INSTALLATION AND CONFIGURATION GUIDE (LINUX)

BIOVIA DIRECT 2021
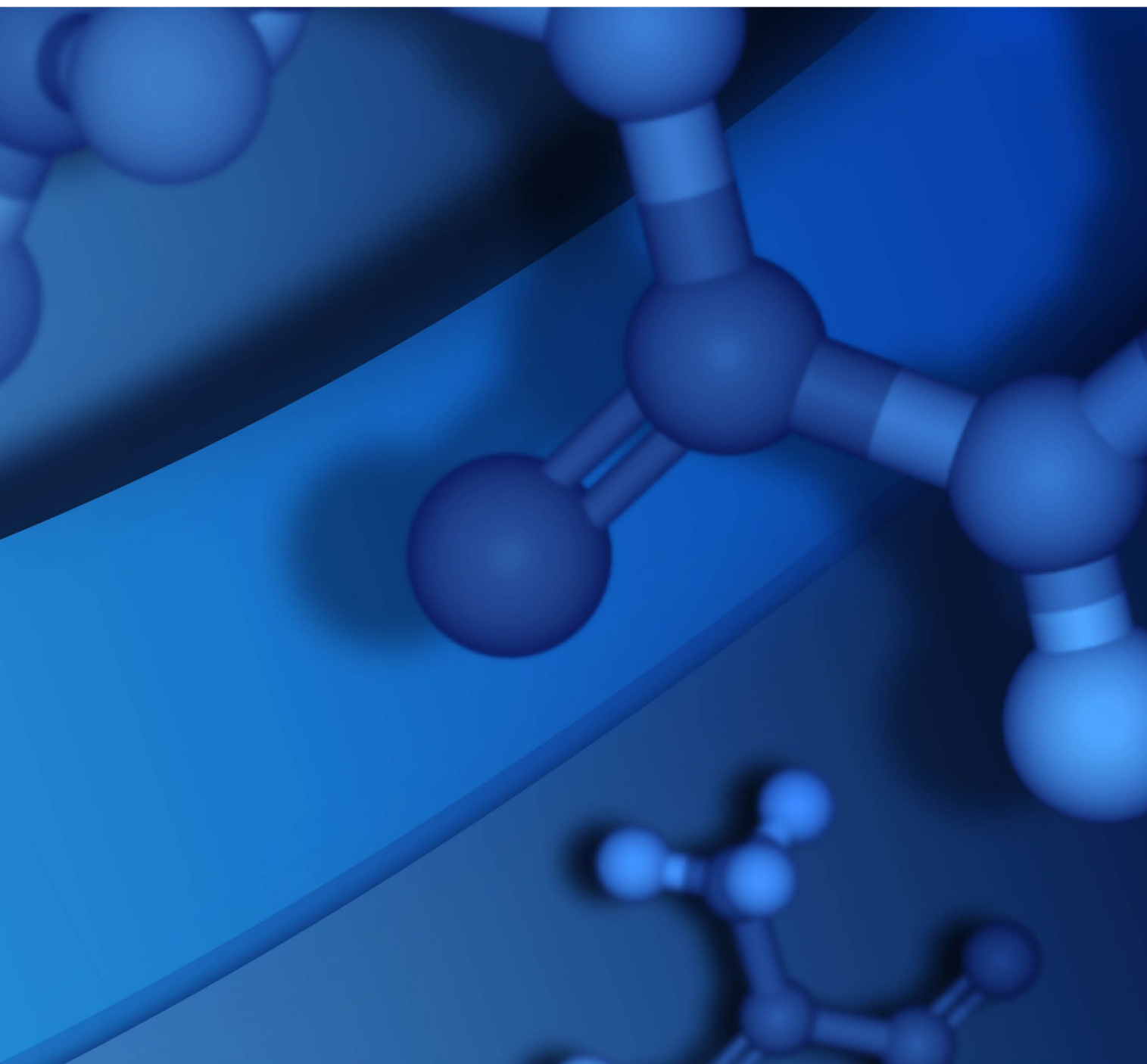
Acknowledgments and References

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Chapter 1:
Introduction to BIOVIA Direct

BIOVIA Direct:

- Uses the extensibility features of Oracle Server to incorporate chemical searching capabilities into Oracle.
- Allows you to use Oracle SQL to perform administrative tasks such as structure registration and searching.

Chapter 2:
Before You Install Direct

This chapter explains the tasks that you must perform before you install Direct, including the prerequisite software that you must install before you can install Version 2021 on an Intel or Intel-compatible host computer that runs the Linux 64-bit operating system.

Before you install Direct, see the Direct System Requirements to verify that you have installed the correct versions of the required software.

Verify Required Hardware and Software

Direct requires that the software for Oracle Server be installed and configured prior to installation.

For more information and a complete list of hardware and software requirements, see *BIOVIA Direct System Requirements*.

System Tasks

Back up any disks involved in the installation.

Verify Disk Space

For more information about disk space requirements for the Direct 2021 application files, see the Direct System Requirements document. Note that this does not include the tablespace required for Oracle databases that use Direct 2021.

To view the space that is available on the file system designated for installation:

1. Start a command prompt on the server.

2. Run the df command to evaluate the available disk space:

```
[biovia@myserver ~]$ df -h /opt
Filesystem                      Size  Used      Avail   Use%    Mounted on
/dev/mapper/rhel-root           151G  92G       59G     61%     /
```

Verify JRE

The standalone UniProt Converter Utility is written in Java, and therefore requires a Java Runtime Environment (JRE). If you want to use the UniProt Converter you therefore must install a 64-bit JRE version 1.8 or later.

Oracle Tasks

Direct 9.1 SP1 and later add support for Oracle 12c, which adds support for Oracle Multitenant / Pluggable databases.

The instructions for installing Direct 9.1 SP1 or later into two or more pluggable databases are the same as when installing Direct into another Oracle instance into the same Oracle Home. Make sure that you install Direct into the pluggable database and not into the container database. For more information, contact Dassault Systèmes Customer Support.

Verify Access to Oracle

You need access to the following:

- listener.ora
- tnsnames.ora

Verify Oracle Instance

For more information, see *BIOVIA Direct System Requirements*.

Verify that You Can Connect to Oracle as a DBA

Log in to SQL*Plus using DBA user name and password, for example:

```
sqlplus DBAname/DBApw
```

If your system login fails, check that the PATH, ORACLE_HOME, and ORACLE_SID are set correctly and that you are using the appropriate user name and password.

Verify Oracle Tablespace

Verify that an Oracle tablespace and a temporary tablespace is available.

For more information, see the Direct System Requirements document.

