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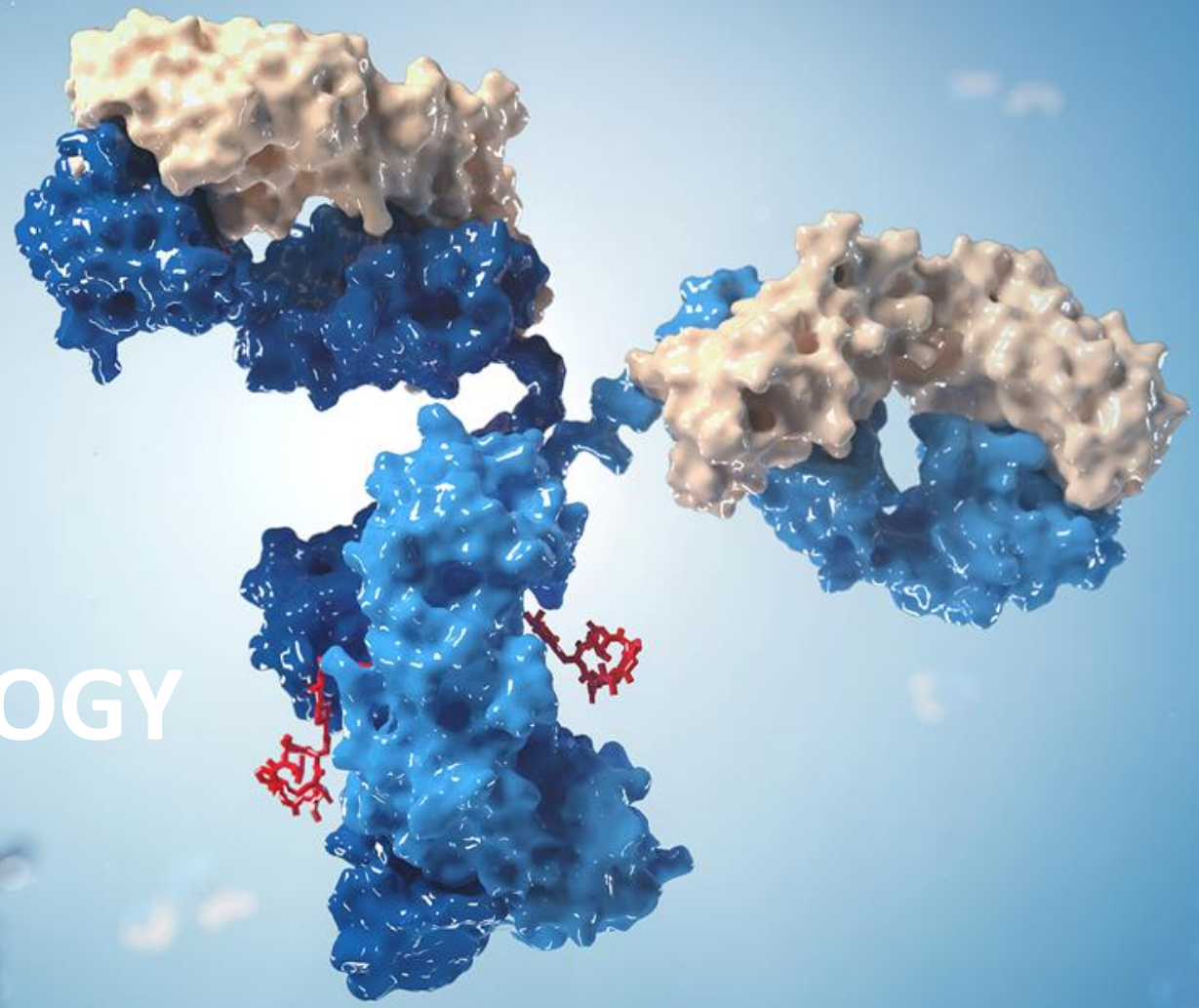

ESTABLISHING AN AI STRATEGY FOR ONCOLOGY CLINICAL TRIALS: WHAT TO CONSIDER

Dec 3, 2024 • CTO Europe 2024 • Sofitel Munich Bayerpost, Munich • Dr Frank Richard, VP Medical

DISCLOSURES

I am an employee at Heidelberg Pharma AG, Germany.

The content of this presentation is my personal view and not intended to make claims about current or future use of AI at Heidelberg Pharma.

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HEIDELBERG PHARMA AT A GLANCE

Differentiated ADC technologies

- In plug & play mode
- 2 years from target to IND

Clinical stage

- HDP-101: 50% ORR in Cohort 5 with no signs of ocular or renal toxicities, myelosuppression or severe liver damage including one **complete remission;** Delivering RP2D in Q2/25
- HDP-102 CTA Q4/2024 & FPI Q1/2025; HDP-103 CTA Q4/2025

GMP manufacturing

- Fully synthetic process for Amanitin

Strong IP including platform, payload, assets, method of use and predictive biomarker

- Several IP families
- Monopoly in the Amanitin/MoA space
- Subcutaneous administration
- Patient stratification with 17p biomarker

Partnerships

- Huadong: China-focused
- Takeda: ATAC technology
- HealthCare Royalty: Telix Pharmaceuticals

Corporate & finance

- Experienced leadership team; 109 employees
- Cash runway: through 2026*

*taking into account the milestone payment of $75 million from HealthCare Royalty

ADC = antibody-drug conjugate | MoA = mode of action | ORR = overall response rate | RP2D = Recommended Phase II Dose | CTA = clinical trial application | FPI = first patient in

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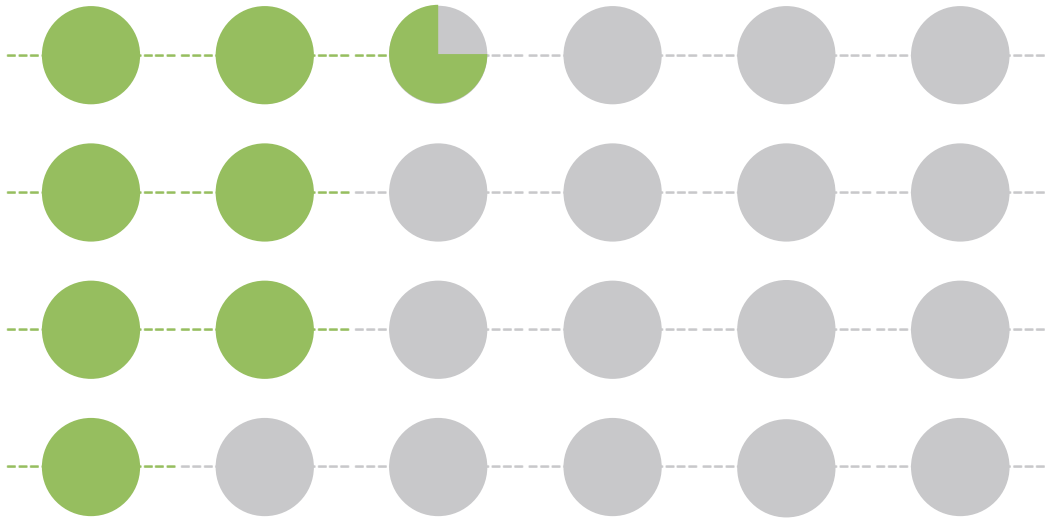
GROWING PIPELINE OF PROPRIETARY PROGRAMS

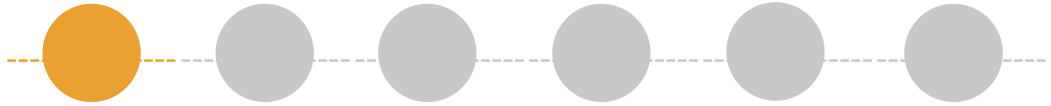
ATAC pipeline

Product	Target	Indication	Partner
HDP-101	BCMA	Multiple Myeloma	Huadong (China+)
HDP-102	CD37	NHL (DLBCL/CLL)	Huadong (Option China+)
HDP-103	PSMA	Prostate cancer	Huadong (China+)
HDP-104	GCC	Gastrointestinal cancers (e.g. CRC)	Huadong (Option China+)



TOPO I

Product	Target	Indication	Partner
HDP-201	GCC	Colorectal cancer	Proprietary



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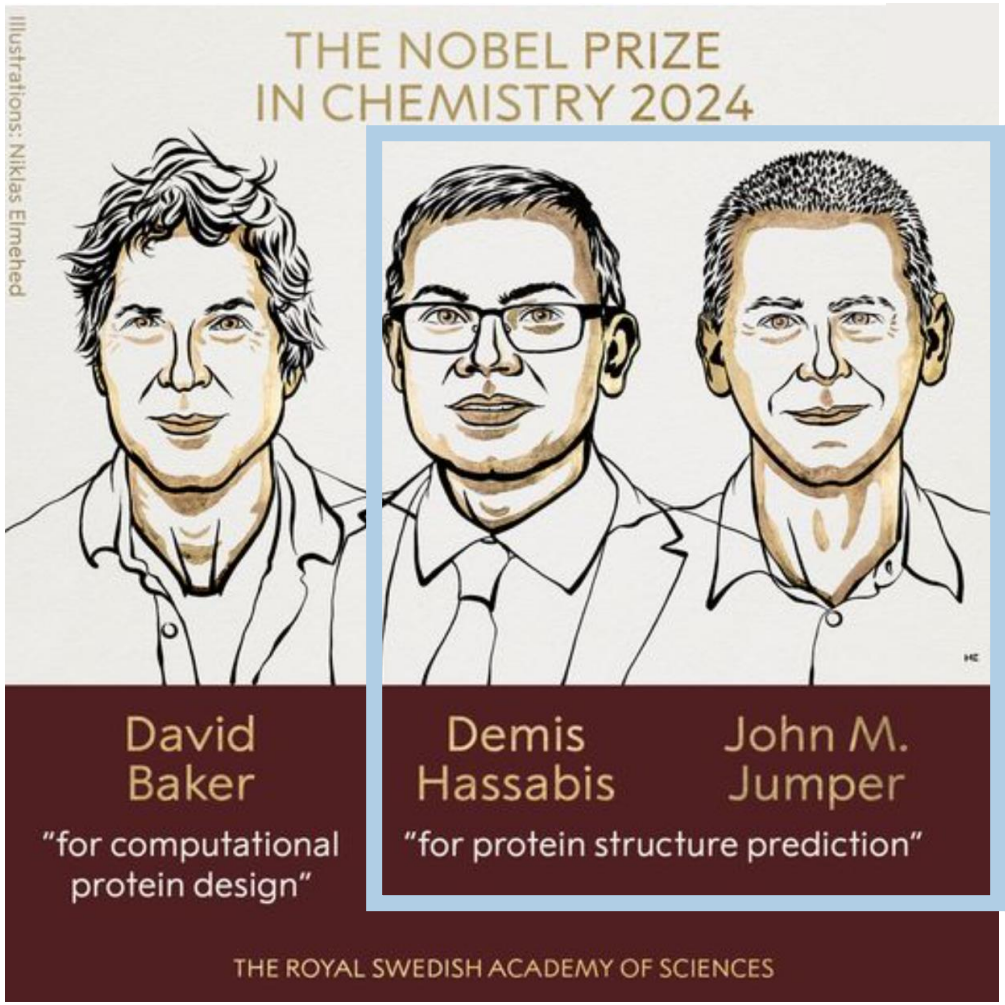
THE NOBEL PRIZE IN CHEMISTRY 2024



DeepMind's AlphaFold learns to **predict protein's 3D shape from its amino-acid sequence**, a 50-year-old Grand Challenge in biology.

