BioPhenom

An evidence-based workflow approach supporting SSbD goals for chemical and materials design

Webinar Series on "Advancing Sustainable Bio-Based Systems: From Safe Design to Circular End-of-Life Solutions"

19 May 2026

Funded by the European Union

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Grant Agreement No: 101135107

Project funded by

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
State Secretariat for Education, Research and Innovation SERI

This work has received funding from the Swiss State Secretariat for Education, Research and Innovation (SERI).
Grant Agreement No: 24.00212

UKRI Innovate UK

This work was supported by UKRI Horizon Europe Underwriting – Innovate UK Council [1005409].

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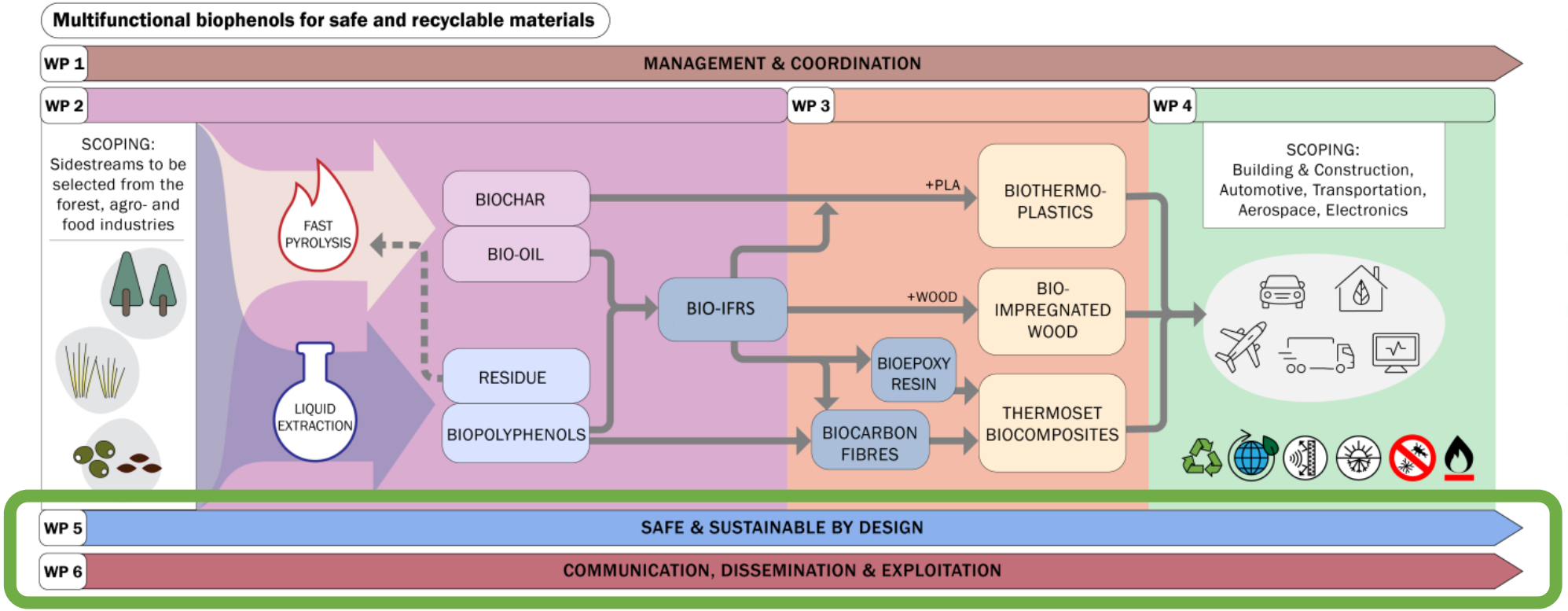
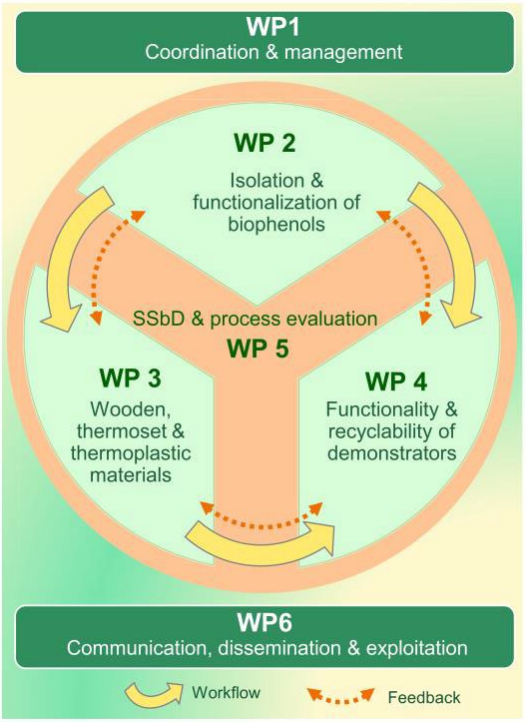
BioPhenom Project Work Activities






Fragmented Clues
NAM data | models | exposure | literature | sustainability
FAIR Knowledge Infrastructure
| metadata | ontologies | knowledge graphs
ASPA Workflow
structured decision gates
AI Evidence Integration
AI +
patterns | read-across | uncertainty
Regulatory-Ready Evidence Package
traceable | reproducible
interpretable
EVIDENCE


ASPA + SaferWorldbyDesign
Creating & Reporting SSbD Evidence Across the Innovation Lifecycle
ASPA
Workflows
SaferWorldbyDesign
Molecular Design
Material Development
FAIR Knowledge Infrastructure
FAIR
FAIR Ontologies
Linked Data Resources
Knowledge Graphs
AI Evidence Integration
AI +
ASPA Algorithms
Mechanistic Models
NGRA / SSBD
Exposure
SaferWorldbyDesign
TRACEABLE EVIDENCE PACKAGE
RELIABLE KNOWLEDGE MANAGEMENT
AI-ASSISTED WORKFLOWS
Molecular Design
Post-Market Monitoring
EVIDENCE

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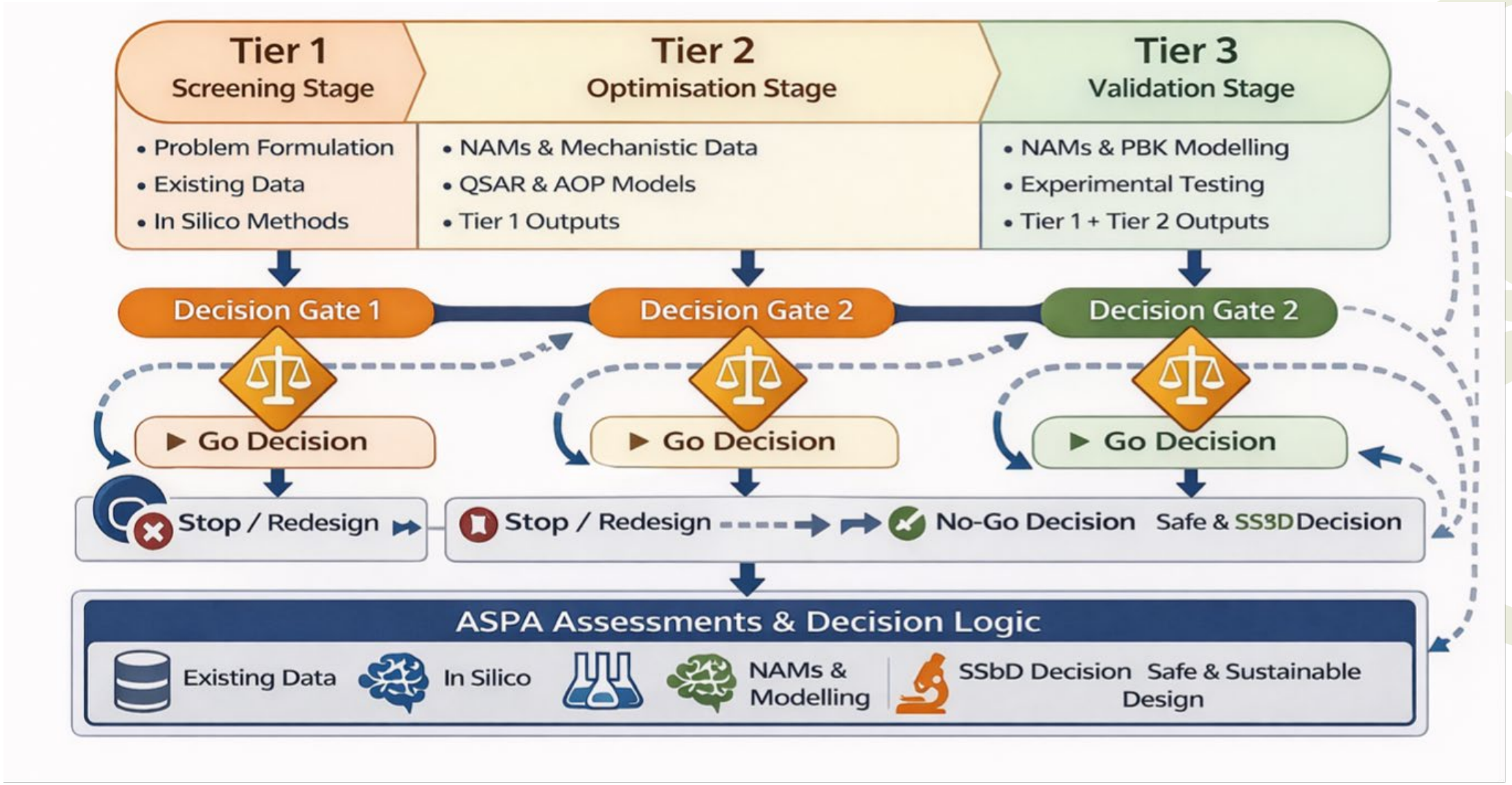
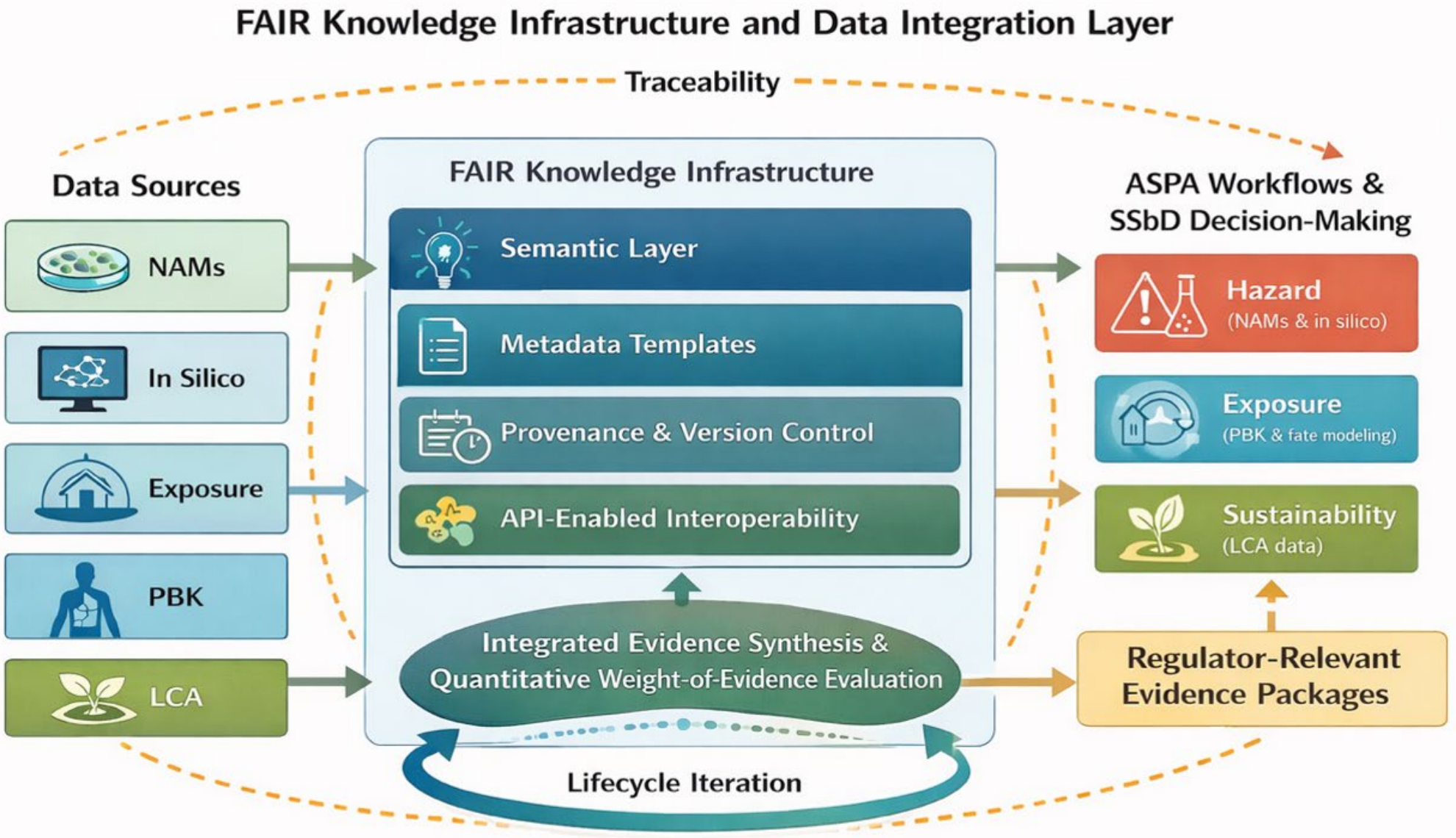
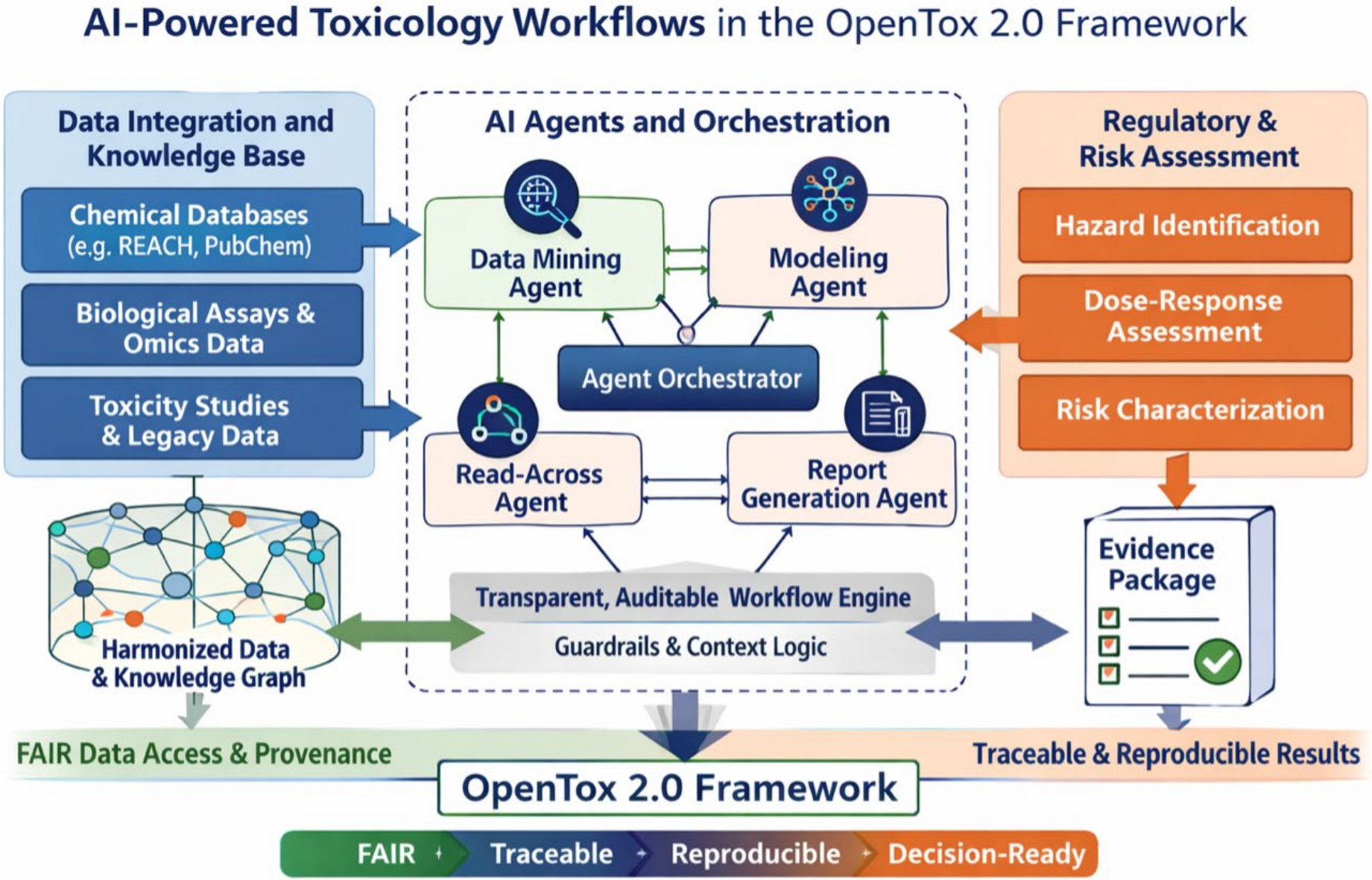

