

SSbD Tools and Use Cases - A walk in the PARC

PARC - Partnership for the Assessment of the Risks from Chemicals - 101057014

Tomas Rydberg, Fotini Nikiforou

SSbD chemicals and materials networking session, 2024-06-17

MaterialsWeek, Limassol, Cyprus

PARC



PARC project

Support to Green Deal and Chemical Strategy for Sustainability

Number of participating countries: 27

Austria (AT), Belgium (BE), Croatia (HR), Cyprus (CY), Czech Republic (CZ), Denmark (DK), Estonia (EE), Finland (FI), France (FR), Germany (DE), Greece (EL), Hungary (HU), Iceland (IS), Ireland (IE), Israel (IL), Italy (IT), Latvia (LV), Lithuania (LT), Luxembourg (LU), Netherlands (NL), Norway (NO), Poland (PL), Portugal (PT), Slovakia (SK), Slovenia (SI), Spain (ES), Sweden (SE), Switzerland (CH), United-Kingdom (UK)

Participating EU agencies/services:

3 agencies: EEA, EFSA, ECHA

and 5 DGs: DG R&I, DG ENV, DG SANTE, DG GROW and JRC



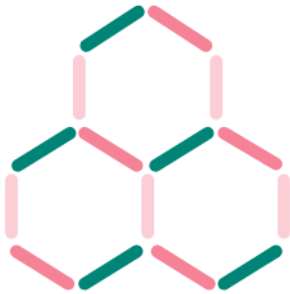



- A public-public **partnership** under Horizon Europe

- 7 years partnership – **400 millions euros co-funded**

- An initiative where the **European Union**, prepared with early involvement of **Member States and Associated Countries**, together with public partners (EU and National Risk Agencies, Universities, Public Research Organisations), commit to **jointly support the development and implementation of a programme** of research and innovation activities in relation with **the assessment of risk of chemicals**.

PARC thematic areas

 <h3>Risk assessment</h3>	 <h3>Tools & resources</h3>	 <h3>Building capacities</h3>	 <h3>Science to policy</h3>
<p>Monitoring +</p>	<p>Innovative tools and methods +</p>	<p>Laboratory networks +</p>	<p>Science to policy dialogue network +</p>
<p>Hazard assessment +</p>	<p>Safe and sustainable by design +</p>	<p>Online catalogues on exposure monitoring +</p>	<p>PARCopedia +</p>
<p>Innovation +</p>	<p>PARC FAIR Data Hub +</p>	<p>Trainings +</p>	<p>PARCroute +</p>
		<p>Skills development for FAIRification of PARC data +</p>	<p>Policy uptake and regulatory achievements +</p>

<https://www.eu-parc.eu/#thematic-areas>

PARC WP8 Tools, Task 8.1 SSbD

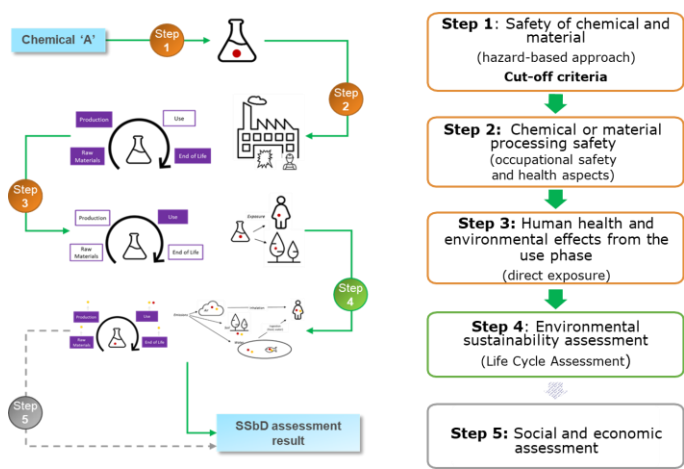
8.1: Supporting the operationalisation of the SSbD criteria and methodology developed by the EC and testing an SSbD toolbox to support the implementation of SSbD by the various users

Aktiviteter:

- 8.1.1 Translate EC SSbD criteria & methodology towards operationalisation
- 8.1.2 Toolbox development
- 8.1.3 SSbD toolbox operationalisation: Use cases & indicators
- 8.1.4 Knowledge sharing & Education
 - as key factors for efficient SSbD operationalisation

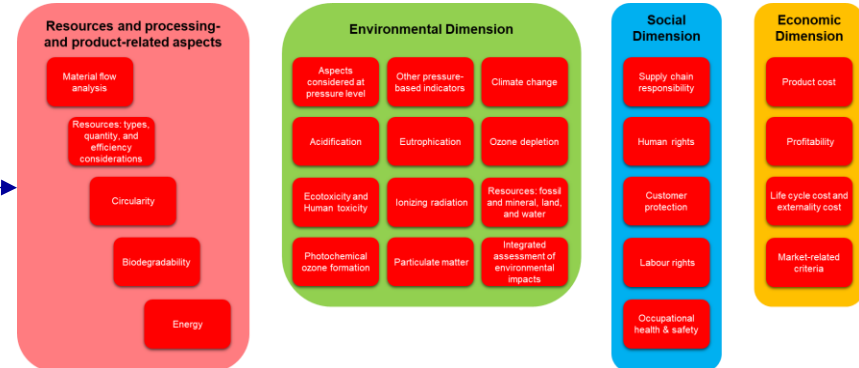
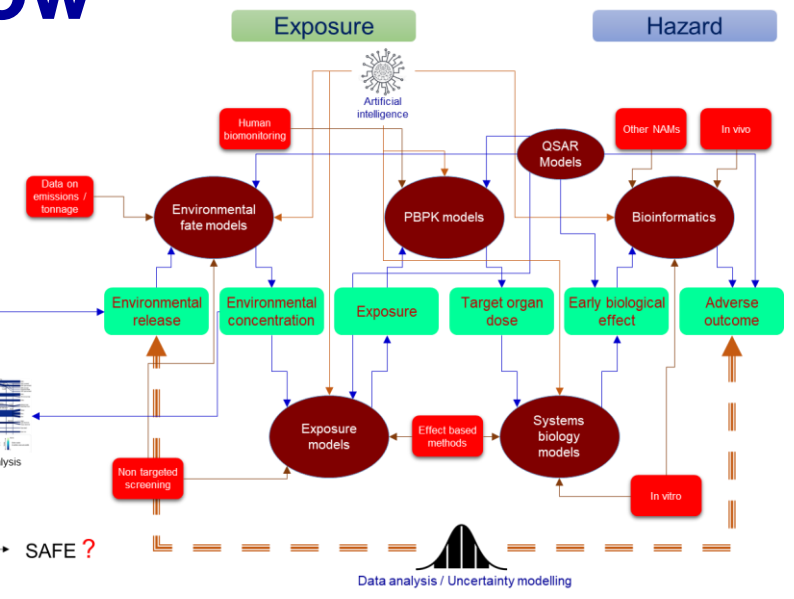
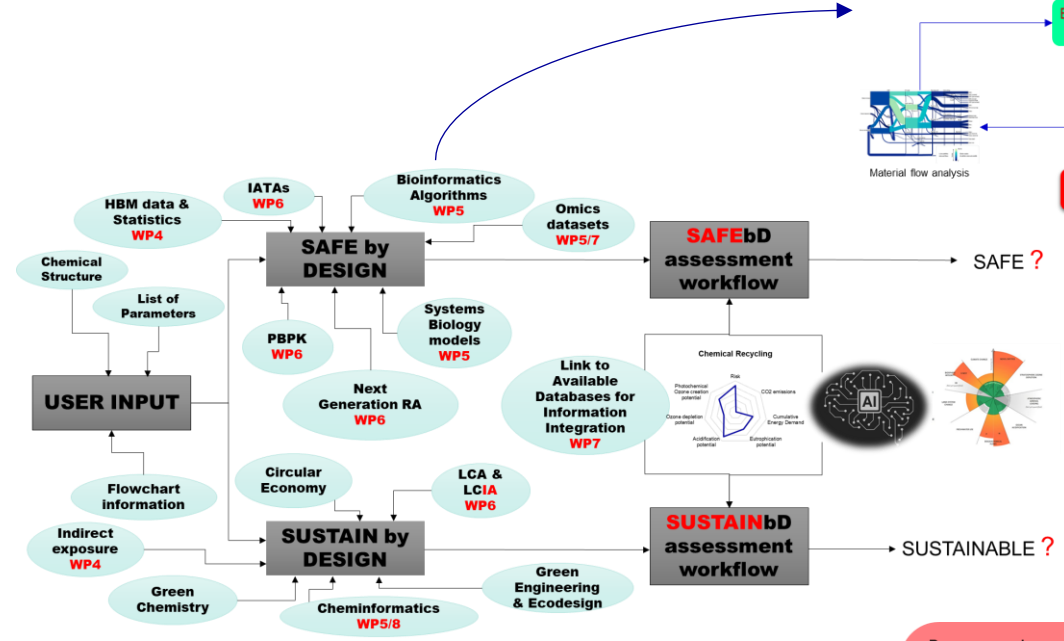
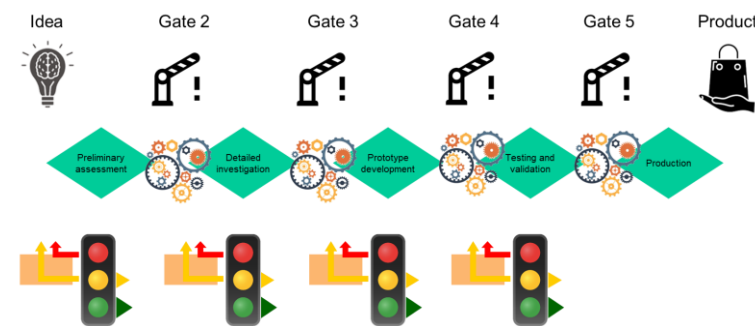
SSbD assessment workflow

