



Pathway Data and Metabolite Prediction in Crop Science R&D

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Agenda

motivation

pathway data

challenges &
opportunities





Why?



Bayer is a life science company with three divisions



Crop Science



Pharmaceuticals



Consumer Health



Represented by
291 consolidated
companies in

80
countries

92.8k
employees worldwide

€6.2bn
investment in R&D

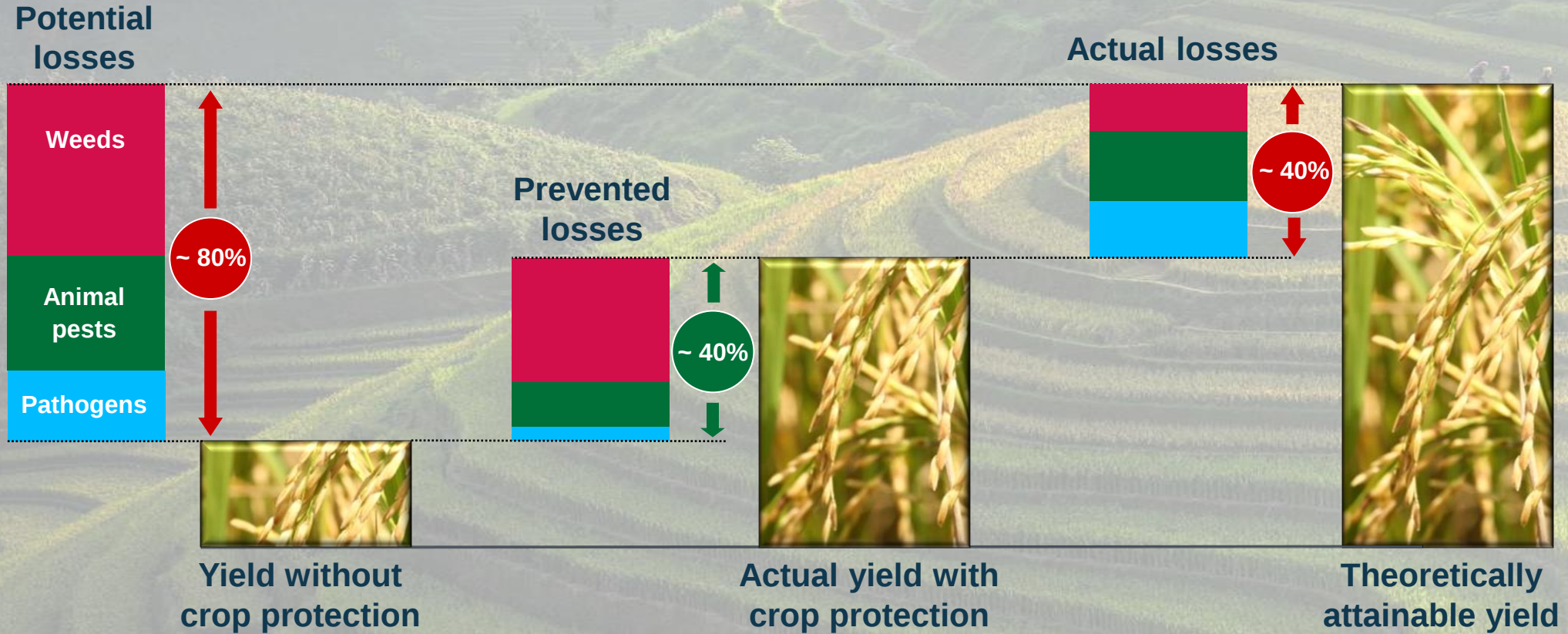
€46.6bn
sales

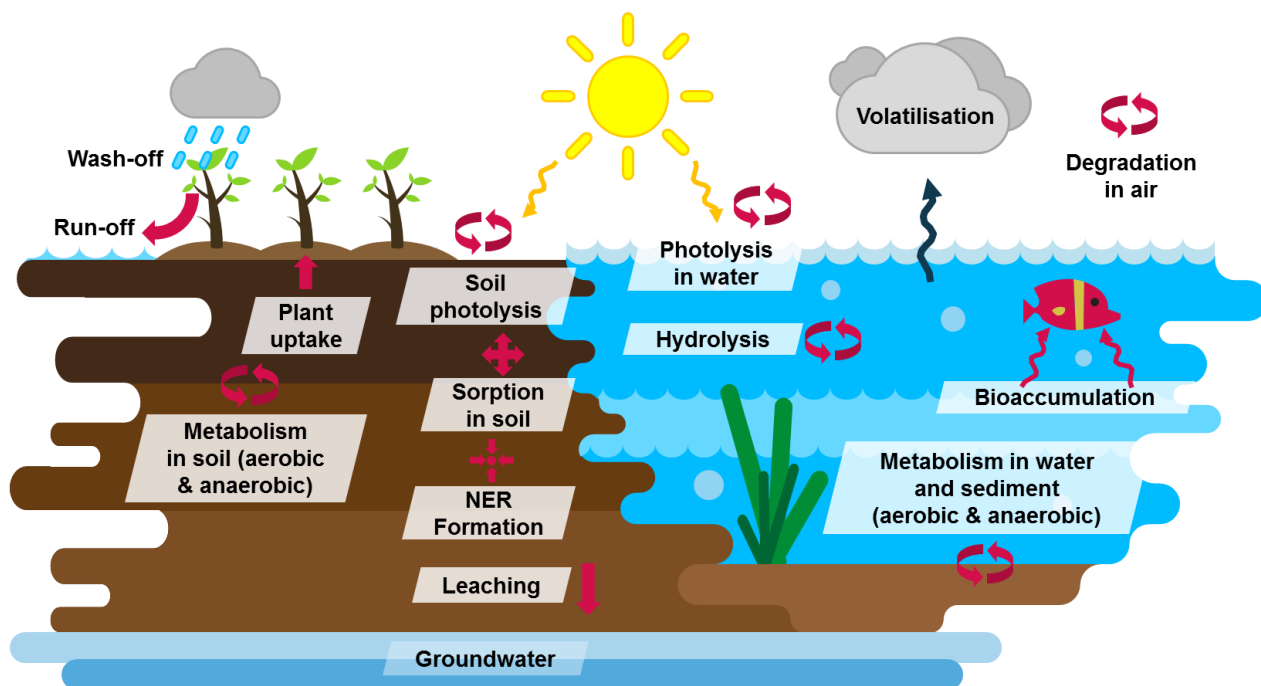
Health for all,
Hunger for none

As of December 31, 2024; employees in full-time equivalents

