INSTALLATION GUIDE
BIOVIA DIRECT COMPATIBLE DATABASES
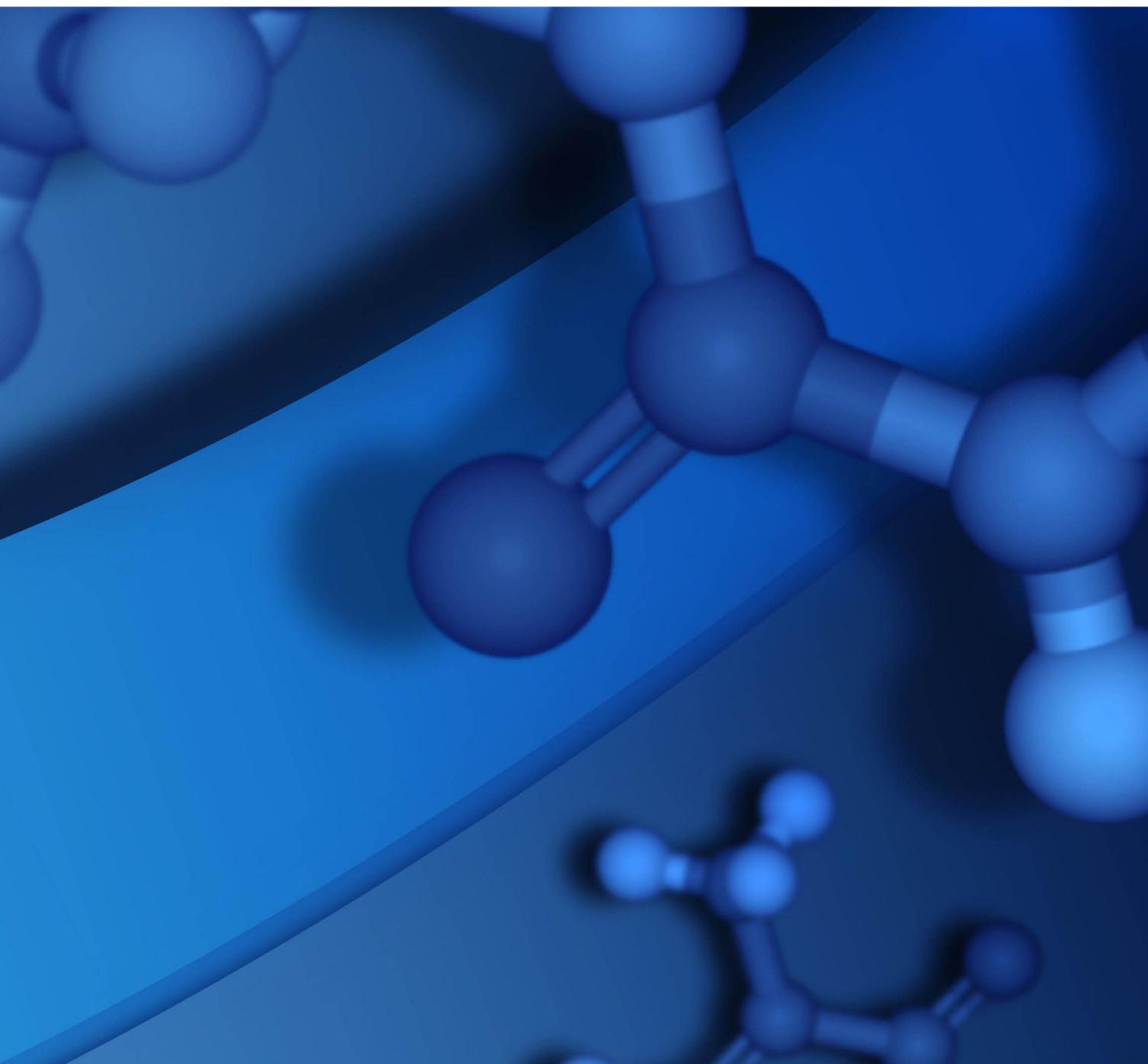
Acknowledgments and References

To print photographs or files of computational results (figures and/or data) obtained by using Dassault Systèmes software, acknowledge the source in an appropriate format. For example:

> "Computational results were obtained by using Dassault Systèmes BIOVIA software programs. DiscoveryGate Web Service was used to perform the calculations and to generate the graphical results."