Installation Parameters for Direct on Oracle

Parameter	Example	Value for your site
Operating system		
BIOVIA Direct installation directory	/opt/BIOVIA/	
Product BIN folder This is the location of the mdldirect.so library (included in the LD_ LIBRARY_PATH for the EXTPROC listener	/opt/BIOVIA/direct2021/bin19 (If you are using Oracle 12, replace /bin19 with /bin12)	
Owner of the BIOVIA Direct application files	biovia	
Oracle environment		
Oracle home folder	/opt/oracle/product/<OracleVersion>/dbhome1	
Oracle user with DBA privileges	system/password	
Oracle SYS password	sys/password	
Oracle Service Name	BIOVIA	
Password for the cartridge schema	direct	
Default tablespace for the Direct 2021 cartridge schema	USERS	
Temporary tablespace for the Direct 2021 schema	TEMP	

Chapter 3:
Installing Direct

Direct Installation Task List

Task	
Ensure that you have completed the pre-installation tasks before starting your installation.	☐
Obtain the Direct Pre-Installation License Validation Tool and Validate the Direct License	☐
Obtain and Unpack the Application GZIP File.	☐
Modify Application Files.	☐
Modify the Oracle Configuration Files.	☐
[Optional] Prepare the EXTPROC listener to run from a non-privileged operating system account.	☐
Start the EXTPROC listener.	☐
Install the Direct Oracle Schema and Cartridge Objects.	☐
Perform the SYS task.	☐

Obtain the Direct Pre-Installation License Validation Tool and Validate the Direct License

Running Pre-Installation License Validation ensures that your Direct license is valid and provides access to the Direct installers.

Direct is supplied as a ZIP file for Windows and a BIN file for Linux. This provides access to a Pre-Installation License Validation tool and, on Windows, supporting files. A license file is provided separately. When the Pre-Installation License Validation tool has validated your license it provides your installation archive(s) which can then be used in the Direct installation procedure.

> **Tip:** When Pre-Installation License Validation has completed successfully you can distribute the installation archive(s) to all machines where Direct should be installed. You do not need to re-validate the license for each machine.

The Direct Pre-Installation License Validation tool will create the installation archives in the specified directory. You should use these archives to continue the installation procedure.

1. On the command line, enter `BIOVIA_Direct_2021_Package.bin` to run the Pre-Installation License Validation process.

2. Enter the full path to your license file and press **Enter**.

3. Enter the full path to the folder to which you want to extract the Direct installation archive and press **Enter**.

The Pre-Installation License Validation process will create Direct installation archives in the specified directory. You should use these archives to continue the installation procedure.

Required Permissions

During the installation of Direct, specific tasks require specific Oracle or system administrator privileges. The following table lists the tasks and the permissions required to perform the tasks.

Task	Owner	Permission required
Install the Direct files.	Administrator	[If required] The administrator must create the Direct installation directory and grant permissions to the user that will own the Direct application files.
Configure the Direct schema	Database DBA	Oracle DBA

Create the Direct Installation Directory

BIOVIA recommends you install Direct from a regular operating system user with no elevated privileges. The following assumes that you have created an operating system user *biovia* as the designated owner of the BIOVIA Direct 2021 files. Furthermore, we assume Direct 2021 will be installed into the directory /opt/BIOVIA/direct2021.

1. Log in as a privileged user who has permissions to create the /opt/BIOVIA directory.

2. Create the /opt/BIOVIA directory.

   ```
   [root@myserver ~]$ mkdir /opt/BIOVIA
   ```

3. Create the /opt/BIOVIA/direct2021 directory.

   ```
   [root@myserver ~]$ mkdir /opt/BIOVIA/direct2021
   ```

4. Recursively change the owner and group of the /opt/BIOVIA directory.

   ```
   [root@myserver ~]$ chown-R biovia:biovia /opt/BIOVIA
   ```

Obtain and Unpack the Application GZIP File

1. Log in as the user who will own the Direct files (e.g. biovia).

2. Copy the Direct installation archive (*direct2021_linux.tar.gz*) to the /opt/BIOVIA/direct2021 directory, as appropriate:

3. Unzip and untar the GZIP file.

   ```
   [biovia@myserver direct2021]$ gunzip direct2021_linux.tar.gz

   [biovia@myserver direct2021]$ tar –xvf direct2021_linux.tar
   ```

4. Change permissions on the files in the bin19 and lib directories so Oracle's extproc listener process can read and execute these files:

   ```
   [biovia@myserver direct2021]$ chmod +rx bin19/* lib/*
   ```

   If you are using Oracle 12, replace bin19 with bin12.

Modify the Application Files

Before you can install the BIOVIA Direct Oracle cartridge objects you must modify specific files in the Direct installation directory. The following steps assume that you have unpacked the Direct 2021 application files into the directory /opt/BIOVIA/direct2021.

1. Make a backup copy of the file /opt/BIOVIA/direct2021/sql/mkdirect.sql. This file is used to create the Oracle schema that holds the Direct 2021 cartridge objects.

2. Open the file /opt/BIOVIA/direct2021/sql/mkdirect.sql in a text editor.

3. Locate the CREATE USER statement in the file:

```
create user C$DIRECT2021 identified by direct
    default tablespace USERS
    quota unlimited on USERS
    temporary tablespace TEMP;
```

   If required modify the user's password, the user's default tablespace and its quota, and the user's temporary tablespace so that they match your Oracle configuration. Do not modify the username C$DIRECT2021!

   For example, if your designated password is password123, your target tablespace is BIOVIA, and your target temporary tablespace is BIOVIA_TMP the modified CREATE USER command will look like this:

```
create user C$DIRECT2021 identified by password123
    default tablespace BIOVIA
    quota unlimited on BIOVIA
    temporary tablespace BIOVIA_TMP;
```

4. Save the modified file.

5. Make a backup copy of the file /opt/BIOVIA/direct2021/sql/mdllibdef.sql. This file will be executed as part of the main installation SQL script.

6. Open the file /opt/BIOVIA/direct2021/sql/mdllibdef.sql in a text editor.

7. Locate the CREATE OR REPLACE LIBRARY statement in the file:

```
create or replace library mdldirect is
    'directory/mdldirect.dll' AGENT 'DIRECT2021_AGENT';
```

8. Replace the path to the BIOVIA Direct library with the respective path of your Direct 2021 installation. For example, if you installed the Direct 2021 files into /opt/BIOVIA/direct2021 the modified CREATE LIBRARY statement will look like this for an Oracle 19 installation:

```
create or replace library mdldirect is
    '/opt/BIOVIA/direct2021/bin19/mdldirect.so' AGENT 'DIRECT2021_AGENT';
```

   If you are using Oracle 12, replace bin19 with bin12.

9. Save the modified file.

Modify the Oracle Configuration Files

Starting with version 2017, each BIOVIA Direct version requires a separate Oracle EXTPROC listener. This allows you to:

- Configure the EXTPROC listener so that it does not interfere with your existing LISTENER configurations.
- Easily configure a non-privileged, secure EXTPROC listener as recommended by Oracle.

- Maintain a listener that is less likely to interfere with the standard database listeners and is easier to troubleshoot in cases of unexpected failures.
- Run multiple versions of Direct 9 or higher in parallel. (Required)

To configure a separate EXTPROC listener Oracle the definition of a public database link and a reference to that link in the library definition of the cartridge is required. Both requirements are already implemented in the installation SQL files provided with Direct 2021.

