SSbD4CheM

From Innovation to Implementation: Applying the SSbD4CheM Toolbox in Case studies for Sustainable Material Design

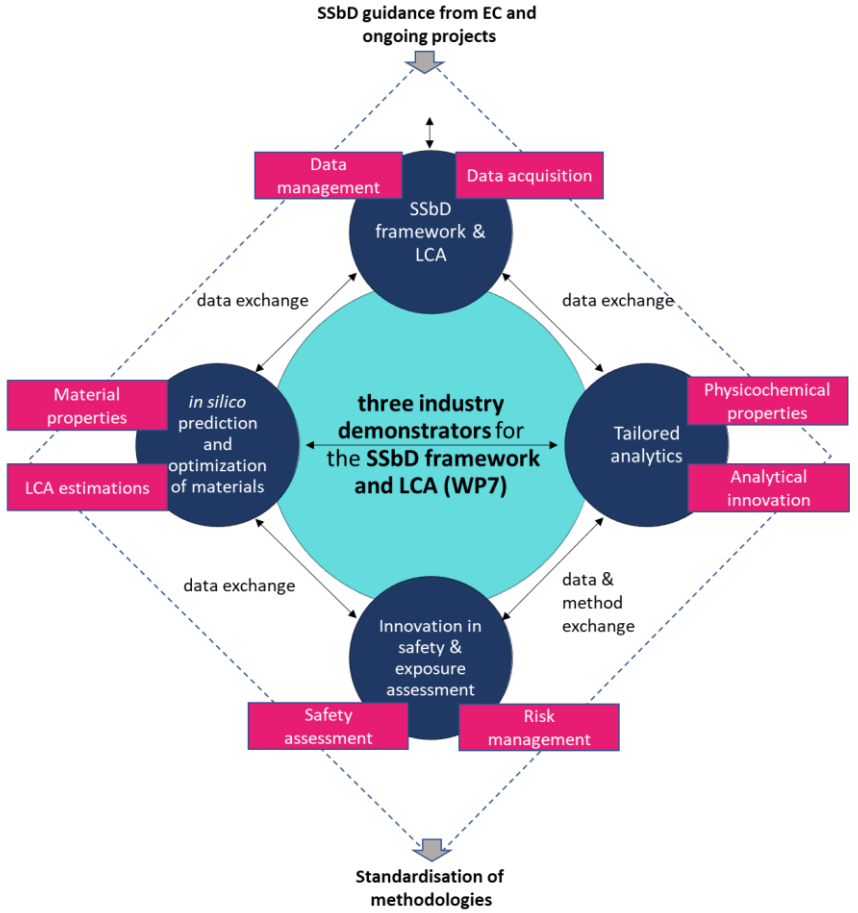
Milica Velimirovic Fanfani

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.

SSbD4CheM: safety and sustainability integrated in the chemical/product development

- 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:
  - 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



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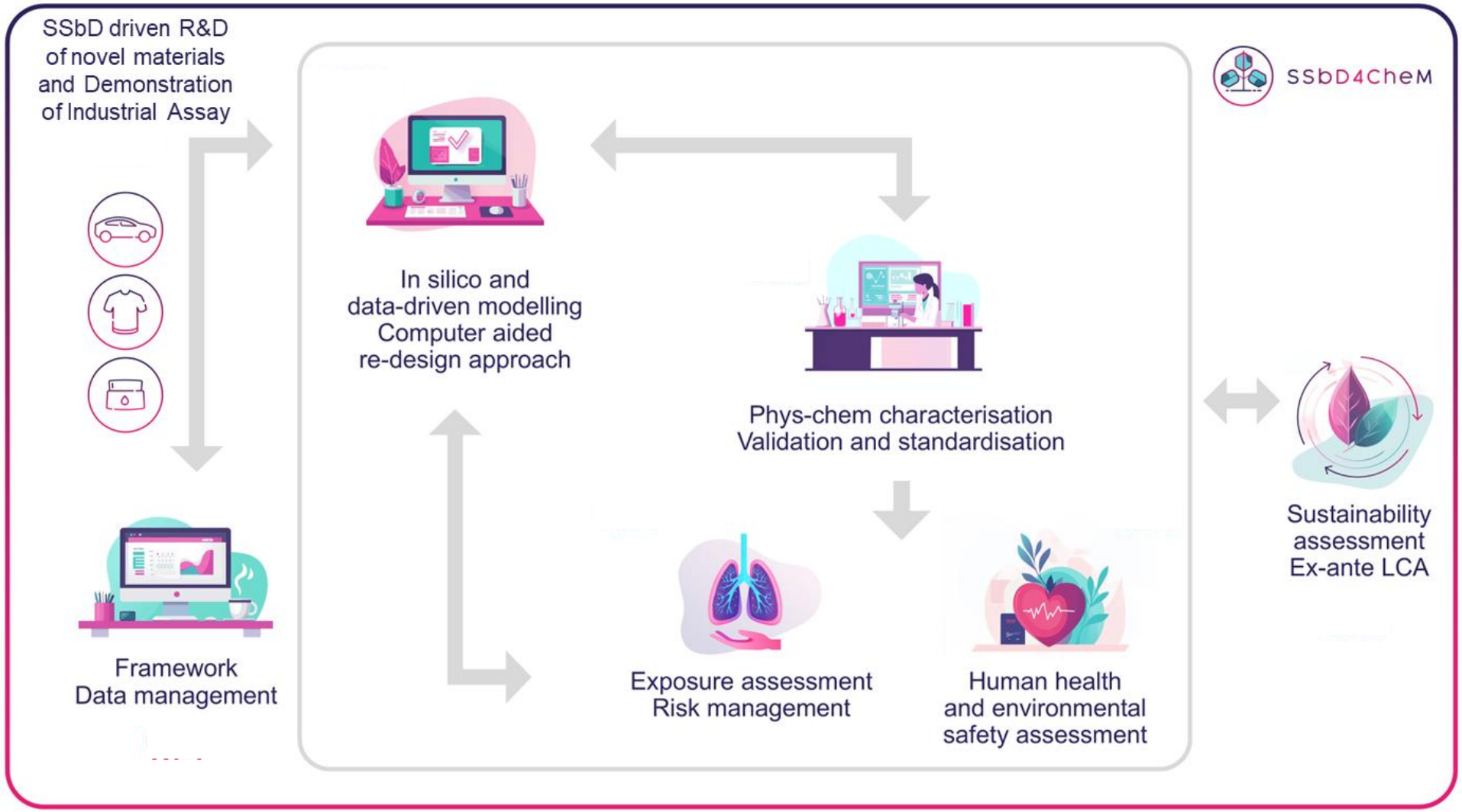
SSbD4CheM in a nutshell