Dassault Systèmes may grant permission to republish or reprint its copyrighted materials. Requests should be submitted to Dassault Systèmes Customer Support, either by visiting https://www.3ds.com/support/ and clicking **Call us** or **Submit a request**, or by writing to:

Dassault Systèmes Customer Support
10, Rue Marcel Dassault
78140 Vélizy-Villacoublay
FRANCE

Contents

Overview

BIOVIA distributes its commercial BIOVIA Direct compatible databases as Oracle export files. BIOVIA database releases are cumulative.

These databases contain chemical structures, reactions, and related data. They can be installed on computers that run Linux or Microsoft Windows operating systems.

For additional details on the hardware and operating systems that are supported for BIOVIA Direct, refer to the *BIOVIA Direct System Requirements* document.

> **Note:** Databases formatted for a particular version of BIOVIA Direct are compatible only with that version of Direct. For example, databases in the Direct 2017 format are compatible only with Direct 2017. Databases in the Direct 2019 format are compatible only with Direct 2019 and so on.

About this Guide

This guide explains how to install databases that are compatible with BIOVIA Direct.

Intended Audience

This document is intended for the system administrator who will install the BIOVIA Direct compatible databases.

Prerequisite Knowledge

This document assumes that you are familiar with the operating system on the computer on which you are installing the BIOVIA Direct compatible databases.

Document Conventions and Special Symbols

Convention or Symbol	Example
Examples of operating-system commands and file listings that form separate paragraphs in the guide use a fixed-width font.	`$ env	grep NLS_LANG`
Examples use italic type to represent information that is variable.	`$ sqlplus` *`username/password`*
Examples that show your dialog with a program use fixed-width font and regular type to represent program prompts and other output. Bold type represents your input.	`SQL>` **`commit;`**
Examples that show your dialog with a program use bold italic type to represent input that is variable.	`$ chown` ***`owner file`***
Examples of commands and other items that you choose graphically when interacting with Direct or respective operating systems are shown in bold font. The greater than sign **>** indicates a cascading menu.	**Start > Programs > Windows Explorer**
This symbol indicates the primary command prompt for the Korn shell for a user other than `root`.	`$`
This symbol indicates the primary command prompt for the C shell for a user other than `root`.	`%`
This symbol indicates the primary command prompt for the Korn shell for the user `root`.	`#`
Command prompt for Windows operating systems. Windows displays the path to the current folder followed by a greater than sign.	`>`

Note: When the same command is valid for both the Korn shell and the C shell, the command is given only once and uses the Korn shell prompts.

Where to Install BIOVIA Direct Compatible Databases

You must install these databases into an Oracle instance that contains the BIOVIA Direct Oracle data cartridge.

Zip File Contents

The first `.zip` file contains this document, one or more Oracle export (`.dmp`) files, and other support files. Any remaining `.zip` files contain `.dmp` files. For more information, see Files Present for all Databases.

Data Pump Import

Data Pump Import is the fastest way to import Oracle export files. Export files suitable for a data pump import are not suitable for a traditional import and export files suitable for a traditional import cannot be imported using the data pump utility. BIOVIA provides data pump import files for all products and the import parameter file (`.par` file) is named *Dbname*`direct_dp.par`.

Files Present for all Databases

After you extract the `.zip` files, you will see the following files:

- *Dbname*`direct`*VersionNumber*`.dmp`

  Oracle export file that contains the tables, indexes, and any views and functions for the database that is being installed.

