

Data Models and Domains

Allotrope Foundation is a consortium of chemical & life sciences companies formed in 2013 to revolutionize the way we acquire, share and gain insights from scientific data through the application of community-derived data standards consistently delivered via an extensible technology framework.

Allotrope Foundation manages and enables a community-led effort to:

1. Standardize vocabularies commonly used in scientific data and experiments
2. Structure vocabularies into taxonomies and ontologies (Allotrope Foundation Ontologies – AFO) to add more context
3. Standardize schema (Allotrope Data Models – ADMs) using AFO terms to create unified descriptions of scientific domains (experiments, techniques, instruments, results, etc)
4. ADMs can be represented as:
 - Allotrope Simple Model (ASM) - standardized JSON files for text based tabular data
 - Allotrope Data Format (ADF) - standardize RDF graphs in an HDF5 container for semantically richer data



VOCABULARY

Collection of terms with agreed upon definitions used to describe things



TAXONOMY

Hierarchical classification of the vocabulary terms



ONTOLOGY

Formal categories, properties, and relationships across taxonomy terms

The Allotrope Framework

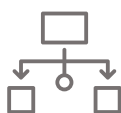
The Allotrope Framework provides a complete toolkit for data standardization to meet a wide range of use cases ranging from consistent data labeling to advanced semantic exploration & data science.

Define



Vocabulary

Classify

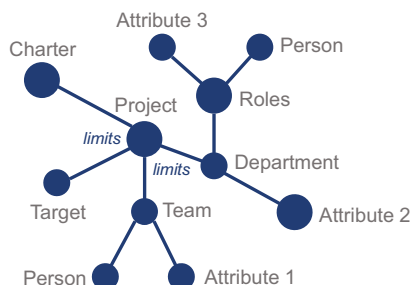


Taxonomy

Relate



Ontology



CSV



ZIP



JSON



HDF5



RDF



XML

CONTEXT

Terminology defined & desired relationships established in well-structured ontologies.

STRUCTURE

Use of ontologies to define data models that are blueprints to consistently describe things.

FORMAT

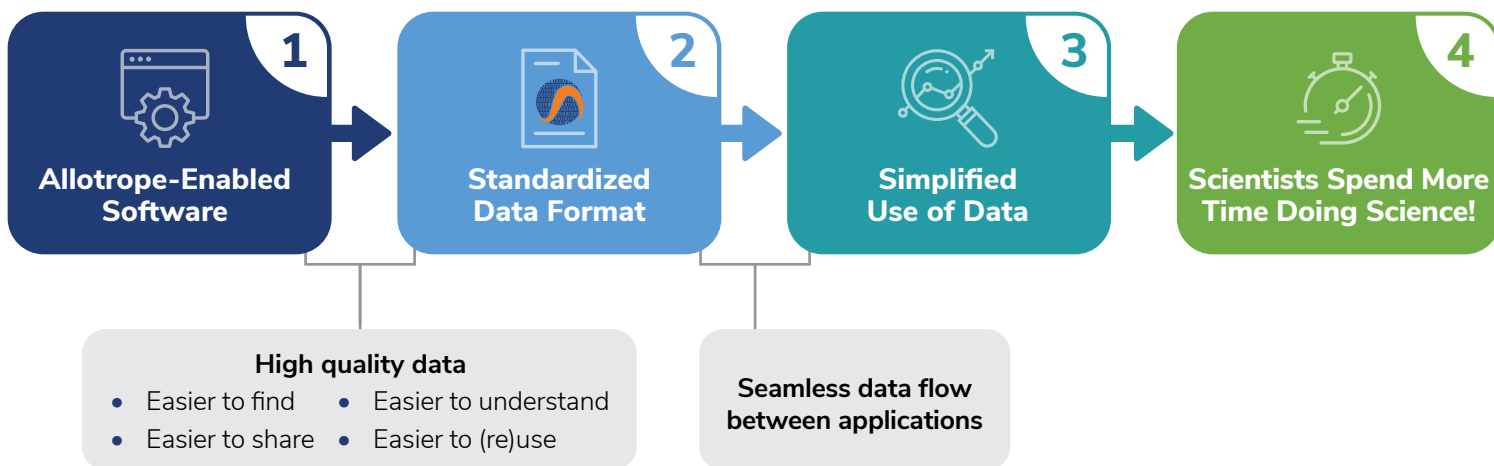
Use data models to create final representation of data used in software applications.

Domain Coverage

The Allotrope Foundation community has released approximately **50 interoperable data models** (as of August 2022) – **and growing**.

- Automated Reactors - PAT
- Balance
- Blood Gas Analyzer (BGA)
- Bulk Density
- Calibration
- Cell Counting
- Cell Culture Analyzer (Metabolite Analyzer)
- Code Reader
- Conductivity
- Differential Scanning Calorimetry (DSC)
- Disintegration
- Dynamic Vapor Sorption Analyzer (DVS)
- Fluorescence
- Foam Height
- Foam Qualification
- FPLC
- FTIR
- Gas Chromatography
- LC-MS
- LC-UV
- Light Obscuration (Liquid Particle Counter)
- Liquid Chromatography
- Loss on Drying
- Luminescence
- Mass Spectrometry
- Mass Spectrometry - Intact Mass
- Methods: LC-UV
- Nephelometry
- Optical Microscopy
- Osmolality
- Oven/Coulometric Karl Fischer (KF)
- Particle Size Distribution (PSD)
- pH
- qNMR
- qPCR
- Raman
- Scanning Electron Microscope (SEM)
- Single Quad-Mass Spec (SQD-MS)
- Specific Rotation
- Supercritical Fluid Chromatography (SFC)
- Surface Area Analysis
- Tablet Hardness (Hardness Tester)
- Tensile Testing
- Thermogravimetric Analysis
- Titration (inclusive of KF)
- Ultraviolet (UV) Absorbance
- X-Ray Powder Diffraction

What Success Looks Like



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Allotrope.org | more.info@allotrope.org



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