

Technical Note T21-2020

(Revised November 2020, Original Technical Note T103-2015)

Creating a Domain Index on BIOVIA Databases for Direct 2017R2, 2018, or Direct 2021

Program

BIOVIA Direct 2017 R2
BIOVIA Direct 2018
BIOVIA Direct 2021

Database

BIOVIA Available Chemicals Directory (ACD)
BIOVIA Screening Compounds Directory (SCD)
MDDR
BIOVIA Toxicity

Operating System

All operating systems supported with BIOVIA Direct

Description

BIOVIA currently provides its chemical sourcing databases (ACD, SCD) and its bioactivity databases (MDDR, Toxicity) in the formats for BIOVIA Direct 2017, 2019 and 2020. If you are running any of these BIOVIA Direct versions you can install the BIOVIA databases in their native formats (see further notes on Direct 2020 below).

If you however are running BIOVIA Direct 2017R2, 2018 (or 2021), you must first install the BIOVIA database in Direct 2017 (or 2020) format and subsequently update the chemistry domain index for your installed BIOVIA Direct version.

The databases in Direct 2020 format apply a **new representation for Haptic Bonds** and use the **Self Contained Sequence Representation (SCSR) for biological sequences**. For more information on these representations, see the *BIOVIA Chemical Representation* document from the BIOVIA Direct documentation package. If you are running BIOVIA Direct 2020 or 2021 but prefer the previous representation of haptic bonds and biological sequences, you must initially install the BIOVIA database in Direct 2019 format and then update the chemistry domain index for Direct 2020 or Direct 2021.

This Technical Note describes the workflow to perform the required domain index upgrades.

Note: BIOVIA databases are released in a particular BIOVIA Direct format only until the support of the particular BIOVIA Direct version in a regulated environment ends. The support timelines for BIOVIA Direct versions are outlined in the respective *BIOVIA Direct Product Release Document* or the BIOVIA Online Support Matrix at <https://supportmatrix01.biovionline.com/SIRMC>.

Resolution

Depending on the BIOVIA Direct version(s) installed in your Oracle database you must follow one of two scenarios. Which scenario to follow is described in the decision matrix below. Based on the decision then follow the detailed steps for either Scenario 1 or Scenario 2.

Table 1: Decision matrix for determining which Scenario to use.

Scenario 1		
This scenario applies under the following conditions		
<ul style="list-style-type: none"> a) The target Direct version is installed but does not match any of the database formats provided by BIOVIA or b) At least one additional Direct version is installed that matches one of the database formats provided by BIOVIA. 		
Target (primary) Direct version	Secondary Direct version	Database format to install
2017 R2 or 2018	Direct 2017 is installed	2017
2020 or 2021 with preference for previous chemical representation	Direct 2019 is installed	2019
2021	Direct 2020 is installed	2020

Scenario 2		
This scenario applies under the following conditions		
<ul style="list-style-type: none"> a) The target Direct version is installed but does not match any of the database formats provided by BIOVIA b) No additional Direct version is installed that matches one of the database formats provided by BIOVIA 		
Target (primary) Direct version	Secondary Direct version	Database format to install
2017 R2 or 2018	Direct 2017 is NOT installed	2017
2020 or 2021 with preference for previous chemical representation	Direct 2019 is NOT installed	2019
2021	Direct 2020 is NOT installed	2020

Scenario 1)

The workflow basically follows the steps as described in the chapter “**Upgrading Indexes**” in the BIOVIA Direct Administration Guide. The steps 2 through 6 should complete very fast in just seconds on most servers. The steps 1 and 7 may take some time to complete.

The following steps upgrade the BIOVIA ACD database as an example.

1. Install the BIOVIA database in the format that matches the secondary BIOVIA Direct installation in your environment. For details on loading the BIOVIA database into Oracle please consult the *BIOVIA_DirectCompatibleDatabases_InstallationGuide.pdf* file provided with the BIOVIA database.

