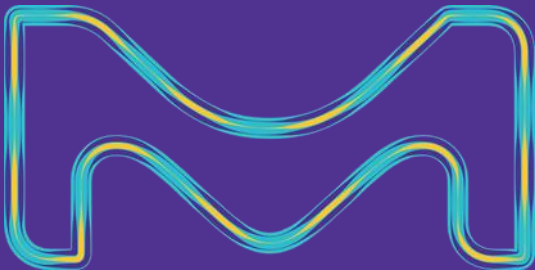


# Revolutionizing Healthcare: Harnessing Digital Innovation for Precision Medicine

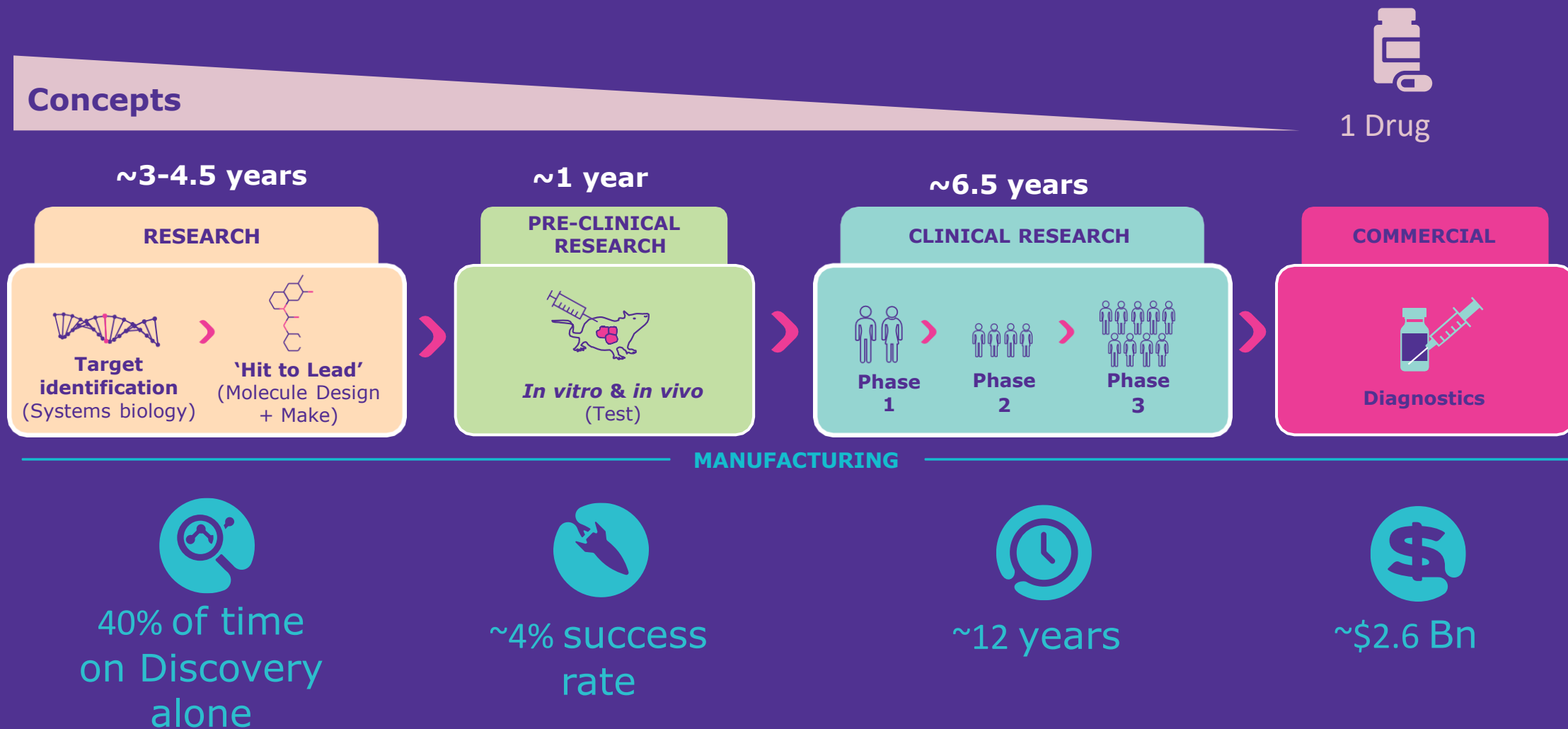
Dr. Laura Matz  
Chief Science & Technology Officer  
September 11, 2024

Intelligent Health



**MERCK**

# Traditional drug discovery and development: time-consuming, expensive and with modest success rate





## Needs in Drug Discovery



Reduce timelines



Increase in "hit rate"



Increase success rate



Increase accessible chemical space



Improve processes for synthesis



Increase target space – beyond small mol inhibition

# Tying together our capability and expertise in **developing molecules** across three industries

## Electronics

Advancing digital living

- Specialty chemicals & gases for semiconductor manufacturing
- OLED
- Liquid crystals



## Life Science

Solving the toughest problems in Life Science

- Biologics and ADC Technologies
- E2E mRNA offering
- High Potency APIs
- Viral & Gene therapies



## Healthcare

As one for patients

- Monoclonal Antibodies
- ADCs & PROTACs
- Small Molecules
- Growth and Fertility hormones

## KEY FIGURES

**62,908**

Employees worldwide

**21.0**

Sales (€ billion)  
in 2023

**2.4**

R&D (€ billion)

**66**

Countries

**1668**

Founded

# Data Revolution: Shaping our future

Innovation powered  
by **Data & Digital**

Automating processes, **analyzing large datasets** for actionable insights, enabling **predictive analytics**, and enhancing **decision-making** across various digital platforms and systems



