



Allotrope Foundation Quarterly Update 2023/06

Dear Allotrope Community,

We have continued our progress this quarter and improved or expanded the AFO, ADM, ASM, and ADF further in the following areas 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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Allotrope Foundation Ontology & Data Models (AFO/ADM/ASM)

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

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

AFO Updates

Following the updated set of ADMs 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 Tools (Term Dictionary and New Term Submission)

Allotrope Term Dictionary: The tool 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](#)

AFO New Terms Submission Tool: This project provides the tools to enable simple (and friendly) new AFO term(s) submissions for governance independent of developing data models. To get started with the AFO New Term Submission, please refer to: <https://gitlab.com/allotrope/afo-new-term-submission>.

Allotrope Foundation Data Models (ADM/ASM)



ASM is Public

Last quarter, the foundation announced the public release of the Allotrope Simple Models. By making ASM available to the public, Allotrope Foundation seeks to enable wide-spread data standardization throughout the scientific community through adoption of this technology. To accommodate the public availability of the ASM artifacts and the training material, a new Allotrope public group was opened on Gitlab (<https://gitlab.com/allotrope-public>) and some of the related ASM projects were moved. For more information on how to access the ASM and licensing terms, please visit the Allotrope Foundation website at <https://www.allotrope.org/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 new location of the directory on the public repository: <https://gitlab.com/allotrope-public/asm/-/blob/main/README.md#allotrope-simple-model-directory>

ADM/ASM Updates

During this quarter, several models were updated to align with a modular structure across techniques. The updated models add a new technique specific parent, to ensure model consistency when writing and querying regardless of whether it's a single contained instrument or a modular stack with multiple detectors, pumps, or anything else. With the updated modular structure, we introduce technique specific parent document at a higher level (e.g., liquid chromatography document), where the measurement aggregate document as well as the device system document, which describes the instrument (e.g., chromatography stack or plate readers with a variety of different detectors attached at the same time) lives under that.

The Allotrope Data Models and Allotrope Simple Model suite release is 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 latest Tabular Model Template in Excel is available for download on GitLab: <https://gitlab.com/allotrope/adm/-/tree/develop/purl/template> or Client Connect: [here](#)

ADM Model Updates

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

ADM Model	Type	Maturity	Path	GitLab Links
Walkup LC/MS	Tabular	CR	New	Diagram Shape
Liquid Chromatography	Tabular	CR	REC to CR	Diagram Shape
Gas Chromatography	Tabular	CR	REC to CR	Diagram Shape

FPLC	Tabular	CR	REC to CR	Diagram Shape
Fluorescence	Tabular	CR	REC to CR	Diagram Shape
Luminescence	Tabular	CR	REC to CR	Diagram Shape
UV Absorbance	Tabular	CR	REC to CR	Diagram Shape
Hot Seal (Hot Tack)	Tabular	CR	REC to CR	Diagram Shape
Gloss	Tabular	CR	REC to CR	Diagram Shape
Tensile	Tabular	CR	REC to CR	Diagram Shape
Foam Height	Tabular	CR	REC to CR	Diagram Shape
Foam Qualification	Tabular	CR	REC to CR	Diagram Shape

ASM Model Updates

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

ASM Model	Type	Maturity	Path	GitLab Links
Walkup LC/MS	Tabular	CR	New	JSON schema Sample file
Liquid Chromatography	Tabular	CR	REC to CR	JSON schema Sample file
Gas Chromatography	Tabular	CR	REC to CR	JSON schema Sample file
FPLC	Tabular	CR	REC to CR	JSON schema Sample file
Fluorescence	Tabular	CR	REC to CR	JSON schema Sample file
Luminescence	Tabular	CR	REC to CR	JSON schema Sample file
UV Absorbance	Tabular	CR	REC to CR	JSON schema Sample file
Hot Seal (Hot Tack)	Tabular	CR	REC to CR	JSON schema Sample file
Gloss	Tabular	CR	REC to CR	JSON schema Sample file
Tensile	Tabular	CR	REC to CR	JSON schema Sample file
Foam Height	Tabular	CR	REC to CR	JSON schema



