Thematic talks

Topic 1: The Safe and Sustainable Approach in Material Science and Technology – **Thomas Exner**, Pink Project

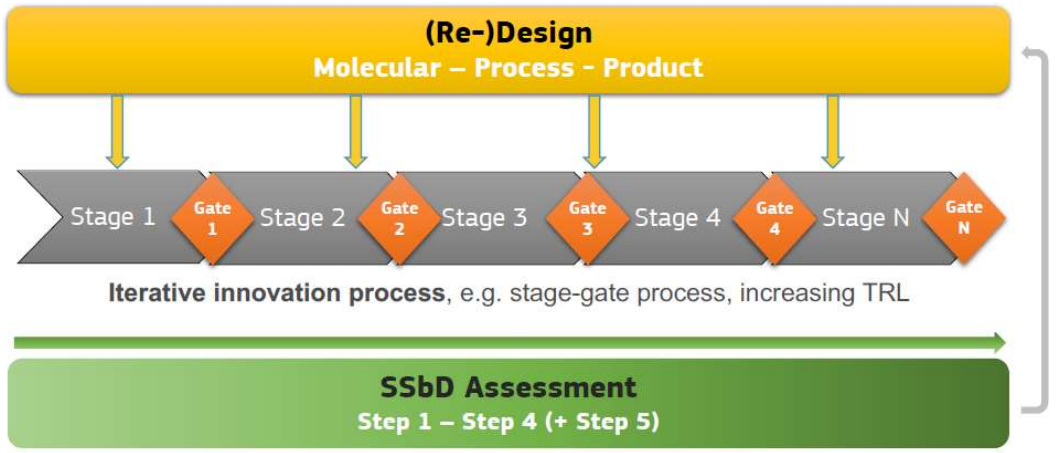
The starting point

European Commission

JRC TECHNICAL REPORT

Safe and Sustainable by Design chemicals and materials

Framework for the definition of



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

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

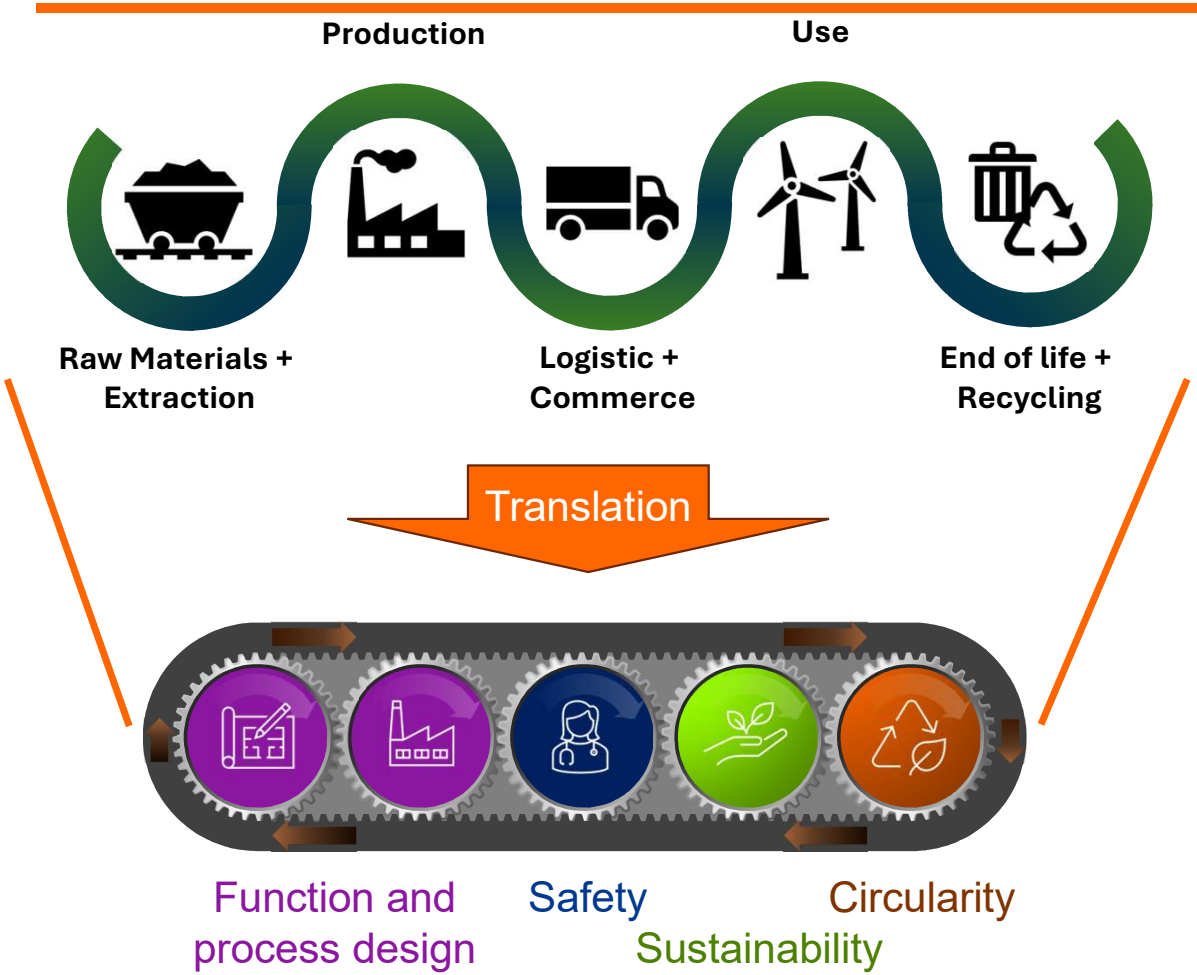
Step 3. Hazards and risks of the final application of the chemical or material in question

Step 4. Environmental impacts throughout the life cycle of the chemical or material in question

