

Technical Note T22-2020

(Revised December 2021, Original Technical Note T77-2017)

Creating a Domain Index on ACD Data Mart 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) Data Mart

Operating System

All operating systems supported with BIOVIA Direct

Description

BIOVIA currently provides ACD Data Mart in the formats for BIOVIA Direct 2019, 2020 and 2021SP1. If you are running any of these BIOVIA Direct versions, you can install the BIOVIA databases in their native formats.

The database 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:

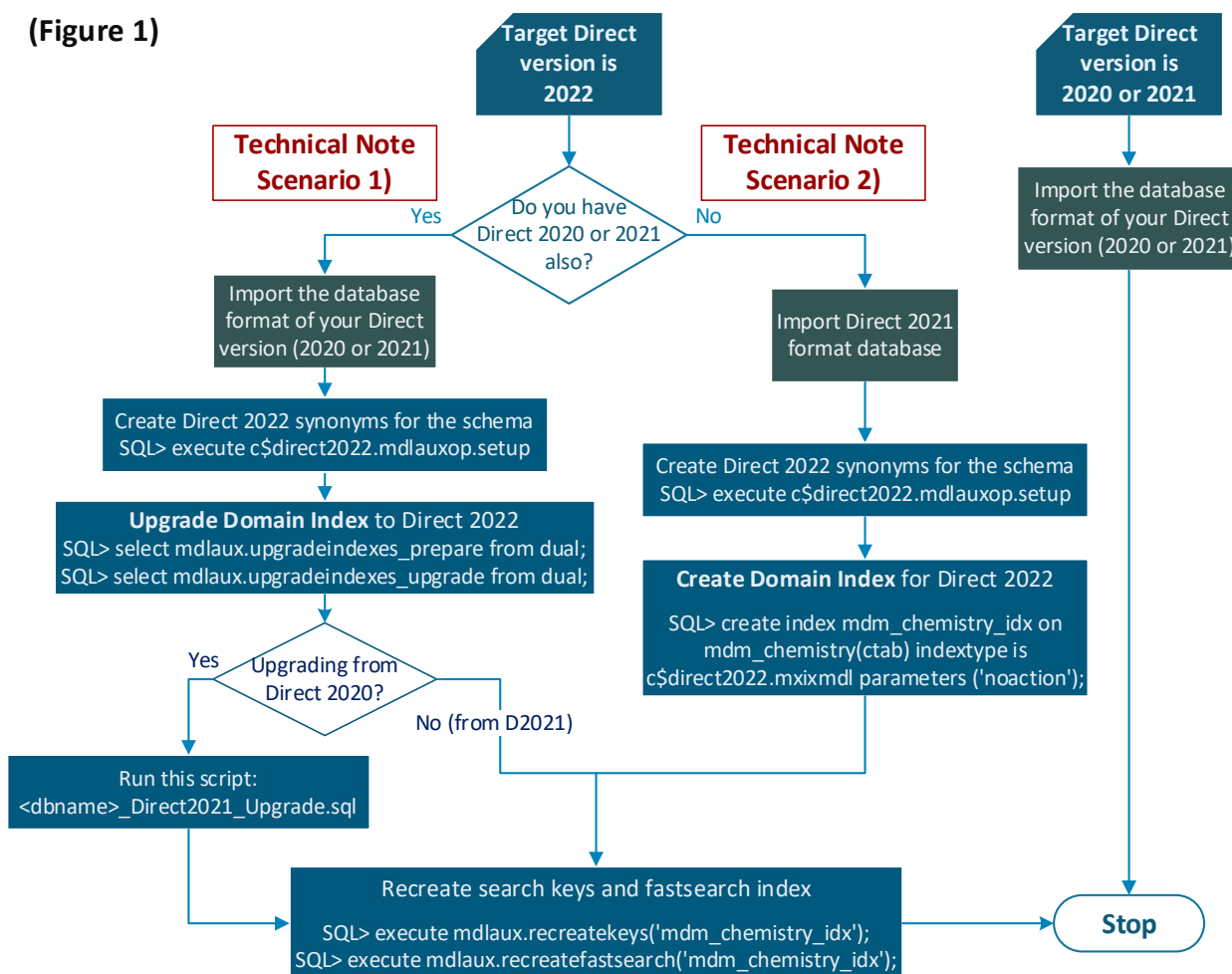
1) **Direct 2021 formats of content databases are built with BIOVIA Direct 2021 SP1.**

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* document page 9, available at https://media.3ds.com/support/DS_LifeCycleInformation.pdf.

