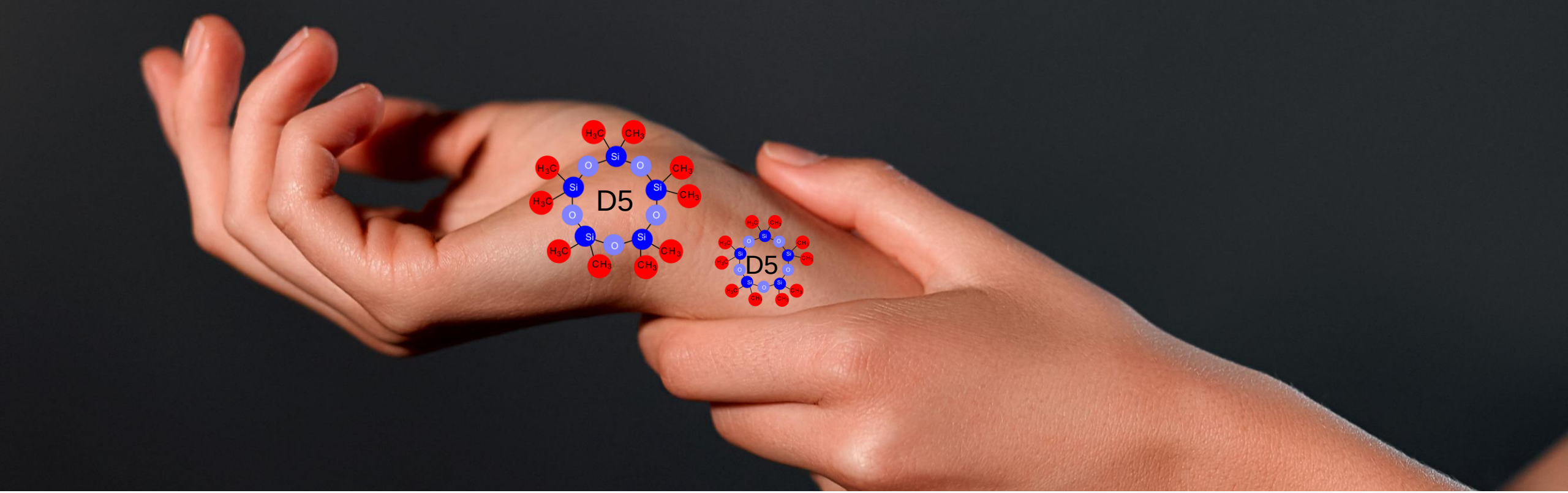
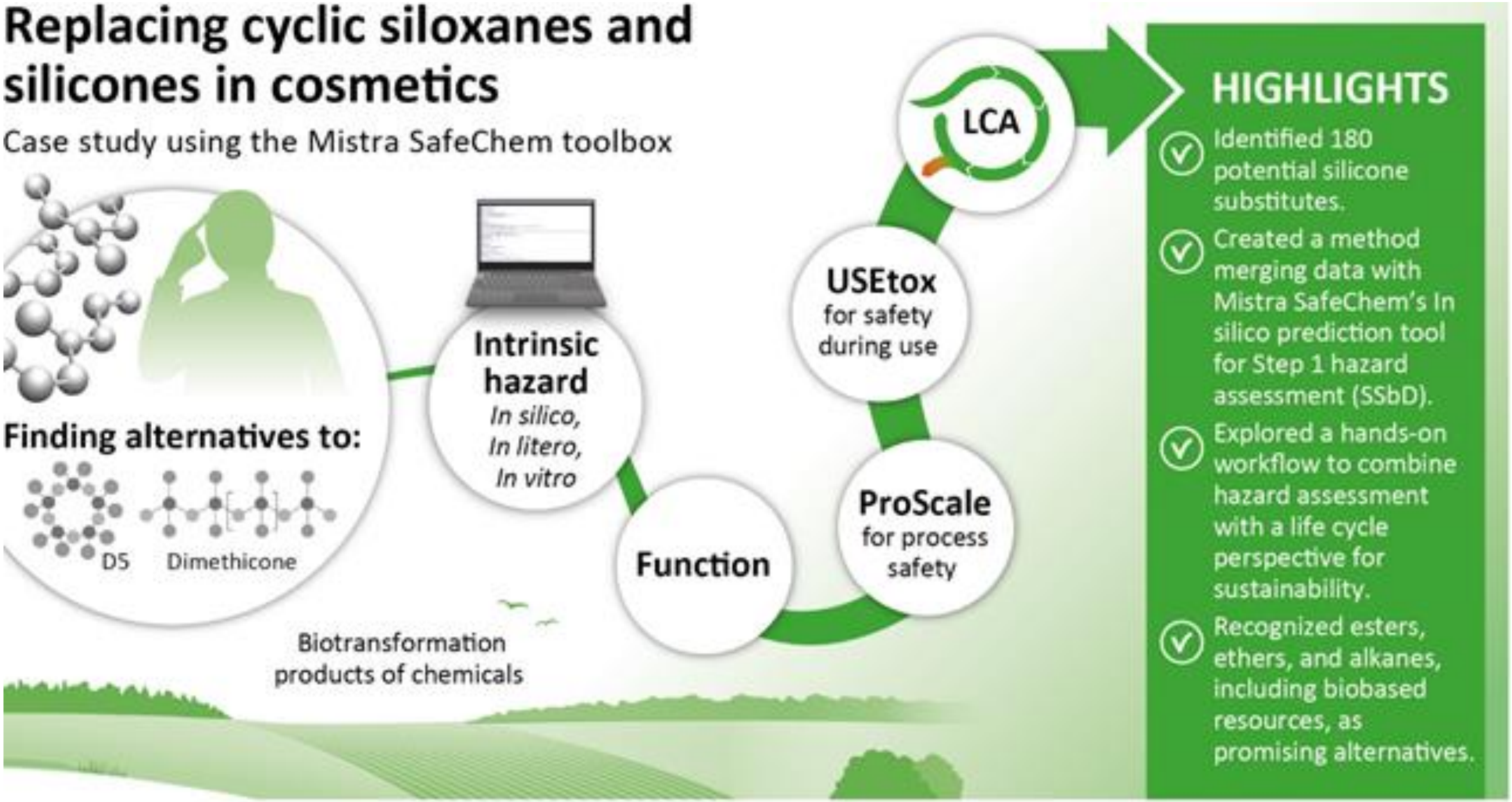


