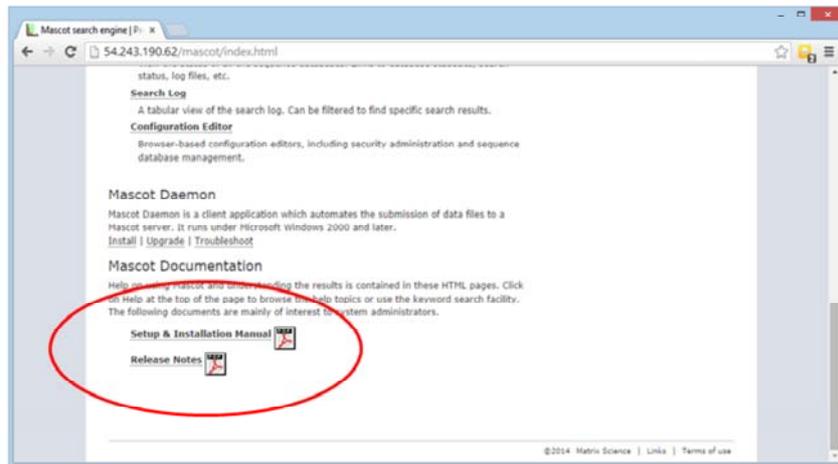


Administration & Configuration

MASCOT



Installation & Setup

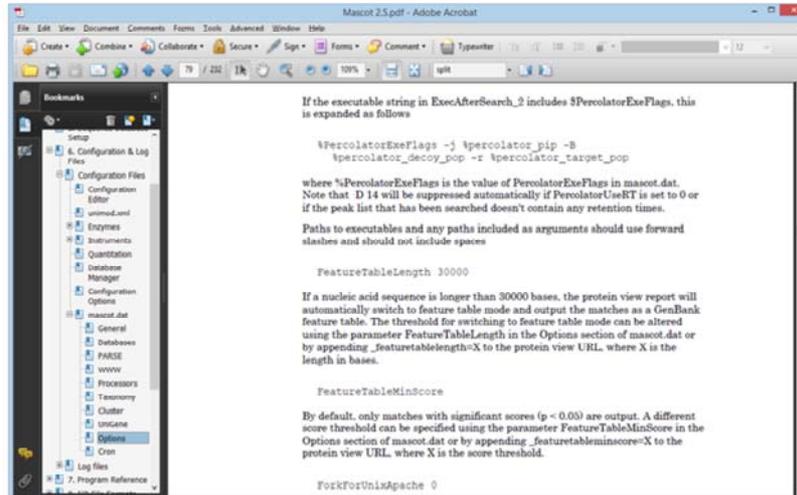


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The Mascot Installation & Setup manual is linked from your local Mascot home page. If you need detailed information on any aspect of Mascot installation or configuration, this is the place to look

Installation & Setup



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This is an administrator's manual, not a user manual. You won't find much relating to how to submit a search or how to interpret the results. User help is in the Mascot HTML pages.

Installation & Setup

- Mascot Security
- Configuration Editor
- Log Files
- Cluster mode

These are the topics we will cover in this presentation

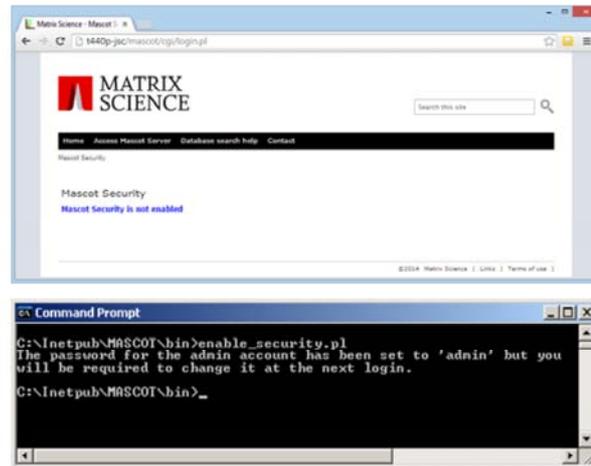
Mascot Security

Examples of how Mascot security can be used:

- Ordinary users can browse configuration files and status screens, but not make changes
- Certain sequence databases are 'private' to a group of users
- Limit some users to one search at a time while others can run many searches simultaneously
- Limit the length of searches from a particular group to 1 hour
- Prevent certain users submitting 'no enzyme' searches
- Let 'customers' view the results of searches run for them without being able to submit searches themselves.

Mascot security is not a substitute for a firewall. It won't stop your server being hacked or infected by a virus. It is a way of managing and allocating the Mascot Server resources.

Mascot Security - enable / disable



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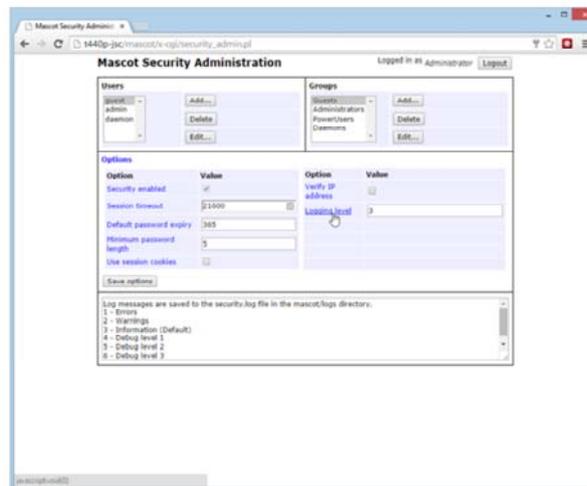


When Mascot is first installed, Mascot security is disabled. So, if you try to log in you will see this message.

