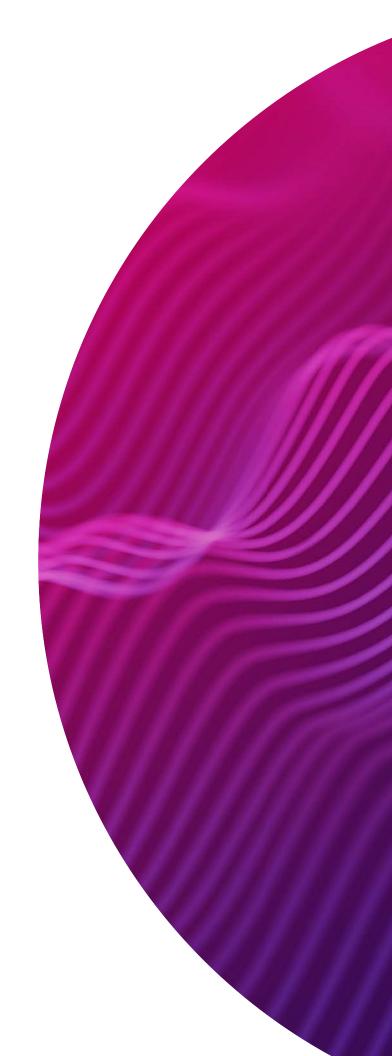


SMRT® Link software installation guide (v11.1)



Research use only. Not for use in diagnostic procedures.

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SMRT® Link software installation guide (v11.1)

Introduction

This document describes the procedure for installing **SMRT Link v11.1**. This document is for Customer IT or SMRT Link administrators.

Note: SMRT Link v11.1 is for use with Sequel[®] II systems and Sequel IIe systems **only**.

SMRT Link is the web-based end-to-end workflow manager for the Sequel II systems and Sequel IIe systems. It includes software applications for designing and monitoring sequencing runs, and analyzing and managing sequence data. SMRT Link provides a web interface that can control **multiple** Sequel II systems and Sequel IIe systems.

SMRT Link is the primary access point for applications used by researchers, laboratory technicians, instrument operators, and bioinformaticians for various interactions with applications related to the Sequel II platform. The applications include:

- Sample Setup: Calculate binding and annealing reactions for preparing DNA samples for use on the Sequel II and Sequel IIe systems.
- Run Design: Design runs and create and/or import sample sheets which become available on the Sequel II
 systems and Sequel IIe systems.
- Run QC: Monitor run progress, status and quality metrics.
- **Data Management**: Create Projects and Data Sets; manage access permissions for Projects and users; generate QC reports for Data Sets; view, import, export, or delete sequence, reference, and barcode files.
- **SMRT**[®] **Analysis**: Perform multiple types of secondary analysis, including sequence alignment, variant detection, *de novo* assembly, structural variant calling, and RNA analysis.

Note: SMRT Link and the Sequel II systems and Sequel IIe systems are for research use only (RUO).

Overview

- 1. Install or upgrade the SMRT Link software. (See "Installation summary" on page 5 and "Configuring LDAP in WSO2" on page 12 for details.)
- 2. **(Optional)** Configure SMRT Link to use an SSL certificate. (See "Step 1: Obtain a domain-specific signed certificate from the appropriate Certification Authority." on page 19 for details.)
- 3. (**Optional**) Add SMRT Link Users and Assign User Roles. (See "Adding SMRT Link users via LDAP integration and assigning user roles" on page 15 for details.)
- 4. **(Optional)** Change the admin and pbicsuser passwords. (See "Changing admin and pbicsuser passwords" on page 11 for details.)
- 5. (Optional) Configure LDAP. (See "LDAP integration" on page 12 for details.)

PacBio Compute Infrastructure Partners (https://www.pacb.com/products-and-services/smrt-compatible-products/analysis-products/) provide HPC solutions designed to support the Sequel II systems.

Note: SMRT Link v10.0 and later offer a SMRT Link Cloud deployment option using AWS as an alternative to installing SMRT Link on a local network. For SMRT Link Cloud compute requirements, see the document **SMRT Link Cloud reference guide (v11.0)**.

Sequel Ile system compute requirements

| Head node | | | |
|---|------------------------|--|--|
| Cores | 32 | | |
| RAM | 64 GB | | |
| Local Storage | 1 TB SSD/Flash storage | | |
| db_datadir (Local Storage) | 250 GB | | |
| Compute nodes | | | |
| Cores (Total) | 64 | | |
| Minimum RAM per Slot (1 slot = 1 core) | >4 GB | | |
| Local Storage | 100 GB | | |
| Shared data storage | | | |
| Sequence Data | 20 TB ^a | | |
| Analysis Data | 40 TB ^a | | |
| Network | | | |
| 10 GBE recommended , 1 GBE required ^b | | | |

- a. Storage is calculated for one Sequel IIe system, assuming 100 human genomes per year at 30-fold coverage, *de novo* assembly.
- b. This information is specific to the network connection between the SMRT Link head node and the Sequel IIe system.

Notes:

- Single-system compute configurations are available contact your Pacbio Bioinformatics Field Application Specialist (FAS) for details.
- For **Sequel II** system compute requirements, see "Appendix C: Sequel II system compute requirements" on page 26 for details.

Data storage

• The SMRT Link software's installation **root** directory **must** be readable and writable by the SMRT Link install user (\$SMRT_USER) and **must** be addressable along the same installation path (\$SMRT_ROOT) on **all** relevant cluster nodes via NFS. PacBio recommends /opt/pacbio/smrtlink for the SMRT Link software's installation root directory (referred to as \$SMRT_ROOT), and smrtanalysis for the SMRT Link install user (referred to as \$SMRT_USER).

- The SMRT Analysis job **output** directory is used to store output from SMRT Analysis jobs. The software accesses this directory through a symbolic link (\$SMRT_ROOT/userdata/jobs_root) that points to the desired job output directory location. The link can be modified by using the installation script. The symbolic link destination should be on a shared file system (NFS); it **must** be writable by the \$SMRT_USER, and it **must** be accessible along the same path on **all** compute nodes. The default is to keep these output directories on the **same** NFS export as the SMRT Link installation, but optionally may be symbolically linked to a larger storage volume.
- The SMRT Analysis database directory is used to store database files and backups. The software accesses this directory through a symbolic link (\$SMRT_ROOT/userdata/db_datadir) that points to the desired database directory location. The link can be modified by using the installation script. This symbolic link destination should be a local directory (not NFS) and be writable by \$SMRT_USER. This directory should exist only on the SMRT Link install host.
- The SMRT Analysis **temporary** directory is used for fast I/O operations during run time. The software accesses this directory through a symbolic link (\$SMRT_ROOT/userdata/tmp_dir) that points to the desired temporary directory location. The link can be modified manually or using the installation script. This symbolic link destination should be a **local** directory (**not** NFS), it must be writable by \$SMRT_USER, and the link destination must exist (or be creatable) as an independent directory on **both** the head node and the compute nodes.

Software prerequisites: Server operating systems

- · SMRT Link server software is supported on:
 - English-language CentOS 7.x, supported until end-of-life 6/30/2024.
 - English-language Rocky Linux 8.x supported until end-of-life 5/31/2029.
 - Ubuntu 18.04 and 20.04 64-bit Linux® distributions.
 - These supported versions **also** apply to SMRT Link compute nodes.
- Note: PacBio advises against new installations of CentOS for use with SMRT Link.
- SMRT Link is **not** guaranteed to work on Linux versions that are no longer supported by the operating systems' vendors.
- SMRT Link server software cannot be installed on systems running other versions of UNIX, macOS[®] or Windows[®].

