# Allotrope Foundation Quarterly Update 2024/03

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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## *Welcoming New Community Members*

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### *Gustavus Adolphus College*

We would like to welcome a new member to the APN – Gustavus Adolphus College

Dr. Dwight Stoll, from the Department of Chemistry at Gustavus Adolphus College is one of the authors of the HPLC Columns website, where he maintains the Column Selectivity Database.

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## *Allotrope Foundation Ontology & Data Models (AFO/ASM/ADM)*

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Modeling teams have continued working to align on proposals to expand the domain coverage of the AFO, ASM and ADM. 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 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 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

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### Allotrope Foundation Data Models (ASM/ADM)

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## 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

## 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.

## ADM/ASM Updates

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

### ASM and ADM Model Updates

Given the growing interest in implementation and usage of ASM (JSON Schema), the Product Team will be generating the ADM specific artifacts (SHACL and  its deployment using ADF)  by request in future releases.

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

| ASM Model | Type | Maturity | Path |
|---|---|---|---|
| Spectrophotometer | Tabular | REC | New |
| Multi Analyte profiling | Tabular | REC | New |
| Tensile test | Tabular | REC | Update |
| Stirring | Tabular | REC | Update |
| Temperature monitoring | Tabular | REC | Update |
| pH monitoring | Tabular | REC | Update |
| Pressure monitoring | Tabular | REC | Update |
| Liquid chromatography | Tabular | REC | Update |
| Gas chromatography | Tabular | REC | Update |
| FPLC | Tabular | REC | Update |

* 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 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.

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### Allotrope Data Format (ADF):

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## ADF Library Version 1.5.6 RF Released

The ADF Library version 1.5.6 RF was released at the middle of this quarter.

ADF Library version 1.5.6RF 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

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

- New feature was introduced with the ability to activate compression during Data Package import in order to minimize the ADF file size was added to the release: More details: Link
- Guidance on how to handle Japanese characters and Unicode characters in general in the file name path was added: More details: Link

- The ADF repository CI pipelines were cleaned up and improved.

## *ADF Library Version 1.5.7 Release Candidate*

The Product Team together with the HDF Group support team was working on library improvements toward the next ADF Library release version 1.5.7

ADF Library version 1.5.7RC (Release Candidate) is available for download via:

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

The improvements and resolutions for version 1.5.7 release can be viewed at the project milestone: [https://gitlab.com/allotrope/adf/-/milestones/15#tab-issues](https://gitlab.com/allotrope/adf/-/milestones/15#tab-issues)

- The HDF Group has updated its underline HDF5 binaries (libhdf5) to version 1.14.x supporting both amd64 and arm64. The 1.5.7 Release Candidate includes libhdf5-1.14.3 (the latest released version at present) and enables the support for MacOS with ARM64 architecture.
- This release candidate includes libhdf5-1.14.3 (the latest released version at present), built with:
  - Threadsafe
  - Zlib compression
  - Computer architectures:
    - Linux x86-64
    - Windows x86-64 and x86
    - macOS x86-64 and aarch64

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

## *ADF Library, Community Support & Maintenance*

The Allotrope Board has decided to support the ADF Library through a community model. The APN was informed about the Allotrope Board decision at the January 2024 APN teleconference.

Following the Allotrope Board decision, as of March 2024, support for the ADF Library will be done through a community model. It can include code contributions or special project funding to support or even enhance the ADF library.

Additionally, as an option, if at any time a subset of the Allotrope Community wishes to fund additional ADF work, the product team can reach out to the HDF group to get an estimate for that work and put an SOW in place.

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.

### Improving PURL (AFO server) stability

The DevOps team is working to improve PURL (AFO server) stability:

- Resolve Fuseki (SPARQL server) database disk space consumption with every update.
- Update Fuseki (SPARQL server) to latest version.
- Create server alerts using AWS Cloud Watch

### Further enhancements to the ADM/ASM automated QA tools using the CI pipelines

Further enhancements to the ADM/ASM automated QA tools using the CI pipelines were designed:

- Check the maturity levels of imports: A new Python tool was created to validate that REC won't import CR etc. https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/239
- Check ASM/ADM manifests import existing AFO files: New checks to the manifest validator, JSON scripts, to ensure the exitance of the referenced .ttl files from the AFO. https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/238
- Add format checking to ASM. https://gitlab.com/allotrope-open-source/allotrope-devops/-/issues/232. It validates formats in ASM JSON files using Python JSON schema validation tool https://python-jsonschema.readthedocs.io/en/latest/validate/#validating-formats

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.

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**Working Group Updates**

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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)

ASM modularization work continues across the different working groups. The Common Hierarchy Schemas is a collection of "Lego" like, reusable  building blocks to create consistent hierarchical structures across the different models.

- A new Spectrophotometer model was released (initiated by Benchling).  It models data from stand-alone UV-VIS-NIR spectrophotometers.
- A new Multi Analyte profiling model was released (initiated by Benchling). The model is intended to capture data from bead-based immunological assays and the associated analyzers. These assays and instruments are often referred to as 'Luminex' - the original company that developed the technique and/or 'xMAP' the brand name of the assay type.

- The team is working on new modular Documents/Schemas:
  - Regression model document
  - Error document
  - image document

## *Plate Reader: (Notes: here)*

As of this year, the Plate Reader WG  meets bi-weekly from 9am to 10am EST on Monday.