**Precision Medicine**



**Supply Chain**



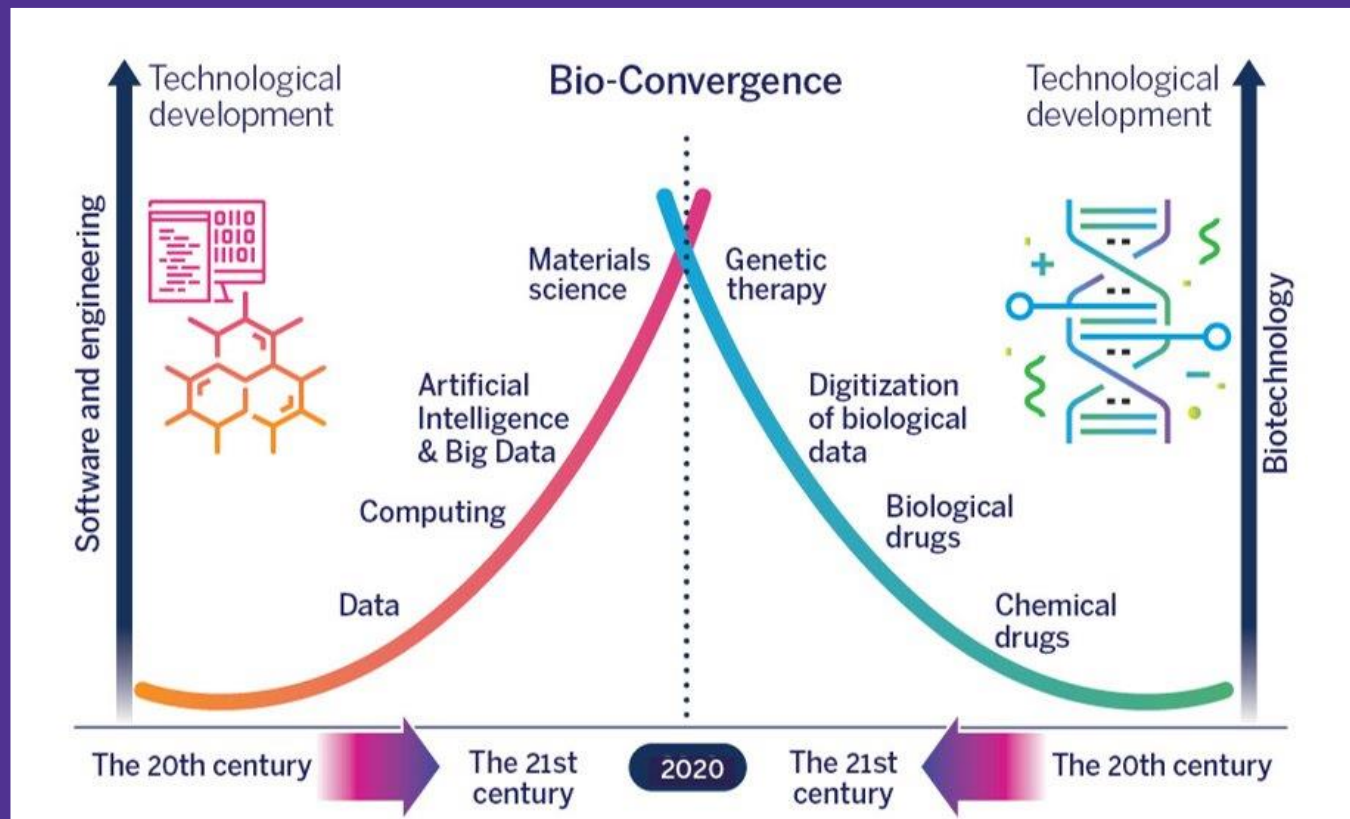
**Sustainability**



**Bioconvergence**

# Bioconvergence: the advancements in engineering, biology and medicine fueled by data & digital!

*"Rapid genome sequencing is one of the reasons that multiple COVID-19 vaccines were developed so quickly."*



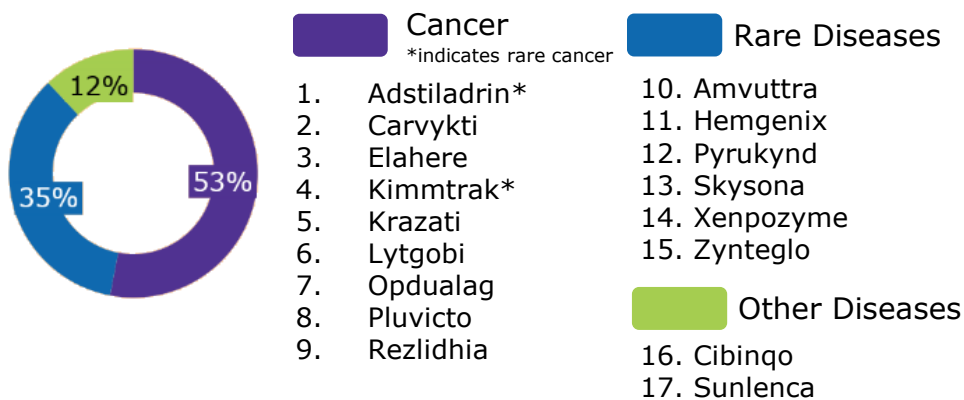
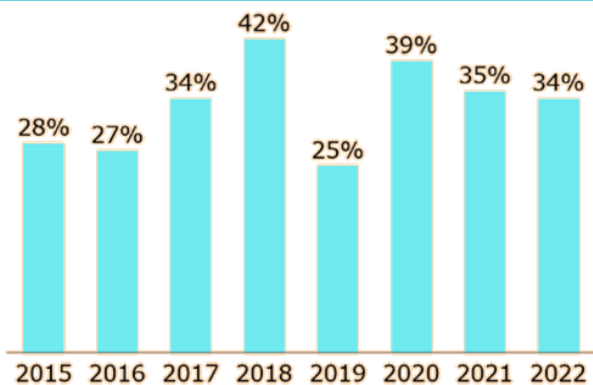
Source: <https://innovationisrael.org.il/en/reportchapter/bio-convergence>, quotes from BICO (<https://bico.com/bio-convergence/>)

*"Bio-convergence is the future of human health, a future that promises targeted, transformative healthcare, cures for illnesses, and hope for better, more accessible care worldwide."*