Software/hardware prerequisites: Client systems

To use SMRT Link on a client operating system:

- SMRT Link **requires** the Google[®] Chrome web browser, version 90 or later.
- SMRT Link **requires** a minimum screen resolution of 1600 by 900 pixels.

Network configuration

- Refer to the IT Site prep guide provided with your instrument purchase for more details.
- For network connectivity considerations, see the network diagram in the **Computer requirements** section of the **IT Site prep guide**.

SMRT Link server environment assumptions

- The SMRT Link server should run on a dedicated 64-bit Linux host with libc 2.17 or greater.
- The installation is performed by the same non-root user (\$SMRT_USER) that will be used to run the SMRT Link
 web services.
- The \$SMRT_USER has full permissions recursively throughout the install directory, and in all linked directories for jobs_root, db_datadir and tmp_dir. (Common problems include NFS setup problems, ACLs, and so on.)
- When running in distributed mode, all other nodes have the same path for \$SMRT_ROOT and for all linked directories. (The NFS exports should have identical mount points on all cluster nodes.)
- No other daemons/services processes are bound to the same ports as the SMRT Link services.

- PacBio highly recommends that the system clock be synchronized to a domain or public NTP time server.
- The \$SMRT_USER service account must have both the nofile and nproc soft user limits set to a minimum of 8192. (See the ulimit(1) and limits.conf(5) Linux man pages for more information.)
- The host operating system must provide the en US.UTF-8 locale/character set.

General security notes

- PacBio recommends that you install the SMRT Link server on networks that are only accessible to trusted
 users, and discourages installing SMRT Link on public networks. You can also install SMRT Link Cloud on
 AWS see SMRT Link Cloud reference guide (v11.0) for details.
- Do not install SMRT Link or run SMRT Link services as the root user.

SMRT Link v11.1 security notes

SMRT Link v11.1 restricts access to the web services API to clients running on localhost (such as the WSO2 server that handles authentication and permissions) or remotely using SSL encryption and password-based authentication.

Starting in v11.0, the WSO2 API Manager can be replaced by a new API gateway that combines the KrakenD, Keycloak, and NGINX servers to provide a nearly identical API and user experience. Some additional setup is required after the installation to use this option. No changes to connected Sequel II systems/Sequel IIe systems are necessary. This new API Gateway will be the default in future SMRT Link releases.

Ports and firewalls: SMRT Link end users **must** be able to access the SMRT Link server on port 8243. This port is also used by the Sequel Instrument Control Software (ICS), so it must be accessible to **any** Sequel II systems or Sequel IIe systems as well.

- If your network configuration already allows access to port 8243, **no additional changes** are required to use SMRT Link v11.1.
- The instrument must have access to port 8243 of the SMRT Link server.
- End users must also have access to port 8243 of the SMRT Link server for access to the browser UI.

Installation/upgrade checklist

Following is a list of items you should have ready **before** starting a new installation or upgrading an existing installation. **Note**: Paths that include spaces are **not** supported.

- Full path to the \$SMRT ROOT directory.
- A service account (called the \$SMRT USER in this document) to install and run the web services.
- Full path to the installation root directory, used for the main installation root.
- · Job Management System settings.
- Full path to a directory on the shared file system the jobs root directory.
- Full path to a directory on the local file system on each node the tmp dir directory.
- Full path to a directory on the local file system on the install node the db datadir directory.
- (Optional) LDAP settings. See "Configuring LDAP in WSO2" on page 12 for details.
- (Optional) SSL certificate for WS02 or NGINX. See "SMRT® Link and SSL certificate procedures" on page 18 for details.

Installation summary

Following are the steps for installing SMRT Link v11.1 on a **new** system. (See "Appendix A: SMRT Link workflow terminology" on page 24 for details.) To upgrade SMRT Link to v11.1 from a **previous version**, follow the upgrade steps on Page 7.

SMRT Link v11.1 can be used with the following supported version of ICS:

v11.0 (Sequel II systems and Sequel IIe systems)

SMRT Link installation options

The following table lists the types of SMRT Link installations and what they include:

| Installation type | GUI | Command- line tools | JMS integration | Sample data | Barcode and reference files | SMRT Link services | Cromwell | Cromwell with call caching |
|-------------------|-----|------------------------|--------------------|----------------|-----------------------------|-----------------------|----------|----------------------------------|
| Full SMRT Link | Υ | Υ | Υ | Υ | Υ | Υ | Υ | Υ |
| SMRT® Tools only | N | Υ | Υa | N | N | N | Υ | N |

a. JMS integration on a SMRT Tools-only installation may be setup using pbcromwell. See **SMRT Tools** reference guide (v11.1) for more information.

| Step | Installation summary - SMRT Link v11.1 | | | |
|------|--|--|--|--|
| 1 | Download SMRT Link software: Download and extract the SMRT Link software installer from here. | | | |
| 2 | Definitions and variables: For clarity, this document uses these conventions to refer to site-specific information: | | | |
| | • \$SMRT_ROOT: The SMRT Link Install Root Directory, such as /opt/pacbio/smrtlink. | | | |
| | • \$SMRT USER: The SMRT Link Install User, such as smrtanalysis. | | | |
| | • smrtlinkhost.mydomain.com: The fully-qualified domain name of the SMRT Link Install Host. | | | |
| | smrtlinkhost: The short host name of the SMRT Link Install Host. | | | |
| | For \$SMRT_ROOT, defining the variable in the shell allows the commands below to be run verbatim. To do so, use something like: | | | |
| | SMRT_ROOT=/opt/pacbio/smrtlink | | | |
| | The fully-qualified domain name of the SMRT Link Install Host may always be used in place of the short host name. But in some cases, particularly when working with WSO2, the fully-qualified domain name is required. | | | |
| 3 | Log onto the SMRT Link Install Host (such as the hostname or IP address) as the SMRT Link Install User (such as \$SMRT_USER.) | | | |
| 4 | Install SMRT Link by invoking the SMRT Link Installer: | | | |
| | ./smrtlink_ <version number="">.runrootdir \$SMRT_ROOT</version> | | | |
| | Note: The \$SMRT_ROOT directory must not exist when the installer is invoked, as the installer will try to create it, and will abort the installation if an existing \$SMRT_ROOT location is found. | | | |
| | If a previous installation was canceled or otherwise failed, the installer can be invoked without extraction. Rerun using theno-extract option: | | | |
| | ./smrtlink_ <version number="">.runrootdir \$SMRT_ROOTno-extract</version> | | | |
| | See "Appendix A: SMRT Link workflow terminology" on page 24 for additional information. | | | |
| 5 | On the instrument, click Install when prompted to install the Sequel Chemistry Update. | | | |

