



Allotrope Foundation Quarterly Update 2022/06

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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Welcoming New Community Members

AgileISR

We would like to welcome AgileISR <http://agileisr.com/>. Here is Steve Hamby from Agile ISR introduction message to the community: “AgileISR brings 20+ years' experience in data and ontology governance to assist Allotrope member organizations in implementing Allotrope ontologies and data models and enhance the trust and usability of the resulting knowledge.”

Steve Hamby serves as the primary business and technical PoC contact (steve.hamby@agileisr.com) and Gabriel Aviles (gabriel.aviles@agileisr.com) serves as an additional technical PoC contact.

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 full list of available models was updated on June 30, 2022.

AFO Updates

Following the updates that were issued to set of ADMs, a new AFO release is published this quarter

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>

New AFO Tools (Term Dictionary and New Term Submission)

Following requests coming from community members, the following new tools were introduced during this quarter:

Allotrope Term Dictionary

We would like to thank John Hollerton from GSK for initiating this project and tool.

Some community applications of AFO may only require simple term/definition look-ups by scientists and non-ontologists who seek the simplest representation of terms for their domain of interest. Those users

may not have access to open source or COTS ontology tools. To address this request, a simplified “dictionary” for term search by anyone was developed. It is a simple alternative to navigating public ontology lookup services which contain a lot more information than needed for some personas. 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. It aims to address members of the community who would like to work with ontologies only or those who need to add a few terms to the ontology and are not yet developing a model. The tool integrates several subsystems and automates the submission with GitLab service desk and Issues notification emails, as well as Google Forms, Sheets, and Apps Script. To get started with the AFO New Term Submission, please refer to: <https://gitlab.com/allotrope/afo-new-term-submission>.

AFO is Available on AberOWL

The latest AFO version was picked up by AberOWL and users can browse it at <http://aber-owl.net/ontology/AFO/#/>. REST API queries to the AFO can be implemented using the AberOWL server. Swagger documentation and testing is available at <http://aber-owl.net/docs/>

AberOWL was jointly developed by researchers from [University of Cambridge](#) (An APN member), [University of Birmingham](#), and [KAUST BORG](#). AberOWL is a framework for ontology-based access to biological data. It consists of a repository of bio-ontologies; a set of webservice which provide access to OWL reasoning over the ontologies, and several frontends which utilize the ontology repository and reasoning services to provide access to specific biological datasets (<http://aber-owl.net/about/>).

Allotrope Foundation Data Models (ADM/ASM)

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

Several updates were issued to set of ADMs following a bug fixing effort. Here is the list of the new set of ADMs released in this quarter.

ADM Model	Type	Maturity	Path	GitLab Links
Mass spectrometry	Tabular	REC	New	Diagram Shape
Gas chromatography	Tabular	REC	New	Diagram Shape
Foam height	Tabular	REC	New	Diagram Shape
FOAM Qualification	Tabular	CR	New	Diagram Shape
Code Reader	Tabular	REC	New	Diagram Shape

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
Mass spectrometry	Tabular	REC	New	JSON schema Sample file
Gas chromatography	Tabular	REC	New	JSON schema Sample file
Foam height	Tabular	REC	New	JSON schema Sample file
FOAM Qualification	Tabular	CR	New	JSON schema Sample file
Code Reader	Tabular	REC	New	JSON schema Sample file

New and Updated ASM Training Materials and Working with the ASM

New and updates 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.

Allotrope Data Format (ADF):

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

First pre-release version of ADF Java Library 1.5.5 is available

The first pre-release version of ADF Java Library 1.5.5 is available for testing purposes. It aims to handle the support for xsd:dateTimeStamp (Jena version 2 limitation)

A dev version labeled "1.5.5-dev.1" was uploaded to jFrog Artifactory. It is available at <https://allotrope.jfrog.io/ui/repos/tree/General/libs-release-internal/org/allotrope>.

In addition, the CI pipeline configuration was extended to allow Artifactory uploads when either not a release or a snapshot release, and the Artifactory upload maven plugin was updated.

