THE FUTURE OF DATA INTEGRATION:

BIOINFORMATICS AND CHEMINFORMATICS

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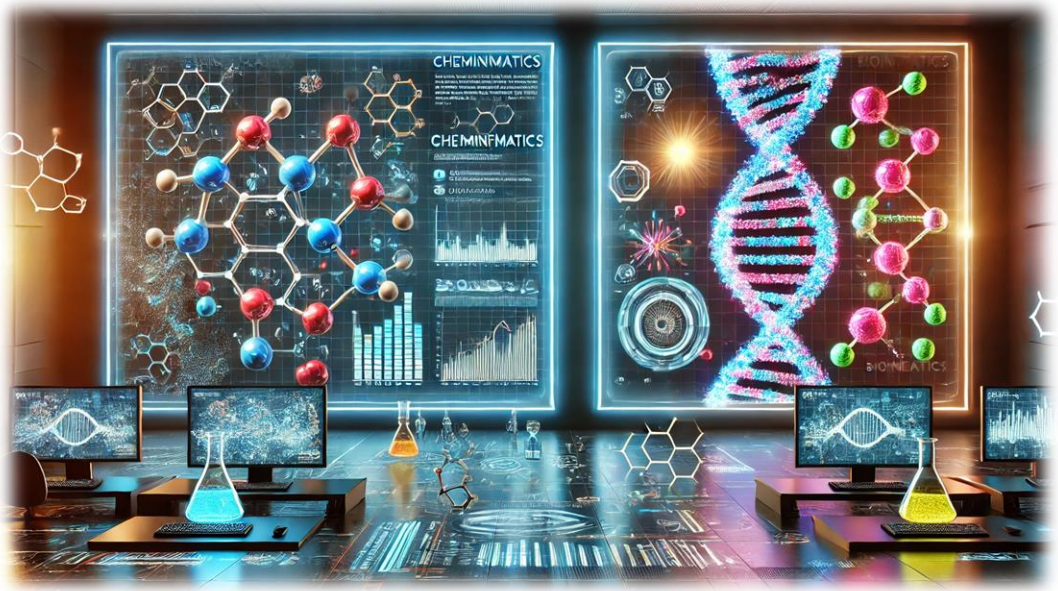
Head of iDATA Unit, EFSA