| Step | Installation summary - SMRT Link v11.1 | | |
|------|---|--|--|
| 6 | Start SMRT Link services: \$SMRT_ROOT/admin/bin/services-start | | |
| | Optionally, you can now migrate to the new API gateway: \$SMRT_ROOT/admin/bin/services-startmigrate | | |
| | The migration launches an interactive CLI tool after the server starts; as this is a new installation very few steps are required. Once migration is finished, SMRT Link automatically starts with the new API gateway in the future. | | |
| 7 | Run the Site Acceptance Test from the command line: | | |
| | \$SMRT_ROOT/admin/bin/run-sat-services Successful completion of run-sat-services indicates that the HPC configuration is functioning correctly. This creates a "PacBio Example SAT Job" analysis entry in the SMRT Analysis section of the SMRT Link GUI. | | |
| 8 | (Optional) Clear the browser cache: | | |
| | This is a good troubleshooting step if needed. | | |
| | 1. Open the Chrome Browser and choose More Tools > Clear browsing data , choose All Time from the Time Range control, then check Cached images and files . Click Clear data . | | |
| | 2. Restart the browser. | | |
| 9 | (Optional) Configure LDAP and/or add local users: | | |
| | See "Configuring LDAP in WSO2" on page 12, "Adding local users to SMRT Link using WSO2" on page 16 for details. | | |
| 10 | (Optional) Configure SMRT Link to use a signed SSL certificate: | | |
| | See "Installing an existing certificate" on page 21 for details. | | |
| 11 | (Optional) Change the admin and pbicsuser passwords: | | |
| | We recommend that you change the admin and pbicsuser account passwords from the default values. See "Changing admin and pbicsuser passwords" on page 11 for details. | | |

Upgrading SMRT® Link

Supported upgrade path

- SMRT Link upgrades to v11.1 are supported from any v8.x, v9.x or v10.x releases.
- You cannot upgrade to SMRT Link from SMRT Analysis v2.3.0 or earlier. Additionally, analysis job
 directories and run history from SMRT Analysis v2.3.0 or earlier are not compatible with SMRT Link and
 cannot be imported.
- SMRT Link v11.1 can be used with the following supported version of ICS:
 - v11.0 (Sequel II systems and Sequel IIe systems)

| Step | Upgrading SMRT Link |
|------|---|
| 1 | Download SMRT Link software: Download and extract the SMRT Link software installer from here. |
| 2 | Definitions and variables: For clarity, this document uses these conventions to refer to site-specific information: |
| | • \$SMRT_ROOT: The SMRT Link Install Root Directory, such as /opt/pacbio/smrtlink. |
| | • \$SMRT_USER: The SMRT Link Install User, such as smrtanalysis. |
| | • smrtlinkhost.mydomain.com: The fully-qualified domain name of the SMRT Link Install Host. |
| | smrtlinkhost: The short host name of the SMRT Link Install Host. |
| | For \$SMRT_ROOT, defining the variable in the shell allows the commands below to be run verbatim. To do so, use something like: |
| | SMRT_ROOT=/opt/pacbio/smrtlink |
| | The fully-qualified domain name of the SMRT Link Install Host may always be used in place of the short host name. But in some cases, particularly when working with WSO2, the fully-qualified domain name is required. |
| 3 | Log onto the SMRT Link Install Host (such as the hostname or IP address) as the SMRT Link Install User (such as \$SMRT_USER.) |
| 4 | Stop the SMRT Link services: |
| | \$SMRT_ROOT/admin/bin/services-stop |
| | Note : Ensure that no active SMRT Link analysis jobs are running before stopping services. |
| 5 | Upgrade SMRT Link by invoking the SMRT Link installer: |
| | ./smrtlink_ <version number="">.runrootdir \$SMRT_ROOTupgrade</version> |
| | Note: The \$SMRT_ROOT directory must be an existing SMRT Link installation. Several validation steps will occur to ensure that a valid \$SMRT_ROOT is being updated. |
| | If a previous upgrade was canceled or otherwise failed, the installer can be invoked without extraction. Rerun using theno-extract option: |
| | ./smrtlink_ <version number="">.runrootdir \$SMRT_ROOTupgradeno-extract</version> |
| | See "Appendix A: SMRT Link workflow terminology" on page 24 for additional information. |
| 6 | On the instrument, click Install when prompted to install the Sequel Chemistry Update. |
| 7 | Start the SMRT Link services: |
| | \$SMRT_ROOT/admin/bin/services-start |
| | Optionally, you can now migrate to the new API gateway: \$SMRT ROOT/admin/bin/services-startmigrate |
| | The migration launches an interactive CLI tool after the server starts; as this is a new installation very few steps are required. Once migration is finished, SMRT Link automatically starts with the new API gateway in the future. |

| Step | Upgrading SMRT Link | | |
|------|---|--|--|
| 8 | Run the Site Acceptance Test from the command line: | | |
| | \$SMRT_ROOT/admin/bin/run-sat-services | | |
| | Successful completion of run-sat-services indicates that the HPC configuration is functioning correctly. This creates a "PacBio Example SAT Job" analysis entry in the SMRT Analysis section of the SMRT Link GUI. | | |
| 9 | (Optional) Clear the browser cache: | | |
| | This is a good troubleshooting step if needed. | | |
| | 1. Open the Chrome Browser and choose More Tools > Clear browsing data , choose All Time from the Time Range control, then check Cached images and files . Click Clear data . | | |
| | 2. Restart the browser. | | |
| 10 | (Optional) Change the admin and pbicsuser passwords: | | |
| | We recommend that you change the admin and pbicsuser account passwords from the default values. See "Changing admin and pbicsuser passwords" on page 11 for details. | | |

Updating the SMRT Link Chemistry and UI Bundles

SMRT Link Bundle updates allow updating of SMRT Link features **without** having to reinstall the SMRT Link software. As of SMRT Link v11.1, there are two Bundle types for which an update indicator may appear:

SMRT Link Chemistry Bundle

• This includes kit and DNA Control Complex names used in the Sample Setup and Run Design modules. The update also updates Sequel[®] Instrument Control Software (ICS).

SMRT Link UI Bundle

This includes changes and fixes to the SMRT Link graphical user interface (GUI).

Updating the SMRT Link Bundles from SMRT Link

Note: Only SMRT Link users with the **Admin** role can perform these updates. In addition, SMRT Link **must** have a route to the internet and update services **must** be enabled.

- 1. In SMRT Link, choose **About SMRT Link** from the Gear menu. (A red circle indicates that one or more Bundle Update(s) are available.)
- 2. Click the **Update Chemistry Bundle** button.
- 3. Click the **Update UI Bundle and Restart UI Server** button, if applicable.
- 4. If there are any problems, clear the browser cache: Choose More Tools > Clear browsing data, choose All Time from the Time Range control, then check Cached images and files. Click Clear data. Refreshing the browser tab or clearing the browser cache may be necessary for the Bundle update(s) to take effect.

Updating the SMRT Link Chemistry Bundle on the instrument

The SMRT Link Chemistry Bundle will also need to be upgraded with the same Chemistry Bundle files used by the SMRT Link web services. Once SMRT Link's Chemistry Bundle is updated, the updates are passed along to any PacBio instruments configured to use that same instance of SMRT Link. Once available, follow the instructions below to update the Chemistry Bundle on the instrument side.

- 1. On the instrument, choose **Admin** from the Main menu. (A red circle indicates that a Chemistry Bundle Update is available.)
- 2. Click the **Updates** tab, then click **Install**. The instrument software then restarts, which will take around 10 minutes.
- 3. Click the **question mark** to check the version number to validate the Chemistry Bundle update.

Rolling back a SMRT Link UI Bundle update

SMRT Link UI Bundle updates allow updating of SMRT Link UI features **without** having to reinstall the SMRT Link software. This includes changes and bug fixes to the SMRT Link graphical user interface. When you upgrade the SMRT Link UI by clicking **Gear > About SMRT Link > Update UI Bundle and Restart UI Server**, the previous version of the UI is saved to a time-stamped folder. For example:

In this example, s1 is the tomcat_current/webapps/ROOT root directory installed by the bundle update, and $s1_20200103_135348$ is the backup of the original UI code.

