

Deployment Manual

CLC WORKBENCHES

Manual for CLC Workbenches: deployment and technical information Windows, macOS and Linux

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This software is for research purposes only.

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Introduction

This manual includes information about installers, licenses and where the files associated with a Workbench installation are put. It is intended for administrators responsible for Workbench installation, configuration and maintenance.

The currently available commercial CLC Workbenches are:

- CLC Genomics Workbench
- CLC Main Workbench

In this manual, we suggest methods for the efficient deployment of CLC Workbenches to multiple machines and describe the files and settings important to Workbench installations and their configuration.

Please contact ts-bioinformatics@qiagen.com if you have questions about Workbench deployment and setup that are not answered by the information in this manual.

For information about installing the *CLC Genomics* Server, please refer to the installation chapter in the CLC Server administration manual: http://resources.qiagenbioinformatics.com/manuals/ clcserver/current/admin/index.php?manual=Install.html.

1.1 Deployment strategies

The steps outlined here can be used when deploying identically configured Workbenches onto multiple machines, decreasing the time needed to configure each Workbench:

- 1. On a single computer that has the same OS as the other computers the Workbench will be installed on, complete a full Workbench installation.
- 2. Launch the newly installed Workbench and complete the initial Workbench setup by doing the following:
 - Set up the licensing. See section 3 for details.
 - Install any desired plugins. Plugins can be downloaded via the Workbench Plugin Manager if the Workbench can connect to the external network. Alternatively, plugin

files can be downloaded on a machine with external network access from https: //www.qiagenbioinformatics.com/plugins, and then copied to the machine with the Workbench, and installed using the "Install from File" functionality of the Workbench Plugin Manager.

- If you have any modules (commercial plugins) you plan to use for analysis work, the licensing can be set up for these now if you wish, but this step can also be done later¹.
 - For a network license setup, the relevant module licenses should be made available from your CLC License Server.
 - For static licenses, a license file for the relevant products needs to be present on each machine where analyses will be carried out.

For further information about plugin installation and licensing, please refer to the individual plugin manuals, available from https://www.qiagenbioinformatics. com/plugins/.

- 3. Configure the settings to be applied to all Workbench users via properties files. See section 10.1 for a list of property files and links to the relevant chapters describing them.
- 4. Run the Workbench installer in silent mode (-q) on each of the other computers to install the Workbench on them. See section 2.3 for details.
- 5. Copy the following files from the initial Workbench installation to the corresponding location on the other computers.
 - All files under the settings folder of the installation directory.
 - The plugins folder and its contents from under the initial Workbench's installation area.

Another option for deployment is to create an image, which is then copied to all the target computers. With this option, though, there are a few routines performed by the Workbench installer that need to be taken into account, such as the creation of short cuts and file associations, and the setting of memory limits, which is described in section 9.1.

1.2 Java

The Workbenches are Java software, which means there must be a Java Runtime Environment (JRE) to run them. The Workbench installers have a built-in JRE that is installed under the installation directory of the Workbench. The advantages of this include that no JRE needs to be downloaded and installed from another source and that compatibility problems due to other JREs on a system are avoided because the Workbench uses its own JRE.

The JRE used for running a Workbench does not interfere with existing JREs on the computer.

¹For CLC Genomics Workbench 10.x, CLC Main Workbench 7.x, and Biomedical Genomics Workbench 4.x and as well as earlier versions of these products, you must install relevant module licenses at this point, even if you do not plan to use the initial installation for analysis work.

1.3 System requirements

The system requirements for Workbenches can be found within the individual Workbench manuals (http://www.qiagenbioinformatics.com/support/manuals/) or online at https://www.qiagenbioinformatics.com/support/manuals/) or online at https://www.qiagenbioinformatics.com/support/manuals/) or online at https://www.qiagenbioinformatics.com/system-requirements/).

Installation of Workbenches

2.1 Getting Workbench installers

Workbench installers are available for Windows, macOS and Linux. How to get installer files is described in our Frequently Asked Questions area "Where can I get installer files for the software?": https://secure.clcbio.com/helpspot/index.php?pg=kb.page&id=156.

2.2 What a Workbench installer does when launched

When the Workbench installer is run, it performs the following tasks:

1. It extracts and copies files to the installation directory The Workbench software is installed into a directory. It is self contained. The suggested folder name to install into reflects the software name and the major version line, for example, for the *CLC Genomics Workbench* version 12.0, the default installation location offered on each platform would be:

Windows C:\Program files\CLC Genomics Workbench 12

macOS /Applications/CLC Genomics Workbench 12

Linux /opt/CLCGenomicsWorkbench12

To install the software into central locations like these generally requires administrator rights.