The World of Crop Science

Rice losses to weeds, animal pests & plant diseases





environmental processes & identification of metabolites



effects in all organism groups





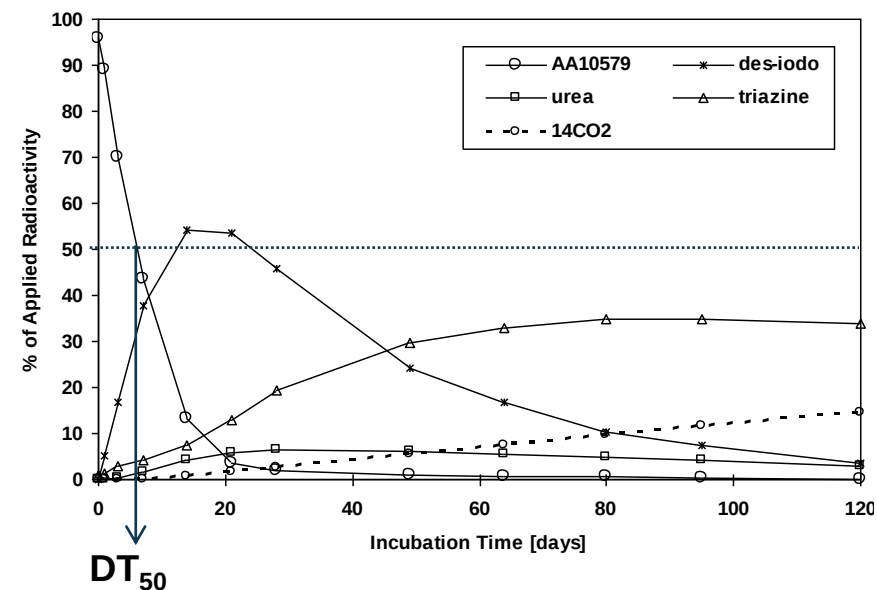
pathway data in R&D

Soil Degradation Studies

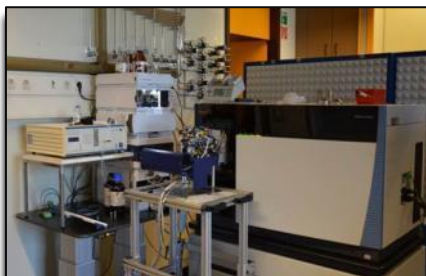
OECD 307

// Study Evaluation:

- // quantification of parent and metabolites in soil extracts
- // complete mass balance (incl. $^{14}\text{CO}_2$, other volatiles, non-extractable radioactivity)
- // identification of metabolites and structure elucidation
- // determination of half-lives and kinetic parameters