Tier 1
Screening Stage
Tier 2
Optimisation Stage
Tier 3
Validation Stage
• Problem Formulation
• Existing Data
• In Silico Methods
• NAMs & Mechanistic Data
• QSAR & AOP Models
• Tier 1 Outputs
• NAMs & PBK Modelling
• Experimental Testing
• Tier 1 + Tier 2 Outputs
Decision Gate 1
Decision Gate 2
Decision Gate 2
▶ Go Decision
▶ Go Decision
▶ Go Decision
Stop / Redesign
Stop / Redesign
No-Go Decision
Safe & SS3D Decision
ASPA Assessments & Decision Logic
Existing Data
In Silico
NAMs & Modelling
SSbD Decision
Safe & Sustainable Design


FAIR Knowledge Infrastructure and Data Integration Layer
Traceability
Data Sources
NAMs
In Silico
Exposure
PBK
LCA
FAIR Knowledge Infrastructure
Semantic Layer
Metadata Templates
Provenance & Version Control
API-Enabled Interoperability
Integrated Evidence Synthesis & Quantitative Weight-of-Evidence Evaluation
Lifecycle Iteration
ASPA Workflows & SSbD Decision-Making
Hazard
(NAMs & in silico)
Exposure
(PBK & fate modeling)
Sustainability
(LCA data)
Regulator-Relevant Evidence Packages



Hardy, B., & Ali, A. (2026). OpenTox 2.0: A Perspective on the Principles for Predictive Toxicology and Risk Assessment Applications in the Era of Integrated New Approach Methods, Computational Modelling and Artificial Intelligence. Zenodo. https://doi.org/10.5281/zenodo.19458289

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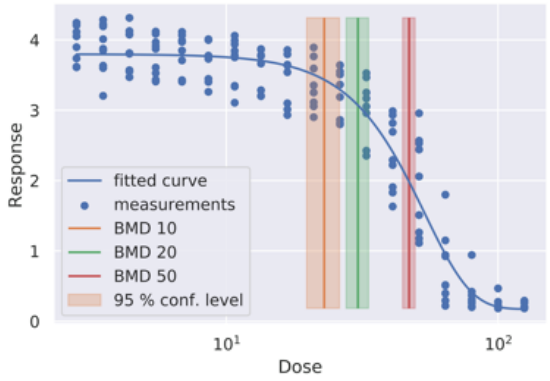
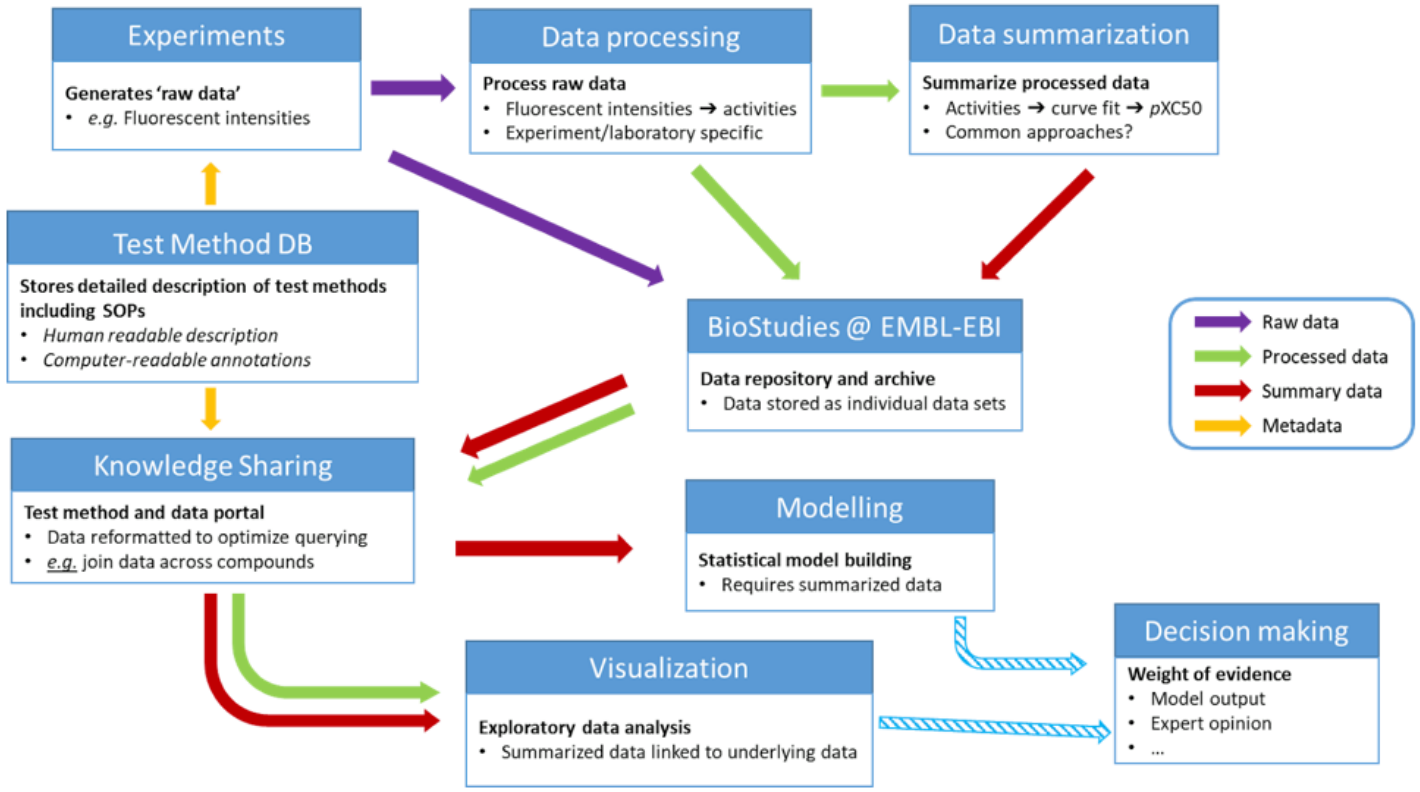
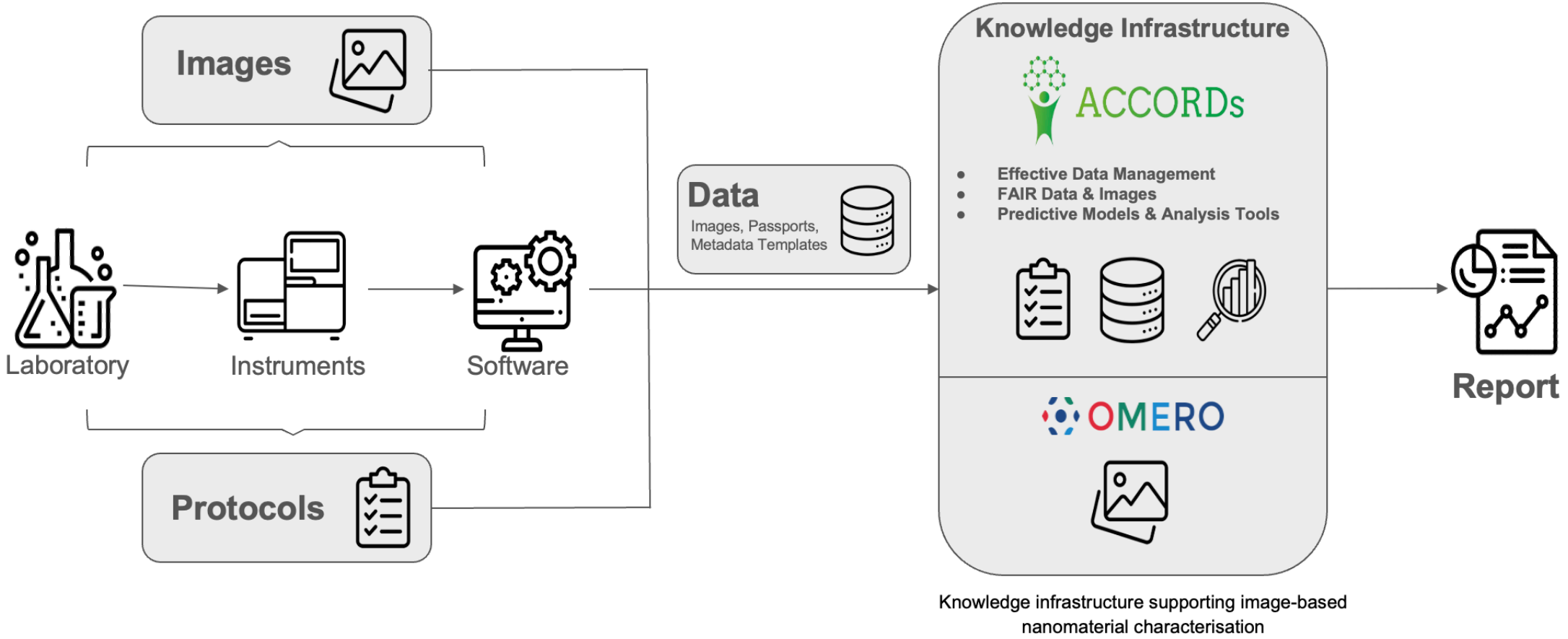


