

Ardia Platform: an open ecosystem for chromatography and mass spectrometry

Stephane Houel – Mark Ressler

 The world leader in serving science



Chromatography & mass spectrometry

Software

What is the Ardia Platform?



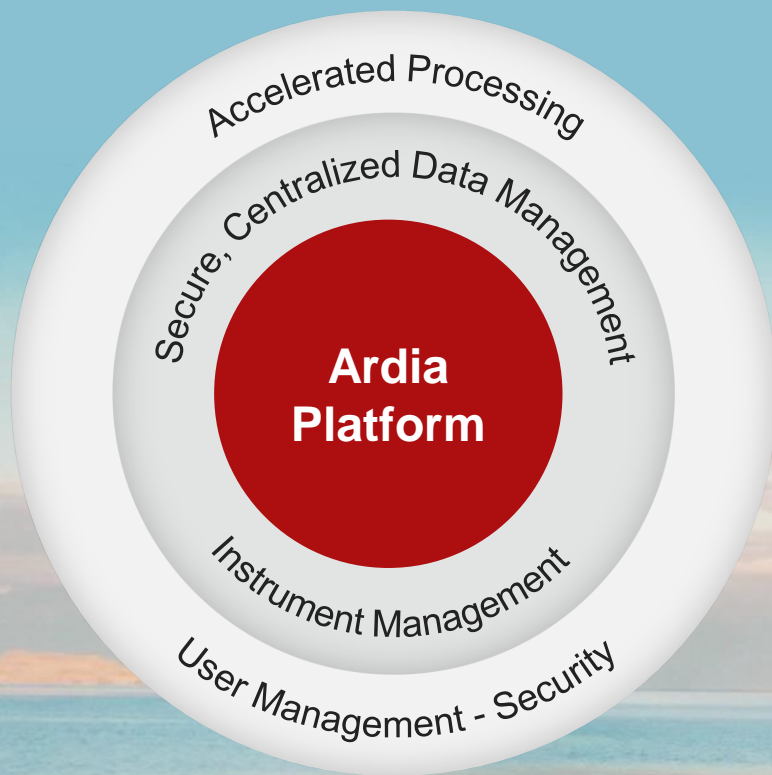
- Introduction to the Ardia Platform
- Core applications: Data Explorer - Data Viewer – Instruments
- New Data Insights application: Instrument utilization

Open platform features

- 3rd party API access: Skyline connection
- Ardia Platform Data Sync
- FAIR data principles: Data catalog – metadata

The Thermo Scientific™ Ardia™ Platform

(Launched in 2023 and installed worldwide)



Software designed for scientists performing chromatography and mass spectrometry analysis evolving with their needs, built on the latest software architecture and technology

Ardia Platform

Collaboration

Bring people, data and instruments together on an intuitive, integrated platform that encourages the sharing of knowledge

Productivity

Efficiently manage assets, automate workflows and speed up processing with fit-for-purpose solutions to accelerate results

Deep insights

Centralized, connected and annotated data enables mining of the information to gain additional insights

Security

Controlled access to centrally stored data and results with audit trails, results versioning and backup, and archive capabilities built in

Connecting instruments



- Centralized data management
- Easy access to data
- Instrument status from anywhere
- Efficient lab operations

Collaboration

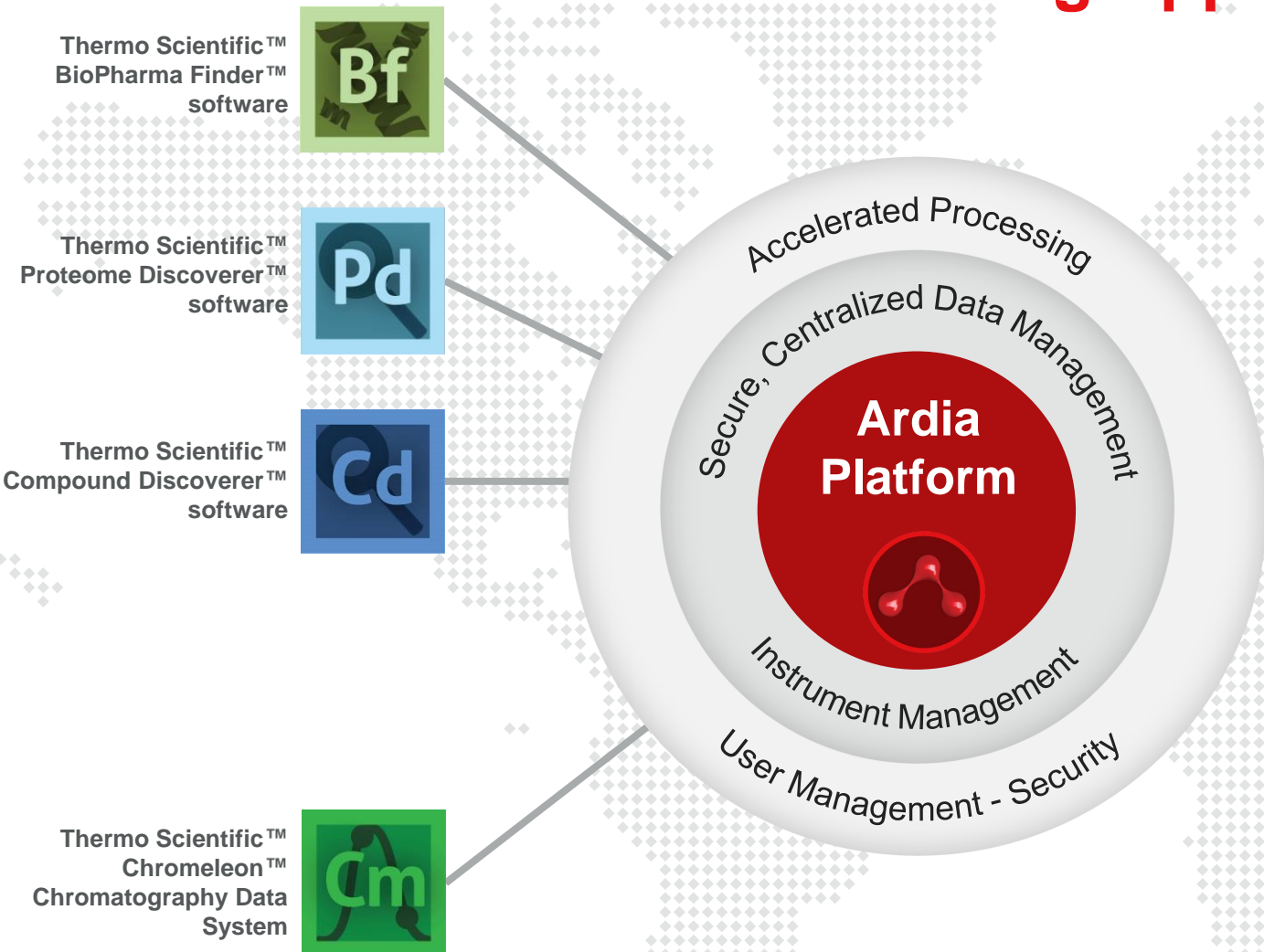
Productivity

Deep insights

Security



Connecting Applications



- User Management
- Audit trials & results versioning
- Automation & performance
- Enhanced reporting

Collaboration

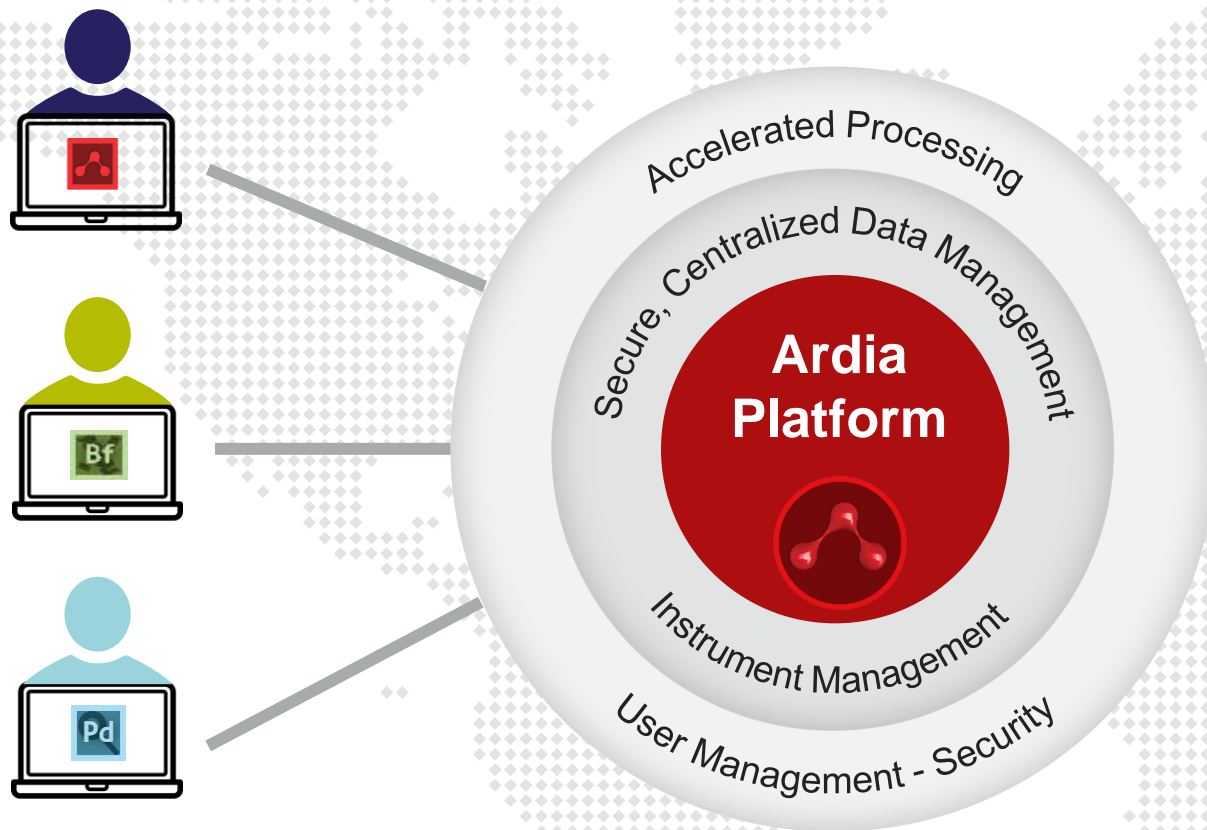
Productivity

Deep Insights

Security



Connecting people and data



- Enhanced collaboration
- Global access to data and results
- Secure, controlled environment
- Holistic instrument view
- Metrics and utilization

