DeconTools_Autoprocessor & DeconConsole.exe

This document contains information on:

▶ DeconTools_Autoprocessor

▶ DeconConsole.exe

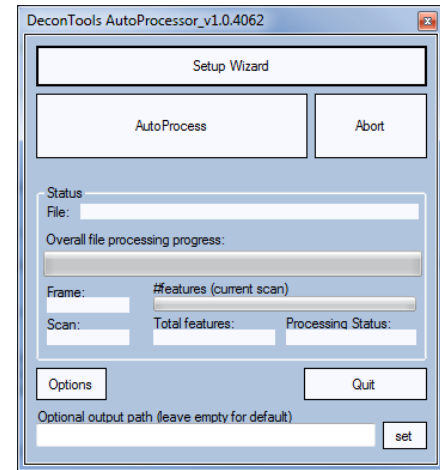▶ The DeconTools parameter file.

Contact:

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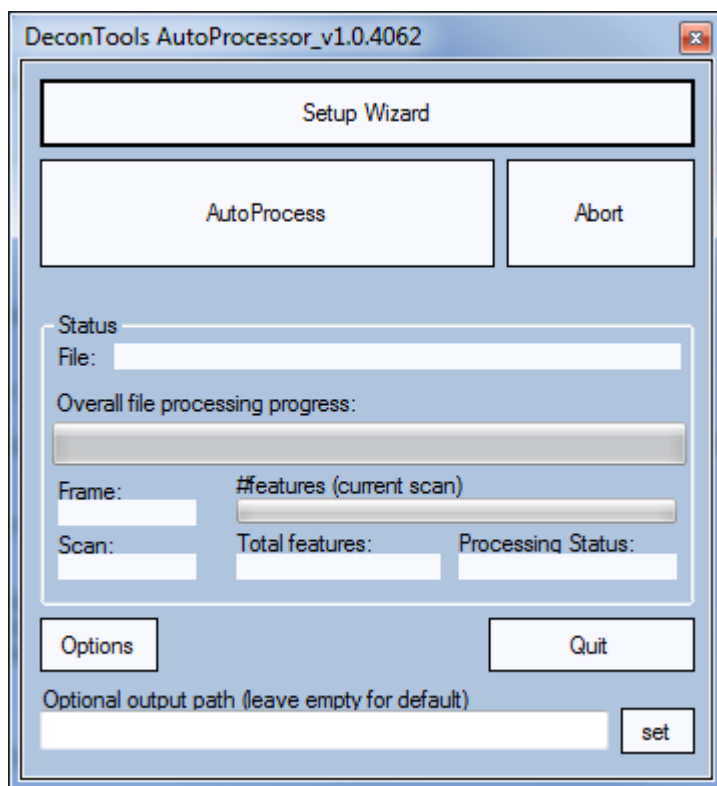
DeconTools_Autoprocessor & DeconConsole.exe