Safe and Sustainable Chemistry by Design: selected case insights from the Mistra SafeChem research programme

MISTRA SAFECHEM

Replacing cyclic siloxanes and silicones in cosmetics

Case study using the Mistra SafeChem toolbox



MISTRA SAFECHEM

Approach

(a) SSbD procedure (draft)

STEP 1– Hazard assessment of the chemical /material (intrinsic properties)

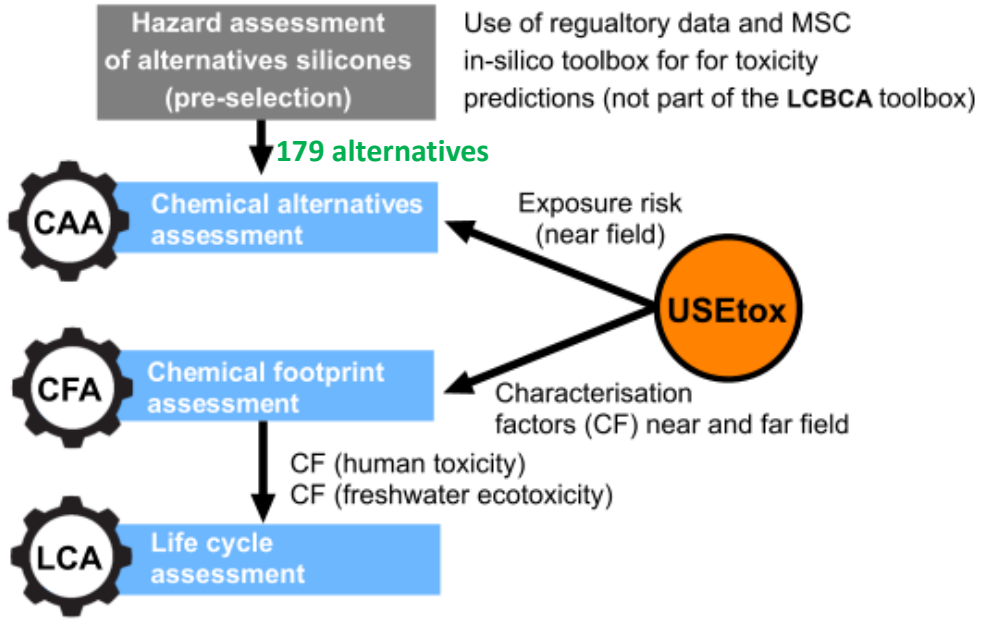
STEP 2– Human health and safety aspects in the chemical/ material production and processing phase

STEP 3–Human health and environmental aspects in the final application phase

STEP4–Environmental sustainability assessment PEF is recommended.

STEP 5– Social and Economic sustainability assessment (Not yet developed)