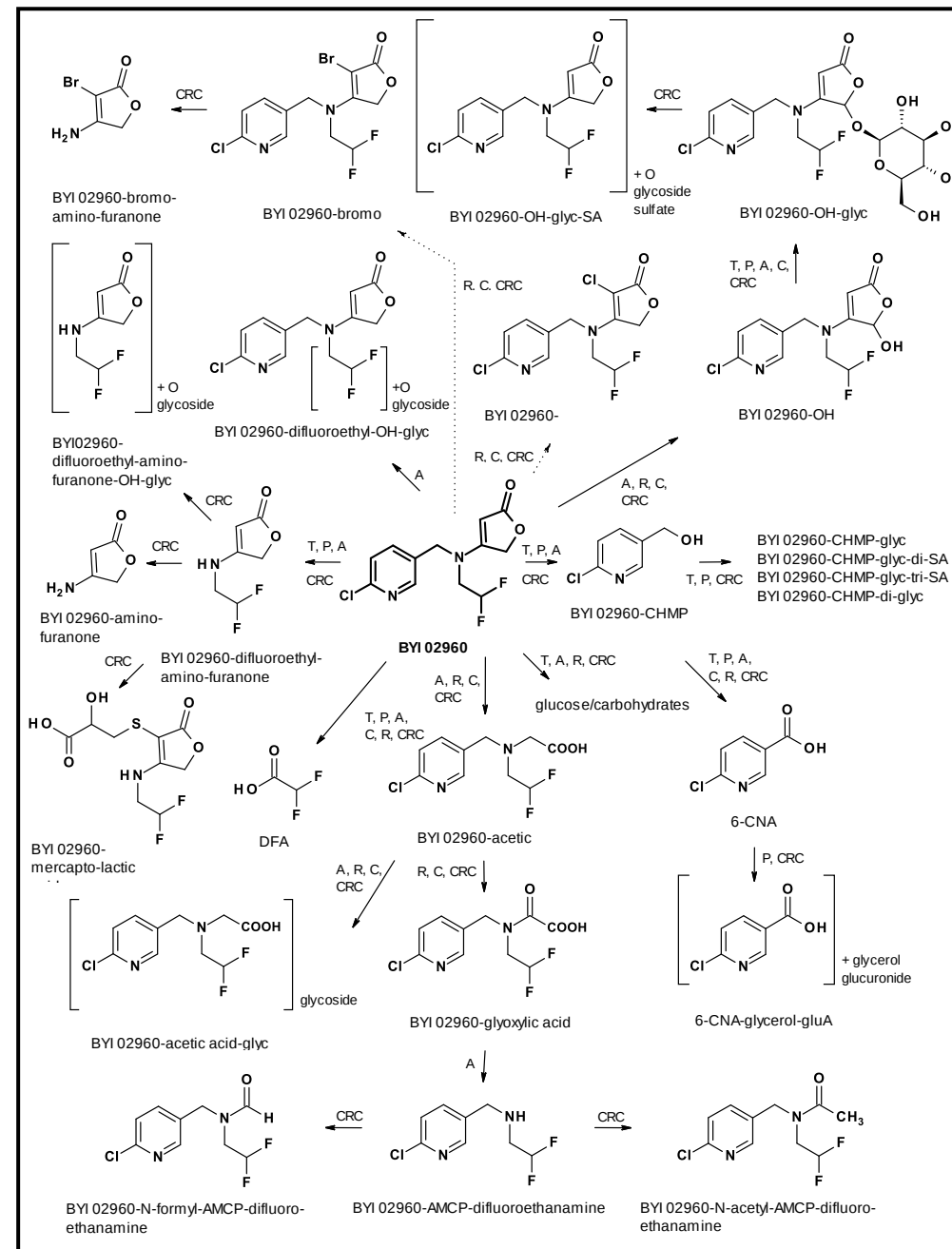


Identification of metabolites

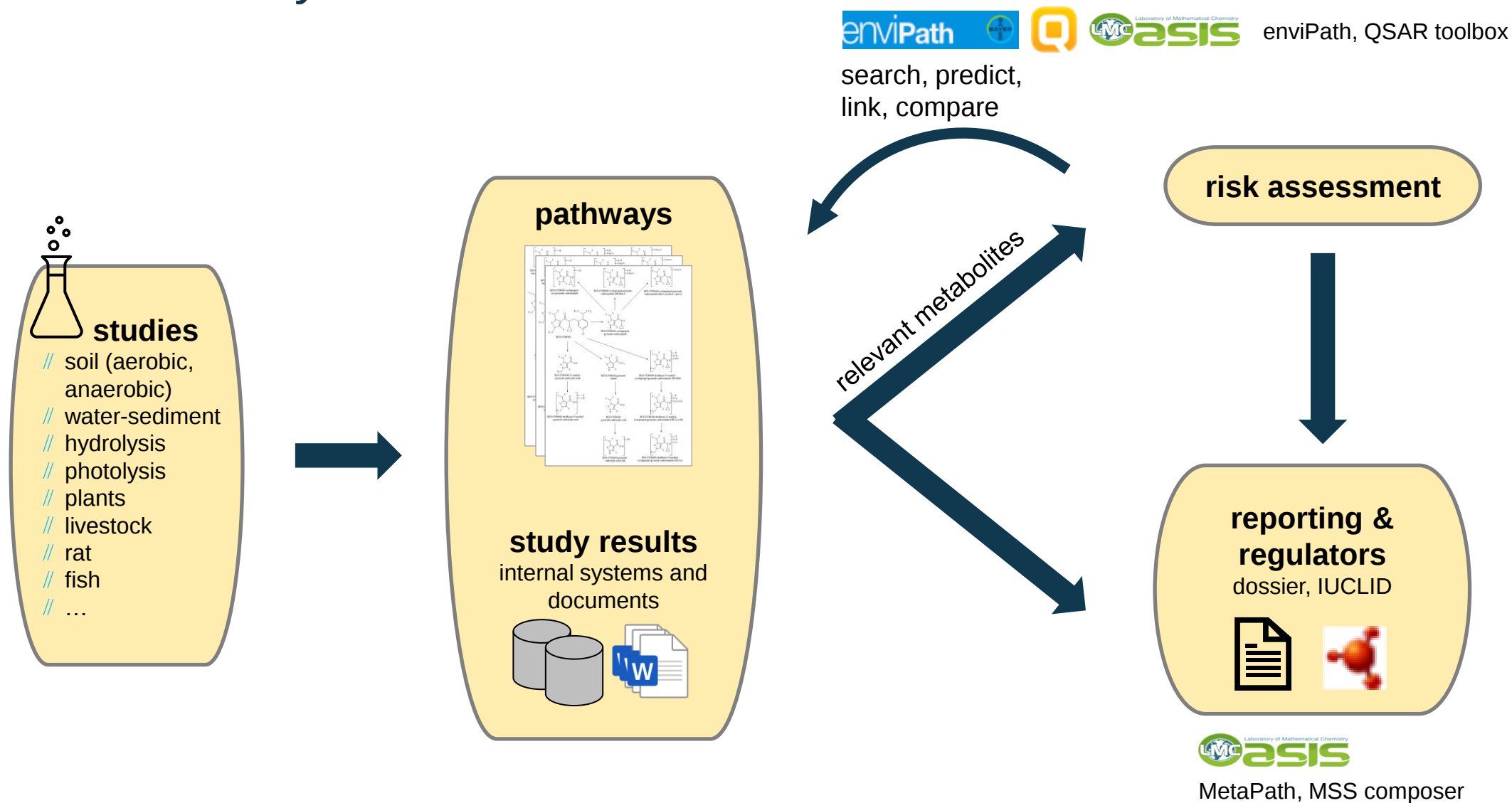


- Nature of residues
- Metabolic pathway

Metabolic pathway in plants:



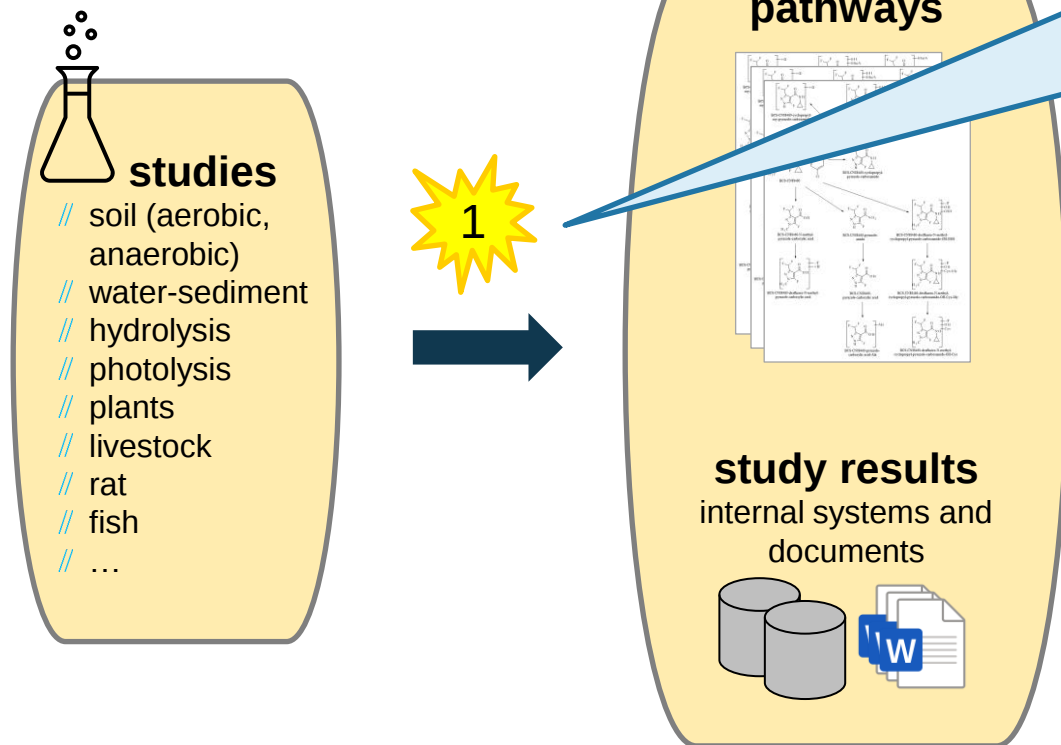
The Pathway Data Process





challenges & opportunities

Challenges

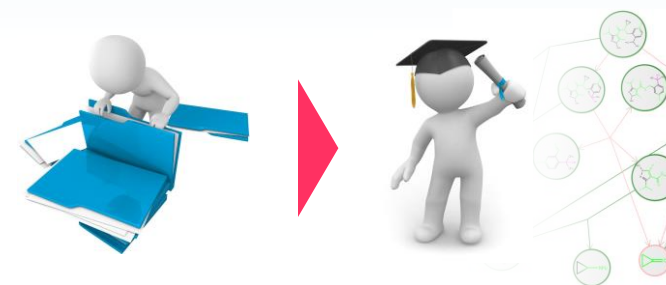


Digitalization Challenges:

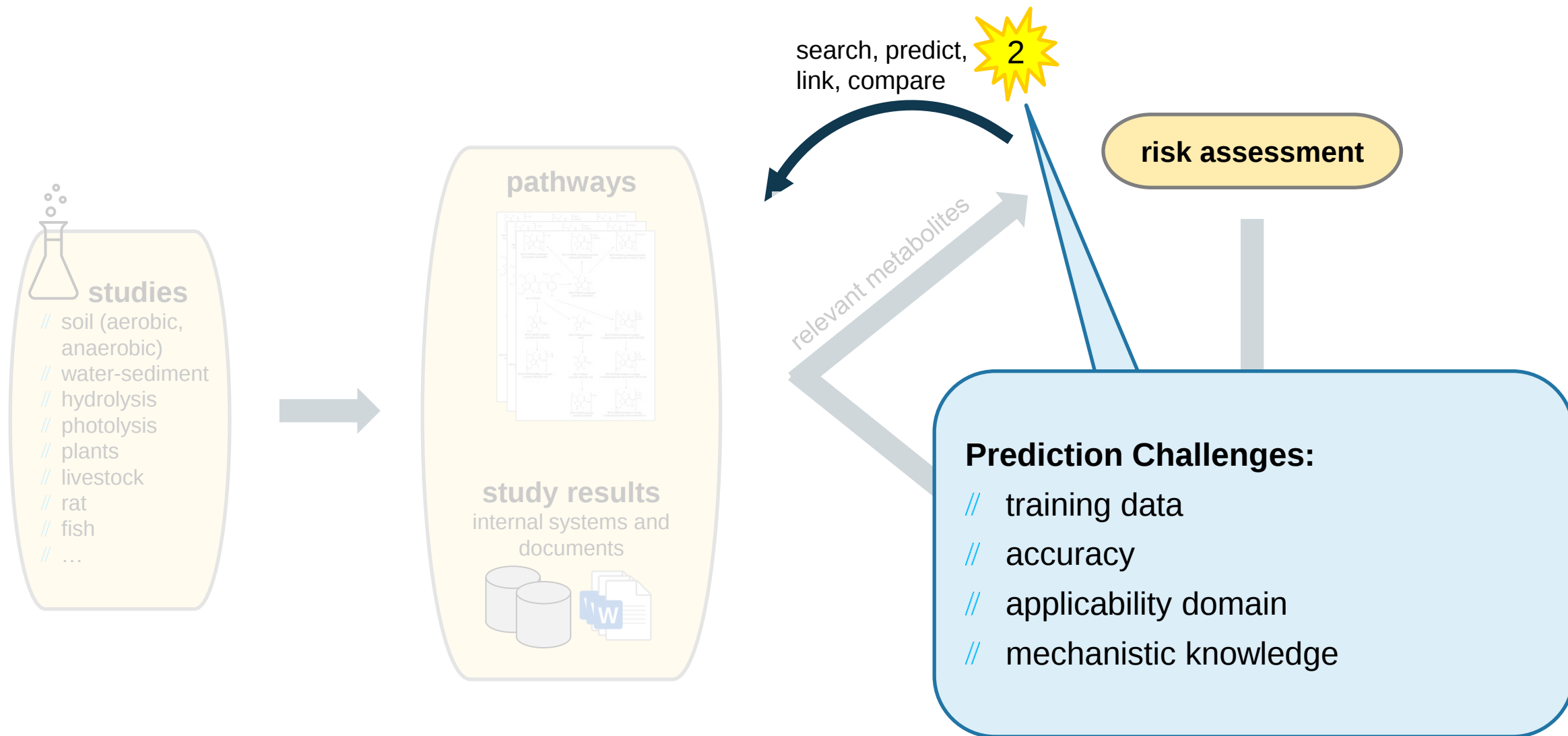
- // lab process integration
- // getting users onboard
- // confidential data
- // connection to internal systems
- // partially elucidated structures

Opportunity:

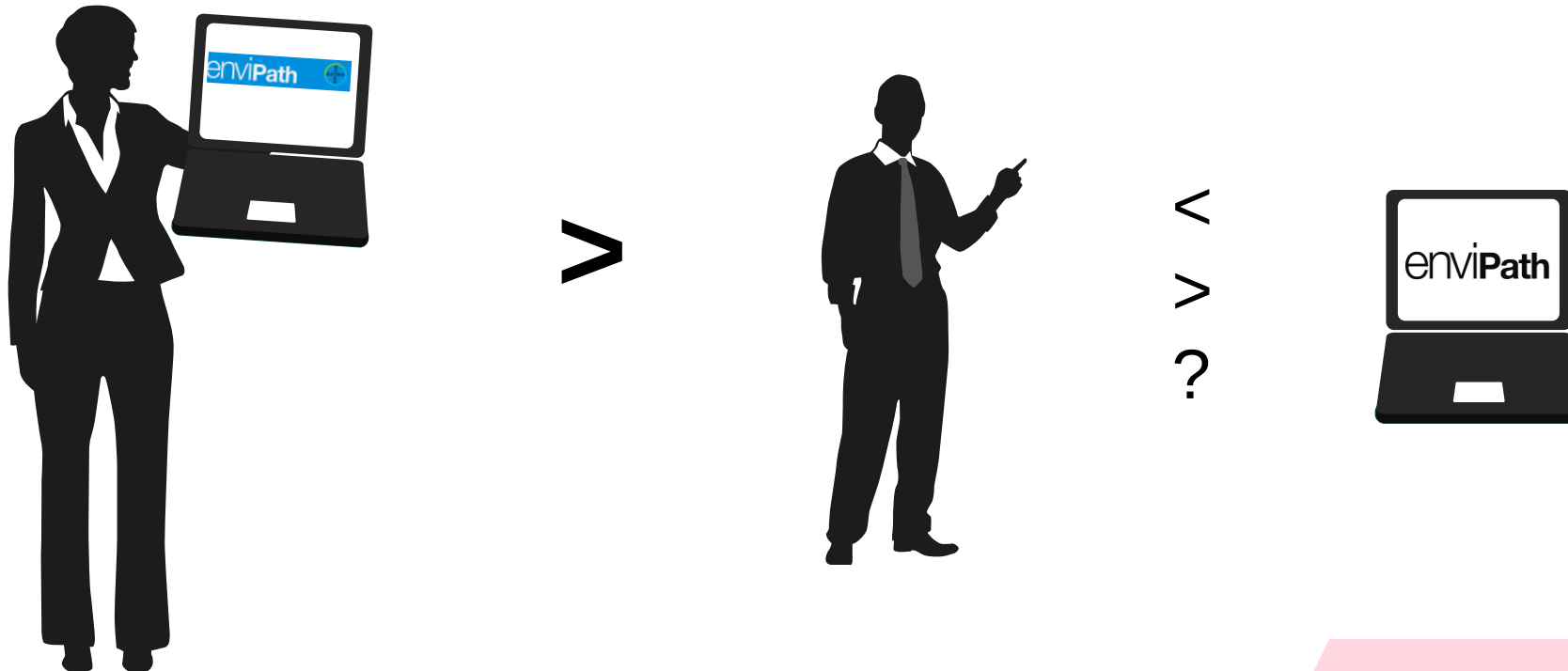
- // valuable knowledge base that can be interlinked with additional information
- // enable efficient, creative and mechanistic thinking



