



Mascot Daemon is our automation client. It's a part of the Mascot package that is only available when you have a Mascot server in-house.

It is only available for Windows because all of the mass spectrometry data systems are Windows packages, so this is always the platform where the data files originate.

Links to install and update Daemon can be found on your local Mascot home page, so that anyone with access to the server can easily get a copy of Daemon. You should try and make sure that you have the same version of Mascot Server and Mascot Daemon installed. An older version of Daemon will probably work, but it won't support features in later versions of Mascot Server.

Installing	g Mascot Daemon	
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	S bogong/mascot_2_4_0_64/daemon_install.html#INST	\$ \$
	local Users group Full Control. This will change the settings for the directory and all the	files it contains.
	executables elevated privileges: Open Vinidovs Explorer and nariquete to the Directory installade (C.Vinoyam / Heldwich Sciencychick and choose Properties: on the Compability on once, and the service is installed, you can back and dear these checkboxes.	where Dearnon is 80 on a 94-bit 6, check <i>Run dhis</i> 8 Deernon has run
	Control Stat de Conservation     Control Index muit france     Control Index muit france     Control Index muit grando Trainingo     Poladog Land     Kontrol Index muit grando Trainingo     Control Index muit grando Trainingo     Control Index muit grando Trainingo	
	Start Mascet Deemon from the Windows Start Menu. Shortly after displaying the splast presented with the Preferences dialog:     More themes Preference     Team and the Preference dialog:     Team and the Preference dialog:	s screen, you will be
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If installing on Windows Vista or later, it is essential to follow the instructions and change the properties of both executables so that they 'Run as Administrator'. Once the Mascot service is installed and the settings saved to the registry, you can revert to running as a standard user, if you wish.

Installing Mascot Daemon
Mascot Daemon: Preferences
Intranet Data import filters ADD connection Timer settings Authentication Mascot server URL, up to and including cgi directory, (e.g. http://your_server/mascot/cgi/)
http://161-jsc/mascot/cgi/
HTTP timeout (seconds) 60 HTTP access type Registry default v HTTP proxy server HTTP protocol C HTTP/1.0 C HTTP/1.1
Cancel
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When Mascot Daemon is first launched, this dialog will be displayed and you have to enter the URL of your local Mascot server to proceed. Note that you cannot enter the public web site URL ... it simply won't work. If Mascot security is enabled, you will also need to enter a valid user name and password on the authentication tab.

Installing Mascot Daemon
Mascot Daemon: Preferences
Intranet Data import filters ADD connection Timer settings Authentication
Web Server Authentication         User name         Password         Proxy Server Authentication         User name         Password         Mascot Security         User name         User name         Password
Save Cancel
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Mascot security is not the same as web server security or having to tunnel through a firewall or authenticated proxy server. There are separate fields for each of these.



Once Daemon has connected to the Mascot server, you will see a display like this. The user interface is a simple, tabbed dialog box



Mascot Daemon has comprehensive, context sensitive help. Just press F1. There is a tutorial to get you up to speed and detailed reference material.



Lets look at the tabs in more detail.

The Task Editor tab is used to define each task. A task defines *what* data will be searched and and *when* the search will take place. A Parameter set is selected that contains the search parameters. This determines *how* the data files will be searched.

Here we have a very simple batch task. A single data file has been selected, a parameter set has been chosen, and the task will run the search as soon as we press run.

The data files can be simple peak lists. In this case, we are using Mascot Distiller as a data import filter and the data file is a RAW file. More about data import filters later.

Note the checkbox at the bottom left. Merging a batch of files into a single search can be very useful. MudPIT fractions, for example

Search Parameter Editor
Mascot Daemon
Search title Submitted from <taskname> by Mascot Daemon on <tocalhout> Taxonotity Part white: Database NA_scratch perf Sexectified V Decoy database  Protein mass kDa</tocalhout></taskname>
Fixed modifications     Carbanidometryl (C)     Monoisotopic Average     C     Enzyme     Trypsin/P       Variable modifications     Oxidation (M)     Select Modifications     Peptide charge     2 •
Peptide tol. ±     20     ppm     # #13C     0       MS/MS     MS/MS tons search     Image: Comparing the search     Quantitation     None     Image: Comparing the search       Error tolerant search     MS/MS tol. ±     0.3     Da     Instrument     ESI-TRAP     Image: Comparing the search
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The parameter editor allows sets of search parameters to be defined and saved to disk, so that they can be used over and over again by tasks. The search parameters define *how* the data will be searched. As you can see, the fields are very similar to those on the web browser search form.