AlphaFold

- A novel **machine learning** approach
- **Deep learning** algorithm based on a **neural network** model
- Incorporates physical and biological knowledge about protein structure

Source: Jumper 2021

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OUTLINE

WHAT AWAITS YOU

AI In Pharma	Reiterating basics of AI and its value in pharma
AI In Clinical Trials	AI use cases and solutions
AI Strategy Development	A holistic approach incorporating tools, ethics and data privacy
Considerations	Challenges and lessons learned to overcome them

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AI IN PHARMA

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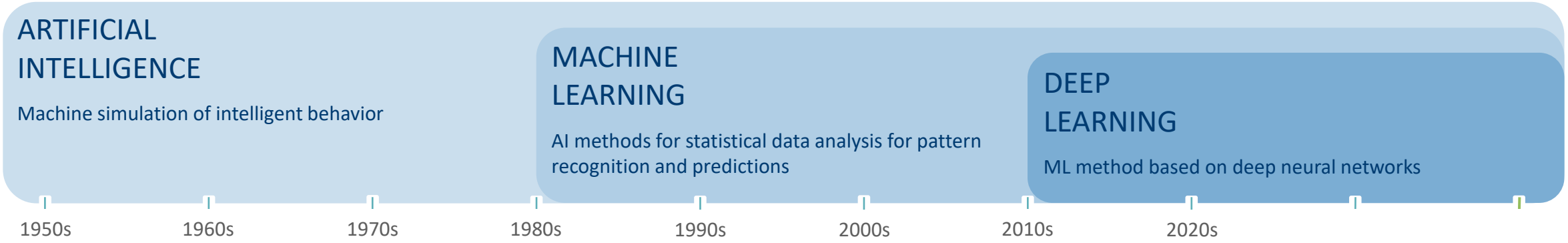
ARTIFICIAL INTELLIGENCE

AI CAN DELIVER ON INDUSTRY EXPECTATIONS THROUGH MACHINE LEARNING AND DEEP LEARNING



Artificial Intelligence (AI)

Intelligence exhibited by machines, whereby machines mimic cognitive functions associated with human minds; cognitive functions include all aspects of learning, perceiving, problem solving, and reasoning.

Machine Learning (ML)

Major approach to realizing AI by learning from, and making data-driven prediction based on, data and learned experiences. ML comprises several categories, including unsupervised learning, supervised learning and reinforcement learning.

Deep Learning (DL)

ML method in which algorithms attend to model high-level abstractions in data. DL connects artificial, software-based calculators that approximate the function of brain neurons. Neural networks, formed by these calculators, receive, analyze, and determine inputs and are informed if determination is correct.

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ARTIFICIAL INTELLIGENCE

CAPABILITIES

Computer Vision

Process visual data and recognize objects

Understand the semantics of images or video sequences

Computer Audition

Process and interpret audio signals

Computer Linguistics

Process, interpret, and render text and speech

Robotics & Control

Analyze, interpret, and learn from data representing physical systems (incl. Internet of Things) and control its behavior

Discovery

Process large amounts of data and find patterns and “logical” relationships

Forecasting

Make predictions about future course of time series or likelihood of events

Planning & Optimization

Look for optimal solutions to problems with large solution space

Creation

Generate images, music, speech, and more based on sample creations

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AI HAS ALREADY DELIVERED VALUE IN PHARMA

AI-DRIVEN INNOVATIONS AND IMPACT ACROSS THE BIOTECH/-PHARMA RESEARCH VALUE CHAIN (EX.)

	Target Identification	Target Validation	Hit Identification	Lead Generation / Optimization	Preclinical
Examples of AI-driven acceleration	Insights from data sources (internal and from vendors) to generate novel target hypothesis Gene network, biochemical pathway, and cellular-response data integration in target identification	In silico, phenotypic, cellular models validate targets/identify biomarkers Disease causality determined within patient groups with significant unmet medical need	Automated image analysis for cellular assays through computer vision technology Molecular property prediction (virtual screening)	Molecular structure and property prediction (e.g., protein binding, logP, toxicity) for novel target proteins Rapid design iteration, across small and large molecules, using e.g., General Adversarial Networks	Safety issues and DMPK prediction using internal and public data Hypothesis-driven dosages for adaptive trials and targeted populations
Examples from industry and observed impact	Biopharma unlocked all-inclusive view of complex indication by attributing disease causality through linkages between genomic data and patient electronic medical records	Biopharma internalized AlphaFold2 and ColabFold to generate 3D models of almost any known, synthesized protein and protein-protein interactions, **reducing access to 3D structures from six months to a few hours**	Biotech saw **significant acceleration of high-throughput sequencing** (HTS) phase (time to 75% hits detected reduced by 50%) with platform-based "compound prioritization" algorithm	Biopharma leveraged generative machine learning model to expand library/optimize promising compounds and predict compound efficacy, **significantly increasing efficiency of library expansion**, with 60.000+ new compounds generated	Biopharma utilized predictive algorithms to **maximize probability of successful PK predictions with 83% of drug development projects** progressing to clinic with no PK issues

Source: DMPK: Drug metabolism and pharmacokinetics; PK: Pharmacokinetic | https://www.mckinsey.com/industries/life-sciences/our-insights/ai-in-biopharma-research-a-time-to-focus-and-scale

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AI AS FEASIBLE PROGNOSTIC TOOL

MONITORING IN MYELOMA

Original Reports | Artificial Intelligence

Check for updates

Machine Learning Approach for Rapid, Accurate Point-of-Care Prediction of M-Spike Values in Multiple Myeloma

Ehsan Malek, MD[1,2,3]; Gi-Ming Wang, MS[3,4]; Curtis Tatsuoka, PhD[4,5]; Jennifer Cullen, PhD, MPH[3,4]; Anant Madabhushi, PhD[6,7]; and James J. Driscoll, MD, PhD[1,2,3]

DOI https://doi.org/10.1200/CCI.23.00078

ABSTRACT

PURPOSE The gold standard for monitoring response status in patients with multiple myeloma (MM) is serum and urine protein electrophoresis which quantify M-spike proteins; however, the turnaround time for results is 3-7 days which delays treatment decisions. We hypothesized that machine learning (ML) could integrate readily available clinical and laboratory data to rapidly and accurately predict patient M-spike values.

METHODS A retrospective chart review was performed using the deidentified, electronic medical records of 171 patients with MM.

RESULTS Random forest (RF) analysis identified the weighted value of each independent variable (N = 43) integrated into the ML algorithm. Pearson and Spearman coefficients indicated that the ML-predicted M-spike values correlated highly with laboratory-measured serum protein electrophoresis values. Feature selected RF modeling revealed that only two variables—the first lagged M-spike and serum total protein—accurately predicted the M-spike.

CONCLUSION Taken together, our results demonstrate the feasibility and prognostic potential of ML tools that integrate electronic data to longitudinally monitor disease burden. ML tools support the seamless, secure exchange of patient information to expedite and personalize clinical decision making and overcome geographic, financial, and social barriers that currently limit the access of underserved populations to cancer care specialists so that the benefits of medical progress are not limited to selected groups.

ACCOMPANYING CONTENT

Appendix

Accepted July 20, 2023
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JCO Clin Cancer Inform
7:e2300078

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Presented by A Madabhushi at International Myeloma Conference 2024, Sep 25-28. Rio de Janeiro, Brazil

AI IN CLINICAL TRIALS

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PHARMA DRUG DEVELOPMENT CYCLE

CLINICAL TRIALS

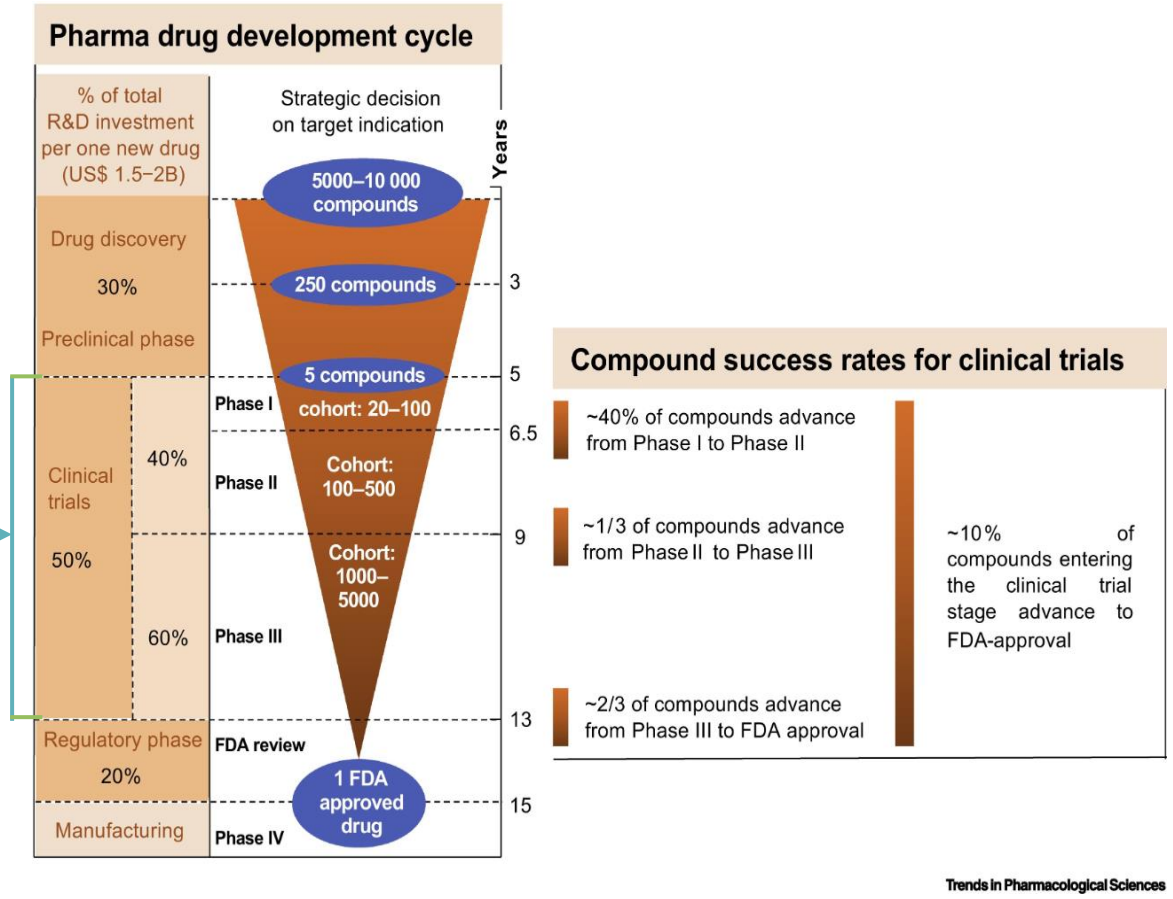
Clinical trials consume the latter half of the 10 to 15 year, 1.5–2.0 billion USD, development cycle for bringing a single new drug to market.

