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Coming of age of Allotrope: Proceedings from the Fall 2020 Allotrope Connect

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The Allotrope Foundation (AF) is a group of pharmaceutical, device vendor, and software companies that develops and releases technologies [the Allotrope Data Format (ADF), the Allotrope Foundation Ontology (AFO), and the Allotrope Data Models (ADM)] to simplify the exchange of electronic data. We present here the first comprehensive history of the AF, its structure, a list of members and partners, and an introduction to the technologies. Finally, we provide current insights into the adoption and development of the technologies by summarizing the Fall 2020 Allotrope Connect virtual conference. This overview provides an easy access to the AF and highlights opportunities for collaboration.

Keywords: Precompetitive consortium; Semantics; Metadata; Standard; Harmonization; Laboratory IT; Allotrope; Digital Lab

Introduction

The analytical laboratory is a complex environment and host to a plethora of computer-supported devices and software solutions to design, execute, and analyze experiments. Unfortunately, most scientific systems are communicating with severe limitations, which inhibit distributing scientific data. A common data exchange format could solve this problem. Although multiple attempts have been made to address the issue of nonstandardized data formats, no single standard has yet emerged that could truly unify the laboratory IT landscape [1–3].

Under the umbrella of the AF, a group of pharmaceutical, device vendor, and software companies has addressed the challenges of the analytical laboratory for the better part of the past decade (Fig. 1). Founded in 2012, the AF has made large strides in addressing the issue of laboratory data exchange. This review describes the history of the foundation, introduces the three main AF technologies (ADF, AFO, and ADM) and summarizes the recent Allotrope Connect Fall 2020 virtual conference.

Although the adoption of ADF is still nascent, the Foundation has reached a level of maturity sufficient to address data-exchange challenges beyond the pharmaceutical industry, such as within academia. Consequently, in this report, we emphasize not only the business value of the AF, but also opportunities for academia to interact and support the initiative. Thus, the key purpose of this report is to introduce the format and to increase awareness of the activities of the AF.

History of the Allotrope Foundation

In 2010, Roberts *et al.* instigated what would become the AF, because they presented in a vision for a new decade the major challenges for IT in analytical laboratories [4]. The first publications by Roberts *et al.* [4,5] introduced a common thread that interweaves throughout all following efforts: the benefits of a standardized and versatile data format. The origins of Allotrope go back to the old, yet unsolved, problems of application-centric infrastructures: time-intensive routine work on data sets,

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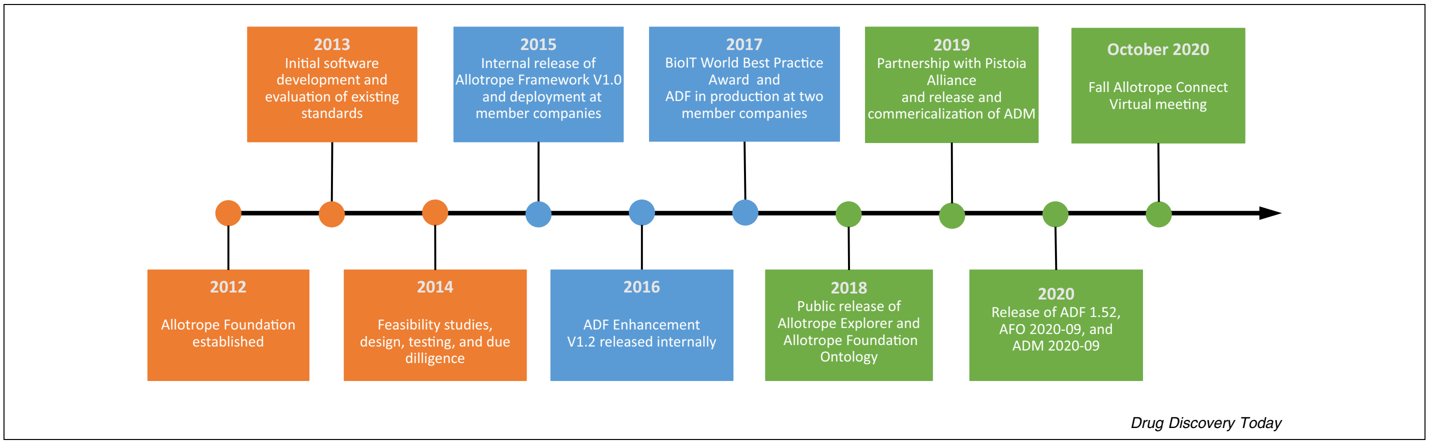