The search title includes some tokens, or variable, that will be replaced when the task runs. Here, for example, <taskname> will be replaced by the name of the task and <localhost> will be replaced by the name of the computer on which Daemon is running. This will make it easy to identify where the searches came from when looking at the Mascot search log on the server. There are many such tokens. You can find details in the help file.



Each search result is added to an Explorer-like tree on the Status tab. There is a minimum of summary information, and a hyperlink to the full result report. Mascot Daemon isn't intended to be an interface to browse Mascot results, it is just a tool to automate search submission and keep track of results

Data files within a particular task are run serially, but multiple tasks can be set running at the same time. This means that several data files can be processed and search the same time.

Data Import Filters	
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Status       Eyent Log       I ask E ditor       Parameter Editor         Owner       Task       United       New       Run         Parameter set       C:Vhogan Files/Matrix Science/Masco       Data inport filer       Options         Data file ist       Data files into the area below or cick on Add       Parameter ist./Masco       Options         Data file ist       Thermofining on LO1 / DECA RAW file Masco       Options       Stating on LO1 / DECA RAW file Masco         Data file ist       Data cycles       Stating on LO1 / DECA RAW file Masco       Options         C:Vbistler test data/Vcalbur/00081585AT       C:Voistler test data/Vcalbur/00081585AT       Follow-up         C:Voistler test data/Vcalbur/00081585AT       Follow-up       Search priority       O         Delete       Add Folder       Add Files       Follow-up       Follow-up         Werge MS/MS files into single search       Pasc data to       None       Image: Pasc data to	
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Going back to the task editor tab. For some file formats, we have data import filters. These allow Daemon to generate peak lists directly from the binary files created by the MS data system.

These data import filters are only listed if the relevant software packages are installed. For Mascot Distiller, you need to have a licence for the Daemon Toolbox

Next to the drop down list, you have a button to view the data import filter options

Data Import Filters
Mascot Daemon: Data import filter options
extract man Micromases and Spiev disalined Data Evidored Macrod Distiller TS2Macrod
All versions First scan Last scan Minimum mass 300 Maximum mass 4000 Grouping tolerance 1.4 Intermediate scans 1 Min. scans / group 1 Precursor charge [AUT0 ]
OK Cancel
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Each filter has different options, and all the options are described in the Mascot Daemon help - just press F1

The extract\_msn filter is a Thermo utility that enables Daemon to create peak lists from Thermo Xcalibur .RAW files. Mascot Daemon simply calls the utility using the parameters specified in this dialog. A brief description of each argument is provided in the Mascot Daemon help. extract\_msn can be downloaded from the Thermo web site, but Thermo is no longer developing it, so it cannot be used with their latest instruments, such as the Q-Exactive.

The Micromass filter was just a way of locating pkl format peak lists and is obsolete now that you can submit searches direct from ProteinLynx Global Server. It will be dropped in a future release

Mascot Search - Options     Mascot parameters     Set default parameters     Set default parameters     Set default parameters     Mascot on this computer     C. Local Mascot     Min. number cycles between groups     Max. number cycles per group     Min. number cycles per group     Ms/MS data processing   Remove peaks if intensity < 0   Z of maximum   IDA survey scan   IDA survey scan   IDA survey scan   IDA survey scan   IDefault precursor charge state from survey scari   Default precursor charge states   ID bisodope MS/MS data   ID claust precursor charge states   ID biscard ions with charge of 5+ or higher   Dther   Use original format for query titles     OK     Cancel
--

The AB Sciex Analyst filter uses the Mascot.dll script that is provided with Analyst and supports the QTrap and QStar families of instruments. If you are using a recent version of the mascot.dll script, the controls in the options dialog will vary slightly according to the version of Analyst.

