SSbD4CheM

Stakeholder Outreach Webinar: Practical application and Case Studies in industrial SSbD

11 June 2025, 15:00 – 16:30h CEST, online

Funded by the European Union

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Program - *Event Program Online (LinkedIn)*

- **SSbD4CheM – Advancing Safe and Sustainable by Design Practices for Chemicals and Materials**, Milica Velimirovic (VITO)
- **Perspective on the Application of SSbD to Cosmetics Products**, Ze'evi Ma'or and Assaf Assis (AHAVA)
- **AI-assistance in Knowledge Collection and Curation supporting SSbD workflows**, Barry Hardy (Edelweiss Connect)
- **Materials Characterisation**, Ondrej Panak (National Institute of Chemistry, Slovenia)
- **Materials Modelling supporting Hazard Profiling**, Panagiotis Kolokathis (NovaMechanics)
- **Use of New Approach Methods in SSbD**, Yvonne Kohl (Fraunhofer IBMT)
- **Life Cycle Assessment**, Nils Thonemann (University of Leiden)
- **Insights from Case Study Applications**, Ivana Burzic (Wood K plus)

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SSbD4CheM – Advancing Safe and Sustainable by Design Practices for Chemicals and Materials

Milica Velimirovic (VITO)

11 June 2025, 15:00 – 16:30h CEST, online

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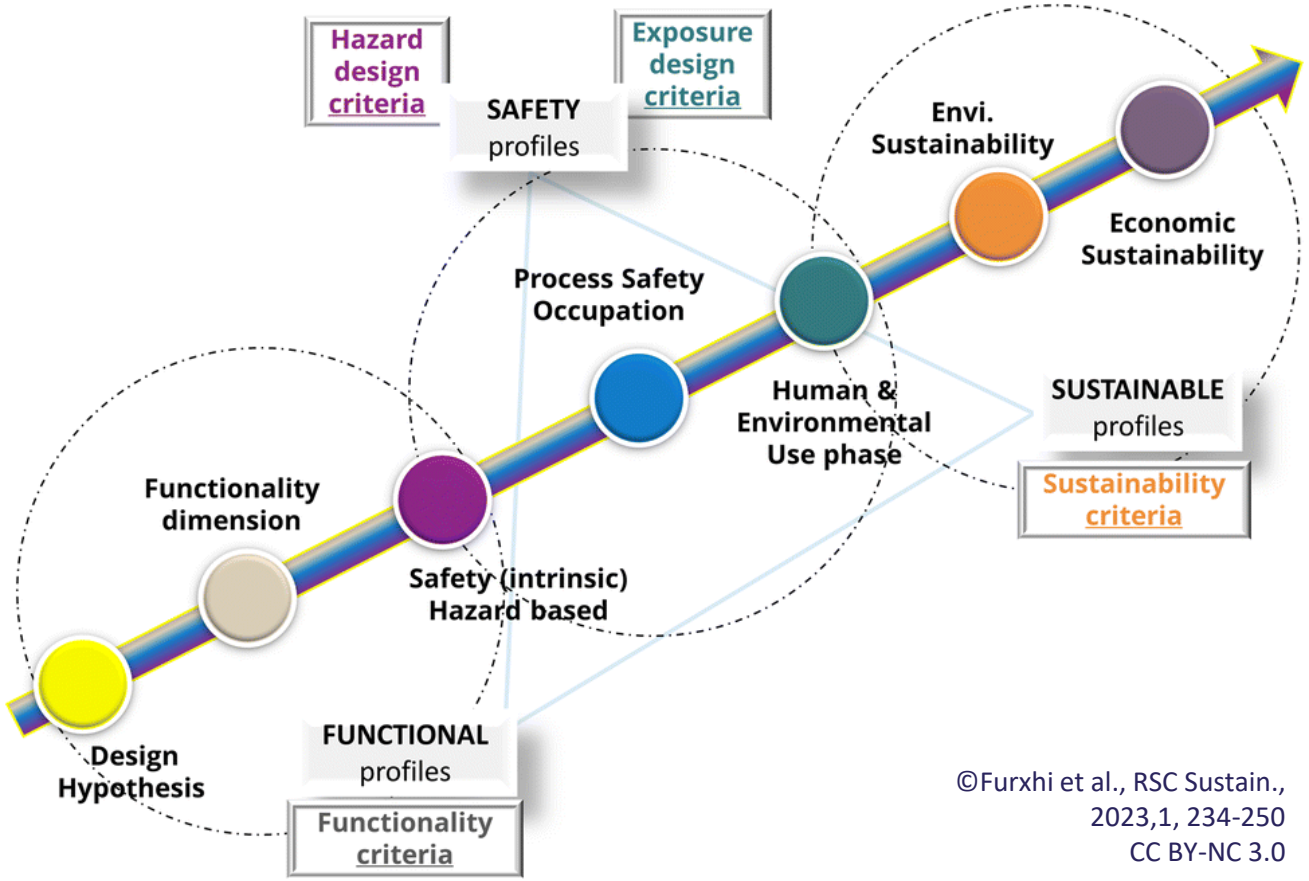
SSbD framework

- Safety and sustainability integrated in the chemical/product development

- Key Principles
  - **Safety:**

    Ensuring that products and processes do not pose risks to human health and the environment.
  - **Sustainability:**

    Minimizing environmental impact and promoting resource efficiency throughout the lifecycle.



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SSbD4CheM project details

Call: **HORIZON-CL4-2023-RESILIENCE-01-21**

Project Number: **101138475**

Start date: **1 January 2024** | End date: **31 December 2027**

Duration: **4 years**

EU contribution: **€ 7 498 762,50**

UK and CH contribution: **€ 1 966 420,00**

Consortium

19 partners | **14** countries

10 research institutes | **3** universities

4 SMEs | **2** LEs

Sister projects:

CHIASMA

CheMatSustain

TOXBOX

Innovative methods for safety and sustainability assessments of chemicals and materials

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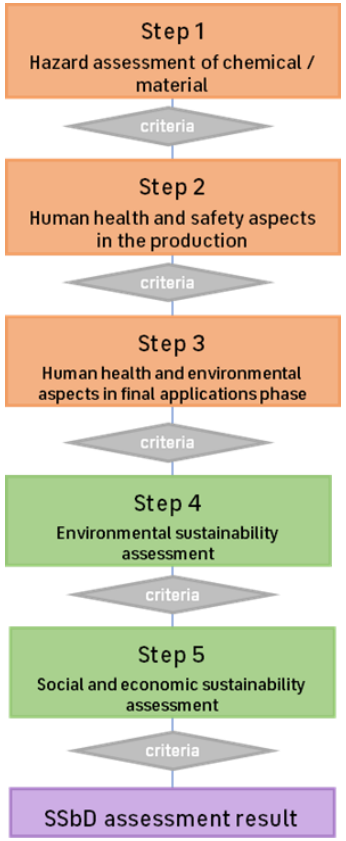
SSbD4CheM ambition

- Develop a SSbD4CheM framework to utilize new science-based approaches and innovative technologies to proactively identify and address hazards and risks, fostering the design of safer, sustainable products, and processes across sectors and value chains:
- This includes:
  - improvement of safety and sustainability assessment along product life cycle
  - alternative methods for safety assessment (e.g., NAMs) without animal models
  - robust, reliable and faster test methods or models, including high-throughput and *in silico* models
  - validated *in vitro* tools for a variety of substances and materials – coatings and composites
  - enhanced international collaboration on uptake of new methods and/or models



The 5 main steps methodology of the SSbD Framework

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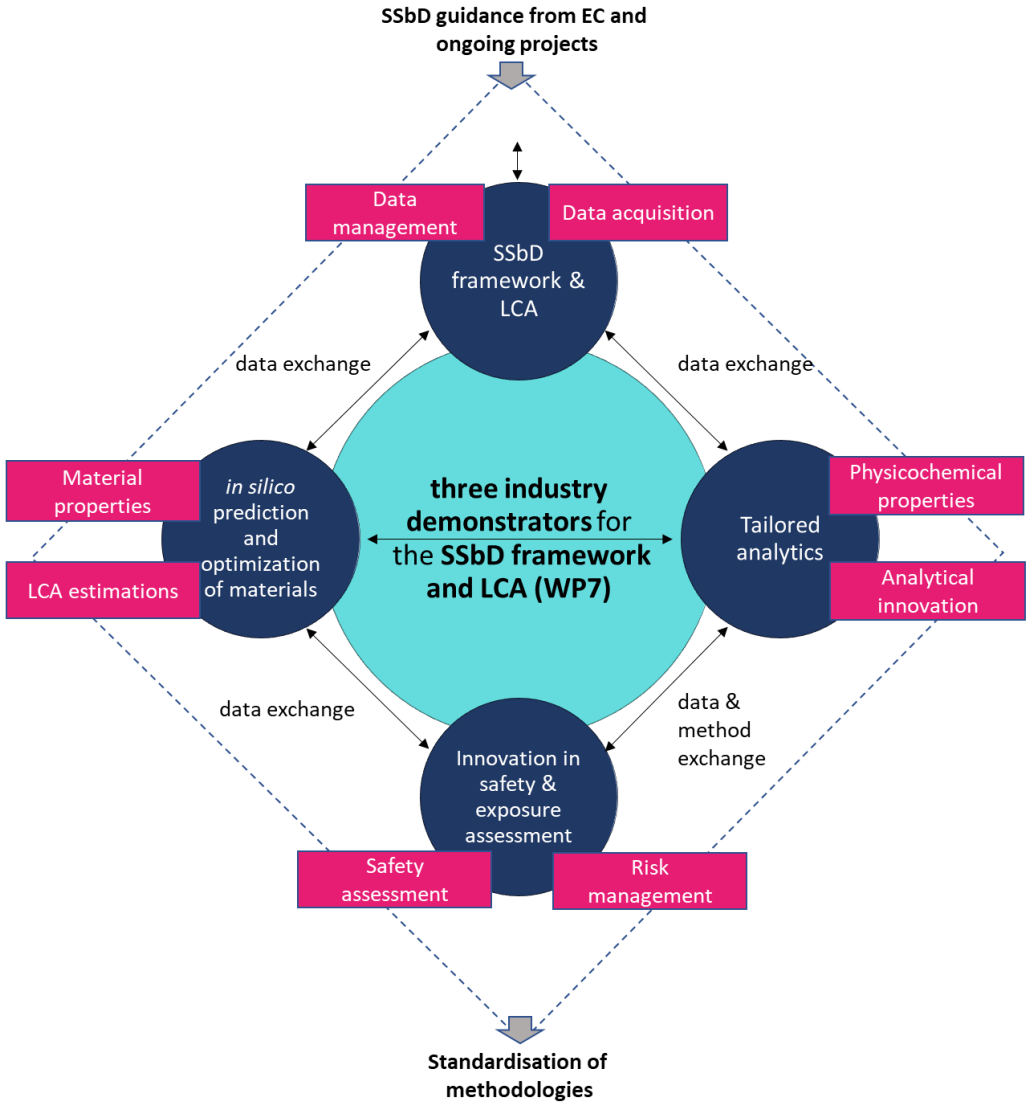
SSbD4CheM methodology

- SSbD4CheM serves as a comprehensive toolbox equipped with resources and tools for developing safe and sustainable products and processes.
- Encompassing a wide array of tools, guidance documents, and databases, the toolbox is designed for versatility.
- Stakeholders in industry, government, academia, and civil society can utilize a range of tools, guidance documents, and databases.



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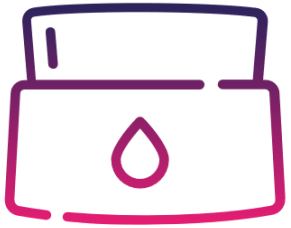
SSbD4CheM demonstrators

Renewable based composites for automotive interior

Bio-based self-cleaning/water repellent & antimicrobial treatments for apparel textiles



Nanocellulose for applications in cosmetics

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SSbD4CheM demonstrators

Renewable based composites for automotive interior

- **Safety Goals:**
  - Hazard assessment of micro fibrillated cellulose (MFC) completed
  - Human health & safety evaluated during MFC production and processing; processes optimized
  - **TVOC emissions reduced** by using MFC vs. wood-based fillers
  - **Formaldehyde release from all formulations < 10 ppm**
  - **Odor level target ≤ 3**

- **Sustainability Goals:**
  - Substitution of mineral based fillers by micro fibrillated cellulose targeting the same **mechanical performances**: Flex Strength & Modulus 20-50 MPa @23°C; 1500-2500 @23°C (ISO178)
  - Development of renewable composite formulations: **renewable feedstock content > 80%**.
  - **Lower environmental impact by 20%:** raw material usage and energy consumption are distinctly reduced
  - **Reduce material weight** (due to lower filler density) composite density target value <1,15 g/cm3 (ISO 1183) allowing reduced fuel consumption.

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SSbD4CheM demonstrators

Bio-based self-cleaning/water repellent & antimicrobial treatments for apparel textiles

- **Safety Goals:**
  - **Reduced water, chemical, and energy use** → lower environmental & health impact.
  - No cross-linkers needed → **minimal VOC emissions**.
  - **Compliance with REACH Article 33** for all chemicals/materials.
- **Sustainability Goals:**
  - Treatment based on renewable and sustainable sources to **substitute fossil-based feedstock**.
  - **≥ 90% biodegradation in soil** absolute or relative to cellulose in 2 years according to EN-13432 / ISO 18606 .
  - Development of bio-based polymer formulations: **biomass content > 50%**
  - **20% lower environmental impact**: raw material usage and energy consumption are distinctly reduced
  - **Coating thickness reduced** from 2–30 µm to ~200 nm
  - Compared to conventional solvent-based coating processes **no energy-intensive application and drying steps are necessary**, leading to small and cost-efficient plant concepts.

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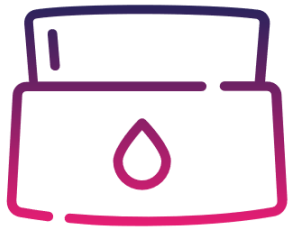
SSbD4CheM demonstrators



Nanocellulose for applications in cosmetics

- **Safety Goals:**
  - **Skin irritation:** safety testing to ensure that nanocellulose is safe for use in cosmetic products.
  - **Inhalation risk:** Human health & safety evaluated during manufacturing or use of cosmetic products; processes optimized
  - **Environmental impact:** assess biodegradability & bioaccumulation
- **Sustainability Goals:**
  - **Resource use:** Nanocellulose can be produced from renewable resources, such as wood pulp, making it a potentially sustainable material.
  - Development of renewable composite formulations: **renewable feedstock content > 80%**.
  - **Biodegradability:** Nano-cellulose is biodegradable, which means that it can break down naturally in the environment, reducing the potential for environmental harm.
  - **Reduced waste:** Nanocellulose can be produced using waste streams from other industries, such as the paper industry, reducing waste and promoting sustainability

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SSbD4CheM framework and workflow

EdelweissConnect · ENTELOS INSTITUTE

Characterization	Computer aided (re)design approach	Human health and environmental safety assessment	Exposure assessment / risk management	Sustainability assessment across the life cycle assessment
AUTOMOTIVE (WOOD KPLUS · STELLANTIS CRF)				
Time-of-flight mass spectrometry (TOFWERK)	Computational Fluids Dynamics (NovaMechanics)	hiPSC-based *in vitro* lung model (Fraunhofer IBMT)	Reduced TVOC emissions (HOCHSCHULE FRESENIUS · WOOD KPLUS · VITO)	LCA, s-LCA, and LCC (Universiteit Leiden · ITENE · VITO)
TEXTILE (CTCR · KORTEKS)				
High resolution chemical imaging (LUXEMBOURG INSTITUTE OF SCIENCE AND TECHNOLOGY LIST)	Molecular simulations (NovaMechanics)	Zebrafish embryo model (VITO)	Characterisation of microfibers and microfibrils release (Loughborough University · VITO)	LCA, s-LCA, and LCC (Universiteit Leiden · ITENE · VITO)
COSMETICS (KEMIJSKI INŠTITUT · AHAVA)				
Field-Flow Fractionation hyphenated to light scattering (POSTNOVA)	Machine learning toxicity models (NovaMechanics)	Human skin *ex vivo* and *in vitro* models (AHAVA)	Fate and the behaviour in the environment (HOCHSCHULE FRESENIUS)	LCA, s-LCA, and LCC (Universiteit Leiden · ITENE · VITO)

D&C&E · BNN

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Perspective on the Application of SSbD to Cosmetics Products

Ze’evi Ma’or and Assaf Assis (AHAVA)

11 June 2025, 15:00 – 16:30h CEST, online

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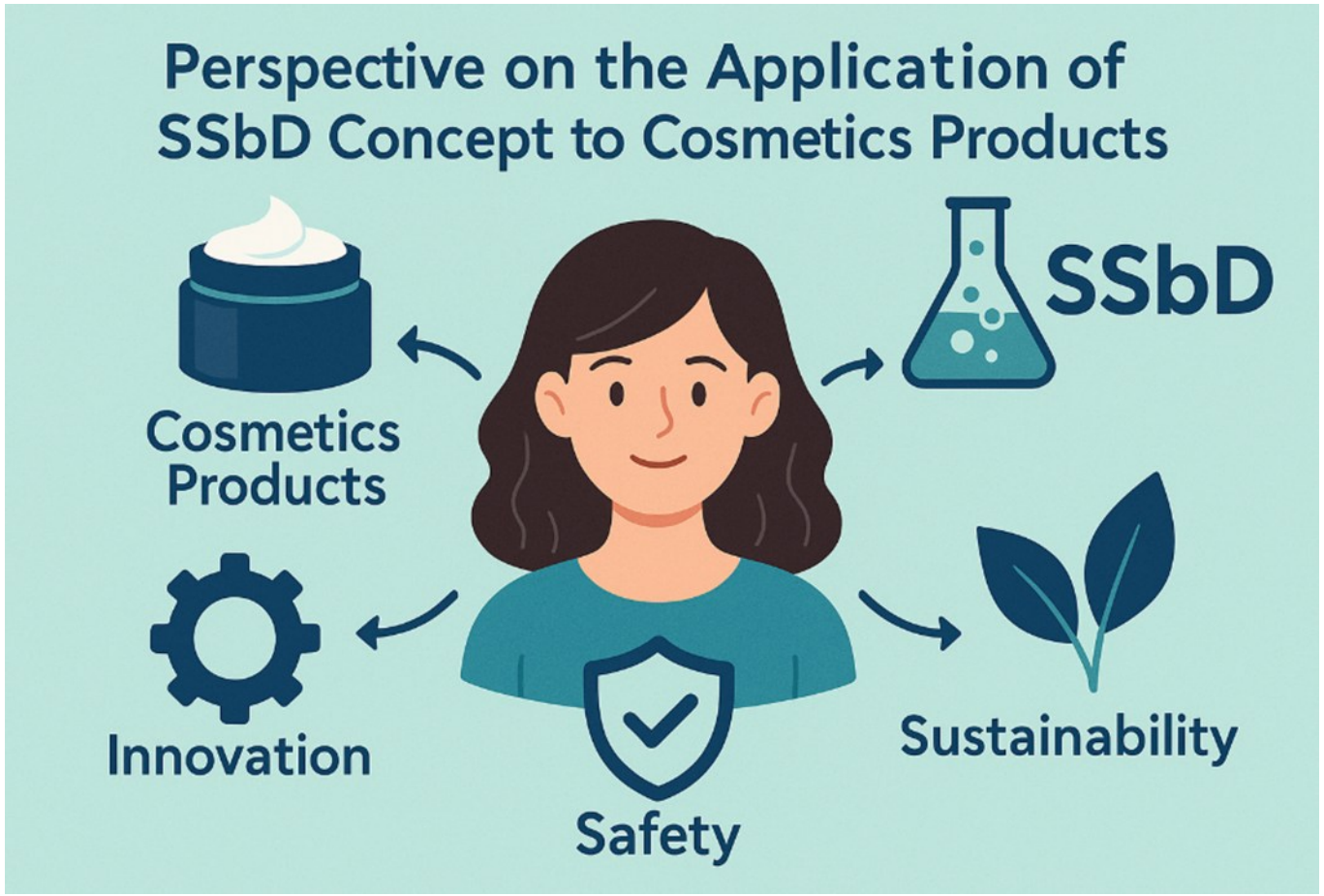
AHAVA



AHAVA Dead Sea Laboratories

Ze’evi Ma’or and Assaf Assis

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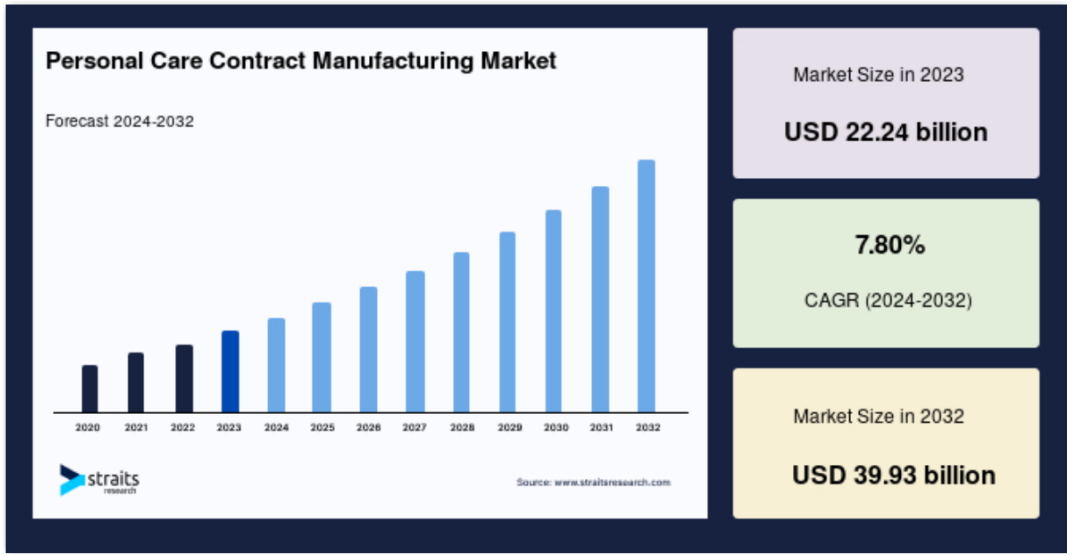
An Industry Perspective on SSbD in Cosmetics

Cosmetics is a mature and competitive industry.



Straitsresearch

SSbD is a new concept in these markets.

Catalisti

Introducing SSbD to the cosmetic markets should be performed in a clever and sophisticated way, taking advantage and benefits for the relevant stakeholders.

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Industry Context

Market Realities

Cosmetics industry operates in saturated, competitive markets.

SSbD represents novel concept requiring sophisticated implementation.

Success Factors

Strategic stakeholder engagement essential.

Value creation across supply chain.

Clear differentiation from "clean beauty" claims.

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Reaching the Consumers

SSbD benefits should be well understood to the end-user

To establish a strong **Reason to Believe** for SSbD new concept for the consumers

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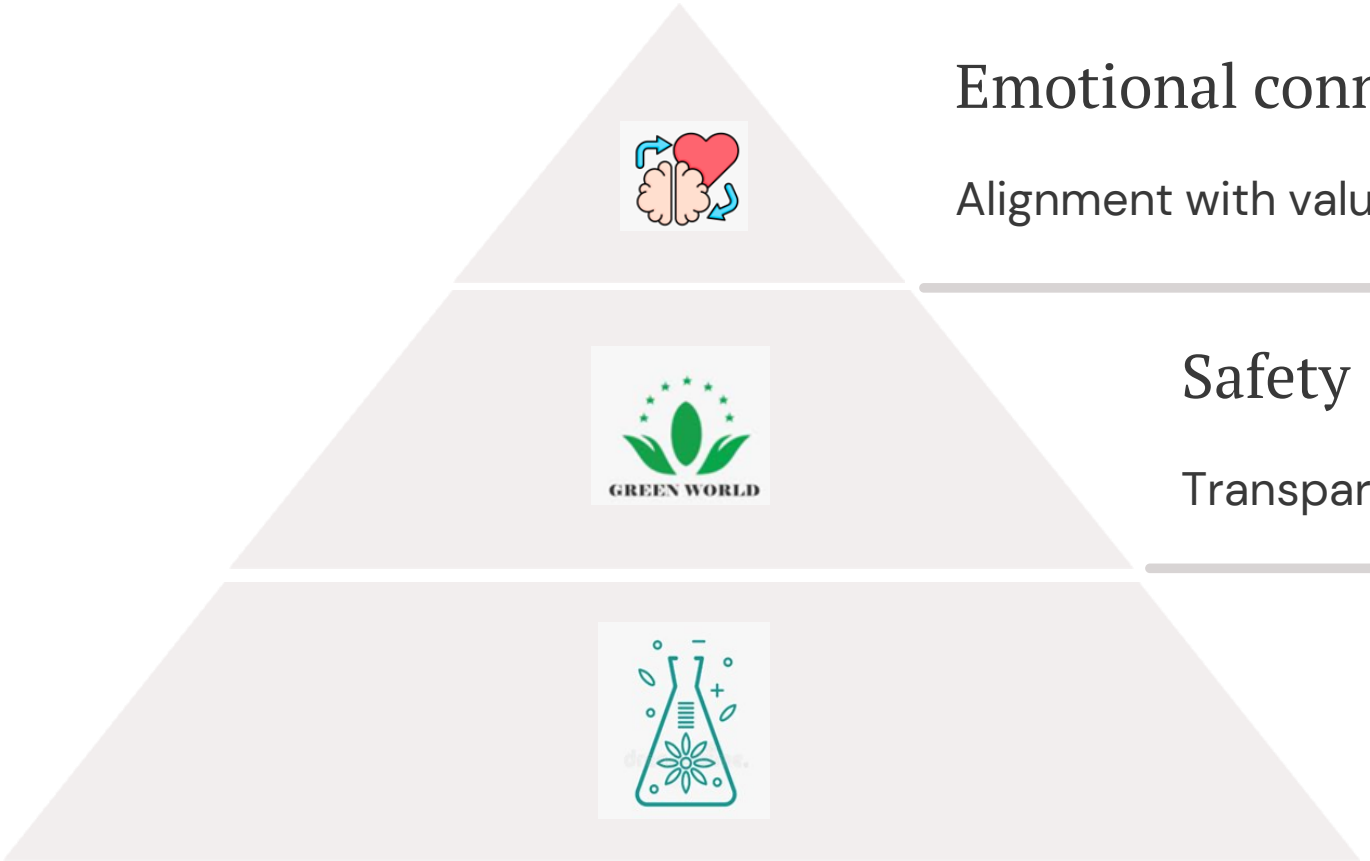
Consumer Priorities



Emotional connection

Alignment with values and identity

Safety & sustainability

Transparent ingredients and processes

Product efficacy

Performance that delivers results

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Retail Strategy

Establish partnerships

Selective distributors as SSbD champions

“Clean Beauty” retailer as pioneers to SSbD claim

In-store experience

Education-focused merchandising

Certification visibility

Clear labeling of SSbD benefits

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Regulatory Engagement

European Green Deal Alignment

Demonstrate SSbD compliance with environmental policies

Formal Accreditation

Develop standardized certification framework for SSbD.

Clean Claims Distinction

Support regulation limiting misleading "**clean beauty**" and "**chemical-free**" marketing claims

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Competitive Landscape – holistic point of view

Identify threats

Monitor established and emerging competitors

Anticipate responses

Prepare for competitive SSbD claims

Protect innovation

Secure intellectual property where possible

Differentiate positioning

Develop unique SSbD value proposition

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Strategic Implementation Roadmap

Phase 1: Foundation

Define SSbD standards specific to cosmetics

Build supplier partnerships

Phase 2: Innovation

Develop flagship SSbD products

Create consumer education materials

Phase 3: Market Entry

Launch with strategic retail partners

Engage opinion leaders

Phase 4: Expansion

Scale across categories and markets

Drive industry-wide SSbD adoption

SSbD4CheM

AHAVA

GREEN WORLD

Nanocellulose for applications in cosmetics

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AI-assistance in Knowledge Collection and Curation supporting SSbD workflows

Barry Hardy (Edelweiss Connect)

11 June 2025, 15:00 – 16:30h CEST, online

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Knowledge Infrastructure and Workflow approach

SSbD4CheM

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).

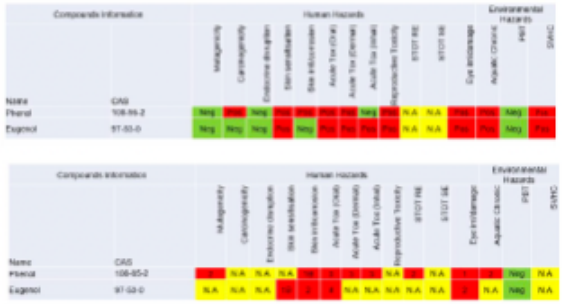
Knowledge Graphs

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).