LCA

Step 5. **Social and economic** sustainability assessment

PINK's holistic approach



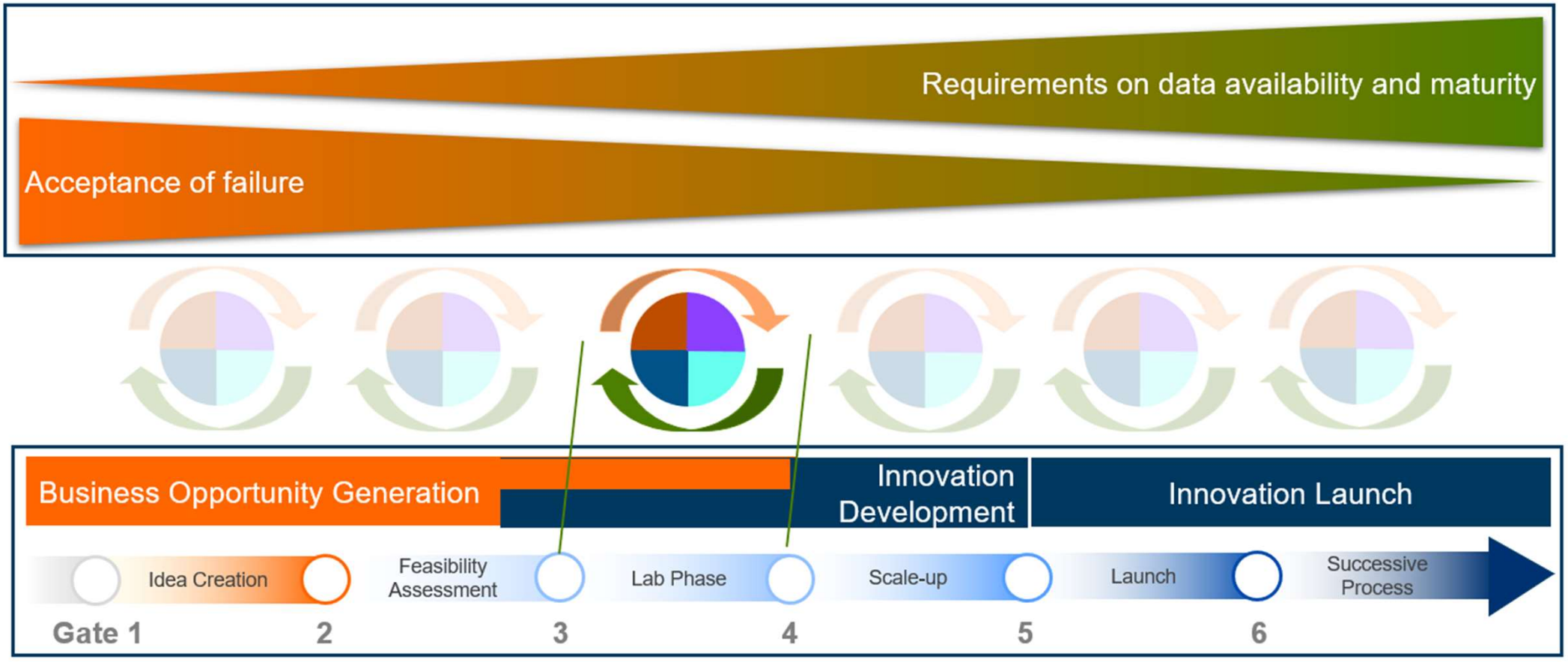
Holistic view on material value chain and life cycle

Tiered list of indicators representing the SSbD dimensions

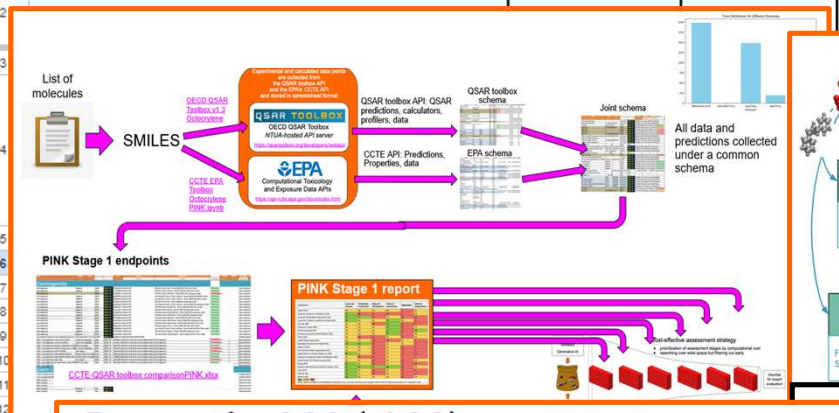
PINK's high-level objectives

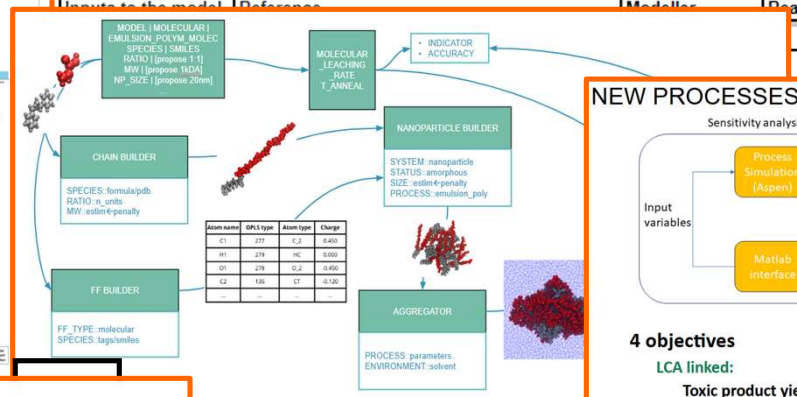
- DEVELOP innovative modelling and simulation approaches addressing industrial SSbD needs
- MAKE the software accessible to SMEs and industry through the open innovation platform ☞ *PINK In Silico Hub - PINKISH*
- VALIDATE the platform on PINK Developmental Case Studies and Industrial Demonstrators provided by SMEs and large industries
- REAL-LIFE industry needs:
  - Assessment challenges in biodegradability of co-polymers in aqueous dispersions (long-term toxicity?)
  - Long-term aquatic environmental effects of organic UV-blocker in cosmetics and personal care products
- Fully IMPLEMENT open science and FAIR principles contributing to establishing a European chemicals and materials data, modelling and software ecosystem
- STRENGTHEN knowledge transfer through collaboration and exploiting synergies
- BOOST the innovative capacity of SMEs and industry and make them more agile to respond to external and internal influences