Recommendations for installation directory locations

- For minor updates, you will be asked whether you wish to:
 - Update the existing installation Generally recommended when installing minor updates New files will be installed into the same directory as the existing installation. Licensing information will generally **not** need to be updated if this option is chosen for minor updates.
 OR
 - Install to a different directory. When installing to a new location, all required configuration will need to be carried out. E.g. licensing will need to be set up,

desired plugins will need to be installed, etc.. The License Manager appears when the Workbench is started up if no license has yet been configured. If you have an older, licensed version of the Workbench software installed, then updating the license can be done by choosing the "Upgrade from an existing Workbench installation" option for static licenses or the "Configure License Server connection" option if using a network license.

- For major updates. The suggested installation directory will reflect the new major version number of the software. *Please do not install a new major version into the same folder as an existing, older version of the Workbench.* All configuration will need to be carried out anew. E.g. licensing will need to be set up, desired plugins will need to be installed, etc..
- 2. It sets the amount of memory available The installer investigates the amount of RAM on the machine during installation and sets the amount of memory that the Workbench can use. Read more in section 9.1.
- 3. It establishes shortcuts if desired On Windows and Mac systems, an option is provided during installation to create a shortcut for starting the Workbench. On Linux systems, this option is also presented, but it has no effect.

2.3 Installation modes - console and silent

Two installation modes are available to support efficient installation of the Workbench software.

- **Console mode** This mode is particularly useful when installing Workbenches onto remote systems. On Linux, this mode is enabled by using the option -c when launching the installer from the command line. On Windows the option is -console.
- Silent mode This mode supports hands-off installation. Default answers to all prompts are used, although a non-default installation directory can specified if desired (see below). Silent mode is activated using the -q parameter when launching the installer from the command line. On Windows, the -console option can be appended after -q, that is, as the second parameter, to ensure output to the console.

If desired, you can **specify the directory to install the software to** when running the installer in silent mode. Do this adding the -dir option to the command line.

On Windows, the -console and the -dir options only work when the installer is run in silent mode.

The following is an example of a command that would install a Workbench into the directory "c:\bioinformatics\clc" on a Windows system using silent mode with console output :

CLCMainWorkbench_8_0.exe -q -console -dir "c:\bioinformatics\clc"

On a Linux system, a similar command to install into the directory "/opt/clcgenomicsworkbench11" could look like:

./CLCGenomicsWorkbench_11_0_1_64.sh -c -q -dir /opt/clcgenomicsworkbench11

The -q and the -console options work for the uninstall program as well.

2.4 Uninstalling a Workbench

For information about uninstalling a Workbench, please refer to our Frequently Asked Questions area "How can I uninstall a CLC Workbench?": https://secure.clcbio.com/helpspot/index.php?pg=kb.page&id=279

Licenses

There are two kinds of licenses for the Workbenches:

- **Static licenses** Static license files are placed under the "licenses" subfolder of the Workbench installation area. A static license is specific to the machine the Workbench software is installed on. Static licenses cannot be used on systems with more than 64 cores and remote use of software with a static license is not supported.
- **Network licenses** Network licenses are hosted by a CLC License Server. Workbenches are configured to contact the CLC License Server on startup to see if licenses for that product are available. Network licenses are a good option for sites where there are many Workbenches. In addition, to run Workbenches remotely or on systems with more than 64 cores, a network license is needed. Network licenses are sometimes also known as floating licenses.

If you are administering network licenses, please also refer to the CLC License Server manual: http://resources.giagenbioinformatics.com/manuals/clclicenseserver/ current/.

Further information about configuring licensing is available in the individual Workbench manuals: http://www.qiagenbioinformatics.com/support/manuals/.

Commercial plugins, or modules, use the same licensing system as the Workbenches, so the concepts described above also apply to plugin licenses. Network licenses are handled exactly the same way that Workbench network licenses are. How to download module static licenses in a Workbench is described in our Frequently Asked Questions area: https://secure.clcbio.com/helpspot/index.php?pg=kb.page&id=351.

3.1 Connecting to a CLC License Server from Workbenches

Setting up a connection from an individual Workbench to a CLC License Server is described in the Workbench manuals: http://www.qiagenbioinformatics.com/support/manuals/. It involves choosing the option "Configure License Server Connection" from the Workbench License Manager. However, when setting up multiple Workbenches, it can be more efficient to configure license server connections without launching each Workbench. To do this:

- Launch a single Workbench and configure the correct license server information using the graphical License Manager tool.
- Find the file called license.properties that will have been created in the settings folder under the Workbench installation area.
- Copy the license.properties into the settings folder of each of the other Workbench installations.

The license.properties file contains the following lines, with the information after the = sign based on what was entered via the Workbench License Manager interface.

```
serverip=your.license.server
serverport=6200
disableborrow=false
autodiscover=true
useserver=true
username=
usecustomusername=false
```

You can download a sample license.properties file from http://resources.qiagenbioinformatics.com/deployment/current/license.properties.