				Sample file
Foam Qualifications	Tabular	CR	REC to CR	JSON schema Sample file

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 Licensing

The ASM is collectively licensed under three licenses, depending on intended usage and membership status:

- a) If your use is non-commercial (e.g., academic research), the ASM is licensed under the [Creative Commons Attribution-NonCommercial 4.0 International](#) License (CC-BY-NC 4.0). This license does not permit commercial use but enables modification* of the ASM.
- b) If your use is commercial (e.g., to incorporate into or to support a commercial product or service), the ASM is licensed under the [Creative Commons Attribution-NoDerivatives 4.0 International](#) License (CC-BY-ND 4.0). This license permits commercial use, but restricts modifications to maintain the Allotrope standards.
- c) Alternatively, if you are a member of the Allotrope Foundation or the Allotrope Foundation Partner Network, the ASM is licensed under the Allotrope Commercial License available to members**. This license allows for commercial use and modification* of the ASM.

*Validation of modifications by Allotrope required to utilize ASM or Allotrope designation.

**<https://www.allotrope.org/membership-and-access-to-framework>

ASM Modeling and Support

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

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.

Allotrope Data Format (ADF):

ADF Library Version 1.5.6

As a further commitment to supporting and maintaining the ADF Library, the Product Team together with the HDF Group support team is working on library improvements toward the next ADF Library release version 1.5.6.

The ADF Library version 1.5.6 targeted release dates:

- A pre-release in Q3 2023
- A final release in Q4 2023

The planned improvements, progress, and resolutions for version 1.5.6 release can be viewed at the project milestone: <https://gitlab.com/allotrope/adf/-/milestones/14#tab-issues>

HDF Group is evaluating the effort of upgrading the ADF Library with the latest maintenance release of the HDF5 library 1.10.10 (released in April 2023). This version includes:

- Bug fixes (memory corruption, variable-length attributes etc.)
- Fixing CVEs (Common Vulnerabilities and Exposures)
- Performance improvements, particularly when working with many datasets.
- For more information, please refer to <https://www.hdfgroup.org/2023/04/release-of-hdf5-1-10-10-newsletter-192/>

We would like to thank Aleksandar Jelenak from the HDF Group engineering team for his dedication and support of the ADF Library.

General ADF Library Information

Latest ADF Library version 1.5.5RF is available for download via:

- Client Connect: [here](#)
- JFrog Artifactory:
 - Java Library: <https://allotrope.jfrog.io/ui/repos/tree/Properties/libs-release-internal>
 - C# Library: <https://allotrope.jfrog.io/ui/repos/tree/Properties/libs-release-internal-net>

Support tickets:

Support tickets can be viewed and opened at the ADF repo ([here](#)). Please select the “new bug” template to describe the issue and attach any supporting artifact.

Tooling, Testing, QA and Automation Pipeline

Updates to the AFO and ADM Pipeline and Tools

- New automation CI pipelines to package and deploy the AFO and ADM release packages as well as the ASM Dictionary (CSV and Excel versions) to JFrog Artifactory was developed and pre-tested.
- New automation CI pipelines to deploy the AFO and ADM to PURL were developed.
- A visual view of the updated AFO CI pipeline is available at: https://gitlab.com/allotrope/afo/-/ci/editor?branch_name=develop&tab=1
- A visual view of the updated ADM CI pipeline is available at: https://gitlab.com/allotrope/adm/-/ci/editor?branch_name=develop&tab=1
- New *csv2xlsx* utility was developed and added to the CI tools to allow the formatting and the filtering feature of the Excel version of the dictionary (written in Python <https://gitlab.com/allotrope/afo/-/blob/develop/ci/tools/csv2xlsx.py>).
- In order to enhance the ASM QA, a new tool *validate_json* was developed for “walking” through the PURL directory and loading the JSON files for validation (written in Python https://gitlab.com/allotrope/adm/-/blob/develop/ci/tools/validate_json.py). The tool is based on the Python package *jsonschema*. The tool includes an option to run only on the current version.
- In order to enhance the ADM QA, a new tool *validate_shacl* was developed for “walking” through the PURL directory and loading the TTL files for validation (written in Python https://gitlab.com/allotrope/adm/-/blob/develop/ci/tools/validate_shacl.py). The tool is based on the Python package *pySHACL*, and it is an alternative replacement to the Allotrope SHACL validator. The tool includes an option to run only on the current version.