Harmonised Data, Protocol and Metadata Management Infrastructure supported by EdelweissData



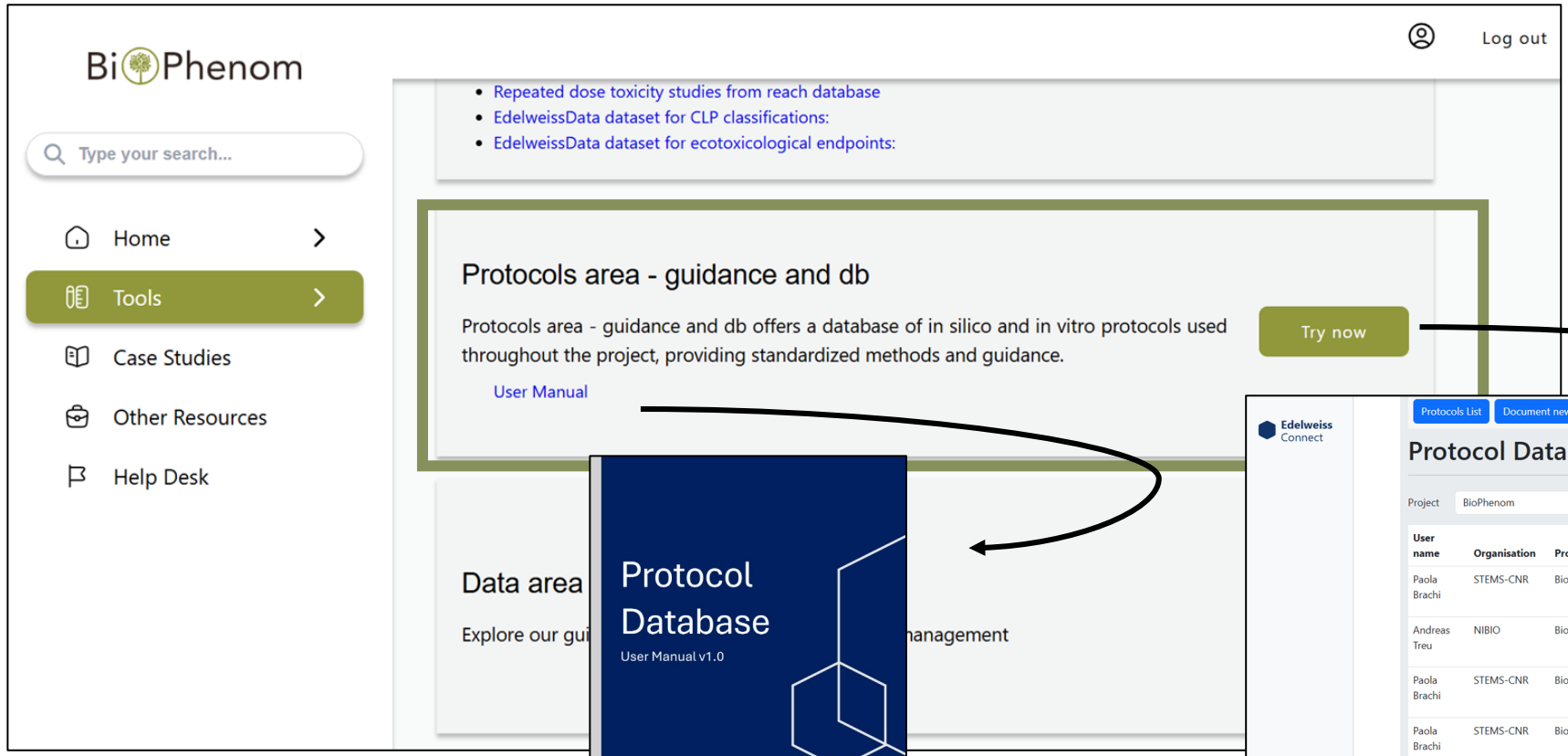
Barry Hardy, Tomaz Mohoric, Thomas Exner, Joh Dokler, Maja Brajnik, Daniel Bachler, Ody Mbegbu, Nora Kleisli, Lucian Farcal, Krzysztof Maciejczuk, Haris Rašidagić, Ghada Tagorti, Pascal Ankli, Daniel Burgwinkel, Divanshu Anand, Ugis Sarkans, Awais Athar, Knowledge infrastructure for integrated data management and analysis supporting new approach methods in predictive toxicology and risk assessment, Toxicology in Vitro, Volume 100, 2024, 105903, ISSN 0887-2333, https://doi.org/10.1016/j.tiv.2024.105903

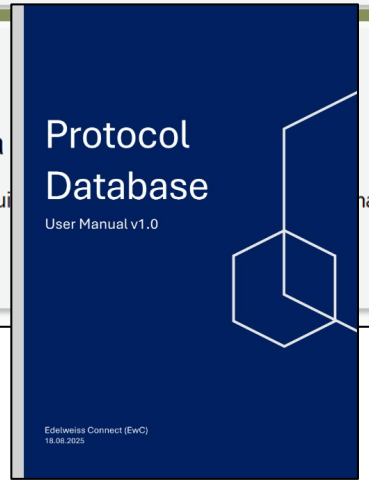
Materials Characterisation Knowledge Infrastructure