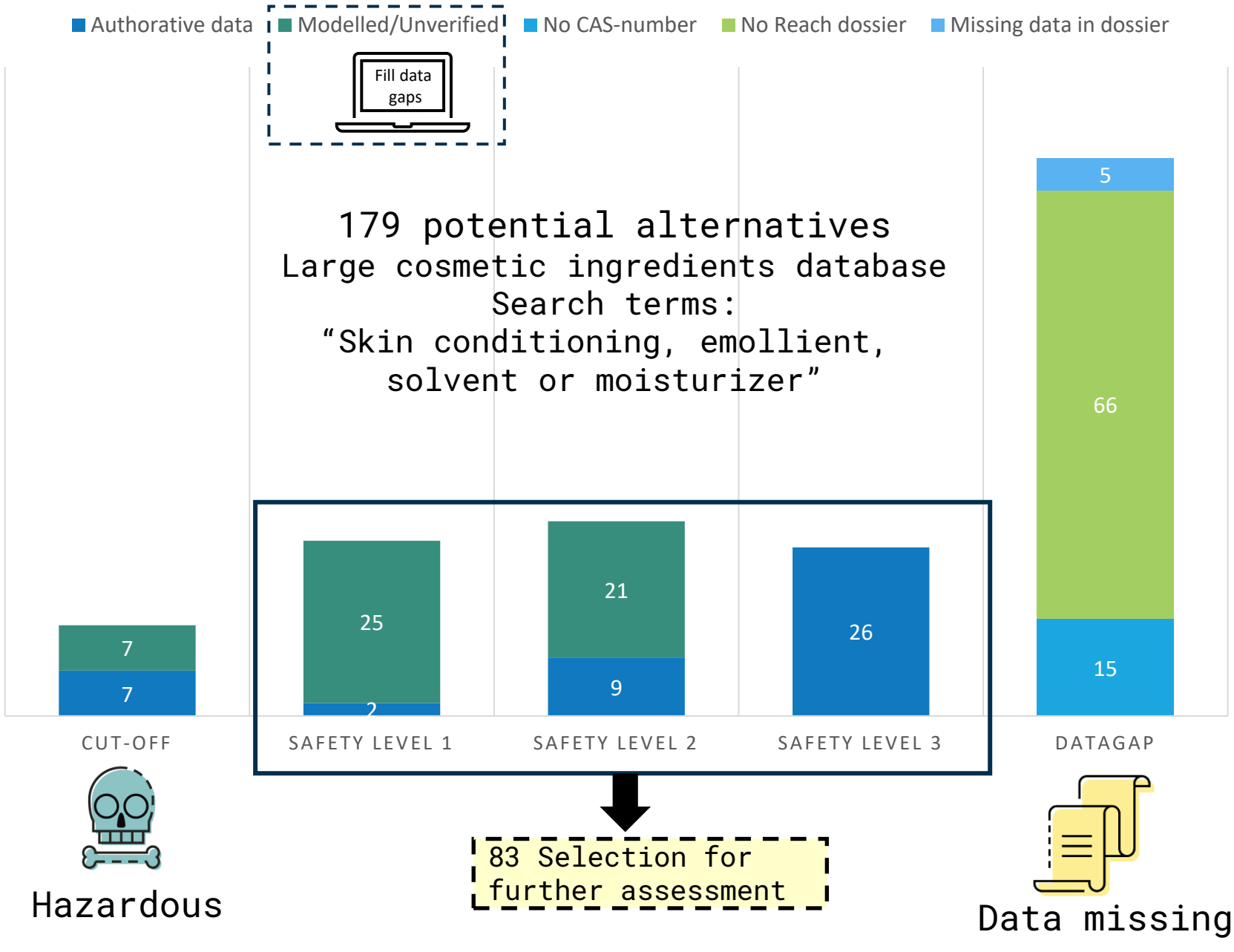
Mirror the SSbD steps and apply the Life Cycle-Based Chemicals Assessment (LCBCA) toolbox

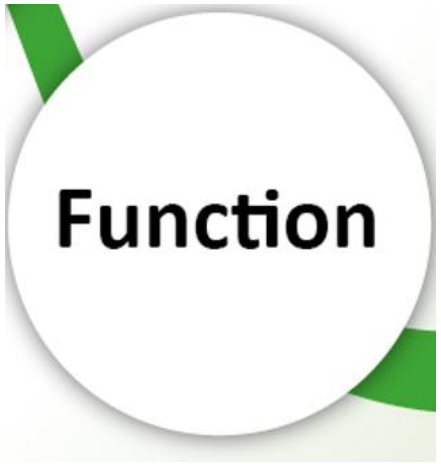


RESULTS OVERVIEW OF INTRINSIC HAZARD SCREEN

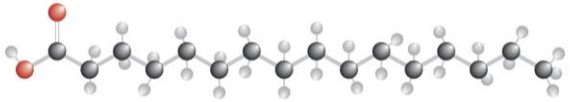
Intrinsic hazard
In silico,
In litero,
In vitro

STEP 1





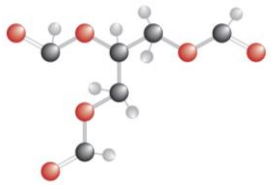
83 Potential alternatives

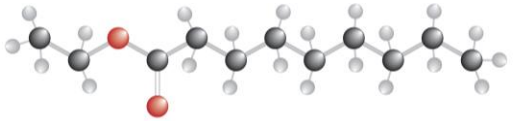


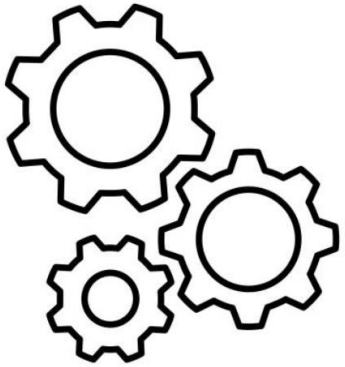
- Large cosmetic database analysis for a description of function
- Expert judgment

Chemical group	Comments
Hydrocarbon solvents	▪ Insufficient function ▪ Reduced spreadability ▪ Flammability
Esters	▪ Good function ▪ Silicone mimics (similar properties as D5) ▪ Defined structures ▪ Biobased, petroleum-based and partly biobased
Natural oils	▪ Function not optimal ▪ Good spreadability but not volatile enough to be used in a face makeup ▪ Contain complex mixtures ▪ Biobased