  For example, `toxdirect20192.dmp`. If there is more than one `.dmp` file, the files will have additional numbering, for example, `scddirect20192-1.dmp`, `scddirect20192-2.dmp`, and so on.

- *Dbname*`direct_dp.par`

  Parameter file that is used for the data pump import. Data Pump Import (invoked with the `impdp` command) is a new utility as of Oracle Database 10g. Although its functionality and its parameters are similar to those of the original Import utility (`imp`), they are completely separate utilities and their files are not compatible.

- `drop_db.sql`

  Oracle SQL script that drops the objects in an existing database.

- `tbl_inddirect.lst`

  Text file that lists the size of each table and index contained in the export file. Use it to estimate the tablespace requirements for the database.

- `readme.txt`

  Text file that contains information specific to the database release.

Additional Files for BIOVIA ACD and BIOVIA SCD

The following additional files are only present for BIOVIA Available Chemicals Directory (ACD) and BIOVIA Screening Compounds Directory (SCD).

- `catalogs.pdf`

  PDF that contains the chemical suppliers' company names and company CODENs. It also contains the names, dates, and versions of the catalogs that were included in the database.

- `catalogs.txt`

Text file that contains the chemical suppliers' company names and company CODENs. It also contains the names, dates, and versions of the catalogs that were included in the database.

- `mdldiff.txt`

  Text file that contains a list of changes, deletions, and additions to MDLNUMBER assignments for each chemical-supplier product and catalog number. The changes are those that were made between the immediately previous version of the database and the current version.

- `acd_scd_direct_book.pdf`

  PDF that explains the data model.

Additional Files for MDDR

The following additional file is present only for MDDR.

- `activity.txt`

  Text file that contains definitions of codes that specify biological and therapeutic activities for chemical substances.

Installing BIOVIA Direct Compatible Databases on Linux-based Servers

This section explains how to install BIOVIA Direct compatible databases on **Oracle Solaris**, **Red Hat Linux**, or **SuSE Linux**.

> **Note:** The text files in the databases use the linefeed convention. That is, the lines are terminated using a single character. You can open text files with the default editor (for example, `vi` for UNIX). If you edit text files through a Microsoft Windows operating environment, you must use WordPad. To open files that use NotePad as the default editor (for example, `.txt` files), open WordPad, and then navigate to the file using the **File > Open** menu commands.

Preinstallation Tasks

Before you install the database, perform the following preinstallation tasks:

Verify the Prerequisites for the Installation

The Oracle instance in which you are installing the database must:

- Contain the appropriate BIOVIA Direct data cartridge
- Have sufficient free space

You can estimate the required tablespace size by referring to the customer letter or to the file `tbl_inddirect.lst`.

> **Note:** Tablespace sizes can vary among different Oracle instances. The amount of free space required to hold the database can be larger if tablespace fragmentation is significant. Therefore, the tablespace requirements mentioned in `tbl_inddirect.lst` and the product release document are estimates taken from our own installations and might underestimate or overestimate those at your site. BIOVIA recommends that you allow 10-20% additional tablespace for each database.

Installing BIOVIA Databases for BIOVIA Direct

BIOVIA delivers Direct compatible databases as `.zip` files. After you unzip the `.zip` file(s), you see the Oracle export file(s) that contain the data for the database and other files.

These topics explain how to install the databases on an **Oracle Solaris**, **Red Hat Linux**, or **SuSE Linux** computer into a directory on a disk to which that computer has access. Perform these tasks in the order in which they appear.

Create an Oracle User Who Will Own the Database

> **Note:** If you have already created an Oracle user who will own the database, you can skip this step.

1. Start SQL*Plus and log in as a user with Oracle DBA privileges. The syntax for the command to run SQL*Plus will differ depending on your operating-system and Oracle version.