Likewise, the EXTPROC configuration in the Oracle configuration files *listener.ora* and *tnsnames.ora* need to include these references. The configuration code listed in the following already includes the required references, so copy it as a whole to your configuration file and make edits only as directed.

To add the separate EXTPROC listener configuration to the Oracle *listener.ora* and *tnsnames.ora* configuration files follow these steps.

> **Note:** The following instructions assume you are using Oracle 19. If you are using Oracle 12, replace `bin19` with `bin12`. It also assumes that your ORACLE_HOME is set to `/opt/oracle/product/19c/dbhome_1`.

1. Make backup copies of the *listener.ora, tnsnames.ora*, and *sqlnet.ora* configuration files located in the `$ORACLE_HOME/network/admin` directory.

2. Open the *listener.ora* file in a text editor.

3. Append the complete following text sections at the end of the file:

```
SID_LIST_DIRECT2021 =
  (SID_LIST =
    (SID_DESC =
      (SID_NAME = PLSExtProc_DIRECT2021)
      (ORACLE_HOME = /opt/oracle/product/19c/dbhome_1)
      (PROGRAM = extproc)
      (ENVS = "EXTPROC_DLLS=ANY,LD_LIBRARY_
PATH=/opt/BIOVIA/direct2021/bin19")
    )
  )
DIRECT2021 =
  (DESCRIPTION_LIST =
    (DESCRIPTION =
      (ADDRESS_LIST =
        (ADDRESS = (PROTOCOL = IPC)(KEY = DIRECT2021))
      )
    )
  )
```

> **Note:** If you have problems copying these text sections you can also find them in the file `unix_add_to_listener.ora.txt` located in the `examples/extproc_configuration_files` subdirectory of the Direct installation directory.

4. Modify the path in the `ORACLE_HOME` line so that it matches your `ORACLE_HOME` directory. Omit a slash at the end of the path.

5. Save the modified *listener.ora* file.

> **Note:** Do not make any changes to other lines of the new listener configuration!

6. Open the *tnsnames.ora* file in a text editor

7. Append the complete following text section at the end of the file:

```
EXTPROC_CONNECTION_DATA_DIRECT2021 =
  (DESCRIPTION =
    (ADDRESS_LIST =
      (ADDRESS = (PROTOCOL = IPC)(KEY = DIRECT2021))
    )
    (CONNECT_DATA =
      (SID = PLSExtProc_DIRECT2021)
    )
  )
```

> **Note:** Note: If you have problems copying this text section you can also find it in the file `add_to_tnsnames.ora.txt` located in the `examples\extproc_configuration_files` subdirectory of the Direct installation directory.

8. Save the modified *tnsnames.ora* file.
9. Open the *sqlnet.ora* file in a text editor.
10. Search the *sqlnet.ora* file for the `SQLNET.INBOUND_CONNECT_TIMEOUT` parameter.
11. If the parameter is present, set the parameter to 0. If not, no modification is necessary.
12. Close or save the modified *sqlnet.ora* file.

[Optional] Prepare the EXTPROC Listener to Run from a Non-privileged Operating System Account

When you are calling BIOVIA Direct functions in Oracle, the Oracle EXTPROC listener starts the Oracle-provided executable EXTPROC which will subsequently load the Direct library into memory. The EXTPROC executable will run from the same operating system account as the EXTPROC listener process so in order to work this requires that the Oracle EXTPROC listener account has read and execute permissions on the Direct files located in the BIOVIA Direct installation directory. These permissions were set in step 6 of Obtain and Unpack the Application GZIP File.

Additionally, on the Linux platform, the operating system account that runs the EXTPROC listener needs to have read access to the Oracle *listener.ora* file that defines the EXTPROC listener. The standard `listener.ora` file, located in `$ORACLE_HOME/network/admin`, only provides read and write access to the owner of the oracle files, typically *oracle*, and additional read access to members of the *oinstall* group. `listener.ora` does not provide any access to world.

If you will be running the EXTPROC listener from the account that owns the Oracle files or from any account that is member of the *oinstall* group, proceed to the next section.

If, however, you plan to run the extproc listener from another operating system account, a *secure extproc listener*, we recommend that you create a `listener.ora` file in a location that is accessible to that account, such as the account's home directory. The following steps assume that you will be running the EXTPROC listener from the *biovia* account.

1. Log in to the *biovia* operating system account.
2. Open a text editor and paste the configuration of the Direct 2021 listener as described in step 3 of the previous chapter Modify the Oracle Configuration Files.
3. Save the files as `listener.ora` into the home directory of the *biovia* user: */home/biovia*

> **Note:** The following alternative solutions are possible but not recommended: Rather than creating a separate `listener.ora` file in the account's home directory, you can add the account to the *oinstall* group, or extend the access permissions on the `listener.ora` file in $ORACLE_ HOME/network/admin so that world has read access.

Start the EXTPROC Listener

With permissions set correctly on the BIOVIA Direct installation directory and all required file modifications made you can now start the new EXTPROC listener.

Using a Privileged Account

If you want to run the EXTPROC listener from the account that owns the Oracle files, or from any account that is member of the *oinstall* group:

1. Log in to the operating system account that owns and runs the Oracle database, such as *oracle*.

2. If required run the `oraenv` script to set the Oracle environment.

   ```
   [oracle@myserver ~]$ . oraenv
   ```

3. Start the EXTPROC listener through the `lsnrctl` command:

   ```
   [oracle@myserver ~]$ lsnrctl start DIRECT2021
   ```

   After the successful start of the service the listener status will be reported as:

```
Connecting to (DESCRIPTION=(ADDRESS=(PROTOCOL=IPC)(KEY=DIRECT2020)))
STATUS of the LISTENER
------------------------
Alias                   DIRECT2021
Version                 TNSLSNR for Linux: Version 12.0.0.0.0 - Production
Start Date              07-AUG-2020 10:09:13
Uptime                  2 days 11 hr. 33 min. 10 sec
Trace Level             off
Security                ON: Local OS Authentication
SNMP                    OFF
Listener Parameter File /opt/oracle/product/19c/dbhome_
1/network/admin/listener.ora
Listener Log File
/opt/oracle/diag/tnslsnr/myserver/direct2021/alert/log.xml
Listening Endpoints Summary...
  (DESCRIPTION=(ADDRESS=(PROTOCOL=ipc)(KEY=DIRECT2021)))
Services Summary...
Service "PLSExtProc_DIRECT2021" has 1 instance(s).
  Instance "PLSExtProc_DIRECT2021", status UNKNOWN, has 1 handler(s) for
this service...
The command completed successfully
```

Using a Non-Privileged Account

If you want to run the EXTPROC listener from a non-privileged account:

1. Log in to the operating system account that will run the non-privileged EXTPROC listener, such as *biovia*.

2. Set the `TNS_ADMIN` environment variable to point to the location of the `listener.ora` file created in the user's home directory. See the [Optional] Prepare the EXTPROC Listener to Run from

a Non-privileged Operating System Account.

```
[biovia@myserver ~]$ EXPORT TNS_ADMIN=/home/biovia
```

3. If required run the `oraenv` script to set the Oracle environment.

```
[biovia@myserver ~]$ . oraenv
```

4. Start the EXTPROC listener through the `lsnrctl` command:

```
[biovia@myserver ~]$ lsnrctl start DIRECT2021
```

After the successful start of the service you should recieve a report similar to the example in step 3 of Using a Privileged Account.