Most promising alternatives from a perspective of function

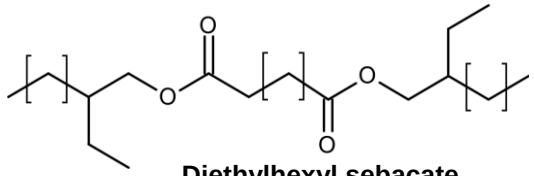






MISTRA SAFECHEM

Alternative selection for USEtox 3.0



Diethylhexyl sebacate
(partly biobased)

Input data:

USEtox input data: ~18.000 substances (partly incomplete)

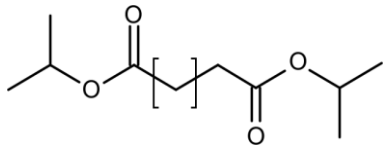
Based on Aurisano et.al
Probabilistic Points of Departure and Reference Doses for Characterizing Human Noncancer and Developmental/Reproductive Effects for 10,145 Chemicals

Match function in Excel to search for alternatives (83) in USEtox input data set

Result

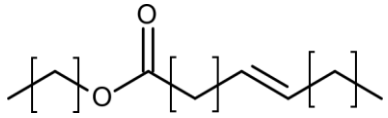
Table 2: *availability of input date for USEtox 3.0*

Chemical group	USEtox 3.0 input data	
Hydrocarbon solvents **(7)**	▪ Physicochemical input data	✓
	▪ Ecotoxicity effect data (HC20) ✓	✓
	▪ Almost complete input data sets for human toxicity effects data, some extrapolations and conversions were necessary	✓
Esters **(3)** (good function)	▪ Physicochemical input data	✓
	▪ Ecotoxicity effect data (HC20) ✓	✓
	▪ Almost complete input data sets for human toxicity effects data, some extrapolations and conversions were necessary	✓
Esters **(9)**	▪ Physicochemical input data	✓
	▪ Ecotoxicity effect data (HC20) ✓	✓
	▪ No human toxicity effects data	X
Natural oils **(0)**	▪ No input data	



Diisopropyl Adipate
(petroleum based)

Focus substances for the Guideline



Decyl oleate
(partly biobased)

- Fill in data gaps with CTV predictions for ED10 and RfD

Use stage assessment:

USEtox interface - Personal care products (PCPs)

Personal care products are consumer products used mainly for personal hygiene or beautification

Download user interface

USEtox was run in batch mode for single substances

Face make up with 20% Solvent/emollient

ASSESSMENT OF CHEMICAL IN PERSONAL CARE PRODUCTS

Fill in the green highlighted cells as input data - other data are automatically calculated

CHEMICAL SELECTION and CONTENT	Unit	Data
CAS RN		123-31-9
Row Number in Substance data		107
Chemical name		Diethylhexyl sebacate
Chemical mass fraction in product	[$kg_{chemical}/kg_{product}$]	2.00E-01

Save current chemical-product for batch run

PRODUCT INPUTS		
Product characteristics	Unit	Default data
Product row number	-	307
Product name	-	face make-up
Product mass	g	0.394899818
Exposure duration	h	16
Show more product inputs		
Product thickness for skin permeation	cm	0.001584795
Product thickness for volatilization	cm	0.001584795
Use mode	-	non-shower
User scenario	-	adult
Age group of child in household	-	2 to <3 years

INDOOR SETTING	Unit	Default data
HomeRowNr		10
HomeName		OECD countries average 2
Volume of house	m^3	236
Ventilation rate of house	h^{-1}	0.79
Total number of adults	-	2
Total number of children	-	1

REGION	Unit	Data
RegionRowNr		7
RegionName		Default USEtox

Results: different human toxicity CFs
Accounting for near-field and far-field exposure

Human tox impacts	CF cancer [DALY/kginventory]	CF noncancer-general [DALY/kginventory]	CF noncancer-rep/dev [DALY/kginventory]
User adult	0	5.17E-05	4.14E-04
User child	0	0	0
Household adult	0	1.13E-05	4.45E-05
Household child	0	6.50E-06	2.56E-05
Cumulative impact results	0	2.19E-07	2.77E-06
Total	0	6.98E-05	4.87E-04

Ecotox impacts	Exposure Cumulative transfer fractions [$kg_{to\ compartment}/kg_{inventory\ mass}$]	Characterization factor Endpoint ecotoxicity potentials [$PDF{\cdot}m^3{\cdot}d/kg_{inventory}$]	Damage Ecotoxixity damage [$PDF{\cdot}m^3{\cdot}d$]
To:	From PCP	From PCP	From PCP
Freshwater	3.98E-03	1.31E+02	1.03E-02

Comment:
The application of USEtox 3.0 without a predefined user stage scenario will be very challenging for less professional USEtox users!