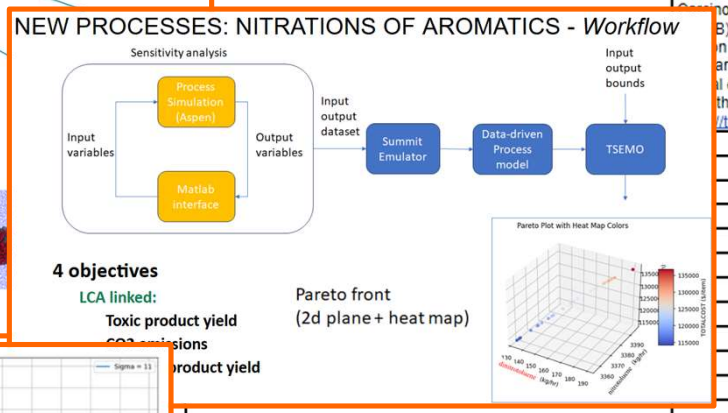
PINK's tiered approach

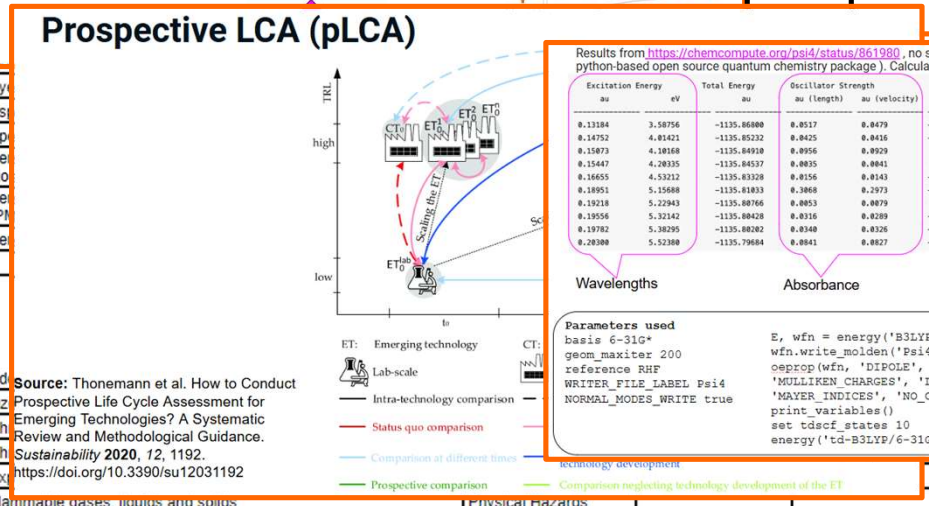


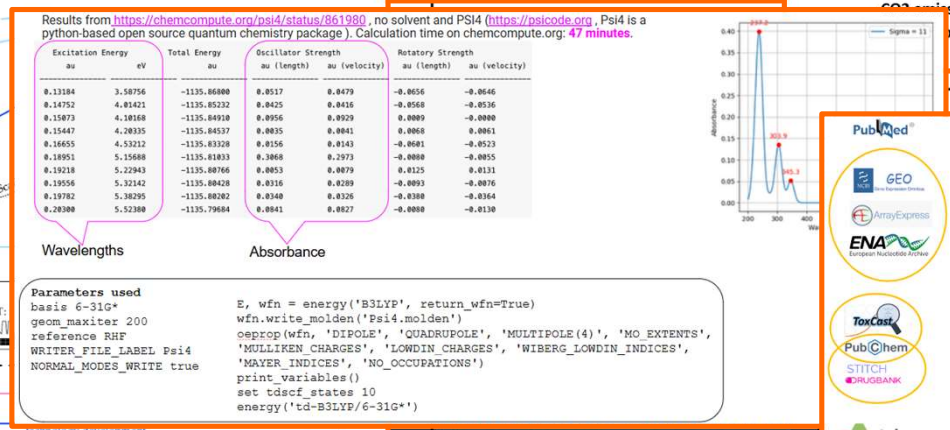
Tools for all SSbD dimensions

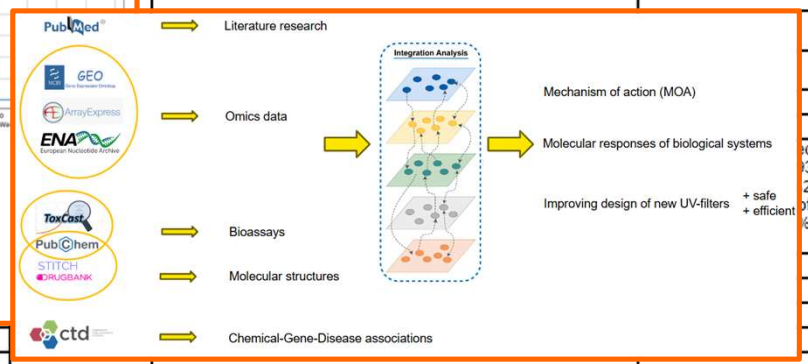




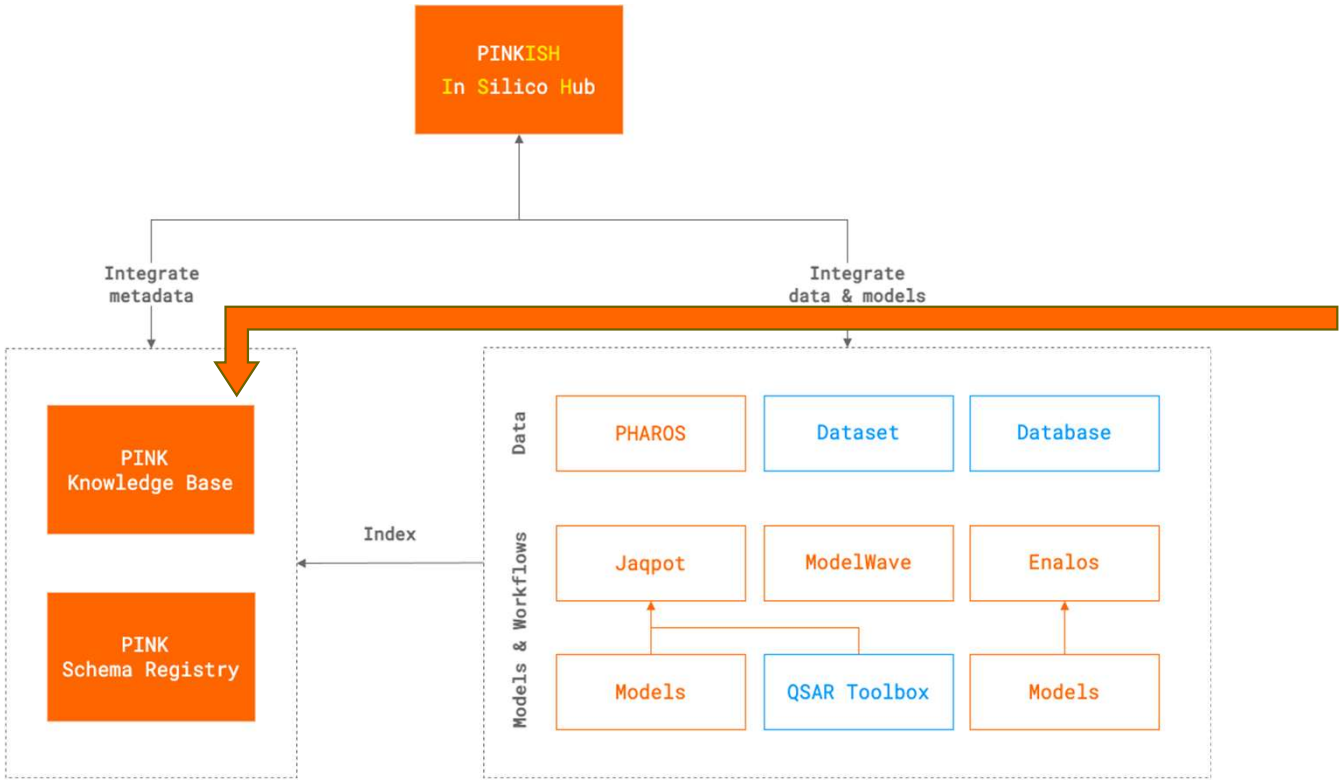






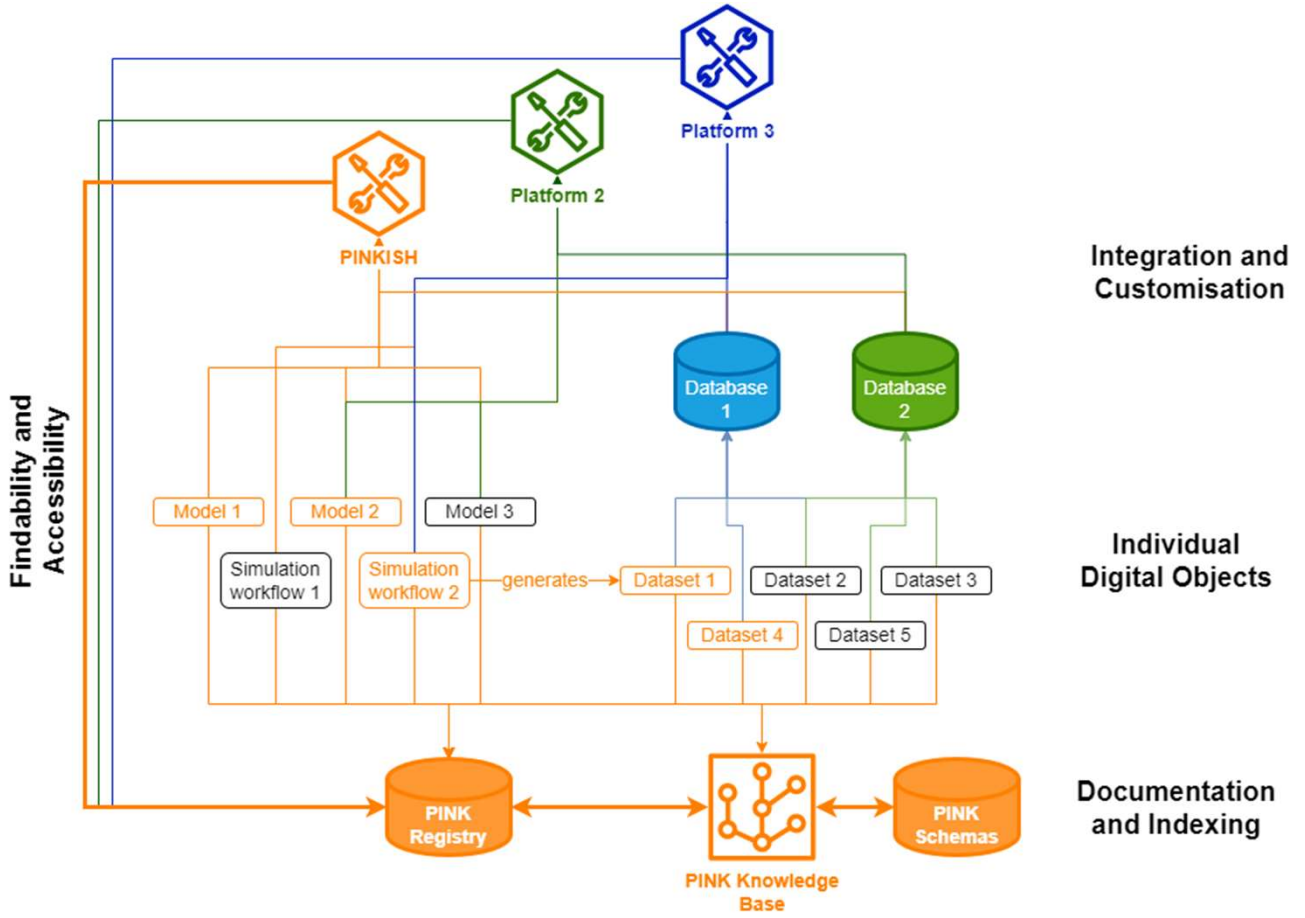


Working towards an interoperable ecosystem

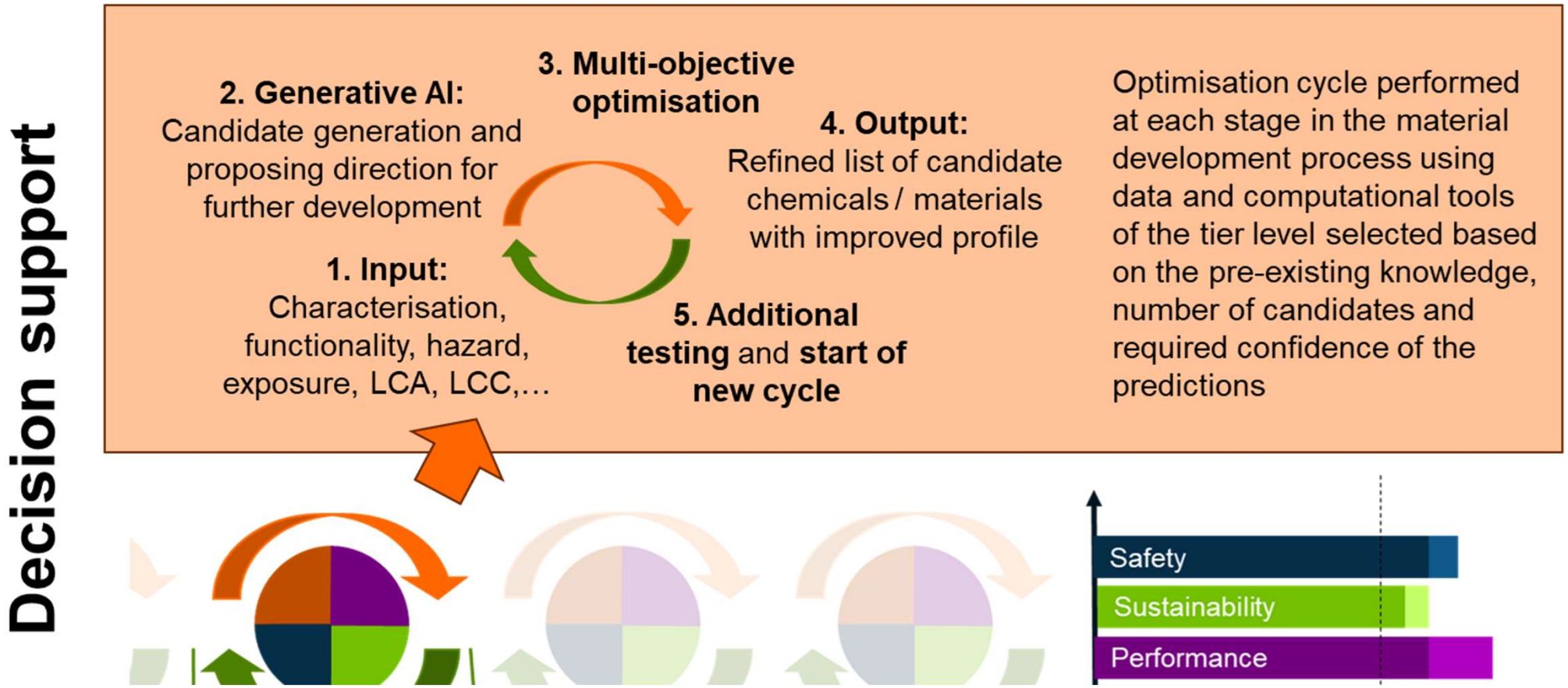


PINK metadata	
SSbD category	Safety
Subcategory	Human Health
Stakeholder in value chain to provide data	Starting material provider
Material life cycle stage	Starting material
Method	QSAR / Random Forest classifi
Method ID	https://app.jaqpot.org/dashbc s/2027
Indicator	Animal Carcinogenicity
Indicator ID	https://bioportal.bioontology. gies/ENM?p=classes&concept %2F%2Fpurl.enanomapper.org 2FENM_0000029
Input indicator	SMILES
Tier level (early, intermediate, late)	early
Chemical name	list of chemicals from training
CAS	list of chemicals from training
SMILES	list of chemicals from training

