



# Allotrope Foundation Quarterly Update 2022/12

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 and Returning Community Members*

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### *BASF*

We would like to welcome a new trial Allotrope Foundation member – BASF

<https://www.basf.com/us/en.html> . BASF Corporation, headquartered in Florham Park, New Jersey, is the North American affiliate of BASF SE, Ludwigshafen, Germany.

BASF is a leading brand in the chemical industry, with a corporate purpose – to create chemistry for a sustainable future.

### *Benchling*

We would like to welcome the back to the APN – Benchling <https://www.benchling.com/> . Benchling's mission is to unlock the power of biotechnology by creating scientifically aware technology that connects R&D data, teams, and processes, all in one place for better data management, improved collaboration, and real-time insights.

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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 December 14, 2022.

### *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: <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 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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### *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: <https://gitlab.com/allotrope/asm-directory>

### *ADM/ASM Updates*

During this quarter the Modeling Working Group together with SMEs support from Dow, was working on the development of:

- New statistic datum pattern for statistical quantity values
- Model alignment on standardized hierarchy for aggregate models

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 Updates*

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

ADM Model	Type	Maturity	Path	GitLab Links
UV Absorbance	Tabular	CR	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
Liquid Chromatography	Tabular	CR	Update	<a href="#">Diagram</a>

				<a href="#">Shape</a>
Gas Chromatography	Tabular	CR	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
FPLC	Tabular	CR	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
Foam Height	Tabular	REC	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
Tensile Test	Tabular	REC	Update	<a href="#">Diagram</a> <a href="#">Shape</a>
Foam Qualification	Tabular	REC	Promoted (CR to REC)	<a href="#">Diagram</a> <a href="#">Shape</a>
Gloss	Tabular	REC	Promoted (CR to REC)	<a href="#">Diagram</a> <a href="#">Shape</a>
Hot Tack	Tabular	REC	Promoted (CR to REC)	<a href="#">Diagram</a> <a href="#">Shape</a>

### *ASM Model Updates*

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

ASM Model	Type	Maturity	Path	GitLab Links
UV Absorbance	Tabular	CR	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Liquid Chromatography	Tabular	CR	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Gas Chromatography	Tabular	CR	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
FPLC	Tabular	CR	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Foam Height	Tabular	REC	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Tensile Test	Tabular	REC	Update	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Foam Qualification	Tabular	REC	Promoted (CR to REC)	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Gloss	Tabular	REC	Promoted (CR to REC)	<a href="#">JSON schema</a> <a href="#">Sample file</a>
Hot Tack	Tabular	REC	Promoted (CR to REC)	<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. The next version is anticipated to be released early next year in order to solve version compatibility problems of ADF Library version 1.5.4 and above with previous versions of the library following some of the latest fixed issues.

The ADF Library 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 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 pipeline was rewritten and tested successfully 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 property labels was added and tested successfully



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 the new structures for hierarchical aggregation patterns of laboratory test models.
- In addition, the team was working on the development of a new approach for modeling statistical features. An overview of representing statistical parameters in a Tabular Model was presented by Ben during the 2022 Fall Allotrope Connect and can be viewed on the Allotrope YouTube channel at [here](#)
- As a result of the new structures for hierarchical aggregation and the statistical pattern, some of the models were updated. FPLC, GC, LC, UV Absorbance, Foam Height, and Tensile Test were updated with latest statistical and hierarchy aggregation patterns. Foam Qualification, Gloss, and Hot Tack aligned as above and were promoted from CR to REC

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

- GC and LC, tabular models were updated with the latest statistics and hierarchy aggregation patterns.

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

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

The team made progress with Quantitation MS tabular model:

- Quantitation of compounds (with generic reusable structure where possible) using MS
- Relying to on partner supplied example data

#### *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>

#### *Lab Interoperability with DLX using ASM-JSON Format*

A new whitepaper written by Daniel DeAlmeida, Scitara’s Head of Product Management, was published on November 2022. The paper discusses the language of automated science. It provides the advantages of using Scitara DLX’s ability to provide data mobility and transform data in flight in combination with the Allotrope’s ASM for the structure of instrument data. By using this mechanism, result data can be automatically standardized before storage in data lakes without need of further interpretation.

The paper is available at: <https://scitara.com/allotrope/>

#### *Open-Source Chromatographic Data Analysis for Reaction Optimization and Screening*

A new project paper was published in ChemRxiv (<https://chemrxiv.org/>). The paper named "Open-Source Chromatographic Data Analysis for Reaction Optimization and Screening", presents an open-source Python project called MOCCA (Multivariate Online Contextual Chromatographic Analysis) for the analysis of open-format HPLC–DAD (photodiode array detector) raw data.

The project includes the use of the Allotrope Framework as well as a Python library that was developed by the HDF5 Group and named h5ld (It enables to read the ADF file Data Description using Python <https://github.com/HDFGroup/h5ld>).

The paper is available at: [here](#)

MOCCA documentation is available at: <https://mocca.readthedocs.io>

The project was supported by Bayer life science collaboration program and by the DARPA accelerated molecular discovery program.

#### *Trends and Developments in Data Handling 2022: Key trends and developments in data handling according to selected panelists from the chromatography sector*

A selected group of panelists from the chromatography sector answers a set of questions on [The Column](#), on October 2022 and discusses: "Trends and Developments in Data Handling 2022." The panel answers questions on data management and handling solutions for chromatographers, as well as the importance of recent developments in “Big Data” and others. Allotrope Foundation is referenced as an initiative to address some of the challenges.

The discussion is available at: [here](#)

#### *Text-to-Ontology mapping via natural language processing models: Attempts to solve text-to-ontology mapping challenges*

A new research paper was published in the CEUR-WS.org (<http://ceur-ws.org/>) which is an online publication service for editors of scientific proceedings, on September 2022: "Text-to-Ontology Mapping via Natural Language Processing Models." The paper presents the work in attempting to solve text-to-



ontology mapping challenges and mentions the Allotrope Foundation Ontology as one of the ontologies that were used during the experiments. The paper is available at: <http://ceur-ws.org/Vol-3226/paper3.pdf>

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### *Allotrope Publications*

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We have published new 2-page summaries:

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

A new 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](#)

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### *AF Community and Events*

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#### *2022 Fall Allotrope Connect*

During the two days of the informative 2022 Fall Allotrope Connect Workshop we had nine presentations covering the following subjects:

- ASM at Scale at Merck & Co, Inc (Merck/Tetra Science)
- Modeling Working Group Update: Models, Statistical Features, Aggregation Patterns, and Converter Implementation (Dow/Allotrope Product Team)
- Allotrope Modelling Domains: Potential opportunities for future expansion (Allotrope Product Team)
- Multivariate Online Contextual Chromatographic Analysis (MOCCA) via ADF data access (Bayer/MIT)
- You have FAIRified your data. Now what? (Zontal)
- Keynote by Dr. Matthias Arnold: LADS OPC UA – The “Common Language” for Lab & Analytical Devices (LADS/Spectaris )
- Lab Interoperability with DLX Using ASM-JSON Format (Scitara)
- The Methods Database: From vision to execution (Pistoia/GSK/Merck)
- Leveraging Allotrope to achieve open-data compliance (IFPEN)

The playlist of 2022 Fall Allotrope Connect Workshop recordings is available on the Allotrope YouTube channel: [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*

The Allotrope YouTube Channel hosts the Allotrope Connect public presentations from 2020 to the latest 2022 Fall 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/>
- 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 year of 2023. 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](mailto:product_team@allotrope.org).

Sincerely,

Allotrope Product Team