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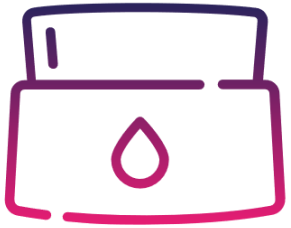
SSbD4CheM demonstrators

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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Renewable based composites for automotive interior parts

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

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

SSbD

In vitro lung model

→Transport, barrier integrity, inflammation, viability

Zebra fish embryo model

→lethality

Worker and consumer exposure and risk assessment:

- measured data;
- exposure models

LCA, s-LCA, and LCC

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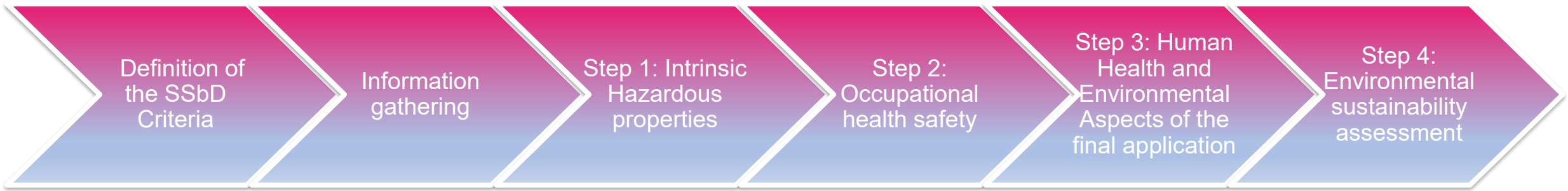
Methodology for the SSbD assessment in SSbD4CheM



- Definition of the criteria for every step

- Information about the materials and chemicals used is being gathered by communication with partners.

- Assessment of the chemicals based on the ECHA, CLP, bibliographic research and SDS.
- Qsar models and Data mining.

- Estimation of the production and processing-related risks. Risk estimated as a combination of chemical and/or material hazards, exposure and risk management measures.

- Likelihood of exposure to the chemical or material, potential exposure routes and related toxicity impacts on human health and the environment.

- Environmental sustainability aspects of the chemical or material.

In vitro tests if data are missing or there are new compounds.

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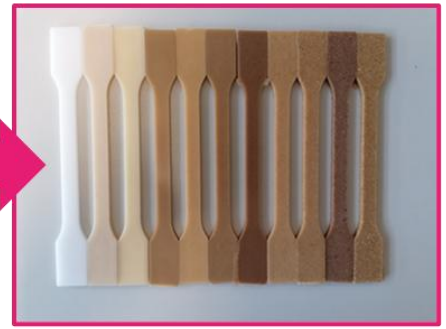
Wood Plastic Composites (WPCs)
Renewable PP
PP heterophasic copolymer
Recycled PP
Ultrafine cellulose
Regenerated cellulose
Soft wood, Hemp fibers
Hybrids
Talc compounds as reference material

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



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

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SSbD Step 1 & Step 2

Step 1. Hazardous properties of the chemical/material in question

Step 2. Human health and safety aspects of production and processing

General information															1st step					Step 2									
Trade Name	Product or chemical name	CAS number(s)	State/form	MSDS	Role in the formulation	Human health hazard	Enviromental hazards	Physical hazards	Human health hazard	Enviromental hazards	Physical hazards	Human health hazard	Enviromental hazards	Physical hazards	Criterium group				Level	Acute human health hazards	Chronic human health hazards	Physical properties	Hazards from release behaviour	Process-realted hazards	Safety		
						SDS information			Harmonized C&L Classification (Annex VI)			Bibliographic research			HHH	EH	PH	Global	Level	Score (0-4)					Total score	OHS Level	Aspect
Daplen EG 108 AI	Polypropylene TPO Compound filled with talc		pellets	N	matrix	Product does not require SDS in accordance with Article 31 of Regulation (EC) No 1907/2006 and ist amendments			-	-	-	NTE found	NTE found	NTE found	-	-	-	-	3	4	4	4	0		12	3	Low-risk
Borcycle™UJ599MO-71	Recycled PP Compound, polypropylene copolymer	9010-79-1	pellets	Y	matrix	Not classified	Not classified	Not classified	-	-	-	NTE found	NTE found	NTE found	-	-	-	-	3	4	4	4	4		16	4	Negligible risk
BJ400HP	Polypropylene		pellets	N	matrix	Product does not require SDS in accordance with Article 31 of Regulation (EC) No 1907/2006 and ist amendments			-	-	-				-	-	-	-	3	4	4	4	0		12	3	Low-risk
		No,																										

