System Requirements

Mascot Distiller requires Microsoft Windows 2000 SP3, XP Professional, Server 2003, Vista, or Server 2008. 64-bit versions of Windows can be used, although Distiller will run as a 32-bit application.

Note: The system locale should be set to English. If not, ensure the decimal separator is set to a period (full stop).

To submit a Mascot or MSBlast search directly from Distiller requires Microsoft Internet Explorer 5.5 or later.

Mascot Server must be 2.0 or later, except for the Quantitation Toolbox, which requires Mascot server 2.2 or later. Batch automation of quantitation requires Mascot Daemon 2.3 or later (to be released Summer 2009).

Note: Ensure you patch your Mascot Server to the latest patch level available. Quantitation using Average or Replicate protocols requires 2.2.06 or later. See the Mascot Server <u>support page</u> for further details.

Note: If you wish to use Mascot Distiller with Mascot Server 2.0, certain files on the server must be updated. These can be downloaded from the Mascot Distiller <u>support page</u> on the Matrix Science web site. Note that these updates are for Mascot Server 2.0 only, Mascot Distiller cannot be used with Mascot Server 1.9 or earlier. No updates are required for Mascot Server 2.1 or later.

For certain mass spectrometry data file formats, Mascot Distiller makes use of library files (*DLL* 's or *OCX* 's) that are supplied as part of the instrument data processing software. Either Mascot Distiller must be installed on the PC where the instrument data processing software is installed, or vice versa. The supported data system file formats are:

Agilent MassHunter (Q-TOF)

No dependency on the instrument data system.

Microsoft .NET Framework 2.0 is required. This is only available for Windows 2000 SP3 and later.

Agilent *wiff* format (LC/MS TOF)

Requires Agilent LC/MSD TOF software to be installed on the same PC as Mascot Distiller. Mascot Distiller has been tested against version A.02.01. Users of earlier software versions will need to upgrade.

• Applied Biosystems Data Explorer (Voyager, 4x00)

No dependency on the instrument data system for *.T2D files exported from 4000 Series Explorer, (TOF-TOF).

For Voyager *.DAT files, Data Explorer is required. This software must be installed on the same PC as Mascot Distiller. Mascot Distiller has been tested with versions 3.5 to 4.9.

If you have the Data Explorer application open while using Distiller, child windows will open, close and change focus. This is caused by the design of the Data Explorer application. It is strongly recommended that you not use Data Explorer at the same time as Distiller. For instance, if you close a file in Data Explorer while it is in use by Distiller, errors may occur.

Applied Biosystems Analyst (QStar, QTrap)

No dependency on the instrument data system.

Bruker / Agilent yep format (Bruker Esquire, Agilent LC/MS Trap)

No dependency on the instrument data system.

● Bruker XMASS / XTOF (Reflex, Biflex, etc.)

No dependency on the instrument data system.

For XMASS FT data, the ambiguous data dialog will be displayed. Always select profile data.

Charge state for PSD files is always set to 1

Bruker baf format (Apex, MicrOTOF)

Some Bruker raw data files contain compressed data to reduce the size of the files. The required compression DLLs are installed with the Bruker-Compass software. If you don't have the Compass software installed on Distiller system, and you are a Bruker customer, you can get a free CD from your local Bruker representitive (CompassXtract Bonus-CD 2.0). Alternatively, you can download the CompassXPort software from the Bruker web site.

(CompassXPort installs the compressor-DIIs at C:\Program Files\Common Files\Bruker Daltonik\AIDA\compression).

• mzXML 🚺

No dependency on the instrument data system.

mzXML files must conform to version 2.0 or 2.1 of the mzXML schema. If you look at an mzXML file in a text editor, the first few lines should look similar to this, referencing a schema called mzXML_2.0 or mzXML_2.1.

<?xml version="1.0" encoding="ISO-8859-1"?> <mzXML xmlns="http://sashimi.sourceforge.net/schema_revision/mzXML_2.1" xmlns: xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:schemaLocation="http://sashimi.sourceforge.net/schema_revision/mzXML_2.1 http://sashimi.sourceforge.net/schema_revision/mzXML_2.1/mzXML_idx_2.1.xsd">

If the first few lines reference a schema called MsXML.xsd, then the file is an earlier format, not supported by Mascot Distiller.

Analyst profile data that has been exported to mzXML format is not supported. This is because the file contains compressed profile data, and there is no way to replace the missing data points.

Shimadzu Kompact (Axima)

No dependency on the instrument data system.

Data files from Axima instruments are supported. Earlier Kompact files are unlikely to work.

To open these files, Mascot Distiller requires the gzip.exe program, supplied with Launchpad, to be on the system path. If Launchpad has been installed in the default location, gzip.exe will be in: c:\Program Files\Kompact\programs

If you are not sure how to add this directory to your system path, simply copy (don't move) this file to your Windows directory.

Many possible calibration methods can be specified for Axima data. Least squares (old and new), quadratic, cubic and two point are supported. Polynomial calibration is not supported. For PSD data, additional fragment correction using cubic spline is supported but quadratic fit is not supported.

A complete LC Maldi run can be opened in Distiller by opening the LCSpots0001.run file. All of the ms spectra in the LCSpots0001 file will be loaded, along with the related ms-ms spectra from the separate run files. All files must be in the same directory. The calibration files Cal1Spots and Cal2Spots will be ignored.

The ms spectrum and all the ms-ms spectra of an auto experiment can be loaded and treated as a single file by loading the 'base' .run file. For example, loading sample_0001.run from an auto experiment might also load sample_0001-N14-1164_0001.run and sample_0001-N14-1440_0001.run which correspond to the ms-ms spectra with m/z precursors of 1164 and 1440 from well N14.