Collaboration

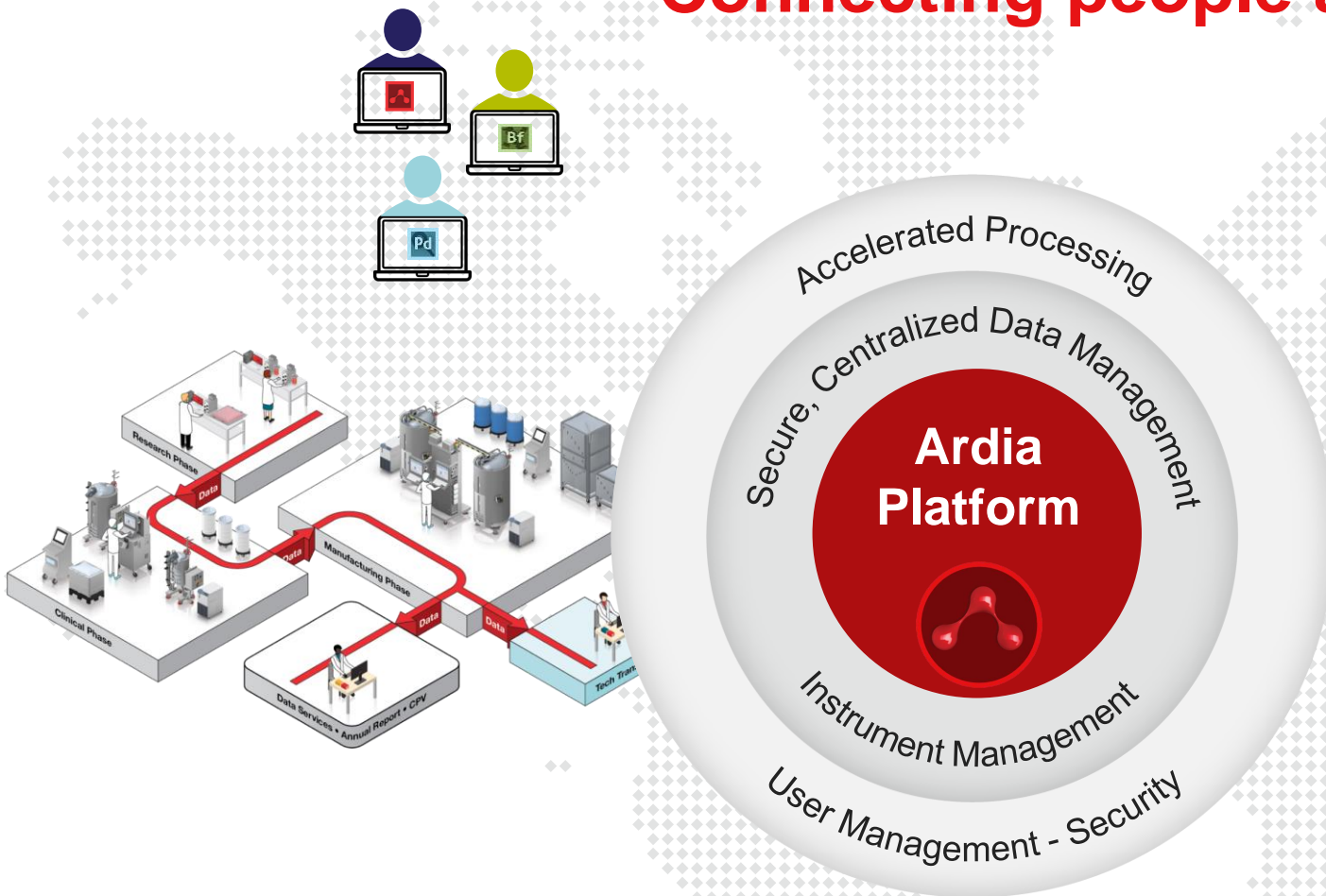
Productivity

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Connecting people and data



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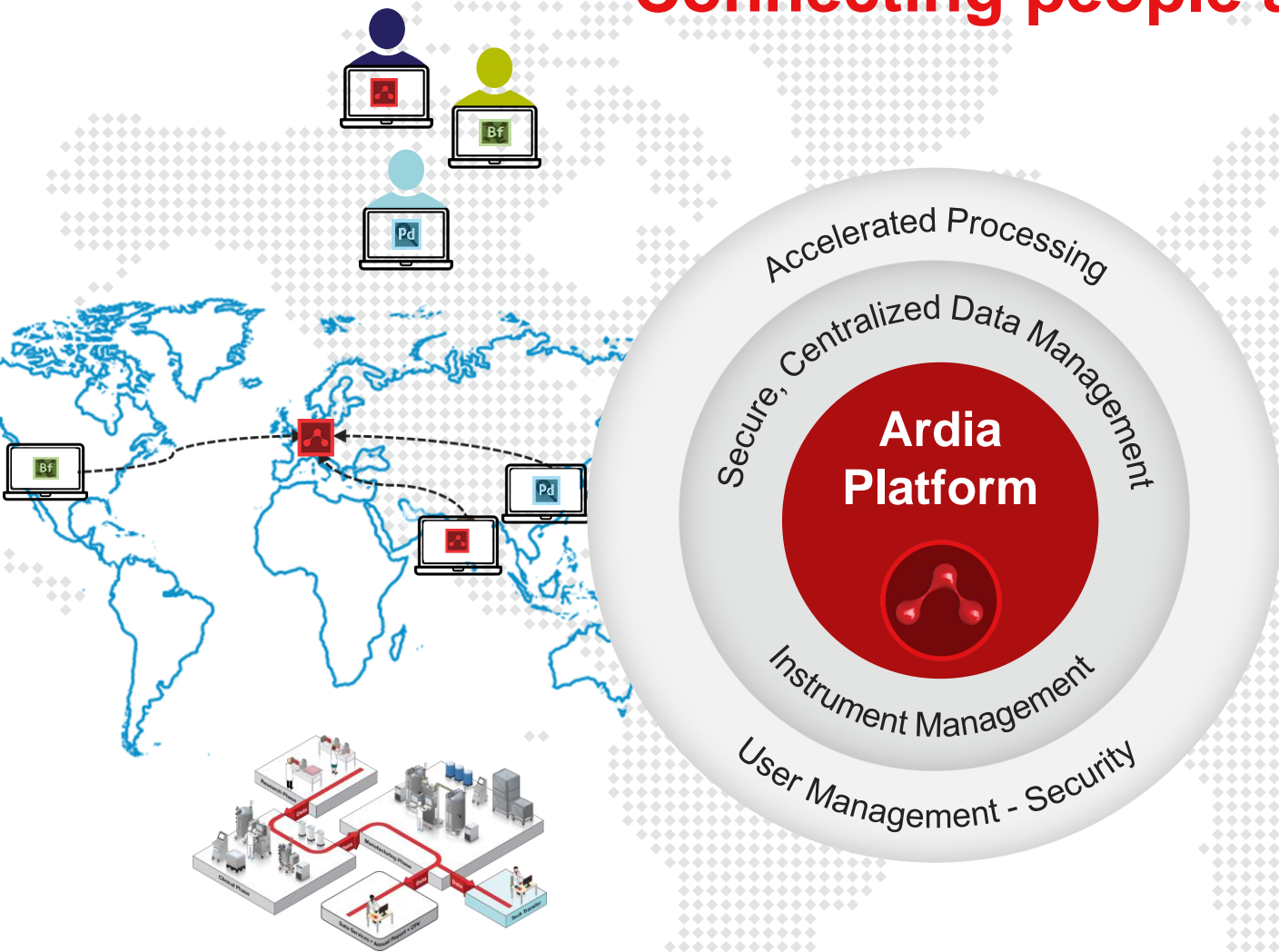
Productivity

Deep insights

Security



Connecting people and data



- Enhanced collaboration
- Global access to data and results
- Secure, controlled environment
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Collaboration

Productivity

Deep insights

Security



Landing page of the Ardia Platform

Thermo Scientific Ardia Platform | Home

Thermo Scientific Ardia Platform

Core applications

- Data Explorer**
Browse and manage folders, files, and data objects stored on the Ardia platform.
- Instruments**
Manage, schedule, and monitor data acquisition of all instruments connected to the Ardia platform.
- Audit Trail Viewer**
Display audit entries generated in the Ardia platform such as user access, data operations, and setting changes.
- Client Registration and Management**
Create and manage application registration codes utilized to connect Thermo Scientific desktop applications to the Ardia platform.
- Global Settings**
Define administrative settings that are applied across the Ardia platform.
- IdP Configuration**
Configure, edit, and remove the identity providers used by the Ardia platform.
- Users and Roles**
Add new users and manage existing users in the Ardia platform. Define roles, users, and configure permissions.

Ardia Platform: Data Explorer



Ardia Repository > BioPharma Finder > Intact

Search Intact



New folder

Upload files



Quick Access



Ardia Repository



Astral



BioPharma Finder

Experiments

Intact

Peptide Mapping

kimys

Tara

CM7 Data Vaults



Storage

939.66 GB of 9.74 TB used

9%

Details

Rename

Delete

Move to

Manage access



1 row selected

#	<input type="checkbox"/>	Name	Type	Date modified	Modified by	Status	
1	<input checked="" type="checkbox"/>	Trastuzumab ADC	Folder	10/22/2024, 11:5...	administrator	Live	
2	<input type="checkbox"/>	Trastuzumab IdeS	Folder	10/22/2024, 11:5...	administrator	Live	
3	<input type="checkbox"/>	Trastuzumab Native	Folder	10/22/2024, 11:5...	administrator	Live	

One place to manage all your data

- Raw data from Xcalibur and Chromeleon are automatically and securely transferred to the Ardia server
- Manually upload data (of any type) to the server
- Built-in versioning, access control, archive, and download tools
- Open object audit trail