Workbench plugins

Plugins extend the functionality of CLC Workbenches and the CLC Genomics Server. Workbench plugins distributed by QIAGEN Aarhus can be downloaded via the Workbench Plugin Manager if the Workbench can connect to the external network. Alternatively, plugin files can be downloaded on a machine with external network access from https://www.qiagenbioinformatics.com/plugins, and then copied to the machine with the Workbench and installed using the Install from File button at the bottom of the Plugin Manager (figure 4.1).

When a plugin is installed, it is put into a folder called plugins within the installation area of a Workbench. For a single Workbench, one would typically use the graphical Workbench Plugin Manager for installing plugins and modules. However, when administering a large number of Workbenches, it can be more efficient to:

- Install the desired plugins and modules on a single Workbench using the Workbench Plugin Manager.
- Copy the plugins folder and its contents from that Workbench's installation area to the same relative location on other machines running the same Workbench version.



Figure 4.1: The Plugin Manager.

Tools delivered as part of a module, i.e. a commercial Workbench plugin, require a module license to be available¹. Please see section **3** for more on licensing.

¹For CLC Genomics Workbench 10.x, Biomedical Genomics Workbench 4.x and CLC Main Workbench 7.x, as well as earlier versions of these products, relevant module licenses must be installed for the module to load when the Workbench starts up.

Workflows

Workflows can be installed and managed using the **Workflow Manager** in the Workbench. See figure **5.1**.

The **Workflow Manager** can be invoked by choosing the option **Manage Workflows...** when you click on the **Workflows** button at the top right of the Workbench toolbar, or from under the main **Help** menu.



Figure 5.1: The workflow manager.

A workflow installed on a Workbench is always installed on a per-user basis. The workflow definition is stored in the user's home area. This is described further in section 10.2.

The ability to install workflows can be disabled by configuring a policy. See section 7 for further details about this.

When the Workbench is part of a *CLC Genomics Server* setup, desired workflows can be installed on the CLC Server. All users logged into the server from their Workbench then have access to the centrally administered workflow. Updating an installed workflow would then take place on the CLC Server, rather than on a per-user basis.

Connecting to a CLC Server

The CLC Server Connection dialog in CLC Workbenches can be used to log into or out of a *CLC* Server, as well as check on the status of a server connection. It is launched from the menu system by going to¹:

File | CLC Server Connection (S)

The location and port of CLC Servers that Workbenches are able to connect to can be pre-configured for all users of a Workbench on a given machine by placing a file called serverinfo.properties into the settings folder under the Workbench installation directory.

A serverinfo.properties file contains two lines for each *CLC* Server that should be listed in the drop down list within the CLC Server connection dialog in the Workbench.

For example, if 2 servers are available, the serverinfo.properties file would take the following form:

```
server.1.host = <hostname>
server.1.port = <portnumber>
server.2.host = <hostname>
server.2.port = <portnumber>
```

where <hostname> should be replaced with the name of the system the CLC Server is running on and <portnumber> by the port number of the CLC Server, typically 7777. The numbers in the parameter names (e.g. server.1.x, server.2.x) are used to specify the order the servers are presented in the dropdown list presented to users connecting from the Workbench. The order of the lines themselves does not matter. Up to 8 servers can be listed.

You can download an example serverinfo.properties file at http://resources.qiagenbioinformatics.com/deployment/current/serverinfo.properties.

If a serverinfo.properties file is present under the settings folder of the Workbench

¹The CLC Server Connection option was introduced in CLC Genomics Workbench 12.0 and CLC Main Workbench 8.1. For connecting to a CLC Server using earlier versions of these programs, or the Biomedical Genomics Workbench, the CLC Workbench Client Plugin needs to be installed. This can be found in the Workbench Plugin Manager of relevant software versions.

installation, the name of the CLC Server entered for the server.1.host parameter in the file, and its port number, are initially presented in the dialog for all users of the Workbench on that system. When multiple servers are available, users can just select the one they want from the drop down list.

Machine level and user level CLC Server settings

To log into a *CLC Server*, Workbench users need to supply the *CLC Server* name and port, as well as a username and password. The server name, port and username will be remembered between Workbench sessions. This information is saved in their user settings file, usersettings.xml, whether or not a serverinfo.properties file exists.

Users can specify if they want their password to be stored. If they do, the encrypted password is saved in the usersettings.xml file. If they choose to save their password, they will also be able to specify if they want the Workbench to log into the CLC Server automatically each time the Workbench starts up.

If server information is present in both a user's usersettings.xml file and the central serverinfo.properties file, then the information from both is presented in the CLC Server Connection drop down list of servers. If the server information is identical in both files, only one item will be listed per server. If there is more than one server, the order they appear in the drop down list is determined by the information in the serverinfo.properties file.