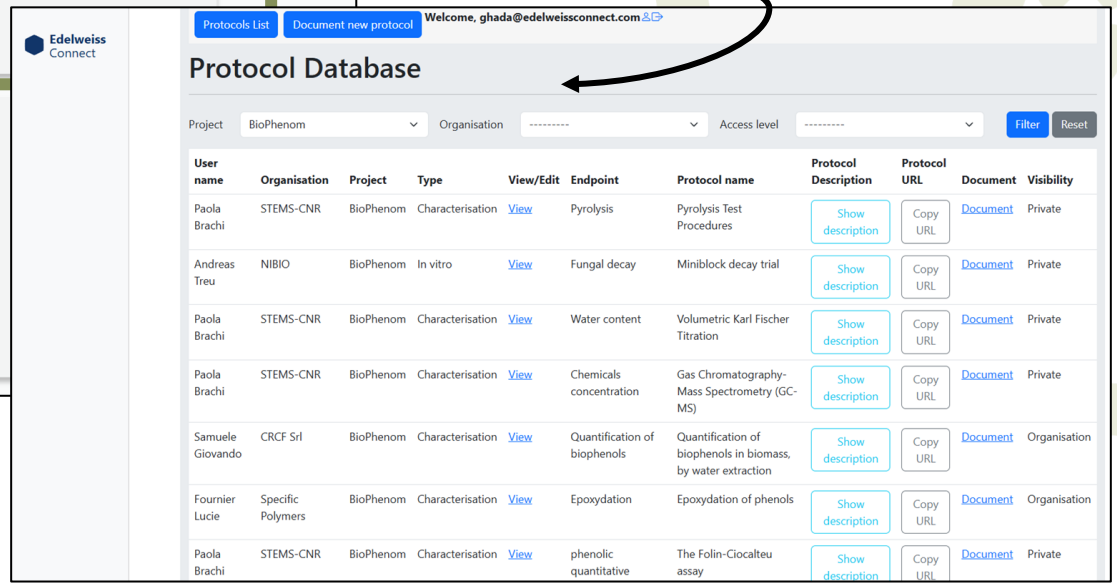


Knowledge infrastructure supporting image-based nanomaterial characterisation

BioPhenom





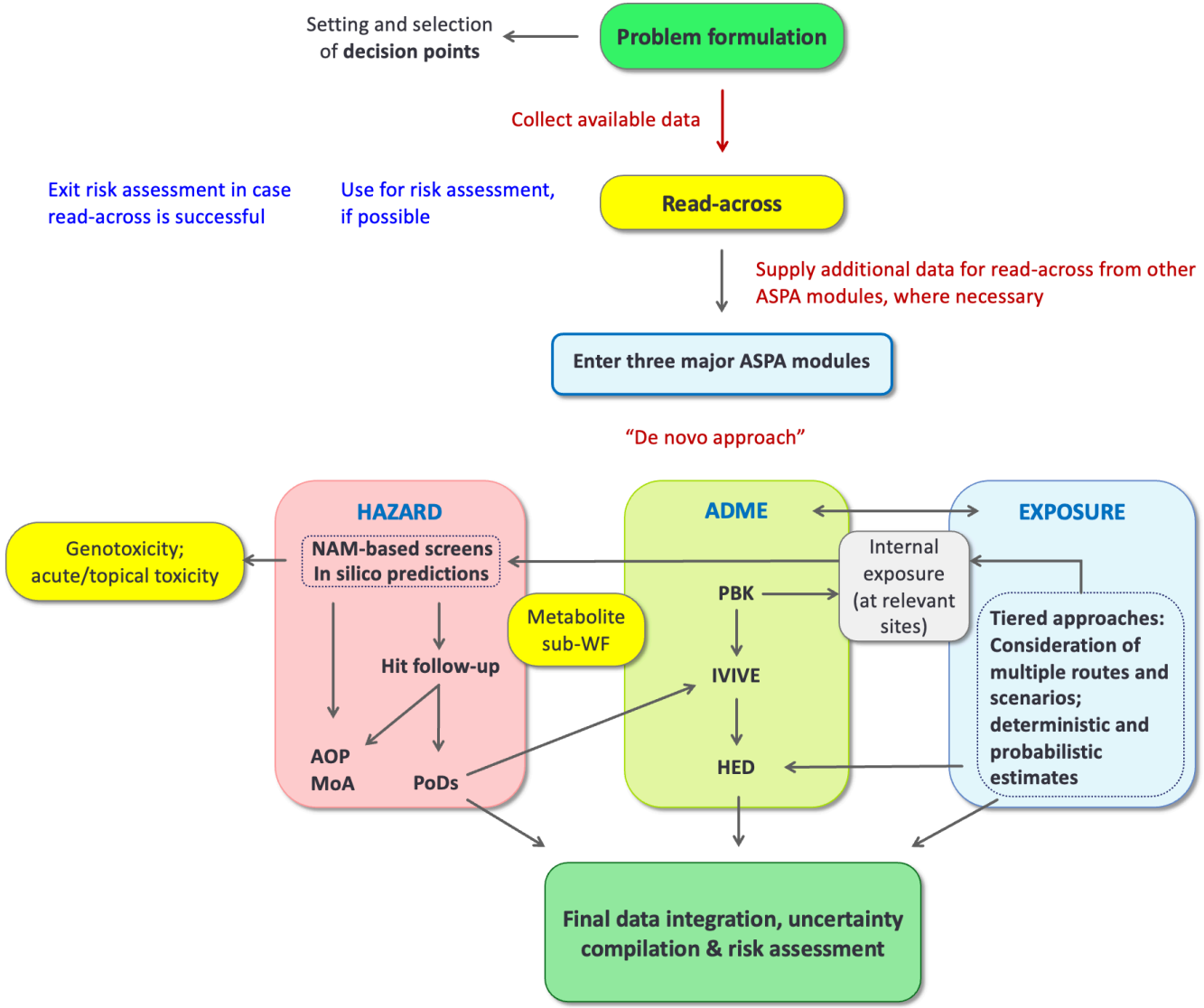


https://biophenom.edelweissconnect.com/tools/

Workflow Approach

An alternative safety profiling algorithm (ASPA) to transform next generation risk assessment into a structured and transparent process, Marcel Leist *et al*; https://zenodo.org/records/16993943

ALTEX. 2025 Oct 16. doi: 10.14573/altex.2509081. Epub ahead of print. PMID: 41099509



https://www.linkedin.com/posts/barryhardy_aspa-ssbd-gsrs25-activity-7385334765064712192-bKa3/

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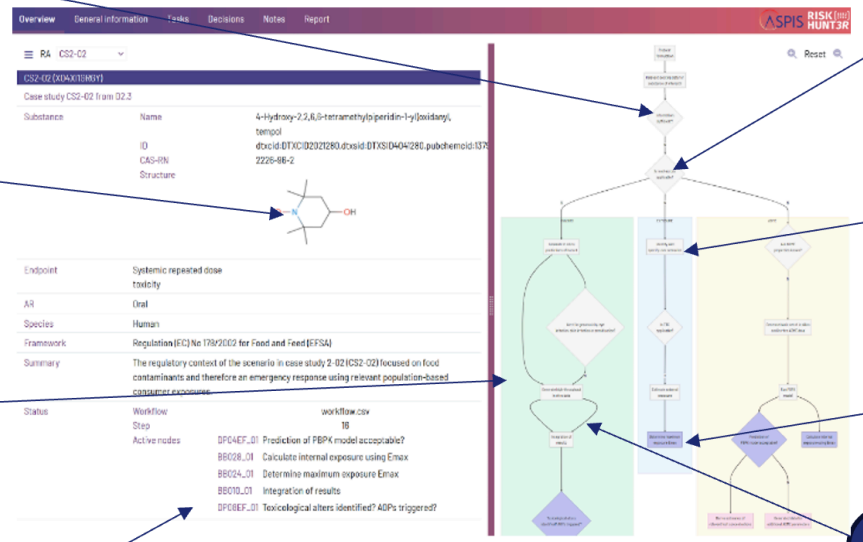
AI-assisted Workflows with Human Interaction, Interpretation and Learning

Biological Data (Biostudies, EdelweissData, Notebooks)

AI assisted

Methods Database (ToxTemp)

Compound Database



AI assisted

Toxicokinetics and Exposure protocols

Knowledge Graphs

AI assisted

OpenModel Repository

Case Study Documentation

Life Cycle Assessment

AI assisted

Prediction and Analysis Tools (QSAR, Molecular Simulations, Metabolism, Omics)

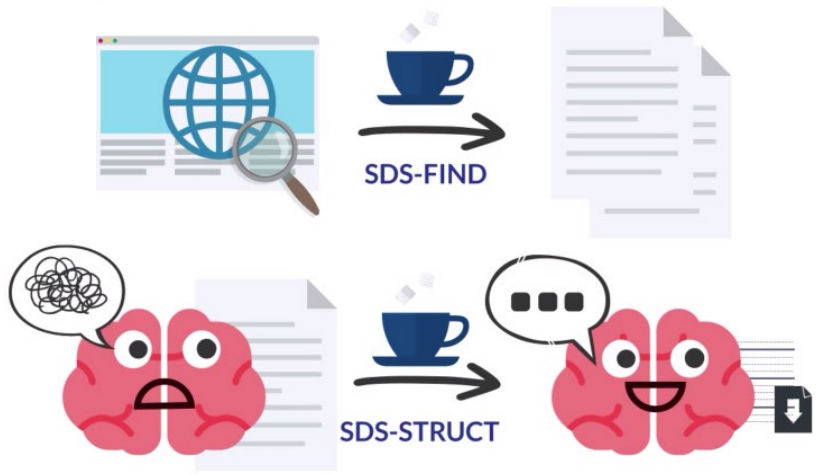
AI Assistance Resource Examples

AI Assistance of data from literature

AI Assistance of collection and curation of data from databases

AI Assistance of data from documents

- **PubMed ChemInsight:** Automated literature mining https://pubmed-cheminsight.edelweissconnect.com/
- **PubChem Pal:** Automated chemical data extraction https://pubchempal.edelweissconnect.com/
- **AI Assistance** of collection, extraction and curation of data from safety data sheets and other legacy documents



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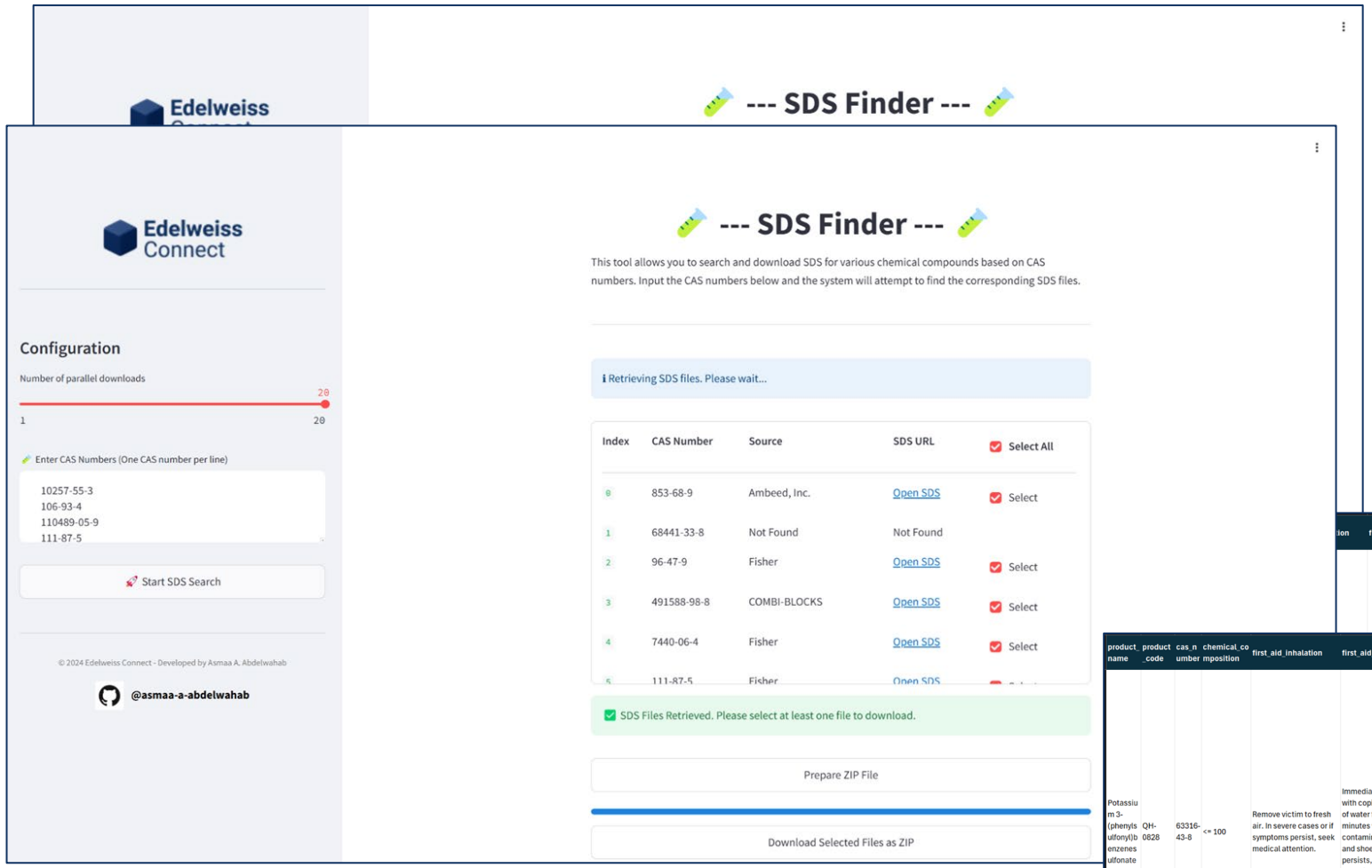

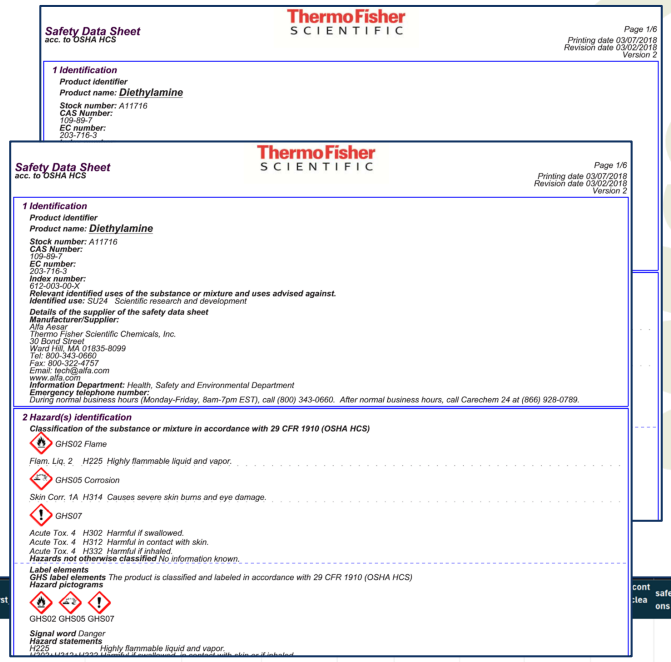

AI

product_name	product_code	cas_number	chemical_composition	first_aid_inhalation	first_aid_skin_contact	first_aid_eye_contact	first_aid_ingestion	suitable_extinguishing_media	fire_hazards	special_firefighting_instructions	personal_precautions	environmental_precautions	methods_containment_cleanup	safe_handling_precautions	storage_conditions
Potassium 3-(phenylsulfonyl)benzenesulfonate	QH-0828	63316-43-8	<= 100	Remove victim to fresh air. In severe cases or if symptoms persist, seek medical attention.	Immediately wash skin with copious amounts of water for at least 15 minutes while removing contaminated clothing and shoes. If irritation persists, seek medical attention.	Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing. Get medical attention.	Wash out mouth with copious amounts of water for at least 15 minutes. Seek medical attention.	Use dry sand, dry chemical or alcohol-resistant foam for extinction.	Carbon monoxide, sulfur oxides	Wear self-contained breathing apparatus for firefighting if necessary.	Ensure adequate ventilation. Use personal protective equipment.	Should not be released into the environment. See Section 12 for additional ecological information.	Sweep up or vacuum up spillage and collect in suitable container for disposal.	Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electro-static charge. For precautions see section 2.2.	Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