Challenges

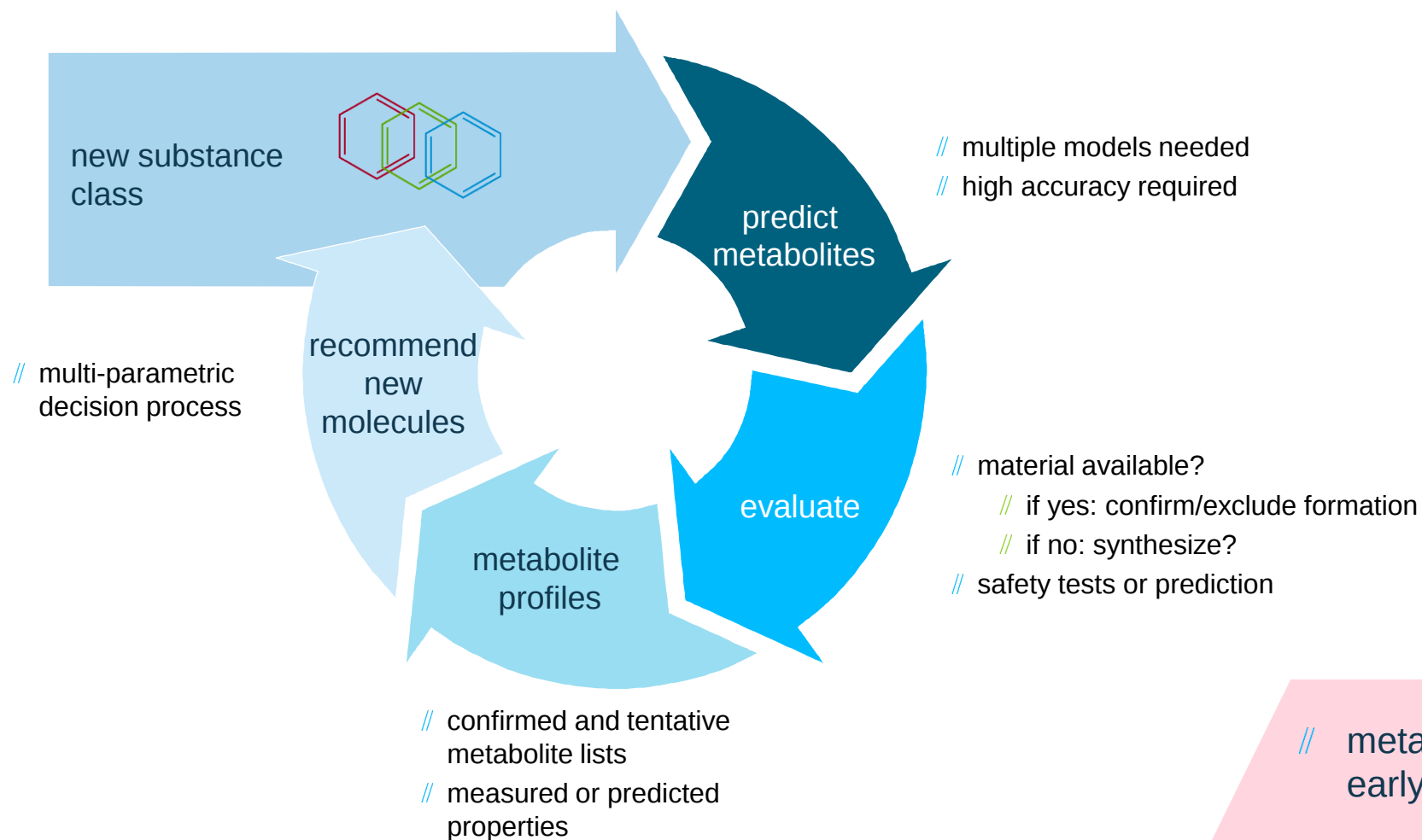


Human Level Performance?

