



# Allotrope Foundation Quarterly Update 2022/09

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)*

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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](http://www.allotrope.org/product-releases) for full list of available models was updated on September 30, 2022.

### *AFO Updates*

Following the new and updated set of ADMs released this quarter, a new AFO release is published.

The Allotrope Merged Ontology Suite release is available on:

- BioPortal, the repository of biomedical ontologies: <https://bioportal.bioontology.org/ontologies/AFO>
- Client Connect: [here](#)
- Gitlab: <https://gitlab.com/allotrope/afo/-/tree/master/afo>
- Allotrope PURL sever: <http://purl.allotrope.org/> (listed under AFO>MERRGED)
- 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 a 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>.

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

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### *New ASM Directory*

Following a community member request, a new ASM Directory for the applicable sample JSON and JSON Schema files per technique was setup for a 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: <https://gitlab.com/allotrope/asm-directory>



### ADM/ASM Updates

The Allotrope Data Models and Allotrope Simple Model Suite release is available with a restricted access to the community members 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 Tabular Model Template in Excel was reformatted, and the latest update is available for download on GitLab: <https://gitlab.com/allotrope/adm/-/tree/develop/purl/template> or Client Connect: [here](#)

### ADM Model Creation or Updates

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

ADM Model	Type	Maturity	Path	GitLab Links
FPLC	Tabular	REC	New	<a href="#">Diagram</a> <a href="#">Shape</a>
Gas Chromatography	Tabular	REC	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
Gloss	Tabular	CR	New	<a href="#">Diagram</a> <a href="#">Shape</a>
Hot Tack	Tabular	CR	New	<a href="#">Diagram</a> <a href="#">Shape</a>

### ASM Model Creation or Updates

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

ASM Model	Type	Maturity	Path	GitLab Links
FPLC	Tabular	REC	New	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Gas Chromatography	Tabular	REC	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Gloss	Tabular	CR	New	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Hot Tack	Tabular	CR	New	<a href="#">JSON schema</a> <a href="#">Sample file</a>

### ASM Training Materials and Working with the ASM

ASM training materials are available on GitLab at the following locations:

- Brief introduction to ASM: <https://www.allotrope.org/allotrope-simple-model>
- ASM Primer: <https://gitlab.com/allotrope/asm-primer/-/wikis/home>



- ASM Jupiter Notebook Demo: <https://gitlab.com/allotrope-open-source/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.

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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The HDF Group engineering team is supporting the ADF Library. The team is working on further maintenance of the ADF Library, which will be released later this year with the minor version of 1.5.5.

#### *A pre-release version of ADF Library 1.5.5RC1 is available*

A pre-release version of ADF Java Library 1.5.5 (both Java and .Net) is available for testing purposes. It aims to fix the following ADF issues:

- [Issue #43](#): Handle the support for xsd:dateTimeStamp (Jena version 2 limitation) and
- [Issue #8](#): Fix the DataCube API qb.order property.
- [Issue #127](#): Support for pre-release ADF packages in C# build and test pipeline jobs

ADF Library version 1.5.5RC1 is available for download via:

- JFrog Artifactory:
  - Java Library (1.5.5-rc.1): <https://allotrope.jfrog.io/ui/repos/tree/Properties/libs-release-internal>
  - C# Library (1.5.5-rc1): <https://allotrope.jfrog.io/ui/repos/tree/Properties/libs-release-internal-net>

Support tickets can be opened at the ADF repo (<https://gitlab.com/allotrope/adf/-/issues>). Please select the “new bug” template to describe the issue and attach any supporting artifact.

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### *Tooling, Testing, QA and Automation Pipeline*

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### *Updates to the AFO and ADM Pipeline and Tools*

During this quarter, we continued with the efforts to improve the quality of our AFO development lifecycle

- The AFO GitLab merge-release job pipelines was rewritten to be more flexible on the ontology merger and inference. This also involved some refactoring of the catalog names to remove some hard-coding from the Python script.
- A SPARQL query to support the BioPortal labels was added

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.

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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](http://www.allotrope.org/working-groups)

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

- The team was working with DOW SMEs on new models and some updates:
  - Hot Tack: A test to determine the strength of a heat seal, while it is still hot
  - Gloss: Measuring the specular reflection (gloss) of a surface
- The team was working with Merck SME on new models:
  - FPLC tabular model

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

- The Gas Chromatography tabular model (modeled with ASM and ADM) was updated
- The WG is evaluating modeling options for future release such as results reproducibility, instrument logbook and activity log
- SMEs can be included in the Bi-Weekly (Monday) Chrom WG invite by contacting the Product Team.

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

We would like to thank Graham McGibbon and Adam Kimball for stepping forward and continue to lead the MS working group.

- The team were evaluating on Mass Spectrometry calibration vs quantitation and analyzed quantitation reports.

#### *Semantic: (Notes: [here](#))*

- Continued discussions related to improving design and functionality.



- The working group discussed the AFO alignment with the OBO Foundry

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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>

*Digitalization of paper-based processes against standardized ontologies: Project digitizes sharing of data to support machine learning and boost cyber resilience*

A new article was published in the R&D World Magazine (<https://www.rdworldonline.com/>) on June 2022: "The Pistoia Alliance is announcing that it has successfully completed a proof of concept (PoC) on the digital transfer via cloud of analytical High Performance Liquid Chromatography (HPLC) methods, proving it is possible to move analytical methods securely between two different vendors and Chromatography Data Systems (CDS) vendors with ease...The Pistoia Alliance collaborated with the Allotrope Foundation, using the Allotrope Framework technology stack to ensure interoperability." The article is available at <https://www.rdworldonline.com/pistoia-alliance-project-digitizes-sharing-of-analytical-methods-data-to-support-machine-learning-and-boost-cyber-resilience/>

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### *Allotrope Publications*

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This quarter we have published new 2-page summaries:

- **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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*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*

The Allotrope YouTube Channel hosts the Allotrope Connect public presentations from 2020 to the latest spring 2022 Connect event (some previous event presentations are available as well). The YouTube Channel is available [here](#) and organized by playlists [here](#).



## 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/](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/](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/](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](mailto:amnon.ptashek@allotrope.org).

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## Looking Forward

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The Allotrope Product Team is looking forward to another very productive quarter and to develop additional improvements to meet the evolving needs of our community.

Please contact us for any questions at [product\\_team@allotrope.org](mailto:product_team@allotrope.org).

Sincerely,

Allotrope Product Team