Data Import Filters	
Mascot Daemon: Data import filter options	3
extract_msn   Micromass.spl   Sciex Analyst   Data Explorer   Mascot Distiller   TS2Mascot	
Processing settings	
VBA macro Baseline VBA macro assigned to button Correct baseline	
Noise filters         Correlation factor         7	
Peak filters     ✓ Only monoisotopic peaks     ✓ Only singly charged peaks	
Intensity filters     C All peaks     (• Select 10 most intense peaks per 100 Da	
Cancel	
	14
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The Data Explorer filter can be used to process data files from AB Sciex Voyager systems or T2D files exported from TOF/TOF data.

Data Import Filters	
Mascot Daemon: Data import filter options	
extract_msn Micromass.spl Sciex Analysi Data Explorer Mascot Distiller TS2Mascot Peak Filtering Mass range 60 Da to 20 Da below precursor Minimum S/N 10 Monoisotopic peaks only ⊽	
OK Cancel	
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TS2Mascot imports AB Sciex TOF/TOF peak lists direct from the Oracle database.

Data Import Filters
S Mascot Daemon: Data import filter options
estract_msn Micromass.spl Sciex Analysi Data Explorer Mascot Distiller TS2Mascot
Mascot Distiller Processing Options  C:\Program Files\Matrix Science\Mascot Distiller\Orbitrap_k Edit Save As
Data File Format         Text Data File (MS only)         Intensity values           Thermo Xcalibur         C Centroided peak list         C Area           C Profile / Lowingson         S 300
Multi-Sample Files     Quantitate Protein Hits       Merge all samples into single search     Image All Image All Image from The samples       Separate search for each samples     Image from The sample from The same from The sam
Scan Range (multi-scan files) Peak List Format Start End Units Minutes  MGF
Output PMF Masses as       Output MS/MS Fragments as       Distiller Project File         C m/z       C MH+       C Mr       IF Save
DK Cancel
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The most powerful data import filter is Mascot Distiller, because it can import all of the major raw file formats. The dialog is simple because most of the peak picking options are contained in the selected processing options file.

The idea is that you adjust the processing options by working interactively with a typical data file in Mascot Distiller Workstation. You then save these options to a file and select it here.

Notice the checkbox at the bottom right. You can ask Daemon to save a project file containing the Peak lists and Mascot search results.

In Mascot Daemon 2.3, you can also batch automate quantitation. We'll be discussing quantitation in detail in a later talk.



If Distiller is used for peak picking, once the search has completed, you get a hyperlink to open the project in Mascot Distiller. Click on the link and ...



Shazam



•Peak lists created by Daemon are always saved to disk. This is the default path, which can be changed in preferences.

•When you delete a task, any peak lists are also deleted. If you have used Mascot Distiller as in import filter, then the distiller project file is also deleted. The raw data files are never deleted.

•In this example, all the tasks between 1 and 32 have been deleted.

•Task 32 was called "t2d using Distiller" and you can see that for each raw data file, a Distiller project file and a Mascot Generic Peak list file has been created



Lets talk in more detail about tasks. Mascot Daemon supports three kinds of task:

A batch task allows you to search one or more specified files immediately or at a defined date and time

A real-time monitor task is the key to real automation. You define a task using a file path for the data file which includes wild cards. Any file that matches this path is picked up and searched.

A follow-up task is a task where the data files are passed to it by another task. This is very powerful because it allows searches to be chained together to implement complex workflows. For example, a batch of data files might be screened against a contaminants database containing entries for keratins, BSA, trypsin, etc. Those data files which fail to find a match can then be automatically searched against a non-redundant protein database. Spectra which are still unmatched can then be searched against a large EST database, etc., etc.

