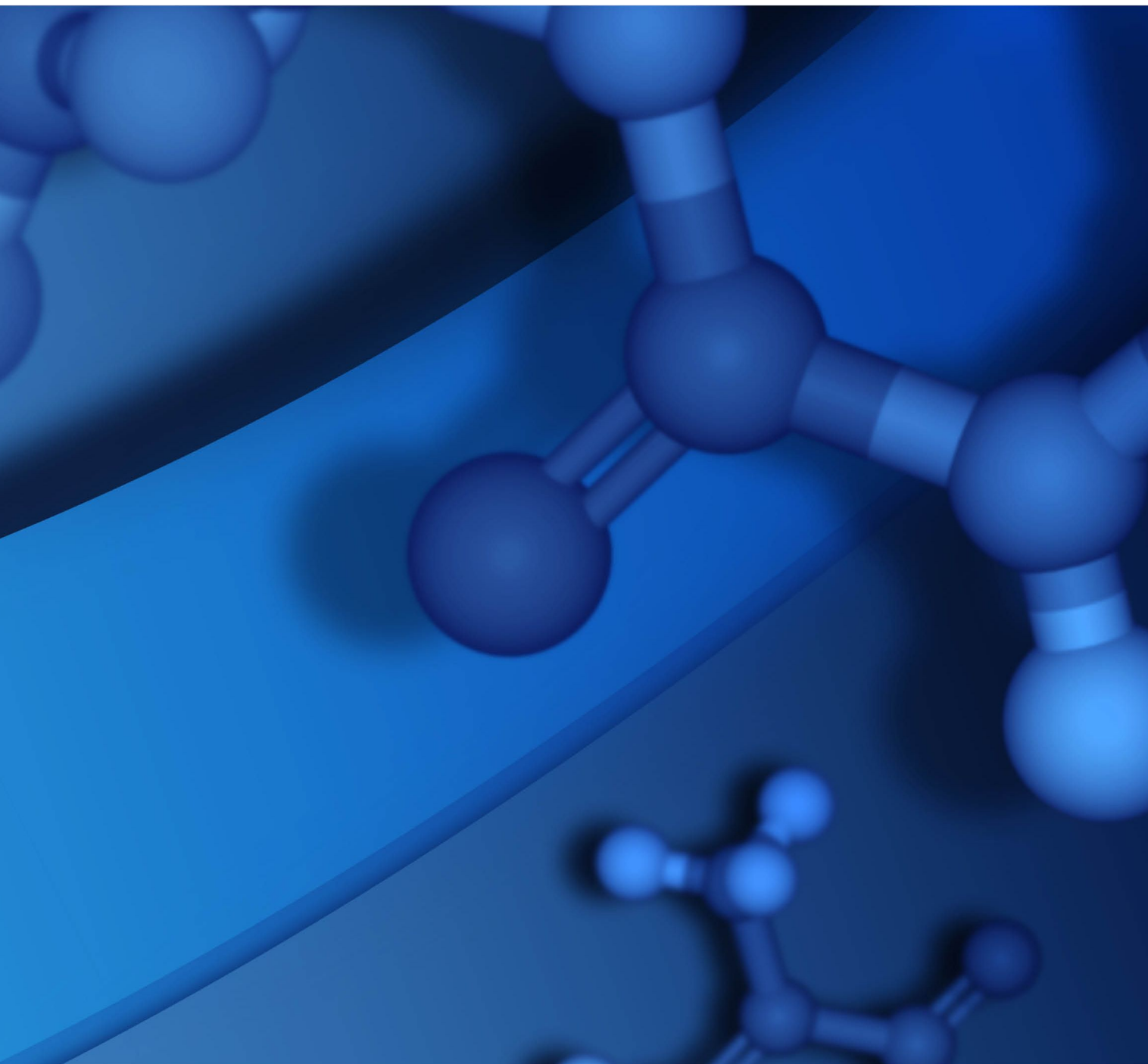


INSTALLATION AND CONFIGURATION GUIDE (WINDOWS)

BIOVIA DIRECT 2021



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Chapter 1:

About This Guide

This guide explains how to install and configure BIOVIA Direct on Intel or Intel-compatible host computers that run on the Microsoft Windows Server 64-bit operating system. For information about how to administer the data cartridge, see the *Direct Administration Guide*.

Introduction to 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.