2. Create the user:

   ```
    SQL> CREATE USER username IDENTIFIED BY password
    2 DEFAULT TABLESPACE tablespace_name
    3 TEMPORARY TABLESPACE temp_tablespace_name;
   ```

3. Grant privileges to the user:

   ```
   SQL> GRANT CONNECT, RESOURCE TO username;
   ```

   ```
   SQL> GRANT CREATE VIEW TO username;
   ```

   ```
   SQL> GRANT CREATE SYNONYM TO username;
   ```

4. Revoke the `UNLIMITED TABLESPACE` privilege from the user:

   ```
   SQL> REVOKE UNLIMITED TABLESPACE FROM username;
   ```

5. Grant use of space in the user's default tablespace to the user:

   ```
   SQL> ALTER USER username QUOTA quota_size ON tablespace_name;
   ```

   where *quota_size* is at least equal to the tablespace size. For example:

   ```
   SQL> ALTER USER acd201907 QUOTA UNLIMITED ON ACD_DATA;
   ```

6. Exit SQL*Plus:

   ```
   SQL> exit
   ```

> **Tip:** If you reuse the database username and password every time you install the database, the Isentris administrator will not need to update the IDS files with each release. See Configuring the Isentris IDS Files

Create a Directory Object for Data Pump File Import

1. Start SQL*Plus and log in as a user with Oracle DBA privileges.
2. Create the Oracle directory object corresponding to the OS directory where data pump dump files are located.

   ```
   SQL>create or replace directory directory_name as '/usr/db/subdir';
   ```

   where *directory_name* is the name given to the Oracle directory object. For example:

   ```
   SQL>create or replace directory dpimp as '/usr/db/direct';
   ```

3. Grant the Oracle directory object Read and Write privileges.

   ```
   SQL>grant read,write on directory directory_name to username;
   ```

   where *directory_name* is the name given to the Oracle directory object and where *username* is the user who will own the database. For example:

   ```
   SQL>grant read,write on directory dpimp to acd201907;
   ```

4. Grant `Read` and `Write` privileges to the operating system directory corresponding to the Oracle directory object.

Empty the Existing Database Schema and Prepare for Data Pump Import

If you have a previous database installation and want to install into the **same schema**, remove the objects before you import the database export files.

> **IMPORTANT!** The SQL script, `drop_db.sql`, is designed to drop all objects from a Direct schema in order to ready it for import of a new database version. Therefore, BIOVIA recommends that you do not store custom objects in your database schema that are meant to persist from release to release. If you do intend to store permanent objects in the database schema, then you must modify `drop_db.sql` not to drop these objects or choose some other means to prepare the schema for import.

1. Start SQL*Plus and log in as the user who owns the database:

   ```
   $ sqlplus username/password
   ```

2. Run the script `drop_db.sql` to drop the schema objects:

   ```
   SQL>@drop_db.sql
   ```

3. *(Optional)* To free tablespace that is occupied by the previous database version, type:

   ```
   SQL>purge recyclebin;
   SQL>exit
   ```

4. Use the correct NFS mount parameters. You can skip this step if the export files (`.dmp`) do not reside on an NFS. If the export files reside on an NFS mount, be sure the NFS mount is mounted with the following parameters so that Oracle will recognize it:

   ```
   $ mount rw,bg,intr, hard,timeo=600, wsize=32768, rsize=32768
   ```

Otherwise, Oracle error `ORA-27054` (`NFS file system where the file is created or resides is not mounted with correct options`) will occur even though the location of the export files was correctly specified when the directory object was created.

5. Verify that Oracle can create the log file. Oracle requires a UNIX user, for example, oradba. The import creates a log file owned by this user. Therefore, this user must have sufficient permission to create the import log file.

   For example, if the UNIX username for Oracle is `oradba`, and the log file is created in directory `/usr/db/direct`, then `oradba` must have write permission on the install directory. If `oradba` is not the owner of the install directory then:

   ```
   $ chmod 777 /usr/db/direct
   ```

   ensures that the log file will be created without problems.