To downgrade to the previous UI version, follow these steps:

- 1. Stop the server: \$SMRT ROOT/admin/bin/services-stop.
- 2. Rename the sl directory to any unique, recognizable name.
- 3. Rename the backup directory to sl.
- 4. Start the server: \$SMRT ROOT/admin/bin/services-start.

Skipping a SMRT Link UI Bundle update

To skip a specific SMRT Link UI Bundle update, use the pbservice skip-update command:

```
$ pbservice skip-update smrtlink-ui --user admin --password admin --host smrtlink-uri -port 8243 Marked bundle update smrtlink-ui/9.0.0.99999 as ignored. Note that you will need to re-login to the SMRT Link UI for this to take effect.
```

```
$ pbservice skip-update smrtlink-ui --user admin --password admin --host smrtlink-uri -port 8243
No upgrades found for bundle smrtlink-ui
```

To **undo** skipping the bundle, run an identical command using unskip-update. Note that the UI will still show the pending update unless you log out and log in again (the bundle's update status is cached upon initial login.)

Installing only SMRT Tools

To install **only** command-line SMRT Tools, use the <code>--smrttools-only</code> switch when calling the installer, whether for a new installation or an upgrade. (This installs the **same** command-line tools as a full installation.) Examples:

```
./smrtlink-11.1.0.xxxxx.run --rootdir smrtlink --smrttools-only ./smrtlink-11.1.0.xxxxx.run --rootdir smrtlink --smrttools-only --upgrade
```

Note: Using --smrttools-only will **only** unpack the command-line applications, and will **not** run through the configuration prompts or provide the web services of a full SMRT Link installation. If command-line only use with JMS integration is desired, see the **SMRT Tools reference guide (v11.1)** on how to setup JMS integration using pbcromwell.

Warning: Sequel II systems and Sequel IIe systems cannot communicate with a --smrttools-only installation.

Updating the SMRT Link Chemistry Bundle on smrttools-only installations

Use this procedure **only** if you have installed the SMRT Link package using the --smrttools-only switch.

Download the Chemistry Bundle from the PacBio website, then unpack the files and place them in a user-defined directory. The value of the \$SMRT_CHEMISTRY_BUNDLE_DIR environment variable then defines where the software finds the updated files. Following are the suggested best practices for installing the Chemistry Bundle:

- 1. Download the Chemistry Bundle from here.
- 2. **(Optional)** Define \$SMRT_ROOT for convenience: SMRT ROOT=/opt/pacbio/smrtlink
- 3. Make directories, unpack, and link:

```
mkdir -p $SMRT_ROOT/userdata/chemistry/chemistry-pb-10.0.0.xxxxx
tar -C $ SMRT_ROOT/userdata/chemistry/chemistry-pb-10.0.0.xxxxx -xf /path/to/chemistry-pb-
11.0.0.xxxxx.tar.gz
ln -s ./chemistry-pb-11.0.0.xxxxx $SMRT ROOT/userdata/chemistry/chemistry-pb-active
```

4. Define and export the \$SMRT CHEMISTRY BUNDLE DIR environmental variable and validate:

```
export SMRT_CHEMISTRY_BUNDLE_DIR=$SMRT_ROOT/userdata/chemistry/chemistry-pb-active
```

5. Define the \$SMRT_CHEMISTRY_BUNDLE_DIR environment variable in the appropriate startup script for your shell to make it permanent. **Example**: Use ~/.bashrc.

Changing admin and pbicsuser passwords

The SMRT Link admin account has full access to SMRT Link, and is used to create users and grant users access.

SMRT Link comes with a default Instrument Control Software (ICS) user account (pbicsuser) which is used by the Sequel II systems to communicate with SMRT Link web services over a secure, encrypted connection. The pbicsuser account is required for instruments to communicate with SMRT Link. (Note that the pbicsuser credentials can only be used to access SMRT Link resources – it is not an LDAP account or a local account on the Linux system.)

The passwords for the admin and pbicsuser accounts are set to default values that are the same for all SMRT Link installations. Because the passwords can be used to access SMRT Link accounts and information, the passwords should be changed and only given to **trusted** users who require access.

To change the admin and phicsuser passwords for WSO2 API Manager, use the following procedure:

```
$SMRT_ROOT/admin/bin/services-stop

$SMRT_ROOT/admin/bin/set-wso2-creds -u admin -p 'NEW-PASSWORD'

$SMRT_ROOT/admin/bin/set-wso2-creds -u pbicsuser -p 'NEW-PASSWORD'
```

If you are using the new API gateway, use the following procedure:

```
$SMRT_ROOT/admin/bin/services-stop

$SMRT_ROOT/admin/bin/set-keycloak-creds -u admin -p 'NEW-PASSWORD'

$SMRT_ROOT/admin/bin/set-keycloak-creds -u pbicsuser -p 'NEW-PASSWORD'
```

To verify the admin and phicsuser passwords, use the following procedure:

```
$SMRT_ROOT/admin/bin/services-start
$SMRT_ROOT/smrtcmds/bin/pbservice status --host localhost --user admin --ask-pass
$SMRT_ROOT/smrtcmds/bin/pbservice status --host localhost --user pbicsuser --ask-pass
```

The pbservice status information should display, before exiting with an exit status of 0 indicating success.

You must **also** change the pbicsuser account password in the Instrument Control Software (ICS) to match the new password. To do so: Select **Menu > Admin > SMRT Link** on the instrument touch screen to change the password.

Warning: When using WSO2, **only** use the set-wso2-creds script to change the password for those accounts.

Note: If you are using the new API gateway, you can use the Keycloak administration interface to change both passwords.

Changing usage tracking settings

When first logging in to the SMRT Link GUI after a successful installation or upgrade, users are prompted to notify PacBio of the upgrade/installation success and whether they wish to share SMRT Link analysis usage information with PacBio. Once set, these settings may **only** be viewed and modified from the command line using the accept-user-agreement tool.

WARNING: To use the accept-user-agreement tool, services must be running:

```
$SMRT ROOT/admin/bin/services-start
```

To set new settings, use the following command, specifying true or false for the options accordingly. For example:

```
$SMRT_ROOT/admin/bin/accept-user-agreement --install-metrics true --job-metrics true
```

PacBio will be notified of a successful installation or upgrade immediately if the install metrics setting is true.

To view the current settings, run the command without any arguments:

```
$SMRT ROOT/admin/bin/accept-user-agreement
```

Note: If accept-user-agreement is run **without** arguments and the settings have not been previously set (either in the GUI or on the command line), **both** the install and job metrics settings will automatically be set to true and PacBio will be immediately notified of the installation or upgrade.

Starting SMRT Link automatically on server boot

To start SMRT Link automatically when the server boots using <code>systemd</code>, refer to the template service file located here:

```
$SMRT ROOT/admin/template/smrtlink.service.tmpl
```

Follow the instructions in the template comments to make site-specific modifications and install as a systemd service file.

LDAP integration

SMRT Link supports integration with LDAP for user login authentication, as well as using local WSO2 users that exist **only** within SMRT Link.

If you are interested in configuring SMRT Link integration with your organization's LDAP, PacBio recommends that you consult your LDAP administrator to help determine the correct LDAP settings.

