Integrating Safe and Sustainable by Design (SSbD) Frameworks for Hazard Characterisation and Risk Profiling of Bio-Based Phenolic Compounds

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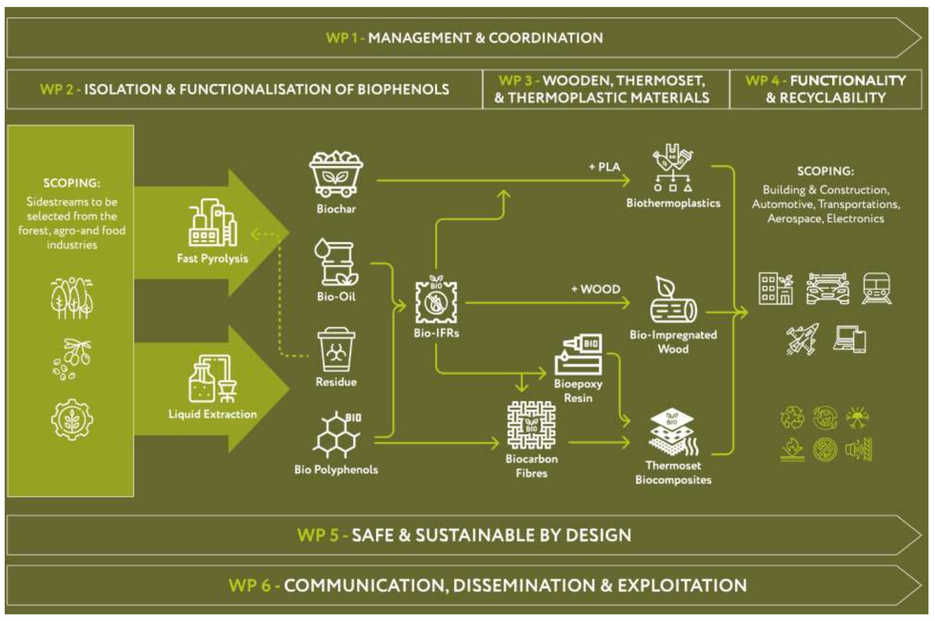
BioPhenom

www.biophenomproject.eu

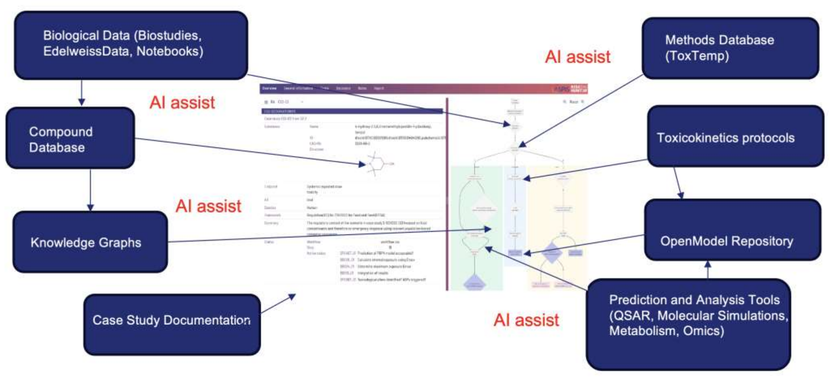
BioPhenom Objectives

The BioPhenom project aims to address the significant challenge posed by the widespread use of unsustainable petrochemicals, many of which are substances of very high concern (SVHC) due to their harmful effects on the environment and human health. These materials are toxic, non-recyclable, and accumulate in our ecosystems, thus prompting an urgent need for safer alternatives. Leveraging advanced technologies and processes (i.e. fast pyrolysis, liquid extraction), the BioPhenom project seeks to exploit biophenols isolated from industrial biomass sidestreams to produce bio-based flame retardants and replace SVHC in the development of safe, sustainable, and recyclable materials (i.e. wood products, CF thermosets, thermoplastic composites) for different applications following the Safe and Sustainable by Design (SSbD) principles established by the JRC Framework.



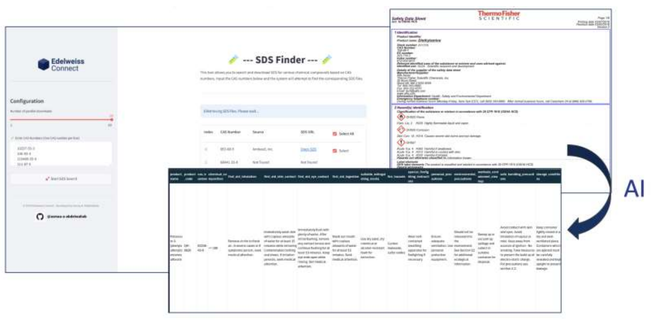
Current Work Activities

Workflows



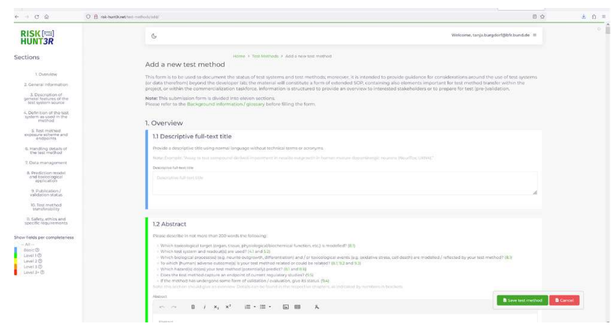
All workflows are well-documented with regards to sources of data and criteria for scoring and decision points.

