



Welcome to the

AiChemist and AIDD School Berlin

from the Machine Learning Research Group at Bayer Pharmaceuticals



Health for all, hunger for none





Bayer Pharmaceuticals R&D

/// Health for all



Oncology



Cardiovascular



Neurology and Rare Diseases



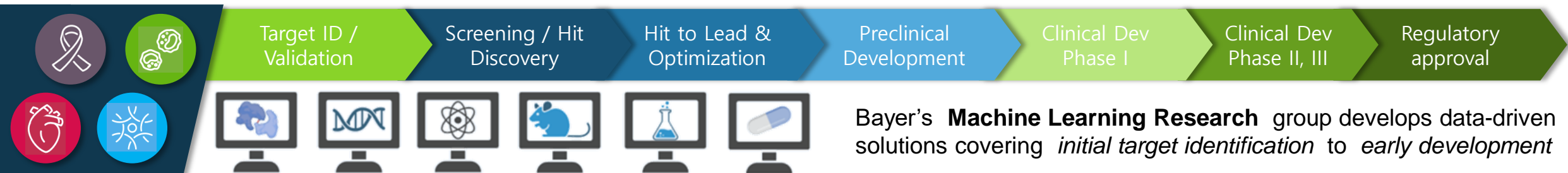
Immunology

- Protein Therapeutics
- Cell Therapies
- Contrast Agents
- Genetic Medicines
- Radionuclide Therapies
- Small Molecules



Machine Learning Research at Bayer Pharmaceuticals

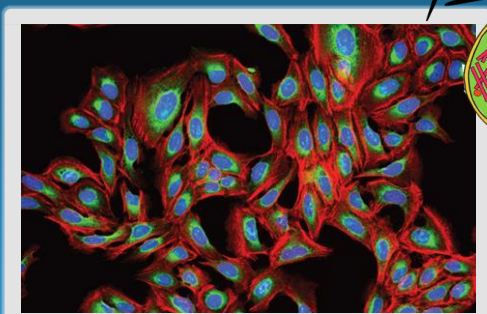
/// We drive fundamental Machine Learning Research with tangible impact on drug development



Bayer's **Machine Learning Research** group develops data-driven solutions covering *initial target identification* to *early development*

Cell painting

/// Adding phenotypic profiling to our toolkit

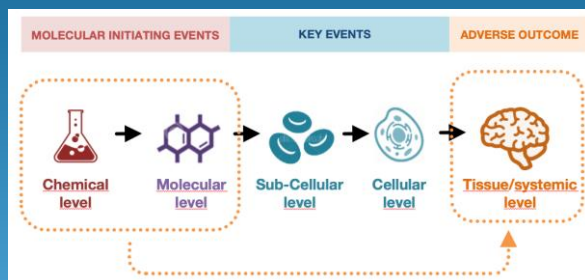


Picasso



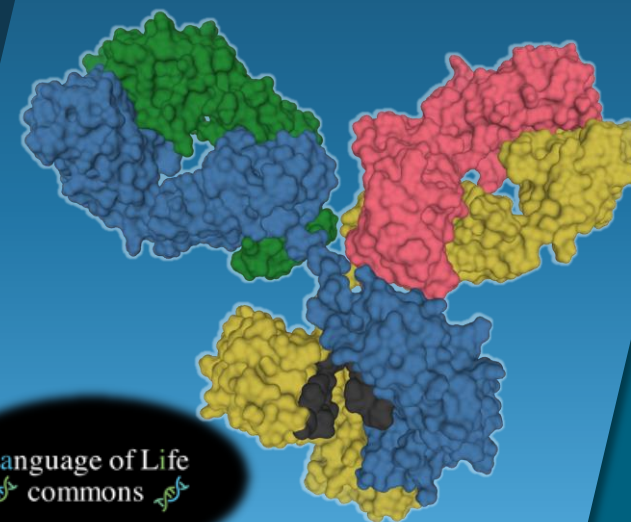
OnTox

/// New approaches to drug safety



Language of Life

/// ML-powered modeling of large molecules



Language of Life commons

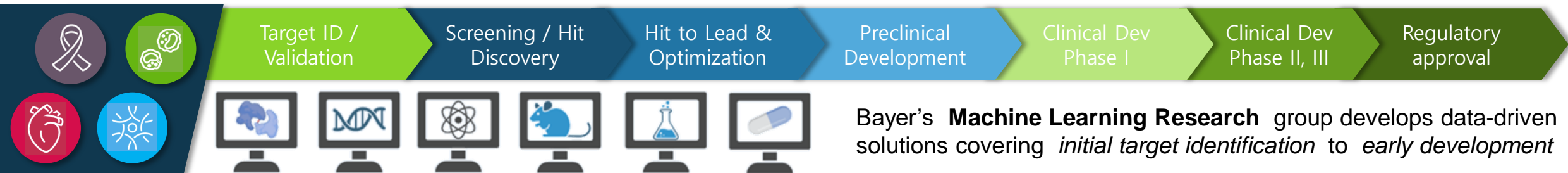
Kim, V., Adaloglou, N., Osterland, M., Morelli, F.M., Halawa, M., König, T., Gnutt, D. and Zapata, P.A.M., 2023. *BioRxiv*, pp.2023-04.

Garcia de Lomana, M., Marin Zapata, P.A. and Montanari, F., 2023. *Chemical Research in Toxicology*, 36(7), pp.1107-1120.



Machine Learning Research at Bayer Pharmaceuticals

/// We drive fundamental Machine Learning Research with tangible impact on drug development



Do we observe desired responses?

/// Adding phenotypic profiling to our toolkit



Paula
Marín Zapata

Modeling **drug response** in **image-based** screens as a function of **chemical space**

Should we expect undesired effects?

/// New approaches to drug safety



Marina
García de Lomana



Matteo
Aldeghi

Advanced ML methods to predict and understand the **toxicity** of **drug candidates**

How do we produce at scale?

/// ML-powered modeling of large molecules



Santiago
Villalba

Generative language models for the **design** of tailored **chemical transformations**



Welcome to the AiChemist and AIDD School Berlin!



Bayer AG
Müllerstraße 178

Tuesday, March 5
8:30-9:30 am

Please make sure to bring your passport!

