



Bayer's Lab of the Future approach



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**Lab of the Future Congress,
Wellcome Genome
Conference Centre,
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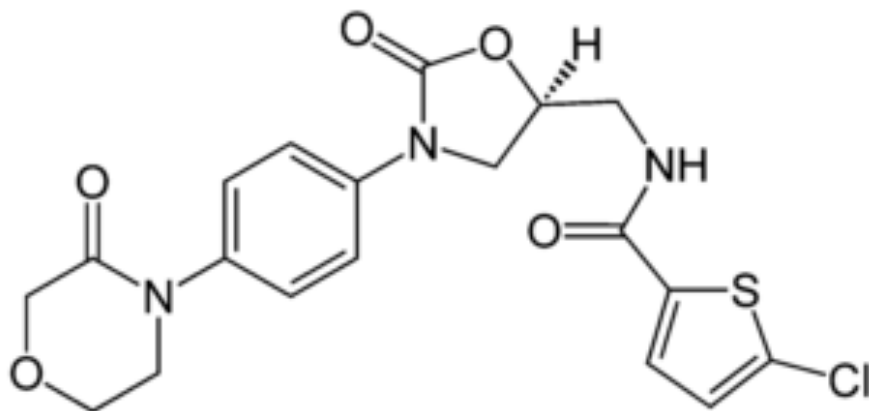
Agenda – Bayer’s Lab of the Future approach

- // Stakeholders and as-is situation
 - // For whom are we working for?
 - // What are current lab digitization obstacles?
- // Bayer’s LotF prototype
 - // High level overview
 - // IoT technology and tablet application
 - // Outlook and results
- // Summary / take home messages



Prolog – The secret code of chemists

The secret code of chemists



and the secret code of IT



A lot of things in common...



Stakeholders and as-is situation

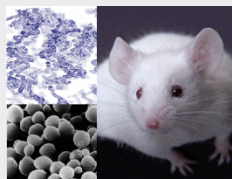
The Bayer example



Research Value Chain – all about generating Data



High-Throughput Screening



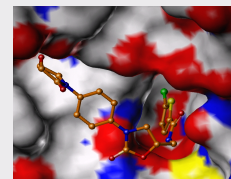
Early ADME/PK



Medicinal Chemistry



Predictive Pharmacology



Computational Chemistry

Target Discovery

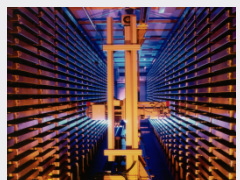
Compound Screening

Lead Generation

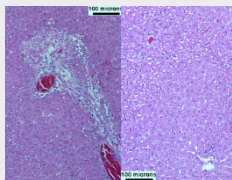
Lead Optimization

Preclinical Development

Clinic Phase I



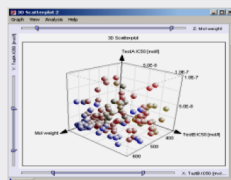
Compound Collection



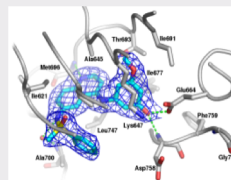
Early Toxicology



Automated Synthesis



Pharmacophore Informatics



Structural Biology

Maximize patient benefit

Increase druggable target space

Leverage digital progress



Laboratory workflows to be improved

- Usage of paper notes in lab
- Real-time and automated documentation is not possible
- Lab devices offer RS-232 or USB-ports, but often it is not used
- Useful information has to be gathered manually
- Already high standard of lab safety, but still room for improvement



Collaboration and journey

*High level
overview*



Cooperation with





Lab of the Future

The evolution of the initiative



Phase 1: Smart Glasses

- UAT in 2015
- Great potential
- Smart glasses not mature
- Support functions needed



Phase 2: Digital support of technician

- Automatic documentation
- Accurate documentation
- Task manager and IoT
- Independence of device

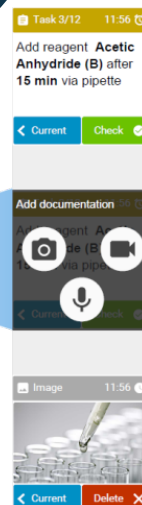


Phase 3: Digital Integrated Lab

- IoT integration of equipment
- Implementation of voice-to-text
- Refinement of smart documentation

Phase 4: Going Productive

- Visualization of lab device data
- Move from PoC to Production
- Establish interfaces to the ELN & chemical inventory system
- Rollout