MISTRA SAFECHEM

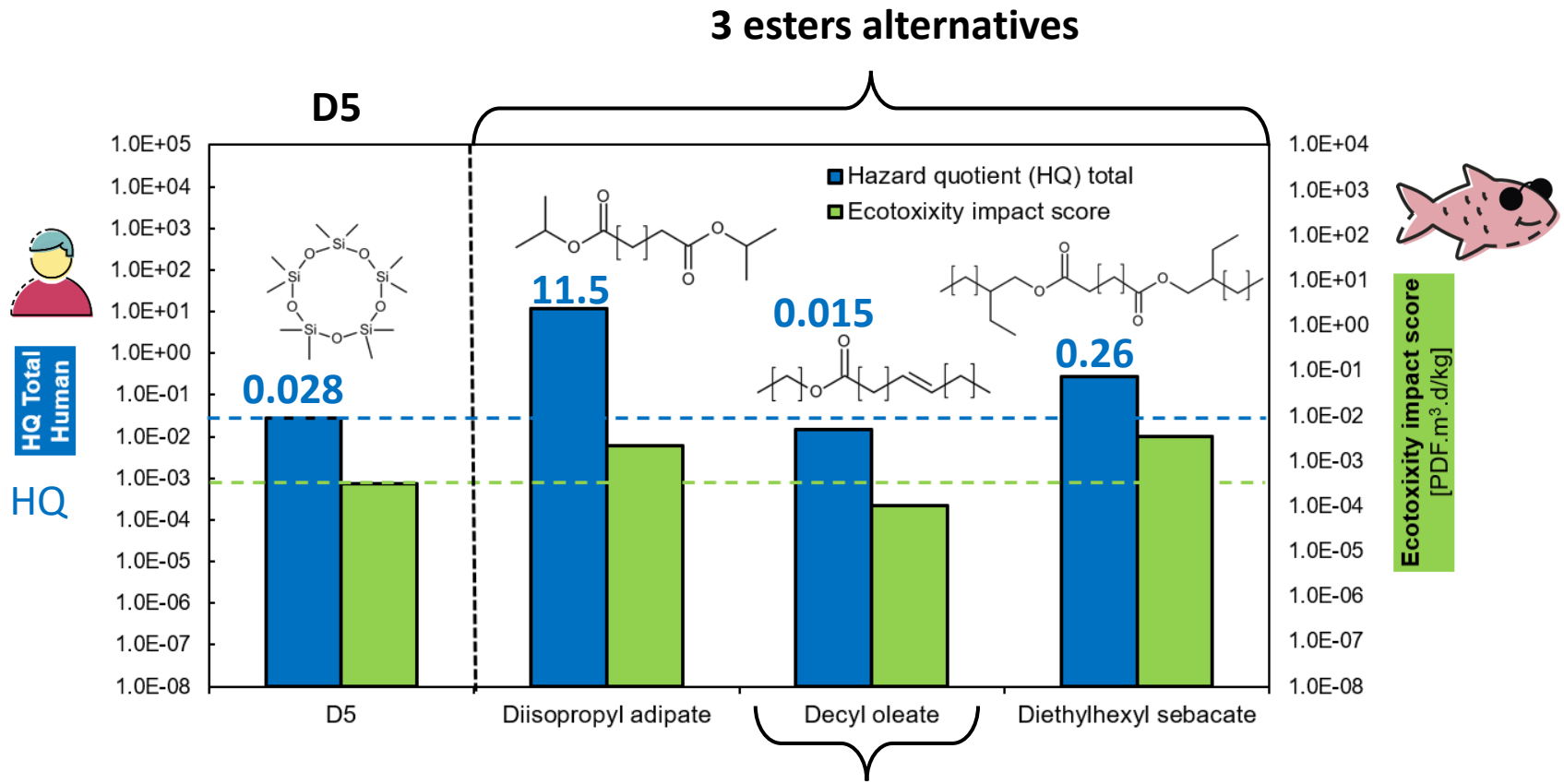
Safety during Use

RESULTS USEtox

- Result of D5 in comparison to three esters with 3 esters comparable performance (assumed)

STEP 3

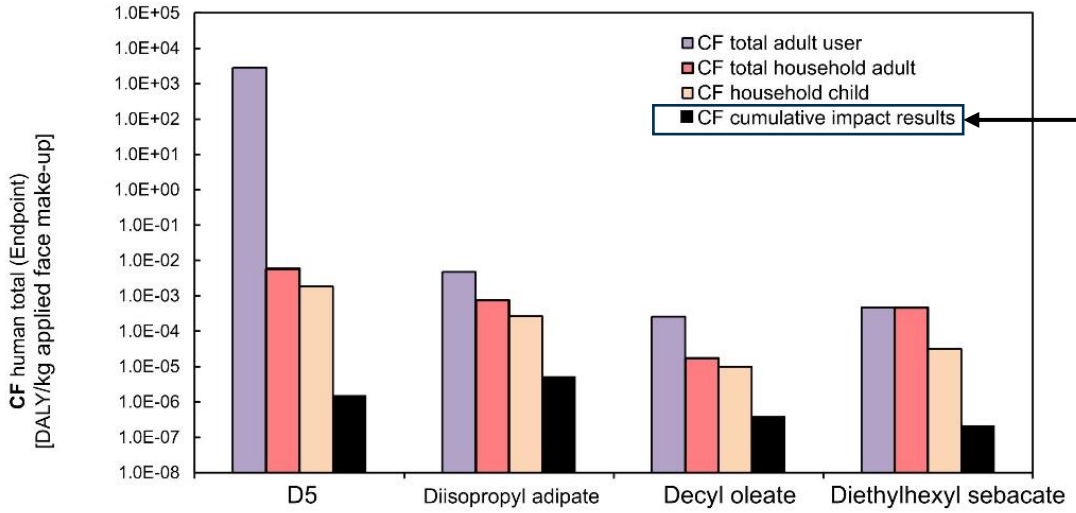
HQ> 1 are considered as high risk



Only one ester had a lower human toxicity exposure risk and a lower ecotoxicity impact score

