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SSbD and LCA

The diagram illustrates the relationship between Safety and sustainability assessment and Life Cycle Assessment (LCA) framework.

Safety and sustainability assessment is divided into five main components:

- HAZARD PROPERTIES OF THE CHEMICAL/MATERIAL**: Represented by a beaker icon.
- HUMAN HEALTH AND SAFETY OF PRODUCTION PROCESSES**: Represented by a person with a skull and crossbones icon.
- ENVIRONMENTAL AND HUMAN HEALTH RISKS IN THE USE PHASE**: Represented by a person with a skull and crossbones icon.
- ENVIRONMENTAL IMPACTS ALONG THE ENTIRE LIFE CYCLE**: Represented by a person with a skull and crossbones icon.
- (S. Socio-economic assessment)**: Represented by a person with a skull and crossbones icon.

These components are interconnected by arrows, indicating a flow and relationship between them. A vertical stack of four colored boxes (red, orange, green, blue) represents the stages of the LCA process: **RAW MATERIALS**, **PRODUCTION**, **USE**, and **END OF LIFE**.

Life Cycle Assessment framework consists of three main stages:

- Goal and scope**
- Inventory analysis**
- Impact analysis**

These stages are interconnected by arrows, indicating a flow and relationship between them. The final output of the LCA framework is **Interpretation**.

Legend:

- CHEMICAL MATERIAL UNDER EVALUATION
- OTHER SUBSTANCES EMITTED DURING THE LIFE CYCLE

A Venn diagram with three overlapping circles. The top-left circle is green and labeled 'Environment'. The top-right circle is blue and labeled 'Economy'. The bottom circle is orange and labeled 'Society'. The orange circle overlaps with both the green and blue circles. A red arrow points from the text 'Life Cycle Sustainability Assessment (LCSA)' to the orange circle. Below the orange circle, the text 'Social Life Cycle Assessment' is written.

Applying LCSA to novel chemicals is often difficult because detailed **Life Cycle Inventory (LCI)** data are unavailable, incomplete, or confidential—particularly for complex and early-stage chemicals. This motivates an automated workflow that uses retrosynthesis to derive synthesis pathways and translate them into model-ready inventories for environmental, economic, and social sustainability assessment.

Following Parvatker et al., data gaps can be filled according to following methods:

- **Method 0:** Uses real plant data (or plant-based LCI datasets) for the chemical
- **Method 1:** Models the full process in simulation software to derive LCI flows, e.g. ASPEN
- **Method 2:** Applies detailed engineering mass/energy balances without full simulation (generic)
- **Method 3:** Uses simplified balances and rule-of-thumb factors for major flows plus energy
- **Method 4:** Estimates inputs/outputs from the balanced reaction equation(s) only
- **Method 5:** Predicts impacts from structure, uses a similar chemical using ML/QSAR methods
- **Method 6:** Using a similar structure as proxy
- **Method 7:** Omit from the product system



LCA Simulation Approach

The diagram illustrates two approaches to Life Cycle Impact Assessment (LCIA): Retrospective and Predictive.

Retrospective LCIA:

- Goal and Scope:** System boundaries and functional unit.
- Future supply network model:** Background LCIA Step.
- Molecular and structural properties:** (SMILES, descriptors).
- Expert Knowledge and Plant Data:**
- Empirical LCIA:** The central process, which leads to **Empirical LCIA** and then **Environmental impact**.
- Environmental impact:** Climate Change, Ozone Depletion, Acidification.

Predictive LCIA:

- Predictive LCIA:** The central process, which leads to **Predictive LCIA** and then **Environmental impact**.
- Environmental impact:** Climate Change, Ozone Depletion, Acidification.

Approach 1:

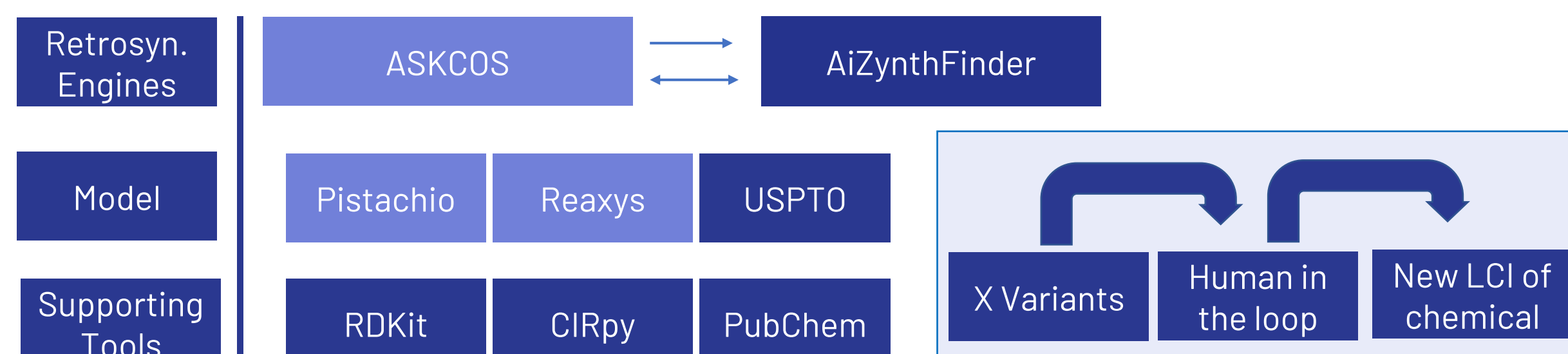
- Predictive Approach 1:**
 - Direct impact estimation (QSAR)
 - Upstream modelling not possible
 - Requires high quality LCIA data for similar molecules

Approach 2:

- Predictive Approach 2:**
 - Inventory construction from predicted data
 - Upstream modelling is possible
 - Expert knowledge can enhance prediction

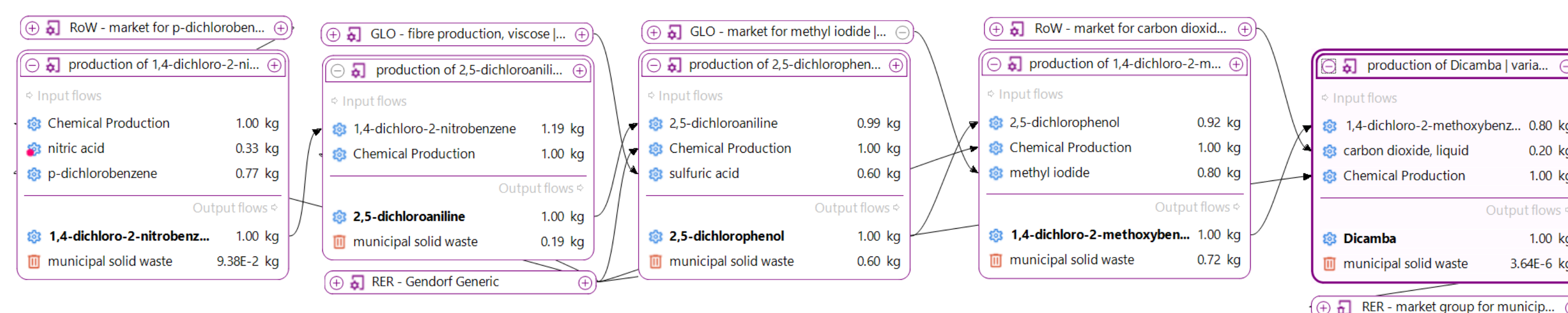
Approach 2: Molecular information is combined with predicted synthesis information, expert knowledge, and background databases to construct an LCI before calculating the LCIA. Using transparent unit-process, synthetic pathways are understood and real impacts can be modelled. Here the “Method 3” from above can be applied. **It also supports LCSA!**

Retrolca: automated LCI generation in openLCA. Our Python-based toolkit transforms retrosynthesis pathways into linked, model-ready process chains directly in **openLCA** via its IPC interface. Starting from a target chemical's **SMILES** code, it obtains alternative reactions from retrosynthesis engines such as **ASKCOS** or **AiZynthFinder**, then **recursively creates foreground production processes for missing intermediates**. Existing **chemical datasets** in the background database, such as ecoinvent, are **automatically identified** and linked wherever suitable providers are available.



