\Mass Hunter\Data\131003 Characterize QC Bariatric Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef True  Automatically increase for isomeric compounds Do not match if score is Reject score threshold Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra Extracted spectrum expansion mode Asymmetric low width Single width Single width Single width Sound Extract MS/MS spectrum False Precursor tolerance Precursor tolerance Diesotope MS/MS spectrum True Include structure Warn if score is Warn single ion threshold True  C:\Mass Hunter\Data\131003 Characterize QC Bariatric Timepoints\140415 QC FBI \notation FBI of Samples Neg Mode.cef True  1rue	Relative Mass Tolerance	20.00
Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg Mode.cef True  Compounds Do not match if score is Reject score threshold On not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra Extracted spectrum expansion mode Asymmetric low width Single width Sing	Single ppm width:	35.0
Automatically increase for isomeric True  Compounds  Do not match if score is True  Reject score threshold 60.00  Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold 300.00  Prefer profile for raw spectra, if available True  Clip extracted raw spectra True  Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Marn if score is True  Warn if the (unobserved) second ion's True  Warn single ion threshold 75.00  Warn single ion threshold 50.000  True	Cef Path	C:\Mass Hunter\Data\131003 Characterize QC Bariatric
Automatically increase for isomeric True  compounds  Do not match if score is True  Reject score threshold 60.00  Do not match if the (unobserved) second True  ion's abundance is expected to be  Reject second ion threshold 300.00  Prefer profile for raw spectra, if available True  Clip extracted raw spectra True  Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  Warn single ion threshold 50.00  Warn single ion threshold 50.00		Timepoints\140415 QC FBI\140415 QC FBI for FBI of Samples Neg
compounds Do not match if score is Reject score threshold Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra True Extracted spectrum expansion mode Asymmetric low width S.0000 Asymmetric low width S.0000 Single width S.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance Display MS/MS spectrum Procursor tolerance Tolerance unit Deisotope MS/MS spectrum True Include structure Warn if score is Warn single ion threshold True		Mode.cef
Do not match if score is Reject score threshold Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra Extracted spectrum expansion mode Asymmetric low width S.0000 Asymmetric high width S.0000 Single width S.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's False Precursor tolerance Deisotope MS/MS spectrum True  Deisotope MS/MS spectrum True True True True False Warn if score is True Warn single ion threshold True  Toue Toue True True True True True True True Tr	Automatically increase for isomeric	True
Reject score threshold Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra True Clip extracted spectrum expansion mode Symmetric (m/z) Asymmetric low width S.0000 Asymmetric high width 10.0000 Single width 5.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's False Precursor tolerance 20.00 Precursor tolerance 0.05 Tolerance unit ppm Deisotope MS/MS spectrum True Unclude structure False Warn if score is True Warn sore threshold T5.00 Warn single ion threshold  50.00  True	compounds	
Do not match if the (unobserved) second ion's abundance is expected to be  Reject second ion threshold 300.00  Prefer profile for raw spectra, if available Clip extracted raw spectra True  Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn single ion threshold 50.00  Warn single ion threshold 50.00  True	Do not match if score is	True
ion's abundance is expected to be  Reject second ion threshold 300.00  Prefer profile for raw spectra, if available True  Clip extracted raw spectra True  Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn single ion threshold 50.00  Marn single ion threshold  300.00  True  True  True  300.00	Reject score threshold	60.00
Reject second ion threshold Prefer profile for raw spectra, if available Clip extracted raw spectra True Extracted spectrum expansion mode Symmetric (m/z) Asymmetric low width 5.0000 Asymmetric high width 10.0000 Single width 5.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance Precursor tolerance Tolerance unit Deisotope MS/MS spectrum True Include structure False Warn if score is True Warn score threshold T5.00 Warn single ion threshold  50.00 True	Do not match if the (unobserved) second	True
Prefer profile for raw spectra, if available Clip extracted raw spectra Extracted spectrum expansion mode Symmetric (m/z)  Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance 20.00  Precursor tolerance 10.05  Tolerance unit 10.0000  True  Include structure False Warn if score is True  Warn if the (unobserved) second ion's True  Warn score threshold  75.00  Warn single ion threshold  True	ion's abundance is expected to be	