FIGURE 1

Development and key achievements of the Allotrope Foundation in three phases. The planning phase is in orange, internal application of Allotrope products in solutions in blue, and public application of Allotrope products in green.

low efficiency and consistency in metadata tagging, and limited communication between programs and applications. Roberts *et al*. called for a modular solution that could render modeling and optimization in the laboratory increasingly feasible, be flexibly extendable, and able to respond to unanticipated needs, such as data science today.

In a subsequent article, Roberts *et al*. expanded on these ideas from a more technical perspective, introducing the concept of a holistic data format [5]. A file in such a format would be created the moment data were generated, be it from a laboratory device or a user, and would evolve with the data as they passed between different systems, such as electronic laboratory notebooks (ELNs), laboratory information systems (LIMS), or scientific data management systems (SDMS). Roberts *et al*. also explored basic formats, such as XML, although the need for specialized services that could enable security and authentication, data validation, instrument control, data acquisition abilities, and random access to data appeared beyond the scope of existing solutions.

The introduction of a holistic data format required a holistic industry approach. In the spring of 2011, a team sponsored by the International Consortium for Innovation & Quality in Pharmaceutical Development (IQ Consortium; https://iqconsortium.org/) was formed to explore the possibility of a collaborative project to realize the vision articulated by Roberts *et al*. In meetings with the IQ-sponsored team, laboratory instrument and software vendors expressed a high level of support and enthusiasm for the vision, as well as a willingness to work together to implement the proposed Framework. In December 2011, the IQ Consortium Board of Directors determined that the initiative should proceed but that it would be better managed and served by creating a separate legal entity, independent of the IQ Consortium; thus, the AF was formed on June 4, 2012.

A report from 2014 provides insights into the first years of the Foundation [6]; it mentions that the consortium comprised Foundation members from biopharma and a partner network of laboratory device vendors, academic institutes, and software companies (Fig. 2). The first deliverable of the Foundation was the AF software suite, version 1.0 in October 2015, which internally released the ADF version 1.0, Allotrope Foundation Taxonomies, and Application Programming Interfaces (APIs).

Here, we shed light on the discussions and decisions that led to the first release of the AF as described by Vergis *et al*. [7]. After organizing the foundation, the member companies initiated a request for proposals for implementing the holistic data format. Over the course of nearly 2 years, they collected user requirements and evaluated existing technologies (e.g., AniML [8]). In an open selection process, the AF decided to partner with Osthus GmbH, a Germany-based scientific informatics company, in December 2013 to implement and deliver the necessary solutions. During this time, it became apparent that requirements, especially around semantic capabilities, necessitated a completely new data architecture. Together, the AF and Osthus decided to build a new data format on the existing HDF5 format [9] and the Resource Description Framework (RDF) [10]. Besides the design of a new ADF and class libraries to read and write the format, the Foundation recognized the need to develop a semantic model to ensure that metadata would be understandable. In a staggered approach, it coordinated with subject-matter experts to develop a list of controlled vocabulary for high-performance liquid chromatography (HPLC) with ultraviolet (UV) absorption detection, and subsequently assembled it into a taxonomy; a complete graph-based ontology for LC-UV would soon follow driven by subject matter experts at GSK and Merck & Co.

We learn from conference abstracts that companies such as Genentech and Bayer started to realize the value of ADF as a long-term data preservation and archiving format (in accordance with the definition of an archival information package within the OAIS Reference Model - ISO 14721) and started first proof-of-concept and small-scale projects. The main benefit of an ADF file as a storage container rests in the open standards that will ensure future readability and high-quality metadata information that enables interpretation of the data for nonsubject-matter experts. This reduces the expected cost of data migration projects, which typically require expensive data transformation and validation efforts.