PARC toolbox concept



Need to integrate the assessment steps of the SSbD framework

Facilitate SSbD assessment at each innovation stage





Brussels, 8.12.2022
C(2022) 8854 final

COMMISSION RECOMMENDATION

of 8.12.2022

establishing a European assessment framework for 'safe and sustainable by design' chemicals and materials

Review of safety and sustainability dimensions, aspects, methods, indicators, and tools



JRC TECHNICAL REPORT

Safe and Sustainable by Design chemicals and materials

Review of safety and sustainability dimensions, aspects, methods, indicators, and tools

Caldeira, C, Farcal, R, Mancini, L, Rasmussen, K, Sala, S.

2022

Framework for the definition of criteria and evaluation procedure for chemicals and materials



JRC TECHNICAL REPORT

Safe and Sustainable by Design chemicals and materials

Framework for the definition of criteria and evaluation procedure for chemicals and materials

Caldeira, C, Farcal, R, Mancini, L, Rasmussen, K, Sala, S.

2022

Application of the SSbD framework to case studies

DRAFT FOR CONSULTATION



JRC TECHNICAL REPORT

Safe and Sustainable by Design chemicals and materials

Application of the SSbD framework to case studies

DRAFT

Caldeira, C, Farcal, R, Mancini, L, Rasmussen, K, Sala, S.

2023



ISSN 1831-9424

Safe and Sustainable by Design chemicals and materials - Methodological Guidance

Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H., Sala, S.

2024



Joint Research Centre

EUR 131942 EN



Joint Research Centre

EUR 30991 EN



Joint Research Centre

EUR 31100 EN



Co-funded by the European Union

8.1.1

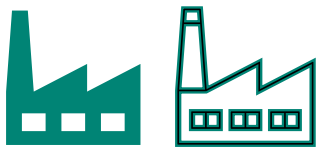
Translate EC SSbD criteria & methodology towards operationalisation

Connecting SSbD Toolbox users



Interview/focus group

- 8 in-depth interviews/focus groups
- open conversations > 3 hours



Companies

- Diverse group of companies
- Developers and producers of base chemicals/materials
- Producers of specialty chemicals/materials
- Formulators of consumer products
- Mainly large companies