# AI-Driven Personalized Healthcare Revolutionizing Drug Development

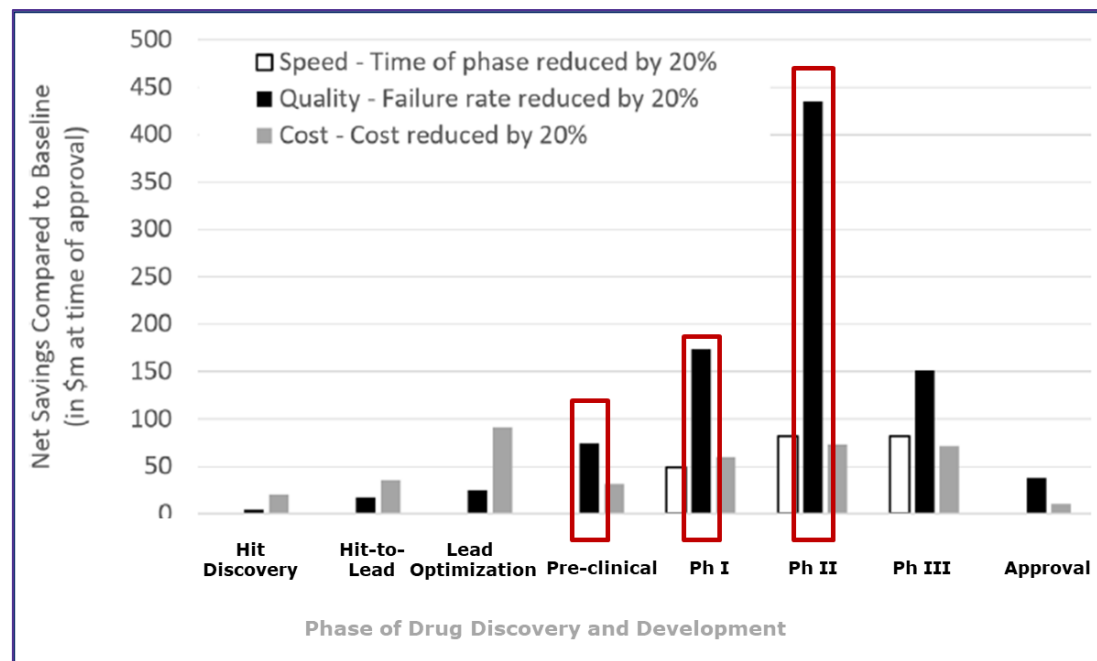
**More than 25% of FDA approvals for the last eight years, were personalized medicines**



- |  |  |  |
|--|--|--|
| <p><b>Cancer</b><br/>*indicates rare cancer</p> <ol style="list-style-type: none"> <li>1. Adstiladrin*</li> <li>2. Carvykti</li> <li>3. Elahere</li> <li>4. Kimmtrak*</li> <li>5. Krazati</li> <li>6. Lytgobi</li> <li>7. Opdualag</li> <li>8. Pluvicto</li> <li>9. Rezlidhia</li> </ol> | <p><b>Rare Diseases</b></p> <ol style="list-style-type: none"> <li>10. Amvuttra</li> <li>11. Hemgenix</li> <li>12. Pyrukynd</li> <li>13. Skysona</li> <li>14. Xenpozyme</li> <li>15. Zynteglo</li> </ol> | <p><b>Other Diseases</b></p> <ol style="list-style-type: none"> <li>16. Cibirgo</li> <li>17. Sunlenca</li> </ol> |
|--|--|--|

Source: <https://www.personalizedmedicinecoalition.org/Userfiles/PMC-Corporate/file/report.pdf>

**Leveraging AI to improve the quality of drug development has the greatest impact on the success of a project**

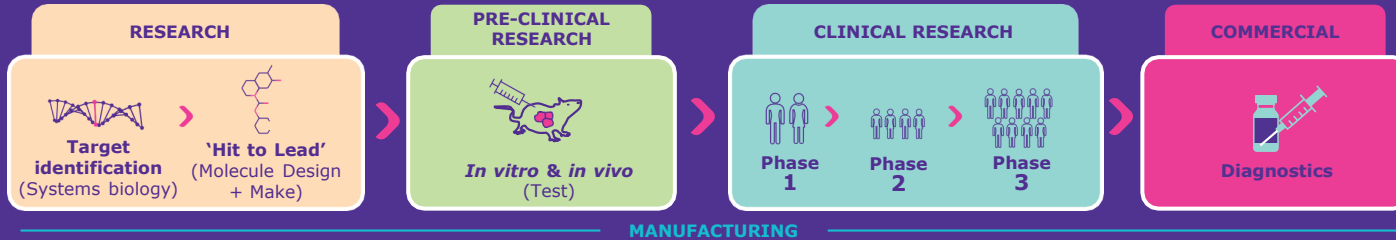


Adapted from Bender and Cortès-Ciriano (2021) Drug Discovery Today 26, 2: 511  
<https://doi.org/10.1016/j.drudis.2020.12.009>

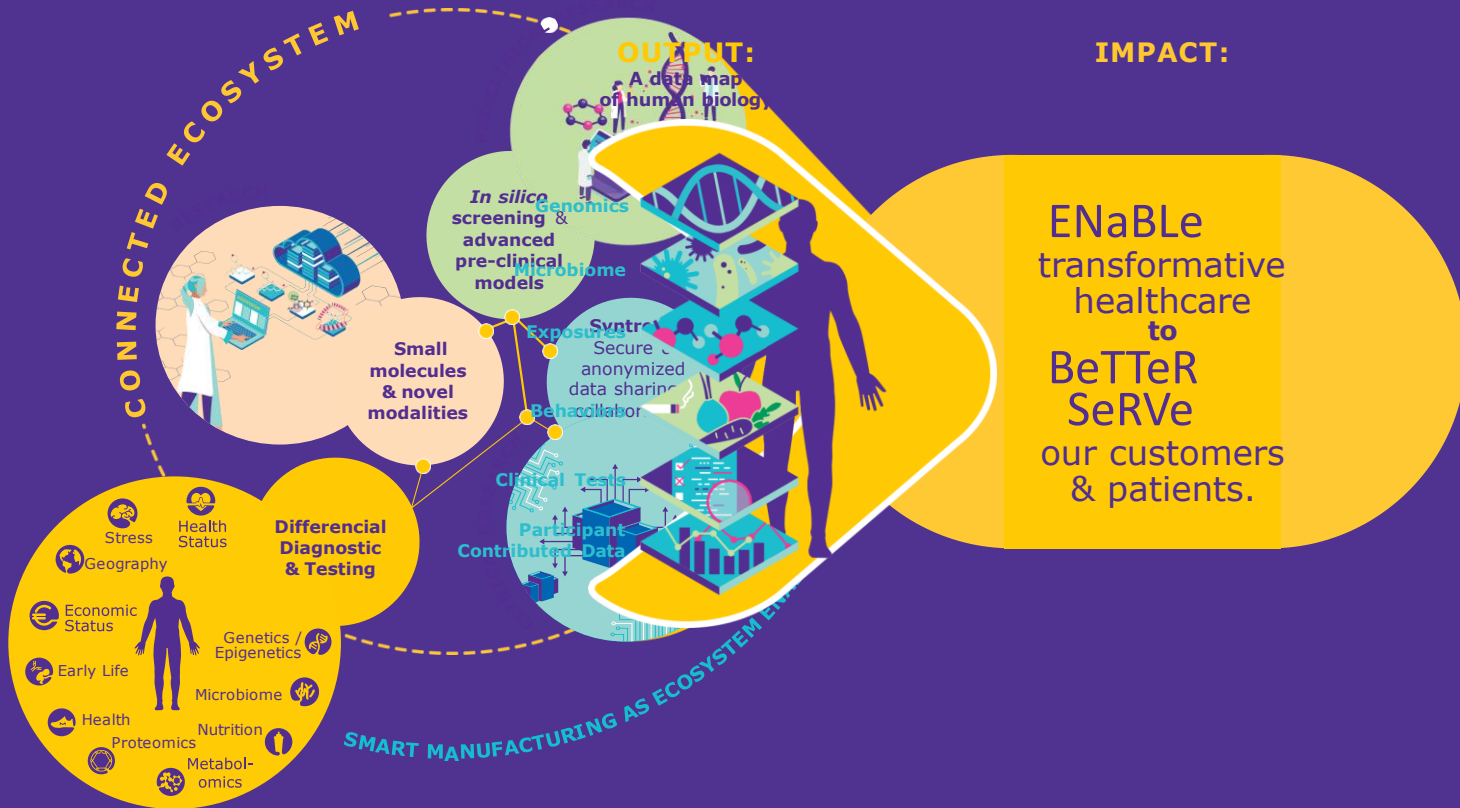
# The “how” of the future drug development