Other precompetitive consortia, such as the Pistoia Alliance [11], started to align their efforts with the Foundation. In a short article from 2015, Vanderwall [12] reported on the synergies between the semantic mapping work of the Pistoia Alliance

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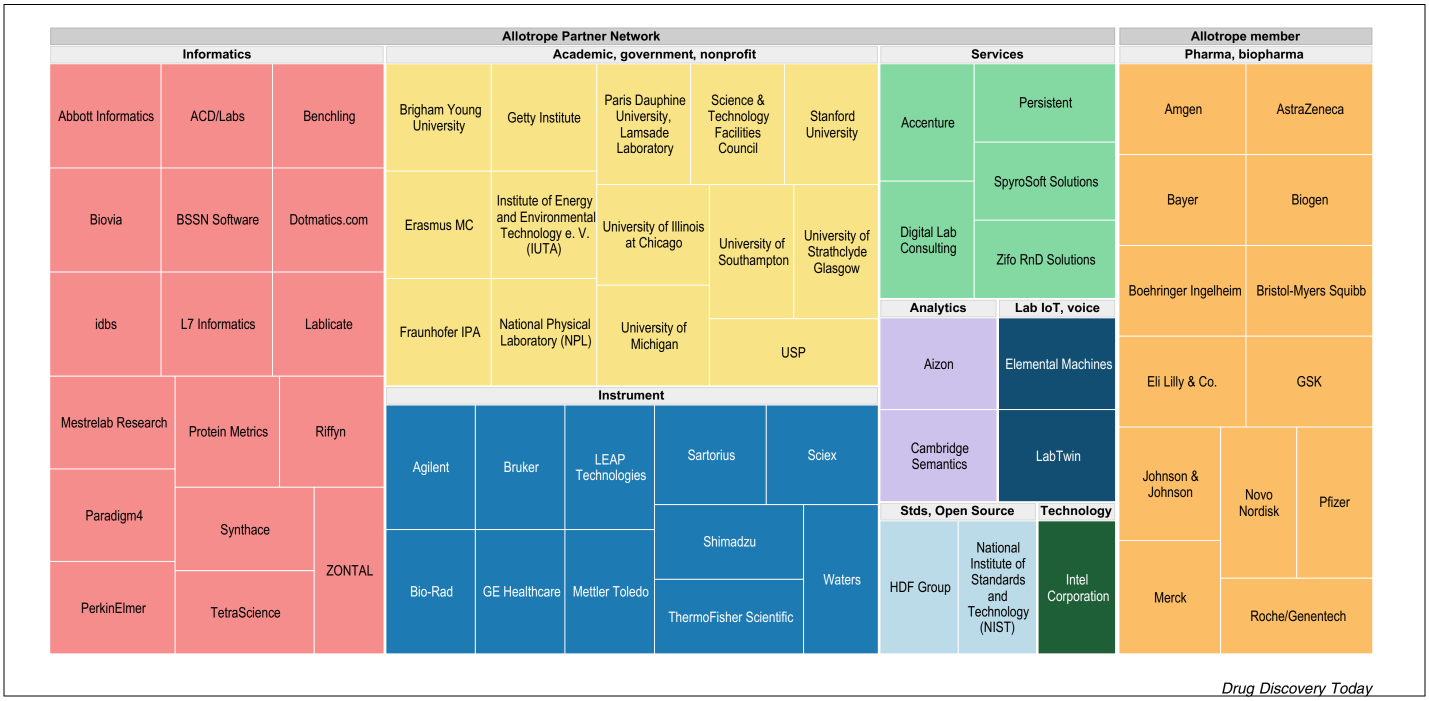

FIGURE 2

Allotrope partner network and member companies as of October 2020.

and the AF and how their complementary focus and collaboration would lead to easily shareable semantic models going forward.