▶ DeconTools_Autoprocessor:
   ■ User interface
   ■ Supports batch processing of files
▶ DeconConsole.exe
   ■ Console-based automated processing
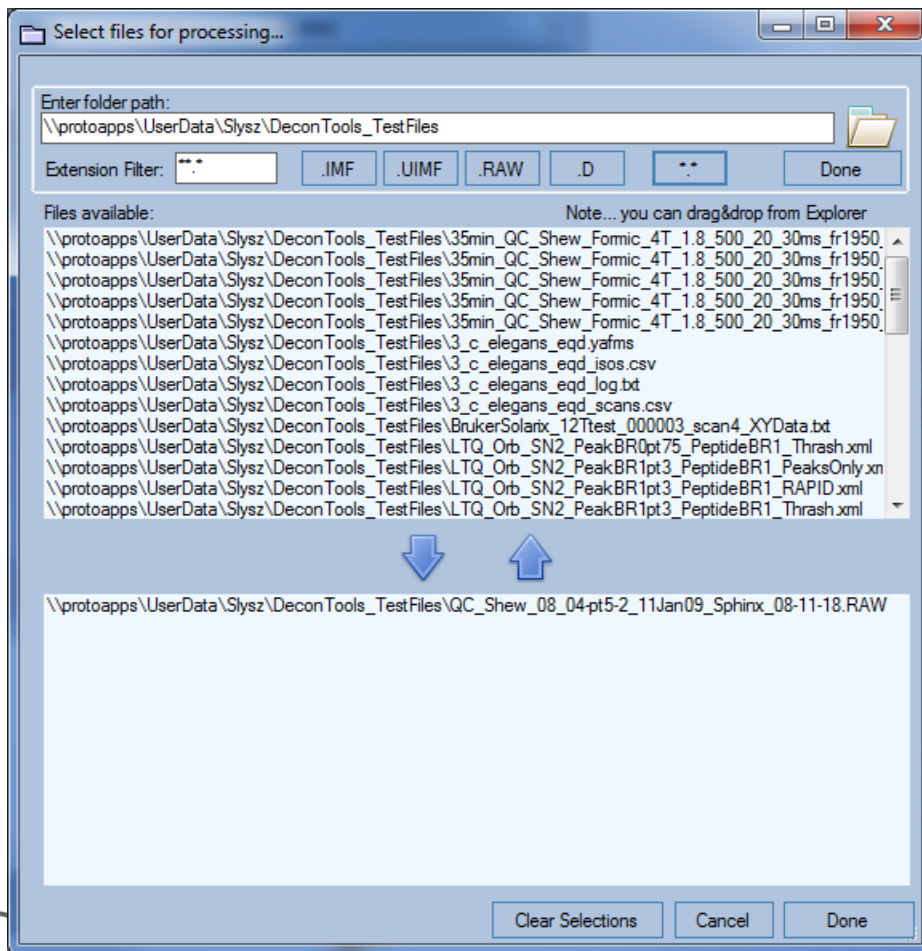   ■ Useful for insertion into multi-step, multi-application workflows

DeconTools_Autoprocessor

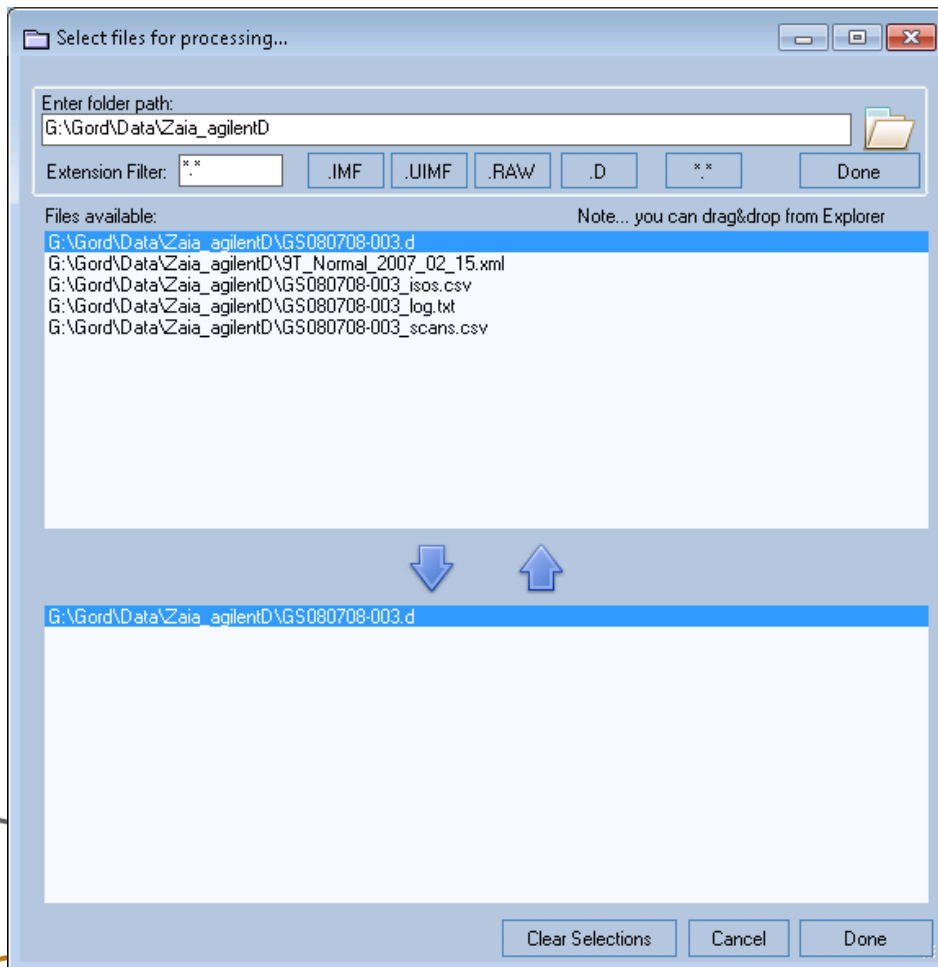▶ For automated MS Feature finding (deconvolution)