## A digital ecosystem to deliver transformative healthcare solutions to patients and healthcare systems faster

TODAY



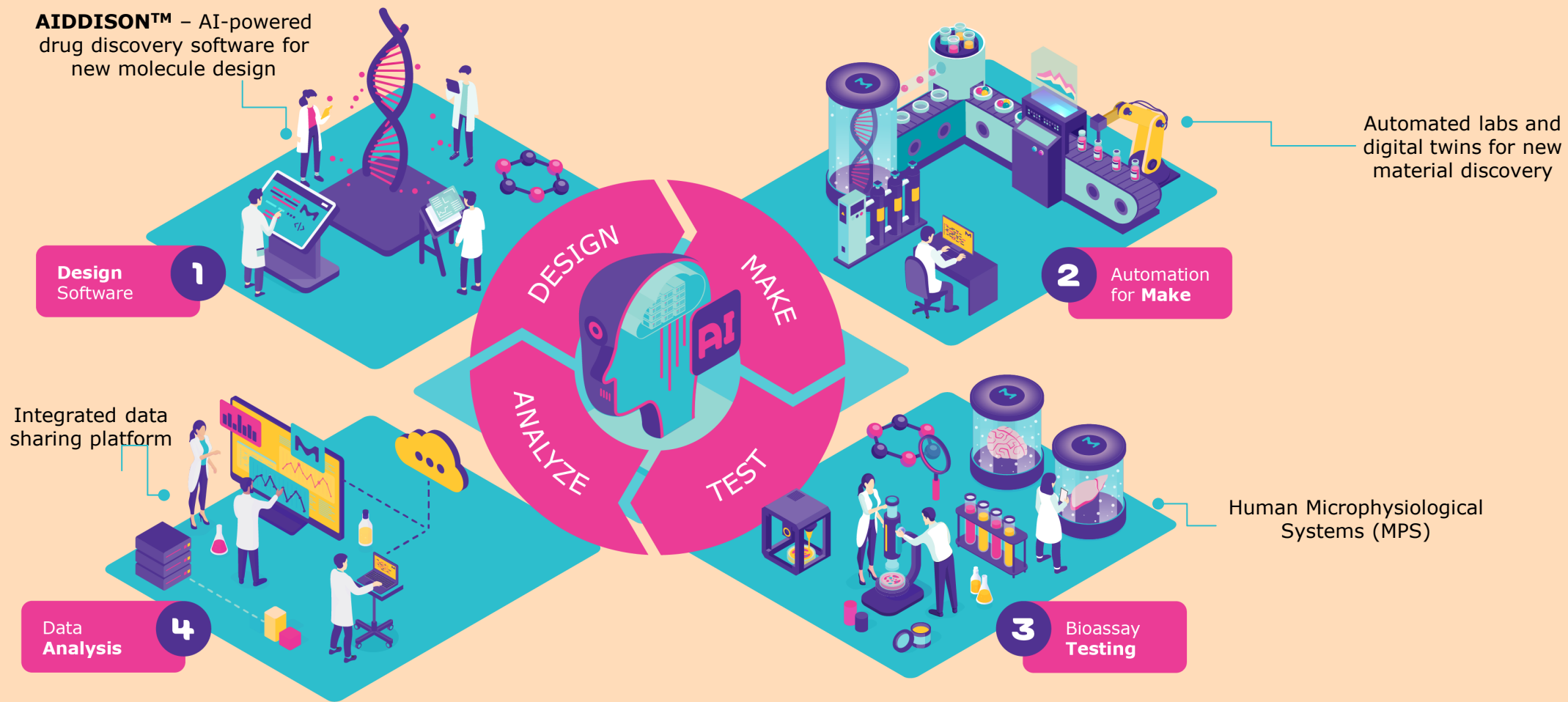
TOMORROW





# AI in Drug Discovery (AIDD)

Combined expertise in drug discovery in **Healthcare** & chemistry leadership in **Life Science**, and data collaboration ecosystems powered **Electronics** chips