2. Log in as your database schema owner:

```
sqlplus acd/*****
```

3. Drop existing synonyms for BIOVIA Direct:

```
SQL> execute mdlaux.unsetup  
PL/SQL procedure successfully completed.
```

4. Create the BIOVIA Direct synonyms for the installed target Direct version (i.e. 2017 R2, 2018, or 2021). Or if you want to upgrade Direct 2019 format to use the old representation with newer Direct versions, setup the synonyms for the target version.

```
SQL> execute c$direct2021.mdlauxop.setup  
PL/SQL procedure successfully completed.
```

5. Verify the version number for the target Direct version by executing the following SQL:

```
SQL> select mdlaux.version from dual;
```

```
VERSION
```

```
-----
```

```
BIOVIA Direct
```

```
Revision 2021 (Microsoft Windows Oracle12) (21.1.0.513)
```

```
Copyright (c) Dassault Systemes, 1999-2020
```

6. Upgrade the domain index:

```
SQL> select mdlaux.upgradeindexes_prepare from dual;
```

```
UPGRADEINDEXES_PREPARE
```

```
-----  
Prepared index for upgrade/recreate: ACD2D_MDLIX Table: ACD2D_MOLTABLE
```

```
SQL> select mdlaux.upgradeindexes_upgrade from dual;
```

```
UPGRADEINDEXES_UPGRADE
```

```
-----  
Created index: ACD2D_MDLIX
```

7. (When Upgrading to Direct 2021)

Run the `<dbname>_Direct2021_Update.sql` that is included in your download package, where `<dbname>` is your database name. The script will address the issue DIR-4107, that is explained in the *BIOVIA Direct 2021 Product Release Document* in more detail.

(When upgrading to Direct 2020 from Direct 2019)

Recreate Fastsearch. This step may take some time to complete.

```
SQL> execute mdlaux.recreatefastsearch('dbname_mdlix');  
where dbname_mdlix is the domain index name. For example,
```

```
SQL> execute mdlaux.recreatefastsearch('ACD2D_MDLIX');  
PL/SQL procedure successfully completed.
```

This completes the upgrade of the domain index to your target Direct version.

Scenario 2)

The following steps upgrade the BIOVIA ACD database as an example.

1. From the [Scenario 2 table](#) in page 2 above, find the database format you need, then download and install it. For details on loading the BIOVIA databases into Oracle please consult the *BIOVIA_DirectCompatibleDatabases_InstallationGuide.pdf* file provided with the BIOVIA databases.

As the database format you import does not match your installed BIOVIA Direct version(s) you will notice some errors during the datapump import of the data into Oracle. All objects will basically import successfully, but the domain index creation step will fail with errors similar to those below as the matching Direct version is not installed:

```
. . .  
Processing object type SCHEMA_EXPORT/TABLE/INDEX/DOMAIN_INDEX/INDEX  
ORA-39083: Object type INDEX:"ACD"."ACD2D_MDLIX" failed to create with error:  
ORA-29833: indextype does not exist  
Failing sql is:  
CREATE INDEX "ACD"."ACD2D_MDLIX" ON "ACD"."ACD2D_MOLTABLE" ("CTAB")  
INDEXTYPE IS "C$DIRECT2017"."MXIXMDL" ...
```

Additionally, you might see the following error if the Oracle schema is already enabled for your target BIOVIA Direct version.

```
ORA-31684: Object type SYNONYM:"ACD"."MDLAUX" already exists
```

2. After the import, verify that the tables with the chemistry index data exist, per the chapter 'Upgrading Indexes' in the Direct Administration Guide. The following statement should

return at least 13 rows. If it returns less than 13 rows please contact BIOVIA Support for assistance with upgrading the database.

```
sqlplus acd/*****
```

```
SQL> select table_name from user_tables where upper(table_name) like  
upper('%_MDLIX_%');
```

```
TABLE_NAME
```

```
-----  
ACD2D_MDLIX_BSQ  
ACD2D_MDLIX_CCLK  
ACD2D_MDLIX_CONV  
ACD2D_MDLIX_CTAB  
ACD2D_MDLIX_FLEX  
ACD2D_MDLIX_FMLA  
ACD2D_MDLIX_FSDL  
ACD2D_MDLIX_FSIX  
ACD2D_MDLIX_FSUP  
ACD2D_MDLIX_IKY2  
ACD2D_MDLIX_LOG  
ACD2D_MDLIX_NEC  
ACD2D_MDLIX_PROP  
ACD2D_MDLIX_SGRP  
ACD2D_MDLIX_SKY2
```

```
15 rows selected.
```

3. If the import created a domain index, it must be dropped with the FORCE option before you continue:

```
SQL> drop index dbname_mdlix force;
```

where `dbname_mdlix` is the domain index name. For example,

```
SQL> drop index acd2d_mdlix force;  
drop index acd2d_mdlix force
```

Note: The drop index command will fail if the import did not create the domain index:

```
ERROR at line 1:  
ORA-01418: specified index does not exist
```

This is normal and the error can be ignored.

