ThermoFisher SCIENTIFIC

Ardia Platform: an open ecosystem for chromatography and mass spectrometry

Stephane Houel – Mark Ressler

The world leader in serving science

Agenda

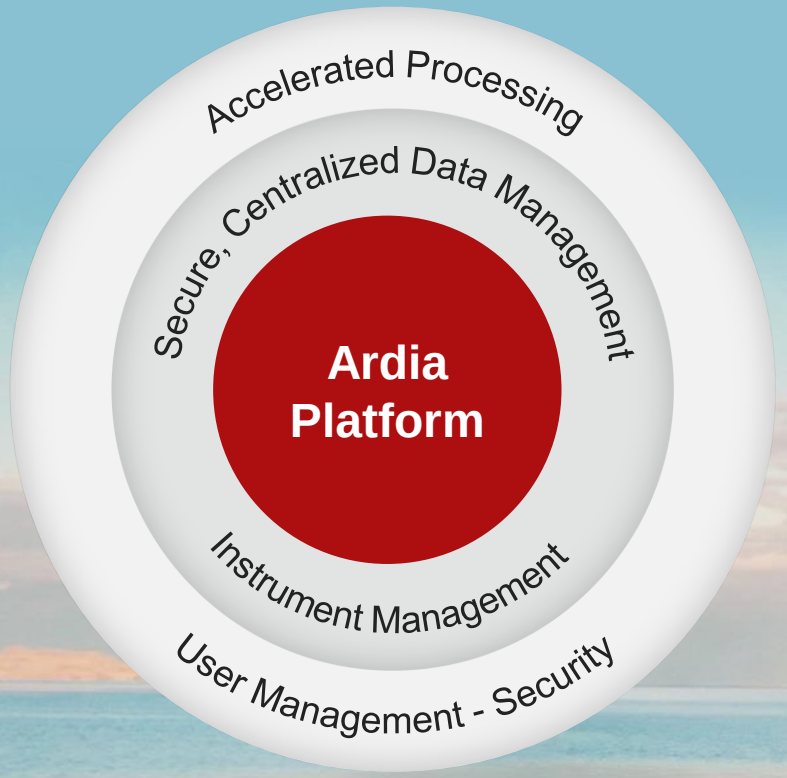
What is the Ardia Platform?

- 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

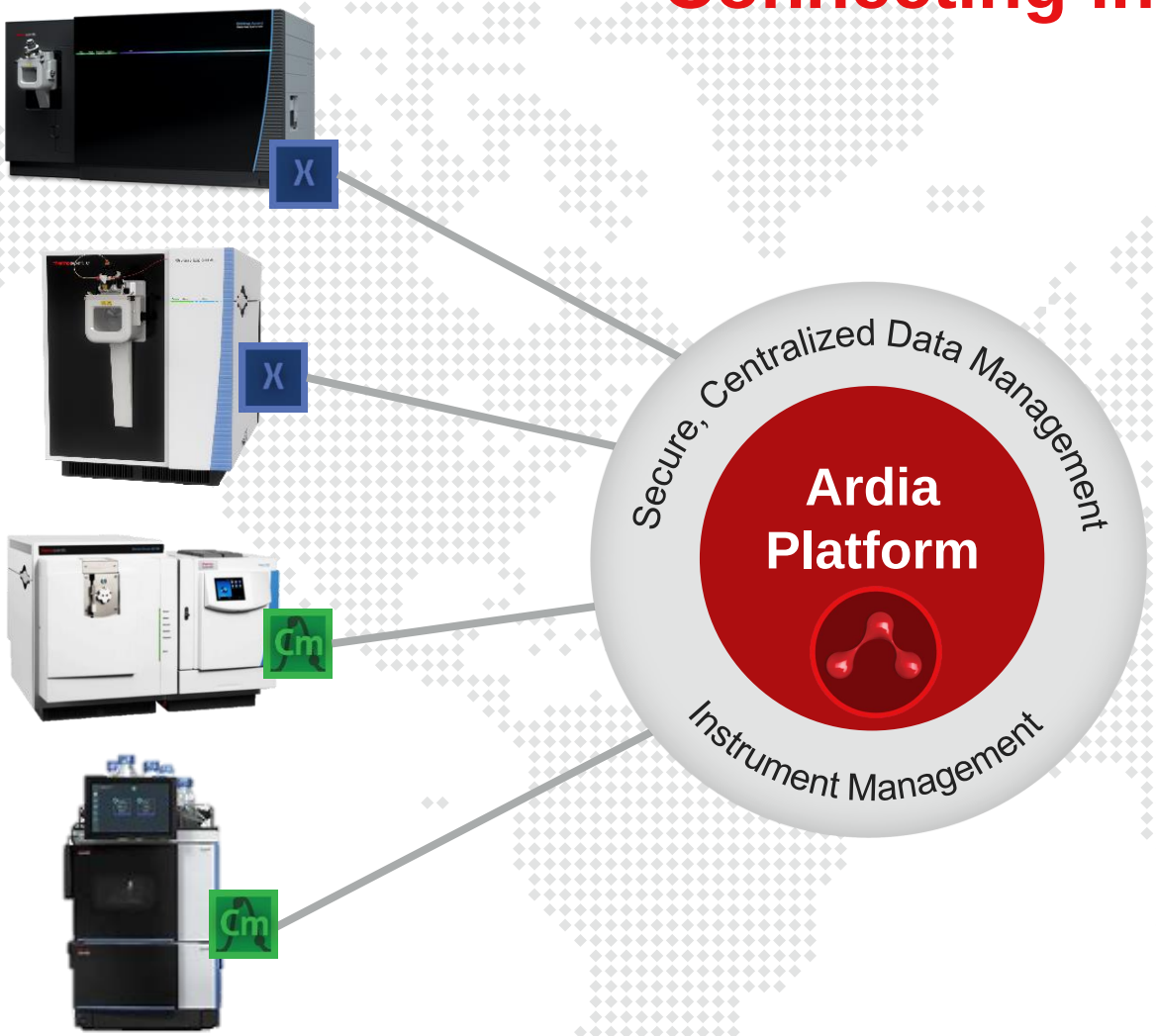
Deep insights

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**

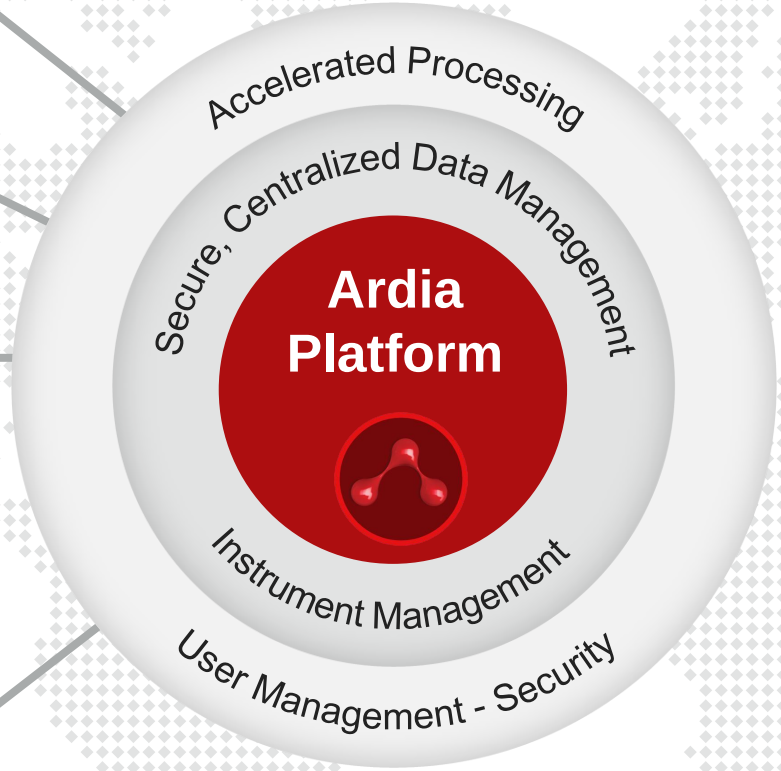
Connecting Applications

Thermo Scientific™ BioPharma Finder™ software

Thermo Scientific™ Proteome Discoverer™ software

Thermo Scientific™ Compound Discoverer™ software

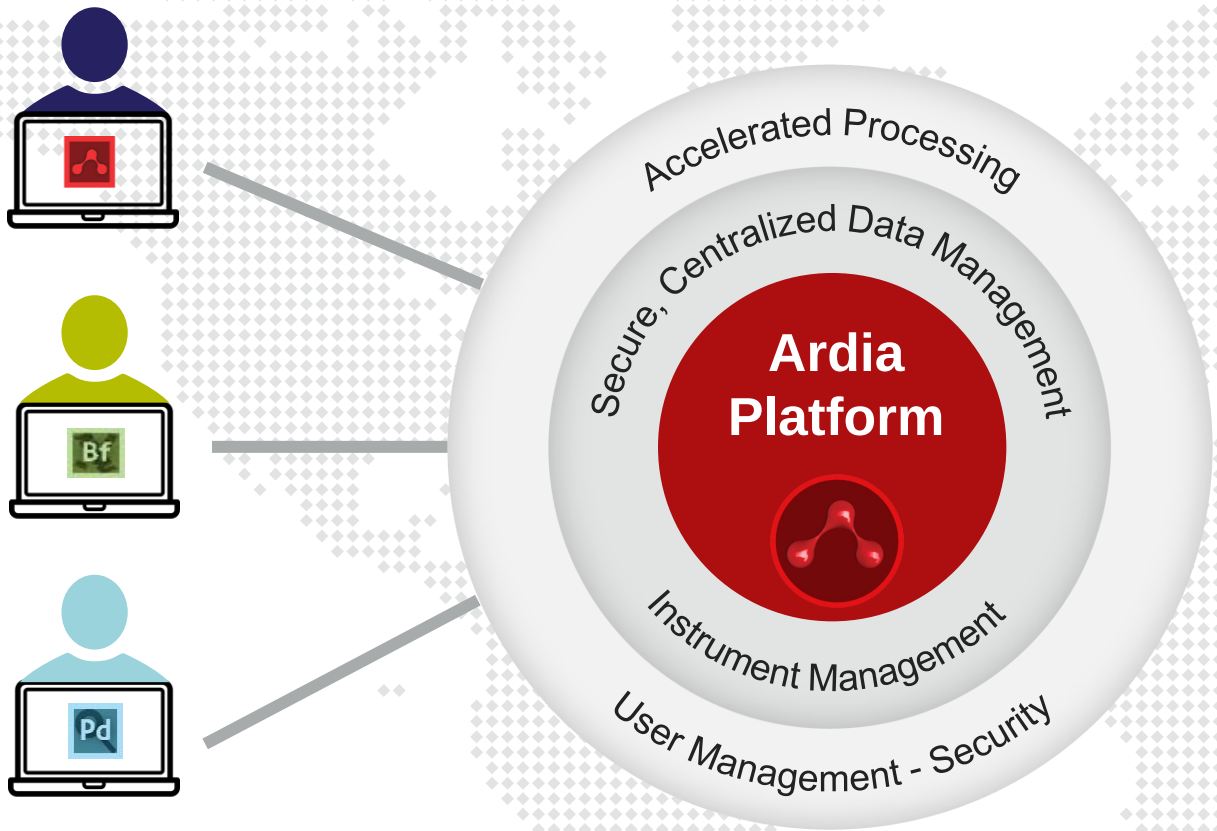
Thermo Scientific™ Chromeleon™ Chromatography Data System



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

Collaboration | **Productivity** | **Deep Insights** | **Security**

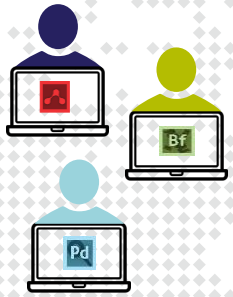
Connecting people and data

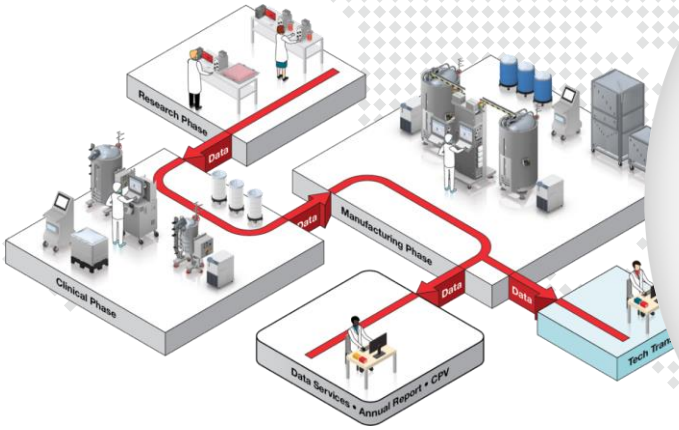


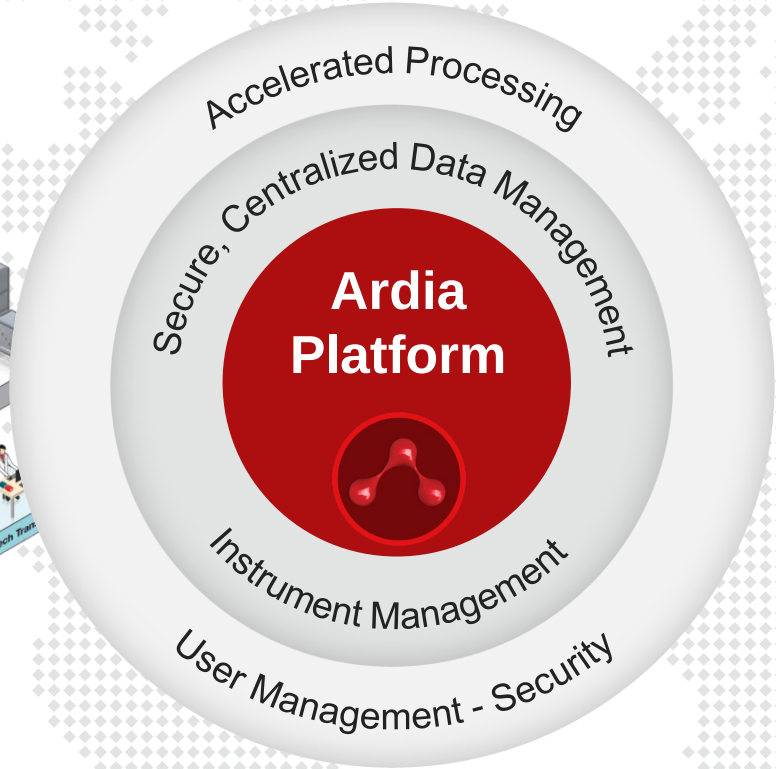
- Enhanced collaboration
- Global access to data and results
- Secure, controlled environment
- Holistic instrument view
- Metrics and utilization

Collaboration | **Productivity** | **Deep insights** | **Security**

Connecting people and data







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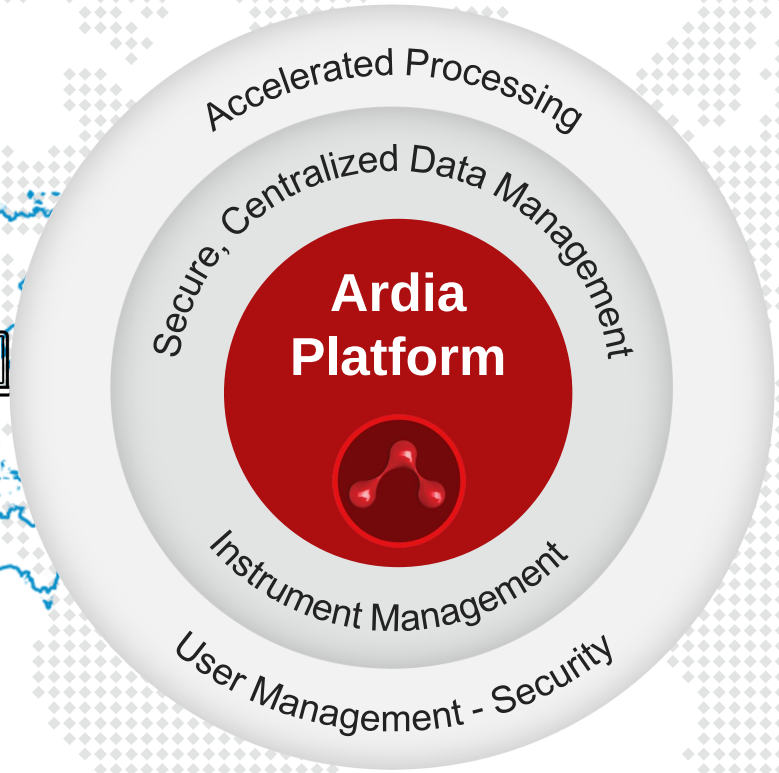
Connecting people and data



