



Allotrope Foundation Quarterly Update 2025/03

Dear Allotrope Community,

We have continued our progress this quarter and improved or expanded the AFO and ASM with updates to share. Please note that access to links may require access to GitLab or other Allotrope Community resources. More details for access [here](#).

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Welcoming New Community Members

Gilead Sciences

We would like to welcome a new member to the Allotrope community – Gilead Sciences
<https://www.gilead.com/>

Gilead Sciences is a biopharmaceutical company that has pursued and achieved breakthroughs in medicine for more than three decades, with the goal of creating a healthier world for all people. The company is committed to advancing innovative medicines to prevent and treat life-threatening diseases, including HIV, liver diseases, cancer and inflammatory diseases.

Allotrope Foundation Ontology & Data Models (AFO/ASM)

Modeling teams have continued working to align with proposals to expand the domain coverage of the AFO and ASM. Easily access files located on Client Connect [here](#) and more granular technical details available on GitLab, <https://gitlab.com/allotrope>.

See www.allotrope.org/product-releases for a full and updated list of available models.

AFO Updates

Following the new and updated set of ASM released this quarter, a new AFO release is published. Please note that QUDT 1.0 is no longer merged into the Allotrope Merged Ontology Suite.

The Allotrope Merged Ontology Suite release is available on:

- BioPortal, the repository of biomedical ontologies published by the National Center for Biomedical Ontology at Stanford University: <https://bioportal.bioontology.org/ontologies/AFO>
- OLS4, the Ontology Lookup Service repository for biomedical ontologies published by the European Bioinformatics Institute: <https://www.ebi.ac.uk/ols4/ontologies/afo>
- Ontobee, Ontologies data server published by the University of Michigan Medical School: <https://ontobee.org/ontology/AFO> (Ontobee generates the AFO list of terms in an Excel spreadsheet as well as Tab Separated Values file)
- Client Connect: [here](#)
- Gitlab: <https://gitlab.com/allotrope/afo/-/tree/master/afo>
- Allotrope PURL sever: <http://purl.allotrope.org/> (listed under AFO>MERGED)
- JFrog Artifactory: <https://allotrope.jfrog.io/ui/repos/tree/General/AFO-release-public>
- Allotrope website: <https://www.allotrope.org/ontologies>



AFO Term Dictionary

Allotrope Term Dictionary is available in both .xlsx (Excel) and .csv (Comma Separated Values) format and can be downloaded from the

- Allotrope website at: <https://www.allotrope.org/ontologies>
- Client Connect: [here](#)
- JFrog Artifactory: <https://allotrope.allotrope.jfrog.io/ui/repos/tree/General/AFO-dictionary-release-public>

Allotrope Foundation Simple Models (ASM)

ASM Directory

ASM Directory for the applicable sample JSON and JSON Schema files per technique is available for convenient viewing of file content using a browser. The directory contains links to the latest sample files and embedded (i.e., standalone) schema for all ASMs in REC (Recommended) status. Please refer to the directory on the public repository: <https://gitlab.com/allotrope-public/asm/-/blob/main/README.md#allotrope-simple-model-directory>

Modularization

JSON Schemas allow for modularization and factoring out commonly used rules by utilizing references to other JSON schema files. The simple model schemas make use of this modular approach. The ASM Schema is defined using:

- Technique specific schema: a JSON Schema that contains the domain specific rules. It references the core declarations instead of each technique defining its own.
- Core schema: a JSON Schema that contains reusable, domain independent rules. The core schema defines value types for all possible values that may be used in tabular models.
- Other reusable schemas: Cube, Hierarchy, Manifest, Units, other future extensions

Having the basic rules factored out in a core and other schemas allows for later extensions without changing each technique specific schema. It ensures consistent writing and querying regardless of whether it's a single contained instrument or a modular stack with multiple detectors, pumps, or anything else. Motivation of the modular pattern is to drive consistent data structures across techniques, enabling data from different models to work seamlessly together.