Ardia Platform: Data Explorer

Easily control who has access to what data

Manage access

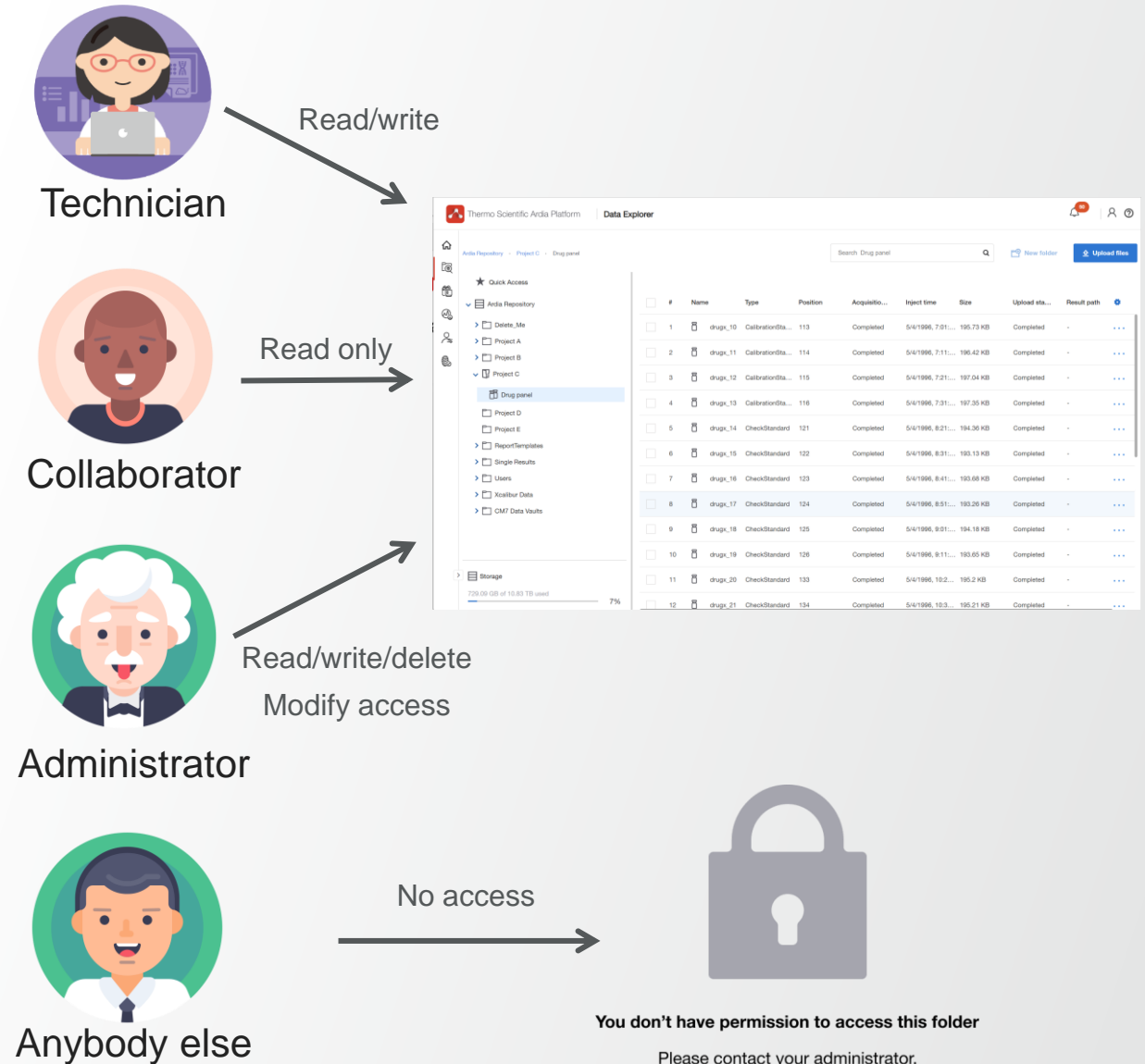
Folder name
Data uploads

Roles Can edit

Users with access Permissions

Roles	Permissions	Actions
Super Admin	Can edit	<input type="button" value="Clear users"/>
Users		
kevin.schauer@thermofisher.com	Full access	<input type="button" value="Clear users"/>

Other registered users



Access can be controlled on a **Role** or **User** level.

Data Explorer: search function

The screenshot displays the Thermo Scientific Ardia Platform Data Explorer interface. At the top, the platform name and 'Data Explorer' are shown. A search bar contains the text 'trastuzumab'. Below the search bar, there are buttons for 'New folder' and 'Upload files'. The main area shows a table of search results with columns for Name, Type, Size, and Path. The search results include folders for 'Trastuzumab ADC', 'Trastuzumab IdeS', and 'Trastuzumab Native', as well as sequence and injection files for 'Trastuzumab_Emtansine_Native_70k'. A storage usage bar at the bottom left indicates 937.94 GB of 9.74 TB used (9%).

Thermo Scientific Ardia Platform | Data Explorer

trastuzumab X

New folder Upload files

Ardia Repository

Quick Access

- Ardia Repository
- Astral
- BioPharma Finder
- kimys
- Tara
- CM7 Data Vaults
- 2022-03-15_8min_2

Name	Type	Size	Path
Trastuzumab ADC	Folder	-	Intact (/BioPharma Finder)
Trastuzumab IdeS	Folder	-	Intact (/BioPharma Finder)
Trastuzumab Native	Folder	-	Intact (/BioPharma Finder)
Trastuzumab_Emtansine_Native_70k	Sequence	9.71 MB	Trastuzumab ADC (/BioPharma Finder/Intact)
Trastuzumab_Emtansine_Native_70k	Injection	9.71 MB	Trastuzumab_Emtansine_Native_70k (/BioPharma Finder/Intact)

- Folder, sequence and injections containing the word trastuzumab are easily located
- The data explorer path for each item is displayed

Storage

937.94 GB of 9.74 TB used 9%

Data Explorer: shareable links

The screenshot shows the Thermo Scientific Ardia Platform Data Explorer interface. The top navigation bar includes the Thermo Scientific logo, the text 'Thermo Scientific Ardia Platform', and 'Data Explorer'. On the right side of the navigation bar are a notification bell, a user profile icon labeled 'SH', and a help icon. The main content area is divided into a left sidebar and a main panel. The sidebar contains a home icon, a search icon, a storage icon, a graph icon, and a folder icon. Below these icons is a 'Storage' section showing '938.17 GB of 9.74 TB used'. The main panel has a breadcrumb 'Ardia Repository > BioPharma Finder', a search box 'Search BioPharma Finder', and two buttons: 'New folder' and 'Upload files'. Below the search box is a 'Quick Access' section with a star icon. The main content area displays a tree view of folders: 'Ardia Repository' (expanded), 'Astral' (expanded), 'Experiments' (expanded), 'Intact' (expanded), 'Trastuzumab ADC' (expanded), and 'Trastuzumab Emtansine Native_70k' (expanded). The 'Trastuzumab IdeS' folder is also visible. A table lists the contents of the 'Trastuzumab ADC' folder:

#	Name	Type	Date m...	Modifie. ⚙
1	Experiments	Folder	11/8/2024, ...	roberto.ζ...
2	Intact	Folder	10/22/2024,...	administ...
3	Peptide Mapping	Folder	11/8/2024, ...	roberto.ζ...

Two shareable links are highlighted with red arrows pointing from the folder names in the tree view to the links:

- A red arrow points from the 'Experiments' folder in the tree view to the link: <https://ardia-demo.thermofisher.net/go/folders%2F0b9fca5d-8011-402c-855f-32ebd63e917c>
- A red arrow points from the 'Trastuzumab Emtansine Native_70k' folder in the tree view to the link: <https://ardia-demo.thermofisher.net/go/standard-sequences%2F0df6a068-10c3-4e8f-9800-a6c863a88409>

A large white box at the bottom of the screenshot contains the text: 'Shareable links make folder and sequence items easily accessible'.

Ardia Platform: Data Viewer

Thermo Scientific Ardia Platform

Home

Thermo Scientific Ardia Platform

Core applications

- Data Explorer**
Browse and manage folders, files, and data objects stored on the Ardia platform.
- Data Viewer**
Visualize and qualitatively analyze chromatography and mass spectrometry data.
- Data Explorer**
Browse and manage folders, files, and data objects stored on the Ardia platform.

Utilities

- Audit Trail Viewer**
Display audit entries generated in the Ardia platform such as user access, data operations, and setting changes.
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Ardia Platform: Data Viewer



File



Data Viewer Version 1.1.0

Qualitatively review, analyze, and compare data collected from Xcalibur and Chromeleon.

Open injection

Help

Open

- Data Viewer allows user to quickly review raw data stored in Ardia without the need to download files locally
- One data viewer for all customers, instruments (LC, GC,UV, MS) and acquisition (Xcalibur – Chromeleon)
- Review data, perform basic peak integration

Trastuzumab IdeS
HER_IdeS_Red_01082016_3
Trastuzumab Native
Peptide Mapping

Currently selected:

Name

Cancel

Open

Ardia Platform: Data Viewer



Ardia Platform: Instruments



Core applications



Data Explorer



Browse and manage folders, files, and data objects stored on the Ardia platform.



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Visualize and qualitatively analyze chromatography and mass data.



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Client Registration and Management



Create and manage application registration codes utilized to connect Thermo Scientific desktop applications to the Ardia platform.



Global Settings



Define administrative settings that are applied across the Ardia platform.



IdP Configuration



Configure, edit, and remove the identity providers used by the Ardia platform.



Users and Roles



Add new users and manage existing users in the Ardia platform. Define roles, users, and configure permissions.

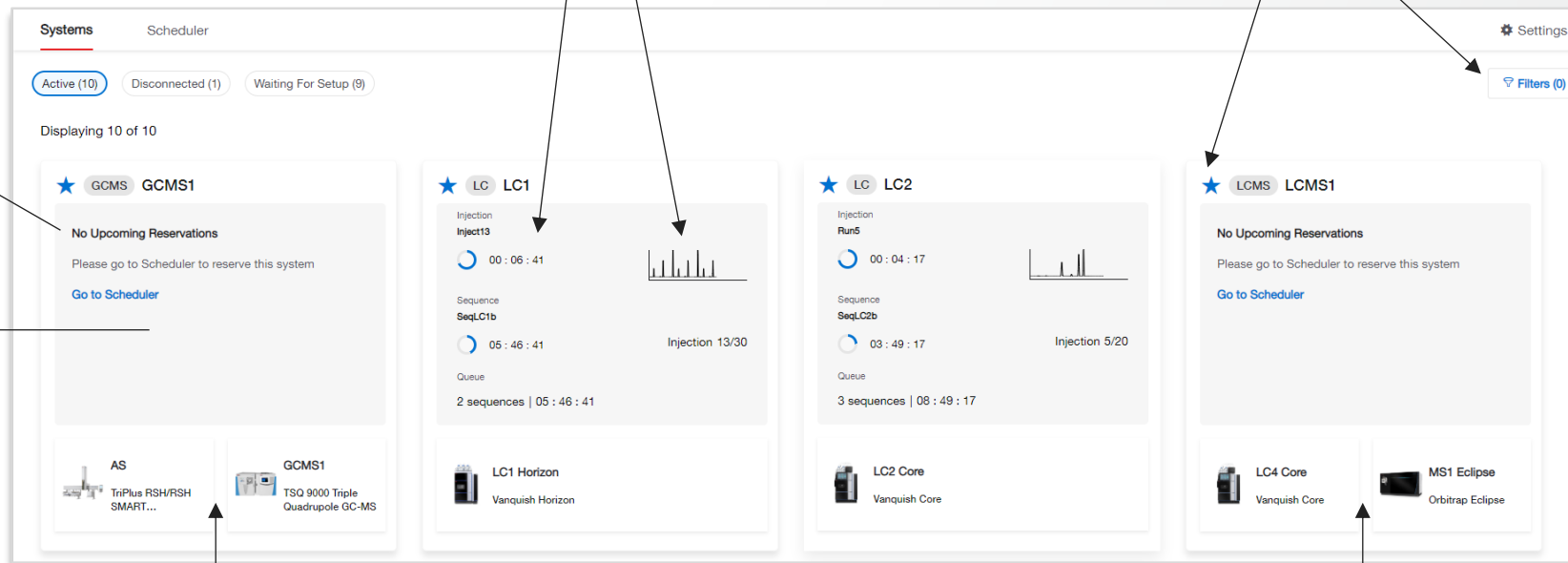
Instruments: Systems View

Monitor systems with a centralized overview

1 Integrates with Scheduler so users can see any upcoming reservations

2 Live acquisition status enables you to harness real-time data to make fast, informed decisions

3 Ability to filter, sort, search and favourite instruments to enhance accessibility and ascertain important information quickly