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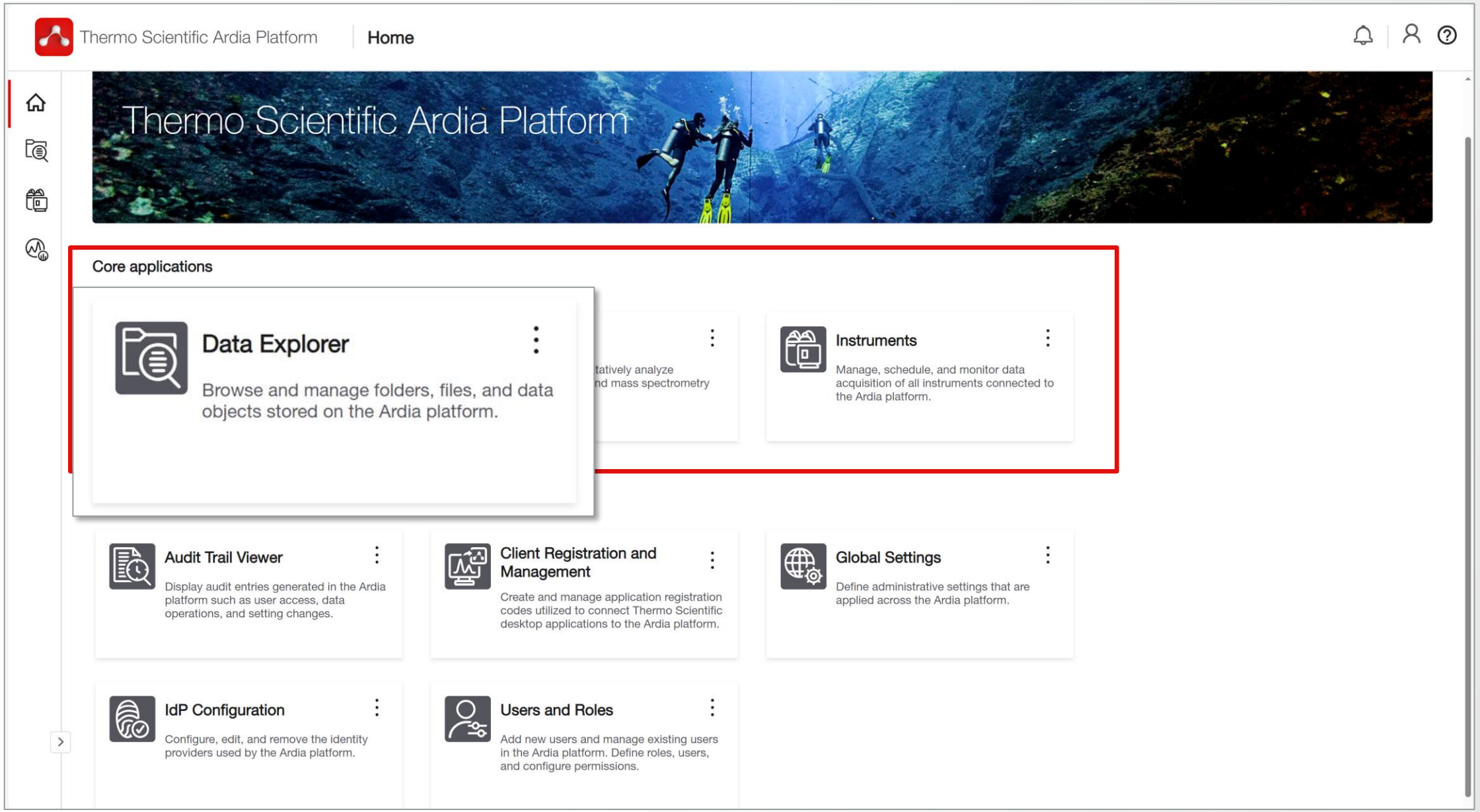
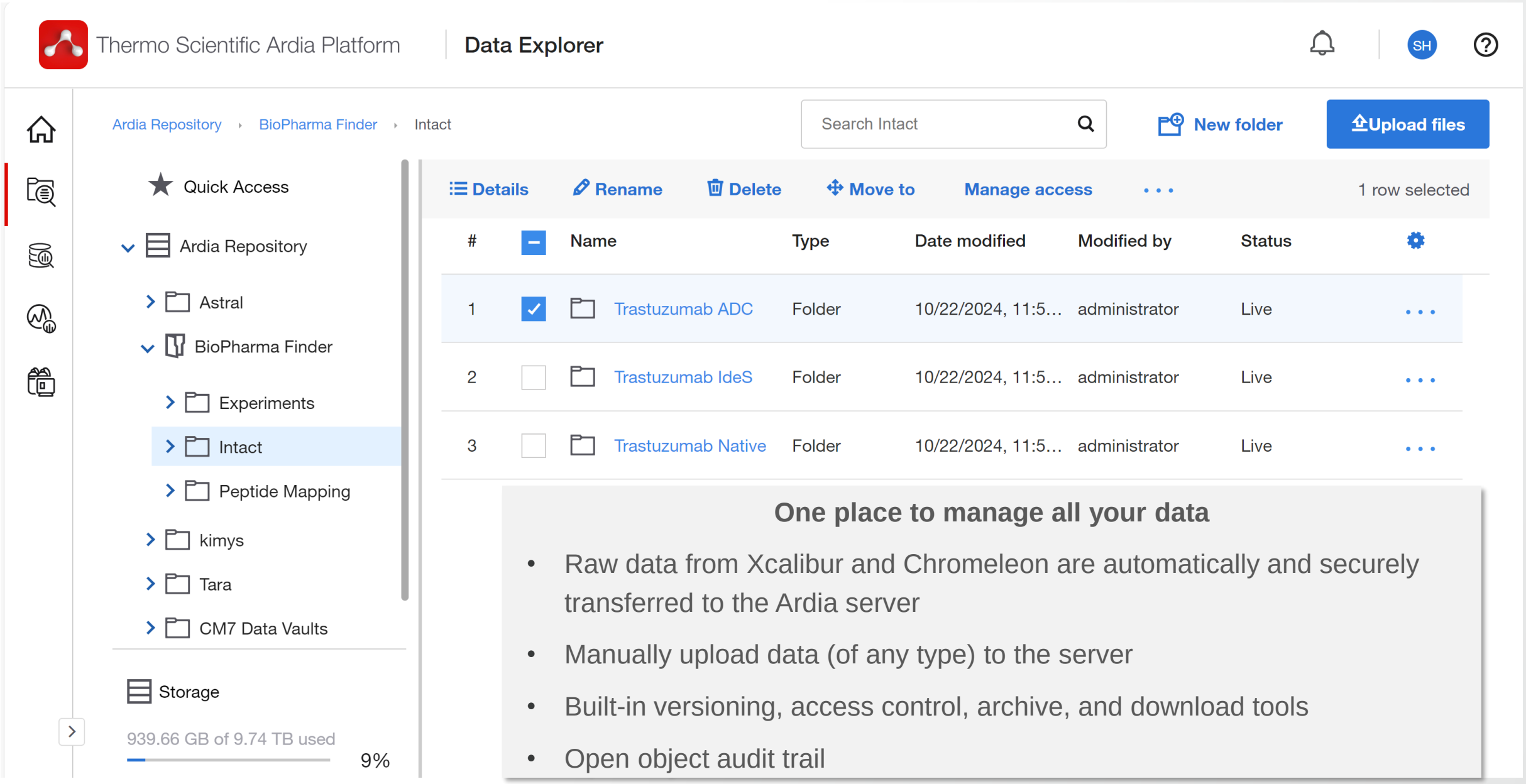
Landing page of the Ardia Platform



Ardia Platform: Data Explorer

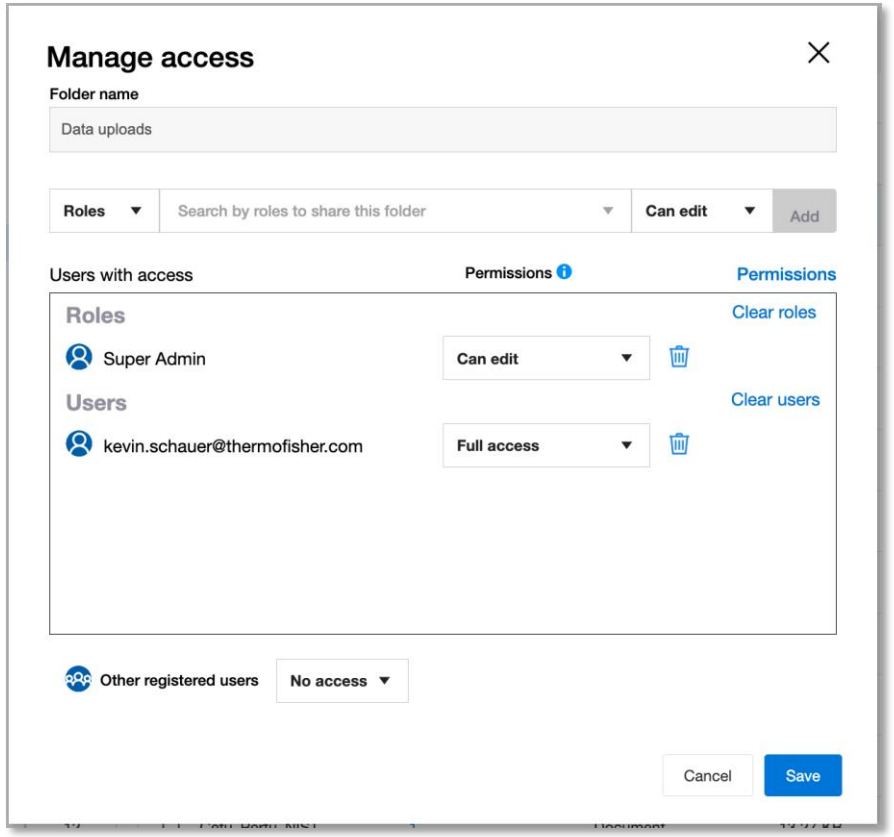


One place to manage all your data

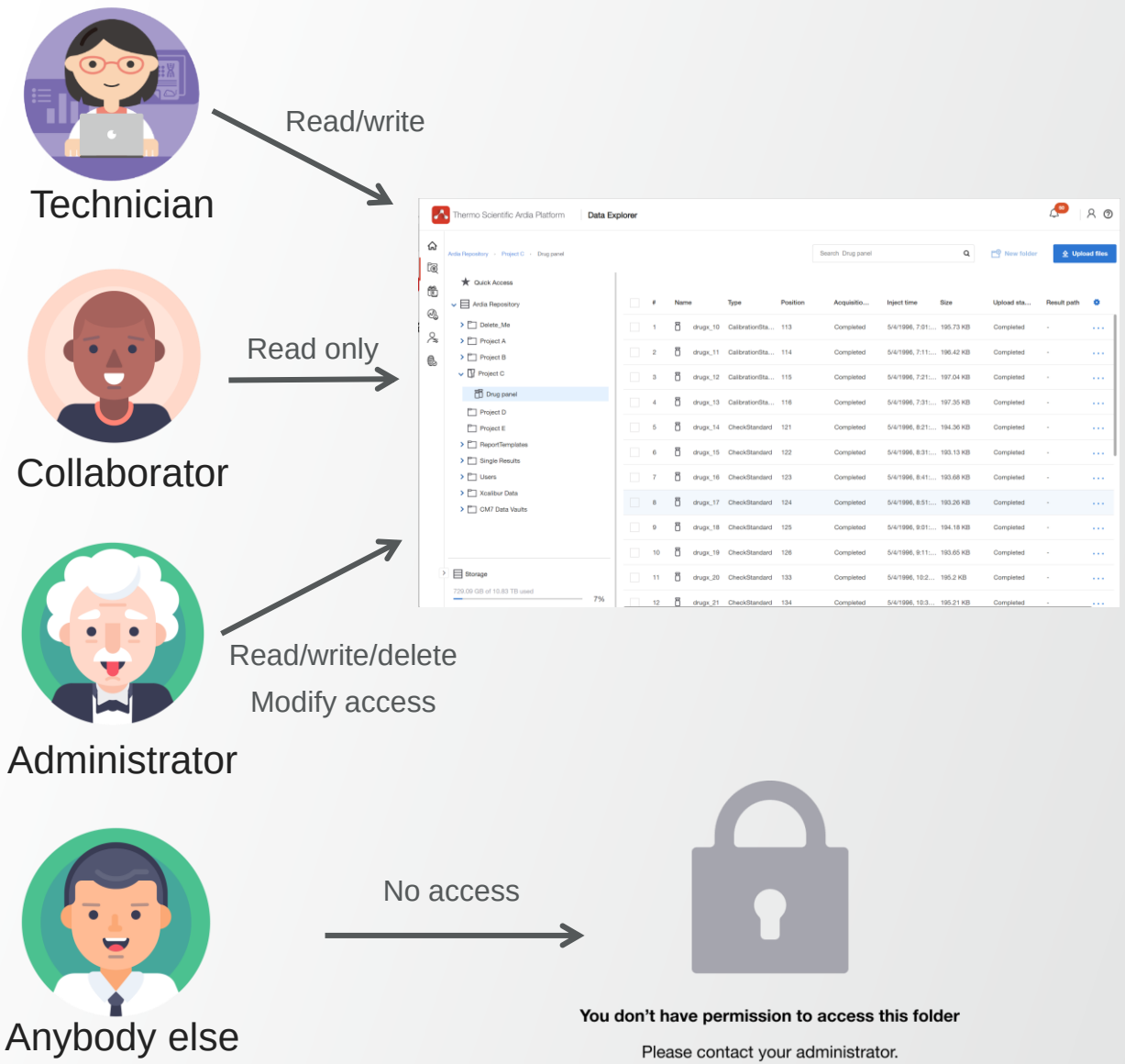
- Raw data from Xcalibur and Chromeleon are automatically and securely transferred to the Ardia server
- Manually upload data (of any type) to the server
- Built-in versioning, access control, archive, and download tools
- Open object audit trail