To enable security, open a command prompt or a shell on the Mascot server, and change to the mascot/bin directory. Type `enable_security.pl` (or `./enable_security.pl` if Linux).

This takes a few seconds. If you forget the administrator password, it can always be reset to 'admin' by running this script again.

Mascot Security - administration



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All security configuration is browser based. The top level page of the security administration utility looks like this.

There is a list of users, a list of groups and a few options.

If you hold the mouse over any of the blue text, help will appear at the bottom of the screen.

The options shown on this page are global options, which apply to all users.

Reference:

You can't disable security from here - it has to be done on the server using the disable security command

The session timeout is in seconds. After this period of inactivity, the user will be required to login again.

The password expiry time is in days. After this period of time, the user will be required to enter a new password. Set to 0 to allow passwords to be permanent

Any new password must be at least this length.

Session cookies are automatically destroyed when the browser is closed. With some browsers, session cookies are not shared when a new instance of the browser is opened, which might mean that a user has to login again for each new window opened.

If verify the IP address is set, then any request to perform a privileged action will compare the IP address that the request is coming from with the one originally used to login.

Logging level should normally be left at 3

Mascot Security - “role based”

Users

- Login name
- Password, password expiry
- Full name, email address
- Account enabled / disabled
- Member of one or more groups.

Groups

- Name
- List of members
- List of allowed tasks.

Mascot security is “role based”. This means that privileges, known as tasks, are assigned to groups, not individual users.

Users gain these privileges by being members of one or more groups.

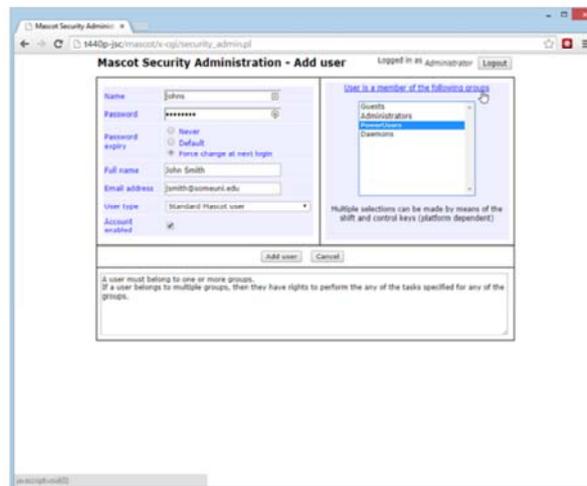
Mascot Security - tasks

For example

- Allow PMF search
- Allow MS/MS search
- Maximum number of queries
- Can view the search log
- Can search specific databases
- Can view other peoples results.

There are 30 different tasks that members of a group can be allowed to perform - for example:

Mascot Security - add user



The screenshot shows a web browser window titled "Mascot Security Administration - Add user". The page is for adding a new user. It includes the following fields and options:

- Name:** john
- Password:** [masked]
- Password expiry:** Never, Default, Force change at next login
- Full name:** John Smith
- Email address:** johnsmith@somewhere.edu
- User type:** Standard Mascot user
- Account enabled:**

On the right side, there is a section titled "User is a member of the following groups" with a list box containing "Guests", "Administrators", "Standard users", and "Deacons". Below this is a note: "Multiple selections can be made by means of the shift and control keys (platform dependent)".

At the bottom of the form are "Add user" and "Cancel" buttons. A footer note states: "A user must belong to one or more groups. If a user belongs to multiple groups, then they have rights to perform any of the tasks specified for any of the groups."

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Adding a new user is very simple.

The Administrator must enter a username and password and it is usually a good idea to force the user to enter a new password when they first login

Enter their full name and email address. The user will be able to change this

I'll return to the choice of user types later - most users should just be standard Mascot users.

Make sure that the account is enabled, and then select one or more groups for the user to belong to.

Example - Core Lab. Customer

If you don't want the customers to be able to do any searches, but just view the results, then just give them the access to tasks:

SEARCH: Allow all fasta databases to be searched
VIEW: See search results from other people in your own group
VIEW: Allow user to view the search log
ADMIN: Allow use of Database Status application

In a core lab., you may want a group that enables customers to view their results. In this case, only give them rights to perform these tasks:

You must allow all fasta databases to be searched, otherwise they won't be able to view reports. However, they can't perform PMF or MS/MS searches, because this task is missing.

Example - Core Lab. Customer

The screenshot displays two overlapping browser windows. The left window, titled 'MASCOT search log', shows a table of search logs with columns for Job ID, Date, and User Name. The right window, titled 'MASCOT Search Result', shows a search result page with a search title, database information, and a list of protein families. Below the search results, there is a table with columns for Job ID, Date, and User Name.