https://sds-finder.edelweissconnect.com/

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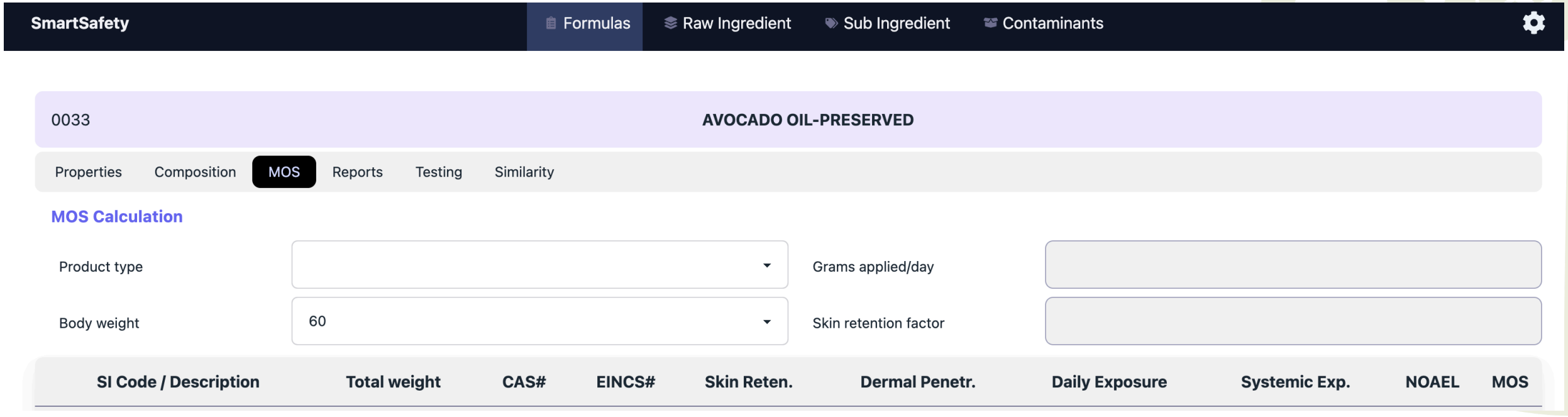
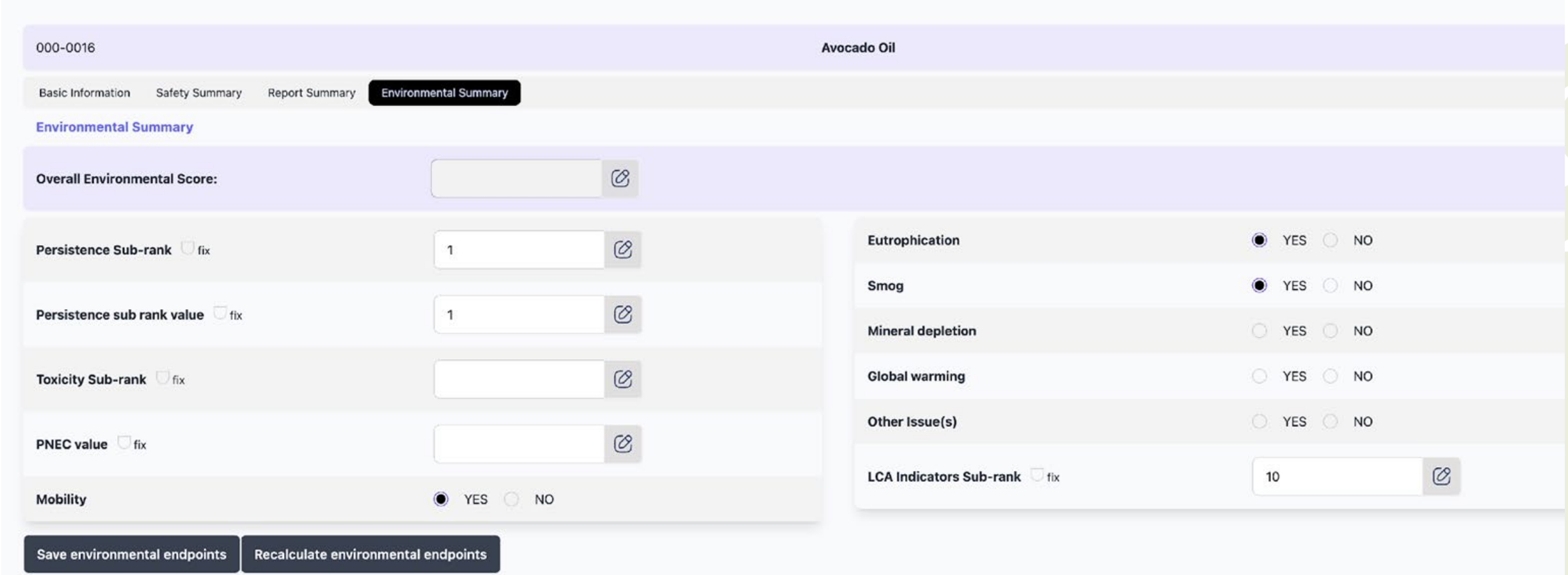
SmartSafetybyDesign Product Assessment and Decision Software for Formulations and Ingredients



SmartSafetybyDesign – Environmental Scoring

BiPhenom



Reference

JK Saxe, L Hoffman, R Labib, Method to incorporate green chemistry principles in early-stage product design for sustainability: case studies with personal care products, *Green Chemistry*, 2022, 24, 4969–4980.
DOI: https://doi.org/10.1039/D2GC00842D

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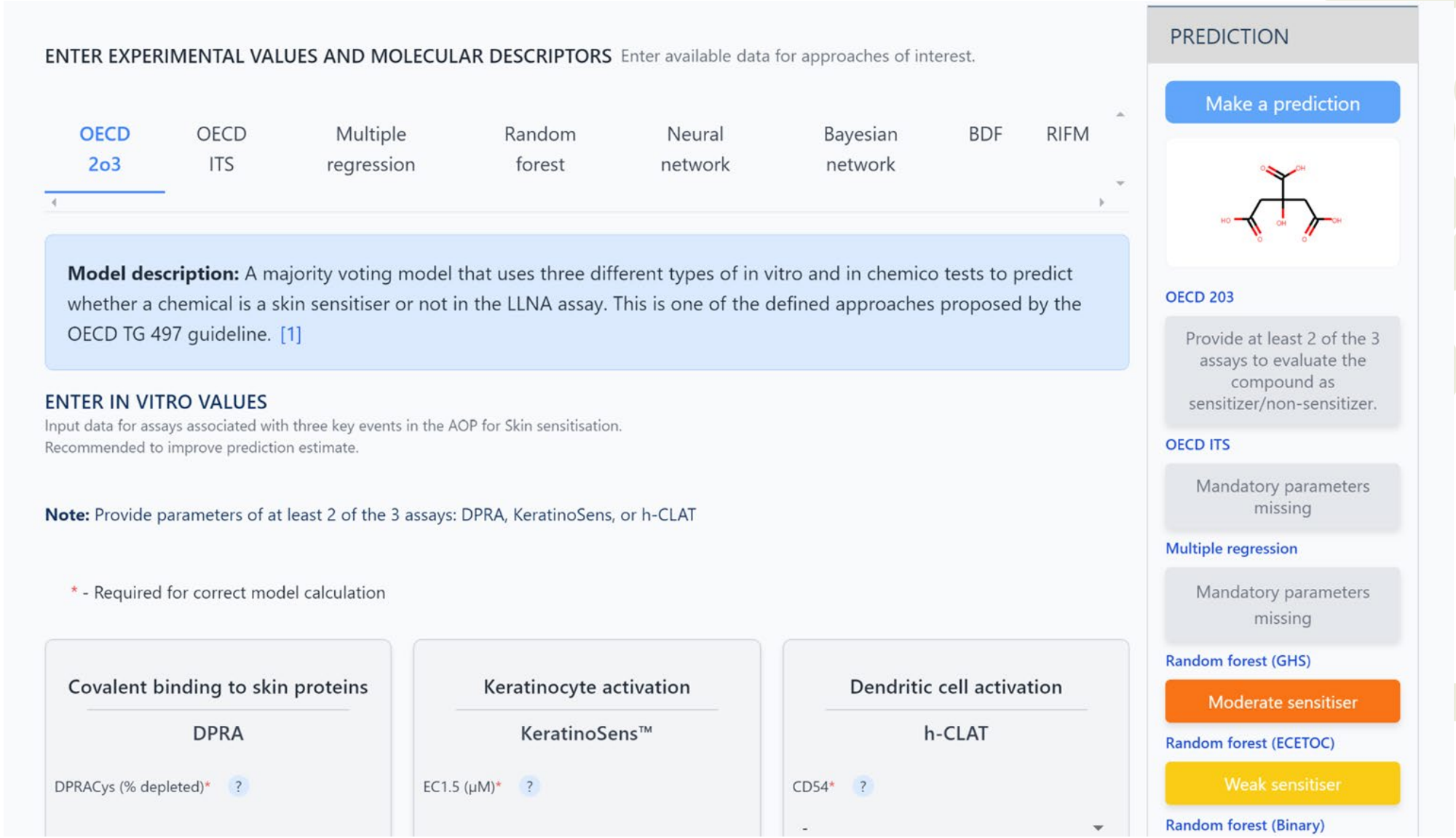
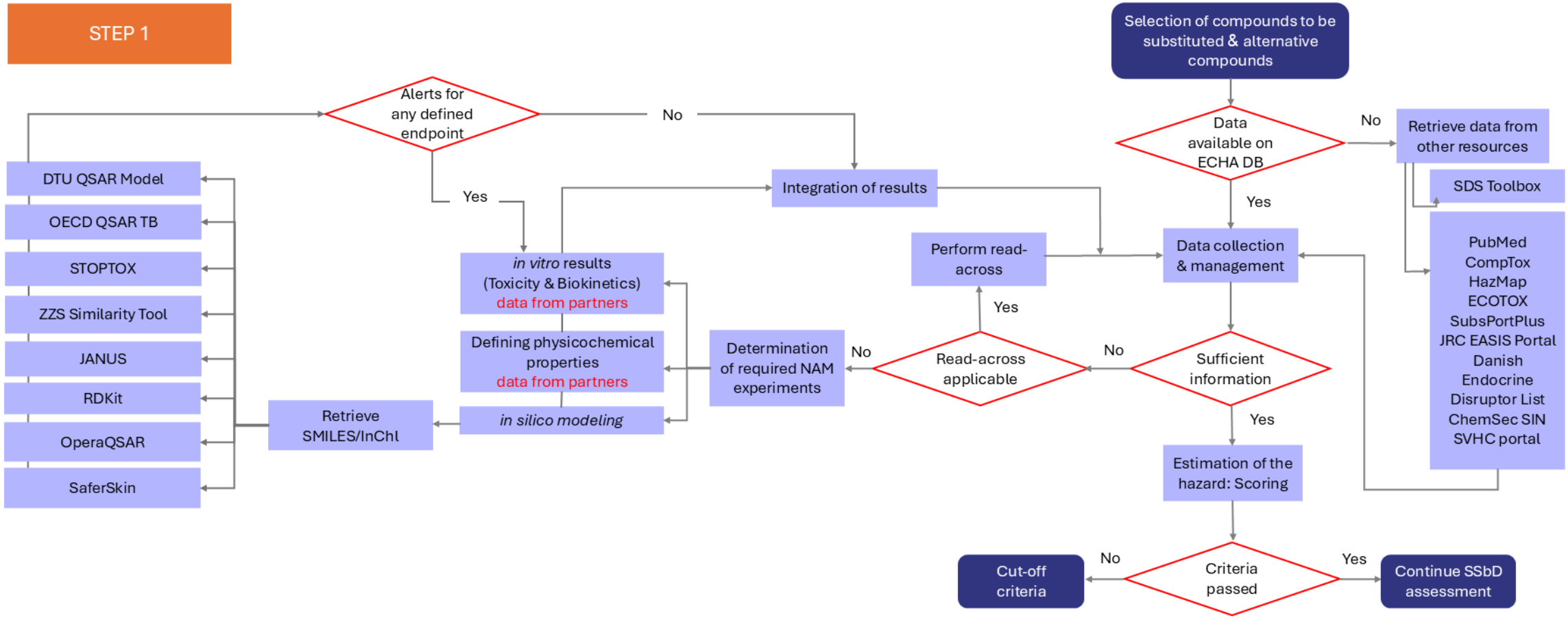
SmartSafetybyDesign – Integration of SaferSkin with Comparison of Different Prediction Models For Skin Safety Assessment