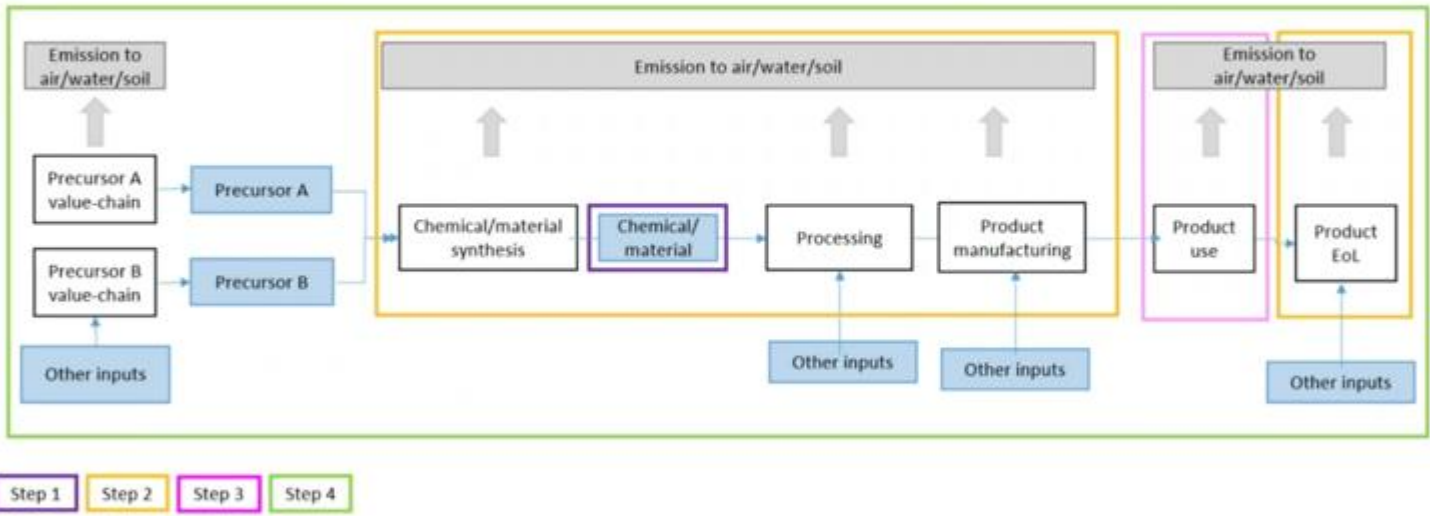


Agenda

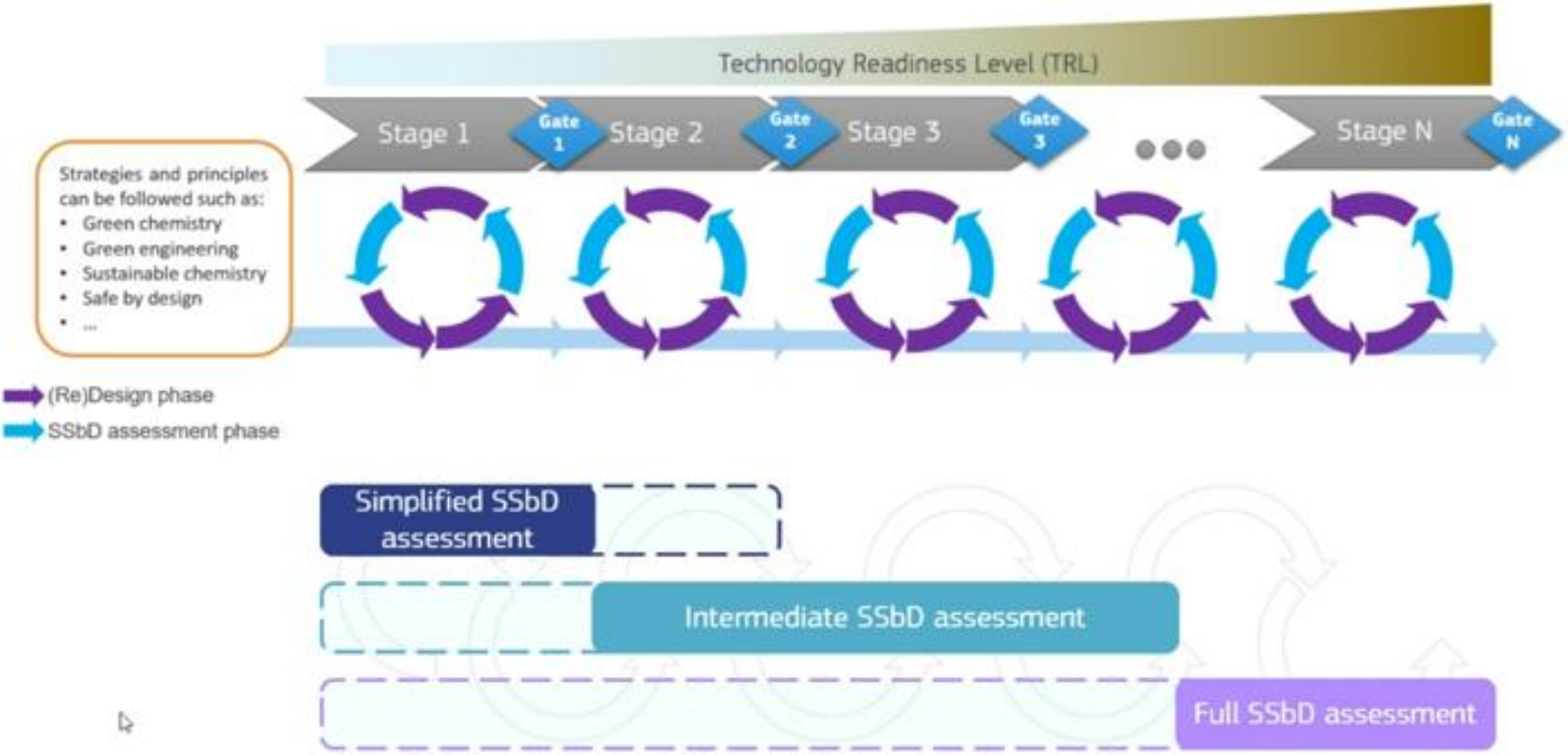
- Agenda topics
 - Innovation
 - Safety, sustainability, socio-economic assessment
 - EU SSbD framework
 - Other

Scoping in the recent EC Guide

SSbD - Overview of the 1st Methodological guidance Scoping analysis: The life cycle



Acknowledging the interactive nature of SSbD



4

Innovation



Increasing TRL/Stage / Increasing information

Exploratory phase

Investment and development phase

Market phase

Exploratory phase

General & feasibility

- Limited time and funding
- “Proof of principle” (Does it work?)
- “Proof of benefit” (Market fit)
- “Fail early, Fail cheap”

Safety

- Basic screening
- Expert judgement
- ‘Red flag’ approach
- Application driven

Sustainability

- Limited
- Company strategy important
- Comparator/in-house
- Portfolio/product group

Investment and development phase

General & feasibility

- Dedicated project time and funding
- Development of proof of context
- Decreasing ‘risk of failure’
- Customer need/Market fit

Safety

- Application based hazard hypothesis formulation and testing
- ‘Red flag’ approach
- Registration/regulation as context

Sustainability

- GHG as a driver
- Screening LCA
- Portfolio/product group
- Value chain collaboration to map cradle to grave

Market phase

General & feasibility

- Proven functionality
- Clear market perspective
- Pilot tests

Safety

- Registration ready/Compliant
- Application as a context

Sustainability

- GHG as focus
- Portfolio/product group
- PEF in limited cases on demand
- Planetary boundaries not mature enough

Some key learnings

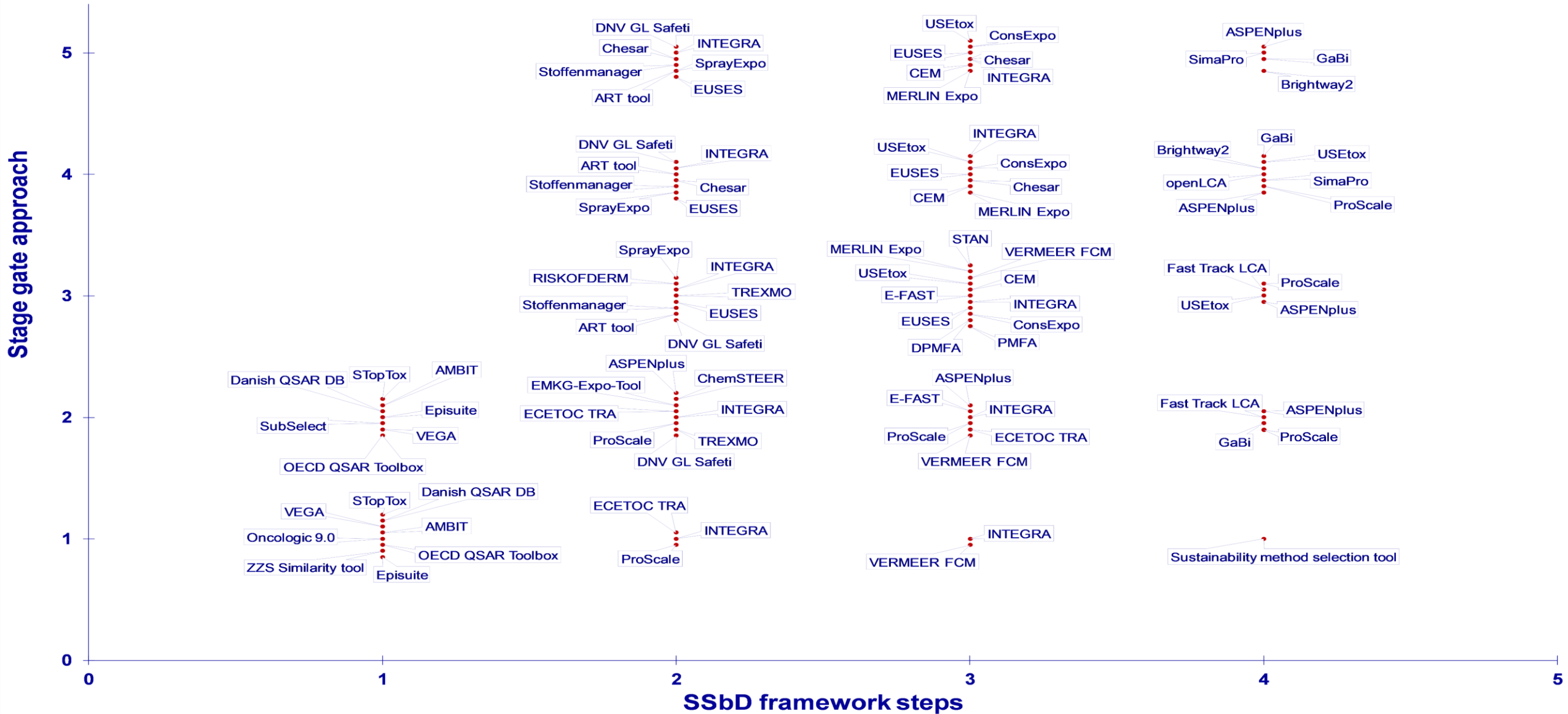
- **Stage gate is very commonly used**
 - Not uniform, non-linear/iterative, either structured process or more informal
- **Starting point of innovation is important**
 - Single chemical – Process – Product – Optimization (– Value chain)
- **Decision making**
 - Team effort – team composition depends on maturity level
 - Balancing act – performance in early stage key
 - Final decision increasingly strategic
- **Industry/sector specificity**
 - Innovation process is company specific
 - Company profile, (corporate) company policy is important in S&S assessment
 - Socio-economic aspects often part of company policy
 - Sector developments – generalized approaches/data sets/models
- **Tools and data**
 - Variety of tools and data: from QSARs to checklists to certification schemes
 - Open to share under conditions