Install the Direct Oracle Schema and Cartridge Objects

Once the EXTPROC listener is configured and started you can install the BIOVIA Direct Oracle schema and cartridge objects.

> **Note:** If you are installing on a multitenant database, make sure that you create the Direct schema and objects in the pluggable database, not in the container database.

Follow these steps:

1. Open a command prompt and change to the SQL subdirectory of your BIOVIA Direct installation directory, such as `/opt/BIOVIA/direct2021/sql`.
2. If required run the `oraenv` script to set the Oracle environment.

```
[biovia@myserver sql]$ . oraenv
```

3. Login to an Oracle DBA account through SQL*PLUS and run the `mkdirect.sql` script to create the user that will hold the Direct cartridge objects:

```
[biovia@myserver sql]$ sqlplus system/systempw @mkdirect.sql
```

4. Run the `mdltestlistener.sql` script to check if the EXTPROC listener is configured and running correctly:

```
SQL>@mdltestlistener.sql
```

This script should not return an error.

5. Login to the Oracle user c$direct2021 that is will hold the BIOVIA Direct cartridge objects, and run the `mdlinst_all.sql` script.

```
[biovia@myserver sql]$ sqlplus c\$direct2021/direct @mdlinst_all.sql
```

> **Note:** The default password for the C$DIRECT2021 user is *direct* but you may have changed it as described in Modify the Application Files. You can check for the password in the `mkdirect.sql` file.

This script should return no error.

> **Tip:** The output of the `mdlinst_all.sql` script is logged to the file `mdlinst_all.log` in the user's current directory. The logged output may be helpful in diagnosing any problems with the installation script.

Perform the SYS Task

This task facilitates rapid import of other Direct 2021 databases and safeguards maintenance operations.

1. Log in to the Oracle SYS account as sysdba through SQL*PLUS.
2. Run the `mdlsysactions.sql` file:

   ```
   [biovia@myserver sql]$ sqlplus sys/syspw as sysdba
   SQL> @mdlsysactions.sql
   ```

3. Log out of SQL*Plus.

Chapter 4:
Verify the Installation

To test the validity of your installation, verify that the objects are valid and that the cartridge can start up:

1. Start SQL*Plus and log in as the user C$DIRECT2021:

   ```
   [biovia@myserver ~]$ sqlplus c\$direct2021/direct
   ```

   where *direct* is the password for the user C$DIRECT2021.

2. Execute the following SQL SELECT command:

   ```
   SQL> SELECT DISTINCT STATUS FROM USER_OBJECTS;
   ```

   This command should display a single row of output:

   ```
   VALID
   ```

   If there is a row of output that displays as INVALID then the installation was not successful.

3. To display the product banner, run the following command:

   ```
   SQL> SELECT MDLAUX.VERSION FROM DUAL;
   ```

4. If the Direct cartridge is installed and configured correctly, a banner screen similar to the screen that follows appears:

   ```
   VERSION
   -------------------------------------------------------------

                            BIOVIA Direct
                Revision 2021 (Linux Oracle19)(21.1.0.x)
                Copyright (c) Dassault Systemes, 1999-2020
   ```

5. Exit SQL*Plus:

   ```
   SQL> EXIT
   ```

If the Installation Fails

If the verification step above yields one or more errors, check the configuration of the listener.ora file.

Chapter 5:
Post-Installation Tasks

After you complete the installation of Direct, you might need to complete the tasks that follow:

- Enable specific accounts to run the Direct cartridge.
- Modify the `UniProtConverter` file.
- Customizing SETPATH
- (Optional) Install Direct in additional Oracle instances.

After you have completed the post-installation tasks, you must set up the demonstration databases for the Direct cartridge if you plan to use the example applications.

Enable Accounts to Run the Cartridge

Perform this task for each Direct user at your site.

> **Note:** The following task requires that you run the package procedures `mdlauxop.setup`, which defines the synonyms `mol` and `rxn`. If tables exist with these reserved words, running the package will fail. Verify that your databases do not contain reserved words in the name before you continue with this task. For more information about reserved words, see your Oracle documentation.

> **Permissions required:** Oracle DBA access to modify the roles and system privileges assigned to BIOVIA Direct users, if required.

1. Identify the Oracle users you want to enable to run BIOVIA Direct using, for example *directuser*. Note that this user must not be the C$DIRECT2021 user.

2. Start SQL*Plus and log in to a DBA account, such as `system`:

   ```
   [biovia@myserver ~]$ sqlplus system/password
   ```

3. Assign the required roles and permissions to the new Direct user:

   ```
   SQL> grant connect to directuser;
   SQL> grant resource to directuser;
   SQL> grant create session to directuser;
   SQL> grant alter session to directuser;
   SQL> grant create synonym to directuser;
   SQL> grant create table to directuser;
   SQL> grant create view to directuser;
   SQL> grant create trigger to directuser;
   SQL> grant create sequence to directuser;
   ```

4. Connect to the user that will be enabled to run Direct:

   ```
   SQL> CONNECT directuser/password
   ```

   where `directuser` and `password` are the user name and password for the Oracle user you want to enable.

5. Enable the Direct 2021 synonyms:

   ```
   SQL> EXECUTE C$DIRECT2021.MDLAUXOP.SETUP;
   ```

If the command is correctly executed, the following message displays:

```
PL/SQL procedure successfully completed.
```

```
SQL> select count(*) from user_synonyms where table_owner like
'C$DIRECT2021'and synonym_name in (select synonym_name from
c$direct2021.mdl_synonym_defs);

  COUNT(*)
----------
      99
```

6. Exit SQL*Plus.

```
SQL> exit
```

Modify the UniProtConverter File

Run this procedure to use the UniProt Converter Utility. You must modify the `UniProtConverter` file with the correct Java executable path:

1. Open and edit the file `/opt/BIOVIA/direct2021/bin19/UniProtConverter`. If you are using Oracle 12, replace `bin19` with `bin12`.

2. Change the value of the environment variable JAVA to the location of your Java executable.

   For example, `/usr/bin/java`

3. Save and close the file.

Customizing SETPATH

To customize the `setpath` file:

1. Open a text editor and edit the file. `setpath` files are placed into the following directory by the installer.

   `/opt/BIOVIA/direct2021/bin19`

   If you are using Oracle 12, replace `bin19` with `bin12`.

2. Replace strings of four letters with path or value customized for the installation:

AAAA	Oracle SID
ZZZZ	Oracle home directory

   Also, check the `PATH` set in `DIRECTBIN` so that it matches the Direct bin directory that applies to your Oracle version.