☒ Open processing *(yes, spray coating and sieve analysis equipped with an external ventilation and an appropriate air exchange)*
☒ Large area application (*yes sufficient enough (space related) to ensure safe application of powders as described in the document shared and once again attached)*

☐ Open design or partially open design, natural ventilation
☐ Partially open design, processing-related opening with simple extraction or open with simple extraction
☒ Closed processing with possibilities of exposure, e.g., during filling, sampling, or cleaning (Compounding areas *are equipped with an external ventilation and an appropriate air exchange)*

☐ Closed design, tightness not ensured, or partially open design with effective
☐ Closed design, tightness ensured, partially closed design with integrated extraction or partially open design with highly effective extraction

Engage 8842	Polyolefin Elastomer, ultra-low density ethylene-octene compolymer, 1-Octene, polymer with ethene	26221-73-8	pellets	Y	in blends with PP and PE, excellent flow characteristics	-	-	Combustible dust	Not classified	Not classified	Not classified	NTE found	NTE found	NTE found	-	-	C	C	2	4	4	3	0		11	3	Low-risk
PP ED007HP	Polypropylene polymer		pellets	Y	raw material for plastics industry	The product is not classified as hazardous accoridng to regulation (EC) No 1272/2008			Not classified	Not classified	Not classified	NTE found	NTE found	NTE found	-	-	-	-	3	4	4	3	0		11	3	Low-risk
Hemp fiber FZ517/150, Schwarzwälder Textilwerke			fibers	Y	filler	Not relevant	Not relevant	Not relevant	-	-	-	NTE found	NTE found	NTE found	-	-	-	-	3	4	4	4	0		12	3	Low-risk

0	Very high risk	0
1-5	High risk	1
6-10	Medium-risk	2
11-15	Low-risk	3
16-20	Neglible risk	4

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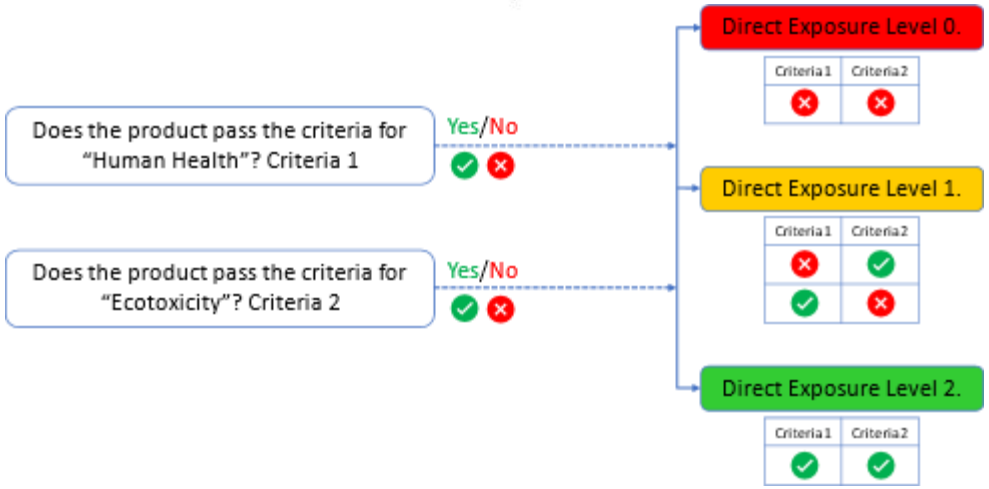
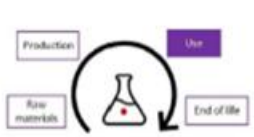
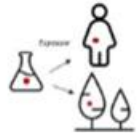
SSbD Step 3

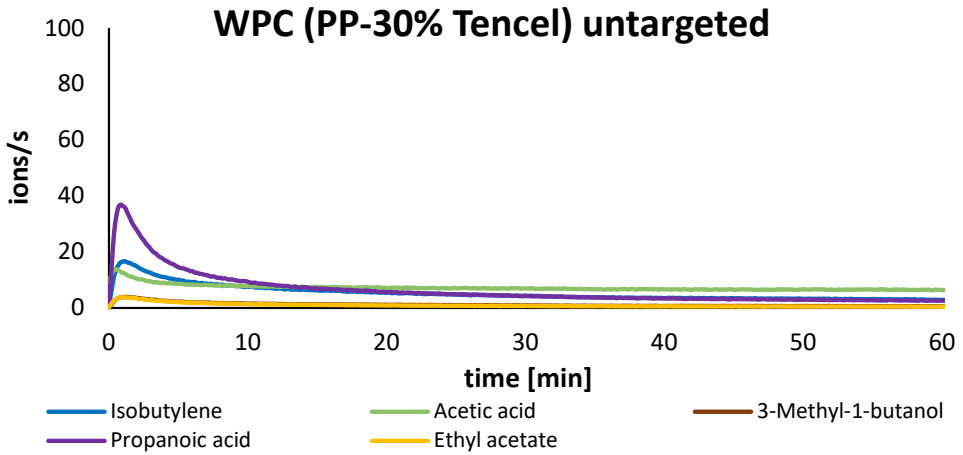
Step 3. Hazards and risks of the final application of the chemical or material in question

