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S-v2_92_NLDM-FHT5-D12-pl4_2__314.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_93_NLDM-FHT5-D12-pl4_3_failedinj-2mm-noWBS_020.mzML</file><file>/
global/project/projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_93_NLDM-FHT5-D12-pl4_3_reinj-postfailed_398.mzML</file><file>/
global/project/projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_94_NLDM-TxCtrl-pl4_1__323.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_95_NLDM-TxCtrl-pl4_2__265.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_96_NLDM-TxCtrl-pl4_3__218.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_97_NLDM-FHT5-F08-pl5_1__188.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_98_NLDM-FHT5-F08-pl5_2__253.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_99_NLDM-FHT5-F08-pl5_3__347.mzML</file><file>/global/project/
projectdirs/metatlas/raw_data/agolini/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_NEG_MSM
S-v2_9_NLDM-AMD436-pl1_3__374.mzML</file></parameter></p></div>

```

batchstep><batchstep
method="net.sf.mzmine.modules.rawdatamethods.peakpicking.massdetection
.MassDetectionModule"><parameter name="Raw data files"
type="ALL_FILES"></parameter><parameter name="Scans"><ms_level>1</
ms_level><scan_definition></scan_definition></parameter><parameter
name="Mass detector" selected="Centroid"><module
name="Centroid"><parameter name="Noise level">10000</parameter></
module><module name="Exact mass"><parameter name="Noise level"></
parameter></module><module name="Local maxima"><parameter name="Noise
level"></parameter></module><module name="Recursive
threshold"><parameter name="Noise level"></parameter><parameter
name="Min m/z peak width"></parameter><parameter name="Max m/z peak
width"></parameter></module><module name="Wavelet
transform"><parameter name="Noise level"></parameter><parameter
name="Scale level"></parameter><parameter name="Wavelet window size
(%)"></parameter></module></parameter><parameter name="Mass list
name">masses</parameter><parameter name="CDF Filename (optional)"
selected="False"></parameter></batchstep><batchstep
method="net.sf.mzmine.modules.rawdatamethods.peakpicking.massdetection
.MassDetectionModule"><parameter name="Raw data files"
type="ALL_FILES"></parameter><parameter name="Scans"><ms_level>2</
ms_level><scan_definition></scan_definition></parameter><parameter
name="Mass detector" selected="Centroid"><module
name="Centroid"><parameter name="Noise level">100</parameter></
module><module name="Exact mass"><parameter name="Noise level"></
parameter></module><module name="Local maxima"><parameter name="Noise
level"></parameter></module><module name="Recursive
threshold"><parameter name="Noise level"></parameter><parameter
name="Min m/z peak width"></parameter><parameter name="Max m/z peak
width"></parameter></module><module name="Wavelet
transform"><parameter name="Noise level"></parameter><parameter
name="Scale level"></parameter><parameter name="Wavelet window size
(%)"></parameter></module></parameter><parameter name="Mass list
name">masses</parameter><parameter name="CDF Filename (optional)"
selected="False"></parameter></batchstep><batchstep
method="net.sf.mzmine.modules.masslistmethods.ADAPChromatogrambuilder.
