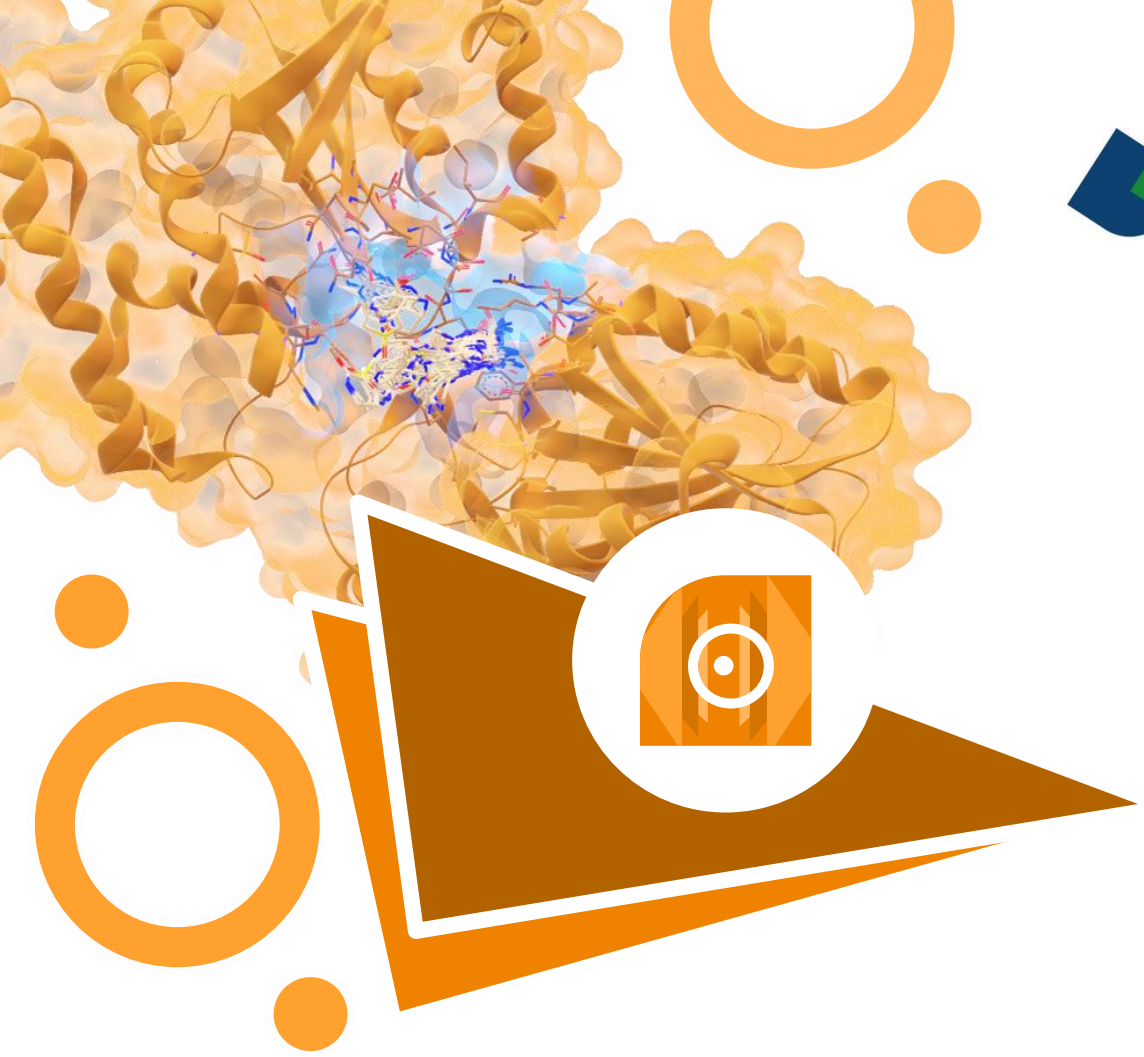


BioSolveIT
expect actives!

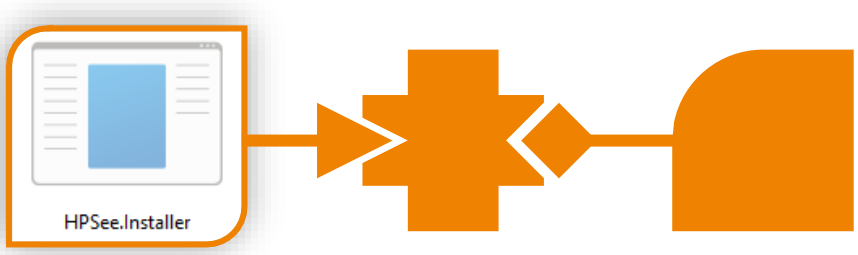
HPSee

Beginner's Guide
Version 1 - Maia

Your ecosystem for large-scale computations.