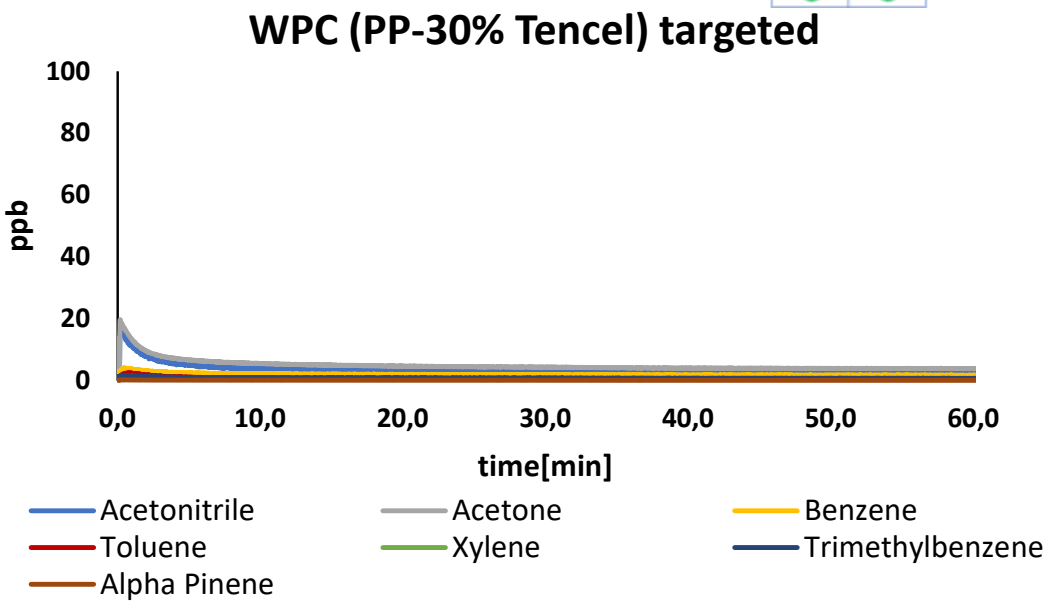


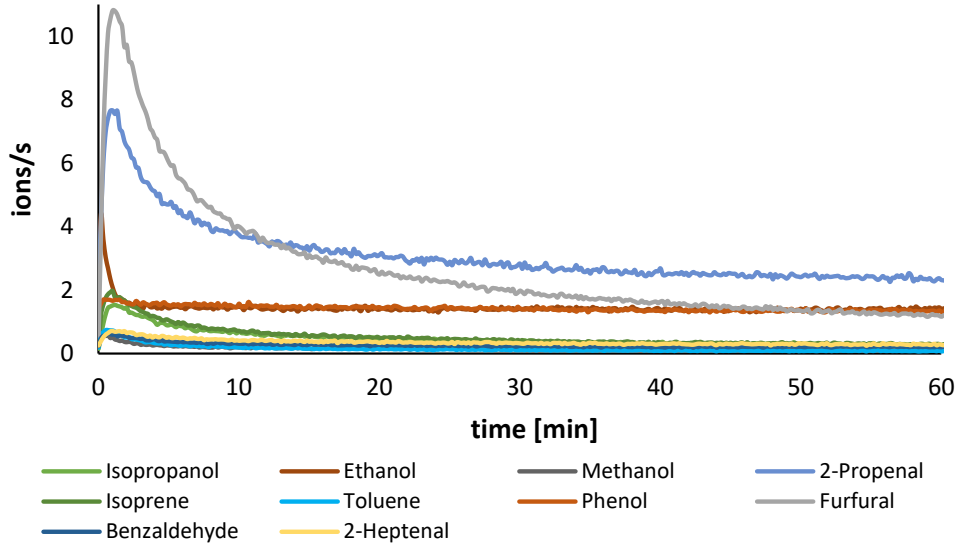




Proton-Transfer-Reaction Time-of-Flight Mass Spectrometry (VOCUS CI-TOF PTR/AIM) : **Heating cycle (4h, 65°C)**







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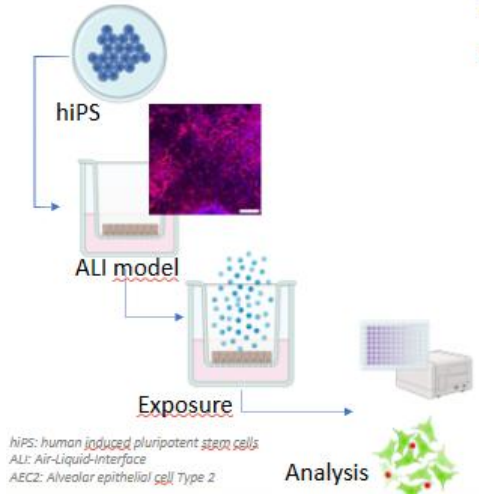
SSbD Step 3 Real-life simulation of chemical release for consumer and occupational setting

