

2022 Fall Allotrope Connect Agenda

Day	time EDT	[M in]	Org,	Title	Presenters	Abstract
1	10:00	5	Allotrope	Event welcome and introduction	- Corey Bakalarski, Ph.D. , Allotrope Chair, Senior Principal Bioinformatics Scientist, Computational Proteomics and Analytical Data Science Group. Depts. of Microchemistry, Proteomics & Lipidomics and Research Informatics & Software Engineering Genentech, Inc.	
1	10:10	30	Merck/ Tetra Science	ASM at Scale at Merck & Co, Inc	Presenters in order: - Wes Schafer , Director, Business/Tech. Analysis, Develop and Make Product, Composition of Matter Product Line, MRL IT - Vincent Antonucci , Composition of Matter Product Line Lead at Merck & Co, Inc., Chair Emeritus, Allotrope Foundation - Evan Anderson , Manager, Data Architects at Tetra Science	Merck has begun a 2 ½ year project with TetraScience to “FAIRify” its instrument data by implementing the Allotrope Simplified Model (ASM) at scale. It will convert data from over 10,000 instruments to ASM and leverages the TetraScience Data Platform to store and serve that data.
1	10:40	30	Dow/ Allotrope Product Team	Modeling Working Group Update: Models, Statistical Features, Aggregation Patterns, and Converter Implementation	Presenters in order: - Amnon Ptashke , Technical Director, Allotrope Product Team - Ben Woolford-Lim , Senior Developer, Allotrope Product Team - Simon Cook , Solution Manager at Dow, Research Data Management - Leo Musters , Solution Manager at Dow, Research Data Management - Vasiliy (Vas) Dulskiy , Informatics on assignment at Dow	The Modeling Working Group and Dow Chemicals will present an update on its recent activity and development. The presentation includes - A short overview of the path for modeling a new technique using Excel. - Statistical features and aggregation patterns - Data Science in the Chemical Industry - Dow developed models - Dow Converter Design and Implementation
1	11:10	10	Allotrope Product Team	Allotrope Modelling Domains: Potential opportunities for future expansion	- Ben Woolford-Lim , Senior Developer, Allotrope Product Team	Brief review and potential gap analysis to suggest new opportunities for modeling domain expansion, and the related domain coverage (Ontologies and Data Models) for E2E laboratory workflow.
1	11:20	30	Bayer- MIT	Multivariate Online Contextual Chromatographic Analysis (MOCCA) via ADF data access	Presenters in order: - Henning Kayser , Digital Transformation Lead, Bayer AG, Research & Development, Crop Science, Small Molecules Technologies - Christian P. Haas , Massachusetts Institute of Technology & Bayer AG, Crop Science Division, Since October 2022, Christian works as an R&D	Providing a closed-loop reaction optimization example, on how HPLC raw data use can open up new ways of innovating in process chemistry and revolutionize analytics by transforming from a post-experiment info into becoming integral part of in-process decision making. Multivariate Online Contextual Chromatographic Analysis (MOCCA) is a recently published

			<p>scientist in the Liquid Phase Separation Division of Agilent Technologies - Laura Di Rocco, Lead Knowledge Engineer, Bayer Pharmaceuticals CMC department.</p> <p>Henning Kayser is heading the Digital Transformation group for Small Molecules Technologies at Bayer Crop Science, leading the transition into new, innovative ways of converting scientific data to knowledge. Henning studied industrial chemistry at RWTH Aachen University & UPMC/Sorbonne Paris before joining Bayer as an R&D IT consultant. He is a recognized leader in lab digitalization combining IT, data and scientific aspects synergistically with a strong track record at Consumer Health and Pharma unlocking their potential by making scientific data accessible applying standards and leveraging central data assets. As part of this role, he is member of Allotrope Foundation's Operations Team on behalf of Bayer and putting Allotrope's vision of a smart analytical laboratory into practice.</p> <p>Christian Haas studied chemistry in Marburg an der Lahn, Germany. During his PhD, his research focused on analytical chemistry, flow chemistry, and automation. His two-year postdoc program on closed-loop reaction optimization led him in the group of Professor Klavs Jensen at MIT and the Process Research division at Bayer Crop Science where he got in contact with Allotrope. Since October 2022, Christian works as an R&D scientist in the Liquid Phase Separation Division of Agilent Technologies in Waldbronn, Germany.</p> <p>Laura Di Rocco works in Bayer Pharmaceutical as Lead Knowledge Engineer for the CMC department. She got her PhD in Computer Science in 2019 from University of Genova, Italy. After 2 years as a PostDoc at Northeastern University in Boston, MA, Laura joined Bayer in the middle of 2021. Since then, her role has been to develop and maintain ontologies for CMC and sponsor FAIR technologies for integration.</p>	<p>https://doi.org/10.26434/chemrxiv-2022-0pv2d open source, Python-based analysis tool of HPLC-DAD raw data directly from crude reaction mixtures, including multidimensional-deconvolution of signals for tracking and quantification of impurities and side products. Access to the DAD raw data from industry-standard Chromatography Data Systems can be challenging. In this work it is shown ADF-data can be read for downstream use within the MOCCA App.</p>
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1	11:50	30	Zontal	You have FAIRified your data. Now what?	- Dennis Della Corte, Chief Science Officer. ZONTAL, INC.	Laboratory data in all its variability and complexity has posed a seemingly insurmountable challenge to those seeking adherence to FAIR data principles. In a concerted effort, together with leading partners from Pharma and Biotech and the Allotrope community, ZONTAL has established a scalable platform that now delivers what seemed only a few years ago Utopia – FAIR data for the modern laboratory. However, FAIR data is a milestone, not the destination. ZONTAL's Digital Lab and Life Science Analytics solutions lead the industry in delivering unmatched instrument connectivity for easy processing and analysis of scientific data that open the door to future advancements in machine learning and artificial intelligence. Join us to learn how we leverage the Allotrope Data Format and Allotrope Foundation Ontologies to pass the FAIR bar and why it is not enough to just store data in the cloud. See how our customers leverage ZONTAL to accomplish unprecedented success in delivering digital transformation and data science at scale. Witness the future of the digital lab, powered by ZONTAL.
1	12:20	5	Allotrope	Day 1 closing and Day 2 short introduction	- Corey Bakalarski	
2	10:00	5	Allotrope	Day 2 Welcome and introduction (Summary of Day 1)	- Corey Bakalarski	
2	10:10	30	LADS-Spectaris	LADS OPC UA – The “Common Language” for Lab & Analytical Devices	<p>Keynote:</p> <p>- Dr. Matthias Arnold, Technical Lead LADS OPC-UA Joint Workgroup “Laboratory and Analytical Device Standard”, SPECTARIS & OPC Foundation</p> <p>- Serial entrepreneur and CTO in the field of laboratory equipment and services for biotechnology research</p> <p>- Research background in industrial connectivity (PhD, RWTH Aachen University of Technology)</p> <p>- Chief architect of product digitalization platform for global laboratory instrument vendor</p>	<p>To date, most laboratory and analytical instruments are hard to integrate into information networks. Typically, they communicate via vendor specific communication protocols, if they provide interfaces at all. This situation hinders digitalization in the laboratory and analytical domain.</p> <p>LADS OPC UA is an upcoming communication standard that aims at plug & play integration of laboratory & analytical devices along the laboratory workflow. It addresses key use-cases such as remote monitoring and control, orchestration, service & asset management.</p> <p>LADS builds on the proven and established OPC UA industrial communication-protocol and will be published as an official OPC UA Companion Specification.</p> <p>Application domain specific ontologies such as the Allotrope Foundation Ontology play an important role with regards to</p>

