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CALIMERO

IMPROVING BIO-BASED INDUSTRIES LIFE CYCLE SUSTAINABILITY

D3.1
Biodiversity assessment methodology definition

Due date of submission: 30/06/2025
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LIST OF ACRONYMS

AoP	Area of protection	**GHS**	Globally Harmonized System
AD	Application Domain	**HF**	Hazard Factor
API	Application Programming Interface	**GP**	Gaussian Process
c	Environmental compartment	**LCA**	Life Cycle Assessment
CAS	Chemical Abstracts Service	**LCI**	Life Cycle Inventory
CCF	Continuous-Cover Forest	**LDI**	Landscape Development Index
CF	Characterization Factor	**LCIA**	Life Cycle Impact Assessment
CLP	Classification, Labelling and Packaging	**LC_{50}**	Lethal Concentration for 50% of the population
ML	Machine Learning	**MF**	Material Flow
DF	Degradation Factor	**ML**	Machine Learning
ECA	Equivalent Connected Area	**NN**	Neural Networks
ECHA	European Chemicals Agency's	**NMD**	Nationella marktäckedata (Swedish National Land-Cover Database)
EF	Environmental Footprint	**NPV**	no-observed-effect concentration
EC_{50}	Effect Concentration for 50% of the population	**PEF**	Product Environmental Footprint
ELU	Exponential Linear Units	**PEFC**	Programme for the Endorsement of Forest Certification

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EL	Effective Loading for 50% of the population	**PSU E**	ProScale E of Unit Process
ERF	Environmental Release Factor	**REACH**	Registration, Evaluation, Authorization and Restriction of Chemicals
ES	Ecosystem Services	**SSbD**	Safe-and-Sustainable-by-Design
EU	European Union	**SMILES**	Simplified Molecular-Input Line-Entry System
FSC	Forest Stewardship Council	**SSbD**	Safe and Sustainable by Design
GMM	Gaussian Mixture Model	**UN**	United Nations

PROJECT INFORMATION

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List of participants:

Partner No.	PARTICIPANT ORGANIZATION | ACRONYM
1 (Coord.)	**Contactica | CTA**
2	WeLOOP | **WELOOP**
3	European Cellulose Insulation Association | **ECIA**
4	Swedish Environmental Research Institute | **IVL**
5	Neovili | **NEOVILI**
6	Cesefor | **CESEFOR**
7	Luxembourg Institute of Science and Technology | **LIST**
8	Technical University of Denmark | **DTU**
9	Techtera | **TECHTERA**
10	Essity | **ESSITY**
11	BIM Kemi AB | **BIMKEMI**
12	Ereks garment| **EREKS**

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DELIVERABLE DETAILS

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Supporting data:	A full overview of the developed ProScaleE characterization factors and input data is provided in Appendix X.1
Abstract:	This report presents methodological developments for assessing biodiversity and related ecotoxicity in the Life Cycle Assessment (LCA) of bio-based value chains, with a focus on alignment with the EU Product Environmental Footprint (PEF) framework. For biodiversity, by IVL, a spatially explicit method based on structural landscape connectivity was developed and tested using Swedish forestry as a demonstration case. The approach quantifies regional risk factors by modelling the effects of land use on ecological connectivity, taking into account both the distribution and conservation value of forest areas. For ecotoxicity, novel Characterization Factors (CFs) were established using two complementary approaches. The ProScaleE method applies regulatory data and hazard classification to derive CFs, as done by IVL, consistent with REACH and the EU CLP Regulation, while machine learning techniques were applied by LIST to extend the coverage of CF for USEtox (as applied in the EF) for certain chemicals relevant to bio-based sectors. Together, these approaches support improved coverage of chemical emissions across multiple environmental compartments. Findings indicate that spatial configuration and conservation value are critical for assessing biodiversity risk, and that further refinement of land use class alignment and data availability is required for operational application at larger scales. The work also identifies ongoing gaps in data and method transferability, particularly for agricultural landscapes and chemicals outside current model domains. Overall, the results provide a basis for additional ecologically relevant and robust assessments of both biodiversity and related ecotoxicity impacts in bio-based industries.

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1 Introduction

1.1 Context

Biodiversity loss is accelerating at an unprecedented rate, posing significant risks not only to ecosystems, but also to economic stability and societal well-being. In this regard, according to the World Economic Forum, more than half of global GDP (Gross Domestic Product) is moderately or highly dependent on nature and its services (WEF, 2020). Consequently, the transition to a bio-based economy introduces opportunities for decarbonization and resource efficiency, apart from bringing new sustainability challenges. Key sectors, such as forestry, agriculture, and chemicals, contribute to biodiversity decline through land transformation, emissions of chemicals, and resource exploitation, as highlighted in D1.2.

The Product Environmental Footprint (PEF) methodology proposed by the European Commission provides a standardized framework for assessing environmental impacts of products. However, several critical gaps persist in the way this method currently characterizes impacts on biodiversity and ecotoxicity. While the methodology has advanced considerably over the past decade, its capacity to reflect certain ecologically relevant damage remains limited. Most notably, the current PEF guidance does not mandate biodiversity indicators. Ecotoxicity modelling under the PEF framework is currently limited to freshwater impacts and does not yet adequately cover other compartments such as soil or marine environments (Sala et al., 2022), nor does it fully align with risk assessment practices under the EU (European Union) chemical legislation, such as the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) regulation. Finally, for many chemicals, ecotoxicity characterization factors are lacking.

The need for improved methodologies is recognized at both policy and scientific levels. For the biobased industry in particular, more robust and comprehensive Life Cycle Assessment (LCA) approaches, able to better represent biodiversity and to expand and refine ecotoxicity characterization, are essential to ensure that growth in this sector is truly sustainable.

1.2 Aim and objectives

The CALIMERO project, funded under Horizon Europe, aims to improve the sustainability performance of industrial bio-based sectors through enhanced LCA methodologies. This report addresses the environmental dimension of sustainability with a specific focus on biodiversity and ecotoxicity. These topics have been identified as critical yet underdeveloped areas within existing Life Cycle Impact Assessment (LCIA) methods, especially in relation to the PEF framework.

The main objective of this report is to present the methodological developments conducted within CALIMERO to address key gaps in current environmental impact modelling for bio-based value chains. This includes the development or refinement of impact assessment methods and characterization factors (CFs) that are applicable within LCA, and that aim to improve spatial, ecological, and regulatory relevance. While not all methods are yet operational for integration into PEF, they represent significant steps forward and provide a basis for future harmonization and policy integration.

Table 1 presents an overview of the environmental topics and corresponding methods addressed in this report. Each method is further described in the following sections, with details on modelling rationale, scope of application, data requirements, and recommendations for implementation.

Table 1. Environmental aspects and impact assessment methods related to biodiversity developed in CALIMERO.

Impact area	Indicator/approach	Scope/application
Biodiversity	Spatially explicit method based on structural landscape connectivity	Forestry systems (Sweden); regional-scale CFs
Ecotoxicity	ProscaleE, novel CFs for chemical compounds related to ecotoxicity	Chemicals used in CALIMERO case studies
	USEtox, novel CFs for chemical compounds related to ecotoxicity	Chemicals used in CALIMERO case studies

1.3 Report structure

This report presents developments of LCIA methods carried out within the CALIMERO project, with the objective of improving the representation of biodiversity, ecosystem services, and ecotoxicity in the assessment of bio-based value chains.

Each thematic section opens with a concise state-of-the art overview (drawing on D1.3), followed by a detailed description of the method development and its rationale within CALIMERO.

Section 2 introduces a new approach to assessing biodiversity impacts with a focus on structural landscape connectivity, as developed by IVL. **Section 3** addresses ecotoxicity modelling. In this regard, **Section 3.2** presents the work conducted using the ProScale methodology, for deriving CFs form regulatory hazard data , research carried out by IVL; **Section 3.3** focuses on the refinement and application of the USEtox via machine-learning models, conducted by LIST.

Finally, **Section 0** summarizes the main findings from the connectivity and ecotoxicity work, discusses key data and methodological limitations, and suggests possible next steps.

2 Biodiversity methodology – LILaC (Land-use Impact on Landscape Connectivity)

2.1 State-of-the-art

Drawing on the systematic review in D1.3, this section summarizes current practices in biodiversity assessment methodology for LCA. Understanding the myriad pressures on biodiversity is crucial for effective mitigation strategies. While habitat change resulting from land use stands as a key driver of biodiversity loss, other factors like climate change, invasive species, overexploitation of resources, and pollution also exert significant influence (Millennium Ecosystem Assessment, 2015). Despite the prevalence of models focusing solely on land-use impacts (Damiani et al., 2023), there is an emerging drive to capture broader biodiversity impacts on the Area of Protection (AoP) 'ecosystem quality', by integrating multiple pressures such as climate change and toxicity along with land use (Verones & Dorber, 2023). Examples include ReCiPe2016, LC-Impact, Stepwise and Impact world+. These models are a step forward in offering more comprehensive biodiversity assessments. However, they face important challenges. The complex interactions between different pressures make it difficult to isolate the contribution of each factor, raising concerns about double counting and reduced transparency in the cause-effect modelling (Jaureguiberry et al., 2022). Moreover, most of the current models still exclude significant drivers like invasive species and overexploitation (Curran et al., 2011) and fall short in environmental relevance due to inadequate incorporation of the multidimensionality of biodiversity (Crenna et al., 2020; Damiani et al., 2023; Marques et al., 2021).