Prefer profile for raw spectra, if available Clip extracted raw spectra Extracted spectrum expansion mode Asymmetric low width Asymmetric high width Incompage width Single width Single width Single width Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance Precursor tolerance O.05 Tolerance unit Deisotope MS/MS spectrum True Include structure False Warn if score is True Warn if the (unobserved) second ion's Tole width True Warn score threshold T5.00 Warn single ion threshold  True  Tru		
Clip extracted raw spectra Extracted spectrum expansion mode Asymmetric low width 5.0000 Asymmetric high width 10.0000 Single width 5.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance Precursor tolerance 0.05 Tolerance unit ppm Deisotope MS/MS spectrum Include structure False Warn if score is Warn if the (unobserved) second ion's True abundance is expected to be Warn sore threshold True Tougon Tougon Tougon True True True True True True True True	Reject second ion threshold	300.00
Extracted spectrum expansion mode Asymmetric low width 5.0000 Asymmetric high width 10.0000 Single width 5.0000 Extract MS/MS spectrum False Average MS/MS spectrum for all CE's Precursor tolerance 20.00 Precursor tolerance 70.05 Tolerance unit ppm Deisotope MS/MS spectrum True Include structure False Warn if score is True Warn if the (unobserved) second ion's True abundance is expected to be Warn score threshold T5.00 Warn single ion threshold	Prefer profile for raw spectra, if available	True
Asymmetric low width 5.0000  Asymmetric high width 10.0000  Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Clip extracted raw spectra	True
Asymmetric high width  Single width  Extract MS/MS spectrum  Average MS/MS spectrum for all CE's  Precursor tolerance  Precursor tolerance  Tolerance unit  Deisotope MS/MS spectrum  True  Include structure  Warn if score is  Warn if the (unobserved) second ion's  abundance is expected to be  Warn single ion threshold  10.0000  5.000  False  Average MS/MS spectrum for all CE's  False  Precursor tolerance  20.00  Precursor tolerance  0.05  True  1. True  True  True  True  True  True  Warn if score is  True  Warn if the (unobserved) second ion's  True  Abundance is expected to be  Warn single ion threshold  50.00	Extracted spectrum expansion mode	Symmetric (m/z)
Single width 5.0000  Extract MS/MS spectrum False  Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Asymmetric low width	5.0000
Extract MS/MS spectrum  Average MS/MS spectrum for all CE's  False  Precursor tolerance  20.00  Precursor tolerance  0.05  Tolerance unit  ppm  Deisotope MS/MS spectrum  True  Include structure  False  Warn if score is  True  Warn if the (unobserved) second ion's  abundance is expected to be  Warn score threshold  75.00  Warn single ion threshold	Asymmetric high width	10.0000
Average MS/MS spectrum for all CE's False  Precursor tolerance 20.00  Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Single width	5.0000
Precursor tolerance 20.00 Precursor tolerance 0.05 Tolerance unit ppm Deisotope MS/MS spectrum True Include structure False Warn if score is True Warn if the (unobserved) second ion's True abundance is expected to be Warn score threshold 75.00 Warn single ion threshold 50.00	Extract MS/MS spectrum	False
Precursor tolerance 0.05  Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Average MS/MS spectrum for all CE's	False
Tolerance unit ppm  Deisotope MS/MS spectrum True  Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Precursor tolerance	20.00
Deisotope MS/MS spectrum True Include structure False Warn if score is True Warn if the (unobserved) second ion's True abundance is expected to be Warn score threshold 75.00 Warn single ion threshold 50.00	Precursor tolerance	0.05
Include structure False  Warn if score is True  Warn if the (unobserved) second ion's True  abundance is expected to be  Warn score threshold 75.00  Warn single ion threshold 50.00	Tolerance unit	ppm
Warn if score is  Warn if the (unobserved) second ion's  True  abundance is expected to be  Warn score threshold  True  75.00  Warn single ion threshold  Toue	Deisotope MS/MS spectrum	True
Warn if the (unobserved) second ion's abundance is expected to be Warn score threshold 75.00 Warn single ion threshold 50.00	Include structure	False
abundance is expected to be Warn score threshold 75.00 Warn single ion threshold 50.00	Warn if score is	True
Warn score threshold75.00Warn single ion threshold50.00	Warn if the (unobserved) second ion's	True
Warn single ion threshold 50.00	abundance is expected to be	
	Warn score threshold	75.00
Smooth EIC before integration False	Warn single ion threshold	50.00
	Smooth EIC before integration	False