6 Systems presented on individual cards for easy navigation and visualization

5 Detail provided on each module of a configured device which is automatically updated if configuration changes

4 Visualize chromatography and mass spectrometry systems running under Chromeleon CDS and Xcalibur software from a single location

Instruments: Logbook

Document events with the Logbook

Allows you to:

- Capture auto-populated events
 - Software upgrades
 - Configuration changes
 - Instrument events
- Capture manual events
 - Routine maintenance
 - Unplanned issues
 - QC results
- Save custom notes/images/small raw files/etc with each entry
- Access service bundles

The screenshot displays the ThermoFisher Logbook interface for a specific instrument. At the top, there are tabs for 'Systems' and 'Scheduler'. The main header shows the instrument ID 'MS THERMO-73HD4FM5_121500' and a star icon. Below this, there is a section for instrument details including 'THERMO-73HD4FM5_121500-MS', 'Orbitrap Ascend', 'Location: Tirupati', 'Room: 你跟我一起去吗?', 'Owner: bobby.lapointe@thermofisher.com', and 'Instrument Tags: My MS'. A calendar for September 2024 is shown, with the 5th of September highlighted. The logbook entries for Thursday, 5 September 2024, include: 1. 'MS | THERMO-73HD4FM5_121500-MS Software Installed' with a sub-entry 'Orbitrap Ascend 4.2.4323.0' and a '+ Add note or attachment' link. 2. 'Configuration MS | THERMO-73HD4FM5_121500-MS New configuration' with sub-entries 'New configuration details', 'MS | THERMO-73HD4FM5_121500-MS', 'Orbitrap Ascend', and 'Orbitrap Ascend: SREE369', also with a '+ Add note or attachment' link. On the right side, a 'Create new entry' modal is open, showing configuration details, event type selection (Predefined event selected), instrument selection, and a 'Create Entry' button. A 'Request Support' button is also visible. The interface includes a 'Settings' gear icon in the top right and a 'Collapse details' link.



Core applications



Data Explorer



Browse and manage folders, files, and data objects stored on the Ardia platform.



Data Insights



Understand trends and derive insights from your data.



Data Viewer



Visualize and qualitatively analyze chromatography and mass spectrometry data.



Instruments



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Utilities



Audit Trail Viewer



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Client Registration and Management



Create and manage application registration codes utilized to connect Thermo Scientific desktop applications to the Ardia platform.



Global Settings



Define administrative settings that are applied across the Ardia platform.



IdP Configuration



Configure, edit, and remove the identity providers used by the Ardia platform.



License Management



Add and manage licenses for applications across the Ardia platform.



Users and Roles

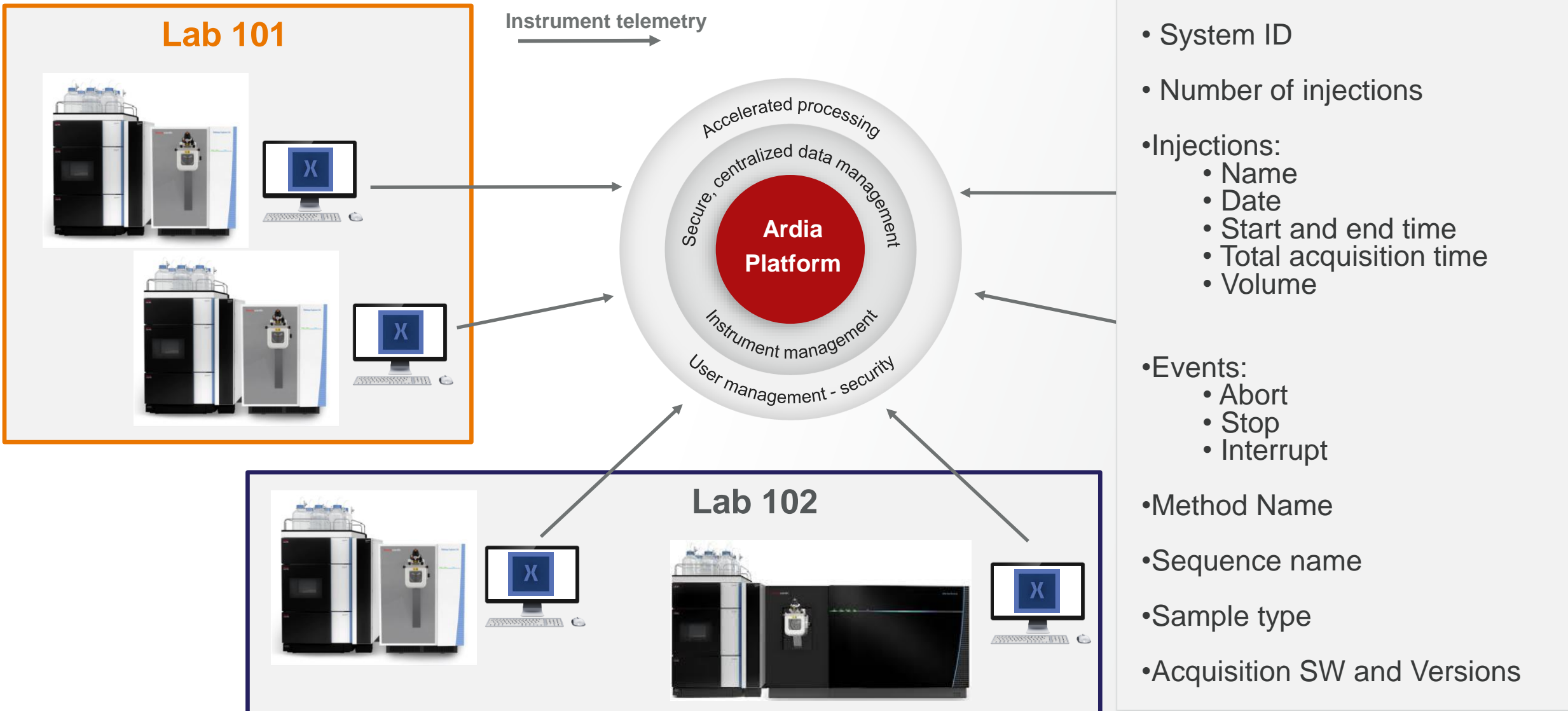


Add new users and manage existing users in the Ardia platform. Define roles, users, and configure permissions.



Data Insights: Instrument utilization

Instrument telemetry is collected in near real-time.



Data Insights: instrument utilization



Data Insights Version 1.0.5

Understand trends and derive insights from your data.

Get started

[+ New dashboard](#)

Administration

[Help](#)

Recently Created

My Dashboards

All Dashboards

Deleted Dashboards

Dashboards

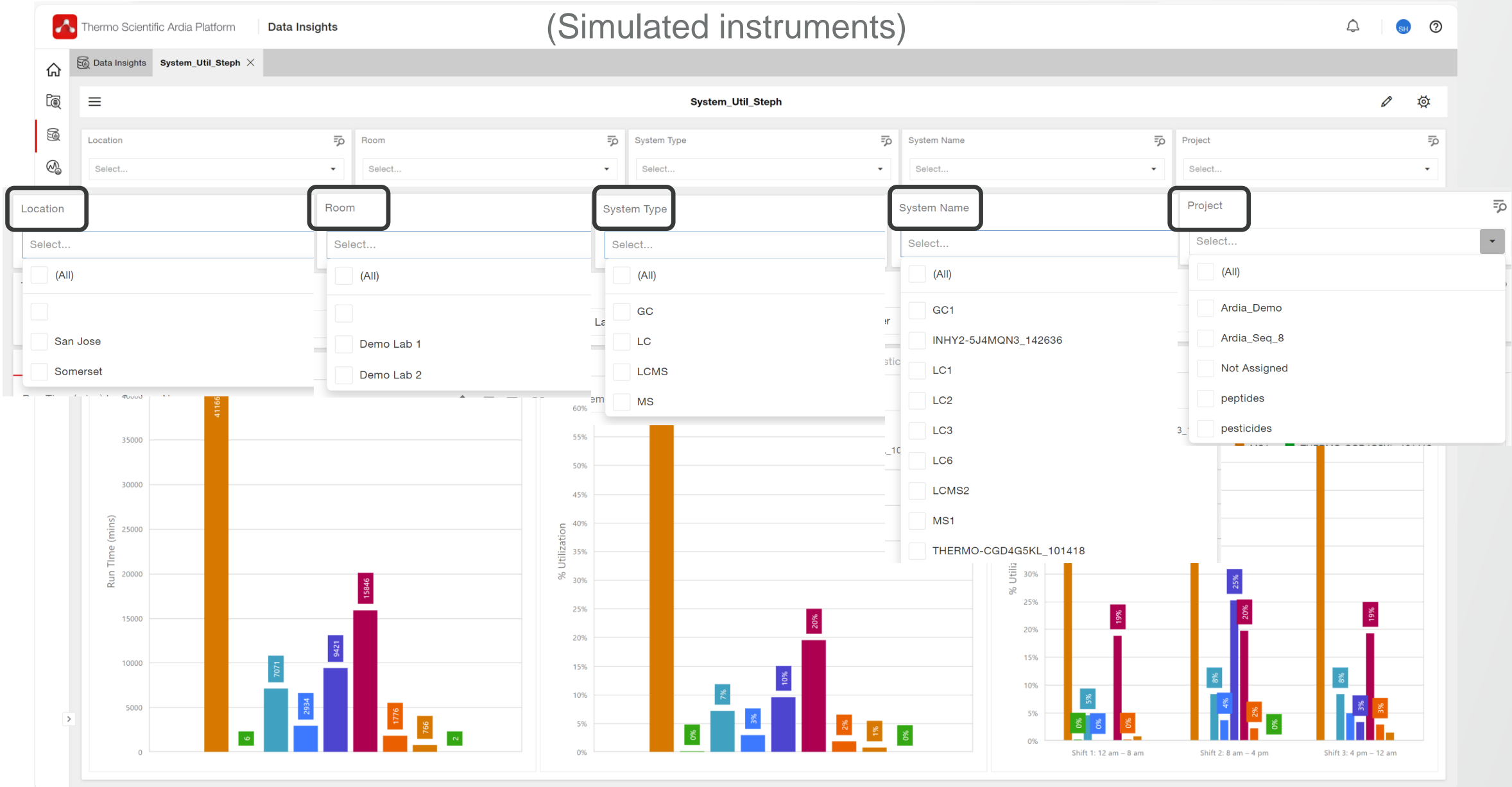
Search dashboards



<input type="checkbox"/>	Name	Author	Data Source	Created	Modified
<input type="checkbox"/>	System_Util_Steph	You	System_Utilization	11/8/2024, 3:57:42 PM	11/8/2024, 3:57:42 PM

