

# Revvity Signals Inventa™ 3.5.1

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Release Notes

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Powered by Spotfire®

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# 1 General Description

Signals Inventa™ powered by Revvity Signals Data Factory and Spotfire® empowers scientific professionals to readily access the scientific data they need to discover better drugs faster. Through Signals Data Factory, structured and unstructured scientific data is normalized and contextualized such that it can be discovered by Signals Inventa™ scientists in an intuitive and efficient workflow. Through Spotfire®, those data are automatically presented in a well-organized SAR workflow that encourages data exploration and drug candidate assessment.

Moreover, Signals Inventa™ includes features to drive the full life cycle of data. Data Generators (assay and analytical scientists) can more easily publish their data with the confidence that those data will be discovered and re-used by the project teams. Data consumers (Signals Inventa project team members) can dedicate their time to understanding the science rather than painstakingly assembling data.

## The Global Search App allows you to:

- Create complex nested queries and interrogate any subset of the stored data of interest.
- Query for Structure, any compound attribute, and any assay or measurement, and query over an expanded set of comparison operators.
- Control system performance directly by choosing estimated vs. precise query result counts at different levels of precision.
- Save queries for easy re-use. Saved searches can be public or private.

## The SAR Analysis App allows you to:

- Define how the Compound and Assay data should be organized (e.g. by Compound or Compound Batch) and summarized (by mean, median, count, standard deviation, etc.).
- Customize long assay names into more meaningful, human-readable abbreviations.
- Configure intuitive tabular and graphical representations of the data through a point-and-click interface.
- Toggle between saved views of the data to easily navigate SAR analyses including many assays.
- Generate and compare compound lists with an interactive Venn diagram.

## The Publish Measurements App allows you to:

- Capture all the descriptive information surrounding data publication
- Automatically configure data coming out of a data processing or screening workflow to be ingested for final review and publication
- Configure and capture the publication information for a Signals VitroVivo Protocol.
- Re-play the publication configuration automatically in all future runs of the Signals VitroVivo Protocol.

## The Target Engagement Profile App allows you to:

- Integrate *in vivo* pharmacokinetics and *in vitro* efficacy data within a single, normalized graph to streamline candidate selection.
- Define relevant time-concentration and PK parameter measurement types
- Define plasma protein binding or other normalizing measurement types
- Integrate with *in vitro* IC50, EC50, AC50 measurements

- Toggle visualization between Concentration vs. Time and % Inhibition vs. Time

**Highlights of Signals Inventa™ 3.5.1 Release:**

- Rebranding to Revvity Signals
- Performance optimization for dataset loading
- ChemCharts 4.4
  - HELM Support and Data Functions, including sequence alignment, similarity search, and property calculations
  - New Biological Sequence data functions, including annotation, motif search, gap removal, and antibody liability prediction
  - Support for embedded PDB files
- Configuration option to specify overwrite behavior of blank values in Data Factory
- Upgraded Data Factory to RKE (v1.5.3)
- Various bugs addressed

## 2 Distribution Limitations

This is a general release for all customers who are running 12.0.x LTS or 14.0.x LTS.

## 3 Release Qualification

### 3.1 Scope of Testing

To assure the quality of Signals Inventa, in depth functional, performance and regression testing was performed throughout the development cycle. Testing was conducted in the environments described below.

### 3.2 Testing Environment

Machine Type	Operating System	Database	Docker	kubern etes	helm	Rancher RKE	Spotfire	Signals VitroVivo	Browser
SIA/SDF Server	Ubuntu 20.04 LTS	MongoDB 5.0.8/ 4.4.1	Docker 20.10.9	NA	NA	NA	NA	NA	NA
Client for SIA/SDF Cluster	Ubuntu 20.04 LTS	NA	NA	12	Helm 3.8.2	RKE 1.5.3	NA	NA	NA
Spotfire Server DB	Windows Server 2019 (64bit)	PostgreSQL L 15	NA	NA	NA	NA	NA	NA	NA
	Windows Server 2019 (64bit)	PostgreSQL L 12	NA	NA	NA	NA	NA	NA	NA