3. Save and close the file.

4. To verify that the file has been modified correctly, source the file in sh, ksh or bash using

   `setpath`

   Then use `ldd` to ensure that none of the dependencies of `mdldirect.so` are missing. There should not be any shared objects which are not found.

> **Note:** The following instructions assume you are using Oracle 19. If you are using Oracle 12, replace `bin19` with `bin12`.

```
ldd mdldirect.so
```

Example

```
# -----------------------------------------------------------
# Environment shell script (Korn or Bourne shell version)
#
# This shell script may be used to set the PATH and LD_LIBRARY_PATH
# needed to run the Direct tools.
#
# Use the command ". setpath" to execute the commands in
# this shell script in the current Korn or Bourne shell.
# -----------------------------------------------------------
#
# Customize this path as required
DIRECTBIN=/opt/BIOVIA/direct2021/bin19
#
# Set this to the Oracle home path
if [ -z "$ORACLE_HOME" ]
then
    ORACLE_HOME=/opt/oracle/product/19c/dbhome_1
    export ORACLE_HOME
fi
#
# Set this to the Oracle SID
if [ -z "$ORACLE_SID" ]
then
    ORACLE_SID=biovia
    export ORACLE_SID
fi
#
ORALIB=$ORACLE_HOME/lib
ORABIN=$ORACLE_HOME/bin
PATH=${DIRECTBIN}:${ORABIN}:$PATH
export PATH
LD_LIBRARY_PATH=${ORALIB}:${DIRECTBIN}:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH
```

Chapter 6:
Setting Up the Direct Demonstration Databases

This chapter explains how to set up the demonstration databases and tables that BIOVIA supplies with Direct.

> **Note:** If you plan to use the example applications, you must perform the procedures in this chapter to view the molecules and reactions through the cartridge.

Introduction to the Sample Databases

The Oracle Data Pump dump file `DCSAMPLES.DMP` contains an export of the `DCSAMPLES` schema. the .dmp file includes:

- a 2D molecule table (`SAMPLE2D`)
- a reaction database containing a reaction table (`SAMPLERX_REACTION`) and hierarchical data tables
- a generic structure table (`SAMPLEGEN`)
- a biopolymer sequence table (`SAMPLEBIO`)
- a single molecule table containing simple molecules, generic structures and biopolymer sequences (`SAMPLEMOL`)

Demonstration Database Task Checklist

Use this checklist to verify that you have performed all the tasks that are required to correctly set up the demonstration reaction table and molecule database for Direct. The procedures that you perform are explained in the corresponding sections.

Task	Details	Done
Create a new Oracle schema to contain the `DCSAMPLES` database tables.	For more information, see Create a New Oracle Schema to Contain DCSAMPLES.	
Import the Oracle `DCSAMPLES.DMP` file.	For more information, see Import the Oracle DCSAMPLES.DMP File.	
Test the `SAMPLE2D` database.	For more information, see Molecule Verification.	
Test the `SAMPLERX` database.	For more information, see Reaction Verification.	

Create Oracle Schema for DCSAMPLES Database Tables

To load the sample database:

1. Connect to Oracle as a database administrator and create a schema to hold the sample databases. The examples assume that the schema is named `DCSAMPLES`, however, you can choose any name. To create the user:

   ```
   sqlplus system/******
   create user dcsamples identified by dcsamples default tablespace users
   ```

```
quota unlimited on users temporary tablespace temp;
grant create session to dcsamples;
grant alter session to dcsamples;
grant resource to dcsamples;
grant connect to dcsamples;
grant create synonym to dcsamples;
grant create table to dcsamples;
grant create view to dcsamples;
grant create trigger to dcsamples;
grant create sequence to dcsamples;
```

2. Connect to the new sample database schema, for example, DCSAMPLES, and enable it for use with Direct by executing C$DIRECT2021.MDLAUXOP.SETUP. For example:

```
connect dcsamples/dcsamples
execute c$direct2021.mdlauxop.setup;
```

The .dmp file was created using the Oracle Data Pump Export utility. This utility does not accept a directory path name. The utility uses an Oracle *directory* object to specify the directory where the dump file is located.

3. Contact your Oracle database administrator and determine what Oracle directory object should be used to import the dump file, and copy the dump file to the location on the disk corresponding to the Oracle directory object.

The DBA system user might need to create a directory object for you, for example:

```
connect system/*****
create or replace directory dpump_dir as '/tmp';
grant read,write on directory dpump_dir to public;
```

Import the Oracle DCSAMPLES.DMP File

Using the Oracle Data Pump Import utility (impdp), import the file DCSAMPLES.DMP.

Note: If you did not name your schema DCSAMPLES in Step 1, use the REMAP_SCHEMA parameter to remap the schema DCSAMPLES stored in the .dmp file to your schema name. If your default tablespace name is not USERS, use the REMAP_TABLESPACE parameter to remap the tablespace USERS stored in the .dmp file to your tablespace name.

■ To import the .dmp file into the schema DCSAMPLES and a tablespace named USERS which already exist, enter:

```
> impdp dcsamples/dcsamples directory=dpump_dir dumpfile=DCSAMPLES.DMP
```

■ To import the .dmp file into the schema DCSAMPLES with the default tablespace named WORK_TABSPACE, enter:

```
> impdp dcsamples/dcsamples directory=dpump_dir dumpfile=DCSAMPLES.DMP
remap_tablespace=users:work_tabspace
```

■ To import the .dmp file into schema OURSAMPLES, with the default tablespace named WORK_TABSPACE, enter:

```
> impdp dcsamples/dcsamples directory=dpump_dir dumpfile=DCSAMPLES.DMP
remap_schema=dcsamples:oursamples remap_tablespace=users:work_tabspace
```

Once imported, the five databases contain the following objects:

Chapter 6: Setting Up the Direct Demonstration Databases

Database and Objects	Description
2D Generic Structure, and Biopolymer Structure Molecule Database	
SAMPLEMOL	Main molecule table
SAMPLEMOL_IX	Direct molecule domain index on CTAB
2D Molecule Database	
SAMPLE2D	Main molecule table
SAMPLE2D_IX	Direct molecule domain index on CTAB
SAMPLE2D_ACTIVITY	Subtable of activities
SAMPLE2D_ALTERNATE_NAMES	Subtable of alternate names
SAMPLE2D_BOILING_POINT	Subtable of boiling points
SAMPLE2D_MELTING_POINT	Subtable of melting points
Reaction Database	
SAMPLERX_REACTION	Main table of reaction variations
SAMPLERX_REACTION_IX	Direct reaction domain index on RCTAB
SAMPLERX_REACTANT_MOLREGNO	Subtable of links to SAMPLERX_MOLTABLE
SAMPLERX_PRODUCT_MOLREGNO	Subtable of links to SAMPLERX_MOLTABLE
SAMPLERX_VARIATION	Subtable of reaction variations
SAMPLERX_CITATION	Subtable of links to SAMPLERX_DOC
SAMPLERX_SYSNO	Subtable of links to SAMPLERX_SYSTEXT
SAMPLERX_RXNREF	Subtable of reaction scheme data
SAMPLERX_REACTANT	Subtable of reactant data and links to SAMPLERX_MOLTABLE
SAMPLERX_PRODUCT	Subtable of product data and links to SAMPLERX_MOLTABLE
SAMPLERX_STEPNO	Subtable of synthesis steps
SAMPLERX_CONDITION	Subtable of searchable condition data
SAMPLERX_AUXMOL	Subtable of solvent, catalyst and reagent data and links to SAMPLERX_MOLECULE
SAMPLERX_SYSTEXT	Text descriptions of reaction keywords
SAMPLERX_DOC	Literature references
SAMPLERX_AUTHOR	Subtable of separate author names
SAMPLERX_MOLTABLE	Molecules that participate as reactants, products,