# **Chromatogram smoothing settings**

Smoothing function:	Gaussian
Function width:	15
Gaussian width:	5.000

#### **MS Integrator selection**

Integrator Selection	Agile	

## **MS ChemStation Integration settings**

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00



Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	1
0: Shoulders Mode	OFF
0: Baseline Now	False

## MS Universal integrator settings

Shoulder detection	OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

# Find by Formula Chromatogram peak filter settings

Peak height (counts) >=	500
Limit to largest:	5
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## Find by Formula - Mass Spectra

## MS Peak spectrum extraction settings

Average scans above (%):	10
TOF saturation limit (%):	10.0
Restrict saturation m/z range:	False
MS background source:	None
Also evaluate with no background	False
Never return an empty spectrum	True
Tof saturation mz range option	In the m/z ranges used in the chromatogram

## MS TOF peak finder settings

Detect Maximum Spike Width	2
Detect Required Valley	0.70

## Charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	1
Limit assigned charge states to a maximum	True
of:	

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Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	True
charged	

## Find by Formula - Sample Purity

# Sample Purity options Compute sample purity False Device delay settings MS1 use delay Exclude mass(es) settings Exclude masses: False MS Integrator selection Integrator Selection Agile

## **MS ChemStation Integration settings**

Tangent skim mode:	Standard
Baseline correction mode:	Classical
Front skim height ratio:	0.00
Tail skim height ratio:	0.00
Skim valley ratio:	20.00
Peak-to-Valley ratio:	500.00
0: Slope Sensitivity	5
0: Peak Width	0.05
0: Area Reject	5
0: Height Reject	1
0: Shoulders Mode	OFF
0: Baseline Now	False

## MS Universal integrator settings

Shoulder detection	OFF OFF
Threshold:	0.00
Area reject:	0.00
Peak width:	0.00
Use Data Scale Factor	False
0: Baseline Now	False

## MS Chromatogram peak filter settings



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Peak area (%) >=	1.000
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

# **Identify Compounds**

## **Search Database**

Database search settings	
Use Absolute Mass Tolerance	False
Relative Mass Tolerance	5.00
Retention Time Tolerance	0.100
Maximum Hits	10
Maximum number of peaks to search when	5
peaks are not specified graphically:	

Search "neutral" database entries for masses from simple ions

# **Database location settings**

Database Path C:\Mass Hunter\PCDL\default.csv

## **Probable Pos Species settings**

Positive ions:	
Modifier	+H
Modifier	+Na
Positive Neutral Loss:	
Positive Charge State Range	1-1
Positive Dimer	False
Positive Trimer	False

# **Probable Neg Species settings**

Negative ions:	
Modifier	<u>-</u> H
Modifier	+Cl
Negative Neutral Loss:	
Negative Charge State Range	1-1
Negative Dimer	False
Negative Trimer	False

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## **Identification Scoring**

