Arcondis BRUKER CHEMSPEED SciY

Autonomous Digital Labs Summit

April 1st, 2025

Agenda

Time	Topic	Speaker
13.30	Arrival, coffee	
14:00	Welcome	Stefan Müller, Chief Commercial Officer, Arcondis Bernd Gleixner, Divisional President Automation, Bruker
14:15	Keynote: Data-driven Automated & High-throughput screening	Paco Laveille, Managing Director SwissCAT+, ETH Zürich
14:45	Break-out sessions block 1	Break-out moderators
15:30	Coffee break	
15:50	Break-out sessions block 2	Break-out moderators
16:30	Keynote: Automation Connectivity and Digitalisation Concept for Roche Labs	Tom Kissling, Global pRED Lab Automation Partner, Roche
17:00	Break-out Summary	Break-out moderators
17:45	Closing	Christian Hebich, CEO, Arcondis
18:00	Networking with drinks and snacks	
19:00	End of the event	

A warm welcome from our side

Stefan Müller

Chief Commercial Officer
Arcondis Holding
Basel

Stefan is Global Chief Commercial Officer and Managing Director Switzerland at Arcondis, with over 18 years of experience in life sciences. He also serves on the board of obvioTec AG, an AI-driven quality control start-up. A former high-performance javelin thrower, Stefan brings a passion for excellence, innovation, and teamwork to his leadership.

Bernd Gleixner

Division President Automation
Bruker BioSpin Group
Zurich & Basel

Bernd held various roles in management, engineering and sales across industries - from Start Up to Corporate. Working for 9 years with Bruker and since March 2024 Managing Director of Chemspeed (a Bruker company). Stalking mountain streams in canton Grisons with a fly rod he learned persistence, resilience and creating opportunities.

The lab of the future is faster, smarter and cheaper

Augments scientist, enabling wider exploration, leading to greater innovation

▼ **25%**	cost reduction[1]
▼ **10-20%**	faster time to market[2]
▲ **30-40%**	increased productivity[3]
▼ **30%**	waste reduction[4]

[1]Baker, L., PhD. (2024, March 12). *Introducing the Lab of the Future*. Informatics From Technology Networks. https://www.technologynetworks.com/informatics/articles/introducing-the-lab-of-the-future-356898
[2]Colback, L. (2024, November 27). AI and the R&D revolution. *Financial Times*. https://www.ft.com/content/648046c1-7fcd-43fb-819b-841f104396d9
[3]Challenges to the Lab of the Future. (n.d.). https://labforward.io/test-blog-labtwin-new-2021/smart-lab-of-the-future-through-digital-transformation-and-lab-automation-0
[4]Baker, L., PhD. (2024c, March 12). *Introducing the Lab of the Future*. Informatics From Technology Networks. https://www.technologynetworks.com/informatics/articles/introducing-the-lab-of-the-future-356898

Six key components of a fully digitized lab

Arcondis provides process/workflow support for most components

01 Fully Integrated Digital Ecosystem

- ◆ Tools, devices and systems are connected
- ◆ Unified platform for data ingestion, curation, analysis and reutilisation
- ◆ AI and automation ready data

02 Data Driven Research (AI/ML)

- ◆ AI-driven insights, experimentation and pattern identification
- ◆ Predictive analytics to optimise and maintain R&D processes

03 Automation and Robotics

- ◆ Automated routine tasks like sample preparation
- Advanced robots for precise and complex tasks

04 Integrated Digital Processes and Workflows

- ◆ Instruments and data systems are seamlessly integrated
- ◆ Integrated workflows that streamline data capture, analysis, reporting and preservation

05 Sustainability and Smart Infrastructure

- ◆ Use of eco-friendly materials and energy-efficient technologies
- ◆ Waste reduction and sustainable resource management. Circular economy

06 Collaborative and Flexible Workspace

- ◆ Modular and collaborative workspaces to support interdisciplinary teams
- ◆ Real time collaboration tools for seamless interaction and joint work

◆ Arcondis support (Process/ Workflow)