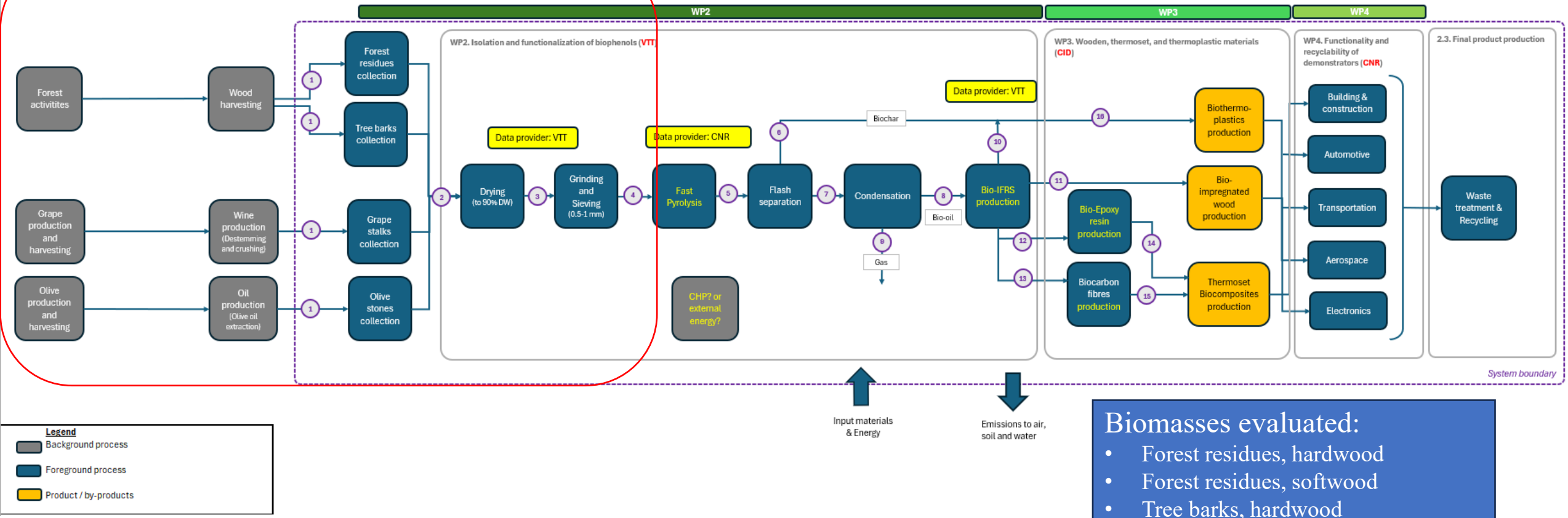
Hazard Characterisation Workflow

BiPhenom



Environmental sustainability assessment

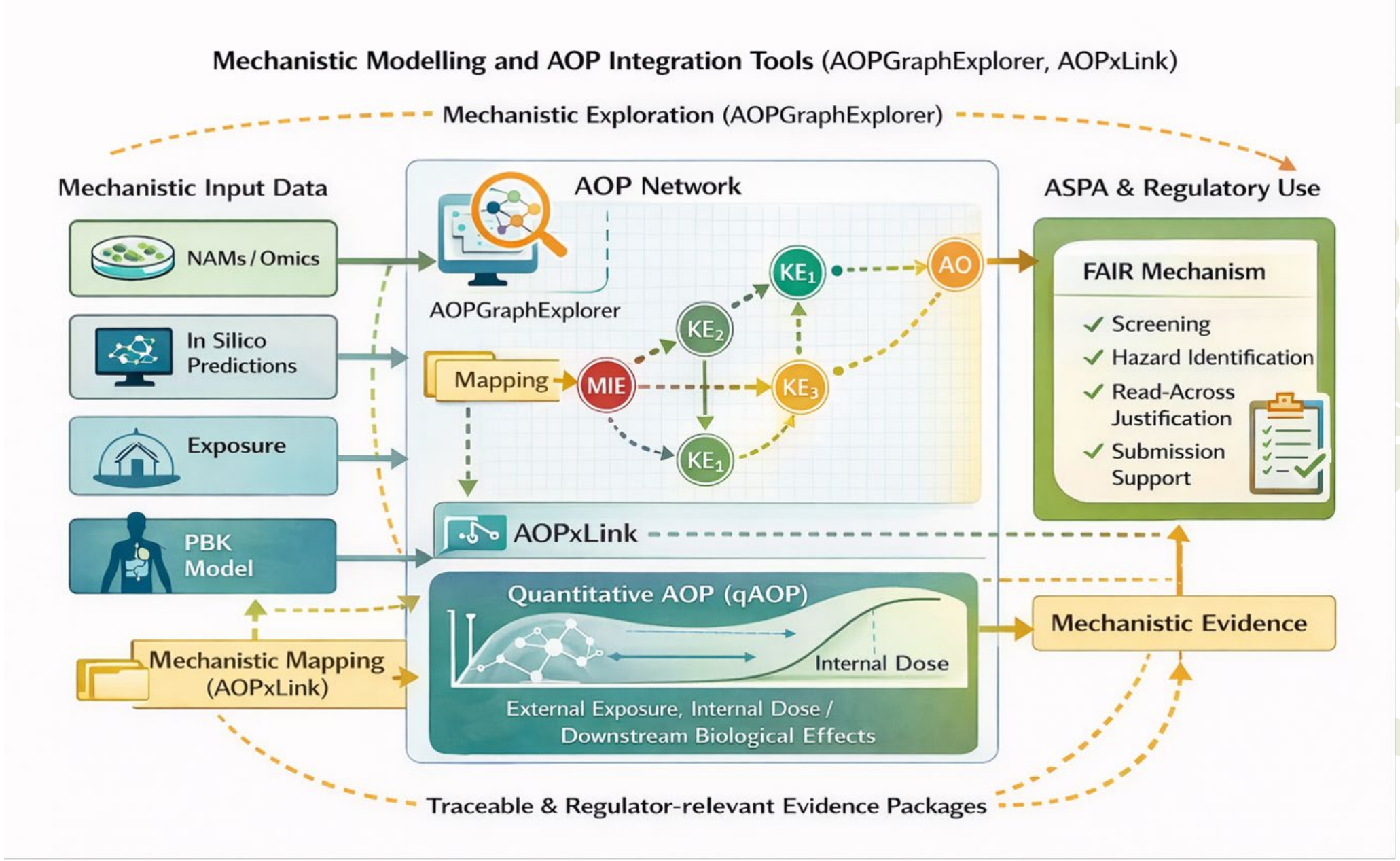
Evaluating potential biomasses



FU: 1 kg biomass 90% DW, 1 mm particle size (grinded and dried)

Biomasses evaluated:

- Forest residues, hardwood
- Forest residues, softwood
- Tree barks, hardwood
- Tree barks, softwood
- Grape stalks
- Olive stones


Mechanistic Modelling and AOP Integration Tools (AOPGraphExplorer, AOPxLink)
Mechanistic Exploration (AOPGraphExplorer)
Mechanistic Input Data
NAMs / Omics
In Silico Predictions
Exposure
PBK Model
Mechanistic Mapping (AOPxLink)
AOP Network
AOPGraphExplorer
Mapping
MIE
KE1
KE2
KE3
KE1
AO
AOPxLink
Quantitative AOP (qAOP)
Internal Dose
External Exposure, Internal Dose / Downstream Biological Effects
ASPA & Regulatory Use
FAIR Mechanism
Screening
Hazard Identification
Read-Across Justification
Submission Support
Mechanistic Evidence
Traceable & Regulator-relevant Evidence Packages

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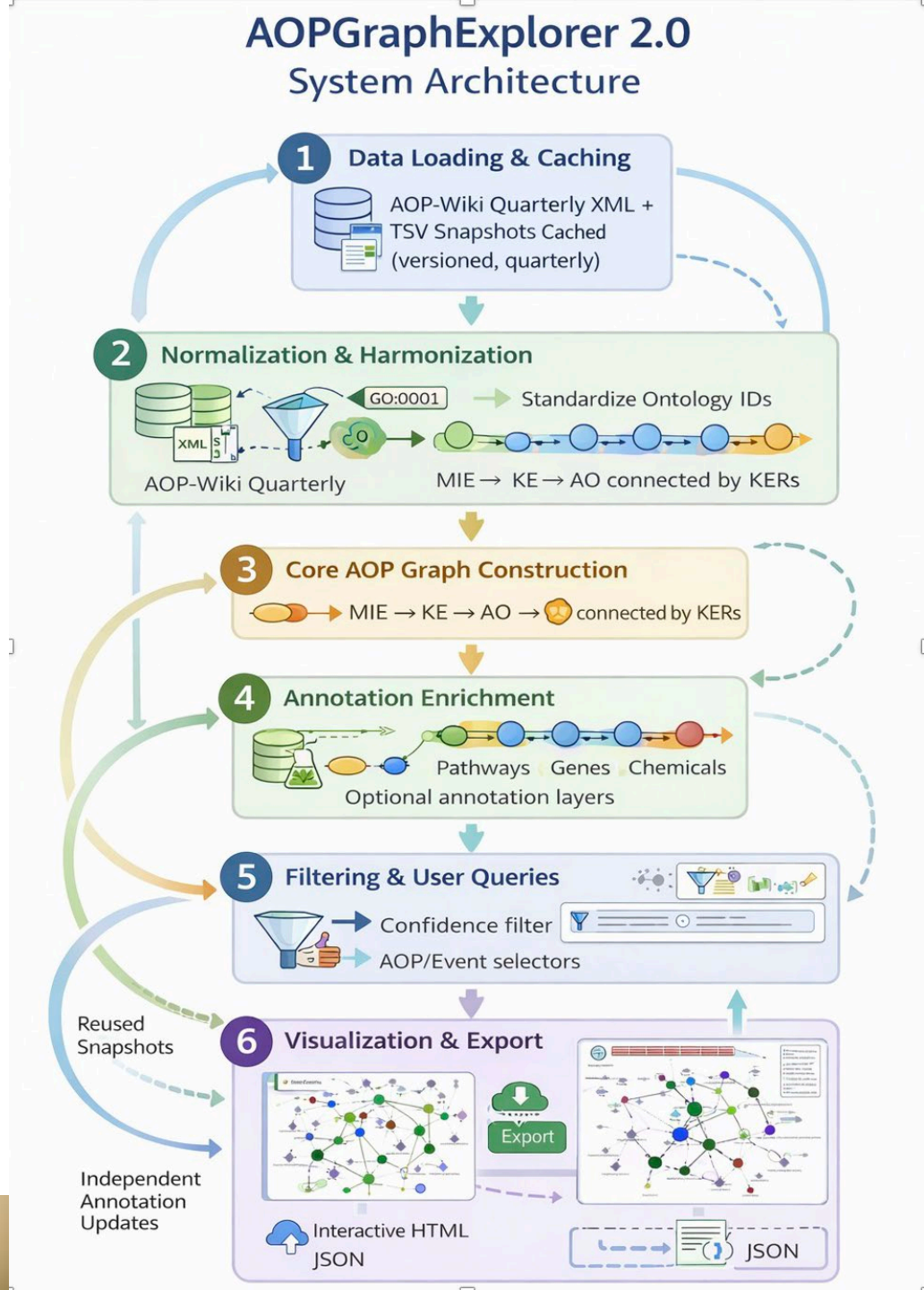
Integrating knowledge to create a model guiding experimental design and interpretation