Hence, a failed trial sinks not only the investment into the trial itself but also the preclinical development costs, rendering the loss per failed clinical trial at 800 million to 1.4 billion USD.

Two of the main causes for high trial failure rates are:

- Suboptimal patient cohort selection and recruiting techniques
- Inability to monitor patients effectively during trials

PHARMA DDC AND COMPOUND SUCCESS RATES



DDC: Drug development cycle; Harrer et. al 2019

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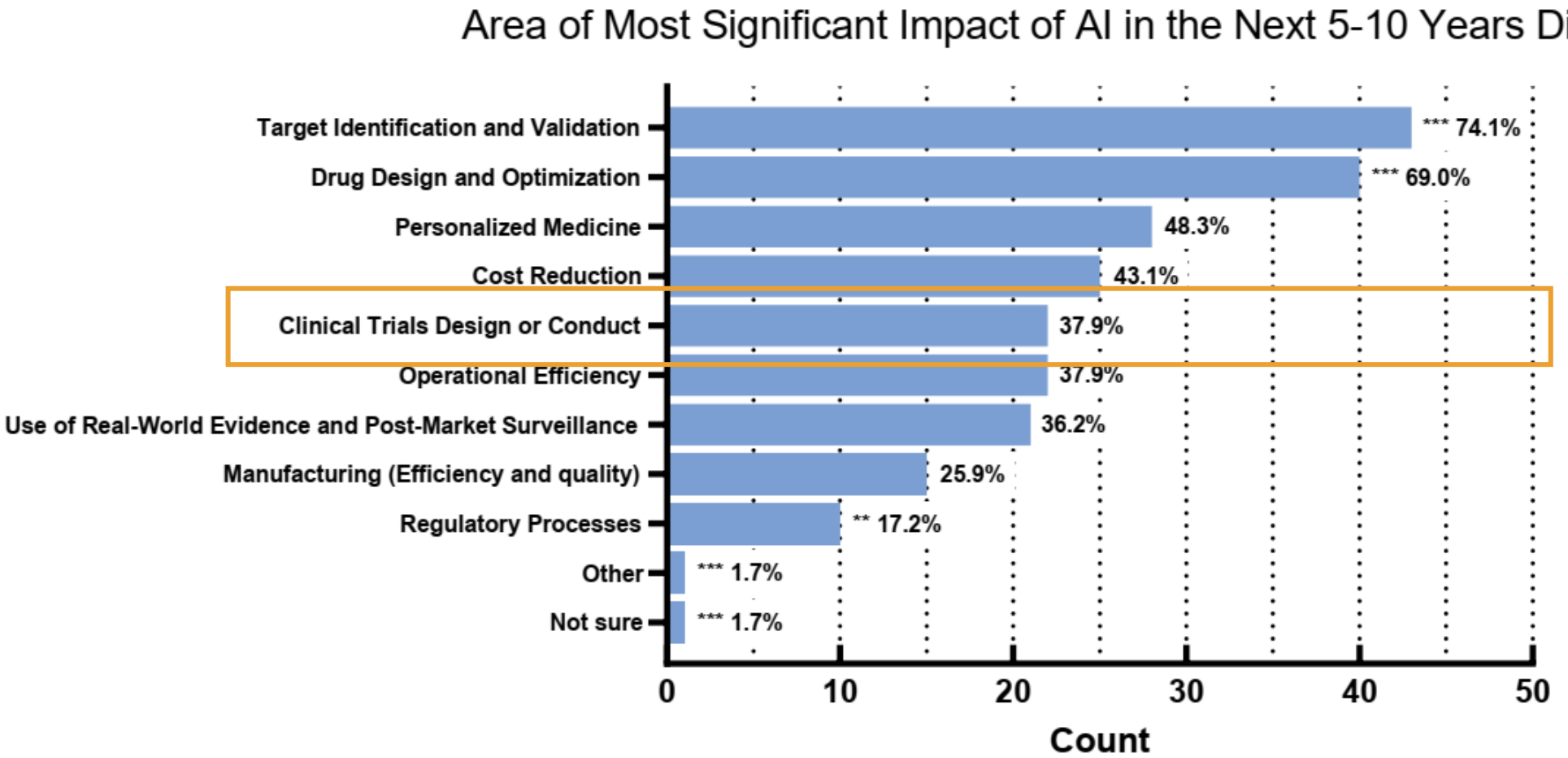
SURVEY ON ADOPTING AI IN PHARMA



Data were analysed by Chi-square goodness of fit testing, which indicated that the overall distribution was significantly different from an equal distribution ($p < 0.0001$; n=58). Asterisks indicate statistical significance based on standardised residuals (**$p < 0.01$, ***$p < 0.001$).

Source: Figure 9 from: Ross, T.; AI Integration in Drug-Development Biotechs: An Analysis of Current Adoption, Challenges, and Competitive Impact. Master Thesis. Aug 2024. Goethe Business School, Frankfurt, Germany. Permission to use has been granted.

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AI IN CLINICAL TRIALS

AI USE CASES AND APPLIED AI CAPABILITIES

AI Use Case	Patient recruitment	Patient monitoring	Clinical trial protocol design and authoring	Patient outcome prediction	Synthetic data generation	Improve pathology analysis
AI Capability	Pattern Recognition Classification	Pattern Recognition Classification	Prediction NLP Generation	Prediction	Generation Creativity	Image analysis Pattern Recognition Classification
Description & Outcomes	**Increasing speed and probability of trial success** by identifying the most suitable and eligible **candidates** quickly and **retaining them on the trial**.	Monitoring patient adherence to trial protocols and identifying deviations. Gathering additional data during trials, including observational studies, for **better outcomes**	Design **efficient clinical trial protocols**, optimizing various parameters to **improve trial outcomes** and **reduce costs**.	Developing personal treatment plans to **reduce patient risk** of exposure to ineffective or harmful treatments. **Enhancing probability of trial success**.	Enhancing trial data with synthetic data, e.g., for under-represented populations or control arm in external comparator studies.	Analysis of medical images or laboratory results.
Reference	Beck et al. 2020 Hassanzadeh, Karimi and Nguyen 2020 Cai et al. 2021	Baig et al. 2017 Abiodun, Okunbor and Osamor 2022	Harrer et al. 2019 Wang and Sun 2022 Wu et al. 2022 Kavalci and Hartshorn 2023 Wang, Xiao and Sun 2023	Beacher et al. 2021 Cui et al. 2022 Feuerriegel et al. 2024	Krenmayr et al. 2022 D'Amico et al. 2023	Wang et al. 2019 Jiang et al. 2020 Sultan et al. 2020

Adapted from Table A1: Ross, T.; AI Integration in Drug-Development Biotechs: An Analysis of Current Adoption, Challenges, and Competitive Impact. Master Thesis. Aug 2024. Goethe Business School, Frankfurt, Germany.

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AI IN CLINICAL TRIALS

AI USE CASES AND AI SOLUTIONS (EXAMPLES)

Patient Recruitment

AiCure H.Code

Patient engagement AI platform

Trial Design & Optimization

StarGPT

Determine the optimal patient population for a trial by analyzing data from previous studies

Data Collection & Analysis

Data Hub

Comprehensive range of solutions to streamline and optimize the clinical trial process

Operational Efficiency

Neuroute AI

AI platform that generates a tailored clinical trial design and operational plan

Regulatory

Cedience

AI platform that helps to leverage past regulatory data to find evidence-backed answers

IND Application

AutoIND

AI-native platform to automate IND drafts, for quality review, editing and refinement

Medical Writing

Yseop Copilot

Generative AI to accelerate medical writing

Data Anonymization

Trusano

AI-powered data & document anonymization, redaction & masking software

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AI STRATEGY DEVELOPMENT

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AI STRATEGY DEVELOPMENT

STRATEGY

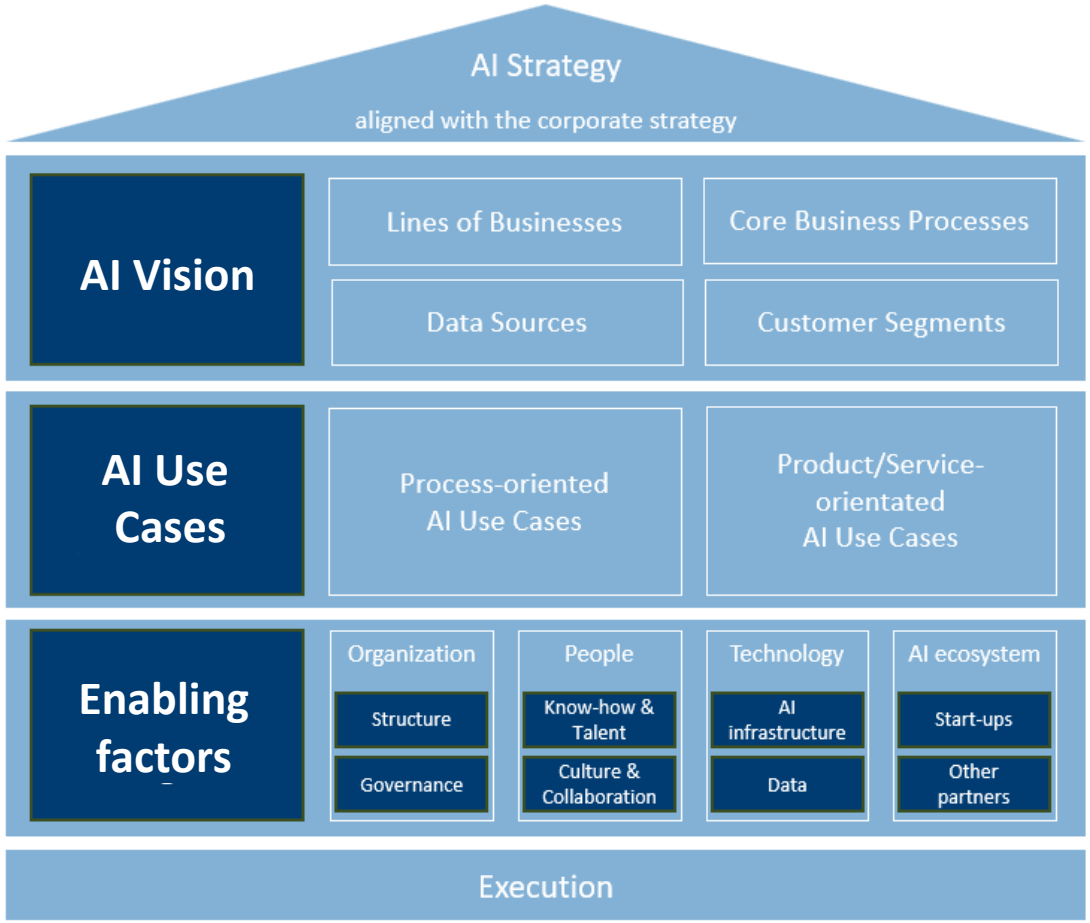
Ansoff 1965

- Strategies are measures to ensure the long-term success of a company.