# AIDDISON™ – AI-powered drug discovery software for new molecule design

**Design  
Software**

1

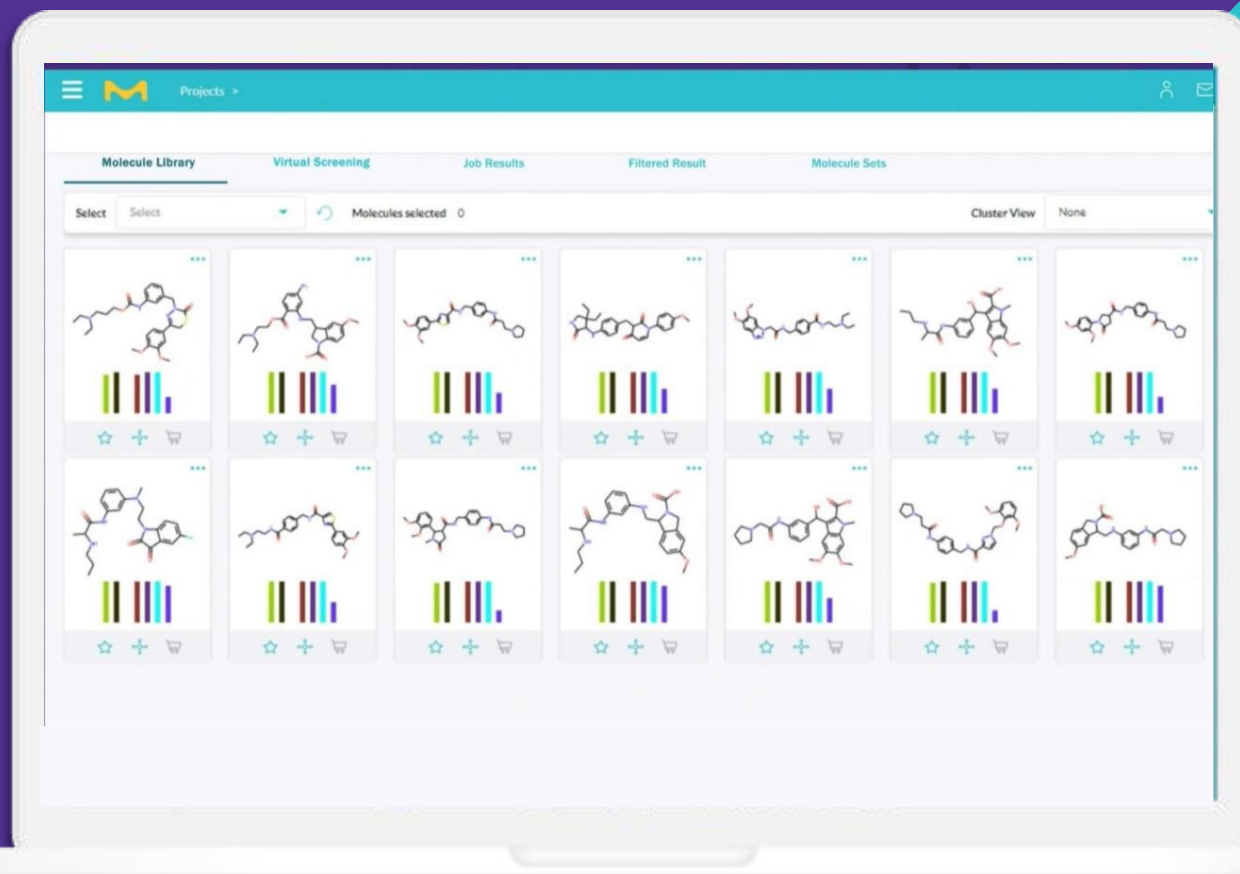


DESIGN

# AIDDISON® Generative AI-Powered Drug Discovery Platform

## Partnership with Life Science and Healthcare for drug discovery

- ✓ External customers signed for 2023 and completed AIDDISON-Synthia Integration!



## ALL-IN-ONE AI FOR DRUG HUNTERS

Design to full retrosynthesis, AIDDISON™ empowers medicinal chemists to make data-driven decisions at every stage of drug discovery.

**64B**

Molecules in  
chemical space

**99%**

Faster than  
screening

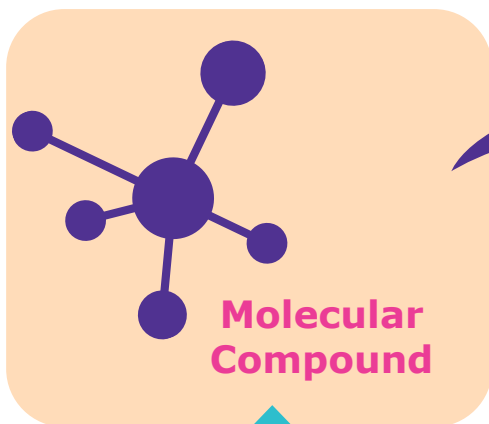
**20 +**

Years of validated  
data models

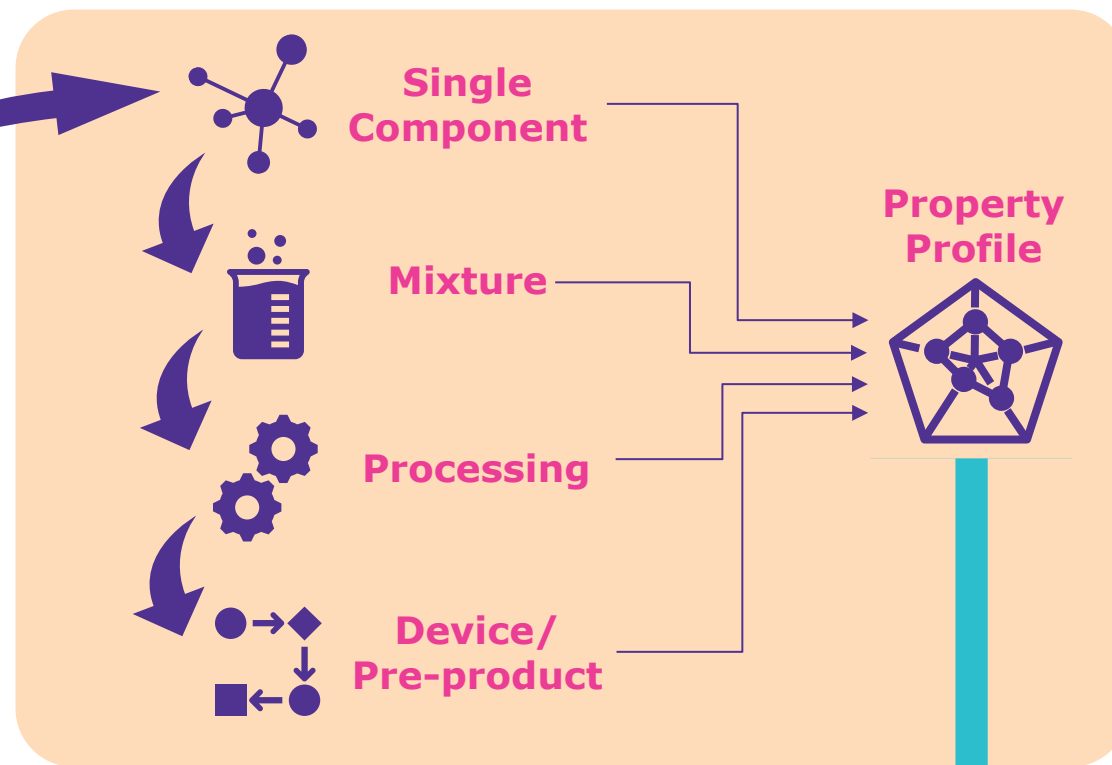
# Accelerating drug discovery

## Generative and predictive models for molecule design

### AI Structure Generator



### Property Prediction



Close-loop structure optimization  
for target property profile

- Critical parameters can be derived from each of the workflow steps
- **Domain-specific**, even product-specific **models** need to be developed **for property prediction**
- Customized machine-learning models are used to **score quality of newly-generated molecules**