MISTRA SAFECHEM

RESULTS: Characterization factors



Far-field Contribution to CFs

Midpoint CFs can be extracted from the result Sheet

Human Toxicity midpoint characterization factors [cases/kg emitted]			*Human Health endpoint (damage-level) characterization factors [DALY/kg emitted]*	*Ecotoxicity midpoint characterization factors [PAF.m³.d/kg emitted]*
Application to Skin surface layer			*Emission to cont. agr*	*Em.Skin surface l*
cancer	nc general	nc rep/dev	total	freshwater
0	2.91E-05	1.10E-05	1.06E-07	2.62E+02

USEtox 3.0
Personal care products interface
Characterization factor output

Endpoint CFs

Human tox impacts	CF cancer [DALY/kginventory]	CF noncancer-general [DALY/kginventory]	CF noncancer-rep/dev [DALY/kginventory]
User adult	0	2.88E+03	3.15E-04
User child	0	0	0
Household adult	0	5.80E-03	4.26E-05
Household child	0	1.83E-03	2.45E-05
Cumulative impact results	0	1.74E-07	1.39E-06
Total	0	2.88E+03	3.84E-04

CF Unit= per kg inventory and not per Functional Unit

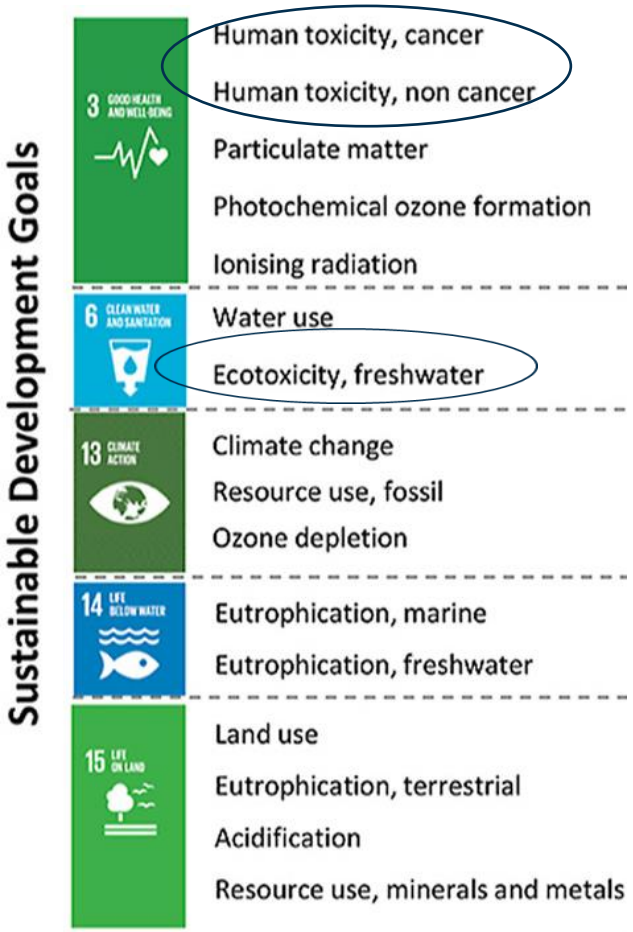
STEP 4: Environmental sustainability assessment
Life cycle impacts for the chemical production

STEP 4

Cradle to gate LCA for silicone and three esters

- Proxy data selected from Ecoinvent 3.9.1 as implemented in SimaPro
- Based on cut-off U (unit process) models, modified
- Dioctyl adipate – modified, isopropanol used to replace octanol part, adjusted based on molar mass
- Stearic acid as proxy for oleic acid
- Sebacic acid modelled with coconut oil