ASM Updates

New and updated Allotrope Simple Models release this quarter are available on:

- Client Connect: [here](#)
- GitLab: <https://gitlab.com/allotrope/adm/-/tree/master/>
- JFrog Artifactory: <https://allotrope.jfrog.io/ui/repos/tree/General/ADM-release-public>

The current Release Notes is available on Client Connect: [here](#)

Here is the list of the new and updated set of ASMs released this quarter.*

ASM Model	Type	Maturity	Path
Binding Affinity Analyzer, SPR (Surface Plasmon Resonance)	Tabular	REC	New
Chrom updates to support Conductance detector module	Tabular	REC	Updates
Electronic Lab Notebook (ELN)	Tabular	REC	CR Upgrade
Flow Cytometry	Tabular	CR	New
Regression model (as part of the Common Hierarchy)	Tabular	CR	New
Mass Spec updates to support MALDI-TOF detector and ionization type terms (and example). Also supports Direct Injection	Tabular	REC	Updates

* To find out how to access the related model's artifacts on GitLab:

<https://gitlab.com/allotrope/adm/-/wikis/Summary-Table-of-the-Governed-ADM-and-ASM-Techniques-Artifacts>

ASM Training Materials and Working with the ASM

ASM training material is available on Allotrope public repository at the following locations:

- Brief introduction to ASM: <https://www.allotrope.org/allotrope-simple-model>
- ASM Primer: <https://gitlab.com/allotrope-public/asm-primer/-/wikis/home>
- ASM Jupyter Notebook Demo: <https://gitlab.com/allotrope-public/asm-jupyter-demo> It is a step-by-step example file for working with ASM files in a Jupyter Notebook. It was also tested with Google Colab.

ASM and ADM Modeling and Support

ASM related support tickets can be opened at the ADM project (<https://gitlab.com/allotrope/adm/-/issues>).

The Product Team can generate ADM specific artifacts (SHACL and its deployment using ADF) by request.

The latest updated set of ASM models is available on Gitlab. New and updated models will be released in conjunction with the release of new tabular models. Adopters can generate example results of tabularized data based on the JSON ASM format.

In cases where there is no tabular model for a chosen instrumentation type or technique, the product team is available to support the drafting of a new tabular model, and the Modeling Working Group is ready to review and govern drafted models.

Tooling, Testing, QA and Automation Pipeline

General Maintenance

- The ID Generator tool for generating sequential IDs in AFT & AFO IRIs went through a security vulnerability update <https://gitlab.com/allotrope-open-source/ontology-qa-tools/-/tree/master/artificial-id-generator>, <https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/265>

Further enhancements and automation of AFO QA

Further enhancements were made to the automated AFO QA tools using the CI pipelines:

- Fixing the AFO Dictionary to populate the Domain column: <https://gitlab.com/allotrope/afo/-/issues/1075>
- Refining regular expression for IRI checks. <https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/253>
- Updating QUDT entities without definition: <https://gitlab.com/allotrope/afo/-/issues/1029>

Further enhancements to the ASM and ADM automated QA using the CI pipelines

Further enhancements were made to the automated ASM and ADM QA tools using the CI pipelines:

- Add format checking to ASM <https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/232>
- Format validation in the ASM JSON files is done using Python JSON schema validation tool <https://python-jsonschema.readthedocs.io/en/latest/validate/#validating-formats>
- Checking the ASM manifests import existing AFO files: New checks to the manifest validator, JSON scripts, to ensure the existence of the referenced .ttl files from the AFO. AFO entities checks was added <https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/238>

We would like to thank Karin Colman from the PharmaLex engineering team for her dedication and commitment to improve the overall tooling, testing, QA and automation pipeline.

Working Group Updates

Please note that the working group meetings are recorded to improve access and transparency for those unable to attend or for members interested in staying informed.

To sign up for any working group, go to: www.allotrope.org/working-groups

Modeling: (Notes: [here](#))

The modularization efforts within ASM are actively progressing across various working groups. The Common Hierarchy Schemas act as a collection of reusables, "Lego-like" building blocks, enabling the consistent development of hierarchical structures across different models.

Initiated by Benchling, the working group was working on developing a Binding Affinity technique with Surface Plasmon Resonance (SPR) as the detection method. Binding affinity techniques are pivotal in



measuring the interaction strength between molecules, such as drugs, and their biological targets, such as proteins. This process is essential in drug discovery and development, as it helps evaluate the efficacy of drug candidates in binding to their targets, optimize their potency, and reduce potential side effects.

Initiated by Merck, the working group began developing a regression model as part of the common hierarchy schema to address a calibration use case. The model has been released at the Candidate Release (CR) maturity level.

Chromatography: (Notes: [here](#))

The Chromatography Working Group added a Conductance Detector schema (measured in siemens units). A conductance detector measures the ability of a solution to conduct an electrical current, which depends on the concentration of ionic species in the mobile phase. It is used in Ion Chromatography (IC) to detect and quantify ionic species in a sample.

Looking ahead, the group anticipates to work on several key areas, including Multi-Angle Light Scattering (Merck), Size Exclusion Chromatography (Merck), and Supercritical Fluid Chromatography (GSK).

Additional efforts may involve incorporating gradients, such as:

- Temperature Gradient: Controlled increases in column temperature during the separation process.
- Solvent Gradient: Gradual changes in the mobile phase composition over time during separation.