## Automated labs and digital twins for new material discovery



2

Automation for **Make**

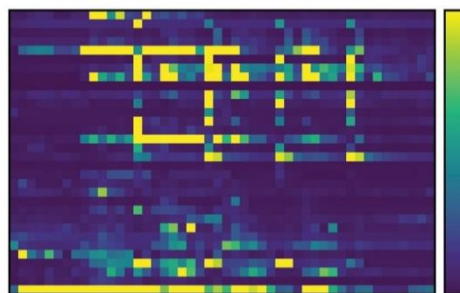
AI  
MAKE

# Autonomous lab driven by AI, automation, and big data Accelerating successful drug discovery

## 1 Miniaturization

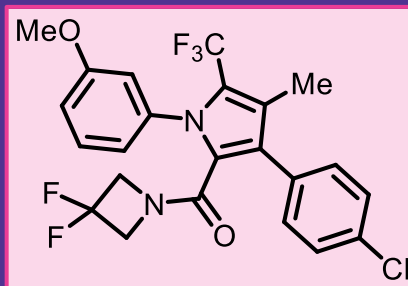
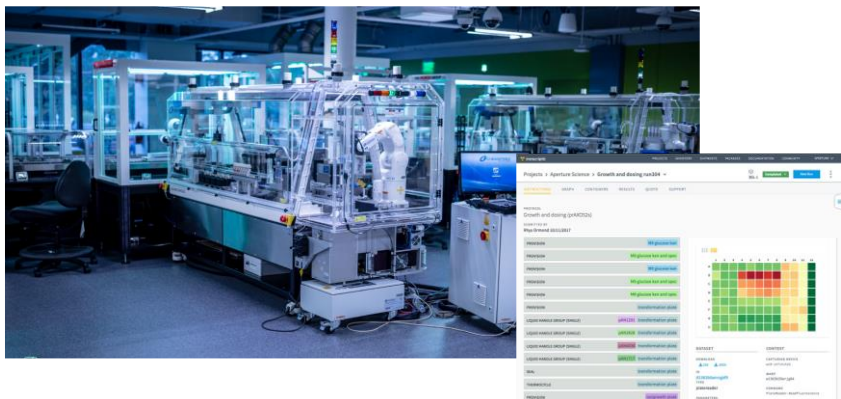


### High throughput



## 2 Fully Automated Labs

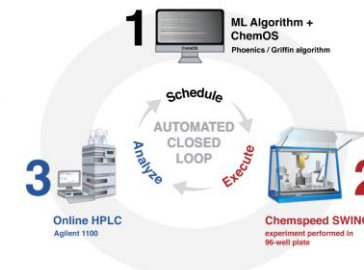
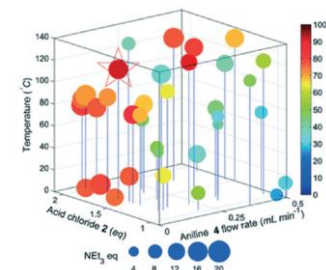
### Human-less laboratory



- ❖ Scale - HTS
- ❖ Faster
- ❖ Increased success

## 3 Closed-Loop Optimization

### Computers decide the experiments





TEST



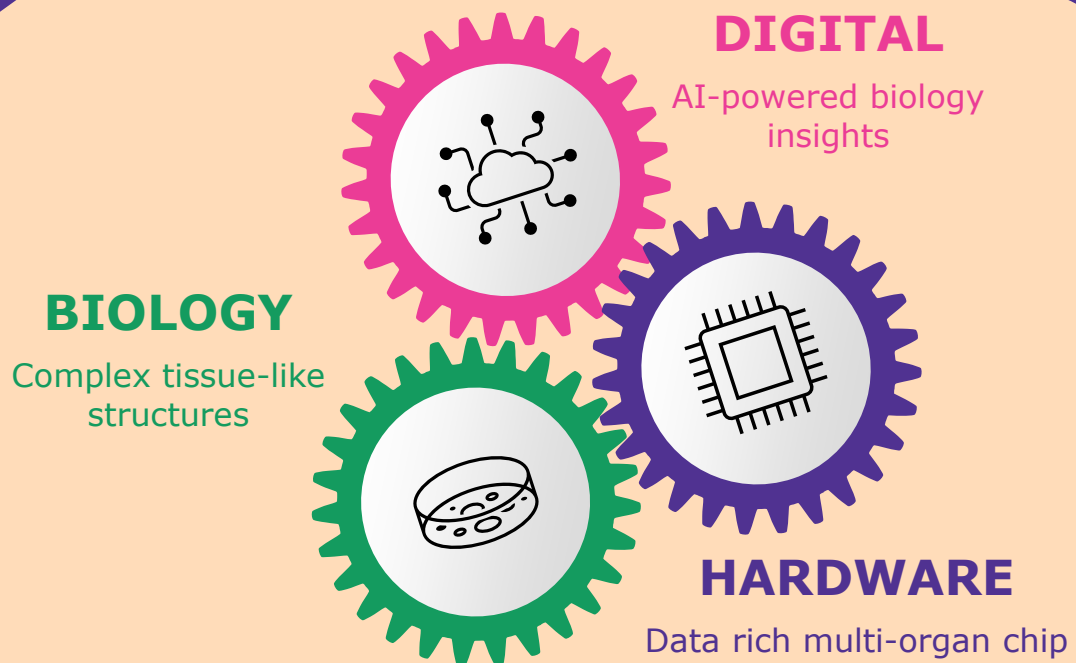
3

Bioassay Testing

Human Microphysiological Systems (MPS)