Ardia Platform: Data Explorer

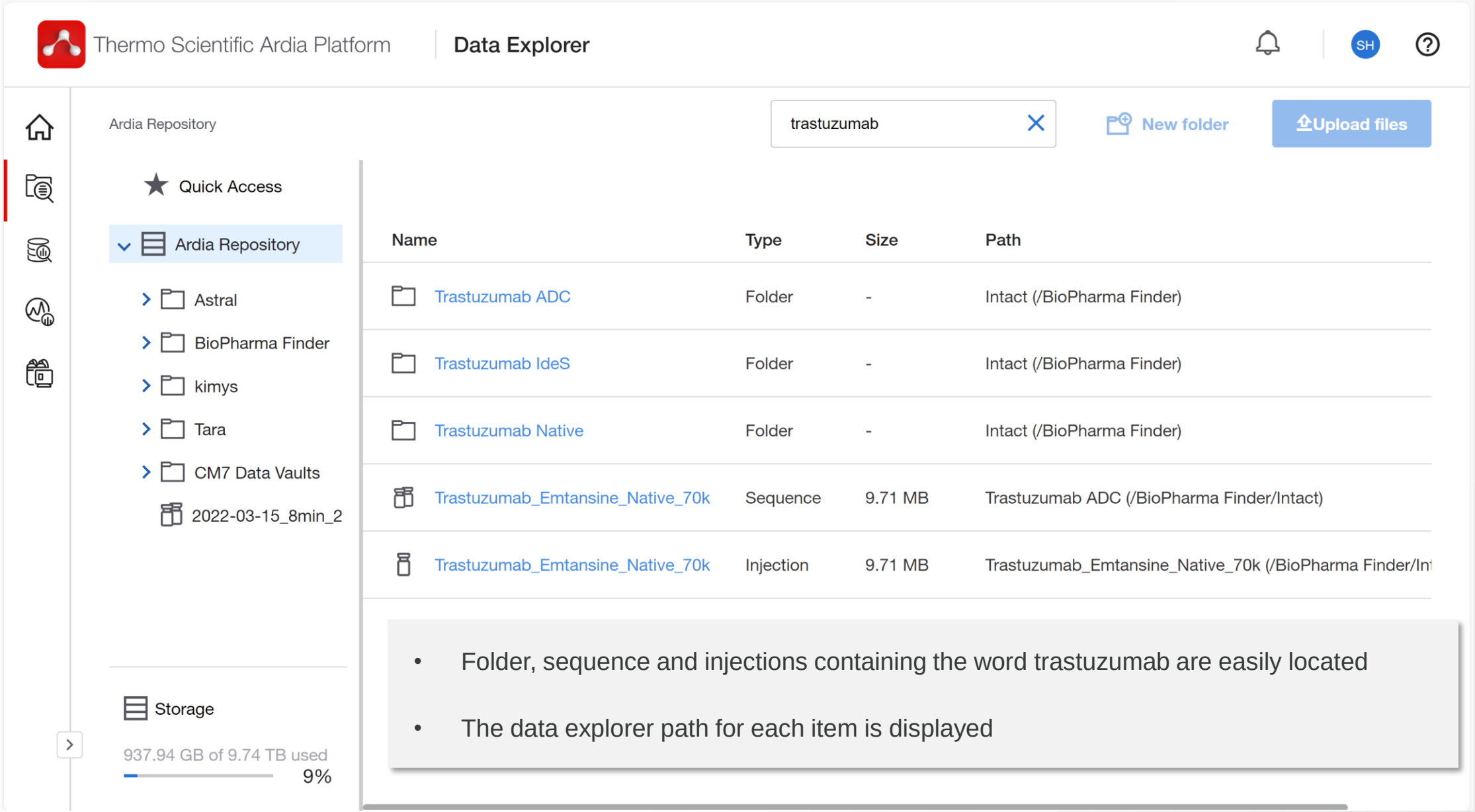
Easily control who has access to what data



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

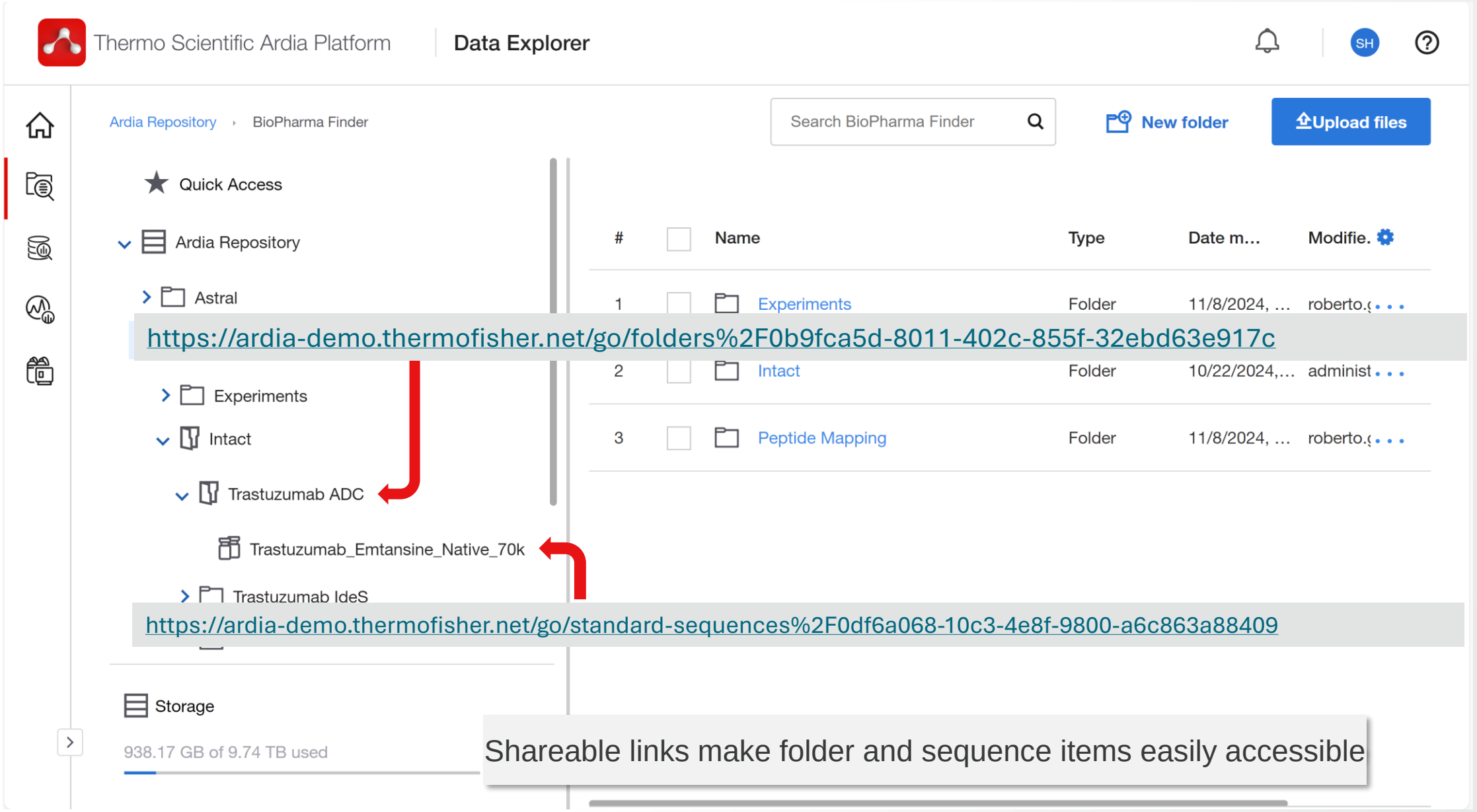


Data Explorer: search function

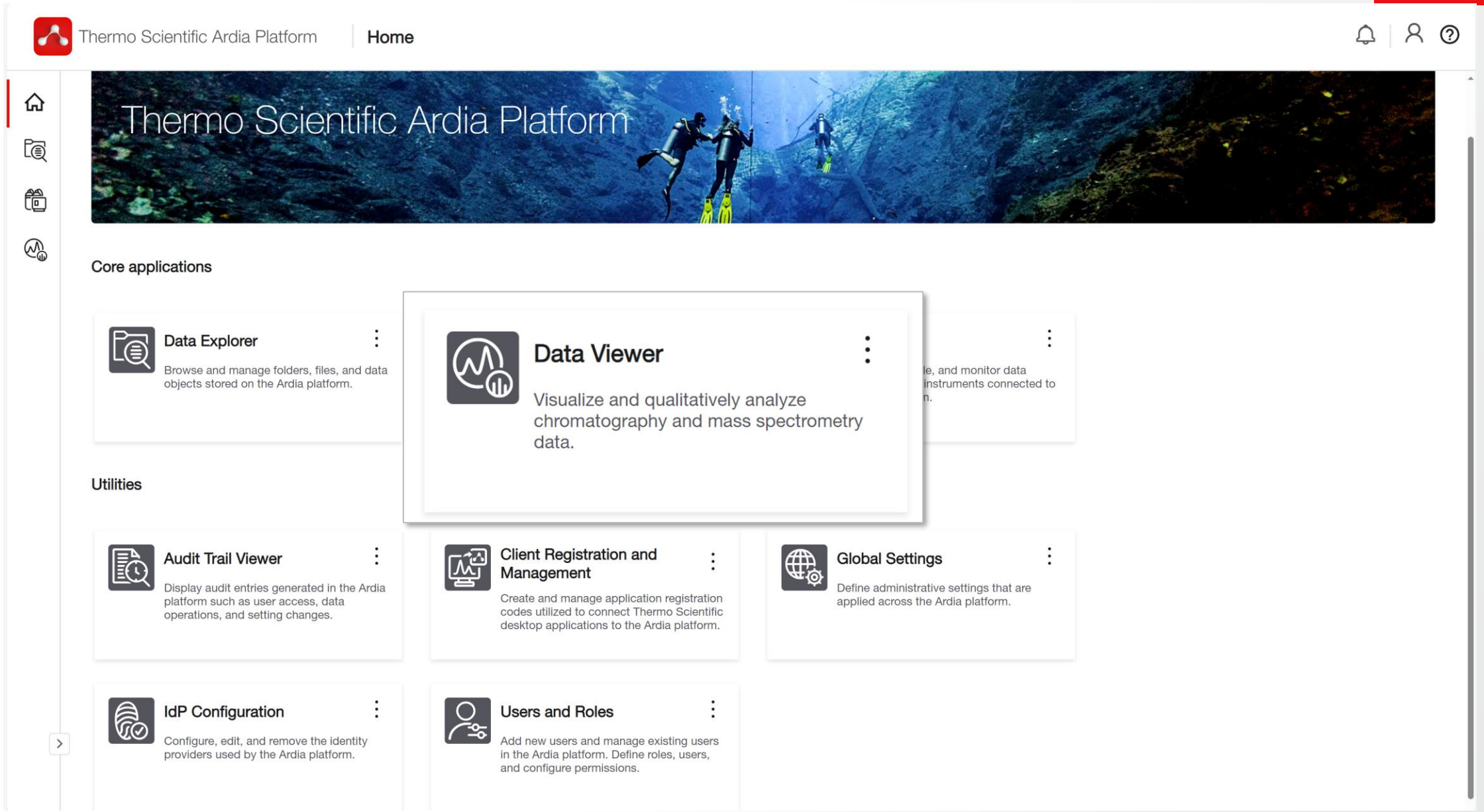


- Folder, sequence and injections containing the word trastuzumab are easily located
- The data explorer path for each item is displayed

Data Explorer: shareable links



Ardia Platform: Data Viewer



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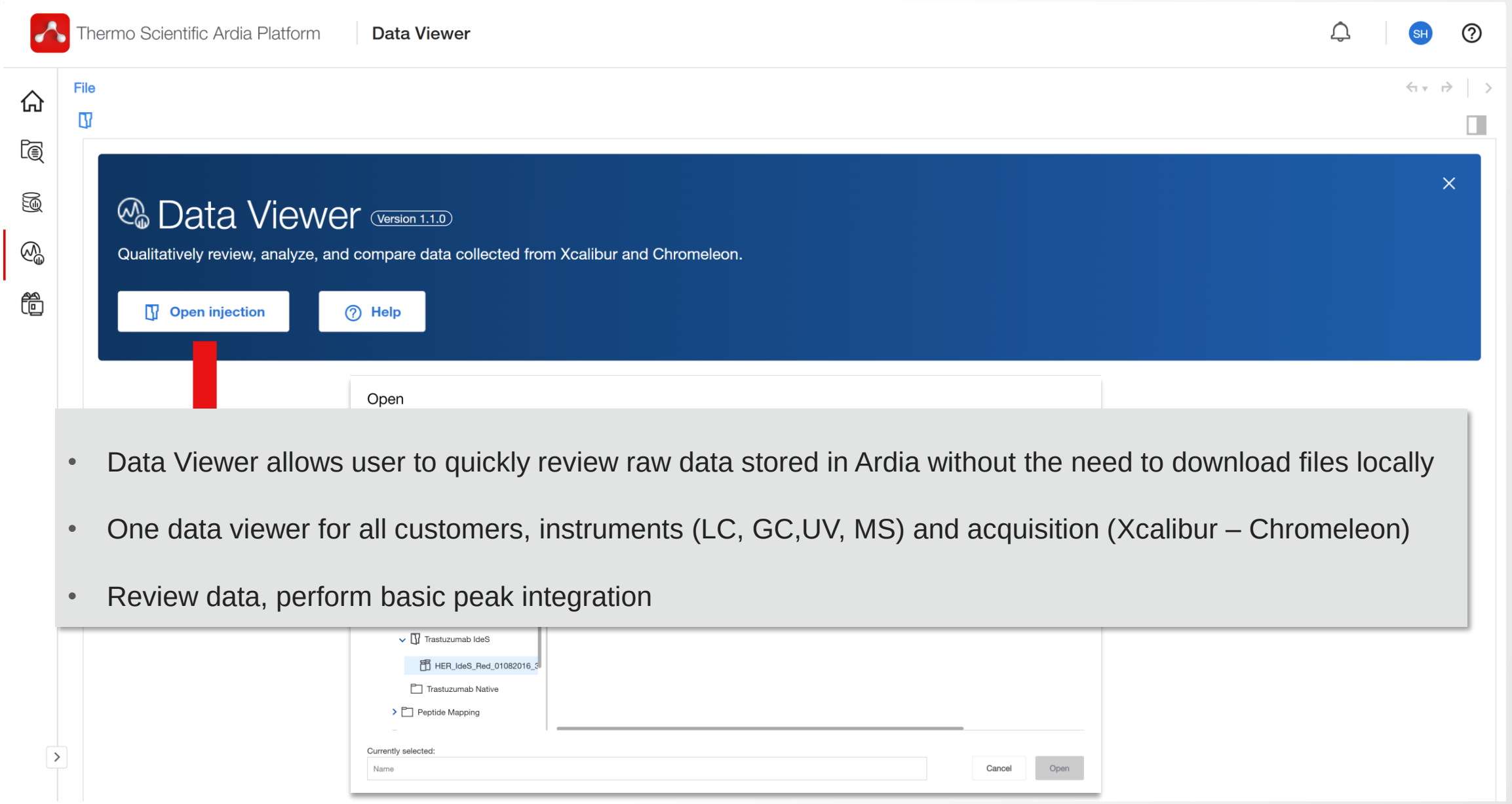
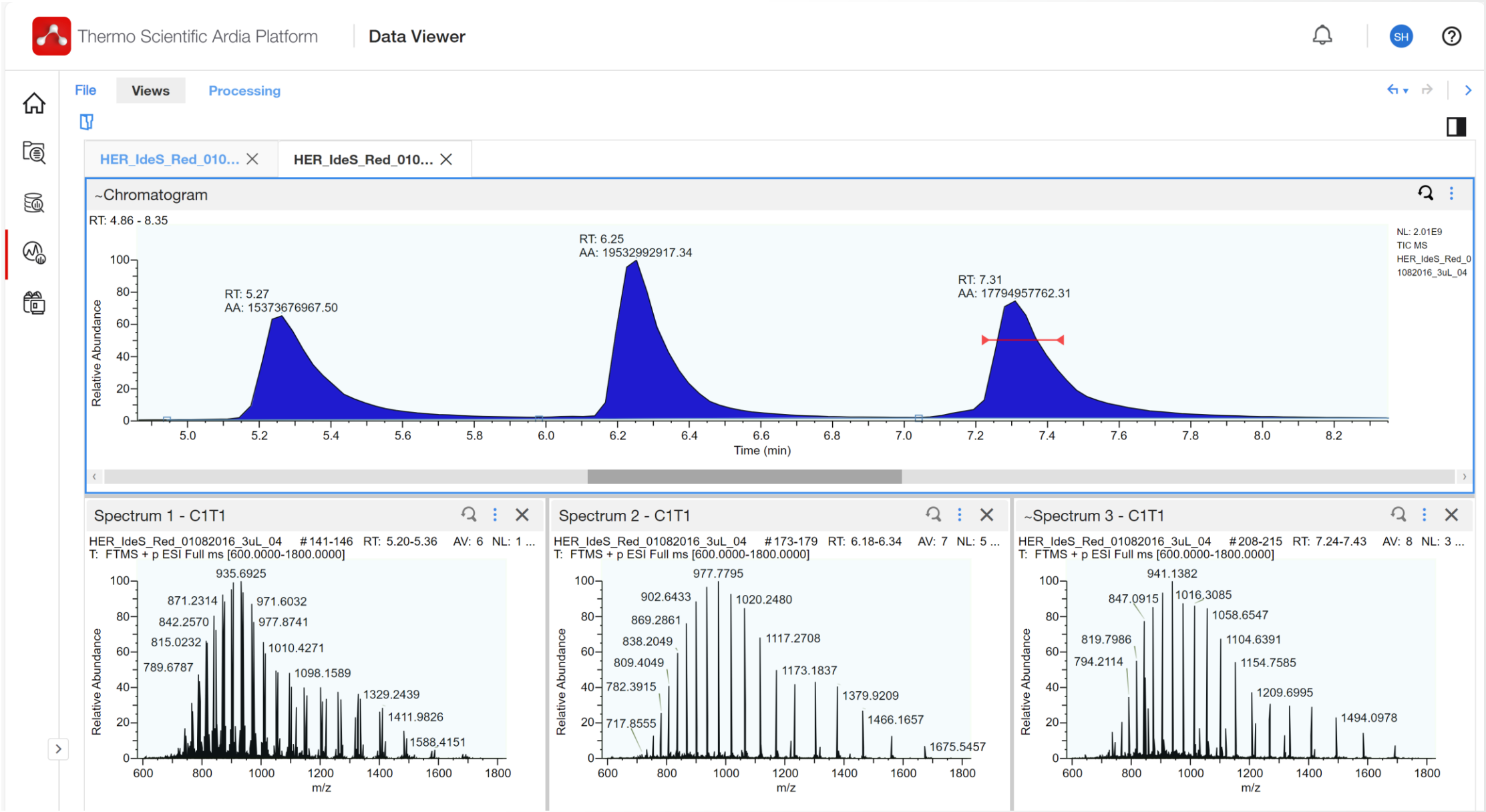
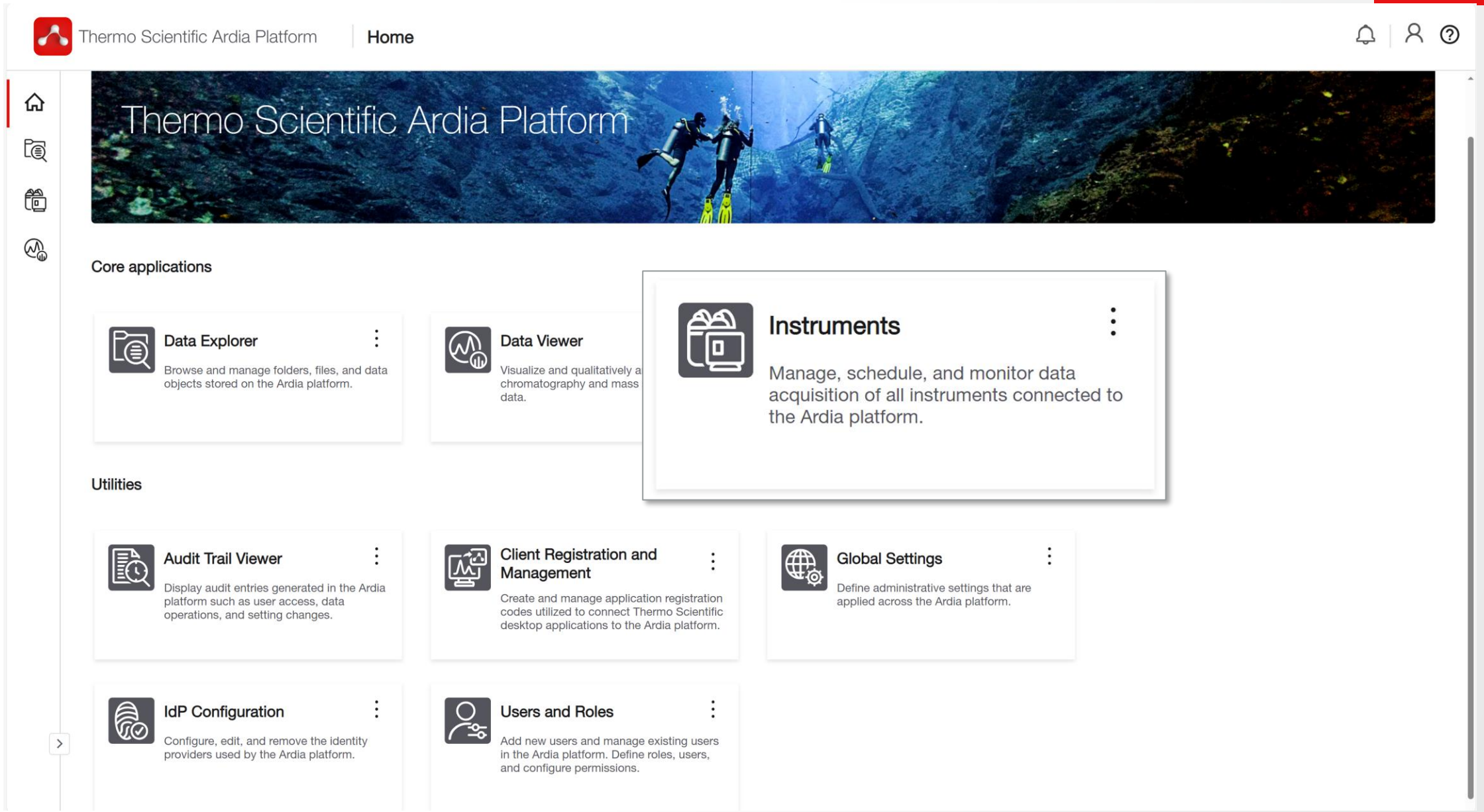