AI STRATEGY DEVELOPMENT

Goals → Pain Points → Current Capabilities → Data Strategy → Resource and Adoption Readiness

THE AI STRATEGY HOUSE



The AI Strategy Roadmap. Microsoft 2024 | The AI Strategy House: DOCULLMANN.AI, modified from AppliedAI

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AI STRATEGY DEVELOPMENT

AI VISION

Strategic anchors

Determine the strategic goals that leadership is striving towards and how AI might enhance, accelerate, or augment existing strategic goals, e.g.:

- 3–5-year goals
- Key differentiators (at a company or product level)
- Current initiatives or thrusts

AI Transformation Vision

- Use the AI Transformation Vision Map
- Find the AI or data-backed capabilities most likely to help the firm succeed in the marketplace in the long term.

AI TRANSFORMATION VISION MAP

Source: AI Transformation Vision Map: DOCULLMANN.AI, based on EMERJ AI Transformation Template

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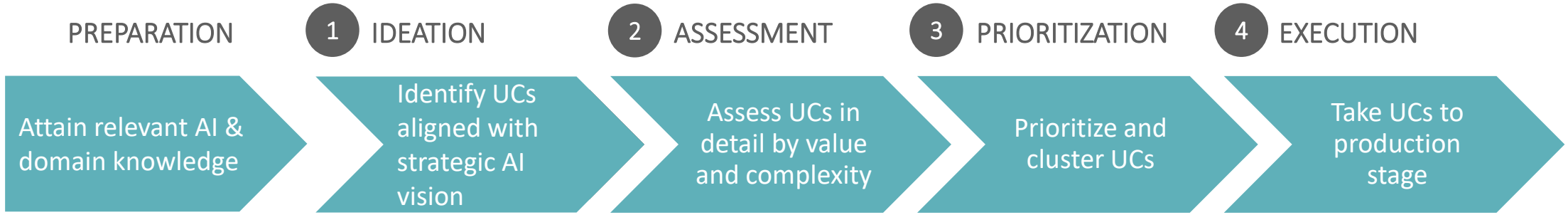
AI USE CASE DISCOVERY PROCESS



	PREPARATION	1 IDEATION	2 ASSESSMENT	3 PRIORITIZATION	4 EXECUTION
CONTENT	• Understanding AI • AI Maturity Assessment • Business Priorities • AI Search Fields	• **Bring together opportunity space** (from process and customer view) **with solution space** (data and AI capabilities) for UC ideas	• **Structured assessment** of all identified UCs, along **with value and ease of implementation** dimensions	• **Prioritization and clustering** of portfolio of use case ideas **based on value and ease of implementation**	• Per UC: Define scope for 1st data exploration and scope for MVP • Data gathering • Model development & validation
PARTICIPANTS	• Business Top Mgt. • AI Strategists (CoE) • Business Owners/ Domain Experts • Data Experts/ Owners		• AI Strategists • AI Engineers • Domain Experts/Owners • Data Experts/Owners		• Business Owner • AI Engineers • External Solution Partners
OUTCOME	• Good AI knowledge • Relevant case studies • Focus areas for AI • AI maturity		• Filled-out **opportunity and solution space cards** per identified use case	• Filled-out **prioritization matrix** (value & ease of implementation) • Draft **roadmap** for prioritized use cases	• Narrow-scope definition for initial data exploration • Broader scope for MVP development

Source: CoE: Center of Excellence; MVP: Minimal viable product; UC: Use case

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Provided by DOCULLMANN.AI

AI Use Case Discovery

Created by:	Area:	Date:	Status:

DEMAND FOR AI | PROBLEM OR OPPORTUNITY

1. What is the problem you want to solve or the opportunity you want to seize?

2. Which services/systems/processes are affected?

3. User Story – Describe how the user carries out the various steps today.

SOLUTION WITH AI | USE CASE HYPOTHESIS

1. Which AI capability(ies) could be used to solve this problem? (Explanation: see separate document)

- ○ Vision
- ○ Audition
- ○ Linguistics
- ○ Robotics
- ○ Forecasting
- ○ Discovery
- ○ Optimize
- ○ Generate

2. How will AI solve this? What is the value and the desired outcome?

3. What information/data is required to train an AI for this?

Provided by DOCULLMANN.AI

AI Use Case Assessment

Created by:	Area:	Date:	Status:

Description of the use case

Trustworthy AI | Assessment of risks required?

- ○ Ethical aspects (e.g. dealing with gender-specific or diverse prejudices)
- ○ Cyber-security risks (e.g., in fully automated processes)
- ○ Regulatory aspects (e.g. upcoming regulatory changes)
- ○ Human-in-the-loop requirement (e. g., black swan resilience)

VALUE | Created business and/or benefit value

1. How does the use case fit in with your AI vision?	2. What strategic advantages does this offer?	3. What are the financial effects (e.g. savings, additional income)?
Score 0 to 10 Weighting 15% ☐	Score 0 to 10 Weighting 25% ☐	Score 0 to 10 Weighting 60% ☐

Score / 10

FEASIBILITY | Ease of implementation

Please enter a value between 0 (strongly disagree) and 5 (strongly agree) in the boxes for the following statements. If you cannot assess a statement, please enter a minus "–".

1. Data/Infrastructure | Score:

- We have access to the required data. ☐
- We have the required amount of data. ☐
- We have the required data quality. ☐

2. Algorithm/Solution | Score:

- We know of technical resources that can lead to a solution. ☐
- A similar problem has already been solved by others. ☐
- We know techniques that could help with this problem. ☐

3. Processes/Systems | Score:

- No/few processes need to be changed. ☐
- No/few systems need to be adapted. ☐
- No/few organizational changes are necessary. ☐

4. Know-how | Score:

- The required technology know-how is available. ☐
- The required domain know-how is available. ☐
- The required trainings can be executed within a reasonable time. ☐

How long does the development of the use case take until the verified PoC (proof of concept)?

○ <3 months (+5 points) ○ 4–6 months (+4 points) ○ 7–9 months (+3 points) ○ 10–12 months (+2 points) ○ >12 months (+1 point)

Score / 65

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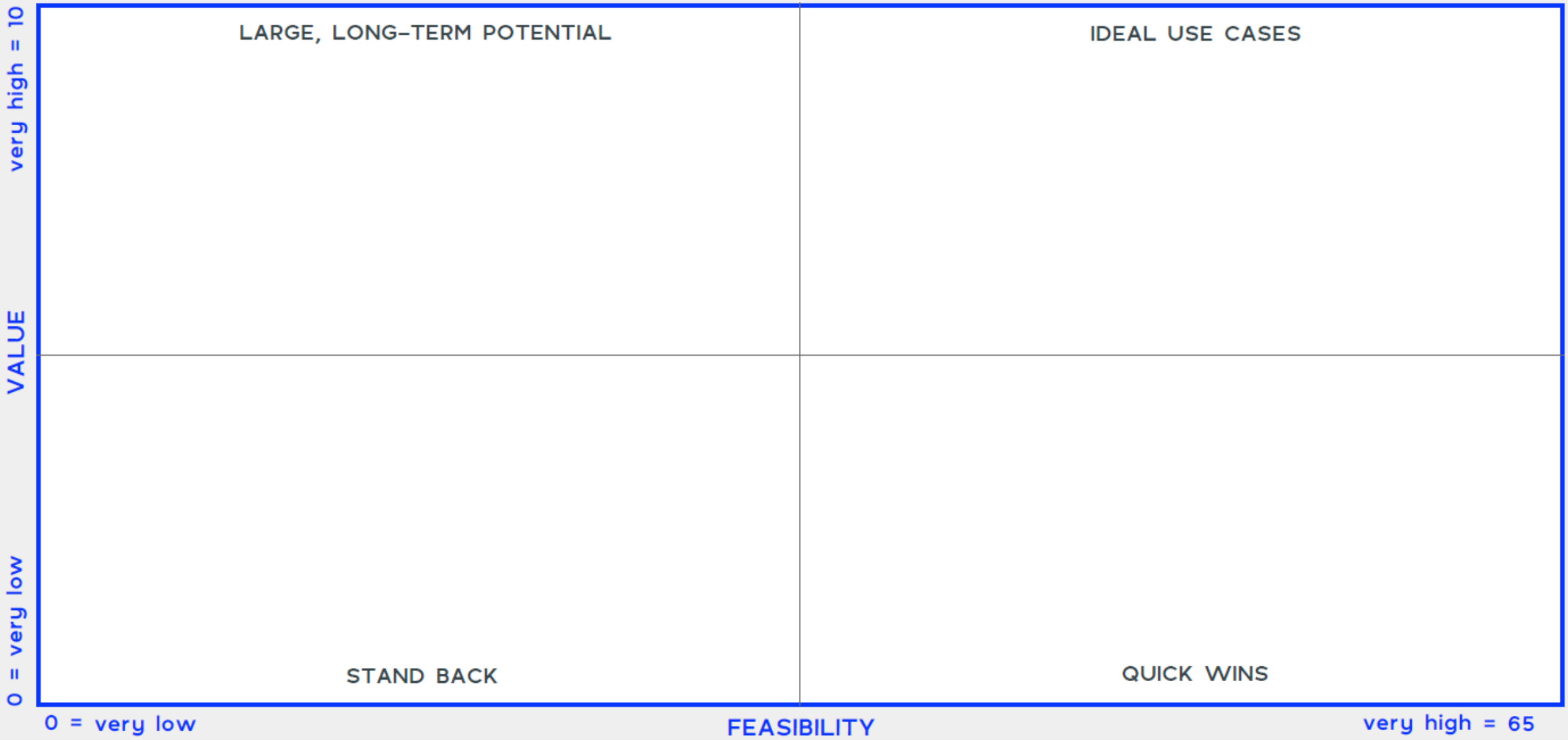
AI Use Case Prioritization

Created by:	Area:	Date:	Status:



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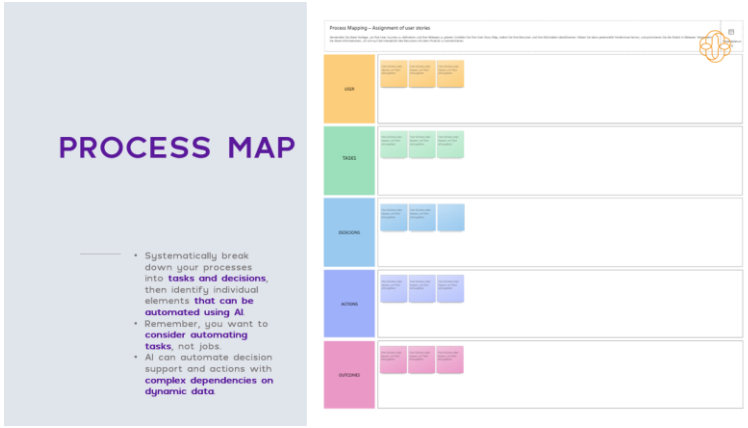
AI Use Case Prioritization

Created by:	Area:	Date:	Status:

REQUIRED INPUT MAPS FOR AI USE CASE IDEATION

PROCESS MAP

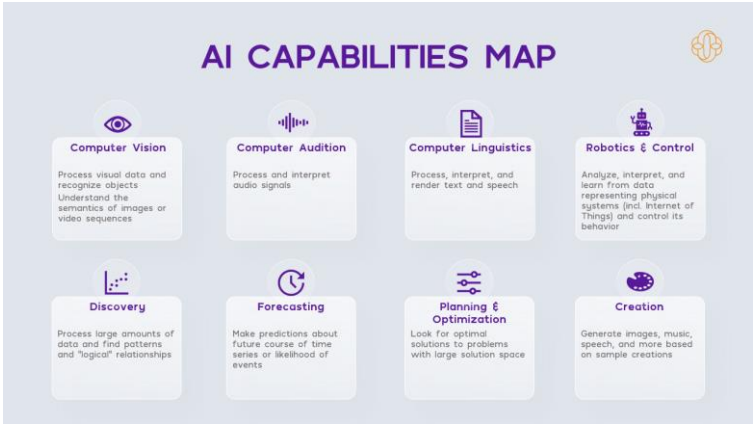


Systematically **break down your processes** into tasks and decisions, then identify individual elements that can be automated using AI.

Remember, you want to consider automating tasks, not jobs.

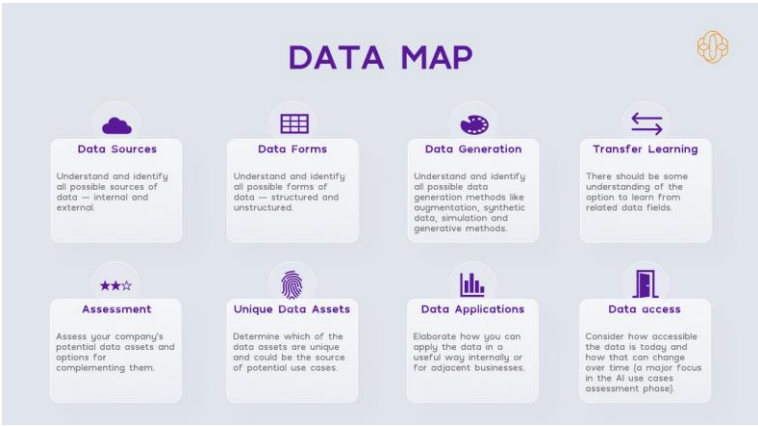
AI can automate decision support and actions with complex dependencies on dynamic data.

AI CAPABILITIES MAP



- Computer vision
- Computer audition
- Computer Linguistics
- Robotics & Control
- Discovery
- Forecasting
- Planning & Optimization
- Generation

DATA MAP



- Data sources
- Data forms
- Data generation
- Transfer learning
- Data assessment
- Unique data assets
- Data applications
- Data access

AI Use Case Ideation Input Maps © DOCULLMANN.AI; All rights reserved

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CONSIDERATIONS

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AI PROJECT CONSIDERATIONS

AI-SPECIFIC CHALLENGES

AI Performance Uncertainty

- For novel AI use cases or untested data repertoires

AI Paradox

- It is deceptively easy to build successful AI prototypes, but fiendishly hard to scale AI.

AI Value Estimate Questions

- What scale (of possibly interacting AI applications) is required?
- What degree of maintenance is needed to adapt to new data requirements?

MAKE OR BUY

AI is NOT Plug-and-Play

- In AI, make-or-buy is more of a continuum than a binary decision.

AI Open-Source Models

- Most raw AI algorithms are (still) open source, available for free, but without immediate business value.

AI Customization

- The best vendors offer pre-trained models with graphical user interfaces to support the further process of customization.

AI-USE FLAGS

Regulatory or Ethic Flag

- Mostly when sensitive people-related data/decisions are involved

Cyber-Security Flag

- Truly critical when processes are fully automated and might get infiltrated

Resilience Flag

- It may be important to expose AI use cases to an extensive test of resilience against future extreme events not represented in the test sets.

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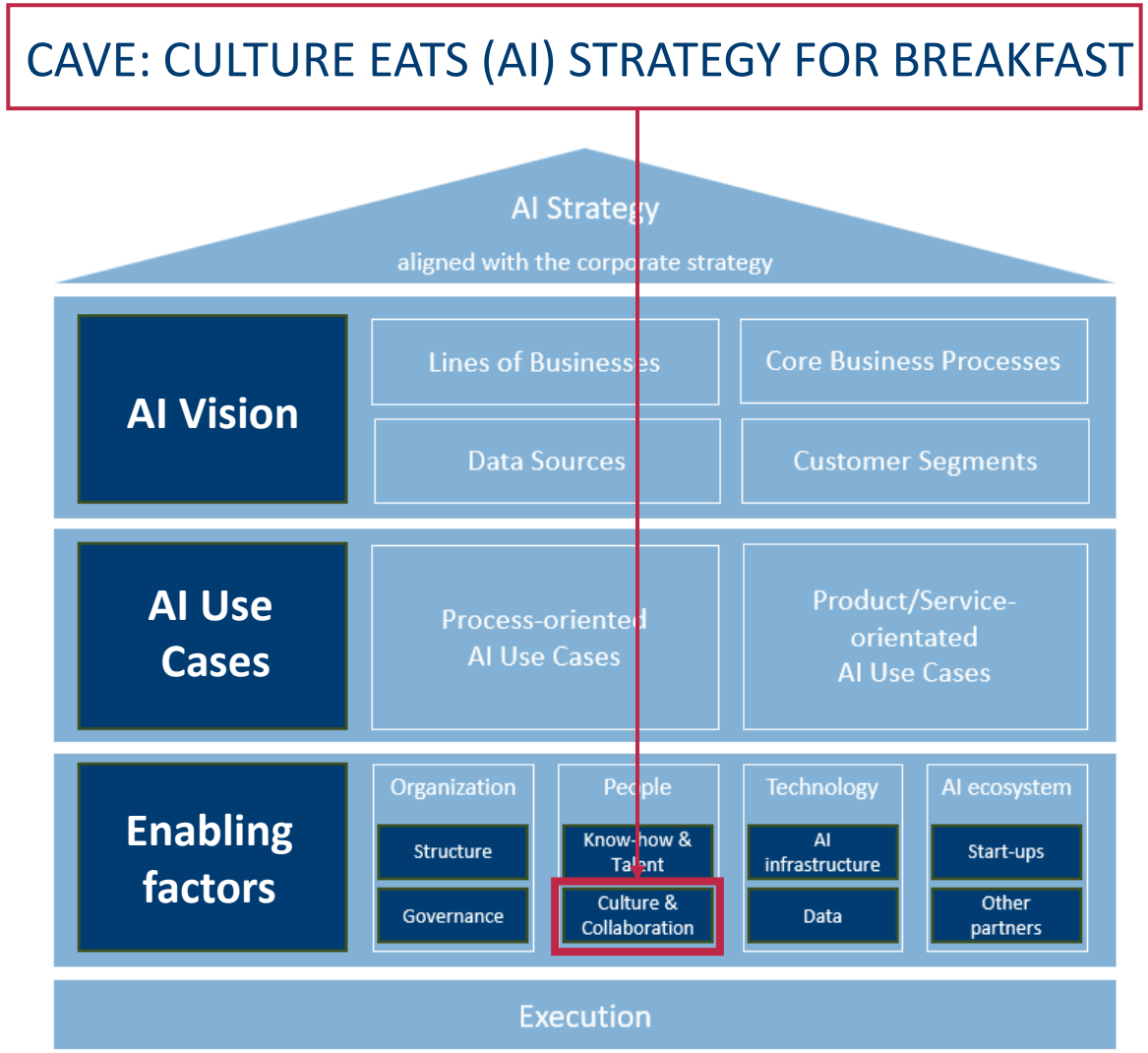
AI STRATEGY AS CONDITIO SINE QUA NON FOR AI SUCCESS

AI PROJECT FAILURE

According to Gartner, approximately 85% of AI projects fail to deliver on their promises, with many either being abandoned or failing to meet their intended objectives.

Most significant barriers for AI project success are:

- Lack of an AI vision and adoption strategy
- Lack of leadership commitment
- Lack of AI talent, AI skills and knowledge
- Inadequate change management
- Data management issues



Source: Gartner 2017, Kar 2022 | The AI Strategy House: DOCULLMANN.AI, modified from AppliedAI

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AI SUCCESS PRINCIPLES

THINK BIG – START SMALL

AI is NOT IT

- Treat AI solutions as product, not project.

Governance

- Set the right balance between **central coordination and decentralized ownership** from the start.

Leadership Commitment & AI Fluency

- Demonstrate powerful leadership and broad **commitment from** an **AI-educated C-Level:**
  - AI transformation vision
  - Conceptual AI understanding
  - AI use case range

Think Big – Start Small

Start with a quick win AI pilot (low hanging fruit).

"MACHINE LEARNING TECHNOLOGY WITHOUT MANAGEMENT AND ORGANIZATIONAL CHANGE WILL BE INEFFECTIVE."

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AI COULD LEAD TO SUBSTANTIAL ADVANCES IN CANCER CARE

COLLABORATIVE EFFORTS ARE NEEDED

"(…) **Education** and **training** are crucial to **increase trust in AI in medicine**. (…) As a community, we **need to demystify AI** and provide **loads of opportunities for oncologists** to familiarise themselves with the basic ideas behind it.(…)", says Dr. Mireia Crispin Ortuzar, University Cambridge, UK, Co-Chair of 1st edition of **ESMO AI& Digital Oncology Congress,** Berlin, November 2025.

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CONCLUSION & RECOMMENDATIONS

AI IMPLEMENTATION SUCCESS PRINCIPLES

AI Vision & Strategy

Develop a clear AI vision and strategy (“Why? What? Who? How?”).

AI Flags

Identify AI use case flags (e.g., GDPR, EU AI Act, ethics& regulation) at an early stage.

Leadership Commitment

Ensure leadership commitment right from the start.

Data Governance

Develop a data strategy and invest in data governance, Quality & Compliance.

