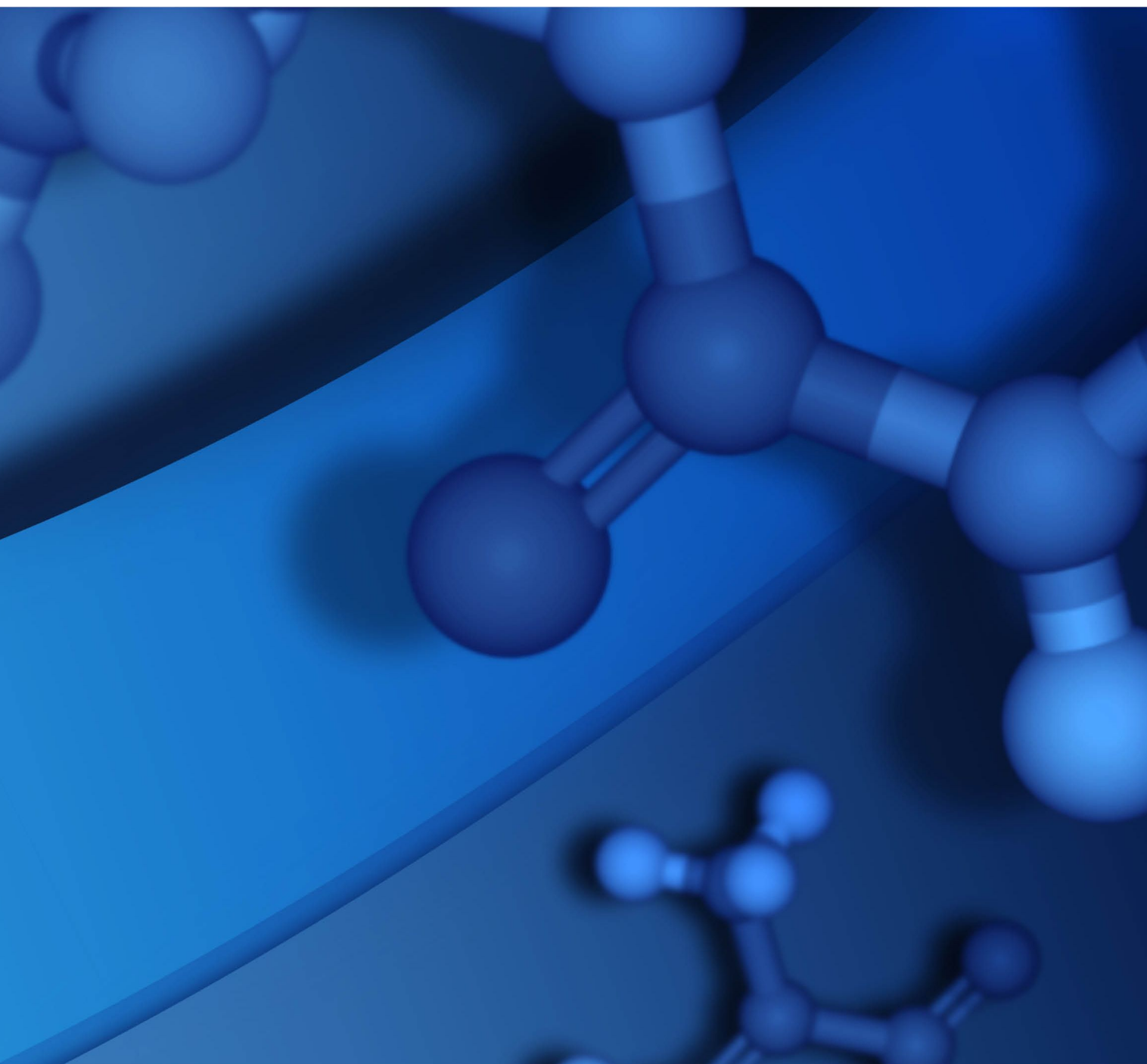


SYSTEM REQUIREMENTS

BIOVIA DIRECT 2021



Copyright Notice

©2020 Dassault Systèmes. All rights reserved. 3DEXPERIENCE, the Compass icon and the 3DS logo, CATIA, SOLIDWORKS, ENOVIA, DELMIA, SIMULIA, GEOVIA, EXALEAD, 3DVIA, 3DSWYM, BIOVIA, NETVIBES, IFWE and 3DEXCITE, are commercial trademarks or registered trademarks of Dassault Systèmes, a French "société européenne" (Versailles Commercial Register # B 322 306 440), or its subsidiaries in the U.S. and/or other countries. All other trademarks are owned by their respective owners. Use of any Dassault Systèmes or its subsidiaries trademarks is subject to their express written approval.

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. BIOVIA Direct 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

Database Tier Requirements	1
Capacity Planning	1
Hardware Requirements	1
Operating Systems	2
Software Requirements	2
Required Software	2
Optional Software	2
Disk Space Requirements and Recommendations	2
Oracle Information and Requirements	4
Supported Versions of Oracle Database Server	4
Supported Character Sets in the Oracle Database Server	4
Oracle Recommendations	5
Storage Parameters	5
Database Initialization Parameters	5

Database Tier Requirements

The Direct 2021 server uses Oracle for data storage, indexing, PL/SQL packages, triggers, and views.

Capacity Planning

The estimates that follow are for planning purposes only. The actual memory requirements for your workload might vary, depending on Oracle parameters, database size, user activity, and other site-specific factors.

