Technical Overview

Agilent OpenLab

Extract Deeper Insights from Your Chromatography Data

Data Accessibility Tool Expands the Power of Agilent OpenLab CDS

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Introduction

The Data Accessibility Tool (DAT) is a add-on tool for the OpenLab ecosystem designed to enhance the capabilities of OpenLab content management systems. The DAT extends the functionalities of OpenLab Server, ECM, and ECM XT by providing a direct Structured Query Language (SQL) interface for interactive exploration of OpenLab CDS chromatography data. The tool utilizes a relational schema tailored to the chromatography domain, making it user friendly for both lab and data scientists. The DAT is compatible with many commercial, open-source data visualization and analytics tools, providing users with choices to interactively explore and visualize their chromatography data. This technical overview presents the DAT, covering its components, deployments, and connectivity to data analytics tools.

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Data Accessibility Tool – An add-on tool for OpenLab CDS

Agilent OpenLab provides a selection of centralized data management solutions for cloud and on-premises storage of scientific data. Using these systems as a single source for laboratory data makes many processes more efficient by enabling centralized management of methods, signatures, and reports. Additionally, OpenLab Server, ECM, and ECM XT offer a full suite of technical controls to support data integrity and security needs to comply with various industry regulations.

The DAT is an addition to OpenLab, extending the OpenLab Server, ECM, and ECM XT capabilities, allowing for a comprehensive interactive exploration of OpenLab CDS chromatography results data. Specifically, key analytical results in addition to sample, instrument, and compound information are made available through the DAT. To enable this, the DAT provides a direct SQL interface to the chromatography data contained inside the centralized data repository. This interface makes the data searchable and allows any data visualization software to query the data interactively.

Figure 1 shows a schematic overview of the system architecture with the DAT. The tool consists of a set of OpenLab services and a database component. It is deployed on a separate machine on the same network as the central data storage. The DAT connects to the server and transforms the chromatography data into a relational database schema. This connection to the source system is one way and the data integrity of the source is always maintained. The synchronization service keeps the information current with the source data and can be scheduled to automatically update. Additionally, the synchronization can be configured to include specific projects or a specific data range for historical analyses.

The DAT is compatible with recent client/server configurations of OpenLab CDS as shown in table 1. OpenLab CDS gas and liquid chromatography (GC, LC) data, as well as GC and LC with mass spectrometry (GC/MSD, LC/MSD), are supported as of OpenLab CDS version 2.0.

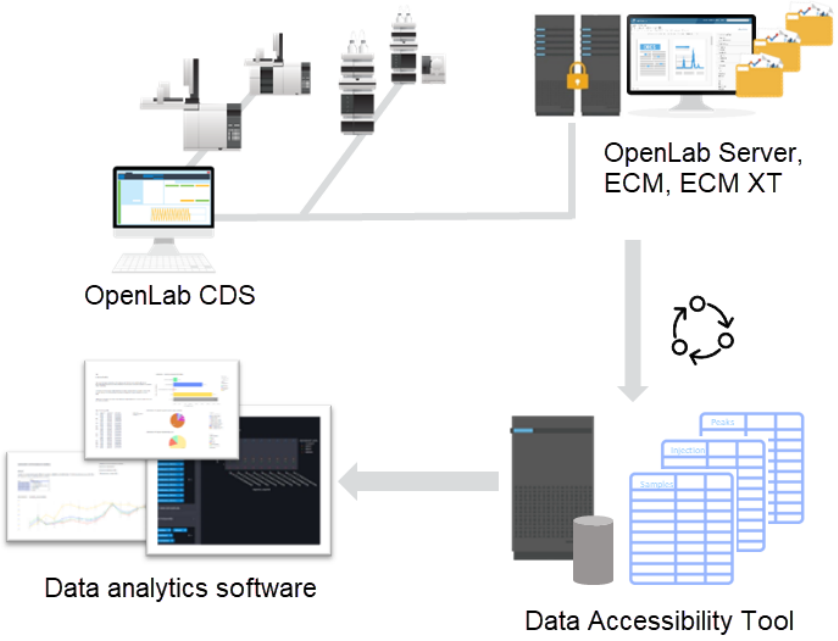

Figure 1. Overview of a OpenLab deployment with the DAT (from top-left clockwise): OpenLab CDS acquires data from a range of instruments and saves to OpenLab Server, ECM, and ECM XT. The DAT connects to the server and unfolds chromatography data into a relational database schema. Data analytics tools connect to the DAT database directly through the standard SQL interface.

Database - Relational schema for chromatography data

The DAT database is implemented in PostgreSQL and uses a relational schema tailored to the chromatography domain. The tables in the database model contain all relevant concepts in chromatography experiments such as samples, sequences, and injections. Table 2 lists the most important tables in the schema with a short description. In total, the schema contains 14 tables with over 200 columns that hold a wealth of information. The information ranges from high-level sample descriptions to details such as the detector serial number.