8.1.2

Toolbox Development

SSbD toolbox implementation

Linking models within the **SSbD framework** and the **stage gate approach**



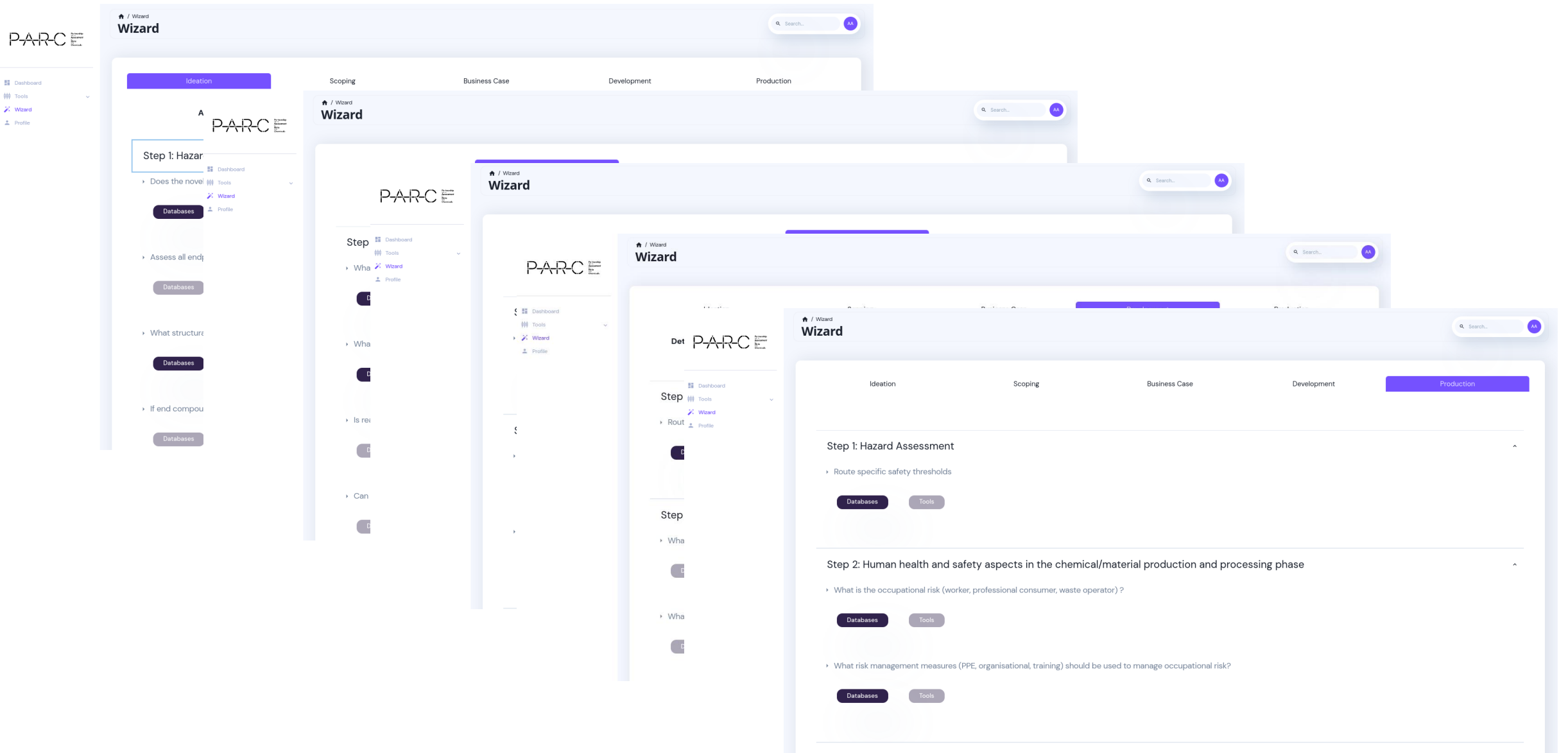
SSbD toolbox implementation

Computational implementation – key features

- **Bring together and develop tools that support safety and sustainability aspects**
 - Cover the needs of all steps (1-5) in the SSbD framework
 - Align them with data needs for the various innovation stages
- **Forge functional links between the available tools**
- Diverse landscape - functional linking will often require **tailored solutions**.
- Develop a choice of (user) interface for the model pipeline;
- Link with different databases
- Blockchain technologies for use of proprietary data