4. Create the synonyms for the target Direct version, for example if you have Direct 2018:

```
SQL> execute c$direct2018.mdlauxop.setup  
PL/SQL procedure successfully completed.
```

5. Verify the version number for the target Direct version by executing the following SQL:

```
SQL> select mdlaux.version from dual;
```

```
VERSION
```

```
-----  
BIOVIA Direct  
Revision 2018 (Microsoft Windows Oracle12) (18.1.0.365)
```

```
Copyright (c) Dassault Systemes, 1999-2017
```

6. Create the domain index using the 'NOACTION' parameter:

```
SQL> create index dbname_mdlix on dbname_moltable(ctab) indextype is  
c$direct2018.mxixmdl parameters ('noaction');
```

where `dbname_mdlix` is the domain index name and `dbname_moltable` is the molecule table name. For example,

```
SQL> create index acd2d_mdlix on acd2d_moltable(ctab) indextype is  
c$direct2018.mxixmdl parameters ('noaction');
```

```
Index created.
```

7. (When upgrading to Direct 2021)

Run the `<dbname>_Direct2021_Update.sql` that is included in your download package, where `<dbname>` is your database name. The script will address the issue DIR-4107, that is explained in the *BIOVIA Direct 2021 Product Release Document* in more detail.

(When upgrading to Direct 2020 from Direct 2019)

Recreate Fastsearch. This step may take some time to complete.

```
SQL> execute mdlaux.recreatefastsearch('dbname_mdlix');  
where dbname_mdlix is the domain index name. For example,
```

```
SQL> execute mdlaux.recreatefastsearch('ACD2D_MDLIX');  
PL/SQL procedure successfully completed.
```

This completes the upgrade of the domain index to your target Direct version.

Note: Molecule table names for BIOVIA databases are:

Database	Table	Structure column name	Domain Index
ACD	ACD2D_MOLTABLE	CTAB	ACD2D_MDLIX
SCD	SCD2D_MOLTABLE	CTAB	SCD2D_MDLIX
MDDR	MDDR2D_MOLTABLE	CTAB	MDDR2D_MDLIX
Toxicity	TOX_STR_MOLTABLE	CTAB	TOX_STR_MDLIX

Optional: You can run queries such as the following if you want to further verify the status of your upgrade or to help troubleshoot any issues:

1. Verify that the status of your domain index(es) is/are VALID, and the ITYP_OWNER is your BIOVIA Direct version for your database. The following section is an example with Direct 2021. Note: All three 'STATUS' columns must be VALID:

```
select index_name, table_name, status, domidx_status, domidx_opstatus,
ityp_owner from user_indexes where index_type = 'DOMAIN';
```

```
index_name  table_name  STATUS  DOMIDX_STATU  DOMIDX  ityp_owner
-----
ACD2D_MDLIX  ACD2D_MOLTABLE  VALID  VALID  VALID  C$DIRECT2021
```

2. Verify that there are no synonyms owned by the previous Direct version. If you have Direct 2021 (or 2020 or 2018 or 2017R2), TABLE_OWNER includes C\$DIRECT2021 (or C\$DIRECT2020 or C\$DIRECT2018 or C\$DIRECT2017R2).

```
SQL> select distinct table_owner from user_synonyms;
TABLE_OWNER
-----
C$DIRECT2021
ACD
```

3. Run a search in the database, for example:

```
SELECT COUNT(*) FROM ACD2D_MOLTABLE WHERE
SSS(CTAB, 'c:\BIOVIA\direct2021\examples\molfiles\didehydroalanine.mol')
=1;
COUNT(*)
-----
279
```

How to contact BIOVIA Support

If you have any questions, please contact [BIOVIA Support](#).