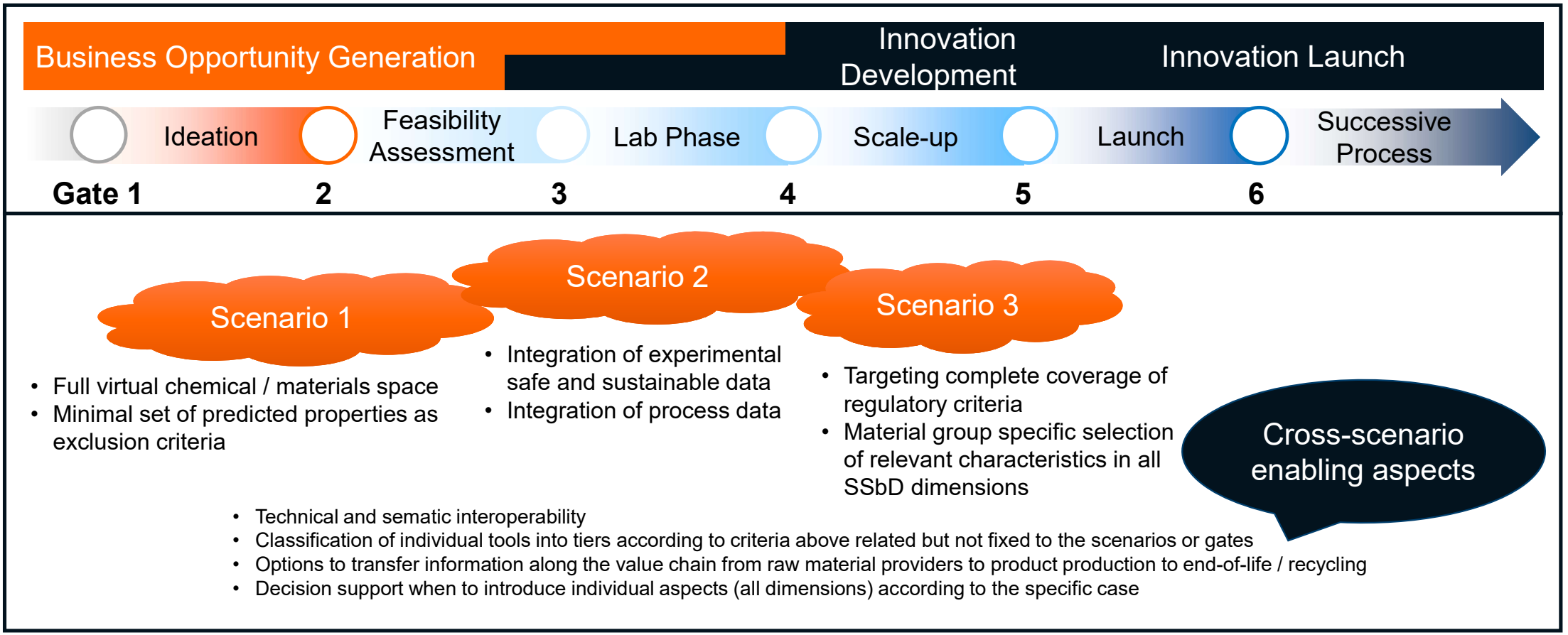
Working towards an interoperable ecosystem



Decision support for (re-)design



PINK's tiered approach



PINK's industry focus

Jan 2024 — June 2025 — Dec 2026 — Dec 2027

1. REFINE and 3. INTEGRATE

Requirement analysis, PINK Platform specification and Developmental Case Study definition

4. VALIDATE and 5. REAL-WORLD

Developmental Case Study execution driving PINK Platform development

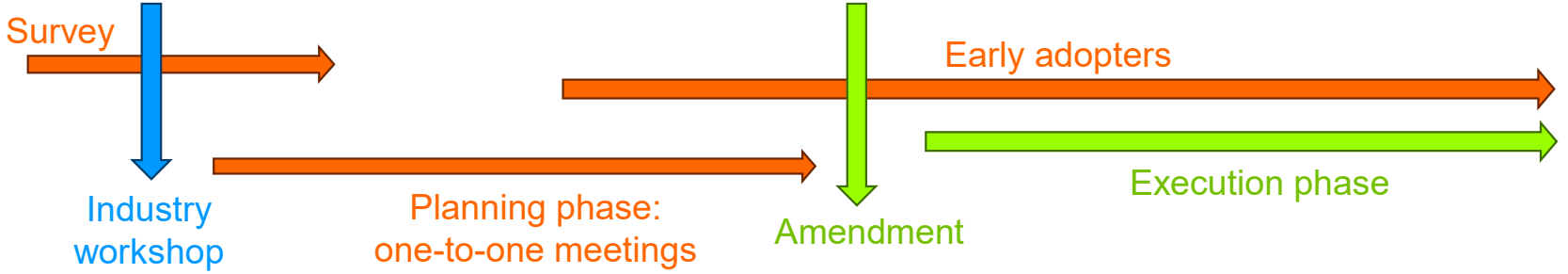
7. STRENGHTEN and 8. BOOST

Onboarding and execution of Industrial Demonstrators

Developmental Case Study 1: styrene/acrylate copolymers
→ low biodegradation

Developmental Case Study 2: organic UVB-filter
→ has to be classified for chronic aquatic effects

Industrial Demonstrators → to be defined



Developmental Case Studies

1. Organic synthetic UVB-filter used in sunscreens

- data-rich
- concentrations up to 10 wt% in cosmetic products
- environmental behaviour re-assessed
- low human health hazard
- **chronic aquatic effects**

2. Styrene/acrylate co-polymers used in aqueous polymer dispersions

- particles diameter 10 – 1500 nm
- important raw materials for industrial processes (Mt dispersions used)
- adhesives, paints, coatings, paper board coating, nonwoven fabrics, carpets, construction materials, textile finishing agents
- low human health and environmental hazard
- low **biodegradation**

Case Study 1

Organic synthetic UV-filter used in sunscreens

Octocrilene

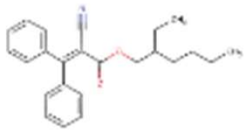
Regulatory process names 13 IUPAC names 20 Trade names 7 Other identifiers 4

Substance identity

EC / List no.: 228-250-8

CAS no.: 6197-30-4

Mol. formula: C24H27NO2



Hazard classification & labelling

According to the classification provided by companies to ECHA in **REACH registrations** this substance is very toxic to aquatic life with long lasting effects.

Properties of concern

PBT — Under assessment as Persistent, Bioaccumulative and Toxic

More details

Important to know

- Substance included in the Community Rolling Action Plan (CoRAP).

How to use it safely

- Precautionary measures suggested by manufacturers and importers of this substance.
- Guidance on the safe use of the substance provided by manufacturers and importers of this substance.

About this substance

This substance is registered under the REACH Regulation and is manufactured in and / or imported to the European Economic Area, at ≥ 1 000 to < 10 000 tonnes per annum.