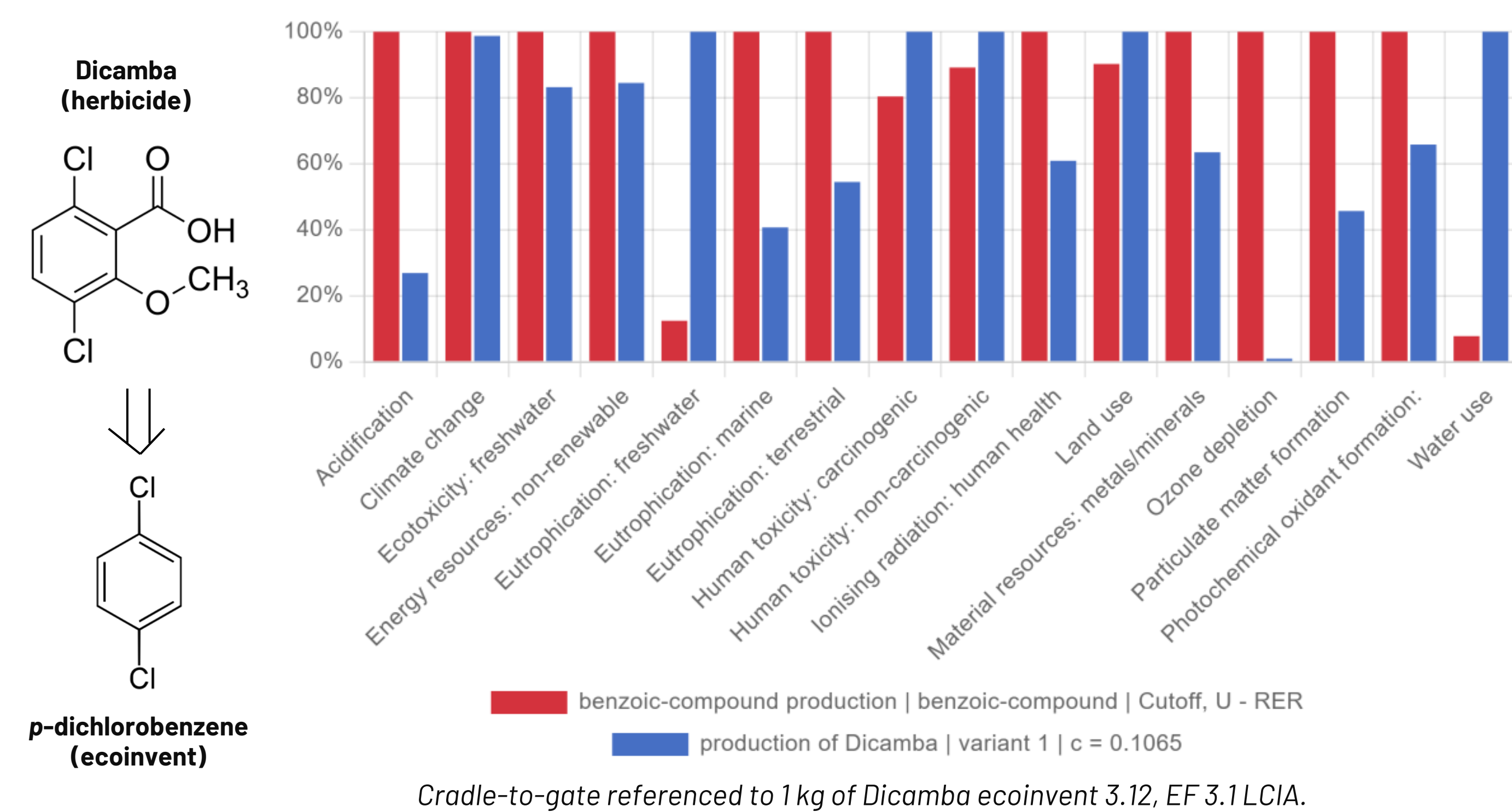
- Retrosynthesis
 - Inbox
 - level 1
 - production of 1,4-dichloro-2-methoxybenzene | variant
 - production of 1,4-dichloro-2-methoxybenzene | variant
 - production of methyl 3,6-dichloro-2-methoxybenzoate
 - production of methyl 3,6-dichloro-2-methoxybenzoate
 - level 2
 - level 3
 - level 4
 - level 5
 - level 6
 - level 7
 - level 8
 - level 9
 - level 10
 - level 11

Configurable, transparent route modelling. Users can define the maximum retrosynthetic depth and number of route variants, select or customise background-data providers, and add generic production or mass-balancing processes where detailed information is unavailable. Generated processes include reaction visualisations and are organised for subsequent review, editing, and completion by the practitioner. This creates a transparent bridge from **molecular structure** → **retrosynthetic route** → **LCI process chain** → **product system** → **LCIA**, enabling systematic comparison of alternative synthesis pathways while retaining expert oversight.



Once a product system is built and the remaining options being removed, the environmental but also socioeconomic impacts of producing a chemical can be assessed. **The data gap has been filled!**

To benchmark our approach, we used the **production of Dicamba** (herbicide) as a benchmark from ecoinvent and simulated its production giving similar values (2 variants, 12 levels, AiZynthFinder). The environmental impacts across most impact categories were comparable:



01 Retrosynthesis can automatically fill missing LCI data gaps for novel and early-stage chemicals lacking real production data.

02 Retolca links molecular structure to retrosynthetic routes to LCI process chains enabling full LCSA within openLCA.

03 Benchmarking against ecoinvent's Dicamba production showed comparable impact results, validating the LCI generation approach.

04 Generated process chains keep the practitioner in the loop, allowing expert review and refinement before final impact assessment