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S-v2_93_NLDM-FHT5-D12-pl4_3_failedinj-2mm-noWBS_019.mzML</file><file>/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
S-v2_93_NLDM-FHT5-D12-pl4_3_reinj-postfailed_397.mzML</file><file>/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
S-v2_95_NLDM-TxCtrl-pl4_2__264.mzML</file><file>/global/project/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
S-v2_97_NLDM-FHT5-F08-pl5_1__187.mzML</file><file>/global/project/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
S-v2_98_NLDM-FHT5-F08-pl5_2__252.mzML</file><file>/global/project/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
S-v2_99_NLDM-FHT5-F08-pl5_3__346.mzML</file><file>/global/project/
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_POS_MSM
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.MassDetectionModule"><parameter name="Raw data files"
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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)"
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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
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width"></parameter></module><module name="Wavelet
transform"><parameter name="Noise level"></parameter><parameter
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(%)"></parameter></module></parameter><parameter name="Mass list
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parameter><parameter name="Suffix">chromatograms</parameter></
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n.DeconvolutionModule"><parameter name="Peak lists"
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name="Suffix">deconvoluted</parameter><parameter name="Algorithm"
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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
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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
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type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">deisotoped</parameter><parameter name="m/z
tolerance"><absolutetolerance>0</absolutetolerance><ppmtolerance>20</
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shape">True</parameter><parameter name="Maximum charge">3</
parameter><parameter name="Representative isotope">Most intense</
parameter><parameter name="Remove original peaklist">True</
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ListsModule"><parameter name="Peak lists"
type="BATCH_LAST_PEAKLISTS"></parameter></batchstep><batchstep
method="net.sf.mzmine.modules.peaklistmethods.alignment.join.JoinAlign

```

```

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parameter><parameter name="Peak list name">Aligned peak list</
parameter><parameter name="m/z tolerance"><absolutetolerance>0.0</
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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
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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
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r.DuplicateFilterModule"><parameter name="Peak lists"
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AVERAGE</parameter><parameter name="m/z
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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
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type="BATCH_LAST_PEAKLISTS"></parameter><parameter name="Name
suffix">gap-filled</parameter><parameter name="Intensity
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```

```

tolerance"><absolutetolerance>0.001</
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parameter><parameter name="Retention time tolerance"
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv
e/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv
e_peak-height.csv</parameter><parameter name="Field separator">,</
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item></parameter><parameter name="Export data file
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AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv
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e/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv
e_MSMS.mgf</parameter><parameter name="Mass list">masses</
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projects/untargeted_tasks/20201218_LZH-
AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv

```


e/20201218_LZH-

AG_MdR_ENIGMA_Atlas_20201111rnd1_QE119_Ag683775-924_USHXG01474_positiv
e_metadata.tab</parameter><parameter name="Presets">HIGHRES</
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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>