Stakeholder Forum, 27 Nov 2024 Brussels

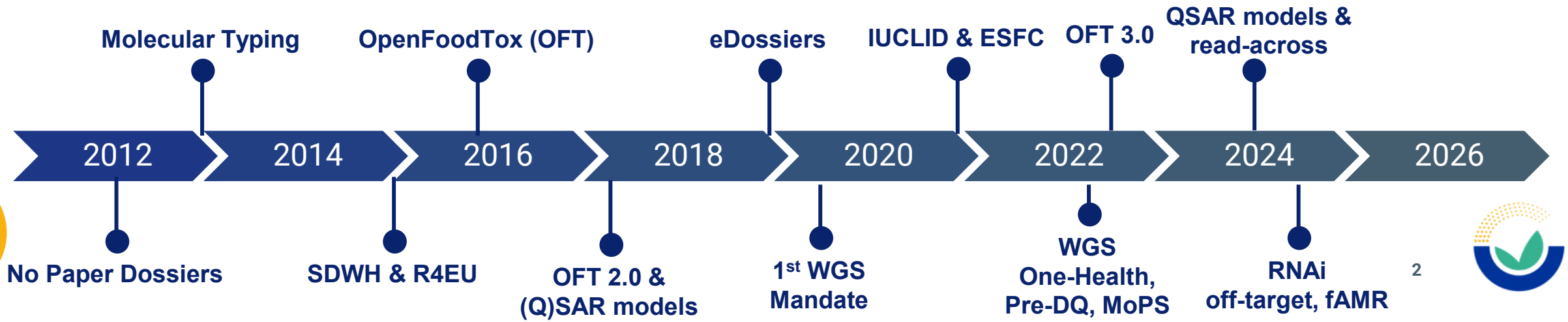
EUROPEAN FOOD SAFETY AUTHORITY

BIOINFORMATICS AND CHEMINFORMATICS @ EFSA



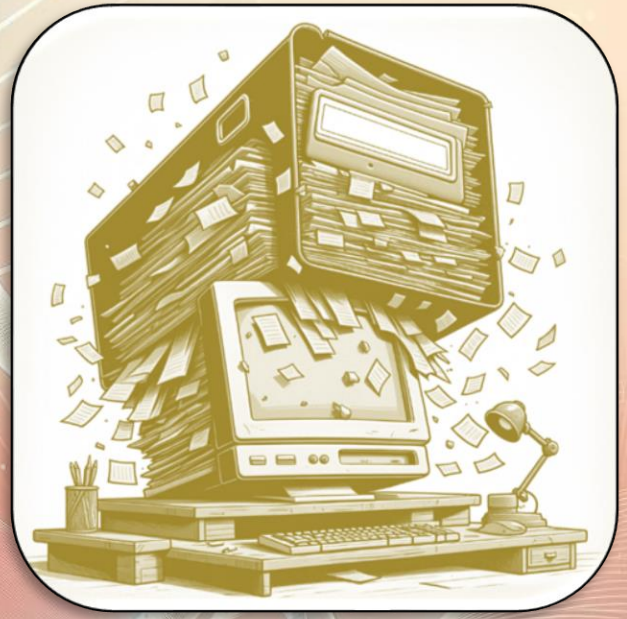
Provide an update on EFSA's progress in developing **bioinformatic** and **cheminformatic** data pipelines and tools (data and code) ensuring interoperability and (re-)use of data at data ingestion, validation and (re-)use stages.

Gather feedback from stakeholders on their requirements and explore the most effective ways to engage them in these initiatives.



BIOINFORMATICS UNTIL 2020: NO WGS STORAGE, NO PIPELINES, NO TOOLS

OFFICERS MANUALLY SCREEN A GENETIC SEQUENCE LETTER BY LETTER

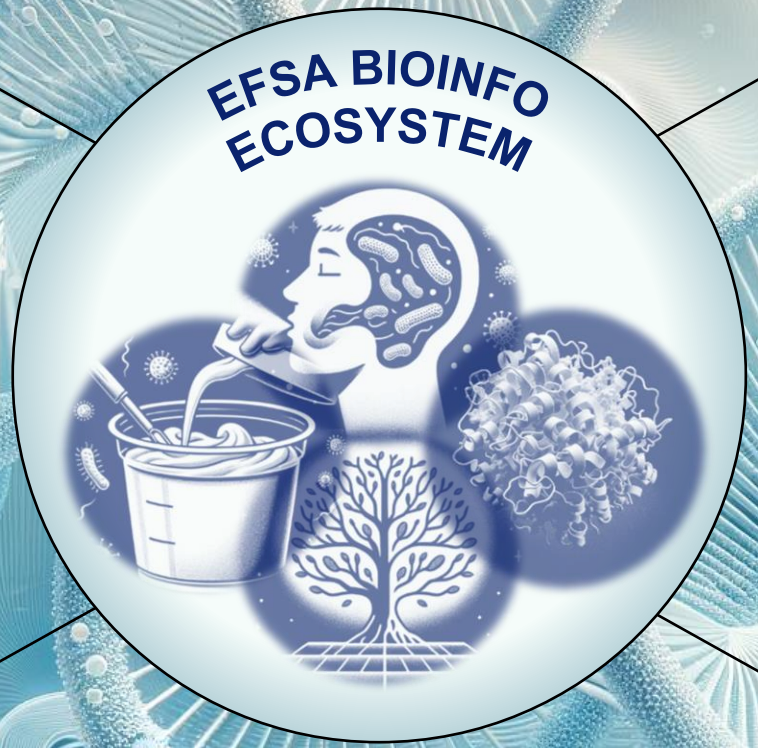


ISSUE TO STORE RAW GENOMICS DATA RECEIVED FROM APPLICANTS

NO PIPELINES
NO TOOLS

MANDATE TO ANALYZE WGS DATA

PRESENT: EFSA INTERNAL BIOINFORMATIC ECOSYSTEM OF TOOLS



WGS REGULATED PRODUCTS

MoPS tool
fAMR tool

WGS FOODBORNE OUTBREKS

WGS ONE HEALTH Tool in collaboration with ECDC

ADVERSE EFFECS PREDICTION

PRE-DQ Tool for Peptides
RNAi off-targets Tool

OTHERS (under development)

Prediction of Protein Toxicity tool

BENEFITS FROM THE USE OF BIOINFORMATICS

Faster risk assessment• Automate data analysis pipelines to deliver immediate results and promptly flag concerns for risk assessors (e.g., WGS One Health and MoPS sequencing analysis).