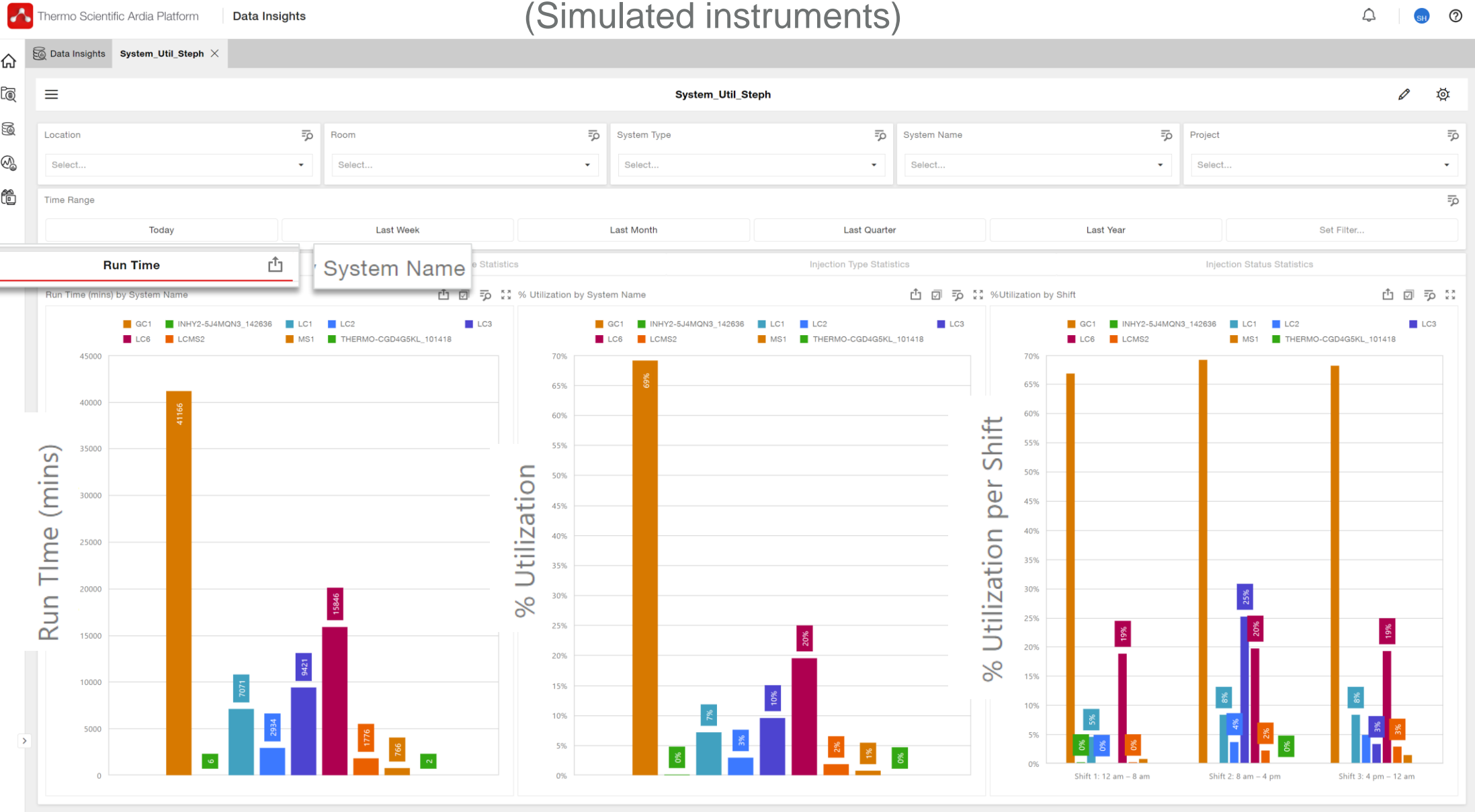
Data Insights: instrument utilization

(Simulated instruments)

