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PROJECT BUDGET	1,135,015€
EU CONTRIBUTION	680,705€
WEBSITE	www.life-combase.com

LIFE15 ENV/ES/416 COMBASE
COMputational tool for the assessment and substitution of **Biocidal Active substances** of Ecotoxicological concern

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COMBASE, FOR THE SUSTAINABLE USE OF
 BIOCIDAL PRODUCTS



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BACKGROUND INFORMATION

Biocides are used in the treatment of damaging biological growth. However, not only do they kill pathogens, they also kill non-pathogens, meaning they may have **undesirable side effects** harming human health and/or the environment. .

The use of **non-animal alternative test methods** has been foreseen in the Biocides Product Regulation, Regulation (EU) 258/2012 (BPR). The widespread use of non-testing methods (NTM) would help SMEs identifying, amongst other, the so called **metabolites of ecotoxicological concern** whereas **facilitating the approval** of biocidal active substances within the BPR and **reducing animal testing**.

PROJECT OBJECTIVES

The **main target** of the LIFE-COMBASE Project is to promote the **sustainable use of biocidal active substances from a life cycle perspective**.

The specific objectives of the project are the following ones:

- ⇒ Contribute to the **fulfilment of the BPR** (Biocides Product Regulation – 258/2012).
- ⇒ **Minimize** the **environmental effects** associated to active substances, metabolites, degradation and reaction products from biocides. Aligned with present target, the human health impacts associated to biocides when indirectly exposed through the environment will be reduced.
- ⇒ **Reduce the need of animal testing** by promoting the use of computational tools for ecotoxicological effects prediction as a non-testing alternative to traditionally used assays.
- ⇒ Demonstrate the **effectiveness of computational models** to minimize the environmental impacts from active substances in biocidal products. Demonstrate the suitability of developed models to alternative products (Plant Protection Products; and chemicals in general –REACH-).
- ⇒ Promote the **standardisation of the use of non-testing methods** by the chemical industry.
- ⇒ Contribute to the consolidation of the knowledge base on the **hazard of biocidal active substances** from a life cycle perspective.

EXPECTED RESULTS

- ⇒ **On-line platform based on computational chemistry** to support decision making on the basis of the ecotoxicological properties of biocide active substances and potential metabolites.
- ⇒ Demonstration of the operability and robustness of the models integrated in the COMBASE DSS in a total of **four trophic levels**: bacteria, algae, *Daphnia* and fish.
- ⇒ **Promotion of *in silico* methods** to scrutinize the ecotoxicological potential of candidate new chemicals before their synthesis.
- ⇒ For industrial stakeholders and regulators:
 - Identification of the **most critical biocides** based on PBT and CMR* criteria: the 10% of the most critical biocides will be identified.
 - Identification of **molecular features responsible for the ecotoxicity** of the most critical biocides: 15 structural alerts, or critical physico-chemical parameters will be identified.
 - Identification of safe moieties which can be used within the **planning of safer biocides**: 15 safe fragments, or critical physico-chemical parameters will be identified.
- ⇒ In relation to consumers, a **new consciousness in the use of biocidal products** will be promoted targeting informed consumers for the **responsible and sustainable use of biocidal active substances** containing products.
- ⇒ The suitability of computational approaches for metabolites derivatization in **alternative chemical products** (PPP and chemicals in general – REACH) will be assessed within the **replicability strategy**.

* PBT: Persistent, Bioaccumulative & Toxic // CMR: Carcinogenic, mutagenic or toxic to reproduction