Our view on total lab connectivity

From atoms to functions

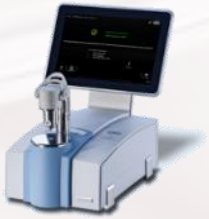
Sample preparation

Synthesis

Formulation

Fluorescence microscopy

Spectroscopy



NMR

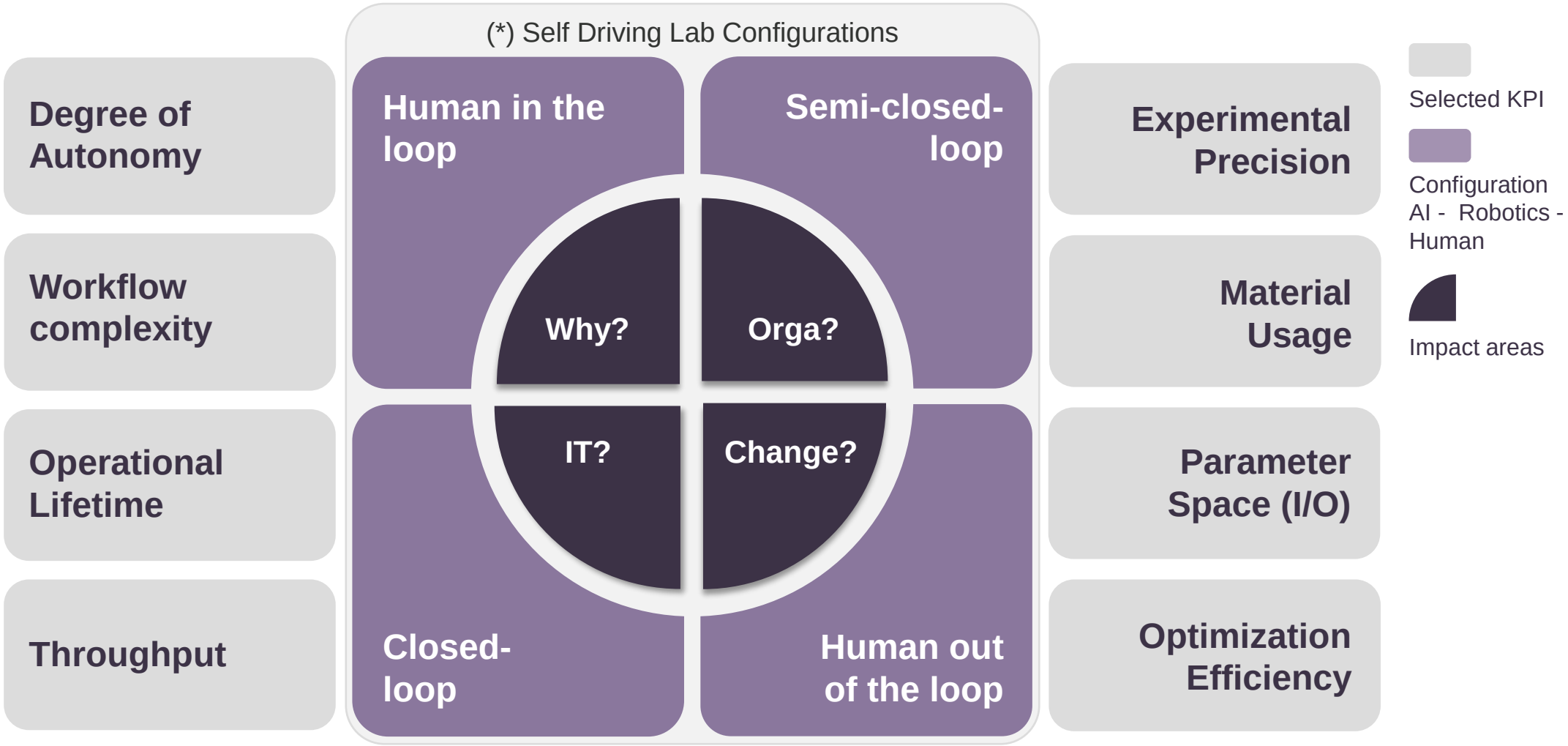
Elemental Analysis

X-ray diffraction

Logistics

AI Readiness

The Rise of SDLs(*): challenges in designing optimal autonomous labs



Build on: Amanda A. Volk & Milad Abolhasani, Performance metrics to unleash the power of self-driving labs in chemistry and materials science, Nature 14. February 2024, Discussion with Pascal Miéville

The next step towards the augmented scientist? AI multi agents in your lab

User (M2M, Human)

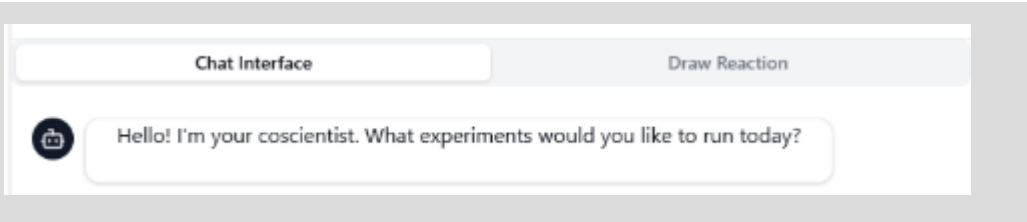
Input / prompt

Supervisor

- LLM Setup
- Agent Orchestration
- Data Loading & Indexing

Agents

- Agent 1 Workflow programming
- Agent 2 Experiment planning
- Agent 3 Retrosynthesis
- Agent 4 …



- Robotic platforms
- Instrument software
- Human and more…

Output

Dynamic hybrid experiment optimization

- «Brute force» BO
- Combi BO w/ LLM
- Hypo-thesis
- Human in the loop

Keynote: Data-driven Automated & High-Throughput Screening

This session will explore the SwissCAT+ East platform at ETH Zurich, a cutting-edge, data-driven facility for catalyst discovery and optimization. We will dive into its high-throughput capabilities in catalyst synthesis, characterization, and testing, highlighting the seamless integration of a robust data management system. A key focus will be on Bayesian Optimization in closed-loop experimentation, accelerating the screening of vast chemical spaces with minimal human intervention. Finally, a compelling case study on CO_2-to-methanol hydrogenation will showcase how this approach condenses years of catalyst development into weeks, paving the way for next-generation AI-driven research workflows.

Paco Laveille

Managing Director
SwissCAT+ ETH Zurich

Break-out and collaborate

TOPIC #1

Automated Qualification & Validation for Digital Labs

MODERATOR
Pascal Lauener,
Chief Digital Officer,
Arcondis

Pascal Lauener

TOPIC #2

Connected & Self-driving Labs Trends

MODERATOR
Anna Codina,
Senior Director,
Strategy @ BD,
SciY

Anna Codina

TOPIC #3

Lab of the Future Data Strategy

MODERATOR
Mark Polinkovsky,
Head of Data Science Services,
Arcondis

Mark Polinkovsky

TOPIC #4

AI for Autonomous Digital Labs

MODERATORS
Mathias Cherbuin
CTO Chemspeed

Loic Roch
CTO/Co-Founder
Atinary

Mathias Cherbuin
Loïc Roch

EXECUTION

- All break-outs repeated twice
- You have pre-registered to two break-outs out of the four, please follow your color codes
- Each break-out lasts 40 minutes
  - Starts with 5 minutes introduction
  - Followed by an interactive discussion about experiences, best-practices, challenges, and opportunities
- Discussion results will be documented and presented at the end of the event

Breakout session #1
Automated Qualification & Validation for Digital Labs

Pascal Lauener

Chief Digital Officer,
Arcondis AG

Director Software Engineering

Senior Vice President Global IT

DevOps Sr Project Lead

Lead DevOps Architect

Computer Science

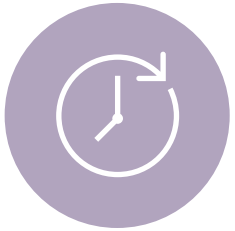
IT Management

Business Process Engineering

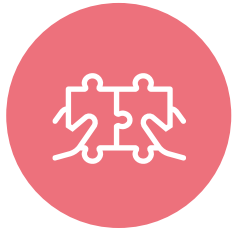
- **We've conquered 99% automation in Computer System Validation for software—so why are labs still stuck in the slow lane? It's time to break through the barriers.**
- In this workshop we will discuss what are the blockers to bring test automation, infrastructure as code, and DevOps best practices like Continuous Integration (CI)/Continuous Deployment (CD) to lab validation.
- Get inspired by real-world success stories, tackle automation roadblocks, and walk away with actionable strategies to revolutionize your lab workflows.
- Whether you are a lab pro, software engineer, or quality specialist, this session is your ticket to the future of validation!

Problem statement

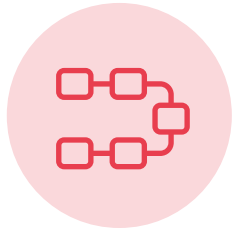
Manual handling of CSV files leading to errors and inconsistencies.



Manual handling of CSV files are time-consuming due to the manual writing, reviewing, and approval of documents.