More consistent risk assessment• Enable standardized approaches for risk assessment by sharing pipelines with industry, ensuring consistent methods of analysis for all stakeholders (e.g., common bioinformatics workflows).

More efficient risk assessment• Utilize predictive tools to forecast adverse effects, enabling a tiered approach to hazard evaluation and improving the efficiency of risk assessment (e.g., in silico toxicity models).

PRESENT: PRE-DQ TOOL OPEN TO EXTERNALS

INDUSTRY APPLICANTS

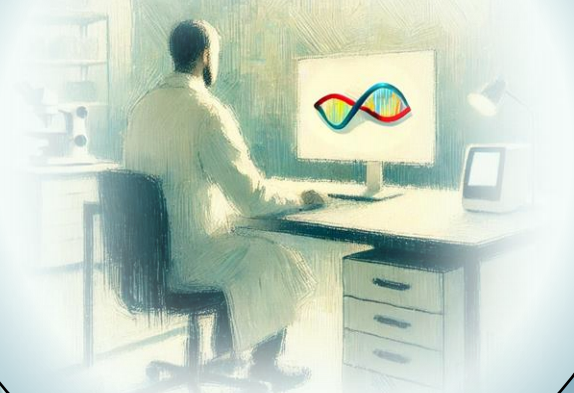
RAW DATA

PRE-DQ TOOL

Adverse effects of peptides in celiacs

RESULTS

EFSA RISK ASSESSORS



RAW DATA IS **NOT** “SENT” TO EFSA, ONLY RESULTS ARE.

FUTURE: MOPS TOOL OPEN TO INDUSTRY

INDUSTRY APPLICANTS

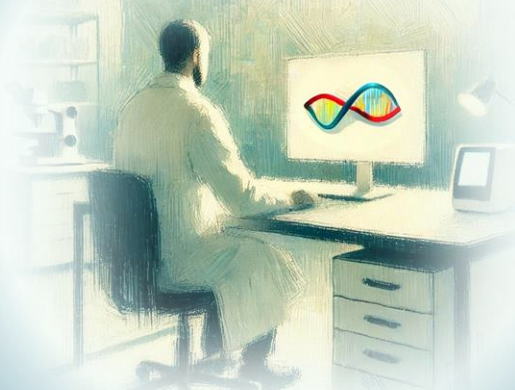
RAW DATA

MoPS TOOL

Safety assessment of microorganisms used in food and feed.

RESULTS

EFSA RISK ASSESSORS



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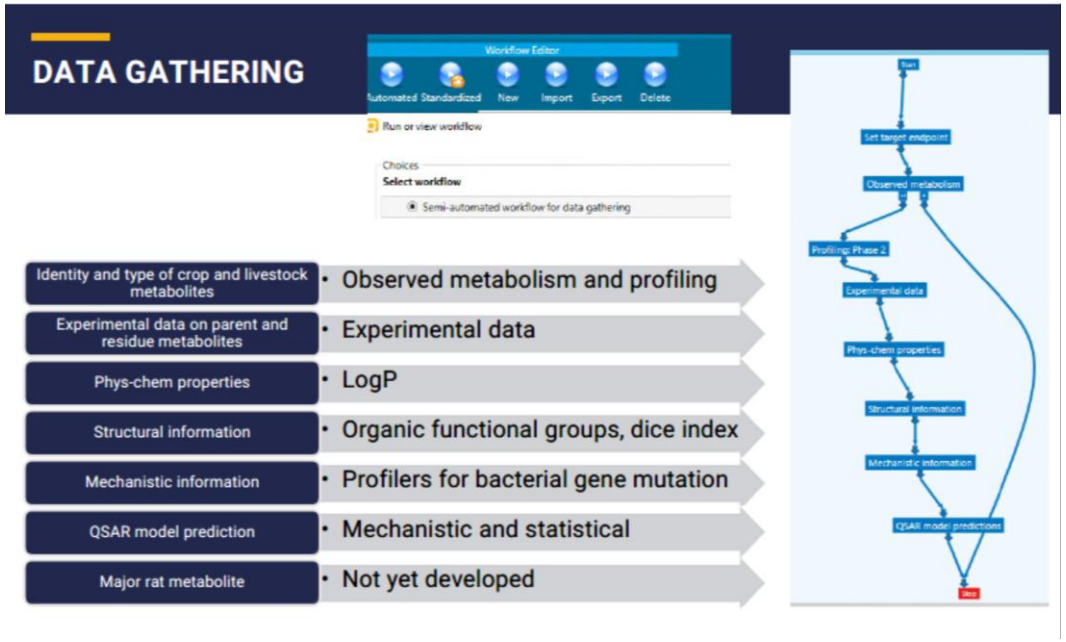
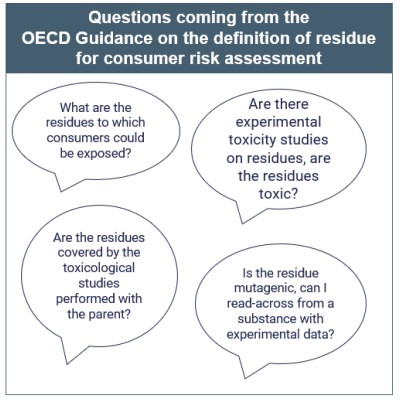
EXAMPLE OF CHEMINFORMATICS APPLICATION AT EFSA