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Database and Objects	Description
	solvents, catalysts, or reagents
SAMPLERX_MOL_IX	Direct molecule domain index on CTAB
SAMPLERX_CAS	Subtable of CAS numbers
SAMPLERX_NAME	Subtable of molecule names
The following tables are present because they are used in the reaction database data model, however for SAMPLERX, they do not contain data.	
SAMPLERX_CHEMNAME	
SAMPLERX_CONTENT_RELEASE	
SAMPLERX_DISCRETE	
SAMPLERX_KEYWORD	
SAMPLERX_MOLCITATION	
SAMPLERX_POLYMER_INFO	
SAMPLERX_POLYMER_NAME	
SAMPLERX_PROT_GP	
SAMPLERX_REACTIONSCHEME	
SAMPLERX_SOLID_SUPPORT_NAME	
SAMPLERX_SS_CONDITION	
SAMPLERX_SS_KEYPHRASE	
Generic Structure Molecule Database	
SAMPLEGEN	Generic structure table
SAMPLEGEN_IX	Direct molecule domain index on CTAB
See the file `testsamplegen.sql` for examples of searching.	
Biopolymer Sequence Molecule Database	
SAMPLEBIO	Biopolymer structure table
SAMPLEBIO_IX	Direct molecule domain index on CTAB
See the file `testsamplegen.sql` for examples of searching.	

Isentris Data Source Definition Files

Isentris data source definition files for SAMPLE2D and SAMPLERX are also included:

- DIRECT_DCSAMPLES_RELATIONAL.XML
- DIRECT_DCSAMPLES_IDS.XML

  The first file defines an Isentris relational datasource. It must be edited to change the values for the username, password, HOST, PORT and SID. The username and password are both set to dcsamples; there are no defaults for the Oracle connection parameters.

  The second file defines a set of Integrating Data Source (IDS) connectors for these databases. The file does not need editing. This file is intended for demonstration purposes only. The connectors do not match the format used for BIOVIA databases, such as the ChemInform Reaction Library database.

To set up the Isentris data source definition files:

1. Copy both files into the /system/config/datasource/dsfiles directory under your Isentris installation. For example:

   /opt/BIOVIA/isentris2020/system/config/datasource/dsfiles

2. After copying, open an XML editor and edit the file direct_dcsamples.relational.xml:

   a. Change the username and password to the correct values for the account created in Create a new Oracle Schema to contain DCSAMPLES > Step 1. If you created the account as DCSAMPLES/DCSAMPLES, no change is required.

   b. Change the HOST string to the appropriate name for the computer running Oracle.

   c. Change the PORT string to the port number on which the appropriate Oracle listener is listening. This is generally 1521.

   d. Change the SID string to the Oracle SID for the database. You also can replace SID=<your-SID> with service_name=<your-service-name>.

3. After you have made your changes, save and close the file.

Verify Demonstration Database and Tables Installation

Molecule Verification

The following tests are listed in the testsample2d.sql file located in the /opt/BIOVIA/direct2021/examples directory. You can run this file instead of running the following tests manually.

Permissions required: Log in to SQL*Plus as the owner of the schema, for example, dcsamples/dcsamples.

Test the SAMPLE2D Database

1. Verify that the SSS operator is working correctly.

   ```
   SQL> SELECT COUNT(*) FROM SAMPLE2D WHERE SSS
   (CTAB,'/opt/BIOVIA/direct2021/examples/molfiles/sssquery.mol')=1;
   ```

   If the command executes correctly, the following message displays:

   ```
   COUNT(*)
   --------
         52
   ```

1. Display cartridge errors.

   ```
   SQL> SELECT MDLAUX.ERRORS FROM DUAL;
   ```

   If the command executes correctly, the following message displays:

   ```
   ERRORS
   -------------
   ```

2. Verify that the MOLSIM operator is working correctly.

   ```
   SQL> SELECT COUNT(*) FROM SAMPLE2D
     2> WHERE MOLSIM(CTAB, 'C1CCNCC1', 'NORMAL')>40;
   ```

   If the command executes correctly, the following message displays:

   ```
     COUNT(*)
   ----------
            3
   ```

3. Verify that the FLEXMATCH operator is working correctly.

   ```
   SQL> SELECT CDBREGNO FROM SAMPLE2D WHERE FLEXMATCH(CTAB,'C1CCCCC1','ALL')=1;
   ```

   If the command executes correctly, the following message displays:

   ```
   CDBREGNO
           27
   ```

4. Verify that the INSERT statement works correctly.

   ```
   INSERT INTO SAMPLE2D(CDBREGNO,CTAB,MOLNAME,CORP_ID) VALUES (1000,MOL
   ('C1CCCCC1'),'INS1','INS1');
   ```

   If the command executes correctly, the following message displays:

   ```
   1 row created.
   ```

5. Verify that the UPDATE statement works correctly.

   ```
   SQL> UPDATE SAMPLE2D SET MOLNAME='INS1' WHERE CDBREGNO=3;
   ```

   If the command executes correctly, the following message displays:

   ```
   1 row updated.
   ```

6. Verify that the DELETE statement works correctly.

   ```
   DELETE FROM SAMPLE2D WHERE CDBREGNO=2;
   ```

   If the command executes correctly, the following message displays:

   ```
   1 row deleted.
   ```

7. Rollback changes.

   ```
   SQL> ROLLBACK;
   ```

   If the command executes correctly, the following message displays:

   ```
   Rollback complete.
   ```

8. Display record count.

   ```
   SQL> SELECT COUNT(*) FROM SAMPLE2D;
   ```

   If the command executes correctly, the following message displays:

```
COUNT(*)
----------
       382
```

Reaction Verification

The following tests are listed in the `testsamplerx.sql` file located in the `/opt/BIOVIA/direct2021/examples` directory. You can run the file or run the tests manually.

The example reaction files must be made read-accessible from the operating system account under which the Oracle extproc listener runs.

> **Permissions required:** Log in to SQL*Plus as the owner of the schema, for example, `dcsamples/dcsamples`.

Test the SAMPLERX Table

1. Verify that the `RSS` operator is working correctly.

    a. Start SQL*Plus and log in as the owner of the schema, for example:

        C:\> sqlplus dcsamples/dcsamples

    b. Verify the RSS operator is working:

        SQL> SELECT RXNMDLNUMBER FROM SAMPLERX_REACTION WHERE RSS(RCTAB,
        '/opt/BIOVIA/direct2021/examples/rxnfiles/rssq1.rxn')=1;

    > **Note:** When typing `rssq1.rxn`, make sure that you type a one (1) not a lowercase L.