Job ID	Date	User Name
1111	12/06	testuser
1112	12/06	testuser
1113	12/06	testuser
1114	12/06	testuser
1115	12/06	testuser

Job ID	Date	User Name
1111	12/06	testuser
1112	12/06	testuser
1113	12/06	testuser
1114	12/06	testuser
1115	12/06	testuser

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A group member will be able to view the search log, see their results, but when they try to do a repeat search, access is denied

Example - Daemon & Distiller



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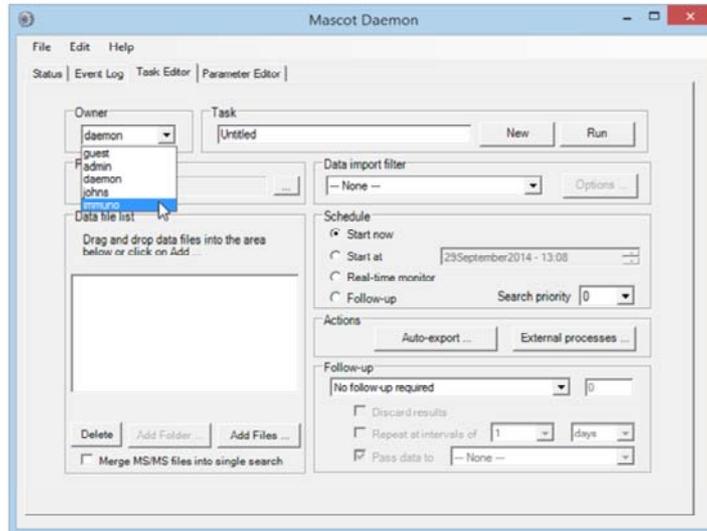


Client software, like Mascot Distiller and Mascot Daemon, requires special privileges. The Mascot Daemon user must have the security token 'Mascot Daemon is allowed to submit searches'. The default daemons group settings shown here are appropriate for either a Daemon or Distiller client.

View config files is required because both clients need to retrieve configuration information from the server, like a list of the databases that are available.

Mascot users can be given the privilege to submit searches under other user names. This is particularly useful in a core lab, when customers only have privileges to see their own search results, so the instrument operator needs to submit their searches under individual customer log-in names. The security task is 'For Mascot Daemon, allow spoofing of another user'.

Example - Daemon & Distiller



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If this has been enabled for the user who is running Mascot Daemon, then a drop down list of other Mascot user names will be enabled on the Task Editor tab.

Example - 3rd party applications

Older applications that submit searches to Mascot won't have their own login

Try logging in using Internet Explorer before running the application - cookies

Use one of the 'special' user types:



The screenshot shows a dialog box for user selection. It has a title bar and several fields: 'Email address' with an empty text box, 'User type' with a dropdown menu showing 'User authenticated using web server', and 'Account enabled' with a checked checkbox. Below these is a list of user types: 'Standard Mascot user', 'Computer name', 'IP address', and 'Agent string'. The 'User authenticated using web server' option is highlighted in blue. To the right of the list is a 'Multiple shift' checkbox. At the bottom right are 'Add user' and 'Cancel' buttons.

There are potential issues with older, legacy applications that interface with Mascot but don't have code to support the security system.

Since session ids are saved as cookies, and since most Windows applications that access web sites use Microsoft Internet Explorer libraries, it may be sufficient just to login from an Internet Explorer browser window before starting the application.

Alternatively, you can use one of the special user types.

Example - 3rd party applications

Computer name / IP address

- Never have to log in from that computer
- Use the computer name / IP address as the 'name'

Agent string

- Can determine the agent string from the web server logs
- Not secure because someone could create another app to use this agent string

Web server authentication.

These methods are less secure than a password protected login, but ensure that all applications are able to connect somehow.

Mascot Security - general tips

- Plan carefully before implementation
- Login as admin to perform admin tasks
- Enabling Mascot security doesn't stop your server from being hacked.
- Moving Mascot to another computer?

Just copy over *user.xml*, *group.xml* and *security_options.xml*.

I can't stress enough that you should plan what you intend to do before you start. Think carefully about what groups you want to create

As any Unix administrator will tell you, it's always best to separate your administration and user tasks. However, we can't force you, but that is why the default admin user cannot submit searches.

It is very important to understand that Mascot security does not provide protection against a malicious hacker. Hackers don't attack a server through Mascot ... they've probably never heard of Mascot. They attack through weaknesses in the operating system and through flaws in well known applications, like the web server. It is still essential to have a dedicated firewall between the Mascot server and the Internet

Configuration Editor

(Almost) everything in Mascot is configured using text files in the config directory

- General settings - *mascot.dat*
- Masses and modifications - *unimod.xml*
- Enzymes - *enzymes*
- MS/MS ions series - *fragmentation_rules*
- Taxonomy categories - *taxonomy*
- Cluster geometry - *nodelist.txt*
- Security - *group.xml*, *user.xml*,
security_options.xml, *security_tasks.xml*

(Almost) everything in Mascot is configured using these text files in the config directory. The syntax for each of these files is described in the manual.

Configuration Editor



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You can edit these files in a text editor, but it is easier and safer to use the browser-based Configuration Editor. The first three entries are interfaces to different sections of unimod.xml.