- Data Viewer allows user to quickly review raw data stored in Ardia without the need to download files locally
- One data viewer for all customers, instruments (LC, GC,UV, MS) and acquisition (Xcalibur – Chromeleon)
- Review data, perform basic peak integration

Ardia Platform: Data Viewer



Ardia Platform: Instruments



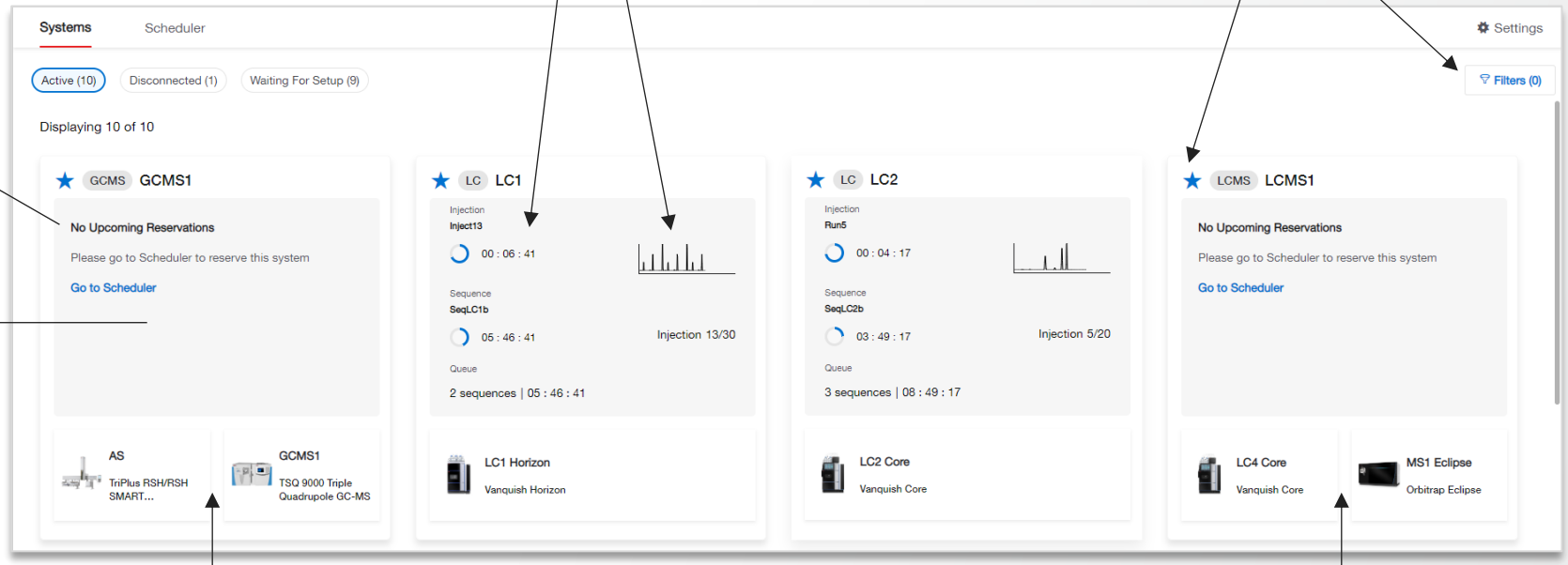
Instruments: Systems View

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

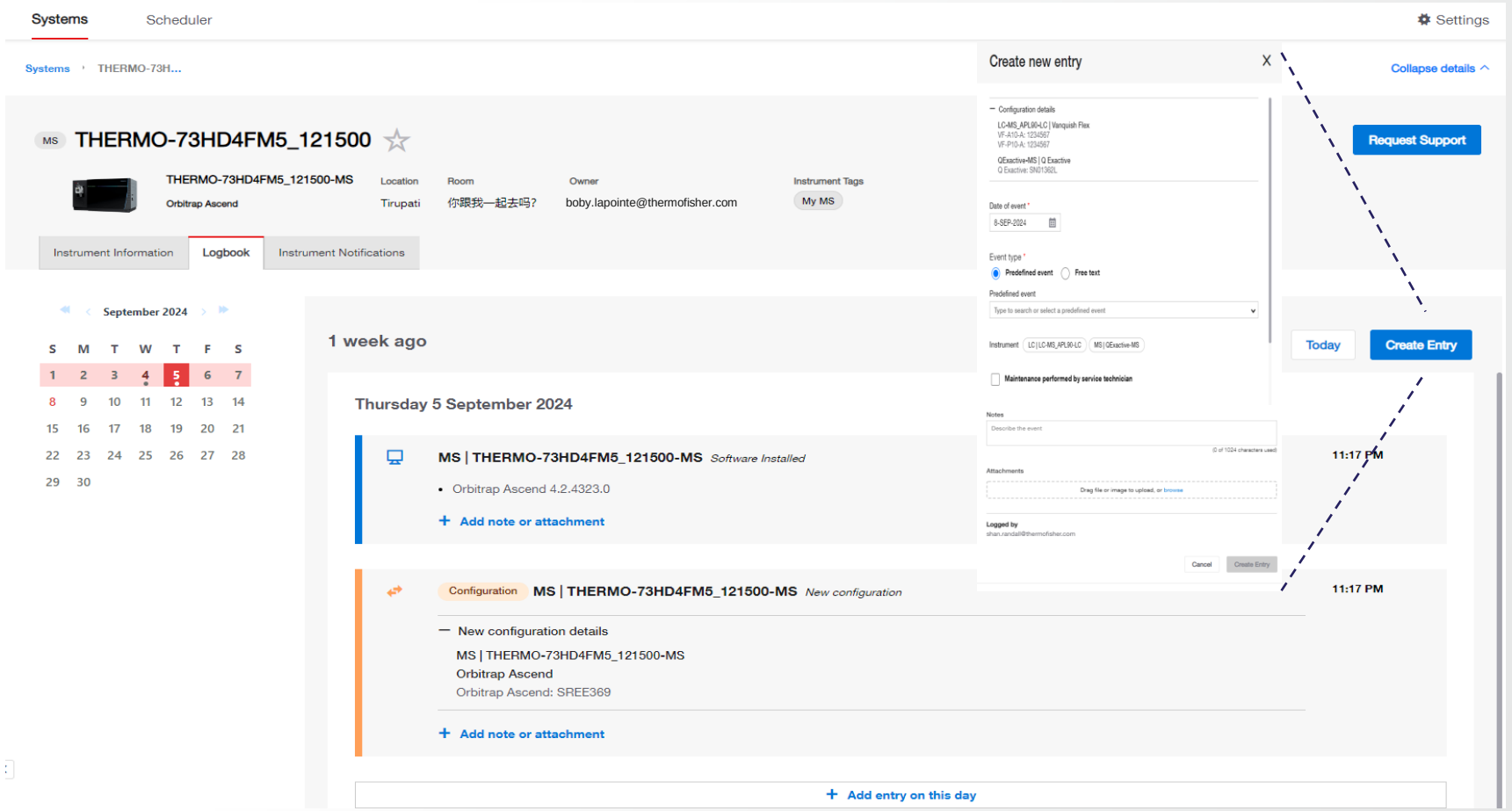
Instruments: Logbook

Document events with the Logbook

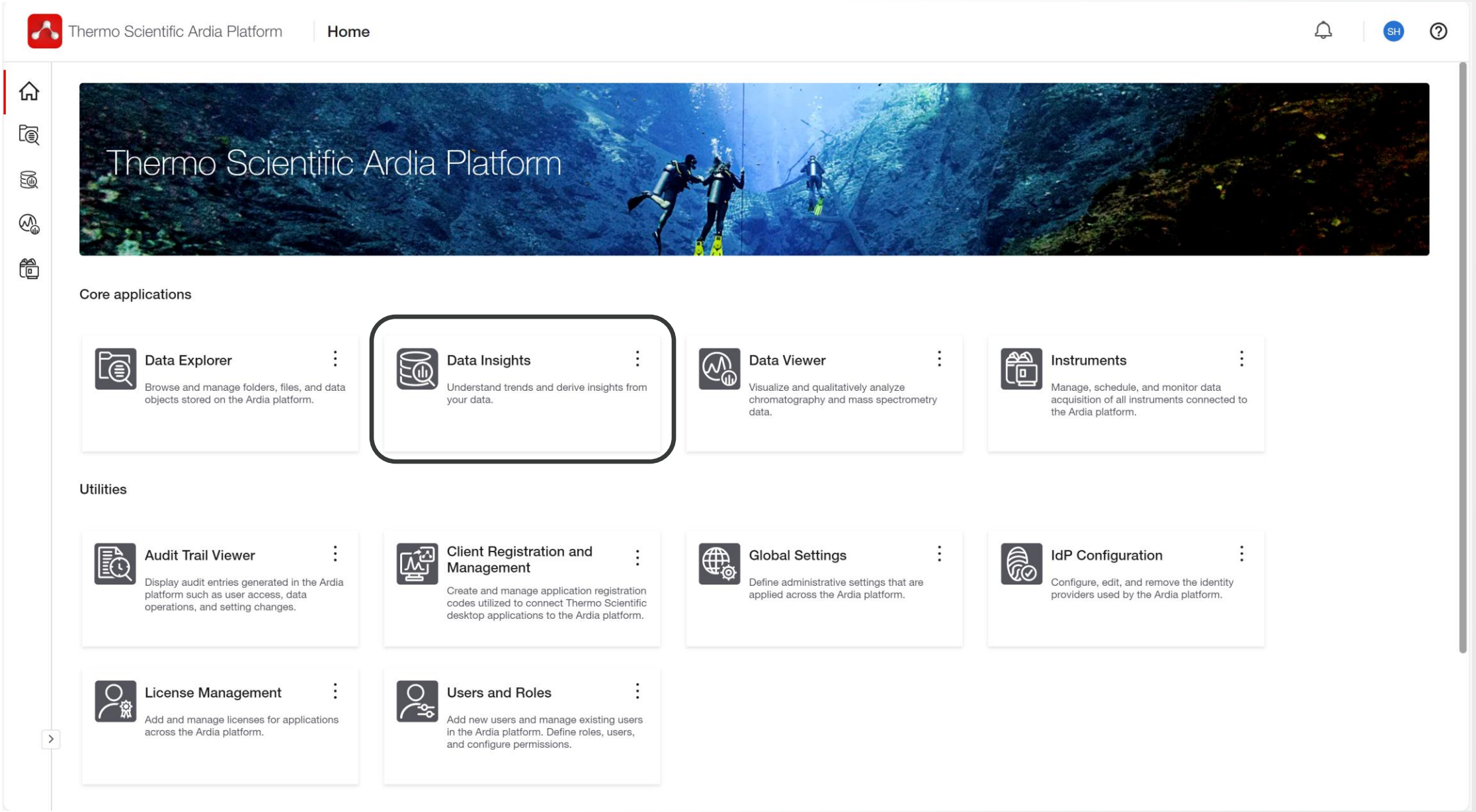
Allows you to:

- 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

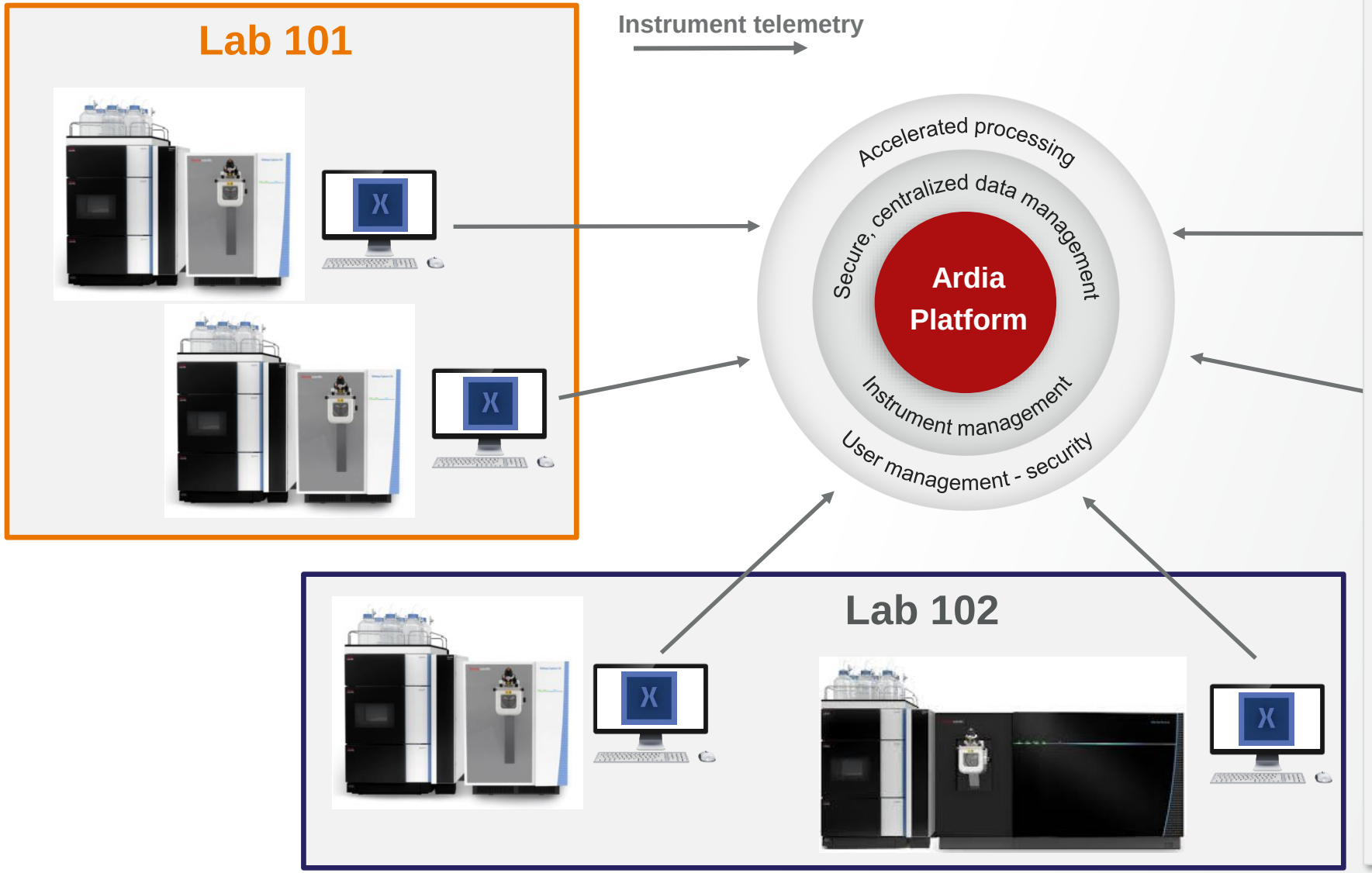


Data Insights



Data Insights: Instrument utilization

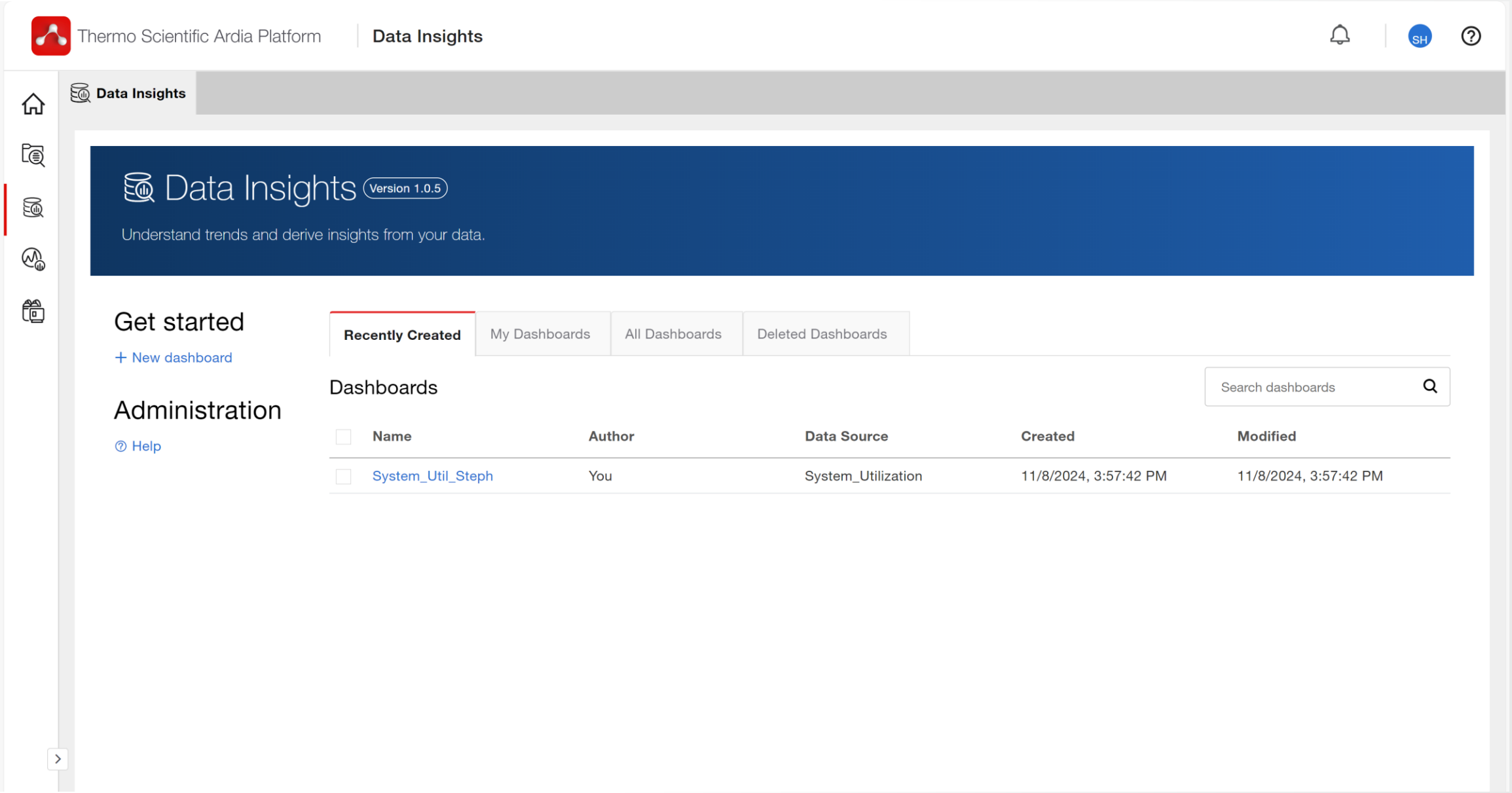
Instrument telemetry is collected in near real-time.



Telemetry recorded (today):

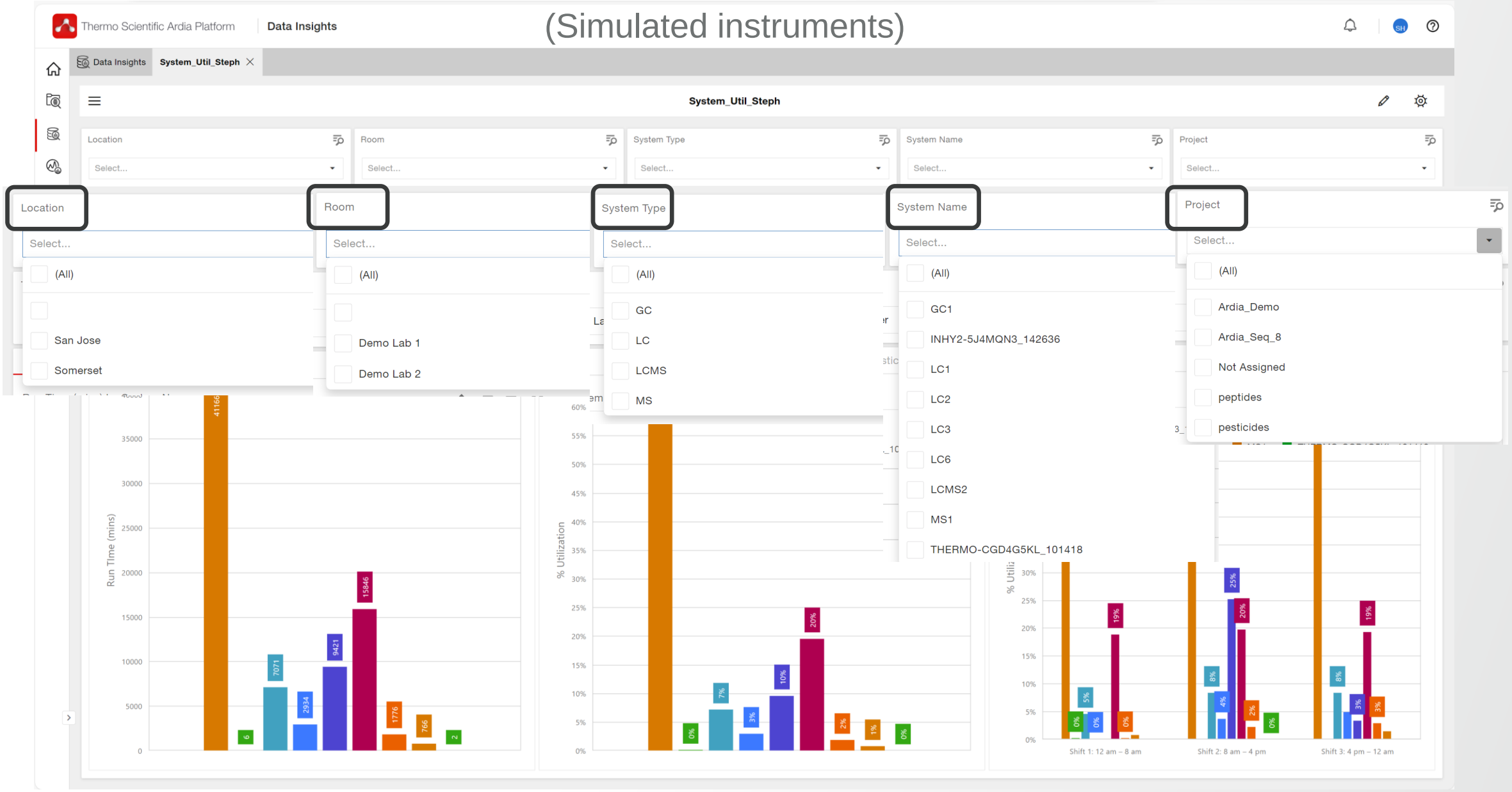
- System ID
- Number of injections
- Injections:
  - Name
  - Date
  - Start and end time
  - Total acquisition time
  - Volume
- Events:
  - Abort
  - Stop
  - Interrupt
- Method Name
- Sequence name
- Sample type
- Acquisition SW and Versions

Data Insights: instrument utilization



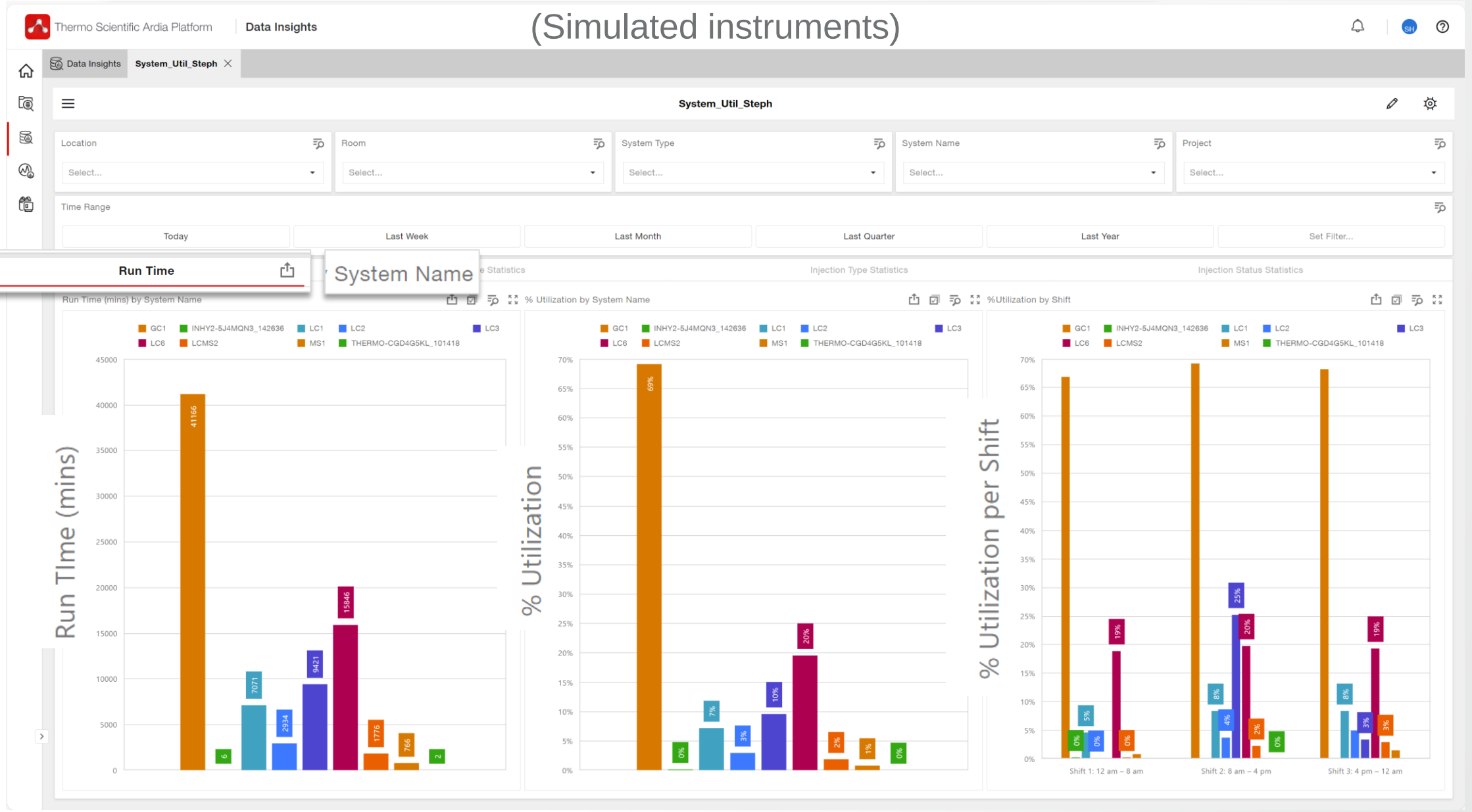
Data Insights: instrument utilization

(Simulated instruments)



