2023 Spring Allotrope Connect Agenda

Day 1 - Public Session: "Allotrope in Action" - Presentations from Allotrope Foundation and Allotrope Partner Network Members

Time (EDT)	Webex, Accessories	Subject/Title	Speaker	Organization
Day 1: Tue, Apr 25		**Day 1: Open to the public - "Allotrope in Action" Presentations**		
8:30-9:30		**Gatherings/networking**		
9:30		**Welcome and short introduction to Allotrope Foundation and Technology**	**Corey Bakalarski**	**Allotrope Foundation**
10:00	Webex (from Europe)	**How open-source projects have been made possible by CC ASM**	**Maxime Visconte**	**IFPEN**
10:25	Webex (from Europe)	**Automatic Sample preparation**	**Diego Olivares Garcia**	**Novo Nordisk**
10:45		**Morning break**		
11:00	Webex (from Europe)	**LC-UV Methods and Results Interoperability using ADF**	**Azzedine Dabo**	**GSK**
11:30	Webex (from Europe)	**Automation: the new frontier for Allotrope?**	**Frederick Francois Chesneau**	**BASF**
12:00		**Lunch**		
1:00	Webex	**Accumulus FHIR Overview for the CMC data**	**Sheetal Gaiki Rita Algorri**	**Johnson & Johnson, Amgen**
1:30		**Advances in Data Utility through Application of Process & Reading Ontologies in BIOVIA ONE Lab**	Kirsten Gesenberg	Biovia
2:00	Webex	**From Chaos to Clarity: ZONTAL's Digital Solutions for Biotech Wizards!**	Dennis Della Corte	Zontal
2:30		**Afternoon break**		
3:00		**Accelerating Bio-Tech innovation through instrument data standards**	**Nick Floeck**	**Benchling**
3:30		**If your strategy depends on data, you need a strategic roadmap to deliver data worthy of the aspirations**	**Dana Vanderwall**	**DLC**
4:00		**Group Discussion: What is your digital strategy? How can Allotrope technology help you realize it?**	**Vinny Antonucci (moderator)**	**Merck & Co, Inc**
4:45		**Closing Remarks**	**Corey Bakalarski**	**Allotrope Foundation**
6:00		**Welcome Reception and Dinner**		

Day 1 Presentations

9:30am - Welcome and short introduction to Allotrope Foundation and Technology (Corey Bakalarski, Allotrope Foundation)

10:00am - How open-source projects have been made possible by CC ASM (Maxime Visconte, IFPEN)

Allotrope Simple Model has been released under the open Creative Commons license. IFPEN demonstrates how this allows the plan to build an open-source library for the ASM written in Java and release it to the public to become a reality. The presentation will feature an overview of the components already publicly available, and a roadmap for the next month.

- **Maxim Visconte:** Director of IT for IFPEN, France's leading research institute on the energy transition. After a M.Eng in Chemical Engineering, and a few years in the industry working as an Advanced Process Control engineer, he is now in charge of facilitating data acquisition across all labs and pilot-scale industrial units for IFPEN researchers.

10:25am - Automatic Sample preparation (Diego Olivares Garcia, Novo Nordisk)

Workcell to automate sample preparation for chromatography analysis.

- **Diego Olivares Garcia:** IT/OT Architect. CMC QC Technology and IT at Novo Nordisk. Background - Mechatronic Engineer, MSc Industrial Engineering and Management, 4 year FAE for factory automation in Mitsubishi Electric, 3 Years as Automation Lead for Omnio a software company for industrial data standardization, 2 years NN IT/OT architect doing lab automation projects.

11:00am - LC-UV Methods and Results Interoperability using ADF (Azzedine Dabo, GSK)

Digitizing Analytical Methods - The methods Hub Project: Currently analytical methods used in the pharmaceutical industry face the twin challenges of interoperability and reproducibility due to the methods being stored and managed in paper form. They also are frequently stored in proprietary software platforms. Improving automation and interoperability of analytical methods may improve quality, enhance efficiency, and reduce cost. Such benefits are expected by enabling digital b2b method transfer (e.g. from CRO to Pharma), reducing manual entry and cost associated with human transcription errors, faster reproducibility, enhancing data use and re-use with thorough contextual meta-data, and improving out of spec (OOS) analysis capability. Looking forward, this infrastructure may help leverage data standard for machine-learning. In essence, easier compliance fosters more science.

- **Azzedine Dabo:** is currently part of GSK's Method Innovation Team based in Stevenage UK with area of interest in in-silico modelling, quality by design (QbD) method development and the transfer of analytical methods and results between chromatography instruments.

11:30am - Automation: the new frontier for Allotrope? (Frederick Francois Chesneau, BASF)

We will walk through a proof-of-concept implementation of Allotrope Simple Models to provide standardized data for synthesis workloads at BASF. In addition, we will go through the motivation and general approach we are currently following with a live demo of the current demonstrator. We will touch on IoT and sensor topics as well.