MS mass coeff (m Da)	2.0
MS mass coeff (ppm)	5.6
MS/MS mass coeff (MDa)	5.0
MS/MS mass coeff (ppm)	7.5
MS isosope abundance	7.5
Retention time:	0.250
Isotope abundance score	60.00
Mass score	100.00
Isotope spacing score	50.00
Retention time score	100.00
MS/MS score weight	50.00

## **Search Accurate Mass Library**

# LC Spectral library search settings

Spectral library path:	
Limit to the best	False
Maximum hits per compound:	10
Search criteria	Collision Energy, Fragmentation Voltage, Polarity, Scan Type,
	Instrument Type, Precursor Ion
Search method	Reverse
Ce Tolerance	2.00
Precursor Ion m/z ppm	10.0
Precursor Ion m/z m Da	2.0000
Product ion m/z ppm	20.0
Product ion m/z m Da	2.0000
Minimum forward match score:	25.00
Minimum reverse match score:	80.00

## **Spectral library selection settings**

Spectral library path:	
Apply to search database path	False

## **Search Library Options**

Perform Unit Mass Library Search False

## Peak filters used by spectral library search

Peak height (counts) >=	100
Peak height (%) >=	0.500
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

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# **Generate Formulas**

Formula	calculator	settinas
---------	------------	----------

MS nitrogen rule:	even electron
Positive ions:	Н
Negative ions:	H
Element Limits	
C	3 to 60
<u>H</u>	0 to 120
0	0 to 30
N	<u>0 to 30</u>
S	0 to 5
Cl	<u>0 to 3</u>
Maximum neutral mass for which formulas	750.0000
should be calculated:	
Minimum score	35.000
Maximum MS mass error	False
Require DBE from	False
Maximum number of hits per charge carrier	False
MS Mass Coeff (MDa)	2.0
MS Mass Coeff (Ppm)	5.6
MS MS Mass Coeff (MDa)	2.5
MS MS Mass Coeff (Ppm)	7.5
MS isotope abundance	7.5
Formula generation rules	<u>B0201</u>
Include target formula in results	False
Target formula	_
Positive ions:	
Modifier	+H
Negative ions:	
Modifier	<u>-H</u>
Group hits with same formula (but different	True
charge carriers)	

# Charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	1
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	True
charged	

## Fragment formula annotation peak filter settings

Peak height (counts) >=	10
Peak height (%) >=	0.100
Limit to the largest:	100
Annotate fragment spectrum peaks with	False
formulas	



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Generate formulas for non-fragment False (unknown) ions

#### **Identification Scoring**

MS mass coeff (m Da)	2.0
MS mass coeff (ppm)	5.6
MS/MS mass coeff (MDa)	5.0
MS/MS mass coeff (ppm)	7.5
MS isosope abundance	7.5
Retention time:	0.250
Isotope abundance score	60.00
Mass score	100.00
Isotope spacing score	50.00
Retention time score	100.00
MS/MS score weight	50.00

## **Combine Identification Results**

## **Combine identification results settings**

DB search score weight:	40.00
MFG score weight:	40.00
Library search score weight:	40.00
Bio Confirm score weight:	40.00
Minimum overall score:	0.00
Autolock score:	60.00
Maximum number of hits:	10

# **Compound Automation Steps**

## (1) Result Options

## **Compound Automation Result Options**

Delete all previous results True

## (2) Find and Identify

## Compound automation processing options

Compound mining algorithm Find by Molecular Feature



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Search a database for each compound	False
Generate formulas for each compound	False
Generate formulas for peaks with no	True
database hits	
Chromatogram Polarity:	Both
TIC	True
BPC	False
TWC	False
Signal A	False
Match sequences for each compound	False
Show only identified compounds	True
Search a library for each compound	False