1. Click 'Setup Wizard'

DeconTools_Autoprocessor: selecting the target MS datafile


1. Click 'Setup Wizard'

2. Navigate to the folder that contains the target MS datafile.

DeconTools_Autoprocessor: selecting the target MS datafile

1. Click 'Setup Wizard'
2. Navigate to the folder that contains the target MS datafile.
3. Select the file/folder and click 'Done'

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DeconTools_Autoprocessor: selecting the parameter file
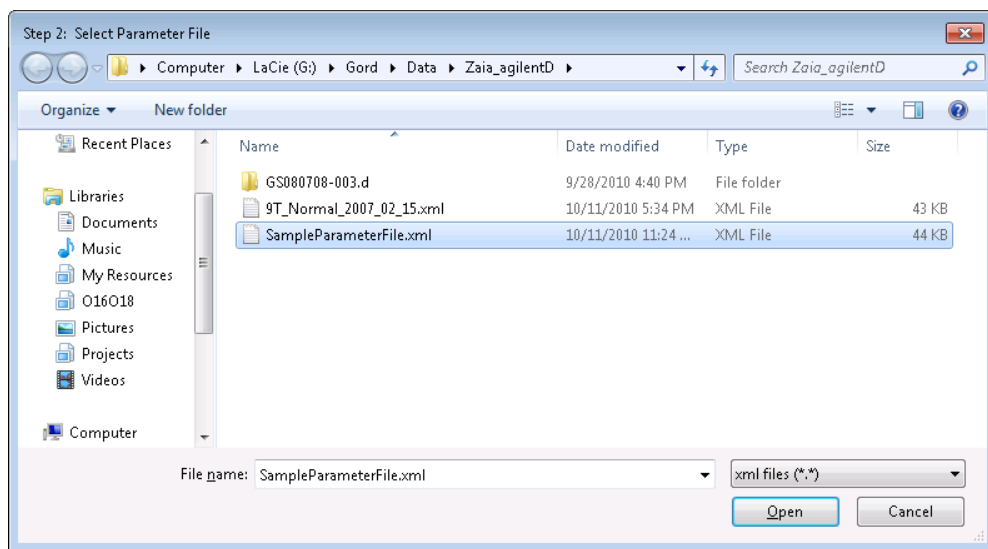
4. Select a .XML parameter file. This parameter file is the same one used in earlier versions of DeconTools.