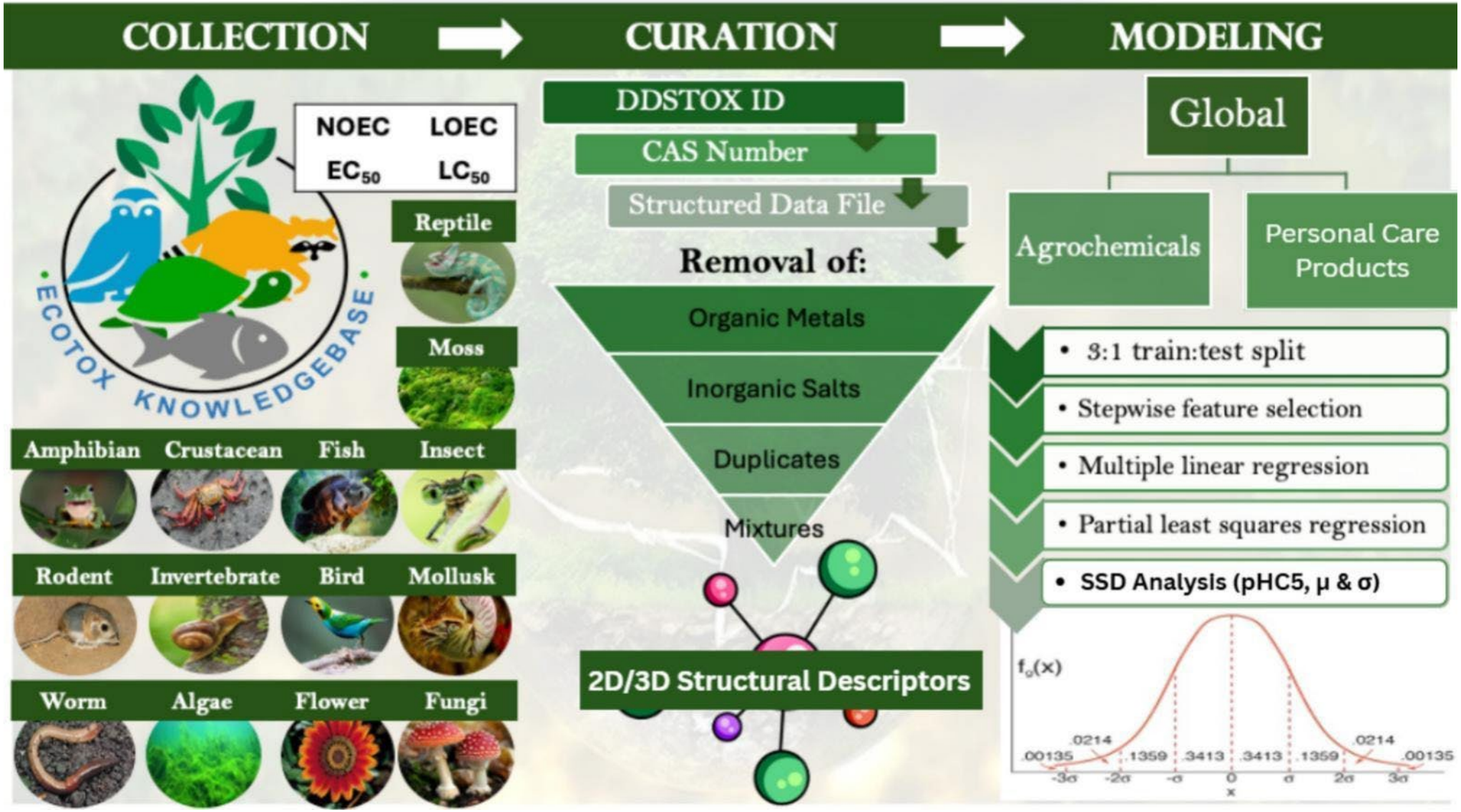
AOPGraphExplorer 2.0
An Interactive Graph-Based Platform for Multi-Domain Mechanistic Annotation and Exploration of Adverse Outcome Pathways
Asmaa A. Abdelwahab, and Barry Hardy

https://doi.org/10.64898/2026.02.27.708648

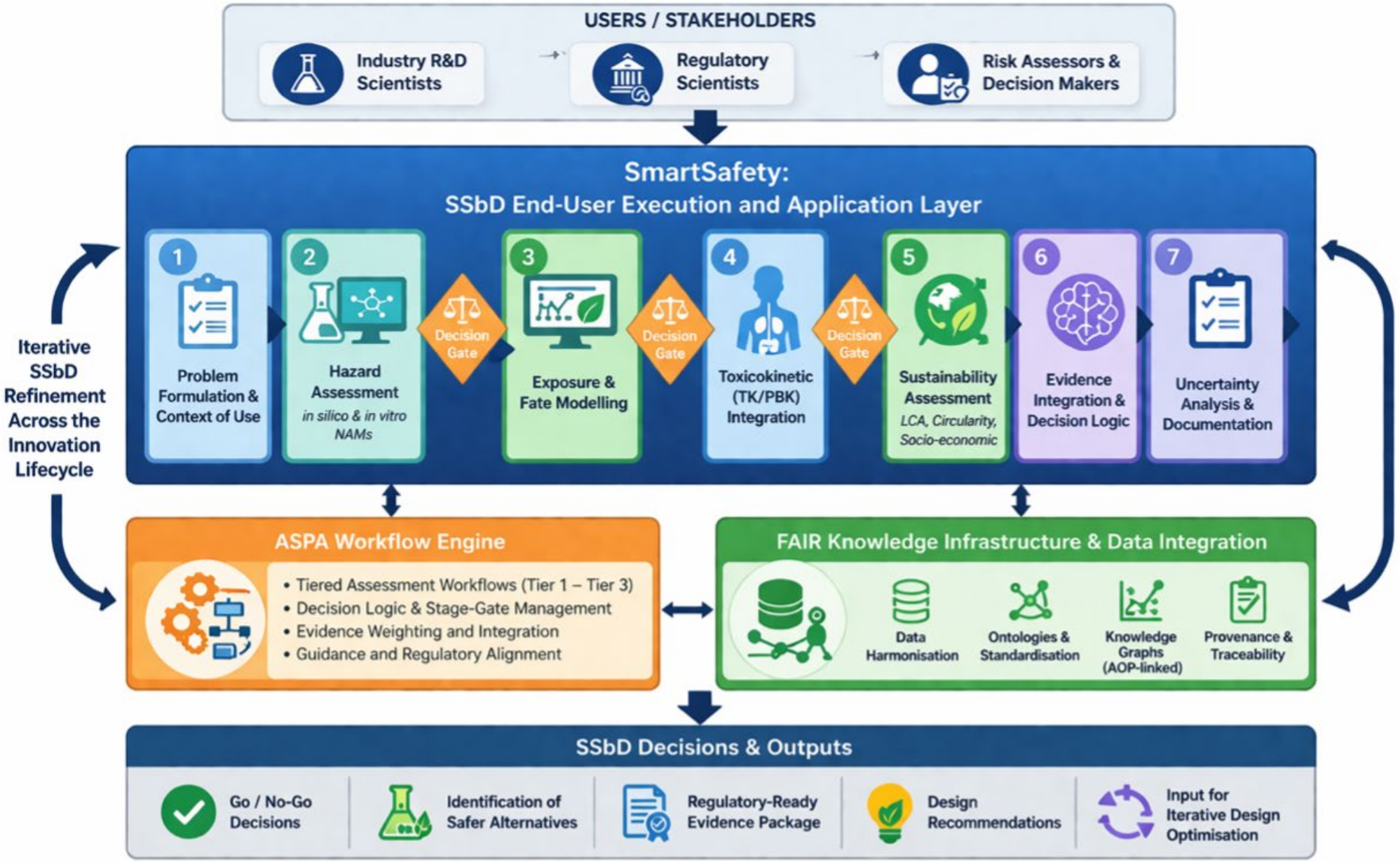


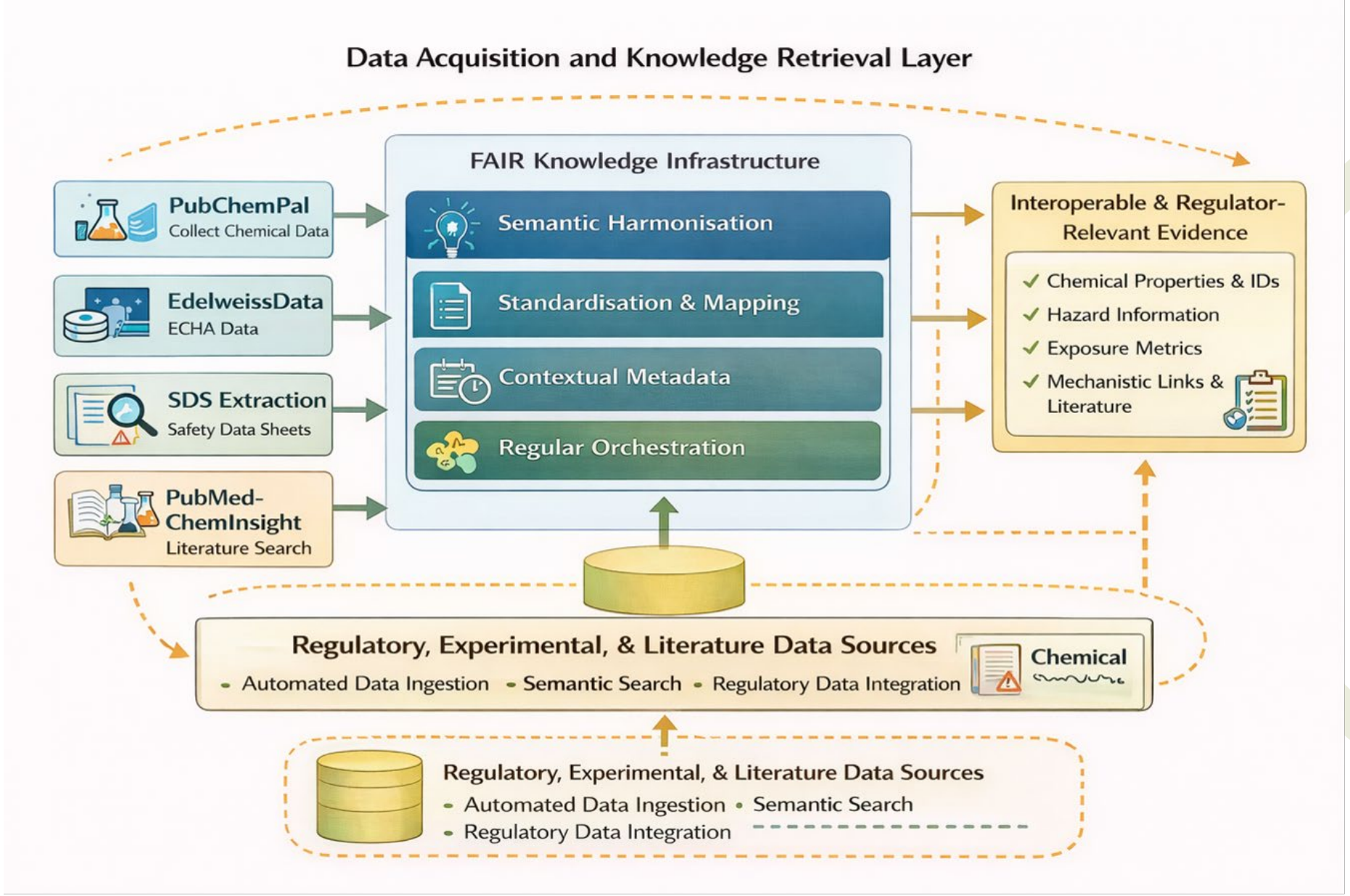
Species Distribution Modelling

Kabiruddin Khan, Nyssa Tucker, Holli-Joi Martin, Varun Gopalakrishnan Nair, Asmaa Ali, Ghada Tagorti, Barry Hardy, Species sensitivity distribution modeling for ecotoxicity prediction of industrial chemicals, Science of The Total Environment, Volume 1006, 2025, 180875, ISSN 0048-9.



