

Creation of Allotrope Ontology and Usage as ELN Metadata



**Allotrope
Foundation**

CASE STUDY

Goals

- Alignment and harmonization of terminology used in biological process development and in respective analytical methods.
- Creation of aligned vocabulary, respective relations and definitions for a metadata ontology.
- Proof of concept for simplified analysis through metadata mapping.

Challenges

- Scope led to involvement of many SME
- Collection of concepts was focused on result data
- Understanding of ontological concepts limited
- Some practical limitations on usability of terms due to architecture of existing application, alternate labels in use.

Results

- Creation of nearly 2500 'concepts' for 14 analytical techniques and 2 process development operations
- Very useful exercise for harmonization of definitions
- Use of many terms / definitions in ELN
- Successful Proof of concept for mapping of terms and results from different data sources with the general ontology.

Goals

During the implementation of an Electronic Laboratory Notebook (ELN) in Biological Process Development, an opportunity was identified to increase system sustainability and data interoperability. This would be done by leveraging the Allotrope Data Framework (ADF) to standardize the vocabulary used in an ELN, which contained a variety of terms and definitions used at multiple sites. The controlled vocabulary implemented as part of the ADF would be used in multiple template-based specific (unit) operations and analytical workflows within the ELN.

As part of developing the taxonomies, harmonized definitions of the terms to be used needed to be established. By defining the terms and concepts, as well as the relationships between them (i.e., creating the ontology), the downstream analyses comparing newly acquired data with respect to other data from other workflows, departments or even from the public domain should be enabled. The scope for the ontology development included 2 biological Process Development operations and 14 related analytical techniques.

Challenges

The scope of the exercise proved to be larger than initially anticipated. With 14 analytical techniques in use, many terms needed to be created and multiple SMEs had to be

involved in this process. Generally, the average SME had limited knowledge of the corresponding ontologies or the concepts required to properly develop them. The use of knowledge engineers (KE) to assist with this task was crucial for a more comprehensive output.

Another particular challenge was that some analytical techniques as well as process operations were comparatively large in scope relative to others. Practically, this led to focusing only on higher order result-oriented terms versus a more comprehensive list.

Due to the architecture and previous work with the ELN, a number of preexisting terms were fixed and

...approximately 2500 concepts for 14 analytical techniques and 2 process development operations were defined.

could not be changed. This needed to be addressed through the additional step of mapping these terms to alternate labels.

Results

With the combined efforts of the SMEs and KEs, approximately 2500 ontological concepts were created across the different techniques and operations and sites. Many of these concepts can be contributed back to Allotrope Foundation for integration within the general Allotrope Ontology. Other terms, which are more company-specific terms are stored as extensions to the Allotrope Ontology.



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As anticipated, the efforts to create this ontology successfully facilitated harmonization between and across sites with regards to alignment of techniques and definitions. This is anticipated to result in long-term operational savings with respect to

There were practical limitations with respect to which terms could be actually used in the specific ELN project since many definitions and terms were already established with the initial implementation of the ELN and this prior effort needed to be

and from other data sources relative to the common ontology allowed us to analyze these varied data in a streamlined, automated fashion.

Proof of concept could show that it is possible to map and analyze ELN data in comparison to outside generated data.

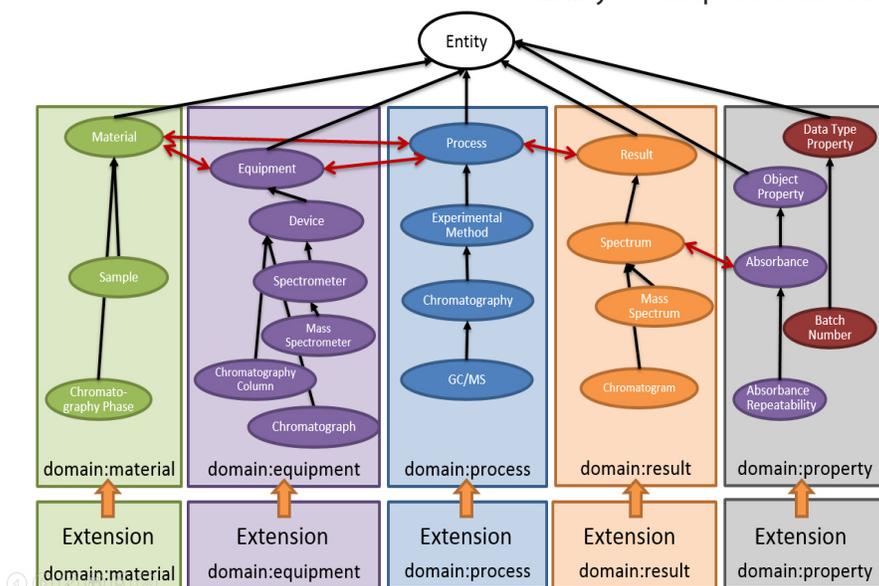
The development of taxonomies, ontologies and data models is enabled by working groups that are comprised of representatives representing both Member and Partner Network companies. For more information click here www.allotrope.org

ongoing systems support and long-term maintenance since the entire functional area is working with one standard from system to system.

considered as immutable. However, the practical use of the developed ontology was demonstrated through this proof of concept project. The ability to map data inside the ELN

Concepts Created

Technique/Operation	# Concepts
HPLC-UV	170
HPLC-MS	100
ELISA	95
HTRF	54
MFI	243
qPCR	44
DSD-Page	64
FTIR	29
Biacore	135
Spectrophotometer	86
Microplate Reader	37
iCE/CE	189
Bioanalyzer	71
Potency	64
Chromatography	741
TFF	327
Total	2449



Schematic representation of the AFO illustrating the use of extensions for company-specific terms.

About Allotrope Foundation

Allotrope Foundation is an international consortium of pharmaceutical & biopharmaceutical companies launched in 2012 with a common vision to develop innovative approaches for handling scientific data. Allotrope Foundation has developed a framework to capture and represent data generated by any analytical device in the laboratory in a standardized format, including more complete metadata related to each test and measurement event, expressed in a standardized vocabulary, which facilitates the exchange, utilization and integration of data beyond the boundaries of the originating instruments and laboratories.

This effort is fully funded by the members of Allotrope Foundation and is rapidly progressing on our common goals to improve data integrity, reduce wasted effort and allow us to realize the full value of our scientific data.

Allotrope Foundation

1500 K Street, NW
Washington, DC 20005
(202) 230-5855

<http://www.allotrope.org>