**Note: A sample parameter file is provided (same folder as DeconToolsAutoprocessor.exe)

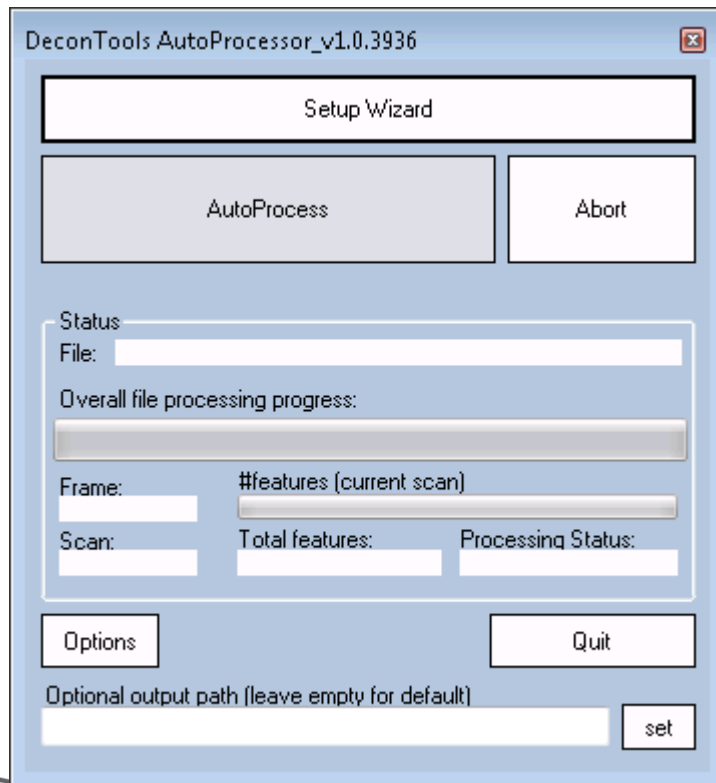Pacific Northwest
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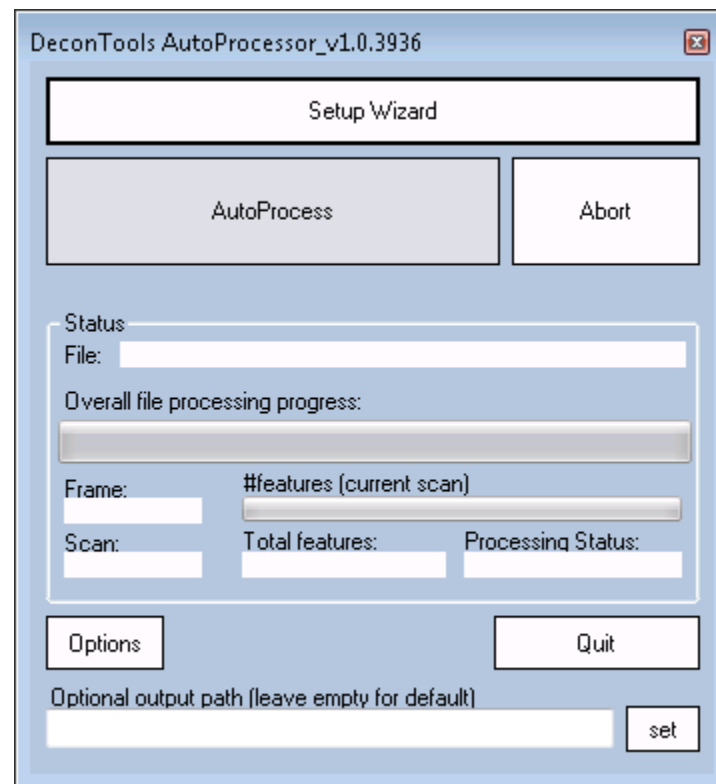*Proudly Operated by* **Battelle** *Since 1965*

DeconTools_Autoprocessor

4. Select a .XML parameter file. This parameter file is the same one used in earlier versions of DeconTools.

5. Click 'AutoProcess'

DeconTools_Autoprocessor

Things to note:

▶ Three files are created in the same folder as the original MS datafile folder:

- the _isos.txt file
- the _scan.txt file
- the _log.txt file
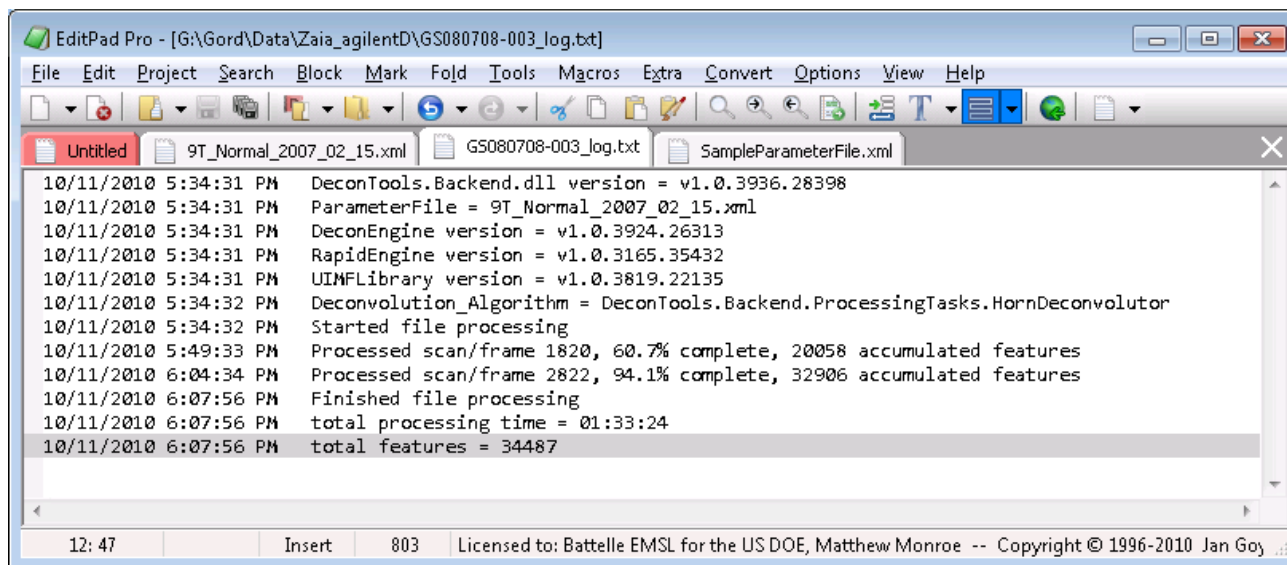
DeconTools_Autoprocessor

▶ Log file is created in the same folder as the raw data file. This can be opened unobtrusively. The log file is updated every 15 minutes, so this is another way of monitoring progress.

DeconConsole.exe

► DeconConsole.exe is console-based means of automating MS_feature extraction.

 ■ requires two arguments:

 ● filename

 ● DeconTools parameter file (.xml). This is the same parameter file used in previous versions of DeconTools.

► Sample command, entered at a DOS prompt:

DeconConsole.exe BSA_TOF4.d SampleParameterFile_Scans10-12.xml

DeconTools Parameter file information

SampleParameterFile.xml

```xml
<?xml version="1.0" encoding="utf-8" standalone="yes"?>
<parameters>
    <version>1.0</version>
    <PeakParameters>
        <PeakBackgroundRatio>1.3</PeakBackgroundRatio>
        <SignalToNoiseThreshold>2</SignalToNoiseThreshold>
        <PeakFitType>QUADRATIC</PeakFitType>
    <WritePeaksToTextFile>False</WritePeaksToTextFile>
    </PeakParameters>
    <DTAGenerationParameters>
        <MinScan>1</MinScan>
        <MaxScan>1000000</MaxScan>
        <MinMass>200</MinMass>
        <MaxMass>5000</MaxMass>
        <MinIonCount>35</MinIonCount>
        <ConsiderCharge>False</ConsiderCharge>
        <ChargeValueToConsider>0</ChargeValueToConsider>
        <CCMass>1.00727638</CCMass>
        <WindowSizeToCheck>5</WindowSizeToCheck>
        <ConsiderMultiplePrecursors>False</ConsiderMultiplePrecu
    <IsolationWindowSize>3</IsolationWindowSize>
    <OutputType>DTA</OutputType>
    <IsProfileDataForMzXML>False</IsProfileDataForMzXML>
    <IgnoreMSnScans>False</IgnoreMSnScans>
    </DTAGenerationParameters>
    <HornTransformParameters>
        <TagFormula />
        <AveragineFormula>C4.9384 H7.7583 N1.3577 O1.4773 S0.0417</AveragineFormula>
        <DeleteIntensityThreshold>1</DeleteIntensityThreshold>
        <MaxFit>0.3</MaxFit>
        <MinIntensityForScore>10</MinIntensityForScore>
```