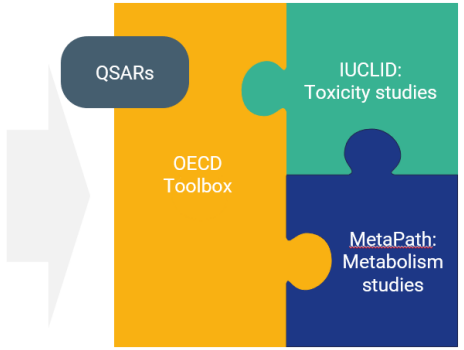
- The OECD QSAR Toolbox is a freely available cheminformatics tool
- EFSA is developing a workflow that will be made publicly available to predict the mutagenicity of pesticide residues using IUCLID data on as input according to a new OECD Guideline

✓ Identification of existing data

✓ Toxicological predictions

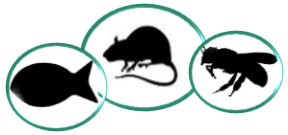






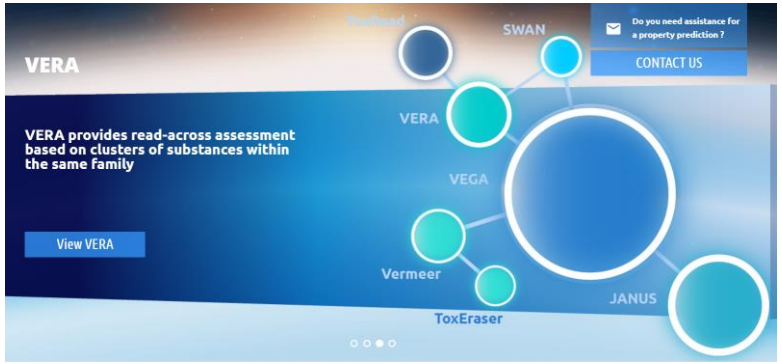
OPENFOODTOX 3.0 AND IN SILICO TOOLS – PUBLICLY AVAILABLE

- **20+ QSAR models** available in VEGA HUB in silico platform to predict chemical properties/toxicity for:
  - Human health
  - Animal health
  - Environment
  - Physico-chemical



https://www.vegahub.eu/portfolio-types/in-silico-models/

- **New software VERA** (Virtual Extensive Read-Across) publicly available to support **read-across** and **grouping** of chemicals