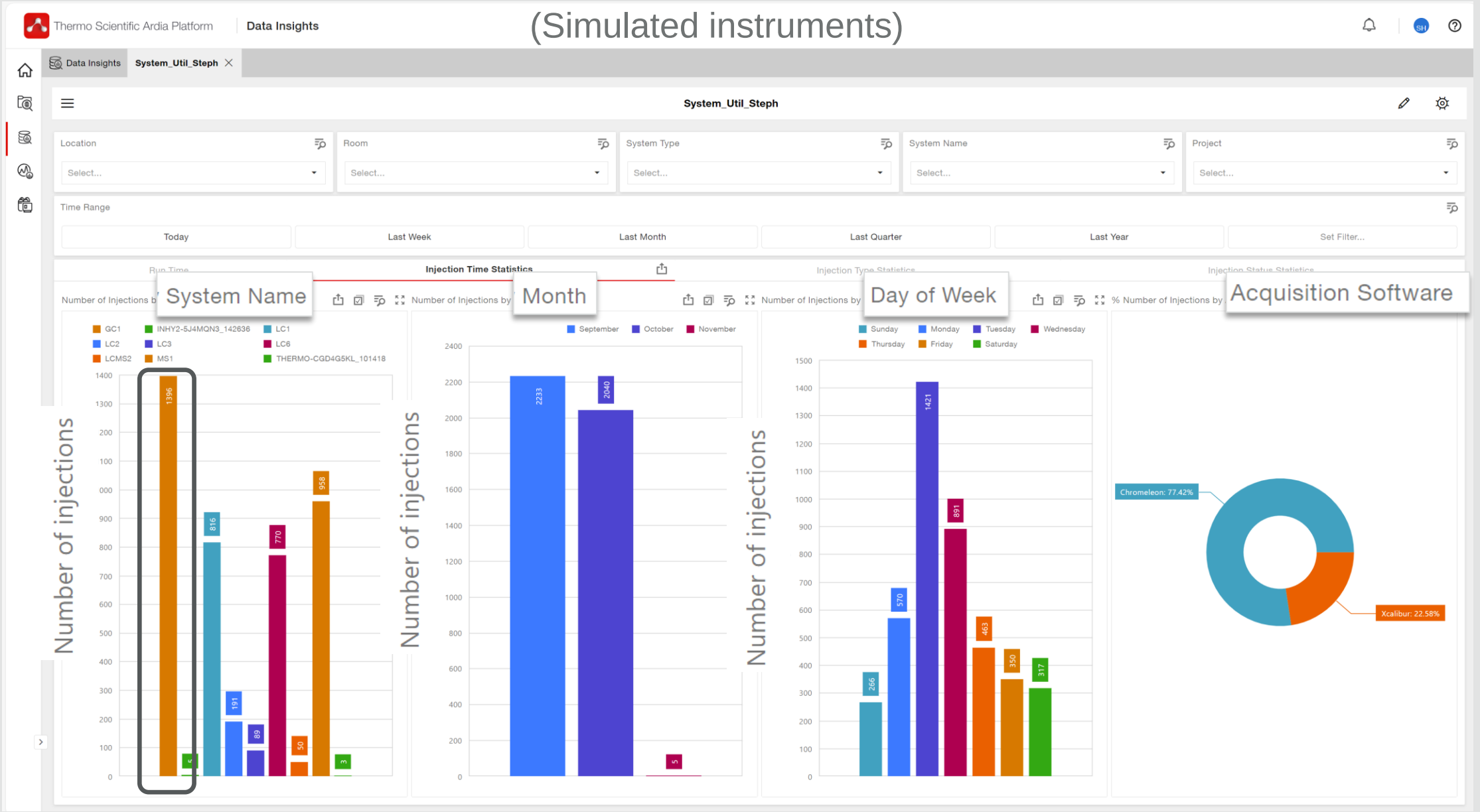
Instrument utilization: Run Time

(Simulated instruments)



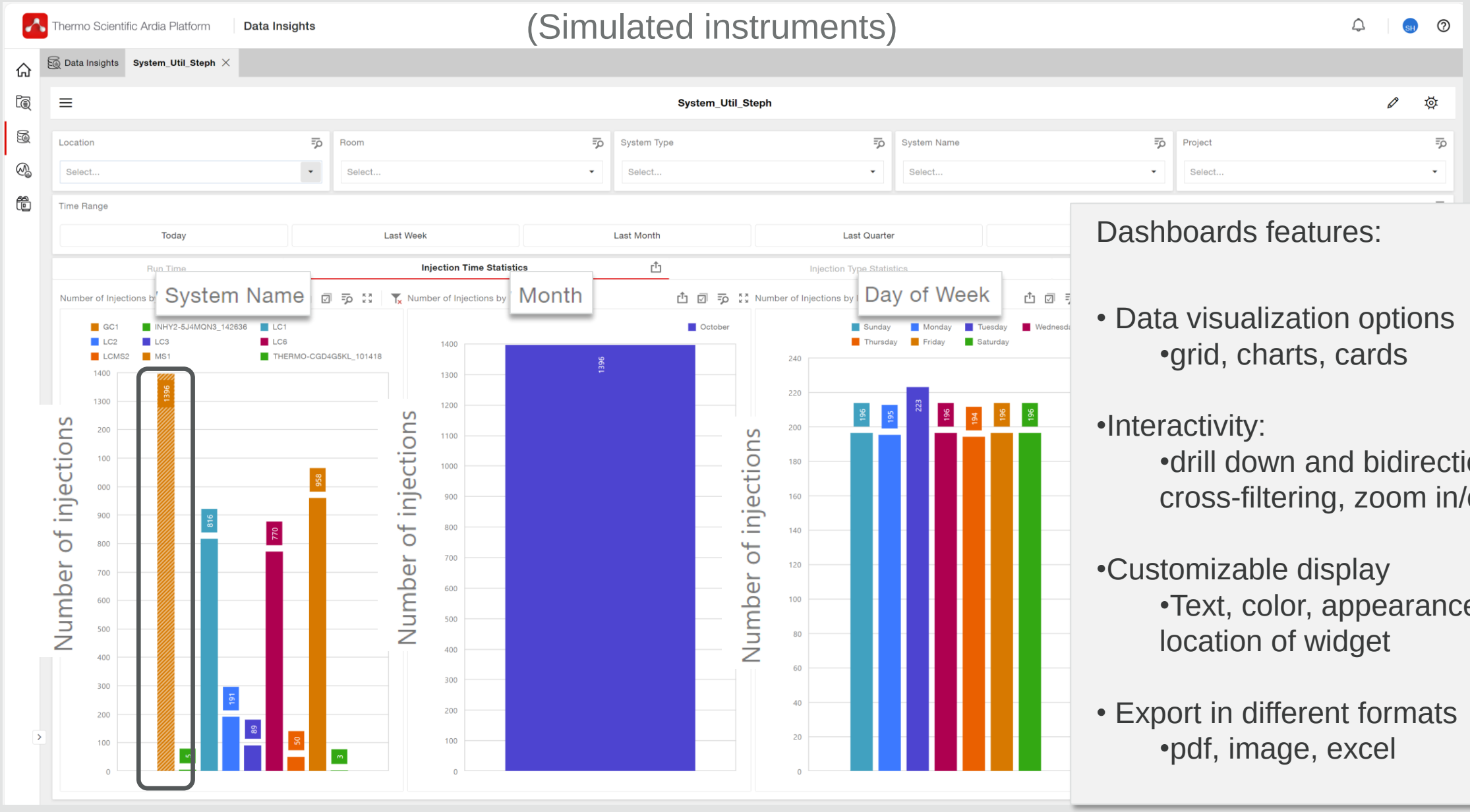
Instrument utilization: Injection Time

(Simulated instruments)



Injection Time: drill down for a specific system

(Simulated instruments)



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

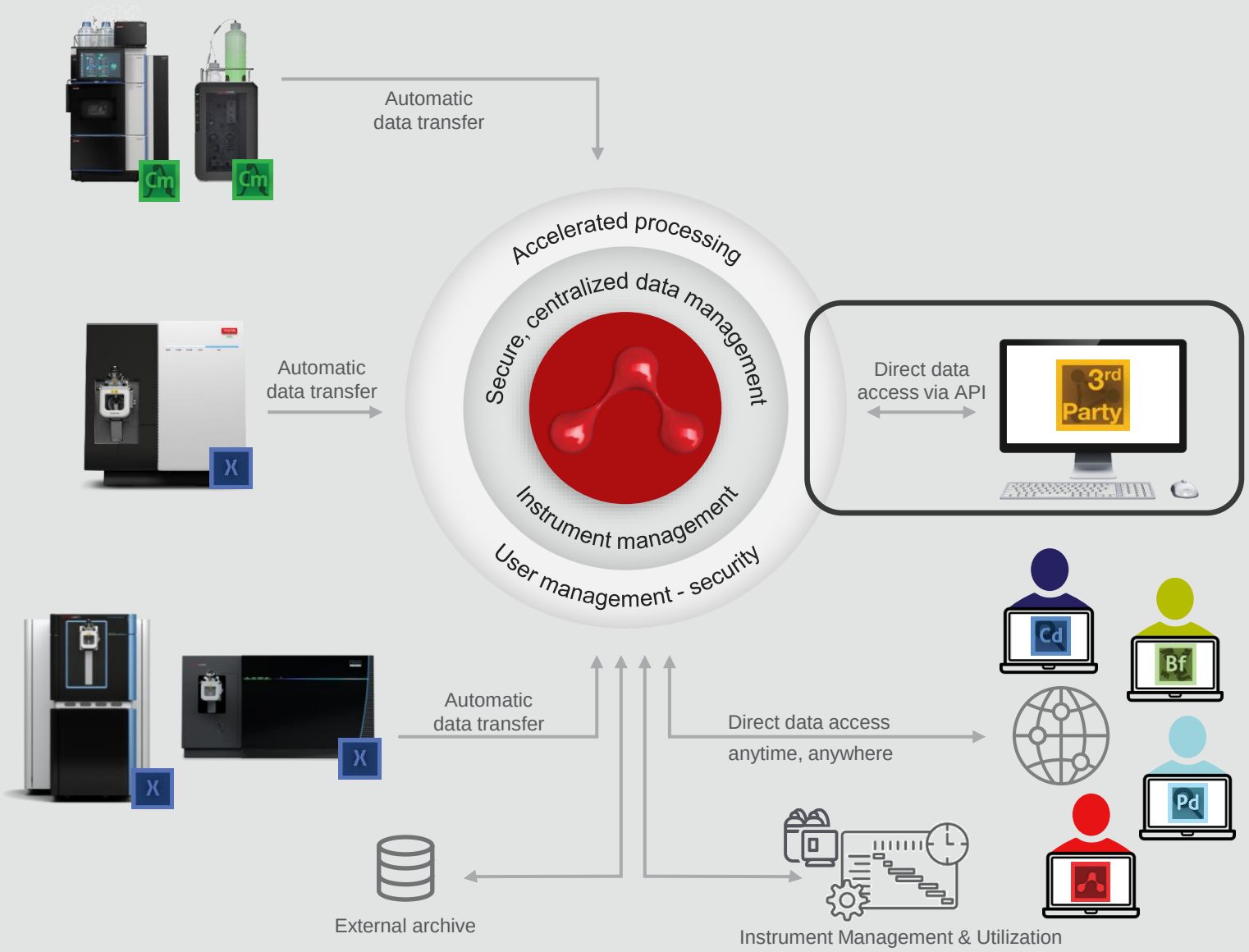
Enhanced resource management

- 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

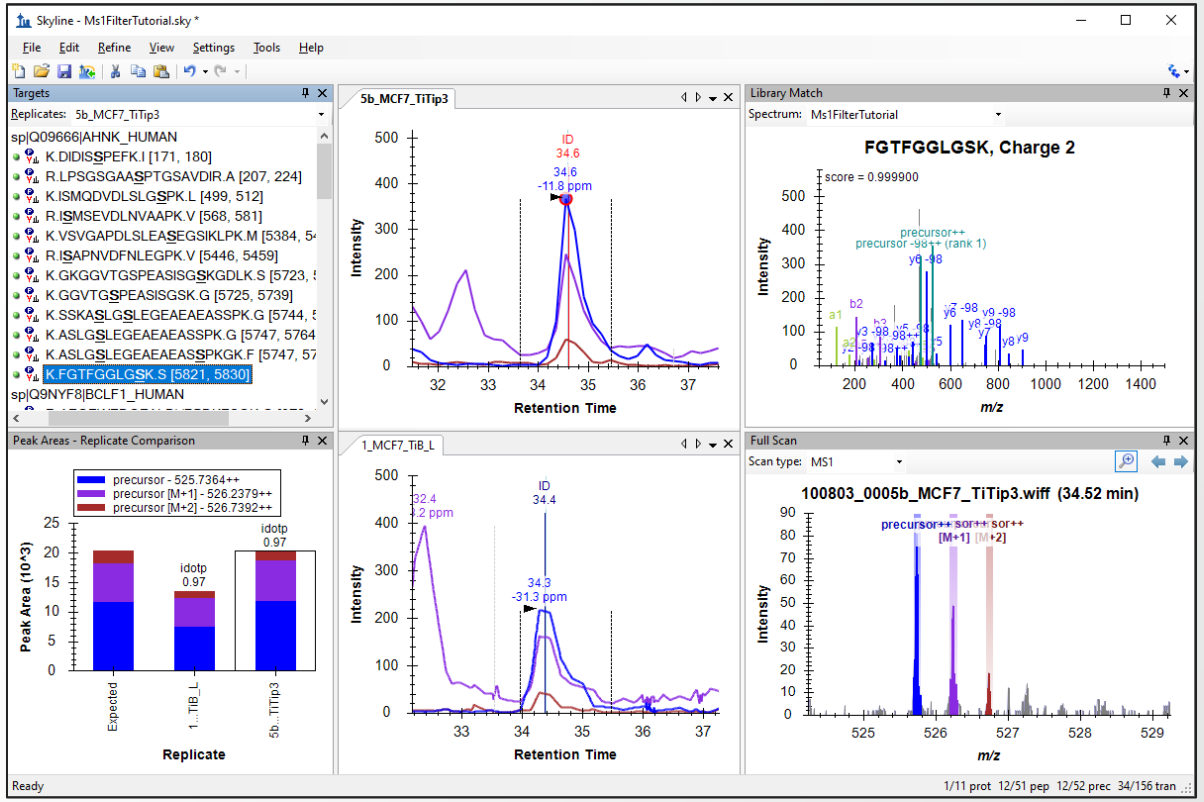
- Register the 3rd party software
  → **Registration Service**
- User connects to Ardia
  → **Identity Service**
- User is connected to Ardia
  → **Session Management Service**
- User selects data via Ardia object picker
  → **Navigation Service**
- User access the selected data
  → **Standard Sequence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

First connection to a third-party software: Skyline

Gold standard software for targeted peptide quantitation

Skyline

- → 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 MS

automatic data transfer

CHIMERYS
Centralized data management
Instrument Management

Ardia Server

Automate PD analysis for PRM discovery data

direct data transfer

store results

Skyline

Data Flow:

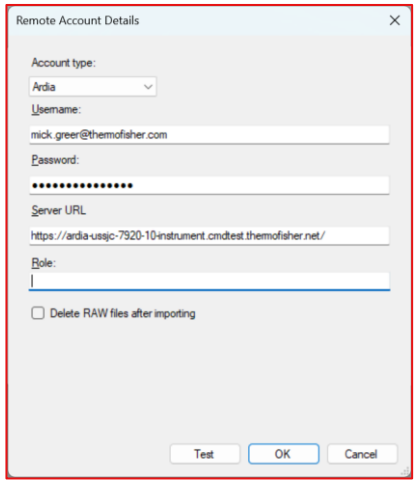
Stellar streams data to Ardia server
(~80TB capacity for advanced tower)