Lab of the Future – Usability Mockup

First concept with Hololens





Lab of the Future

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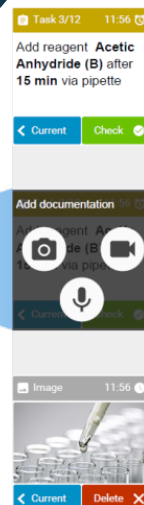
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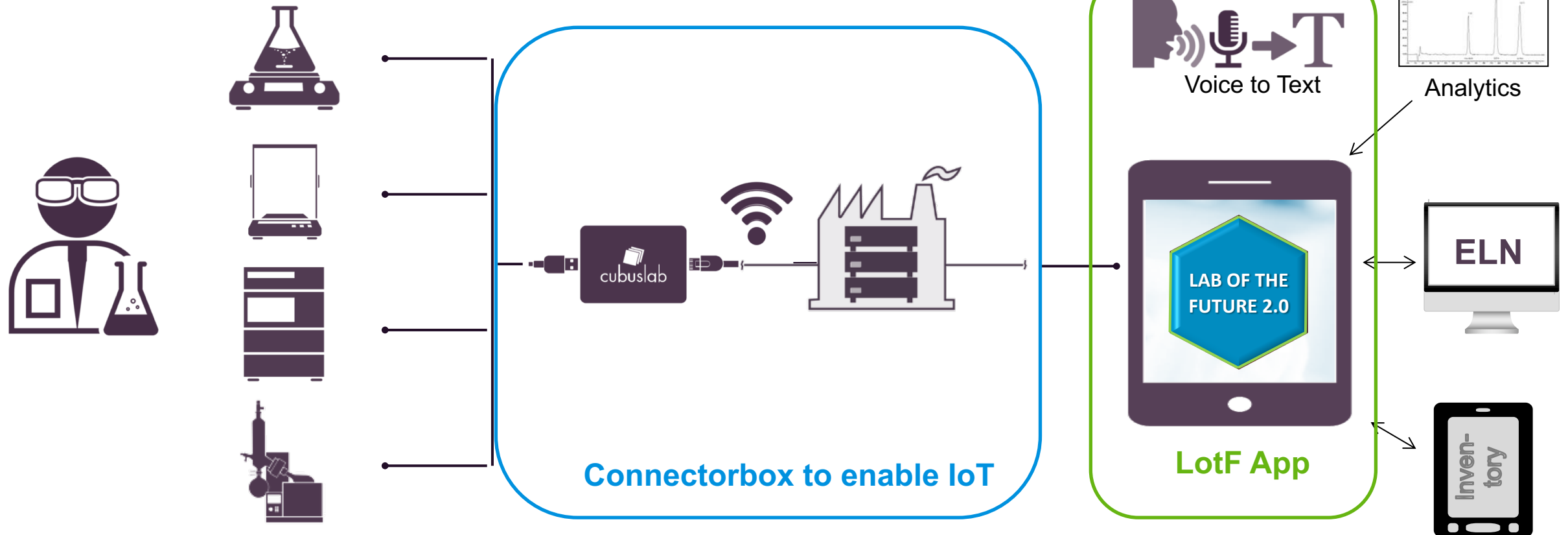
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General Setup – IoT platform and IT architecture

„IT should follow me & not vice versa“
(Lab Technician)





Redesigned workflows

*Prototype
application*



Paperless laboratory: mobile ELN

- ✓ Web-based application to display current experiments with:
 - ✓ Structures / chemical equation
 - ✓ Protocol text
 - ✓ Reagents parameter (e.g. weighing amount)

- ✓ Strip down mobile solution to fit purpose
 - ✓ Communication / synchronization through API to ELN

- ✓ Modern, intuitive UI that follows user (not vice versa)

The screenshot displays the Bayer mobile ELN application interface. At the top, there is a navigation bar with the Bayer logo and the text "DIGITAL LAB OF THE FUTURE". The main title is "Experimente". Below the title, there are four tabs: "NEU" (highlighted in green), "LAUFEND", "BEENDET", and "ALLE". A search bar is located on the right side of the navigation bar.

The main content area is divided into four panels, each representing an experiment:

- HAHN 69.0:** Shows a chemical reaction between a substituted benzimidazole derivative and a piperazine derivative, resulting in a complex product. The status is "Neu" and the timestamp is "12.02.2019 08:40:15 Uhr".
- HAHN 68.0:** Shows a chemical reaction between a substituted benzimidazole derivative and a piperazine derivative, resulting in a different product. The status is "Neu" and the timestamp is "12.02.2019 13:09:58 Uhr".
- HAHN 67.0:** The content is partially obscured.
- HAHN 66.0:** The content is partially obscured.

At the bottom of the interface, there is a field for "Name of laboratory technician" and two buttons: "AKTUALISIEREN" (refresh) and "ABMELDEN" (logout).

Interactions with lab devices

- ✓ Read/write access to:
 - ✓ Set temperature profile, transmit data, etc.
 - ✓ Easy stoichiometry adjustment while weighing
 - ✓ Protocol templates

- ✓ Interactions with lab devices through IoT
 - ✓ One solution regardless of manufacturer or device type
 - ✓ Requirement: RS232 or USB port
 - ✓ Provision of structured data (SiLA / Allotrope)

← ≡ DIGITAL LAB OF THE FUTURE

Mischen/Rühren Aufgabe

★ HAHN 69.0 - Neu

Chemical reaction scheme showing the synthesis of a complex molecule from two reactants.

bei Aktiviere Heizer

▲ Bitte überprüfen Sie, ob ein externer Temperatursensor angeschlossen ist.

für hinterher weiter rühren (ohne zu heizen, bis ich stopp drücke)

bei

Substanzen
Elemente mit Drag and Drop verschieben.