   > **Note:** Oracle error `ORA-29283` (`invalid file operation`) indicates that a permission problem occurred when creating the log file.

Import the Database Export Files

> **Tip:** To install BIOVIA ACD and SCD, 1 GB of rollback is required. For other BIOVIA Direct compatible databases, less than 150 MB is required.

> **Note:** Verify that you have extracted all the files. All of the `.dmp` files are required for the import to succeed. Use the Oracle Import utility to import the database export files:

1. Edit the parameter file:

   > **Note:** The parameter file is named *Dbname*`direct_dp.par.`

   a. For each export file, precede the name with the full path, if the location of the export file is different than that of the parfile.

   b. Specify the name of the log file. Precede the name with the full path, if you want the log file location to differ from that of the parfile.

   c. Specify *username* in the `REMAP_SCHEMA` parameter and specify `tablespace_name` in the `REMAP_TABLESPACE` parameter.

   For example, if your ACD schema name is `acd` and the tablespace name is `acd_dbs`, the first two lines of `acddirect_dp.par` must be:

   ```
   remap_schema=acd201907:acd
   remap_tablespace=mdl_data:acd_dbs
   ```

2. Import the export files by entering the appropriate command at the operating-system prompt.

   ```
   $ impdp userid=username/password parfile=parameter_filename
   directory=dpimp
   ```

   where *username* is the Oracle username and *password* is the Oracle password, dpimp is the name of the Oracle directory object created in the previous procedure called Create directory object for data pump file import.

   If the import displays the warning message `ORA-30036`, this indicates that one or more tables failed to load due to insufficient rollback space and you must redo the import. To enable the import to succeed, increase the rollback.

The following errors will appear if you try to use the traditional import (`IMP`) utility on data pump dump files:

```
IMP-00010: not a valid export file, header failed verification
IMP-00000: Import terminated unsuccessfully
```

You can ignore the following message if it appears during import.

```
Note: table contains ROWID column, values may be obsolete 107490 rows
imported
```

3. After you have successfully created the database, you can delete the export files from your system.

> **Tip:** Importing the database could take a few minutes to many hours. If importing the database seems to take an excessive amount of time, adjusting the Oracle parameter `sort_area_size` could improve performance.

Post-Installation Tasks

If there are users who access the databases using Isentris and/or Insight, the administrators for those systems may need to perform additional configuration tasks. Therefore, it is a best-practice recommendation for the database administrator to notify the Isentris and Insight administrators after any database update.

For more information, see Configuring Isentris and Insight for BIOVIA Direct Compatible Databases.

Installing BIOVIA Direct Compatible Databases on Microsoft Windows Server

This section explains how to install BIOVIA Direct compatible databases on Microsoft Windows Server.

Additional details on the Windows operating systems that we support for BIOVIA Direct are in your BIOVIA Direct System Requirements document.

> **Note:** The text files in the BIOVIA Direct compatible databases use the UNIX linefeed convention. That is, the lines are terminated using a single character. You can open the text files with the default editor (for example, `vi` for OpenNT). If you edit text files through a Microsoft Windows operating environment, you must use WordPad. To open files that use NotePad as the default editor (for example, `.txt` files), open WordPad, and then navigate to the file using the **File > Open** menu commands.

Preinstallation Tasks

Before you install the database, perform the following preinstallation tasks:

Verify the Prerequisites for the Installation

The Oracle instance in which you are installing the database must:

- Contain the appropriate BIOVIA Direct data cartridge
- Have sufficient free space

You can estimate the required tablespace size by referring to the customer letter or to the file `tbl_inddirect.lst`.

> **Note:** Tablespace sizes can vary among different Oracle instances. The amount of free space required to hold the database can be larger if tablespace fragmentation is significant. Therefore, the tablespace requirements mentioned in `tbl_inddirect.lst` and the product release document are estimates taken from our own installations and might underestimate or overestimate those at your site. BIOVIA recommends that you allow 10-20% additional tablespace for each database.