Configuration Editor

Mascot Configuration: Symbols

Symbol	Name	Molecular Weight	Average	Composition
13C	Carbon 13	13.003355	13.0034	13C
15N	Nitrogen 15	15.000109	15.0001	15N
18O	Oxygen 18	17.999160	17.9992	18O
2H	Deuterium	2.014102	2.0141	2H
Ac	Acetate	42.010565	42.0267	C(2) H(3) O(2)
Ag	Silver	106.905092	107.8682	Ag
As	Arsenic	74.921594	74.9216	As
Au	Gold	196.966542	196.9666	Au
B	Boron	11.009306	10.811	B
Br	Bromine	79.903336	79.904	Br
C	Carbon	12	12.0107	C
Ca	Calcium	39.962491	40.078	Ca
Cd	Cadmium	112.903357	112.411	Cd
Cl	Chlorine	34.968852	35.453	Cl
Co	Cobalt	58.933198	58.9332	Co
Cr	Chromium	51.940310	51.9961	Cr
Cu	Copper	62.929599	63.546	Cu
dHex	Deoxy-hexose	146.057908	146.1412	C(6) H(10) O(5)
F	Fluorine	18.998403	18.9984	F
Fe	Iron	55.845209	55.845	Fe
H	Hydrogen	1.007825	1.0079	H
Hep	Heptose	182.063388	182.1666	C(7) H(12) O(6)
Hex	Hexose	162.052024	162.1466	H(2) C(6) O(5)
Hexa	Hexanamide	176.020086	176.1491	C(6) H(13) N(1)
HexNAc	N-Acetyl Hexosamine	203.079373	203.1925	C(8) H(13) N(1) O(3)
Hg	Mercury	200.592447	200.59	Hg
I	Iodine	126.904473	126.9045	I
K	Potassium	39.098307	39.0983	K
Kdo	3-deoxy-D-glycero-D-galacto-nonulosonic acid	250.048868	250.2027	C(9) H(14) O(8)
Kdu	2-keto-3-deoxyribulosonic acid	226.050383	226.1787	C(8) H(12) O(7)
Li	Lithium	7.016003	6.941	Li
Me	Methyl	14.015650	14.0266	C H(2)
Mg	Magnesium	24.304094	24.305	Mg
Mn	Manganese	54.938047	54.9380	Mn
Mo	Molybdenum	97.956107	97.94	Mo

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You may need to add or edit an element or an amino acid, but its fairly unlikely.

Configuration Editor

Accession #	PSI-MS Name	Interim name	Description	Monoisotopic mass	Average mass	Composition
267	Label:13C(6)15N(4)	13C6-15N4	13C(6) 15N(4) Side label	10.000269	9.9296	C(-6) 13C(6) N(-4) 15N(4)
452		Ser->Pro	Ser->Pro substitution	10.020735	10.0379	HE2 C(2) O(-1)
269	Label:13C(9)15N(1)	13C9-15N1	13C(9) 15N(1) Side label	10.027228	9.9273	C(-9) 13C(9) N(-1) 15N
444		Thr->Ile	Thr->Ile substitution	12.036386	12.0538	HE4 C(2) O(-1)
440		Thr->Asn	Thr->Asn substitution	12.995249	12.9988	H(-1) N
337	Methylamine	MethylamineST	Michael addition with methylamine	13.031634	13.0418	HE3 C N O(-1)
359	Pro->iso-Glu	Pyroglutamic	proline oxidation to pyroglutamic acid	13.979265	13.9835	HE(-2) O
288	Trp->>Oxalathione	oxalathione	Tryptophan oxidation to oxalathione	13.979265	13.9835	HE(-2) O
34	Methyl	Methyl	Methylation	14.015458	14.0264	HE2 C
338		Asp->Glu	Asp->Glu substitution	14.015458	14.0268	HE2 C

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The modifications file, unimod.xml, is an XML representation of a public database called Unimod. This is the interface to the public database. From time to time, you should update your local file by downloading the latest file using the links in the Unimod help

Configuration Editor

Mascot Configuration: Modifications

Displaying 994/994

Visibility: Short list Long list Mixed Not listed

Error tolerant: Yes No Mixed

Classifications: Post-translational Co-translational Pre-translational CHEMICAL derivative Artifact

Sources: Unimod Edited Unimod Local

Name	Mascotopic	Average	Composition	Source	Visibility	Err Tol			
2-dimethylsuccinyl	144.042239	144.1253	HC3 C18 O4	Unimod	long	yes Copy Print			
2-methylsuccinyl	136.026809	136.2897	HC3 C18 O4	Unimod	long	yes Copy Print			
2-ribitolbutyl	135.032028	135.1201	HC3 C17 N O2	Unimod	short	yes Copy Print			
2-succinyl	116.019939	116.0722	HC4 C14 O4	Unimod	long	yes Copy Print			
2MG	282.052824	282.2476	HC10 C14 O3	Unimod	long	yes Copy Print			
3-deoxyglycerone	144.042239	144.1253	HC3 C18 O4	Unimod	long	yes Copy Print			
3-phenylglyoxal	167.082375	168.0420	HC3 C13 O8	P	Unimod	long	yes Copy Print		
acetyl	183.062829	184.3392	HC4 C17 O4	S	Unimod	long	yes Copy Print		
4-OH	154.009380	154.2063	HC4 C18 O2	Unimod	long	yes Copy Print			
4-OH-Delta-9C-2(OH-1)	136.088815	136.1910	HC22 C9	O	Unimod	long	yes Copy Print		
4ketylal	372.142033	372.3671	HC24 C17	O8	Unimod	long	yes Copy Print		
4-type-iso	-46.005479	-46.0254	HC-21 C1-21	O0-21	Unimod	long	yes Copy Print		
AcetylTag	170.048013	170.1674	HC6 C130	HC21	O	Unimod	long	yes Copy Print	
Acetyl	42.010505	42.0367	HC21 C22	O	Unimod	mixed	yes Copy Print		
Acetyl-13C(1)	44.017274	44.0226	HC21 13C(2)	O	Unimod	long	yes Copy Print		
Acetyl-2NC(1)	45.029395	45.0552	HC-1 2NC(2)	C22	O	Unimod	long	yes Copy Print	
Acetyldeoxyribose	97.089149	97.1582	HC11 C18	N	Unimod	long	yes Copy Print		
Acetylribose	113.084064	113.1576	HC11 C18	N	O	Unimod	long	yes Copy Print	
ADP-Ribosyl	941.061110	941.3005	HC21 C115	HC31	OC13	PL2	Unimod	long	yes Copy Print
ADRS	183.035399	183.2276	HC3 C18	N	OC23	S	Unimod	long	yes Copy Print