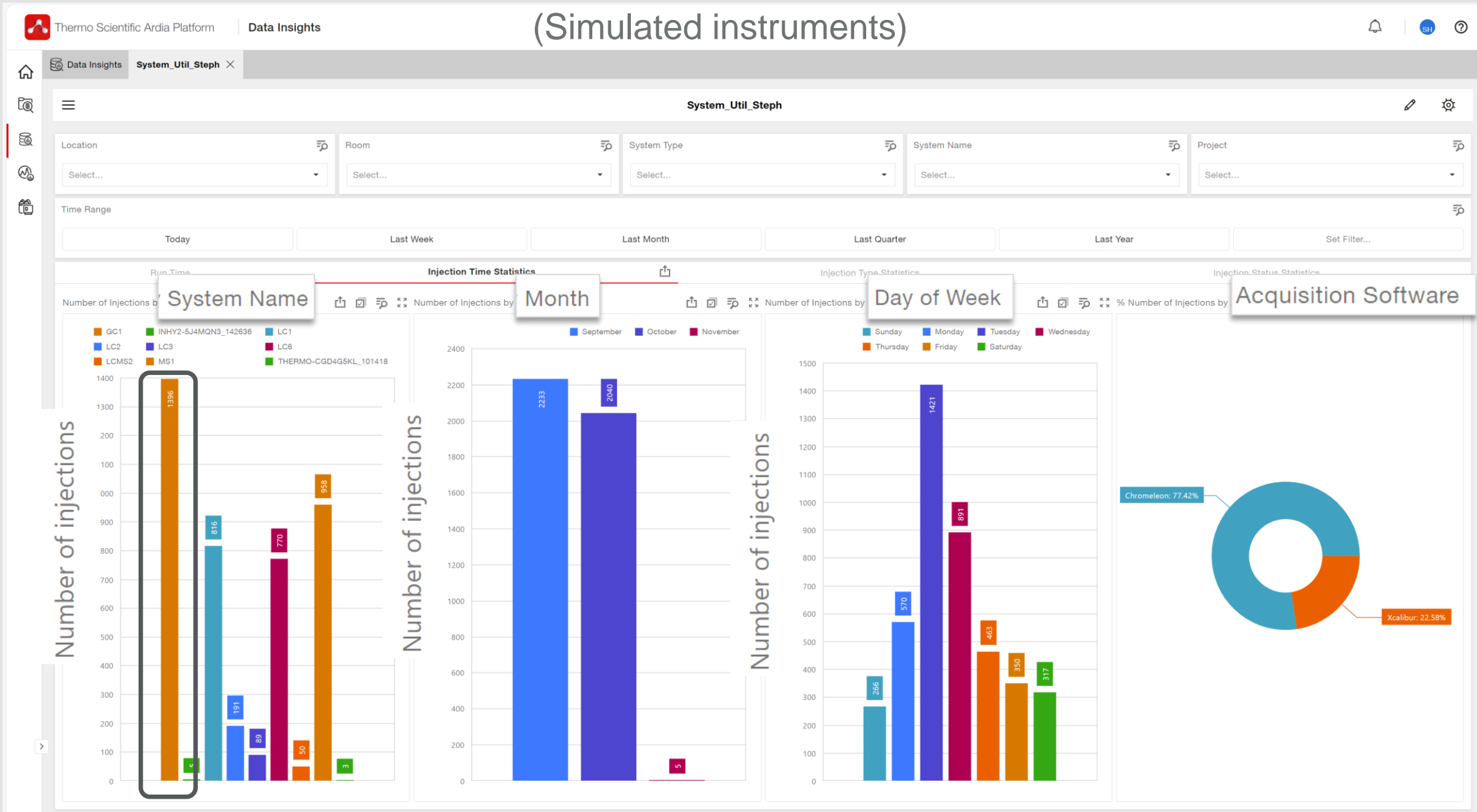


Instrument utilization: Run Time

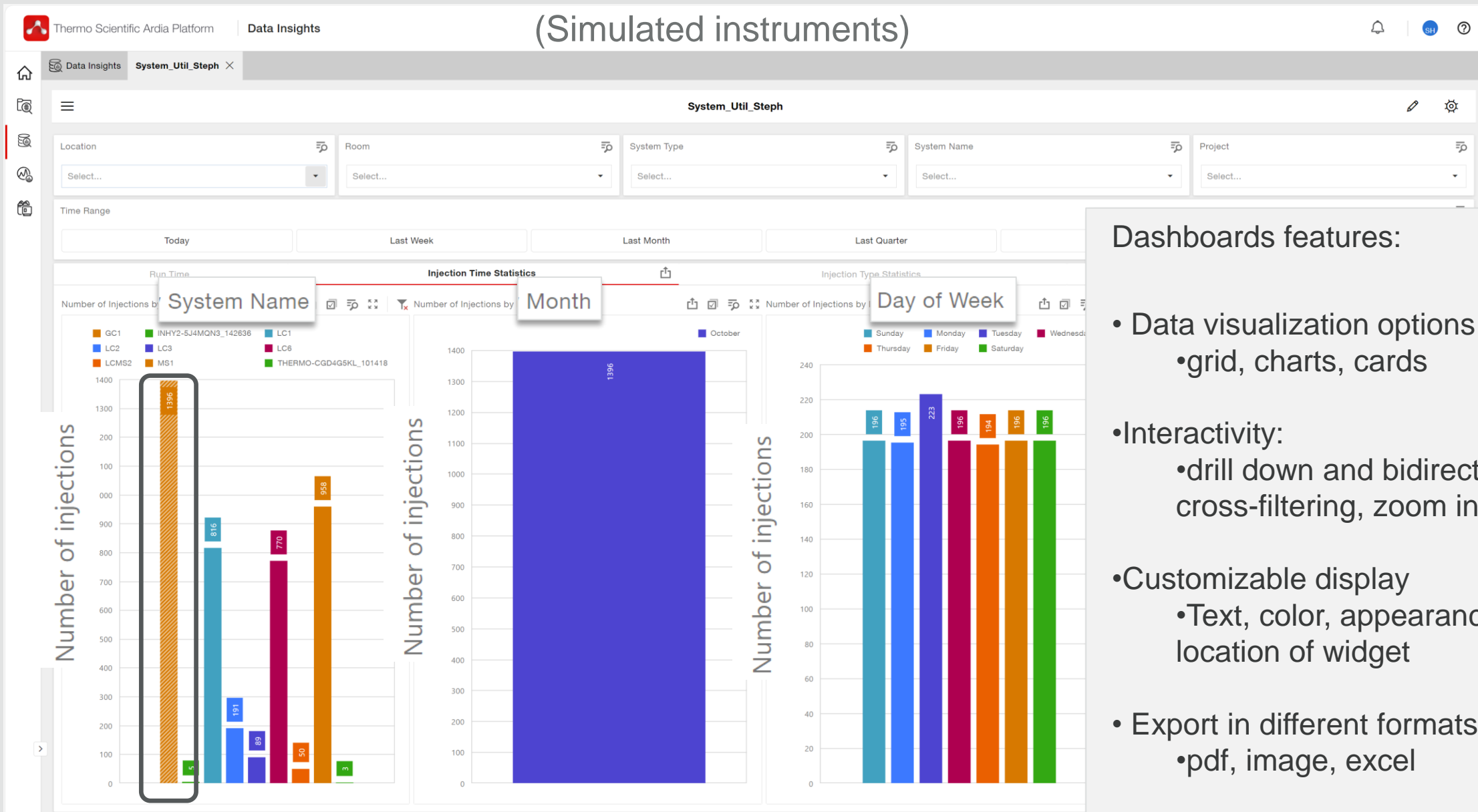
(Simulated instruments)



Instrument utilization: Injection Time



Injection Time: drill down for a specific system



- Dashboards features:
- Data visualization options
 - grid, charts, cards
 - Interactivity:
 - drill down and bidirectional cross-filtering, zoom in/out
 - Customizable display
 - Text, color, appearance, location of widget
 - Export in different formats
 - pdf, image, excel

Benefits of instrument utilization dashboards

Improved decision-making

- With access to detailed usage statistics, managers can make informed decisions regarding maintenance schedules, equipment purchases, and resource allocation, leading to better overall operational efficiency

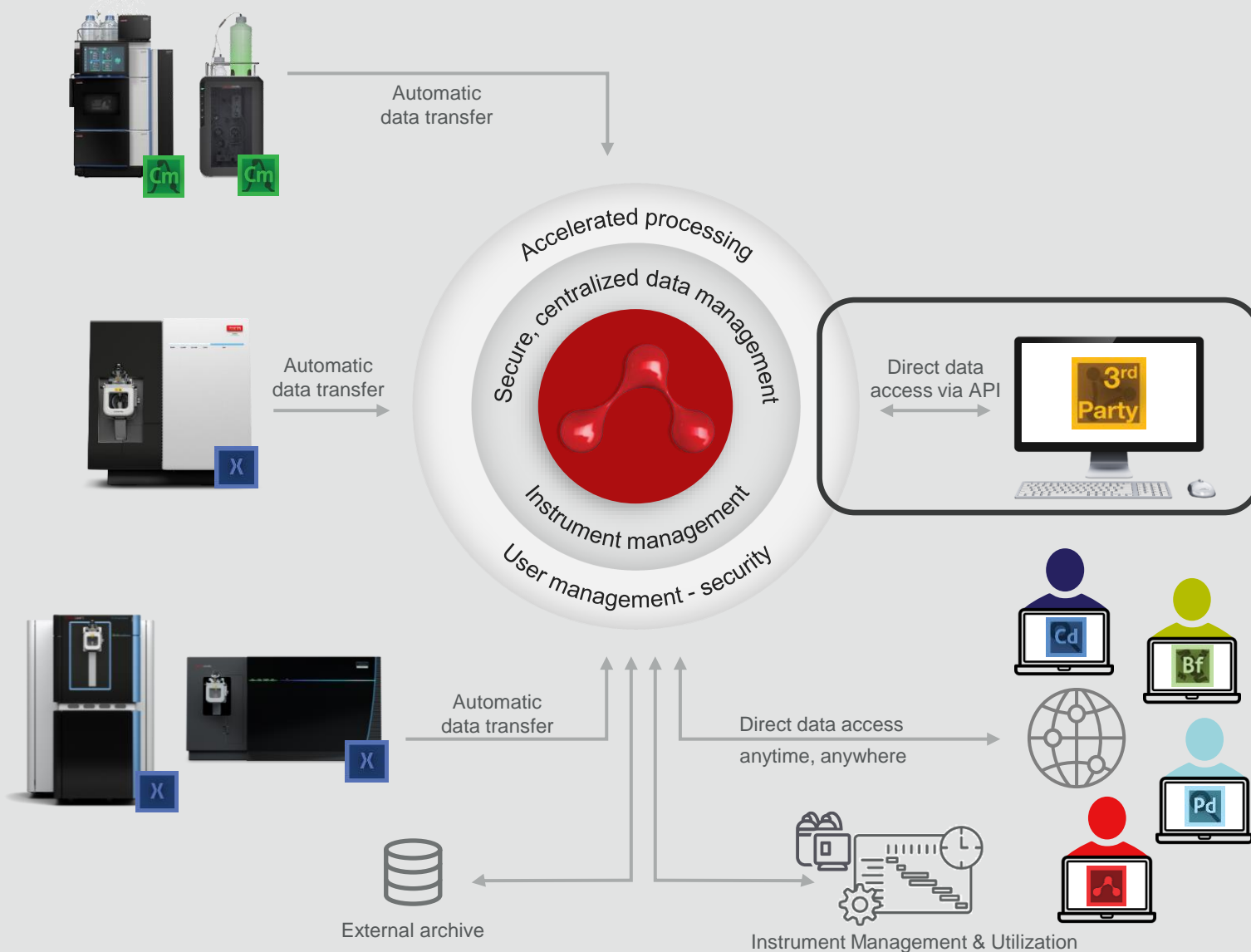
Enhanced resource management

- By providing real-time data on the usage of instruments, these dashboards help organizations optimize the allocation of resources, ensuring that equipment is used efficiently and downtime is minimized

Increased productivity

- With a clear view of instrument availability and usage patterns, staff can plan their work more effectively, reducing wait times and increasing overall productivity

Open platform: third party API for data access



Direct data access via API for third party software

- Register the 3rd party software
→ **Registration Service**
- User connects to Ardia
→ **Identity Service**
- User is connected to Ardia
→ **Session Management Service**
- User selects data via Ardia object picker
→ **Navigation Service**
- User access the selected data
→ **Standard Sequence Service**
→ **Raw Data Service**

First connection to a third-party software: Skyline

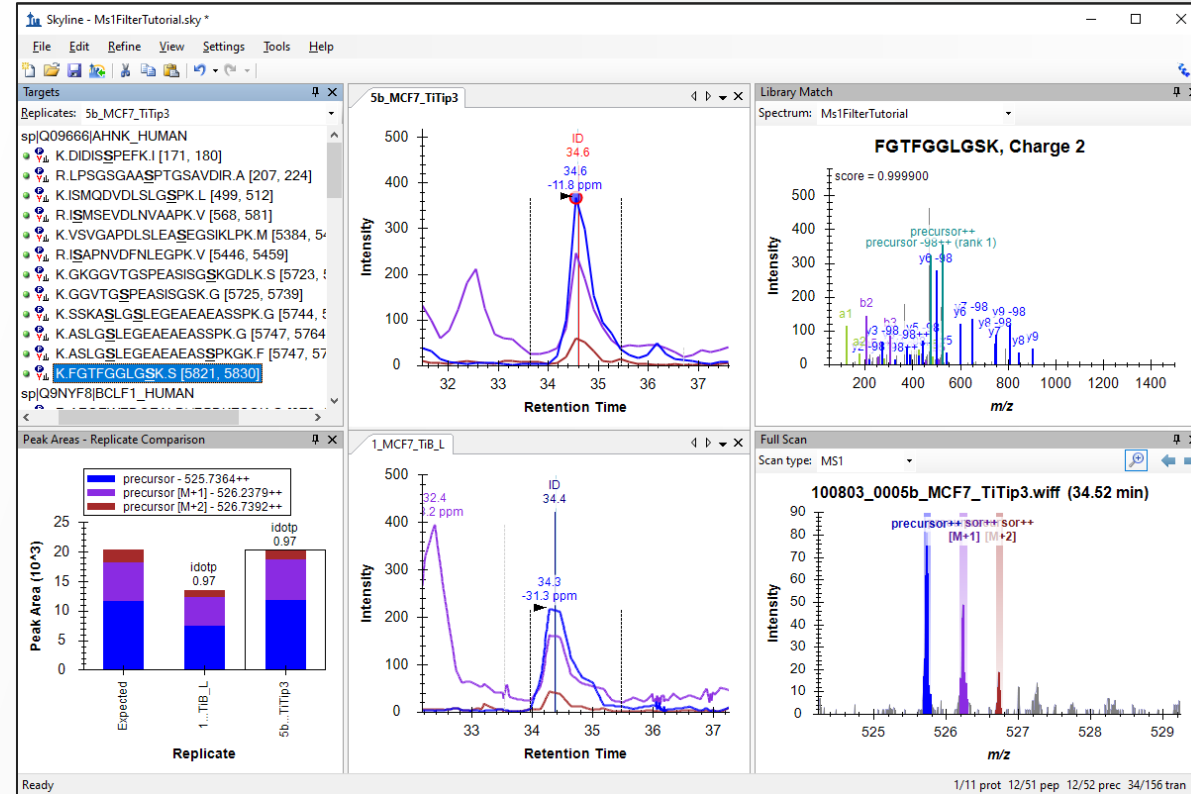
Gold standard software for targeted peptide quantitation