Another report by Colsman and Uphill captured the quintessence of producing ‘actionable scientific knowledge’ and indicated a growing interest from other industries in the Allotrope standard [13]. Throughout 2016 and 2017, the Foundation released quarterly updates and public versions of the AFO and the Allotrope Explorer, a basic viewer for ADF files. Biannual Allotrope Connect meetings were introduced, which featured public days for non-members to explore progress of the foundation. However, during this period, only commentary on initiatives by the US Food and Drug Administration (FDA) were published [14,15]. A great achievement for the Foundation was the 2017 BioIT World Best Practice Award.

The AF released the first ontological models publicly in March 2018, introduced a simplified tabular model (equivalent to a key-value pair in a semantic model), and enhanced the ADF with audit trail functionality. Although the Foundation did not directly publish further advancements, it grew into a more mature organization by adding three full-time staff members. Although the organizational size and maturity is an important factor to gauge longevity, success needs to be measured by adoption rate. Agilent released the first commercial product supporting ADF in August 2018 [16], ZONTAL released the first enterprise digital hub built on ADF in November 2018 [17], and the Pistoia Alliance announced a method exchange database based on ADF in 2019 [18]. Other solutions included large-scale nuclear magnetic resonance (NMR) data migration projects at Boehringer Ingelheim and Pfizer, Allotrope-based data lakes at Amgen, ADM application to data-rich experimentation at Merck & Co, and ADF archiving at Bayer and Genentech. Two publications by Della Corte *et al.* showed the usability of ADF outside the pharmaceutical industry because it enables effective electronic archiving at a large university library [19], and proposed ADF as a solution that could enable the data-centric lab of the digital age [20]. A current overview of the structure and organization of the Foundation is given in Supplemental Information 1 in the supplemental information online, and a detailed listing of all companies, academic institutes, and software partners is given in Fig. 2.

The Allotrope framework

The Allotrope Data Format

The AF releases updated documentation about the Framework through a public website (docs.allotrope.org) and we present here a short summary of the key technologies. The ADF enriches the HDF5 file format ((https://www.hdfgroup.org/), which was designed to organize large amounts of data for supercomputing environments. ADF is well suited for the same environment but has additional features, organized by layers, that enable it to fill a broader use-case. Although implementations may vary, the ADF specification calls for four layers. The data description, data cubes, and data package layers specifically support scientific work. A data provenance layer contains the audit trail and checksums, which make ADF well suited for long-term archiving (Fig. 3).

The data description layer acts as a map for the contents of the file and makes it easy to navigate the contents, whether navigation happens from a desktop viewer application or from a web application. Stored in TTL, a compact equivalent of RDF, the data description can contain information about the instruments used, the process conducted, and the samples used, as well as many

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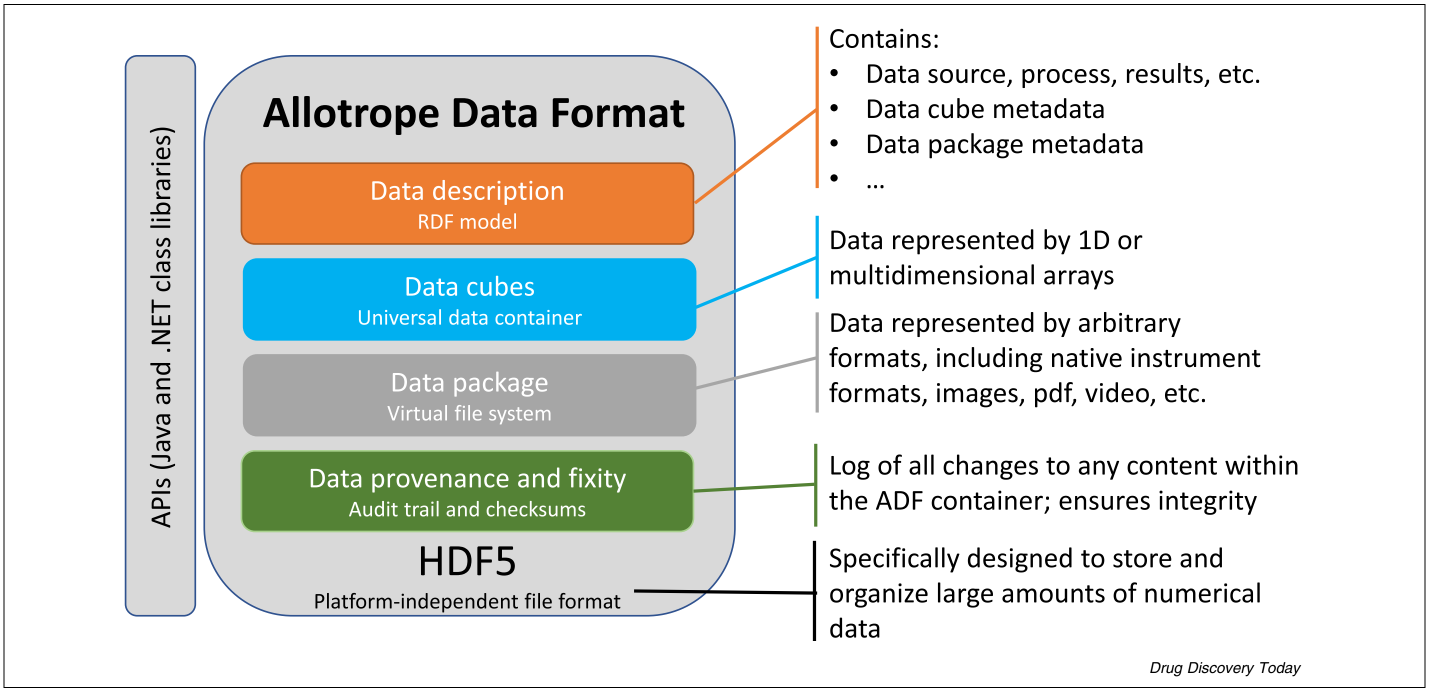