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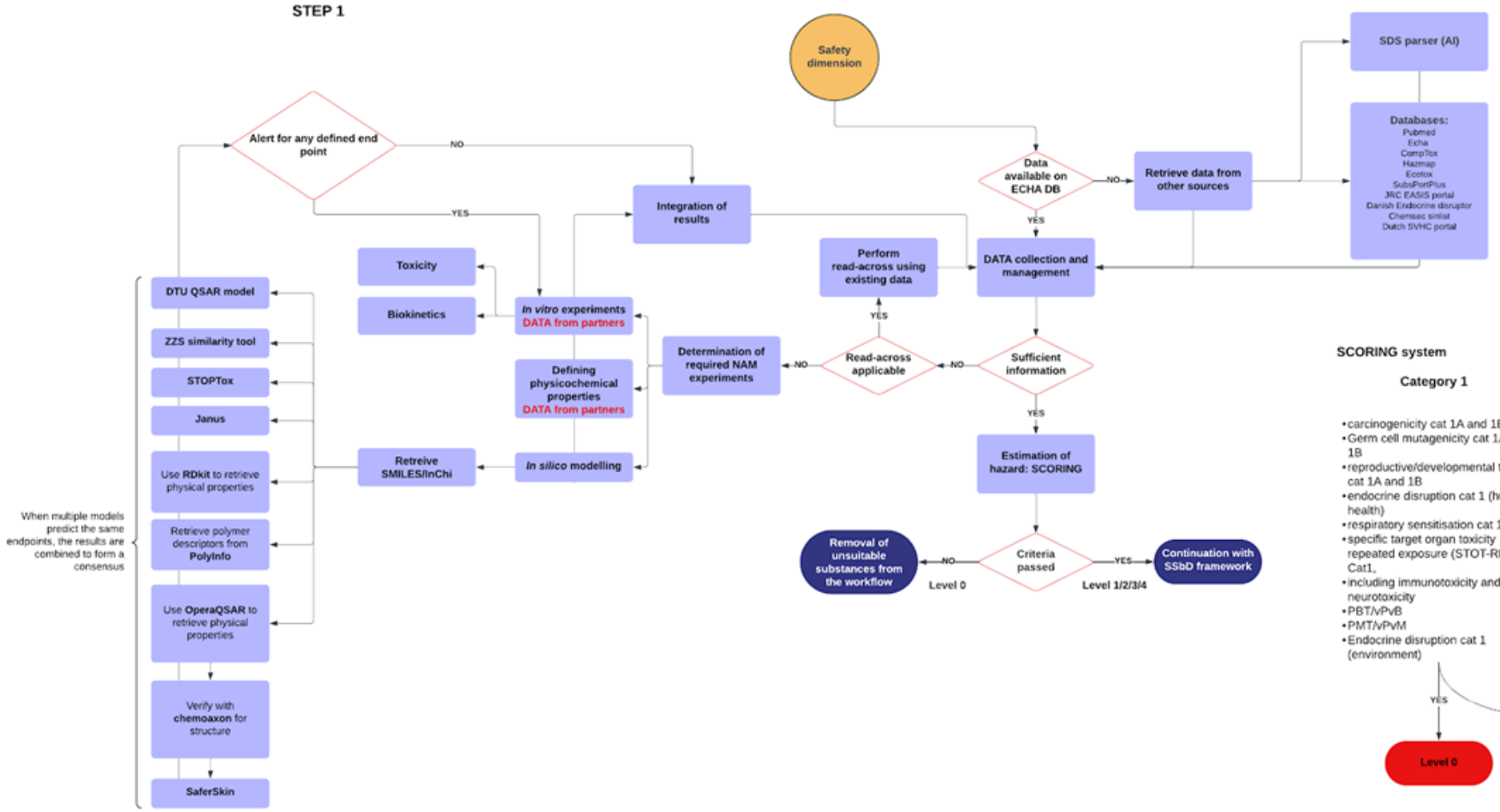
Tier 0/1 workflow



Retrievable data from ECHA DataBase

Human hazard endpoints	Environmental hazard endpoints	Physical hazards endpoints
• carcinogenicity • Mutagenicity • reproductive toxicity • ED (human) • respiratory sensitisation • STOT-RE • Skin sensitisation • Acute toxicity oral • Acute toxicity dermal • acute toxicity inhalation • skin corrosion/irritation • eye damage/irritation • aspiration hazard • STOT-SE	• PBT/vPvB • PMT/vPvM • ED (environment) • Ozone • Chronic aquatic toxicity • Acute aquatic toxicity	• explosive • flammable • aerosols • oxidizing • gases under pressure • self-reactive • pyrophoric liquids/solids • self-heating • emits flammable gas • organic peroxides • corrosivity • desensitized explosives

SCORING system

Category 1	Category 2	Category 3
• carcinogenicity cat 1A and 1B • Germ cell mutagenicity cat 1A and 1B • reproductive/developmental toxicity cat 1A and 1B • endocrine disruption cat 1 (human health) • respiratory sensitisation cat 1 • specific target organ toxicity repeated exposure (STOT-RE) Cat1, • including immunotoxicity and neurotoxicity • PBT/vPvB • PMT/vPvM • Endocrine disruption cat 1 (environment)	• Skin sensitisation cat1 • carcinogenicity cat2 • germ cell mutagenicity cat2 • reproductive/developmental toxicity cat2 • specific target organ toxicity-repeated exposure (STOT-RE) cat2 • specific target organ toxicity-single exposure (STOT-SE) cat1 and 2 • endocrine disruption cat2 (human health) • hazardous for the ozone layer • chronic aquatic toxicity • endocrine disruption cat2 (environment)	• acute toxicity • skin corrosin/skin irritation • eye damage/eye irritation • aspiration hazard (cat1) • STOT-SE cat3 • acute aquatic toxicity • explosives • flammable • aerosols • oxidising • self reactive • pyrophoric liquids, solids • self-heating • in contact with water emits flammable gas • organic peroxides • corrosivity • desensitised explosives

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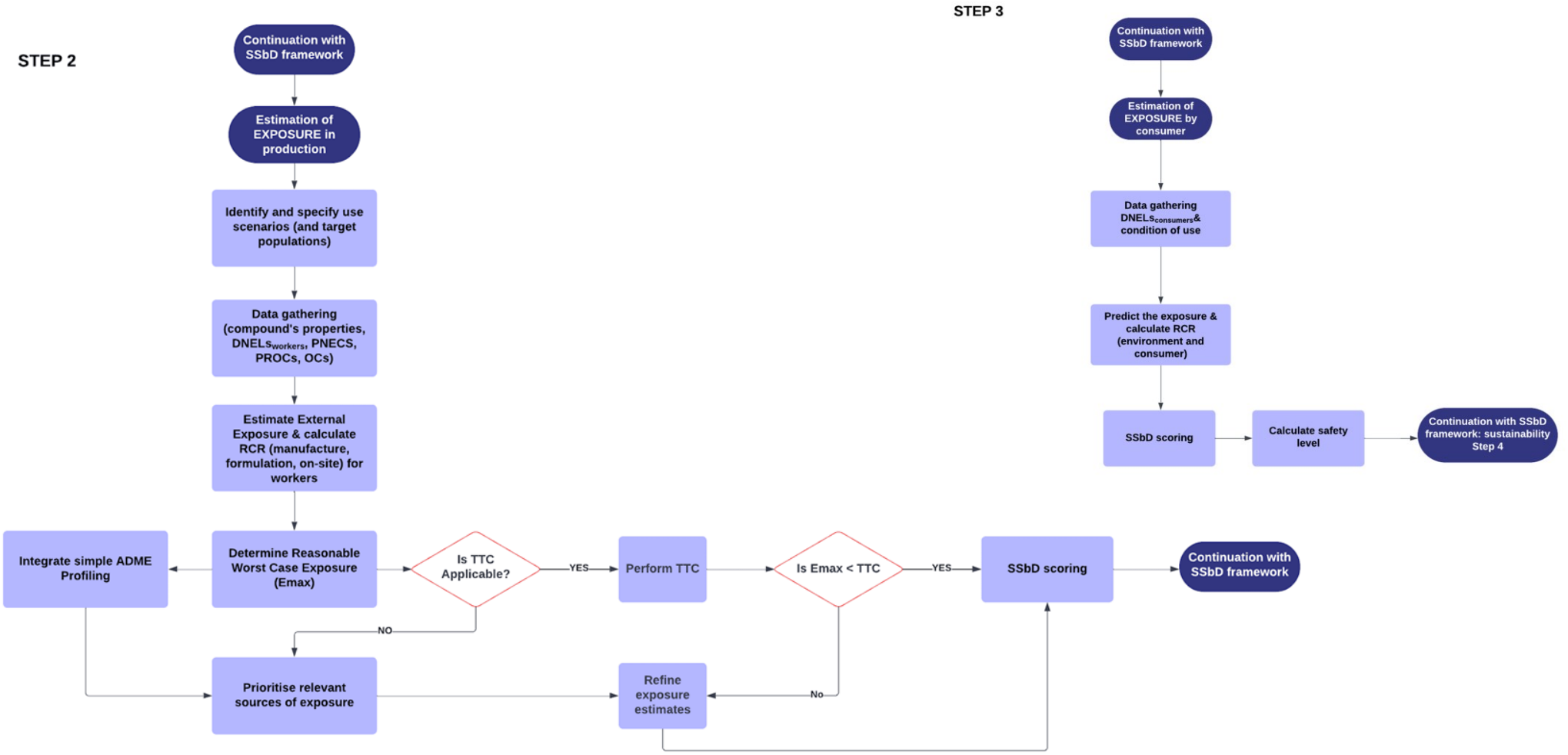
Tier 0/1 workflow



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Step 1 Hazard Characterisation

Group definition	Human health hazards	Environmental hazards	Physical hazards
Includes the most harmful substances (according to CSS (EC, 2020a)), including the substances of very high concern (SVHC) according to REACH Art. 57(a-f)[20,21] (EU, 2006). These hazard properties form Criterion H1.	• Carcinogenicity Cat. 1A and 1B • Germ cell mutagenicity Cat. 1A and 1B • Reproductive / developmental toxicity Cat. 1A and 1B • Endocrine disruption Cat. 1 (human health) • Respiratory sensitisation Cat 1 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 1, including immunotoxicity and neurotoxicity	• Persistent, bioaccumulative and toxic / very persistent and very bioaccumulative (PBT/vPvB) • Persistent, mobile and toxic / very persistent and mobile (PMT/vPvM) • Endocrine disruption Cat. 1 (environment)	
Includes substances of concern, as described in CSS (EC, 2020a), defined in the Article 2(28) of SPI proposal (EC, 2022b)[22] and that are not already included in Criterion H1. These hazard properties form Criterion H2.	• Skin sensitisation Cat 1 • Carcinogenicity Cat. 2 • Germ cell mutagenicity Cat. 2 • Reproductive / developmental toxicity Cat. 2 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 2 • Specific target organ toxicity - single exposure (STOT-SE) Cat. 1 and 2 • Endocrine disruption Cat. 2 (human health)	• Hazardous for the ozone layer • Chronic environmental toxicity (chronic aquatic toxicity) • Endocrine disruption Cat. 2 (environment)	
Includes the other hazard classes not part already in Criteria H1 and H2. These hazard properties form Criterion H3.	• Acute toxicity • Skin corrosion • Skin irritation • Serious eye damage/eye irritation • Aspiration hazard (Cat. 1) • Specific target organ toxicity - single exposure (STOT-SE) Cat. 3	• Acute environmental toxicity (acute aquatic toxicity)	• Explosives • Flammable gases, liquids and solids • Aerosols • Oxidising gases, liquids, solids • Gases under pressure • Self-reactive • Pyrophoric liquids, solid • Self-heating • In contact with water emits flammable gas • Organic peroxides • Corrosivity • Desensitised explosives

Used databases :
PUBCHEM
ECHA
HAZ-MAP
COMPTOX
CAMEO CHEMICALS

Used tools :
JANUS
OECD QSAR TB
VEGA
STOPTOX
SAFERSKIN
ZZS SIMILARITY

EC, JRC; 2022. Available from: doi/10.2760/487955

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Step 1 Hazard Characterisation

Compounds Information		Human Hazards												Environmental Hazards		
Name	CAS	Mutagenicity	Carcinogenicity	Endocrine disruption	Skin sensitisation	Skin irrit/corrosion	Acute Tox (Oral)	Acute Tox (Dermal)	Acute Tox (Inhal)	Reproductive Toxicity	STOT RE	STOT SE	Eye irri/damage	Aquatic Chronic	PBT	SVHC
Phenol	108-95-2	2	N.A	N.A	N.A	1B	3	3	3	N.A	2	N.A	1	2	Neg	N.A
Eugenol	97-53-0	N.A	N.A	N.A	1B	2	4	N.A	N.A	N.A	N.A	N.A	2	N.A	Neg	N.A

From databases

Compounds Information		Human Hazards												Environmental Hazards		
Name	CAS	Mutagenicity	Carcinogenicity	Endocrine disruption	Skin sensitisation	Skin irrit/corrosion	Acute Tox (Oral)	Acute Tox (Dermal)	Acute Tox (Inhal)	Reproductive Toxicity	STOT RE	STOT SE	Eye irri/damage	Aquatic Chronic	PBT	SVHC
Phenol	108-95-2	Neg	Pos	Neg	Pos	Pos	Pos	Pos	Neg	Pos	N.A	N.A	Pos	Pos	Neg	Pos
Eugenol	97-53-0	Neg	Neg	Neg	Pos	Neg	Pos	Pos	Pos	Pos	N.A	N.A	Pos	Pos	Neg	Pos

From in silico tools

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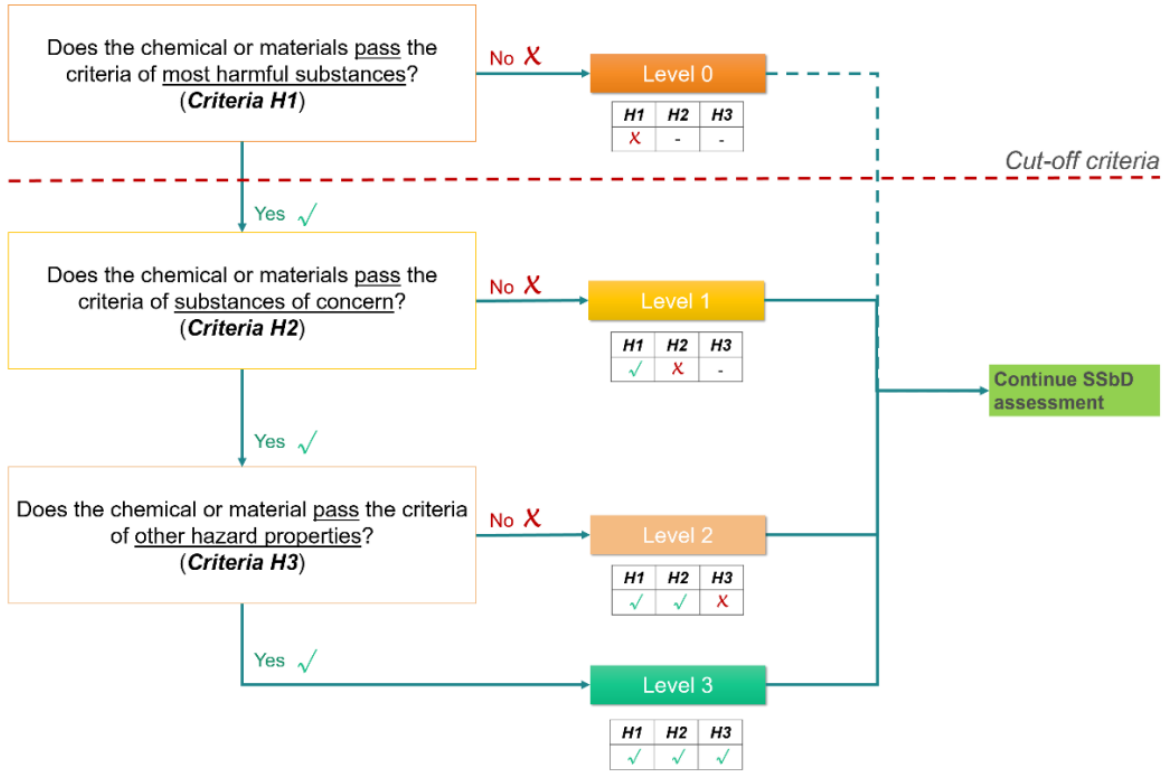
Step 1 Hazard Characterisation

Compound	SSbD level step 1	Reason
Phenol	1	Mutagenicity Cat 2 (Criteria H2)
Eugenol	1	Skin sensitisation Cat 1B (Criteria H2)

Continue SSbD Assessment



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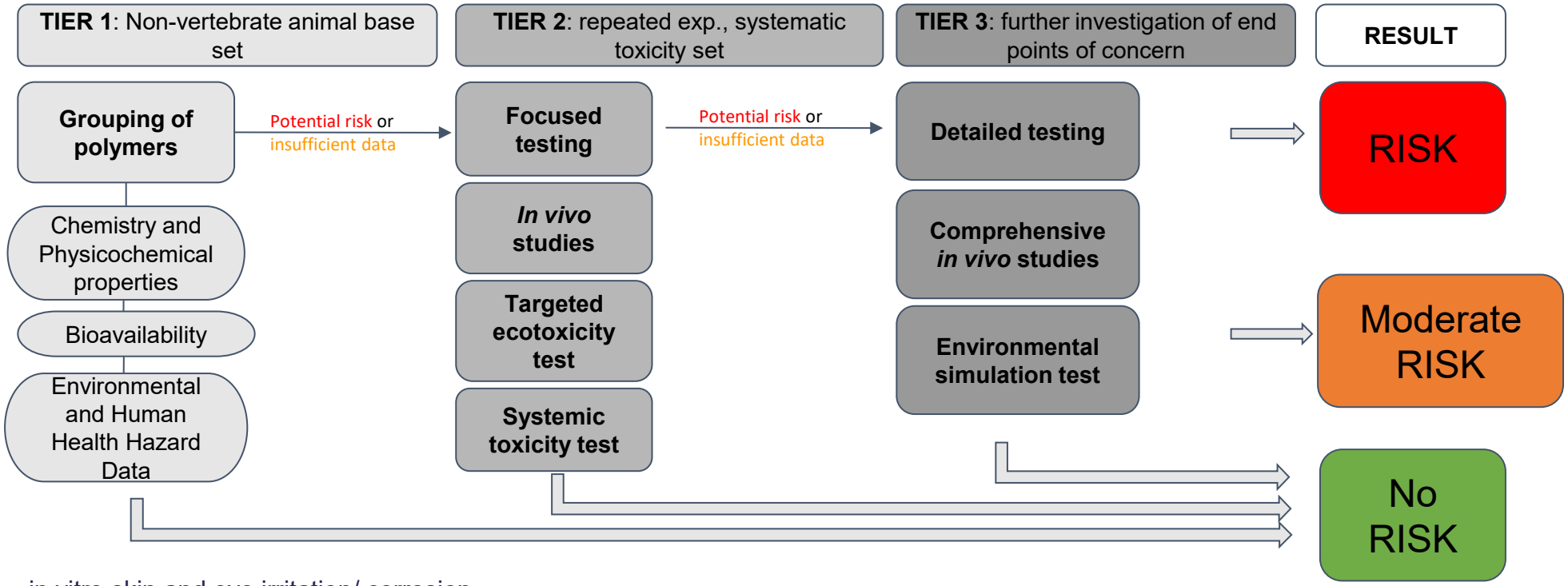
Current Workflow for Polymers suggested by REACH



- in vitro skin and eye irritation/ corrosion
- in chemico/in vitro skin sensitization and in vitro genotoxicity
- in vitro local effects on respiratory epithelia, gastrointestinal epithelia
- systemic bioavailability assessment
- environmental fate and distribution
- aquatic environment, acute
- terrestrial environment, acute
- bioavailability

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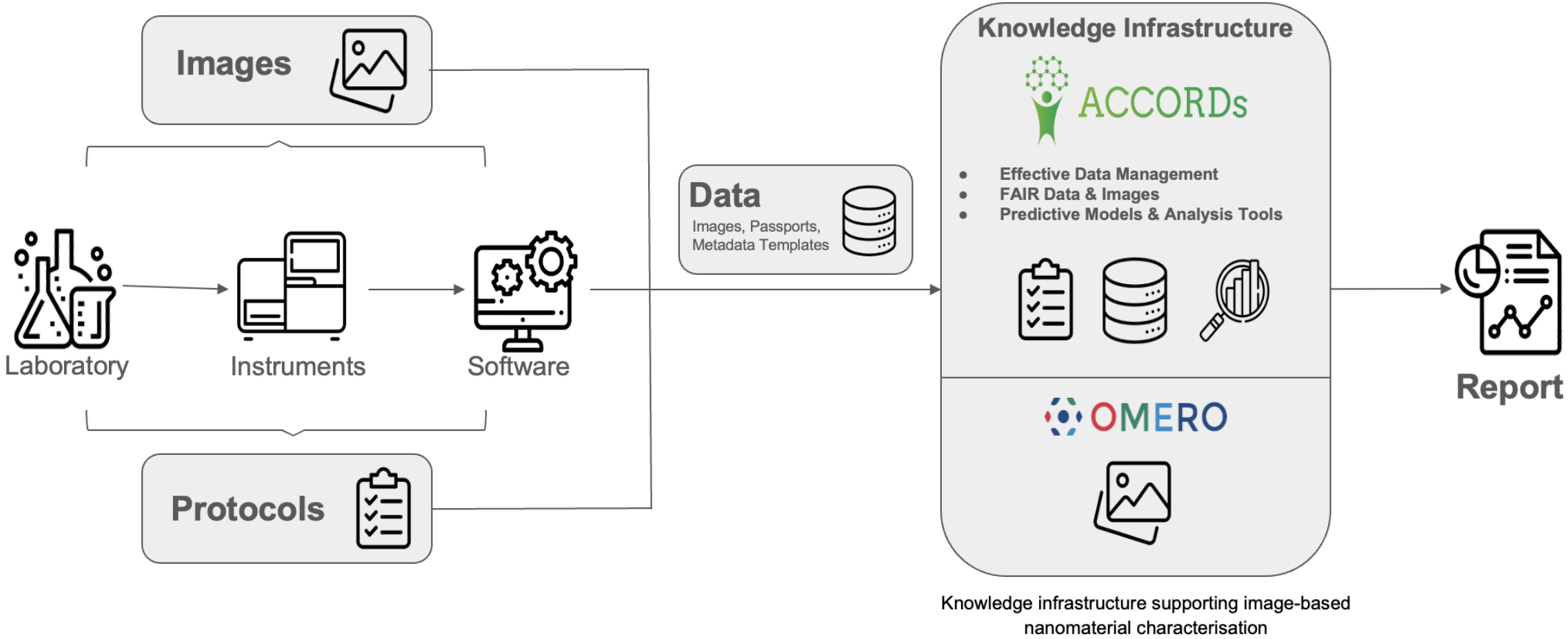
Characterisation Workflow (based on ACCORDs)



Knowledge infrastructure supporting image-based nanomaterial characterisation

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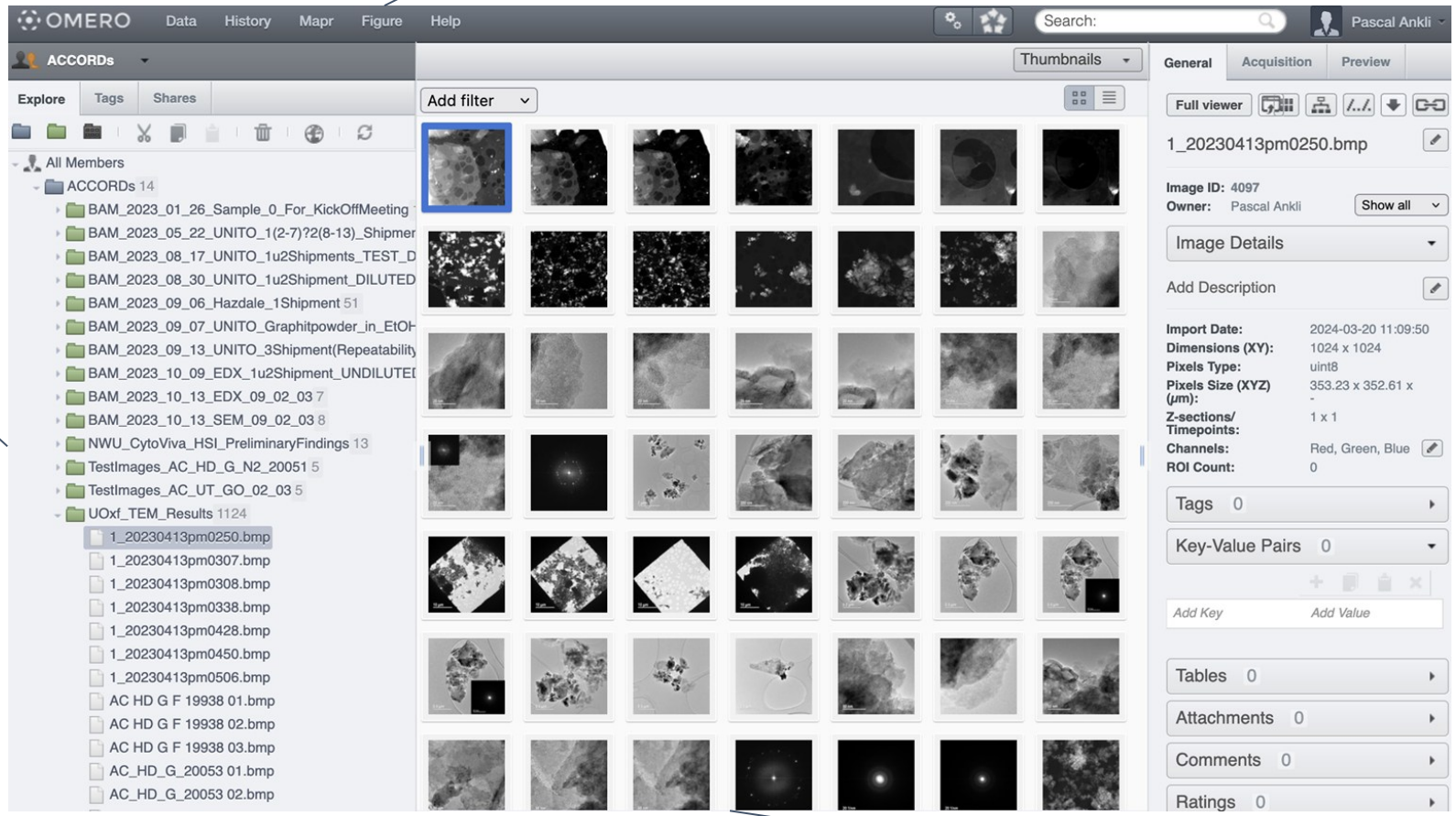
SSbD4CheM

Easy figure creation for publication



Organised folder structure

Data and metadata overview

Analysis, Editing etc.

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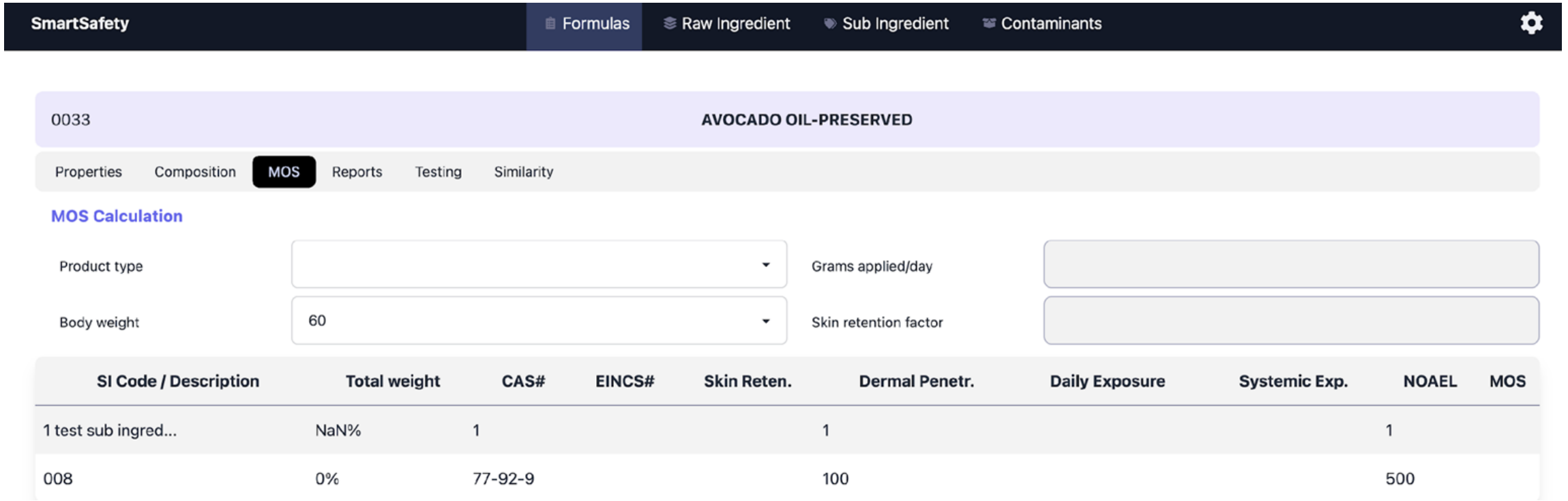
SmartSafety: Formulation and Ingredient Risk Assessment and SSbD modules



- Application Software and Database Modules for Sub-Ingredients, Raw Ingredients, Contaminants and Formulas
- Extraction of INCI profile documents for Cosmetic Ingredients to create a reference Sub-Ingredient Database for SmartSafety
- Formula Compare (identification of most similar formulas) and Margin of Safety calculations
- Generate CPSR, CSAR and other reports (with variations)
- Deployment onto cloud infrastructure

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SaferSkin Integration with SmartSafety supporting NAMs-based Skin Safety Assessment of Ingredients in Formulation

Edelweiss Connect

ENTER EXPERIMENTAL VALUES AND MOLECULAR DESCRIPTORS Enter available data for approaches of interest.