How to Use the Installation Guide

Prerequisite Knowledge

This guide assumes that you are familiar with:

- Windows Server 64-bit operating system
- Windows system administration
- Oracle database administration

Related Documents

Document	Purpose
<i>BIOVIA Direct System Requirements</i>	Lists hardware and software requirements for BIOVIA Direct 2021.
<i>BIOVIA Direct Administration Guide</i>	Administering the Direct cartridge.
<i>BIOVIA Direct Developers Guide</i> <i>BIOVIA Direct Reference Guide</i>	Developing applications using Direct.
<i>BIOVIA Chemical Representation Guide</i>	Reference information on BIOVIA Chemical Representation.
<i>BIOVIA Direct Error Messages Guide</i>	Contains errors messages that might occur in using Direct, when upgrading databases to Direct 2021, and common Oracle errors.
<i>CTFile Formats</i>	Describes the file formats used to represent structures.

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 Direct on an Intel or Intel-compatible host computer that runs the Microsoft Windows Server 64-bit operating system.

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

Pre-Installation Task Checklist

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 the *BIOVIA Direct System Requirements* document.

Fonts

The following system fonts are required to render images:

- Arial
- Courier New

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 drive:

Permissions required: Log in as an Administrator.
--

1. Start Microsoft Windows Explorer.
2. Select the drive on which you will install Direct.

Microsoft Windows displays the amount of free space at the bottom of the window.

Verify the Required Hardware and Software

See the *BIOVIA Direct System Requirements* Document.

To install the **Visual C++ Redistributable Packages for Visual Studio 2013** onto the Oracle server Windows computer:

1. Go to <https://www.microsoft.com/en-us/download/details.aspx?id=40784>.
2. Download and run `vcredixt_x64.exe`. This will install the runtime libraries needed by Direct:
 - `msvcr120.dll`
 - `msvcpr120.dll`

Verify that JRE is Installed

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 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 the *BIOVIA Direct System Requirements* document.

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 *BIOVIA Direct System Requirements* document.

Chapter 3:

Installation Parameters Worksheet

Use the Installation Parameters Worksheet to consolidate information needed for the installation.
The installation worksheet specifies the information required when you install the Direct program files.

Installation Parameters for Direct on Oracle

Parameter	Example	Value for your site
Operating System		
BIOVIADirect installation directory	<i>C:\BIOVIA\direct2021</i>	
Product BIN folder ¹	<i>C:\BIOVIA\direct2021\bin12</i>	
Owner of the BIOVIA Direct application files	<i>BIOVIA</i>	
Oracle Environment		
Oracle home folder	<i>C:\Oracle\product\<Oracleversion>\dbhome</i>	
Oracle user with DBA privileges	<i>SYSTEM/password</i>	
Oracle SYS password	<i>SYS/password</i>	
Oracle Service Name	<i>BIOVIA</i>	
Password for cartridge schema	<i>direct</i>	
Default tablespace for the Direct schema	<i>USERS</i>	
Temporary tablespace for the Direct Oracle database schema	<i>TEMP</i>	
¹ The location of <code>mdldirect.dll</code> . This is included in the PATH for the EXTPROC listener. The number used for the bin folder folder corresponds with the version of Oracle you are using. For example: use <code>bin19</code> with Oracle 19 and <code>bin12</code> with Oracle 12.		

Chapter 4:

Direct Installation Task List

Task	Done
Ensure that you have completed the pre-installation tasks before starting your installation.	<input type="checkbox"/>
Obtain the Direct Pre-Installation License Validation Tool and Validate the Direct License	<input type="checkbox"/>
Obtain and Unpack the Direct 2021 Application ZIP file.	<input type="checkbox"/>
Modify Direct 2021 Application Files.	<input type="checkbox"/>
Modify the Oracle Configuration Files <i>listener.ora</i> and <i>tnsnames.ora</i> .	<input type="checkbox"/>
Check Required Permissions on the Installation Directory.	<input type="checkbox"/>
Install the EXTPROC Listener as a Windows Service.	<input type="checkbox"/>
Install the Direct Oracle Schema and Cartridge Objects.	<input type="checkbox"/>
Perform the <u>SYS</u> task.	<input type="checkbox"/>

Chapter 5:

Installing Direct

This chapter explains the tasks required to install Direct 2021 on an Intel or Intel-compatible computer that runs the Microsoft Windows Server 64-bit operating system.

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 installer(s).

Direct is supplied as a ZIP file. This provides access to a Pre-Installation License Validation tool and 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.