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

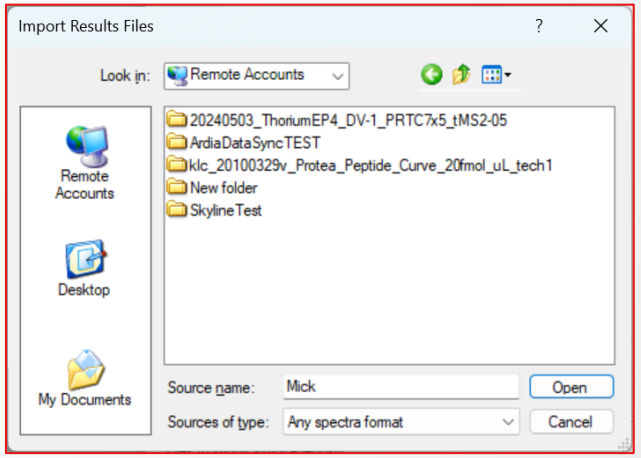


Login to Ardia via IdP

Create Ardia registration code

Input code via Skyline UI

Access Ardia

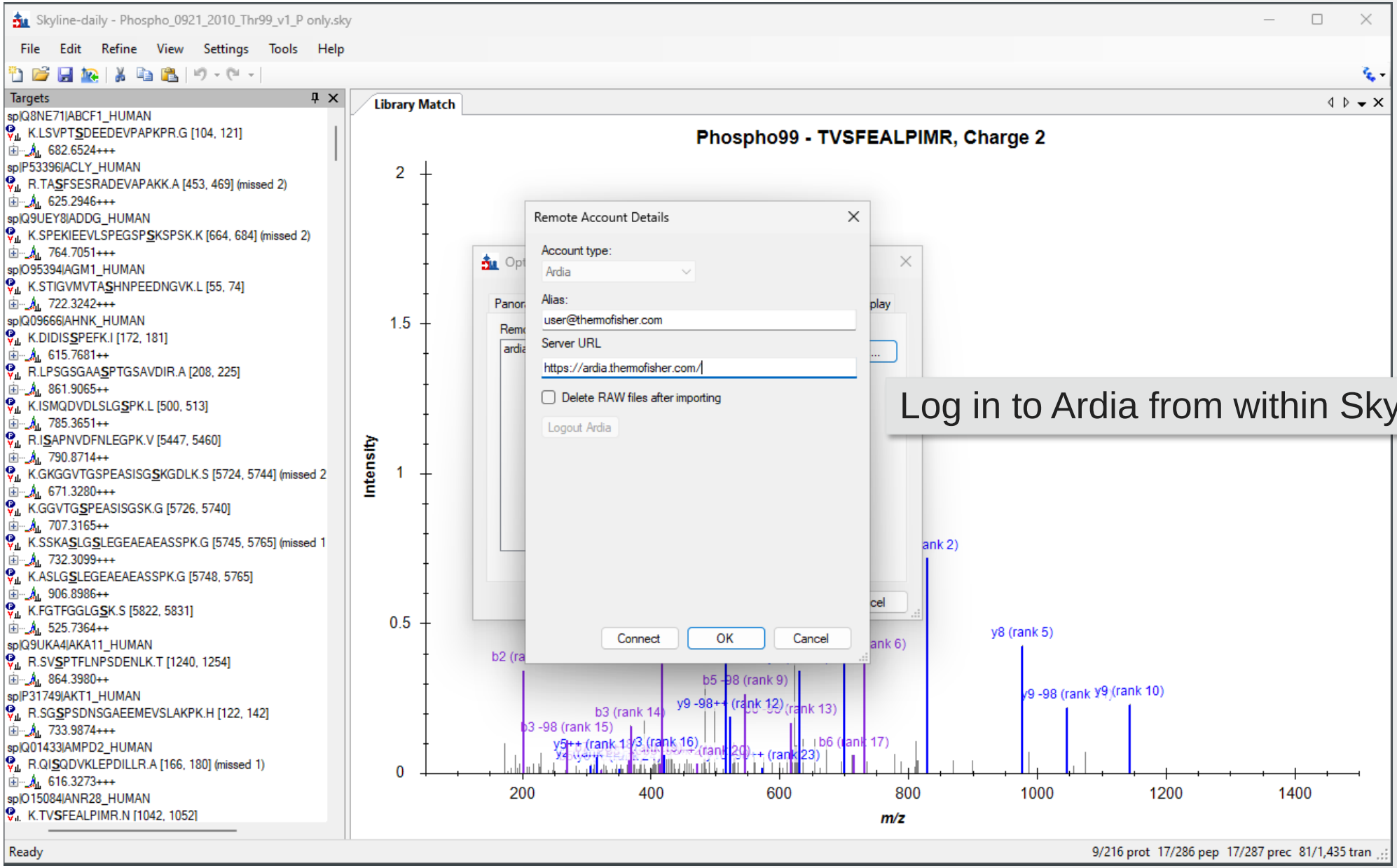


Select RAW files to analyze

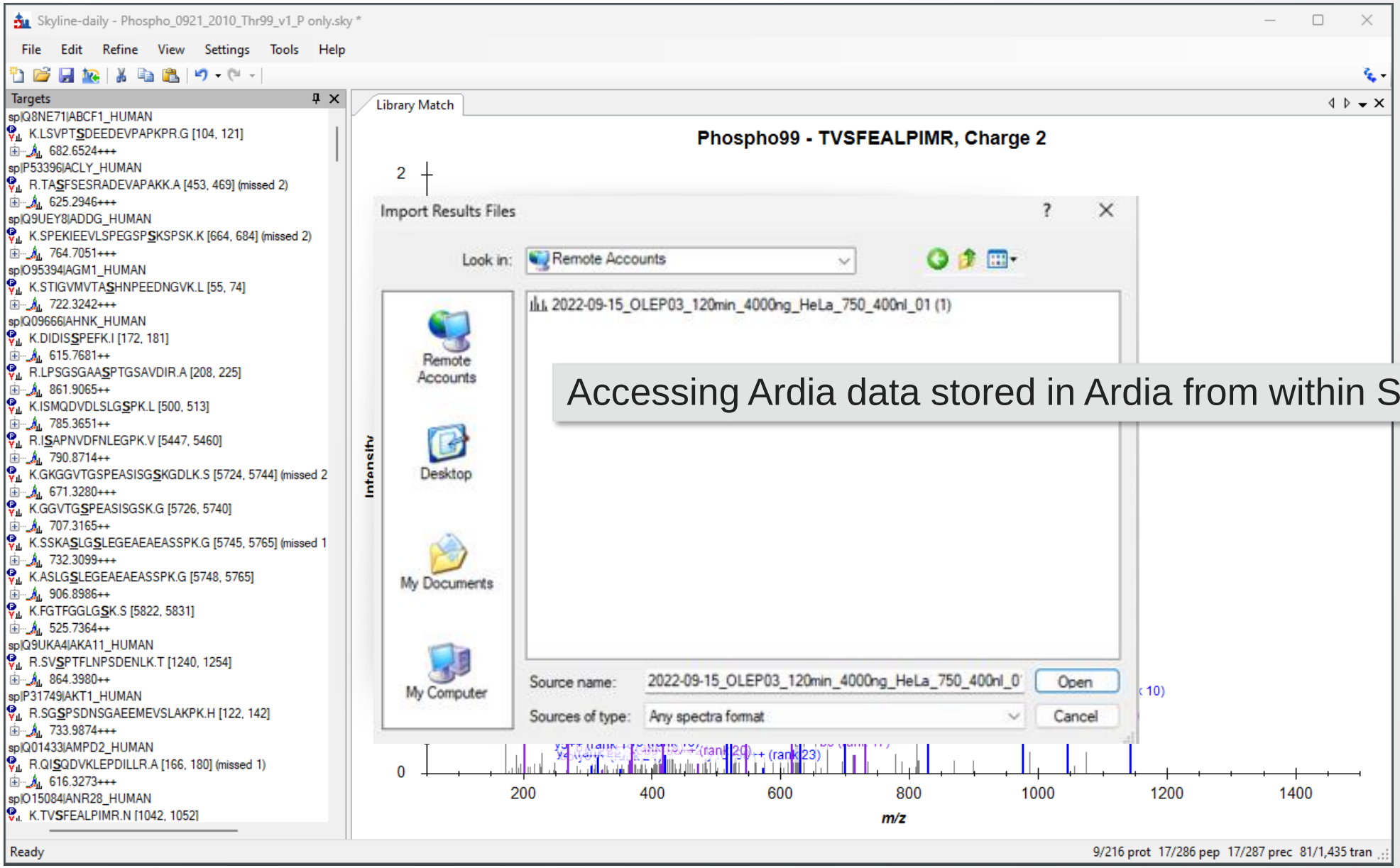
Process via local Skyline

Store/access Skyline results

Ardia – Skyline: how does it look?

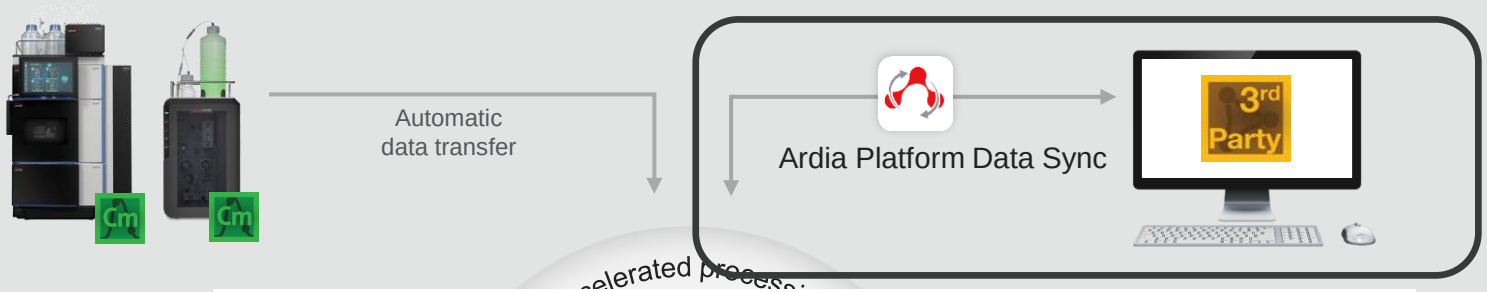


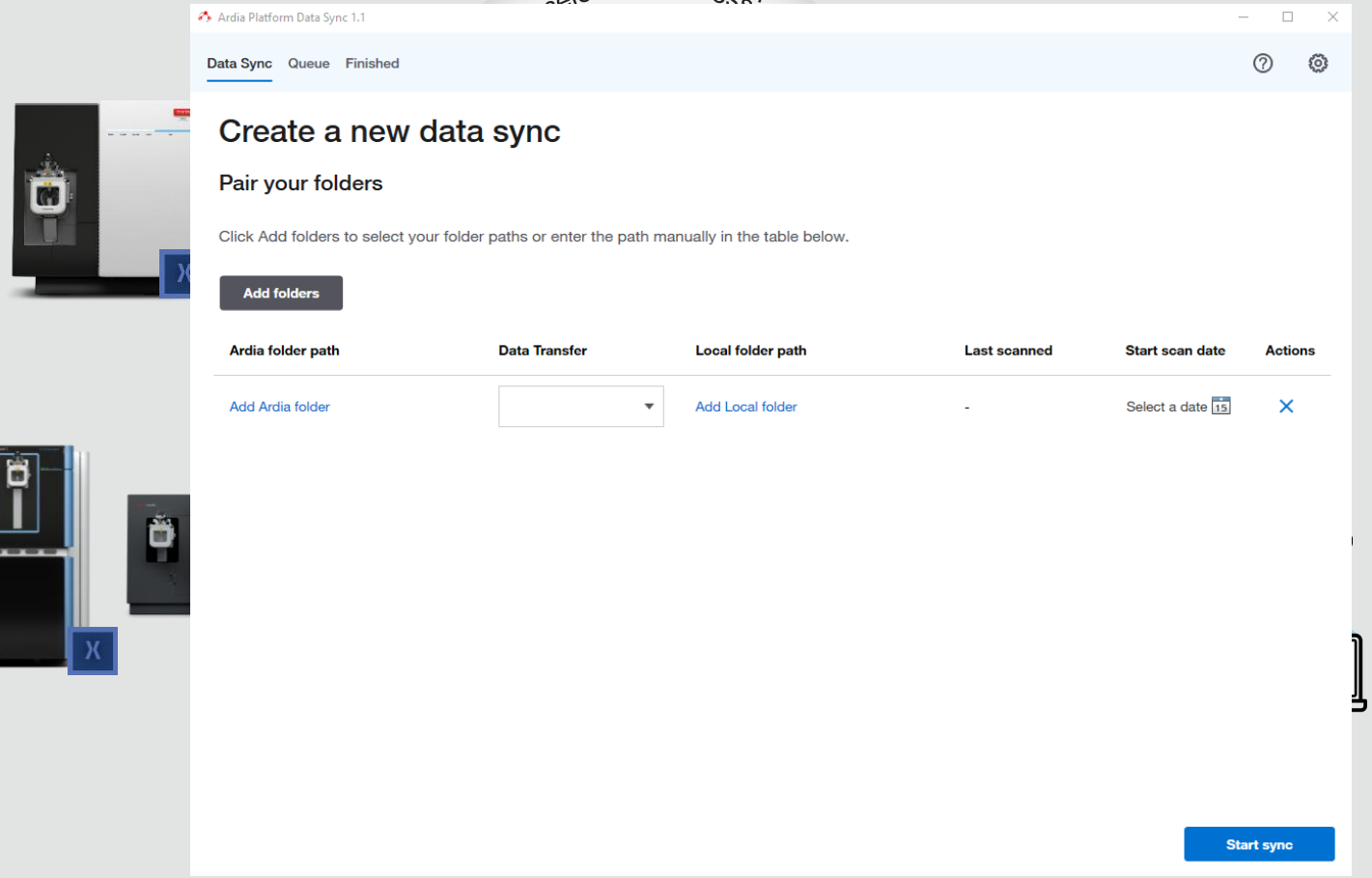
Ardia – Skyline: how does it look?



Accessing Ardia data stored in Ardia from within Skyline

Open platform: Ardia Platform Data 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

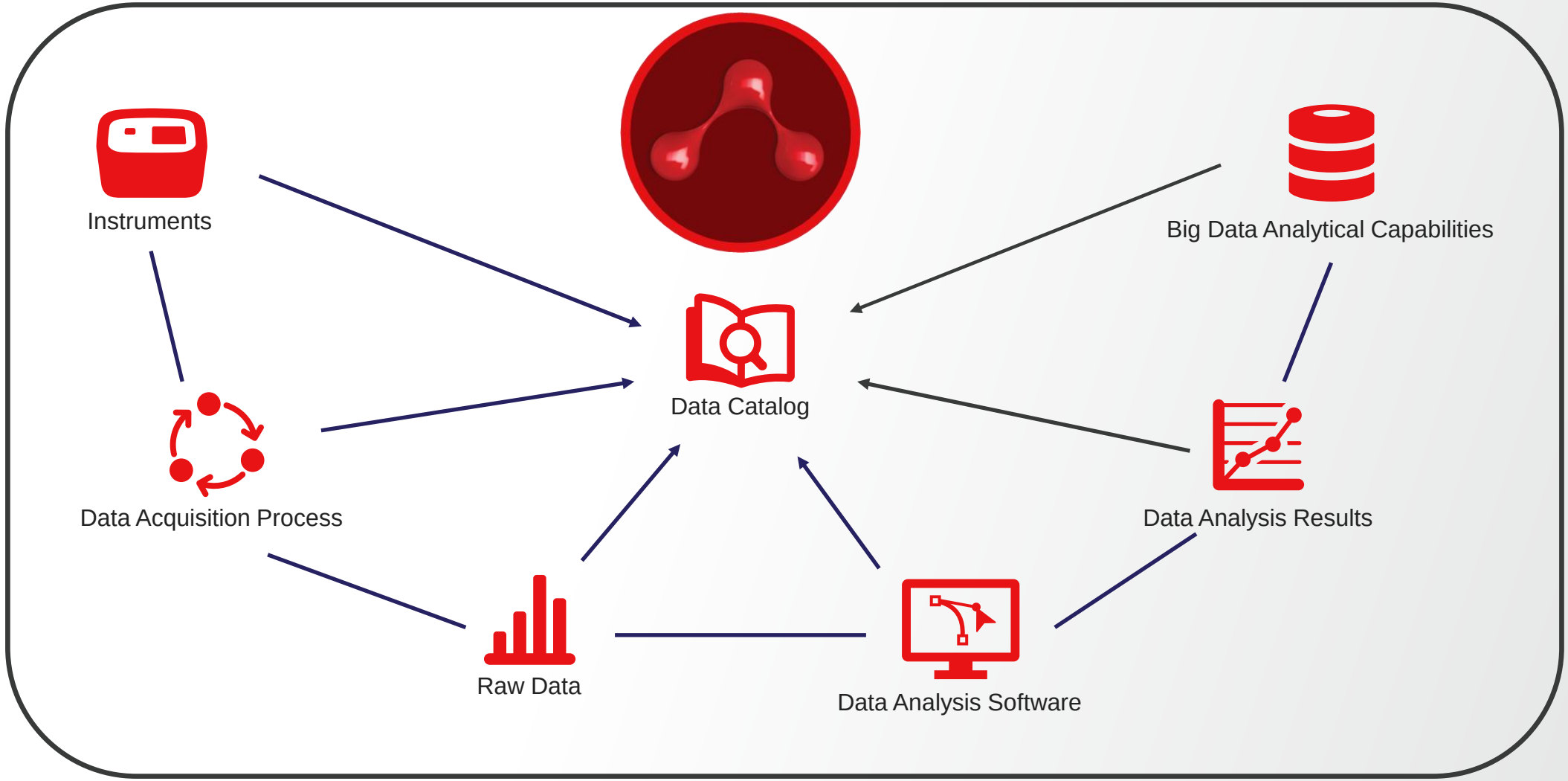
- **Metadata is linked to major ontologies, such as Allotrope**