Enhancing the ADM and ASM QA

ASM and ADM artifacts are now going through additional validations:

- Check all TTL files are valid (shapes/test/manifests).
- Check all JSON files are valid (JSON schemas (including core, units, embedded, reference)/test/manifest).
- Apply shsh checks to all shape files to confirm valid SHACL. (<https://www.w3.org/ns/shacl-shacl> , <https://www.w3.org/TR/shacl/#shacl-shacl>)
- Apply meta-schemas check to all JSON schemas to confirm valid schemas. <http://json-schema.org/specification.html#meta-schemas>. It will make sure the schema is valid as far as possible, but not that it makes sense or isn't illogical or impossible.
- Run validation of test TTL files against appropriate shape files (via reading of manifest entries to identify shapes and vocabularies to test against; dependent on AFO artifacts being available).
- Run validation of test JSON files against appropriate schema files (via reading of manifest entries to identify schemas to test against).

PURL Enhancements

PURL stability (CPU and Memory limits) was improved by enhancing the search PHP script.

We would like to thank Karin Colman from the OSTHUS 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 groups meetings are recorded to improve access and transparency for those unable to attend or for the folks that are just interested in what's going on. To sign up for any working group, go to: www.allotrope.org/working-groups

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

- The Plate Readers tabular models, and the original DOW initiated tabular models were updated to align with a modular structure across techniques.
- Some of the future models expected to be developed include:
 - Capillary Electrophoresis (initiated by Merck)
 - Multi-angle light scattering – MALS (initiated by Merck)
 - Liquid handlers (initiated by Benchling)

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

- GC, LC, and FPLC tabular models were updated to align with a modular structure across techniques.
- The Chromatography Working Group is expected to work on the development of a Chromatography Column model.

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

We would like to thank Graham McGibbon (ACD/Labs) for stepping forward and continuing to lead the MS working group.

- A new Walkup LC-MS model was developed.
- Future work may include the development of a new Tubular model (ASM/ADM) for Purity.

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>

Which challenges in the laboratory are solved with data standards?

Adesso Group (<https://www.adesso.de/en/index.jsp>), a large German IT service provider, published on June 2023 an article which discusses "Which challenges in the laboratory are solved with data standards?" It summarizes the principles to ensure data integrity and mentions the standardization work done by Allotrope.

The article is available at: <https://www. adesso.de/de/news/blog/welche-herausforderungen-im-labor-werden-mit-datenstandards-geloest.jsp>

Benchling Creates Open-Source Library of Lab Instrument Data Converters

SAN FRANCISCO, May 16, 2023 (Announced at the Bio-IT World Conference). Benchling partners with Allotrope, backing industry standards and making library of open source industry data converters freely available to the scientific community. Benchling is contributing to industry standards as an active member of the Allotrope Foundation Partner Network (APN) and is also creating a library of open source converters that format instrument-generated data to the Allotrope Simple Model (ASM) standard to help organizations to put these standards into practice.

