



# Launch Discovery Studio On the Cloud Tutorial

**Molecular Sciences and Digital Innovation Center, GGA Corp.**



Kindly enter your assigned username



## Welcome to the 3DEXPERIENCE platform

Sign in to continue

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***\*Note: see email for assigned username and password***

 English

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Login with assigned username and password

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My Roles

 3DSwyrmer

 Collaborative Industry Innovator

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Getting Started

Learn the Experience

New Tab 1






3DEXPERIENCE


Welcome to the 3DEXPERIENCE platform


The 3DEXPERIENCE platform is a BUSINESS EXPERIENCE platform

It provides software solutions for every organization in your company - from marketing to sales to engineering - that help you, in your value creation process, to create differentiating consumer experience. With a single, easy-to-use interface, it powers Industry Solution Experiences, based on 3D design, analysis, simulation and intelligence software in a collaborative interactive environment.

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discovery studio simulation


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Discovery Studio Simulation

Click here

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Wait a minute for the 3DE Launcher to launch the Discovery Studio Simulation

Discovery Studio Simulation Client

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

MacromoleculesSimulationReceptor-Ligand InteractionsPharmacophoresSmall MoleculesX-rayMy Tools

New

ToolsFiles

DS Welcome

Sketch Molecules

Build Fragment

Prepare or Filter Ligands

Search Small Molecule Conformations

Minimize Ligands

Align Small Molecules

Calculate Molecular Properties

Study SAR

Design and Analyze Libraries

Select Subset Libraries

Molecule Browser

Materials Registration

Model Repository Management

Publish

Publish to the Model Repository.

Publish Pharmacophore to Model Repository...

Publish Docking to Model Repository...

Manage

Browse or retrieve models in the Model Repository.

Manage Model Repository...

BIOVIA | Discovery Studio Simulation

What's New

Actions

My Recent Actions

Publish Docking to Model Repos...

Open URL...

Prepare Ligands...

Dock Ligands (CDOCKER)...

Open..

Ligand Profiler...

PharmaDB Profiler...

PharmaDB Filter...

My Recent Tool Panels

Model Repository Management

Prepare or Filter Ligands

Dock Ligands

Define and Edit Binding Site

Model Protein Structures

Predict Protein Formulation Pr...

Design Protein

Dock and Analyze Protein Compl...

Data

My Recent Files

MAPK14\_4AA5.dsv

Molecule.sd

4AA5.dsv

Protocol.pr\_xml

Protocol.pr\_xml

Molecule.sd

7WVU.dsv

Details.csv

Details.csv

exportedIteration9\_Round5\_Mol3...

exportedIteration9\_Round5.sdf

exportedIterationStructures2.s...

exportedIterationStructures.sd...

Structure2D\_COMPOUND\_CID\_5154....

Q5\_FPR1\_pharma10.ds\_chm

241.dsv

PIInteractions.csv

Pose1.dsv

HydrogenBonds.csv

Notifications

My Recent Jobs

Publish Docking to Model Repos...

Success Oct-28 12:06

Publish Docking to Model Repos...

Success Oct-28 12:01

Dock Ligands (CDOCKER)

Success Oct-02 13:46

PharmaDB Profiler

System Error Oct-02 08:25

Publish Pharmacophore to Model...

Success Oct-01 10:29

Publish Pharmacophore to Model...

Success Oct-01 10:28

Publish Docking to Model Repos...

Success Oct-01 10:15

Jobs

Protocol Name	Saved	Status	Details	Elapsed Time	Start Date	Server Location	Category	Description
> Publish Dock	Yes	Success	Published MAPK13_5EKN_doc	0:00:28	週二 十月 28 12:0	3DEXPERIENCE C	base	Publishes docking methods and models to the model repository
> Publish Dock	Yes	Success	Published MAPK11_3GP0_doc	0:00:39	週二 十月 28 12:0	3DEXPERIENCE C	base	Publishes docking method
> Dock Ligand	Yes	Success	10 poses: Structure2D_COMP	0:02:02	週四 十月 2 13:43	3DEXPERIENCE C	singlecore	Docks ligands into an activ
> Publish Pharm	Yes	Success	Published FPR2_7WVV_Pharm	0:00:23	週三 十月 1 10:28	3DEXPERIENCE C	base	Publishes pharmacophore(s) into the model repository

Successfully connected to cloud server

novelynk@3DEXPERIENCE Cloud



# THANK YOU