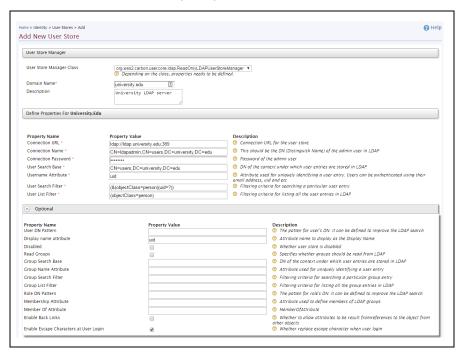
Note: Existing LDAP configurations are **automatically** migrated during upgrade.

Configuring LDAP in WSO2

- LDAP is configured after SMRT Link v11.1 is installed, using the WSO2 API Manager software, as shown below. If you have migrated to the new API gateway, see instructions below for configuring the Keycloak server
- SMRT Link must **first** synchronize with your organization's LDAP objects before any directory accounts can be enabled and given a role to facilitate SMRT Link access.
- 1. Enter the following in your browser: https://<hostname>:9443/carbon/ where <hostname> is the host where SMRT Link is installed.
- 2. Login using admin/admin.
- 3. Click User Stores > Add.



4. Edit the fields as necessary for your site.



The following fields are **required**. (**Note**: Values provided in the example above are listed below for clarity. Actual values should be provided by your LDAP administrator):

- User Store Manager Class: org.wso2.carbon.user.core.ldap.ReadOnlyLDAPUserStoreManager
- Domain Name: university.edu
- Connection URL: ldap://ldap.university:389 (The port is required in the URL.)
- Connection Name: CN=ldapadmin, CN=users, DC=university, DC=edu (This is the bind DN, which is used to authenticate to the LDAP environment.)
- Connection Password: <password>
- User Search Base: CN=users, DC=university, DC=edu
- Username Attribute: uid
- User Search Filter: (&(objectClass=person)(uid=?))
- User List Filter: (objectClass=person)
- Display name attribute: uid

For more information on LDAP, consult the following web pages:

https://en.wikipedia.org/wiki/Lightweight_Directory_Access_Protocol https://en.wikipedia.org/wiki/LDAP_Data_Interchange_Format https://msdn.microsoft.com/en-us/library/ms677605%28v=vs.85%29.aspx

Problems with the LDAP server may be debugged by looking at the log file located here:

\$SMRT ROOT/userdata/log/smrtlink-analysisservices-gui/wso2/wso2-apigw-errors.log

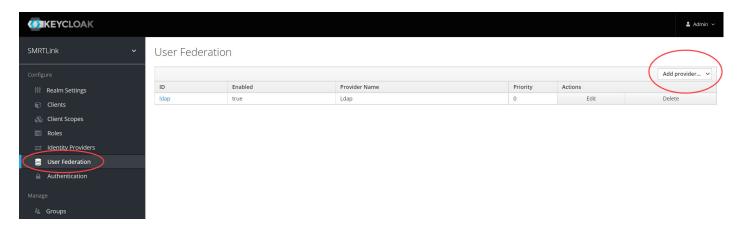
The client-truststore.jks file can be found in the following location:

\$SMRT_ROOT/current/bundles/smrtlink-analysisservices-gui/current/private/pacbio/smrtlink-analysisservices-gui/wso2am-2.0.0/repository/resources/security/client-truststore.jks

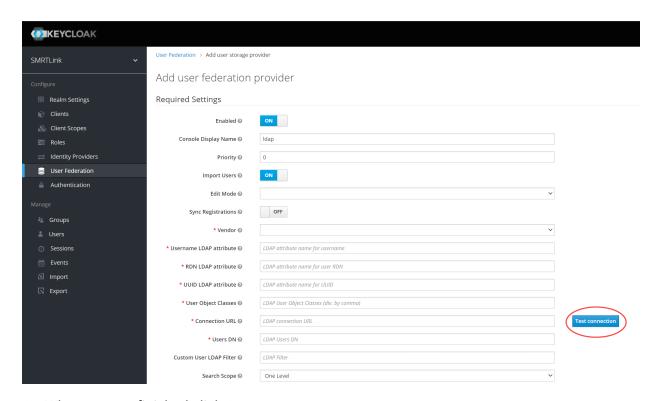
Note: If LDAPS needs to be used, simply change the Connection URL to use ldaps and adjust the port (LDAPS uses 636 by default). Then, use keytool to add the LDAPS X.509-formatted public certificate to the client-truststore.jks file and enter yes to force trust when prompted.

Configuring LDAP in Keycloak

- 1. Enter the following in your browser: https://<hostname>:9443/auth/admin/ where <hostname> is the host where SMRT Link is installed.
- 2. Login using admin/admin (unless you have changed the password).
- 3. Under **Configure** on the left hand side of the window, click **User Federation**.



- 4. On the right hand side of the window, click **Add provider...** and select the **Idap** option.
- 5. Enter the required fields (and any others necessary for your LDAP server) and verify that you can connect to the server using the **Test connection** and **Test authentication** buttons.



- 6. When you are finished click Save.
- 7. After you save the LDAP configuration, additional buttons display at the bottom of the window. Clicking **Synchronize all users** imports **all** users to the Keycloak database **without** assigning them SMRT Link roles.

Save Cancel Synchronize changed users Synchronize all users Remove imported Unlink users

8. Enable SMRT Link users individually as described in the next section.

SMRT Link user roles

SMRT Link supports three user roles: **Admin**, **Lab Tech**, and **Bioinformatician**. Roles define which SMRT Link modules a user can access. The following table lists the privileges associated with the three user roles:

| Tasks/privileges | Admin | Lab Tech | Bioinformatician |
|---------------------------------|-------|----------|------------------|
| Add/delete SMRT Link users | Υ | N | N |
| Assign roles to SMRT Link users | Υ | N | N |
| Update SMRT Link software | Υ | N | N |
| Access Sample Setup module | Υ | Υ | N |
| Access Run Design module | Υ | Υ | N |
| Access Run QC module | Υ | Υ | Υ |
| Access Data Management module | Υ | Υ | Υ |
| Access SMRT Analysis module | Υ | Υ | Υ |

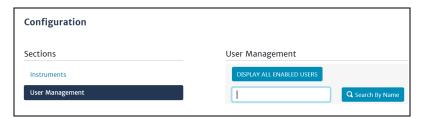
PacBio recommends the following role assignments:

- Assign at least one user per site to the Admin role. That individual is responsible for enabling and disabling SMRT Link users, as well as specifying their roles. The Admin can also access all SMRT Link modules, as well as every file in the system. (Note: SMRT Link supports multiple users with the Admin role per site.)
- Assign users who work in the lab preparing samples and performing runs the Lab Tech role. Lab Tech can also access all SMRT Link modules.
- Assign users who work only on data analysis the Bioinformatician role. Bioinformatician can only access
 the Run QC, Data Management and SMRT Analysis modules; this is the lowest access level.

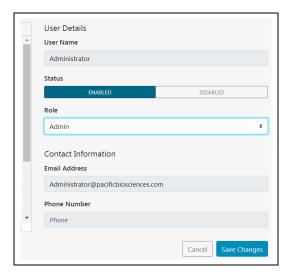
Note: The Admin role only allows a user account to administer the configuration options available through the SMRT Link browser UI. It does **not** provide access to the WSO2 API Management interface, which is intentionally restricted to the built-in admin user **only**.