(A) HAHE739

(B) Ethylpiperazin

Dichlormethan

ABBRECHEN



What else?

- ✓ On-the-fly documentation / smart assistant:
 - ✓ Voice-to-text already implemented
- ✓ Enhance lab safety:
 - ✓ Instant validation of chemical identity upon weighing (scanning)
 - ✓ Advance monitoring of your lab devices and visualization of important parameter
 - ✓ Secure laboratory network through hardened connector boxes





Redesigned workflows

*Outlook and
results*



The Lab of the Future is a never ending story

- ✓ How to handle GxP requirements?
- ✓ How can we automate our inventory?
 - ✓ Keep track of your substances and stock amounts
- ✓ How to extend to non-chemistry labs?
- ✓ How to support automation / robotics?





Lab of the Future shows overall benefit in the long run

For the company:



- How can we generate **more data** in the labs?
- How can we increase the **quality** of the data?
- How can we make the data machine readable?

For the lab technician:



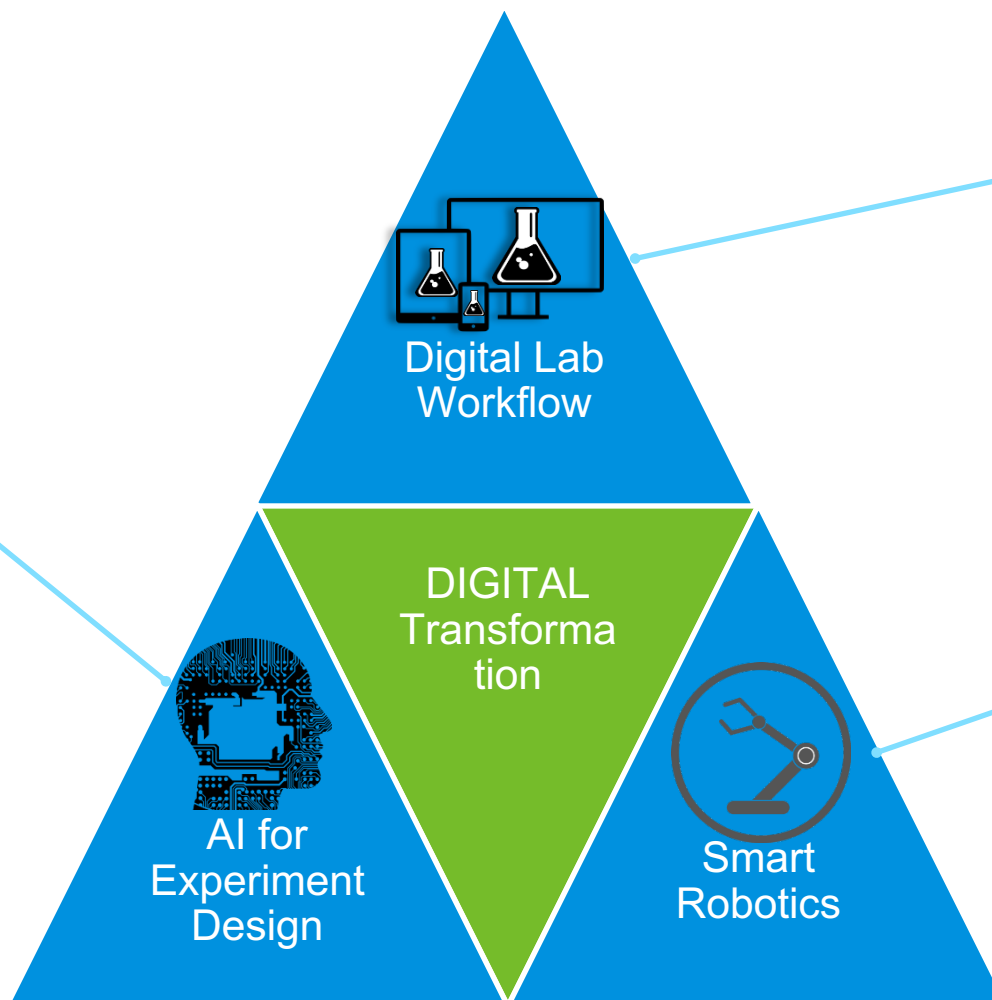
- What will **my workplace** look like?
- How can „digital“ **make my life easier** ?
- What „**boring**“ tasks can be automated for me?



Digital Transformation fuses emerging technologies into tangible changes

Quality

- Reduce the number of wet lab experiments through in silico predictions



Lab of the Future

- Reduce the effort needed for experiment documentation by 50%
- Improve the quality of the experiment documentation

Automation

- Automate standardized activities



Take home messages

- IoT in the lab can be a major leverage to improve data quality
- Through balance of user needs and business goals we developed a modular solution fitting in our IT landscape
- IoT needs long term commitment over short term goals
- Adapt the new standards for open and FAIR data
- Automate routines, empower people for value-adding activities
- Never rest - think big in terms of lab digitization!



*Thank you
for your attention!*