Note: The Pre-Installation License Validation Wizard requires Visual C++ 2013 runtime library or later on Windows systems. If this is not available on the machine where you run the wizard it will be installed automatically before license validation proceeds. If there are restrictions on installing additional libraries on the machines where Direct will be installed you can perform the license validation on another machine and subsequently transfer the resulting installer archive(s).

1. Log on to the destination computer as an administrator.
2. Extract BIOVIA_Direct_2021_Package.zip to unpack the Pre-Installation License Validation Wizard.
Navigate to the extracted directory.
3. Double-click on the BIOVIA_Direct_2021_Package.exe to run the Pre-Installation License Validation Wizard.
4. Click **Next** to begin the license validation.
5. If the wizard detects that Visual C++ 2013 or later is not available:
 - a. Ensure that the "Visual C++ Redistributable for Visual Studio" checkbox is checked and click **Next** to install it.
 - b. Review the terms and conditions and, if you are satisfied, check the "I agree to the License terms and conditions" checkbox, and click **Install**.
 - c. Wait for the installation of Visual C++ 2013 to complete, then click **Close**.
6. Click **Browse...** and select your license file, click **Next** to check that you are licensed to install Direct. If the validation fails, a message reports the reason for failure. Reasons for failure to validate include:
 - License file does not apply to the product.
 - The license file has expired.

- The file specified is not a valid license.

Tip: If you attempt to run the Pre-Installation License Validation Wizard without having extracted it from the ZIP archive, the license file will fail validation.

- To extract the installation archive(s) to a location other than the default, click **Browse...** and choose the destination folder.
- Click **Next**.
- Click **Extract** to complete the wizard and obtain the installation archive(s).
The wizard will report its progress.
- When the process is complete, click **Finish**.

The Direct Pre-Installation License Validation Wizard will create the installation archive(s) in the specified directory. You should use these archive(s) to continue the installation procedure.

Permissions Required to Install Direct

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

Task	Owner	Permission required
Install the Direct files.	User who will own the Direct 2021 files	The User who will own the Direct 2021 application files must have read and write permissions on the directory into which Direct will be installed.
Configure the Direct Oracle schema.	Oracle DBA	Oracle DBA

Install Direct

Unpack the Direct 2021 Application ZIP File

Permissions required: Log in as the user who will own the Direct files, for example BIOVIA.

- Extract the `direct2021_windows.zip` file to your BIOVIA Direct2021 installation directory.
BIOVIA recommends that you use the directory name `direct2021` for the installation directory.

Modify the Direct Application Files

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

- Make a backup copy of the file `C:\BIOVIA\direct2021\sql\mkdirect.sql`. This file will be used to create the Oracle schema that holds the BIOVIA Direct 2021 cartridge objects.
- Open the file `C:\BIOVIA\direct2021\sql\mkdirect.sql` in a text editor.
- 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.

IMPORTANT! 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*, then 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 `C:\BIOVIA\direct2021\sql\mdl1libdef.sql`. This file will be executed as part of the main installation SQL script.
6. Open the file `C:\BIOVIA\direct2021\sql\mdl1libdef.sql` in a text editor.
7. Locate the CREATE OR REPLACE LIBRARY statement in the file:

```
create or replace library mdlirect is
'directory/mdlirect.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 `C:\BIOVIA\direct2021` the modified CREATE LIBRARY statement will look like this:

```
create or replace library mdlirect is
'C:\BIOVIA\direct2021\<binNumber>\mdlirect.dll' AGENT 'DIRECT2021_
AGENT';
```

Depending on which version of Oracle you run, replace *<binNumber>* with a directory with the corresponding version number. For example, use *bin19* with Oracle 19 and *bin12* with Oracle 12.

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, 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 these required references, so copy it to your configuration file and make edits to it only where directed.

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

1. Make backup copies of the *listener.ora* and *tnsnames.ora* files. These files are located by default in the %ORACLE_HOME%\network\admin directory, but might be in a different directory in your environment.
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 = c:\Oracle\product\<OracleVersion>\dbhome_1)
      (PROGRAM = extproc)
      (ENVS = "EXTPROC_DLLS=ANY,PATH=C:\BIOVIA\direct2021\<binNumber>")
    )
  )
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 `windows_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 backslash at the end of the path.
5. The PATH environment variable entry in the ENVS line includes the path to the BIOVIA Direct 2021 bin directory (<binNumber>). This path must be modified to match your Direct bin directory. For example, use bin19 with Oracle 19 and bin12 with Oracle 12. Omit the backslash at the end of the path entry.
6. Save the modified *listener.ora* file.

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

7. Open the *tnsnames.ora* file in a text editor
8. 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: If you have problems copying these text sections you can also find them in the file `add_to_tnsnames.ora.txt` located in the `examples\extproc_configuration_files` subdirectory of the Direct installation directory.

9. Save the modified file.

Check Required Permissions on the Installation Directory

When calling BIOVIA Direct functions in Oracle, the Oracle EXTPROC listener starts the Oracle-provided executable EXTPROC which subsequently loads the Direct library into memory. The Oracle EXTPROC process must have read and execute permissions on the Direct files located in the installation directory to function. You must therefore grant read and execute permissions on the Direct installation directory and its sub-directories to the operating system user that runs the Oracle EXTPROC listener.

On the Windows platform, Oracle enforces the installation of the database into a particular operating system account, such as *Oracle*, and runs the database and its listeners from this account by default. Oracle also allows you to run the database and listeners from the privileged SYSTEM account.

Identify the user that runs the database and grant read and execute privileges on the Direct installation directory and all of its subfolders and files to that user.

Install the EXTPROC Listener as a Windows Service

With all required file modifications made and permissions set correctly on the BIOVIA Direct installation directory, you can now install the new EXTPROC listener as a Windows Service.

1. Open a command prompt with Administrator privileges.
2. Run the command:

```
C:\>lsnrctl start DIRECT2021
```

You will be prompted to enter the password of the user that runs the Oracle database. The `lsnrctl` program then creates the Windows listener service for Direct and configures it to run from the Oracle database user account. It then starts the service. After the successful start of the service you get the following output:

```

Connecting to (DESCRIPTION=(ADDRESS=(PROTOCOL=IPC)(KEY=DIRECT2021)))
STATUS of the LISTENER
-----
Alias                     DIRECT2021
Version                  TNSLSNR for 64-bit windows: Version 19.0.0.0.0 -
Production
Start Date               07-AUG-2020 16:05:34
Uptime                   1 days 10 hr. 58 min. 27 sec
Trace Level              off
Security                 ON: Local OS Authentication
SNMP                     OFF
Listener Parameter File  c:\Oracle\product\19c\dbhome_
1\network\admin\listener.ora
Listener Log File        c:\Oracle\diag\tnslsnr\myserver\direct2021>alert\log.xml
Listening Endpoints Summary...
  (DESCRIPTION=(ADDRESS=(PROTOCOL=ipc)(PIPENAME=\\.\pipe\DIRECT2021ipc)))

```

```

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

```

You can now start the Windows Services console and configure the new EXTPROC Windows service to run from a non-privileged account, a *secure extproc listener*. If you do so, confirm that you have set the read and execute permission on the Direct installation directory as described in [Check Required Permissions on the Installation Directory](#). You might also want to configure the service to start up automatically at system startup. The Windows service name is typically `OracleOraDb12g_home1TNSListenerDIRECT2021`.

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.

To do so follow these steps:

1. Open a command prompt and change to the SQL subdirectory of your Direct installation directory, for example, `C:\BIOVIA\direct2021\sql`.
2. Login to an Oracle DBA account using `SQL*PLUS` and run the `mkdirect.sql` script to create the user that will hold the Direct cartridge objects:

```
C:\BIOVIA\direct2021\sql>sqlplus system/systempw @mkdirect.sql
```

3. 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.

4. Login to the Oracle user `c$direct2021` that holds the BIOVIA Direct cartridge objects, and run the `mdlinst_all.sql` script.

```
C:\BIOVIA\direct2021\sql>sqlplus c$direct2021/direct @mdlinst_all.sql
```

Note: The default password for the `C$DIRECT2021` user is *direct* but you might have changed it as described in [Modify the Direct Application Files](#). 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 databases and safeguards maintenance operations.

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

```
C:\BIOVIA\direct2021\sql> sqlplus sys/syspw as sysdba
SQL> @mdlsysactions.sql
```
3. Log out of SQL*Plus.

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:

```
> 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;
```

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

```

                                VERSION
-----
                                BIOVIA Direct
                                Revision 2021 (Microsoft windows Oracle19) (21.1.0.x)

                                Copyright (c) Dassault Systèmes 1999-2020
```

4. Exit SQL*Plus:

```
SQL> EXIT
```

If the Installation Fails

If the verification step above yields one or more errors, then the error is most likely in the configuration of the `listener.ora` file.

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
- [Verify the Direct installation](#)
- [Modify the UniProtConverter.bat file](#)

- [Customizing SETPATH](#)
- (Optional) Install Direct in additional Oracle instances

These tasks are explained in the sections that follow.

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

Enable Oracle Users to Run Direct

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*:

```
C:\> 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$DIRECT2021'
2      and synonym_name in (select synonym_name from c$direct2021.mdl_
synonym_defs);
```

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

6. Exit SQL*Plus.