Mascot Daemon         Fle Edit Help         Statue       Event Log         Issk Editor       Parameter Editor         Overet:       Task.         Parameter set       Real time monitor example         Parameter set       Options         CVProgram Files/Matrix Science/Mascr       Data import filter         Optional Files/Matrix Science/Mascr       Import filter         Optional Files/Matrix Science/Mascr       Schedule         Specity path to root folder       Stat at 181615         Jata file fist       Suble 2012         Choose       Stat at 181615         Browse       Stat at 181615         Optional wild card file or folder name       Stat at 181615         Follow-up       Search priority         Auto-print results       External processes         Follow-up       No follow-up required         No follow-up required       Implemented         Include sub-folders       Implemented         Implementer       New files only	Real-t	ime Monitor Tasks
	Fid	Bascot Daemon         Edx       Help         Status       Event Log         Task       Real time monitor example         Parameter set       Data import filter         CVProgram Files/Matrix Science/Masco       Data import filter         Optional Relative root folder       Schedule         Specify path to root folder       Schedule         Browne       Schedule         Optional wild card file or folder name       Follow-up         Search priority       Image: Search priority         Follow-up       Search priority         Follow-up       Search priority         Follow-up       Search priority         Include sub-folders       Image: State to         Verw files only       Pass date to

When you select real-time monitor in the schedule frame, the task editor tab looks like this. Here, we are looking in the specified directory and all its subdirectories, for any file called peaklist.

Note that the final part of the path says "file or folder name". This is because some raw files are actually folders, not files.

If Include sub-folders is checked, then Daemon will search down through all sub-directories of the root folder

If new files only is checked, then any files that exist when the task is started will be ignored. A common problem when using real-time monitor like a batch task is to have this checked and then wonder why nothing is happening

Follow-up Tasks	
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Ele Edit Help	
Status Event Log Iask Editor Parameter Editor	
Owner Task	
jootireli 🔄 JEST mouse follower New Run	
Parameter set Data import filter	
Jance Mascel Daemonivet_mouse.par None Uptions	
Data file list       Schedule         A follow-up task does not have a pre-defined fit of data files. It runs continuously, waiting to receive data from other tasks.       Start at 092833 + 10 July 2012 + C         C Start at 092833       C Start at 092833 + 10 July 2012 + C         C Reaktime monitor       C Follow-up	
Actions	
Followup	
No follow-up required	
Discard results	
Repeat at intervals of 1 v days v	
Pass data to None	
	1/2
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Follow-up tasks are a little more difficult to explain. Any task can pass data to a follow-up task to be searched again in a different way. Only follow-up tasks can receive data from other tasks in this way.

Lets illustrate with an example. Imagine we want to search our MS/MS data files against the mouse sequences plus a contaminants database as a first pass search. We then want to search all spectra that fail to get a significant match against a database of mouse EST sequences.

We start at the end of the chain, and define the EST search as a follow-up task. We just choose Follow-up in the schedule frame and a parameter set, created earlier in the parameter editor, that contains the required search parameters.



We press run, and we see our Follow-up task running. Although the task is running, nothing will happen until we feed some data into it

Follow-up Tasks	
Mascot Daemon      Fie Edit Help      Status     Event Log      Jask Editor      Parameter Editor      Owner      Control      Data files into the area     below or tack on Add      C.\Downloads\\iptg2008.mgf      C.\Downloads\\iptg2008.mgf      Follow-up      Search prionly      Total files      Follow-up      Search prionly      Total      Follow-up      Search prionly      Total      Follow-up      Follow-up	
Delete       Add Files       If Code Sea My Hist match is sendong > 1 in to days         Merge MS/MS files into single search       If Code Sea My Hist match is sendong > 1 in to days         MASCOT       : Automation with Mascot Daemon       © 2007-2012 Matrix Science	MATRX

We go back to the task editor and create a simple batch task. There is one data file and the search parameters are a different set, in which the databases are SwissProt with a taxonomy filter of rodents plus second database of contaminant sequences.

Before pressing Run, we have to link this task to the follow-up task. We need to specify a condition for passing the data to the follow-up task. This can be score based or probability based.

Follow-up Tasks			
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File Edit Help			
Status Event Log Iask Editor Parameter Editor			
Owner Task			
jcottrell VissProt mouse trypsin/p New Run			
Parameter set Data import filter			
Mascot Daemon\swissprot_mouse.par None Options			
Data file list			
Drag and drop data files into the area G Start now			
below or click on Add			
C:\Downloads\iprg2008.mgf C Real-time monitor			
C Follow-up Search priority 0			
Actions			
Auto-print results External processes			
Follow-up			
If probability that match is random > 1 in v  20			
Discard results			
Delete Add Folder Add Files   Repeat at intervals of days Y			
Merge MS/MS files into single search			
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For this example, we will use the default significance threshold of 5%. If the score a peptide match in the first search is below a 5% significance threshold, then the spectrum will be passed to the follow-up task we created earlier. Note that you also have the option to repeat the search at intervals, maybe to see whether a better match can be found in some future update to the sequence database. The task is now configured, and we can press Run.