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A recurring limitation is the lack of attention to spatial landscape structure. Most existing models do not account for how the physical configuration of habitats influences ecological functions such as dispersal and gene flow. Acknowledging biodiversity's inherent spatial and regional dependency, several initiatives have called for more regionally differentiated methods. Scherer et al. (2023), as part of the GLAM Phase 3 project, introduced an improved model that combines land use intensity with fragmentation effects. This approach builds upon earlier models developed by Chaudhary & Brooks (2018) and Kuipers et al. (2021), and incorporates the Equivalent Connected Area (ECA) concept. However, these approaches still rely on average land use categories and do not capture spatial detail specific to different systems or land use classes.

Among recent developments, the BioMAPS method by Maier (2024) stands out by offering biodiversity CFs at local, regional, and global scales, and is included in the ORIENTING project as addition to the LANCA® soil quality model (Pihkola et al., 2022). While the method shows high flexibility, its regional component, the Landscape Development Index (LDI), has been identified as a methodological weakness. The LDI aggregates land use types and their associated local risks, reflecting land use intensity rather than true spatial heterogeneity. By reusing local risk factors, it places proportionally greater emphasis on the risk of local biodiversity loss than on global biodiversity loss, without a clear scientific basis. Most critically, it does not account for the spatial layout of landscapes, and their role in shaping ecological connectivity. As such, it overlooks a critical dimension of ecological integrity: whether the landscape allows species to move, disperse, and maintain viable populations (Crawford et al., 2016; Haddad et al., 2015).

To address this gap, IVL has developed LILaC, a connectivity-based regional indicator intended to replace BioMAPS' LDI.

2.2 Methodological framework for LILaC

2.2.1 Indicator rationale and scope

Building on the limitations identified for the LDI, IVL is developing LILaC - Land use Impact on Landscape Connectivity as a novel regional biodiversity indicator. Rather than quantifying impacts on local species richness or direct biological effects, LILaC focuses on the spatial arrangement of the landscape; and how well that configuration supports ecological flows such as dispersal and gene flow. The resulting structural connectivity metric will provide regional CFs that can complement existing local and global biodiversity layers in BioMAPS once the development is complete.

Structural landscape connectivity refers to the degree to which habitat patches are physically connected within a landscape, based on their spatial arrangement and intervening land use types. It is a key determinant of ecological functioning, influencing species migration, gene flow, and resilience to disturbances (Crawford et al., 2016; Haddad et al., 2015; Phillips et al., 2021). Unlike functional connectivity, which requires species-specific data on behavior and mobility, structural connectivity offers a generalized, spatially explicit proxy, and was considered more feasible for integration into LCIA.

To operationalize this, we apply circuit theory-based modelling through the Omniscape tool (Anantharaman et al., 2020; Landau et al., 2021). In this approach, movement paths are treated as electrical currents flowing through a resistance surface, with pathways of lower resistance being preferred. These resistance values represent the ease or difficulty with which species can move through different land cover types. The model compares baseline scenarios that reflect current land use with counterfactual scenarios in which, for example, resistance in production forests is reduced to simulate natural, high conservation-value conditions. This comparison isolates the marginal contribution of each land-use flow to overall regional connectivity.

The goal is to provide a spatially explicit method that:

- Improves the regional granularity of biodiversity assessments in LCA,
- Provides a more ecologically meaningful interpretation of landscape structure than aggregated land use shares,
- Is methodologically compatible with the BioMAPS framework,
- Is applicable in the case-study on pulp&paper production in Sweden, as explored in the CALIMERO project,
- And can be expanded to different geographies and land use classes.

This approach builds on growing recognition that biodiversity impacts cannot be meaningfully assessed without considering the spatial organization of ecosystems. By refining the LDI to reflect landscape connectivity, the method strengthens the scientific robustness and policy relevance of regional biodiversity indicators used in LCIA.

2.2.1 Inventory-flow delineation

To link the regional connectivity indicator directly to Life Cycle Inventory (LCI) datasets, each forestry scenario is expressed as a distinct land-use elementary flow. The flow names follow the convention 'Forestry, [intensity], [qualifier]', so that the resulting CFs can be matched one-to-one with LCI data.

Because forest certification (i.e. FSC; Forest Stewardship Council and PEFC; Programme for the Endorsement of Forest Certification) is a potential lever for more sustainable sourcing in LCA supply-chain modelling, the method distinguishes certified and non-certified intensive forestry: separate CFs allow practitioners to test whether purchasing certified wood products can measurably reduce regional biodiversity risk.

The present deliverable defines three intensive-rotation flows: Forestry, intensive, not otherwise specified (FIN_{nos}), Forestry, intensive, non-certified (FIN_{nc}), Forestry, intensive, certified (FIN_{cert}) and lists Forestry, extensive (FEX) for completeness (not modelled). A synopsis of the underlying map layers is given in **Table 2**; **Table 3** then summarizes each flow, its plain-language description and the area equation.

Set-asides, certification and the flow hierarchy

LCI records rarely indicate whether roundwood is FSC or PEFC-certified; they typically report only *Forestry,* or *Forestry, intensive*. For that reason, FIN_{nos} serves as the default, catch-all flow: every productive forest pixel that is not an impediment, potential primary forest or Continuous-Cover Forest (CCF) stand, or strictly protected area is assigned to FIN_{nos}, even if that pixel might later function as a conservation set-aside.

Swedish FSC and PEFC standards require 5–10 % of the managed forest to be retained as conservation set-asides where harvesting is prohibited (Forest Stewardship Council (FSC), 2020). Together with legally protected forests, these areas maintain structural habitat features such as old trees, dead wood and riparian buffers, and thereby mitigate some connectivity losses caused by harvesting elsewhere. Because spatial data on certified holdings are not publicly available, the model approximates set-asides with key biotopes mapped by the Swedish Environmental Protection Agency.

The set-aside layer is applied differently in the two split flows:

- FIN_{nc} removes the set-aside pixels from FIN_{nos} (Eq. 2.2), representing uncertified intensive forestry, consisting only forest in rotation.
- FIN_{CERT} retains the same area for production forest in rotation, and considers the set-asides a part of the production system that is protected from harvesting. The connectivity loss caused by the

production forest in rotation is therefore divided by the combined area of forest land in rotation *plus* the mandatory set-asides, reflecting their shared responsibility for landscape integrity (See risk factor calculations in **Section 2.2.2**).

Throughout this subsection, A denotes area (m^2); subscripts in the area equations refer to map layers listed in **Table 2**.

Table 2. Spatial layers for the extraction of forestry inventory flows.

Subscript	Meaning
Forest	Total forest land
Impediment	Non-productive forest (e.g. mires, boulder fields)
Primary, CCF	Potential primary or Continuous-Cover Forest
Protected	Strictly protected areas (e.g. National parks)
Set-asides	Set-asides patches as mandated by FSC/PEFC schemes, here approximated with data on Key Biotopes

Table 3. Forestry land-use flows and their spatial delineation.

Code	**Land-use flow**	**Area definition**	**Equation**
FIN_{NOS}	*Forestry, intensive, not otherwise specified*	Managed rotation forestry after removing impediments, potential primary / continuous-cover stands and protected areas	$A_{FIN_{nos}} = A_{forest} - (A_{Impediment} + A_{Primary,CCF} + A_{Protected})$ (2.1)
FIN_{NC}	*Forestry, intensive, non-certified*	FIN_{NOS} minus set-aside patches	$A_{FIN_{NC}} = A_{FIN_{nos}} - A_{set-asides}$ (2.2)
FIN_{CERT}	*Forestry, intensive, certified*	Managed rotation forestry as in FIN_{nc} , plus mandatory set-asides (The reference treats only $A_{FIN_{NC}}$ as production forest in rotation, while $A_{set-asides}$ remain unchanged to reflect FSC/PEFC rules. See eq. 2.5)	$A_{FIN_{cert}} = A_{FIN_{NC}} + A_{set-asides}$ (2.3)
FEX	*Forestry, extensive*	In Sweden defined as Continues cover forestry (Excluded due to lack on data)	A_{CCF}

The definitions established here provide the basis for the modelling workflow described in the next subsection.

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2.2.2 Modelling workflow

The modelling pipeline consists of four sequential steps: (i) construction of the resistance layer, (ii) reference-scenario construction, (iii) connectivity modelling with Omniscape, and (iv) calculation of risk factors. **Figure 1** provides a visual summary of this process (illustrated for the municipality of Lerum); the steps are then explained in turn below.