```
SQL> exit
```

Modify the UniProtConverter.bat File

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

1. Open and edit the file `drive:\BIOVIA\direct2021\<binNumber>\uniprotconverter.bat`. The `<binNumber>` corresponds with the version of Oracle you are using. For example, use `bin19` with Oracle 19 and `bin12` with Oracle 12.
2. Change the value of the environment variable `JAVA` to the location of your Java executable, for example, `C:\Program Files\Java\jre1.7.0_10\bin\java`.
3. Save and close the file.

Customizing SETPATH

1. Open a text editor and edit the `setpath.bat` file.

The `setpath` file is placed into the following directory by the installer:

```
C:\BIOVIA\direct2021\<binNumber>
```

Replace `<binNumber>` with the corresponding Oracle version. For example, use `bin19` with Oracle 19 and `bin12` with Oracle 12.

2. If the path name to the `<binNumber>` directory is not correct in the second line of `setpath.bat`, replace it with the correct path.
3. Save and close the file.

Chapter 6:

Setting Up the Direct Demonstration Database

This chapter explains how to set up the demonstration databases and tables that BIOVIA supplies with Direct 2021.

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 file DCSAMPLES.DMP contains a user export of the DCSAMPLES schema. The .dmp file includes a:

- 2D molecule table (SAMPLE2D)
- reaction database that includes a reaction table (SAMPLERX_REACTION) and hierarchical data tables
- generic structure table (SAMPLEGEN)
- biopolymer sequence table (SAMPLEBIO)
- 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.

Do This	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 database tables	<input type="checkbox"/>
Import the Oracle DCSAMPLES.DMP file	For more information, see Import the Oracle DCSAMPLES.DMP file	<input type="checkbox"/>
Test the SAMPLE2D database	For more information, see Molecule verification	<input type="checkbox"/>
Test the SAMPLERX database	For more information, see Reaction verification	<input type="checkbox"/>

Each of these tasks is explained in detail in the sections that follow.

Create a New Oracle Schema for the 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, use any name you choose. To load 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 'C:\temp';
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 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.

- For example, 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_tablespace
```
- 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_tablespace
```

Once imported, the five databases contain the following objects:

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_MOLTABLE
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,

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 <code>testsamp1egen.sql</code> for examples of searching.	
Biopolymer sequence molecule database	
SAMPLEBIO	Biopolymer structure table
SAMPLEBIO_IX	Direct molecule domain index on CTAB
For examples of searching, see the file <code>testsamp1egen.sql</code> .	

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 DataSource connectors for these databases. It does not need editing. This file is intended for demonstration purposes only, its 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:
`C:\BIOVIA\isentris2020\system\config\datasource\dsfiles`
2. After copying, open any editor that allows you edit XML, 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.

Note: 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.

Verifying Demonstration Database and Tables Installation

Molecule verification

The following tests (and more) are listed in the `testsample2d.sql` file located in the `C:\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, 'C:\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

Tip: The following tests (and more) are listed in the `testsamplerx.sql` file located in the `C:\BIOVIA\direct2021\examples` directory. You can run this file instead of running the following tests manually.

Note: The example reaction files must be made read-accessible from the operating system account under which the Oracle extproc listener run. Errors occur if this is not done.

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,
'C:\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,
'C:\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, 'C:\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('C:\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, 'C:\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
```

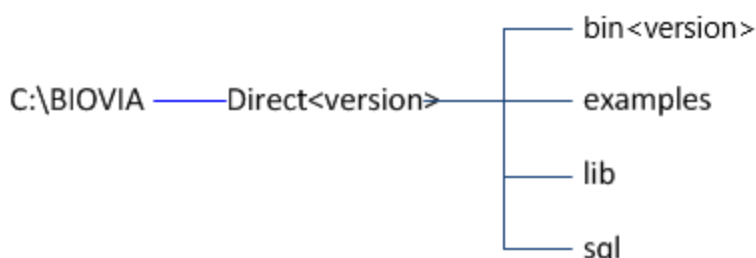
Chapter 7:

Direct File Configuration on Windows

This chapter explains the configuration of the molecule and reaction cartridge files on Microsoft Windows, assuming that you have installed BIOVIA Direct to C:\BIOVIA\direct2021.