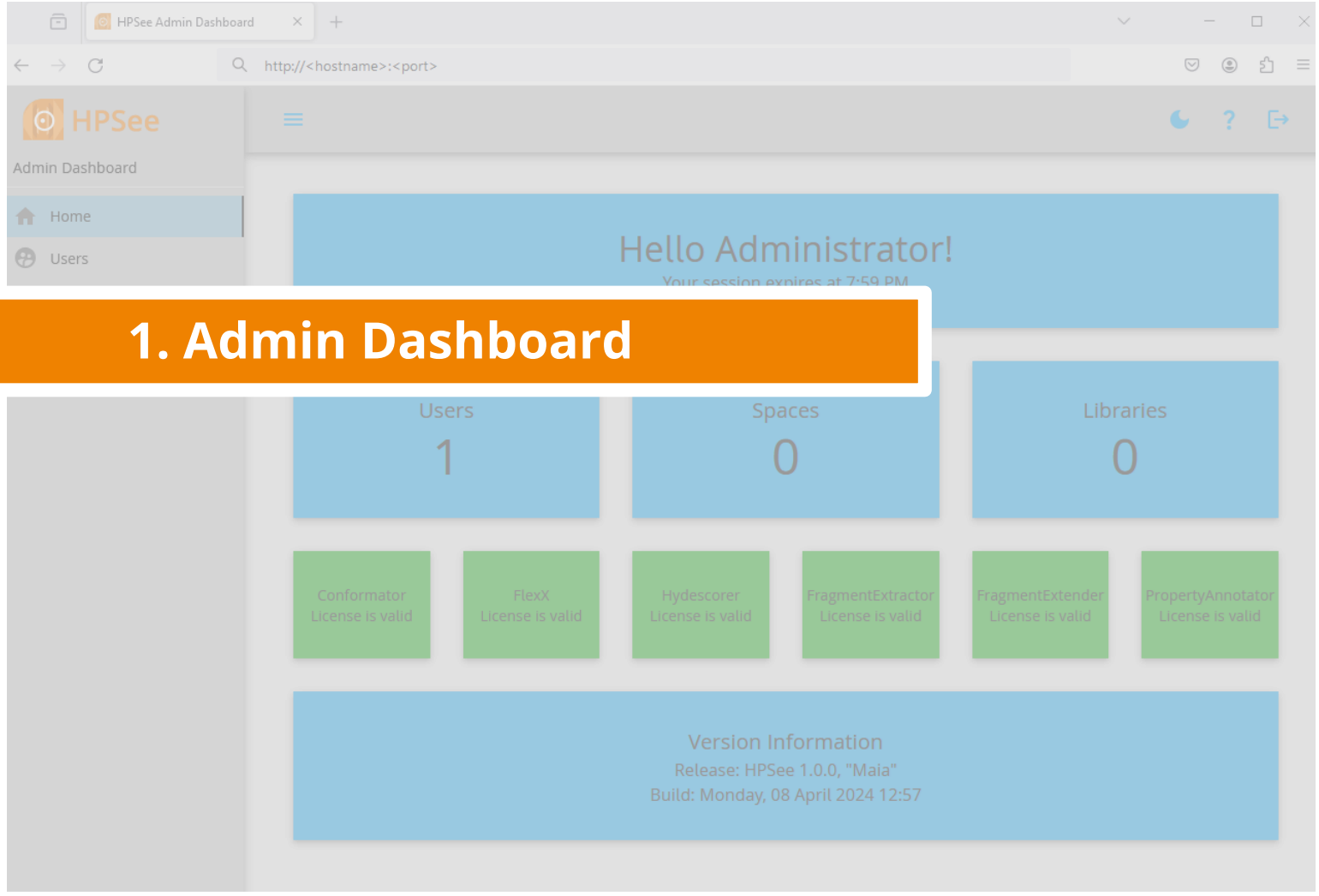
Content

0. Before You Start

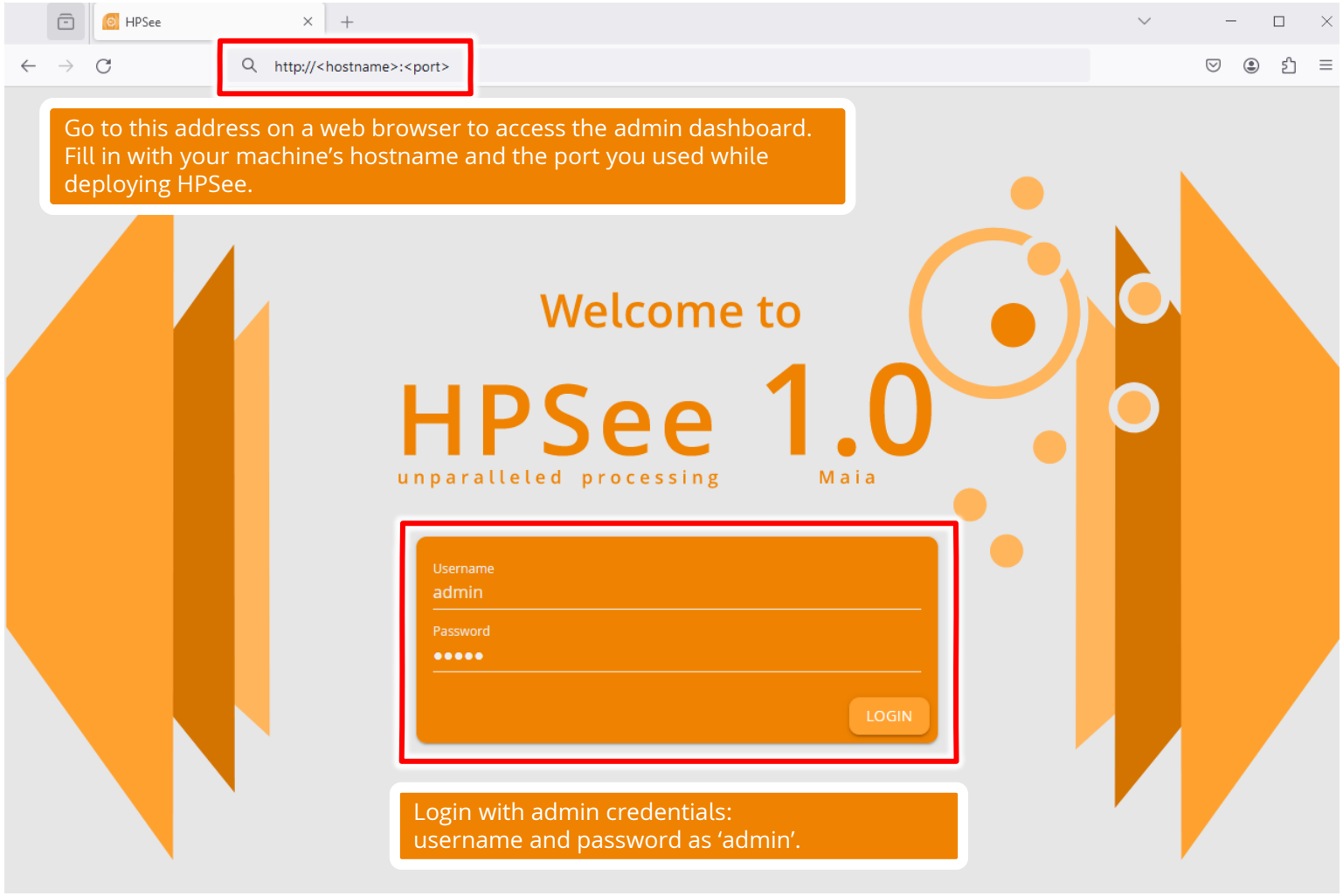


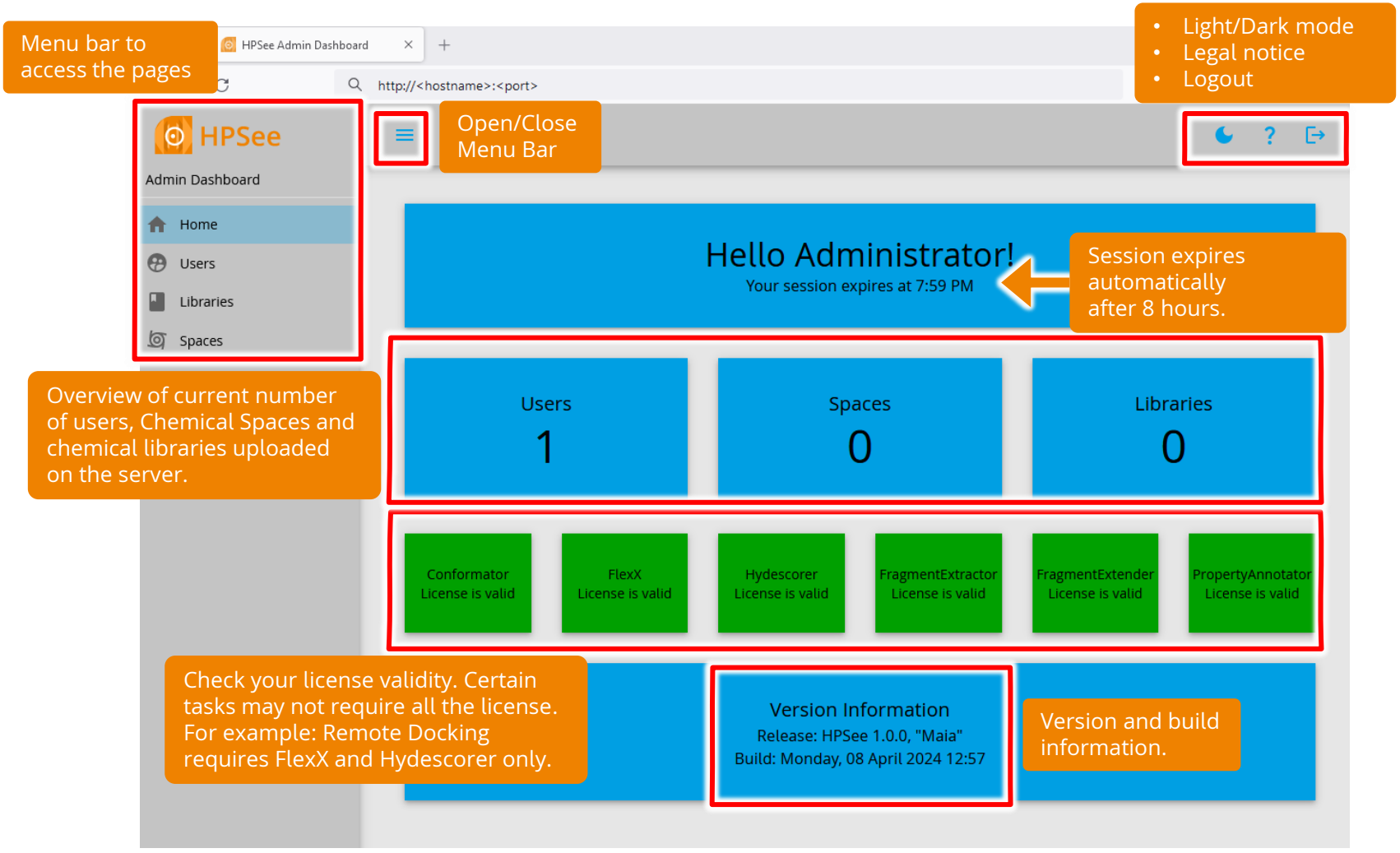
Your container should be deployed and running

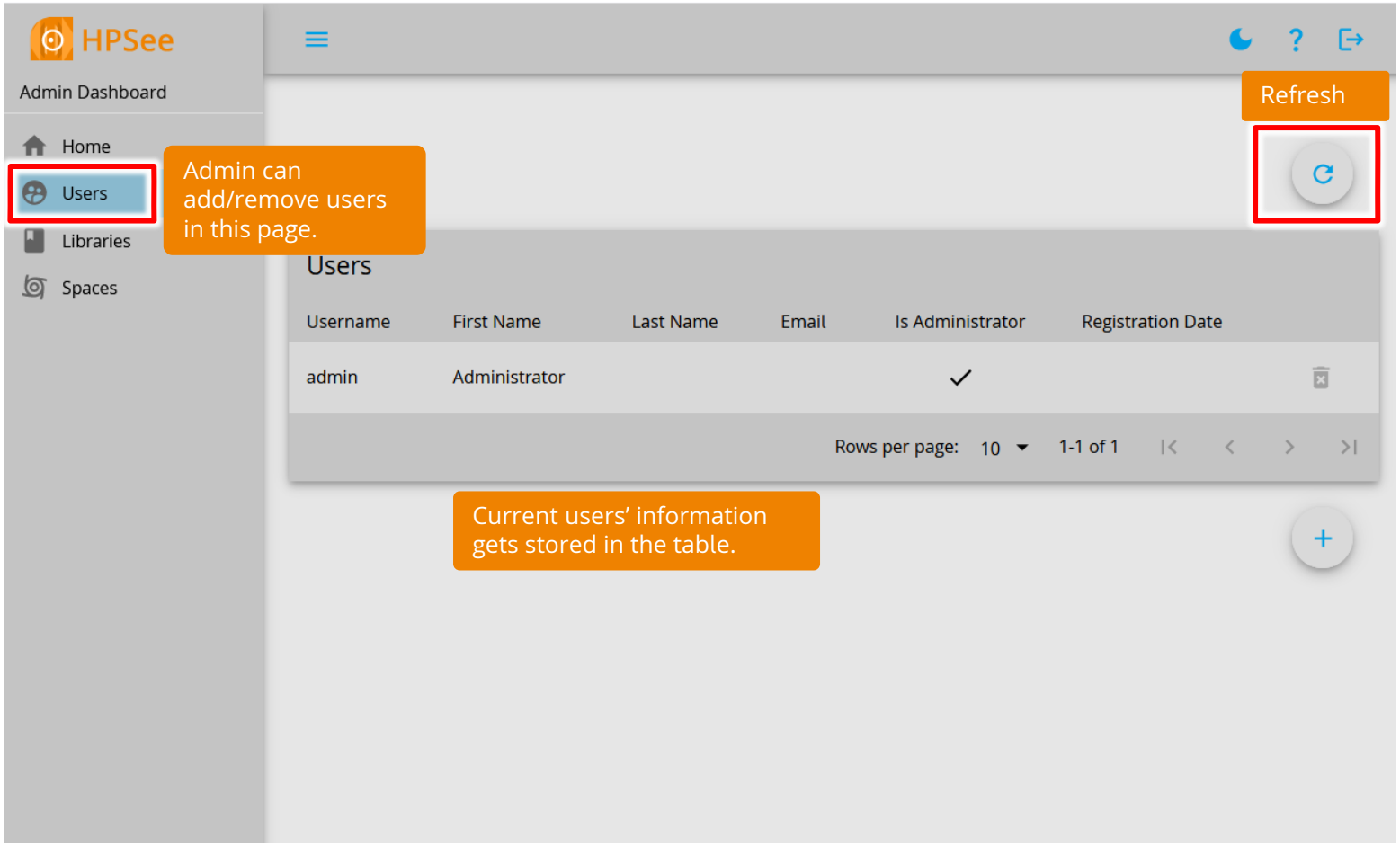
If you are not familiar with installation or deployment of HPSee, refer to the “HPSee Deployment Guide”