AI Fluency

Educate your staff about the benefits of AI in your organization and implement AI training.

Change Management

Engage and incorporate employees early in the AI implementation process.

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ACKNOWLEDGEMENT

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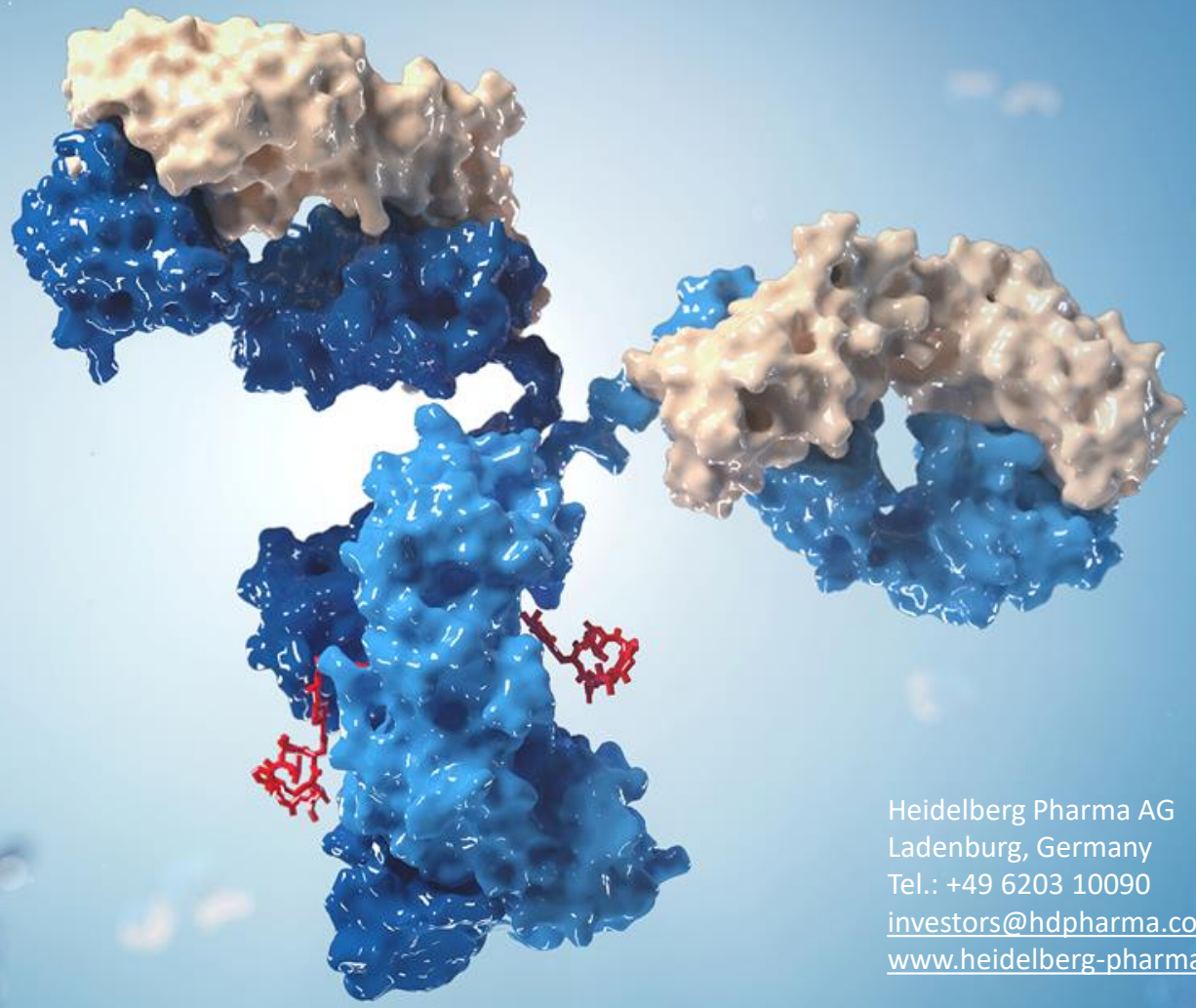

THANK YOU!

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Q&A

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BACKLOG

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AI IN CLINICAL TRIAL SCREENING & DATA MANAGEMENT

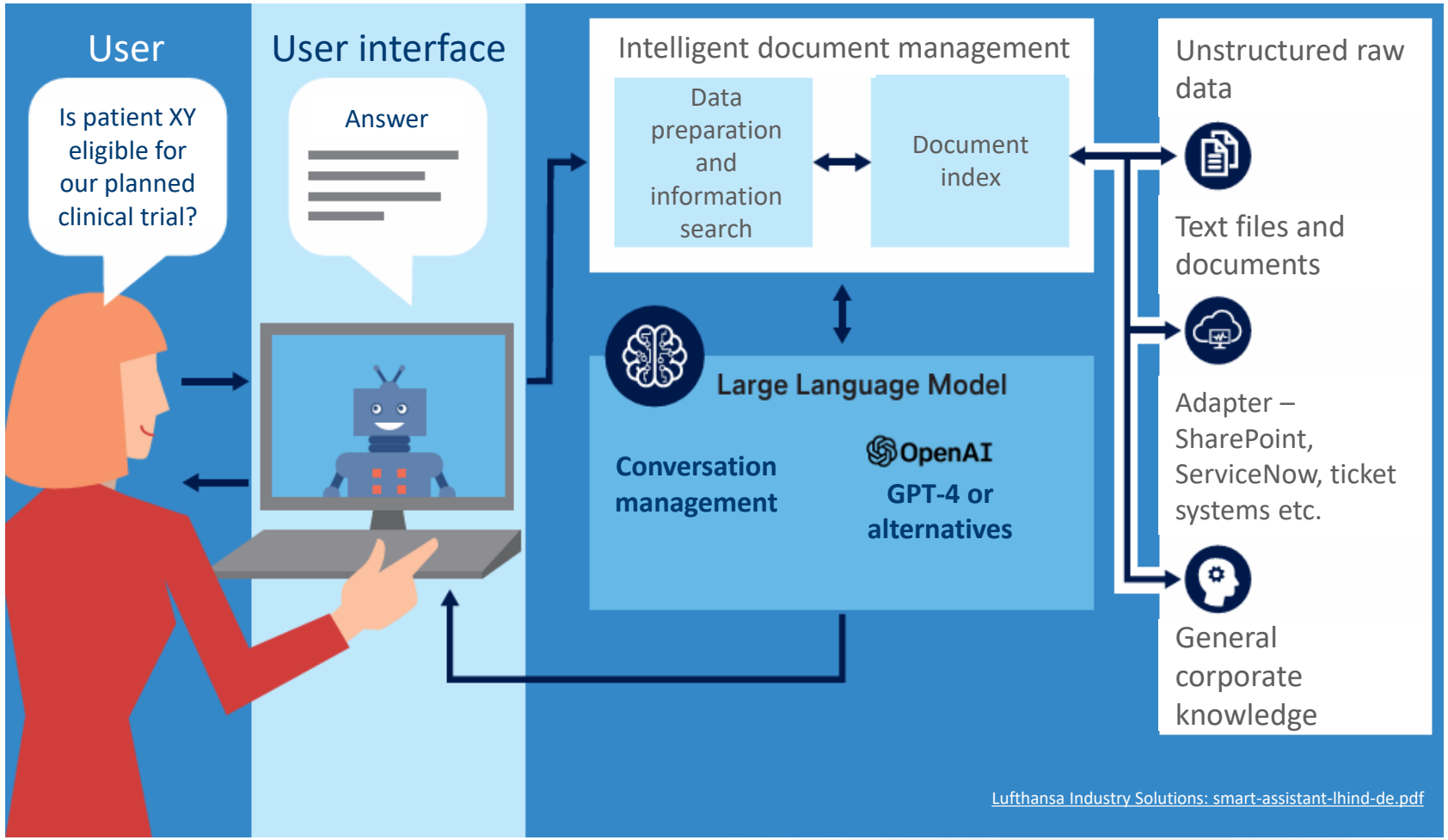
RETRIEVAL-AUGMENTED GENERATION (RAG)

Clinical trial screening process:

- Currently manual
- Error-prone
- Costly

RAG based on LLMs like GPT-4 can **significantly enhance** clinical trial **screening performance** and **reduce costs** by automating the screening process.

Careful consideration of potential hazards is required and should include safeguards such as **final clinician review**.



Source: GPT: Generative pre-trained transformer; LLM: Large language model; Tan et. al 2024, Onlu et al. 2024

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AI-DRIVEN FUTURE FOR ONCOLOGY

IMPACT ON THE PRACTICE OF ONCOLOGY THROUGH MANY DIFFERENT APPLICATIONS

npj | precision oncology

Perspective

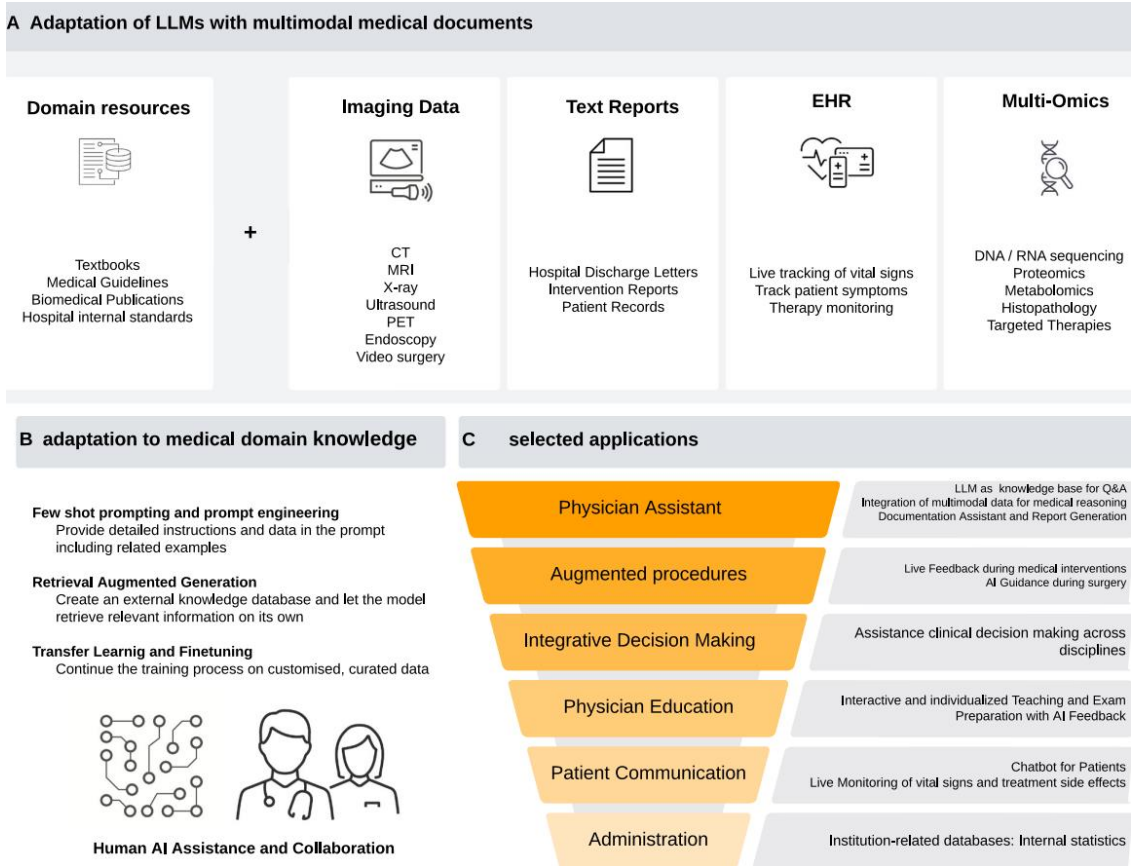
Published in partnership with The Hormel Institute, University of Minnesota

https://doi.org/10.1038/s41698-024-00573-2

Large language models and multimodal foundation models for precision oncology

Check for updates

Daniel Truhn[1], Jan-Niklas Eckardt[2,3], Dyke Ferber[4,5] & Jakob Nikolas Kather[2,3,4,5]



Source: Truhn et al.2024 Fig 1: Overview of medical adaptations of LLMs.