FIGURE 3
The Allotrope Data Format (HDF) comprises multiple modules based on HDF5 that are accessible through Application Programming Interfaces (APIs). The Data Provenance and Fixity layer contains the audit trail and checksums.

other relevant descriptors of an experiment. The data cube is a multidimensional array optimized for high-throughput and analytic applications. It is included as a separate layer to allow better machine access for big-data processing and deep learning applications. The data package is a virtual filesystem, allowing compressed storage of all folders and filetypes, delivered as part of a single portable file. The final two layers support long-term storage and archiving. The audit trail layer tracks all changes made to the data with useful descriptions attached to each change. The checksum layer acts as a check for file degradation, providing a fingerprint of the contents of the file at creation time.

The Allotrope Foundation Ontology

An ontology bridges the gap between the specialized vocabulary in a field of research and the rigid digital encodings of computer data. AFO grew from the need to make data reproducible across laboratories, the inability to concretely define and label archived data, and the need to interface more deeply with digital systems. Using an ontology ensures unambiguous sharing and recall of information. Allotrope was granted permission to include terminology from IUPAC [21], the authoritative source of chemistry terminology and definitions. By synthesizing research-specific vocabulary into a machine-understandable format, experimental processes, materials, equipment, and results can be more easily transferred, allowing greater collaboration and reducing the overhead for reproducing results. AFO helps define descriptive properties to help better organize and index large volumes of laboratory data. The Foundation currently advertises 39 rigorously defined and vetted ontology domains, as listed in Supplemental Information 2 in the supplemental information online, with new additions on a quarterly release cycle.

Developing an ontology requires literature reviews, expert opinions, existing ontologies, lists and references, and quality assurance. The AF enthusiastically accepts inputs from laboratory experts regarding meaningful terms to include in an ontology, and the AFO (https://bioportal.bioontology.org/ontologies/AFO) standards currently boast > 2200 unique terms that can be easily translated across human and machine languages. As part of this need-centered discussion, the Allotrope governance model ensures that each ontology is consistent, follows appropriate style guidelines [22], is useful for interoperability [23], and follows general best practices [24].

The Allotrope Data Model

Ontologies provide a dictionary of terms, but the grammar and structure of scientific interoperable data requires additional constraints, which are defined in ADMs. By mixing ontology terms as needed, and designating hierarchical relationships, the ADM takes ontologies from the realm of the abstract into a fluid and practical format.