Some time later, the status tab looks like this. The results for the first search appear under task 14. Those spectra that failed to obtain a significant match were passed to the follow-up task, task 13, where the result information appears once the search has completed



•One follow-up task can pass data to another follow-up task, creating a chain of tasks to implement a complex workflow. Thresholding applies to individual spectra. If there are 1000 spectra, and 100 get a good match, we take the 900 that didn't get a match and pass them to the follow-up task. You can think of the chain of tasks as a series of finer and finer sieves.

•Remember that, when you define the chain, you have to start at the end of the chain, with the last task, and work forwards to the first task in the chain

•Having created a follow-up task, or a chain of follow-up tasks, multiple batch or real-time monitor tasks can feed into it. It just sits there, waiting

•Note that any result node can be dragged and dropped onto a follow-up task node to repeat the search using a different parameter set

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External Pr	ocesses	
C	🛾 Mascot Daemon: External processes 🛛 🛛 📉	
Ele Edit Help	Before starting task	
Status	··· No external process ···	
Owner	Wait for completion Halt on error	
icottrell	Before each search	
Parameter set	··· No external process ···	
AMascot Dae	Wait for completion Halt on error	
Data file list	After each search	
Drag and drop below or click	wscript c:\temp\simple.vbs " <resultfilename>" "<resulturb"< th=""><th></th></resulturb"<></resultfilename>	
C:\Download	Wait for completion Halt on error	
	After completing task	
	··· No external process ···	
	Wait for completion Halt on error	
Dalata		
	IS files into sincle search V Pass data to 13 EST mouse follower	
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We'll briefly touch on a few other features of Daemon. The task editor tab includes a button labelled 'External processes'. A Mascot Daemon task can execute external processes at one or more of the following time points:

- •At the start of a task
- •Before submitting each search in a task
- •After completion of each successful search in a task.
- •At the end of a task

A process is a one line command. This could execute a Windows program, or it could be a batch file or script to perform some more complex procedure. You can pass arguments to the commands by including tokens, such as <taskname>



The help file contains a list of all the available tokens. It also gives examples of how to use External processes, such as a script to build an HTML page in real-time that contains hyperlinks to the search results.



Mascot Daemon is divided into two components: a Graphical User Interface (GUI) and a Service. We have been looking at the GUI, which is used to configure Daemon, edit tasks, view search results, etc. The service is responsible for executing the tasks, in the background, whether the GUI is running or not. It will continue to run tasks even if you close the GUI and log out of Windows

If something goes horribly wrong, you may need to stop and start the service to clear the problem

To access data files across the LAN, you will need to configure the Daemon service to log in as a Windows user. In most cases, you will want to have the service use the same Windows log-in as you do. Full details in the help file.

Remember that services don't recognise drive letter mappings. For files on remote computers, Daemon will use UNC paths and must be able to access these files without being challenged for a password

If this proves impossible, for example, if the files are on a SAMBA server, you can run both Daemon components on the desktop by setting the service to disabled



To change the service login you need to use the services control panel. Find and select the MascotDaemonService in the list. You can stop or start the service using the controls at the top, or by right clicking to get the context menu. To change the user, click properties and then, on the log on tab choose "This account" and enter your user name and password. Remember that if you change your password, you will also need to come back to this screen and also change it here.



Under the hood, Mascot Daemon stores information in a Microsoft Access Database called taskdb.mdb. It is possible to use other databases, and this should be setup in the "ADO Connection" tab of the Mascot Daemon Preferences.

Multiple Mascot Daemon clients can share the same task database. Each task is "owned" by the client that created it. Clients can only Pause, Resume, Cancel, or Delete their own tasks. However, any client can Clone any task and can transfer data files to any follow-up task, either by dragging and dropping the result node or by specifying the task in follow-up criteria.