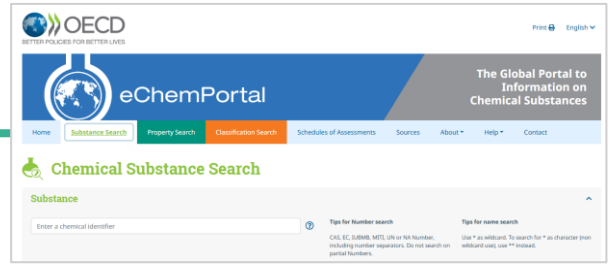


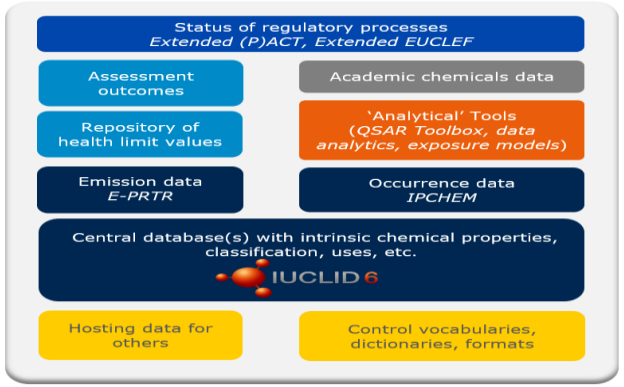
(EFSA contract OC/EFSA/SCER/2018/01)

EXTENDING THE USE OF IUCLID FORMAT

Structured data in **IUCLID** enables interoperability with **cheminformatics** and **dissemination** tools

IUCLID 6





OECD
BETTER POLICIES FOR BETTER LIVES

efsa

ECHA
EUROPEAN CHEMICALS AGENCY

EUROPEAN MEDICINES AGENCY
SCIENCE MEDICINES HEALTH

European Environment Agency

EU Common Data Platform on Chemicals

BENEFITS FROM THE USE OF CHEMINFORMATICS

Faster risk assessment Facilitate the identification and use of chemicals data (identification of common pesticides metabolites) with similar structure and toxicological profile that could be assessed and managed in groups improving efficiency of risk assessment

More consistent risk assessment EFSA will develop and make available models and tools that follow OECD Guidelines and increase the regulatory certainty of the validity of the approach (e.g. assessment of pesticide residues using a workflow developed by EFSA in the QSAR Toolbox).

More efficient risk assessment Using computational tools to predict chemical properties when experimental data are not available. Predict toxicity with Quantitative Structure Activities Relationships (QSAR) models.

ASSESSMENT OF PESTICIDE RESIDUES USING QSAR TOOLBOX

METABOLIC DATA

IUCLID 6

QSAR TOOLBOX

Identification of existing data and toxicological predictions

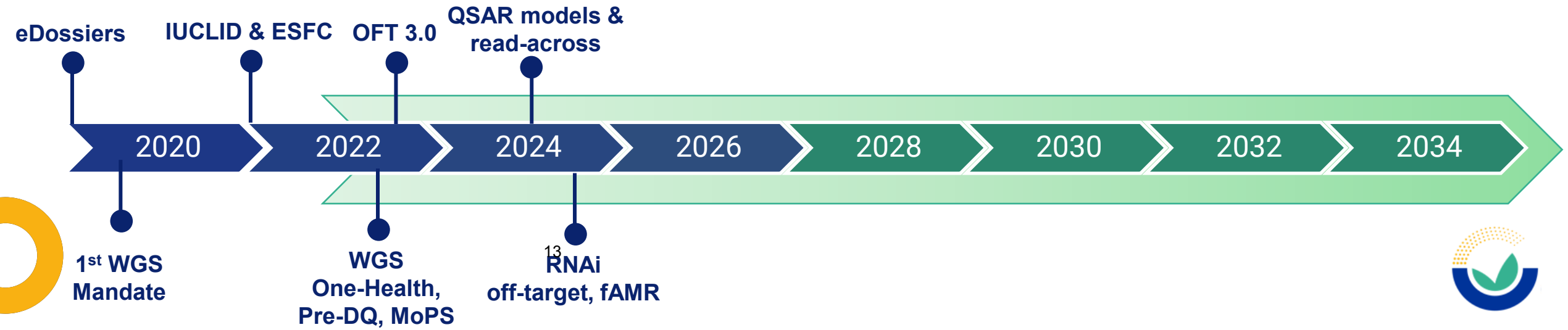
RESULTS

OECD QSAR Toolbox will read data on metabolites in IUCLID format and generate predictions for risk assessment

CHEMINFORMATICS AND BIOINFORMATICS @ EFSA

By augmenting ***Chemistry*** and ***Biology*** with ***Informatics***
we have enabled **ChemInformatics** and **BioInformatics** pipelines, models and tools
with concrete benefits for regulators, industry and academia.

With the advent of AI we can further augment what we have created
so far in BioInformatics and ChemInformatics



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