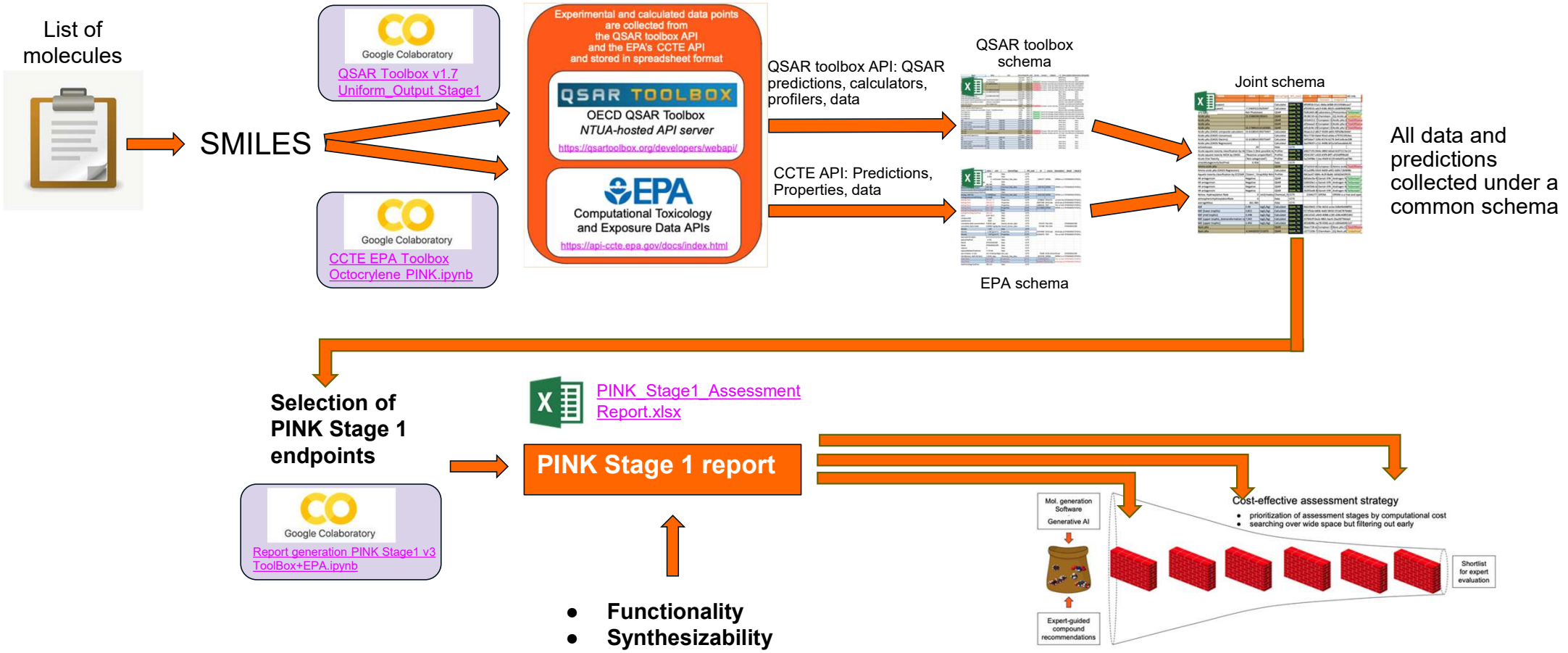
This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Source: ECHA substance information

Group definition	Human health hazards	Environmental hazards	Physical hazards
H1 Includes the most harmful substances (according to CSS), including the substances of very high concern (SVHC) according to REACH Art. 57(a-f).	❑ 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)	
H2 Includes substances of concern, as described in CSS, defined in the Article 2(28) of SPI proposal and that are not already included in Criterion H1.	❑ 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)	
H3 Includes the other hazard classes not part already in Criteria H1 and H2.	❑ 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

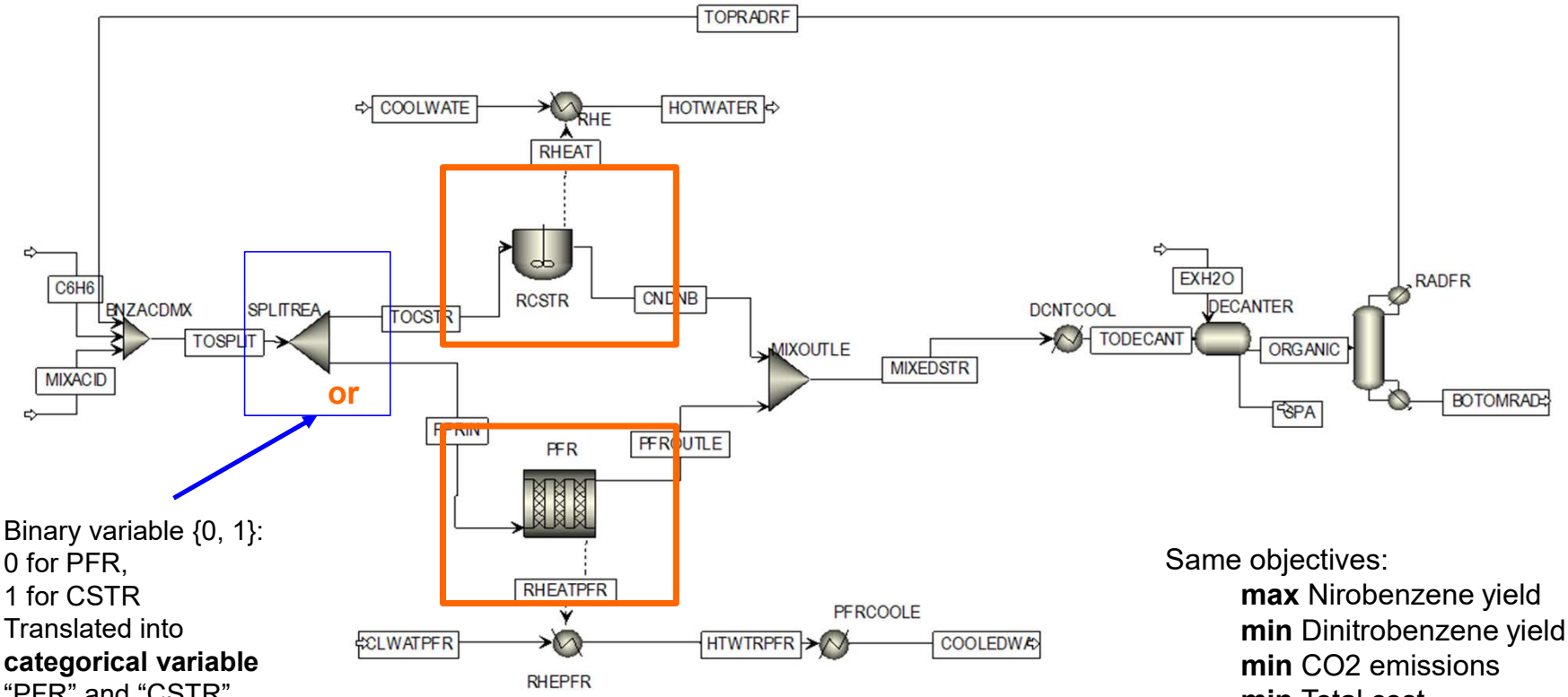
Drop-in replacement of SVHC, SHC, SoC

Workflow for SSbD



Process optimisation

Example process: nitration of benzene **Design options for reactor:** PFR or CSTR