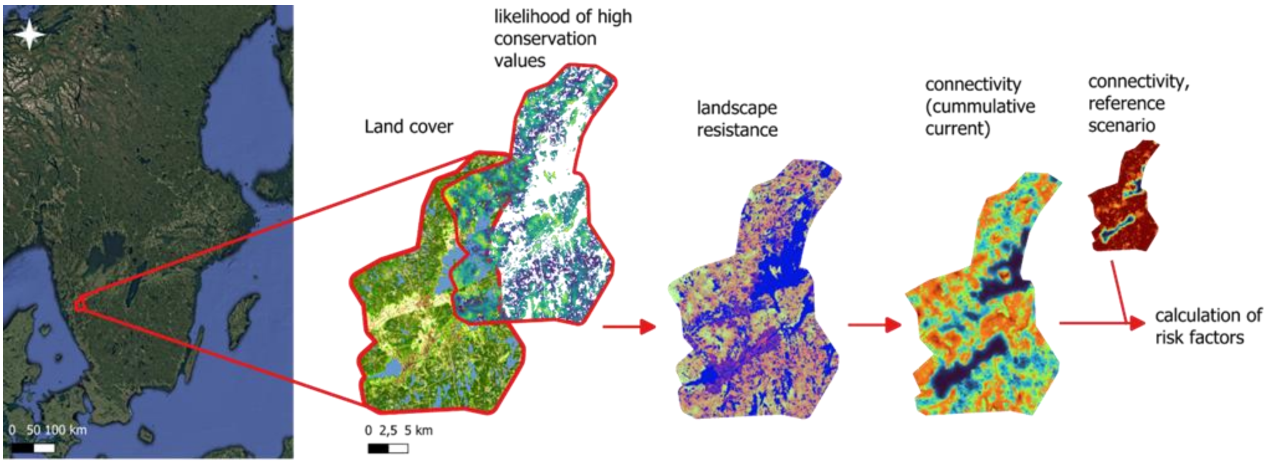

Figure 1. Workflow for constructing connectivity maps and risk factors. Illustrated for the Swedish municipality Lerum. Land cover and the likelihood of high conservation values were used to generate a landscape resistance layer. Connectivity was then calculated based on this resistance, and the resulting connectivity layers—both for the current state and a reference scenario—were used to derive risk factors.

1. Construction of the resistance layer

Using Nationella marktäckedata (NMD, the Swedish National Land-Cover Database; Swedish Environmental Protection Agency, 2018), each land use class was assigned a resistance value that reflects the relative difficulty for species movement, informed by literature (Nilsson & Englund, 2024). Resistance values for forests were then refined with the NVK Skog model (Bubnicki et al., 2024), which predicts, at 1 ha resolution, the probability that a pixel harbours high conservation values, even in areas where direct conservation data are lacking. We converted this probability inversely and linearly into resistance: a 100% likelihood was assigned the minimum resistance (1), whereas very low probabilities approached the maximum (100), with intermediate values scaled proportionally. A full list of land cover classes and their assigned resistance values is provided in **Table 4.**

Table 4. Resistance values assigned to land cover classes.

Land cover, NMD code	Land cover, class	Resistance value
111-117	Forest not on wetland	1-100 (depending on conservation value)
118	Temporarily non-forest not on wetland	300
121-127	Forest on wetland	1-100 (depending on conservation value)
128	Temporarily non-forest on wetland	100
2	Open wetland	40
3	Arable land	300
41	Non-vegetated other open land	40
42	Vegetated other open land	40
51	Artificial surfaces, building	600
52	Artificial surfaces, not building or road/railway	600
53	Artificial surfaces, road/railway	600
61	Inland water	600
62	Marine water	600
-	Extra resistance in densely populated areas	+200

2. Reference scenario

To isolate the risk factors of specific land use types, such as production forests, reference scenarios are constructed. In this reference scenario, as a presumption, the resistance values for the land use in question were lowered to 1, simulating an idealised natural situation.

3. Connectivity modelling

The resistance maps for both the baseline (current land use) and the reference scenario were processed in Omniscape. Omniscape treats movement as electrical current that seeks paths of least resistance, producing cumulative current density maps for the baseline $C_{baseline,x}$ and the reference $C_{reference,i,x}$

where:

- i = land use flow
- x = region

Structural connectivity is expressed as the mean current density across the landscape, which serves as a proxy for ecological flow.

Omniscape settings used:

- Search radius: 100
- Block size: 21
- r-cutoff: 50
- Buffer zone: 1000 m (to minimise edge effects)

4. Risk-factor calculation

For each land-use flow, the connectivity loss is the difference between baseline and reference cumulative current. This loss is normalised by the mapped area of the flow $A_{i,x}$, to give a risk factor per square meter:

$$Risk\ factor_{i,x} = \frac{C_{baseline,x} - C_{reference,i,x}}{A_{i,x}} \tag{2.4}$$

For the certified flow, the connectivity loss is divided between the production forest in rotation *plus* its set-asides patches. Hereby, we recognize set-asides as integral parts of the certified production system. In this way, both the production forest in rotation and conservation set-asides, share the resulting connectivity burden.

$$Risk\ factor_{FIN_{cert},x} = \frac{C_{baseline,x} - C_{reference,FIN_{cert},x}}{A_{FIN_{NC},x} + A_{set-asides,x}} \tag{2.5}$$

Where:

i = land use flow
x = region
$C_{baseline,x}$ = Cumulative current density in the baseline map, in region x
$C_{reference,i,x}$ = Cumulative current in the reference map for land use type i in region x
$A_{i,x}$ = Area of flow i in region x (in m^2)
$A_{set-asides,,x}$ = Area conservation set-asides in region x

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2.2.3 Software and tools

The workflow runs on open-source software, supplemented by project specific Python and Julia code:

- GIS software: GRASS GIS 8.4.0
- Connectivity Modelling Tool: Omniscape v0.6.2
- Scripting languages: Python 3.12.4 and Julia 1.10

A practical execution guide, complete with step-by-step instructions and links to the script repository, will be delivered in one public report of WP5. Full technical documentation of the code will be released at the same time. In parallel, the method (including extended validation) will be prepared for submission to a peer-reviewed scientific journal.

Together, the inventory-flow definitions, resistance-layer specification, reference-scenario protocol and risk-factor equations (Equations 2.1-2.4) constitute the full technical set-up. **Section** Error! Reference source not found. applies this workflow in a pilot analysis of four Swedish municipalities.

2.3 Pilot application: four Swedish municipalities

The pilot applies the connectivity workflow to the Swedish municipalities Vara, Lerum, Hofors and Bjuv. Its purpose is illustrative only; to show how landscape-level risk factors emerge from the method, not to establish definitive CFs. The analysis cover the three intensive forestry flows defined earlier (FIN_{NOS} , FIN_{NC} and FIN_{CERT}); Continuous-cover forestry (FEX – Forestry, extensive) was excluded because it represents only ≈ 3.6 % of Sweden's productive forest land (Skogsstyrelsen, 2023) and spatial data on this management system was unavailable.

2.3.1 Landscape context

The proportion of forested cover varies substantially among the four municipalities (**Table 5**). Bjuv, which is largely agricultural, has the lowest forest share (10.9 %), while Hofors is the most forested at 27.8 %. Yet, forest extent alone does not predict connectivity; Hofors, records the lowest mean current-density (0.18), indicating a spatially fragmented forest of low conservation value.

By contrast, Lerum, with a forest share similar to Hofors (27%) achieves highest connectivity (0.58). The difference is explained by a more cohesive patch mosaic and the municipality's comparatively high probability of forests with high conservation value (also reflected in the share of strictly protected forests and key biotopes found in Lerum), thereby increasing its capacity to sustain ecological flows.

Vara and Bjuv show numbers in between. Vara's 15% forest cover yields intermediate connectivity (0.21), while Bjuv's small but relatively well-situated forest remnants (10.9% cover) give a slightly higher connectivity score (mean current density: 0.29). Taken together, these findings confirm that regional connectivity depends more on the spatial distribution and conservation quality of forest patches than on total forest area alone.

Table 5. Municipal variations in forestry landscapes in the test-case study.

Municipality	Vara	Lerum	Bjuv	Hofors
Total area (ha)	124 660	70 427	24 491	91 379
Forest area (ha)	19 078	19 002	2 681	25 380
Productive forest (ha)	17 934	17 803	2 660	24 199
of which strictly protected (%)	0.8%	3.3%	3.6%	1.2%
of which key-biotopes (not on protected land; %)	0.3%	1.9%	0.8%	0.3%
Connectivity (mean current density)	0.21	0.58	0.29	0.18

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2.3.2 Risk-factor results

Figure 2 presents the connectivity-based risk factors for the three intensive forestry flows. In all municipalities the ranking is the same: FIN_{cert} >FIN_{nos} >$FIN_{nc,}$ meaning certified management consistently showing the lowest negative values, i.e. least loss in connectivity. This reduction arises because changes in connectivity between the baseline and the reference situation are distributed over a larger area compared to non-certified forestry, including mandatory set-aside required by FSC/PEFC that are considered a part of the production system. FIN_{nc} lacks this buffering area. Even so, the certification benefit is modest, a consequence of the limited spatial coverage of key biotopes (0.3-1.9% of productive forest, **Table 5**) used here as set-aside proxies.