The ADM organizes ontological terms via a tabular model or a graph model (Fig. 4). A tabular model is well suited to describe key-value data and can show relationships between nodes in a one-to-one hierarchical relationship. The tabular model is deemed sufficient to describe most laboratory work that only requires mining of entity–result relationships. The graph model includes more complicated relationships (including one-to-many and many-to-many) and visualizes these relationships in a fully connected graph. Often, a tabular model will act as the basis for developing a full graph model as the need arises to support these additional relationships and complex data exploration.

The AF has developed a set of mature models that are available and ready to use by Foundation members. Publicly accessible information is limited but becoming a Foundation member is free for academic and nonprofit users, which grants full access to internal documentation and training materials. A current list-

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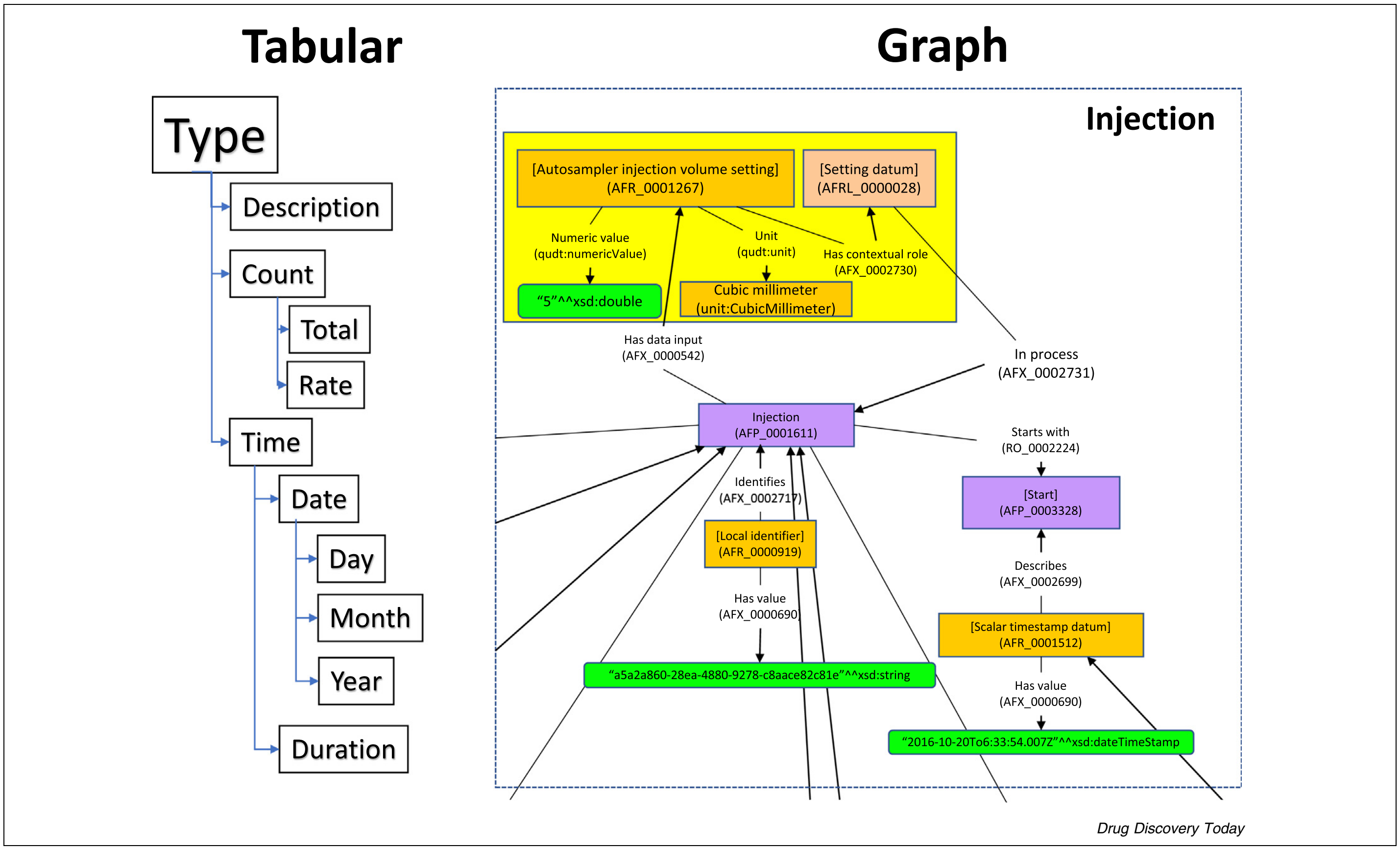