## Exclude mass(es) settings

Exclude masses:	False

## (3) Compound Report

## **Compound report settings**

Show compound table	True
Sort compound table in increasing order:	True
Show user chromatogram(s)	False
Show compound chromatogram(s)	True
Overlay compound chromatogram(s)	False
Show MS spectrum	True
Show library spectrum	False
Show difference spectrum	False
Show MS peak table	True
Show predicted isotope match table	False
Show MS spectrum (zoomed in on special	True
peaks)	
Overlay predicted isotope distribution	True
Show MS/MS spectrum	True
Show MS/MS peak table	True
Left zoom limit	30.0
Right zoom limit	30.0
Sort compound table by	Retention Time
Exclude details for unidentified compounds	False

# **Worklist Automation**

## **Reporting Options**



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## **Worklist print report options**

Content to include	Include all results
Print report	False
Save report as Excel file	False
Save report as PDF file	False
Separate report per data file	True

## **Worklist Actions**

#### **Worklist actions**

1) Find Compounds by Formula

2) Export to CEF

## **Selected Ranges**

#### Selected time ranges for automation

Limit operations to specific retention times: False

# **Export**

## **ASR Options**

## **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## **ASR** export options

Peak window: 0.04

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## **CEF Options**

## **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## **Compound Summary CSV Options**

#### **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## **MGF Options**

## **Export content settings**

Export entire data file	True
·	

## **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## mzData export settings

MS level type	All
MS storage mode to use	Peak Detected
Compute deisotope	False

#### mzData export TOF peak finder settings

Detect Maximum Spike Width	2
Detect Required Valley	0.70

## mzData export MS/MS peak filter settings



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Peak height (counts) >=	10
Peak height (%) >=	0.100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## mzData export MS/MS charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	2
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	False
charged	

# mzData Options

## **Export content settings**

Export entire data file	True

## **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## mzData export settings

MS level type	All
MS storage mode to use	Peak Detected
Compute deisotope	False

## mzData export TOF peak finder settings

Detect Maximum Spike Width	2
Detect Required Valley	0.70

## mzData export MS peak filter settings

Peak height (counts) >=	10
Peak height (%) >=	0.100
Annotate fragment spectrum peaks with	False

formulas

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Generate formulas for non-fragment	<u>False</u>
(unknown) ions	

## mzData export MS charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	2
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	False
charged	

## mzData export MS/MS peak filter settings

Peak height (counts) >=	10
Peak height (%) >=	0.100
Annotate fragment spectrum peaks with	False
formulas	
Generate formulas for non-fragment	False
(unknown) ions	

## mzData export MS/MS charge state assignment settings

Isotope spacing tolerance(m/z)	0.0025
Isotope spacing tolerance(ppm)	7.0
Maximum charge state	2
Limit assigned charge states to a maximum	True
of:	
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-	False
charged	

## **MS/MS Inclusion List Options**

# **Export content settings**

Export entire data file	True

## **Export destination settings**

Export to the batch location	False
One export file per data file	True
At the location of the data file	True
Overwrite existing export file	False

## **Export Inclusion List options**



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Retention time window:	0.00
Retention time window:	0.25
Limit number of precursor ions per	1
compound to	
Limit number of precursor ions per	True
compound to	
PSet Export Inclusion List_Minimun Ion	2000
Abundance	
Minimum ion abundance:	True
Export monoisotopic m/z	True
Specify charge state preference order	False
Method path:	C:\Mass Hunter
Only highlighted compounds	False
PSet Export Inclusion List_Selected Charge	2
States	
PSet Export Inclusion List_Selected Charge	3
States	
PSet Export Inclusion List_Selected Charge	>3
States	
Modifier	+H
Modifier	-Н
Charge State Priorities	Agilent.Mass Spectrometry.Data Analysis.Collection
	Parameter`1[Agilent.Mass Spectrometry.Data
	Analysis.Qualitative.PSet Charge State Priority]
Sort exclusion list by:	Retention Time
Export inclusion list format	Auto MS/MS preferred list
Sort Ascending	True

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