In silico models for exposure analysis

hiPSC-based in vitro lung model

Worker (Step 2) and consumer exposure (Step 3) and risk assessment

SSbD Toolbox developed within PARC: www.parc-ssbd.eu/



STEP 2

Stoffenmanager
RISKOFDERM
Advanced REACH -Tool
ProScale
EMKG-Expo-Tool
TREXMO
PMFA
INTEGRA
Spray Expo
E-FAST
ChemSTEER
Beat
MEASE
DNV GL Safeti

STEP 3

ConsEXPO
MERLIN-Expo Tool
Vermeer FCM
DPMFA
Consumer Exposure Model (CEM)

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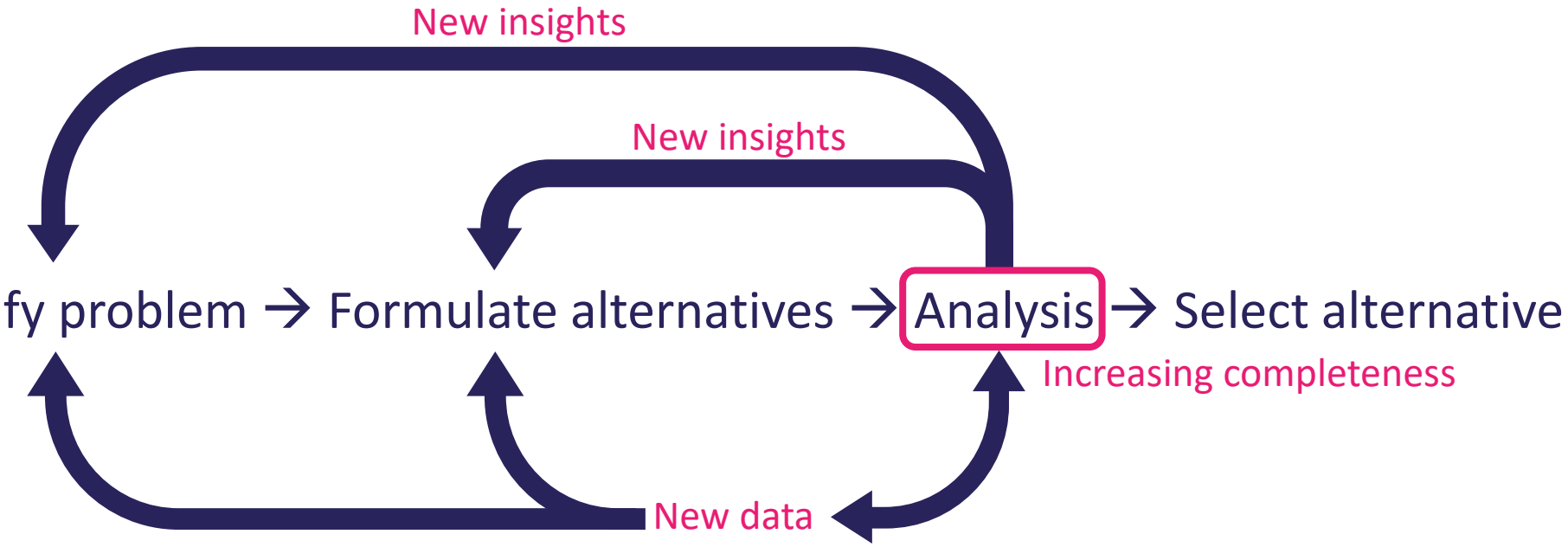
SSbD Step 4 LCA in SSbD: ex-ante & tiered