OECD 2o3 | OECD ITS | Multiple regression | Random forest | Neural network | Bayesian network | BDF | RIFM

Model description: A majority voting model that uses three different types of in vitro and in chemico tests to predict whether a chemical is a skin sensitiser or not in the LLNA assay. This is one of the defined approaches proposed by the OECD TG 497 guideline. [1]

ENTER IN VITRO VALUES

Input data for assays associated with three key events in the AOP for Skin sensitisation.
Recommended to improve prediction estimate.

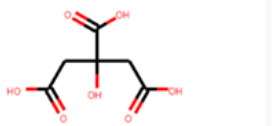
Note: Provide parameters of at least 2 of the 3 assays: DPRA, KeratinoSens, or h-CLAT

* - Required for correct model calculation

Covalent binding to skin proteins	Keratinocyte activation	Dendritic cell activation
DPRA	KeratinoSens™	h-CLAT
DPRACys (% depleted)* ?	EC1.5 (µM)* ?	CD54* ?
		-

PREDICTION

Make a prediction



OECD 203

Provide at least 2 of the 3 assays to evaluate the compound as sensitizer/non-sensitizer.

OECD ITS

Mandatory parameters missing

Multiple regression

Mandatory parameters missing

Random forest (GHS)

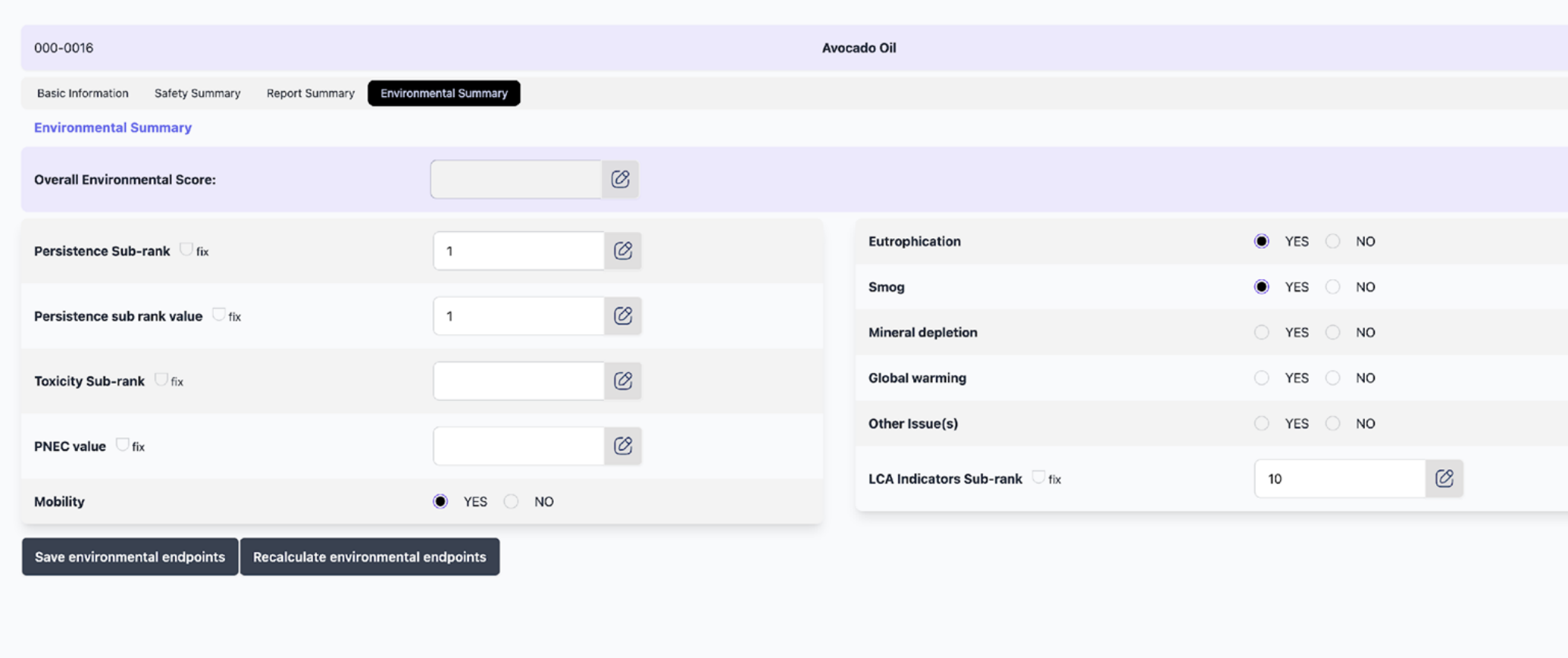
Moderate sensitiser

Random forest (ECETOC)

Weak sensitiser

Random forest (Binary)

SmartSafety – Environmental Scoring of Ingredients in Formulation



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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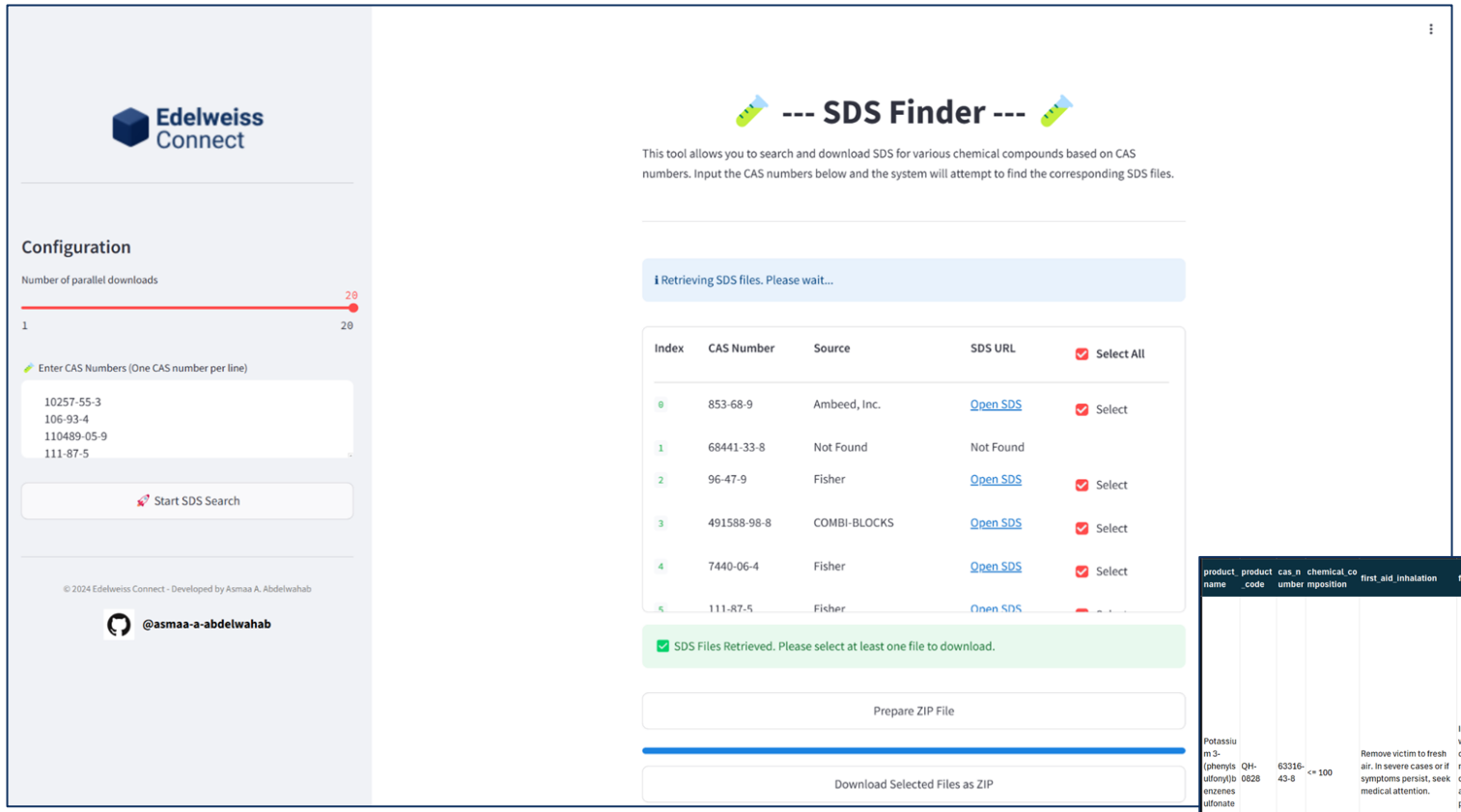
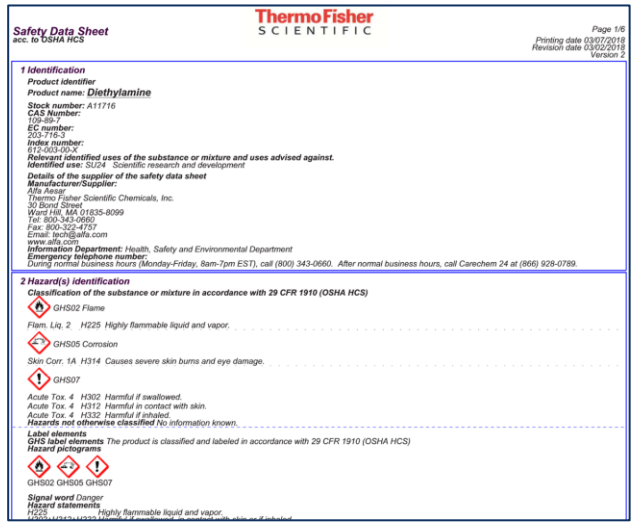
Automated AI-assisted Safety Data Sheet Retrieval





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/

Software for documenting workflows

Biological Data (Biostudies, EdelweissData, Notebooks)

Compound Database

Knowledge Graphs

Case Study Documentation

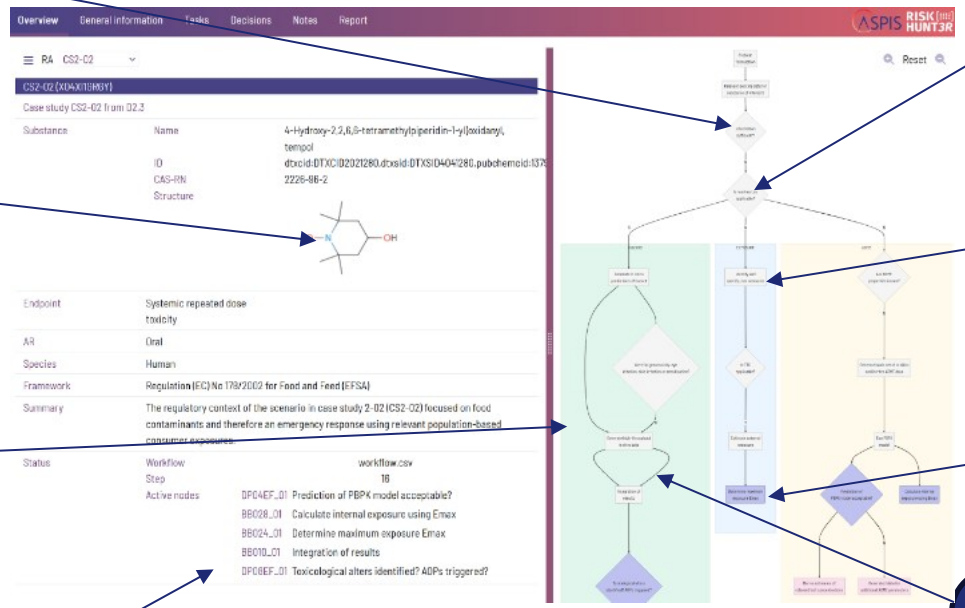
Life Cycle Assessment

AI assisted

AI assisted

AI assisted

AI assisted



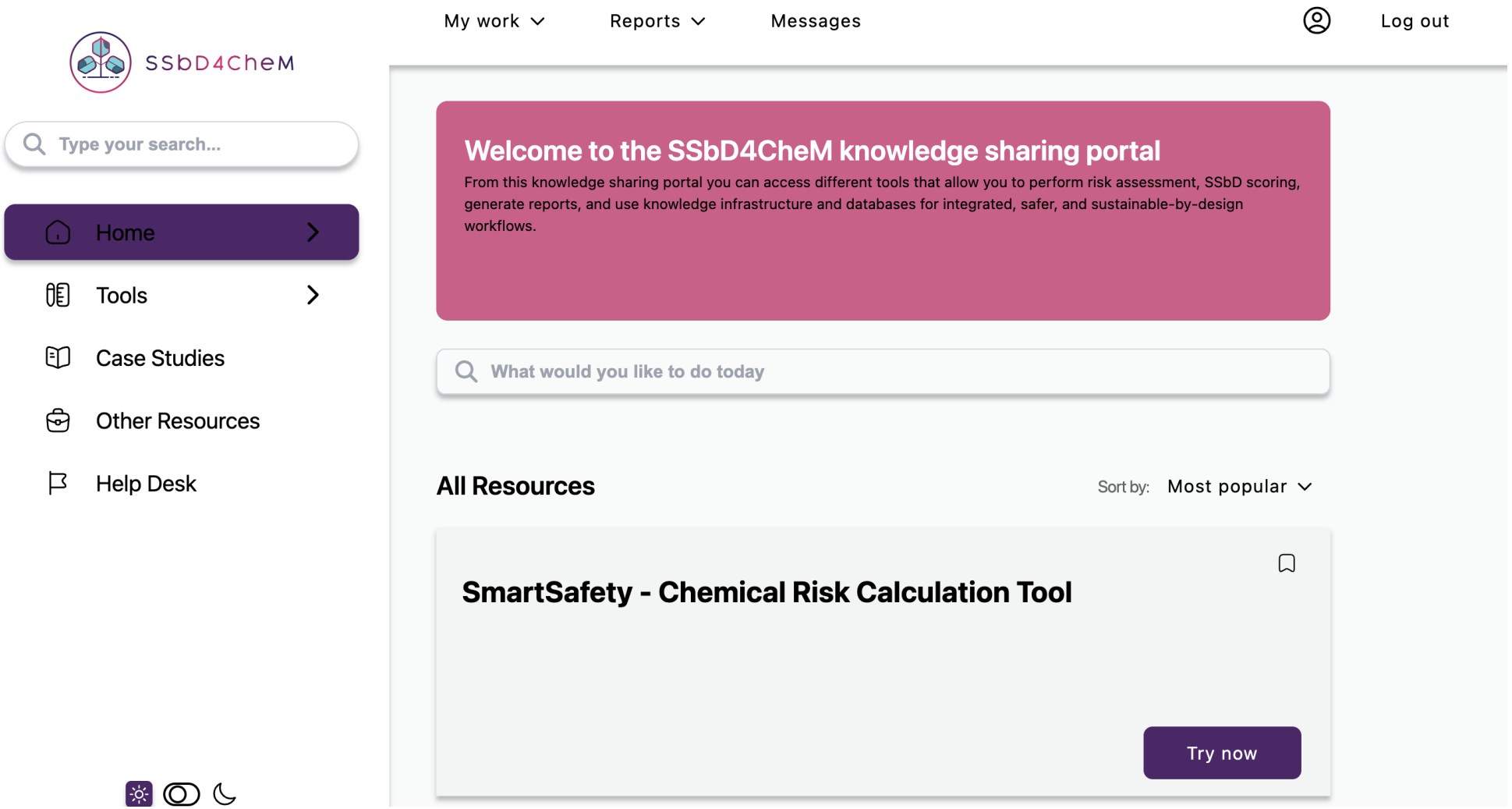
Methods Database (ToxTemp)

Toxicokinetics and Exposure protocols

OpenModel Repository

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

Demonstration



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Test Methods

Home › Test Methods

This material is to be used to document the status of test systems and test methods; moreover, it is intended to provide guidance for considerations around the use of test systems (or data therefrom) beyond the developer lab; the material will constitute a form of extended SOP, containing also elements important for test method transfer within the project, or within the commercialization taskforce. Information is structured to provide an overview to interested stakeholders or to prepare for test (pre-)validation.

EWC Test methods

Add a new test method

TEST METHOD	DESCRIPTION	PUBLIC	STATUS / COMPLETENESS LEVEL	ACTIONS	
EWC11_ADME_BPR_fs_1	sdf		Rejected / basic	Actions	
EWC1a_Liver_HepG2_Diff_6D_exp24h_1	Test ToxTemp Barry		In progress / None	Actions	
EWC1b_Liver_HepG2_Diff_6D_exp24h_1	Test ToxTemp Barry 1b		In progress / None	Actions	
EWC1b_Liver_HepG2_Diff_6D_exp24h_2	Test ToxTemp Barry 1b version 2		In progress / basic	Actions	barry@edelweissconnect.com
EWC22_Liver_HepG2_Diff_6D_1	Test Method BH Apr 2025		In progress / None	Actions	

Test Methods from Other Partners

Test system: Calu - airway epithelial cells; MucilAir - airway epithelium; BIP - BIP; BPR - blood plasma ratio; MCF7 - breast cancer cells

Intended uses: 4stressors; Absorbtion; ADME; Autophagy; control

Organisations: ARTTIC; BASF; Bayer; BDS; BioGlavia

Filter | Reset | Export to Excel

TEST METHOD	DESCRIPTION	ORGANISATION	PROJECT	INTENDED USE	TEST SYSTEM

Demonstration

SSbD4ChemM

Would you like to make Opera your everyday browser? How do I do that? Yes, set it as default browser

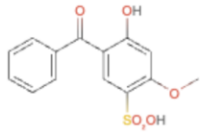
Overview | General information | Tasks | Decisions | Notes | Report

ASPIS RISK HUNT3R

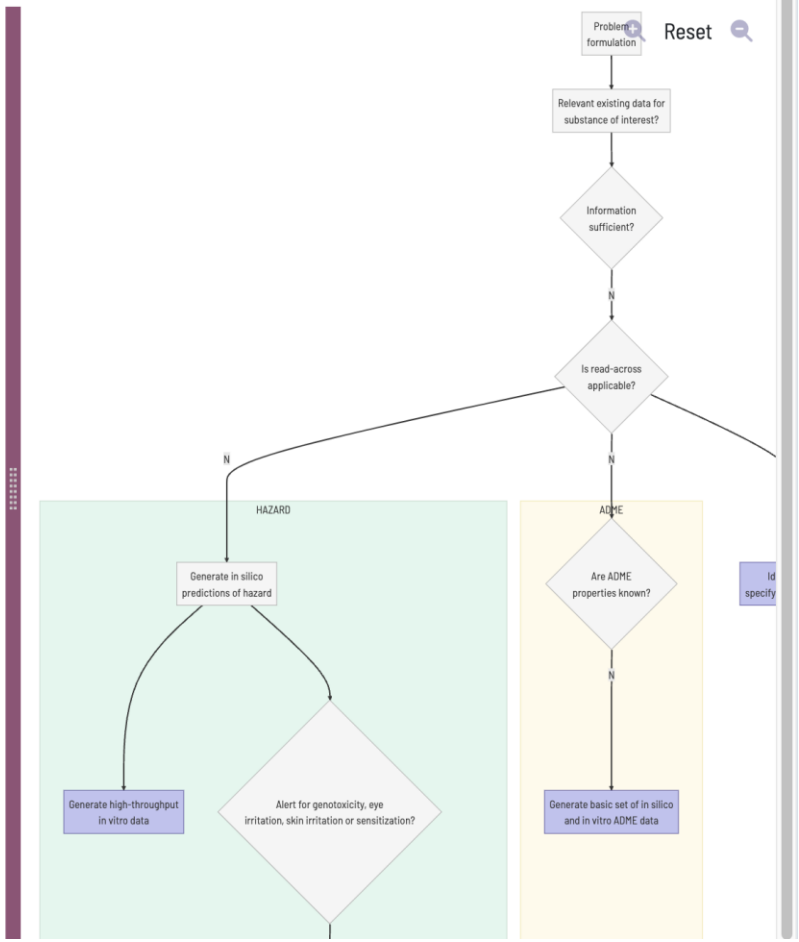
RA BP4 Case Study

BP4 Case Study (L11BOYQPGK)

Case Study for BP4

Substances	Name	CAS-RN	Structure
	Benzophenone-4	4065-45-6	

Endpoint	Systemic		
AR	Dermal		
Species	human		
Framework	?		
Summary	testing out workflow		
Status	Workflow		workflow.csv
	Step		10
	Active nodes	BB003_01	Generate basic set of in silico and in vitro ADME data
		BB022_01	Identify and specify user scenarios
		BB009_01	Generate high-throughput in vitro data
		DP07EF_01	Information sufficient?



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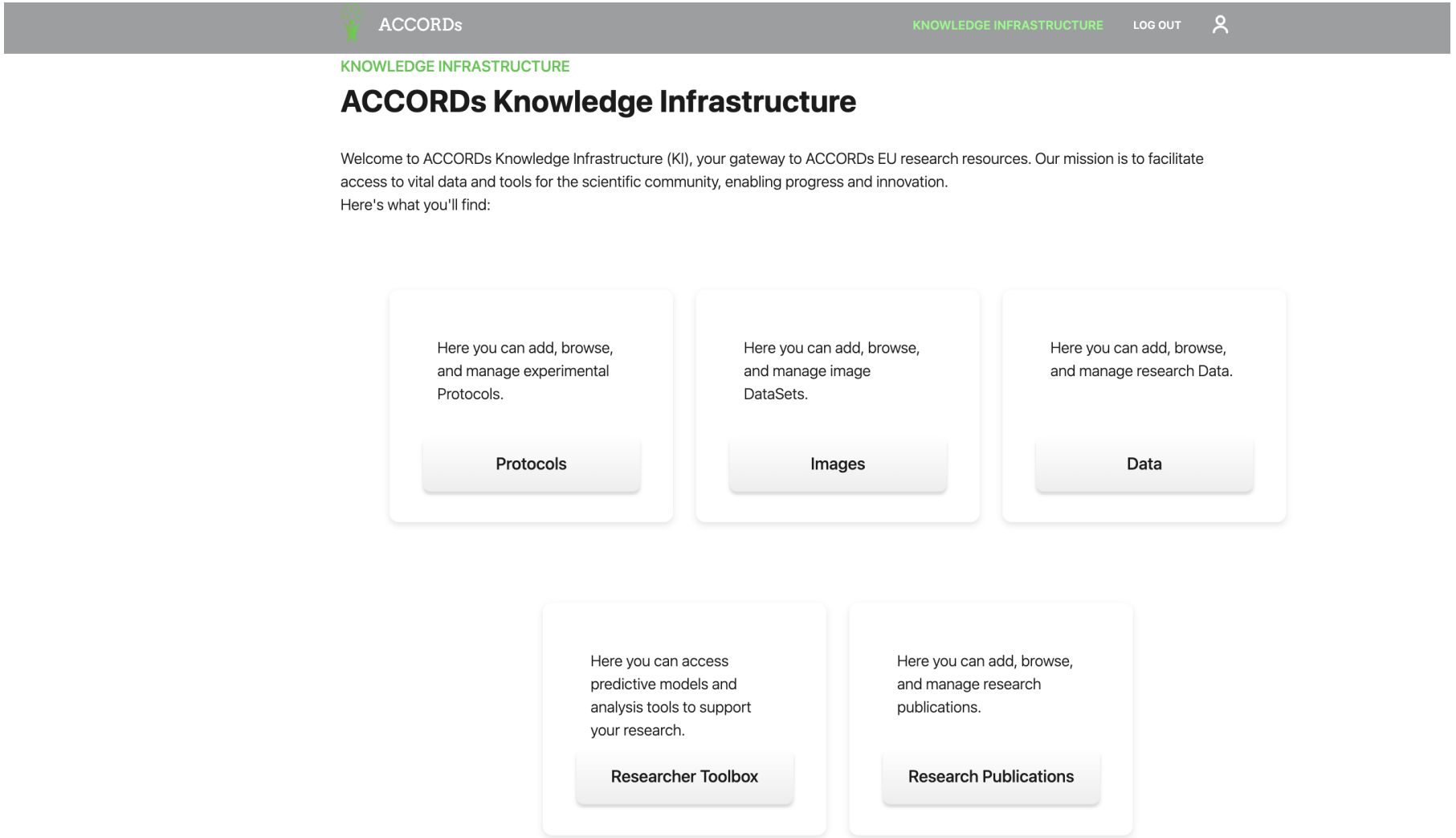

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Demonstration

SSbD4CheM

Edelweiss Connect | SDS-TOOLBOX

SDS-FIND

Enter your email to receive results

🧪 Enter CAS Number or IUPAC Name (One value per line)

77-92-9
Aspirin

🚀 Start SDS Search

🧪 --- SDS Find --- 🧪

This tool enables you to search for and download Safety Data Sheets (SDS) for chemical compounds using their CAS numbers or IUPAC Names.

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Demonstration

SSbD4CheM

Edelweiss Connect | DOI 10.5281/zenodo.14771565

📧 Enter your email address

🔑 Enter your NCBI API key (Preferred)

Create NCBI API key for a better performance

Number of Synonyms per Compound

5

Number of Synonyms per Target

5

Number of Articles per Compound-Target Pair

10

Start Year

2000

End Year

2025

PubMed ⚗️ ChemInsight

📄-Unlock Insights from PubMed-📄

This tool allows you to search PubMed for Scientific Articles Specific to your Compounds of Interest.

🧪 Enter Compounds (One Chemical Name or CAS Number per Line)

Ibuprofen
Metformin
Atorvastatin
Omeprazole

🔍 Retrieve Synonyms for Compounds

📌 Enter Interaction Targets (One Target per Line in the format of 'target, type')

BRAF, protein
TP53, gene
aspirin, chemical
GABA receptor, receptor
Apoptosis, pathway

🔍 Retrieve Synonyms for Targets

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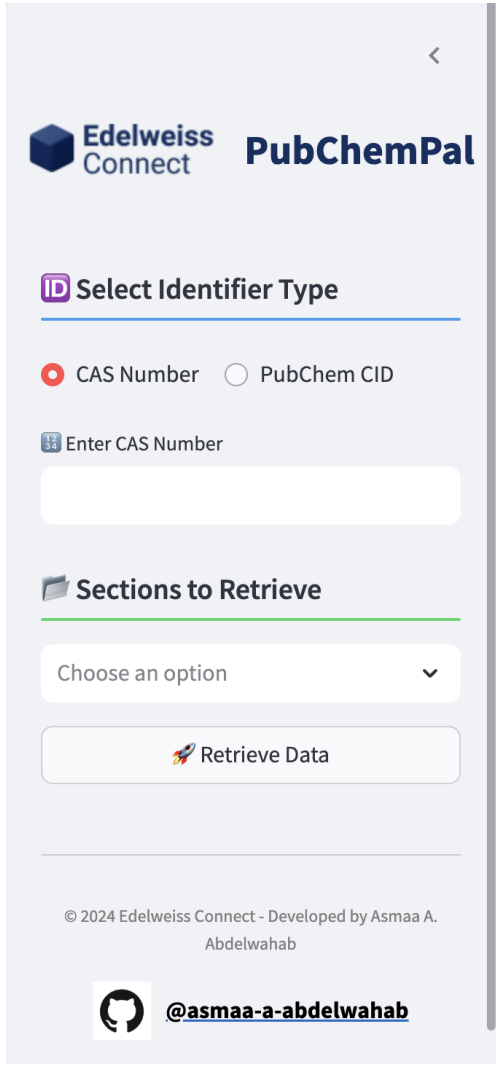

PubChemPal: Compounds

An interactive, user-friendly application that allows scientists, researchers, and regulatory professionals to retrieve, clean, and explore structured PubChem compound data using CAS numbers or PubChem CIDs.

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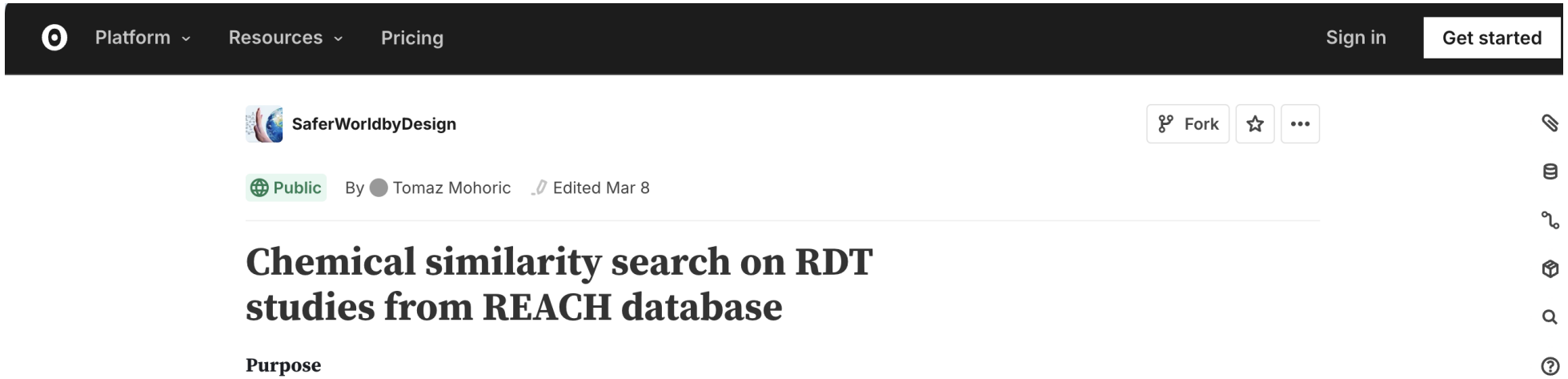

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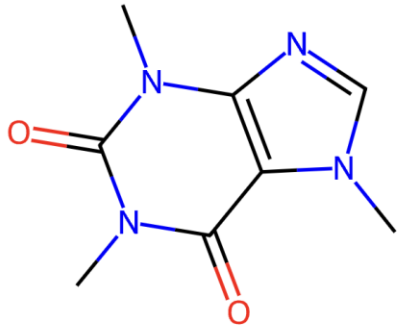
Demonstration

(1) Enter compound name. Chemical structure (SMILES) will be automatically inferred from PubChem.