Regional landscape structure exerts a stronger influence than management class: Hofors shows the most negative risk factors across all flows, while Lerum showed the least negative factors, benefiting from better baseline connectivity and higher protection share. Vara end Bjuv occupy the middle ground. In Bjuv, a relatively high protection share and the higher probability of forests with high conservation values, might compensate for the limited forest extent.

A greater proportion of protected forests means that a smaller percentage of the land remains available for commercial forestry, which, in turn, contributes to lower risk factors in Lerum and Bjuv. However, whether there is a direct correlation between the extent of protected areas and population density remains an open question, as land-use priorities often differ between urban and rural municipalities.

Together, these results illustrate that (i) the indicator responds sensitively to spatial pattern and protection status, and (ii) certification measures reduce risk, but this effect is modest, particularly when set-aside implementation is incomplete in the underlying data.

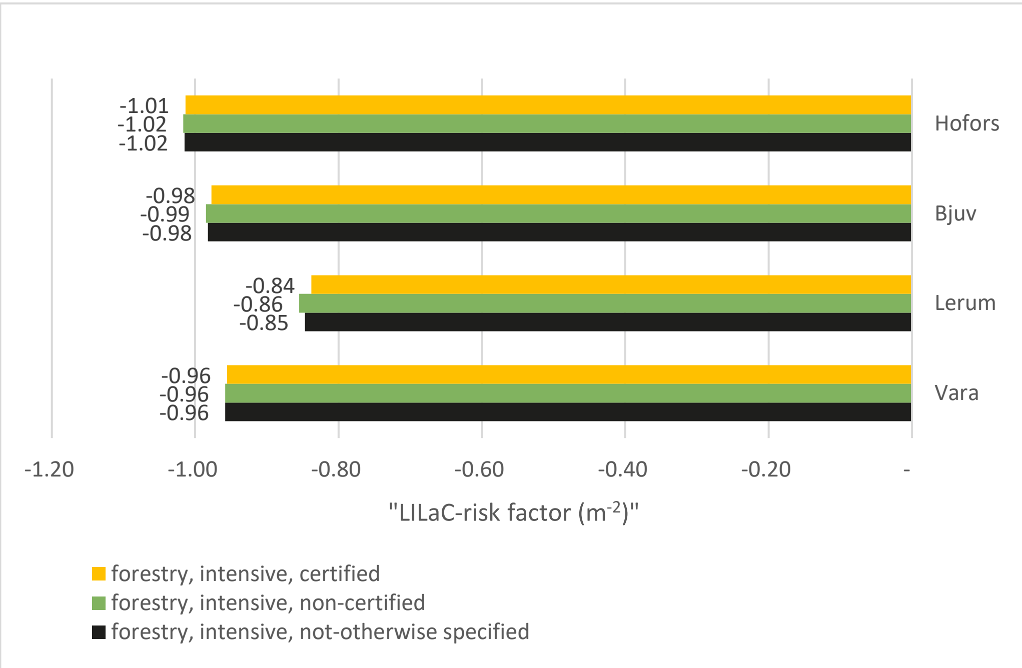

Figure 2. Risk factors (per m^2) for the three forest management systems in the test-case study, across four Swedish municipalities. The risk factor is calculated as the unitless connectivity loss divided by the mapped land area of the production system; hence the resulting values are expressed per square meter (m^{-2})

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2.4 Discussion and implementation

While the case study demonstrates the application of connectivity-based risk factors for forestry in four Swedish municipalities, several limitations constrain both the current findings and broader applicability. Most notably, the actual CFs are still under development. These will be calculated in the context of Swedish pulp and paper case study as part of the CALIMERO project and are intended for publication in the forthcoming D5.3. The calculated CFs will represent regionalized biodiversity risks of forestry in different regions in Sweden, for the land use flow: *Forestry, intensive, not otherwise specified*.

Differentiating certified from non-certified forestry is attractive in principle, because certification schemes may, if properly implemented, lower the risk that forest management poses to structural connectivity.
In practice, three obstacles currently prevent a robust split between the systems:

- The current model underestimates set-aside areas in certified forests considerably. For example, key biotopes, used as proxy for set-aside patches, accounted for only 0.3-1.9% of the non-protected productive forest land in the test study, whereas certification schemes such as FSC and PEFC typically require 5-10% of the forest area to be set-aside for conservation (Forest Stewardship Council (FSC), 2020).
- Spatial data on certified forest land is not publicly available, making it difficult to accurately distinguish certified from non-certified areas at landscape scale.
- Certification requirements do not always translate into practice. Audits and field studies have found no evidence that certification increased the proportion of set-asides, retention trees, or high stumps left standing compared to non-certified forests (ASI, 2023; Villalobos et al. 2018). This questions the assumption that certification alone actually reduces biodiversity risk in intensive forestry systems.

Given these constraints, the forthcoming case study will treat intensive forestry as a single management archetype. FIN_{cert} and FIN_{nc} will nevertheless be retained to test the mechanics of the indicator. Prior to publishing the final CFs in D5.3, a sensitivity analysis will be conducted in which certified forestry is assumed to include the full 5–10 % set-aside share required by FSC/PEFC. High-probability conservation forest (as flagged by NVK Skog) will be added as set-aside areas until that target percentage is met, and the effect on risk factors will be reported. This exercise will illustrate how much the indicator might shift if comprehensive, spatially explicit data on set-asides were available.

2.4.1 Opportunities and next steps

The results also highlight that a greater proportion of forest cover does not automatically result in higher ecological connectivity. The spatial arrangement and quality of forest patches are critical. This underscores the value of a connectivity-based approach, which looks beyond simple land cover statistics.

To make this method truly operational for LCA and PEF, several key issues should be addressed:

- There is a need to map land cover classifications onto harmonized, multi-level land use typologies, such as those proposed by Koellner et al. (2013). This will enable proper matching of characterization factors with elementary flows, also for land use types other than forestry.
- While land cover and protection status data are generally available in Europe, reliable information on conservation value is less widespread. Ongoing work aims to adapt and validate the conservation value model for other countries. Where detailed data is unavailable, global datasets such as HILDA+ and GLOBIO 4 (cf. Scherer et al., 2023) may offer a practical alternative, though with less ecological detail.
- Assigning generalized resistance values may overlook region- and habitat-specific conditions, particularly in landscapes and ecosystems that differ markedly from Swedish forests. Careful

adjustment for regional context, while maintaining comparability, will be crucial for broader application.

3 Ecotoxicity assessement methodology

3.1 State-of-the-art

Currently, the USEtox model provides ecotoxicity CFs for slightly more than 2,000 substances. One of the latest Environmental Footprint updates (i.e., EF v3.0) has expanded this to 6,038 chemicals (Sala et al., 2022). Douziech et al. (2024) recently extended the CFs for freshwater ecotoxicity to more than 9,000 chemicals. However, a first gap is that this still represents only a small portion of the chemicals humans and ecosystems may be exposed to, limiting the effectiveness of LCA and Safe-and-Sustainable-by-Design (SSbD) in real-world applications (Wang et al., 2020). To bridge this gap, data-driven approaches like Machine Learning (ML) can support fast and cost-effective screening of chemical hazards (Hou et al., 2020). However, while existing efforts mainly focus on predicting intermediate parameters such as HC50 before calculating CFs, this stepwise approach is hard to scale for CF prediction due to data gaps and uncertainty.

Moreover, the ProScale methodology has been proposed as an alternative or complementary approach to USEtox and EF as the first version of ProScale provides a life cycle approach covering workers exposure, which is typically not included in other tools (Lexén et al., 2021), representing a second gap. Additionally, the tool is built to utilize data derived under already existing regulatory policies such as the REACH regulation. In a recent development, the ProScale methodology has been extended to also cover ecotoxicity. Further developments are expected in the future focused on some aspects like covering the service life of products (Halling, 2024).

3.2 ProScale E

3.2.1 Background methodology explanation

ProScale E, recently developed by IVL as an extension built on the ProScale framework, enables the calculation of ecotoxicity CFs (Rydberg et al., 2024; Lexén et al., 2021). The ProScale E approach follows the established ProScale methodology used for human toxicity and is thus also based on the use of information reported under the REACH regulation including hazard phrases (H-phrases) from the EU Classification, Labelling and Packaging (CLP) Regulation. A major difference between the use of classifications under the CLP regulation is that for ProScale H the H3XX-phrases covering human toxicity is used, while for ProScale E the ecotoxicity series, H4XX-phrases, are applicable.