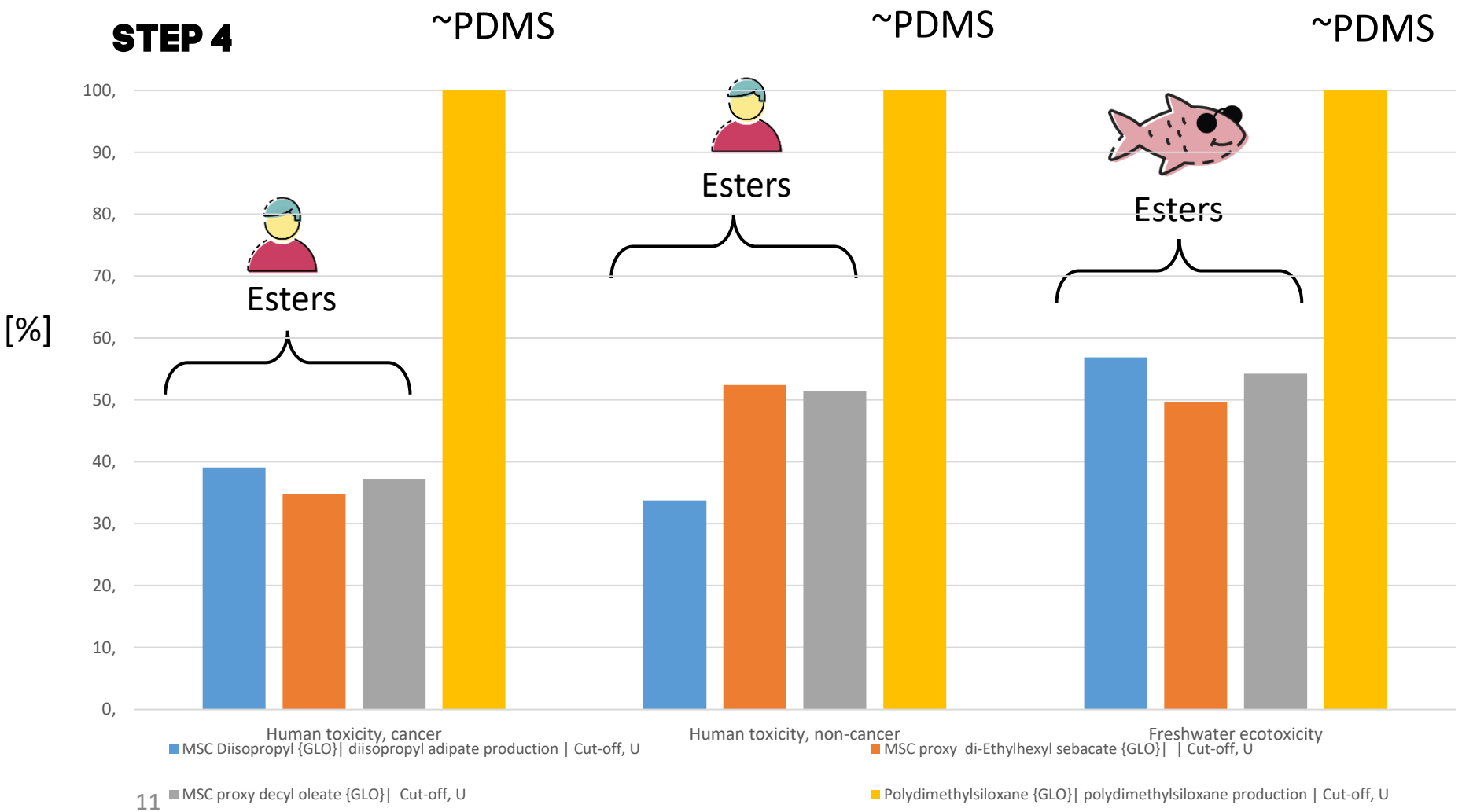
Environmental Footprint 3.1 categories; Usetox 2.13



RESULTS Life cycle impacts for chemical production

Method: USEtox 2.13

STEP 4



siloxane has higher human and freshwater ecotoxicity impacts than the alternatives

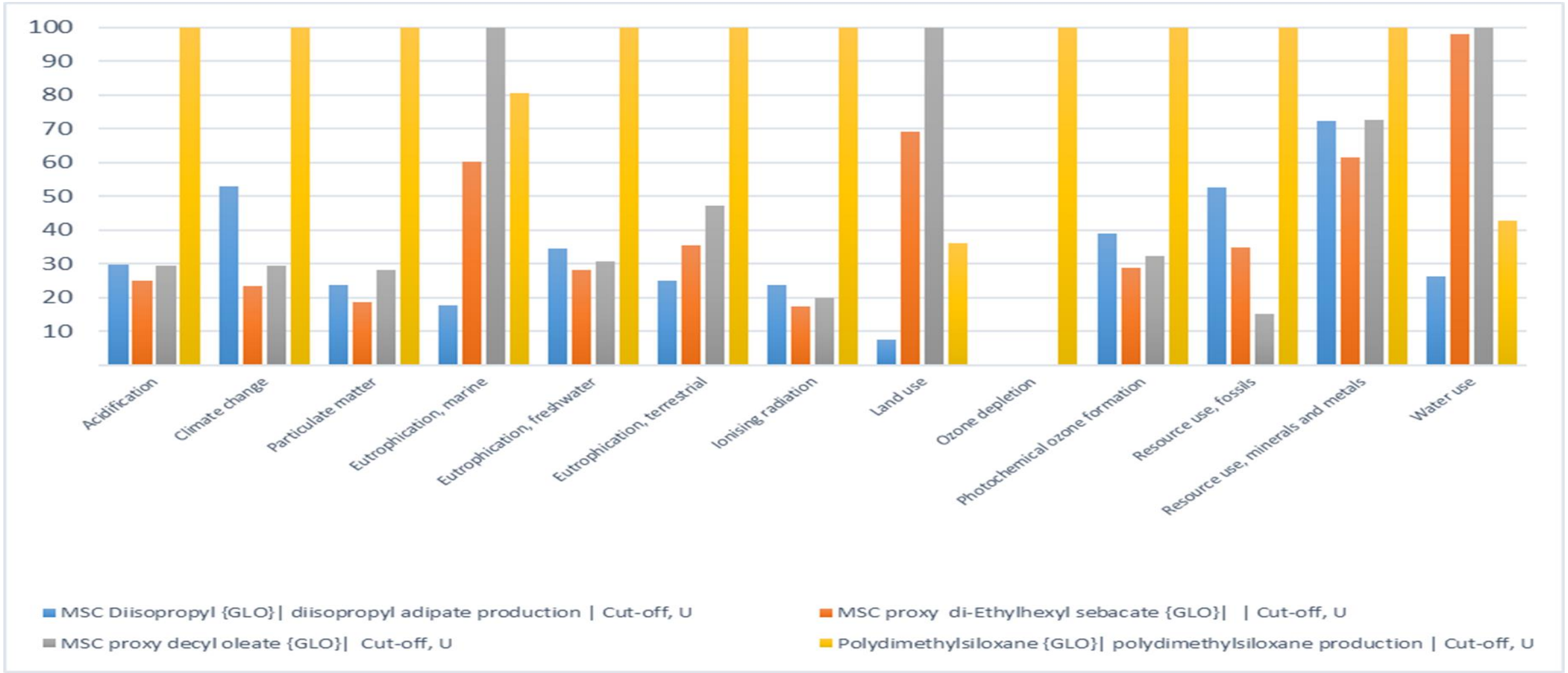
Esters (alternatives):