Search by name: caffeine Submit

(2) Confirm/modify SMILES. You can modify the SMILES that was suggested based on the compound name or keep it unchanged. The final SMILES will be used.

SMILES string: CN1C=NC2=C1C(=O)N(C(=O)N2C)C



(3) Set the similarity threshold. By default value of 0.7 is used for threshold Tanimoto similarity.

0.7

(4) Results In total 14 RDT oral studies related to chemically similar compounds. The studies with their key properties and effect levels are displayed below.

CAS	SMILES	Similarity	Species	Reliability	GLP	Duration	Endpoint	Effect level from	Effect level to	Unit
58-08-2	Cn1c(=O)c2c(ncn2C)n(C)c1=O	1	rat	1 (reliable without restriction)	yes	90 days	NOAEL	1500		ppm
58-08-	Cn1c(=O)c2c(ncn2C)n(C)c1=O	1	mouse	1 (reliable without	not specified	90 days	NOAEL	167.4		mg/kg bw/day

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SSbD4CheM

Materials Characterisation

Ondrej Panak (National Institute of Chemistry, Slovenia)

11 June 2025, 15:00 – 16:30h CEST, online

Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101138475. UK participants in SSbD4CheM project are supported by UKRI. CH participants in SSbD4CheM project receive funding from the Swiss State Secretariat for Education, Research and Innovation (SERI). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

Ingredients and raw materials

Safety Data Sheet,
Product Data Sheet
Databases/literature

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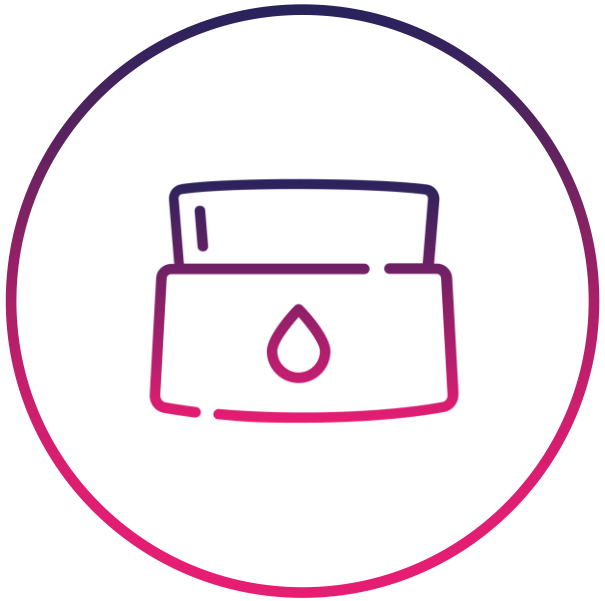
Products



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Properties

Chemical

- Molecular composition
- Functional groups
- Purity
- Reactivity

spectroscopy (IR, NMR, UV-Vis, XPS), chromatography, mass spectrometry, elemental analyses, ...

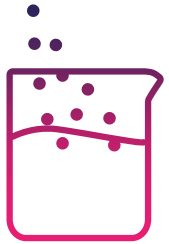
Physical and physico-chemical

- Size
- Morphology
- Porosity
- Crystalinity
- Thermal properties

SEM, TEM, AFM, DSC, TGA, XRD, DLS, ...

- Solubility
- pH and conductivity
- Surface tension / surface free energy
- Viscoelastic properties

...



Mechanical and Organoleptic

- Hardness
- Tensile strength
- Stability / Durability
- Color
- Smell

...

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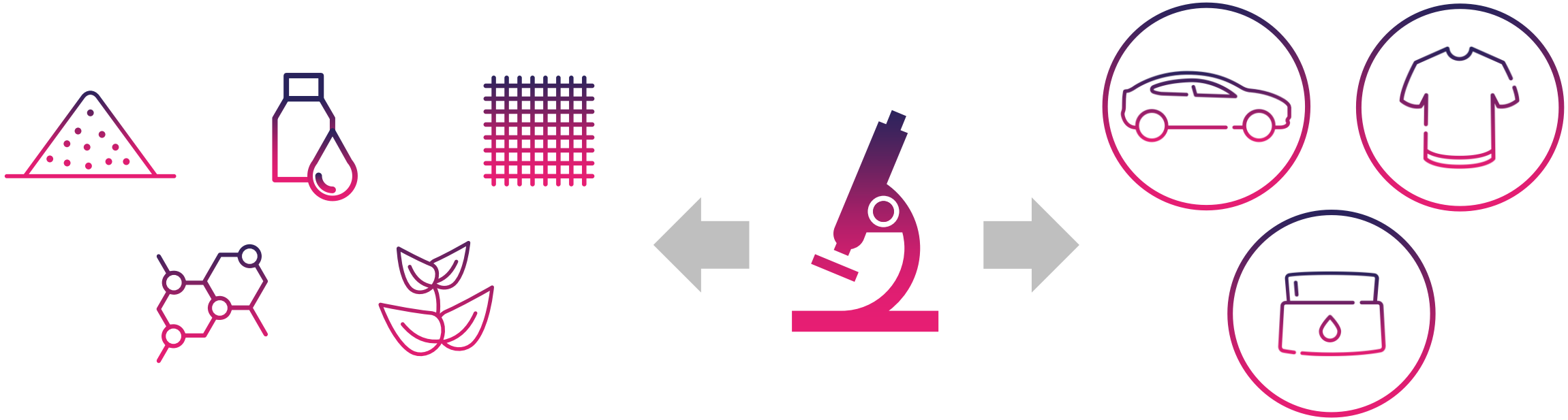
What methods to chose?

- What do I need and for what?
- What is missing?
- What is feasible?

- Who performs the measurement?
- What data form? (FAIR principles)

  Findable, Accessible, Interoperable and Reusable



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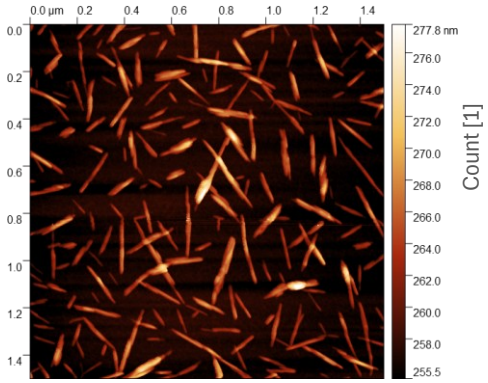
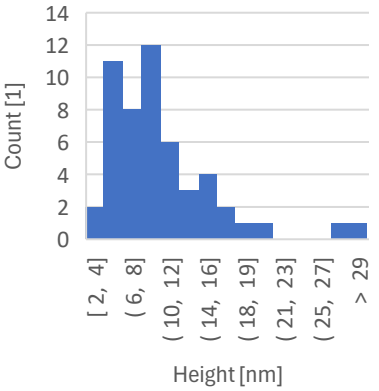
Nanocellulose in cosmetic products

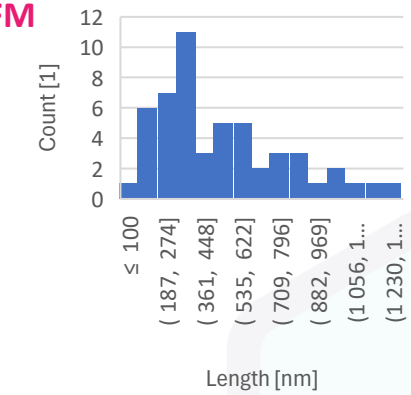
Source material

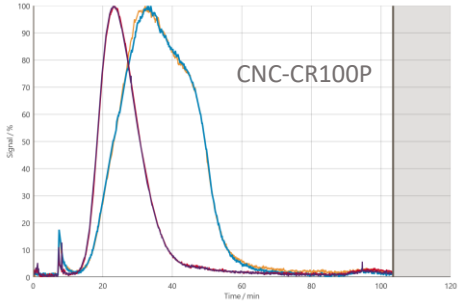
- Particle size
  - DLS – Dynamic Light Scattering
  - **AF4-MALS** (Asymmetric Flow Field-Flow Fractionation with Multi-Angle Light Scattering)
  - High resolution imaging
    - **SEM** – Scanning Electron Microscopy
    - TEM – Transmission Electron Microscopy
    - AFM – Atomic Force Microscopy
- Particle surface: BET
  - Brunauer-Emmett-Teller theory, gas adsorption
- Functional groups:
  - FTIR – Fourier Transformation Infrared Spectroscopy
- Dispersion stability:
  - Zeta potential
  - Attachment Efficiency (α)



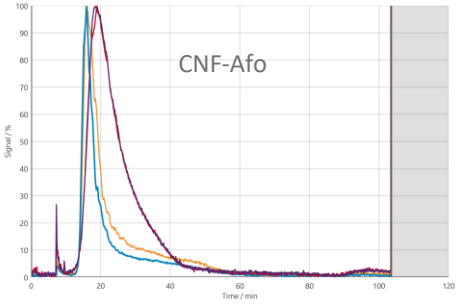


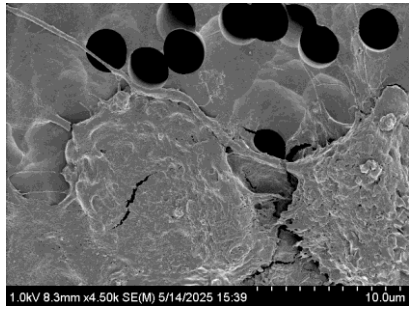
AFM

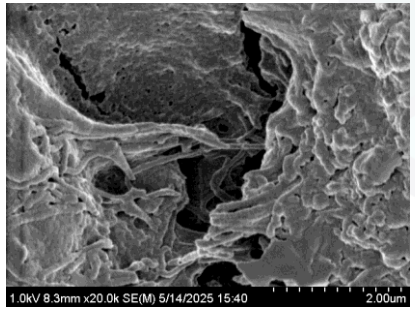




AF4-MALS







SEM

CNF and cell cultures

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Nanocellulose in cosmetic products

Products

- Viscosity
- pH
- Organoleptic properties
- Stability (3 temperatures)
- Texture

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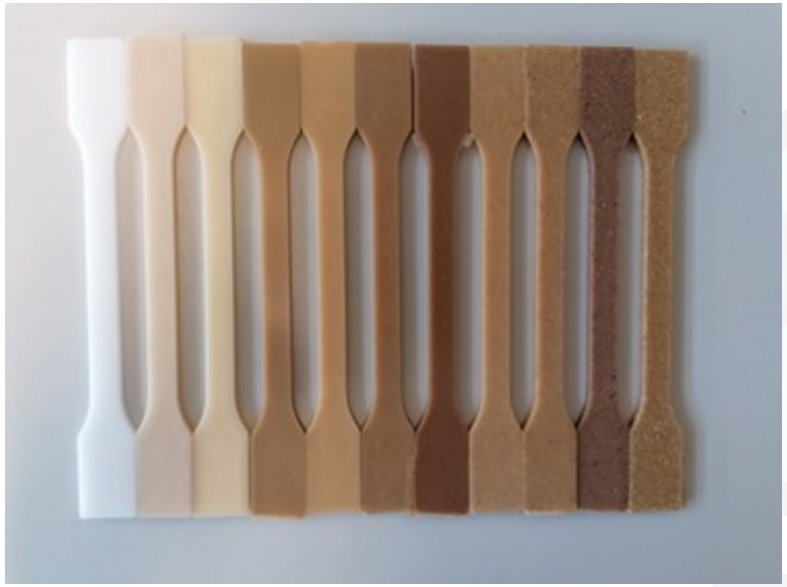
Wood Plastic Composites in automotive interior trims

Products testing (double bone specimens and prototypes)

- Tensile and Flexular properties according to ISO 178 standards
- Impact strength ISO 179-1 standard
- Density ISO 1183 standard
- Melt Flow Index (WPC compounds) ISO 1133 standard
- Weathering Testing according to SAE J2412 standard
- **TVOC emission** testing according to VDA 278
  - Total Volatile Organic Compound
  - Thermal Desorption
  - Gas Chromatography-Mass Spectrometry technique



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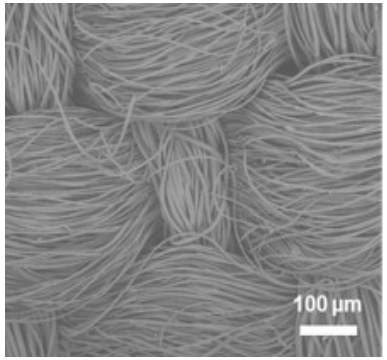
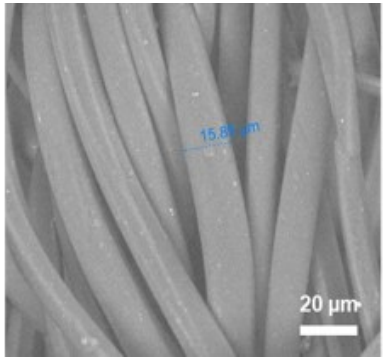
Functional coatings using plasma tehnology for textiles

Products

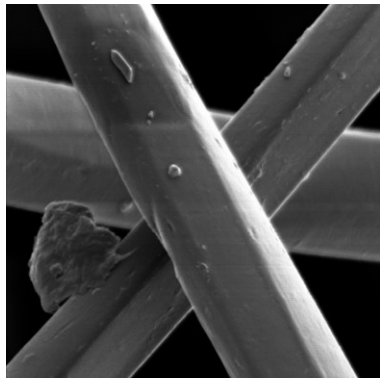
- Surface analysis
  - SEM – Scanning Electron Microscopy
- Elemental distributions
  - FIB-SIMS – Focused ion beam-Secondary Ion Mass Spectrometry
- Chemical composition
  - DART-MS – Direct Analysis in Real Time Mass Spectrometry
  - Py-GC-MS – Pyrolysis-Gas Chromatography-Mass Spectrometry

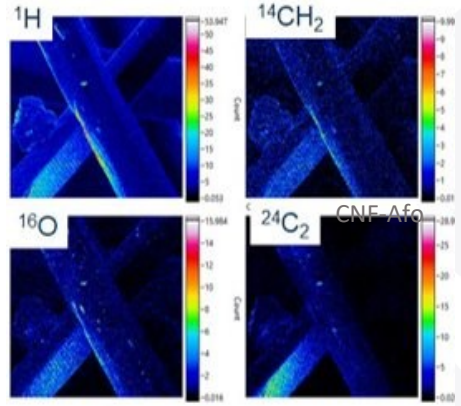
SEM



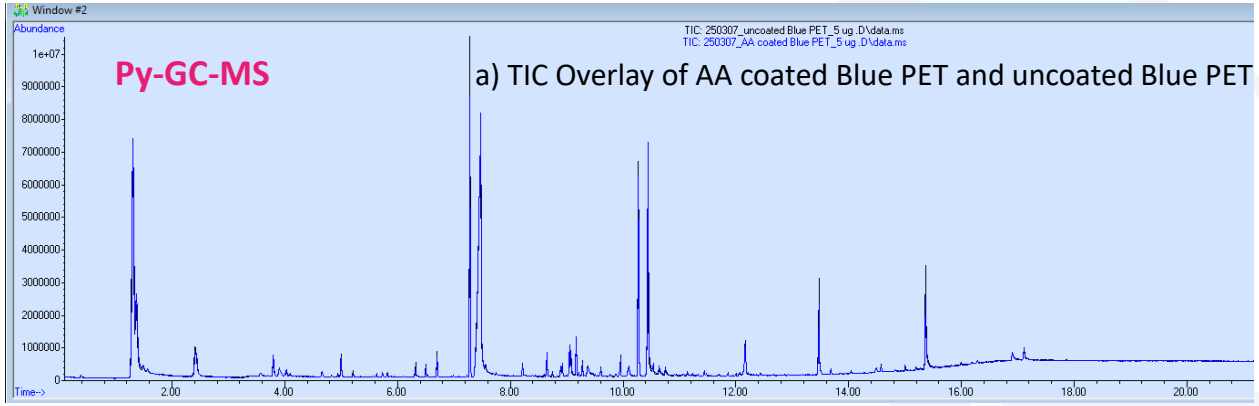


FIB-SIMS





Py-GC-MS



a) TIC Overlay of AA coated Blue PET and uncoated Blue PET

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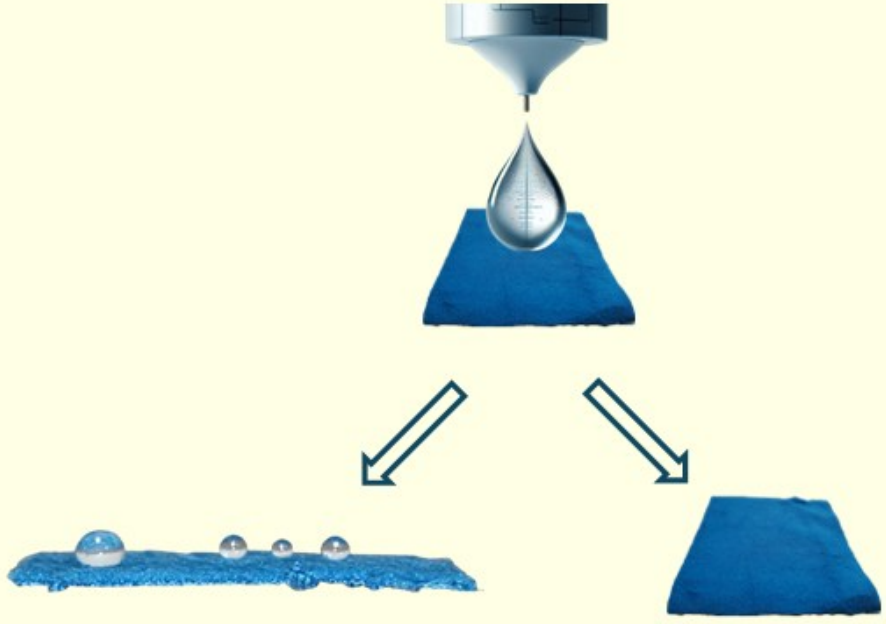
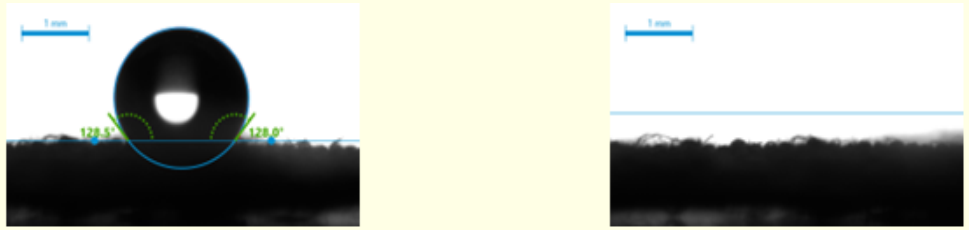
Functional coatings using plasma tehnology for textiles

Products

- Water repelency – contact angle
  - Sessile drop method
- Antimicrobial activity
  - based on the ISO 20743 transfer method





Coated fabric
(hydrophobic WCA>120°)

Control fabric
(hydrophilic)

Drop Shape Analysis

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SSbD4CheM

Materials Modelling supporting Hazard Profiling

Panagiotis Kolokathis (NovaMechanics)

11 June 2025, 15:00 – 16:30h CEST, online

Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101138475. UK participants in SSbD4CheM project are supported by UKRI. CH participants in SSbD4CheM project receive funding from the Swiss State Secretariat for Education, Research and Innovation (SERI). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

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SSbD4ChemM

SSbD4ChemM SbD4Skin: Safe by Design for Skin
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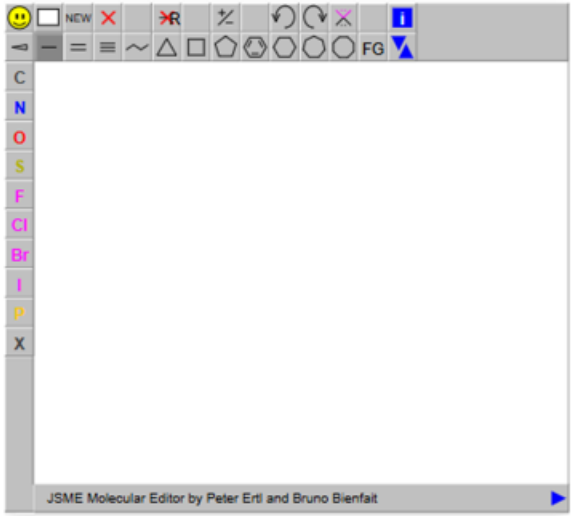
About | Sketcher Mode | Virtual Screening Mode

Chemical Sketcher



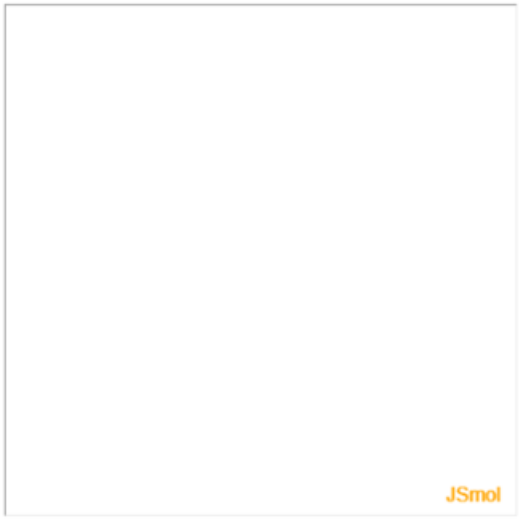
SMILES, Visualize in 3D

List of SMILES

SMILES

Import Smile | Delete Selected

3D Visualization



Open in NGL viewer

Execute

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ChemPharos Database

SSbD4CheM

chemPharos: Developed by Scientists, Curated for Excellence

Curated Datasets ready for Modelling

ID	Dataset
ds6	Blood-brain barrier (BBB) permeability of small molecules
ds7	Free energy of small molecules in water
ds8	Enriched dataset for agonist activity of small molecules against PPARδ
ds9	Enriched dataset for antagonist activity of small molecules against PPARγ
ds10	Boiling point of small molecules
ds11	Ames mutagenicity of small molecules
ds12	Computationally derived descriptors and binding activity of 1442 small, natural compounds as inhibitors of CYP2A6
ds13	Acute dermal toxicity of small molecules
ds14	Skin irritation potential of small molecules
ds15	Skin sensitization potential of small molecules

Description

SSbD4CheM

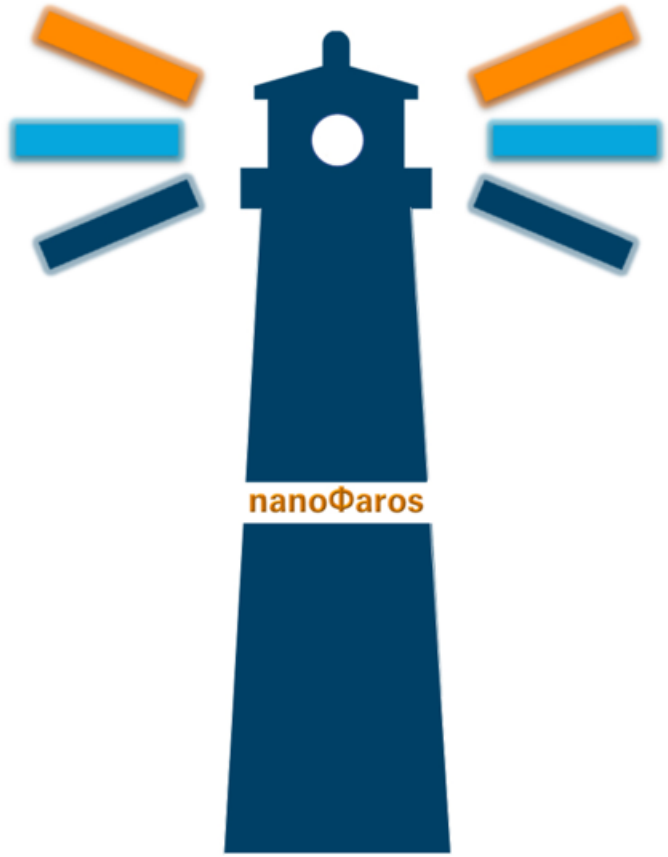
A curated and enriched dataset focused on the acute dermal toxicity of small organic molecules. The data were sourced from the REACH Study Results Database, ToxValDB, and relevant scientific literature, and were curated as part of the study by Borba et al. (https://ehp.niehs.nih.gov/doi/10.1289/EHP9341). The final dataset includes 2,616 compounds, enriched with 1,003 Mordred descriptors, as well as MACCS and Morgan fingerprints derived from their 2D molecular structures. Each compound is labelled as either "1" (toxicant) or "0" (non-toxicant), indicating its classification based on acute dermal toxicity. Information on the compounds CAS, CID, InChIKey etc. are also included whenever possible, retrieved from the PubChem database.