A ProScale E score (PSU E) for a given unit process, *u*, for each substance, *i*, is based on four factors: (i) Material Flow (MF), (ii) Environmental Release Factor (ERF), (iii) Degradation Factor (DF), and (iv) Hazard Factor (HF), and calculated for each environmental compartment, *c*, of interest, as shown in **Equation 3.1**.

$$PSU\ E_{u,c} = \sum_{i} \underbrace{HF_i \cdot DF_i}_{\text{CF}} \cdot MF_i \cdot ERF_{i,c} \tag{3.1}$$

The MF captures the material flow for a unit process while the ERF accounts for the emissions related to that specific MF, in instances where the specific emission flows are already known those can be used. The DF is assigned based on the biodegradability in water as determined by screening tests as well as the persistence of the substance, see **Table 6**. For this work it was decided that when ProScale E is applied to inorganic substances, they are assigned DF = 1. The reason for this is that the tests for biodegradation and persistence are not applicable to inorganics.

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Table 6. Overview of DFs for ProScale E assessment.

Degradation factor (DF)	
Readily biodegredable	0.01
Inherently/Rapidly biodegredable	0.1
Persistent/Not biodegradable	1
Very persistent	
Inorganic substance	

When performing ProScale E assessments the HFs are derived differently from how it is done in a ProScale H assessment, apart from being based on the 4XX-phrases the multiplying factors (M-factors) are used. M-factors are reported alongside H-phrases for substances which are highly toxic and is a way to increase the weight of the toxicity for such substances in mixtures, even at low concentrations (UN, 2023). In ProScale E assessments the M-factor is accounted for in a way by using it as a modification factor when converting H-phrases into HFs. A conversion table from the relevant CLP hazard categories (here also referred to as H4XX-phrases), with or without M-factors, into harmonized HF_e:s can be seen in **Table 7.**

Table 7. Overview of ProScale E HF_e:s as derived based on the CLP regulation.

ProScale hazard class	CLP hazard categories (H4XX-phrases)	Environmental hazard factor (HF_e)
E (10 000 - 100 000)	PBT/vPvB	100 000
	PMT/vPvM	100 000
	ED, env cat 1	100 000
	Chronic aquatic 1 (H410), M-factor ≥ 10 000	100 000
	Chronic aquatic 1 (H410), M-factor = 1000	30 000
D (1000 - 10 000)	ED, env cat 2	10 000
	Chronic aquatic 1 (H410), M-factor = 100	10 000
	Acute aquatic (H400), M-factor ≥ 10 000	10 000
	Chronic aquatic 1 (H410), M-factor = 10	3000
	Chronic aquatic 1 (H410), M-factor = 1	1000
	Acute aquatic (H400), M-factor = 1000	3000
C (100 - 1000)	Chronic aquatic 2 (H411)	1000
	Acute aquatic (H400), M-factor = 100	1000
	Acute aquatic (H400), M-factor = 10	300
B (10 - 100)	Chronic aquatic 3 (H412)	100
	Acute aquatic (H400), M-factor = 1	100
A (1 - 10)	Chronic aquatic 4 (H413)	10
No hazard	No class ("regarded as safe")	-

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3.2.2 Method for data collection

With inputs from the CALIMERO project partners 105 substances were identified for which it was deemed relevant to derive ProScale E CFs. The MFs and ERFs are context-dependent parameters that fall outside the scope of this task. Consequently, each CF is limited to the product of DF and HF_e, as shown in **Equation 3.1**.

The first step of the assessment was therefore to collect all H4XX-phrases and M-factors for each of the substances. For every substance the ECHA CHEM portal (https://chem.echa.europa.eu/) was consulted, focusing on lead joint registration dossiers, with preference given to full registrations over intermediate ones. If a substance was not available in the ECHA CHEM portal, the old website "Search for chemicals" (https://echa.europa.eu/information-on-chemicals) was checked too. In instances where no H4XX-phrase was available, the Mistra SafeChem prediction models were run, to generate a predicted H4XX-phrase. For additional M-factors both experimental and predicted data was used. More detailed descriptions for running and using prediction tools and calculations for H4XX-phrases and M-factors are provided in **Section 3.2.3**.

For assigning the degradation factors, the REACH dossier sections "5.2 Biodegradation in water: screening tests" and "2.3 PBT assessment" were searched. If the criteria for persistence were fulfilled, but not for biodegradation and/or toxicity, persistence was still assumed. For inorganic substances DF was set to 1, reflecting the limited applicability of tests for degradation and persistence. In cases were biodegradation and persistence were missing in the ECHA REACH dossiers, predicted persistence was used, as described in **Section 3.2.3**.

3.2.3 Prediction and treatment of data for ProScale E assessment

Persistence factors for ProScaleE were predicted by the soil persistence and biodegradability models in Mistra SafeChem in silico Toolbox (v1.0). All compounds predicted to be persistent in soil were assigned a persistence factor of 1. Compounds predicted to be non-persistent in soil but not readily biodegradable were assigned 0.1, whereas those predicted to be non-persistent and readily biodegradable were assigned 0.01.

The H4XX-phrases were predicted using the H-statement models developed by Mistra SafeChem: one for acute aquatic toxicity (H40X) and one for chronic aquatic toxicity (H41X). The models were trained and validated with H4XX-phrases extracted from REACH dossiers (Norinder et al., 2025). Predictions labelled "likely positive" were accepted for subsequent calculations. Additionally, M-factors were predicted with ecotoxicity models in VEGA. Twelve models, including four fish acute LC_{50} (lethal concentration 50%) models, two *Fathead minnow* LC_{50} models, four *Daphnia magna* acute LC_{50}/EC_{50} (effective concentration 50%) models and two algae acute EC_{50} models were used to calculate M-factors for acute toxicity. Three models, including a fish chronic no-observed-effect concentration (NOEC) model, a *Daphnia magna* chronic NOEC model and a algae Chronic NOEC model, were used to calculate M-factor for chronic toxicity. The resulting acute LC_{50}/EC_{50} and chronic NOEC values were converted to M-factors in accordance with the criteria set out in the UN Globally Harmonised System (GHS) 'Purple Book' (**Table 8**), (UN, 2023).

Table 8. M-factor conversion according to the UN GHS Purple Book.

Acute toxicity	M-factor	Chronic toxicity
$L(E)C_{50}$ value		NOEC value
$L(E)C_{50}$>0.1	1	NOEC>0.01
0.01<$L(E)C_{50}$≤0.1	10	0.001< NOEC ≤0.01
0.001<$L(E)C_{50}$≤0.01	100	0.0001< NOEC≤0.001
0.0001<$L(E)C_{50}$≤0.001	1000	0.00001< NOEC≤0.0001
(Continue in factor 10 intervals)		

The ECHA database was used to collect the EC_{50} values for acute and chronic toxicity in three different trophic levels (aquatic invertebrates, algae, and fish) for calculation of M-factors from experimental data. For most of the chemicals, EC_{50} values that were obtained from ECHA were experimental data. However, for a few poorly soluble chemicals EL_{50} (Effective Loading for 50% of the population) were used. The EC_{50} and EL_{50} values were later used to calculate the M-factor for each chemical.

The M-factor is applied to substances that are highly toxic to the aquatic environment, specifically those with LC_{50} or EC_{50} values less than 1 mg/L. Under the GHS of classification, substances falling under Acute Aquatic Toxicity Category 1 or Chronic Aquatic Toxicity Category 1 typically require assignment of an appropriate M-factor. This is a mandatory requirement under the EU CLP Regulation.

The primary purpose of the M-factor is to amplify the contribution of highly toxic components when determining the environmental hazard classification of a mixture. This ensures that even low concentrations of highly toxic substances are properly accounted for in the overall hazard assessment. The value for a calculated M-factor based on experimental values for a substance are also assigned according to **Table 8**.

The M-factors obtained from ECHA follow a similar model for M-factor calculation for each chemical. Two different M-factors (one for acute toxicity and the other for chronic toxicity) were calculated based on the data available in ECHA. This is because in annex VI in the CLP regulation (EU's harmonized substance classification list) M-factors can be assigned to Aquatic Acute 1 or Aquatic Chronic 1 or both. The M-factors for Aquatic Acute 1 and Aquatic Chronic 1 do not have to be the same. The table with background data and M-factor calculations is included in **Appendix X.1**.

The use of predicted data was always considered to have lower reliability in a ProScale E assessment; thus, the following hierarchy was applied generally to all types of utilized predictions:

1. Data from ECHA CHEM dossiers
2. Other sources for measured data
3. Predicted data

There are several potential combinations of lower priority data which can be used for the assigning of HF. Thus, a specific hierarchy for the various combinations was used in relevant cases:

1. H-phrase available in ECHA CHEM + Collected M-factor from ECHA CHEM
2. Predicted H-phrase + Calculated M-factors
3. Predicted H-phrase + Predicted M-factors

In the case of predicted H-phrases and calculated or predicted M-factors, only the highest possible HF was assigned, in line with the precautionary principle.