# Human Microphysiological Systems (MPS)

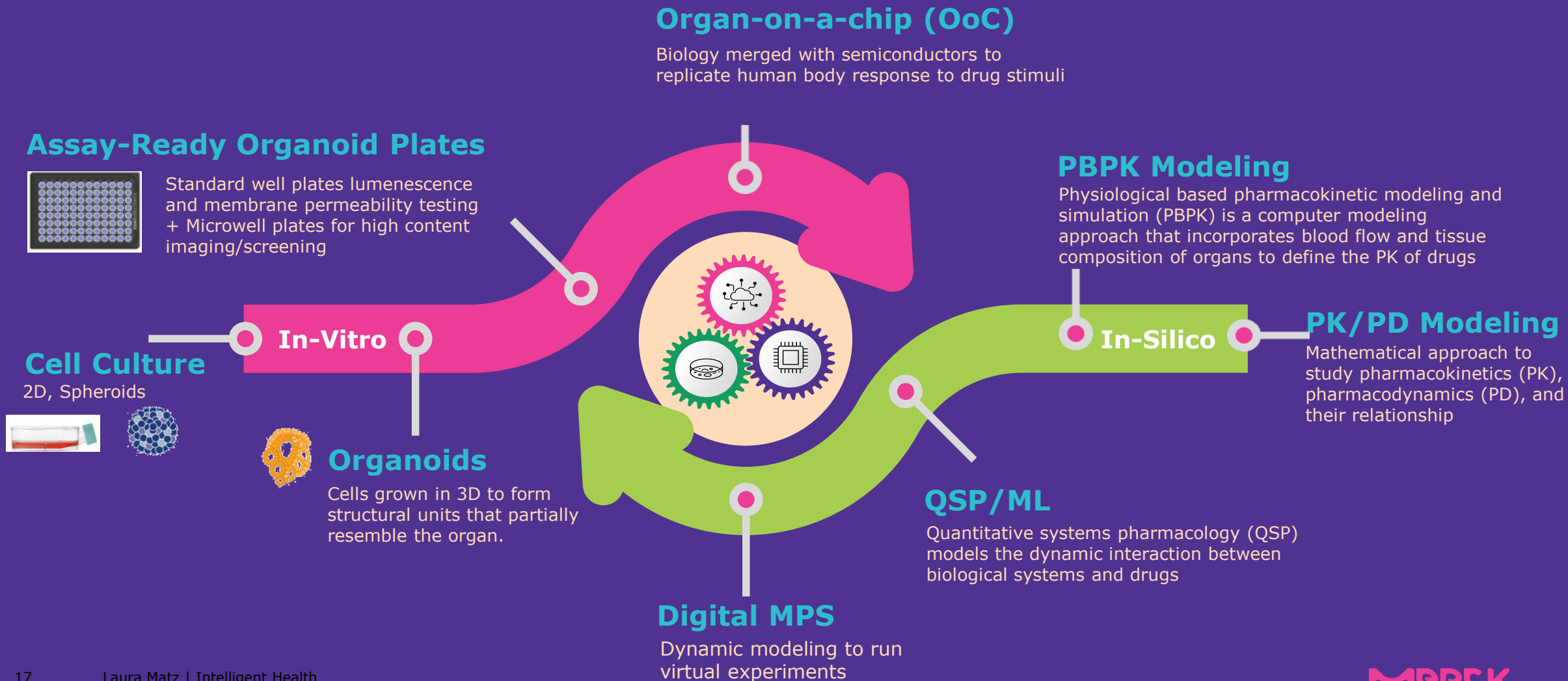
## Transforming the drug development testing process



A ONE Merck Program to transform drug discovery and development processes by enhancing translatability, increasing the development speed and prioritizing animal welfare.

## Our MPS vision

# A set of connected and synergistic in-vitro & in-silico MPS capabilities



**Data Analysis**

**4**

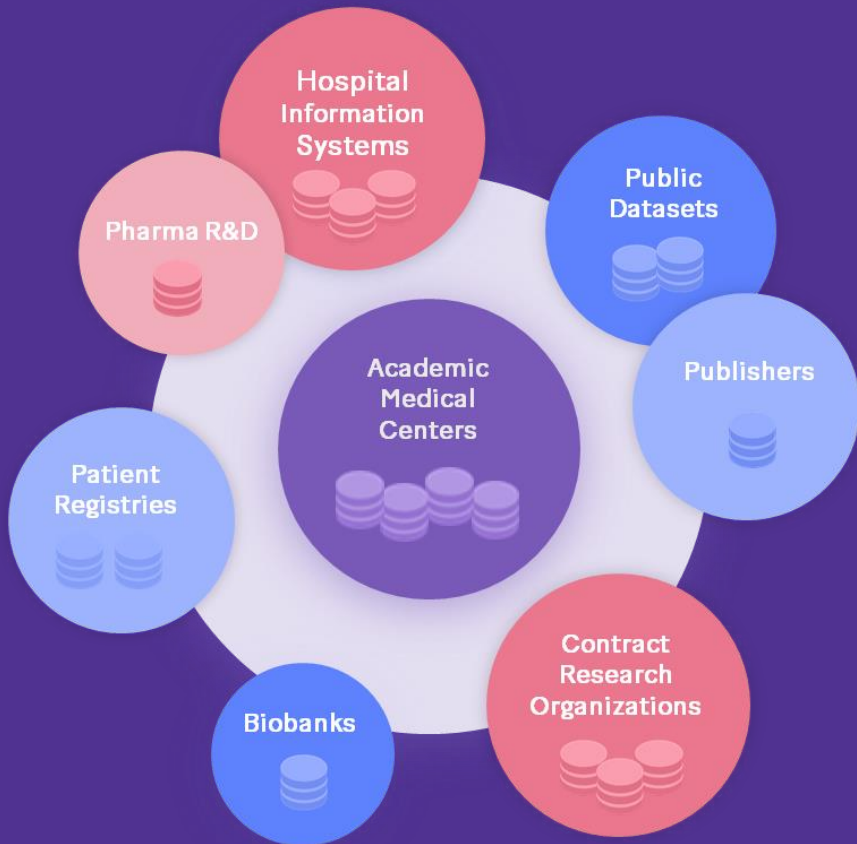


**Integrated data sharing platform**

# Pharma have complex ecosystems

Need to break through the data-silos to improve Data quality & availability

**Biomedical data is siloed across the Healthcare ecosystem**



**Siloed data makes insights harder & slower to find and collaboration difficult**

~80%

of biomedical researchers' time is **spent sourcing and preparing data**<sup>1</sup>

>40%

of large pharma companies consider **data quality the largest barrier** to conducting remote clinical trials<sup>2</sup>



**Researchers want to collaborate** but proliferation of available data, data silos between and within institutions, and **lack of incentives to share** have been huge barriers