FIGURE 4

High-level comparison between **(a)** tabular- and **(b)** graph-based data models. In **(b)**, only a portion is shown to illustrate complicated relationship modeling through use of nodes and arcs. These are given as a visual representation of data organization concepts, with **(a)** Tabular showing hierarchical relations and **(b)** Graph showing more elaborate relations. A step-by-step guide for how to resolve the labels is given in Supplemental Information 3 in the supplemental information online.

ing of available ADMs can be found at www.allotrope.org/product-releases. Requests to prioritize additional data models can be submitted to the AF for consideration at any time.

Summary of the Allotrope Connect Fall 2020

Allotrope development progress

In the recent Allotrope Connect in October 2020 [25], Vincent Antonucci and Matthew Fox announced seven new Allotrope Partner Network companies: Intel, Benchling, Dotmatics, LabTwin, Digital Lab Consulting, SpyroSoft Solutions, and Protein Metrics. They also disclosed two upcoming projects: Python bindings for the Allotrope Data Format, and a high-level API for Tabular Graph Models. In their conclusion, they presented a workflow for successful implementation of the Allotrope Technology, with support opportunities from the foundation.

With growing interest in ADF, new member companies need access to training resources. Amnon Ptashek explained the principles [26] of the basic formal ontology (BFO) [27] and how the AFO (https://bioportal.bioontology.org/ontologies/AFO) extends these. A presentation by Karen Colsman [28] further expanded on these ideas and introduced quality assurance tools to ensure high-quality extension of the AFO.

Wes Schafer and Oliver He further elaborated on the importance of developing and extending ontologies [29] with process chemistry as a use-case for Merck & Co. This combined effort from industry and academia produced a new ontology, which provides a clean means for extracting and aggregating analytical data from experimental and process data and succinctly archives dissimilar data.

Dennis Della Corte [30] discussed that the Foundation currently impacts scientific publications in a minor way, but business-driven evaluation of the ADF, additional technical review reports, and successful use for FAIR data [31] adoption will benefit projects within industry and subsequent academic investigation will increase the visibility of ADF in the scientific community.

The concluding panel discussion [32] re-emphasized that the AF has matured into a strong and diverse community of supporters. To continue on the path of success, Graham McGibbon highlighted that communication between the Allotrope community and suppliers remains vital to achieve strategic objectives. The focus in the future will be less on the development of the format and ontology, but rather on the application of the associated technologies. Supplemental Information 4 in the supplemental information online outlines an adoptions process for interested parties.

Reports on pharma and business use-cases

The Allotrope Framework is a mature technology stack and an increasing number of companies within and outside of the AF

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reported on successful business cases using ADF, AFO, and ADM. Novartis demonstrated how an Allotrope-powered digital integration hub reduced the administrative overhead for data scientists from months to hours [28]. An end-to-end approach connected laboratory instruments with data analytics tools. They achieved this by using ZONTAL, a digital integration hub, to convert the raw data into Allotrope files and leveraged the data description layer to store semantic metadata about the experiments. The data scientists used this system see the full context from the metadata without needing to enter long discussions with the data creators.

Macromoltek, a biotech company that focuses on *in silico* drug discovery, presented another use-case [33]. As frequently reported by biotechs [34], numerous data-quality issues, such as finding important data sets, understanding legacy data, or integrating various data sources, reduce operational efficiency. The presentation introduced a new ADF-based workflow that allowed a data scientist to rapidly build dashboards with ZONTAL to execute project-wide analysis. The conversion of raw data from an ELISA assay [35] to ADF created a FAIR [31] representation of the data that could be used to drive high-value analysis.