Direct Folder Hierarchy

When you unpack the Direct 2021 files, files are placed into the folder hierarchy shown below.



Files and Folders

This section explains the case sensitivity and limitations in using file names and folder names.

Case Sensitivity of File Names and Folder Names

References to file names and folder names on Windows are not case sensitive.

Mixed case names are used in Windows to improve readability. File names read into the Direct are not altered with respect to case. Windows also accepts file names and folder names that contain mixed case letters (that is, both uppercase and lowercase).

You must not include spaces in the names of files or folders that are created by or used by the data cartridge as this will cause erratic program behavior. To improve readability, use underscores in file names and folder names.

Explanation of Folders and Files

Directory or file	Contents
%ORACLE_HOME%\network\admin	Oracle listener configuration directory
listener.ora tnsnames.ora	Oracle network administration files that must be present for use with the extproc listener
C:\BIOVIA\direct2021	Direct 2021 cartridge files
C:\BIOVIA\direct2021\bin12	Binary executable files for Oracle 12c installation
directupgrade.exe	The utility to use when migrating Direct 6, 7, or 8 databases to 2021.

Directory or file	Contents
mdlirect.dll	Primary shared object library that contains the Direct cartridge routines.
exportRDFFile.exe exportSDFFile.exe importRDFFileEx.exe importRDFFile.exe importSDFFile.exe setpath.bat	Import and export utilities for SDFiles and RDFiles.
UniProtConverter.bat	Batch file to run the UniProt Converter Utility
pilot.dll pilotCore.dll ppChemNema.dll ppChemSageCoords.dll ppOpenEye.dll	Foundation files
C:\BIOVIA\direct2021\examples	Sample applications and demonstration databases
DCSAMPLES.DMP	Demonstration database import file
direct_dcsamples_ids.xml direct_dcsamples_relational.xml	Data source definition files for use with Isentris applications
rdcapps.sql	SQL script that runs sample applications to read a RDFFile and create a cross-reference trigger
readme_dcsamples.txt	Instructions on setting up the DCSAMPLES dump file
testsample2d.sql testsamplelx.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 molfiles used in testsamplelx.sql
rxnfiles	Directory containing rxnfiles used in testsamplelx.sql
extproc_configuration_files	Example EXTPROC configuration files
C:\BIOVIA\direct2021\lib	Shared objects
ccatlib.dll Cheshire.jar CheshireJNI.jar ojdbc6.jar UniProtConverter.jar	Cheshire shared library and jar files used by UniProt Converter
C:\BIOVIA\direct2021\sql	Direct 2021 SQL files
mkdirect.sql	SQL used to create the cartridge user and public database link.

Directory or file	Contents
mdl1libdef.sql	Contains the path to mdlldirect.dll and is used to create the shared object library that uses the public database link.
mdl1inst_all.sql	Install all components of the Direct 2021 data cartridge.
mdluninst.sql	Uninstalls the Direct 2021 data cartridge.

Chapter 8:

Removing Direct

Before Removing Direct

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

- [Alert Users That Direct Will Not Be Available](#)
- [Close Any Applications That Use Direct](#)
- [Back Up Direct Files](#)
- [Removing Direct](#)

Alert Users

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 all applications that use Direct.

Back Up Direct Files

Make a back up copy of the Direct files prior to removing 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 2021 schema owner.

1. From a Command Prompt window, log into SQL*Plus:
`C:\ sqlplus c$direct2021/password`
2. Run `mdluninst.sql`:
`SQL> @C:\BIOVIA\direct2021\sql\mdluninst.sql`

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

1. Drop the `c$direct2021` user and the schema objects:
`SQL> drop user c$direct2021 cascade;`
2. Drop the public database link:
`SQL> drop public database link DIRECT2021_AGENT;`

3. Exit SQL*Plus.

```
SQL> exit
```

Drop the Demonstration Database Schema

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

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

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

```
C:\ 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 Direct 2021.

IMPORTANT! If you have files that you have modified in any of the files in the folders under C:\BIOVIA\direct2021, that you want to keep for later installations, be sure to save a copy of the file before you delete the folder.

Chapter 9:

Setting 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 a Direct Installation During an 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.

How to Protect Your Direct Databases 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. Remove Direct 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 `c$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

Back up 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. Remove 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:

Configuring Multiple Direct Versions on the Same System

BIOVIA Direct 2021 is installed 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

An Oracle user account can only be set up to run 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 will invoke only the Direct 2021 cartridge, regardless of the presence of other versions of Direct in the Oracle instance.