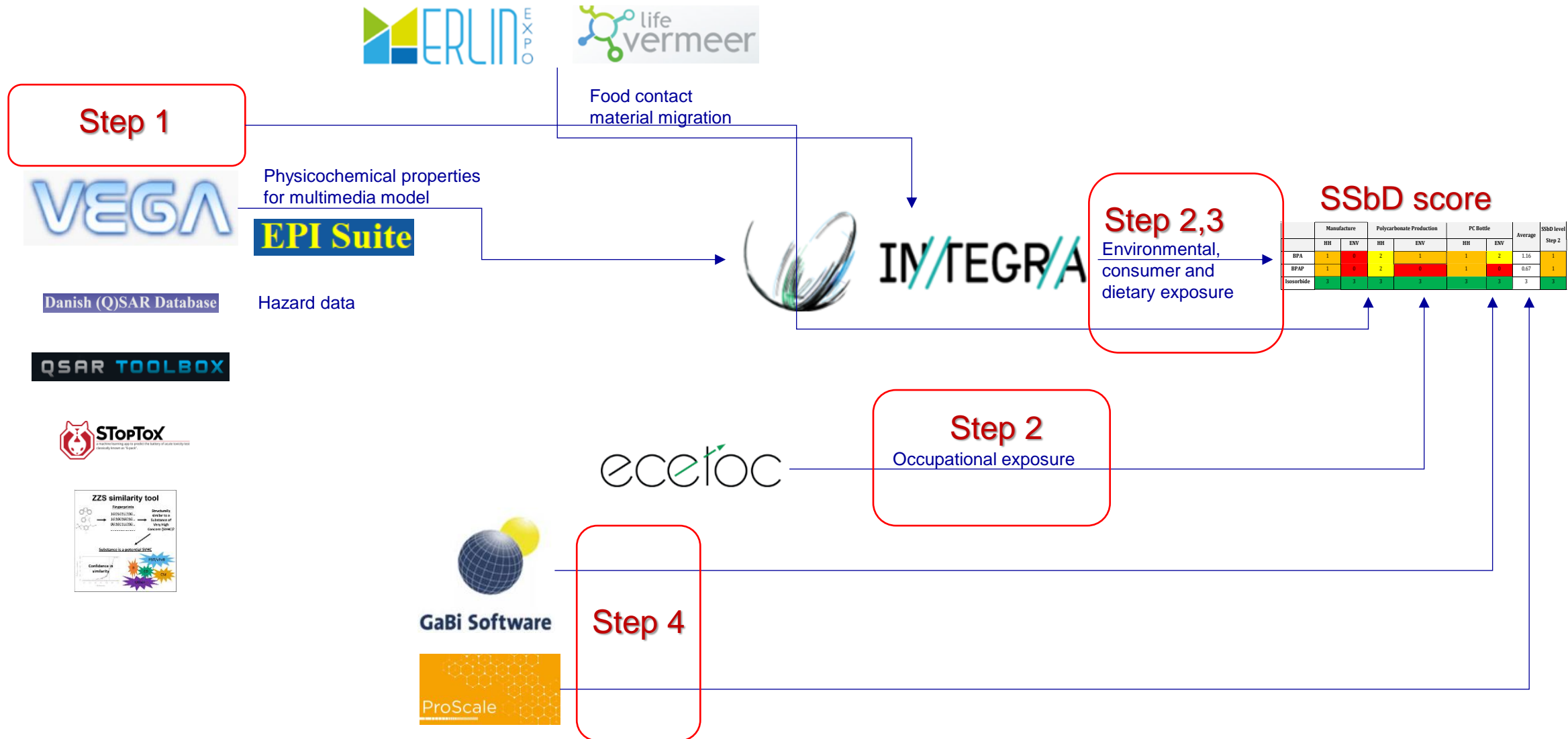
SSbD toolbox implementation

Next steps – Implementation of the interface



PARC SSbD toolbox – first tools

BPA and alternatives case study – Model pipeline



Step 1 - summary

How to use the PARC SSbD toolbox

BPA and alternatives case study – Step 1

Human health hazards

Chemicals	Chronic toxicity	Subacute toxicity	Reproductive toxicity	ED (Hazard)	STP/RE	Acute toxicity (oral)	Acute toxicity (inhalation)	Acute toxicity (dermal)	STP/RE
BPA									
BPAP									
Isosorbide									

Environmental hazards

Chemicals	STP/PvB	PMV/PvM	ED (ENV)	Hazards to ozone layer	Chronic aquatic toxicity	Acute aquatic toxicity
BPA						
BPAP						
Isosorbide						

Physical hazards

Chemicals	Explosives	Flammable	Aerosols	Oxidizing	Gases under pressure	Self-heating	Pyrrophoric when wet	Self-heating	Ecotoxic (aquatic)	Organic peroxides	Corrosivity	Dispersed response
BPA												
BPAP												
Isosorbide												

Required input: SMILES Code

VEGA

Danish (QSAR Database) | QSAR TOOLBOX | StopTox

Co-funded by the European Union

How to use the PARC SSbD toolbox

BPA and alternatives case study – Step 1

<https://www.parc-ssbd.eu/>

ECHA CHEM
ECHA CHEMICALS DATABASE

Co-funded by the European Union

Steps 2 and 3- summary

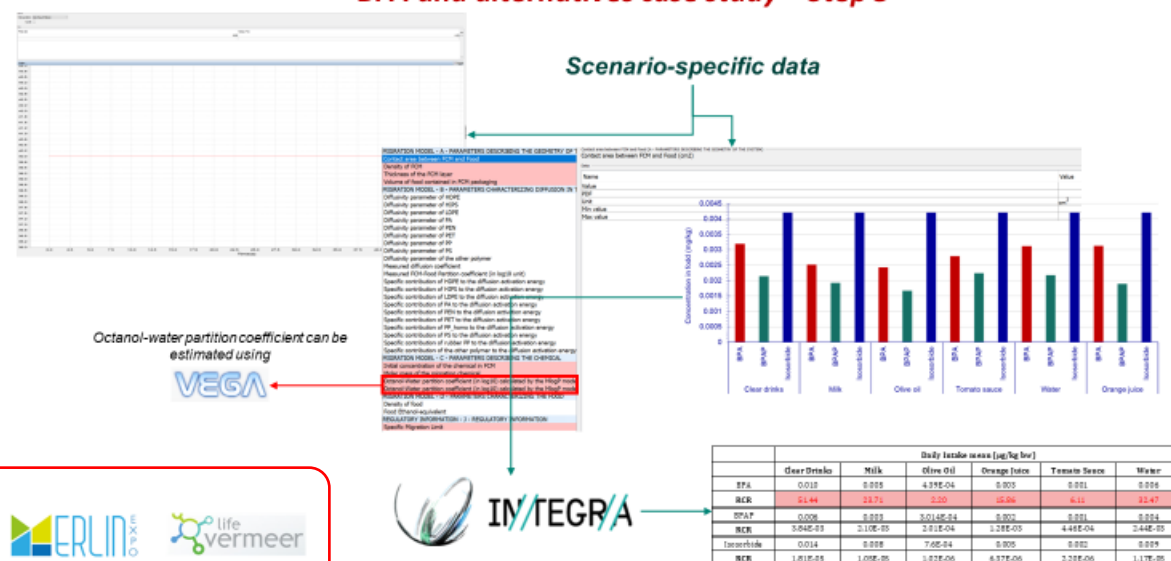
How to use the PARC SSbD toolbox

BPA and alternatives case study – Steps 2 and 3



How to use the PARC SSbD toolbox

BPA and alternatives case study – Step 3



PARC

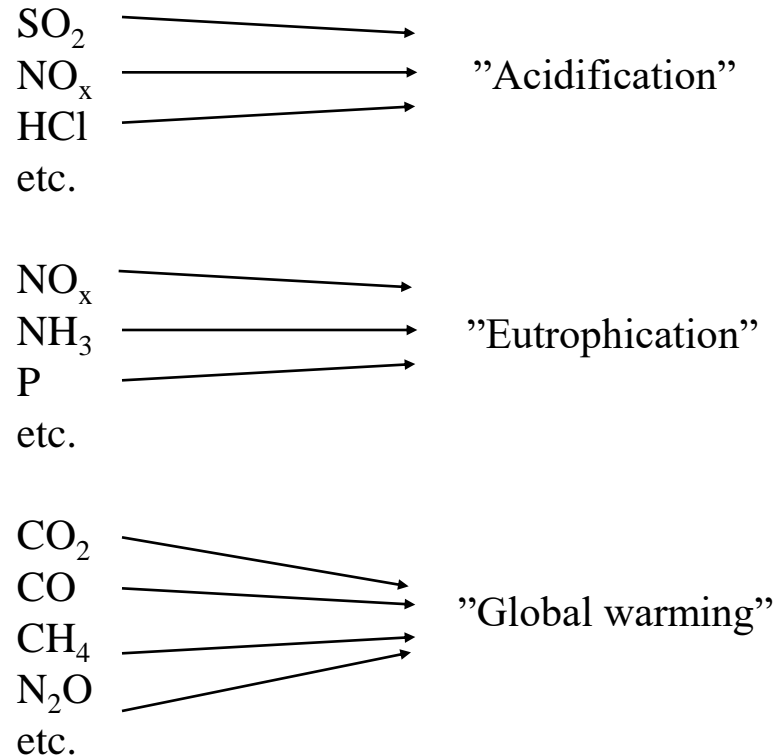
Co-funded by the European Union

Step 4. LCA – “midpoint indicators”

*Inventory
parameters*

“Midpoint indicators”

Classification / characterisation



Our set of indicators for the BPA case:
(**selection** of indicators/models as
recommended in PEF + ProScale indicators):

- Climate change
- Ozone depletion
- Resource use, fossil
- Resource use, minerals/metals
- Water use
- Land use
- Human toxicity, cancer effects (environment mediated/USEtox)
- Human toxicity, non-cancer (environment mediated/USEtox)
- Human direct inhalative exposure impact potentials/ProScale
- Human direct dermal exposure impact potentials/ProScale
- Ecotoxicity, aquatic/Usetox
- (Ecotoxicity /ProSaleE)
- Acidification
- Eutrophication
- Photooxidant formation