3.2.4 Results and Discussion

Our objective was to develop ProScale E CFs for a set of 105 substances. Given that only 18 of these substances are classified with H4XX-phrases in their REACH dossiers, prediction tools were used for the remaining chemicals to expand coverage. An additional 16 substances received H4XX-phrases via *in silico* prediction methods. Together, these 34 substances form the subset for which any acute or chronic ecotoxicity classification could be obtained. For the remaining 71 substances, no H4XX classification was available. Because the prediction tools distinguish only between acute and chronic H4XX-phrases, they do not assign the numerical M-factors required to convert an H-phrase into a HF using **Table 7.** Overview of ProScale E HFe:s as derived based on the CLP regulation Accordingly, we derived M-factors by consulting measured toxicity data or, when such data was not available, by applying prediction tools. Once an M-factor for a given H4XX-phrase was obtained, it was combined with the acute/chronic distinction to yield an HF according to the prescriptive rules in **Table 7**. The collected, calculated, or predicted data used in this assessment are available in **Appendix X.1**.

Similarly, for Degradation Factors (DFs), when information on persistence or biodegradation was available via ECHA, this empirical data was preferred. In cases where ECHA data was absent or ambiguous, we used calculated/predicted values. Given that standard biodegradation and persistence tests are not applicable to inorganic substances, we defaulted to a precautionary DF = 1 for all 40 inorganics in our list, even when ECHA dossiers indicated otherwise.

Of these 34 substances, three lacked at least one required input (H4XX-phrase, M-factor, or DF), further reducing our list of substances for which CFs could be calculated to 31. The remaining 71 substances lacked any H4XX-phrase and, under the current ProScale E version, were treated as "regarded as safe", meaning no CF was assigned. In total, this report therefore provides 31 provisional CFs (**Table 9**), while 74 substances remain without a CF assignment. Because the present workflow cannot yet determine how to handle substances that lack complete hazard data, the 31 CFs reported here should be regarded as interim values.

*Table 9. Interim ProScale E characterization factors. Substances that have H4XX-phrases in ECHA CHEM have been marked with *, the remaining CFs are calculated based on predictions. "-" indicates that no CFs could be calculated.*

Chemical Name	CAS	ProScale E CF
Boric acid	10043-35-3	1000
Calcium chloride	10043-52-4	-
4,4'-Diisocyanatodiphenylmethane	101-68-8	1000
Nitric oxide	10102-43-9	1000
Triethanolamine	102-71-6	-
Ceric sulfate tetrahydrate*	10294-42-5	1000
Butyric acid	107-92-6	-
Diisobutyl ketone	108-83-8	-
Dipotassium phosphate	7758-11-4	-
Cyclohexane*	110-82-7	10
Borax pentahydrate	12179-04-3	-
2-Phenoxyethanol	122-99-6	-
Carbon dioxide	124-38-9	-
Sodium oxide	12401-86-4	-
Flumexol WDN*	126-71-6	1
Cobalt Molybdenum Alloy	12604-58-9	-
Boric oxide	1303-86-2	-
Sodium tetraborate decahydrate	1303-96-4	-
Calcium hydroxide	1305-62-0	-
Calcium oxide/Lime/Quicklime	1305-78-8	-
Potassium hydroxide	1310-58-3	-
Caustic soda	1310-73-2	-
Sodium oxide	1313-59-3	-
Zinc oxide*	1314-13-2	1000

Zirconium dioxide	1314-23-4	-
H-Mordenite	1318-02-1	-
Zeolite	1318-02-1	-
Gypsum	13397-24-5	-
Aluminum oxide	1344-28-1	-
Monoethanolamine*	141-43-5	1
Ethyl acetate	141-78-6	-
Aluminium hydroxide	21645-51-2	-
Polyethylene glycol dimethyl ether	24991-55-7	-
Poly(oxy-1,2-ethanediyl),α-hydro-ω-hydroxy- Ethane-1,2-diol, ethoxylated	25322-68-3	-
Methylisothiazolinone*	2682-20-4	1000
Tungstic acid	7783-03-01	-
Tris (2.4-ditert-butylphenyl)	31570-04-4	-
(2-methoxymethylethoxy)propanol	34590-94-8	-
Calcium carbonate	471-34-1	-
Sodium Carbonate	497-19-8	-
Formaldehyde	50-00-0	-
Glucose	50-99-7	-
Rucholase HCH	56-81-5	-
Urea	57-13-6	-
Toluene diisocyanate/Toluene, 2,4-diisocyanate*	584-84-9	100
Platinum	7440-06-04	-
Ethylenediaminetetraacetic acid	60-00-4	-
Cobalt acetate*	6147-53-1	3000
Ethanol	64-17-5	-
Acetic acid	64-19-7	-
Prestogen FCB	6419-19-8	-
Hydroxymethylfurfural (HMF)	67-47-0	-
Methanol	67-56-1	-
Acetone	67-64-1	-
Chloroform	67-66-3	-
Dimethyl sulfoxide	67-68-5	-
Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts*	68411-30-3	1
Molasses	68476-78-8	-
Isotridecanol, ethoxylated/Poly(oxy-1,2-ethanediyl), α-tridecyl-ω-hydroxy-, branched*	69011-36-5	1
Butanol	71-36-3	-
Methane	74-82-8	-
Ethylene	74-85-1	1
Nickel*	7440-02-0	100
Boron	7440-42-8	-
Magnesium sulfate	7487-88-9	-
Dichloromethane	1975-09-02	-

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Hydrochloric acid	7647-01-0	100
Sodium Chloride	7647-14-5	-
Phosphoric acid	7664-38-2	-
Ammonia*	7664-41-7	1000
Sulphuric acid	7664-93-9	-
Sodium hypochlorite*	7681-52-9	100
Disodium disulphite	7681-57-4	-
Sulphur	7704-34-9	100
Iron sulfate	7720-78-7	-
Potassium permanganate*	7722-64-7	3000
Hydrogen peroxide*	7722-84-1	100
Sodium persulfate	7775-27-1	-
Chlorine*	7782-50-5	1000
Ammonium sulfate	7783-20-2	-
Diammonium phosphate	7783-28-0	-
Diisocyanates	822-06-0	1000
2,6-Bis(2-isocyanato-3-((2-isocyanatophenyl)methyl)benzyl)phenyl isocyanate	85423-11-6	3000
Hexane, 1,6-diisocyanato-	88357-62-4	-
Sulfur dioxide	7446-09-5	-
Octadecane -1-ol ethoxylated*	9005-00-9	10
Cellulase	9012-54-8	-
Glucoamylase	9032-08-0	-
Kieralon MWF (hostapal MWF, soap)	9043-30-5	-
1,1,1-Tris(4-cyanatophenyl)ethane	N/A	300
(2Z)-2-[(10E)-10-[cyano(isocyano)methylidene]-3-(3-methyloxiran-2-yl)-2,7,8-tris(oxiran-2-yl)-4b,9b-dihydroindeno[2,1-a]inden-5-ylidene]-2-isocyanoacetonitrile	N/A	3000
2,2'-Methylenebis(6-(o-isocyanatobenzyl)phenyl) diisocyanate ($C_{31}H_{20}N_4O_4$)	85392-14-9	1000
2,6-Bis(o-isocyanatobenzyl)phenyl isocyanate ($C_{23}H_{15}N_3O_3$)	21132-81-0	1000
Alcohols, C16-18, ethoxylated*	68439-49-6	10
Amylase	9000-90-2	-
Anionic polyacrylamide	9003-0-8	-
Fatty alcohol ethoxylate	78330-20-8	1000
Fodder yeast	8013-01-02	-
Formic acid (CH_2O_2)	64-18-6	-
Lubricating oil	74869-20-0	-
Polyaluminium chloride	1327-41-9	-
Polyester copolymer	139755-78-5	-
Propionic acid ($C_3H_6O_2$)	79-09-04	-
Sodium hydroxide	215-185-5	-
Sulfuric acid	7664-93-9	-

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To determine whether the list of CFs for the 105 substances in question is complete, additional research on the most suitable methodologies for collecting and predicting H-phrases is needed. Currently, the suggested procedures and hierarchies for H-phrases collection from ECHA differ between ProScale E and ProScale H. One reason for this difference is ECHA's ongoing transfer of their database and, possibly, the way harmonized H-phrases, H-phrases from dossiers and notified H-phrases are displayed. Just within the last few weeks of finalizing this work, ECHA launched the first version of its new Classification and Labelling Inventory overview, which displays H-phrases in multiple views. This new interface would be suitable to test for inclusion in our H-phrase collection methodology (European Chemicals Agency, 2025). Further research and testing of the tool are also needed to confirm whether the current methodology for obtaining DFs is most suitable, or if other measures must be taken to accurately cover the impacts of inorganics.