Memory	Estimate	Comments
Virtual Memory	At least 4 GB + 80 MB per connected Direct user	This estimate does not include virtual memory that is required for other applications. Add more memory if individual users will attempt operations that could fill up the available space.
Physical Memory	At least 4 GB + 80 MB per connected Direct user	This estimate does not include any additional physical memory needed by the operating system, Oracle, or other applications.
Temporary Disk Space	At least 20 GB	Additional space is required if you have molecules that are 700 bytes (or larger), or reactions that are 2000 bytes (or larger).

Hardware Requirements

BIOVIA recommends the following minimum hardware on the database tier for proper operation of Direct.

Recommended Configuration	
Processor	Intel or Intel-compatible (EM64T or AMD64) computer 64-bit Note: Intel IA64 (Itanium) is not supported.
Hard disk space	Any standard hard disk with adequate disk space.
Network	Ethernet

Operating Systems

BIOVIA supports the installation of Direct on the following database tier only operating systems.

Operating System	Version	Comments
Microsoft Windows Server	2019, 2016	64-bit only is supported; English and Japanese are supported
Red Hat Enterprise Linux or Oracle Linux	8.1+, 7.5+	64-bit only is supported; English and Japanese are supported

Software Requirements

This section lists the required and optional software in order to operate Direct on the database tier.

Required Software

Software	Version	Comments
Java Runtime Environment (JRE)	64-bit 1.8 or higher	Required to run the UnitProtConverter utility; you do not need to run this utility to access Direct.
Visual C++ Redistributable Packages	2015 2013	Required for Windows Installations
Required Linux Packages	Latest version	audit-libs.x86_64, expat.x86_64, fontconfig.x86_64, freetype.x86_64, glibc.x86_64, keyutils-libs.x86_64, krb5-libs.x86_64, libaio.x86_64, libcap-ng.x86_64, libcom_err.x86_64, libgcc.x86_64, libselinux.x86_64, libstdc++.x86_64, libuuid.x86_64, libx11.x86_64, libxau.x86_64, libxcb.x86_64, libxext.x86_64, libxrender.x86_64, pam.x86_64, pcre.x86_64, zlib.x86_64

Optional Software

Software	Version
BIOVIA Foundation and Pipeline Pilot	2021, 2020, 2019, 2018, 2017 R2, 2017, 2016

Disk Space Requirements and Recommendations

The figures that follow do not include the disk space required to install the Oracle RDBMS, any proprietary Oracle databases, or any other software that you might want to use with Direct.

Software	Space Requirements	Comments
Temporary disk space	Linux: 270MB, Windows: 150MB	This includes Direct files that are required for installation.
	200MB	Required during installation.
Oracle database		For details about administering molecule or reaction databases, see <i>BIOVIA Direct Administration Guide</i> .
Oracle tablespaces		See Oracle Recommendations .

Oracle Information and Requirements

Direct 2021 operates with either Oracle Enterprise Edition or Oracle Standard Edition 2. However, there are Oracle features that are limited in the Standard Edition 2, such as replication. For information on the differences between Enterprise and Standard Editions, see the Oracle documentation.

Supported Versions of Oracle Database Server

BIOVIA supports the installation of Direct with the following Oracle versions in conjunction with the corresponding operating systems.

Supported Oracle Version	Supported Operating System	Notes
Oracle 19c (19.7.0.0.0)	<ul style="list-style-type: none">■ RHEL 7.5 or higher■ Oracle Linux 7.5 or higher■ RHEL 8.1 or higher■ Oracle Linux 8.1 or higher	Requires the SQLNET.INBOUND_CONNECT_TIMEOUT parameter in sqlnet.ora to be set to 0.
	<ul style="list-style-type: none">■ Windows Server 2016■ Windows Server 2019	
Oracle 12c R2 (12.2.0.1)	<ul style="list-style-type: none">■ RHEL 7.5 or higher■ Oracle Linux 7.5 or higher	Requires the SQLNET.INBOUND_CONNECT_TIMEOUT parameter in sqlnet.ora to be set to 0.
	<ul style="list-style-type: none">■ Windows Server 2016	

Some Oracle Enterprise Edition features are not available in the Standard Edition 2. For more information, see the Oracle documentation.

Supported Character Sets in the Oracle Database Server

The following Oracle database character sets are tested and supported with Direct 2021.

- WE8ISO8859P1
- WE8ISO8859P15
- JA16SJIS
- AL32UTF8

Note: Direct supports only US ASCII characters for the content of molfiles and rxnfiles.

Oracle Recommendations

Storage Parameters

BIOVIA recommends the following storage parameters.

Tablespaces	Parameters	Recommendations
Temporary	INITIAL	1 MB
	Next	5MB
	MAXEXTENTS	500KB
Data	INITIAL SHARED_ POOL-SIZE	Two times the size of the database block size in bytes, for example, 4 KB (for a 2 KB database block size) or 16 KB (for an 8 KB database block size). Increase the default value by a factor of four. This value depends on the number of users, amount of data, and other such site-dependent factors.
Rollback	INITIAL	500 KB to 2 MB

Database Initialization Parameters

BIOVIA recommends the following database initialization parameters.

Parameter	Setting or Value	Comments
Open cursors	320 or more	
Cache size		Choose the parameter that is appropriate for your site.
DB_8K_CACHE_SIZE	20 MB (minimum)	Use this parameter if your default block size is NOT 8K.
DB_CACHE_SIZE		Use this parameter if your default block size IS 8K.
DB_SECUREFILE	PERMITTED (recommended)	Values of ALWAYS or FORCE are not recommended.