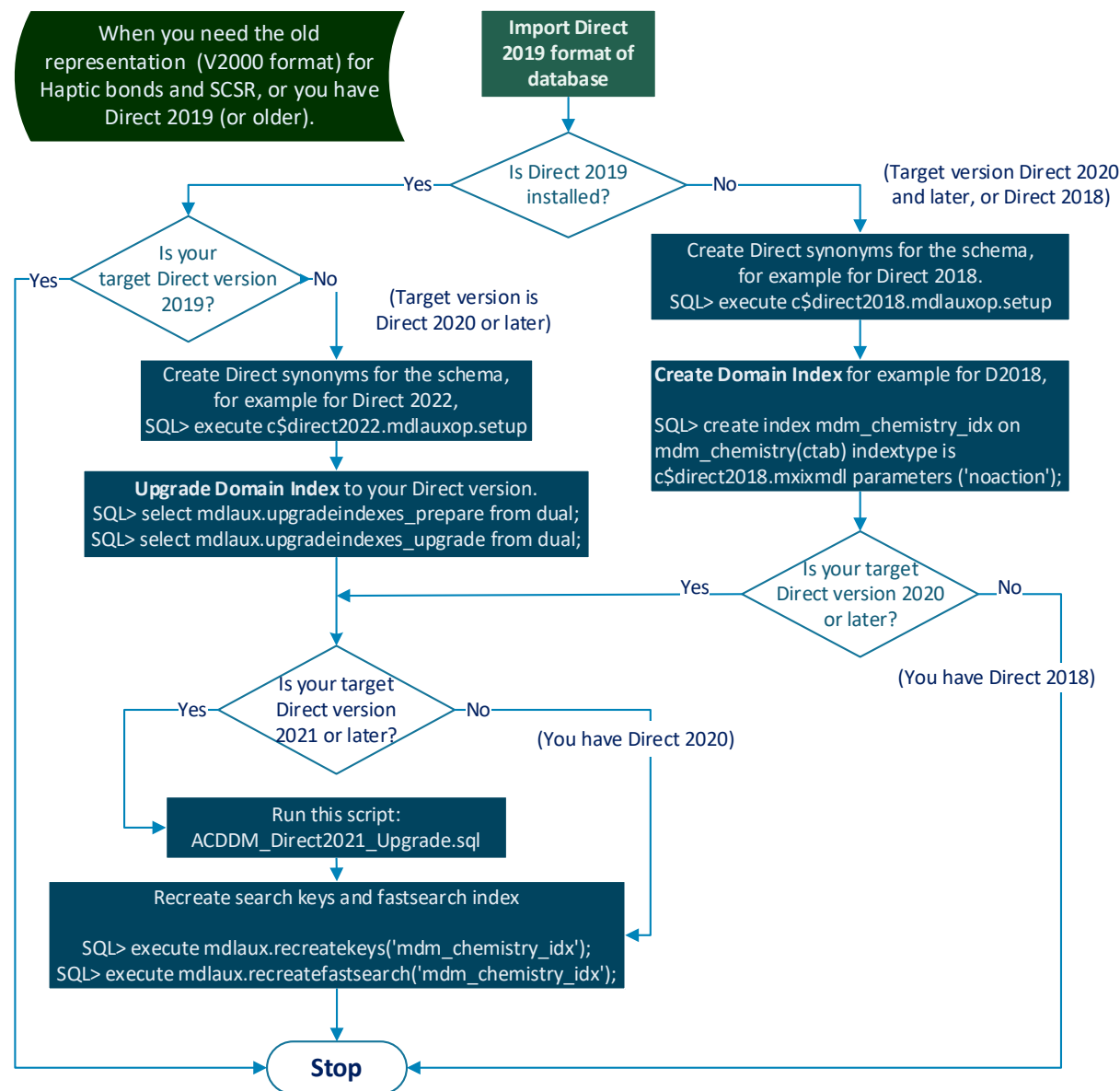
This Technical Note includes **two scenarios** to upgrade the domain index to Direct 2022 (Figure 1). If you however are running BIOVIA Direct 2020 or 2021 but prefer the previous representation of haptic bonds and biological sequences, you must initially install the ACD Data Mart of the Direct 2019 format and 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 ACD Data Mart of your Direct format (Direct 2021 or 2020). The domain index was created for Direct 2021 (or 2020) successfully. For the details on loading the database into Oracle, please consult *install_datamart.pdf*, which is included in the ACD Data Mart download zip file.
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.