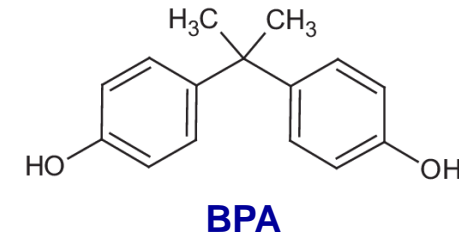
8.1.3

SSbD toolbox operationalisation: Use cases & indicators

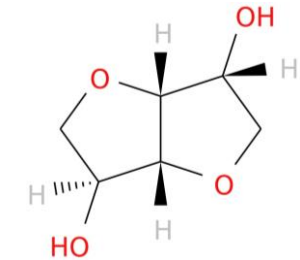
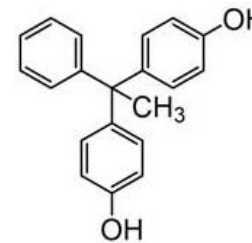
SSbD tool test

Bisphenols case study

Scenario 1 – Replacing BPA in polycarbonate bottles



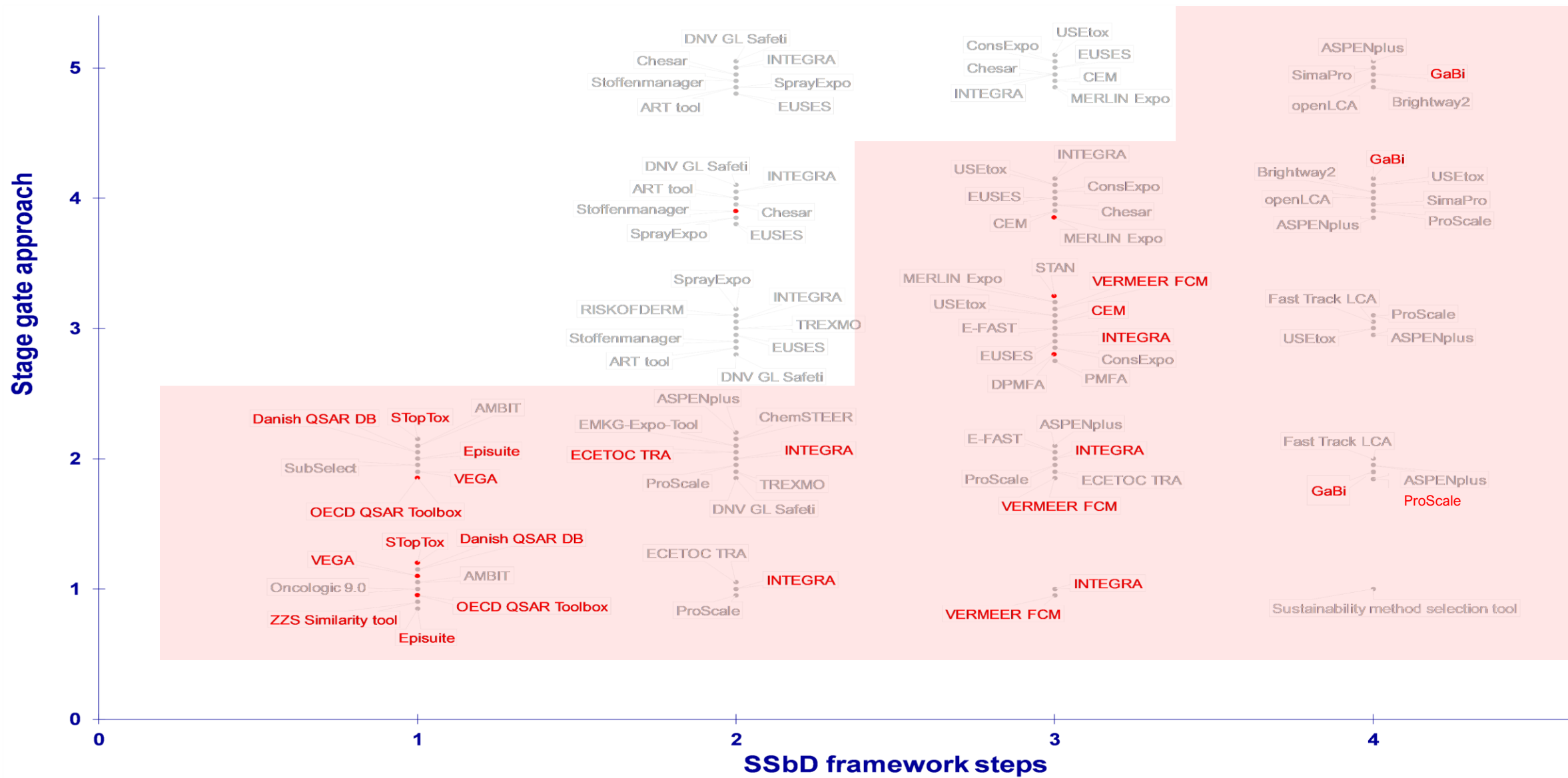
Scenario 2 – Replacing BPA in epoxy resin paints



Name	Acronym	EC	CAS	Molecular weight (g/mol)	ECHA dossier
4,4'-isopropylidenediphenol	BPA	201-245-8	80-05-7	228.28	https://echa.europa.eu/el/registration-dossier/-/registered-dossier/15752
1,1-bis(4-hydroxyphenyl)-1-phenylethane	BPAP	433-130-5	1571-75-1	290.36	https://echa.europa.eu/el/registration-dossier/-/registered-dossier/9115/1/1
1,4:3,6-dianhydro-D-glucitol	Isosorbide	211-492-3	652-67-5	146.14	https://echa.europa.eu/el/registration-dossier/-/registered-dossier/5661/1/1

SSbD toolbox application

Bisphenols case study – tested tools



Contributors to tools testing

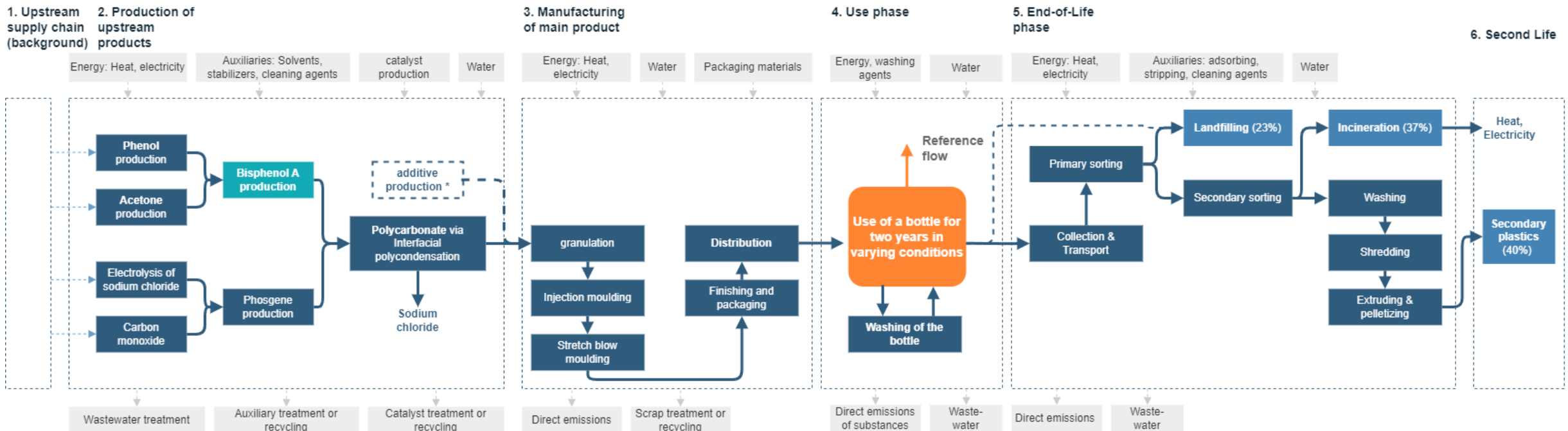
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Bisphenol and substitutes case study

Step 4

Semi-specific flow diagrams – BPA-PC



1. Multiple possible synthesis routes and scenarios possible
2. Most substances along the supply chain are known, including Life Cycle Inventory (LCI) datasets.
3. Several data points are not exactly known, but in practice a baseline scenario can be (and has to be) imagined and formulated, in which “reasonable” assumptions are put in place

Flow diagram: Martijn van Bodegraven, RIVM

Bisphenol and substitutes case study

Step 4

What to do for new or unknown processes ?