- Toxicity impacts for cancer and ecotoxicity are more even.
- Differences for non-cancer human toxcity impacts

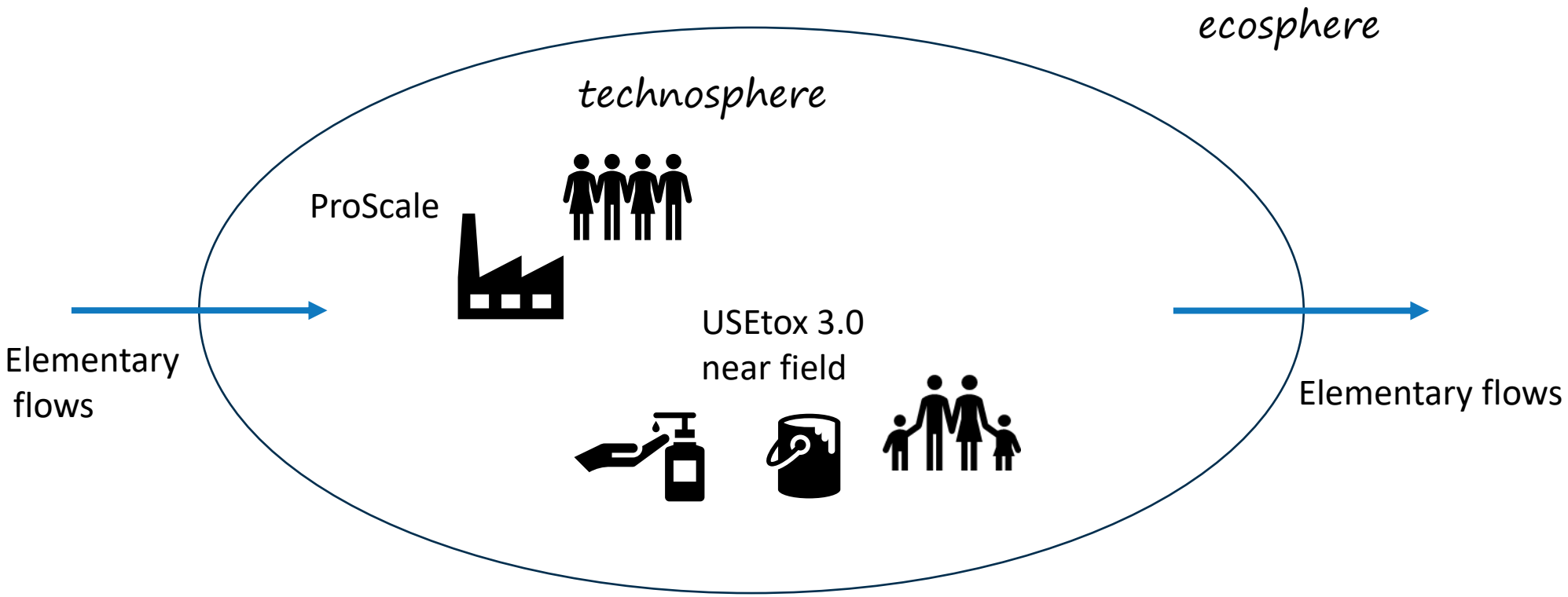
RESULTS Life cycle impacts for chemical production

STEP 4

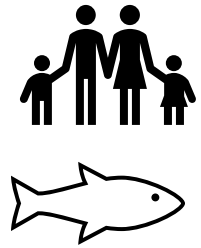
Lower impact of alternatives



Toolbox to populate the technosphere



USEtox 3.0
far field



MISTRA SAFECHEM

Contributions

- RISE – Lisa Skedung (case study lead), Nina Melander (CAA), Swapnil Chavan (computational toxicology), Steffen Schellenberger, Anna-Karin Hellström, Jutta Hildenbrand (CFA, LCA)
- IVL – Hanna Holmquist (WP 5 lead), Tomas Rydberg and Therese Kärnman (ProScale)
- DTU – Peter Fantke, Kerstin von Borries (Usetox 3.0)

MISTRA SAFECHEM

MISTRA SAFECHEM

INDUSTRY PARTNERS

RESEARCH PARTNERS

FINANCIER