Download dataset

Synthesizing Knowledge, Curating Insights:

NovaMechanics Cheminformatics & Nanoinformatics Excellence

ENTELOS INSTITUTE



https://pharos.novamechanics.com/index.html

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SSbD4ChemM

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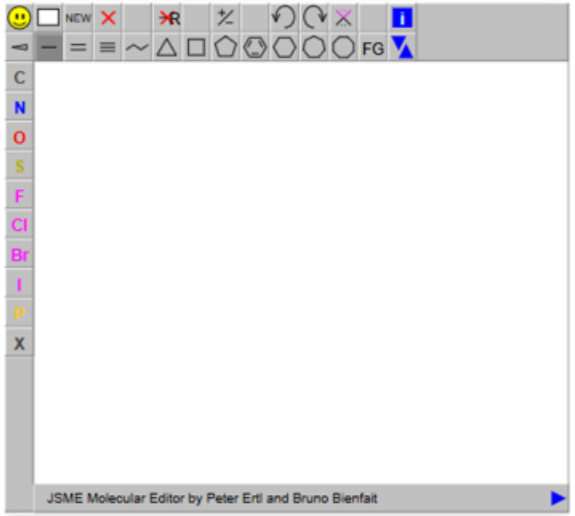
Chemical Sketcher



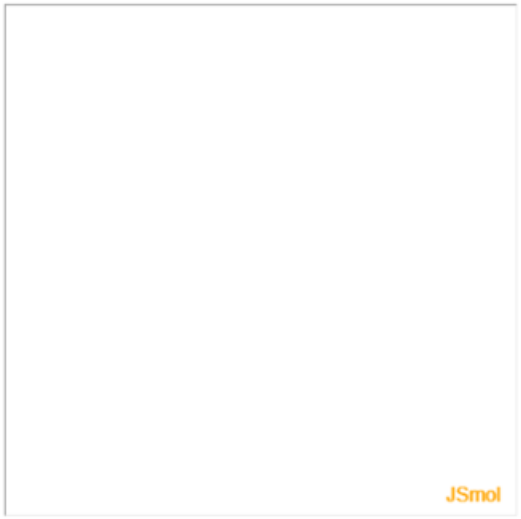
SMILES, Visualize in 3D

List of SMILES

SMILES

Import Smile | Delete Selected

3D Visualization



Open in NGL viewer

Execute

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SSbD4CheM SbD4Skin: Safe by Design for Skin
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Upload and Convert

Valid file extension: .sdf

List of uploaded SMILES

Execute

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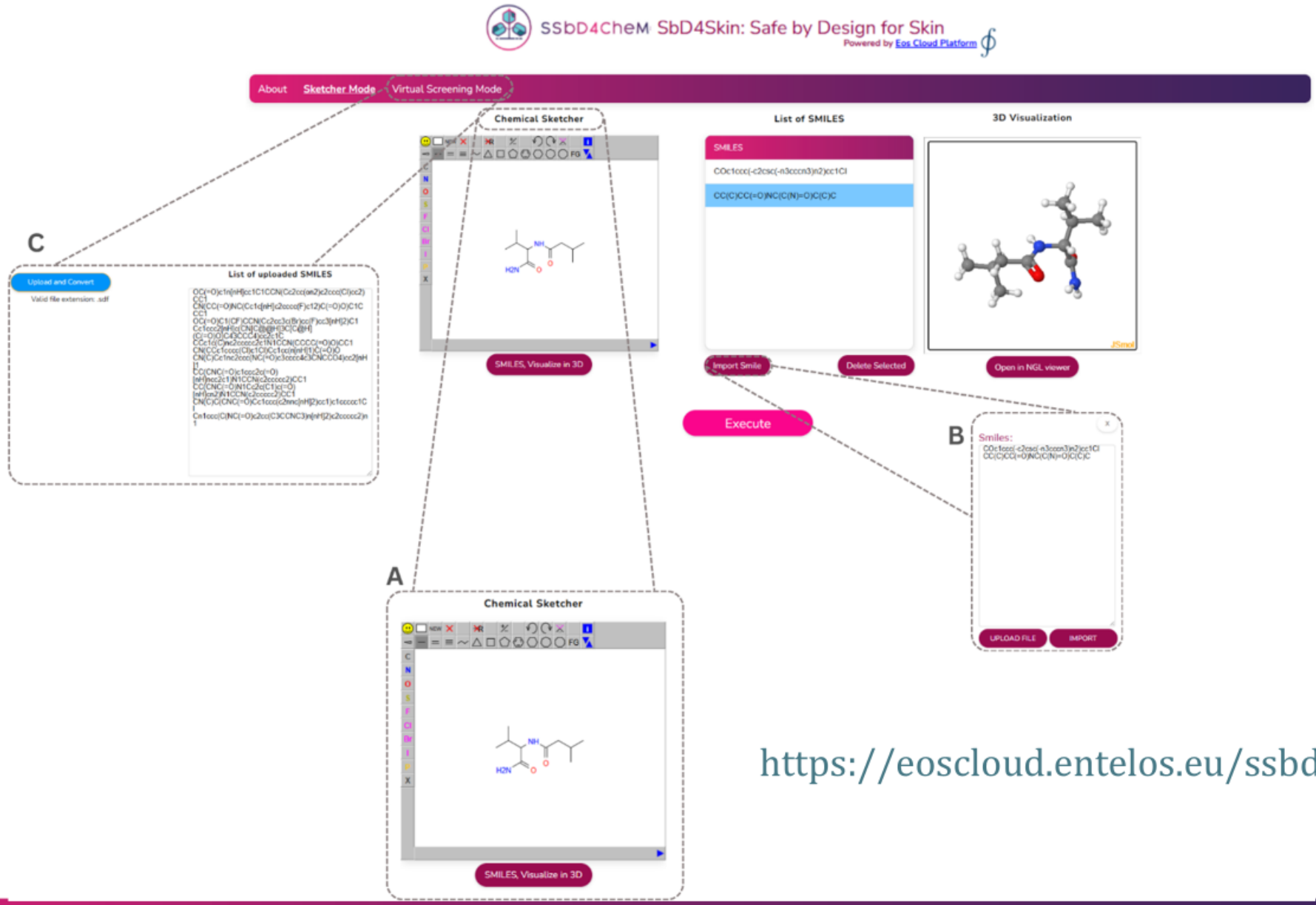

https://eoscloud.entelos.eu/ssbd4chem/sbd4skin/

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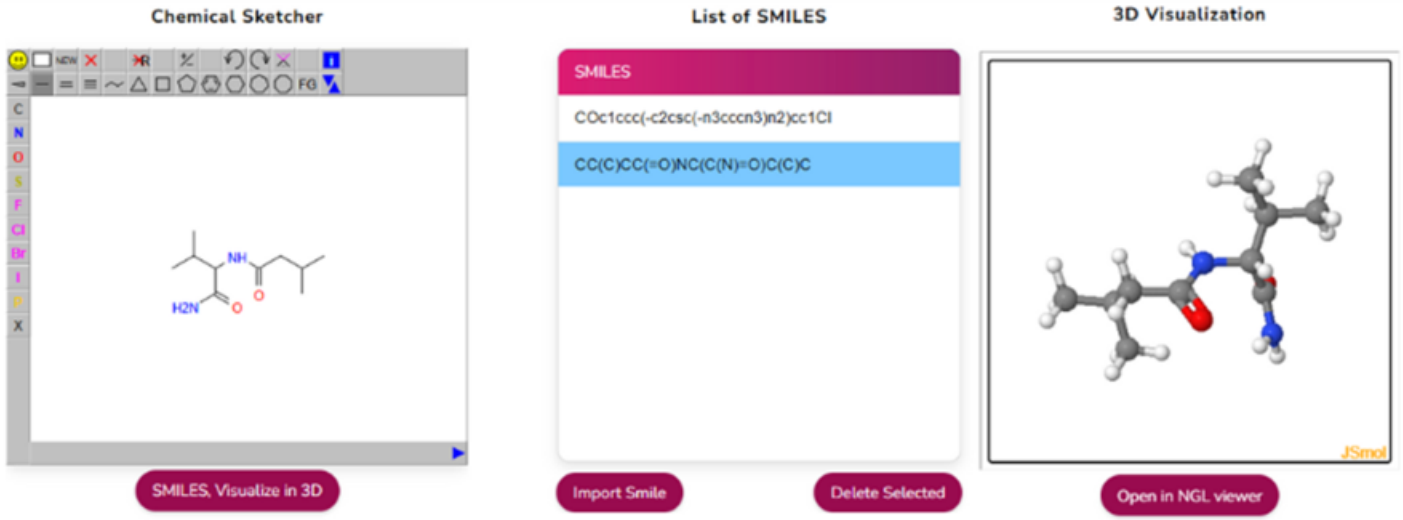

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SSbD4CheM SbD4Skin: Safe by Design for Skin
Powered by Eos Cloud Platform

Molecule	Acute Dermal Toxicity	Acute Dermal Toxicity Probabi	Acute Dermal Toxicity	Sensitization Class	Sensitization Probabi	Sensitization Reliabil	Irritation Class	Irritation Probi
COc1ccc(-c2csc(-n3cccn3)n2)cc1Cl	non-toxic	0	Reliable	non-sensitizer	0.202	Reliable	non-irritant	0.022
CC(C)CC(=O)NC(C(N)=O)C(C)C	non-toxic	0.016	Reliable	non-sensitizer	0.308	Reliable	non-irritant	0.211

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	A	B	C	D	E	F	G	H	I	J	K	L	M
1	SMILES	Predicted_	Predicted_	Avg_Tanin	Similarity_	Inside_AD	Avg_Tanin	Similarity_	Inside_AD	Euclidean	Distance_	Inside_AD	Mordred
2	COc1ccc(-c2csc(-n3cccn3)n2)cc1Cl	non-toxic	0.000205	0.63118	0.354032	TRUE	0.247131	0.136843	TRUE	9.379481	37.21939	TRUE	
3	CC(C)CC(=O)NC(C(N)=O)C(C)C	non-toxic	0.016235	0.503695	0.354032	TRUE	0.249413	0.136843	TRUE	4.332148	37.21939	TRUE	
4													

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Molecule	Acute Dermal Toxicity C	Acute Dermal Toxicity P	Acute Dermal Toxicity R	Sensitization Class	Sensitization Probability	Sensitization Reliability	Irritation Class	Irritation Probability	Irritation Reliability
C=O	toxic	1	Unreliable	sensitizer	0.745	Reliable	irritant	0.939	Reliable
Oc1ccc(cc1)O	toxic	0.981	Reliable	sensitizer	0.975	Reliable	irritant	0.727	Reliable
c1ccccc1	toxic	1	Reliable	sensitizer	0.658	Reliable	irritant	0.981	Reliable
Cc1ccccc1	toxic	0.995	Reliable	sensitizer	0.955	Reliable	irritant	0.939	Reliable
c1ccc(cc1)O	toxic	0.998	Reliable	sensitizer	0.97	Reliable	irritant	0.863	Reliable
CCCCCCCCCOOS(=O)(=O)[O-]	non-toxic	0.001	Reliable	sensitizer	0.813	Reliable	irritant	0.595	Reliable
CO	toxic	0.999	Reliable	non-sensitizer	0.102	Reliable	irritant	0.928	Reliable
CC(=O)C	toxic	0.953	Reliable	non-sensitizer	0.037	Reliable	irritant	0.95	Reliable
ClC(Cl)Cl	toxic	1	Reliable	non-sensitizer	0.056	Reliable	irritant	0.993	Reliable
C1COCC1	toxic	0.991	Reliable	non-sensitizer	0.151	Reliable	irritant	0.981	Reliable

« ‹ 1 / 2 › » [1 - 10 / 13]

Molecule	Acute Dermal Toxicity C	Acute Dermal Toxicity P	Acute Dermal Toxicity R	Sensitization Class	Sensitization Probability	Sensitization Reliability	Irritation Class	Irritation Probability	Irritation Reliability
OC1OC(CO)C(OC2OC(C	non-toxic	0.002	Reliable	non-sensitizer	0.006	Reliable	non-irritant	0.009	Reliable
OC1OC(CO)C(OC2OC(C(=O)=O)C(O)C(O)C2O)C(	non-toxic	0	Reliable	non-sensitizer	0.008	Reliable	non-irritant	0.004	Reliable
OC1OC(CO)C(OC2OC(C	non-toxic	0.001	Reliable	non-sensitizer	0.012	Reliable	non-irritant	0.004	Reliable

« ‹ 2 / 2 › » [11 - 13 / 13]

Download files

Nicotine:

Highly toxic if absorbed through the skin, potentially causing respiratory failure or death.

Pure nicotine may not cause significant skin irritation itself, but systemic toxicity can be fatal

Molecule	Acute Dermal Toxicity C	Acute Dermal Toxicity P	Acute Dermal Toxicity R	Sensitization Class	Sensitization Probability	Sensitization Reliability	Irritation Class	Irritation Probability	Irritation Reliability
CN1CCCC1c1cccnc1	toxic	1	Reliable	sensitizer	0.928	Reliable	non-irritant	0.484	Reliable

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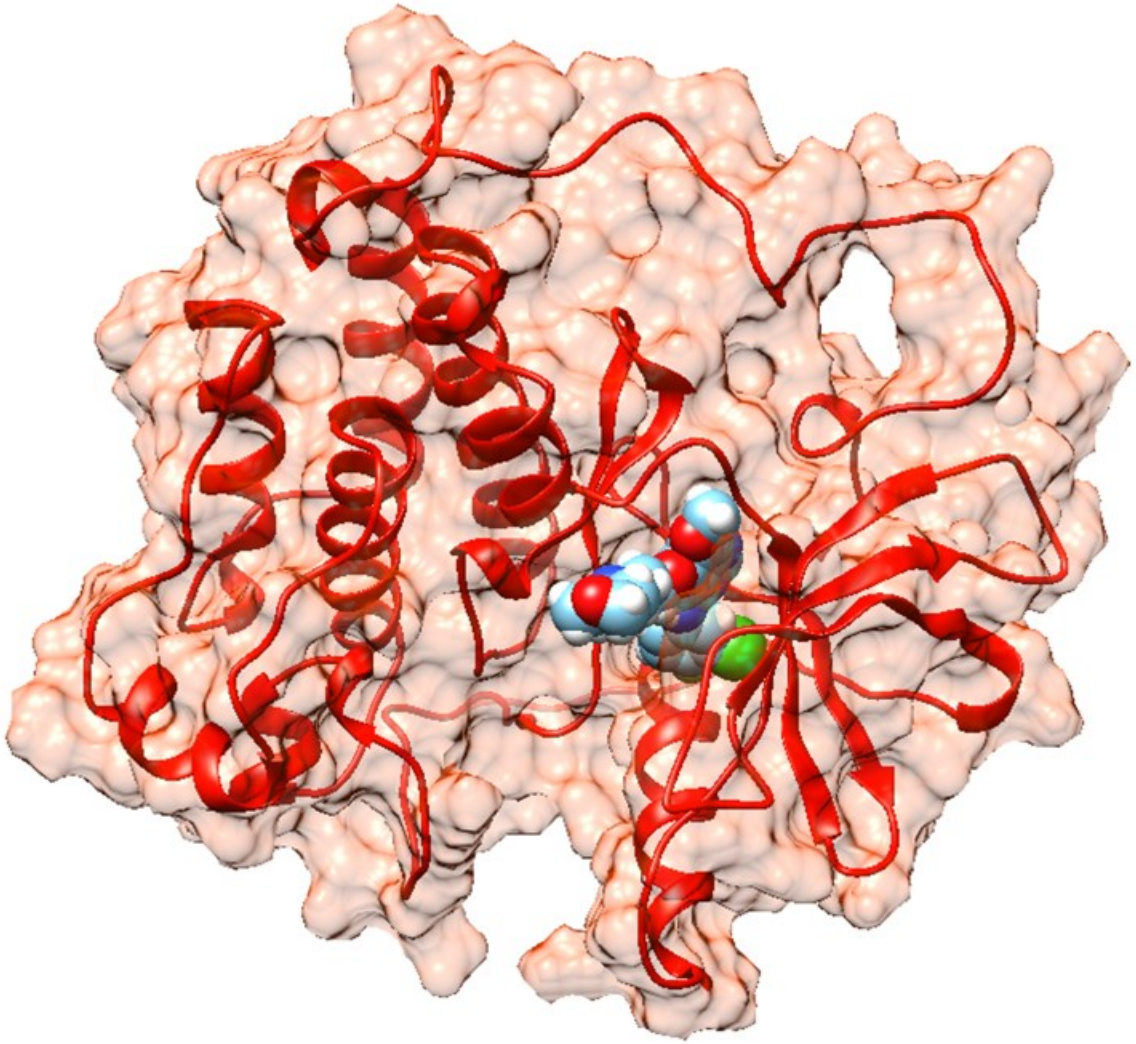
SSbD4CheM

- **Protein Target – EGFR (Epidermal Growth Factor Receptor):**
- EGFR is a transmembrane receptor that plays a crucial role in the regulation of cell proliferation, differentiation, and survival.
- Abnormal activation or inhibition of EGFR is associated with various skin disorders, and its perturbation may be indicative of toxic responses when exposed to certain compounds.
- Molecular docking is a computational method used to predict the binding affinity and orientation of compounds to target proteins.
- High binding affinity scores may point to a compound's capability to interfere with EGFR function, potentially leading to skin toxicity.
- It provides valuable insights into potential interactions that could lead to toxicological effects.

The **Enalos Asclepios KNIME pipeline** ensures streamlining accurate molecular docking.



EGFR kinase domain with gefitinib

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SSbD4CheM

- **Protein Target – EGFR (Epidermal Growth Factor Receptor):**
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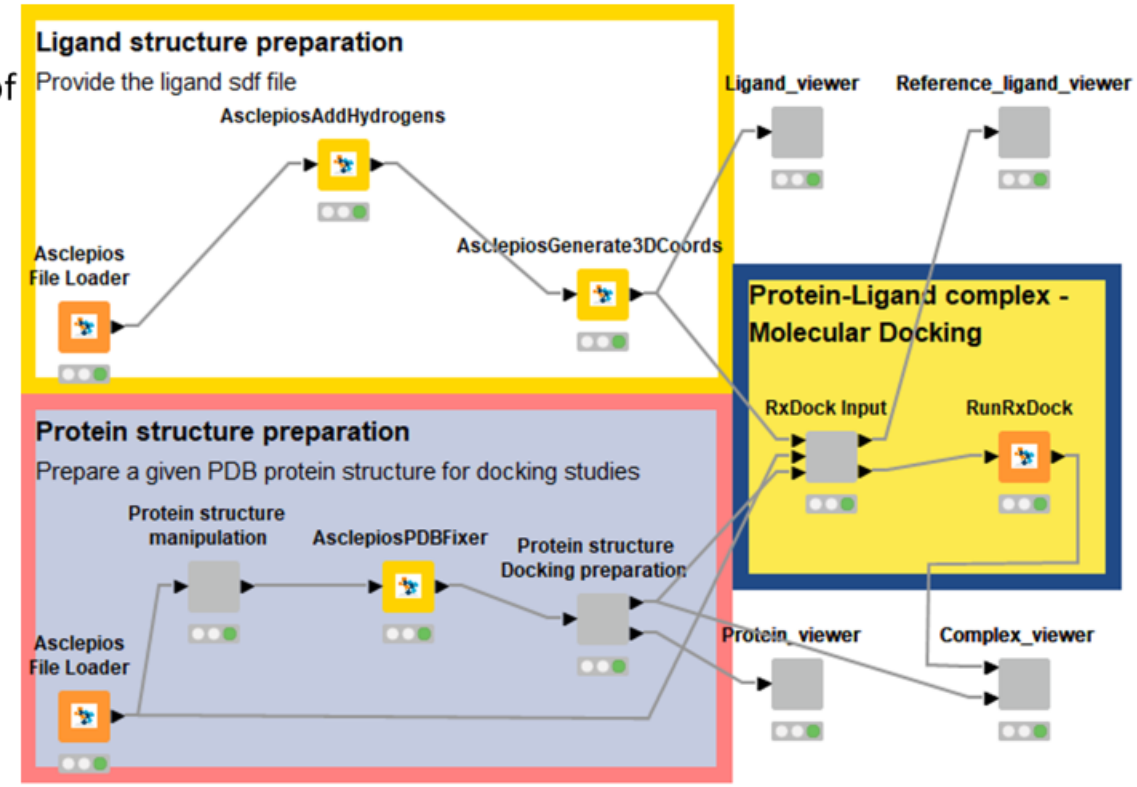

The Asclepios KNIME pipeline employed for the present work.

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Titania: Suite for In Silico Property Prediction and NAM-Based Modeling

Powered by Enalos Cloud Platform

About | Sketcher Mode | Virtual Screening Mode

Within this web-tool, users can import compounds of interest by either drawing molecules using an integrated sketcher or uploading a list of molecules in SMILES format. Users can also inspect a 3D visualization of their molecular structures post-drawing. The platform can be used for high-throughput virtual screening through batch processing: users can upload SDF files and process multiple compounds with one query. Then the users should select one or more endpoints from the available checkbox list. Upon submission, predictions are generated within seconds. The results include the predicted property value(s) and/or toxicity class. All results can be downloaded per model for further analysis, enhancing flexibility and usability for diverse research applications. Apart from the predictions for each model their reliability according to the corresponding applicability domain is presented. Especially for the developed kNN models, in the downloaded results the training neighbours and their distances from the input substances are presented, allowing the evaluation of structural similarity patterns.

Endpoint	Description
logS	A kNN/read-across model for the prediction of water solubility at 25°C (expressed as logS) of small molecules based on their 2D structural descriptors. The dataset used for model development can be found in the ChemPharos DB.
logP	A kNN/read-across model for the prediction of the octanol/water partition coefficient at 25°C (expressed as logP) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
logBCF	A kNN/read-across model for the prediction of the bioconcentration factor (expressed as logBCF) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
logVP	A kNN/read-across model for the prediction of the vapour pressure at 24°C (expressed as logVP, units: mm Hg) of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
BP	A kNN/read-across model for the prediction of the boiling point in °C of small molecules based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
BBB	A kNN/read-across model for the prediction of the blood-brain barrier permeability of small molecules based on their 2D structural characteristics. Compounds are classified as either "permeable (BBB+)" - Class 1 or "non-permeable (BBB-)" - Class 0. The dataset used for model development can be found in the ChemPharos DB.
FreeSolv	A kNN/read-across model for the prediction of the experimental hydration free energy of small molecules in water based on their 2D structural characteristics. The dataset used for model development can be found in the ChemPharos DB.
Cytotoxicity	A kNN/read-across model for the cytotoxicity to NIH/3T3 cells (mouse embryonic fibroblast cell line) prediction of small molecules, based on their 2D structural properties. Compounds are classified as either "Active"—indicating cytotoxicity to NIH/3T3 cells—or "Inactive", signifying non-cytotoxicity to these cells. The dataset used for model development can be found in the ChemPharos DB.
Mutagenicity	A QSAR random forest model for the prediction of small molecules mutagenicity to *Salmonella typhimurium* based on their 2D structural properties. Compounds are classified as either "positive" -indicating mutagenic compounds- or "negative" -indicating non-mutagenic substances. The dataset used for model development can be found in the ChemPharos DB.

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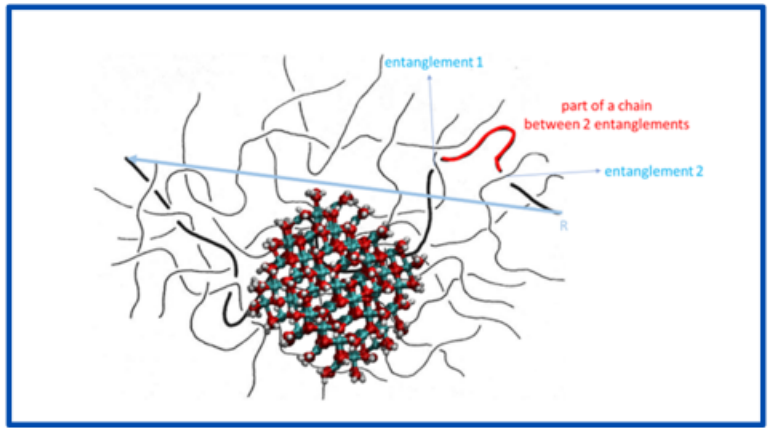
Nanocomposites Polymer Builder powered by EosCloud

SSbD4CheM

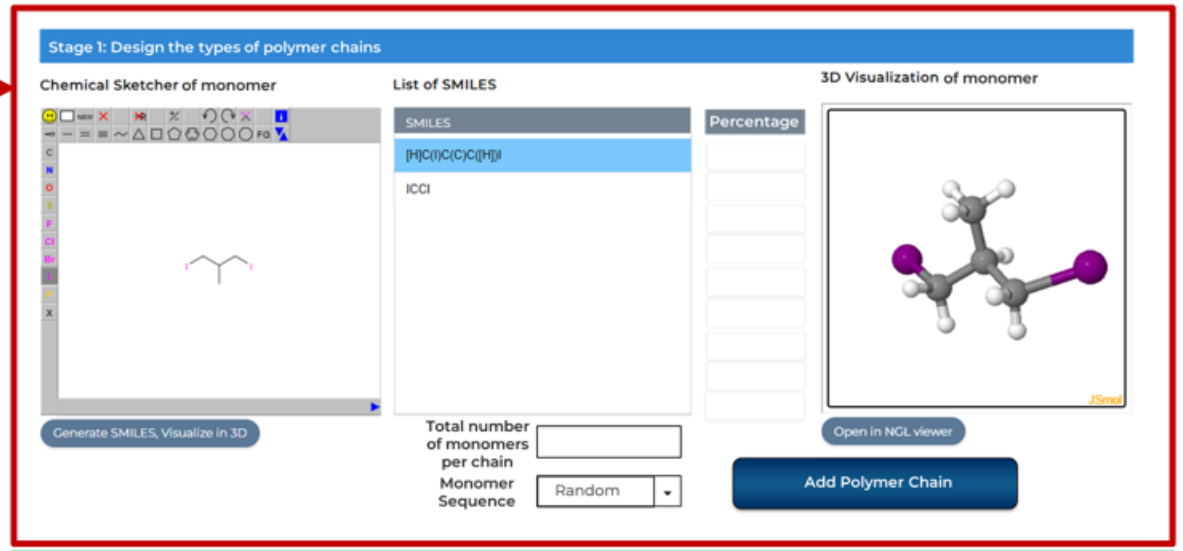
Stage 1: Definition of the types of polymer chains

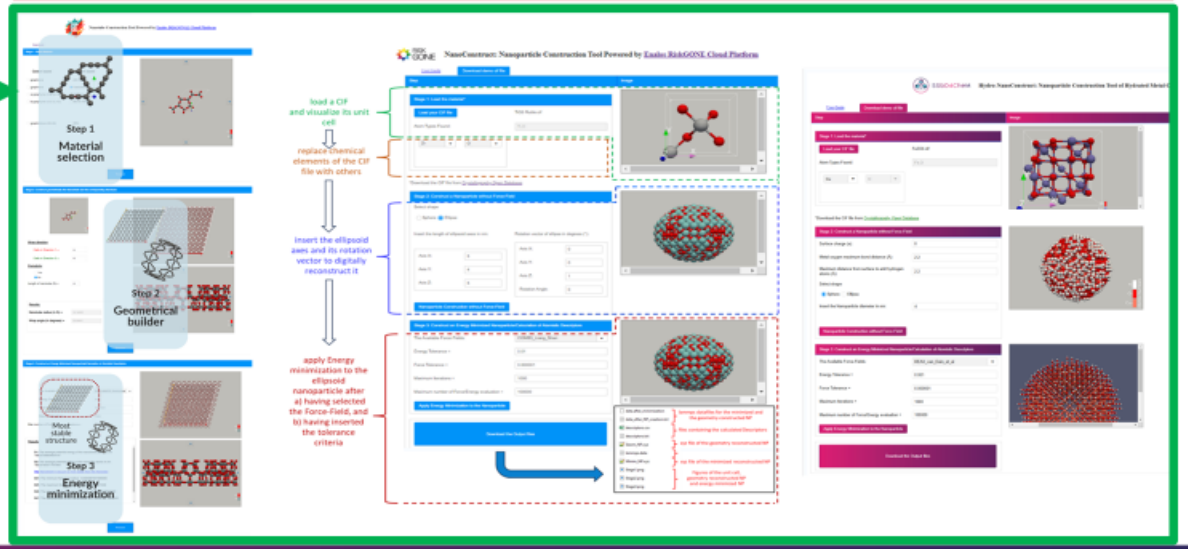
Stage 2: Addition of Nanomaterials from other builders

Stage 3: Geometrical Construction of a Polymer Network in the Simulation Box



Stage 4: Energy Minimization/Relaxation of the Polymer Network





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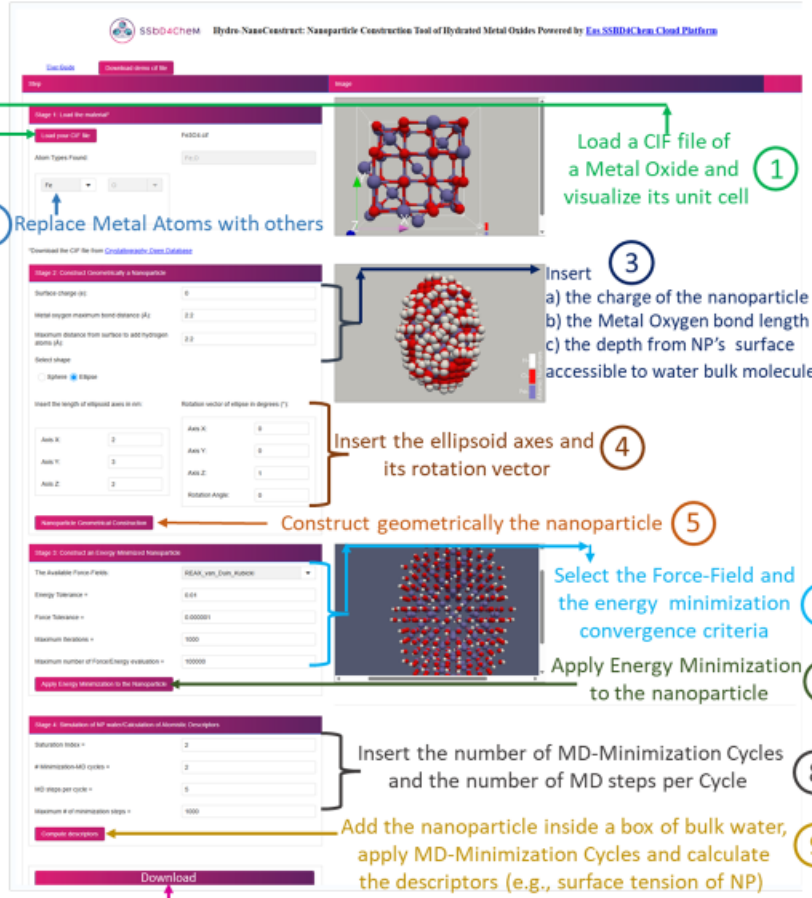
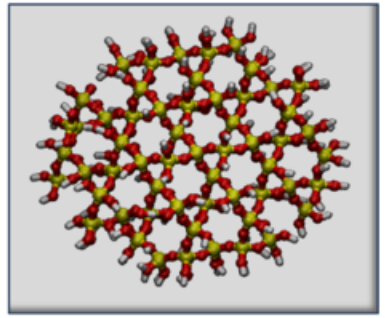
HydroNanoConstruct: Digital Costruction of hydrated Nanoparticles

SSbD4CheM

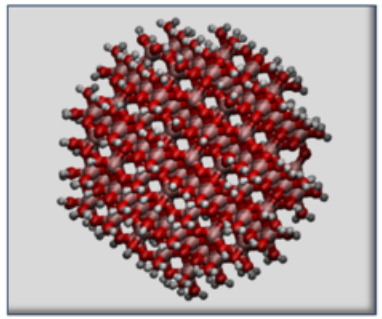


INPUT

- Metal Oxide's CIF File
- NP's ellipsoid axes lengths
- Metal Oxygen bond length
- Depth from NP's surface accessible to water bulk molecules



HydroNanoConstruct



OUTPUT

- Geometrical construction of hydrated Nanoparticles
- Energy minimised hydrated Nanoparticles
- Surface tension of NP in vacuum and water
- List of atomistic descriptors for Machine Learning
- Crystal Growth

Hybrid Composites:
Cellulose based-fillers combined with Metal Oxide, graphene sheets and carbon nanotubes