Adding SMRT Link users via LDAP integration and assigning user roles

- To enable users via LDAP integration, you must first configure LDAP before you can manage users and assign SMRT Link roles to users.
- After LDAP is configured, if you do not assign a SMRT Link role to a user, that user will not be able to login to SMRT Link.
- 1. Access SMRT Link: Enter https://<hostname>:8243/sl/home, where <hostname> is the host where SMRT Link is installed.
- 2. Choose **Configure** from the **Gear** menu and click **User Management**.
- 3. There are 2 ways to find users:
 - To display all SMRT Link users: Click Display all Enabled Users.
 - To find a specific user: Enter a user name, or partial name and click Search By Name.



- Click the desired user. If the Status is Enabled, the user has access to SMRT Link; Disabled means the user cannot access SMRT Link.
 - To **add** a SMRT Link user: Click the **Enabled** button, then assign a role. (See Step 5.)
 - To disable a SMRT Link user: Click the Disabled button.
- Click the Role field and select one of the three roles. (A blank role means that this user cannot access SMRT Link.)
- 6. Click Save. The user now has access to SMRT Link, based on the role just assigned.

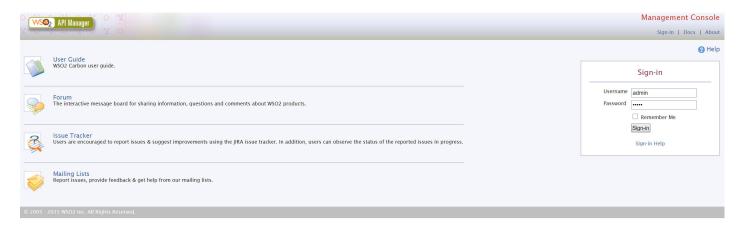


Adding local users to SMRT Link using WSO2

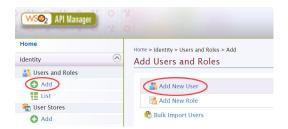
SMRT Link is designed to integrate with an LDAP server to provide user account information, but it is also possible to add **local** user accounts using the WSO2 API Manager that handles authentication and API access.

To add a local account:

1. Access the WSO2 management console at https://<servername>:9443/carbon and log in with SMRT Link's built-in admin account credentials (admin/admin by default.)



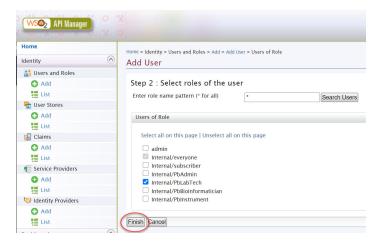
- On the left-hand menu, under Claims, click List.
- 3. Click the item labeled http://wso2.org/claims.
- 4. Scroll to the bottom, find Username, then click Edit.
- Check the box Supported by Default, then click Update. The Username field will display as part of the local user profile.
- 6. Under Users and Roles, click + Add, then click Add New User.



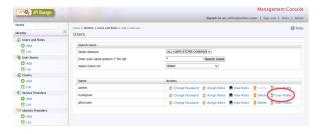
Enter the User ID and password of the new user, then click Next. (Make sure to use a unique password for the User ID that is not used elsewhere.)



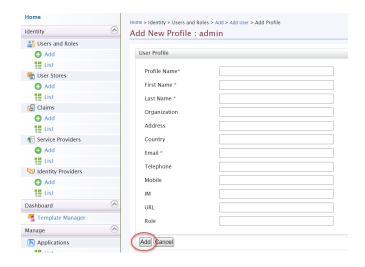
8. Select the appropriate role for the new user. (See "Adding SMRT Link users via LDAP integration and assigning user roles" on page 15 for details.) Click **Finish** to register the new user.



9. (Recommended) Click User Profile for the new user, then click Add New Profile.



- 10. Enter user information such as name and email address. The starred fields are used by the SMRT Link UI user management features. **Note**: Filling in the **Username** field is **required** for the user search in the Configuration and Project pages to find local users.
- 11. Click Add.



12. Click Sign-out. The new user can then log into SMRT Link using the credentials just added.

Ensuring that SMRT Link users are assigned only one role

In some cases, changing a user's role in SMRT Link can cause that user to have **multiple** WSO2 roles. That can lead to accounts remaining enabled when an administrator tries to disable the user. Disabling a user with multiple roles may also still leave the user active. To ensure that users are only assigned **one** role:

- Access the WSO2 management console at https://<servername>:9443/carbon and log in with your site administrator credentials.
- 2. Under **Users and Roles**, click **List** and find the user in question.
- Click View Roles.
- Uncheck one of the redundant roles and click Update.



SMRT® Link and SSL certificate procedures

SMRT Link v11.1 uses SSL (Secure Sockets Layer) to enable access via HTTPS (HTTP over SSL), so that your SMRT Link logins and data are encrypted during transport to and from SMRT Link. SMRT Link includes an Identity Server, which can be configured to integrate with your LDAP/AD servers and enable user authentication using your organizations' user name and password. To ensure a secure connection between the SMRT Link server and your browser, a domain-specific SSL certificate may be installed **after** completing SMRT Link installation.

It is important to note that PacBio will **not** provide a CA-signed SSL certificate. However, once your site has obtained a CA-signed SSL certificate, PacBio's tools can be used to install it for use with SMRT Link web services. (**Note**: PacBio recommends that you consult your IT administrator about obtaining an SSL certificate.) You will need a certificate issued by a certificate authority (CA, sometimes referred to as a **certification authority**.) PacBio has tested SMRT Link with certificates from the following certificate vendors: VeriSign, Thawte and DigiCert.

If your site does **not** provide an SSL certificate, SMRT Link v11.1 will use a PacBio self-signed SSL certificate. If you use the self-signed SSL certificate, **each** user will need to accept the browser warnings related to access in insecure environment. You can also have your IT administrator configure desktops to **always trust** the provided self-signed certificate. Note that SMRT Link is installed within your organization's secure network, behind your organization's firewall.

See "Using SMRT Link with a PacBio self-signed SSL certificate" on page 22 for details on how to handle the security warnings when accessing SMRT Link.

Use the following procedures **only** if your site provides an SSL certificate. These procedures are **not** applicable if you are using PacBio's self-signed SSL certificate.

Note: If you have **already** setup an SSL certificate in SMRT Link v4.0.0 or later, those settings will be carried over **automatically** when upgrading to SMRT Link v11.1.

Installing an SSL certificate for WSO2

Prerequisites: The keytool program is supplied with the SMRT Link installation, and can be found here: \$SMRT ROOT/admin/bin/keytool.

Step 1: Obtain a domain-specific signed certificate from the appropriate Certification Authority.

Step 2: Download the new certificate in .p12 or .p7b format from the DigiCert website: hostname domain com.p12.

Step 3: Combine the CA signed certificate and the keystore key that was generated alongside the CSR:

```
$ keytool -import -trustcacerts -alias server -file ${KEYNAME}.p7b -keystore ${KEYNAME}.jks
Enter keystore password:
Certificate reply was installed in keystore
```

Step 4: Generate an intermediate file in .pem format:

```
$ keytool -export -alias server -keystore ${KEYNAME}.jks -file ${KEYNAME}.pem
Enter keystore password:
Certificate stored in file <hostname domain com.pem>
```

Step 5: Import the .pem file into the client-truststore .jks, which will be created if it does not exist:

```
$ keytool -import -alias server -file ${KEYNAME}.pem -keystore client-truststore.jks -storepass
$KEYPW

<Miscellaneous keytool output>
Trust this certificate? [no]: y
Certificate was added to keystore
```

Step 6: Stop the services by entering \${SMRT ROOT}/admin/bin/services-stop.