Difficulties in the M-Factor Characterization for Single Substances in Environmental Risk Assessment:

1. *Data gap limitations*
Determining an M-factor (Mixture Assessment Factor) for individual substances requires comprehensive toxicity data, yet many substances lack life-cycle hazard endpoints or robust ecotoxicity studies. In the absence of empirical measurements, assigning M-factors based on predictive models introduces uncertainty, especially when a variety of toxicity endpoints demand interpretation within the substance's specific use and release context. In particular, the assessed substance can be unapplicable (e.g., inorganics, ionized compounds or large molecules) or outside of applicability domains of the predictive models. In such cases, both empirical and reliable prediction data are lacking, then a strategy needs to be developed based on other approaches (e.g. read-across or expert judgement).

2. *Toxicological assessment complexity*
M-factor attribution depends on a substance's toxicity profile, encompassing relevant endpoints and, where appropriate, interactions with co-occurring substances. Regulatory frameworks such as GHS and the CLP Regulation provide structured criteria for defining toxicological hazards, however, they may not cover all environmental risks – particularly for novel chemicals and/or non-standard endpoints.

3. *Definitions of hazard potential in context*
Another layer of complexity arises from the fact that the M-factor is not a single, context-independent value but rather depends heavily on the substance-use scenario and the associated environmental release pathways. For example, a compound used only within a closed industrial process may present low risk to the environment, while the same compound, if released to aquatic environmental media, may yield severe eco-toxicological impacts. So, the environmental risk (or "hazard potential") of a chemical substance cannot be determined solely by its intrinsic toxicity or properties. Contextual factors like how, where, and under what conditions the chemical is used or released into the environment are equally important in determining the meaning of environmental risk of a chemical.

4. *Mixture toxicity assessment uncertainties*
Further uncertainty stems from mixture toxicity considerations. Although M-factors are typically estimated for individual chemicals, real environmental exposures almost always involve complex mixtures. The combined toxicological effect of multiple substances may be synergistic, antagonistic, or simply non-additive and extrapolating a single-chemical M-factor to predict mixture-level hazard assessments is fraught with error. Not accounting for interactions among co-released compounds can lead to significant misrepresentations of environmental impacts.

5. *Regulatory and methodological considerations*
Applying M-factors within frameworks such REACH or CLP demands expert judgement and access to high-quality, up-to-date data. Guidance documents exist, but variations in interpretation and application are likely

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to occur, influenced by ongoing ECHA database updates, changes in procedures, and disparate national or regional implementation practices. Each of these aspects complicates the uniform calculation of M-factors, especially for chemicals with limited data or unclear hazard classifications.

In closing, it can be concluded that the use of REACH and the CLP system is appealing due to the availability of data. However, as illustrated here, it may be complicated and not as straight forward as initially expected, both because of how the CLP system works and due to ongoing technical updates in the ECHA database. Until these complexities are addressed, M-factor discrepancies and interim CF values should be expected, underscoring the need for further harmonization between REACH database content and predictive methods.

3.3 Ecotoxicity assessment methodology for PEF/USEtox

3.3.1 Methods

As described in Deliverable 3.4 (section 2.3.3), LIST developed and applied a workflow for direct CF prediction using open-source ML tools and the expanded EF v3 dataset. The approach is designed for high-throughput screening and ease of integration into early-stage innovation processes. Specifically, the pipeline operates in training and prediction modes, with the latter enabling the estimation of CFs for chemicals lacking data. In training mode, the pipeline starts by taking Chemical Abstracts Service numbers (CAS number hereafter) along with their known CF values as inputs using data from the EF v3 database. Then, for each chemical, the pipeline retrieves the corresponding SMILES (Simplified Molecular-Input Line-Entry System) strings based on their CAS numbers and computes a range of molecular descriptors from them. Such descriptors capture the physicochemical and structural properties of these chemicals. After data processing steps, including log-transformation, scaling, and outlier removal, the curated data (i.e., descriptors and CFs), were used to train ML models. In parallel, a Gaussian Mixture Model (GMM) clusters similar chemicals into the same group. The prediction mode also starts by taking a target CAS number as an input to generate SMILES and descriptors. Consequently, the pipeline will check if the new chemical is within the Application Domain (AD) of the trained ML models, and assign a cluster number if within the AD based on GMM results. Finally, the pipeline selects the best ML model for the chemical's assigned cluster to predict the new CF.

This developed workflow has been applied to predict both human toxicity (Deliverable 3.4) and ecotoxicity CFs for different bio-based sectors (This deliverable). Note that the results presented in Deliverable 3.4 focus on two compartments of human toxicity, i.e., household indoor air and industrial indoor air. Moreover, in D3.4XGBoost and Gaussian Process regression were selected based on their performance and suitability for the available dataset. Subsequently in this Deliverable 3.1, which extended the work to ecotoxicity covering CF for eight compartments (See **Table 10**), LIST further explored the use of deep neural networks (NN) in addition to XGBoost and Gaussian Process. This expansion reflects methodological improvements and broader algorithmic testing for enhanced performance and robustness. As a result, while the methodological core remains consistent as described in Deliverable 3.4, readers should be aware that using the ML model set developed in this work to predict human toxicity leads to different prediction results compared to the Deliverable 3.4.

While the description of XGBoost and Gaussian Process regression is described in Deliverable 3.4, we present here the method of NN. A deep neural network is a foundational architecture in machine learning (ML) where data flows in a single direction—from input to output—through multiple layers of interconnected neurons (Sazlı, 2006). Each neuron processes inputs using a weighted sum followed by a non-linear activation function, enabling the network to learn complex patterns. The training involves two key phases: a forward pass to generate predictions and a backpropagation phase where the prediction error is used to update the weights using gradient descent. In this work, LIST implemented a feedforward neural network using the Keras Sequential API (Application Programming Interface) (Ketkar, 2017)The model begins with an input layer corresponding to the dimensionality of the features, followed by batch normalization and dropout

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for regularization. It consists of four hidden layers with decreasing units (100, 50, 35, and 10), each using the Exponential Linear Units (ELU) activation function (Clevert et al., 2016) and L2 regularization (Lewkowycz & Gur-Ari, 2020) to prevent overfitting. A final dense layer maps to the desired output size, followed by a LeakyReLU activation function to allow small gradient flow even for negative inputs.

3.3.2 Results and Discussion

The results (**Table 10**) show that the performances of the models varied across compartments. XGBoost consistently outperforms GP and NN. NN generally showed the weakest results. Sea water compartment exhibits the most predictable performance with an R^2 value of 0.65, while soil compartments, including agricultural and natural soils, exhibited the lowest predictive performance (average R^2 is 0.36). These values of R^2 are within the range of the results obtained by other studies for toxicity prediction and illustrate reasonable predictive performance across several environmental compartments (Hou, Jolliet, et al., 2020; Hou, Zhao, et al., 2020).

Table 10. XGBoost, Gaussian Process Regression, and Neural Network Performance (R^2 and MSE) for Ecotoxicity Across Various Environmental Compartments. MSE: Mean Squared Error.

Ecotoxicity	Compartments	R^2			MSE		
		XGBoost	Gaussian Process	Neural Network	XGBoost	Gaussian Process	Neural Network
Ecotoxicity	Air, continent	0.56	0.55	0.51	1.27	1.28	1.34
	Air, urban	0.54	0.52	0.46	1.24	1.26	1.34
	Household air, indoor	0.55	0.53	0.50	1.25	1.28	1.32
	Industry air, indoor	0.58	0.56	0.52	1.20	1.23	1.28
	Freshwater, continent	0.48	0.47	0.41	1.09	1.11	1.15
	Sea water, continent	0.65	0.63	0.57	2.79	2.87	3.11
	Agricultural soil, continent	0.37	0.37	0.27	1.31	1.31	1.39
	Natural soil, continent	0.35	0.35	0.29	1.31	1.31	1.36

Table 11 presents the R^2 values of XGBoost, Gaussian Process (GP), and NN models across different clusters for ecotoxicity CFs, covering multiple emission compartments. These results illustrate the variability in predictive performance among clusters for each model type. Overall, XGBoost consistently achieved the highest predictive accuracy across most clusters, while NN generally showed lower performance, with some exceptions where GP outperformed in specific clusters (e.g., cluster 7 for the Agricultural soil, continent compartment).

Table 11. XGBoost, Gaussian Process Regression, and Neural Network Performance (R^2) for Ecotoxicity Across Various Environmental Compartments and Clusters.