Python package for reading the Data Description (HDF5 Linked Data Support for ADF)

Last year Aleksandar Jelenak from the HDF Group, developed a Python package for reading the Data Description layer of the ADF file. The Python package provides readers for HDF5-based formats with such metadata that is stored in an RDF Linked Data structure. The entire Data Description content is read in one operation and made available as an [rdflib](#) graph object. The package was recently used successfully by one of the Allotrope members and is available on GitHub at: <https://github.com/HDFGroup/h5ld>

Tooling, Testing, QA and Automation Pipeline

Updates to the AFO and ADM Pipeline and Tools

Issues with limits on utilizing the Docker images for the pipeline were resolved with an authenticated Docker Hub account. For more information, please refer to: <https://gitlab.com/allotrope-internal/purl.allotrope.org/-/wikis/home#authenticating-with-docker-hub>

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 team was working with Dow SMEs on new models:
 - Foam Height testing is one of the measurements to test foaming behavior. The test is using image processing techniques.
 - Foam Qualification test measures the rise process of polyol (<https://en.wikipedia.org/wiki/Polyol>) in foam formulations.
- The team was working with Novo Nordisk SME on new models as it relates to Lab Automation. The first one is the Bar Code Scan reader.
- The working group is anticipating a new set of tabular models during the next quarter including few models in the domain of Lab Automation.

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

- The group was working on a Gas Chromatography tabular model (modeled with ASM and ADM). This initial scope of the model is results interpretation. Next quarter the WG will extend the work to results reproducibility
- Few SMEs from Bayer and IFPEN (The French Institute of Petroleum) were reviewing the Gas Chromatography tabular model
- At the beginning of the year, the WG had a discussion around modeling the sample/compound in chromatography and decided that it needs to be modeled under a new working group activity.
- 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 is working on Mass Spectrometry Tabular/Aggregation Model (a generic model)

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

- Continued discussions related to improving design and functionality.
- The working group will be discussing a strawman proposal to support Knowledge Graph.

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>

Applying the FAIR principles to data in a hospital: challenges and opportunities in a pandemic

A new article was published in the Journal of Biomedical Semantics (<https://jbiomedsem.biomedcentral.com/>) on April 2022: “Applying the FAIR principles to data in a hospital: challenges and opportunities in a pandemic”. It was written by a team in the Department of Human Genetics, Leiden University Medical Center, Leiden, The Netherlands. The article discusses the fragmentation of health data that is not interoperable for analysis with the various heterogeneous information systems that are used in hospitals. It suggests applying the Findable, Accessible, Interoperable and Reusable (FAIR) principles. As part of the suggested metadata modelling, it references and uses properties from the Allotrope Foundation Ontology (AFO). The article can be downloaded freely from the Journal of Biomedical Semantics publications at:

<https://jbiomedsem.biomedcentral.com/track/pdf/10.1186/s13326-022-00263-7.pdf>

American Chemical Society: Now Is the Time to Build a National Data Ecosystem for Materials Science and Chemistry Research Data

A new article was published in ACS Omega (<https://pubs.acs.org/journal/acsofd>) on April 2022: “Now Is the Time to Build a National Data Ecosystem for Materials Science and Chemistry Research Data”. The article makes a viewpoint about the urgent need of a long-term solution in the United States for data in chemistry and materials. It is giving the Allotrope Foundation as an example in the pharmaceutical industry. The article can be downloaded freely from the ACS Omega publications at:

<https://pubs.acs.org/doi/pdf/10.1021/acsomega.2c00905>

New Article Published on Nature Chemistry

New article was published in Nature Chemistry in April 2022: “*Making the collective knowledge of chemistry open and machine actionable*”. The article mentions an effort spearheaded by the pharmaceutical industry to develop a unified data model (the Allotrope data format is mentioned).