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MACHINE LEARNING

AI METHODS FOR STATISTICAL DATA ANALYSIS FOR PATTERN RECOGNITION AND PREDICTIONS

PATTERN

- ML enables computers **to recognize patterns** and correlations in data and to learn from them.

LEARNING

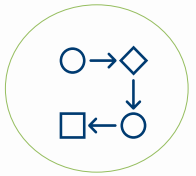
- ML models use algorithms to **learn**.
- This process involves **analyzing** large amounts of data (big data).

DATA

- Data (**big data**) is the basis for machine learning.
- It can be text, images, numbers or almost any other form of data.

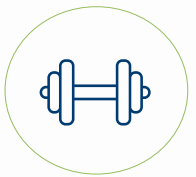
ALGORITHM

- Specific **mathematical models and methods** that enable machine learning.
- Examples include decision trees and **neural networks**.



TRAINING

- The process by which an ML model analyzes data and learns from it.
- The result is a trained model that can be used for **predictions** or decisions.



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DEEP LEARNING

MACHINE LEARNING METHOD BASED ON NEURAL NETWORK

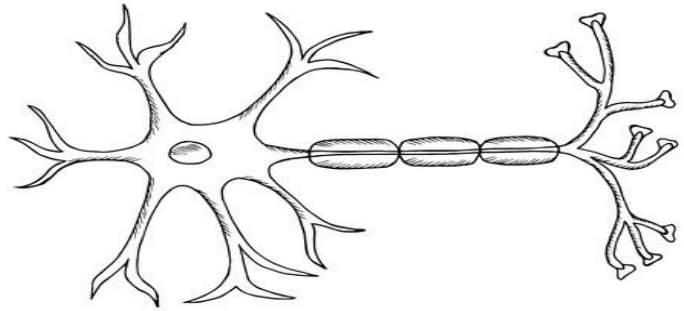
Since the 1940s

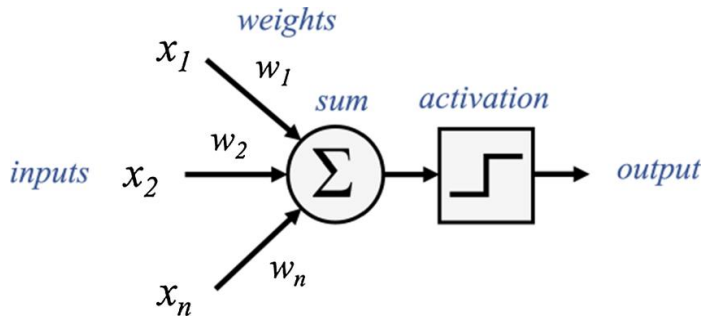
Reproduction of the network of neurons in the human brain

Consists of nodes (neurons) and layers

Three learning methods

- Unsupervised learning
- Supervised learning
- Reinforcement learning





DEEP NEURAL NETWORK

REPRODUCTION OF THE NETWORK OF NEURONS IN THE HUMAN BRAIN

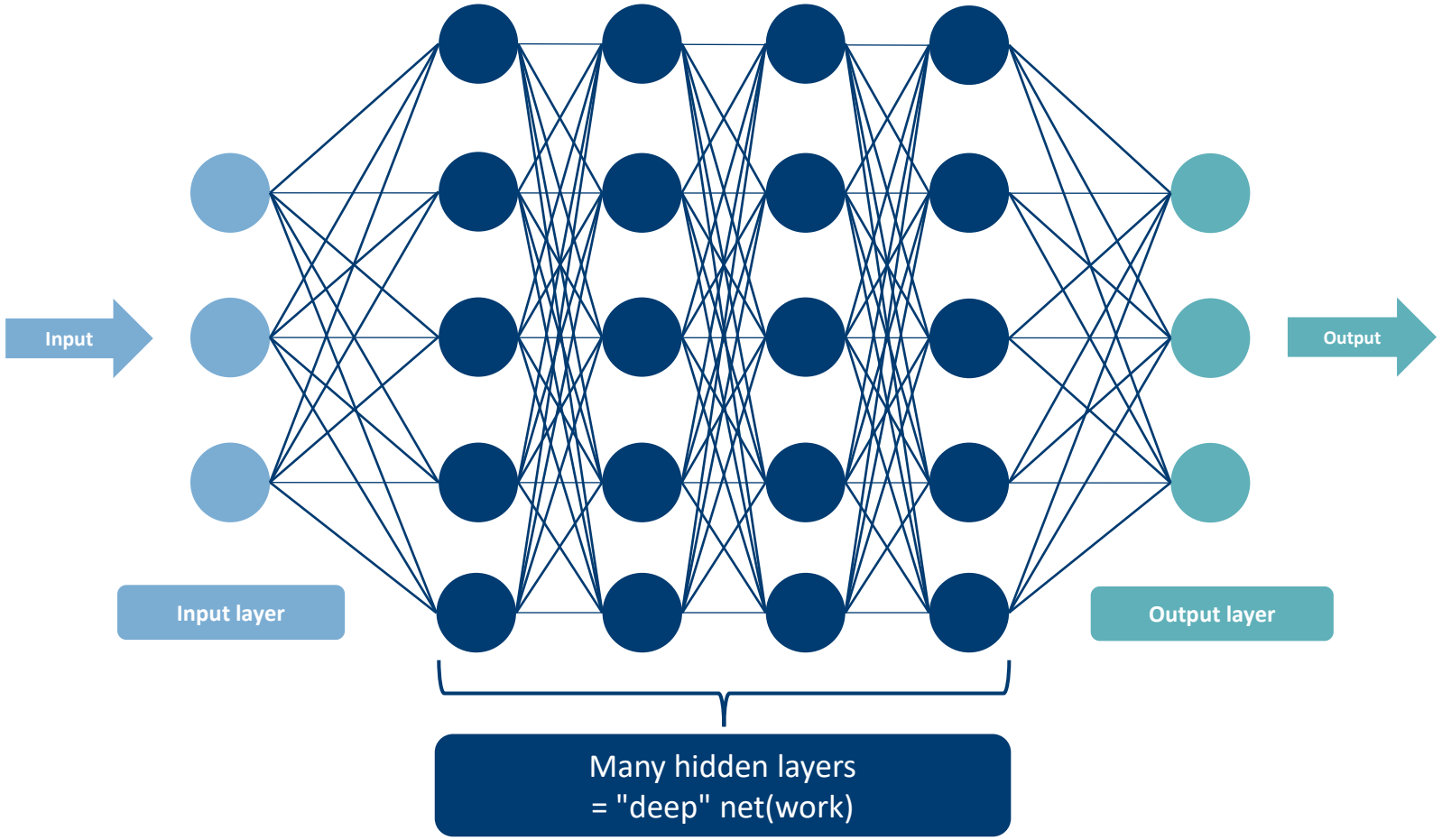


Illustration: DOCULLMANN.AI

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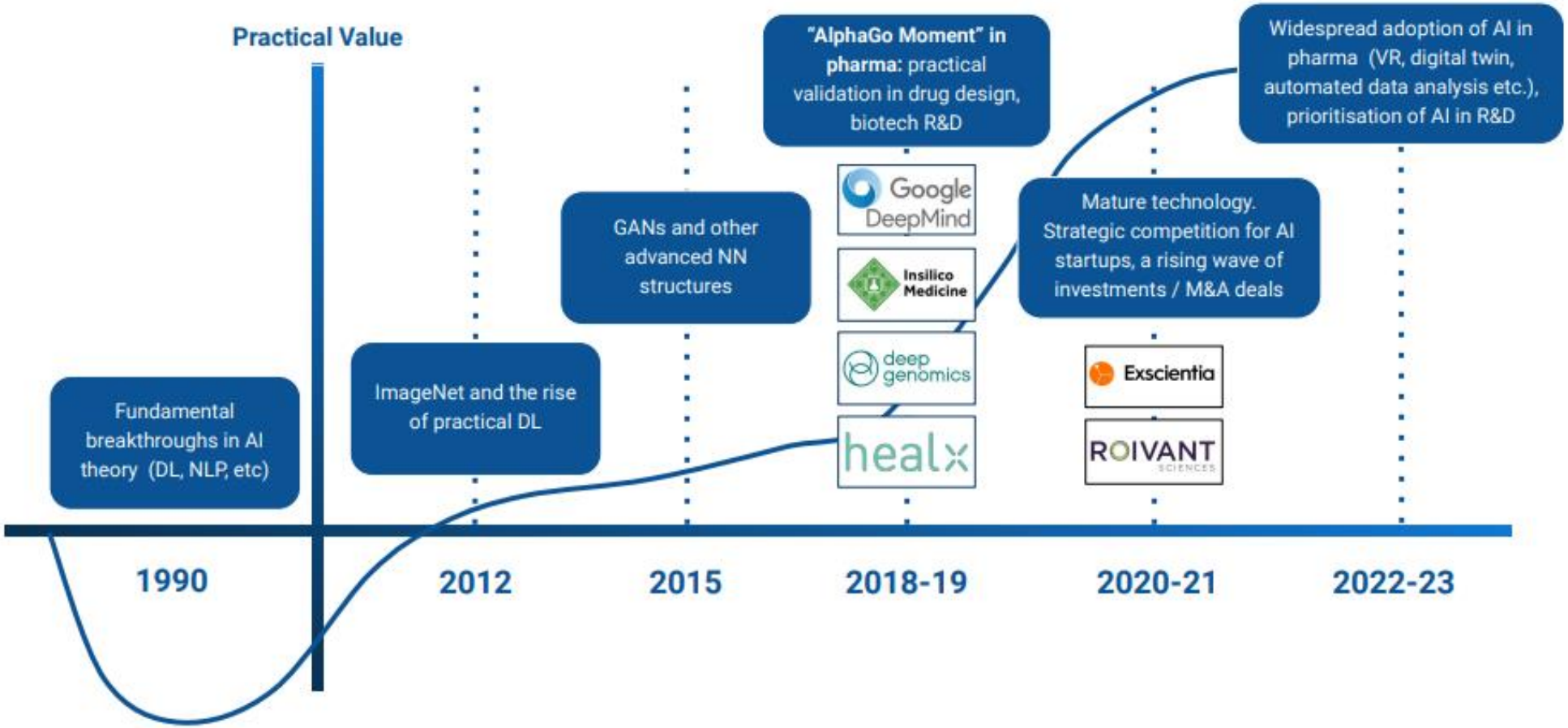
„ALPHAGO MOMENT“ IN PHARMA