The peak parameters. The PeakBackgroundRatio is a key parameter. A low value will result in many peaks being detected. Too many peaks greatly slow down deconvolution (THRASH)

Set this to 'TRUE' to export all detected peaks. Look for a _peaks.txt file.

The DTAGenerationParameters are not currently used.

Deconvolution parameters. HornTransform = THRASH.

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DeconTools Parameter file information

```
</DTAGenerationParameters>
<HornTransformParameters>
    <TagFormula />
    <AveragineFormula>C4.9384 H7.7583 N1.3577 O1.4773 S0.0417</AveragineFor
    <DeleteIntensityThreshold>1</DeleteIntensityThreshold>
    <MaxFit>0.3</MaxFit>
    <MinIntensityForScore>10</MinIntensityForScore>
    <MaxCharge>10</MaxCharge>
    <MaxMW>10000</MaxMW>
    <NumPeaksForShoulder>1</NumPeaksForShoulder>
    <O16O18Media>False</O16O18Media>
    <PeptideMinBackgroundRatio>1</PeptideMinBackgroundRatio>
    <UseAbsolutePeptideIntensity>False</UseAbsolutePeptideIntensity>
    <AbsolutePeptideIntensity>0</AbsolutePeptideIntensity>
    <ThrashOrNot>True</ThrashOrNot>
    <CheckAllPatternsAgainstCharge1>False</CheckAllPatternsAgainstCharge1>
    <CompleteFit>False</CompleteFit>
    <CCMass>1.00727649</CCMass>
    <IsotopeFitType>AREA</IsotopeFitType>
    <UseMercuryCaching>True</UseMercuryCaching>
<SumSpectra>False</SumSpectra>
<SumSpectraAcrossScanRange>False</SumSpectraAcrossScanRange>
<NumberOfScansToSumOver>1</NumberOfScansToSumOver>
<NumberOfScansToAdvance>0</NumberOfScansToAdvance>
<SumSpectraAcrossFrameRange>True</SumSpectraAcrossFrameRange>
<NumberOfFramesToSumOver>3</NumberOfFramesToSumOver>
<IsActualMonoMZUsed>False</IsActualMonoMZUsed>
<LeftFitStringencyFactor>1</LeftFitStringencyFactor>
<RightFitStringencyFactor>1</RightFitStringencyFactor>
<UseRAPIDDeconvolution>False</UseRAPIDDeconvolution>
    <ReplaceRAPIDScoreWithHornFitScore>False</ReplaceRAPIDScoreWithHornFit
    <NumPeaksUsedInAbundance>1</NumPeaksUsedInAbundance>
    </HornTransformParameters>
<Miscellaneous>
    <UseScanRange>False</UseScanRange>
```

THRASH deconvolution parameters

Summing parameters. Set SumSpectraAcrossScanRange to 'TRUE' to sum across scans. NumberOfScansToSumOver represents the +/- number of scans to sum.