Cluster	XGBoost	Gaussian Process	Neural Networks	Compartment
0	0.35	0.34	0.32	Agricultural soil, continent
1	0.31	0.3	0.18	Agricultural soil, continent
2	0.26	0.24	0.18	Agricultural soil, continent
3	0.22	0.2	0.18	Agricultural soil, continent
4	0.28	0.28	0.26	Agricultural soil, continent
5	0.24	0.24	0.1	Agricultural soil, continent
6	0.32	0.32	0.25	Agricultural soil, continent
7	0.4	0.42	0.33	Agricultural soil, continent
8	0.12	0.2	-0.16	Agricultural soil, continent
0	0.69	0.63	0.56	Air, continent
1	0.68	0.67	0.63	Air, continent
2	0.45	0.4	0.35	Air, continent
3	0.41	0.35	0.33	Air, continent
4	0.43	0.38	0.4	Air, continent
5	0.36	0.36	0.31	Air, continent
6	0.38	0.4	0.37	Air, continent
7	0.37	0.44	0.42	Air, continent
8	0.32	0.34	0.22	Air, continent
0	0.65	0.59	0.52	Air, urban
1	0.67	0.63	0.59	Air, urban
2	0.46	0.38	0.42	Air, urban
3	0.41	0.42	0.34	Air, urban
4	0.36	0.32	0.29	Air, urban
5	0.45	0.39	0.34	Air, urban
6	0.37	0.41	0.35	Air, urban
7	0.4	0.46	0.16	Air, urban
8	0.24	0.19	0.09	Air, urban
0	0.28	0.32	0.3	Freshwater, continent
1	0.45	0.45	0.41	Freshwater, continent
2	0.4	0.42	0.35	Freshwater, continent
3	0.42	0.45	0.44	Freshwater, continent
4	0.33	0.25	0.16	Freshwater, continent
5	0.45	0.48	0.42	Freshwater, continent

6	0.36	0.37	0.33	Freshwater, continent
7	0.47	0.51	0.51	Freshwater, continent
8	0.33	0.43	0.23	Freshwater, continent
0	0.59	0.54	0.51	Household air, indoor
1	0.62	0.55	0.54	Household air, indoor
2	0.45	0.42	0.36	Household air, indoor
3	0.36	0.37	0.33	Household air, indoor
4	0.44	0.42	0.38	Household air, indoor
5	0.27	0.24	0.23	Household air, indoor
6	0.46	0.44	0.4	Household air, indoor
7	0.44	0.55	0.42	Household air, indoor
8	0.25	0.25	0.25	Household air, indoor
0	0.6	0.54	0.51	Industry air, indoor
1	0.63	0.59	0.6	Industry air, indoor
2	0.47	0.46	0.44	Industry air, indoor
3	0.46	0.4	0.36	Industry air, indoor
4	0.4	0.42	0.4	Industry air, indoor
5	0.41	0.36	0.36	Industry air, indoor
6	0.5	0.5	0.44	Industry air, indoor
7	0.55	0.55	0.45	Industry air, indoor
8	0.28	0.27	0.14	Industry air, indoor
0	0.35	0.34	0.33	Natural soil, continent
1	0.31	0.3	0.22	Natural soil, continent
2	0.25	0.25	0.22	Natural soil, continent
3	0.21	0.2	0.12	Natural soil, continent
4	0.26	0.28	0.22	Natural soil, continent
5	0.24	0.25	0.18	Natural soil, continent
6	0.32	0.33	0.27	Natural soil, continent
7	0.41	0.42	0.41	Natural soil, continent
8	0.08	0.18	-0.16	Natural soil, continent
0	0.72	0.7	0.67	Sea water, continent
1	0.77	0.72	0.68	Sea water, continent
2	0.59	0.51	0.46	Sea water, continent
3	0.67	0.62	0.6	Sea water, continent
4	0.43	0.46	0.44	Sea water, continent
5	0.69	0.71	0.59	Sea water, continent
6	0.52	0.53	0.43	Sea water, continent
7	0.65	0.59	0.52	Sea water, continent
8	0.46	0.48	0.19	Sea water, continent

Finally, the predicted CFs for ecotoxicity in eight compartments using the best model selected from the pipeline are presented in **Table 12** for the chemicals that were used in the CALIMERO cases and had missing CF.

Table 12. Predicted CFs for the missing chemicals in the CALIMERO project, PAF.m3.d/kg emitted (agrsoilC: Agricultural soil, continent; frwaterC: Freshwater, continent;seawaterC: Sea water, continent; natsoilC: Natural soil, continent; homairI: Household air,

indoor; airC: Air, continent; airU: Air, urban; indairI: Industry air, indoor).

Chemical Name	CAS	agrsoilC	frwaterC	Sea-waterC	natsoilC	homairI	airC	airU	indairI
Nitric oxide	10102-43-9	2.06	28.66	0.47	1.92	6.35	7.68	5.79	7.18
Dipotassium phosphate	7758-11-4	7.96	11.60	0.00	7.89	5.64	5.52	5.50	5.95
Carbon dioxide	124-38-9	3.27	22.94	0.02	3.27	1.57	2.33	2.18	3.29
Potassium hydroxide	1310-58-3	7.26	20.23	0.00	8.12	8.50	6.03	12.22	7.05
H-Mordenite	1318-02-1	8.85	18.91	0.00	7.58	12.21	5.65	18.22	4.34
Gypsum	13397-24-5	7.76	17.93	0.00	9.09	4.96	6.06	5.60	4.50
Tungstic acid	7783-03-1	5.58	37.97	0.00	5.94	13.00	10.56	13.97	9.61
Cobalt Molybdenum Alloy	39422-44-1	4.29	111.1	0.00	6.21	34.19	24.24	43.71	22.93
Glucose	50-99-7	2.11	2.84	0.00	2.13	1.47	1.78	1.14	1.40
Platinum	7440-06-4	2.39	21.71	0.00	2.31	12.29	8.71	22.19	13.05
Cobalt acetate	6147-53-1	7.51	40.49	0.12	7.47	5.86	7.81	5.03	6.50
Sulfur dioxide	7446-09-5	4.54	22.26	0.03	4.29	1.10	3.38	0.94	3.22
Hydrochloric acid	7647-01-0	17.82	84.96	0.11	21.13	15.05	20.03	16.81	24.96
Borax pentahydrate	12179-04-3	2.06	6.16	0.00	2.10	2.65	2.60	3.44	3.01
Sodium tetraborate decahydrate	1303-96-4	6.52	9.56	0.00	5.78	4.71	4.41	5.90	5.02
Sodium oxide	1313-59-3	7.08	18.55	0.00	7.44	5.96	4.06	9.41	4.80
Kieralon MWF (hostapal MWF, soap)	9043-30-5	6.82	18.98	0.02	4.27	6.05	2.02	3.57	2.86
Ceric sulfate tetrahydrate	10294-42-5	7.56	18.33	0.00	7.75	9.28	6.31	7.42	10.19
Alcohols, C16-18, ethoxylated	68439-49-6	0.71	14.27	0.08	1.82	0.49	1.80	1.84	0.50
Sulfuric acid	7664-93-97	6.46	46.00	0.00	6.33	28.40	19.22	25.36	18.05
Fatty alcohol ethoxylate	78330-20-8	0.71	14.27	0.08	1.82	0.49	1.80	1.84	0.50
Cellulase	9012-54-8	8.95	5.65	0.00	9.30	2.28	5.09	2.75	2.32
2,6-Bis(o-isocyanatobenzyl)phenyl isocyanate (C23H15N3O3)	21132-81-0	0.16	21.82	0.04	0.16	1.34	0.87	2.54	1.30
2,2'-Methylenebis(6-(o-	85392-14-9	0.18	11.73	0.00	0.18	0.83	0.66	2.40	0.83

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isocyanatobenzyl)phenyl) diisocyanate (C31H20N4O4)									
2,6-Bis(2-isocyanato-3-((2-isocyanatophenyl)methyl)benzyl)phenyl isocyanate (C39H25N5O5)	85423-11-6	0.12	3.59	0.00	0.12	0.39	0.37	1.16	0.47

4 Conclusions

This report sets out to address methodological challenges in LCA for bio-based industries, with a focus on the environmental dimensions of biodiversity and ecotoxicity. For biodiversity, a spatially explicit, connectivity-based risk indicator was developed as an alternative to the LDI in the BioMAPS framework. Unlike LDI, which aggregates land use intensity and local risk, this approach quantifies the structural connectivity of landscapes and considers how the spatial arrangement and conservation value of habitats shape ecological flows and potential risks. The intention is for this regional risk factor to complement existing global and local indicators, supporting a more nuanced assessment of biodiversity in LCA.

For ecotoxicity, the report describes the parallel development of CFs using two complementary pathways: (i) ProScale E, which translates REACH hazard data into LCA-ready CFs, and (ii) ML models to extend USEtox to substances lacking empirical data. Nevertheless, data completeness remains a critical bottleneck: Full input data (H-phrase, M-factor and degradation factors) were available for only 31 of the 105 compounds to be calculated with ProScale E. Provisional CFs could be calculated for these compounds, while the remaining 74 substances currently lack CF assignments and fall under the 'regarded as safe' category in ProScale E. Integrating hazard classification data through ProScale E facilitates closer alignment with EU chemical legislation, without additional demands for datapoints. However, the quality of the available data or the lack of reported data needs further investigation before stronger conclusions about the alignment are drawn. Meanwhile, the ML extension of USEtox offers a practical route to broader coverage, together providing a foundation for more comprehensive ecotoxicity assessment in bio-based value chains.

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