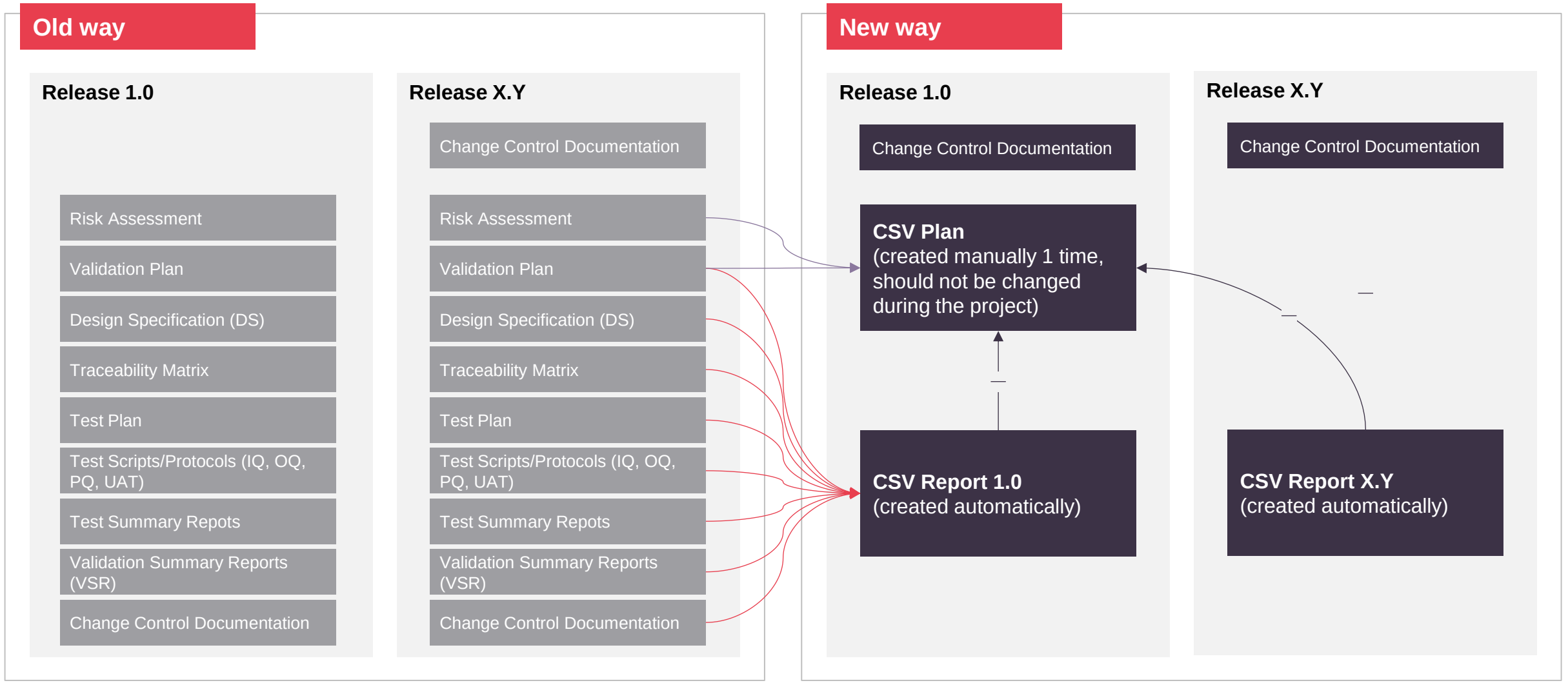
Normally, a lot of CSV-related data is already produced during the software development process, but it is not used for the CVS documents.



The manual process hinders the ability to release or update more frequently.

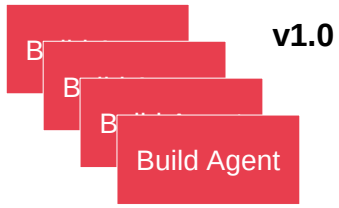
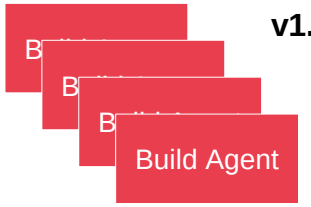
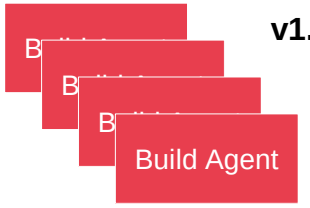
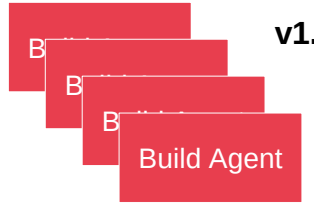
Old way vs new way of CSV example