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

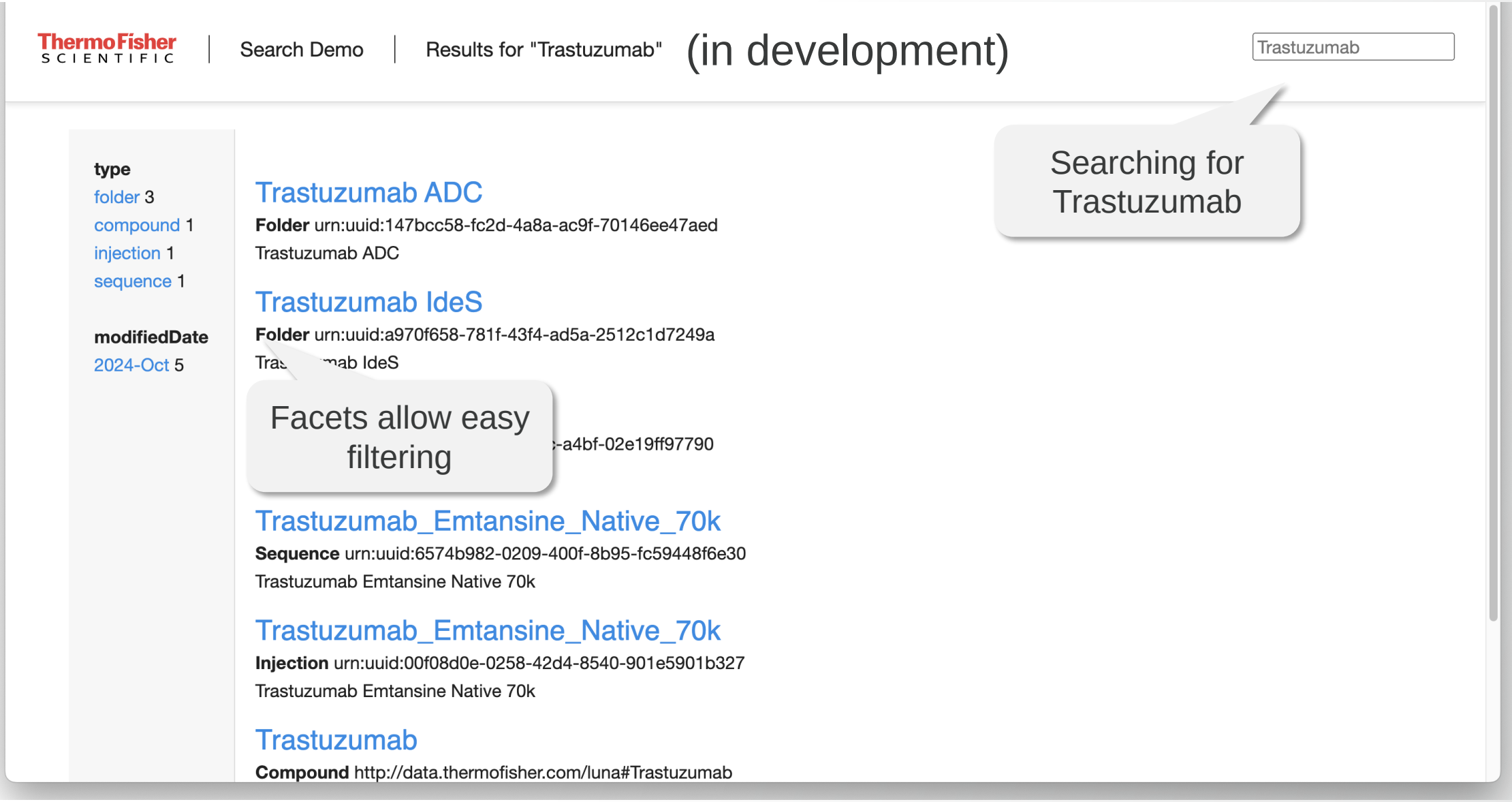
Data Catalog View

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

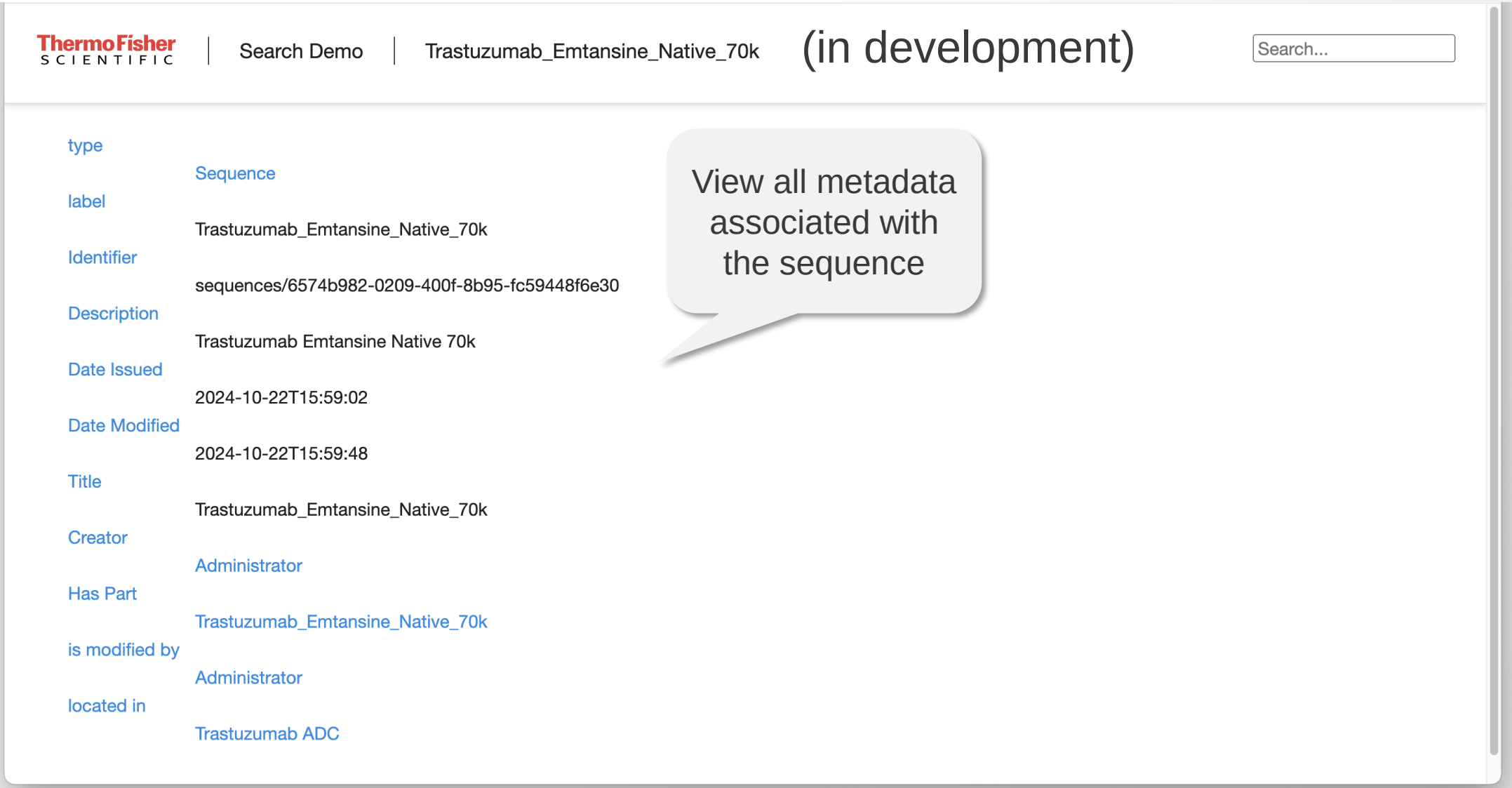
Knowledge Graph View

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

Data Catalog View

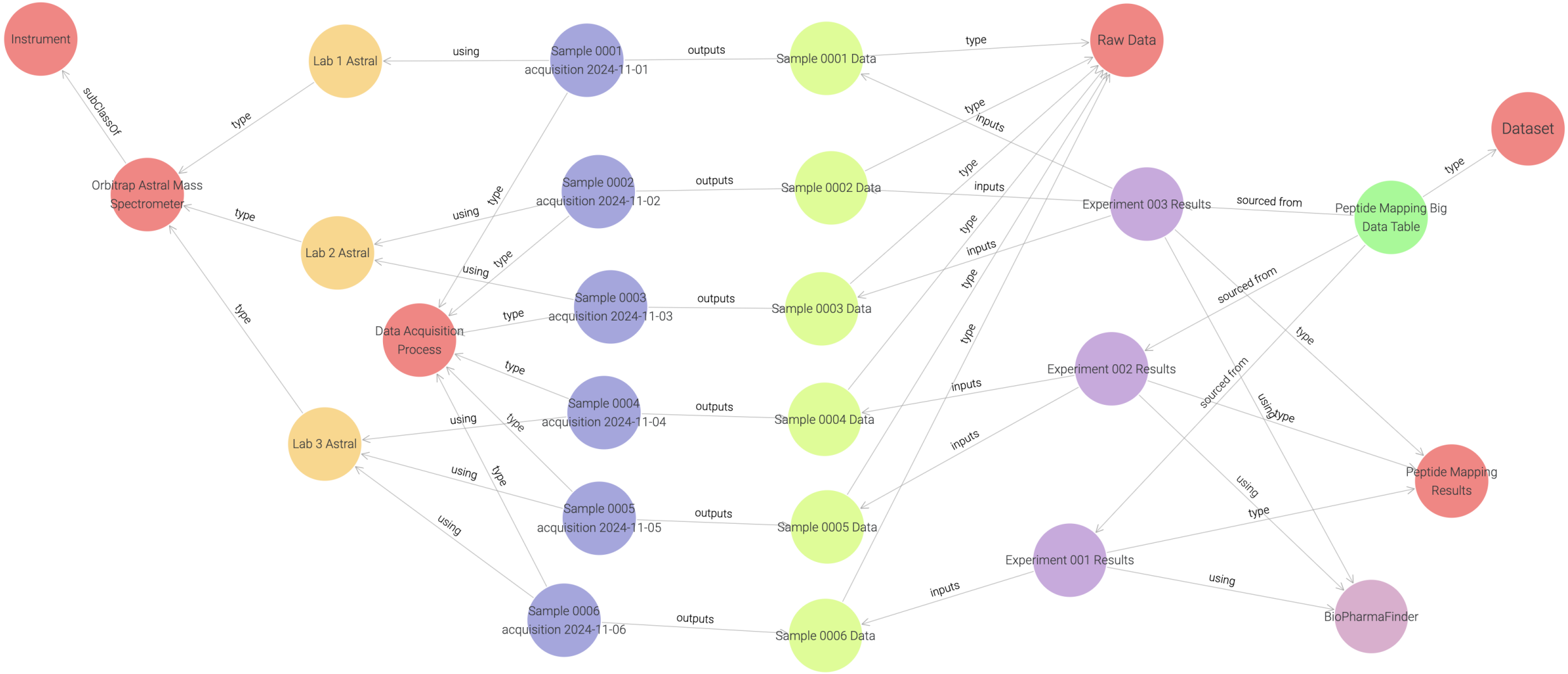


Data Catalog View



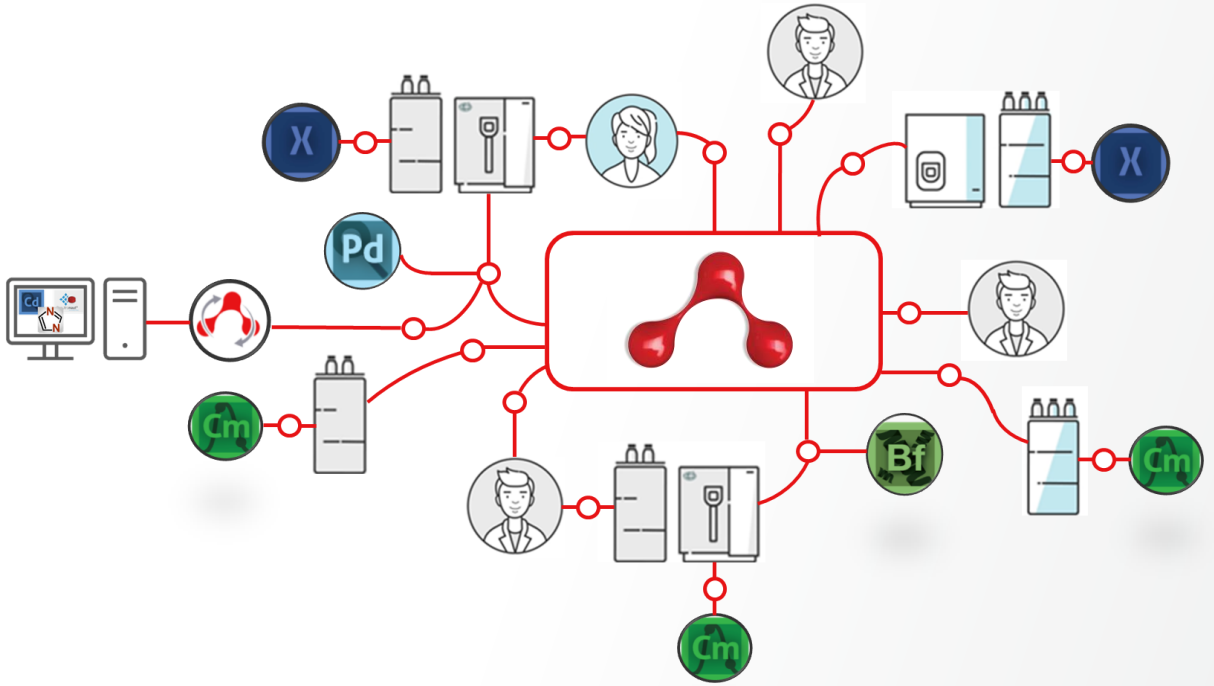
Knowledge Graph View

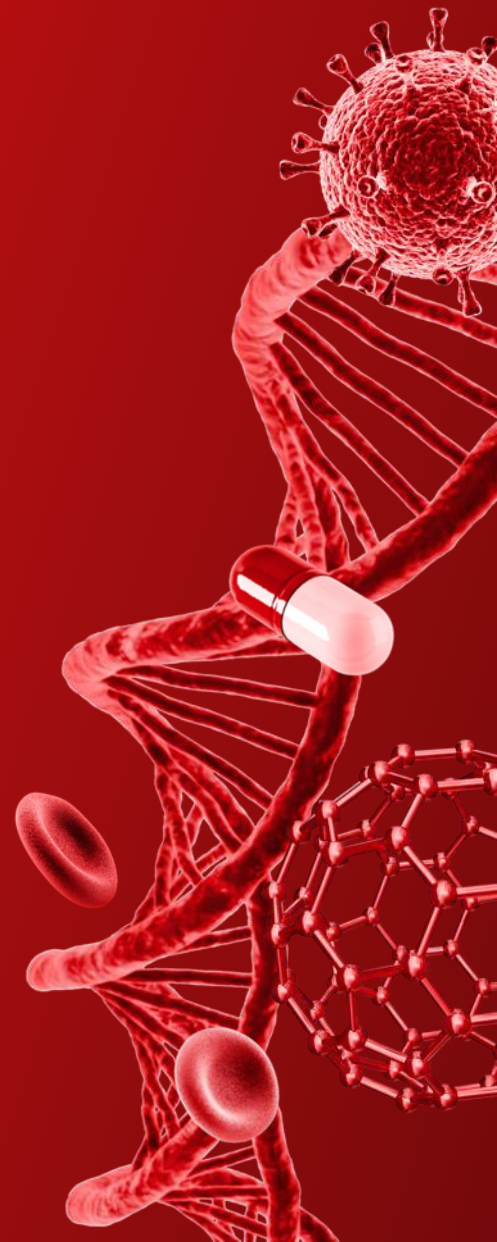
Visualize data context and connections



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