The article can be downloaded freely at: <https://www.nature.com/articles/s41557-022-00910-7.pdf>

Methods Database PoC: Fully Automated and Interoperable Import and Export of HPLC-UV Methods

In its April 2022 newsletter, the Pistoia Alliance (<https://www.pistoiaalliance.org/>) published that it has successfully completed a PoC on the digital transfer of analytical HPLC-UV methods between two different



Chromatographic Data Systems (CDS) based on a data standard and ontology for semantic representation of the method parameters along with adapters allowing for seamless transfer of analytical method information.

The work started in 2019 when Pistoia Alliance, jointly with the Allotrope Foundation, built a data model for HPLC-UV method parameters (the 'Methods Database'). Further information is available at <https://www.pistoiaalliance.org/methods/april-2022-methods-database-hplc-uv-methods/>

Automation & Control Trends: The Digitalization Dozen

Automation.com a subsidiary of ISA, the International Society of Automation (<https://www.isa.org/>) published a special 2021 summary report and analysis on "Automation & Control Trends: The Digitalization Dozen"

Allotrope work is mentioned under the 5th trend "Open Standards: Essential for Innovation". The report can be downloaded from [here](#)

NFDI4chem Published an Analysis of Chemical Ontologies

The [NFDI4chem](#) is an initiative to build an open and FAIR infrastructure for research data management in chemistry. It is funded by the [German Research Foundation](#) – DFG. An analysis of chemical ontologies was published where the comprehensive coverage of the Allotrope Foundation Ontology - AFO is demonstrated in the graphical chart. The analysis can be found at the NFDI4chem website https://knowledgebase.nfdi4chem.de/knowledge_base/docs/topics/ontology/

Research Ideas and Outcomes Journal: Towards a National Research Data Infrastructure for Chemistry in Germany

The [Research Ideas and Outcomes Journal](#) published a grant proposal that describes the vision of the [NFDI4chem](#) initiative to digitize all key steps in chemical research. Part of its strategy is to develop standards and interfaces for data exchange in cooperation with organizations such as Allotrope Foundation. The grant proposal can be downloaded freely from the Research Ideas and Outcomes Journal at <https://riojournal.com/article/55852/download/pdf/>

AF Community and Events

New APN Co-Leaders

We are pleased to inform that Tony Camisa from Accenture and Kashef Qaadri from Bio-Rad has agreed to take on the APN Co-Leaders position. Thank you both for volunteering for this important position and looking forward to your leadership.



2022 Spring Allotrope Connect Workshop

This time, the 2022 Spring Allotrope Connect event was running in a workshop format and was focused on AFO (the first day) & ASM (the second day) as the simplest foundational Allotrope Products to implement.

Some of the key takeaways from the first day workshop:

- Integrating Allotrope's ontologies into your organization's data systems and products presents a simple way to introduce standardization
- New methods of accessing the ontologies (including a new dictionary form on the Allotrope website) make it easy to use ontologies regardless of semantic expertise
- A new term proposal system is coming later this month to allow submission of small numbers of missing terms (not connected to a specific model) by the community
- A variety of methods exist to include IRIs (URLs) for terms into systems without native support, but building systems which can add IRIs as metadata systematically provide the best flexibility
- Many organizations are using AFO in conjunction with other ontologies and standards – can we learn from each other and curate a list of best practices and other ontologies which play well with AFO and are needed to solve core data standardization problem statements (community ontology federation strategies) ?

Experiences with ASM Applications were presented during the second day of the workshop:

- Automatic Instrument Results Capture / Parsing Leveraging ASM: Presented by Johnson & Johnson
- Experience of working with FTIR ASM in Java: Presented by IFPEN
- Creating ASM for Lab Automation: Presented by Novo Nordisk
- Scalable pattern for instrument integration using ASM: Presented by Merck & Co

A recording of the ASM introduction during the second day is available at the allotrope YouTube channel:

- Link to the 2022 Spring AC Day 2-1 Introducing the Allotrope Simple Mode recording: [here](#)

The entire 2022 Spring Allotrope Connect Workshop recordings and slides are 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

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/
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).

Looking Forward

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.

Sincerely,

Allotrope Product Team