Shimadzu LCMSSolution (LCMS-IT-TOF)

Requires Shimadzu LCMS-IT-TOF Data Export Library (TTFLDataExport) 1.02 to be installed on the same PC as Mascot Distiller.

• Thermo Xcalibur (LCQ, LTQ, Orbitrap)

No dependency on the instrument data system.

Waters MassLynx (QTof, M@ldi, TofSpec)

No dependency on the instrument data system.

Installing Mascot Distiller

- 1. Close all programs.
- 2. Insert the **Mascot Distiller** CD into your CD-ROM drive. If Autorun is enabled on your system, the installation starts automatically and you can skip steps 3 and 4. Under Windows Vista, you will be offered the choice of running setup.exe or viewing the files. Choose to view files, open the distiller directory, right click setup.exe and choose **Run As administrator**.
- 3. From the Start menu, select Run.
- 4. Type **D:\distiller\setup.exe** (substitute the appropriate letter of your CD-ROM drive for D) and choose **OK**.
- 5. Follow the **InstallShield Wizard** instructions. Note that support for Agilent MassHunter raw files and the Mascot Distiller Developer Toolbox (MDRO SDK) are options that can be selected on the custom setup page.

By default, GUI files are installed in C:\Program Files\Matrix Science\Mascot Distiller and processing library files in C:\Program Files\Common Files\Matrix Science\MDRO. (Under 64-bit Windows, the default path uses Program Files (x86)).

Note: If your licence includes the Mascot Distiller Quantitation Toolbox, the Adobe SVG Viewer 3 plug-in for Internet Explorer is required. If you are not sure whether this is installed or what version is installed, go to the Windows Control Panel; *Add or Remove Programs*, and look for Adobe SVG Viewer 3.0. The installer can be downloaded from <u>Adobe</u>. (At time of writing, Adobe have ceased to support this plug-in, but it is still available for download and works with Internet Explorer 6, 7, and 8. If this should change, check the <u>Distiller support</u> page for a recommended alternative.)

Note: If you install under Vista or Server 2008, you should make the following change after installation: • In Windows Explorer, select the Mascot Distiller application folder (e.g. C:\Program Files\Matrix Science\Mascot Distiller).

- Right click and choose Properties
- On the Security tab, choose Edit
- Select the local Users group and check Modify in the Allow column
- Choose OK twice to exit from both dialogs

Otherwise, you will find that changes to options files or new options files that you create are only visible to you, and not to anyone logging in under a different Windows user name, which may include Mascot Daemon. Also, you would not be able to load a quantitation report into an external browser.

Licence Registration

The first time you use Mascot Distiller, a dialog box will be displayed requesting you to register the software



If you want to upgrade Mascot Distiller, by adding a new Toolbox, this dialog can also be invoked by choosing **Enter Serial Number** from the Help menu.

View-only mode

If you do not wish to register a licence key, or if your evaluation licence has expired, choose this button to continue in view-only mode. You can open Distiller project files, but cannot modify them or create new ones. More details <u>here</u>.

On-line registration

If your PC has a web browser installed, and can connect to the internet, choose **Register on-line**. Your default web browser will be launched, and the on-line licensing form loaded from the Matrix Science web site.

Matrix Science Licence	: Generator - Mozilla Firefox	
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Licence Generator		
Use this form to ger number on your ins asterisk*. Note that supply below.	nerate a Mascot Distiller licence file from the serial tallation CD. Required fields are marked with an t the licence will be sent to the email address you	
Key 1	a009edff	
Key 2	Distiller-PC	
Key 3	001f3ba054af	
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Name*		
Organisation*		
Address1*		
Address2		
City*		
Zip / Postcode		
State / region		
Country*	V	
Phone*		
Fax		
	Generate Licence	
	Copyright 🐵 2003 Matrix Science Ltd. All Rights Reserved.	
Done		

Required fields are marked by an asterisk^{*}. Enter your contact details, along with your product serial number. Usually, this can be found on a sticker attached to the CD container. Alternatively, it may have been supplied by email or in a printed document. A serial number looks similar to this: **68E9-3233-73A7**.

This information will only be used for verifying registration and providing technical support. It will not be disclosed to any third party.

When the completed form is submitted, if the information is valid, a permanent licence will be sent by **email** to the address supplied on the form.

If you have to reinstall the software on a different PC, or if the original PC is changed in such a way as to invalidate the licence, you will need to repeat this procedure. Instead of a permanent licence, only a 30 day licence will be issued automatically. You will need to contact <u>Matrix Science</u> to request a permanent licence before the temporary one expires.

Registration by fax or post

If you are unable to connect to the internet, choose **Print registration form**. This will load a Rich Text Format document into Word or WordPad. This form should be completed and sent by fax or mail to <u>Matrix Science</u>. A licence will be returned to you by email.

Saving the licence data

Distiller can capture licence data from the Windows clipboard. When you receive your licence by email, proceed as

follows:

- 1. In your email client, select all the text by first clicking in the message body, then choosing **Select All** from the Edit menu (or press Ctrl+A).
- 2. Choose the **Copy** command from Edit menu (or press Ctrl+C) to place the message text onto the Windows Clipboard.
- 3. Launch Mascot Distiller, or switch back to it if already running. For a new license, the licence data will be saved automatically. If this is an upgrade licence, choose **Enter Licence Data** from the Mascot Help menu.

If this procedure fails for some reason, simply save the email message to a plain *ASCII* text file in the folder - C:\Program Files\Common Files\Matrix Science\licdb. (This is the default path to the licdb folder, you may have chosen a different location during installation). The name of the file is not important, but the extension must be .lic.