- Windows client application
- Build quantitative methods for MS data analysis
- Broadly adopted (1000's of installations)
- Vendor neutral software
- Academic software
- <https://skyline.ms>

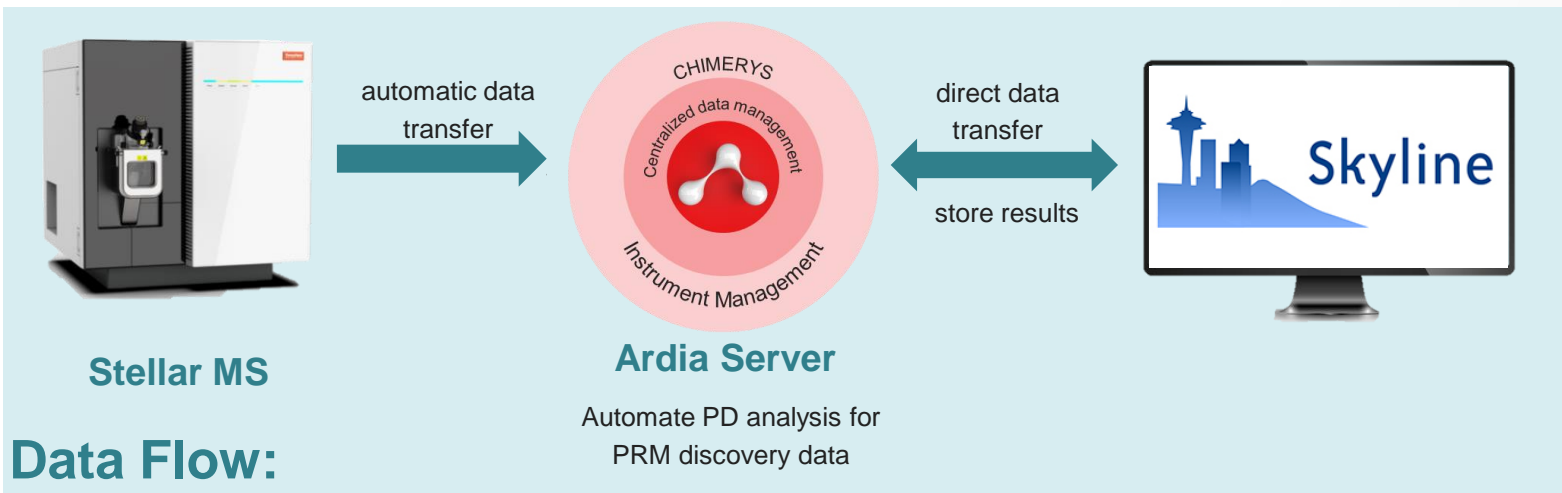
- over 21,000 registered users
 - >4300 registered for Skyline-daily
- ~10,000 instances started each week
- over 160,000 downloads
- over 4000 citations

*User metrics from the Skyline user group
ASMS 2023*



Ardia-Skyline Connection

Brief overview



Stellar streams data to Ardia server
(~80TB capacity for advanced tower)

Skyline installed on PC w/access to Ardia server
*Available to remote users as well

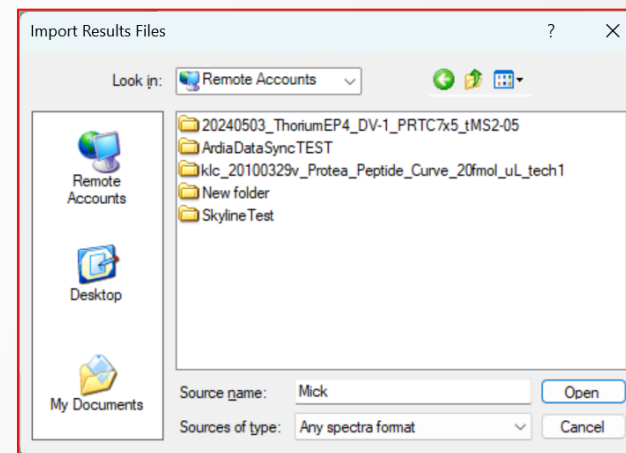
The user runs Skyline as usual
Ardia behaves as the data location and result file destination (optional)

How To:

Register Skyline to Ardia

Login to Ardia via IdP
Create Ardia registration code
Input code via Skyline UI

Access Ardia



Select RAW files to analyze
Process via local Skyline
Store/access Skyline results

Ardia – Skyline: how does it look?

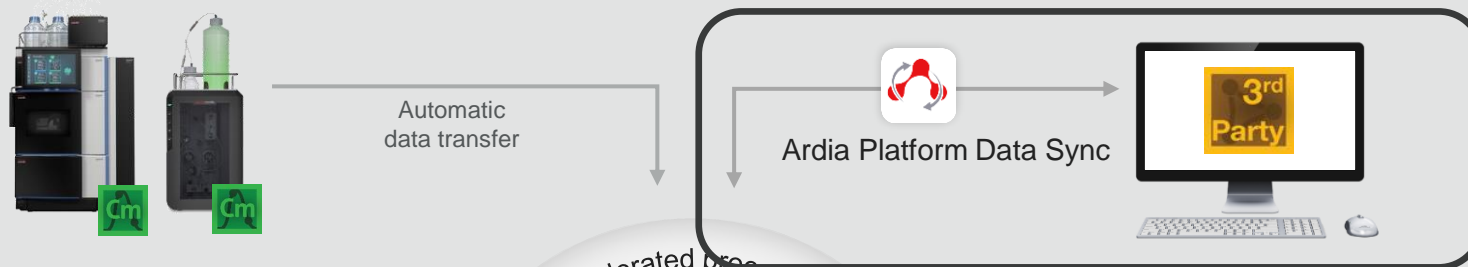
The screenshot displays the Skyline software interface. On the left, a 'Targets' list shows various protein sequences and their corresponding mass-to-charge ratios (m/z). The main window shows a mass spectrum plot titled 'Phospho99 - TVSFEALPIMR, Charge 2'. The x-axis is labeled 'm/z' and ranges from 200 to 1400. The y-axis is labeled 'Intensity' and ranges from 0 to 2. The plot shows several peaks, with some labeled as 'b2 (rank 12)', 'b3 (rank 14)', 'b5-98 (rank 9)', 'b6 (rank 17)', 'y5++ (rank 13)', 'y4 (rank 16)', 'y9-98++ (rank 12)', 'y9-98 (rank 10)', 'y8 (rank 5)', and 'y9 (rank 10)'. A 'Remote Account Details' dialog box is open in the center, with the following fields: 'Account type: Ardia', 'Alias: user@themofisher.com', and 'Server URL: https://ardia.themofisher.com/'. There is also a checkbox for 'Delete RAW files after importing' and a 'Logout Ardia' button. The dialog box has 'Connect', 'OK', and 'Cancel' buttons at the bottom. A text box on the right side of the plot says 'Log in to Ardia from within Skyline'. The status bar at the bottom of the window shows '9/216 prot 17/286 pep 17/287 prec 81/1,435 tran ...'.

Ardia – Skyline: how does it look?

The screenshot displays the Skyline software interface. On the left, a 'Targets' list shows various protein entries with their accession numbers and molecular weights. The main window is titled 'Phospho99 - TVSFEALPIMR, Charge 2'. An 'Import Results Files' dialog box is open, showing a file named '2022-09-15_OLEP03_120min_4000ng_HeLa_750_400nl_01 (1)' selected from the 'Remote Accounts' location. The dialog includes fields for 'Source name' and 'Sources of type', and 'Open' and 'Cancel' buttons. A mass spectrum plot is visible at the bottom of the main window, showing intensity versus m/z.

Accessing Ardia data stored in Ardia from within Skyline

Open platform: Ardia Platform Data Sync



Ardia Platform Data Sync 1.1

Data Sync Queue Finished

Create a new data sync

Pair your folders

Click Add folders to select your folder paths or enter the path manually in the table below.

Add folders

Ardia folder path	Data Transfer	Local folder path	Last scanned	Start scan date	Actions
Add Ardia folder	<input type="text"/>	Add Local folder	-	Select a date <input type="text" value="15"/>	X

Start sync

Ardia Platform Data Sync features:

- Automatically transfer files to and from an Ardia Server
- Supports multiple file paths for data transfer
- Automated transfer of additional file formats: Proteome Discoverer, Compound Discoverer, BioPharma Finder, Xcalibur, Chromeleon, Tracefinder
- 3rd party software (SN, DIA-NN, Skyline)
- Generic file formats .txt, .pdf, .doc (specified under Ardia global settings)
- Support mixed file folders
- Different destination folders can be used for each source
- Audit trail provides traceable information regarding synced files

FAIR Data principle on the Ardia Platform

In development

Findable

- Search for data anywhere in the Ardia platform, regardless of where files are located

Accessible

- Shareable links make data items easily accessible, subject to security constraints