ADAPChromatogramBuilderModule"><parameter name="Raw data files"
type="ALL_FILES"></parameter><parameter name="Scans"><ms_level>1</
ms_level></parameter><parameter name="Mass list">masses</
parameter><parameter name="Min group size in # of scans">5</
parameter><parameter name="Group intensity threshold">200000.0</
parameter><parameter name="Min highest intensity">500000.0</
parameter><parameter name="m/z tolerance"><absolutetolerance>0.002</
absolutetolerance><ppmtolerance>10</ppmtolerance></
parameter><parameter name="Suffix">chromatograms</parameter></
batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.peakpicking.deconvolutio
n.DeconvolutionModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter
name="Suffix">deconvoluted</parameter><parameter name="Algorithm"

```

```

selected="Wavelets (ADAP)"><module name="Baseline cut-off"><parameter
name="Min peak height"></parameter><parameter name="Peak duration
range (min)"><max>10</max><min>0</min></parameter><parameter
name="Baseline level"></parameter></module><module name="Noise
amplitude"><parameter name="Min peak height"></parameter><parameter
name="Peak duration range (min)"><max>10</max><min>0</min></
parameter><parameter name="Amplitude of noise"></parameter></
module><module name="Savitzky-Golay"><parameter name="Min peak
height"></parameter><parameter name="Peak duration range
(min)"><max>10</max><min>0</min></parameter><parameter
name="Derivative threshold level"></parameter></module><module
name="Local minimum search"><parameter name="Chromatographic
threshold">0.3</parameter><parameter name="Search minimum in RT range
(min)">0.05</parameter><parameter name="Minimum relative
height">0.05</parameter><parameter name="Minimum absolute
height">1000000</parameter><parameter name="Min ratio of peak top/
edge">2</parameter><parameter name="Peak duration range
(min)"><max>2</max><min>0.05</min></parameter></module><module
name="Wavelets (XCMS)"><parameter name="S/N threshold">10</
parameter><parameter name="Wavelet scales"><max>5</max><min>0.25</
min></parameter><parameter name="Peak duration range"><max>10</
max><min>0</min></parameter><parameter name="Peak integration
method">Use smoothed data</parameter><parameter name="R
engine">RCaller</parameter></module><module name="Wavelets
(ADAP)"><parameter name="S/N threshold">10</parameter><parameter
name="S/N estimator" selected="Intensity window SN"><module
name="Intensity window SN"></module><module name="Wavelet Coeff.
SN"><parameter name="Peak width mult.">3</parameter><parameter
name="abs(wavelet coeffs.)">True</parameter></module></
parameter><parameter name="min feature height">10</
parameter><parameter name="coefficient/area threshold">110</
parameter><parameter name="Peak duration range"><max>10</max><min>0</
min></parameter><parameter name="RT wavelet range"><max>0.2</
max><min>0</min></parameter></module></parameter><parameter
measure="MEDIAN" name="m/z center calculation"
weighting="NONE">CenterFunction</parameter><parameter name="m/z range
for MS2 scan pairing (Da)" selected="True">0.025</parameter><parameter
name="RT range for MS2 scan pairing (min)" selected="True">0.2</
parameter><parameter name="Remove original peak list">False</
parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.isotopes.deisotoper.Isot
opeGrouperModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">deisotoped</parameter><parameter name="m/z
tolerance"><absolutetolerance>0</absolutetolerance><ppmtolerance>20</
ppmtolerance></parameter><parameter name="Retention time tolerance"
type="absolute">0.1</parameter><parameter name="Monotonic
shape">True</parameter><parameter name="Maximum charge">3</
parameter><parameter name="Representative isotope">Most intense</
parameter><parameter name="Remove original peaklist">True</

```

```

parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.orderpeaklists.OrderPeak
ListsModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.alignment.join.JoinAlign
erModule"><parameter name="Peak lists" type="BATCH_LAST_PEAKLISTS"></
parameter><parameter name="Peak list name">Aligned peak list</
parameter><parameter name="m/z tolerance"><absolutetolerance>0.0</
absolutetolerance><ppmtolerance>20</ppmtolerance></
parameter><parameter name="Weight for m/z">50</parameter><parameter
name="Retention time tolerance" type="absolute">0.2</
parameter><parameter name="Weight for RT">50</parameter><parameter
name="Require same charge state">False</parameter><parameter
name="Require same ID">False</parameter><parameter name="Compare
isotope pattern" selected="False"><parameter name="Isotope m/z
tolerance"><absolutetolerance>0.001</
absolutetolerance><ppmtolerance>20</ppmtolerance></
parameter><parameter name="Minimum absolute intensity"></
parameter><parameter name="Minimum score"></parameter></parameter></
batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.filtering.rowsfilter.Row
sFilterModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">filtered</parameter><parameter name="Minimum peaks in a row"
selected="True">2</parameter><parameter name="Minimum peaks in an
isotope pattern" selected="True">2</parameter><parameter name="m/z"
selected="False"></parameter><parameter name="Retention time"
selected="False"></parameter><parameter name="Peak duration range"
selected="False"><max>10</max><min>0</min></parameter><parameter
name="Chromatographic FWHM" selected="False"><max>1</max><min>0</
min></parameter><parameter name="Parameter">No parameters defined</
parameter><parameter name="Only identified?">False</
parameter><parameter name="Text in identity" selected="False"></
parameter><parameter name="Text in comment" selected="False"></
parameter><parameter name="Keep or remove rows">Keep rows that match
all criteria</parameter><parameter name="Keep only peaks with MS2 scan
(GNPS)">False</parameter><parameter name="Reset the peak number
ID">False</parameter><parameter name="Remove source peak list after
filtering">False</parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.filtering.duplicatefilte
r.DuplicateFilterModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">filtered</parameter><parameter name="Filter mode">NEW
AVERAGE</parameter><parameter name="m/z
tolerance"><absolutetolerance>0.0001</
absolutetolerance><ppmtolerance>10</ppmtolerance></
parameter><parameter name="RT tolerance" type="absolute">0.05</
parameter><parameter name="Require same identification">False</
parameter><parameter name="Remove original peaklist">False</
parameter></batchstep><batchstep

```

```

method="net.sf.mzmine.modules.peaklistmethods.gapfilling.peakfinder.multipthreaded.MultiThreadPeakFinderModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">gap-filled</parameter><parameter name="Intensity
tolerance">0.05</parameter><parameter name="m/z
tolerance"><absolutetolerance>0.001</
absolutetolerance><ppmtolerance>10</ppmtolerance></
parameter><parameter name="Retention time tolerance"
type="absolute">0.2</parameter><parameter name="Remove original peak
list">False</parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.io.csvexport.CSVExportModule"><parameter name="Peak lists" type="BATCH_LAST_PEAKLISTS"></
parameter><parameter name="Filename">/project/projectdirs/metatlas/
projects/untargeted_tasks/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e_peak-height.csv</parameter><parameter name="Field separator">,</
parameter><parameter name="Export common elements"><item>Export row
ID</item><item>Export row m/z</item><item>Export row retention time</
item></parameter><parameter name="Export data file
elements"><item>Peak height</item></parameter><parameter name="Export
quantitation results and other information">False</
parameter><parameter name="Identification separator">;</
parameter><parameter name="Filter rows">ALL</parameter></
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parameter><parameter name="Filename">/project/projectdirs/metatlas/
projects/untargeted_tasks/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e_peak-area.csv</parameter><parameter name="Field separator">,</
parameter><parameter name="Export common elements"><item>Export row
ID</item><item>Export row m/z</item><item>Export row retention time</
item></parameter><parameter name="Export data file
elements"><item>Peak area</item></parameter><parameter name="Export
quantitation results and other information">False</
parameter><parameter name="Identification separator">;</
parameter><parameter name="Filter rows">ALL</parameter></
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method="net.sf.mzmine.modules.peaklistmethods.io.gnpsexport.GNPSEExport
AndSubmitModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Filename">/
project/projectdirs/metatlas/projects/untargeted_tasks/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negativ
e_MSMS.mgf</parameter><parameter name="Mass list">masses</

```



```
parameter><parameter name="Filter rows">ONLY WITH MS2</parameter><parameter name="Submit to GNPS" selected="False"><parameter name="Meta data file" selected="True">/project/projectdirs/metatlas/projects/untargeted_tasks/20201218_LZH-AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negative/20201218_LZH-AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_negative_metadata.tab</parameter><parameter name="Presets">HIGHRES</parameter><parameter name="Email">ben.bowen@gmail.com</parameter><parameter name="Username">bpbowen</parameter><parameter name="Password (unencrypted)">notapassword</parameter><parameter name="Open website">False</parameter></parameter><parameter name="Open folder">False</parameter></batchstep></batch>
```