Allotrope Foundation Release Notes 2021/06

Dear Allotrope Community,

We have continued our progress this quarter and improved or expanded the AFO, ADM and ADF in the following areas with updates to share:

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(Please note that access to links may require access to GitLab or other Allotrope Community resources. More details for access here.)

**Allotrope Data Format (ADF):**

**ADF Support & Maintenance**

The HDF group support team was working on an improved .Net product versioning. A pre-release of the C# package 1.5.4 is available for testing. Please contact the Product Team if you are a C# user and willing to volunteer and test the pre-release version.

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

**Allotrope Data Modeling and the new Allotrope Simplified Model (ASM):**

**Project Progress Update**

The development will enable the use of a simplified syntactic representation of the current governed Allotrope Data Models (ADMs). The simplified representation of the current ADM is an extension to the Allotrope Framework product line.

After a detailed due diligence as well as several discussions with the AF Community a JSON style schema definition was selected as the optimal representation to meet the specific needs of simplified product use. The project is expected to be completed by mid-to-late September with a target of being completed prior to Fall Allotrope Connect. The project has met the first milestone of a defined JSON schema now available for testing.

**Call to APN Partners for Early PoC and Beta Testing of the ASM**

The Product Team is seeking beta testers (instrumentation vendors and solution providers) from the APN to support testing the new JSON Simple Model (ADM-Lite), currently targeted for September launch.

The goal of the beta testing is to generate example results of tabularized data based on the new JSON ASM format, typically using REST interfaces. We encourage participation in beta testing so that APN members...

- ...can gain an early assessment for use and product integrations in advance of the targeted September release.
- ...have an opportunity to demonstrate progress towards your company’s ASM solution at the Allotrope Connect in September

In cases where there is no model for a chosen instrumentation type, the Product Team is happy to support drafting a new tabular model and the Modeling WG is ready to review drafted models.
Intermediate Chromatography ADMs Release – REC/2021/04
Following a community request, the set of Chromatography ADMs were further developed, tested and promoted from CR to REC status. The interim release included the promotion of chromatography models: LC, GC, & SFC including all dependencies (Chromatography, Liquid-Chromatography, UV-detection, and core) from CR/2021/03 to REC/2021/04 status.

Allotrope Foundation Ontology & Data Models (AFO/ADM)

AFO Updates
The current Allotrope Merged Ontology Suite release is available on BioPortal, a repository of biomedical ontologies: [https://bioportal.bioontology.org/ontologies/AFO](https://bioportal.bioontology.org/ontologies/AFO)

Model Creation or Updates
Modeling teams have continued working to align on proposals to expand the domain coverage of the AFO and ADM. Easily access files located on Client Connect [here](https://bioportal.bioontology.org/ontologies/AFO) and more granular technical details available on GitLab, [here](https://bioportal.bioontology.org/ontologies/AFO).

New or Updated Data Models in Recommended (REC) status below:

<table>
<thead>
<tr>
<th>Model</th>
<th>Type</th>
<th>Maturity</th>
<th>Path</th>
<th>Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluorescence</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Luminescence</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Scanning Electron Microscopy (SEM)</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Hardness Tester</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Disintegration</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Oven/coulometric KF</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Light Obscuration (Liquid Particle Counter)</td>
<td>Tabular</td>
<td>REC</td>
<td>WD&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Specific Rotation</td>
<td>Tabular</td>
<td>CR</td>
<td>CR&gt;REC</td>
<td>Diagram Shape</td>
</tr>
<tr>
<td>Loss on Drying</td>
<td>Tabular</td>
<td>CR</td>
<td>CR&gt;REC</td>
<td>Diagram Shape</td>
</tr>
</tbody>
</table>

New Data Models in Candidate Recommendation (CR) status which are now ready for review are listed below as well as Working Draft models which are actively being worked on.
• Comments are accepted before feature freeze date noted below in Development Timelines section

<table>
<thead>
<tr>
<th>Model</th>
<th>Type</th>
<th>Maturity</th>
<th>Path</th>
<th>Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>FPLC</td>
<td>Graph</td>
<td>CR</td>
<td>WD&gt;CR</td>
<td>Diagram Shape</td>
</tr>
</tbody>
</table>


You can also find the 2021/09 ADM release plan on GitLab [here](http://example.com).