Further details about the serverinfo.properties file

Only servers for which there is complete information (both a host and port setting) are presented in the CLC Server Connection drop down list of servers. If incomplete information is found in the serverinfo.properties file, (e.g. a host name setting with no corresponding port setting or vice versa), an error will be written to the CLC Workbench log file (clc-workbench.log), but any complete entries found in the property file will still be listed.

After a serverinfo.properties file is in place, server entries can be added or removed by directly editing the file.

Server details can also be added to serverinfo.properties indirectly: if the configured servers were read from the serverinfo.properties file **and** a user successfully logs into a *CLC Server*, **and** that user has write permission for the properties file, the server name and port used when logging in will be written back to the file as the first server in the list. I.e. that server's details will be entered as the server.1.host, and server.1.port settings, with other servers' details moved down in priority. This server will then be the first one listed in the drop down list in the CLC Server Connection dialog for all users of the Workbench on that system.

The format of the serverinfo.properties files for CLC Genomics Workbench 11.x and earlier, CLC Main Workbench 8.0.x and earlier, and all versions of Biomedical Genomics Workbench software was different to the format described above. For those software versions, only a single server was supported. An example file for those versions can be found at http://resources.giagenbioinformatics.com/deployment/4/serverinfo.properties.

Security policies

The Workbench has a security policy configuration that enables administrators to restrict users' access to things like:

- Tools accessing services on the internet
- Notifications about updates
- Plugin and Workflow management

Policies are specified in a file called policy.properties that needs to be placed within the settings folder under the Workbench installation directory. Users without administrator access typically would not be able to change the contents of this file.

Each of the following keys within a policy.properties file can be followed by either = *allow* or = *deny*. No policy.properties file is present in a default Workbench installation, and thus by default, all the policies listed below are allowed.

- **workbench_version_check** Controls whether notifications for Workbench updates should be shown.
- plugin_version_check Controls whether notifications for plugin updates should be shown. Note that if plugin_download is set to "deny", plugin update notifications will not be shown, regardless of this setting.
- online_search Controls access to online sequence and structure search engines and databases via the tools under the Download menu. Depending on the Workbench being used, this includes tools like Download Genome (
), Search for Sequences at NCBI (
), Search for Reads in SRA (
) and Search for Sequences in UniProt (
).
- **online_ncbi_blast** Controls whether tools performing BLAST at NCBI's servers should be available to users. This includes **NCBI BLAST** () run from the **Toolbox** and also from sequence selections.
- ncbi_blast_download Controls whether the Download BLAST databases () tool, which allows download of BLAST databases from NCBI's servers, should be available.

- plugin_manage Controls whether the Plugin Manager should be available. Users will still be able to install plugin updates if plugin_download and plugin_version_check are allowed.
- plugin_file_install Controls whether plugins can be installed from a local file.
- **plugin_download** Controls whether plugins can be downloaded and installed via the Download Plugins tab of the Workbench Plugin Manager. Setting this policy to deny also stops checks for for updated plugins and the display of notification dialogs about available plugin updates during Workbench startup.
- workflow_manage Controls whether the Manage Workflows dialog should be available.
- workflow_file_install Controls whether workflows can be installed from a file.
- sequence_to_structure Controls access to the Link Variants To Structure (^{sh}) and Download 3D Protein Structure Database (^{sh}) tools, as well as whether the 'Link to Structure' links in variant tables should be enabled or not.
- **usage_information_collection** Controls whether anonymous information about the usage of the workbench is shared with QIAGEN, helping us improve our products. It is also possible to opt out of providing usage information on a per-user basis via a setting in the General section of the Preferences dialog.
- **welcome_center** Controls whether the Workbench should contact the server that distributes content for the Welcome Center. Only pertinent to the CLC Genomics Workbench 12 and later versions of that product.

A sample policy.properties file can be downloaded from

http://resources.giagenbioinformatics.com/deployment/current/policy.properties. This can then be placed in the settings folder and edited to contain the relevant values. The new policy will take effect next time the Workbench is started.

Storing and backing up data

This chapter explains how data is stored, outlines configuration changes useful for setups where analyses will be run on large amounts of data, and gives general guidance on backups and data sizes.

8.1 Storing data

8.1.1 Data structure

The data in the **Navigation Area** is organized into a number of **Locations**. When the *CLC Workbenches* is started for the first time, there will be a location called *CLC_Data* (unless your computer administrator has configured the installation otherwise).

A Workbench data location represents a folder on the computer: The data shown under a Workbench location in the **Navigation Area** is stored on the computer, in the folder the location points to.

This is explained visually in figure 8.1. The full path to the system folder can be seen by mousing over the data location folder icon as shown in figure 8.2.