Step 7: Install the new .jks files and update the configuration files:

```
\{SMRT_ROOT\}/admin/bin/install_ssl_cert.sh $\{FQDN\} $\{KEYSTORE\} $\{KEYPW\}\}
```

This script installs a CA-signed SSL certificate to SMRT Link, removing the browser warnings that occur when using the default certificate. To run this script, you will need the fully-qualified domain name of the SMRT Link server, the two private/public keystore files in Java Key Store (.jks) format, and the common passphrase used for the key and both keystores. The two keystores include:

- A domain-specific keystore, containing the encryption keys and private CA certificate.
- A separate client-truststore.jks required by the authentication manager.

Usage: \${SMRT_ROOT/admin/bin/install_ssl_cert.sh \$FQDN \$KEYSTORE \$TRUSTSTORE \$KEYPW where the four required arguments include:

- \$FQDN is the fully-qualified domain name appropriate to the signed SSL certificate, such as smrtlink.university.edu.
- \$keystore is the path to the keystore file generated from the SSL certificate (.jks extension); this will be copied to the SMRT Link installation.
- \$TRUSTSTORE is the path to client-truststore.jks; this will be copied to the SMRT Link installation.
- \$keypw is the password used for generating keys.

The FQDN must match the <code>dnsname</code> specified in the SMRT Link configuration. The shorthand unqualified subdomain name, hostname, or alias (such as "smrtlinkhost" and not the FQDN of "smrtlink.university.edu") will not work because the certificate is configured to match a specific fully-qualified domain name, and not an unqualified host name. When running the SMRT Link installer, the FQDN is set during the installer's configuration prompts, or by passing the arguments <code>--dnsname</code> <code>\$FQDN</code> to the installer.

Note: If you are using LDAP authentication, the BIND distinguishedName account password is stored encrypted with the SSL certificate key, which has now changed. The BIND distinguishedName service account password for the LDAP integration must be reentered and saved in the WSO2 API Management interface following services startup (https://smrtlink.example.com:9443/carbon.)

Step 8: Start SMRT Link services by entering \$SMRT ROOT/admin/bin/services-start.

Step 9: Final check:

Go to https://hostname.domain.com:8243/sl/home and login as admin/admin (if LDAP is not enabled). You should see a padlock sign in front of the URL. This indicates that the CA certificate was validated and that the site is secure. This may require clearing the browser cache.

Viewing a Java keystore file

The keystore files for SSL certificates are binary files. Use the following command to verify if the same password was used in the SSL certificate generation and install process. If the same password was **not** used in the certificate installation process, this command will give an error. To list the contents of a Java keystore file, use the keytool -list command, as shown below:

```
Usage: keytool -list -v -keystore keystore.jks
```

Example: keytool -list -v -keystore smrtlink example com.jks

```
Enter keystore password:
Keystore type: JKS
Keystore provider: SUN
Your keystore contains 1 entry
Alias name: server
Creation date: Feb 13, 2017
Entry type: PrivateKeyEntry
Certificate chain length: 3
Certificate[1]:
Owner: CN=smrtlink.example.com, O="Pacific Biosciences of California, Inc.",
L=Menlo Park, ST=CA, C=US
Issuer: CN=DigiCert SHA2 Secure Server CA, O=DigiCert Inc, C=US
```

Errors/logs related to certificate installation can be found here:

\$SMRT ROOT/userdata/log/smrtlink-analysisservices-qui/wso2/

Installing an existing certificate

If you **already** have a complete .jks file (suitable for Apache Tomcat in a Java Key Store format), including the signed certificate, you just need to change the alias of the keystore/certificate to server using the keytool command (-keyclone or -changealias subcommands).

Set the password to whatever you will supply to the install script in SMRT Link. Then, follow the instructions in "Adding the public key to client-truststore.jks" in https://docs.wso2.com/display/IS500/Creating+New+Keystores again with the same changes.

If you already have the SSL key in a .jks file and have obtained a certificate for this key in either PKCS #7 (.p7b) or PKCS #12 (.p12) certificate format, the command below is an example of how combine them:

```
$ keytool -import -trustcacerts -alias server -file star.university.edu.p7b -keystore
star.university.edu.jks
```

Then follow the instructions above to generate the client-truststore.jks keystore, and finally run the install ssl cert.sh script as shown in the above certificate installation steps.

Restoring the default WSO2 self-signed SSL certificate

It may sometimes be necessary to uninstall the user-provided SSL certificate and restore the default certificate. The following steps will revert changes made by \$SMRT ROOT/admin/bin/install ssl cert.sh:

1. Stop SMRT Link services:

```
$SMRT ROOT/admin/bin/services-stop
```

- 2. Check that all SMRT Link processes have terminated by running ps -ef | grep smrtlink. Remaining processes should be terminated with kill <PID> or kill -9 <PID>.
- 3. Restore backup settings:

```
cd ${SMRT_ROOT}/current/bundles/smrtlink-analysisservices-gui/current/private/pacbio/smrtlink-analysisservices-gui/wso2am-2.0.0/repository
mv ./conf/ ./conf.new/
mv ./cert-config.backup/orig/conf./conf
mv ./resources/security/client-truststore.jks ./resources/security/client-truststore.jks.save
mv ./cert-config.backup/orig/resources/security/client-truststore.jks./resources/security/
client-truststore.jks
```

4. Start SMRT Link services:

```
${SMRT ROOT}/admin/bin/services-start
```

Installing an SSL certificate for NGINX

In the new API gateway, SSL transport is handled by the NGINX web server, which uses a much simpler configuration consisting of a plain-text certificate and private key. By default SMRT Link will generate a self-signed certificate and key the first time you start the new API gateway:

```
$SMRT_ROOT/userdata/config/security/pb-smrtlink-default.crt
$SMRT_ROOT/userdata/config/security/pb-smrtlink-default.key
```

To install a custom certificate for NGINX

1. Stop SMRT Link services:

```
SMRT ROOT/admin/bin/services-stop
```

2. Copy the certificate and private key files to these paths:

\$SMRT_ROOT/userdata/config/security/smrtlink-site.crt \$SMRT_ROOT/userdata/config/security/smrtlink-site.key

3. Start SMRT Link services:

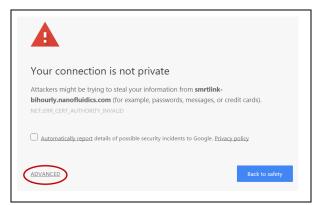
\${SMRT ROOT}/admin/bin/services-start

Using SMRT Link with a PacBio self-signed SSL certificate

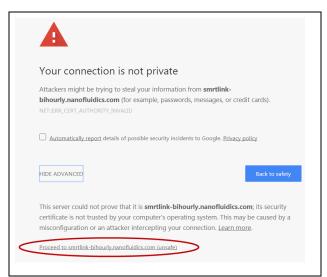
SMRT Link v11.1 uses self-signed SSL certificate provided by PacBio. If your site does **not** have a signed SSL certificate **and** you use the self-signed SSL certificate, **each** user will need to accept the browser warnings related to access in insecure environment. You can also have your IT administrator configure desktops to **always trust** the provided self-signed certificate. Note that SMRT Link should be installed within your organization's secure network, **behind** your organization's firewall.