Binary variable {0, 1}:
0 for PFR,
1 for CSTR
Translated into
categorical variable
"PFR" and "CSTR"

Same objectives:

- **max** Nirobenzene yield
- **min** Dinitrobenzene yield (toxic)
- **min** CO2 emissions
- **min** Total cost

PFAS replacement in food packaging

Coated paper substrate and thermoformed coated paper

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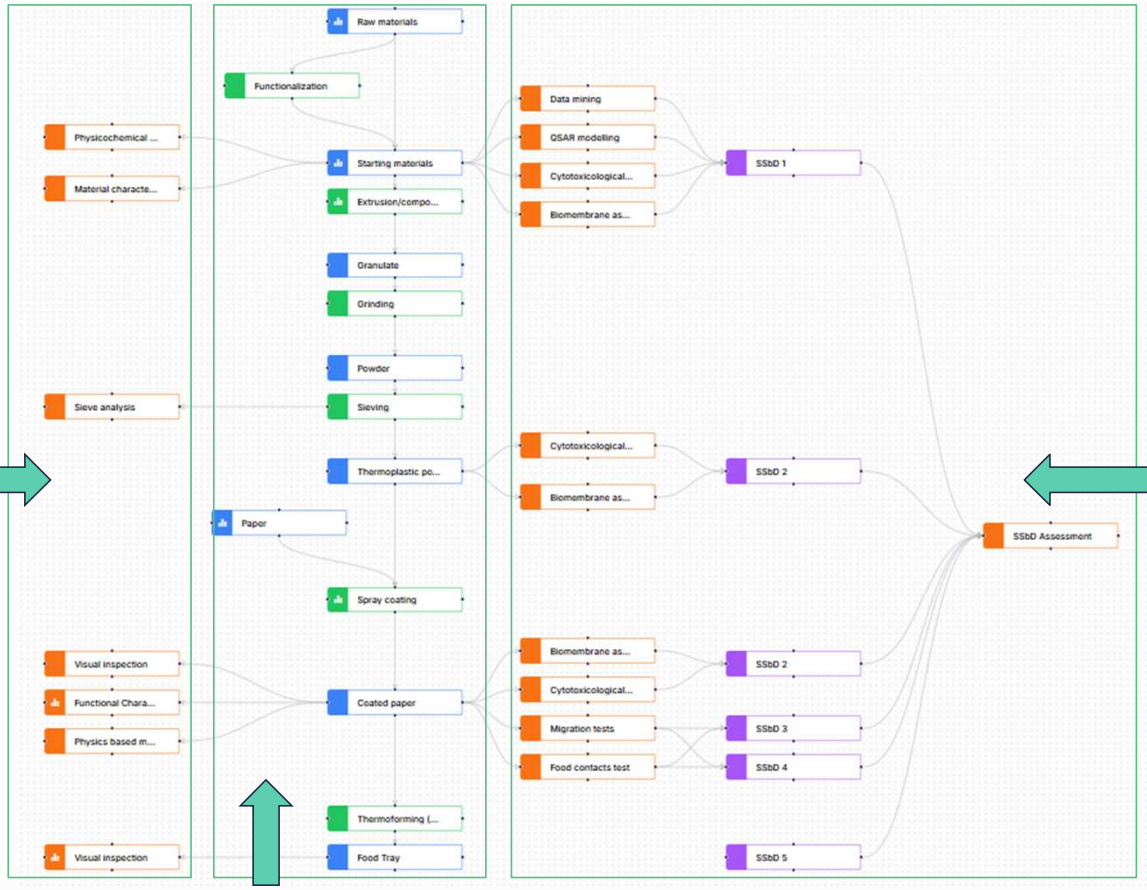
Study Design Maps

Characterisation, assessment of functionality



SSbD assessment

Coating development steps

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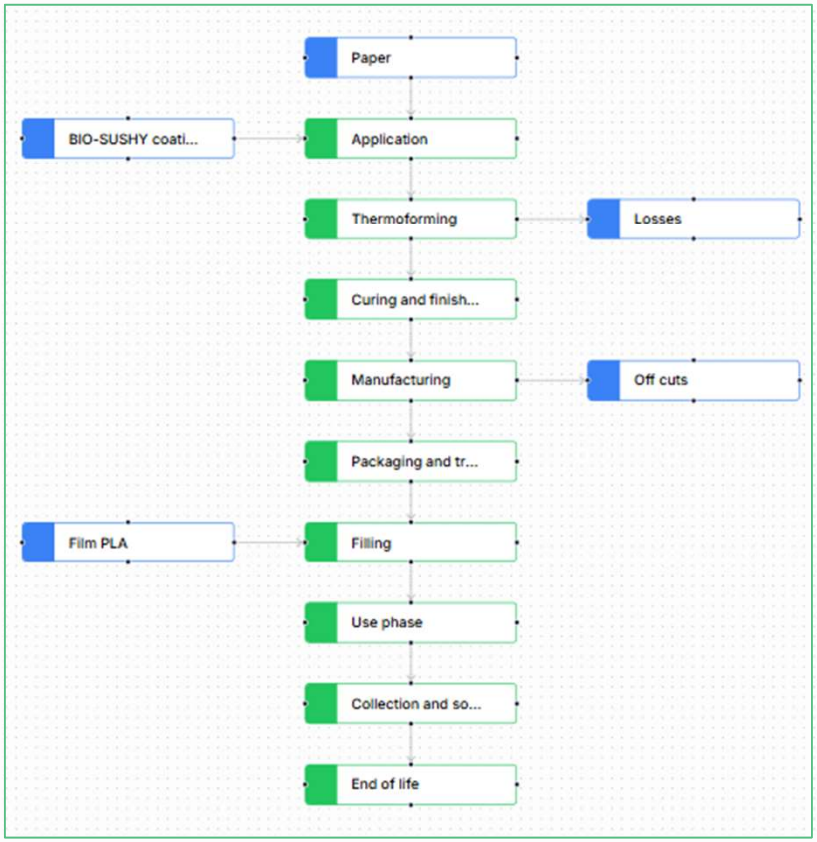
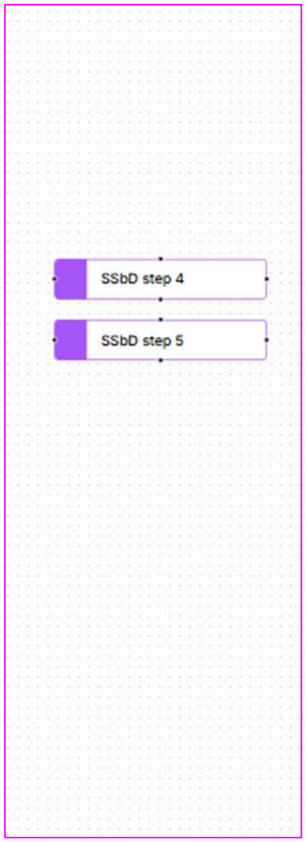
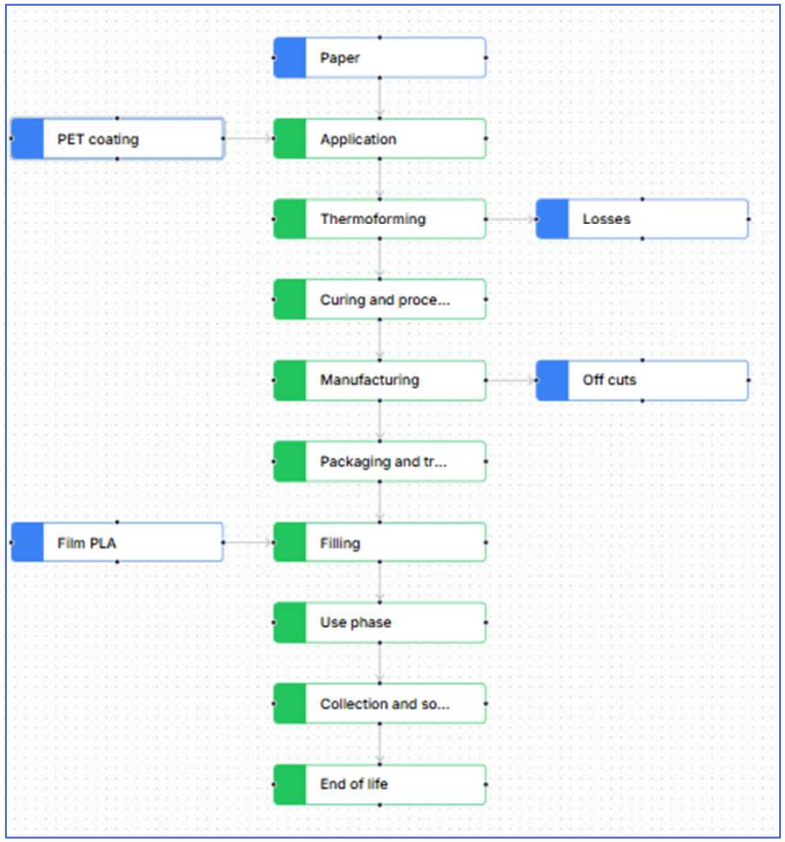
Comparative LCA