# Building data ecosystems through industry collaboration

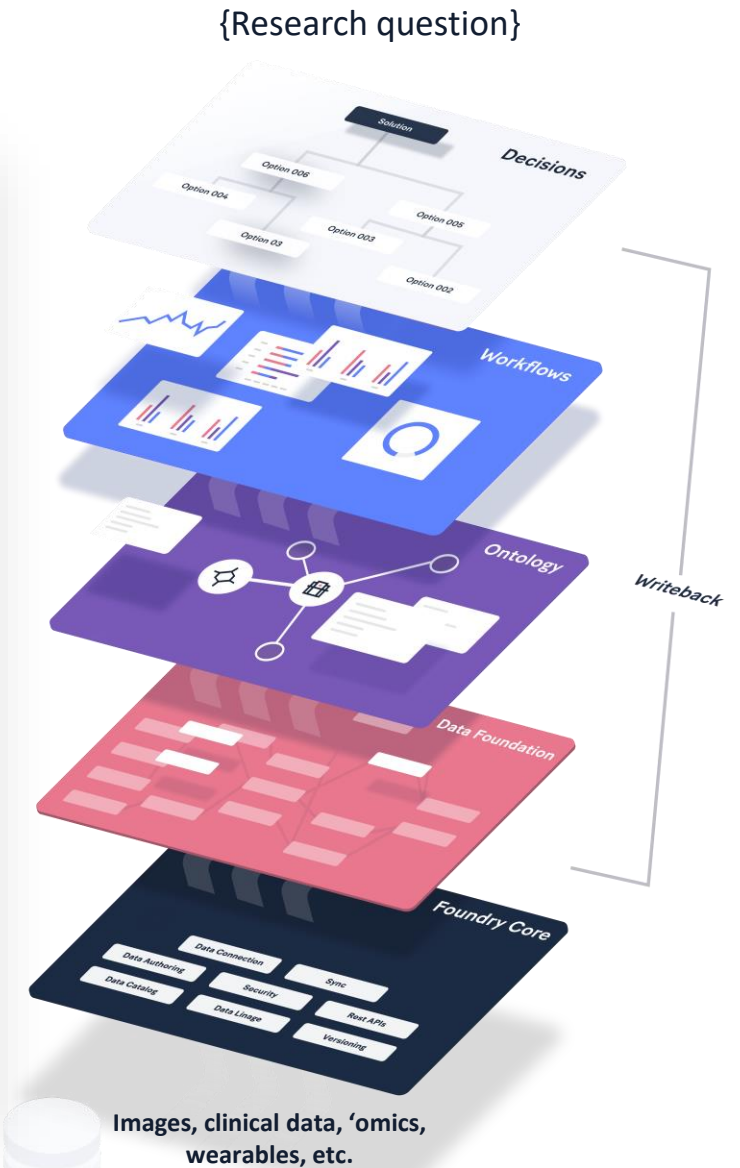
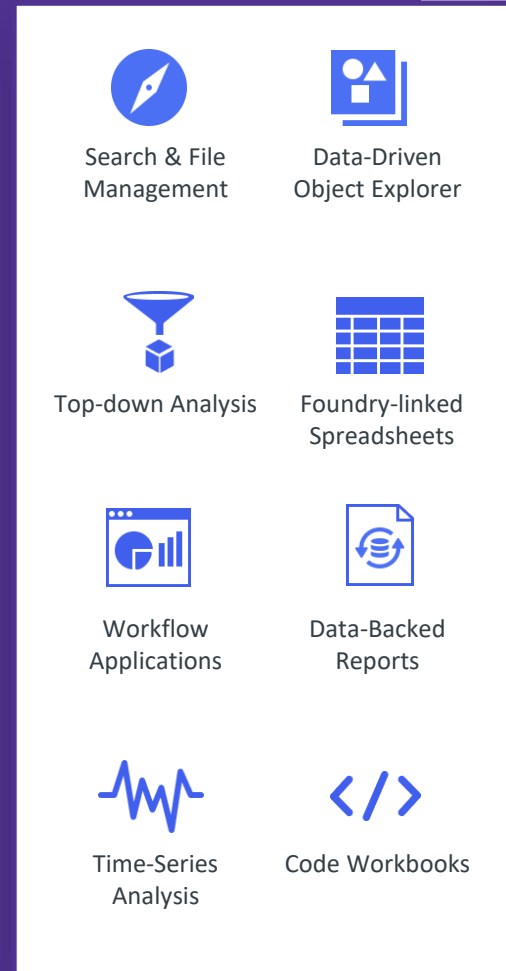


In partnership with:  
 Palantir

A secure & collaborative ecosystem that empowers researchers to work together across organizational boundaries to ask tough questions and solve hard problems

Rapidly bringing data sources together to:

- ❖ Drive meaningful, scalable & data-driven Clinical research
- ❖ Accelerate research, data collaboration and empower an AI OS for Healthcare







# UCI – MITRE Case Study

Powered by Syntropy®

Data Integration

Data Transformation

Data Lineage

Multi-Institution  
Collaboration

Data Security &  
Privacy

## Challenge

- **Integrate patient data** across the University of California, Irvine, and its co-collaborators
- **Standardize data** across the institutions based on a data schema distributed by MITRE
- **Analyze patient outcomes** for patients that received monoclonal antibody treatment for COVID-19

## Solution

- Syntropy® platform:
  - Provided **data pipelines and data exchange**
  - Allowed for **scalable, robust, and flexible** mapping of UCI patient data to MITRE schema
  - Facilitated **data linking, cleaning, and validation**
- UCI standardized and submitted data to MITRE much faster and more securely

## Impact

- **Fastest implementation** of data schema (~2 months faster)
- Explicit data capture through **traceability elements** baked into the workflow
- **Automated, modular data pipeline** and validation scripts
- **Zero PHI leaked**

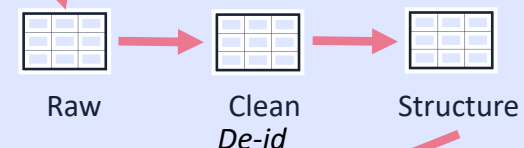
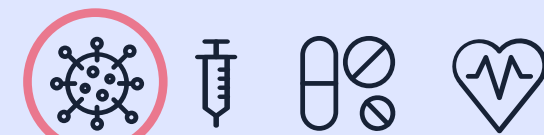
University of  
California,  
Irvine



Data Source Systems



Secure UCI Environment



MITRE  
Environment



Analyze Patient  
Outcomes

MITRE



# Our investment in automation for drug and material development

PRESS RELEASES /

## Merck Invests in State-Of-The-Art Biotech Development Facility in Switzerland

Merck today announced an investment of € 250 million in a new facility in Corsier-sur-Vevey, Switzerland – the Merck Biotech Development Center.



PRESS RELEASES /

## Merck Introduces Modular Automation for Laboratories – A First for the Chemical Industry

Merck today announced its intention to automate the global laboratory environment of its Electronics business sector in addition to digitalizing production.



# Key takeaways

1

At Merck, our full capacity and expertise in developing molecules across three industries enables us to **accelerate innovation**.

2

Our **Bioconvergence** approach merges digital, biotech, and engineering innovations to advance human biology understanding and shape the future of precision medicine and transformative healthcare.

3

The cutting-edge **AI for Drug Discovery program** integrates AI and automation, accelerating early drug discovery while enhancing safety and cost-effectiveness.

4

**Syntropy® data ecosystem** enables a new era of scientific discovery through collaboration and the power of data, driving transformative change across the industry with unprecedented interoperability and insights.





Thank you  
Let's drive innovation together!