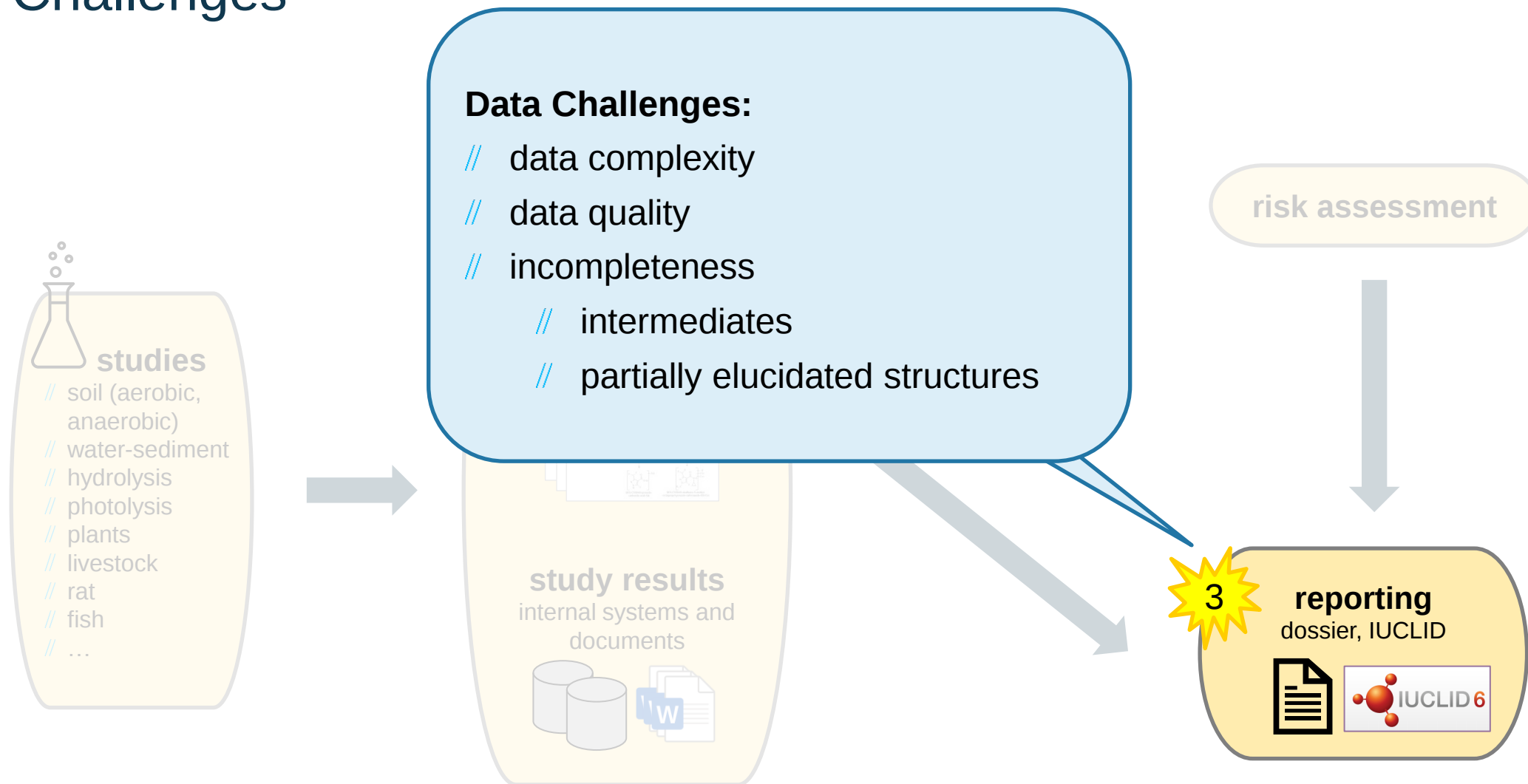


// prediction models can be used to make better decisions

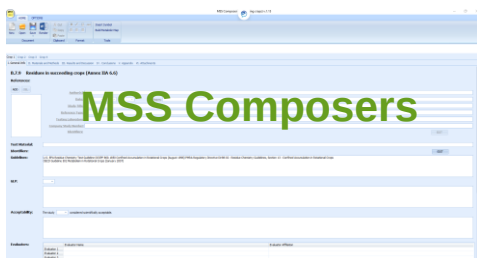
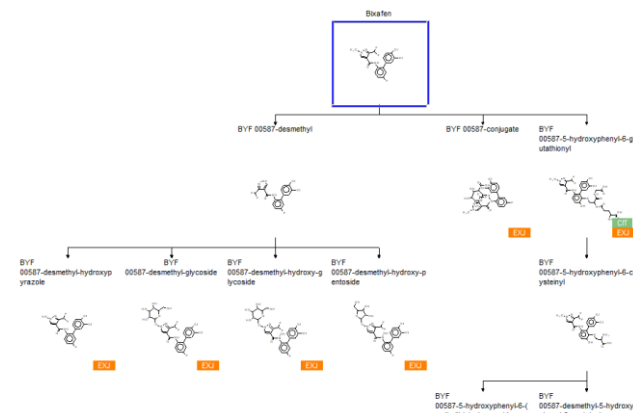
Outlook: Research Optimization Cycle



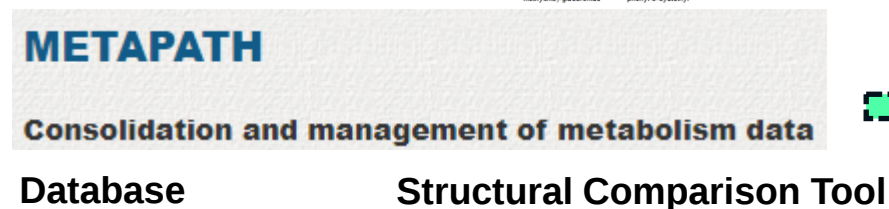
Challenges



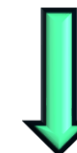
Summary of Characterization and Identification of Radioactive Residues in Plant Matrices Fol				
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- Connectivity between IUCLID and MetaPath