BIO-SUSHY coating LCA Benchmark

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PINK in two words

INTEGRATE

+ BALANCE

The PINK team

12 Beneficiaries - 2 Affiliated Entities - 2 Associated Partners

Jan 2024 - Dec 2027

1 Thomas Exner

2 Seven Past Nine

>PINK

>THANK YOU!

WWW.PINK-PROJECT.EU

BIO-SUSHY

MACRAMÉ

THE PINK PROJECT HAS RECEIVED FUNDING FROM THE EUROPEAN UNION'S HORIZON EUROPE RESEARCH AND INNOVATION PROGRAMME UNDER GRANT AGREEMENT NO. 101137809.

ASSOCIATED PARTNERS (I.E. (A) SWISS PARTNERS AND (B) UK PARTNERS) HAVE RECEIVED NATIONAL FUNDING FROM (A) THE SWISS STATE SECRETARIAT FOR EDUCATION, RESEARCH AND INNOVATION (SERI), AND (B) INNOVATE UK.

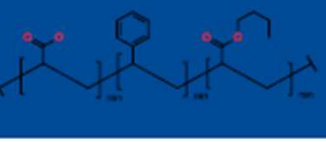
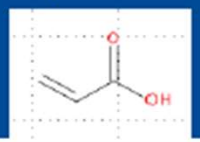
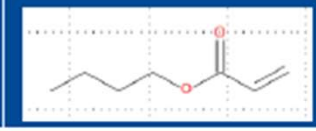
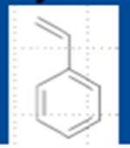
Case Study 2

Styrene/acrylate copolymers used in aqueous polymer dispersions

Styrene/acrylate copolymers are structurally similar polymers that result from the polymerisation of acrylate, methacrylate and styrene monomers.

Acrylate polymers biodegrade slowly under environmental conditions

Generic examples:

		2-Propenoic acid 	butyl 2-propenoate 	ethenylbenzene 
	coatings for paper & board	Approx. 5 %	Approx. 50 %	Approx. 45 %
	building adhesives and sealants	Approx. 3%	Approx. 68 %	Approx. 28 %
	architectural coatings	Approx. 3 %	Approx. 49%	Approx. 46%
	overprint varnishes & inks	Approx. 5%	Approx. 45%	Approx. 50%

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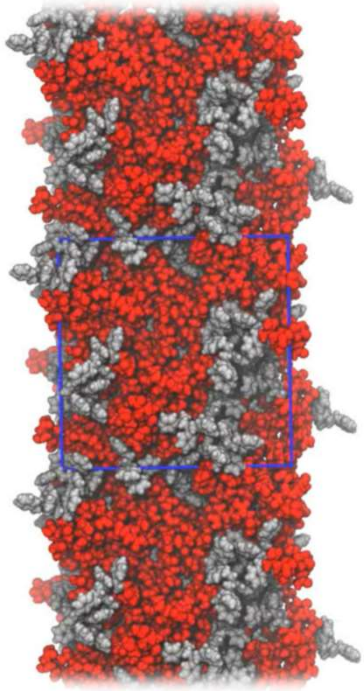
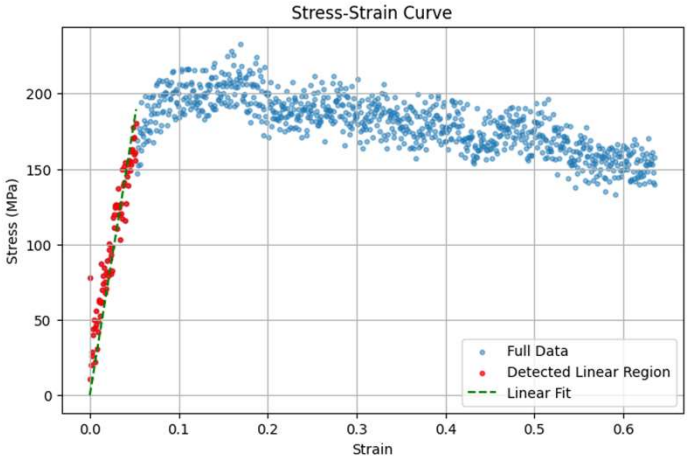
Workflow development – PS-PAA degradation

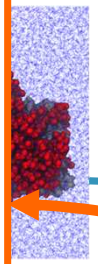
· **INDICATORS**



MD stress simulation



- Young's Modulus
- Yield Strength
- Fracture Strain



HYDROLITIC DEGRADATION

PROCESS::parameters
CONDITIONS::temperature

MECHANICAL DEGRADATION

PROCESS::parameters
ENVIRONMENT::solvent

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Tiered LCA

SSbD step 4: Life Cycle Assessment