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DeconTools Parameter file information

```xml
</DTAGenerationParameters>
<HornTransformParameters>
    <TagFormula />
    <AveragineFormula>C4.9384 H7.7583 N1.3577 O1.4773 S0.0417</AveragineFo
    <DeleteIntensityThreshold>1</DeleteIntensityThreshold>
    <MaxFit>0.3</MaxFit>
    <MinIntensityForScore>10</MinIntensityForScore>
    <MaxCharge>10</MaxCharge>
    <MaxMW>10000</MaxMW>
    <NumPeaksForShoulder>1</NumPeaksForShoulder>
    <O16O18Media>False</O16O18Media>
    <PeptideMinBackgroundRatio>1</PeptideMinBackgroundRatio>
    <UseAbsolutePeptideIntensity>False</UseAbsolutePeptideIntensity>
    <AbsolutePeptideIntensity>0</AbsolutePeptideIntensity>
    <ThrashOrNot>True</ThrashOrNot>
    <CheckAllPatternsAgainstCharge1>False</CheckAllPatternsAgainstCharge1>
    <CompleteFit>False</CompleteFit>
    <CCMass>1.00727649</CCMass>
    <IsotopeFitType>AREA</IsotopeFitType>
    <UseMercuryCaching>True</UseMercuryCaching>
<SumSpectra>False</SumSpectra>
<SumSpectraAcrossScanRange>False</SumSpectraAcrossScanRange>
<NumberOfScansToSumOver>1</NumberOfScansToSumOver>
<NumberOfScansToAdvance>0</NumberOfScansToAdvance>
<SumSpectraAcrossFrameRange>True</SumSpectraAcrossFr      >
<NumberOfFramesToSumOver>3</NumberOfFramesToSum
<IsActualMonoMZUsed>False</IsActualMonoMZ
<LeftFitStringencyFactor>1</LeftFitStr  gencyFactor>
<RightFitStringencyFactor>1</Rig   FitStringencyFactor>
<UseRAPIDDeconvolution>False</UseRAPIDDeconvolution>
    <ReplaceRAPIDScoreWithHornFitScore>False</ReplaceRAPIDScoreWithHornFit
    <NumPeaksUsedInAbundance>1</NumPeaksUsedInAbundance>
    </HornTransformParameters>
<Miscellaneous>
    <UseScanRange>False</UseScanRange>
```

RAPID deconvolution. See Park et al (2008). Set this to 'True' to override THRASH deconvolution.

Miscellaneous section.

DeconTools Parameter file information

```
<ReplaceRAPIDScoreWithHornFitScore>False</ReplaceRAPIDScoreWithHornFi
<NumPeaksUsedInAbundance>1</NumPeaksUsedInAbundance>
</HornTransformParameters>
<Miscellaneous>
<UseScanRange>False</UseScanRange>
<MinScan>5000</MinScan>
<MaxScan>6000</MaxScan>
<UseMZRange>True</UseMZRange>
<MinMZ>200</MinMZ>
<MaxMZ>2000</MaxMZ>
<ApplySavitzkyGolay>False</ApplySavitzkyGolay>
<SGNumLeft>2</SGNumLeft>
<SGNumRight>2</SGNumRight>
<SGOrder>2</SGOrder>
<ZeroFillDiscontinousAreas>False</ZeroFillDiscontinousAreas>
<NumZerosToFill>3</NumZerosToFill>
<ProcessMSMS>False</ProcessMSMS>
<ExportFileType>TEXT</ExportFileType>
<DetectPeaksOnly_NoDeconvolution>False</DetectPeaksOnly_NoDeconvoluti
<Process_MS>True</Process_MS>
</Miscellaneous>
<ElementIsotopes>
</parameters>
```

Set 'UseScanRange' to 'True' if you want to restrict processing to a certain region of the MS data file. Then set the boundaries "MinScan" and "MaxScan" .

Setting this to 'TRUE' means that the mass spectrum will be Savitzky-Golay smoothed.

Setting this to 'TRUE' will result in zero-filling. Good to use for sparse raw data (e.g. TOF-MS).

Setting this to 'TRUE' means that only peaks will be detected and no deconvolution will be performed. Ensure that you set the 'WritePeaksToTextFile' set to 'True

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