    If the command executes correctly, the following message displays:

        MDLNUMBER

        RXCI92065766

2. Display cartridge errors.

        SQL> SELECT MDLAUX.ERRORS FROM DUAL;

    If the command executes correctly, the following message displays:

        ERRORS

3. Verify that the `RXNSIM` operator is working correctly.

        SQL> SELECT RXNMDLNUMBER FROM SAMPLERX_REACTION WHERE RXNSIM(RCTAB,
        '/opt/BIOVIA/direct2021/examples/rxnfiles/query2.rxn', '80 20')=1
        ORDER BY RXNMDLNUMBER;

    If the command executes correctly, the following message displays:

        RXNMDLNUMBER

        RXIC92000009
        RXIC92000010
        RXIC92000013
        RXIC92000014
        RXIC92050814
        RXIC93003231
        6 rows selected.
```

4. Verify that the RXNFLEXMATCH operator is working correctly.

   ```
   SQL> SELECT RXNMDLNUMBER FROM SAMPLERX_REACTION WHERE RXNFLEXMATCH
   (RCTAB,'/opt/BIOVIA/direct2021/examples/rxnfiles/query.rxn',
   'match=all')=1;
   ```

   If the command executes correctly, the following message displays:

   ```
   MDLNUMBER
   --------------
   RXCI94006733
   ```

5. Verify that the INSERT statement works correctly.

   ```
   SQL> INSERT INTO SAMPLERX_REACTION (RXNMDLNUMBER,RCTAB) VALUES
   ('NEW',RXN('/opt/BIOVIA/direct2021/examples/rxnfiles/newrxn1.rxn'));
   ```

   If the command executes correctly, the following message displays:

   ```
   1 row created.
   ```

6. Verify that the reaction was inserted.

   ```
   SQL> SELECT RXNMDLNUMBER FROM SAMPLERX_REACTION WHERE RXNFLEXMATCH
   (RCTAB,'/opt/BIOVIA/direct2021/examples/rxnfiles/newrxn1.rxn',
   'match=all')=1;
   ```

   If the command executes correctly, the following message displays:

   ```
   RXNMDLNUMBER
   ----------------------------
   NEW
   ```

7. Rollback changes.

   ```
   SQL> ROLLBACK;
   ```

   If the command executes correctly, the following message displays:

   ```
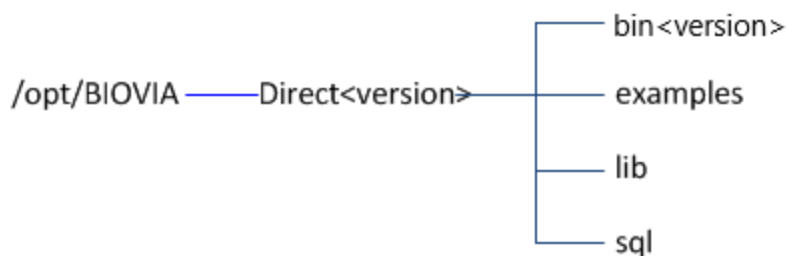   Rollback complete.
   SQL> EXIT
   ```

Chapter 7:
Direct File Configuration on Linux

This chapter explains the configuration of Direct cartridge files on Red Hat Linux or SUSE Linux.

Direct Hierarchy

When you install Direct cartridge files on Linux computers, the installation program places files into the directory hierarchy shown below.

Explanation of Directories and Files

References to file names and directory names on Linux are case sensitive.

Do not include spaces in the names of files that are created by or used by the cartridge, such as `mdldirect.so`. File and directory names that contain spaces might cause erratic program behavior. To improve readability, use underscores in file names and directory names.

Directory or File	Contents

`$ORACLE_HOME/network/admin`
 	
`listener.ora`
`tnsnames.ora`
	Oracle listener configuration directory
	
	Oracle network system configuration listener files that must be present for use with the extproc listener

`/opt/BIOVIA/direct2021`	Direct cartridge files
`/opt/BIOVIA/direct2021/bin19`	Binary executable files for the Oracle 19c installation
`/opt/BIOVIA/direct2021/bin12`	Binary executable files for the Oracle 12c installation
`directupgrade`	
`mdldirect.so`	

`exportRDFile`
`exportSDFile`
`importRDFileEx`
`importRDFile`
`importSDFile`
`setpath`
`setpath.csh`
	Import and export utilities for SDFiles and RDFiles.

Directory or File	Contents
`UniProtConverter`	Batch file to run the UniProt Converter Utility

`libQtCore.so.4`
`libQtGui.so.4`
`liboemetachem-1.5.0.so`
`libpilot.so`
`libpilotcore.so`
`libppchemcip.so`
`libppchemfs.so`
`libppchemmdl.so`
`libppchemnema.so`
`libppchemsagecoords.so`
`libppopeneye.so`
`libsciexpat.so`
`libsciinchi.so`
`libsciz.so`
`libuwin32.so`
`libvcbaseclient.so`
`libvccore.so`
`libvcdm.so`
`libvcdmutil.so`
`libvcmath.so`
`libvcparser`
	BIOVIA Foundation files

`/opt/BIOVIA/direct2021/examples`	Sample applications and demonstration databases
`DCSAMPLES.DMP`	Demonstration database import file
`direct_dcsamples_ids.xml` `direct_dcsamples_relational.xml`	Files for use with BIOVIA Isentris applications
`rdcapps.sql`	SQL script that runs sample applications to read a RDFile and create a cross-reference trigger
`readme_dcsamples.txt`	Instructions on setting up the DCSAMPLES dump file

`testsample2d.sql`
`testsamplerx.sql`
`testsamplebio.sql`
`testsamplegen.sql`
	Script to test the SAMPLE2D database
	Script to test the SAMPLERX database
	Script for examples of searching biopolymer structures
	Script for examples of searching and enumeration of generic structures

`molfiles`	Directory containing molecule files used in `testsamplerx.sql`
`rxnfiles`	Directory containing reaction files used in `testsamplerx.sql`
`extproc_configuration_files`	Directory containing example EXTPROC configuration files
`/opt/BIOVIA/direct2021/lib`	Shared objects
`ccatlib.so`	Cheshire shared library and jar files used by UniProt

Directory or File	Contents

`Cheshire.jar`
`CheshireJNI.jar`
`ojdbc6.jar`
`UniProtConverter.jar`
	Converter

`/opt/BIOVIA/direct2021/sql`	Direct SQL files
`mkdirect.sql`	SQL used to create the cartridge user and public database link.
`mdllibdef.sql`	Contains the path to `mdldirect.so` and is used to create the shared object library that uses the public database link.
`mdlinst_all.sql`	Install all components of the Direct data cartridge.
`mdluninst.sql`	Uninstalls the Direct data cartridge.

Chapter 8:
Removing Direct

Removing Direct involves the following tasks. Each task is explained in detail in the sections that follow.

Alert Users That Direct Will Be Unavailable

Direct is not available once you begin removing Direct files. Notify users:

- They cannot access the version of the program you plan to remove.
- The removal of the version from the system is permanent.

Close Applications That Use Direct

Prior to uninstalling, close any applications that use Direct.

Back Up Direct Files

Back up all files prior to unintalling Direct.

Remove Direct

This section explains how to remove Direct from your server. The following procedure completely removes all installation files. You must manually drop the Direct schema owner and schema objects.

Drop the Direct Schema

Permissions required: Log in to SQL*Plus as the Direct schema owner.

1. From a Command Prompt window, log into SQL*Plus:

   `[biovia@myserver ~]$ sqlplus c\$direct2021/password`

2. Run `mdluninst.sql`:

   `SQL> @/opt/BIOVIA/direct2021/sql/mdluninst.sql`

   Permissions required: Log in to SQL*Plus as the Oracle DBA who configured the schema.