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If you need to add a new modification that will be of interest to others, it's best to add it to the public Unimod database, so that the information is available to all Mascot users. If you want to create a local definition, because the modification is confidential or because you are just experimenting. If so, use the Modifications section of the configuration editor

Configuration Editor

View Modification : Piperidine Administrator [Logout](#)

Name:
Title: Piperidine
Formula: Piperidinium

Delta: [Specify](#) [Ignore Names](#) [View](#) [References](#)

Monoisotopic	66.063000
Average	66.1170
Composition	H8 C10

[OK](#) [Make editable](#)

The chemical composition of the modification as a delta between the modified and unmodified residue or terminal.
For example, if the modification removes an H and adds a CH3 group, the Composition could be shown as HC2 C.
The formula is displayed and entered as 'atoms', optionally followed by a number in parentheses. The number
may be negative and, if there is no number, 1 is assumed. Hence, HC2 C is the same as HC2 C(1)

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The user interface is fairly self explanatory, and help is displayed for each field when you mouse over the label. If the modification is from the downloaded unimod.xml file, and you want to make changes, click on the 'Make editable' link

Configuration Editor

The screenshot displays a web browser window titled 'Mascot configuration' with the URL '1440p-jsc/mascot/xcpl/mc-config.exe/hu=1411992791'. The page is titled 'Edit Modification : Piperidine' and includes a 'Logout' link for the 'Administrator' user. The form is organized into several sections:

- Name:** Includes a 'Title' field with the value 'Piperidine' and a 'Fullname' field with the value 'Piperidine'.
- Data:** A section with tabs for 'Specify', 'Specify Masses', 'Mass', and 'References'.
- Delta:** A section containing 'Monoisotopic' (68.062600) and 'Average' (66.1179) values, and a 'Composition' field with the value 'M(R) C(S)'. Below this is a 'Symbols' dropdown menu set to '13C' and an 'Add' button.
- Buttons:** A row of buttons including 'Save changes', 'Cancel', 'Update', 'Revert to Unimod', and 'Show differences'.
- Help Window:** A large empty text area at the bottom of the form.

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All aspects of the modification become editable. If you want to see the differences between the original Unimod entry and the local entry, choose 'Show differences'. If you want to discard your changes, choose 'Revert to Unimod'

Configuration Editor

The screenshot displays the 'Mascot Configuration: Modifications' page. The interface includes a sidebar with filters for visibility (Short list, Long list, Mixed, Not listed) and error tolerance (Yes, No, Mixed). The main content area features a table with columns for Title, Monotopic, Average, Composition, Source, Visibility, and Edit. The table lists four modifications, all of which are local definitions. Below the table, there are buttons for 'Add new modification', 'Main menu', and 'Check Unmod'. The page also shows a 'Page 1/3' indicator and a 'Page size' dropdown set to 20.

Title	Monotopic	Average	Composition	Source	Visibility	Edit
HexNAc(4)Hex(5)Hex(1)HexAc(1)	2059.734933	2060.8689	Hex(5) HexNAc(4) HexAc(1)	local	long	yes Copy Print
HexNAc(4)Hex(5)Hex(1)HexAc(2)	2350.830350	2352.1234	Hex(5) HexNAc(4) HexAc(2)	local	long	yes Copy Print
HexNAc(4)Hex(5)HexAc(1)	1913.677025	1914.7277	Hex(5) HexNAc(4) HexAc(1)	local	long	yes Copy Print
HexNAc(4)Hex(5)HexAc(2)	2204.772441	2205.8822	Hex(5) HexNAc(4) HexAc(2)	local	long	yes Copy Print

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The top level page allows you to filter the listing. Here, we have checked the box to show only local definitions

Configuration Editor

The screenshot shows a web browser window titled "Mascot Configuration: Enzymes". The browser address bar shows "1440p-jsc/mascot/tx.cgi/mc.config酶hu=1411992791&ENZYMES_SHOW=1". The page content includes a table with the following columns: Title, Name, Class, at, Restrict, Independent, and Specificity. Below the table are buttons for "Add new enzyme" and "Main menu".