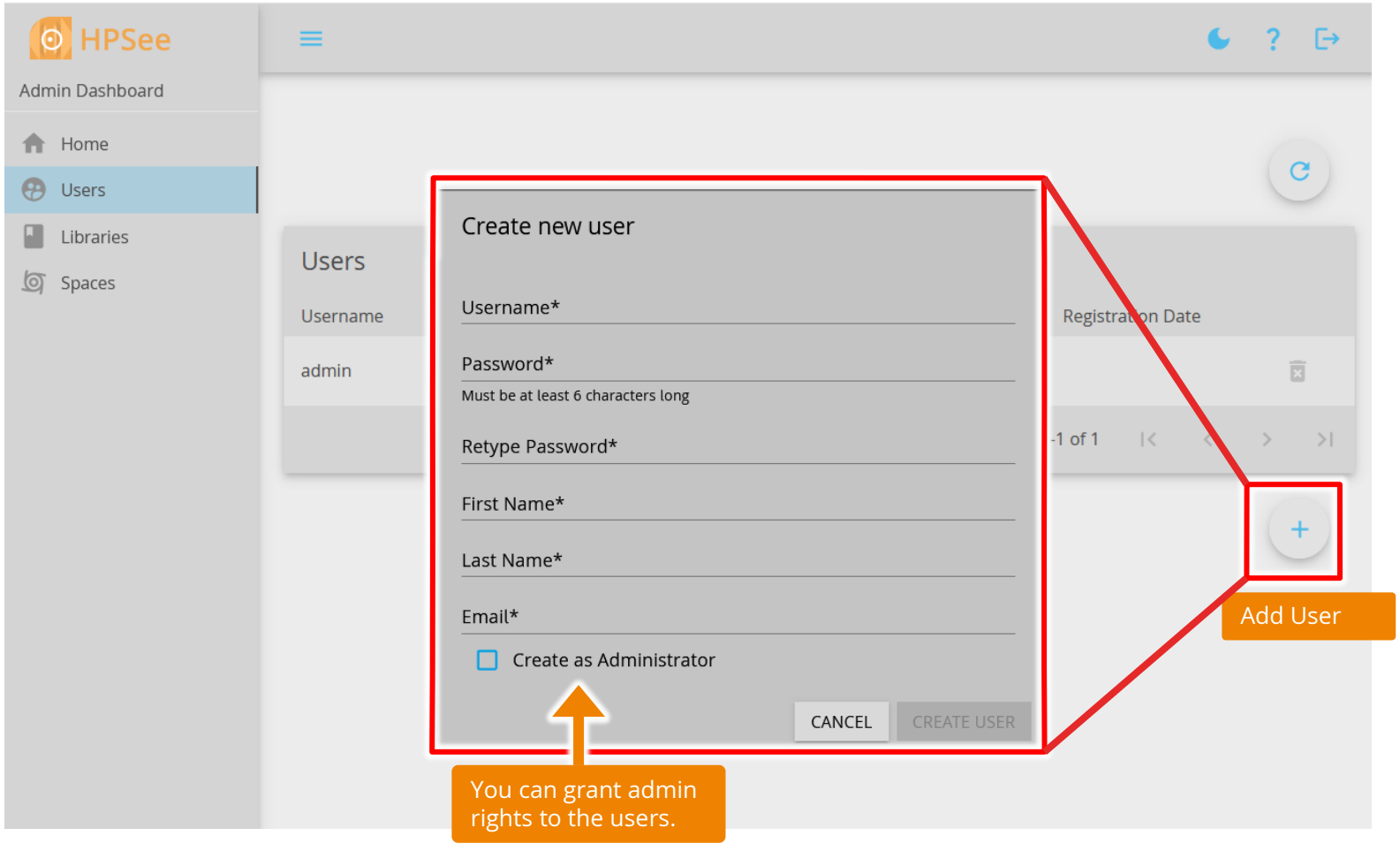


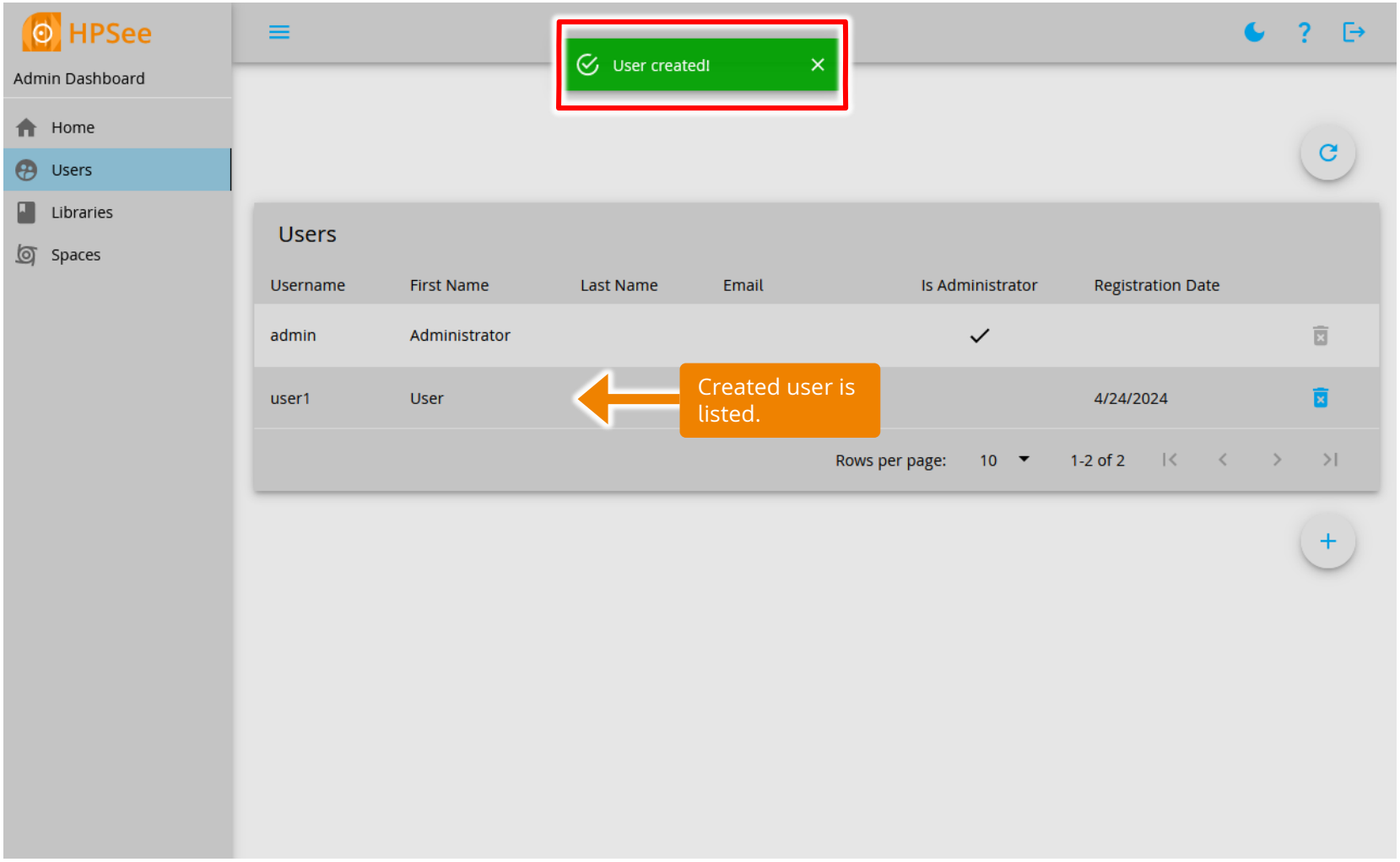
1. Admin Dashboard

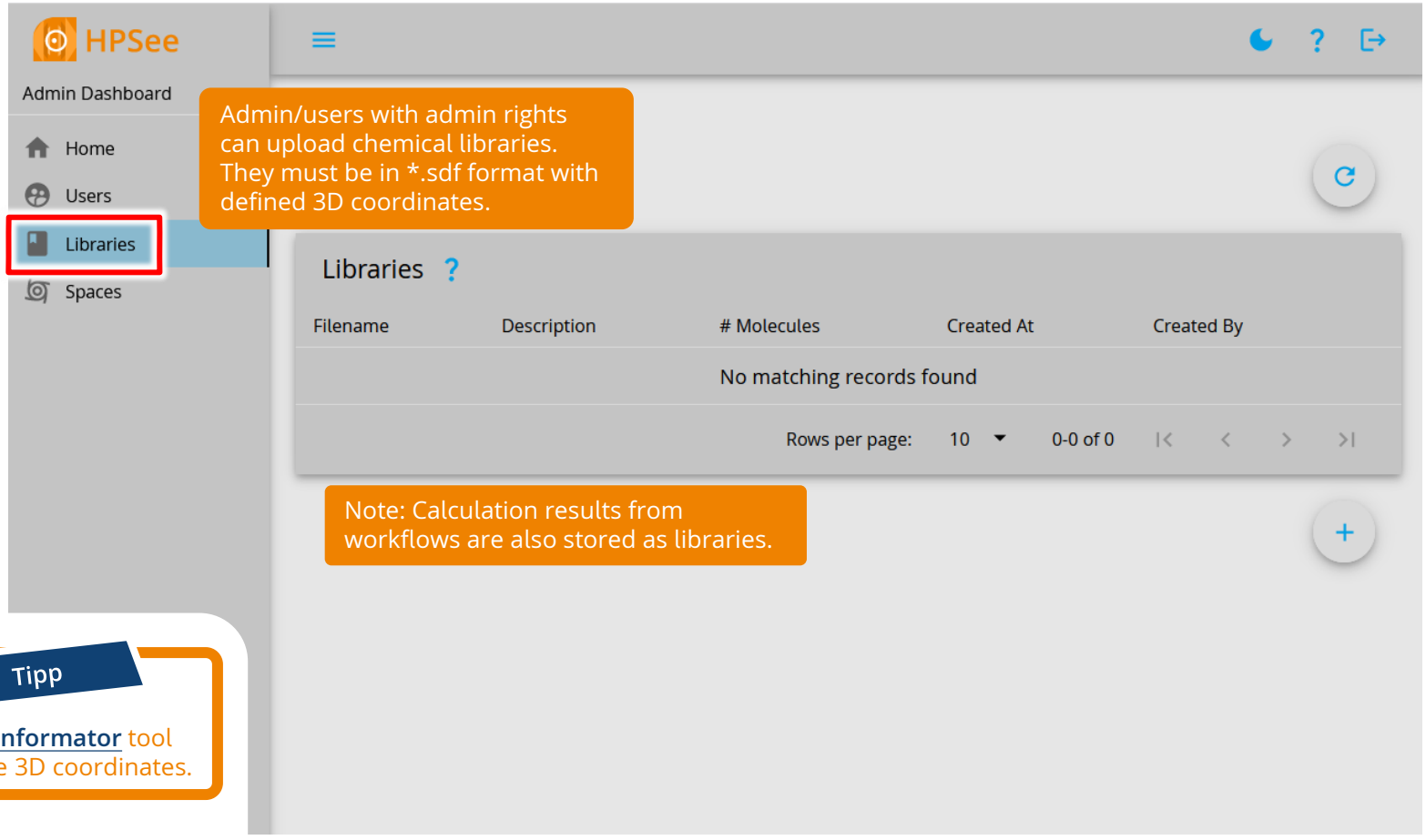

HPSee
http://<hostname>:<port>
Go to this address on a web browser to access the admin dashboard. Fill in with your machine's hostname and the port you used while deploying HPSee.
Welcome to
HPSee 1.0
unparalleled processing
Maia
Username
admin
Password
LOGIN
Login with admin credentials:
username and password as 'admin'.


Menu bar to access the pages
HPSee Admin Dashboard
http://<hostname>:<port>
Light/Dark mode
Legal notice
Logout
HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
Open/Close Menu Bar
Hello Administrator!
Your session expires at 7:59 PM
Session expires automatically after 8 hours.
Overview of current number of users, Chemical Spaces and chemical libraries uploaded on the server.
Users
1
Spaces
0
Libraries
0
Conformator License is valid
FlexX License is valid
Hydescorer License is valid
FragmentExtractor License is valid
FragmentExtender License is valid
PropertyAnnotator License is valid
Check your license validity. Certain tasks may not require all the license. For example: Remote Docking requires FlexX and Hydescorer only.
Version Information
Release: HPSee 1.0.0, "Maia"
Build: Monday, 08 April 2024 12:57
Version and build information.


HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
Admin can add/remove users in this page.
Refresh
Users
Username
First Name
Last Name
Email
Is Administrator
Registration Date
admin
Administrator
Rows per page: 10
1-1 of 1
Current users' information gets stored in the table.

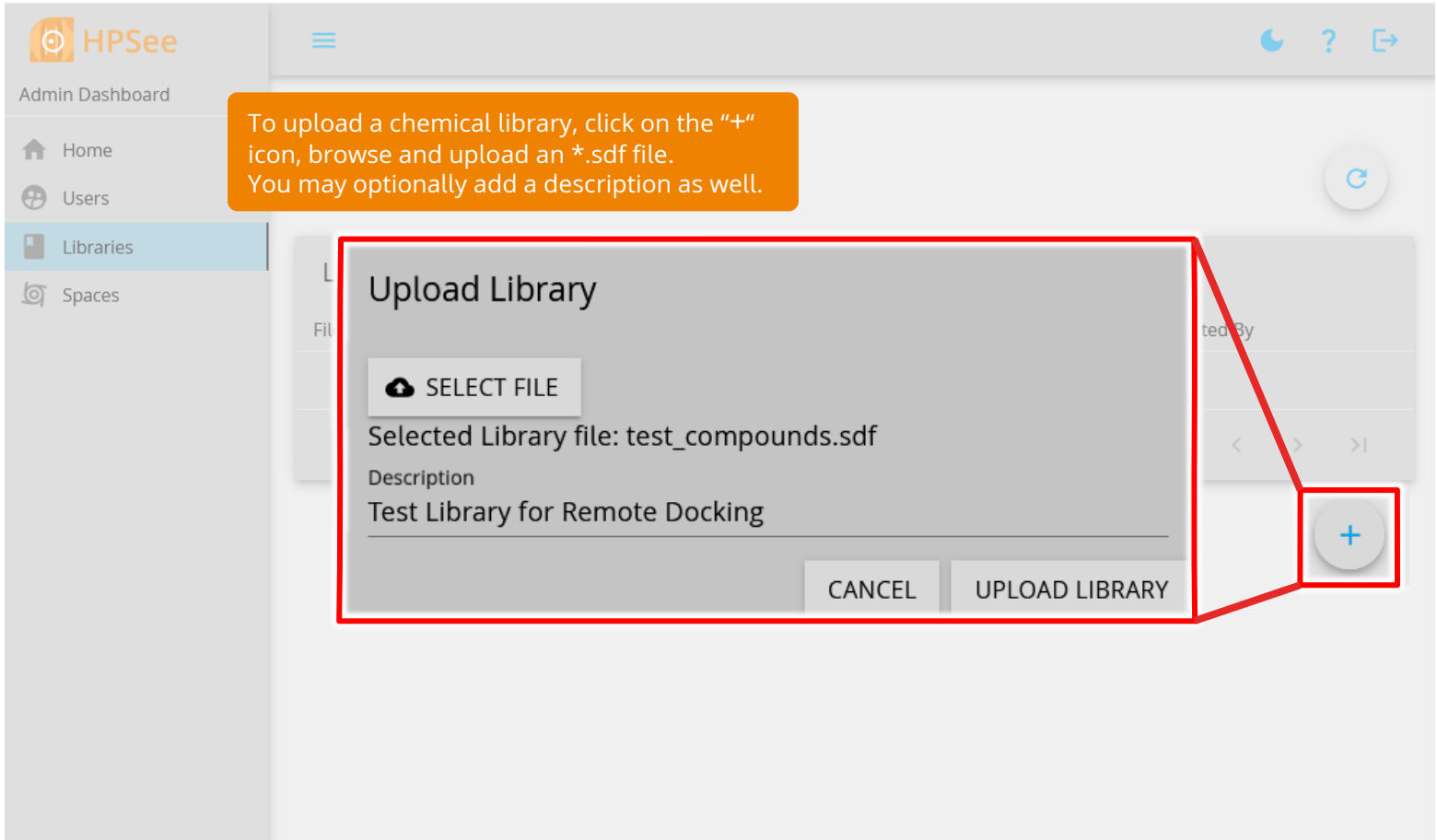

HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
Users
Username
admin
Registration Date
-1 of 1
Create new user
Username*
Password*
Must be at least 6 characters long
Retype Password*
First Name*
Last Name*
Email*
Create as Administrator
CANCEL
CREATE USER
Add User
You can grant admin rights to the users.

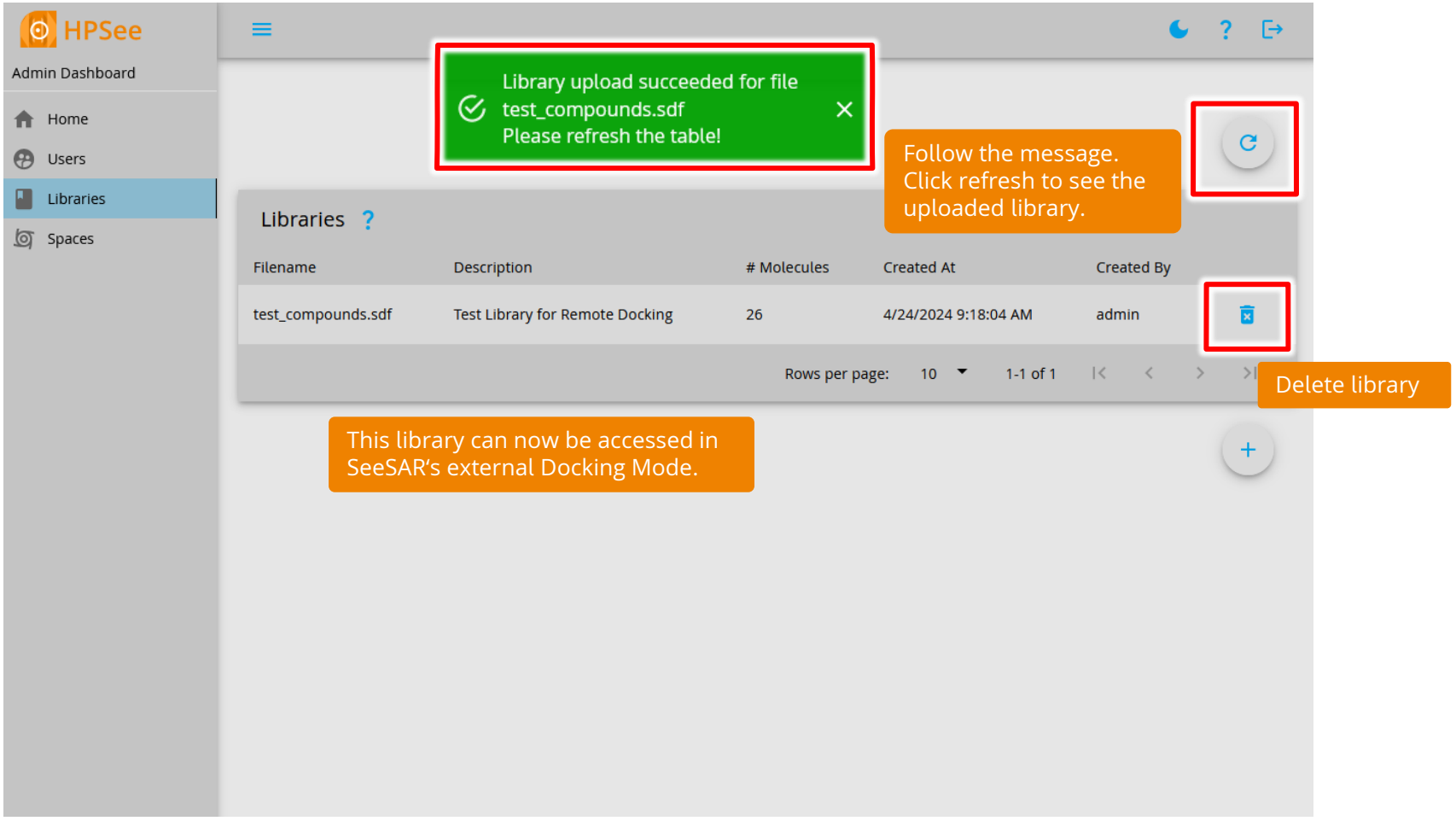

HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
User created!
Users
Username
First Name
Last Name
Email
Is Administrator
Registration Date
admin
Administrator
user1
User
4/24/2024
Created user is listed.
Rows per page:
10
1-2 of 2