- Read-across principles are applicable for chemicals as well as processes
 - Similar chemical structure -> similar hazard properties
 - Similar process conditions -> similar emission and exposure characteristics

Bisphenol and substitutes case study

Step 4

What to do for new or unknown processes

1 Identify the synthesis route

2 Identify the bill-of-material

Precursors, product, byproducts, possible intermediates, etc
(include the "relevant" ones)

3 Envision the process in industry scale and create a preliminary process design

Includes separation steps, effluent treatments etc

simple- rule-of thumb based /rough estimates – ERC, SpERC, etc

More advanced, engineering based, in a relevant tool (e.g. Aspen, Matlab or similar)

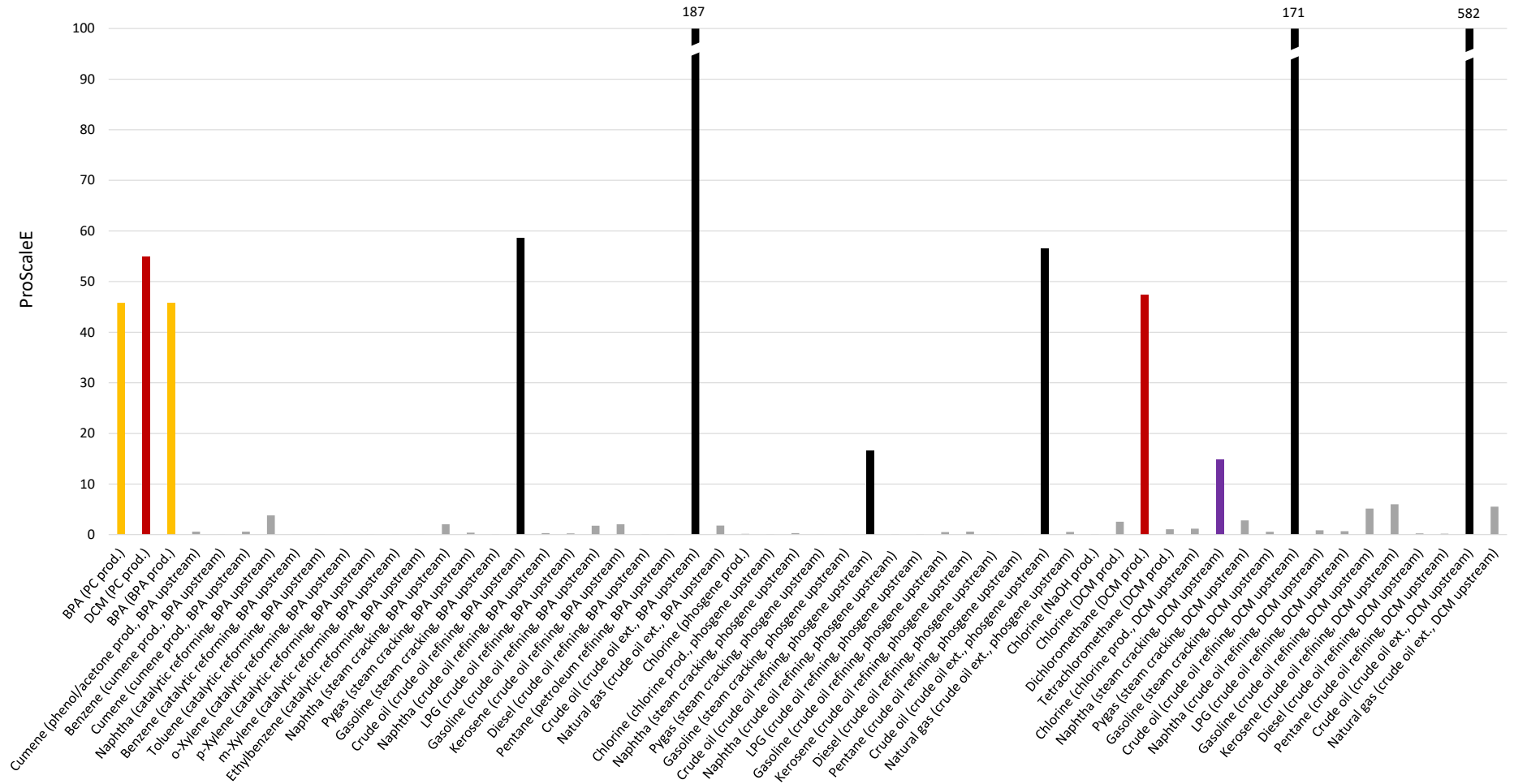
Include and calculate/estimate relevant emissions

5 Insert it into your LCA

Example result for illustration - using ERCs and SPERCs allow for a rough modelling of substance release to air, water and soil

Emissions to air

- Crude oil
- Bisphenol A (BPA)
- Dichloromethane (DCM)
- Naphtha

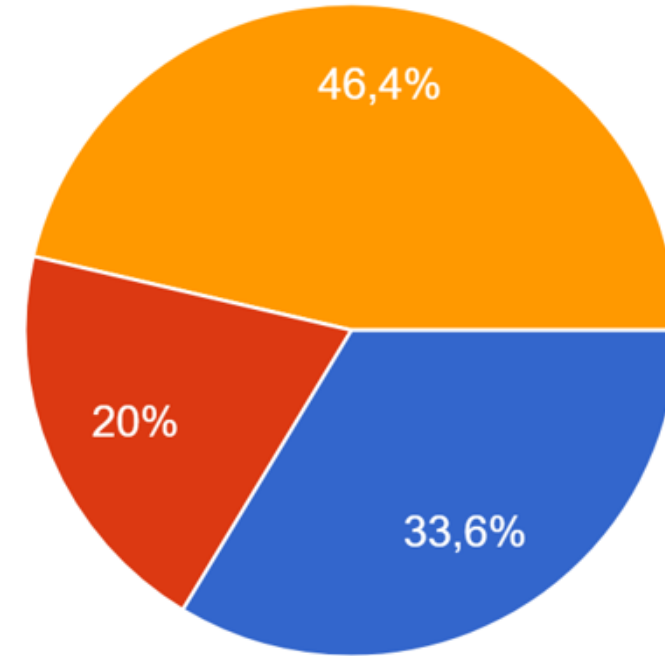
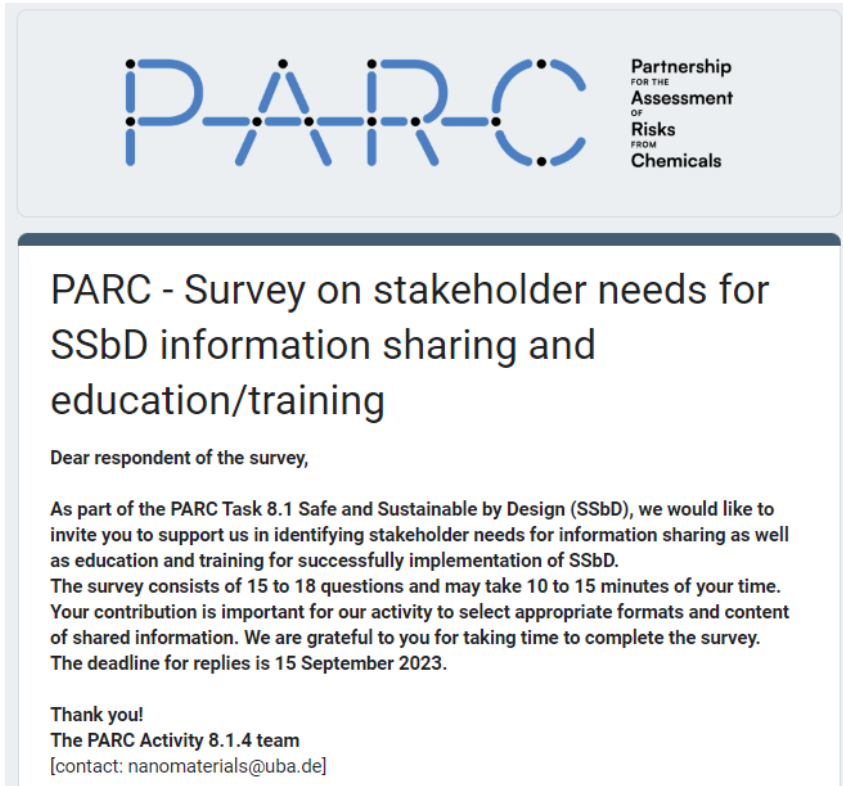