2016: ALPHAGO FROM DEEPMIND BEATS THE KOREAN GO WORLD CHAMPION LEE SEDOL



DL: Deep Learning; GAN: Generative Adversarial Network; NLP: Natural Language Processing; NN: Neural Network, VR: Virtual Reality

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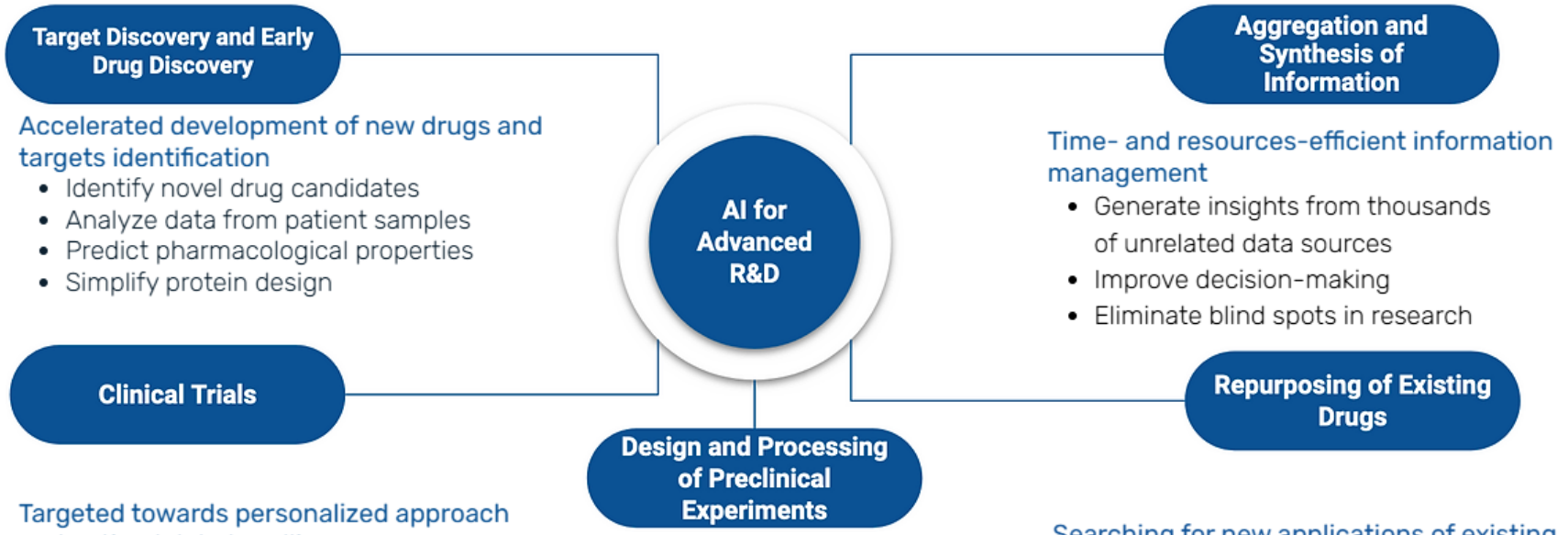
AI APPLICATIONS IN PHARMA

AI IN COMPUTER-AIDED DRUG DISCOVERY (CADD) AND ADVANCED R&D



Target Discovery and Early Drug Discovery

Accelerated development of new drugs and targets identification

- Identify novel drug candidates
- Analyze data from patient samples
- Predict pharmacological properties
- Simplify protein design

Aggregation and Synthesis of Information

Time- and resources-efficient information management

- Generate insights from thousands of unrelated data sources
- Improve decision-making
- Eliminate blind spots in research

Clinical Trials

Targeted towards personalized approach and optimal data handling

- Optimize clinical trial study design
- Patient-representative computer models
- Define best personalized treatment
- Analyze medical records
- Improve pathology analysis

Design and Processing of Preclinical Experiments

Optimization of experiments and data processing

- Reduce time and cost of planning
- Decode open- and closed-access data
- Automate selection, manipulation, and analysis of cells
- Automate sample analysis with a robotic cloud laboratory

Repurposing of Existing Drugs

Searching for new applications of existing drugs at a high scale

- Rapidly identify new indications
- Match existing drugs with rare diseases
- Testing 1000+ of compounds in 100+ of cellular disease models in parallel

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MACHINE LEARNING MODELS FOR DRUG R&D

LIST OF AI-BASED SOFTWARE FOR DRUG DISCOVERY, DEVELOPMENT & ANALYSIS (MAINLY OPEN SOURCE)

Reference	Description	Source code
AlphaFold2 [35]	Deep learning based model for 3D structure prediction of proteins from amino acid sequences	https://github.com/deepmind/alphafold/
DeepChem [80]	A deep learning library for drug discovery and computational chemistry	https://github.com/deepchem/deepchem
DeepBind [81]	A computational tool to analyze binding between the protein and DNA/RNA	https://github.com/MedChaabane/DeepBind-with-PyTorch
DeepBar [82]	A method for accurate and fast prediction of binding free energy	https://fastmbar.readthedocs.io/en/latest/
Deep-Screening [83]	Web-server based in deep learning for virtual screening of compounds	http://deepscreening.xielab.net/
DeepScreen [84]	High performance drug target interaction	https://github.com/cansyl/DEEPScreen
DeepConv-DTI [45]	A convolutional neural network based model for predicting drug-target interactions	https://github.com/GIST-CSBL/DeepConv-DTI
DeepPurpose [24]	A Deep learning library for drug-target interaction, drug-drug interaction, protein-protein interaction and protein function prediction	https://github.com/kexinhuang12345/DeepPurpose
DeepTox [85]	A deep learning model for toxicity prediction of chemical compounds	http://www.bioinf.jku.at/research/DeepTox/
AtomNet [86]	A deep convolutional neural network for bioactivity prediction	github
PathDSP [87]	A deep learning method for predicting drug sensitivity using cancer cell lines	https://github.com/TangYiChing/PathDSP
Graph level representation [88]	Learning graph representation for drug discovery	https://github.com/ZJULearning/graph_level_drug_discovery
Chemical VAE [89]	An auto-encoder based framework to generate new molecules	https://github.com/aspuru-guzik-group/chemical_vae/
DeepGraphMol [87]	A computational method for molecule generation with desired properties using graph neural networks and reinforcement learning	https://github.com/dbkgroup/prop_gen
TorchDrug [26]	A pytorch based flexible framework for drug discovery models	https://torchdrug.ai/

Qureshi R et al. AI in drug discovery and its clinical relevance. Heliyon 9 (2023) e17575; https://doi.org/10.1016/j.heliyon.2023.e17575

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AI TRANSFORMATION

AI TRANSFORMATION PLAN

Step 1 – Begin with the End in Mind

- Strategic anchors (3-5-year goals, key differentiators)
- AI Transformation Vision

Step 2 – The AI Opportunity Discovery Process

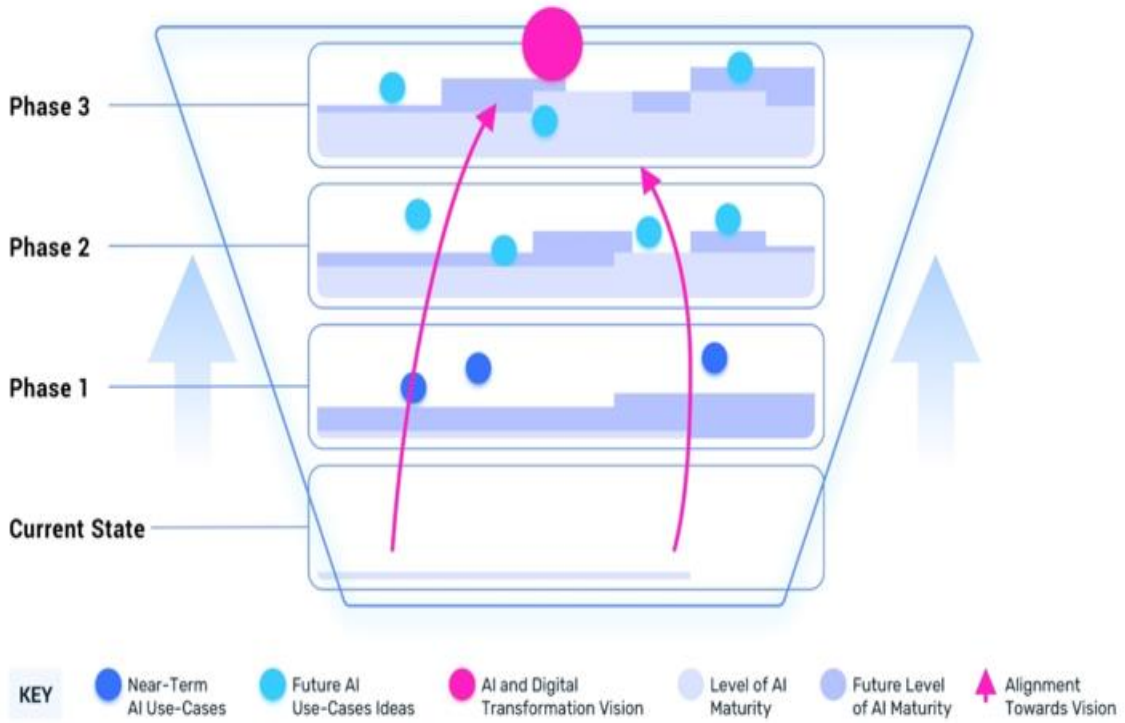
- Approach 1: Beginning with Workflows
- Approach 2: Beginning with Data

Step 3 – Assess Your Current State of AI Maturity

Step 4 – Drafting a Phasic AI Roadmap (top-down)

- AI Vision: Use AI Vision map for brainstorming
- Phase 3: long-term core AI-enabled capabilities
- Phase 2: possible use-cases in the next 1-2 years
- Phase 1: near-term pilot project(s)

THE AI PHASIC ROADMAP MODEL FOR AI TRANSFORMATION



Emerj's Phasic AI Roadmap model (Source: Emerj Plus AI Best Practice Guides

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