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

```
-----
Prepared index for upgrade/recreate: MDM_CHEMISTRY_IDX Table: MDM_CHEMISTRY
```

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

```
-----
Created index: MDM_CHEMISTRY_IDX
```

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

Run the *ACDDM_Direct2021_Update.sql* that is included in the download package. 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('mdm_chemistry_idx');
PL/SQL procedure successfully completed.
```

```
SQL> execute mdlaux.recreatefastsearch('mdm_chemistry_idx');
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 ACD Data Mart. 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:"ACDDM"."MDM_CHEMISTRY_IDX" failed to create
with error:
ORA-29833: indextype does not exist
Failing sql is:
CREATE INDEX "ACDDM"."MDM_CHEMISTRY_IDX" ON "ACDDM"."MDM_CHEMISTRY"
("CTAB") INDEXTYPE IS "C$DIRECT2019"."MXIXMDL" ...
```

Additionally, you might see the following errors if the Data Mart schema is already enabled for your Direct version.

```
ORA-31684: Object type SYNONYM:"ACDDM"."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 statement below should return at least 13 rows. If it returns fewer than 13 rows, please contact BIOVIA Support for assistance with upgrading the database. (Your Data Mart schema name may be inv_datamart if you are using CISPro MSB.)

```
sqlplus acddm/*****
```

```
SQL> select table_name from user_tables where table_name like '%_IDX_%';
```

```
TABLE_NAME
```

```
-----
MDM_CHEMISTRY_IDX_SKY2
MDM_CHEMISTRY_IDX_SGRP
MDM_CHEMISTRY_IDX_PROP
MDM_CHEMISTRY_IDX_NEC
MDM_CHEMISTRY_IDX_LOG
MDM_CHEMISTRY_IDX_IKY2
MDM_CHEMISTRY_IDX_FSUP
MDM_CHEMISTRY_IDX_FSIX
MDM_CHEMISTRY_IDX_FSDL
MDM_CHEMISTRY_IDX_FMLA
MDM_CHEMISTRY_IDX_FLEX
MDM_CHEMISTRY_IDX_CTAB
MDM_CHEMISTRY_IDX_CRCV
```

```
MDM_CHEMISTRY_IDX_CONV  
MDM_CHEMISTRY_IDX_CCLK  
MDM_CHEMISTRY_IDX_BSQ
```

16 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 mdm_chemistry_idx on mdm_chemistry(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('mdm_chemistry_idx');  
PL/SQL procedure successfully completed.
```

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

This completes the domain index upgrade to Direct 2022 format.

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 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
MDM_CHEMISTRY_IDX	MDM_CHEMISTRY	VALID	VALID	VALID	C\$DIRECT2022

2. Verify that there are no synonyms owned by the previous Direct version.

```
SQL> select distinct table_owner from user_synonyms;
```

TABLE_OWNER
C\$DIRECT2022

3. Run a search in the database and verify that it returns hits with no errors, for example:

```
SQL> SELECT COUNT(*) FROM MDM_CHEMISTRY 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](#).