These developments aim to further refine and standardize chromatography models.

Mass Spectrometry: (Notes: [here](#))

This quarter, the team worked on updates to the general MS model to support MALDI-TOF detector, and ionization type terms. The team also worked on a draft for database search (the process of comparing acquired mass spectra against reference databases to identify unknown compounds, proteins, peptides, or microorganisms). The model supports Direct Injection as well.

The addition of ionization type terms to the ontology, addresses the lack of a well-structured ontological classification for ionization methods. Additionally, the team reviewed Lablicate's proposed draft for modeling MALDI-TOF (Matrix-Assisted Laser Desorption/Ionization Time of Flight), a mass spectrometry technique widely used for analyzing biomolecules such as proteins, peptides, DNA, and large organic molecules. A MALDI-TOF example was added.

Plate Reader: (Notes: [here](#))

Initiated by Merck, the working group started to work on a regression model as part of the common hierarchy schema which will be addressing a calibration use case. Merck provided an example of Plate Reader enzyme-linked immunosorbent assay (ELISA). A Plate Reader ELISA is commonly used in diagnostics, pharmaceutical research, food safety testing, and immunological studies due to its efficiency, accuracy, and scalability.



Flow Cytometry: (Notes: [here](#))

The team has reached a significant milestone in developing and releasing a tangible model for flow cytometry data, utilizing established standards such as FCS (Flow Cytometry Standard) and Gating-ML 2.0. Mapping of FCS Keywords to Allotrope Foundation Ontology (AFO) terms has been developed and reviewed.

The working group has been focused on resolving and aligning the ASM model by analyzing and applying example data from FlowJo and incorporating data regions to capture gating analysis.

ELN: (Notes: [here](#))

This quarter, the team was working to review and enhance the initial model use case: Archiving complete ELN entries to a data lake. Merck and ZONTAL provided the model designed to capture this data. The model, while highly generic with minimal semantic details, served as the foundation for developing model patterns.

The team reviewed the current CR model toward a REC release in Q1:

- Archiving complete ELN entries to a data lake.
- Proposed elements of generic field and value types (by ZONTAL)
- Representing material transformation, molecular structures, reactions, and formulations.

If you or a colleague are interested in contributing to this initiative, or if you are a subject matter expert (SME), please feel free to reach out to the Allotrope Product Team for more details and involvement opportunities.

Allotrope Framework Implementations Within and Outside the Allotrope Community

Sample Implementations with the Allotrope Framework

- **EPFL Swiss Cat+ and Agilent: Advancing a Fully Autonomous Laboratory with ASM**

The École Polytechnique Fédérale de Lausanne (EPFL) Swiss Cat+ has built a cutting-edge, data-driven infrastructure to accelerate catalyst discovery and optimization. In collaboration with Agilent Technologies, the initiative integrates Agilent instrumentation into the laboratory's planning architecture. This transformative project employs ASM as a standardized data format. Additionally, it drives innovation through the progressive development of robotic interfaces for scientific equipment, paving the way for a fully autonomous laboratory.

Learn more about the collaboration at [Link](#)

- **Merck Manufacturing Division (MMD) adopting ASM**

Merck Manufacturing Division (MMD) is working on a project utilizing the ASM as a standard across their instrument integration program

- **Scitara utilizes ASM with its DLX platform**

[Scitara](#) DLX platform supports three core functions: Connect, Automate, and Monitor in a single platform to support centralized management of all integrations and orchestrations across a diverse lab ecosystem. It eliminates manual transcription errors, ensures data integrity, and standardizes data collection and workflow practices for time and cost savings. Scitara can now implement FAIR Data Stream utilizing ASM.

- **Ganymede cloud-based data platform processes ASM**

[Ganymede](#) is a cloud-based data platform, engineered to streamline the capture and processing of data between lab instruments, ELN/LIMS/analytical applications. Ganymede can convert instrument data files into the Allotrope format using ASM mapper.

- **Lablicate OpenChrom plugins**

[Lablicate](#) implemented an ASM plugin for MALDI-TOF (Matrix-Assisted Laser Desorption/Ionization Time of Flight), an MS technique used primarily for the analysis of biomolecules like proteins, peptides, DNA, and large organic molecules.