- **Frederick Francois Chesneau:** Head of Laboratory Data Solutions - Digital Laboratory, BASF Digital Solutions. After having lead material research laboratories for 5 years, Frederick has been driving digitalization at BASF for the past 7 years, currently leading a global team of 15 developers focusing on software for the laboratory, from experiment planning to laboratory automation systems.

1:00pm - Accumulus FHIR Overview for the CMC data (Sheetal Gaiki, Johnson & Johnson, and Rita Algorri, Amgen)

FHIR's capability for enabling exchange of data across a variety of formats and systems has many use cases including for CMC regulatory submissions. For this paradigm shift to occur, industry sponsors must match the investments in structured and standardized data put forth by health authorities. One such initiative includes HL7's BR&R DX-PQ initiative spawned from the sponsor companies supporting the non-profit organization Accumulus Synergy, which is developing a FHIR Implementation Guide for Quality Data.

- **Sheetal Gaiki, M. Pharm:** is an Associate Director in CMC Regulatory Submissions, Janssen Pharmaceuticals based in NJ, with industry experience in development of biologics, combination products and small molecules. In her current role, Sheetal is responsible for developing content strategy and delivering biologic and combination product dossiers for global submissions. She is also involved, and leading various internal and external efforts related to CMC data standardization, structured digital submissions through intelligent automation using scalable and sustainable data strategy, modernization of regulatory information management using emerging technologies. She is a Core Team member of CMC Data Exchange platform currently being developed by Accumulus Synergy.
- **Rita Algorri, PhD**: is a Manager, Regulatory Affairs CMC at Amgen Inc. in Thousand Oaks, CA. In this role, her responsibilities include leading and orchestrating internal and external engagement activities relating to regulatory modernization, digitization, automation, and emerging technologies. Rita is the Product Team Lead for the CMC Data Exchange platform currently under development by Accumulus Synergy. Rita is a microbiologist by training and holds a PhD in Clinical and Experimental Therapeutics and M.S. in Regulatory Science from the University of Southern California School of Pharmacy.

1:30pm - Advances in Data Utility through Application of Process & Reading Ontologies in BIOVIA ONE Lab (Kirsten Gesenberg, Biovia)

In the past, when capturing and working with experimental data produced by instruments, the limited application of ontologies has resulted in complex, poorly defined data structures that inhibit the constructive use of the data produced. Early efforts at improvement required complex, ad hoc application of parameter naming and tagging. At BIOVIA, the recent application of more carefully defined result and process ontologies creates a much cleaner, more well-defined approach to structured data, providing a more accessible and reusable data format.

- **Kirsten Gesenberg**: is the Portfolio lead for the BIOVIA Laboratory suite of products. She has been with Dassault Systems for 16 years, first in Professional Services, implementing BIOVIA Workbook across the pharmaceutical industry and now leading the Product Management organization in the Laboratory and ELN space.   Kirsten is passionate about shining a light on dark data while keeping the BIOVIA applications user-focused and intuitive.

2:00pm - From Chaos to Clarity: ZONTAL's Digital Solutions for Biotech Wizards! (Dennis Della Corte, Zontal)

Welcome to our talk about the ZONTAL Application Hub, the innovative digital solution that is designed to streamline data management and analysis for biotech companies. Our platform leverages the Allotrope Data Format, Ontology Model, and the Simple Model, providing new applications that are bundled into tailored solutions for biotech companies. In this presentation, we will highlight some key applications of ZONTAL that can help to enhance the daily activities of biology and chemistry laboratories. Our user stories will showcase how our platform can offer you a competitive edge and enhance your productivity. One of our major focuses will be on the Flow Cytometry application, which is an essential tool for analyzing cells and their properties. Flow Cytometry generates complex data, which can be challenging to manage. Our platform provides a user-friendly interface for data management and analysis, which can help researchers streamline their workflows and make better use of their data. Overall, our presentation will provide an overview of the ZONTAL platform and its applications, highlighting how our innovative solution can help to enhance your laboratory's efficiency and productivity.

- **Prof. Dr. Dennis Della Corte**: serves as Chief Science Officer at ZONTAL and Director of the Consortium of Molecular Design at BYU. His research applies artificial intelligence and advanced analytics in the fields off protein engineering, drug discovery, augmented pathology, and laboratory automation.

3:00pm - Accelerating Bio-Tech innovation through instrument data standards (Nick Floeck, Benchling)

Join us in this session to learn how instrument data standards can enhance scientific workflows & drive more efficient & automated research and development processes. Explore how Benchling can help the Allotrope community to operationalize Allotrope standards as part of a modern, end to end, smart R&D workflow that helps accelerate Bio-Tech innovation.

- **Nick Floeck:** is head of automation & analytics at Benchling. He joins us with over 15 years of experience leading development of data platform & operationalized analytic products & services that help customers transform their business.