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



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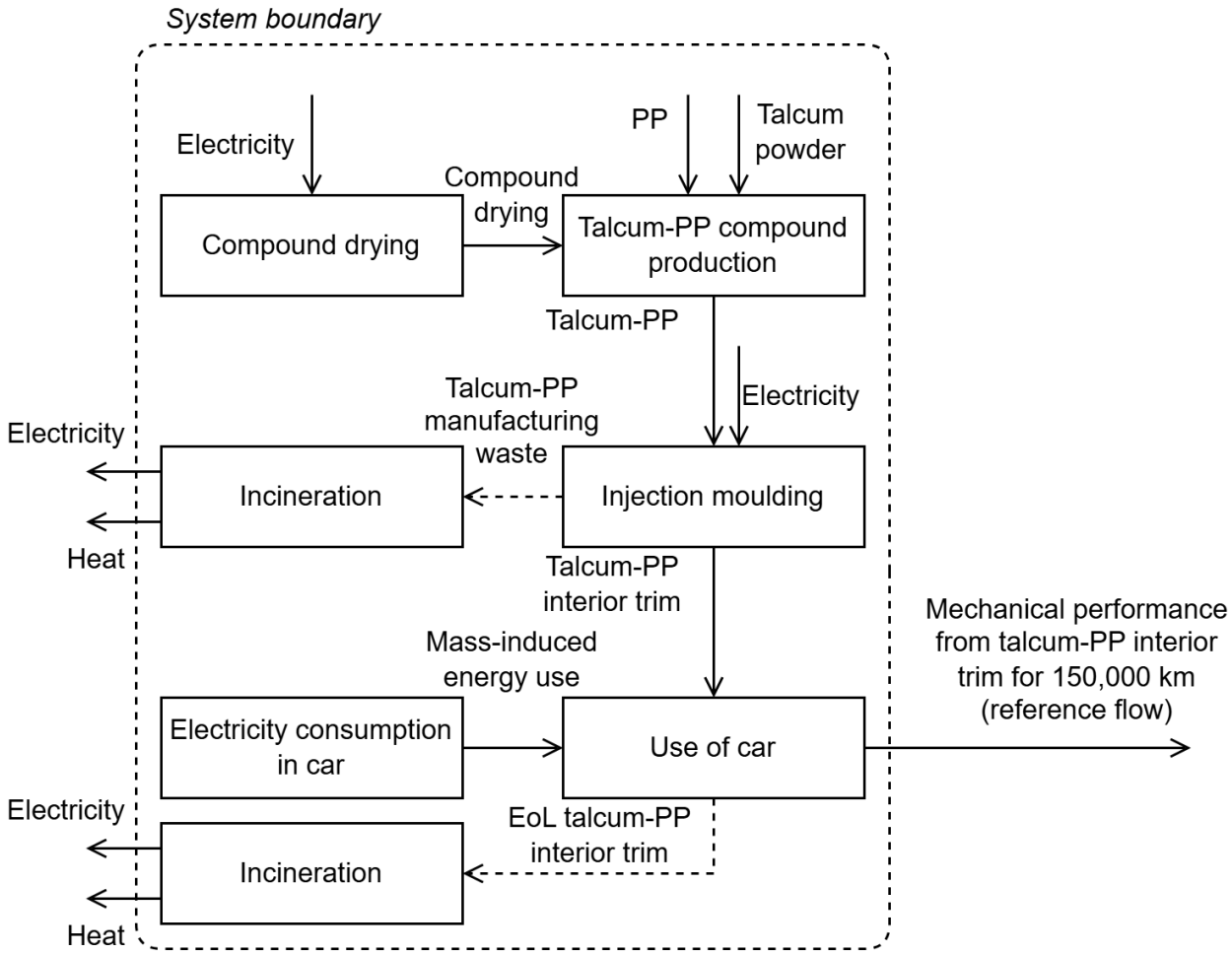
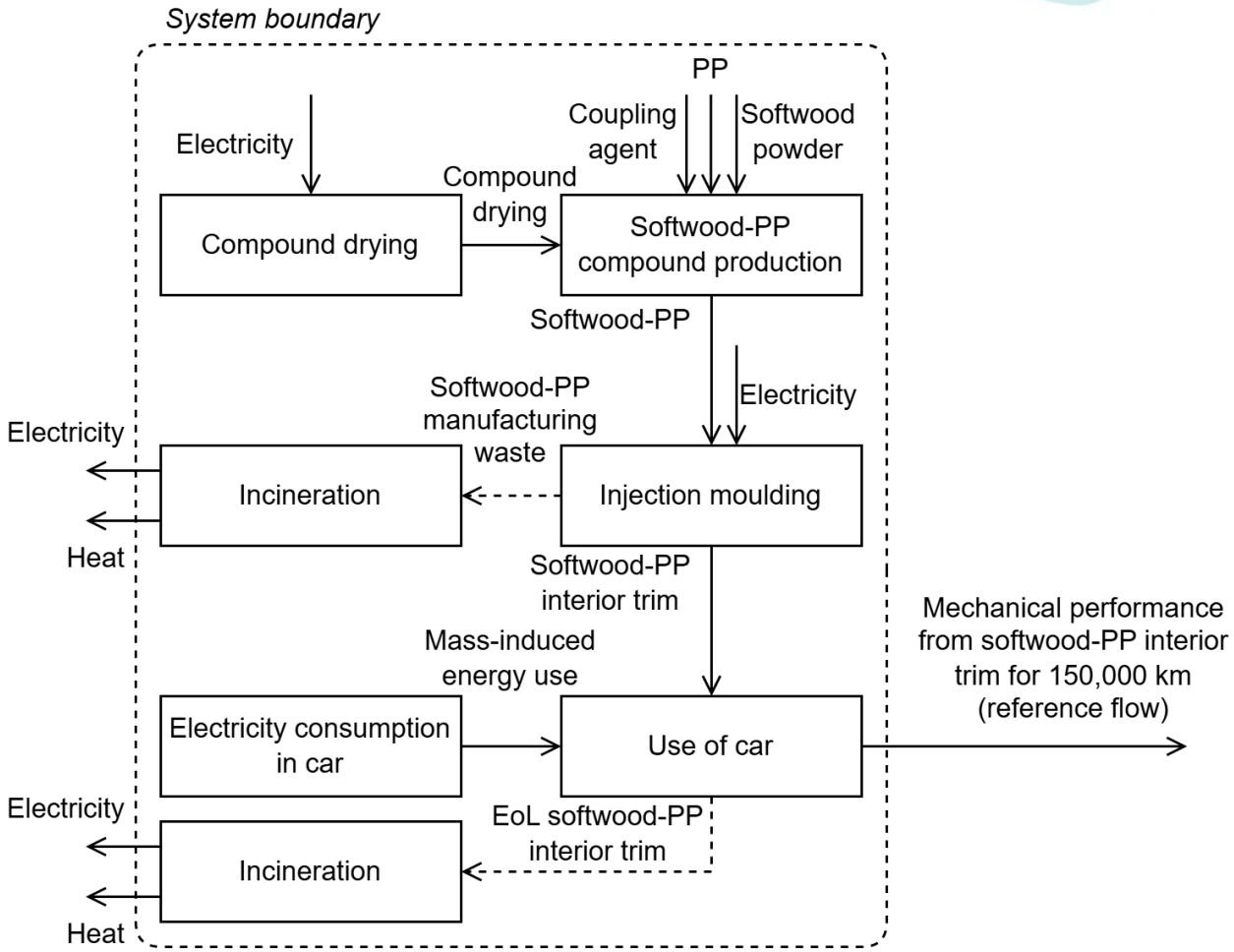
SSbD Step 4 Cradle-to-grave *ex-ante* LCA