Installing BIOVIA Databases for BIOVIA Direct

BIOVIA delivers BIOVIA Direct databases as `.zip` files. After you unzip the `.zip` file(s), you see the Oracle export file(s) that contain the data for the database and other files.

This section explains how to install BIOVIA databases from a **Microsoft Windows Server** computer to a folder on a disk to which that computer has access. Perform these tasks in the order in which they appear.

Create an Oracle User Who Will Own the Database

> **Note:** If you have already created an Oracle user who will own the database, you can skip this step.

1. Start SQL*Plus and log in as a user with Oracle DBA privileges. The syntax for the command to run SQL*Plus will differ depending on your operating-system and Oracle version.

2. Create the user:

   ```
    SQL> CREATE USER username IDENTIFIED BY password
    2 DEFAULT TABLESPACE tablespace_name
    3 TEMPORARY TABLESPACE temp_tablespace_name;
   ```

3. Grant privileges to the user:

   ```
   SQL> GRANT CONNECT, RESOURCE TO username;
   ```

   ```
   SQL> GRANT CREATE VIEW TO username;
   ```

   ```
   SQL> GRANT CREATE SYNONYM TO username;
   ```

4. Revoke the `UNLIMITED TABLESPACE` privilege from the user:

   ```
   SQL> REVOKE UNLIMITED TABLESPACE FROM username;
   ```

5. Grant use of space in the user's default tablespace to the user:

   ```
   SQL> ALTER USER username QUOTA quota_size ON tablespace_name;
   ```

   where *quota_size* is at least equal to the tablespace size. For example:

   ```
   SQL> ALTER USER acd201907 QUOTA UNLIMITED ON ACD_DATA;
   ```

6. Exit SQL*Plus:

    `SQL> exit`

> **Tip:** If you reuse the database username and password every time you install the database, the Isentris administrator will not need to update the IDS files with each release. See Configuring the Isentris IDS Files

Create a Directory Object for Data Pump File Import

1. Start SQL*Plus and log in as a user with Oracle DBA privileges.

2. Create the Oracle directory object corresponding to the OS directory where data pump dump files are located.

    `SQL>create or replace directory directory_name as 'C:\db\subdir';`

    where *directory_name* is the name given to the Oracle directory object. For example:

    `SQL>create or replace directory dpimp as 'C:\db\direct';`

3. Grant the Oracle directory object Read and Write privileges.

    `SQL>grant read,write on directory directory_name to username;`

    where *directory_name* is the name given to the Oracle directory object and where *username* is the user who will own the database. For example:

    `SQL>grant read,write on directory dpimp to acd201907;`

4. Grant `Read` and `Write` privileges to the operating system directory corresponding to the Oracle directory object.

Empty Existing Database Schema

If you have a previous database installation and want to install into the **same schema**, remove the objects before you import the database export files.

> **IMPORTANT!** The SQL script, `drop_db.sql`, is designed to drop all objects from a Direct schema in order to ready it for import of a new database version. Therefore, BIOVIA recommends that you do not store custom objects in your database schema that are meant to persist from release to release. If you do intend to store permanent objects in the database schema, then you must modify `drop_db.sql` not to drop these objects or choose some other means to prepare the schema for import.

1. Start SQL*Plus and log in as the user who owns the database:

    `$ sqlplus username/password`

2. Run the script `drop_db.sql` to drop the schema objects:

    `SQL>@drop_db.sql`

3. *(Optional)* To free tablespace that is occupied by the previous database version, type:

    `SQL>purge recyclebin;`

    `SQL>exit`

Import the Database Export Files

> **Tip:** To install BIOVIA ACD and SCD, 1 GB of rollback is required. For other BIOVIA Direct compatible databases, less than 150 MB is required.