The press release is available at: <https://www.benchling.com/news/benchling-open-source-library-lab-instrument-data-converters>

The LinkedIn post is available at: https://www.linkedin.com/posts/benchling_benchling-creates-open-source-library-of-activity-7064195283236048896-xdU6

An article on Scientific Computing World is available at: <https://www.scientific-computing.com/press-releases/elc-provider-creates-open-source-library-laboratory-instrument-data-converters>

An article on Laboratory Talk is available at: <https://laboratorytalk.com/article/2093440/lab-roundup-22-may-data-conversion-dna-synthesis-bbb-preeclampsia-testing-and-more>

A summary on BioIT World is available at: <https://www.bio-itworld.com/news/2023/05/24/dna-printing-bioengineered-kidney-constructs-in-space-revity-s-big-pharma-agreements-more>

Projects within the Allotrope Community

Instrument Data Converters to ASM (Open Source)

[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 instrument. 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: <https://github.com/ifpen>
- A set of utilities, shared between all the ASM converters were pushed to the Maven central repository: <https://central.sonatype.com/artifact/fr.ifpen.allotropeconverters/ASMUtils/1.0>
- A presentation of this project is available on our YouTube channel: [here](#)

Allotrope Publications

We have published 2-page summaries:

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

A step-by-step guide to a Tabular Model creation using Excel was written by the Product Team:

- **Tabular Model Creation with Excel:** is available for download from Client Connect within the Modeling WG folder: [here](#)
-

AF Community and Events

2023 Spring Allotrope Connect

During the three days of the informative 2023 Spring Allotrope Connect Workshop we had many presentations covering the following subjects:

- Welcome and short introduction to Allotrope Foundation and Technology (Corey Bakalarski, Allotrope Foundation)
- How open-source projects have been made possible by CC ASM (Maxime Visconte, IFPEN)
- Automatic Sample preparation (Diego Olivares Garcia, Novo Nordisk)
- LC-UV Methods and Results Interoperability using ADF (Azzedine Dabo, GSK)
- Automation: the new frontier for Allotrope? (Frederick Francois Chesneau, BASF)
- Accumulus FHIR Overview for the CMC data (Sheetal Gaiki, Johnson & Johnson, and Rita Algorri, Amgen)
- Advances in Data Utility through Application of Process & Reading Ontologies in BIOVIA ONE Lab (Kirsten Gesenberg, Biovia)
- From Chaos to Clarity: ZONTAL's Digital Solutions for Biotech Wizards! (Dennis Della Corte, Zontal)
- Accelerating Bio-Tech innovation through instrument data standards (Nick Floeck, Benchling)
- If your strategy depends on data, you need a strategic roadmap to deliver data worthy of the aspirations (Dana Vanderwall, DLC)
- SoftMax output results standardization (Mike McGorry, Johnson & Johnson)

The playlist of the first day of the 2023 Spring Allotrope Connect Workshop recordings is available on the Allotrope YouTube channel: [here](#)

A copy of the final agenda including the presentation abstract and the speakers bio is available: [here](#)



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 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 2023 Sprint Connect event. The YouTube Channel videos are organized by playlists at: <https://www.youtube.com/@allotropefoundation/playlists>.

Community Website

A reminder that the Allotrope Foundation Community website is an effort to improve and centralize the non-public knowledge and communication with the community. The GitLab-hosted website can be accessed <http://community.allotrope.org> Note this requires GitLab access.

Some of the pages to look for:

- Allotrope Foundation Data Models (ADMs):
https://community.allotrope.org/resources/reference/semantic/allotrope_data_models/
The page includes information about the structure of ADM repository under the section “ADMs artifacts repository”
- ADF Application Programming Interface (API):
<https://community.allotrope.org/resources/reference/adf/api/>
- [ADF Specification: https://docs.allotrope.org/](https://docs.allotrope.org/)
- Allotrope Framework Semantic Style Guide:
https://community.allotrope.org/resources/reference/semantic/style_guide/afo_style_guide/
- Allotrope Foundation Data Model and Ontology Governance Process:
https://community.allotrope.org/resources/reference/semantic/governance/afo_adm_governance_process/

If you would like access to GitLab, please fill out our onboarding questionnaire, [here](#) – It’s a Google Form. If your firewall denies access to Google drive links, please contact amnon.ptashek@allotrope.org.

Looking Forward

The Allotrope Product Team is looking forward to another productive quarter. 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