## DeconTools\_Autoprocessor & DeconConsole.exe

This document contains information on:

- DeconTools\_Autoprocessor
- DeconConsole.exe
- The DeconTools parameter file.



# 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





#### For automated MS Feature finding (deconvolution)

DeconTools AutoProcessor_v1.0.4062	<b>×</b>	
Setup Wizard		
AutoProcess	Abort	1. Click 'Setup Wizard'
Status File: Overall file processing progress:		
Frame: #features (current scan) Scan: Total features: Processing Status:		
Options [ Optional output path (leave empty for default)	Quit	
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#### **DeconTools\_Autoprocessor: selecting the** target MS datafile

Select files for processing         Enter folder path:         \vprotoapps\UserData\Slysz\DeconTools_TestFiles         Extension Filter:	<ol> <li>Click 'Setup Wizard'</li> <li>Navigate to the folder that contains the target MS datafile.</li> </ol>
Clear Selections Cancel Done	
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# DeconTools\_Autoprocessor: selecting the target MS datafile

Enter folder path: G:\Gord\Data\Zaia_agilentD		
Extension Filter:	ne 1	Cli
Files available: Note you can drag&drop from Explor G:\Gord\Data\Zaia_agilentD\GS080708-003.d	rer	
G:\Gord\Data\Zaia_agilentD\9T_Normal_2007_02_15.xml G:\Gord\Data\Zaia_agilentD\GS080708-003_isos.csv G:\Gord\Data\Zaia_agilentD\GS080708-003_log.txt G:\Gord\Data\Zaia_agilentD\GS080708-003_scans.csv	2.	Na tha MS
	3.	Se
↓ ①		an
G:\Gord\Data\Zaia_agilentD\GS080708-003.d		

. Click 'Setup Wizard'

 Navigate to the folder that contains the target MS datafile.

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 Select the file/folder and click 'Done'

#### **DeconTools\_Autoprocessor: selecting the parameter file**

🖉 💭 🗢 🚺 🕨 Corr	nputer	▶ LaCie (G:) ▶ Gord ▶ Data ▶ Zaia_agilentE	) 🕨 👻 🖣	Search Zaia	_agilentD	۶
Organize 👻 New	folder	,				
🗓 Recent Places	*	Name	Date modified	Туре	Size	
🚝 1 thurster		🐌 GS080708-003.d	9/28/2010 4:40 PM	File folder		
De sum sute		📄 9T_Normal_2007_02_15.xml	10/11/2010 5:34 PM	XML File		43 KB
Documents		SampleParameterFile.xml	10/11/2010 11:24	XML File		44 KB
My Resources O16018 Pictures Projects Videos Computer	H .					
F	ile <u>n</u> a	me: SampleParameterFile.xml	•	<ul> <li>xml files (*.*)</li> </ul>		•

 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)

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Setup Wizard				
	AutoProcess		Abor	t
Status File: Overall file proc	essing progress:			
Frame: Scan:	#features (current sca Total features:	n) Proc	essing Statu	8:
Options ptional output p	bath (leave empty for defa	ult)	Quit	set

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

5. Click 'AutoProcess'

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#### 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 Aut	coProcessor_v1.0.3936 🛛 🔯						
	Setup Wizard						
	AutoProcess Abort						
Status File: Overall file pro	Status File: Overall file processing progress:						
Frame: Scan:	Total features: Processing Status:						
Options Optional output	Quit path (leave empty for default) set						



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.

🕢 EditPad Pro - [G:\Gord\Data\Zaia_agilentD\GS080708-003_log.txt]	
<u>F</u> ile <u>E</u> dit <u>P</u> roject <u>S</u> earch <u>B</u> lock <u>M</u> ark Fo <u>l</u> d <u>T</u> ools M <u>a</u> cros E <u>x</u> tra <u>C</u> onvert <u>O</u> ptions <u>V</u> iew <u>H</u> elp	
D + 💩 🚹 + 🗟 🎕 👖 + 🕒 + 🖸 + 🥝 + 🛷 D 🖻 🌮 🔍 🍳 🔍 🗟 🛃 T + 📃 +	
Untitled 📋 9T_Normal_2007_02_15.xml 📋 G5080708-003_log.txt 📋 SampleParameterFile.xml 🗮 X	
10/11/2010 5:34:31 PM DeconTools.Backend.dll version = v1.0.3936.28398	
10/11/2010 5:34:31 PM ParameterFile = 9T_Normal_2007_02_15.xml	
10/11/2010 5:34:31 PM DeconEngine version = v1.0.3924.26313	
10/11/2010 5:34:31 PM RapidEngine version = v1.0.3165.35432	
10/11/2010 5:34:31 PM UIMFLibrary version = v1.0.3819.22135	
10/11/2010 5:34:32 PM Deconvolution_Algorithm = DeconTools.Backend.ProcessingTasks.HornDeconvolutor	
10/11/2010 5:34:32 PM Started file processing	
10/11/2010 5:49:33 PM Processed scan/frame 1820, 60.7% complete, 20058 accumulated features	
10/11/2010 6:04:34 PM Processed scan/frame 2822, 94.1% complete, 32906 accumulated features	
10/11/2010 6:07:56 PM Finished file processing	
10/11/2010 6:07:56 PM total processing time = 01:33:24	
10/11/2010 6:07:56 PM total features = 34487	
12: 47 Insert 803 Licensed to: Battelle EMSL for the US DOE, Matthew Monroe Copyright © 1996-2010 Jan Go	
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- 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