Interoperable

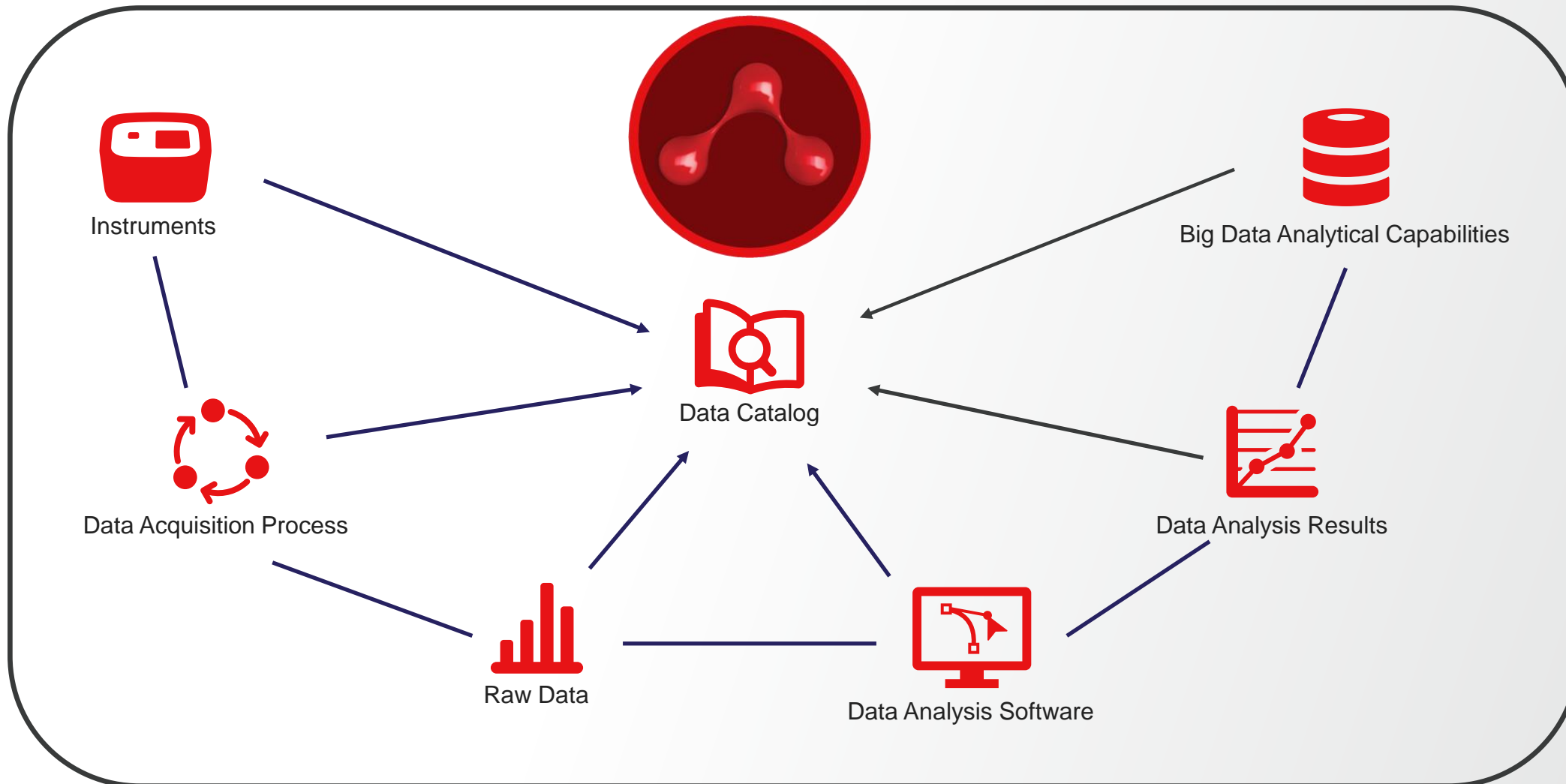
- Metadata is linked to major ontologies, such as Allotrope

Reusable

- Import and export capabilities for Allotrope and other standard formats

Ardia Data Catalog Provides Context

The goal of the data catalog is to create a comprehensive, organized, and searchable inventory of data assets



Three Different Views on Ardia Data

Different approaches to work with the same data – easily switch between views



Data Explorer View

- Navigate through folder hierarchy
- Copy, move, and rename data items
- Manage access to files



Data Catalog View

- Faceted search to find data elements
- View all metadata
- Get data definitions



Knowledge Graph View

- Navigate through graph structures
- View relationships between data
- Query based on data relationships

Data Catalog View

type

folder 3

compound 1

injection 1

sequence 1

modifiedDate

2024-Oct 5

Trastuzumab ADC

Folder urn:uuid:147bcc58-fc2d-4a8a-ac9f-70146ee47aed
Trastuzumab ADC

Trastuzumab IdeS

Folder urn:uuid:a970f658-781f-43f4-ad5a-2512c1d7249a
Trastuzumab IdeS

Facets allow easy
filtering

urn:uuid:4a4bf-02e19ff97790

Trastuzumab_Emtansine_Native_70k

Sequence urn:uuid:6574b982-0209-400f-8b95-fc59448f6e30
Trastuzumab Emtansine Native 70k

Trastuzumab_Emtansine_Native_70k

Injection urn:uuid:00f08d0e-0258-42d4-8540-901e5901b327
Trastuzumab Emtansine Native 70k

Trastuzumab

Compound <http://data.thermofisher.com/luna#Trastuzumab>

Searching for
Trastuzumab

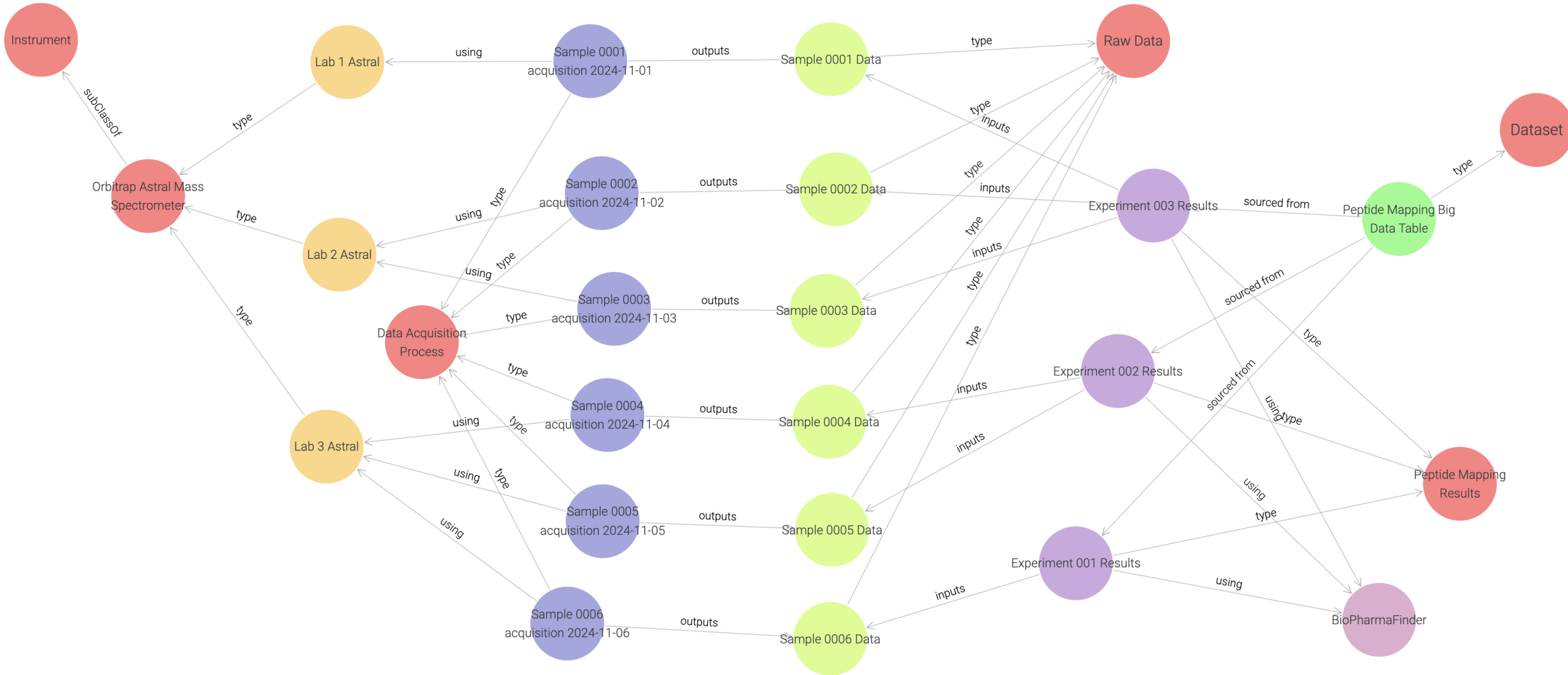
Data Catalog View

type	Sequence
label	Trastuzumab_Emtansine_Native_70k
Identifier	sequences/6574b982-0209-400f-8b95-fc59448f6e30
Description	Trastuzumab Emtansine Native 70k
Date Issued	2024-10-22T15:59:02
Date Modified	2024-10-22T15:59:48
Title	Trastuzumab_Emtansine_Native_70k
Creator	Administrator
Has Part	Trastuzumab_Emtansine_Native_70k
is modified by	Administrator
located in	Trastuzumab ADC

View all metadata
associated with
the sequence

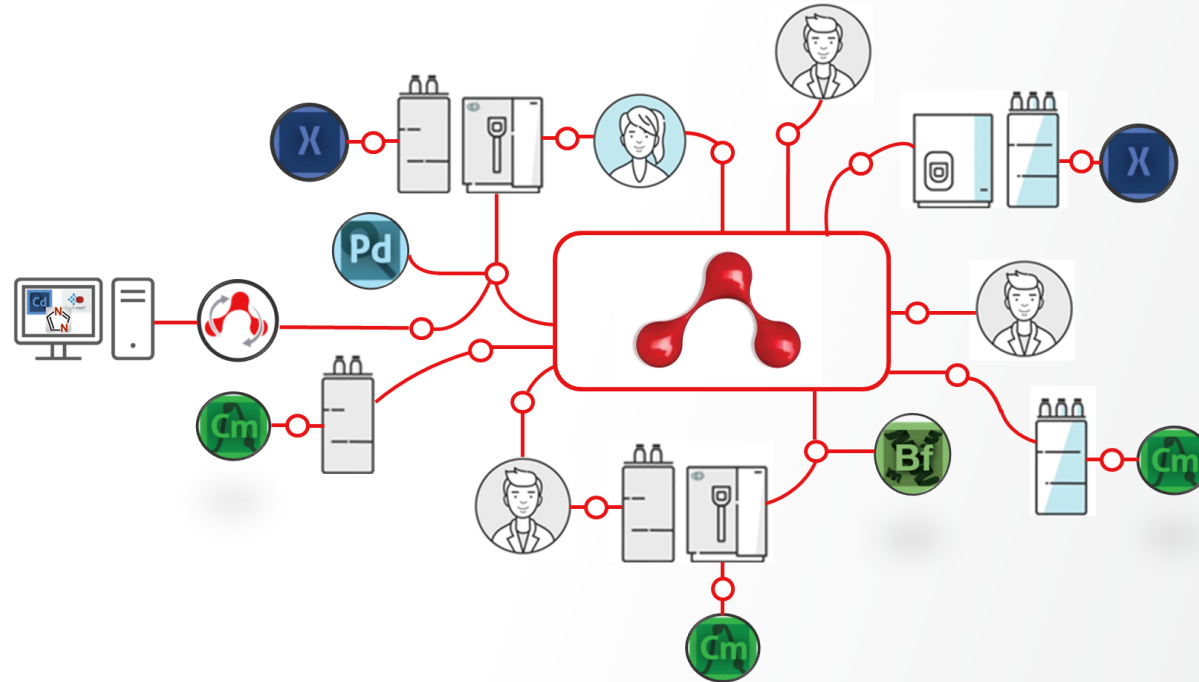
Knowledge Graph View

Visualize data context and connections



Summary

The Thermo Scientific Ardia Platform is a software solution for modern chromatography and mass spectrometry environments



Driving towards an open ecosystem that supports our users' needs, grounded in FAIR principles.

Thank you