Changing the way of SDE Validation



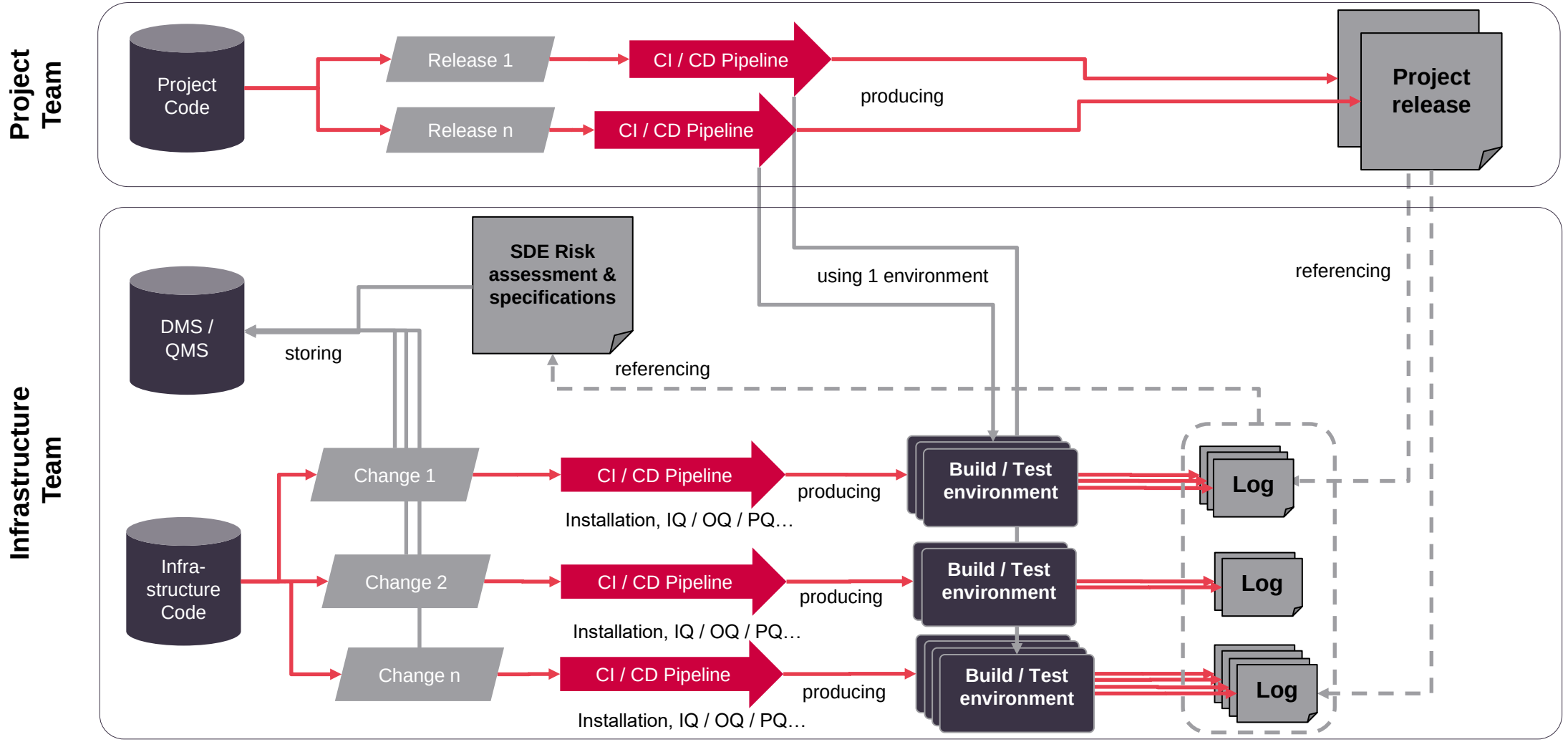
Old way vs new way of CSV example

Changing the way of SDE Validation

SDE Validation Process	**SDE Lifecycle**			
SDE Occasions	**Initial**	**Change 1**	**Change 2**	**Change 3**
Builds	 **v1.0**	 **v1.1**	 **v1.2**	 **v1.3**
Effort currently	Full CSV document stack	New version of many CSV documents	New version of many CSV documents	New version of many CSV documents
Effort future	2 Documents 1 document (DMS) 1 automated (log)	2 Documents 1 Change (Ticket) 1 automated (log)	2 Documents 1 Change (Ticket) 1 automated (log)	2 Documents 1 Change (Ticket) 1 automated (log)

Best practice for automated CSV in software development

Detailed project setup and approach



Questions for Discussion

TOPIC #1

What do you think is the biggest blocker to do automated validation right now?

TOPIC #2

What do you think will be tricky to automate (from a technical point of view)?

TOPIC #3

What do you think would be the biggest issue with this approach during an external audit?

TOPIC #4

What do you think would be the biggest challenge in changing internal processes to enable automation validation?

Breakout summary

TOPIC #1

- **Change & Compliance**: Managing change, knowledge fluctuation, and regulatory sharing is essential.
- **Human Involvement**: Employees need to understand, support, and oversee changes.
- **Resources & Support**: Financial and managerial backing is necessary for success.

TOPIC #2

- **IT Security**
- **System Compatibility**
- **Validation Complexity**: IQ is easy, OQ is medium, and PQ is difficult.

TOPIC #3

- **Regulatory & Audit Complexity**: Automation may be difficult for auditors to understand.

TOPIC #4

- **People & Systems**: Dedicated experts, proper system validation, cross-department integration, and clear QA control are required.
- **Costs vs. Saving:** When does it make sense to implement?

Breakout session #2
Connected & Self-Driving Lab Trends

Anna Codina

Senior Director Strategy & Business Development, SciY

Senior Director Biopharma

Principal Scientist, Analytical R&D

Structural Biology (PostDoc)

Antibody Structure Characterisation

Quality Control (Internship)

PhD in Chemistry and Structural Biology

- **Imagine a lab that thinks, learns, and optimises itself—a true self-driving laboratory! The age of autonomous labs is here, powered by cutting-edge AI, automation, and next-gen data systems.**
- In this electrifying session, we will reveal how smart labs are augmenting scientist, slashing inefficiencies, and delivering significant return of investment.
- But it’s not all smooth sailing—what are the biggest adoption hurdles, and how can you overcome them?
- If you’re looking to future-proof your lab and stay ahead of the innovation curve, don’t miss this session!

WHAT IS A CONNECTED SELF-DRIVING LAB?