Sample Open Source Implementations with ASM

- **Benchling Connect Platform:** [Benchling](#) is developing its platform for lab instrument connectivity and data management, Benchling Connect. It performs instrument data conversion to ASM. Benchling confronts industry-wide challenges with proliferation of proprietary instrument data models and vendor lock-in by mapping all instrument output to the Allotrope Simple Model (ASM) and making the converter codes open source and freely available on GitHub. The Python project is called Allotropy. For an up-to-date list of available instrument converters please refer to the following GitHub page: https://github.com/Benchling-Open-Source/allotropy/blob/main/SUPPORTED_INSTRUMENT_SOFTWARE.adoc
- **Lablicate OpenChrom plugins:** [Lablicate](#) is working on ASM plugins for its OpenChrom platform (a multivendor CDS platform with additional spectroscopy and molecular biology support). Plugins convert data to and from ASM.
- **ASM as a series of Validators:** [Ganymede](#) is a cloud-based data platform, engineered to streamline the capture and processing of data between lab instruments, ELN/LIMS/analytical applications. Ganymede can convert instrument data files into the Allotrope format using ASM mapper. Its SDK utilizes ASM as a series of validators built in the Pandera framework
- **chromeConverter - Open-Source R Tool for Chromatography Data Analysis:** chromeConverter is an open-source R tool (a language and environment for statistical computing and graphics)



designed to streamline the conversion of chromatography data into formats easily readable in R for advanced analysis. It features internal parsers written in R and bindings to external libraries, now including support for the Allotrope ASM format.

For more information, visit the [GitHub project site](#) or the [R Package Documentation README](#)

- **ASM Converters in Java:** [IFP Energies Nouvelles](#) (IFPEN), a French public research, innovation and training organization in the fields of energy, transport and the environment is developing a set of open-source converters to several ASM models and several instruments. The project is managed and developed by Maxime Visconte, Industrial and lab IT manager at IFPEN. More information can be found on [IFPEN's GitHub repository](#). A set of utilities, shared between all the ASM converters were pushed to the [Maven central repository](#). A presentation of this project is available on our YouTube channel: [here](#)

Allotrope Publications and Media

We have published 2-page summaries and updated the introductory presentation:

- **Allotrope Introductory Slide Deck:** can be downloaded from [here](#)
- **Allotrope Models & Domains:** can be downloaded from [here](#)
- **Allotrope Data Strategies:** can be downloaded from [here](#)

Allotrope YouTube Channel

Our YouTube channel has new a handle: <https://www.youtube.com/@allotropefoundation>. The Allotrope YouTube Channel hosts a technical playlist as well as the Allotrope Connect public presentations from 2017 and 2020 to the latest 2024 Fall Connect event.

The YouTube Channel videos are organized by playlists at:
<https://www.youtube.com/@allotropefoundation/playlists>.

Allotrope on LinkedIn

The Allotrope LinkedIn page is very active, with frequent updates and new posts. We encourage you to stay connected and follow us at: <https://www.linkedin.com/company/allotrope-foundation>

Allotrope Data Framework Onboarding Guide

The Allotrope Onboarding Guide wiki page was updated. Please refer to the following link: [Allotrope Data Framework Onboarding Guide](#)

Allotrope in the News

For the latest list of “Allotrope in the News”, please visit our website at:

<https://www.allotrope.org/allotrope-in-the-news>

Here is the listed recent news:

- Modularization in Allotrope Data Modeling: The "Building Blocks" Foundation for Scalable, Reusable, Interoperable, Extensible, and Maintainable Data Structures in Life Sciences, Pharma, and Chemical Labs: [Link](#)
- End-to-end FAIR instrument data with a cloud-based ASM data lake, showcased at Bio-IT World 2025: [Link1](#), [Link2](#)
- Digital evolution: Novo Nordisk’s shift to ontology-based data management: [Link1](#), [Link2](#)
- 5 ways to unlock IT productivity with the Benchling Developer Platform: [Link1](#), [Link2](#)
- The Importance of Connectivity and Data Model Standards: [Link1](#), [Link2](#)
- Elevating Digital Data Governance in Biopharma at 2025 ISPE Biotechnology Conference: [Link1](#), [Link2](#)
- Lab automation isn't keeping pace with AI advancement at DARPA: [Link1](#), [Link2](#)
- How ZONTAL is Shaping the Future of Scientific Data Management: [Link1](#), [Link2](#)
- Data harmonisation, standardisation across analytical instruments: [Link](#)
- New Data Standard on the Horizon: The Allotrope Simple Model: [Link](#)
- Data Normalization: Laying the Foundation for AI-Powered Drug and Material Discovery: [Link](#)
- Harmonizing Regression Data Across Analytical Instruments: [Link](#)
- The ASM plugin in OpenChrom is now available for free via the Lablicate marketplace: [Link1](#)
- Achieving AI Readiness in Scientific Research - A new white paper by ZONTAL: [Link1](#), [Link2](#)
- Harmonizing Analytical Data from Flow Cytometry: Ongoing Standardization by the Allotrope Flow Cytometry Working Group: [Link](#)
- The R&D Data Journey: Understanding Your Scientific Data’s Lifecycle: [Link1](#), [Link2](#), [Link3](#)
- Harmonizing Analytical Data from MALDI-TOF: Ongoing Standardization by the Allotrope Mass Spectrometry Working Group: [Link](#)
- ZONTAL at SLAS Event: [Link](#)
- Enhancing OpenChrom UI for Allotrope Foundation Files: [Link](#)
- 2024: ZONTAL Year in Review: [Link](#)
- Harmonizing Analytical Data from Binding Affinity Analyzers: Ongoing Standardization by the Allotrope Modeling Working Group: [Link](#)
- What are the Key Artifacts of ASM?: [Link](#)
- OpenChrom Supports MALDI-TOF Mass Spectrometry with ASM: [Link1](#), [Link2](#)
- chromConverter: Advancing Chromatography Data Science with ASM in R: [Link](#)
- Raman Spectroscopy ASM with OpenChrom: IUTA and Lablicate Project: [Link](#)
- ZONTAL Webinar: Supercharge your Chromatography Workflows with FAIR Data Use Cases: [Link1](#), [Link2](#), [Link3](#), [Link4](#)
- Improve Lab Productivity and Build a Foundation for AI-Powered Innovation; Standardization of Analytical Data: Best Practices: [Link1](#), [Link2](#), [Link3](#)
- Gen AI, digital twins, and data privacy: Assessing healthcare transformation trends and imperatives in 2025: [Link1](#), [Link2](#)

- Streamlining Analytical Method Validation for ICH Compliance and Standardized Data Integration: [Link](#)
- chromConverter: Open-Source R Tool for Chromatography Data Analysis: [Link1](#), [Link2](#)
- Merck to Present Its Use of ASM at Bio-IT World 2025: [Link1](#), [Link2](#)
- Agilent Roundtable Discussion at Analytica China: Exploring the Future of Digital Laboratories - Focusing on "Digitalization and Intelligence": [Link1](#), [Link2](#)
- EPFL Swiss Cat+ and Agilent: Advancing a Fully Autonomous Laboratory with ASM: [Link](#)
- Virscidian Supports Vendor-Neutral Solutions: [Link](#)
- Lab Instrument Integration to Knowledge Graph Development: Enabling Seamless Data Flow in Laboratory Spaces with Allotrope: [Link](#)
- Beyond ELN: Simplifying Experimental Data Through Standardization: [Link](#)
- From Electronic Documents to Executable Methods: USP's Digital Transformation Journey: [Link](#)
- Exploring Investigational New Drug (IND) Treatment: A Comprehensive Guide: [Link](#)
- Expert Voices: Why Aren't QC Labs Fully Automated Yet?: [Link1](#), [Link2](#)
- Vendor-Neutral Electronic Lab Notebook (ELN) Data Model Debuts in Allotrope Foundation's Q4 Release!: [Link](#)
- Optimizing Pharmaceutical Operations: A Deep Dive into an E2E Request-to-Result Workflow: [Link](#)
- Data collection and formats in drug discovery: [Link1](#), [Link2](#)
- From research to manufacturing: Overcoming data challenges in the drug development lifecycle: [Link](#)

AF Community and Events

End-to-End FAIR instrument data with a cloud-based ASM data lake, showcased at Bio-IT World 2025

A session titled 'Enabling Automated End-to-End Chromatographic Data Workflows and Accelerated Data Insights with the Allotrope Simple Model Vendor-Neutral Data Format' was presented at Bio-IT World 2025 on April 4, showcasing practical examples of how ASM is applied.

Learn more about the event at [Bio-IT World Conference & Expo](#)

Elevating Digital Data Governance in Biopharma at 2025 ISPE Biotechnology Conference

Digital data governance is key to Pharma 4.0, and Allotrope Foundation ontologies play a crucial role in ensuring data consistency, traceability, and usability. By structuring data at its source, Allotrope enables seamless integration, enhanced security, and smarter operations across biopharma.

This discussion will take place at the 2025 International Society for Pharmaceutical Engineering (ISPE) Biotechnology Conference (June 3, 2025 9:30-10:00 AM EST). More information at [Link](#)



Looking Forward

The Allotrope Product Team is looking forward to another productive 2nd quarter of 2025. We are looking to develop additional improvements to meet the evolving needs of our community.

Please contact us for any questions at product_team@allotrope.org.

Sincerely,

Allotrope Product Team