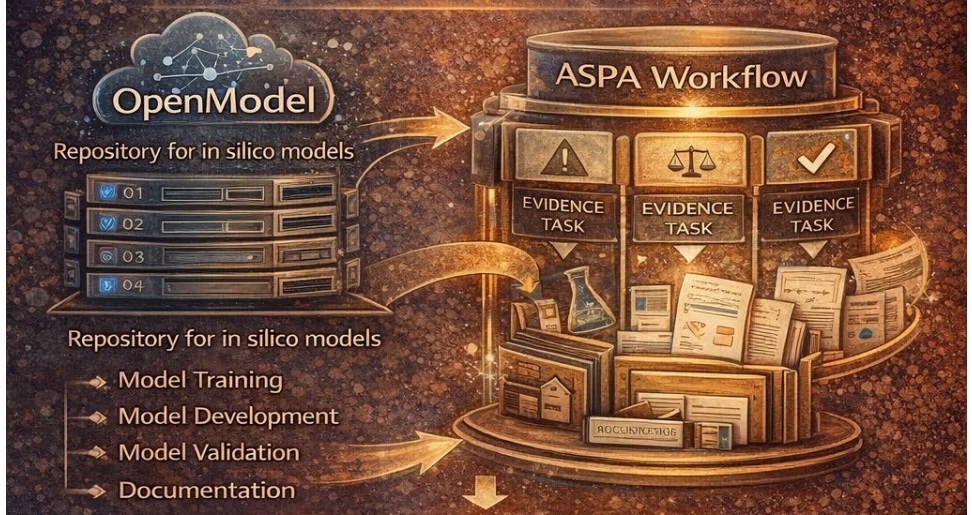
https://www.sciencedirect.com/science/article/pii/S004896972502515X


USERS / STAKEHOLDERS
Industry R&D Scientists
Regulatory Scientists
Risk Assessors & Decision Makers
SmartSafety:
SSbD End-User Execution and Application Layer
1
Problem Formulation & Context of Use
2
Hazard Assessment
in silico & in vitro NAMs
Decision Gate
3
Exposure & Fate Modelling
Decision Gate
4
Toxicokinetic (TK/PBK) Integration
Decision Gate
5
Sustainability Assessment
LCA, Circularity, Socio-economic
6
Evidence Integration & Decision Logic
7
Uncertainty Analysis & Documentation
Iterative SSbD Refinement Across the Innovation Lifecycle
ASPA Workflow Engine
• Tiered Assessment Workflows (Tier 1 – Tier 3)
• Decision Logic & Stage-Gate Management
• Evidence Weighting and Integration
• Guidance and Regulatory Alignment
FAIR Knowledge Infrastructure & Data Integration
Data Harmonisation
Ontologies & Standardisation
Knowledge Graphs (AOP-linked)
Provenance & Traceability
SSbD Decisions & Outputs
Go / No-Go Decisions
Identification of Safer Alternatives
Regulatory-Ready Evidence Package
Design Recommendations
Input for Iterative Design Optimisation


Data Acquisition and Knowledge Retrieval Layer
PubChemPal
Collect Chemical Data
EdelweissData
ECHA Data
SDS Extraction
Safety Data Sheets
PubMed-ChemInsight
Literature Search
FAIR Knowledge Infrastructure
Semantic Harmonisation
Standardisation & Mapping
Contextual Metadata
Regular Orchestration
Interoperable & Regulator-Relevant Evidence
Chemical Properties & IDs
Hazard Information
Exposure Metrics
Mechanistic Links & Literature
Regulatory, Experimental, & Literature Data Sources
Automated Data Ingestion
Semantic Search
Regulatory Data Integration
Chemical
Regulatory, Experimental, & Literature Data Sources
Automated Data Ingestion
Semantic Search
Regulatory Data Integration

An In Silico Protocol for Weight of Evidence

(including conflicting evidence)



Repository for in silico models

- Model Training
- Model Development
- Model Validation
- Documentation

+ ASPA Workflow

- Documentation of Conflicting, Supporting & Inconclusive Results
- Results and Interpretation Provided to Task in Decision Workflow

OpenModel

- Repository for in silico models
- Model Training
- Model Development
- Model Validation

Weights of Evidence for Regulatory Task

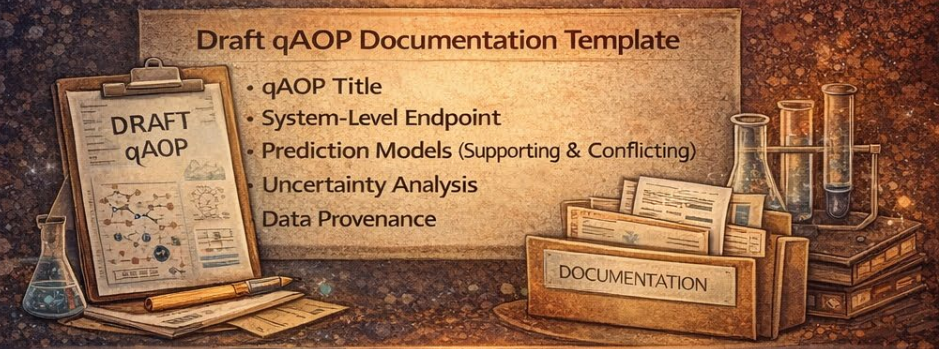
- Interpretation of Results
- Regulatory Presentation
- Defensible Decisions

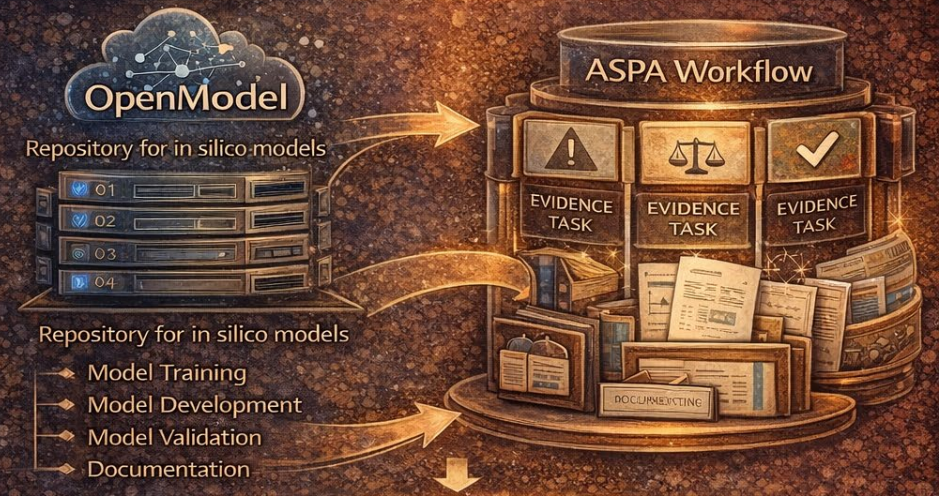
An In Silico Protocol for Weight of Evidence

(including conflicting evidence)

Draft qAOP Documentation Template

- qAOP Title
- System-Level Endpoint
- Prediction Models (Supporting & Conflicting)
- Uncertainty Analysis
- Data Provenance





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- Documentation

Weights of Evidence for Regulatory Task

- Interpretation of Results
- Regulatory Presentation
- Defensible Decisions

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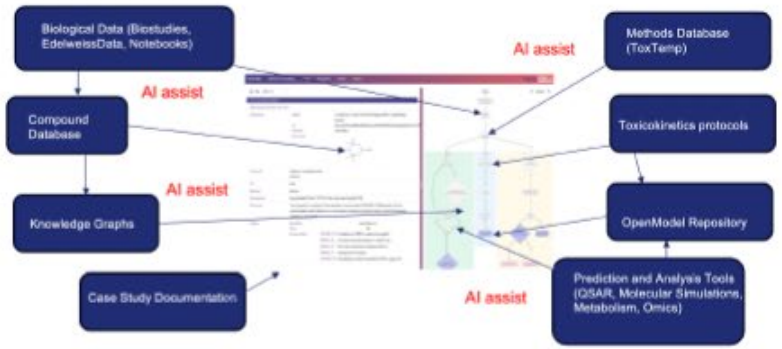
Workflows

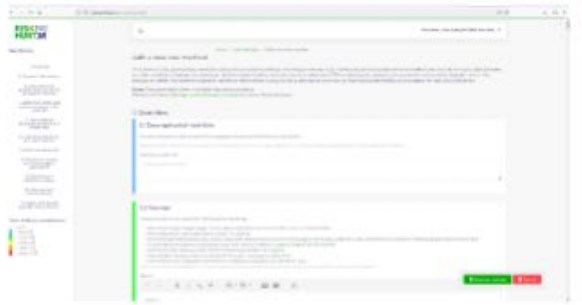


All workflows are well-documented with regards to sources of data and criteria for scoring and decision points.

AI-Assisted Knowledge Mining

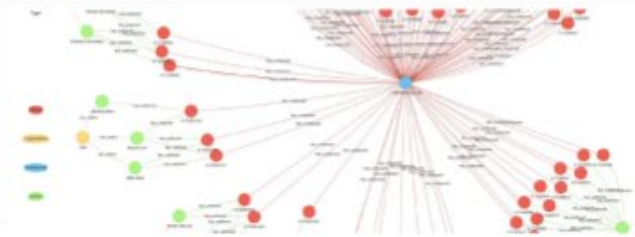
AI resources are used for background knowledge mining of databases, literature and safety data sheets (shown).

Methods Documentation



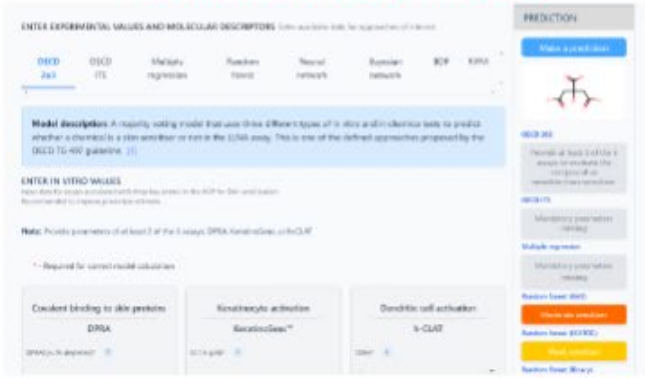
Test methods used to generate data required for SSbD workflows are documented for completeness (ToxTemp shown).

Knowledge Graphs



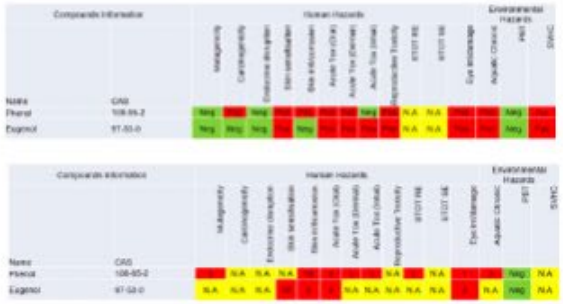
Knowledge graphs are used to define relationships between information assisting search and analysis.

Assessment Tools



Our software toolbox brings information together that is required by the assessor for a particular SSbD task (SaferSkin IATA incorporated here into our SSbD assessment tool shown above).

SSbD Results Profiling



Profiling results for different ingredients are compared based on data from different sources (phenol hazard data profiling from databases and models shown).

Thank you!

VTT

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Grant Agreement No: 101135107

Project funded by

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
State Secretariat for Education, Research and Innovation SERI

This work has received funding from the Swiss State Secretariat for Education, Research and Innovation (SERI).
Grant Agreement No: 24.00212

UKRI Innovate UK

This work was supported by UKRI Horizon Europe Underwriting – Innovate UK Council [1005409].