Qualitative Data Analysis Method Report

Method Name : **140421 Urine Bariatric Study MSMS.m**
Method Path: **C:\MassHunter\Methods\B.06.00\140421 Urine Bariatric Study MSMS.m**

Chromatogram

Integrate (MS)

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

MS Chromatogram peak filter settings

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

MS System Suitability

Enable system suitability calculations	False

Integration Results settings

Clear previous peak spectra	True
Highlight all peaks	False

Integrate (MS/MS)

MS/MS Integrator selection

Integrator Selection	Agile

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

MS/MS Chromatogram peak filter settings

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

MS System Suitability

Enable system suitability calculations	False

Integration Results settings

Clear previous peak spectra	True

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 chromatograms are integrated	False
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)

1-Single m/z width:	0.5000

Exclude mass(es) settings

Exclude masses:	False

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

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 formulas	False
Generate formulas for non-fragment (unknown) ions	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 of:	True
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-charged	True

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:	25
Annotate fragment spectrum peaks with formulas	False
Generate formulas for non-fragment (unknown) ions	False

MS/MS Charge state assignement 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 of:	True
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-charged	False

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 formulas	False
Generate formulas for non-fragment (unknown) ions	False

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 of:	True
Isotope model	Peptides
Treat ions with unassigned charge as singly-charged	True

Extraction Data Format

Data storage options

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

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

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 peaks)	True
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 :	Acq 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

Find Compounds

Find by Auto MS/MS

Find compounds Auto MS/MS settings

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 collision energy	True

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	Agile

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

Targeted MS/MS processing settings

Maximum chromatogram peak width	0.30
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 collision energy	True
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

Annotate fragment spectrum peaks with formulas	False
Generate formulas for non-fragment (unknown) ions	False

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

MFE processing and ion species settings

Restrict retention times:	False
Restrict m/z range:	False
Use peaks with height >=	500
Positive ions:	
Modifier	+H
Modifier	+Na
Negative ions:	
Modifier	-H
Modifier	+Cl
Modifier	+CH3COO
Salt dominated positive ions:	False
Include representative raw spectrum for each compound	False
Assume unidentified ions are radical ions	False
Target data type	Small molecules (chromatographic)
Neutral Species Definitions	
Modifier	
Modifier	
Include representative raw spectrum for each compound	False
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 of:	True
Isotope model	Common organic molecules

Treat ions with unassigned charge as singly-charged	True

MFE result filters

Restrict retention times:	False
Restrict charge states:	False
Restrict to neutral losses:	False
Mass Tolerance	5.000
Filter optionis for mass(es)	Include only these mass(es)
Database	True
Quality score	50.00

Mass defect filter settings

Filter results on mass defects	False

MS/MS spectrum peak filter settings

Limit to the largest:	25
Annotate fragment spectrum peaks with formulas	False
Generate formulas for non-fragment (unknown) ions	False

MFE result options

Delete previous compounds	True
Highlight all compounds	True

MFE database location

Database Path	C:\Mass Hunter\PCDL\UMDB_v3.5.cdb

Find by MRM

MS/MS Integrator selection

Integrator Selection	Agile

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

Annotate fragment spectrum peaks with formulas	False
Generate formulas for non-fragment (unknown) ions	False

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 are integrated	False
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

Integrator Selection	Agile

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 formulas	False
Generate formulas for non-fragment (unknown) ions	False

Chromatogram extraction options

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

Generate formula for each peak	False
Chromatogram used to find mass spectra	Total Ion
Get Signal A from	DAD
Signal Device Name	
Signal Ordinal Number	1

Exclude mass(es) settings

Exclude masses:	False

Device delay settings

MS1 use delay	False

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

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

Find compounds results settings

Delete previous compounds	True
Highlight all compounds	False

Find Compounds by Formula

Find by Formula - Options

Find Compounds by Formula options

Formula source to confirm	Database
Use Absolute Mass Tolerance	False
Retention Time Tolerance	0.500
Single Mz expansion mode:	Symmetric (ppm)
Expected retention time	2.00
Relative Mass Tolerance	5.00
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 Pos Mode.cef
Automatically increase for isomeric compounds	True
Do not match if score is	False
Reject score threshold	60.00
Do not match if the (unobserved) second ion's abundance is expected to be	False
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	False
Warn if the (unobserved) second ion's abundance is expected to be	False
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\UMDB_v3.5.cdb

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	-H
Modifier	+Cl
Modifier	+CH3COO
Negative Neutral Loss:	
Modifier	
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, otherwise use average fragment spectrum	True
Number of most abundant ions from spectral library	5
Number of most abundant ions from average fragment spectrum	7
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	Database
Use Absolute Mass Tolerance	False
Retention Time Tolerance	0.500
Single Mz expansion mode:	Symmetric (ppm)
Expected retention time	2.00
Relative Mass Tolerance	5.00
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 Pos Mode.cef
Automatically increase for isomeric compounds	True
Do not match if score is	False
Reject score threshold	60.00
Do not match if the (unobserved) second ion's abundance is expected to be	False
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	False
Warn if the (unobserved) second ion's abundance is expected to be	False
Warn score threshold	75.00
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 formulas	False
Generate formulas for non-fragment (unknown) ions	False

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

Find by Formula - Sample Purity

Sample Purity options

Compute sample purity	False

Device delay settings

MS1 use delay	False

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
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 formulas	False
Generate formulas for non-fragment (unknown) ions	False

Identify Compounds

Search Database

Database search settings

Use Absolute Mass Tolerance	False
Relative Mass Tolerance	5.00
Retention Time Tolerance	0.100
Maximum Hits	4
Maximum number of peaks to search when peaks are not specified graphically:	5
Search "neutral" database entries for masses from simple ions	False

Database location settings

Database Path	C:\Mass Hunter\PCDL\UMDB_v3.5.cdb

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	-H
Modifier	+Cl
Modifier	+CH3COO
Negative Neutral Loss:	
Modifier	
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

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 formulas	False

Generate formulas for non-fragment (unknown) ions	False

Generate Formulas

Formula calculator settings

MS nitrogen rule:	even electron
Positive ions:	H
Negative ions:	H
Element Limits	
C	3 to 60
H	0 to 120
O	0 to 30
N	0 to 30
S	0 to 5
Cl	0 to 3
Maximum neutral mass for which formulas should be calculated:	750.0000
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	B0201
Include target formula in results	False
Target formula	
Positive ions:	
Modifier	+H
Negative ions:	
Modifier	-H
Group hits with same formula (but different charge carriers)	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 of:	True
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-charged	True

Fragment formula annotation peak filter settings

Peak height (counts) >=	10
Peak height (%) >=	0.100
Limit to the largest:	100
Annotate fragment spectrum peaks with formulas	False
Generate formulas for non-fragment (unknown) ions	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

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
Search a database for each compound	False
Generate formulas for each compound	False
Generate formulas for peaks with no database hits	True
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 peaks)	True
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

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 Targeted MS/MS
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

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

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

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

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 formulas	False
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mzData export MS charge state assignment settings

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mzData export MS/MS peak filter settings

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Peak height (%) >=	0.100
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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 of:	True
Isotope model	Common organic molecules
Treat ions with unassigned charge as singly-charged	False

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

Retention time window:	0.00
Retention time window:	0.25
Limit number of precursor ions per compound to	1
Limit number of precursor ions per compound to	True
PSet Export Inclusion List_Minimun Ion Abundance	2000
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 States	2
PSet Export Inclusion List_Selected Charge States	3
PSet Export Inclusion List_Selected Charge States	>3
Modifier	+H
Modifier	-H
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