- The Plate Reader tabular models are updated to align with a modular structure across techniques. It allows multimode detection in a single run for several Plate Reader techniques such as: Absorbance, Luminescence, and Fluorescence.
- The team is working on Kinetic Data Cube (sample data is available on Client Connect here) for Kinetic reads (the reading or measurement of kinetic data in a plate reader). In plate readers, a kinetics read involves taking measurements at multiple time points to observe changes in a sample over time.
- In the previous quarter, a Well Plate Identifier to enable associating data with specific plate was established as well as alignment on Sample Group Identifier, Acquisition Mode and Plate Definition. Additional detection and acquisition modes and set backlog for inclusion were discussed.

## *Chromatography: (Notes: here)*

The Chromatography Working Group is working on the development of a new Chromatography Column model. The work extends the current Chromatography Column model in the general LC model. Support for the following external detectors was added (with data cube measuring units):

- Fluorescence
- Evaporative Light Scattering Detector (ELSD)
- Refractive Index Detector (RID)
- Radioisotope Flow Detector
- Polarimetry

The team is working on a new Substrate document and Stationary Phase document.

The working group was joined by Dr. Dwight Stoll from the Department of Chemistry at Gustavus Adolphus College. Dr. Dwight maintains the Column Selectivity Database
https://www.hplccolumns.org/about/index.php

## *Mass Spectrometry: (Notes: here)*

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

- Quantitation MS tabular model in progress. It is the quantitation of compounds (with generic reusable structure where possible) using MS.
- During this quarter, Agilent demonstrated a prototype of LC-MS for centroid data ASM.
- The team is analyzing the use of adducts in the LC-MS model.

- The team is looking for data for MS purity as well as getting more MS data and reports to further develop related models of interest (MS quantitation, Proteomics (e.g., peptide mapping), and other MS analyses).
- Few reported MS data files were shared by Genentech.
- Future work may include the development of a new Tubular model (ASM/ADM) for Purity.

## *Flow Cytometry: (Notes: here)*

The Flow Cytometry Working Group was established this quarter following the 2023 Fall Connect Workshop technical meetings. The WG meets bi-weekly from 11am to 12pm EST on Friday, and it is chaired by Joe Negri from Benchling. Community members are welcome to join.

The working group is discussing the scope of the initial model, and reuse of existing standards. Existing ones are Flow Cytometry specific, but they are not cross cutting techniques like ASM. A skeleton for an ASM Flow model was suggested and presented by Joe Negri from Benchling. Some of the members will provide sample Flow Cytometry data.

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### *Allotrope in the News*

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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:

- BASF Digital Solutions hosts the Allotrope Foundation's Allotrope Connect Spring 2024 event in Ludwigshafen, Germany: Link
- The Rise of the Allotrope Simple Model and Allotrope Foundation's Evolution: Link
- Pharmaceutical CMC process ontology Community of Interest Meeting: Link
- A lot is happening in terms of communication standardization and data formats next to the Rhine river in Germany this year!: Link
- Rise of the Allotrope Simple Model: update from 2023 Fall Allotrope Connect: Link
- Inside the Minds of SLAS Scientists: Bridging the Gap in Data Standardization: Link
- Delivering a Standards Based Framework that Enables the Lab of the Future: Interoperability & Connectivity: Link
- Allotropy: Python package for converting instrument data into ASM is on PyPI: Link
- Panel Discussion: Leaders in Biotech and Engineering: Link, YouTube
- 5 changes underway for R&D IT shifting to advanced modalities and biologics: Link
- Pharmaceutical CMC Process Ontology: Link
- Data Centricity: Key for the Successful Digital Journey towards a Digital Lab: Link

## *Sample of Projects with the Allotrope Framework*

- Lablicate Is working on Allotrope ASM/ADF plugin for OpenChrom:
    - Currently a prototype for demonstrated to the Working Group
    - qPCR, FT-IR, MS and GC-FID and HPLC-DAD in various stages of completeness
- Merck is populating a Knowledge Graph with ASM instance data. The project was first presented during the 2023 Spring Connect.
    - Merck is using the $asm.pattern Keyword within the ASM Schema to populate the Knowledge Graph and NOT using any ADM/SHACL/RDF equivalent.
- BASF demonstrated an ASM importer from GitLab
    - Internal microservice that searches for ASM models on Allotrope ADM GitLab repository. It lists the most current ones and delivers their schema on demand.

## *Instrument Data Converters to ASM (Open Source)*

- Benchling is growing its platform for lab instrument connectivity and data management, Benchling Connect. With Connect, 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.
    - Benchling's blog: https://www.benchling.com/blog/benchling-connect
    - "allotropy", open source, Python library repository on GitHub: https://github.com/Benchling-Open-Source/allotropy
    - "allotropy", Python package for converting instrument data into ASM is on PyPI: https://pypi.org/project/allotropy/

- 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

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### *Allotrope Publications*

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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

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### *AF Community and Events*

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#### *Spring 2024 Allotrope Connect*

The registration page for the Spring 2024 Allotrope Connect event is now live and can be accessed here!!

See the Allotrope website for more information 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 Fall 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/
- 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.

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## *Looking Forward*

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The Allotrope Product Team is looking forward to another productive 2nd quarter of 2024. 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