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						Navigation Area	•
Computer + Windows (C:) + Users	CLC_Data	▼ Searce	h CLC_Data		Q	▶協告 ♥	T
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a 🐌 CLC_Data	Name	Date modified	Туре	Size	^	MGM	
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						Q+ <enter search="" term=""></enter>	1

Figure 8.1: In this example the location called "CLC_Data" points to the folder at C:\Users\<username>\CLC_Data.

Data held on a CLC Server



Figure 8.2: Mousing over the location called 'CLC_Data' shows the full path to the system folder, which in this case is C:\Users\<username>\CLC_Data.

If you have logged into a *CLC Server* from your Workbench, then data stored on the *CLC Server* will also be listed in the Workbench Navigation Area, as illustrated in figure 8.3.



Figure 8.3: Data areas on the CLC Server are highlighted with blue square icons in the Navigation Area.

Adding locations

When a Workbench is first installed it will have one data area aleady configured and visible in the **Navigation Area** By default, this is a folder called CLC_Data. It points to the following folder on the underlying system:

- Windows: C:\Users\<your_username>\CLC_Data
- Mac: ~/CLC_Data
- Linux: /homefolder/CLC_Data

You can easily add more locations, which will then be visible in the Navigation Area. Go to:

File | New | Location (

Navigate to the folder you want to add as a data location (see figure 8.4).

When you click **Open**, the new location is added to the **Navigation Area** as shown in figure 8.5.

The name of the new location will be the name of the folder selected. To see the full path to the folder on the file system, hover the mouse cursor over the location icon (_____).

You can configure any folder on a network drive or a removable drive as a location. The only restrictions are that you need permissions to access that folder, and it should **not** be a subfolder of an area already being used as a CLC Workbench or CLC Server location.

Look in:	🧮 Desktop			- 🔹 🖄 🔁	۶ 🛄 ۲
Recent Items	1♥ Compute 한 Network	r			
	4				
Desktop					
Desktop	Folder name:	C:\Users\	\Desktop		Add

Figure 8.4: Navigating to a folder to use as a new location.

Navigation Area 》函嵒の	ৰ প

Figure 8.5: The new location has been added.

Locations appear inactive in the **Navigation Area** if the relevant drive is not available when you start up the Workbench. Once the drive is available, click on the Update All symbol () at the top of the Navigation area. This refreshes the view of the Navigation Area, and all available locations will then be shown as active. There can be sometimes be a short delay before the interface update completes.

Sharing data is possible when a network drive is available to multiple Workbenches. In this case, you can add the same folder as a Data Location on each Workbench. However, it is important to note that data sharing is not actively supported: we do not support concurrent alteration of data and while the software will often detect this situation and handle it appropriately, by for example only allowing read access to all but the one party editing the file, we do not guarantee this. In addition, any functionality that involves using the data search indices, (e.g. search functionality, associating metadata with data), will not work properly for shared data locations. Re-indexing a Data Location can help in the short term, but as soon as a new file is created by another piece of software, the index will be out of date. If you decide to share data via Workbenches this way, it is vital that any Workbench that adds a Data Location already used by other Workbenches uses as a Data Location **the exact same folder from the network drive file system hierarchy as the other Workbenches have used**. Indicating a folder higher up or lower down in the hierarchy will cause problems with the indexing of the files, meaning that newly created objects by Workbench A will not be found by Workbench B and vice versa.

The list of Workbench Data Locations is stored in a file called model_settings_300.xml. The location of this file depends on the operating system being used. Please see section 10.2 for details. We recommend that this file is **not** manually edited.

8.2 Special configurations for large amounts of data

8.2.1 Temporary data

The Workbench writes temporary files to the disk during some types of analysis. Depending on the data set, these temporary files can take up a lot of disk space.

By default, temporary files generated by the Workbench are written to the standard temporary file area on the machine. However, space may be limited there, in which case, a different location for Workbench temporary files should be specified. This is done by creating a text file called path.properties and saving it in the settings folder in the Workbench installation directory. Please ensure this file does **not** have a name with an additional extension, e.g. ".txt".

The path.properties should include a line like this:

```
tmpdir = /path-to-temp
```

where "/path-to-temp" should be the absolute path to the new tmp directory. When the Workbench is restarted, it will start using this configured directory for storing temporary data.

You can download a sample path.properties file at http://resources.qiagenbioinformatics.com/deployment/current/path.properties.

Important: Temp space should be located on the local system. For acceptable performance data transfer to the temp directory must *not* be over a network connection. The Workbench spends a lot of time reading and writing these temporary files, so the data access speed has a great impact on overall performance when working with large data sets.

8.2.2 Default Workbench data storage

On all CLC Workbenches, the default folder for storing Workbench data is called $\tt CLC_Data,$ placed under the user's home area.

On CLC Genomics Workbench, there is additionally a default folder for storing reference data¹ called CLC_References, placed under the user's home area.

If a default folder is not already present under the user's home area, it will be created on the file system when the Workbench starts up, and the corresponding Workebench file locations will be visible in the Workbench Navigation Area.