					<p>semantic contextualization and enable transparent integration of "data in motion" (communication networks) with "data at rest" (database, files, ..).</p> <p>LADS OPC UA was established as an OPC Joint Workgroup (JWG). Its initial nucleus was formed by the SPECTARIS association, and its members. It was supplemented by VDMA and the OPC Foundation. In the meantime, many associations, global instrument vendors as well as software solution providers from the laboratory and analytical domain joined the LADS OPC UA JWG. The setup is complimented by groups representing international end users and implementers.</p>
2	10:40	30	Scitara	<p>Lab Interoperability with DLX Using ASM-JSON Format</p> <p>- Dan DeAlmeida, Head of Product Management, Scitara. Dan is a Scientist and Product Executive with decades of experience connecting technology and business to deliver customer-focused solutions in the laboratory industry. (BIOVIA- Dassault Systèmes & LabVoice)</p>	<p>Scientists across the world find a common language of science. With the increasing number of software, instruments, and devices being utilized in the lab, the amount of data has grown exponentially, meaning more resources are required to collate and interpret data. In addition, the current silos and fragmented data infrastructure make streamlining the laboratory workflows challenging. The deployment of traditional application-centric architecture has created an enterprise environment where new solutions require complex integrations and many data transformations.</p> <p>A new paradigm of data mobility where data are a key asset of any organization, enables applications to visit the data, perform their magic, and express the results of their process back into the data layer for all to share. With the combination Scitara DLX's ability to provide data mobility and transform data in flight as well as the Allotrope's ASM for the structure of instrument data, result data can be automatically standardized before storage in data lakes without need of further interpretation.</p>
2	11:10	30	Pistoia/ GSK/ Merck	<p>The Methods Database: From vision to execution</p> <p>Presenters in order:</p> <p>- Birthe Nielsen, Life Sciences & Biotechnology, Pistoia Alliance</p> <p>- Azzedine Dabo, Method Development and In silico Modelling, GSK</p> <p>- Pankaj Aggarwal, Associate Principal Scientist, Merck</p>	<p>Currently, liquid chromatography analytical methods used in the pharmaceutical industry face the twin challenges of interoperability and reproducibility due to the methods being stored in paper form or electronically in proprietary file format. Improving automation and interoperability of analytical methods using standard ontologies and with data stored in central location will eliminate manual and time consuming steps of the method transfer. This will not only improve the method transfer efficiency but also reduce the number of OOS results and enable on-demand data analytics. In this presentation, we will share work done through this consortium and participating pharma companies demonstrating the successful bidirectional exchange of methods and data between different</p>

						chromatography data systems and different instruments using machine-readable representations of LC-UV methods. Data analytics using data and meta data stored in methods database will also be showcased. The next step of the project includes method transfer across different manufacturers' hardware and invite other pharma members to join this collaborative effort.
2	11:40	30	IFPEN	Leveraging Allotrope to achieve open-data compliance	- Maxime 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.	IFPEN is a public research institute, and as such, must release its experimental data to the public. This presentation will demonstrate how IFPEN leveraged Allotrope to achieve open-data compliance for its gas chromatography data, for the creation of the ASM model to the archival of the experimental data on an agnostic database, through a technical deep-dive into the development of a Java connector for ChemStation data (including the libraries used to parse the ASM JSON schema, map the experimental data, export and validate the experimental data against the standard schema – and the compromises required along the way).
2	12:10	5	Allotrope	Event closing	- Corey Bakalarski	