

Technical Note T21-2020

(Revised December 2021, Original Technical Note T103-2015)

Creating a Domain Index on BIOVIA Databases for Direct 2022, Direct 2018, or a previous representation needed for Direct 202x

Program

BIOVIA Direct 2018

BIOVIA Direct 2020 (only when you want previous representation of Haptics and SCSR)

BIOVIA Direct 2021 (only when you want previous representation of Haptics and SCSR)

BIOVIA Direct 2022

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 to work with BIOVIA Direct 2019, 2020 or 2021SP1. If you are running any of these BIOVIA Direct versions, you can install the BIOVIA databases in their native formats.

The databases in Direct 2020 and 2021 formats 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 and prefer the updated representation of these chemical entities, download and install the database version that matches your installed Direct 2020 or 2021 version. There is no need to follow the steps in this Technical Note.**

Notes:

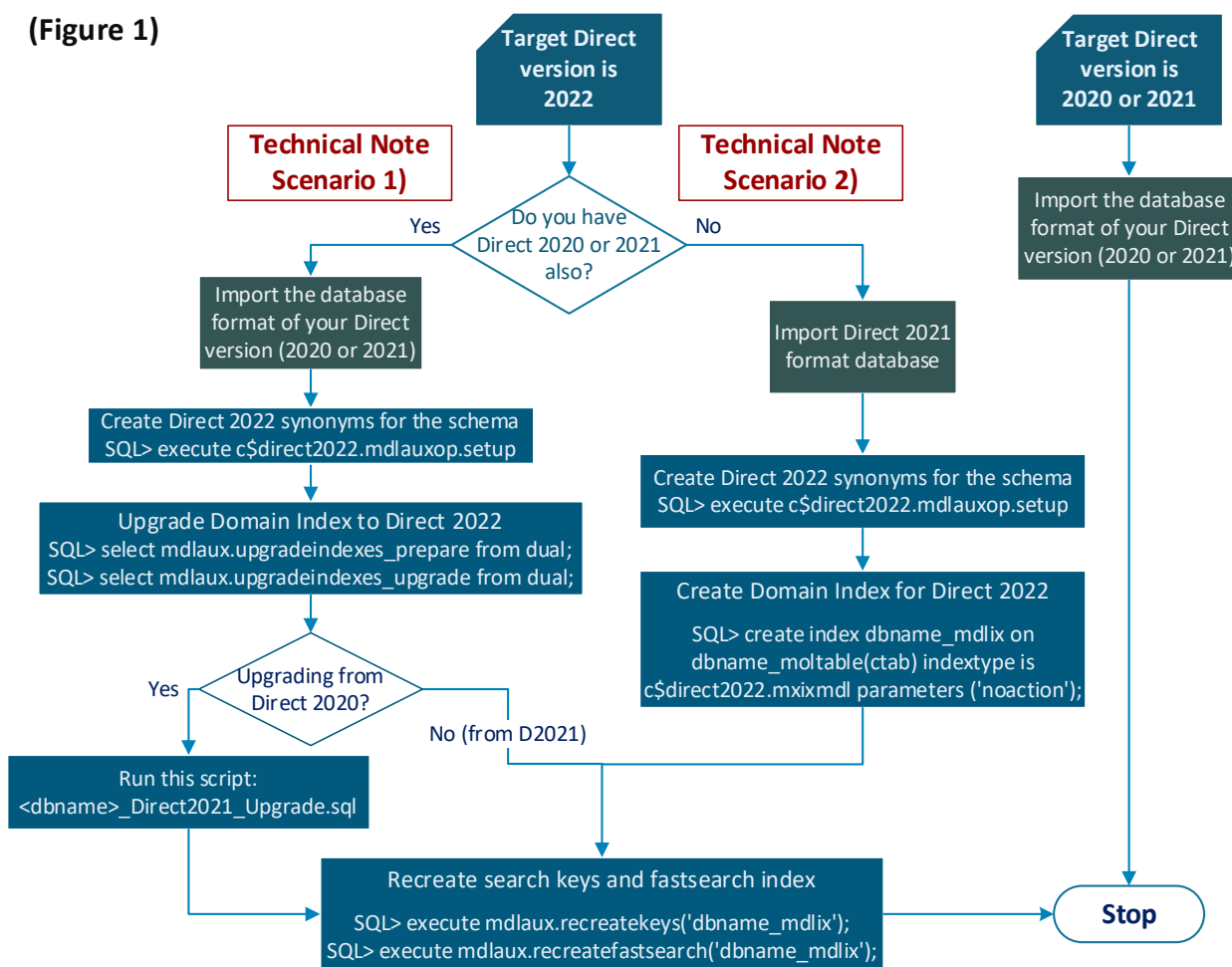
1) **Direct 2021 formats of content databases are built with BIOVIA Direct 2021 SP1.**

If you install the Direct 2021 format database, download the BIOVIA Direct 2021 SP1 from the BIOVIA download platform at the Level – BIOVIA 2021 Refresh2.