Machine Type	Operating System	Database	Docker	kubern etes	helm	Rancher RKE	Spotfire	Signals VitroVivo	Browser
Spotfire Server	Windows Server 2019 (64bit)	NA	NA	NA	NA	NA	Spotfire Server & Node Manager 12.0.8 LTS	NA	NA
	Windows Server 2019 (64bit)	NA	NA	NA	NA	NA	Spotfire Server & Node Manager 14.0.2 LTS	NA	NA
Client	Windows 11 Enterprise version 23H2 (64bit)	NA	NA	NA	NA	NA	Spotfire Analyst & Web Client 14.0.2 LTS HF-007	Signals VitroVivo 3.5.1	Google Chrome 122, Mozilla Firefox 123, MS Edge 122
	Windows 10 Enterprise version 22H2 (64bit)	NA	NA	NA	NA	NA	Spotfire Analyst & Web Client 12.0.8 LTS HF-028		
		NA	NA	NA	NA	NA	Spotfire Analyst & Web Client 14.0.2 LTS HF-007		
	macOS Sonoma 14.4 (64bit)	NA	NA	NA	NA	NA	Spotfire Web Client 12.0.8 LTS HF-028		
		NA	NA	NA	NA	NA	Spotfire Web Client 14.0.2 LTS HF-007		

## 4 Installation Instructions

### 4.1 Installation

Follow the installation instructions provided within the documentation in “*Revvity Signals Inventa v3.5.1 Installation Guide (Bare-Metal Kubernetes).pdf*”.

**Note:** If you want to deploy Revvity Signals VitroVivo with Signals Inventa v3.5.1, it is recommended that you install Signals VitroVivo v3.5.1 for integration.

## 4.2 Prerequisites

The Installation Guide explains the steps required to deploy and set up Signals Inventa, based on the assumption that you have previously performed the following tasks:

- Installed the Spotfire Server 12.0.x LTS or 14.0.x at your site.

## 4.3 Manifest

This package includes:

### SignalsInventa\_3.5.1\_installer:

- Server
  - sdf-standalone-cluster-deployment-ansible-sld.zip
  - sia-cluster-deployment.tar.gz
- Spotfire Distribution
  - SignalsInventa-3.5.0.21.sdn
  - Signals\_Srp\_Client-3.5.0.2.spk
  - Signals.Apps\_5.5.9156.0.spk
  - LeadDiscovery-8.6.3.8.spk
  - LeadDiscovery-NoCDAX-8.6.3.8.spk
  - SarSolution-1.1.4.575.spk
  - ScientificUtilities\_6.0.0.237.spk
  - LeadDiscoveryChemCharts\_4.4.0.9.sdn
- Additional Software
  - siautils-linux-x64-3.5.1.3.zip
  - siautils-win-x64-3.5.1.3.zip
  - cdjs##22.7.0-5075.war
  - ChemCharts4.4.0.9.war

### SignalsInventa\_3.5.1\_documentation:

- Revvity Signals Inventa v3.5.1 Release Notes.pdf
- Revvity Signals Inventa v3.5.1 User Guide.pdf
- Revvity Signals Inventa v3.5.1 Installation Guide (Bare-Metal Kubernetes).pdf
- Revvity Signals Inventa v3.5.1 System Requirements.pdf
- Revvity Signals Inventa v3.5.1 Command Line Utilities User Guide.pdf
- sia-example-datasets-3.5.0.zip (contains supporting files for OotB Dashboards including Quick Start Guides)
- Revvity Lead Discovery Premium v3.5 Release Notes.pdf
- Revvity Lead Discovery Premium v3.5 Installation Guide.pdf
- Revvity Lead Discovery Premium v3.5 System Requirements.pdf
- Revvity Lead Discovery Premium v3.5 Smart Cell Guide.pdf
- Revvity Lead Discovery Premium v3.5 User Guide.pdf
- Data Function Python Library.pdf

- Data Function User Guide.pdf
- Data Function YAML file specification.pdf
- Lead Discovery ChemCharts User Guide.pdf
- Rename Columns from CSV Transformation User Guide.pdf
- ScriptSync User Guide.pdf
- marvinjs