The location of default data areas can be changed, which can be useful in a number of circumstances, for example when quotas are applied to user home areas or where roaming user profiles are used. This is done by specifying the folders to use in a file called path.properties and placing this file in the settings folder of the Workbench installation. If this file is in place before the Workbench is started up, folders are not created in the original default locations, but are only created, if not already present, according to the information specified in this file.

Changing the default data locations

The settings for configuring default locations in a path.properties file are:

• datadir For all CLC Workbenches: the full path to the default data location. The folder

¹This feature was added in CLC Genomics Workbench 11.0.

specified is created if it does not already exist.

• refdir For CLC Genomics Workbench: Either the full path to a folder called CLC_References, or the path under which a folder called CLC_References is present or should be created.

Important: The default data folder (*datadir*) is fully specified by the path given in the path.properties file, whereas if the reference data area (*refdir*) does not end with CLC_References, a folder of that name will be created under the path specified.

The following variables can be used when specifying the desired path:

\$user the user name of the current user

\$home the home directory of the current user

\$product the short name of the workbench (clcgenomicswb or clcmainwb)

You can use either forward slashes (normally used on Mac and Linux) or backslashes (normally used on Windows) in the configuration file. The Workbench will use the appropriate type of slash character depending on the platform.

Some examples:

```
datadir = $home/CLC_Data (the default)
datadir = X:\clcstorage\$user
refdir = X:\clcstorage\$user\CLC_References
refdir = /scratch/$user (equivalent to /scratch/$user/CLC_References)
```

You can download a sample path.properties file from http://resources.giagenbioinformatics.com/deployment/current/path.properties.

Where Workbench location information is stored

When the Workbench is shut down for the first time, a file called model_settings_300.xml is created in user level settings folder. Data location information is read from this file when starting up the Workbench again.

If the model_settings_300.xml file is deleted, then the next time the Workbench starts up it will again look for the datadir property in the path.properties file.

The location of the $model_settings_300.xml$ file depends on the operating system being used. See section 10.2 for details.

8.3 Backup of Workbench information

We recommend backing up the following areas related to a Workbench installation:

Data: Workbench Data Locations are folders under which data are stored as files, often within a file hierarchy. If Workbench data needs to be restored from a backup, simply copy the restored files/folders back to the place they were originally located and start up the Workbench.

User level settings: See section 10.2 for a list of the user level settings files that can be useful to back up. When restoring from backup, close the Workbench if it is running and then place

these files in the same place they were backed up from. The Workbench will use the restored settings when next started up.

Global settings: If customized policy files have been created, these may be useful to back up. Any that exist will be located under the settings folder under the Workbench installation area. See section 10.1 for detail of files that may be present. When restoring from backup, place restored properties files into the settings of the Workbench, overwriting any earlier files of the same name. Workbenches must be restarted to pick up the new policy details.

8.4 Disk space requirements

It is difficult to give general guidance on disk space requirements, but below, we describe some considerations relating to space requirements for sequencing reads and mappings, as these are typically the largest datasets generated when working with NGS data.

- After import, the reads will be in a Sequence List. Details relating to the size of Sequence Lists are below. The original sequence file (e.g. fasta, fastq, etc.) is not needed by the Workbench after import is complete.
- After import, reference sequences take up space. The original reference sequence files (e.g. fasta, embl, genbank), are not needed by the Workbench after import is complete.
- Reads mapped against a reference take up space within the mapping results. This is in addition to space taken up by the reads stored in a Sequence List.
- References also take up space within mapping results.
- Space is needed for temporary files created during analyses. Once an analysis is complete, the associated temporary files are deleted. Temporary files usually do not take up more space than the final result of the analysis. We highly recommend that temporary files are written to an area on the same machine as the Workbench is installed on. See section 8.2.1 for further details.

The formula for disk space usage relating to read sequences in a Sequence List is:

Bytes per read: $28 + (\text{length of read name}) + 0.25 \times (\text{length of read})$

Note that you can discard read names during import to save some space.

If quality scores are present and imported, add: 6 + (length of read)

As an example, a data set of 5.2 million 35 bp reads imported by *CLC Genomics Workbench* using the **Discard sequence names** option and including quality scores would take up:

5,244,764 x ((28 + 0 + 0.25 x 35) + (6 + 35)) = 389 MB

For a stand-alone read mapping that included a 4.7 Mbp annotated reference sequence, this would take up 473 MB.

System resources

You can specify the number of CPU and the amount of memory that the Workbench java process is allowed to use.

9.1 Setting the amount of memory available for the JVM

The Workbench Java Virtual Machine (JVM) needs to know how much memory it can use. The default value is 50% of the computer's RAM or 50GB, whichever is smaller. This is determined during Workbench installation. We recommend sticking with the default value for reasons described later in this chapter. However, it can be changed.