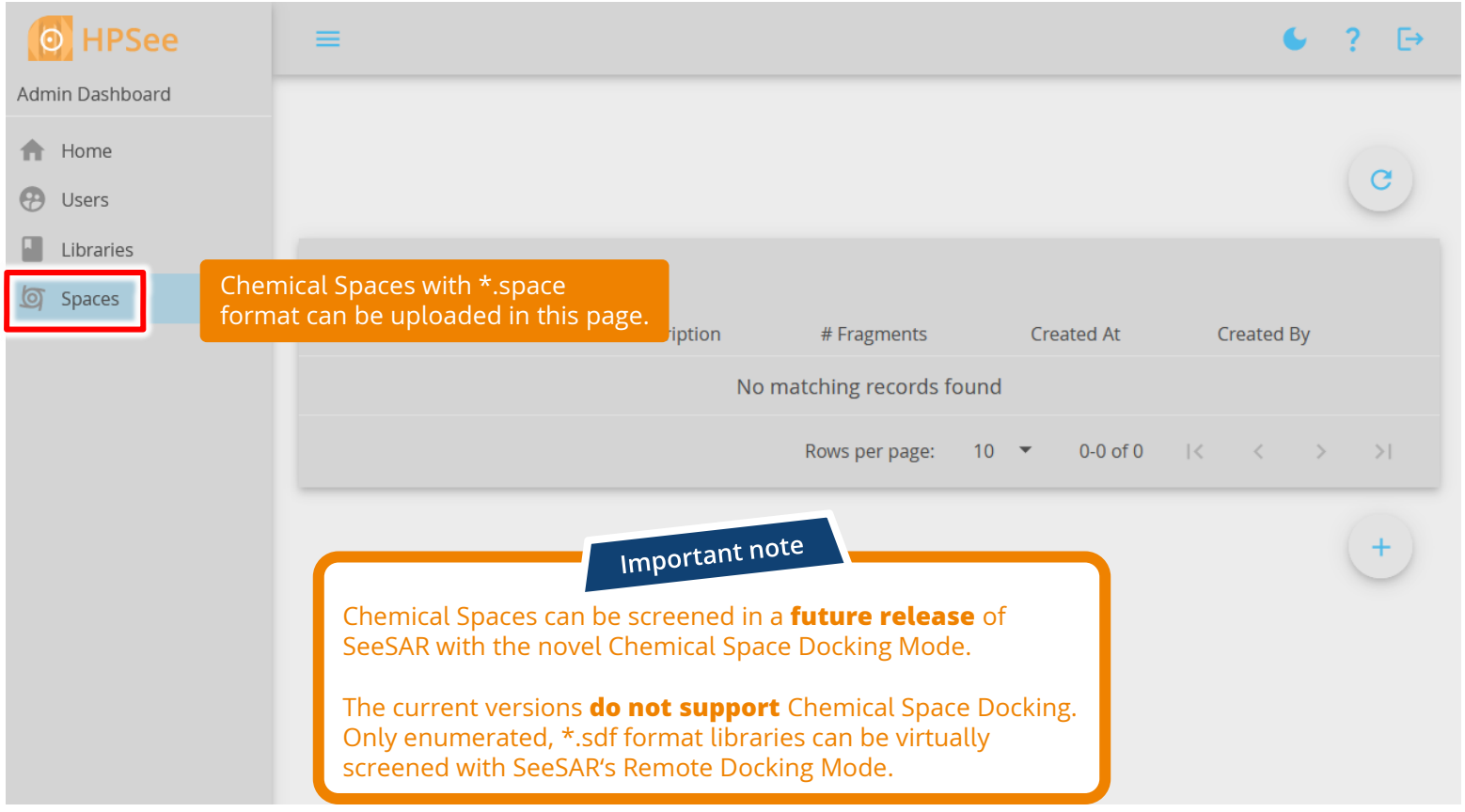


Tipp

Use the **Conformator** tool to generate 3D coordinates.

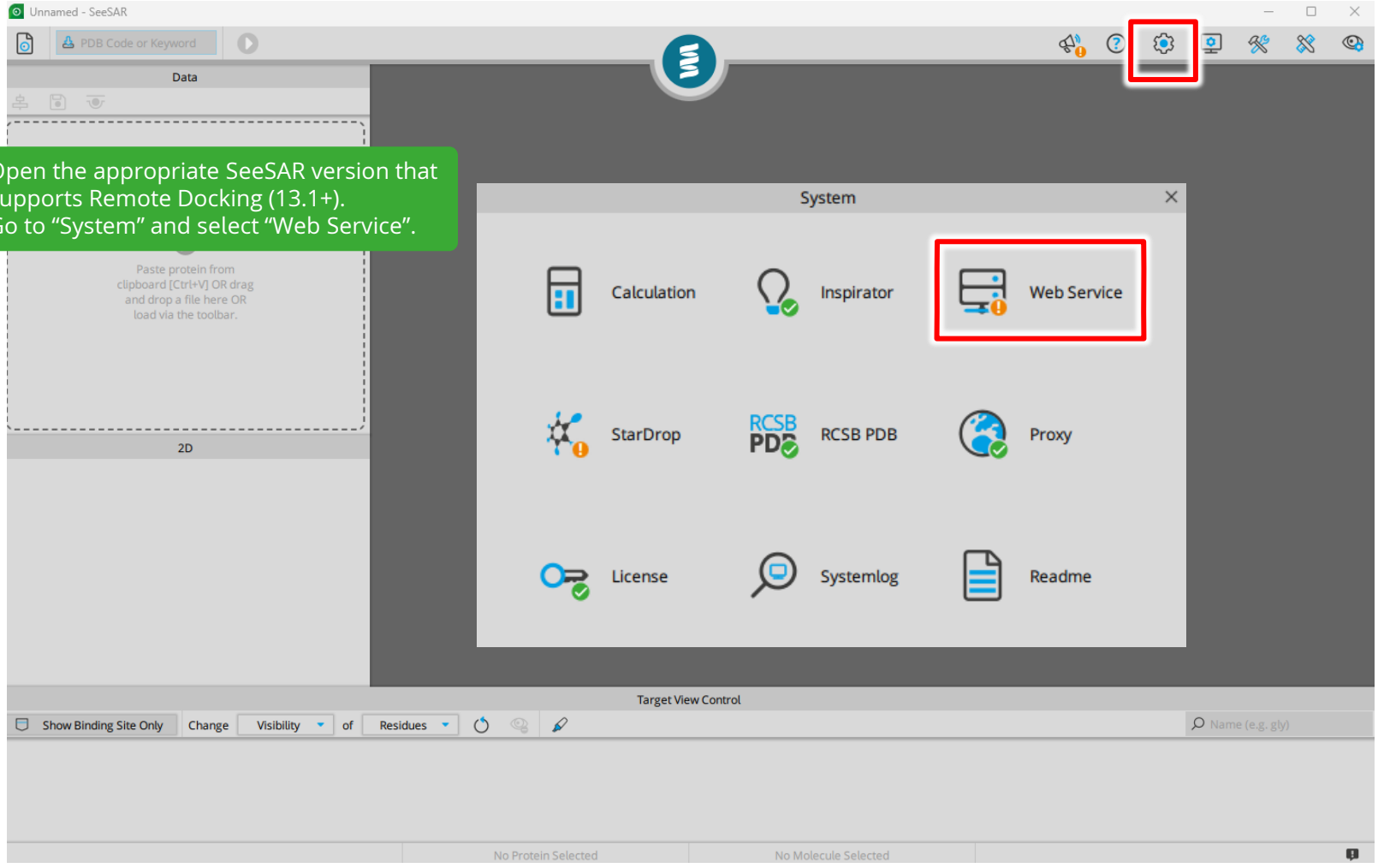

HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
To upload a chemical library, click on the "+" icon, browse and upload an *.sdf file.
You may optionally add a description as well.
Upload Library
SELECT FILE
Selected Library file: test_compounds.sdf
Description
Test Library for Remote Docking
CANCEL
UPLOAD LIBRARY

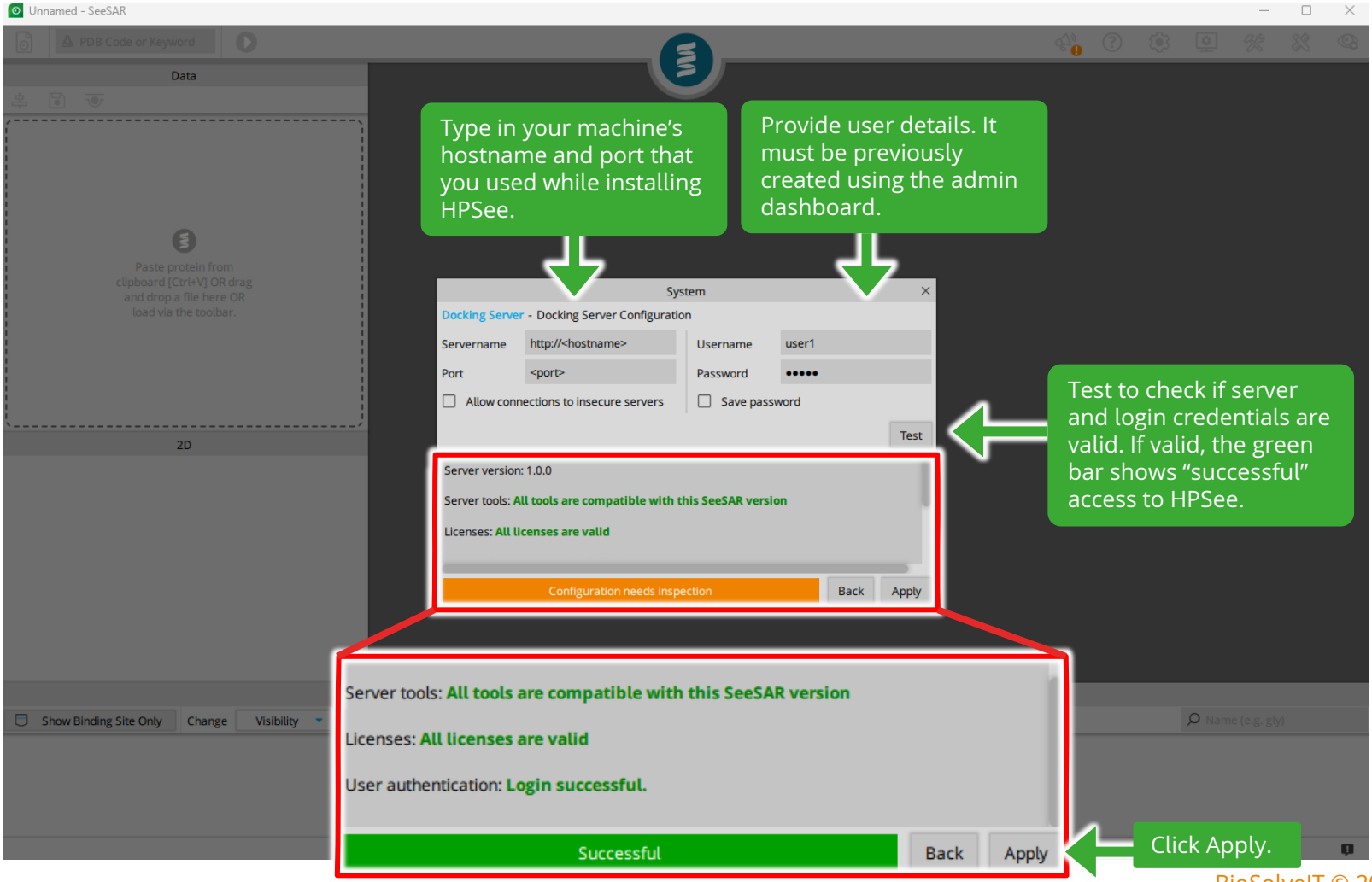

HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
Library upload succeeded for file
test_compounds.sdf
Please refresh the table!
Follow the message.
Click refresh to see the
uploaded library.
Libraries
Filename
Description
Molecules
Created At
Created By
test_compounds.sdf
Test Library for Remote Docking
26
4/24/2024 9:18:04 AM
admin
Rows per page:
10
1-1 of 1
Delete library
This library can now be accessed in
SeeSAR's external Docking Mode.