## 5 Limitations, Known Issues and Workarounds

- Export Assay Details visualization to PDF in Spotfire Analyst is not supported.
- Print Assay Details visualization in Spotfire Analyst is not supported.
- Can only export the first 100 assay result data of Table layout in Edit Assay Details page.
- Add more than 200 measurement types to Assay Details visualization one time may be slow.
- 'Show Title Bar' option change will close the Assay Details Properties dialog and refresh the visualization.
- Spotfire Redo/Undo operations are partially supported.
- Custom theme is partially supported.
- Spotfire Analyst may crash if two visualizations use different data table and one of tables deleted.
- Substructure search with Tautomeric flag misses some tautomers.
- Measurement Condition does not work when one letter name of h1/h2/h3 in assay tree
- Open saved \*.dpx under different SDF projects or environments will cause data inconsistent in some cases.  
**Workaround:** Click 'Reload' button in Global Search.
- A user with Read permission can add new Signals Apps into analysis in Spotfire Web Client.
- Downloaded Global Search results fail to be binned to SAR Analysis App in some cases.  
**Workaround:** Reopen the saved \*.dpx.
- New Spotfire window in SAR Analysis App is not supported.
- An SAR Analysis App page will be reloaded each time with no resource cached when you switch it between other pages in Spotfire Web Client.
- Signals Apps page will be always in processing status in some cases.  
**Workaround:** Reopen the saved \*.dpx.
- Publish data in publish tool by 'Add to data set' option will also add the duplicated rows of data.
- The selection of renamed columns in SAR Analysis App are not persistent after reopening an analysis file in some cases.  
**Workaround:** Select the columns and save the analysis file again.
- Manage Measurement Types cannot work in Spotfire Client when opening in Chrome v76+.
- The field 'Measurement Type' (h1) in Signals Inventa v2.1 or earlier versions has been changed to Assay Type, and a new field. With the name 'Measurement Type' is added, user needs to correct the mapping when opening a dpx file saved in previous versions.
- The Assay Endpoint Result measurement should not be set as a Parent Measurement Type for mapping.
- When migrating Saved Searches from Signals Inventa v2.0, the Structure condition will not show the SMILES value but '...' only.  
**Workaround:** Open ChemDraw editor to save the Structure value, and then save the Search.
- The fixed rows and columns of ChemCharts Table are not supported for filtering in SAR Analysis App.
- The window is not closed in some cases after sign-in succeeds.  
**Workaround:** To close the sign-in window and click Sign In button again
- The Group and Layout items in SAR Analysis App are not displayed in some cases.  
**Workaround:** To switch Spotfire pages to refresh.
- A condition removed by clicking 'x' button will be displayed again after refreshing in some cases.
- Spotfire bookmark is partially supported in SAR Analysis App.

- The upgrade of an analysis file created in a previous SIA version may cause the Structure column settings in some visualizations lost.  
**Workaround:** To do the settings for the Structure column again in the visualizations.
- Some of data in a big dataset may fail to be downloaded in a poor network.
- Duplicate of SAR Analysis app page is not supported.  
**Workaround:** To add more SAR Analysis apps from menu.
- Delete Marked Rows window shows up when deleting the contents in aggregation.  
**Workaround:** To close the pop-up window.
- No standardized endpoint value is calculated if selecting batch attribute as molecular weight in TEP app.
- Data publication is avoided if saving a measurement type map with empty expression in Publish tool.
- Loading status shows up when changing mapping column for an attribute in Publish tool.
- 'Add Match Columns' icon on Configuration tab is disabled when opening TEP app from workflow.  
**Workaround:** Switch to a different measurement type.
- Only "http" and "https" types of URL are supported for the search in Global Search.
- Endpoints named with expressions fail to appear in Global Search when attribute is not mapped.
- Spotfire v14.0 becomes no response for some cases when the option 'Close when finished' checkbox of a pop-up dialog is checked.  
**Workaround:** Upgrade Spotfire v14.0 client to HF-007 or later.

**Note:** Please refer to the limitations and known issues of Lead Discovery Premium in *Revvity Lead Discovery Premium v3.5 Release Notes.pdf*.

## 6 Technical Support

This software is supported by Revvity Signals Software Support.

### Revvity Signals Software Inc.

940 Winter Street | Waltham, MA 02451

<https://support.revvitysignals.com/hc/en-us>

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