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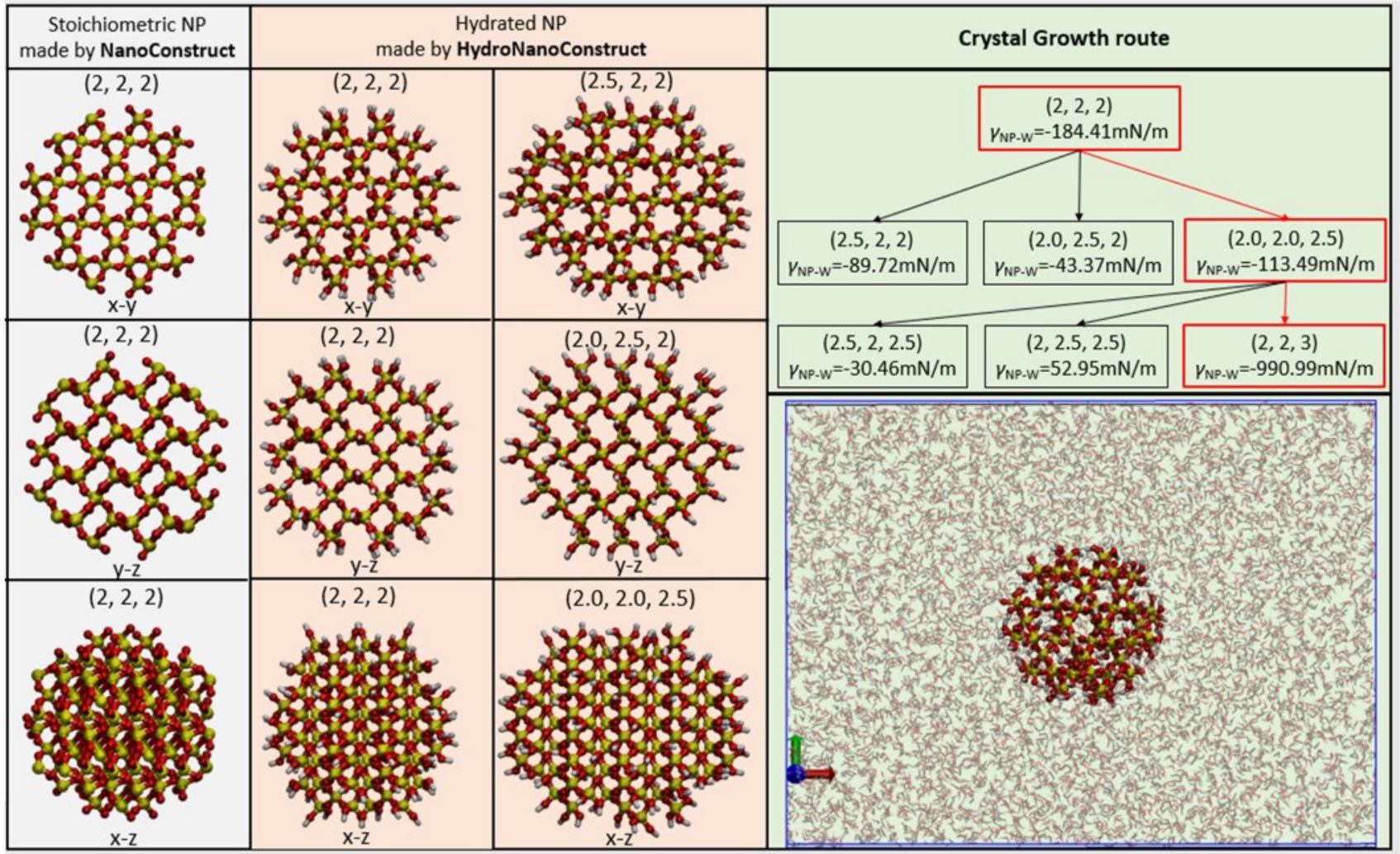
HydroNanoConstruct: Digital Costruction of hydrated Nanoparticles



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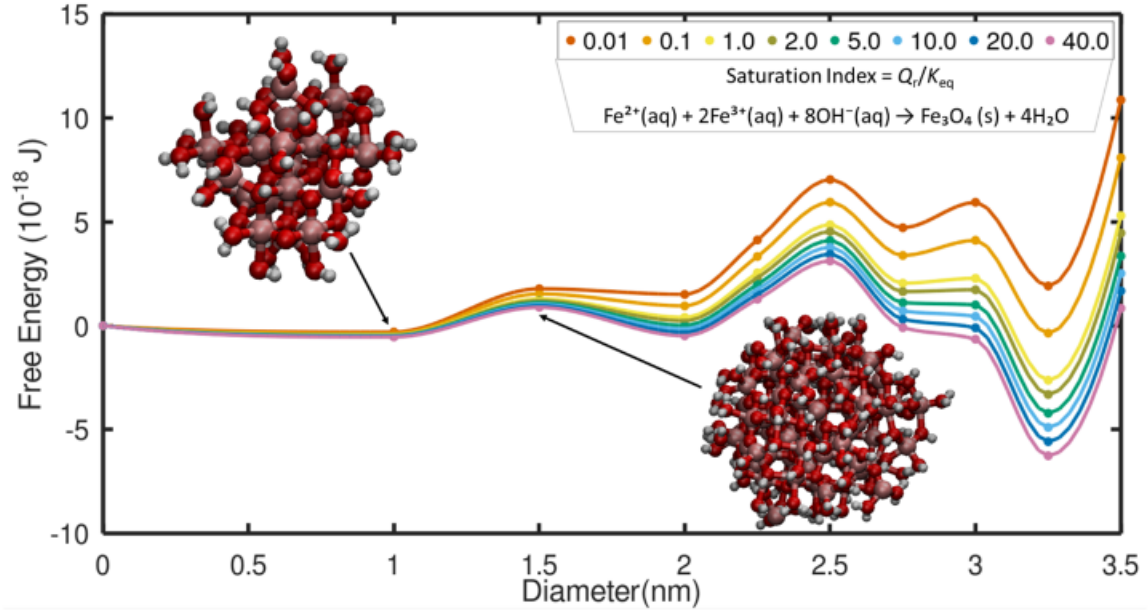
HydroNanoConstruct: Digital Costruction of hydrated Nanoparticles

SSbD4CheM

```
D1:  The max diameter along x axis of the NP in A is: 16.241894042237085
D2:  The max diameter along y axis of the NP in A is: 17.41975661690762
D3:  The max diameter along z axis of the NP in A is: 15.974550362693847
D4:  The Saturation Index is : 1.0
D5:  The surface area of the NP in A^2 is: 859.7529138726339
D6:  The volume of the NP in A^3 is 2366.497342028486
D8:  The Number of Atoms in the Metal Oxide Nanoparticle : 182
D9:  The Number of Atoms of Water in the Simulation Box : 17022
D10:  The average potential energy per Water bulk atoms in eV is : -3.7548521535438133
D11:  The average potential energy per Metal Oxide bulk atoms in eV is : -5.035115950712126
D12: The average potential energy per Metal Oxide NP atoms in vacuum in eV is : -4.870927182749452
D13: The average potential energy per Metal Oxide NP atoms in water in eV is : -6.315677119834228
D14: The average surface energy per Metal Oxide NP atoms in eV is : -0.22072321096145964
D15: The average free energy difference per Metal Oxide NP atoms between the system of Metal Oxide NP in water and its diluted state  in eV is : -0.0036931415571428575
D16: The total potential energy of Metal Oxide NP atoms when NP is in vacuum in eV is : -886.5087472604002
D17: The total potential energy of Metal Oxide atoms if it was in bulk state in eV is : -18045.855567352235
D18: The Free energy difference in eV between the system of Metal Oxide NP in water and its diluted state is : -40.84377615838566
D19: The Free energy in eV between the system of bulk Metal oxide and its diluted state is : -0.6721517634
D20: The Surface energy of NP in eV is : -40.171624394985656
D21: The Surface tension of the Metal Oxide NP in water in eV per square Angstrom is : -0.04672461558058387
D22: The Surface tension of the Metal Oxide NP in vacuum in eV per square Angstrom is : 0.034756911302115744
D23: The Surface tension of the liquid water in vacuum in eV per square Angstrom is : 0.004544319600499376
D24: Wetting in eV per square Angstrom : 0.07693720728220024
D25: Total Potential Energy of the simulation box in eV : -64871.65608504738
D26: Total Potential Energy of the remaining waters in the simulation box in eV : -63722.202849237554
```

Descriptors needed to enrich the dataset



Extension of this tool for cellulose Nanofibers/nanoparticles

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SSbD4CheM

Use of New Approach Methods in SSbD

Yvonne Kohl (Fraunhofer IBMT)

11 June 2025, 15:00 – 16:30h CEST, online

Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101138475. UK participants in SSbD4CheM project are supported by UKRI. CH participants in SSbD4CheM project receive funding from the Swiss State Secretariat for Education, Research and Innovation (SERI). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

What are NAMs – New approach methodologies

NAMs can be defined as any *in vitro, ex vivo, in chemico, in silico* but also alternative *in vivo* method that when used alone, or in concert with others, enable improved saftey assessment through more protective and /or relevant models and as a result, contribute to the reduction or replacement of animal models.

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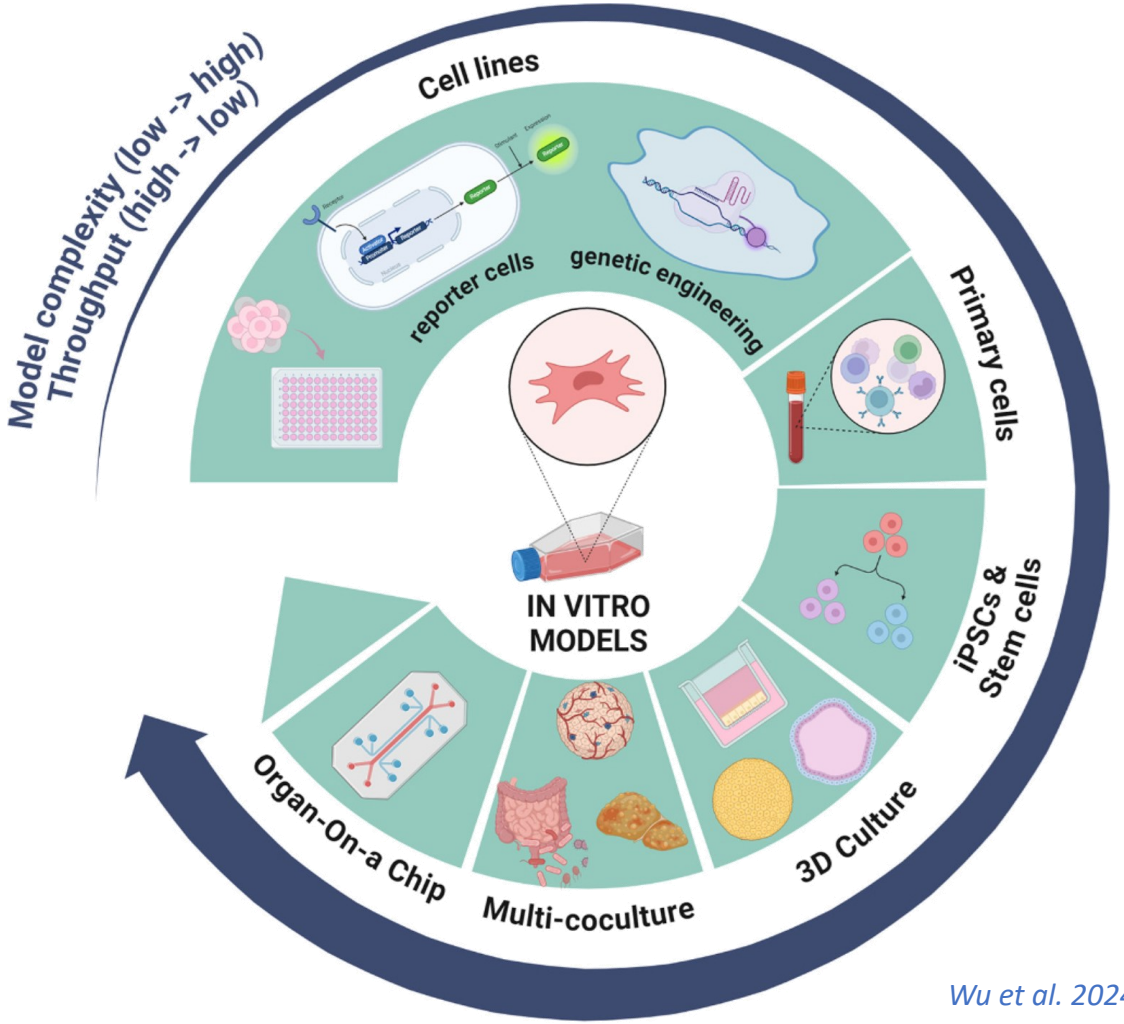
What are NAMs – New approach methodologies

in vitro NAMs



Follow tiered approach and combine data

Wu et al. 2024, doi: 10.1016/j.impact.2024.100533

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IATA - Integrated Approaches for Testing and Assessment

to support material safety

IATA combine multiple sources of information to conclude on the toxicity of chemicals or materials.

IATAs may include

(1) Existing information from the scientific literature or other resources

along with

(2) newly generated data resulting from traditional toxicity testing methods or NAMs

to fill data gaps.

These approaches are developed to address a specific regulatory scenario or decision context.

https://www.oecd.org/en/topics/sub-issues/assessment-of-chemicals/integrated-approaches-to-testing-and-assessment.html

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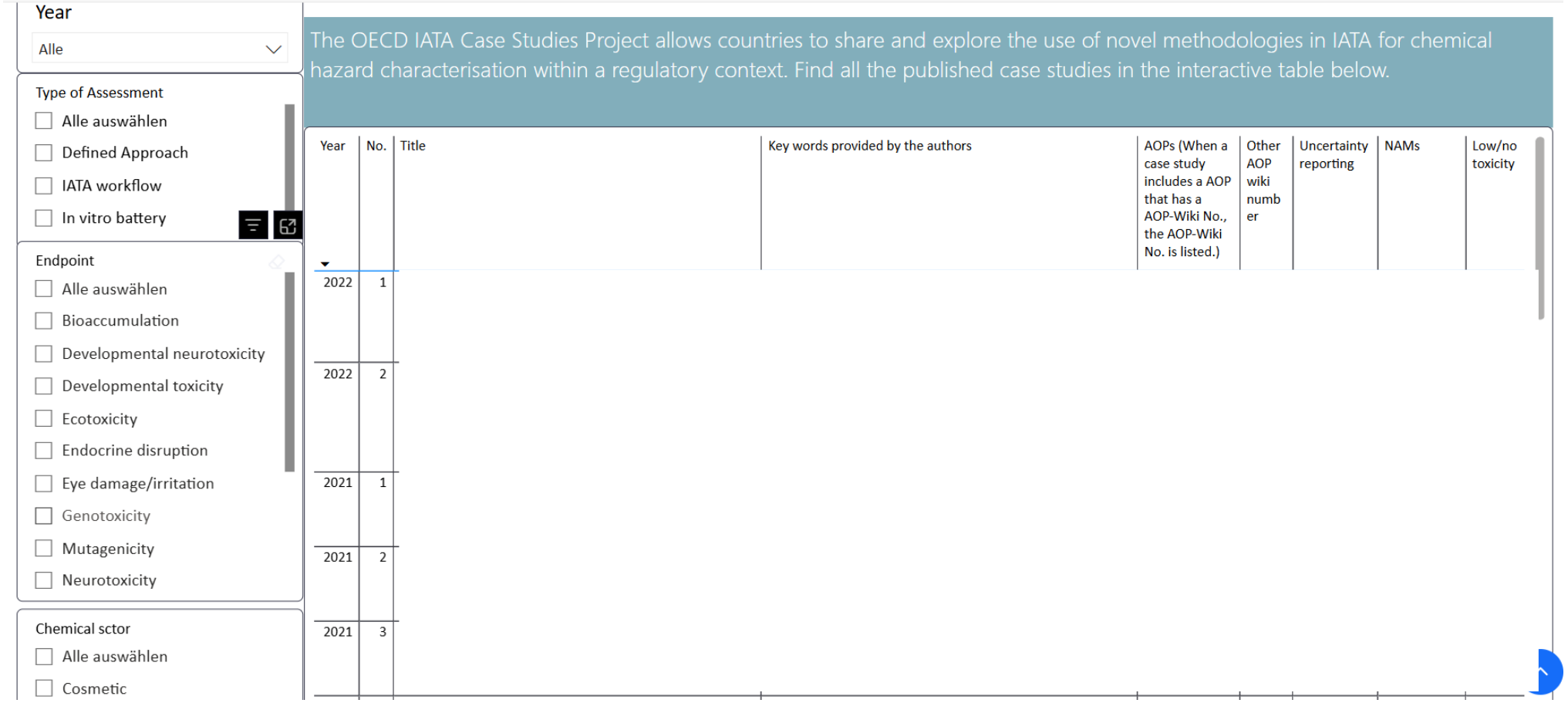
IATA - Integrated Approaches for Testing and Assessment

to support material safety

OECD IATA Case Studies Project



https://www.oecd.org/en/topics/sub-issues/assessment-of-chemicals/integrated-approaches-to-testing-and-assessment.html

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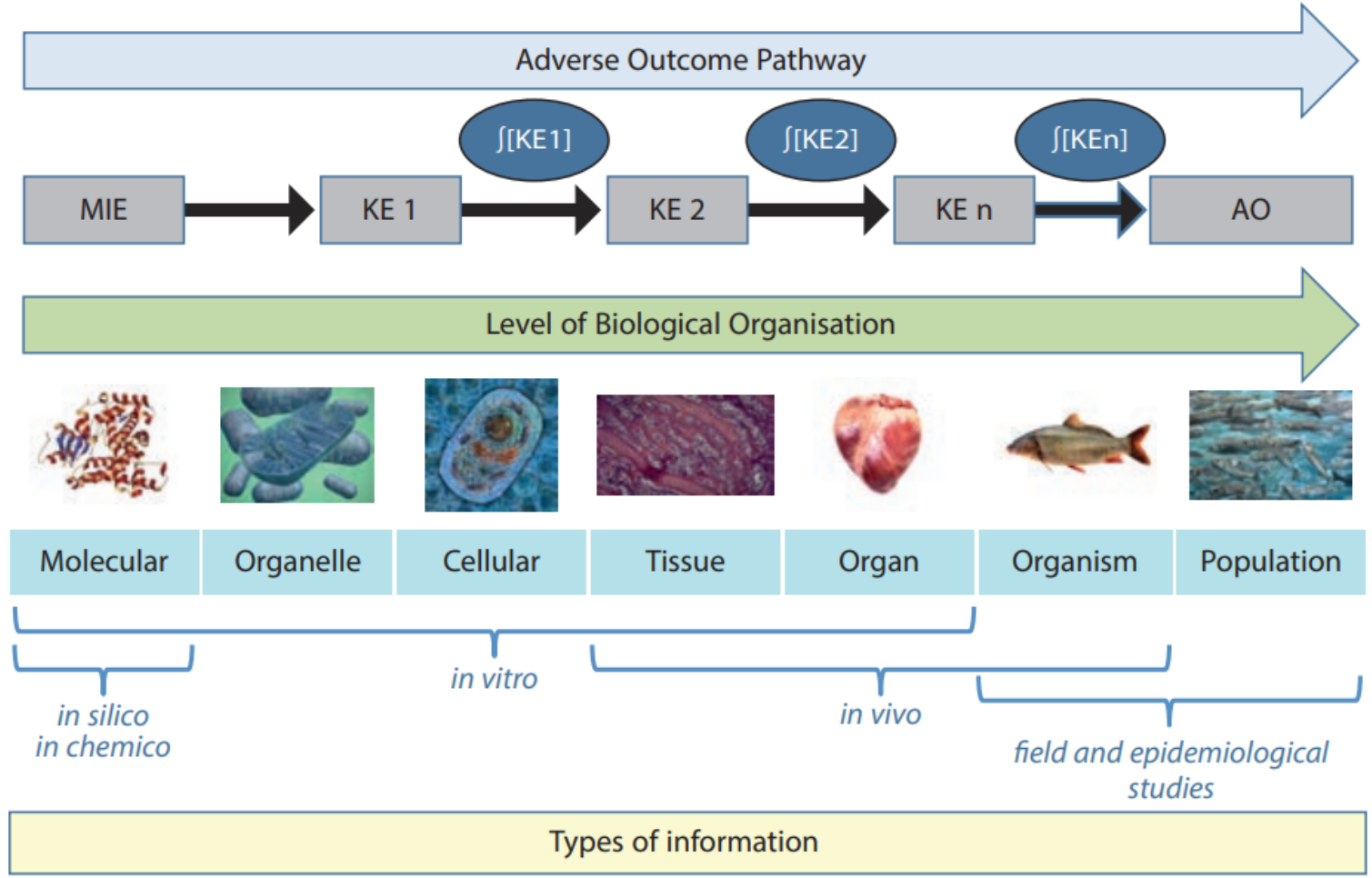
IATA based on AOP concept

AOP:
Adverse Outcome Pathway

MIE:
Molecular Initiating Event

KE:
Key Event



OECD guidance N°260 (2017)

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Are IATAs New Approach Methods?

IATAs are frameworks for integrating information

IATAs often include data from NAMs.

Need for Next Generation Risk Assessment approaches for advanced materials:

- Transition towards a flexible and adaptive Next Generation Risk Assessment (NGRA) approach
- Enabling implementation of NGRA in the current legislative frameworks (e.g., REACH, CLP)
- Adaption of related regulatory guidance to NAMs
- Continuous dialogue and collaboration among all stakeholders to promote change from risk assessments based on apical effects towards more mechanistic safety assessments based on NAMs.

Hristozov et al. 2024, doi: 10.1016/j.impact.2024.100523

https://www.oecd.org/en/topics/sub-issues/assessment-of-chemicals/integrated-approaches-to-testing-and-assessment.html

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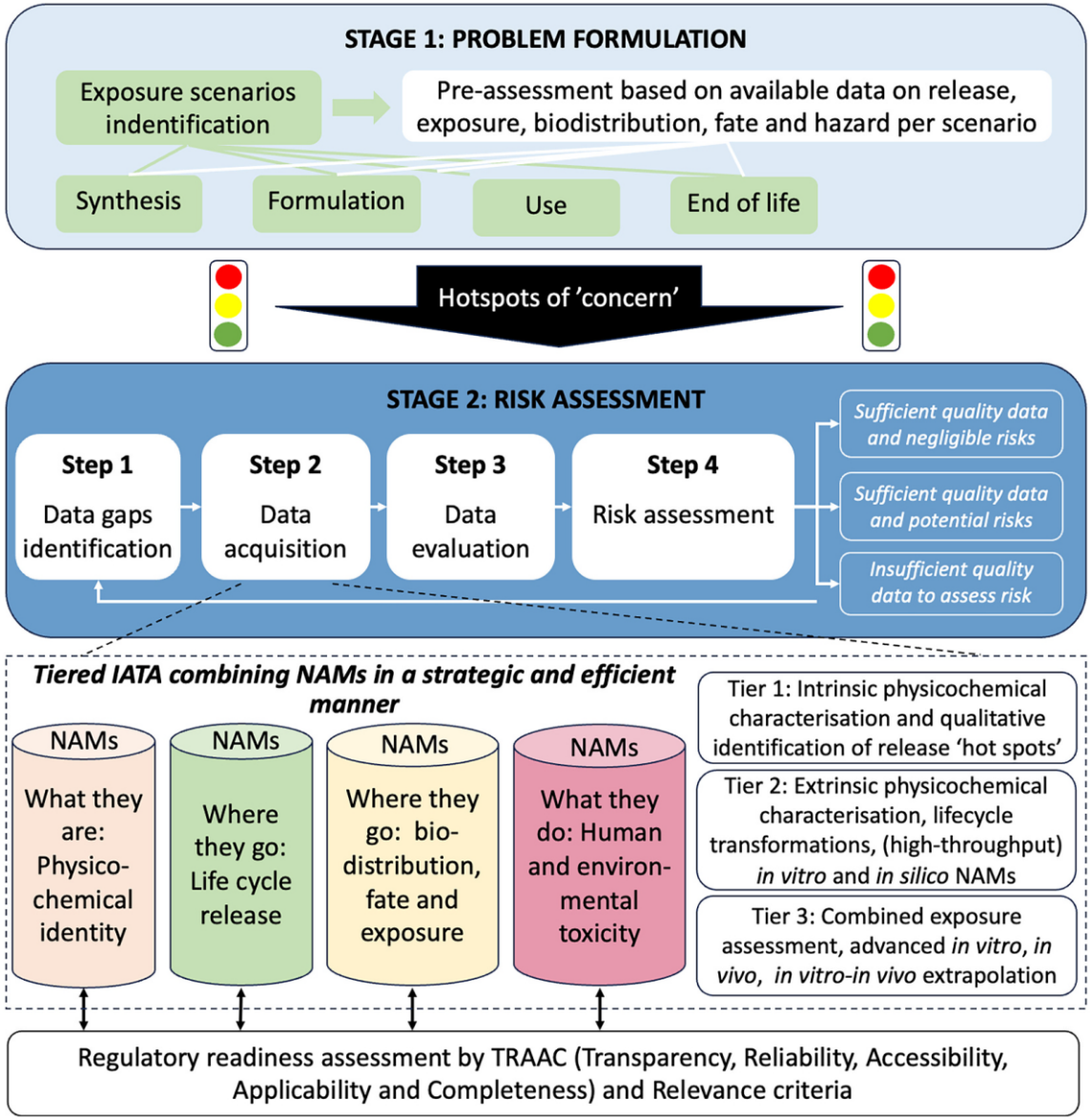
Next Generation Risk Assessment

Conceptual framework for exposure-driven Next Generation Risk Assessment of Advanced Materials



Hristozov et al. 2024, doi: 10.1016/j.impact.2024.100523

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NAMs /Innovative models in SSbD4CheM

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NAMs /Innovative models in SSbD4CheM

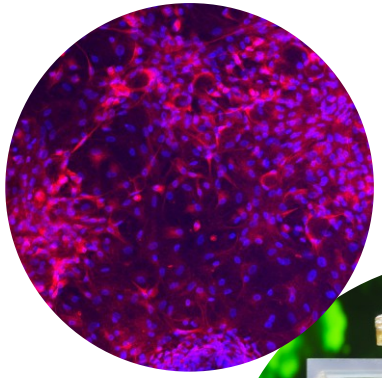
Inhalation studies *in vitro*

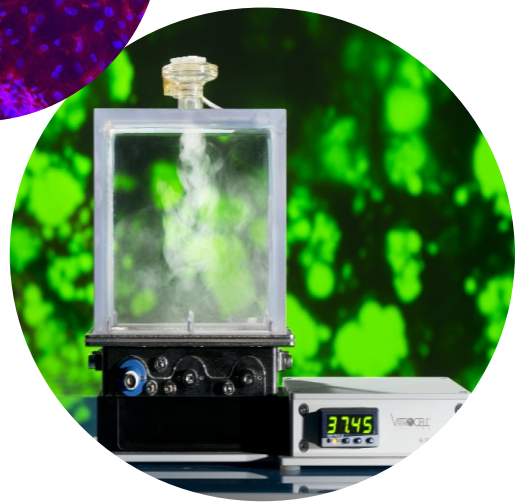
hiPSc-based lung model

Transport

Barrier integrity, Inflammation

Viability





Oral uptake studies *in vitro*

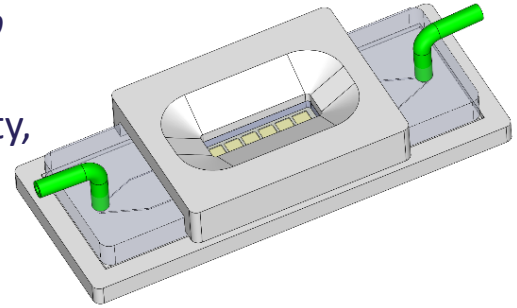
fluidic GIT model

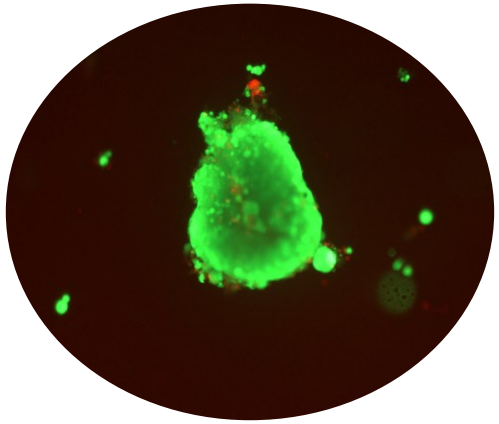
Mucus-on-chip

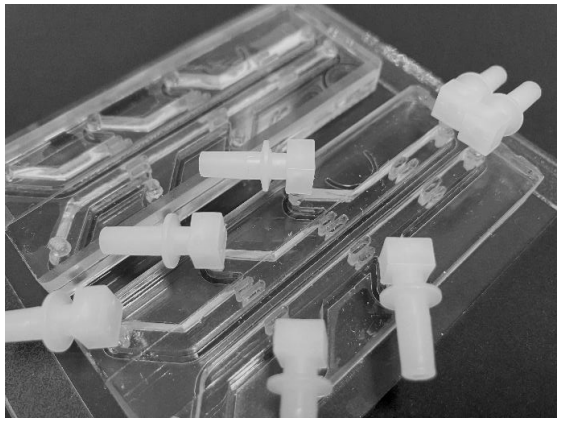
Transport

Barrier integrity, Inflammation

Viability







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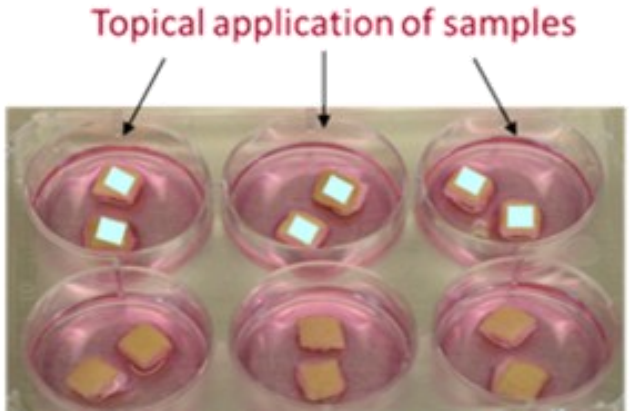
NAMs /Innovative models in SSbD4CheM