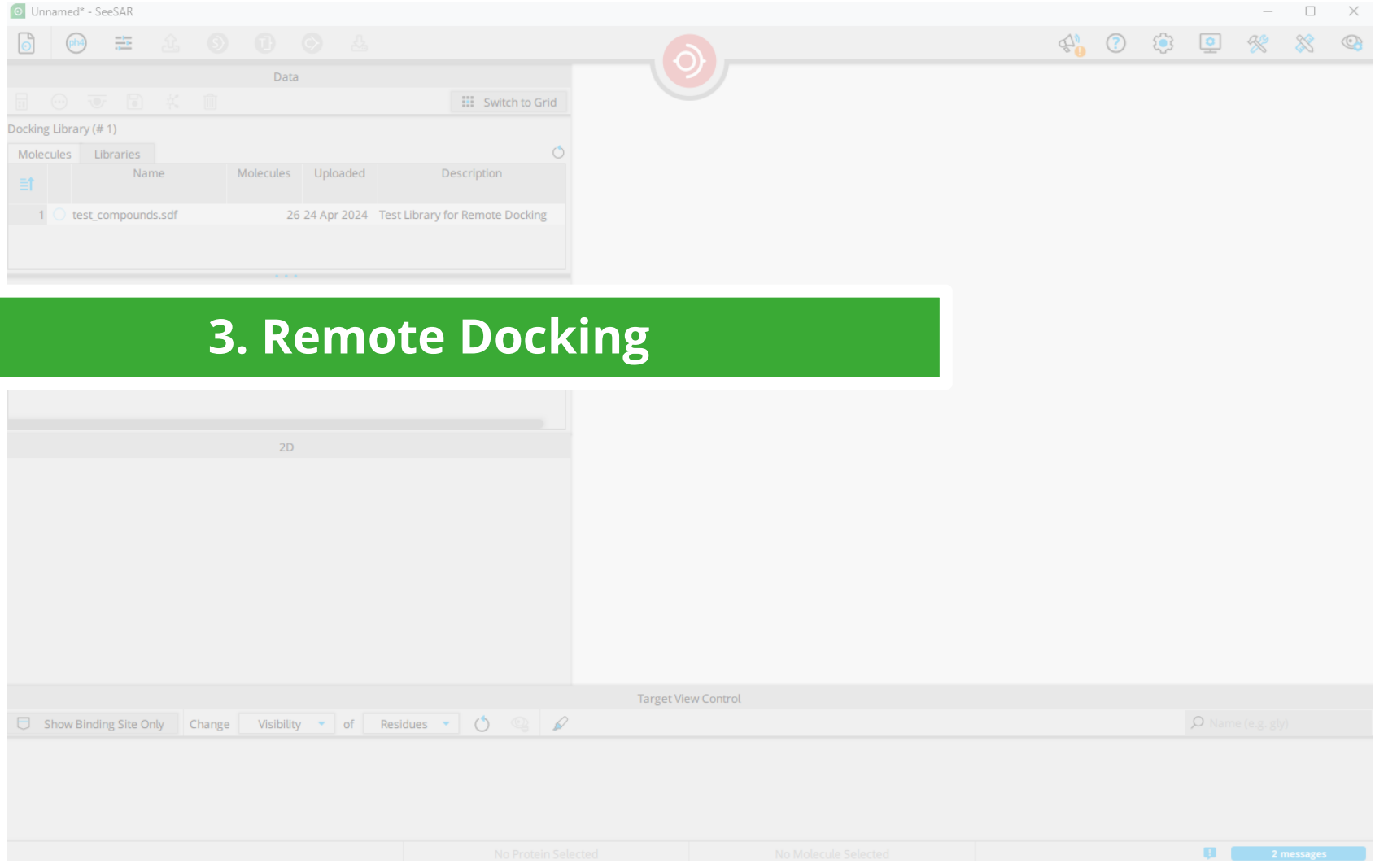

HPSee
Admin Dashboard
Home
Users
Libraries
Spaces
Chemical Spaces with *.space format can be uploaded in this page.
Fragments
Created At
Created By
No matching records found
Rows per page: 10
0-0 of 0
Important note
Chemical Spaces can be screened in a future release of SeeSAR with the novel Chemical Space Docking Mode.
The current versions do not support Chemical Space Docking. Only enumerated, *.sdf format libraries can be virtually screened with SeeSAR's Remote Docking Mode.

2. Connect to SeeSAR

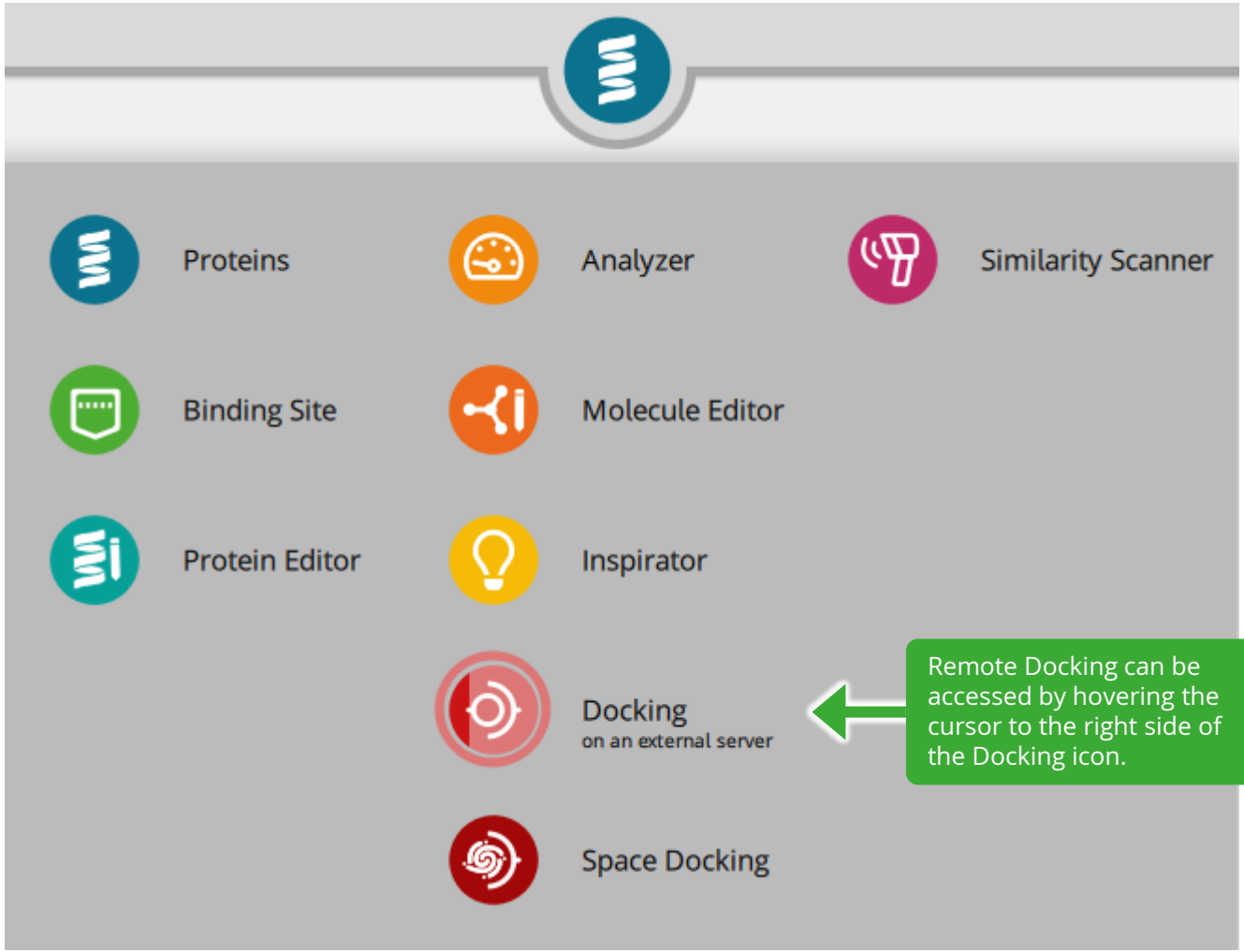
To perform Remote Docking from SeeSAR, it must be first connected to the HPSee server.

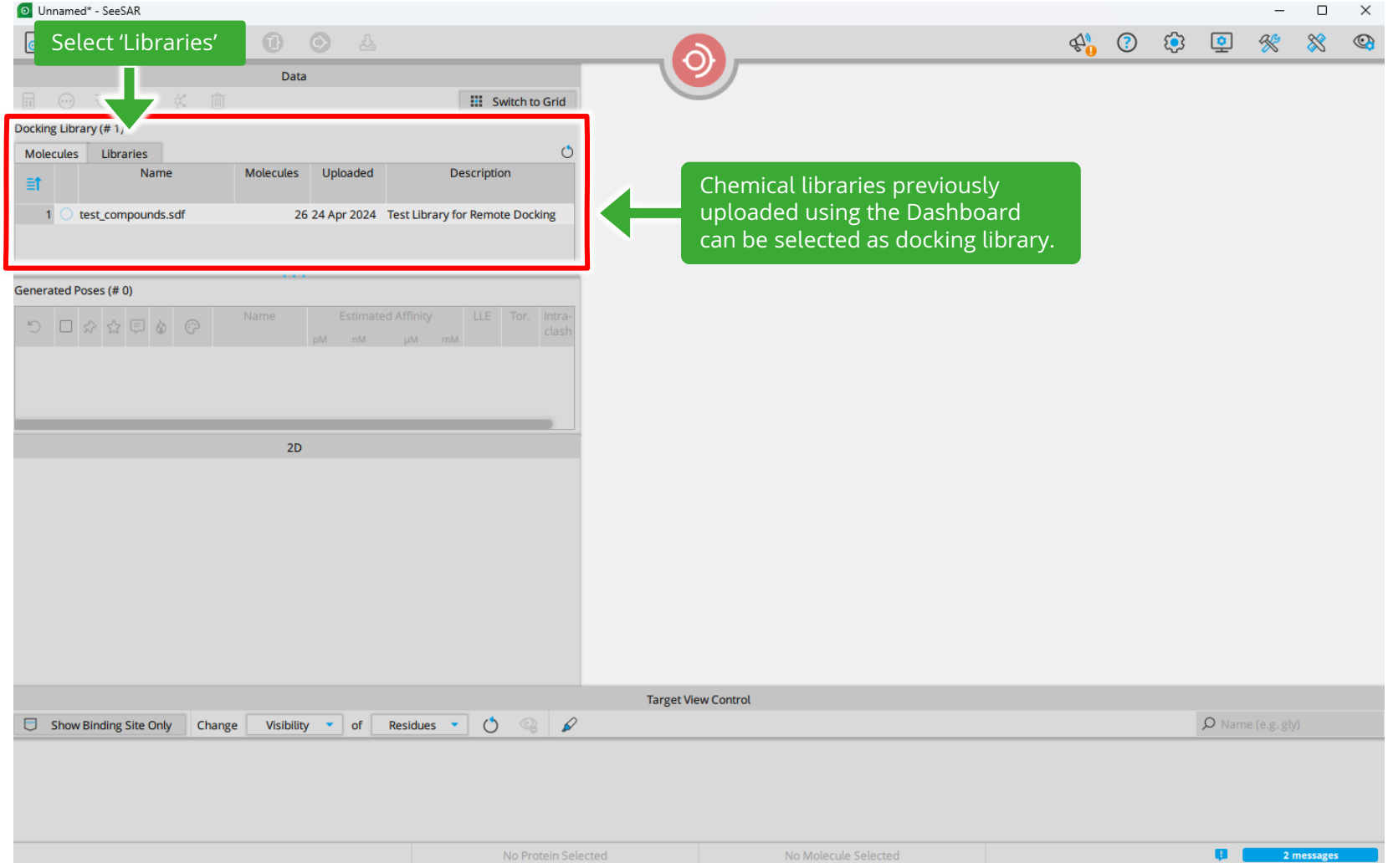

Unnamed - SeeSAR
PDB Code or Keyword
Data
Paste protein from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.
2D
Open the appropriate SeeSAR version that supports Remote Docking (13.1+).
Go to “System” and select “Web Service”.
System
Calculation
Inspirator
Web Service
StarDrop
RCSB PDB
Proxy
License
Systemlog
Readme
Target View Control
Show Binding Site Only
Change
Visibility
of
Residues
Name (e.g. gly)
No Protein Selected
No Molecule Selected

