Welcome to Allotrope Connect Spring 2023
We are a consortium of chemical & life sciences companies, instrument & software vendors, and academic & government institutions formed from IQ Consortium in 2013.

We revolutionize the way we acquire, share and gain insights from scientific data through application of community-derived data standards consistently delivered via an extensible technology framework.
New Paradigm: Data-Centric Environment

- Data are a key asset of any organization
- Data are self-describing and do not rely on an application for interpretation & meaning
- Data are expressed in open, non-proprietary formats
- Access to and security of the data is a responsibility of the data layer, and not managed by applications
- Applications are allowed to visit the data, perform their magic and express the results of their process back into the data layer for all to share

http://www.datacentricmanifesto.org
Impact of R&D Current State on IT

The high cost of being application-centric

- Custom integrations
- Endless relational data mappings
- Lack of modularity
- Technology incompatibilities
- Vendor lock-in with proprietary formats
- Custom data analysis tools
- Complex data sharing
- Complex data migrations
- Wasting valuable resources
- Less bandwidth to drive modeling & data science
Data Standardization Creates FAIR Data

- FAIR provides principles, data standards provide the blueprint for a solution
- Defines data quality goals across all solutions
  - Context
  - Structure
  - Format
- Can standardize anywhere in data lifecycle, but is foundational if done at data capture
- Standardization across domains creates data interoperability and ease of (re)use by design
# Allotrope Framework Products

<table>
<thead>
<tr>
<th>AFO</th>
<th>ADM</th>
<th>ADF</th>
<th>ASM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Allotrope Foundation Ontologies</td>
<td>Allotrope Data Models</td>
<td>Allotrope Data Format</td>
<td>Allotrope Simple Models</td>
</tr>
<tr>
<td>Defines terms &amp; their relationships consistently across laboratory domains</td>
<td>Establishes schema for consistent use of ontologies to describe laboratory items</td>
<td>Provides standardized data format (RDF) to semantically represent laboratory data</td>
<td>Provides standardized text-based representation (JSON) of laboratory data</td>
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©2023 - An Introduction to Allotrope Foundation
Allotrope Data Models (ADM)

- Scope determined by what information is needed within a use case(s)
- Leverages terms and relationships found in Allotrope Foundation Ontologies (AFO)
- Provides a schema to consistently structure data to describe something in the lab (e.g., an instrument or result)
- Simplest application is to create an Allotrope Simple Model (ASM) via automation
The Allotrope Catalog Today

57 domain models available today as ADM and/or ASM

- Automated Reactors / PAT
- Dissolution
- **Liquid Chromatography**
- Oven/Coulometric KF
- Specific Rotation
- Balance
- Blood Gas Analyzer
- Electrochemical Tester
- Liquid Particle Counter
- **pH Sensor**
- LC-MS
- Osmolality
- Surface Area Analysis
- Bulk Density
- **FPLC**
- Live-cell imaging
- qNMR
- **Hot Tack**
- Temperature Monitoring
- Calibration
- FTIR
- Loss on Drying (Moisture Analysis)
- qPCR
- Cell Counting
- **Fluorescence**
- **Luminescence**
- Raman
- **UV Absorbance**
- **Gas Chromatography**
- Methods: LC-UV
- Water Activity Tester
- Conductivity
- Hardness Tester
- Nepholometry
- **Foam Height**
- **Foam Qualification**
- Stirring
- Titration (inclusive of KF)
- X-Ray Powder Diffraction
- Differential Scanning Calorimetry (DSC)
- High Resolution MS
- Optical Microscopy
- Single Quad-Mass Spec (SQD-MS)
- Disintegration
- **Pumping**
- Sample Preparation Process Workflow
- Light Obscuration (Liquid Particle Counter)
- Cell Culture Analyzer (Metabolite Analyzer)
- Size Exclusion Chromatography
- Dynamic Vapor Sorption Analyzer
- Particle Size Distribution (PSD)
- Supercritical Fluid Chromatography
- Scanning Electron Microscope (SEM)
- Thermogravimetric Analysis
- **Pressure Monitoring**
- **Tensile Testing**

*New or Updated in last 6 months

...and more added each quarter! **Allotrope Data Models (ADM)**
Allotrope Foundation Taxonomies (AFT) define and classify terms into five domains.

Allotrope Foundation Ontologies (AFO) link terms across domains for deeper context.

AFO assigns unique identifiers to terms so software can unambiguously track their use.

AFO is conveniently available through your web browser at the Public Bioportal Link.

Can be used to enrich existing data sets.

Available on OLS, Ontobee, and as a Thesaurus.
Allotrope Simple Models (ASM)

- Bidirectionally compatible with the corresponding Allotrope Data Model (ADM)
- Leverages JSON, a preferred data format of data scientists, that works with any programming language and has many publically-available software tools to support its use
- Both human and machine readable
- Easy to directly apply to use cases where simple data structures are sufficient (e.g., associate parameter with result)
Allotrope Simple Models are open to all!

https://www.allotrope.org/asm
Establishing Data Standards as a Community

Allotrope works with other standards – and works as a community to solve data challenges.
The Allotrope Journey

Establishing Technology for Standardization
- ADF
- AFO

Modeling as a Standardizable Practice
- ADM
- ASM

Adopting and Promoting Standards to Solve Problems
- Implementation
- Integration
The Allotrope Community Today (as of March 29, 2023)

Allotrope Foundation

Allotrope Partner Network Members

• Dotmatics
• Erasmus MC
• Fraunhofer IPA
• NIST
• Stanford University
• University of Illinois at Chicago
• University of Michigan
• University of Southampton
Allotrope Foundation Organizational Structure

A consortium managed by industry with dedicated product team

- Allotrope Foundation (AF)
  - Board of Directors (Strategy)
    - Chairperson | Vice-Chairperson
  - Executive Committee (Strategy Execution)

- Allotrope Partner Network (APN)
  - APN Working Group
    - Co-Leads

- Product Team (Product Strategy)
  - Product Owner / Technical Director
  - Senior Developer / Semantics Engineer

- Support, Maintenance, & Governance

- Technical Working Groups
  - Modelling, Semantics, Tool & Product Development, and Domain-Specific Teams (as needed)
Agenda

• Day 1: Allotrope in Action (Public)
  • Presentations by members on Allotrope use in their own hands

• Day 2: A Community Focus on Adoption (Allotrope Members & APN)
  • Community meetings focusing on implementation and adoption of Allotrope, lessons learned, and exploring new opportunities

• Day 3: Moving Allotrope Forward (Allotrope Members & APN)
  • Working Group meetings, Technical office hours and discussions, Board meeting
Allotrope In Summary

Allotrope Foundation Ontology (AFO) provides a common terminology foundation across techniques / domains

Allotrope Data Models (ADM) and Allotrope Data Format (ADF) provide semantically-rich & interconnected data when you need it

Allotrope Simple Models (ASM) make it easy to get started in any environment and solve many problems

A true community-driven standard driven by use cases, representing over 50 organizations