Crade-to-gate system model
for BPA,
here using ProScaleE for
impact scoring

8.1.4

Knowledge sharing & Education

Survey on stakeholder needs for SSbD information sharing and education/training



- Regulators, Risk Assessors
- Industry, SME, CROs
- Science and education

109 responses

- Run time from mid July – end September 2023
- Set of general questions on **information sharing**
- Specific questions on **education/training needs** for regulators/risk assessors, industry (incl. SME, CROs), science and education

Draft Report on survey responses and conclusions for the SSbD knowledge sharing platform



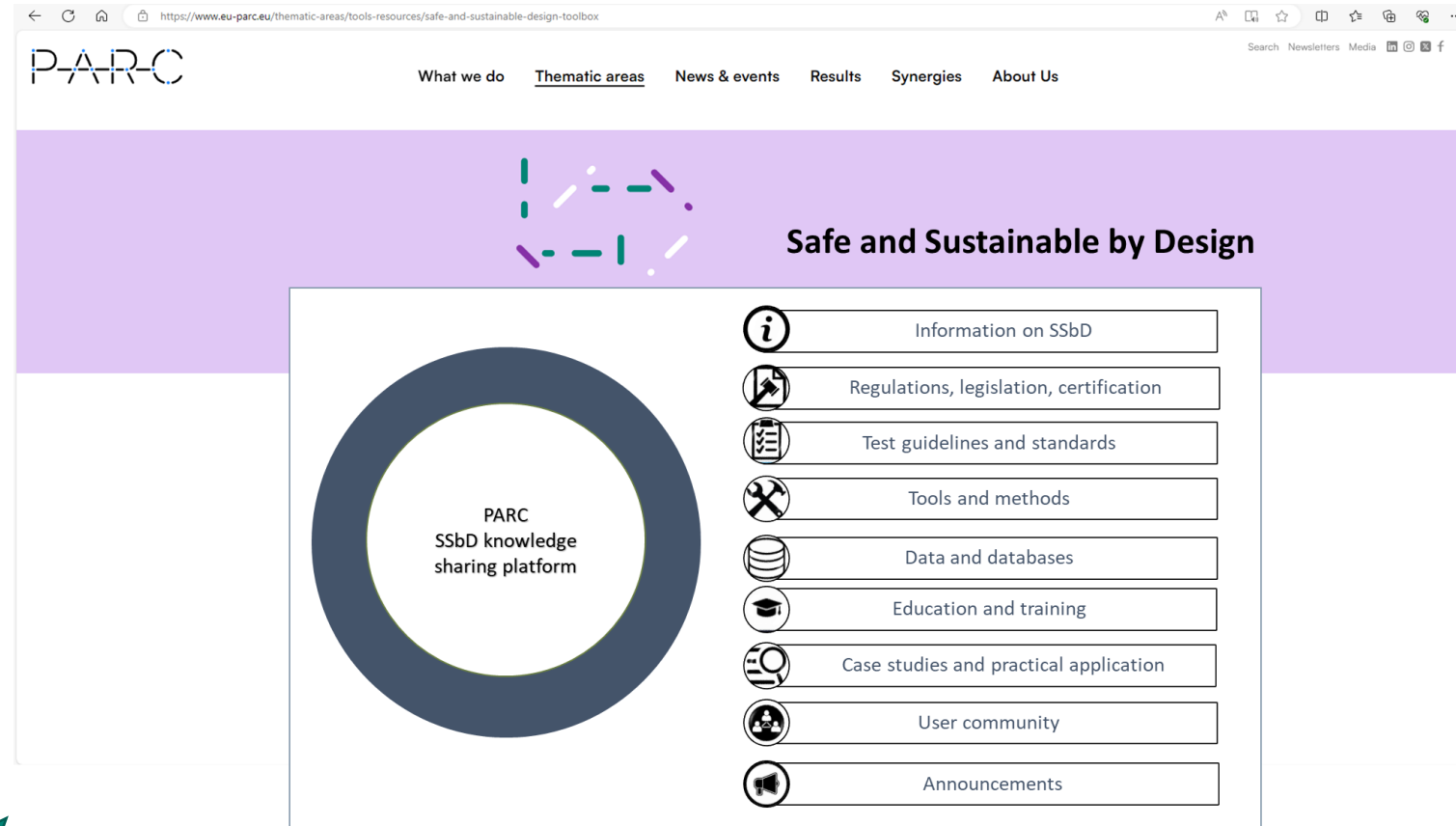
Table of contents

- Introduction
 - Methodology
 - Results
 - No. and distribution of responses (regulators/risk assessors, industry (SME, CROs), science and education)
 - Responses to questions
 - on information sharing
 - on education and training material (separately for the three different stakeholder groups)
 - on education and training material (specific questions to stakeholders on science and education)
 - “any other remarks”
 - Overall conclusions for the knowledge sharing platform
 - Material for information sharing, for education and training
 - Content and format of the knowledge sharing platform
 - Annex with full list of questions
- as Annex to the Inception Plan Y2, check if report can be published at PARC website
- conclusions will also be used for the paper on education framework
- please review and leave your comments until 05 Feb 2024

[Summary of Survey SSbD Stakeholder needs for education for IncPlan_report_draft.docx \(sharepoint.com\)](#)

Idea of realisation of the SSbD knowledge sharing platform via the PARC website

- Start of thematic area with figure of the SSbD KSP and its relevant elements
- By clicking on the elements, users are navigated to the different landing pages
- Landing pages will include introductory text, relevant links and documents
- Landing page on „user community“ will provide link to a dedicated „group“ on SSbD in PARCopedia (to be developed)
- Drafts of landing pages will be developed in the coming months with support of colleagues involved in the corresponding topics (e.g. on tools, case studies)
- This proposal will be discussed with Task 3.2, then Task 2.2



Support will be needed!

8.1

Plan forward

Other issues & Work ahead – PARC SSbD

Overall methodology

Sustainability assessments

Risk or safety assessments

Added value for users

Other uptake

Connecting SSbD
Toolbox users

Outreach to other
projects

Linking new SSbD
projects/tools to the
PARC toolbox

Technical expert
group

Utility of SSbD tools
in the decision
making process of
chemical substitution