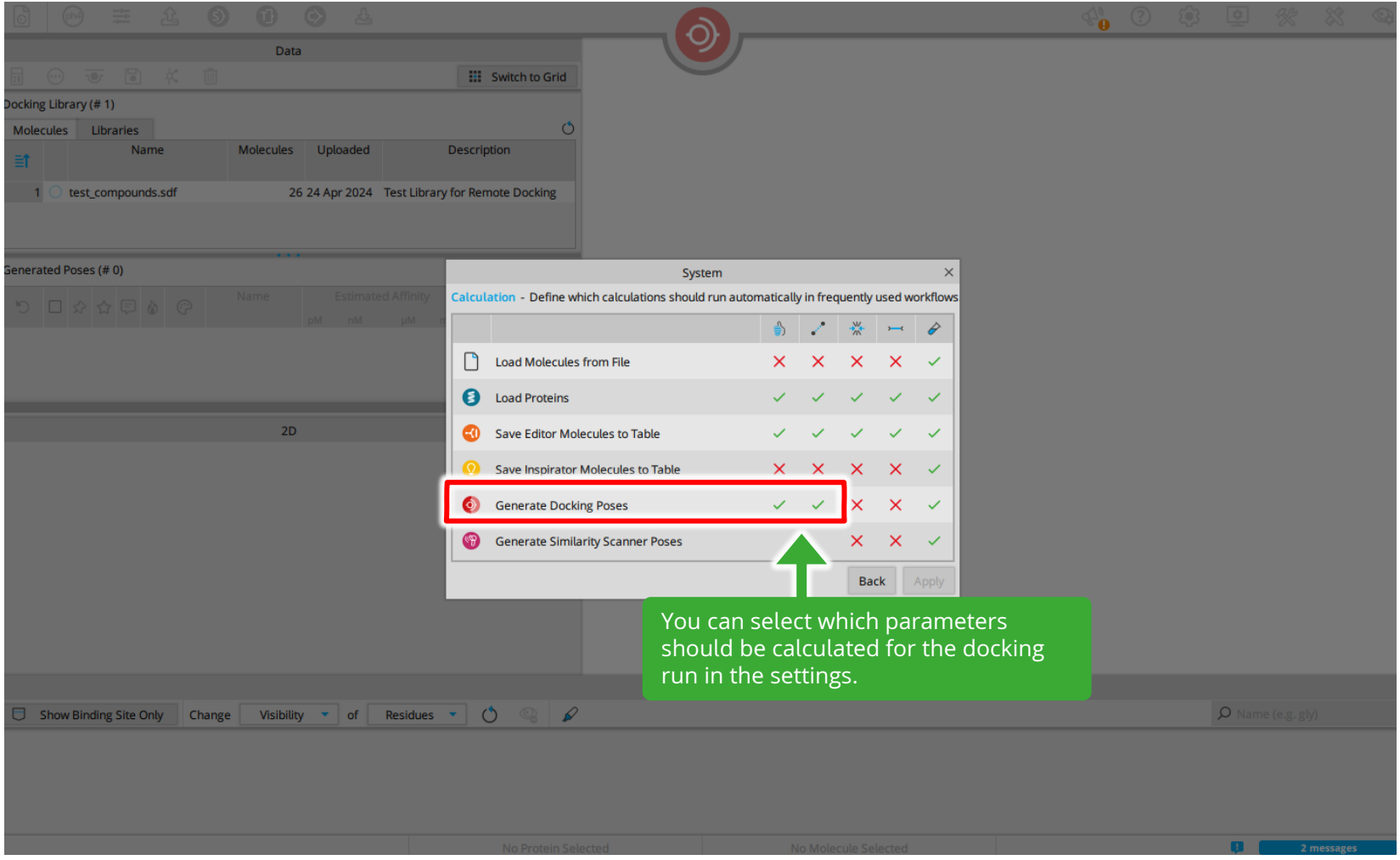

Unnamed - SeeSAR
PDB Code or Keyword
Data
Paste protein from clipboard [Ctrl+V] OR drag and drop a file here OR load via the toolbar.
2D
Show Binding Site Only
Change
Visibility
Type in your machine's hostname and port that you used while installing HPSee.
Provide user details. It must be previously created using the admin dashboard.
System
Docking Server - Docking Server Configuration
Servername
http://<hostname>
Port
<port>
Username
user1
Password
Allow connections to insecure servers
Save password
Test
Server version: 1.0.0
Server tools: All tools are compatible with this SeeSAR version
Licenses: All licenses are valid
Configuration needs inspection
Back
Apply
Test to check if server and login credentials are valid. If valid, the green bar shows "successful" access to HPSee.
Server tools: All tools are compatible with this SeeSAR version
Licenses: All licenses are valid
User authentication: Login successful.
Successful
Back
Apply
Click Apply.

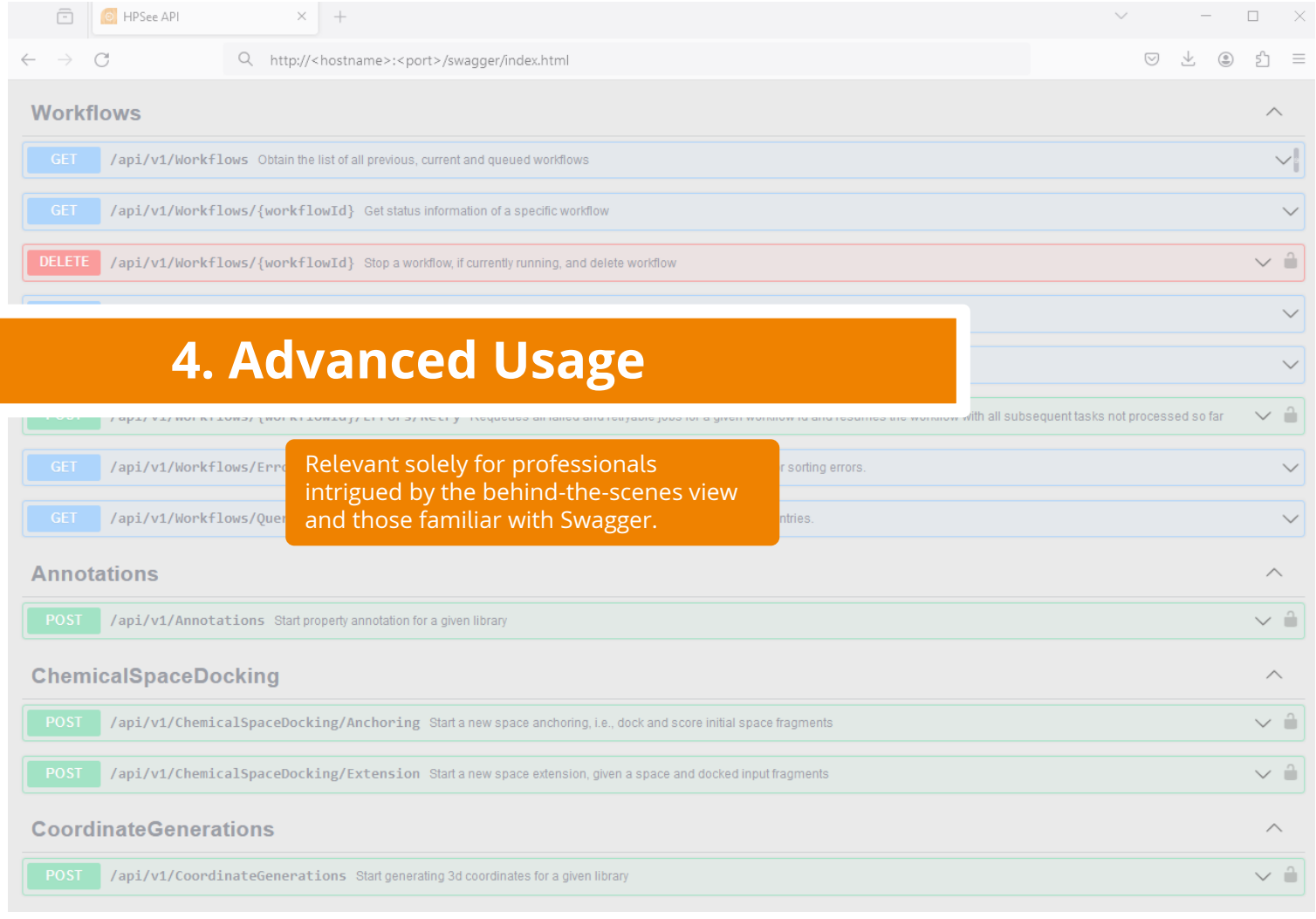


3. Remote Docking


Proteins
Analyzer
Similarity Scanner
Binding Site
Molecule Editor
Protein Editor
Inspirator
Docking
on an external server
Space Docking
Remote Docking can be accessed by hovering the cursor to the right side of the Docking icon.