Biogen showed their roadmap toward Allotrope adoption [36]. They initially used Allotrope ontologies to enrich data from PCRs and ensure future readability by various scientific instruments. Instead of converting all data to ADF, Biogen used a platform by TetraScience to create intermediate files in JSON. Future projects will convert the interoperable JSON data format into the ADF for long-term storage and recall.

Technical presentation and demos

Member and partner companies showcased new and exciting developments around the ADF. SCIEX presented, with Bayer and Boehringer Ingelheim [37], a newly developed ADF export and visualization tool for the SCIEX Analyst software designed for mass spectrometry. Whereas SCIEX-specific vocabulary powers their viewer, the unit and vocabulary URIs allow customizations. The viewer can read SCIEX ADF files and display data in tabular and hierarchical formats. Additionally, it can display total ion and extracted ion chromatograms. The data it reads can be exported in the TTL and XML format. Plans for the further development of the SCIEX ADF viewer involve integration into the existing ADF Explorer, harmonization with the mass spectrometry date shape, and Good-Laboratory-Practice support.

Agilent and ZONTAL showed how an ADF-powered Pistoia Alliance Method Database can interact with OpenLab [38]. Their integration of OpenLab CDS and ZONTAL Space replaces paper-based method description with a digital form for automated interfacing between LIM systems and laboratory instrumentation. This solution increases data integrity, improves process efficiency, increases cyber resiliency, and ultimately enables digital analytical method sharing across laboratories.

Boehringer Ingelheim and Pfizer set out to develop a rapid ADF converter framework for instruments [39]. They automated the building of initial data models, writing of code as reusable modules, and testing the output. Their conversion tool requires a vendor file parser that sends data to an aggregator tool to produce ADF files. Future plans include development from a series of command-line programs into microservices with REST endpoints.

As soon as a company has millions of ADF files under management, the task of high-performance data analysis will become more urgent. A presentation by Paradigm4 introduced currently available big data tools and suggested that these might be used to manage ADF files [40].

Accurids and Agilent described the functional capabilities for integrated publication of AFO with vendor-specific extensions focused on analytical models [41]. Although AFO provides the standardized vocabulary, there is still a need for vendor-specific extensions to capture instrument sub-types with corresponding process parameters. Given a lack of integration and scalable publication mechanisms, unpublished private extensions remain a barrier to adoption for vendors. They also demonstrated software that combines terminology-browsing capabilities with Persistent Uniform Resource Locator (PURL) mechanisms, which are a web link intended almost exclusively for machine consumption (see https://archive.org/services/purl/help for more information on PURL, and http://purl.allotrope.org/ for Allotrope PURL resources).

Concluding remarks and outlook

The AF is a vibrant group of pharmaceutical companies, software and service vendors, and academic partners. The regularly released Allotrope Framework technologies have found their way into the first commercial products and are being evaluated in various proof-of-concept stages at large pharma companies. Throughout the past decade, the goal of the consortium has remained the same, but the strategies and tactics for achieving it are continuously evolving. For example, the idea of a comprehensive graph model was initially considered as the Holy Grail of data exchange, but now we observe a trend toward the development of simpler, table-based models for many use cases focused on trending and basic analytics of experimental results.

The number of member and partner companies has increased with the availability of new and matured software products. The current level of adoption of the standard is still limited, but the recent Allotrope Connect showed at least two cases of biopharma companies beginning to adopt the standard without being as yet official members of the consortium. The development of a FAIR data representation is a frequently encountered buzzword, and ADF has shown potential to qualify as a reasonable container to implement FAIR self-reporting data assets.

The laboratory informatics market is a lucrative niche for many service and solution providers, which could be impacted by a successful data exchange standard. Although the influence of digital transformation and AI strategies in industry will increase demand for native support for ADF and drive market penetration, academia and nonprofits can benefit from free membership of the consortium and leverage the network to give students insights into pharmaceutical business problems and access to a broad range of its major companies. We expect to see more academic collaborations around the Allotrope Framework technologies and additional proofs of value in other industries in the near future.

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Declaration of Competing Interest

T.M. and D.D.C. are also employed by ZONTAL, Inc. D.V. is board member of the Allotrope Foundation.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.drudis.2021.03.028.

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