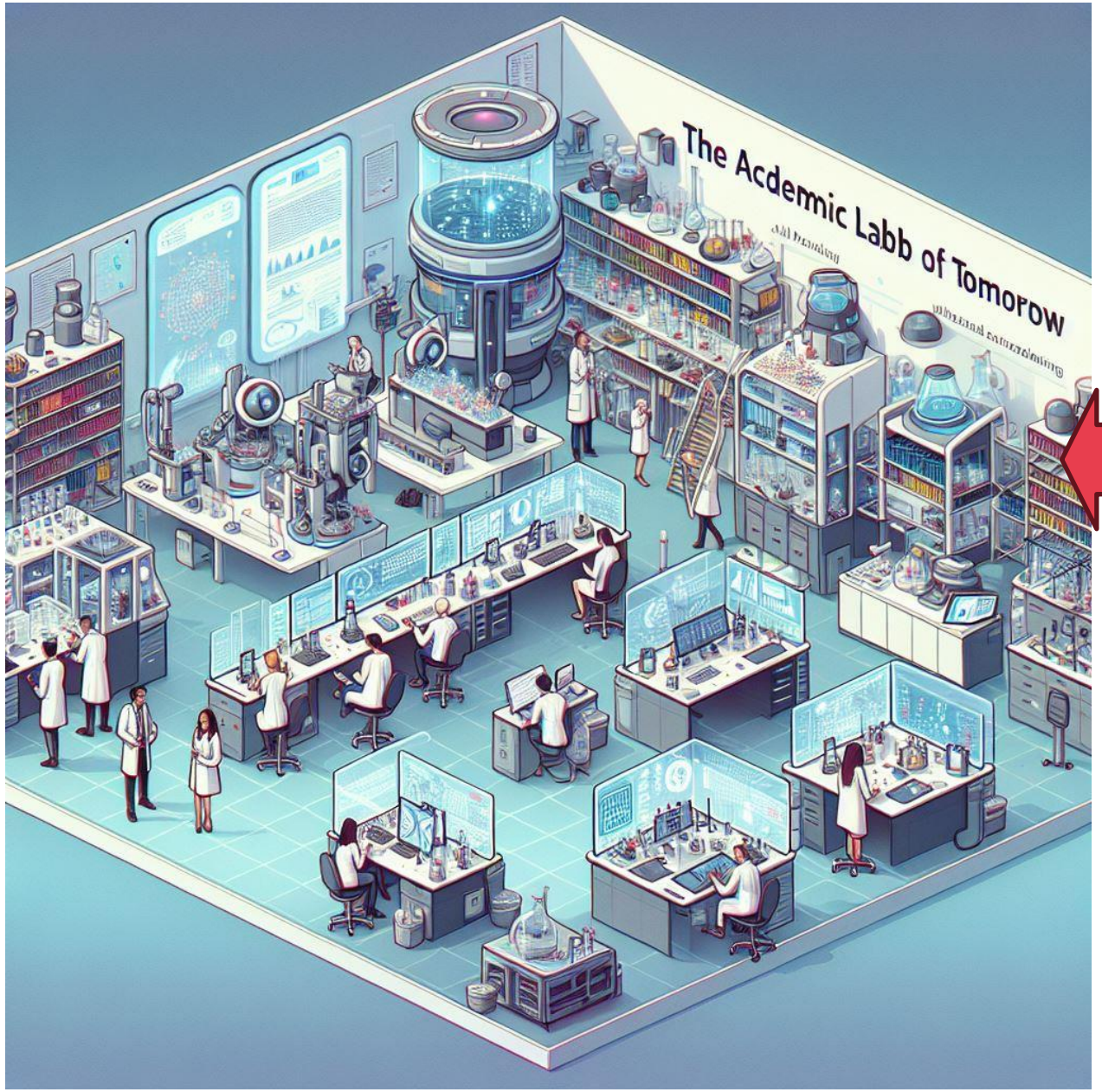


Image AI generated (01Apr25) to illustrate content of the following paper:

Adam, D., The Automated Lab of Tomorrow, PNAS, 121(17), 2024

A different, interesting concept is described in “Digitalization, automation and online testing: Embracing smart quality control”, McKinsey & Company, 2021

WHAT IS A CONNECTED SELF-DRIVING LAB?

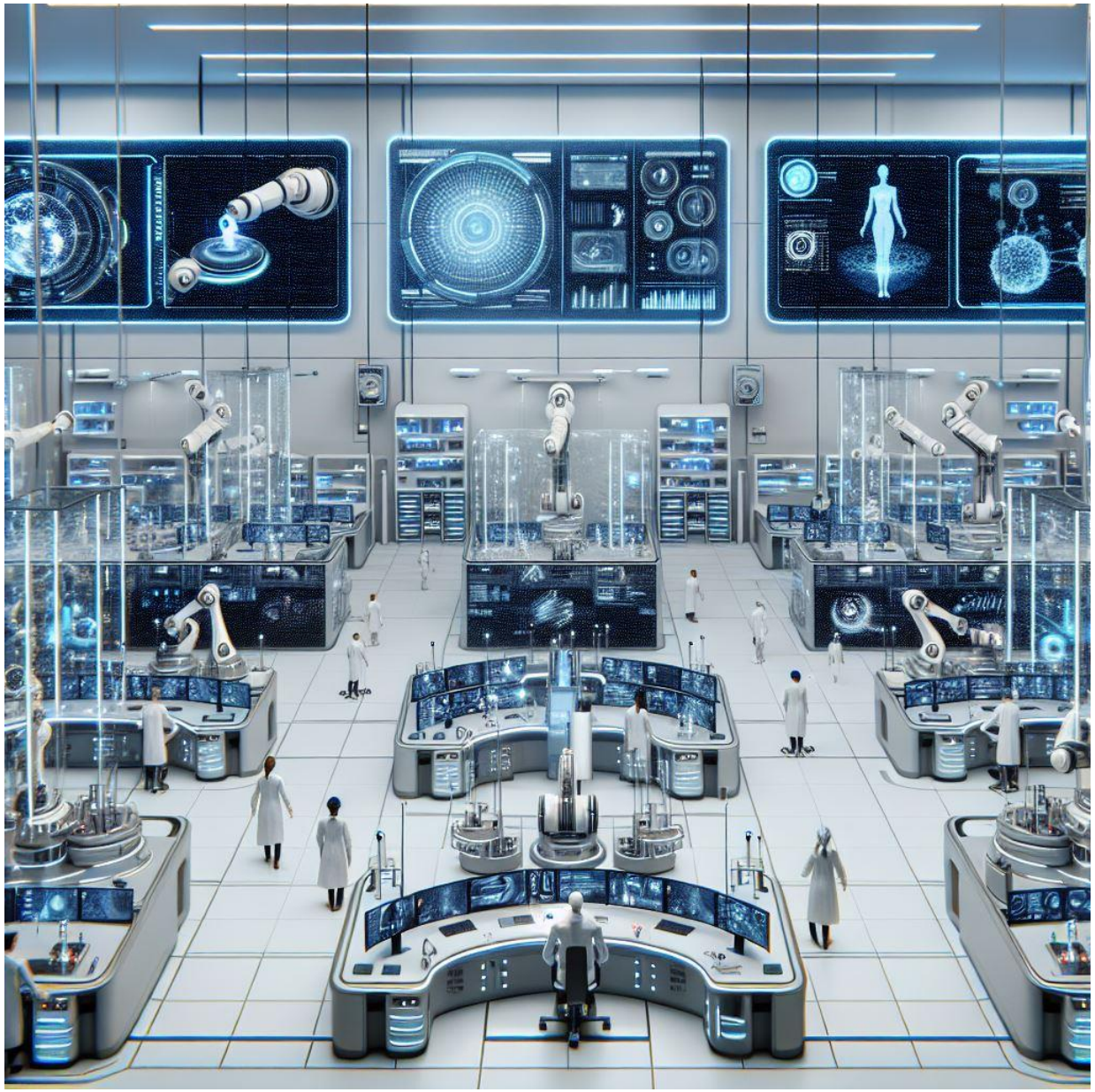


Image AI generated (01Apr25) to illustrate content of the following article:

A Blueprint for Supporting Self-Driving Labs in the UK, UKDayOne, 2024

ACCELERATED TIME TO MARKET

OPTIMIZED COSTS

REDUCES HUMAN ERRORS AND RISKS

ENHANCED PRODUCTIVITY AND REPRODUCIBILITY

INCREASED APPROVAL RATES

IMPROVED COMPLIANCE

STRENGTHENED SUSTAINABILITY

AI-driven high throughput

Synthetic biology for drug discovery and development

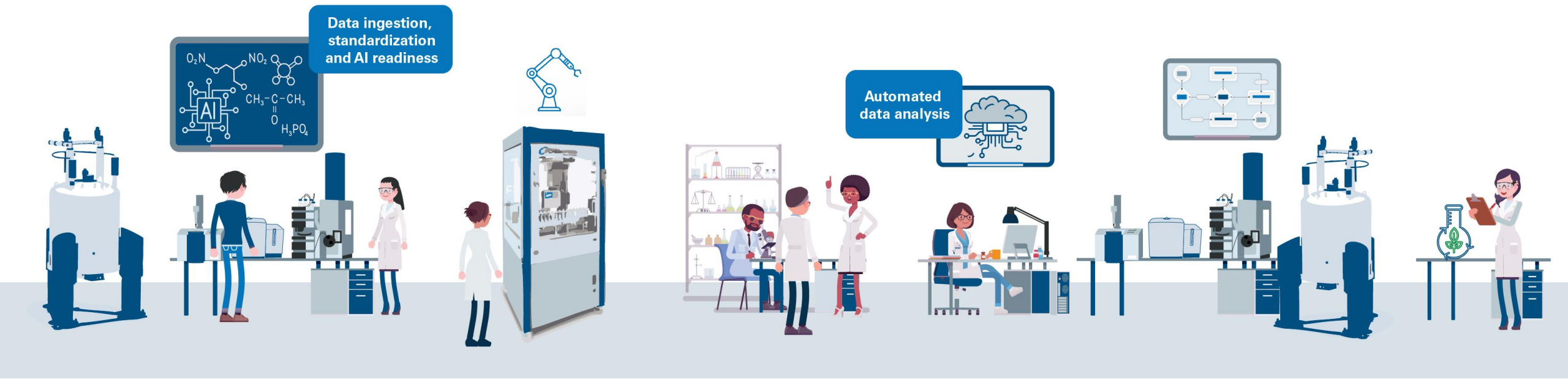
Robotics for automated sample preparation and synthesis

Data and sample management

Digitalization data platform

Automated workflows

Green Chemistry



Automation & Digitalization for R&D / QC | Bruker

THE ULITMATE SUSTAINABLE LAB

Images AI generated (01Apr25) to illustrate content of the article:

The 2050 Lab of the Future: Sustainability, The Analytical Scientist

Questions for Discussion

TOPIC #1

MACRO TRENDS

What are the scientific and technology macro/mega trends in your industry/area?

What are the connections between the macro trends and self-driving labs?

TOPIC #2

TRENDS in SDL

What are the trends with respect to connected and self-driving labs?

Where are were today?

Where are the gaps between today and tomorrow? How do we fill the gap?

TOPIC #3

BARRIERS in SDL

What are the adoptions barriers towards SDL?

How do we win? (decrease the adoption barriers) and what are the gains? What if we do not do it?

What strategies and partnerships?

TOPIC #4

HUMANS in SDL

How do you see the role of humans in the SDL today?

How do you see the role of humans in the SDL of tomorrow / the future? (e.g., in 10 years, time)

Breakout summary

TOPIC #1

- **Automation**
- **Miniaturization**
- **Connectivity**
- **AI**

TOPIC #2

- **Trends:**
  - Automation
  - Data Strategy
- **Status:**
  - Island w/o connectivity
  - Lack of data management / digitalization
- **Gaps:**
  - Connectivity
  - Data standards
  - Skills / Knowledge
  - Cost

TOPIC #3

- **Barriers:**
  - Change mgmt
  - Regulations
  - Equipment reliability
  - Cost
  - No data standards
  - No proof of value
  - Instrument orchestration
  - Skills
- **Proposed approach:**
  - Modularity
  - Partnership

TOPIC #4

- Humans will not be eliminated
- Humans are augmented, focus on strategic and intellectual tasks
- Processes which are not yet automatable

Breakout session #3
Lab of the Future Data Strategy

Mark Polinkovsky

Global Head of Data Excellence,
Arcondis AG

Director of Science and Technology

Data, Innovation, and Automation Investigator

Physics BS – Caltech

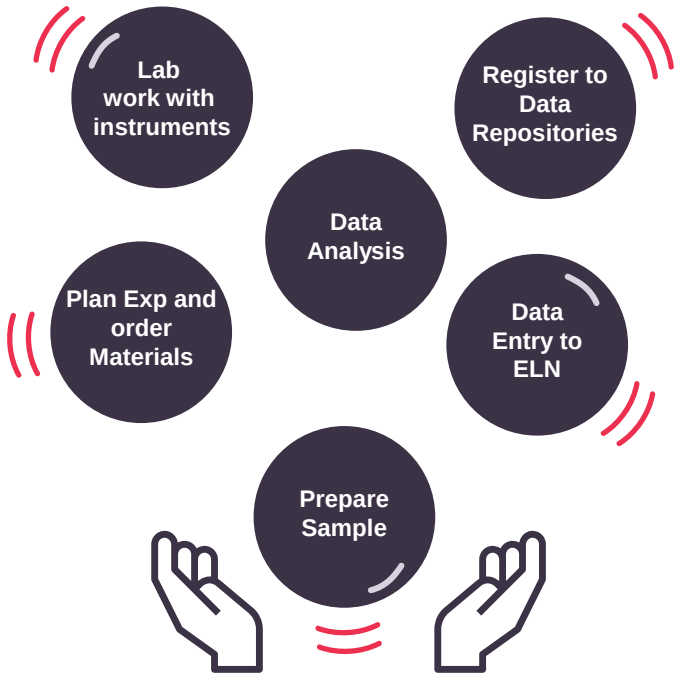
Biophysics PhD – UCSD

- **Your lab's data should work for you, not against you. But too many labs are drowning in disconnected, unstructured, and underutilized data. It's time to fix that.**
- In this power-packed session, we will show you how to build a future-proof data strategy—one that enables seamless system integration, bulletproof governance, and real-time AI-driven insights.
- We will also tackle compliance pitfalls and regulatory must-knows, ensuring your lab stays ahead in a fast-evolving digital landscape.
- Ready to take control of your data and accelerate your lab's transformation? Join us!

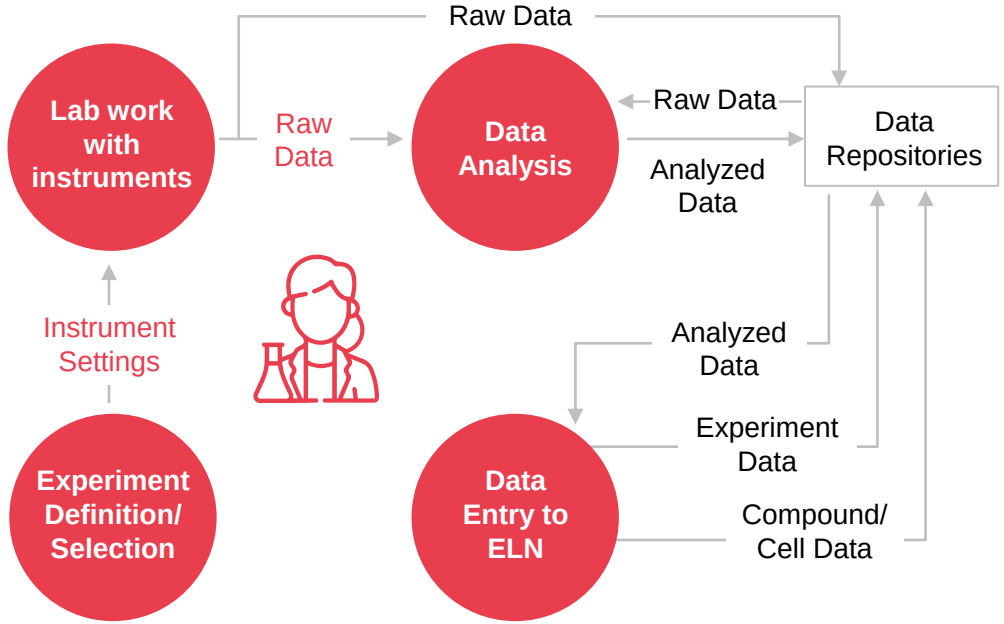
Data Strategy as a Prerequisite for the Digital Lab