Toxicity evaluation of metabolites



Residue Definition

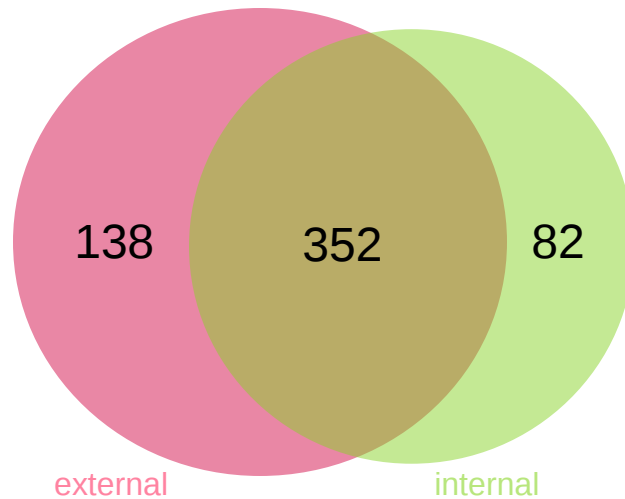
Risk Assessment

Hazard Identification

Help predict whether a metabolite is important for risk assessment

Data Quality

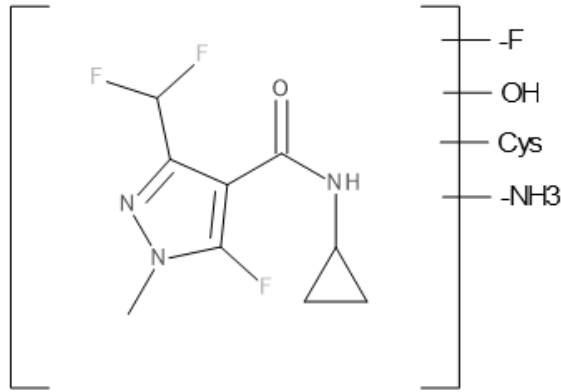
comparison of internal and external data base:



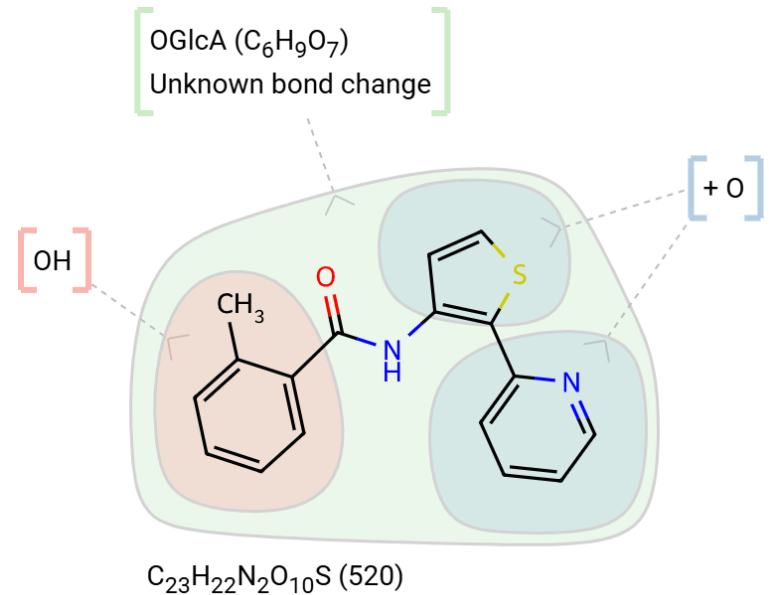
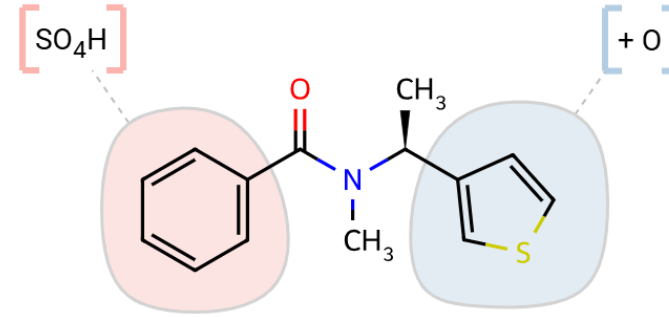
- // 35 pathways compared
- // 62% of metabolites present in both data bases
- // most mismatches due to incompletely elucidated structures (but they were not consistently labelled as such)

// data quality and reporting standards required

The “partially elucidated structure” problem



- // Not properly registered
- // Not searchable
- // Not comparable
- // Not interoperable





Summary

motivation

- // sustainability
- // degradation
- // transformation products

pathway data in R&D

- // laborious studies and elucidation
- // data process from study to dossier

challenges & opportunities

- // Digitalization enables better decisions.
- // For better pathway data we need collaboration across communities.



Thank You!

sebastian.schmidt1@bayer.com

thanks to...

- // the enviPath team:
Tim Lorschbach, Jörg Wicker, Jason Tam, Jasmin Hafner,
Athira Shankar, Albert Anguera, Kunyang Zhang
- // Kathrin Fenner (Eawag, UZH)
- // Bayer colleagues: Jan Schurkemeyer, Andreas Lagojda,
Mark Ott, Lionel Carles, Jana Ferber, Erik Gilberg, Janet
Gamlin, Marc Lamshoef and many others