If you plan install Workbenches on multiple machines using an image, then either all the target computers should have the same amount of RAM, or the memory value specified should be set to 50% of the RAM on the computer with the smallest amount of memory.

Changing the memory setting for the Workbench JVM

The memory limit is configured in a property file by giving a numeric value and unit after the setting -Xmx. For example, this could look like:

-Xmx8000m

with 8000m indicating that the maximum amount of memory the Workbench java process is allowed to use is 8000Mb.

If a new memory limit is configured, it will be applied the next time the Workbench is started up.

The location of the relevant property file depends on the operating system being used:

- Windows and Linux The property file is called <workbenchname>.vmoptions, so for a CLC Main Workbench installation, this would be clcmainwb.vmoptions. It is found under the installation area of the Workbench. For example, on Windows, this would be a location like: C:\Program Files\CLC Main Workbench 8\clcmainwb.vmoptions. Edit the -Xmx setting in this file.
- **macOS** The property file is called vmoptions.txt and can be found in the application bundle. Edit the -Xmx setting in this file.

To find this file in the application bundle, open a Finder window and navigate to the Workbench application. Right click on it, or click on it while holding the Ctrl key down (Ctrl-click), and choose "Show Package Contents" from the menu that appears. The vmoptions.txt is within the Contents folder¹.

If you prefer this sort of information to be configured within the Info.plist file, also available under the Contents folder. This can be done using the following steps:

- 1. Add the following line into the Info.plist file, under the 'VMOptionArray' section: -Xmx4100m, adjusting the numeric value to the amount of memory you want.
- 2. Remove the -Xmx setting from within the vmoptions.txt. If this is not done, this "-Xmx" value will overwrite the setting in the Info.plist. file.

Default memory setting recommendations explained

We suggest an upper limit of 50GB for the memory allocation because there are generally limited gains if the value is increased beyond this, and this limit helps ensure that the JVM does not spend too much time running garbage collection (GC) processes.

The GC is a memory handling subsystem of the JVM that scans through the currently used heap and frees up memory by removing contents no longer in use. The larger the maximum heap, which is what this memory setting is affecting, the longer each check through the heap will take. The JVM has to suspend all other activities while running the GC. These suspensions are normally on the scale of milliseconds to a few seconds, and in this range, they are generally not noticeable. In combination with the GC subsystem of the JVM, the CLC Workbenches and Servers use a sophisticated caching system, moving unneeded data out of memory and into temporary disk storage. The result of this caching system means that there will not be any noticeable performance improvement with a Java heap space larger than 50GB, while GC pauses may become more noticeable.

The suggestion to limit memory use to a maximum of 50% of the physical RAM is made because most CLC Workbenches and CLC Servers have some optimized external binaries responsible for compute-heavy tasks such as read mapping and de novo assembly. These external binaries are not affected by the maximum heap space limit. They request memory from the OS, just like any other executable. Thus, the suggested 50% limit for the heap space setting for the Java Virtual Machine (JVM) is to try to ensure that the machine will have sufficient free memory to run the external binaries.

9.2 Setting the number of cores to use

Some Workbench algorithms can use all the cores available on your system for large jobs to make the analysis as fast as possible. This is particularly relevant for some NGS analysis tools.

You can restrict the number of cores that can be used by:

• Creating a text file called cpu.properties and saving it under the settings folder in the Workbench installation directory.

¹For releases before CLC Genomics Workbench 8.0, Biomedical Genomics Workbench 2.1 and CLC Main Workbench 7.6, the -Xmx setting for macOS was in the Info.plist file, which is also under the Contents folder.

• Editing that file, entering a single line like this:

maxcores = 3

where 3 should be replaced by the maximum number of cores to be used by a given instance tool, like read mapping or de novo assembly. If several such analyses are run concurrently on the Workbench, each of these would be able to use up to this maximum number of cores if needed.

• Restart the Workbench.

Please note that configuring the maxcores setting is **not** a guarantee that the Workbench will never use more than the number of cores specified. However, the use of any higher number of cores would be for very brief and infrequent peaks and should not affect performance of other applications running on your system.

You can download a sample cpu.properties file from http://resources.qiagenbioinformatics.com/deployment/current/cpu.properties.

Overview - where do we put things?

This section provides an overview of the parts of a CLC Workbench installation. Some are global, affecting all Workbench users on that computer, while some are set at a per-user level.

10.1 Per-computer Workbench information

Files relating to the following areas are, unless otherwise specified, located under the *Workbench installation directory* and affect all Workbench users on a given system.