2) BIOVIA databases are released in a particular BIOVIA Direct format only until the full support of the particular BIOVIA Direct version in a regulated environment ends. The support timelines for BIOVIA software are outlined in the “Dassault Systèmes Products Lines Releases Support Life Cycle Dates” page 9, available at https://media.3ds.com/support/DS_LifeCycleInformation.pdf.

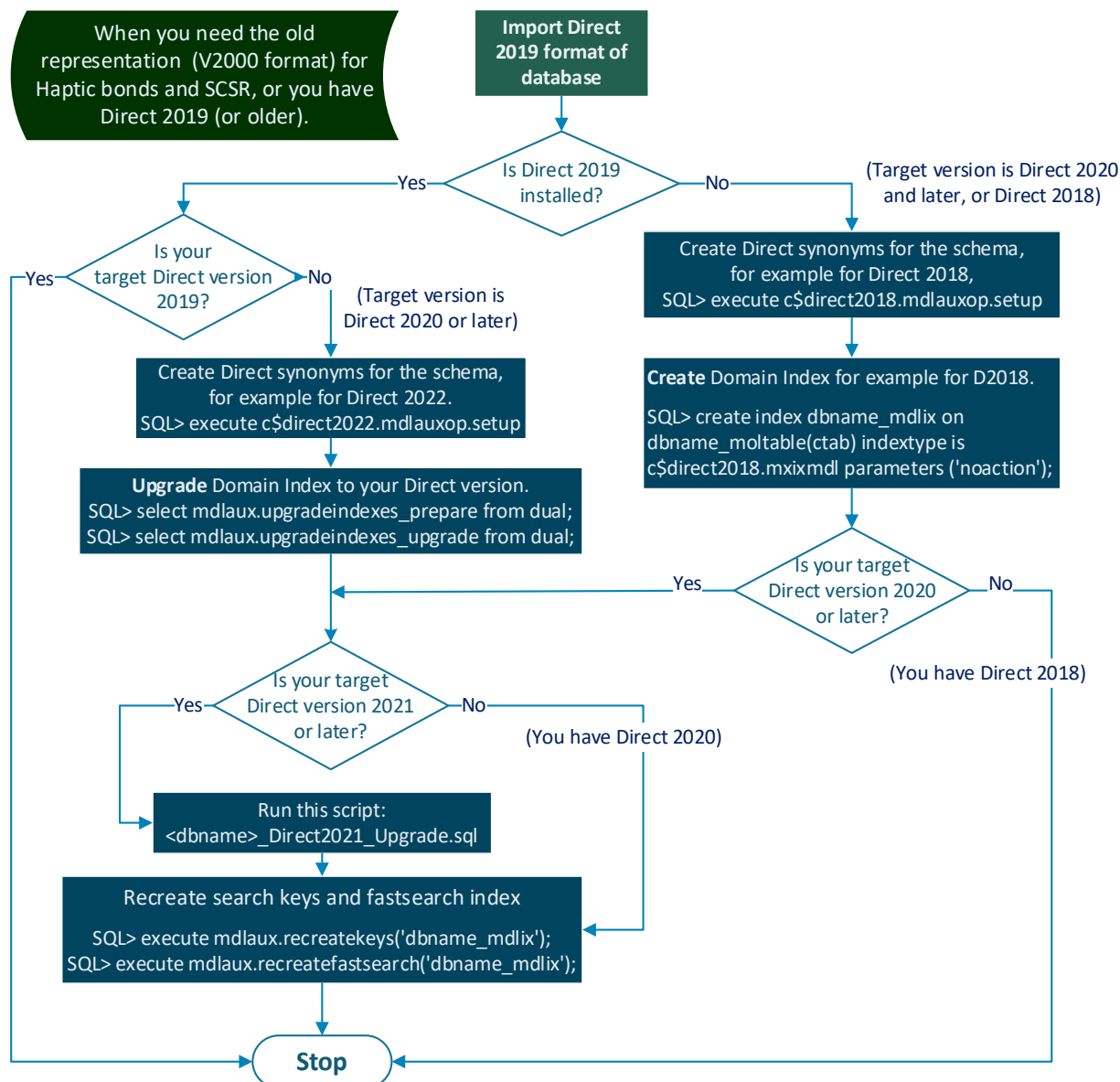
This Technical Note includes **two scenarios** to upgrade the domain index to Direct 2022 (Figure 1). If you however are running BIOVIA Direct 2020 or 2021 but prefer the previous representation of haptic bonds and biological sequences, you must initially install the BIOVIA database in Direct 2019 format and then update the chemistry domain index for Direct 2020 or Direct 2021 (Figure 2).