> **Note:** Verify that you have extracted all the files. All of the `.dmp` files are required for the import to succeed.

Use the Oracle Import utility to import the database export files:

1. Edit the parameter file *Dbname*`direct_dp.par`.

   a. For each export file, precede the name with the full path, if the location of the export file is different than that of the parfile.

   b. Specify the name of the log file. Precede the name with the full path, if you want the log file location to differ from that of the parfile.

   c. Specify *username* in the `REMAP_SCHEMA` parameter and specify *tablespace_name* in the `REMAP_TABLESPACE` parameter.

   For example, if your ACD schema name is `acd` and the tablespace name is `acd_dbs`, the first two lines of `acddirect_dp.par` must be:

   ```
   remap_schema=acd201907:acd
   remap_tablespace=mdl_data:acd_dbs
   ```

2. Import the export files by entering the appropriate command at the operating-system prompt.

   ```
   > impdp userid=username/password parfile=parameter_filename
   directory=dpimp
   ```

   where *username* is the Oracle username and *password* is the Oracle password, dpimp is the name of the Oracle directory object created in the previous procedure called Create directory object for data pump file import.

   If the import displays the warning message `ORA-30036`, this indicates that one or more tables failed to load due to insufficient rollback space and you must redo the import. To enable the import to succeed, increase the rollback.

   The following errors will appear if you try to use the traditional import (`IMP`) utility on data pump dump files:

   ```
   IMP-00010: not a valid export file, header failed verification
   IMP-00000: Import terminated unsuccessfully
   ```

   You can ignore the following message if it appears during import.

   ```
   Note: table contains ROWID column, values may be obsolete 107490 rows
   imported
   ```

3. After you have successfully created the database, you can delete the export files from your system.

> **Tip:** Importing the database could take a few minutes to many hours. If importing the database seems to take an excessive amount of time, adjusting the Oracle parameter `sort_area_size` could improve performance.

Post-Installation Tasks

If there are users who access the databases using Isentris and/or Insight, the administrators for those systems may need to perform additional configuration tasks. Therefore, it is a best-practice recommendation for the database administrator to notify the Isentris and Insight administrators after any database update.

For more information, see Configuring Isentris and Insight for BIOVIA Direct Compatible Databases.

Configuring Isentris and Insight for BIOVIA Direct Compatible Databases

This section explains the configuration tasks that Isentris and Insight administrators may need to perform after a database administrator installs the latest BIOVIA Direct compatible databases.

- If you are installing the database and accessing it with Isentris or Insight for the first time, contact Customer Support for more information on how to configure these applications.

- If you are installing a database update and the schema name, password, or Oracle database has changed, Isentris and Insight administrators must perform the configuration tasks outlined in this section.

- If the schema name, password, and Oracle instance are the same as for the previously installed database, Isentris and Insight administrators do not need to perform any configuration tasks.

Configuring Isentris IDS Files

When a database update is installed into Oracle, the Isentris administrator might need to update the IDS files with the latest information. For example:

- If the schema of the new release differs from that of the previous release, the schema name must be updated in the IDS files.
- If the database is installed into a different Oracle instance than the previous release, the Oracle connection information must be updated in the appropriate IDS file.

It is a best-practice recommendation for the database administrator to notify the Isentris administrator after any database update.

See the Isentris Administration documentation for information on configuring the IDS files.

Configuring Insight IDS and Forms

When a database update is installed into Oracle, the Insight administrator might need to update the relational data source (REL) files with the latest information. For example:

- If the schema of the new release differs from that of the previous release, the schema name must be updated in the REL files.
- If the database is installed into a different Oracle instance than the previous release, the Oracle connection information must be updated in the REL files.

It is a best-practice recommendation for the database administrator to notify the Insight administrator after any database update.

BIOVIA content database IDS files and Search and Browse forms are available at the
3DS Download Center, https://software.3ds.com, with BIOVIA Insight.