Licenses License information depends on the kind of license being used:

- **Static licenses** These are stored as files within the licenses folder. A license file is specific for the computer it was downloaded for.
- **Network licenses** License server connection information is stored in the <code>license.properties</code> file under the <code>settings</code> folder. See section 3.1 for further details. Example file for download:

http://resources.qiagenbioinformatics.com/deployment/current/license.
properties

- **Plugins** Installed plugins and modules are stored in the plugins folder. The plugins folder and its contents can be copied to other computers running the same version of a Workbench.
- **Memory allocation** This is configured in the file <workbenchname>.vmoptions file under the installation area of the Workbench on Windows and Linux. On macOS, it is stored in vmoptions.txt file in the application bundle. See section section 9.1 for details.
- **Property files** A Workbench installation can be fine tuned by placing one or more of the following properties files under the settings folder of the Workbench installation area.
 - policy.properties This can be used to restrict particular Workbench functionality such as installing plugins or using certain tools that download information from online sites. See section 7 for details. Example file for download: http://resources.giagenbioinformatics.com/deployment/current/policy.properties
 - path.properties This is used to configure a non-default location for data and for temporary
 data. See sections 8.2.2 and 8.2.1 for details. Example file for download:
 http://resources.giagenbioinformatics.com/deployment/current/path.properties

- proxy.properties Proxy server settings are configured in this file. The easiest way to set up this file is using the Preferences dialog of a Workbench, as described here: http://resources.qiagenbioinformatics.com/manuals/clcgenomicsworkbench/current/ index.php?manual=Network_configuration.html. Proxy settings are saved in the proxy.properties file under the settings folder of the Workbench installation area, and thus apply to all users of the Workbench on that system. To apply the same proxy settings to other Workbench installations, simply copy this file to the corresponding location on the other machines.
- cpu.properties The maximum number of cores to be used by the Workbench is configured here. See section 9.2 for details. Example file for download: http://resources.qiagenbioinformatics.com/deployment/current/cpu.properties
- serverinfo.properties The host and port to use when connecting to a CLC Server are configured here. See section 6 for details. Example file for download: http://resources.giagenbioinformatics.com/deployment/current/serverinfo. properties.

The format of the serverinfo.properties file changed with CLC Genomics Workbench 12.0 and CLC Main Workbench 8.1. Please refer to Connecting to a CLC Server for a link to an example file relevant for older versions of the software.

In addition to the above, file associations for .clc files are stored in the registry database on Windows.

10.2 Per-user Workbench information

Workbench settings that apply to each user, as well as log files, are found under the user's application data folder. Particularly useful files and areas are described below.

User settings

The usersettings.xml file stores information such as view settings, parameters, workspaces, username and password for CLC Server connections and other settings customized by the user. When an upgraded version of the Workbench is launched for the first time, the user settings file for the most recent older version on the system is copied and used for the new Workbench installation.

The usersettings.xml file is found under:

macOS

```
/Users/<username>/Library/Application Support/CLC bio/Workbench/ \
settings/<wbname>/<version>/
Linux
```

Linux

<userhome>/.clcbio/workbench/settings/<wbname>/<version>/

Windows 7, 8 and 10

```
C:\Users\username\AppData\Roaming\CLC bio\Workbench\ \
Settings\wbname\version\
```

Data Locations

Information about data locations a user has added via the Workbench **Navigation Area** is stored in the model_settings_300.xml file, found under:

macOS

/Users/<username>/Library/Application Support/CLC bio/Workbench/settings/ Linux

<userhome>/.clcbio/workbench/settings/

Windows 7, 8 and 10

C:\Users\username\AppData\Roaming\CLC bio\Workbench\Settings\

Log Files

If problems arise, log file are useful to our Support team for troubleshooting the issue. How to contact the QIAGEN Bioinformatics Support team with the relevant log information is covered in our FAQ area at https://secure.clcbio.com/helpspot/index.php?pg=kb.page&id=73. If you wish to investigate the logs yourself, the key log files are called clc-workbench.log, output.log and error.log. These files can be found under:

macOS

```
/Users/<username>/Library/Application Support/CLC bio/Workbench/log/
```

<userhome>/.clcbio/workbench/log/

Windows 7, 8 and 10

C:\Users\username\AppData\Roaming\CLC bio\Workbench\log\

Workflows

Workflows are saved under:

macOS

```
/Users/<username>/Library/Application Support/CLC bio/Workbench/ \
workflows/<wbname>/<version>/
Linux
```

<userhome>/.clcbio/workbench/workflows/<wbname>/<version>/

Windows 7, 8 and 10

```
C:\Users\username\AppData\Roaming\CLC bio\Workbench\ \
workflows\wbname\version\
```

When an upgraded version of the Workbench is launched for the first time, a user's old workflows are copied into the corresponding folder for the new Workbench unless there are major changes to the workflow framework that break compatibility. If you are using a *CLC Genomics Server*, it can decrease overhead related to upgrading, and maintaining consistent versions of workflows for all users if workflows are deployed and maintained on the *CLC Genomics Server* rather than on the Workbench.

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