3:30pm - If your strategy depends on data, you need a strategic roadmap to deliver data worthy of the aspirations (Dana Vanderwall, DLC)

The aspirations to be more data driven, or leverage predictive capabilities more heavily, are inescapably tied to the quality and availability of that organization's data. To go beyond targeted PoCs or prototypes and enable data across the enterprise to fuel those aspirations requires a strategic view of the full breadth of data across R&D and a roadmap for transformation of the lab data architecture and systems. This presentation will outline an approach to (1) assess the current state, with its bottlenecks, gaps and pain points; (2) define a data centric future state, including the opportunities to implement data standards, like the AFO, ASM, ADF and others; and (3) create an actionable roadmap to deliver the changes and capabilities that power the execution of a data dependent strategy.

- **Dana Vanderwall:** (B.S., Ph.D. Biochemistry) is Senior Director at Digital Lab Consulting. He was previously Executive Director of Enterprise Informatics at Schrödinger, following 26 years in the pharmaceutical industry at Merck, GSK and BMS in Computational Chemistry, Cheminformatics, and R&D IT. His extracurricular activities include contributor and leadership roles in Allotrope Foundation, the Society for Lab Automation & Screening (SLAS), Pistoia Alliance, and IUPAC.

4:00pm - Group Discussion: What is your digital strategy? How can Allotrope technology help you realize it? (Moderated by Vinny Antonucci, Merck & Co, Inc)

Day 2 - Allotrope Foundation and Allotrope Partner Network Members

Time (EDT)	Webex, Accessories	Subject/Title	Speaker	Organization
Day 2: Wed, Apr 26		**Day 2: Allotrope Foundation and Allotrope Partner Network Members**		
9:00		**Gatherings/networking**		
9:30		**Day 2 Opening Remarks** **- Day one reflections and day two introduction**	**Corey Bakalarski**	**Allotrope Foundation**
9:45	Mural board	**Learning from AFO/ASM implementation** **- building new content** **- extending existing content** **- governance** **- improving QA of content** **- building data pipelines** **- implementing cloud solutions** **- integration with downstream applications** **- consuming ASM files in your ecosystem**	**Vinny Antonucci (moderator)**	**Merck & Co, Inc**
10:45		**Morning break**		
11:00	Webex (from Europe)	**SoftMax output results standardization**	**Mike McGorry**	**Johnson & Johnson**
11:30	Mural board	**What are the key problem statements in your organization that require more FAIR data ? Which problem statements should Allotrope focus on in the near future ?**	**Janet Cheetham (moderator)**	**Amgen**
12:15		**Lunch**		
1:15	Webex (MS WG update)	**Working Groups updates** **- Mass Spectrometry Working Group** **- Chromatography Working Group** **- Modeling Working Group**	**Graham McGibbon, Ben Woolford-Lim**	**ACD Labs, Allotrope Foundation**
1:45	Mural board	**Domain coverage – which domains should Allotrope create content to support next to support some of the key problem statements identified in the morning ? Should Allotrope consider partnerships with other organizations to effectively achieve these goals ?** **- prioritizing remaining instrument types (we will review current catalog and planned roadmap for input) ?** **- materials ?** **- processing equipment ?** **- experiment design and procedures ?** **- common bioassays ?** **- digital specifications ?** **- regulatory content ?** **- something else ?**	**Corey Bakalarski (moderator)**	**Genentech**
2:30		**Afternoon break**		
2:45	Mural board	**Community projects – based on the discussions, are there areas of high common interest that we should explore creating community projects to execute this year ?** **- Open sourcing the ASM converter library**	**Gang Xue (moderator)**	**Johnson & Johnson**
4:00		**Closing Remarks**	**Corey Bakalarski**	**Allotrope Foundation**

Day 2 Presentations

11:00am - SoftMax output results standardization (Mike McGorry, Johnson & Johnson)

Currently it is very difficult to integrate data output from Softmax to 3rd party applications such as LIMS and integrated data lakes due to non standardization of templates. An overview of these issues around standardization of Softmax data with initial thoughts and opportunities to improve with harmonization across the industry will be presented.

- **Michael McGorry**: holds a Bachelors Degree in mathematics and Statistics. He has over 20 years' experience in the Pharmaceutical and Biotechnology industry covering a wide range of disciplines; Data analytics, LIMS and ELN system management, computer systems validation. His current passion is accessibility to analytical systems data to enable automated data analytics, reporting such as method validation, analysis, method performance analysis as well as automating data reports for BLA submissions. He was born and raised in New Zealand but has been an Irish resident for the last 25 years. Michael has 3 boys and is now an Avid supporter of Irish Gaelic football and hurling.

Day 3 - Allotrope Foundation and Allotrope Partner Network Members

Time (EDT)	Webex, Accessories	Subject/Title	Speaker	Organization
Day 3: Thu, Apr 27		Day 3: Allotrope Foundation and Allotrope Partner Network Members		
8:30		Board of Directors Meeting (Allotrope Board members only)		
9:00-12:00		A Combined meeting of the technical Working Groups: in-person/remote hybrid session		
		Technical meetings and Product Team office hours		