Automated data movement between systems allows scientists to focus on their research

Laboratory Data Flow Diagram - Current State



Laboratory Data Flow Diagram – Future State

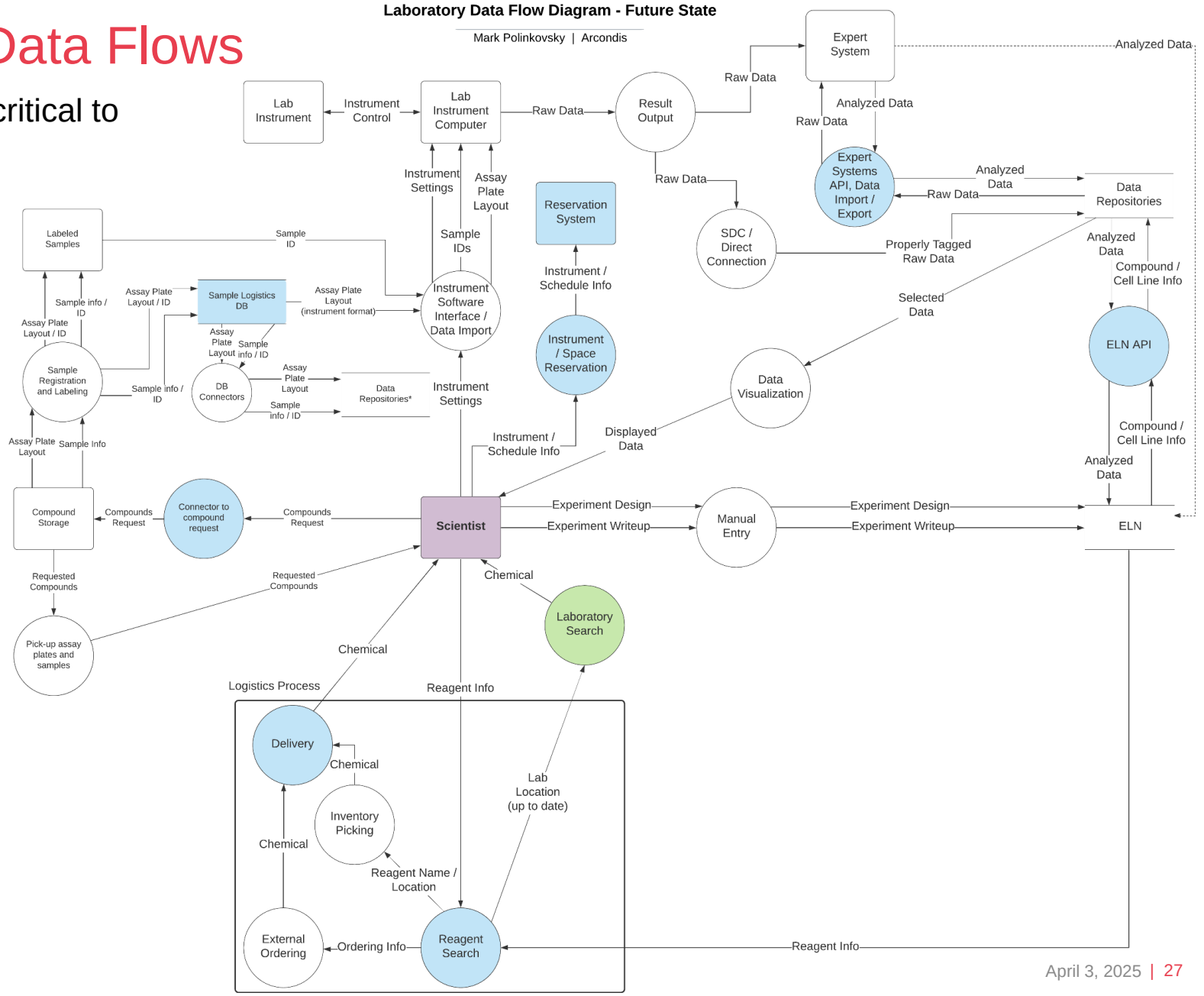


More Details of Future Lab Data Flows

How and why systems use and share data is critical to the functioning of the Digital Lab

Lab-specific Data Strategy components to consider

- **Instrument & System Integration** – Seamless connectivity between lab instruments, sensors, and software
- **Regulatory Compliance & Data Integrity** – Adherence to FDA 21 CFR Part 11, ISO 17025, ALCOA+ principles, and other regulations
- **Lab Workflow Automation** – Automating sample tracking, experiment logging, and approvals
- **Data Standardization & FAIR Principles** – Ensuring consistent data formats and metadata
- **Real-Time Data Processing & Analytics** – AI/ML-driven insights, dashboards, and predictive analytics
- **Cybersecurity & Data Protection** – Encryption, access controls, and cyber threat mitigation
- **Scalability & Future-Proofing** – Cloud-based infrastructure, multi-site collaboration, and emerging tech adoption
- **Data Utilization for Scientific Insights** – AI-driven research, digital twins, and cross-functional collaboration



Elements and Process for Creating the Data Strategy

Elements to Consider:

Data Integration:
Labs often generate data from various sources and formats, making it difficult to integrate and analyze comprehensively. How to get data from instruments in a reasonable way?

Data Quality:
Ensuring the accuracy, reliability, and consistency of data is crucial for meaningful analysis and reproducibility. (e.g. Does “sample” have the same meaning for all systems?)

Data Security and Privacy:
Protecting sensitive data from unauthorized access and ensuring compliance with regulatory standards is essential

Data Storage:
Managing large volumes of data and ensuring secure, long-term storage can be challenging

Data Sharing:
Facilitating seamless data sharing among researchers and systems while maintaining data integrity and security is vital

Process for creating the data strategy:

Questions for Discussion

TOPIC #1

How do you gain support for modifying the existing lab data strategy?