Skin contact studies *in vitro*

Ex vivo skin model

- *UV damage*
- *Allergen / Irritant contact dermatitis*

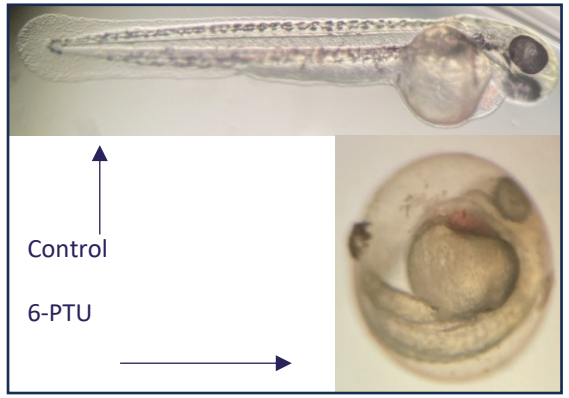
Inflammation
Viability
Apoptosis



Developmental studies *in vitro*

Zebrafish embryo assay

Embryonic development
Larvae death



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Incorporation of data from NAMs into SSbD workflows

NAMs in SSbD

To fill data gaps

in case of new substances, which lack CLP data

Experimental NAMs, for mixtures (e.g. bio-based alternatives) where QSARs are not applicable

To prioritize new chemicals/products **in early design phase**

Assessment relative to benchmark In parallel to technical performance

To support safe materials from early design phase to product application

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FAIR data

to optimize the reuse of data

Findable – data should be included in searchable repositories

Accessible – data should be open available

Interoperable – standard vocabularies

Reusable – reproducible workflows

Koelewijn et al. . 2024, doi: 10.1016/j.impact.2024.100533

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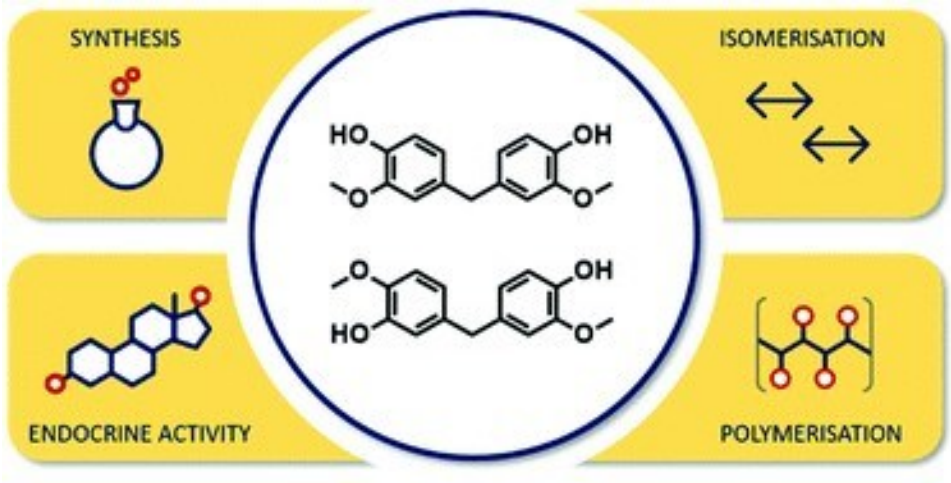
NAMs for SSbD: An example

Safer and renewable bisphenol A (BPA) replacement



Step 1: *In silico* analysis based on chemical structure and properties

→ Vallinyl alcohol: A structural analogue

Step 2: *In vitro* screening of prioritized substances

Koelewijn et al. . 2019, https://doi.org/10.1039/C9GC02619C

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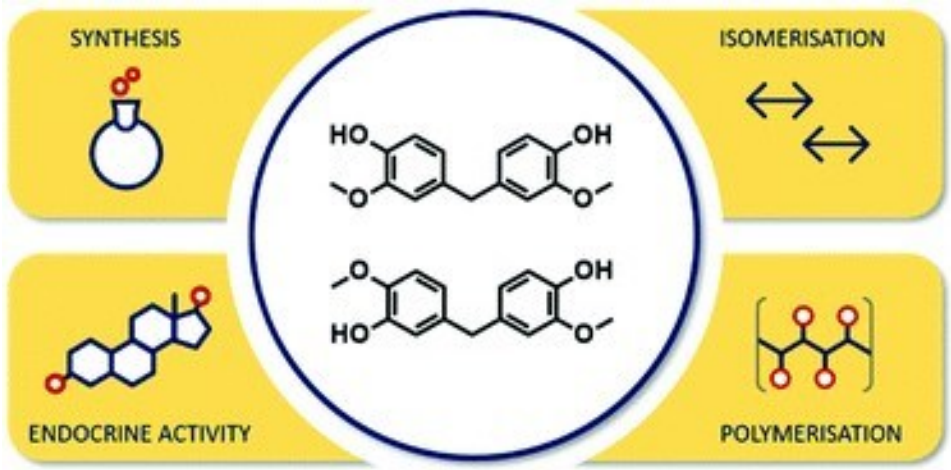
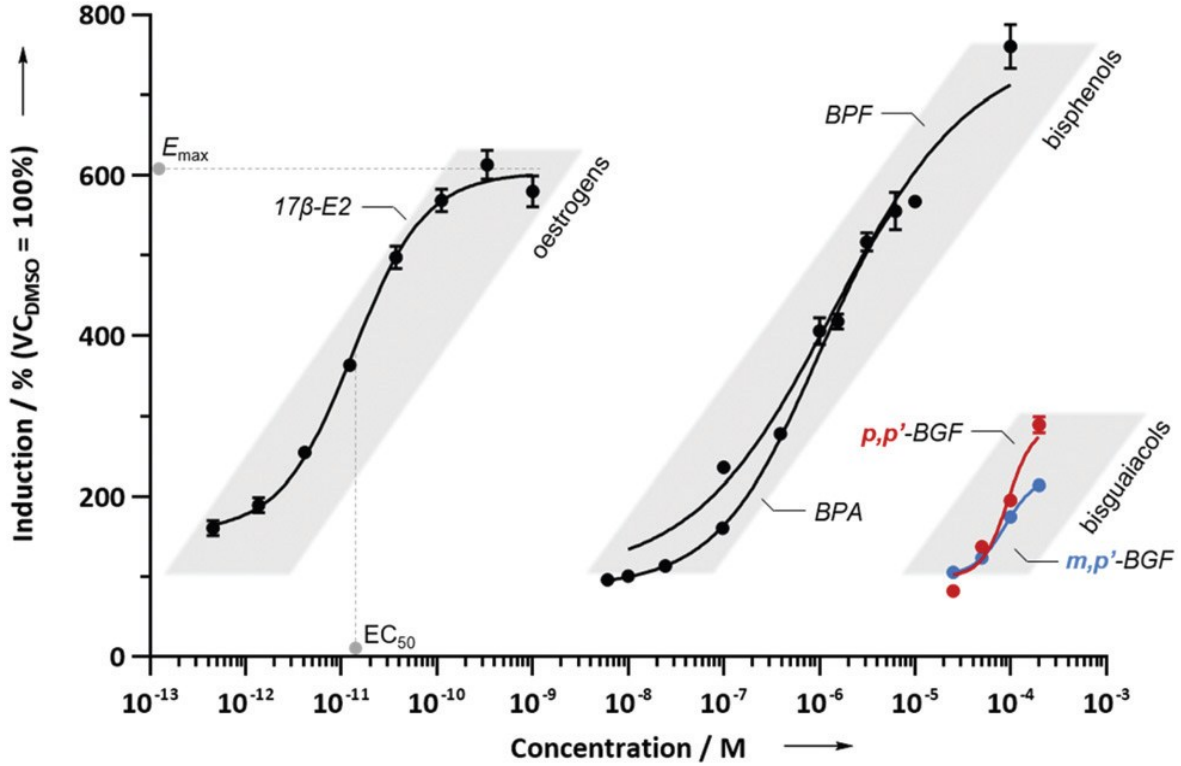
NAMs for SSbD: An example

Safer and renewable bisphenol A (BPA) replacement



- 17β-E2, BPA, and BPF fully activated hERα in a dose-dependent manner
- biobased alternatives did show lower estrogenic potency compared to the fossil-based chemicals

→ **Using NAM-based screening prior to higher tier testing**



Concentration-dependent in vitro transcriptional induction of luciferase by 17β-E2, BPA, BPF, and p,p'-BGF and m,p'-BGF in hERα cells (MELN).

Koelewijn et al. . 2019, https://doi.org/10.1039/C9GC02619C

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SSbD4CheM

Life Cycle Assessment

Nils Thonemann (University of Leiden)

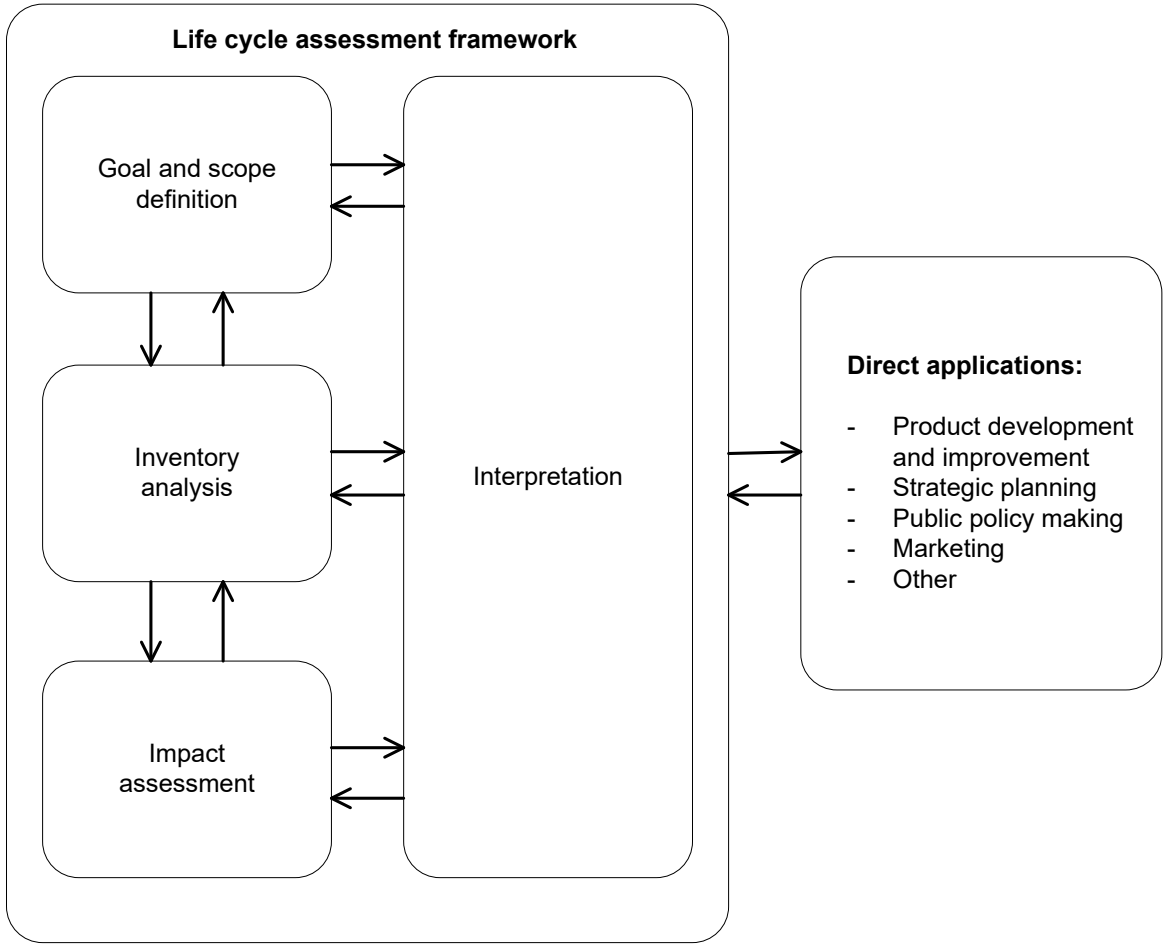
11 June 2025, 15:00 – 16:30h CEST, online

Funded by the European Union

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101138475. UK participants in SSbD4CheM project are supported by UKRI. CH participants in SSbD4CheM project receive funding from the Swiss State Secretariat for Education, Research and Innovation (SERI). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

What is LCA?

- General framework and guidelines defined in ISO14040 and ISO14044
- **Life cycle**: comprehensive perspective of process, product, service, etc. from cradle to grave
- **Quantified impacts**: diverse impact categories calculated from emissions to, and extractions from, the environment



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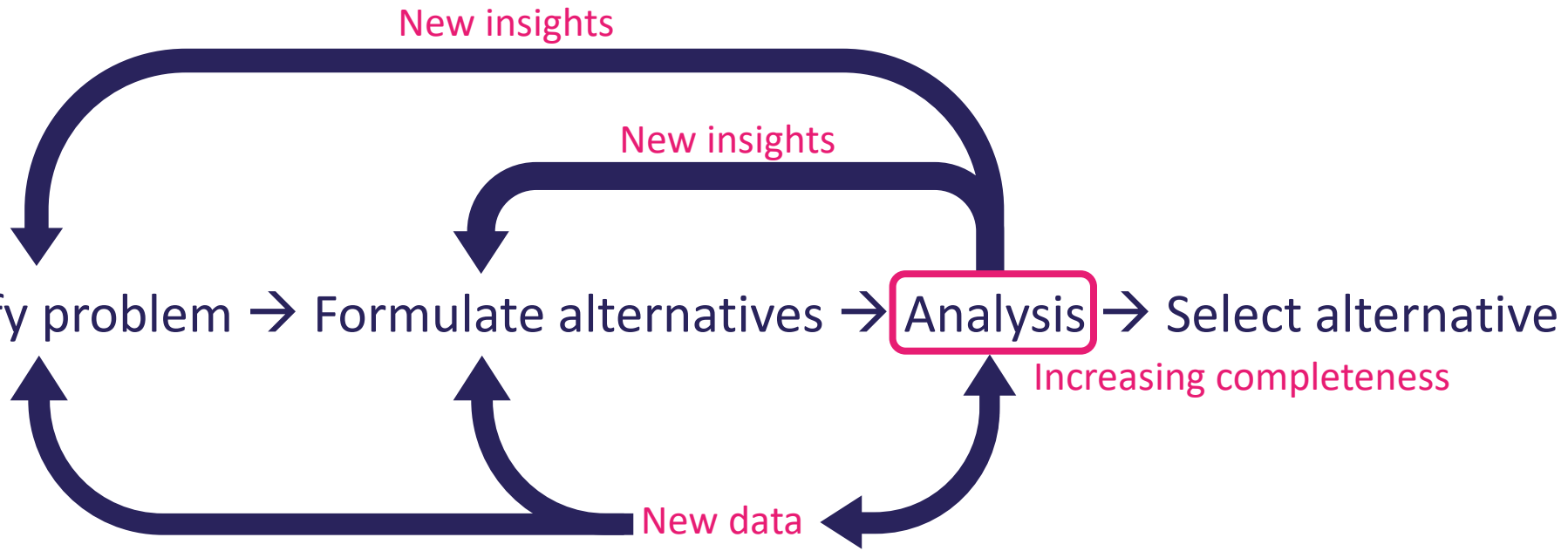
LCA in SSbD: ex-ante & tiered

- Conventional pathway to decision making:
  - Identify problem → Formulate alternatives → Analysis → Select alternative
- Decision making in SSbD:



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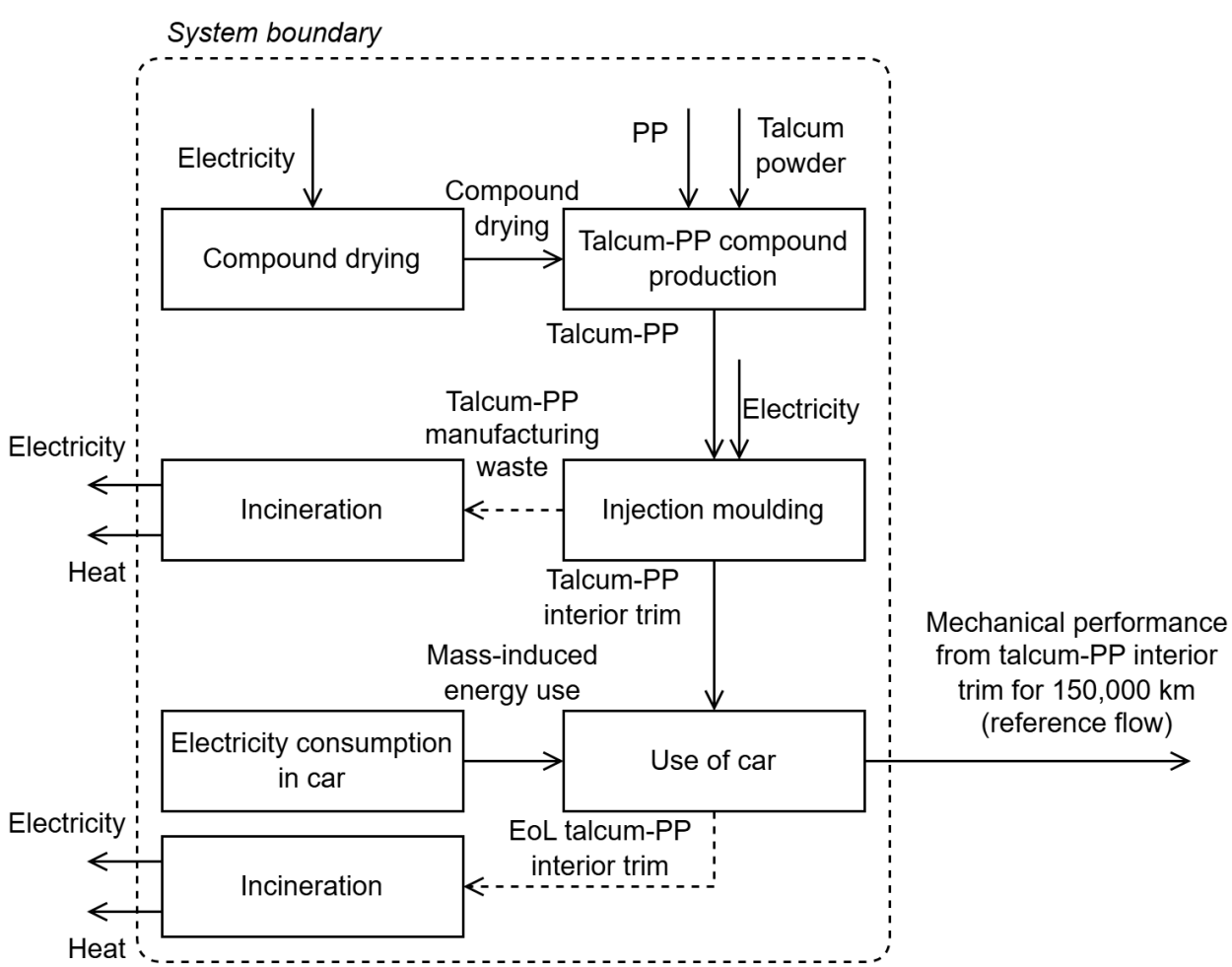
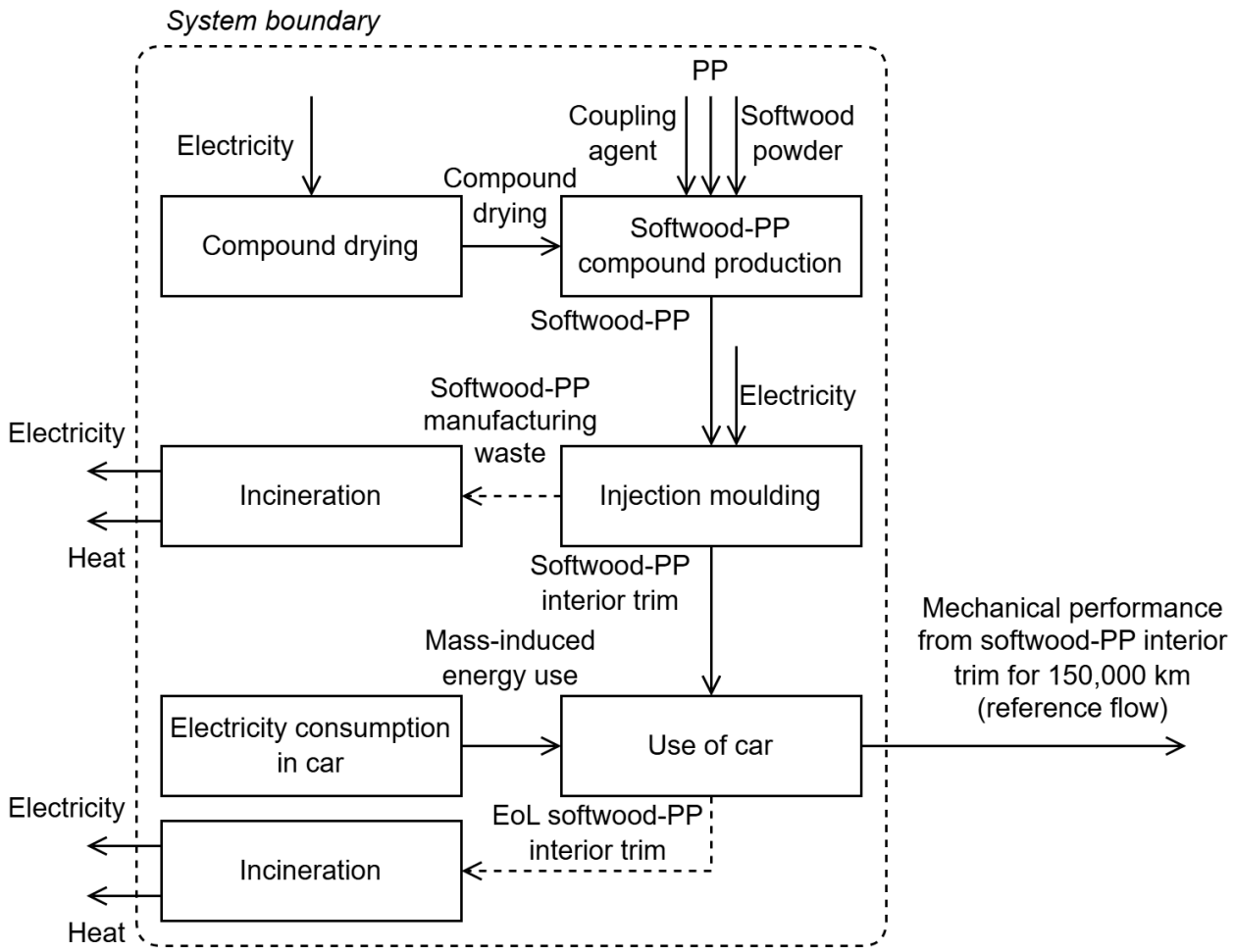
SSbD Step 4 Cradle-to-grave *ex-ante* LCA





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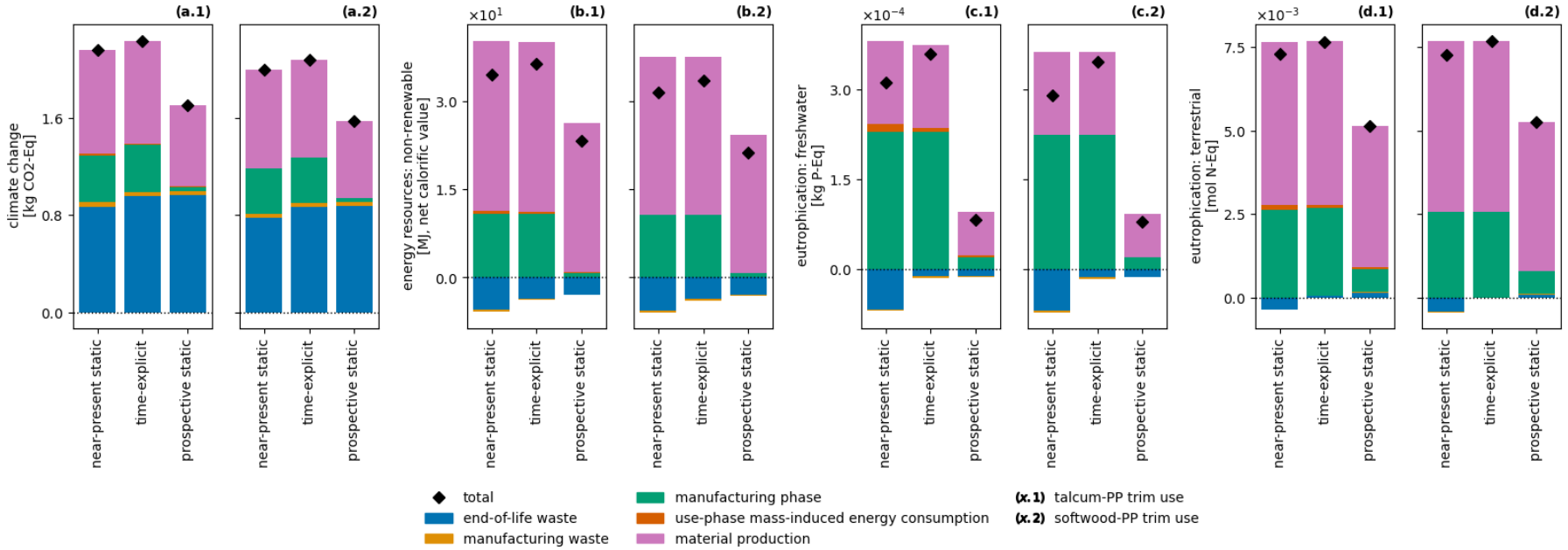
SSbD Step 4 Contributions & comparison

- Material production often has the highest contribution due to high impact of PP.
- When comparing temporal perspectives:
  - Often, large reductions to one or more phases.
  - However, **comparative performances** remains similar.
  - Potential conclusion: for early-stage decision making, a temporally simplified assessment is sufficient.



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Conclusion: what LCA adds to SSbD

- Qualitative & quantitative insight into the broader system
- Perspectives for leveraging (deep) uncertainty
- A growing ex-ante LCA toolbox

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SSbD4CheM

Insights from Case Study Applications

Ivana Burzic (Wood K plus)

11 June 2025, 15:00 – 16:30h CEST, online

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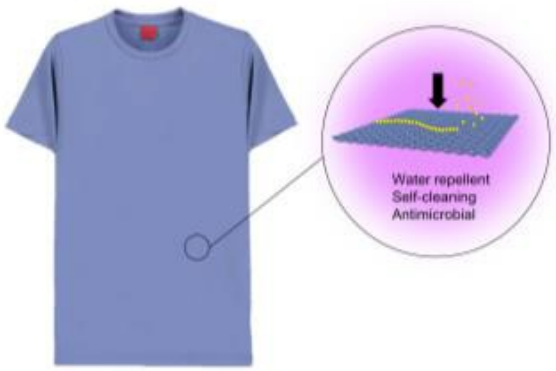
Case studies Objectives

- Development and validation of 2 wood plastics composites with optimised VOC emissions and Odour & improved environmental impact for interior car trims
- Development and validation of 2 organic monomers self-cleaning / water repellent and antimicrobial coatings for textiles
- Introducing and standardize 4 added value SSbD nanocellulose applications to the skin care cosmetics (face cream, body lotion, facial mud mask, dead sea mud)
- Prototyping and validation of composites, coatings and nanocellulose according to use case requirements (automotive, textile, cosmetics) with fulfilled sustainability and safety aspects.