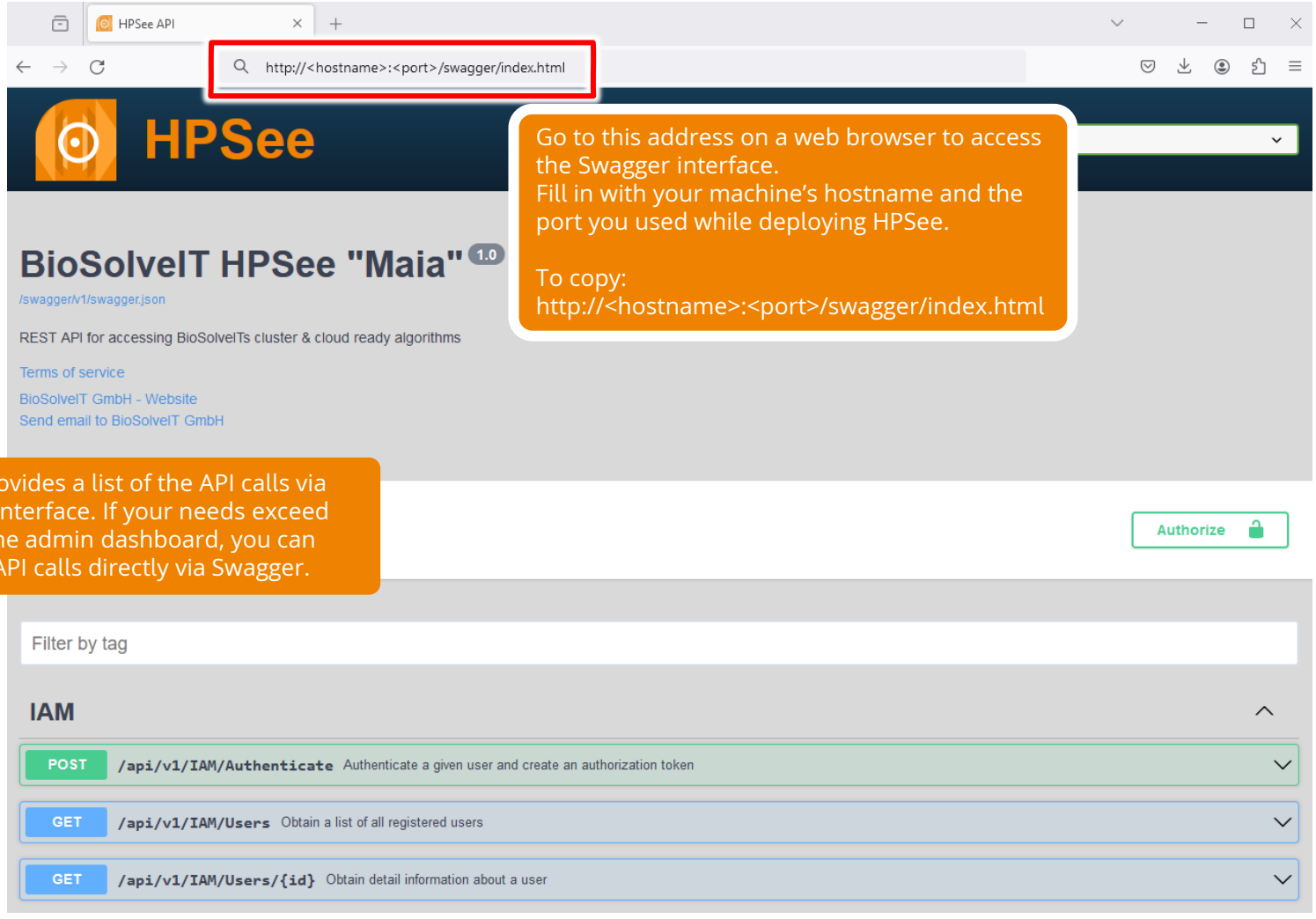

Unnamed* - SeeSAR
Select 'Libraries'
Data
Switch to Grid
Docking Library (# 1)
Molecules
Libraries
Name
Molecules
Uploaded
Description
1
test_compounds.sdf
26 24 Apr 2024
Test Library for Remote Docking
Chemical libraries previously uploaded using the Dashboard can be selected as docking library.
Generated Poses (# 0)
Name
Estimated Affinity
pM
nM
µM
mM
LLE
Tor.
Intra-clash
2D
Target View Control
Show Binding Site Only
Change
Visibility
of
Residues
Name (e.g. gly)
No Protein Selected
No Molecule Selected
2 messages

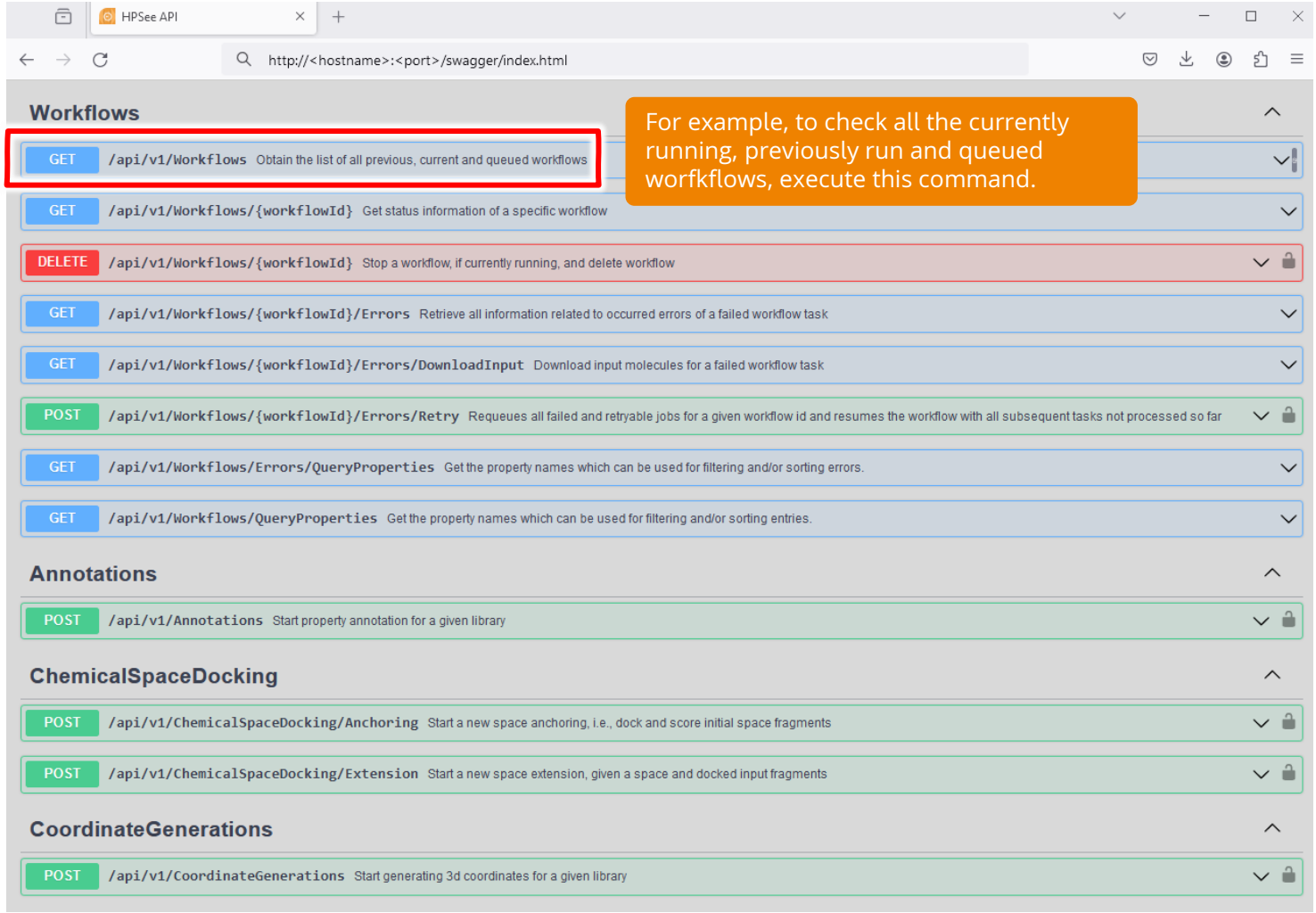

Data
Switch to Grid
Docking Library (# 1)
Molecules
Libraries
Name
Molecules
Uploaded
Description
1
test_compounds.sdf
26 24 Apr 2024
Test Library for Remote Docking
Generated Poses (# 0)
Name
Estimated Affinity
2D
System
Calculation - Define which calculations should run automatically in frequently used workflows
Load Molecules from File
Load Proteins
Save Editor Molecules to Table
Save Inspirator Molecules to Table
Generate Docking Poses
Generate Similarity Scanner Poses
Back
Apply
You can select which parameters should be calculated for the docking run in the settings.
Show Binding Site Only
Change
Visibility
of
Residues
Name (e.g. gly)
No Protein Selected
No Molecule Selected
2 messages



4. Advanced Usage

Relevant solely for professionals intrigued by the behind-the-scenes view and those familiar with Swagger.


HPSee API
http://<hostname>:<port>/swagger/index.html
HPSee
Go to this address on a web browser to access the Swagger interface.
Fill in with your machine's hostname and the port you used while deploying HPSee.
To copy:
http://<hostname>:<port>/swagger/index.html
BioSolveIT HPSee "Maia" 1.0
/swagger/v1/swagger.json
REST API for accessing BioSolveITs cluster & cloud ready algorithms
Terms of service
BioSolveIT GmbH - Website
Send email to BioSolveIT GmbH
HPSee provides a list of the API calls via Swagger interface. If your needs exceed beyond the admin dashboard, you can perform API calls directly via Swagger.
Authorize
Filter by tag
IAM
POST /api/v1/IAM/Authenticate Authenticate a given user and create an authorization token
GET /api/v1/IAM/Users Obtain a list of all registered users
GET /api/v1/IAM/Users/{id} Obtain detail information about a user


HPSee API
http://<hostname>:<port>/swagger/index.html
Workflows
GET /api/v1/Workflows Obtain the list of all previous, current and queued workflows
GET /api/v1/Workflows/{workflowId} Get status information of a specific workflow
DELETE /api/v1/Workflows/{workflowId} Stop a workflow, if currently running, and delete workflow
GET /api/v1/Workflows/{workflowId}/Errors Retrieve all information related to occurred errors of a failed workflow task
GET /api/v1/Workflows/{workflowId}/Errors/DownloadInput Download input molecules for a failed workflow task
POST /api/v1/Workflows/{workflowId}/Errors/Retry Requeues all failed and retryable jobs for a given workflow id and resumes the workflow with all subsequent tasks not processed so far
GET /api/v1/Workflows/Errors/QueryProperties Get the property names which can be used for filtering and/or sorting errors.
GET /api/v1/Workflows/QueryProperties Get the property names which can be used for filtering and/or sorting entries.
Annotations
POST /api/v1/Annotations Start property annotation for a given library
ChemicalSpaceDocking
POST /api/v1/ChemicalSpaceDocking/Anchoring Start a new space anchoring, i.e., dock and score initial space fragments
POST /api/v1/ChemicalSpaceDocking/Extension Start a new space extension, given a space and docked input fragments
CoordinateGenerations
POST /api/v1/CoordinateGenerations Start generating 3d coordinates for a given library
For example, to check all the currently running, previously run and queued worfkflows, execute this command.

Enjoy your high-performance computing adventures with HPSee!

Have fun and enjoy your interactive drug discovery journey with SeeSAR!

If you have any problems, please reach out to us:
support@biosolveit.de