Table 1. DAT compatibility with server backend

OpenLab CDS version	Backend version
2.7	OpenLab Server and ECM XT 2.7*
2.8	OpenLab Server and ECM XT 2.8 OpenLab ECM 3.6 Update 7 and ECM Web Interface 3.10
3.0	OpenLab Server and ECM XT 2.8 Update 10 OpenLab ECM 3.6 Update 7 and ECM Web Interface 3.10

*OpenLab ECM/XT server 2.7 scalable topology not supported.

The database schema is modeled after the actual entities and relationships in a chromatography laboratory to make it intuitive for lab and data scientists alike. As an example, a query for all injections per instrument can be achieved by joining the “injections” table together with the “instruments” table. To extend such a query to compounds found in each injection, the “compounds” table can be used, and the desired columns selected.

To further enhance the usability of the DAT in a laboratory setting, the system gracefully handles multiple versions of data. In a typical chromatography experiment, a result might appear in multiple states. Immediately after sample data is acquired, an automatic processing is often applied. In the next step, a technician might review and further process the results to create a finished version. By default, the database will reliably return the most recent revision of a dataset and hide previous versions. This feature prevents duplication issues that are common to many other data export workflows and eliminates the need for time-consuming data reconciliation steps.

Connectivity – Data visualization tools

Data visualization and analytics tools can interface with the DAT database through a standard SQL interface. Both commercial and open-source data analysis packages usually include standard connectors for PostgreSQL by default. These connections make the system broadly compatible with many popular solutions such as Spotfire, Qlik, and Tableau. Table 3 shows a non-exhaustive list of data visualization tools known to work with the DAT.

Table 2. Common data analyis and visualization tools that work with the DAT database.

Category	Software Package
Commercial	Spotfire
	PowerBI
	Excel
	Qlik
	Tableau
Open source	Grafana
	Metabase
	Apache Superset

The standard SQL interface and broad compatibility with established data analytics tools allow users to choose their preferred tool and leverage existing expertise. Together with the intuitive schema of the database, this choice of tools helps to speed up the development of customized dashboards for the specific use-case.

To illustrate the ease of use in creating a dashboard from the DAT, Figure 2 gives an example of the few steps required to connect using Spotfire. The first step is to enter the details of the DAT server in the PostgreSQL adapter included in the software. After successful connection, the desired tables can be selected in the user interface and the data become available in the main interface. Lastly, filters, tables, and graphs can be dragged onto the canvas to create a rich interactive dashboard. This process applies similarly to the other data visualization tools mentioned in Table 2.

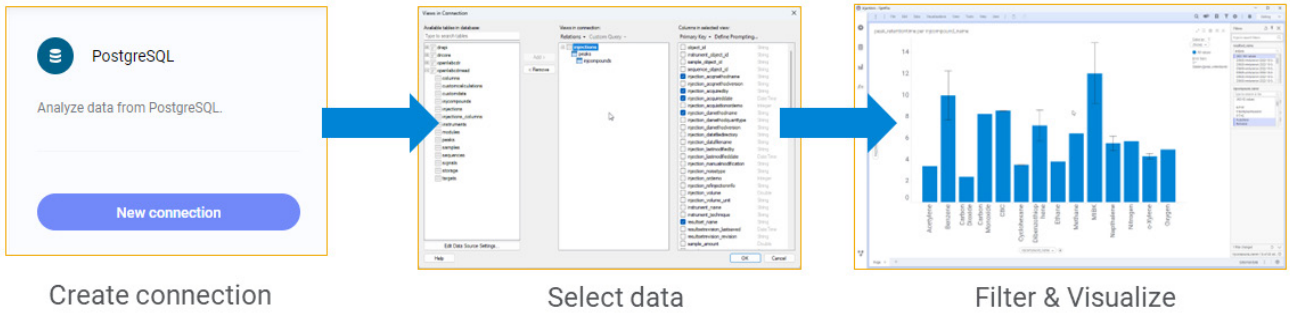

Figure 2. The DAT readily connects to commercial data visualization tools. Left to right the steps to connect to Spotfire: Connect to the DAT using a built-in connector for PostgreSQL. Select the tables of interest through the user interface. Drag and drop visualizations on the canvas and configure axis. The example shows a bar plot with average retention time per compound including standard deviations.

Summary

The Data Accessibility Tool (DAT) is a add-on for the OpenLab ecosystem. It provides a user-friendly SQL interface to the chromatography results data, extending the capabilities of Agilent OpenLab Server, ECM, and ECM XT. As shown with the example dashboard created in Spotfire, selecting data, and beginning a visualization can be achieved in a few easy steps. DAT is also compatible with a wide range of data tools allowing users to leverage their preferred visualization software to get faster results. In this way the DAT helps extract deeper insights from chromatography data, unlocking the full potential of your OpenLab system.

To learn more about the Data Accessibility Tool, visit:

https://www.agilent.com/en/product/software-informatics/chromatography-software/chromatography-add-on/data-accessibility-tool-for-openlab-cds

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