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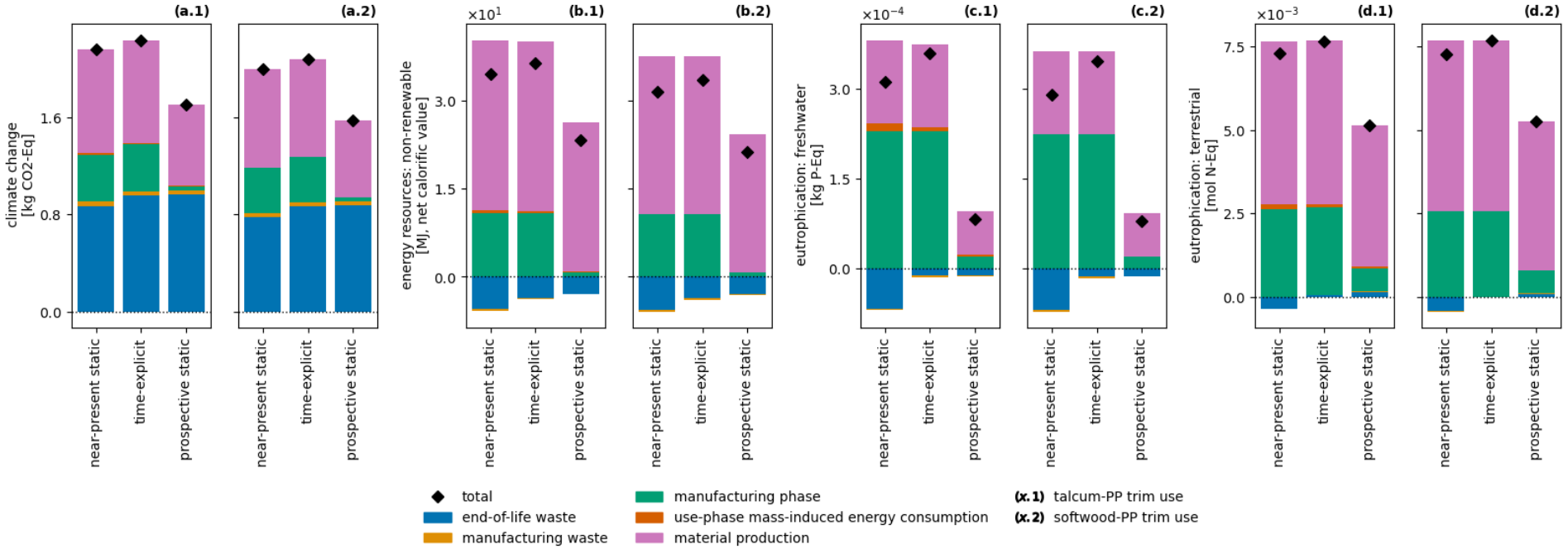
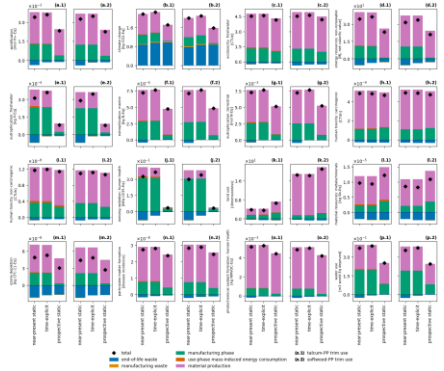
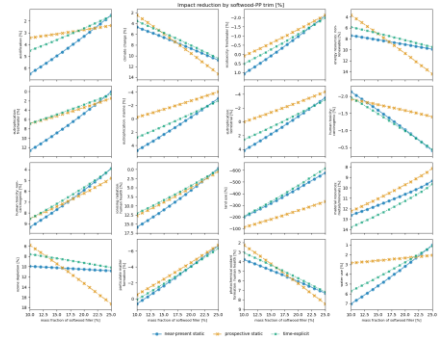
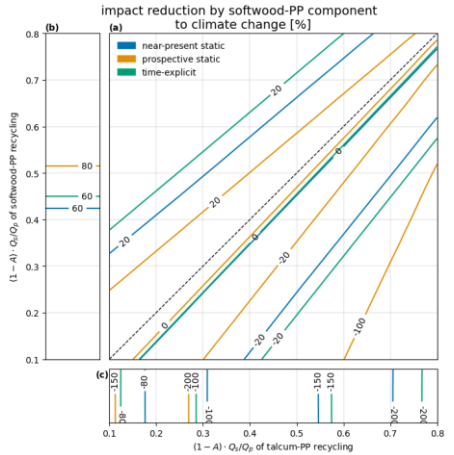
SSbD Step 4 Prospective & time-explicit LCA

- 16 mid-point impact categories assessed.
- Future activities modelled in a future economy.
- Exploring diverse scenarios for robust decision making: insights on material composition, use phase, and circularity.