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TRL 6 — Technology demonstrated in a relevant environment

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SSbD4CheM

Automotive case study

STELLANTIS CRF

Highlights

WOOD KPLUS

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Renewable based composites for automotive interior parts

WP3

Non-target & target TVOC analyis

Following GS 97014-3

(VDA 278)

odor characteristic

(VDA 270)

→ method development for specific aldehyde emission analysis

→ Vocus CI-TOF thermodesoption system to be coupled with the Vocus CI-TOF no chromatography needed

→ the limit values in GS97014-3 are different

→ Aim to standardize the VOC tests

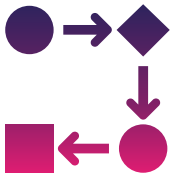
experimental and computational descriptors

WP2

Modelling of data gap for LCA analysis

Modelling of data gap related to human exposure – e.g. inhalation

Modelling of skin irritation in respect to MFC cellulosic fillers



WP1

WP4

In silico models for exposure analysis

hiPSC-based in vitro lung model

WP5

Worker and consumer exposure and risk assessment: - measured data; - exposure models

WP6

LCA, s-LCA, and LCC

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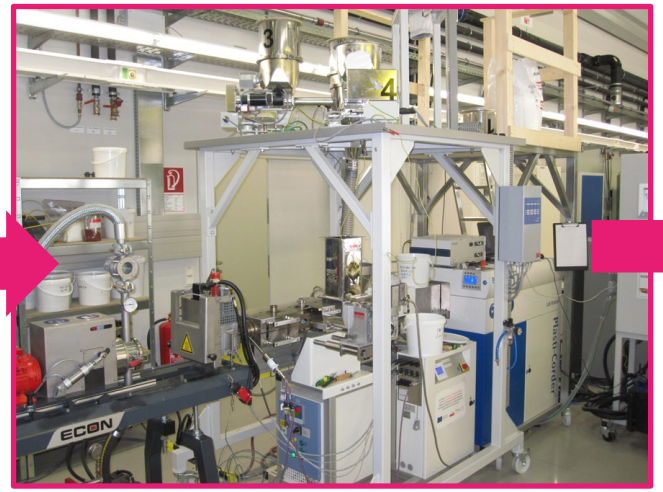
SSbD4CheM

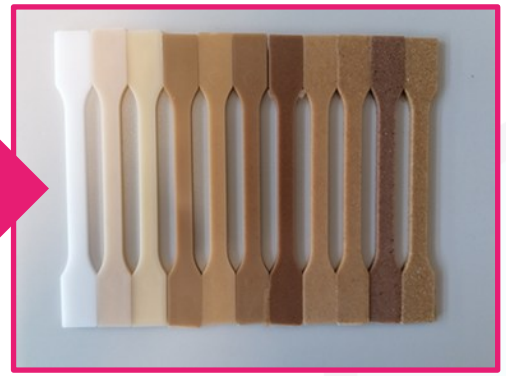
WP7

Wood Plastic Composites (WPCs)

Renewable PP
PP heterophasic copolymer
Recycled PP
Ultrafine cellulose
Regenerated cellulose
Soft wood, Hemp fibers
Hybrids
Talc compounds as reference material

Processing technology: ***Compounding/ Twin screw extrusion/Injection moulding***





WP3

Material & prototypes characterization
Mechanics, MFI
TVOC & FOG emissions testing after processing (granulates and injection moulding)
TVOC emission testing depending on weathering behavior
Odour testing

WP7

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Renewable Composites (WPC) for automotive interior parts – selected results

SSbD4CheM

WP7

New best samples & reference	Density [g/cm³]	Fmod [MPa]	Tstr [MPa]	Impact strength acN(23°C) [kJ/m²]	Impact strength acU(23°C) [kJ/m²]	MFI (190°C, 5 kg) g/min
Targets or reference (Talcum-filled) – all 190°C	0.998	1294	17.1	to maximize, tbd	to maximized, tbd	44 (Talcum filled) Target tbd
PP-CM2_15C400_3Sc_3E	0.970	1347	20.2	**16.1**	30	22.4
PP-CM2_15C400_3Sc_4E_5PP-ED	0.963	1264	19.6	17.0	34	20.2
PP-CM2_15FCP_3SC_3E	0.959	1180	24.4	15.7	53	**5.6**
PP-CM2_15Hemp_3Sc_2E	0.969	**1436**	21.8	14.9	32	17.4
PP-CM3_15UFC_3Sc	0.955	1182	18.9	6.7	**133**	tbd

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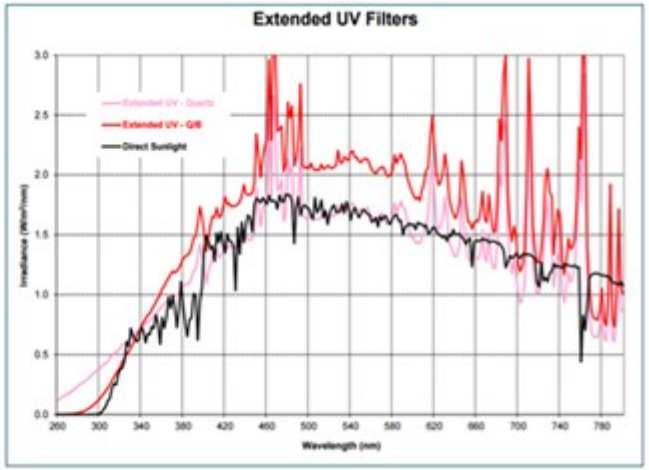
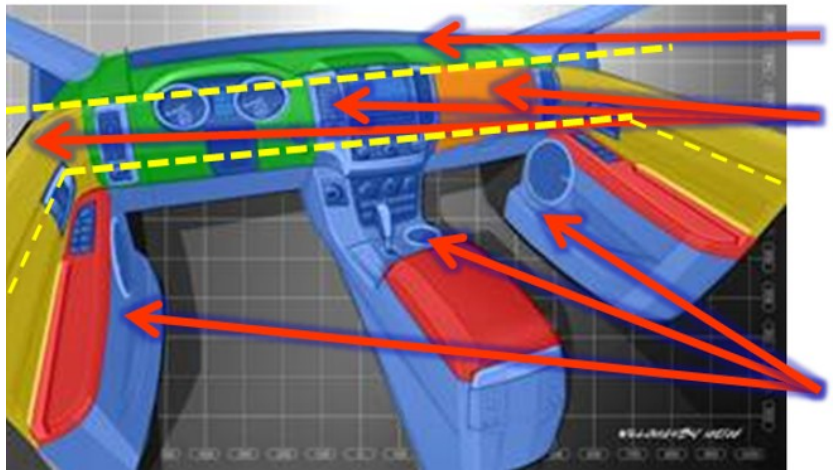
Renewable Composites (WPC) for automotive interior parts – Weathering Testing

WP7





1240 kJ/m²
Instrument Panel Horizontal Surfaces

601 kJ/m²
Upper Pillar trim, Instrument Panel vertical surfaces, Package Tray & Door Roll-over trim materials

225 kJ/m²
Seating trim, Door Trim, Floor Console, Lower Pillar / Cowl trim, Overhead Console / Trim materials

- Light ageing test is carried out according to SAE J2412 standard.
- Artifical light is emitted from Xenon lamp, Quartz/Boro (Q/B) filters system is used to simulate the spectra of the incident sunlight inside the cars.
- Level of radiation depend on the interior part we are considering!
- At CRF 3 level of irradiation can be considered: 225-601-1240 kJ/m^2
- Prepared WPCs will be tested for all 3 level of irradiation to understand in which parts the WPC material can be used – **good input for prototyping besides obtained mechanics!**
- The acceptance criteria (comparing the sample before and after the test) is:
  - $\Delta E \leq 3$
  - Minimum of 4 on AATCC Gray

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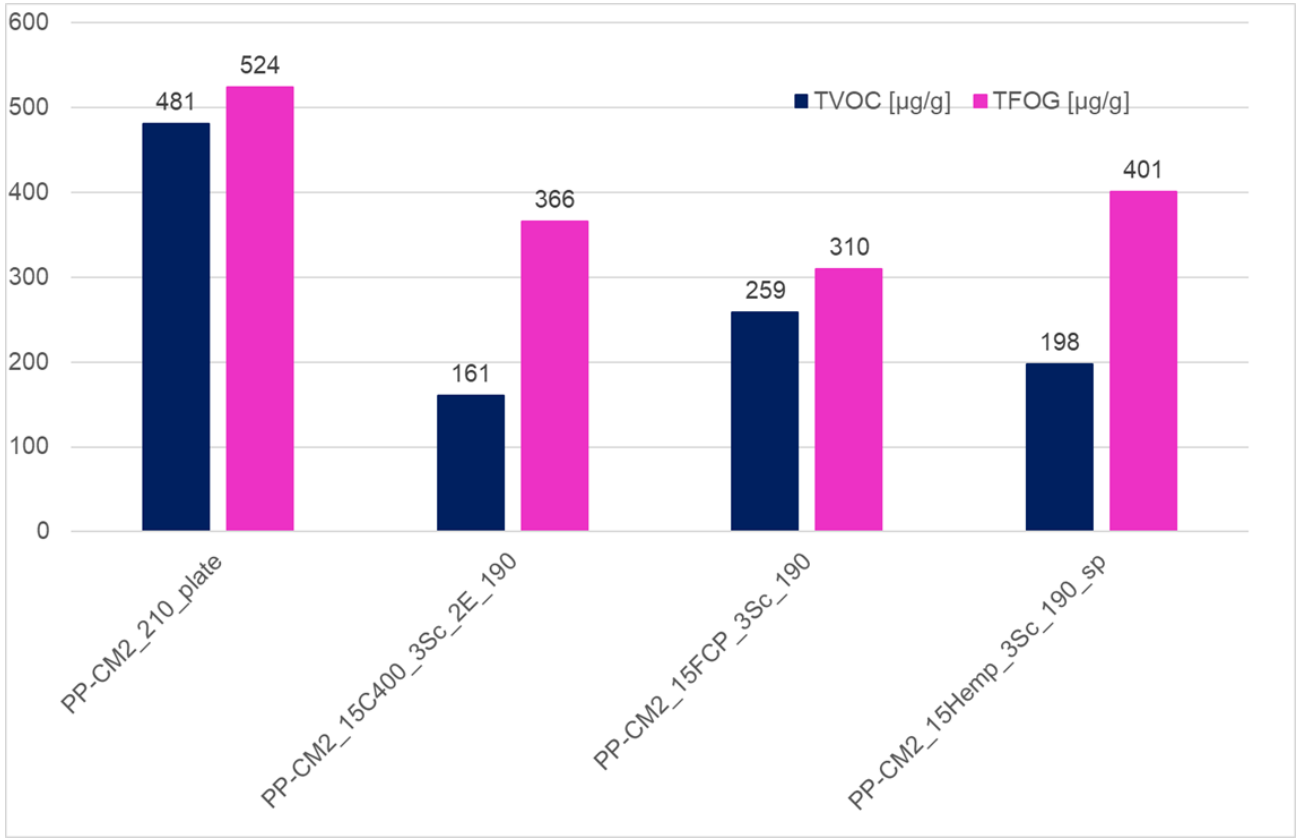
TVOC-Emission testing – data input for potential worker & consumer exposure

WP3

- **Standard emission testing (Aldehydes / TVOC) of Wood Plastic Composites (WPCs)**
  - VDA 278, VDA 275 (EU), ISO 12219-3 (US)
  - Define target list (focus on cellulosic fillers) for VOCUS CI-TOF (PTR /AIM)
- **Coupling of µ- and emission test chambers with VOCUS CI-TOF (PTR/AIM)**
  - Target - Rapid screening (Broad variety of substances→ flexible)
  - Online monitoring of standard emission testing (e.g. influence of temperature profiles – Safety by process design (SbD))



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SSbD4CheM

Textile case study

Highlights

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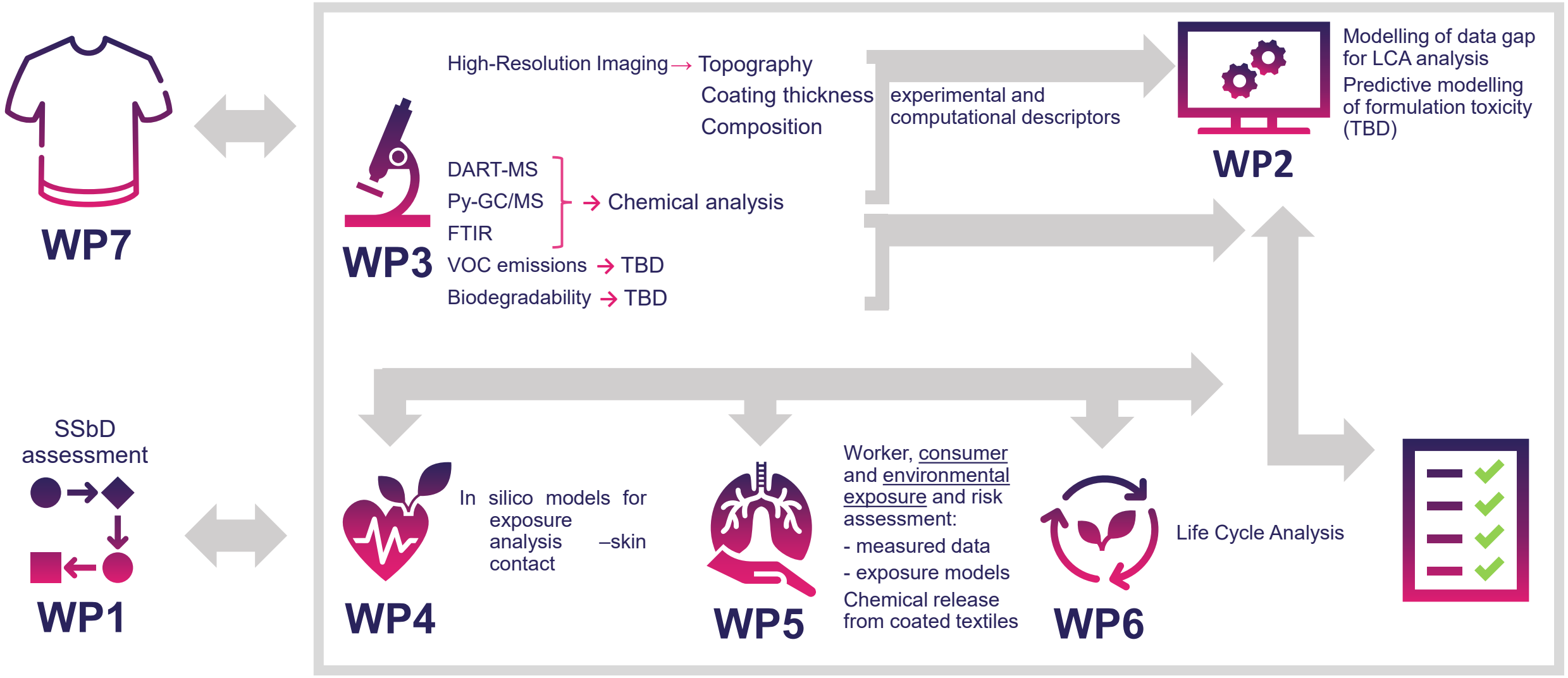
Organic monomers and their compounds as self-cleaning/water repellent and antimicrobial coatings



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Screening of hydrophobic precursors: soybean oil (SO), squalane (SQA), squalene (SQE) and oleic acid (OA)

Analysis of Deposition on Silicon Wafers (Si-W)

Precursor	Parameters				Result
SO	200	80	1.0	10	Wet deposition
SO	400	80	1.0	10	Wet deposition
SO	600	80	1.0	10	Wet deposition
SO	600	80	0.8	10	Wet deposition
SO	600	80	0.8	2	Wet deposition
SO/HDODA (70:30)	600	80	0.8	2	Homogeneous thin film
SO/HDODA (70:30)	600	80	0.8	10	Homogeneous thin film
SO/HDODA (70:30)	400	80	0.8	10	Irregular film
SO/HDODA (70:30)	200	80	0.8	10	Wet deposition
SQA	200	80	1.0	10	Wet deposition
SQA	400	80	1.0	10	Wet deposition
SQA	600	80	1.0	10	Wet deposition
SQA	600	80	0.8	10	Wet deposition
SQA	600	80	0.8	2	Wet deposition
SQA/HDODA (70:30)	600	80	0.8	2	Wet deposition
SQA/HDODA (70:30)	600	80	0.8	2	Wet deposition
SQE	200	80	1.0	10	Wet deposition
SQE	400	80	1.0	10	Wet deposition
SQE	600	80	1.0	10	Wet deposition
SQE	600	80	0.8	10	Wet deposition
SQE	600	80	0.8	2	Wet deposition
SQE/HDODA (70:30)	600	80	0.8	2	Wet deposition
SQE/HDODA (70:30)	600	80	0.8	2	Wet deposition

✔ SO/HDODA: homogeneous thin film

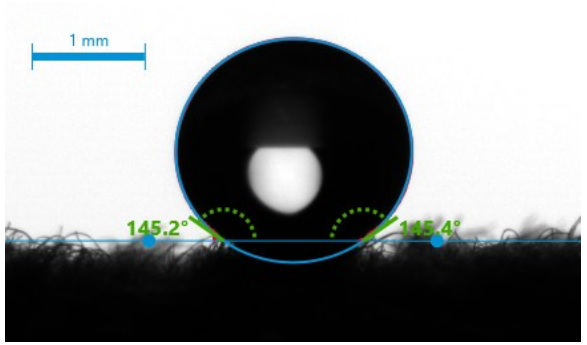
✘ SO, SQA, SQA/HDODA, SQE, SQE/HDODA: oily

Analysis of water repellency on textiles (B-PET)

Reference	Parameters				WCA (°)
	600	80	0.8	2	>150
	600	80	0.8	2	>150
	100	80	1.0	10	>150
	100	80	1.0	10	>150
	-	-	-	-	0

Soybean Oil (**SO**)
Squalene (**SQE**)
Squalane (**SQA**)
Oleic Acid (**OA**)
1,6-Hexanediol diacrylate (**HDODA**)
Divinylbenzene (**DVB**)

✔ SO, SO/HDODA, SQA, SQE: hydrophobic coatings ✘ OA



Selected candidates

a) SO 100%

b) SO 70% / HDODA 30%

Outstanding water repellency with a uniform and homogeneous thin film

Fluoropolymer benchmark: **NUVA N2155 liq**

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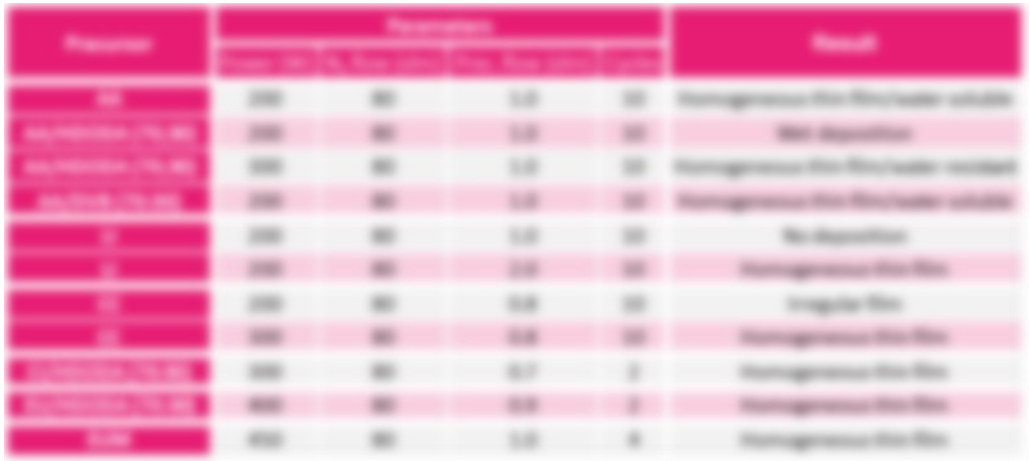
Screening of antimicrobial precursors: acrylic acid (AA), carvacrol (CC), limonene (LI), citronellal (CI) and eugenol (EU)

Analysis of Deposition on Silicon Wafers (Si-W)



Acrylic acid (**AA**)

Carvacrol (**CC**)

Limonene (**LI**)

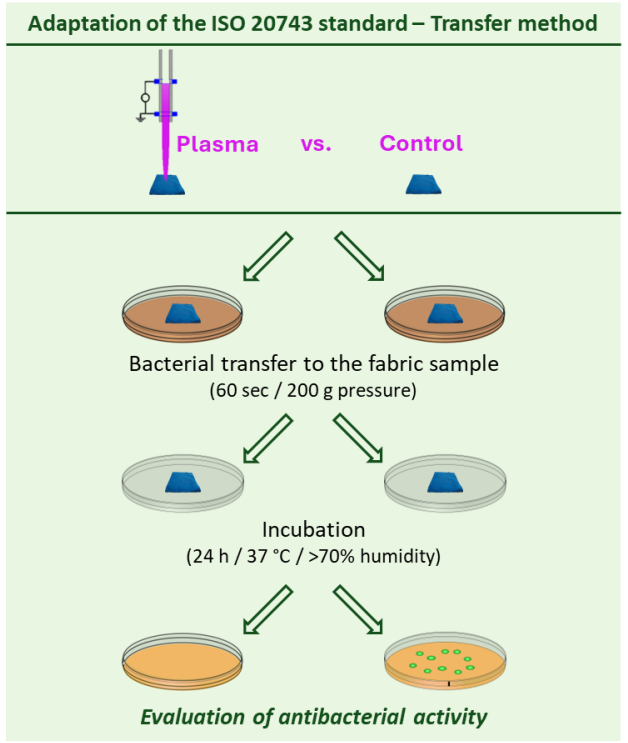
Citronellal (**CI**)

Eugenol (**EU**)

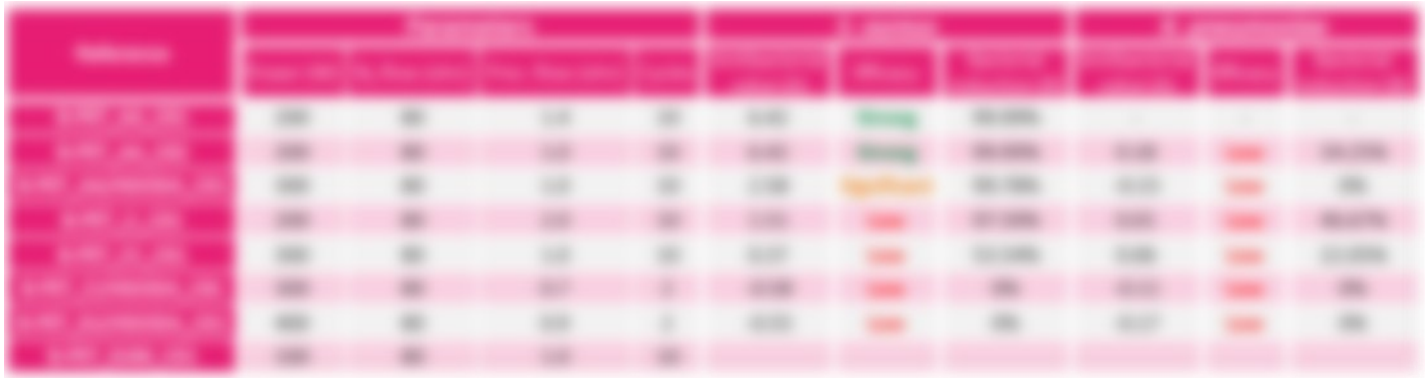
Eugenyl methacrylate (**EUM**)

1,6-Hexanediol diacrylate (**HDODA**)

Divinylbenzene (**DVB**)



Analysis of antimicrobial activity on textiles (B-PET)



✓ **AA and AA/HDODA (strong efficacy)**

✗ **LI, CC, EU and EUM (low efficacy)**

No effect against *K. pneumoniae*

Selected candidates for now

a) AA 100% and **b) AA 70% / HDODA 30%**

Effective against *S. aureus* with a uniform thin film

Ag-based benchmark: **SANITIZED T27-22 Silver**

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Cosmetic case study

Highlights

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Cellulose nanofibers as added value fillers in the skin cosmetics

WP7

IR, titration	→ chem. structure
AFM, SEM, TEM	→ size
MALS/DLS, FFF	→ size
XRD, NMR	→ crystallinity
GCMS, TOFMS	→ impurities
zeta potential	→ stability
surface charge (tit)	→ stability
FIB-SIMS	→ penetration

experimental and computational descriptors

- modelling of stability in electrolyte
- modelling of membrane penetration
- modelling of toxicity (metric is needed)
- modelling of sustainability (metric is needed)

SSbD

ex vivo skin models (healthy & stressed/ stressors: allergene, irritation, UV)	→ inflammation, viability, apoptosis
in vitro GIT model *in vitro* lung model	→ transport, barrier integrity, inflammation, viability
GIT mucus model	→ transport, viscosity
Zebra fish embryo model	→ developmental toxicity

worker, consumer and environmental exposure and risk assessment:
– measured data
– exposure models

future-oriented assessments of environmental, social, and economic sustainability

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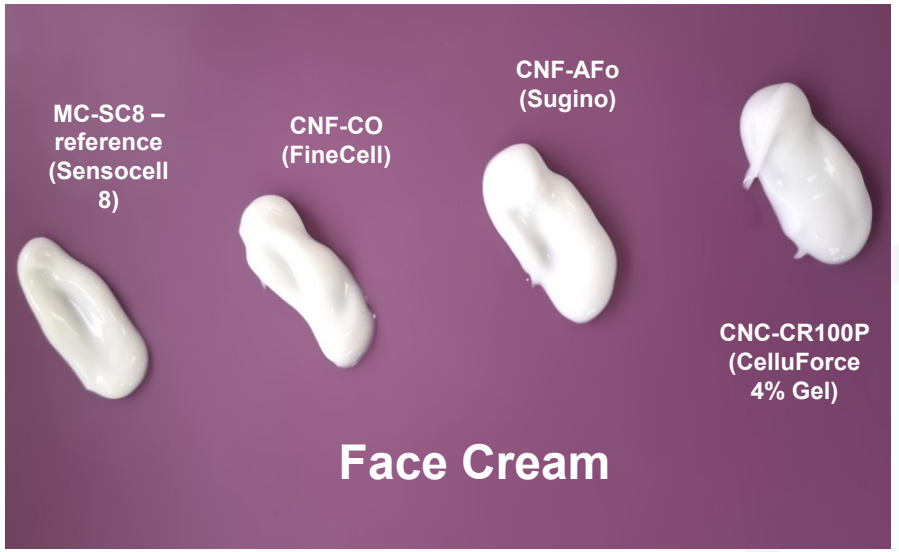
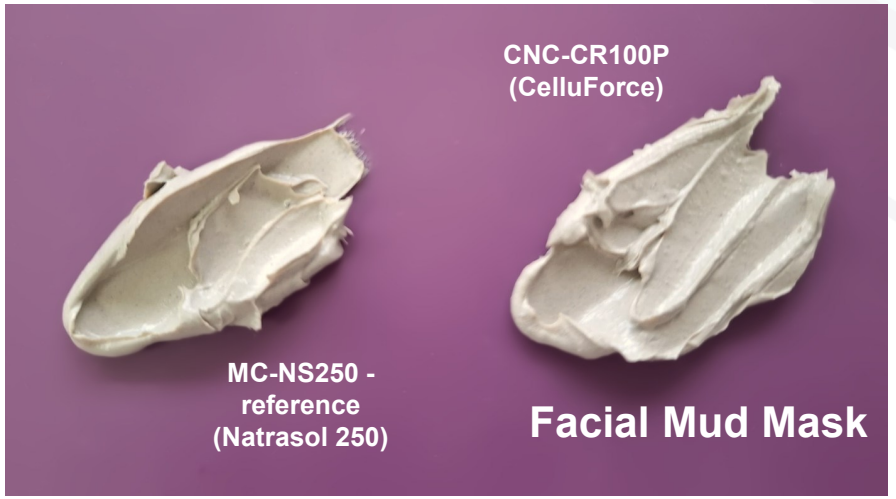
Cellulose nanofibers as added value fillers in the skin cosmetics

- Face cream
  - CNC-CR100P
  - CNF-AFO
  - CNF-CO
- Facial Mud Mask
  - CNC-CR100P
  - CNF-AFO
  - CNF-CO
- SPF lotion
  - CNC-CR100P
  - CNF-AFO
  - CNF-CO
- Dead Sea Mud
  - CNC-CR100P
  - CNF-AFO
  - CNF-CO





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Cellulose nanofibers as added value fillers in the skin cosmetics

- Face cream

Additive	Comment
CNC-CR100P 4% Gel (CelluForce)	Stability 3 months– OK Compared to the reference, it feels more "flowing", more surface area to apply on the skin, slightly improved application, better absorption, lighter feeling.
CNF-Afo 2% (Sugino)	1 month stability – OK Compared to the reference, it feels more "flowing", more surface area to apply on the skin, slightly improved application.
CNF-CO 2% (FineCell)	Stability 3 months – OK Compared to the reference, it feels more "flowing", more surface area to apply on the skin, slightly improved application.

AHAVA

- Facial Mud Mask

Additive	Comment
CNC-CR100P (CelluForce)	Compared to the original, the application is better, less sticky, and easier to wash. It smells the same as the original. 1 Month stability – free water occurs at Cycle and Heat (40 °C) env.
CNC-CR100P 4% Gel (CelluForce)	Will be prepared during May
CNF-CO 2% (FineCell)	Compared to the original, the same feeling.
CNF-Afo 2% (Sugino)	Compared to the original, the application is better, less sticky, and easier to wash. Smell is the same as the original. Stability 1 month – OK, continuing stability test

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Cellulose nanofibers as added value fillers in the skin cosmetics

- Dead Sea Mud

Additive	Comment
CNC-CR100P 4% Gel (CelluForce)	Good, feeling like reference, smooth texture. No water separation. Only visual tests. All tests will be done on a Pilot trial.
CNF-CO 2% (FineCell)	Good, feeling like reference, smooth texture. No water separation. Only visual tests. All tests will be done on a Pilot trial.
CNF-Afo 2% (Sugino)	Good, feeling like reference, smooth texture. No water separation. Only visual tests.

AHAVA

- SPF lotion

Additive	Comment
CNC-CR100P (CelluForce)	Stability 3 months done. OK at all temperatures. Feeling is better than reference with Xanthan Gum Pilot WAS done with suspension and with good results.
CNF-CO 2% (FineCell)	1 month stability - OK The texture is greasier. Not as good at spreading as Celluforce.
CNF-Afo 2% (Sugino)	The stability process started. The texture is greasier. Not as good at spreading as Celluforce.

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SSbD4CheM Case studies key takeaways

- Novel antimicrobial self cleaning coatings following processing requirements of Atmosferic Plasma Polymerization (APP).
- Studied precursors: SO, SO/HDODA, SQA, SQE showed hydrophobic coatings.
- Acrylic acid (AA) showed strong antimicrobial activity on textiles.

- Implementation of different cellulose materials
- CNF, CNC available at commercial and pre-commercial scale are tested addressing the safety and sustainability targets for 4 different cosmetic products.
- CNC & CNF tested showed good stability in e.g Face cream and Facial Mud Mask.
- Margin of Safety (MoS) for 4 CNF will be defined addressing different safety testing.

- Implementation of different WPCs as part of different car interior trims addressing the safety (emissions) and sustainability targets (recycled materials) set by automotive industry.
- Tested soft wood (Arbocel) and Hemp fibers are showing promising results addressing the set KPIs.
- Weathering tests followed by TVOC emission testing would ensure SSbD prototyping phase of selected car interior trims.

Novel NAMs developed within SSbD4CheM project will ensure safer production and application of SSbD4CheM coatings, composites and cellulosic materials following SSbD principles

PTR/TOF (Proton Transfer Reaction/Time of Flight, Vocus CI-TOF simulating a realistic exposure scenario (like a hot car in summer, 65°C for 4 hours; ISO 12219-3).

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