<pre>SampleParameterFile.xml  <?xml version="1.0" encoding="utf-8" standalone="yes"?>  <pre>context</pre> </pre> <pre>context</pre> <pre>co</pre>	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)
<pre><writepeakstotextfile>False</writepeakstotextfile>                           </pre>	Set this to 'TRUE' to export all detected peaks. Look for a _peaks.txt file.
<pre></pre>	
<pre><li><ignoremsnscans>False</ignoremsnscans> <!--/DTAGenerationParameters-->    C4.9384 H7.7583 N1.3577 01.4773 S0.0417 1 0.3<!--/maxFit--> 10 </li></pre>	Deconvolution parameters. HornTransform = THRASH.
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L.		
Ė	<horntransformparameters></horntransformparameters>	
	<pre><morntransformarameters> </morntransformarameters></pre> </th <th>THRASH deconvolution parameters</th>	THRASH deconvolution parameters
	<pre><sumspectra>False</sumspectra> <sumspectraacrossscanrange>False</sumspectraacrossscanrange>FalseFalse <numberofscanstoadvance>@</numberofscanstoadvance> <sumspectraacrossframerange>True</sumspectraacrossframerange> <numberofframestosumover>3</numberofframestosumover> <isactualmonomzused>False</isactualmonomzused> <leftfitstringencyfactor>1</leftfitstringencyfactor> <rightfitstringencyfactor>1</rightfitstringencyfactor> <userapiddeconvolution>False</userapiddeconvolution> <replacerapidscorewithhornfitscore>False<numpeaksusedinabundance>1</numpeaksusedinabundance> </replacerapidscorewithhornfitscore></pre>	Summing parameters. Set SumSpectraAcrossScanRange to 'TRUE' to sum across scans. NumberOfScansToSumOver represents the +/- number of scans to sum.
	<pre><miscellaneous>     False    </miscellaneous></pre>	Pacific Northwest

</th <th>DTAGenerationParameters&gt;</th> <th></th>	DTAGenerationParameters>	
<h< td=""><td>ornTransformParameters&gt;</td><td></td></h<>	ornTransformParameters>	
	<tagformula></tagformula>	
	AveragineFormula>C4.9384 H7.7583 N1.3577 01.4773 S0.0417	
	<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>	
	<pre><checkallpatternsagainstcharge1>False</checkallpatternsagainstcharge1></pre>	
	<completefit>False</completefit>	
	<ccmass>1.00727649</ccmass>	
	<isotopefittype>AREA</isotopefittype>	RAPID deconvolution. See Park et al
	<usemercurycaching>True</usemercurycaching>	(2008). Set this to 'True' to override
<\$	umSpectra>False	THRASH deconvolution.
<\$	umSpectraAcrossScanRange>False	
<n< td=""><td>umberOfScansToSumOver&gt;1</td><td></td></n<>	umberOfScansToSumOver>1	
<n< td=""><td>umberOfScansToAdvance&gt;0</td><td></td></n<>	umberOfScansToAdvance>0	
<\$	umSpectraAcrossFrameRange>True <td></td>	
<n< td=""><td>umberOfFramesToSumOver&gt;3<td></td></td></n<>	umberOfFramesToSumOver>3 <td></td>	
<b>&lt;</b> I	sActualMonoMZUsed>False <td></td>	
<l< td=""><td>eftFitStringencyFactor&gt;1</td><td></td></l<>	eftFitStringencyFactor>1	
<r< td=""><td>ightFitStringencyFactor&gt;1</td><td></td></r<>	ightFitStringencyFactor>1	
<b>&lt;</b> U	seRAPIDDeconvolution>False	
	<replacerapidscorewithhornfitscore>False<td></td></replacerapidscorewithhornfitscore>	
	<numpeaksusedinabundance>1</numpeaksusedinabundance>	Miscellaneous section.
		1
<m< td=""><td>iscellaneous&gt;</td><td></td></m<>	iscellaneous>	
	<usescanrange>False</usescanrange>	

<pre><replacerapidscorewithhornfitscore>False1 </replacerapidscorewithhornfitscore></pre>	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 "MayScan"
E KMiscellaneous>	MINSCAN AND MAXSCAN .
<pre></pre>	
<maxscan>6000</maxscan>	
<usem7range>True</usem7range>	Sotting this to 'TPLIE' means that the mass
<pre><minmz>200</minmz></pre>	security this to TROE means that the mass
<maxmz>2000</maxmz>	spectrum will be Savitzky-Golay smoothed.
<pre><applysavitzkygolay>False</applysavitzkygolay></pre>	
<sgnumleft>2</sgnumleft>	Setting this to 'TRUE' will result in zero-
<sgnumright>2</sgnumright>	filling Good to use for sparse, raw data
<sgorder>2</sgorder>	
<zerofilldiscontinousareas>False<td></td></zerofilldiscontinousareas>	
<numzerostofill>3</numzerostofill>	
<processmsms>False</processmsms>	
<exportfiletype>TEXT</exportfiletype>	
<pre><detectpeaksonly_nodeconvolution>False</detectpeaksonly_nodeconvolution></pre>	
<process_ms>True</process_ms>	
<pre></pre>	Setting this to 'TRUE' means that only
± <elementisotopes></elementisotopes>	peaks will be detected and no
<pre></pre>	deconvolution will be performed. Ensure
	that you set the 'WritePeaksToTextFile' set
	that you set the whiter eaks for exit lie set
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