3. Drop the c$direct2021 user and the schema objects:

   `SQL> drop user c$direct2021 cascade;`

4. Drop the public database link:

   `SQL> drop public database link DIRECT2021_AGENT`

5. Exit SQL*Plus.

   `SQL> exit`

Drop the Demonstration Database Schema

If you set up the demonstration databases, follow this procedure to drop the user and schema that were created.

> **Permissions required:** Log in to SQL*Plus as the Oracle DBA who can drop user accounts.

1. From a Command Prompt window, log into SQL*Plus:

   ```
   [biovia@myserver ~]$ sqlplus username/password
   ```

2. Drop the demonstration database schema:

   ```
   SQL> drop user dcsamples cascade;
   ```

   where `dcsamples` is the name of the demonstration database schema.

3. Exit SQL*Plus.

   ```
   SQL> exit
   ```

Remove the Direct Files

> **Permissions required:** Log in as the user who installed Direct or as an Administrator.

Delete the directory into which you installed Direct2021.

> **IMPORTANT!** If you have files that you modified in the folders under `/opt/BIOVIA/direct2021` that you want to keep for later installations, save a copy of the file before you delete the folder.

Chapter 9:
Set Up an Oracle RAC Environment

> **IMPORTANT!** The path to the Oracle LIB folder and the path to the Direct installation must be the same on all RAC nodes. There is no provision in Oracle RAC for the Direct executables to be located in different directory names or on different devices. BIOVIA recommends installing Oracle and Direct on a shared disk. If you do not use a shared disk, must take additional steps to copy the required files to locations that can be accessed on all nodes using the same path names.

The installation of BIOVIA Direct into a RAC environment follows the same steps as for a single-node Oracle instance. In particular, the configuration of the Direct EXTPROC in the `listener.ora` and `tnsnames.ora` configuration files in an Oracle RAC environment is identical to the single-node configuration. The configuration of the EXPROC listener must be executed on each individual node.

For details on installing Direct into a single-node Oracle instance, see Installing Direct.

> **IMPORTANT!** Make sure that the Direct EXTPROC listener is configured and started on ALL RAC nodes before you install the schema and cartridge objects. For more information, see Install the Direct Oracle Schema and Cartridge Objects.

Appendix A:
Maintaining an Installation During a Major Oracle Upgrade

The Direct executables are Oracle-version specific, so when you upgrade your database to a new Oracle version, the Direct installation no longer runs.

- Direct requires `MDLAUX.PREPAREINDEXEXPORT` before you perform a database export to efficiently perform an import.
- The Oracle import does not restore the Direct schema properly and as a result the import might result in invalid objects.
- The Oracle import might not import the `C$DIRECT2021` schema before it imports schemas that have domain indexes which depend on the Direct schema existing in order for the import to work properly.

Protect Your Direct Data During a Major Oracle Upgrade

- From Direct, run `MDLAUX.PREPAREINDEXEXPORT` in each schema that has a Direct domain index before you export the Oracle database for backup.
- Before performing a major Oracle upgrade and after completing Step 1, uninstall Direct.

There two upgrade scenarios:

1. Upgrade in place (no backup and restore).
2. Backup (full export), upgrade, and restore (full import).

Upgrade Scenario 1 - Upgrade in Place

1. Uninstall Direct.
   This must be done before the Oracle upgrade.
2. Upgrade to the new version of Oracle.
3. Reinstall Direct.
4. For each schema that owns a domain index:
   a. Execute `direct2021.mdlauxop.setup` to define the Direct synonyms.
   b. Select `mdlaux.recreateindexes from dual`.

Direct now functions properly in the upgraded Oracle version.

Upgrade Scenario 2 - Backup, Upgrade, and Restore

Backup with the old version of Oracle, upgrade Oracle, and then restore the database with the new version of Oracle.

1. Run `MDLAUX.PREPAREINDEXEXPORT` in each schema that has a Direct domain index.
2. Export the `ORACLE` database.
3. Uninstall Direct.
4. Install the new version of Oracle.

5. Restore the Oracle database infrastructure, that is, restore any schemas that *do not* have Direct domain indexes.

6. Install Direct.

7. Run `mdlsysactions.sql` as sysdba

8. In each schema that will have Direct domain indexes:

   a. Execute `c$direct2021.mdlauxop.setup` to define the Direct synonyms.

      This step ensures that the version of Direct that you have installed is the version that will be used during import.

   b. Import the contents of the schemas that contain domain indexes, using the `indexes=y` and `ignore=y` options.

   c. For each schema that contains Domain indexes, enter
      `SELECT STATUS,DOMIDX_STATUS, DOMINDX_OPSTATUS, ITYP_OWNER FROM USER_ INDEXES WHERE INDEX_TYPE='DOMAIN'`

If any of the Direct domain indexes do not show all three status columns as `VALID`, then run `MDLAUX.RECREATEINDEXES` in that schema. Any Direct domain indexes that are not repaired by this command needs to be dropped and created again.

> **Note:** The speed of the import and the speed of `MDLAUX.RECREATEINDEXES` depends on `mdlsysactions.sql` having been run in the `SYS` schema. If `mdlsysactions.sql` is not run, the result can be many extra hours of runtime.

Appendix B:
Configure Multiple Direct Versions on the Same System

BIOVIA Direct 2021 installs with a separate listener and therefore does not interfere with existing listener configurations for other Direct versions installed on the system. You therefore can install Direct 2021 in addition to other Direct versions following the standard installation instructions.

User Account Issues with Multiple Cartridge Versions

You can set up an Oracle user account to run only one Direct cartridge version at a time. This means that all the Oracle databases stored in one schema must use the same cartridge version.

End-user accounts must have the Direct cartridge synonyms defined explicitly. To set up an Oracle account for a specific cartridge version, the user needs to execute the `MDLAUXOP.SETUP` procedure. For example:

```
SQL> EXECUTE C$DIRECT2021.MDLAUXOP.SETUP;
```

Thereafter, the synonyms of this user invoke only the Direct 2021 cartridge, regardless of the presence of other versions of Direct in the Oracle instance.