(Figure 1)



If you intend to use the previous representation, or if you are running BIOVIA Direct 2018, use the flowchart below (Figure 2) to create the domain index after importing the Direct 2019 format database. This Technical Note does not include the detailed steps to use the old representation. Please contact BIOVIA Support if you need further assistance.

(Figure 2)



Resolution

Scenario 1) BIOVIA Direct 2022 is installed, and either Direct 2021 or 2020 is installed on the same Oracle instance.

1. Download and import the BIOVIA Content database of your Direct format (Direct 2021 or 2020). The domain index was created for Direct 2021 (or 2020) successfully.
2. Login to the database schema and create the synonyms for the installed BIOVIA Direct 2022.

```
SQL> execute c$direct2022.mdlauxop.setup
PL/SQL procedure successfully completed.
```

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

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

VERSION
-----
                                BIOVIA Direct
                                Revision 2022 (Microsoft Windows Oracle19) (22.1.0.551)
                                Copyright (c) Dassault Systemes, 1999-2021
```

4. Run these commands to upgrade the domain index to Direct 2022, for example for ACD.

```
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
```

5. (Upgrading from Direct 2020 only. If you are upgrading from Direct 2021, skip this and go to Step 6.)

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

6. Recreate search keys and fastsearch indexing data. These commands take some time to complete.

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

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

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

This completes the upgrade of the domain index to Direct 2021 (or 2020) to 2022.

Scenario 2) Your Oracle instance has BIOVIA Direct 2022 only.

1. Download and import the Direct 2021 format of BIOVIA Content databases. The import may return some errors. All objects will basically import successfully, but the domain index creation step will fail with errors similar to those below, when 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$DIRECT2021"."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, login to your BIOVIA content database schema and 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 table_name like '%_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. Create the synonyms for the installed BIOVIA Direct 2022.

```
SQL> execute c$direct2022.mdlauxop.setup
PL/SQL procedure successfully completed.
```

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

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

```
VERSION
```

```
-----
                                BIOVIA Direct
Revision 2022 (Microsoft Windows Oracle19) (22.1.0.551)

Copyright (c) Dassault Systemes, 1999-2021
```

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

```
SQL> create index dbname_mdlix on dbname_moltable(ctab) indextype is
c$direct2022.mxixmdl parameters ('noaction');
```

where dbname_mdlix is the [domain index name](#) and dbname_moltable is the molecule table name. For example for ACD,

```
SQL> create index acd2d_mdlix on acd2d_moltable(ctab) indextype is
c$direct2022.mxixmdl parameters ('noaction');
```

Index created.

6. Recreate search keys and fastsearch indexing data. These commands take some time to complete.

```
SQL> execute mdlaux.recreatekeys('dbname_mdlix');
SQL> execute mdlaux.recreatefastsearch('dbname_mdlix');
```

where dbname_mdlix is the domain index name. For example for ACD,

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

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

This completes the domain index upgrade to Direct 2022 format.

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 is VALID, and the ITYP_OWNER is your BIOVIA Direct version for your database. The following section is an example with ACD Direct 2022. Note: All three 'STATUS' columns must be VALID:

```
SQL> 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\$DIRECT2022

2. Verify that there are no synonyms owned by the previous Direct version. If you have Direct 2022, TABLE_OWNER includes C\$DIRECT2022.

```
SQL> select distinct table_owner from user_synonyms;
TABLE_OWNER
-----
C$DIRECT2022
ACD
```

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

```
SELECT COUNT(*) FROM ACD2D_MOLTABLE WHERE
SSS(CTAB, 'c:\BIOVIA\direct2022\examples\molfiles\didehydroalanine.mol')=1;
COUNT(*)
-----
299
```

How to contact BIOVIA Support

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