Security messages display when users try to login to SMRT Link for the **first time** using the Chrome browser. These messages may also display **other times** when accessing SMRT Link. **Each** SMRT Link user in your organization should address these browser warnings following the procedure below.

1. The first time you start SMRT Link after installation, you see the following text. Click the **Advanced** link.



2. Click the **Proceed...** link. (You may need to scroll down.)



3. Close the window by clicking the **Close** box in the corner.



4. The **Login** dialog displays, where you enter the User Name and Password. The next time you access SMRT Link, the Login dialog displays **directly**.

Importing data into SMRT® Link

If you have a Sequel II system/Sequel IIe system installed and it is linked to the SMRT Link software during the instrument installation, your data will be **automatically** imported into SMRT Link.

You can **manually** import the following types of files directly, using the Data Management module of the SMRT Link GUI:

- Continuous Long Reads: XML file (.subreadset.xml) or ZIP file containing information about subreads from Sequel II systems, such as paths to the BAM files.
- **HiFi reads**: XML file (.consensusreadset.xml) or ZIP file containing information about HiFi reads (reads generated with CCS analysis whose quality value is equal to or greater than 20.)
- Barcodes: FASTA (.fa or .fasta), XML (.barcodeset.xml), or ZIP files containing barcodes.
- **References**: FASTA (.fa or .fasta), XML (.referenceSet.xml), or ZIP files containing a reference sequence for use in starting analyses.

You can also import data in SMRT Link using the pbservice command-line utility, as shown below.

- The host and port for the analysis services are optional and default to localhost:8070. You can change these settings using the --host and --port arguments or by using the \$PB_SERVICE_HOST and \$PB_SERVICE_PORT environment variables.
- If using the authenticated port 8243, valid user credentials must also be supplied. Use the --user and --password switches (or --ask-pass), or set the \$PB_SERVICE_AUTH_USER and \$PB_SERVICE_AUTH_PASSWORD environment variables to specify the credential details.

| Importing | Commands | | |
|---------------------------------------|--|--|--|
| BAM Data Sets | Import individual SubreadSet XML files: | | |
| generated by the Sequel II systems | <pre>\$> pbservice import-datasethost \$HOSTport \$PORTuser \$USERask-pass /path/to/subreads.subreadset.xml</pre> | | |
| | Import a directory of SubreadSet XML files: | | |
| | <pre>\$> pbservice import-datasethost \$HOSTport \$PORTuser \$USERask-pass /path/to/tree/containing/subreadssets.xml/</pre> | | |

Sending log files to Technical Support

Troubleshooting information can be sent to PacBio Technical Support multiple ways. If there is a connection to the PacBio Event Server, do the following:

- From the SMRT Link menu: About > Troubleshooting Information > Send.
- From a SMRT Link "Failed" analysis Results page: Click **Send Log Files**.

If there is connectivity to the PacBio Event Server, run the following command to generate the information and automatically send it to PacBio Technical Support:

```
$SMRT ROOT/admin/bin/tsreport-install --bundle --upload
```

If there is **no** connectivity to the PacBio Event Server, run the following command to generate a .tgz file and email the file to support@pacb.com to file a case:

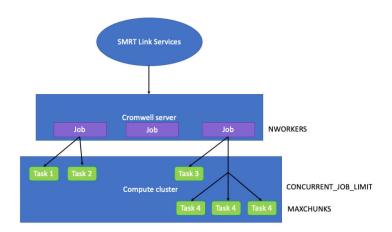
```
$SMRT ROOT/admin/bin/tsreport-install --bundle
```

The generated file can be found here: \$SMRT ROOT/userdata/tsreport/data/ts-install.tgz.

Note: The SMRT Link logs archive bundle will be limited to logs from approximately the past 24 hours. Ensure the above tsreport-install options and SMRT Link menu's **Send** button are run within **one day** of experiencing the issue being addressed.

Appendix A: SMRT Link workflow terminology

Management of all SMRT Link activity is handled by the SMRT Link services. In SMRT Link v8.0 and later, the pbsmrtpipe workflow engine was replaced by Cromwell, an open-source engine developed by the Broad Institute (https://cromwell.readthedocs.io/en/stable/). A continually-running Cromwell server is launched at the same time as SMRT Link services, which executes all jobs directly without spawning new processes. Several user-configurable settings control the use of compute resources by Cromwell. A representation of the SMRT Link services hierarchy is shown below.



NWORKERS: A SMRT Link services setting that specifies the maximum number of simultaneous analysis jobs (or workflows, as Cromwell refers to them) that may be run.

CONCURRENT_JOB_LIMIT: A Cromwell configuration setting that limits the total number of job submissions to a specific backend, across all running workflows.

MAXCHUNKS: A Cromwell workflow that limits the maximum number of pieces a large Data Set may be broken into for parallelized analysis.

NPROC (Not shown in diagram): A Cromwell workflow setting that limits the maximum number of slots that any single JMS cluster submission may request.

Appendix B: Distributed computing setup

PacBio supports the following Job Management Systems (JMS): **Sun Grid Engine (SGE)**, **PBS**, **LSF**, and **SLURM**. You may attempt to manually configure for alternate job management systems, but these are **not** guaranteed to work.

A Job Management System may be used to dispatch jobs to a distributed compute environment. If **no** Job Management System is specified, the system will run in non-distributed mode, and **all** compute jobs will be run locally on the install host.

Available Job Management Systems are detected from the PATH environment variable, but may also be selected manually.

For more information on customizing all of the Job Management Systems, see the comments in the file \$SMRT_ROOT/userdata/user_jmsenv/user.jmsenv.ish. Note that changes to this file will apply to every job submitted to the cluster.

Appendix C: Sequel II system compute requirements

| Head node | | | | |
|--|--|--|--|--|
| Cores | 32 | | | |
| RAM | 64 GB | | | |
| tmp_dir (Local Storage) | 1 TB recommended, 500 GB minimum | | | |
| db_datadir (Local Storage) | 250 GB | | | |
| Compute nodes | | | | |
| Cores (Total) | 384 ^a | | | |
| Minimum RAM per Slot (1 slot = 1 core) | 4 GB/8 GB de novo assembly large complex genomes | | | |
| tmp_dir (Local Storage) | 100 GB | | | |
| Shared d | Shared data storage ^b | | | |
| Sequence Data | 40 TB | | | |
| (jobs_root) Analysis Data | 70 TB | | | |
| Network | | | | |
| 10 GBE recommended, 1 GBE required | | | | |

- a. For a standard CCS sequencing collection (415 GB sequencing data, 25 GB Unique Molecular Yield, 15 kb insert size, 30-hours movie), CCS analysis takes 6.5 hours on this configuration. SMRT Link will work on less powerful compute configurations, however analysis time will be significantly longer.
- b. Storage is calculated for one Sequel II system, assuming 100 human genomes per year at 50-fold coverage, *de novo* assembly.

Data examples

Human assembly

• Genome size: 3.3 GB; sequence data 400 GB; analysis data 700 GB; analysis time: 72 hours wall. This is 50-fold coverage human genome analyzed on the compute configuration listed above.

Rice assembly

Genome size: 0.43 GB; sequence data 55 GB; analysis data 90 GB; analysis time: 20 hours wall. This is 50-fold coverage rice genome analyzed on the compute configuration listed above.