Allotrope Foundation Quarterly Update 2025/06

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.

Welcoming New Community Members

University of Amsterdam

We would like to welcome a new member to the Allotrope community – University of Amsterdam https://www.uva.nl/en - the Van 't Hoff Institute for Molecular Sciences (HIMS)

The University of Amsterdam is ambitious, creative and committed: a leader in international science and a partner in innovation, the UvA has been inspiring generations since 1632.

HIMS is a research institute within the University of Amsterdam with the mission to push the boundaries of chemistry by performing internationally recognized scientific research that is curiosity driven as well as application driven. HIMS strives at utilization and expansion of its knowledge and expertise by engaging in collaborative research efforts that address challenges in society and industry.

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. Easy access to the released artifacts is available from different resources, and they are detailed below. 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)
- FOCUS-SharePoint: Current (Release) Version
- 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

  The current Release Notes is available on FOCUS-SharePoint: Current (Release) Version

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
- FOCUS-SharePoint: Current (Release) Version
- JFrog Artifactory: https://allotrope.jfrog.io/ui/repos/tree/General/AFO-dictionary-release-public

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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 released this quarter are available on:

- FOCUS-SharePoint: Current (Release) Version
- 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 FOCUS-SharePoint: Current (Release) Version

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

ASM Model	Type	Maturity	Path
Plate Reder, Area Scan	Tabular	REC	New
Plate Reder, Fluorescence Polarization	Tabular	REC	Updates
Chrom updates to support Fluorescence detector module	Tabular	REC	Updates
Flow Cytometry	Tabular	REC	Promotion
Regression model (as part of the Common Hierarchy)	Tabular	REC	Promotion
Tandem MS	Tabular	REC	New

* 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.

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Tooling, Testing, QA and Automation Pipeline

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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

AFO errors cleanups (work in progress):
- Duplicate definitions in Working Drafts (WD): https://gitlab.com/allotrope/afo/-/issues/1087
- Semantic Error clean-ups to conform to Style-Guide: Vet new definition sources in Working Drafts (WD) https://gitlab.com/allotrope/afo/-/issues/637

We would like to thank Karin Colsman 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:** The recently developed Regression model schema as part of the Common Hierarchy designed to support calibration use cases, was promoted to a RECommended status

- **Chromatography:** Updates to support a Fluorescence detector. It is used to detect and quantify compounds that naturally fluoresce or can be chemically modified to fluoresce, offering high sensitivity and selectivity for trace-level analytes.

- **Electronic Lab Notebook:** The working group has begun work on Connecting Domains. Please see the "*Call to Action*" section on the monthly newsletter or here.

- **Flow Cytometry:** The recently developed Flow Cytometry model, was promoted to a RECommended status. It is an initial model for flow cytometry data, utilizing established standards such as FCS and Gating-ML 2.0.

- **Plate Reader:**

  o Updates to support an Area Scan detector. It is used to measure optical signals, such as absorbance, fluorescence, or luminescence, across multiple wells in microplates, enabling high-throughput analysis of biological or chemical samples.

  o Updates to support a Fluorescence polarization. It is used to measure molecular interactions and binding events in solution by detecting changes in the rotational motion of fluorescently labeled molecules.

- **Mass Spectrometry:**

- o Updates to support Tandem MS (initiated by Lablicate), an analytical technique that involves multiple stages of mass spectrometry to identify and quantify compounds by fragmenting selected ions and analyzing their product ions.
- o Additional work was done on Matching Database as part of the Common Hierarchy designed to identify database search (the process of comparing acquired mass spectra against reference databases to identify unknown compounds, proteins, peptides, or microorganisms).

Allotrope Framework Implementations Within and Outside the Allotrope Community

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Sample Implementations with the Allotrope Framework

- **Allotrope Simple Model for NMR Experiments with Mnova 16:** Mestrelab Research's Mnova 16, a multi-vendor analytical chemistry software suite designed for processing and analyzing data from various analytical techniques, now supports data exchange for NMR experiments in the Allotrope Simple Model (ASM) format—making it easier to integrate NMR results into standardized, interoperable scientific data ecosystems. Users can now both import and export NMR data in ASM format, enhancing compatibility with Allotrope-compliant systems and workflows. Learn more about Mnova 16 features: Link

- **Spectaris LADS Showcases Integration of OPC UA with Allotrope Standards:** Spectaris, Allotrope Foundation and the OPC Foundation are proud to announce a major milestone in smarter labs by advancing semantic interoperability and structured data standards in laboratory environments: At the most recent, and now 8th hackathon, which took place on April 11, 2025 in Germany and once again featured various companies, from device manufacturers, software providers to even laboratory operators, a successful demonstration showcased the integration of Allotrope Foundation Ontologies (AFO) and the Allotrope Simple Model (ASM) into the OPC UA (Unified Architecture) framework. Read the press release at EIN Presswire (Full PDF version)

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

- **LADS Showcase:** A collection of LADS-compliant OPC UA server implementations is now available on GitHub, demonstrating integration with Allotrope Foundation Ontologies (AFO) and the Allotrope Simple Model (ASM) across a range of laboratory device classes. Access the code on GitHub

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Allotrope Publications and Media

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

- **Allotrope Introductory Slide Deck**: can be downloaded from FOCUS-SharePoint: Overview Slides
- **Allotrope Models & Domains**: can be downloaded from FOCUS-SharePoint: Summary Documents
- **Allotrope Data Strategies**: can be downloaded from FOCUS-SharePoint: Summary Documents

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

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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:

- To what extent is big data relevant for electronic long-term archives in the pharma GLP laboratory?: Link1, Link2
- Fully automated Swiss Cat+ west hub laboratory at EPFL Chemistry: Link
- Are you ready to revolutionize your laboratory's data management?: Link
- Lab Sustainability: From Paperless Workflows to Energy-Wise Labs - Top Tips for Going Paperless in the Lab: Link1, Link2
- From Peaks to Patterns: AI's Transformation of Separation Science: Link1, Link2
- Sharing Is Caring—Especially in Drug Development: Link1, Link2
- Get Ready with Discovery Questions - 2025 July Allotrope® Connect Workshop: Link
- Shaping the Future of Analytical Labs @ HPLC 2025: Link
- Making chromatography smarter with integrated data platforms: Link
- OpenChrom Supports FAIR Data with ASM Export: Link1, Link2
- OpenChrom with ASM at HPLC 2025: Link
- 2025 July Allotrope® Connect Workshop - Join us in shaping the future!: Link
- Digital Transformation of the Analytical Lab – It's Mind Over Matter! at HPLC 2025: Link
- Networked laboratory: Seamlessly integrate data and communication data: Link

- Reproducibility issues in R&D due to poor data management - But it's not all doom and gloom!: [Link](#)
- Transforming and Automating Online Process Monitoring in BioPharma Manufacturing with Allotrope ASM and OPC UA: [Link](#)
- Lablicate Showcases Allotrope Standards-Based Data at the 2025 American Society for Mass Spectrometry (ASMS) Annual Conference: [Link](#)
- LADS Showcase – OPC UA Integration with Allotrope Standards: Now Available on GitHub: [Link](#)
- Allotrope at OPC Day International 2025: See the links ot the "Allotrope in the News" page
- Allotrope Simple Model for NMR Experiments - Now in Mnova 16: [Link1](#), [Link2](#), [Link3](#)
- Smarter Laboratories Need Smart Standards: [Link](#)
- Streamlining ASM Lab Instrument Data with Benchling Connect: [Link](#)
- Interoperability for the Lab — Built on Proven Standards at OPC Day 2025 International: [Link](#)
- Integration of AFO and ASM in OPC UA: [Link](#)
- LADS OPC UA and Allotrope Foundation: Enabling Seamless, Interoperable Laboratory-Data Infrastructures: [Link](#)
- Breakthrough in Smarter Labs: Spectaris LADS Showcases Integration of OPC UA with Allotrope Standards: [Link1](#), [Link2](#), [Link3](#), [Link4](#), [Link5](#)
- Driving Digital Transformation in BioPharma Manufacturing and Lab Automation: (LADS) OPC UA Exposing Allotrope Vendor-Neutral Data for BioPharma Manufacturing and Standardized Access in Automated Offline Labs: [Link1](#), [Link2](#)
- The Next-Generation Lab is Here (and in Action): LADS Live Demo of Allotrope Standards + OPC UA Integration: [Link](#)
- Where Are We on the Digital Road Map?: [Link1](#), [Link2](#)
- We need to build the data that chemistry deserves - here's how we can do it: [Link1](#), [Link2](#)
- Breaking Data Silos: [Link1](#), [Link2](#)
- Laboratory Automation in Pharmaceutical Research: Accelerating Innovation Through Data-Driven: [Link1](#), [Link2](#)
- The Citizen Data Science program at Dow: [Link1](#), [Link2](#)
- 2025 USP Convention Meeting: [Link](#)
- Shepherding your Data with the FAIRy ALCOA+: [Link1](#), [Link2](#)
- chromConverter 0.7.5 is available on CRAN: [Link1](#), [Link2](#), [Link3](#)
- The Pistoia Alliance's Methods Database Project: Instrument, Chromatographic Data System, and Vendor-agnostic Digital Transfer of Machine-readable High-Performance Liquid Chromatography-Ultraviolet Methods Using the Allotrope Data Format: [Link1](#), [Link2](#)
- Enhancing Research Data Management in Chemistry: A Collaborative Approach for Catalyzing Innovation in Germany and the Netherlands: [Link1](#), [Link2](#), [Link3](#)
- 2025/03 Allotrope Product Release is Out!: [Link1](#), [Link2](#)

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](#)

Read the post on [LinkedIn](#)

LADShack #8 Hackathon

At the "LADShack" #8 Hackathon—hosted this year at Infoteam Software in Germany—members of the Spectaris LADS community demonstrated the use of Allotrope products (AFO/ASM) as an Information Model within the OPC-UA framework. This milestone reflects ongoing progress in the alignment between Spectaris and Allotrope, built over several years of collaborative efforts.

LADShack [event page](#)

2025 USP Convention Meeting

Allotrope Foundation participated in the 2025 USP Convention Meeting on May 5-8, which gathered representatives from across the health and science ecosystem to shape the future of trust in medicines, dietary supplements, and food ingredients. Delegates played a key role in discussions and decision-making, including electing leadership and adopting resolutions to guide USP's direction for the next five years. More information at [Link](#)

Allotrope at OPC Day International 2025

LADS OPC UA and Allotrope Foundation: Enabling Seamless, Interoperable Laboratory-Data Infrastructures. (*Presented by Dr. Matthias Arnold, AixEngineers*)

Driving Digital Transformation in BioPharma Manufacturing and Lab Automation: (LADS) OPC UA Exposing Allotrope Vendor-Neutral Data for BioPharma Manufacturing and Standardized Access in Automated Offline Labs. (*Presented by Heiko Fessenmayer, R&D Lab Informatics System Architect at Agilent Technologies*)

More information at [OPC Day International 2025, Day 5, May 23](#)

Allotrope at the 2025 American Society for Mass Spectrometry (ASMS) Annual Conference

Lablicate showcases Allotrope standards-based data at the 2025 American Society for Mass Spectrometry (ASMS) Annual Conference. For more information, read the post on [LinkedIn](#)

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 took 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

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Looking Forward

The Allotrope Product Team is looking forward to another productive 3rd 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