**Term Mapping Database**

Allotrope’s collating instrument term mappings (to the standardized AFO) that already exist in the Community and housing them in a single central database.

The Term Mapping database will:

• Support Allotrope Partners and Members by reducing the tedious efforts often required by teams to map terms
  o Provide direct value to the entire Community by reducing the time needed to harmonize data

Allotrope Product Team will coordinate with Members and Allotrope’s Partner Network to gather mapping information to ensure consistency of mapping across vendors.

**Upcoming Development and Testing Timelines**

*Development*

• Product development for the next quarter has the following applicable dates:
  o Feature freeze of September 2nd
    ▪ Final date for submitting issues for consideration to be included in the pending release
  o Code Freeze of September 16th
    ▪ Updates to code shall not be changed after this date.

*Working Group Updates*

Please note that the Semantic and Modeling WGs have begun to record their meetings each time 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)

*Sample Prep: (Notes: https://highq.in/6ih7dea62a)*

• Initial draft for modeling of workflows can be found [here](http://example.com) and the group is planning to set up a workshop with more details to come soon.
Chromatography: (Notes: https://highq.in/1xgh2gjurj)

- The working group is working on a new LC-UV tabular model to be implemented as part of the new ASM JSON representation

MS: (Notes: https://highq.in/6igryjhpus)

- The team aligned on base model use case of measuring the intact mass of proteins and it is in 2021/09 planned release.

Semantic: (Notes: https://highq.in/6ihpr1kx5x)

- Continued discussions related to improving design and functionality.

Communications: (Folder https://highq.in/4e2l76eqo9)

- WG moved to Friday’s at 9am ET.
- In alignment with Board priorities the Product Team, in coordination with the WG, will be creating new material for distribution throughout the year.
- Team had initial working session to review format comparisons
- Prioritized definition of user personas

Operations: (Folder https://highq.in/4e2l76eqo9)

- Executing planning for Fall Allotrope Connect

Modeling: (Notes: https://highq.in/5hj7qpacex)

- Progress noted in AFO/ADM section

Events and Public Presentations and Other

Upcoming Fall 2021 AF Virtual Connect Event
Event page: https://www.allotrope.org/2021-fall-allotrope-connect

Connect Categories by Date:

- Sept. 13th: Implementations of Allotrope Strategy and Vision
- Sept. 15th: Use cases and Proof-of-Concepts
- Sept. 20th: More Use Cases & Proof-of-Concepts as well as Technical Presentations

Reminder call for abstracts due by August 2nd.

Recent Spring 2021 AF Virtual Connect Event
Event page: https://www.allotrope.org/2021-spring-allotrope-connect

Event presentations are available on the AF YouTube Channel, here

YouTube Channel
A reminder that the public sessions from the latest fall Allotrope Connect are uploaded to our YouTube Channel, here
Community Collaborations

Pistoia Method Hub Project

Lots of progress was made in the Pistoia Methods Hub project seeks to build a bridge for analytical methods to transition from text-based information to fully digitized, machine-readable instruction sets. Natural Language processing tools are used to pre-populate a standard format for a fully digital representation of the method. Alternatively, well-implemented methods can be exported from a Chromatography Data System (CDS) and just validated by comparison to the text-based description. USP, CAS and Elsevier sources for Analytical Method information are evaluated in terms of their information structure from free-text, via semi-structured to fully digital information e.g. based on the Allotrope Foundation Ontology (AFO) and other available ontology providers. Project page: https://www.pistoiaalliance.org/projects/current-projects/methods-on-demand/

AF Community

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 here (http://community.allotrope.org). Note this requires GitLab access > go here to request access.

Some of the pages to look for:

- **Allotrope Foundation Data Models (ADMs):**
  https://community.allotrope.org/resources/reference/semantic/governance/allotrope-data-models/ The page includes information with regard to the structure of ADMs artifacts repository in the table at the bottom of the page
- **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, so if your firewall denies access to Google drive links, please contact matthew.fox@allotrope.org for a current PDF).

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