Title	Name	Class	at	Restrict	Independent	Specificity	
Trypsin	C-Term	KR		F	no	no	Edit Delete
Trypsin/P	C-Term	KR			no	no	Edit Delete
Arg-C	C-Term	R		F	no	no	Edit Delete
Arg-B	N-Term	BD			no	no	Edit Delete
Arg-N_ambic	N-Term	DE			no	no	Edit Delete
Chymotrypsin	C-Term	FLWY		F	no	no	Edit Delete
Chtr	C-Term	H			no	no	Edit Delete
Chtr	C-Term	H			no	no	Edit Delete
Chtr+Trypsin	C-Term	KR		F	no	no	Edit Delete
Familic_acid	N-Term	D			no	no	Edit Delete
Familic_acid	C-Term	D			no	no	Edit Delete
Lys-C	C-Term	K		F	no	no	Edit Delete
Lys-C/P	C-Term	K			no	no	Edit Delete
Lys-C+Argly	N-Term	BD			no	no	Edit Delete
Lys-C+Argly	C-Term	K		F	no	no	Edit Delete
Lys-R	N-Term	K			no	no	Edit Delete
Lys-R	C-Term	FL			no	no	Edit Delete
MSM/Trypsin	C-Term	KR		F	no	yes	Edit Delete
ProteChyma	C-Term	AKLKVY		F	no	no	Edit Delete
ProteChyma	N-Term	J			no	no	Edit Delete
Trypsin/HSP90	C-Term	KR		F	no	no	Edit Delete
Trypsin/HSP90	N-Term	J			no	no	Edit Delete
Trypsin/HSP90/P	C-Term	AKL			no	no	Edit Delete
V8-DE	C-Term	DEEZ		F	no	no	Edit Delete
V8-E	C-Term	EZ		F	no	no	Edit Delete
NuClear	C-Term	J	ABCDEFGHIKLNQKORSTUVWY		no	no	Edit Delete
None							

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Similarly for Enzymes and Instruments. The other sections: Quantitation, Database Manager, and Security, have been touched on in earlier presentations.

Configuration Editor

The screenshot shows a web browser window titled "Configuration Editor: Edit Mascot Options". The page contains several configuration fields and radio buttons. The fields are:

- Proxy Type: Auto (dropdown)
- proxy_server host: proxy (text input)
- proxy_server port: 3128 (text input)
- proxy_username: (text input)
- proxy_password: (text input)
- UseHTTPProxyForFTP: yes no clear
- SaveLastQueryAsc: yes no clear
- SaveEveryLastQueryAsc: yes no clear
- LastQueryAscFile: ../logs/lastquery.asc (text input)
- Interf@basePath: ../inetpub/mascot/data (text input)
- Interf@dataPath: ../data (text input)
- ResultsPerScript: ../cgi/master_results.pl (text input)

There is a "Test Proxy Settings" button next to the proxy configuration fields.

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The Configuration Options section deals with various global settings stored in mascot.dat. Remember that all the sections of mascot.dat that deal with sequence database configuration may be re-written at any time by Database Manager. If you've been in the habit of editing mascot.dat in a text editor, only the Options and Cluster sections can be modified safely unless you decide never to use Database Manager.

There are two configuration files that are missing from the configuration editor: Taxonomy categories (taxonomy) and Cluster geometry (nodelist.txt). If you need to make changes to these, you still have to use a text editor. You can find full details of the file formats in the manual.

Log Files - Troubleshooting

The files in the logs directory are the first place to look if there is a problem

- Installation - *install.log* (Windows only)
- General errors - *errorlog.txt*
- Database update utility - *ftp_log.txt*
- Mascot Monitor events - *monitor.log*
- Security events - *security.log*
- Cluster bootstrapping - *load_node.log* (Unix only)
- Cluster communication - *ipc.log*.

The log files are the first place to look if there is a problem. Most of these files can be accessed from a browser via links in the database status utility, which we'll come to in a minute

Log files - *searches.log*

- May need to split / roll over the log if it gets very large
- Can be recreated using *ms-makesearchlog.exe*
- If you move Mascot to a new machine, transfer *searches.log* and *mascot.job* along with the search results files
- Tab separated values; easily transferred to spreadsheet or relational database.

Every Mascot search adds a new line to the searches log. If the server is busy, the log files can get very large. For most of the logs, you'll probably want to delete the file from time to time. The searches log is different, and you'll probably want to keep all entries indefinitely. Best idea is to rename the file periodically. For example, *searches.log.20060301*. The system will then create a new one automatically.

If the search log is accidentally damaged, a new one can be created by scanning all the result files on the disk

If you move Mascot to a new machine, you'll probably want to transfer or rebuild *searches.log*. The other important file is *mascot.job*, which contains the "next" job number. If you don't copy this across, your job numbers will start all over and you'll have to sort the search log by descending start time to locate the most recent searches.

Some people import the search log into a database application so as to make it easier to search or filter, especially if it gets very large

Log files - database status



The screenshot shows a web browser window displaying the 'MASCOT search status page'. At the top, it indicates 'Version 2.4.0 - Matrix Science in-house test (LOC7-XXBP-QN77-7MTS-YQJH) Licence Info' and 'Logged in as John Costwell - Logout'. Below this, it states 'Using 5 nodes and 10 processors: [0 searches running]'. A navigation bar contains links for 'Search log', 'monitor log', 'error log', 'Error message descriptions', 'node list', and 'Do not auto refresh this page'. The main content area displays a list of database entries with the following details for each:

- apple**: Family = /usr/local/mascot_2_4_0_64/sequence/apple/current/apple_1.fasta, Filename = apple_20120411.fasta, Pathname = /usr/local/mascot_2_4_0_64/sequence/apple/current/apple_20120411.fasta, Status = In use, State Time = Mon May 14 19:11:02 # searches = 0, Men mapped = YES, Request to men map = YES, Request unmap = NO, Men locked = NO, Number of threads = -1, Current = YES.
- CONTAMINANTS**: Family = /usr/local/mascot_2_4_0_64/sequence/contaminants/current/contaminant, Filename = contaminants_20120206.fasta, Pathname = /usr/local/mascot_2_4_0_64/sequence/contaminants/current/cont, Status = In use, State Time = Mon May 14 19:11:02 # searches = 0, Men mapped = YES, Request to men map = YES, Request unmap = NO, Men locked = NO, Number of threads = -1, Current = YES.
- EST_MOUSE**: Family = /usr/local/mascot_2_4_0_64/sequence/EST_mouse/current/EST_mouse_*.fa, Filename = EST_mouse_20120429.fasta, Pathname = /usr/local/mascot_2_4_0_64/sequence/EST_mouse/current/EST_mouse_*.fa, Status = In use, State Time = Mon May 14 19:11:04 # searches = 0, Men mapped = YES, Request to men map = YES, Request unmap = NO, Men locked = NO, Number of threads = -1, Current = YES.
- Human_EST**: Family = /usr/local/mascot_2_4_0_64/sequence/Human_EST/current/Human_EST_*.fa, Filename = Human_EST_111.fasta, Pathname = /usr/local/mascot_2_4_0_64/sequence/Human_EST/current/Human_EST_111.fasta, Status = In use, State Time = Mon May 14 19:11:04 # searches = 0.

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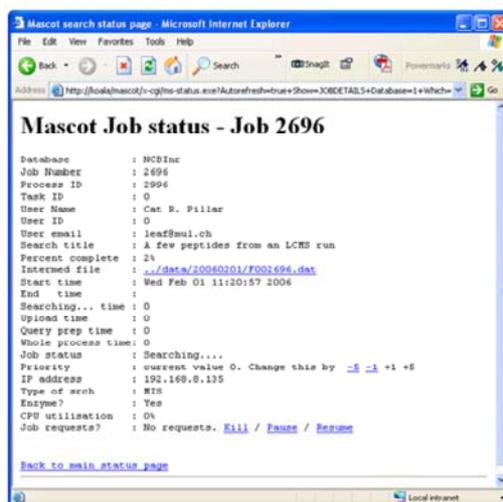


The database status page has links to many of the log files mentioned earlier.

This is the starting point for troubleshooting problems, especially those connected with database updates

When Mascot Monitor first starts, there is a single entry per database. Once a database has been updated, there are two entries, one for the “old” file and one for the ‘new’. We need this double view, because of the way databases can be updated in the background, without interrupting searches. During database exchange, while the new file is compressed and tested, searches can still be submitted to run against the old file. Once the new file is ready, all new searches are run against the new file. So, on a busy server, there may be a period when you have searches running against both the old and new files. As soon as the last search on the old file has completed, the old database can be taken out of use. Mascot monitor takes care of all of this automatically.

Log files - database status



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You can drill down from the database status page to a list of searches for each database, and then down to the details of an individual search, as shown here.

If necessary, you can kill or pause a search from this page, or change its priority

Log files - search log viewer

The screenshot shows the MASCOT search log viewer interface. The browser title is "MASCOT SearchLog - Windows Internet Explorer". The page title is "MASCOT search log". Below the title, it says "Version: 2.3.0 - Licensed to Matrix Science in-house DELL5000, (1 processor)".

Callouts point to the following features:

- Select log file:** Points to the "Log File" dropdown menu.
- Set range:** Points to the "Start at" and "how many" input fields.
- Uncheck to hide column:** Points to the checkboxes in the column headers.
- Sort on column:** Points to the radio buttons in the column headers.
- Filter:** Points to the "Filter" input field.

Job#	ID	abase	User Name	Email	Ti	In	start time	Dur	
16202	4920	SusaiPro			Pe		Tue Mar 23 13:50:42 2010	11	User read re:
16208	4724	SusaiPro			Pe		Tue Mar 23 13:49:55 2010	19	User read re:
16203	4736	SusaiPro			C		Mon Mar 22 22:47:33 2010	19	User read re:
16202	5988	SusaiPro			Pe		Tue Mar 23 13:50:42 2010	11	User read re:
16192	4188	IFI_huma			Ra		Tue Mar 23 13:50:42 2010	11	User read re:
16198	4312	IFI_huma			Pe		Tue Mar 23 13:50:42 2010	11	User read re:
16197	5908	IFI_huma			HU		Thu Mar 11 11:09:30 2010	348	User read re:
16195	4304	SusaiPro	Anna Lazer	alazer@do-olite.edu	HU		Thu Mar 11 11:00:53 2010	379	User read re:
16194	2168	SusaiPro			Pe		Tue Mar 09 09:12:44 2010	16	User read re:
16193	3248	NCElar	Anna Lazer	alazer@do-olite.edu	Fr		Thu Mar 04 11:00:00 2010	1114	User read re:
16191	4428	SusaiPro	Anna Lazer	alazer@do-olite.edu	MS		Thu Mar 04 11:00:00 2010	642	User read re:
16190	4360	SusaiPro	Anna Lazer	alazer@do-olite.edu	MS		Wed Mar 03 11:25:08 2010	22	User read re:
16189	4136	SusaiPro			MS		Tue Mar 02 18:57:27 2010	129	User read re:
16188	4136	SusaiPro			Su		Tue Mar 02 16:00:26 2010	1112	User read re:
16188	4500	SusaiPro			Su		Tue Mar 02 15:45:27 2010	6	User read re:

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This is the search log viewer. You can sort on any of the columns using the radio buttons and then pressing Sort / filter.