What stakeholders in the organization need to be involved?

TOPIC #2

How do you ensure having the right resources for the data strategy implementation?

What new skills do you need from the people implementing the strategy?

TOPIC #3

What needs to change in traditional data strategies to prepare for the autonomous lab?

How do you make sure that those points are considered?

TOPIC #4

What special considerations are there for GxP labs?

High-throughput or other specialty labs?

Breakout summary

TOPIC #1

- Needs to be top-down driven, but involve people in the lab
- Demonstrate Value / ROI
- Involve multiple sites
- Compatibility vs Compartmentalization

TOPIC #2

- Change Management is essential
  - Proactive communication
  - Show benefits
- Involve support / service groups – IT, solution providers, professional service co's

TOPIC #3

- Strategy needs to be E2E
- Governance, Standardization, controlled vocabulary
- Unified Data model
- FAIR, digital data by first intent
- Getting support – demonstrate the benefits, OCM

TOPIC #4

- Strict documentation, validation processes and qualified personnel is needed in GxP labs to ensure compliance
- Human accountability at end
- Different levels of compliance requirements → different strategies
- Which data to store and how for future use?

Breakout session #4
AI for Autonomous Digital Labs

Mathias Cherbuin
Chief Technology Officer,
Chemspeed

Chief Technology Officer (CTO)

Researcher

MsC Engineering & Robotics

Loïc Roch
Co-founder, CTO and Board Member
Atinary Technologies

ML for self-driving labs

AI development for chemistry

SW development for self-driving labs

Chemical app predictability

Molecule computer simulation

MsC Computational Chemistry

BsC Chemistry & Chemical Eng

- **AI isn't just hype—it's radically transforming lab automation and scientific discovery. But how can you make AI work for your lab?**
- This interactive session dives deep into machine learning for experimental design, AI-driven workflows, and the biggest challenges in AI adoption.
- You will get insider insights, real-world case studies, and a chance to collaborate with industry pioneers who are pushing the boundaries of lab automation.
- Whether you are exploring AI or scaling up existing solutions, this session is your roadmap to the AI-powered Lab of the Future.

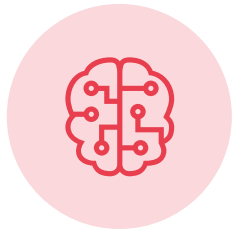
AI for Autonomous Digital Labs

Problem Statement

The complexity and volume of scientific data is outpacing traditional analysis methods

Manual laboratory processes remain time-consuming and error-prone

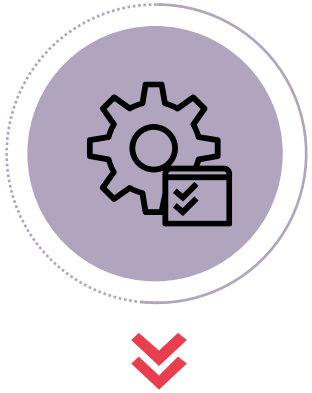
Decision-making in experiments often relies on human intuition rather than data-driven approaches



Labs struggle to implement AI solutions that are both effective and validated for scientific use

Methodological Approach (Part 1)

Integration of machine learning algorithms for experimental design and optimization



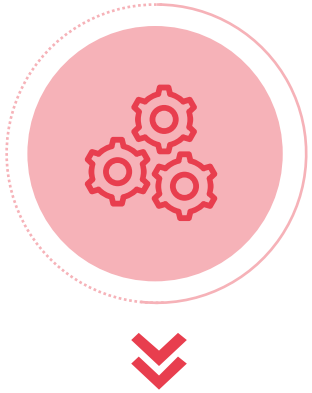
Automated data analysis pipelines that identify patterns human researchers might miss

Predictive modeling to forecast experimental outcomes and suggest refinement

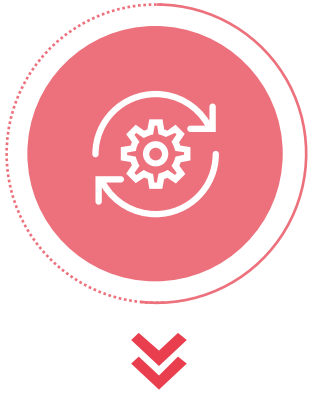
Real-time decision-making systems that adapt protocols based on incoming results

Methodological Approach (Part 2)

Implementation framework for validated AI solutions in regulated laboratory environments



Data management strategies ensuring quality inputs for reliable AI outputs



Hybrid approaches combining expert knowledge with machine learning capabilities

Validation methodologies for AI-driven experimental results

Questions for Discussion

TABLE #1

How have AI technologies already changed your laboratory workflows, and which specific AI applications have delivered the most tangible value in your autonomous lab environment?

TABLE #2

What skills and team compositions do you find most effective when integrating AI into traditional lab environments, and how are you addressing the talent gap in this specialized intersection of domains?

TABLE #3

How can we establish effective human-AI collaboration models where LLMs propose novel experimental designs while scientists maintain appropriate oversight and validation of the process?

TABLE #4

What advancements in AI technology could further revolutionize autonomous labs/your lab and how might AI-driven autonomous labs/your lab impact the future of scientific research and discovery including risks and limitations?

Breakout summary

TOPIC #1

- Still some work to become robust and reliable
- Data needs to be in AI-ready format to maximize efficiency

TOPIC #2

- Identify internal champion to support the implementation of automation and AI learning path
- Lack of broad implementation of AI tools

TOPIC #3

- Increasing confidence in models with time and transparency
- Need to integrate validation checkpoints

TOPIC #4

- 'We are dreaming big but living in a paper world'
- Explainability

Keynote: **Automation Connectivity and Digitalisation Concept for Roche Labs**

The session will dive into the transformative power of lab digitalization, showcasing how cutting-edge technologies are revolutionizing R&D. We will discover the critical role of industry standards in lab automation for seamless integration and scalability. You will gain insights into the key success factors for implementing AI in R&D—turning potential into real-world impact. Explore finally a compelling case study on Roche's AC/DC Concept, revealing how it accelerates digital adoption and drives more efficient, effective lab operations.

Tom Kissling

Global pRED

Lab Automation Partner, Roche

Closure

- A big thanks to all participants, speakers and the org team
- Key take-aways
  - Digitalisation will not go away & automation will be a substantial part of future labs
  - There is an important human factor to take into account
  - Capacity building and change management are key
- Let’s work together to make Autonomous Digital Labs a reality. We – Arcondis and Bruker – are here to support you.
- Stay and join us for refreshments!

Christian Hebich

Chief Execution Officer
Arcondis AG, Basel