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Computational and Structural Biotechnology Journal 29 (2025) 60–71

Contents lists available at ScienceDirect

Computational and Structural Biotechnology Journal

journal homepage: www.elsevier.com/locate/csbj

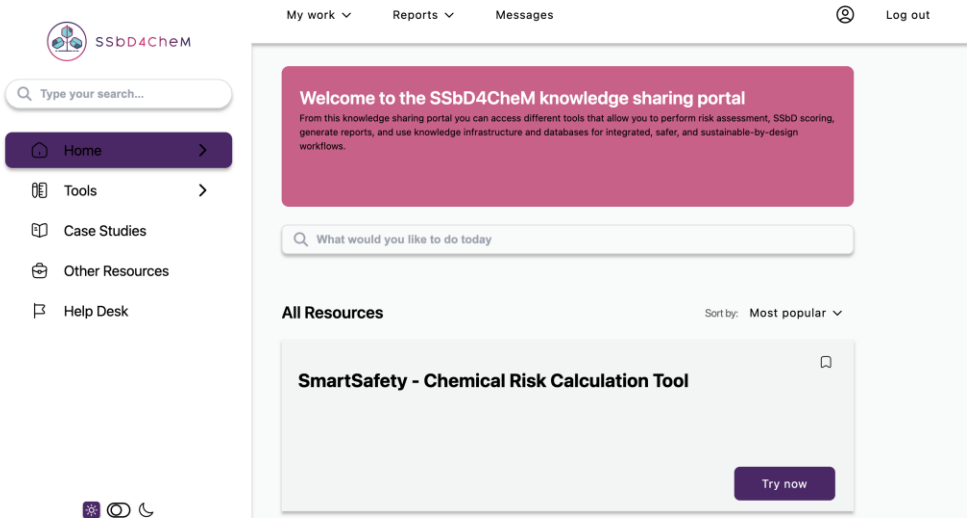
Innovation report

Safe and sustainable by design of next generation chemicals and materials: SSbD4CheM project innovations in the textiles, cosmetic and automotive sectors

Mansoor Ahmad Bhat [a], Tanja Radu [a], Ignacio Martín-Fabiani [b], Panagiotis D. Kolokathis [c], Anastasios G. Papadiamantis [d], Stephan Wagner [e], Yvonne Kohl [f], Hilda Witters [g], Wouter A. Gebbink [g], Yentl Pareja Rodriguez [g], Giuseppe Cardelini [h], Roel Degens [h], Ivana Burzic [i], Beatriz Alfaro Serrano [j], Claudia Pretschuh [i], Eduardo Santamaría-Aranda [k], Elena Contreras-García [k], Judith Sinic [i], Christoph Jocham [i], Dror Cohen [l,w], Ze'evi Maor [w], Assaf Assis [l,w], Ondrej Panák [m], Uroš Novak [m], Sukriti Hans [n], Antje Biesemeier [n], Pau Camilleri [o], Fruela Pérez Sánchez [o], Thomas Arblaster [p], Nils Thonemann [p], Jeroen Guinée [p], Andrea Pipino [q], Onur Çelen [r], Hariprasad Alwe [s], Roland Drexel [t], Roland Welz [t], Florian Meier [t], Indre Piragyte-Langa Oliva [u], Ghada Tagorti [u], Barry Hardy [u], Milica Velimirovic [v,*]

[a] School of Architecture, Building and Civil Engineering, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom
[b] Department of Materials, Loughborough University, Loughborough LE11 3TU, United Kingdom
[c] NovaMechanics MIKE, Piraeus 18545, Greece
[d] Entelos Institute, Nicosia 1065, Cyprus
[e] Institute for Analytical Research, Hochschule Fresenius, Limburger Str. 2, Idstein 65510, Germany
[f] Fraunhofer Institute for Biomedical Engineering IBMT, Joseph-von-Fraunhofer-Weg 1, Sulzbach 66280, Germany
[g] Health Unit, Flemish Institute for Technological Research (VITO), Boeretang 200, Mol 2400, Belgium
[h] VITO-EnergyVille, Boeretang 200, Mol 2400, Belgium
[i] Wood K plus-Kompetenzzentrum Holz GmbH, Division Biobased Composites and Processes, Altenberger Strasse 69, Linz 4040, Austria
[j] BioNanoNet Forschungsgesellschaft mbH, Kaiser-Josef-Platz 9, Graz 8010, Austria
[k] Department of Sustainability and Advanced Materials, Footwear Technology Center of La Rioja (CTCR), Raposal 65, Arnedo, La Rioja 26580, Spain
[l] Ahava Dead Sea Laboratories Ltd., Dead Sea, Israel
[m] Department for Catalysis and Chemical Engineering, National Institute of Chemistry, Hajdrihova 19, Ljubljana 1000, Slovenia
[n] Advanced Instrumentation for Nanoanalytics group, Scientific Instrumentation and Process Technology Unit, Luxembourg Institute of Science and Technology (LIST), Belvaux 4422, Luxembourg
[o] Instituto Tecnológico del Embalaje, Transporte y Logística (ITENE), Carrer d'Albert Einstein, 1, ValenciaPaterna46980 Spain
[p] Institute of Environmental Sciences (CML), Leiden University, Einsteinweg 2, Leiden 2333 CC, the Netherlands

https://doi.org/10.1016/j.csbj.2025.03.022



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Funding acknowledgements

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