The checkboxes determine whether a column is shown or hidden. The two hidden columns are Ti for title and In for intermediate file. This is a hyperlink to display the raw mascot result file, but you can only see the first two characters of the file name, which are “..”. The hyperlink in the first column displays the formatted result report.

You can set the number of lines to display, and whether to start at the beginning or end of the file.

You can also filter the display by entering text into the edit boxes. For example, your user name or a word from the search title

If you have split the search log into sections, then you can choose which file to display by entering the path

Log Files - Troubleshooting

Other useful files

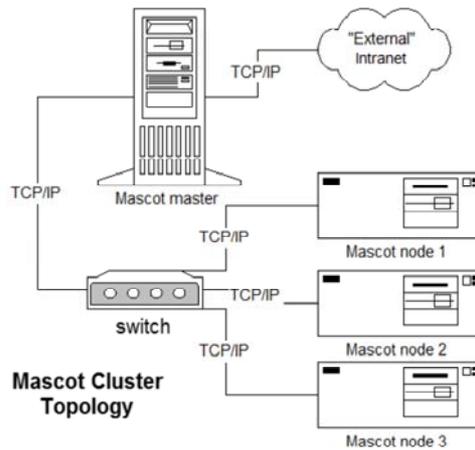
- Database compression
<database>/current/<database>.errors
- Database taxonomy
<database>/current/<database>.NoTaxonomyMatch.txt
- Database statistics
<database>/current/<database>.stats
- Web server access and error logs
- System event or message log.

The first three files are most easily viewed using the links in database status.

Sometimes, there will be nothing in the Mascot logs because the problem is external to Mascot. Sometimes, it can be useful to look at the web server logs or even the operating system logs.

The Windows Event Viewer (control panel; administrative tools) allows you to browse Windows system messages

Cluster mode



Just a few words about Mascot cluster mode

Mascot supports cluster operation using a Beowulf-like topology. Mascot supports cluster mode as standard, whenever the licence is for 4 CPU's or more. You just have to hook up an appropriate number of PC's on a local LAN

Cluster mode

- **Every search is distributed to all the cluster nodes**
 - Each node searches a portion of the sequence database
 - Get the parallel processing advantage for a single spectrum
 - Search results are returned to the master, which merges them, and writes the result file to disk
- **All master - node communication is via TCP/IP**
 - Simple, socket-based communication
 - No parallel operating system required
- **Configuration and program files are distributed and updated automatically from the Master node**
 - A cluster behaves and looks like a single server
- **Need dedicated or partitioned hardware**
 - Cannot allocate machines dynamically
 - General purpose server farm usually not cost effective

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In cluster mode, every search is distributed to all the cluster nodes, and each node searches a portion of the sequence database. This means that you get the parallel processing advantage for a single spectrum. Search results are returned to the master, which merges them, and writes the result file to disk

All master - node communication is via TCP/IP. This uses simple, socket-based communication. A parallel operating system is not required

Configuration and program files are distributed and updated automatically from the Master node, so the cluster behaves and looks like a single server

Sometimes, we are asked about running Mascot on a general purpose server farm, that is being used for other applications.

For standard PC hardware, the cost of the Mascot licence is greater than that of the hardware. For a given capacity, the lowest cost route will always be a minimum number of licences on dedicated hardware. If you want to run Mascot on machines that are part of a larger cluster, best to partition off a number of nodes, either for exclusive Mascot use, or where Mascot has absolute priority over other processes.

Mascot cluster nodes cannot be dynamic because of the size of the database files. The time taken to move these files between machines, or even just in and out of memory, would always be unacceptable

Cluster mode



The screenshot displays the Mascot search status page in a browser window. The page shows search results for three different files, each with details on its status, search time, and thread count. Below the search results is a table titled 'Cluster Nodes' which provides an overview of the search nodes, including their IP addresses, OS, response status, physical memory usage, swap file usage, and disk space.

Node	IP Address	OS	Responding	Physical Memory	Swap file	Disk space
node01	10.251.1.1	Linux	OK	80% Free	100% Free	15% Free
node02	10.251.1.2	Linux	OK	81% Free	100% Free	19% Free
node03	10.251.1.3	Linux	OK	81% Free	100% Free	19% Free
node04	10.251.1.4	Linux	OK	81% Free	100% Free	19% Free
node05	10.251.1.5	Linux	OK	82% Free	100% Free	23% Free

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If you have a Mascot cluster, it is almost as easy to administer as a single machine. Everything is reported and controlled through the master node. The Cluster Nodes table provides an overview of the search nodes; smiley faces or green unhappy faces. If you need a closer look at one of the search nodes, follow the links to view the search node log files.

Sources of Information

Using Mascot Server

- The HTML help pages

Mascot Server installation, configuration, and troubleshooting

- Installation & Setup Manual
- Support pages on www.matrixscience.com

Using Mascot Daemon

- Online help (F1)

Using Mascot Distiller

- Online help (F1)

Anything not answered by the above

- support@matrixscience.com

Finally, a reminder of where you can find technical information about Mascot