AI-Assisted Knowledge Mining



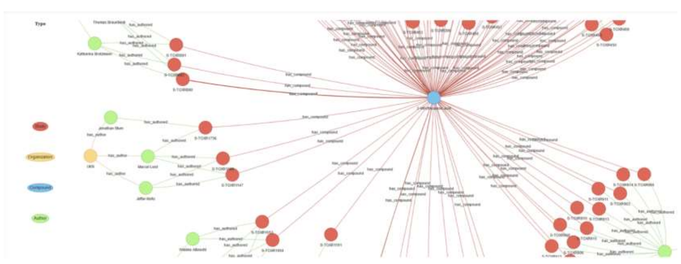
All resources are used for background knowledge mining of databases, literature and safety data sheets (shown).

Methods Documentation



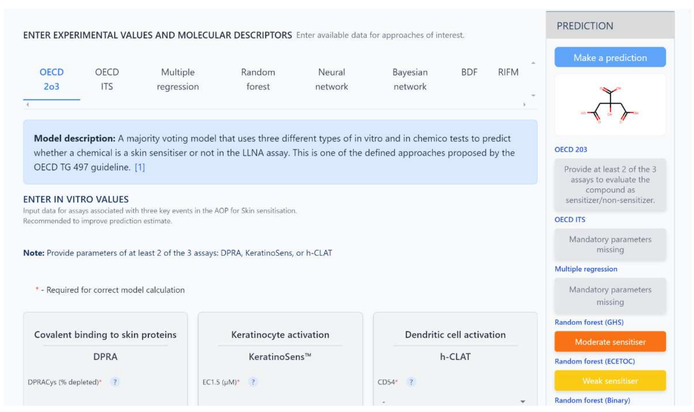
Test methods used to generate data required for SSbD workflows are documented for completeness (ToxTemp shown).

Knowledge Graphs



Knowldedge graphs are used to define relationships between information assisting search and analysis.

Assessment Tools



Our software toolbox brings information together that is required by the assessor for a particular SSbD task (SaferSkin IATA incorporated here into our SSbD assessment tool shown above).

SSbD Results Profiling

Compounds Information		Human Hazards											Environmental Hazards		
		Mutagenicity	Carcinogenicity	Endocrine disruption	Skin sensitisation	Skin irritcorrosion	Acute Tox (Oral)	Acute Tox (Dermal)	Acute Tox (Inhal)	Reproductive Toxicity	STOT RE	STOT SE	Eye irridamage	Aquatic Chronic	PBT	SVHC
Name	CAS															
Phenol	108-95-2	Neg	Pos	Neg	Pos	Pos	Pos	Neg	Pos	N.A	N.A	Pos	Pos	Neg	Pos	
Eugenol	97-53-0	Neg	Neg	Neg	Pos	Neg	Pos	Pos	Pos	N.A	N.A	Pos	Pos	Neg	Pos	

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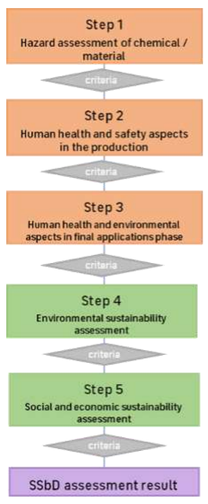
Name	CAS															
Phenol	108-95-2	2	N.A	N.A	N.A	1B	3	3	3	N.A	2	N.A	1	2	Neg	N.A
Eugenol	97-53-0	N.A	N.A	N.A	1B	2	4	N.A	N.A	N.A	N.A	N.A	2	N.A	Neg	N.A

Profiling results for different ingredients are compared based on data from different sources (phenol hazard data profiling from databases and models shown).

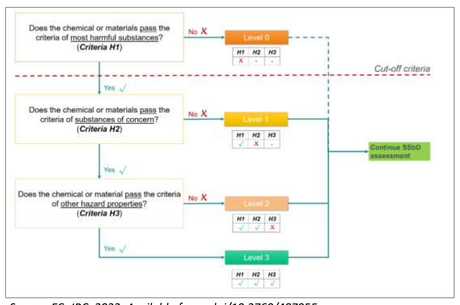


The SSbD framework involves five main steps (L) which can be tiered and phased and progressing in parallel in a particular phase. A case study (below) was conducted to demonstrate the implementation of the Safety dimension of the framework.

Case Study: Phenol vs Eugenol
Implementation of the SSbD framework
Application: Wood Adhesives

Step 1. Hazard Assessment

Compound	SSbD level step 1	Reason
Phenol	1	Mutagenicity Cat 2 (Criteria H2)
Eugenol	1	Skin sensitisation Cat 1B (Criteria H2)



Source: EC, JRC; 2022. Available from: doi/10.2760/487955

Risk Characterisation Ratio (RCR) Scoring System

Score	Description
0	Total RCR>1 and more than one individual RCRs>1
1	Total RCR>1 but at least 1 individual RCRs>1
2	Total RCR>1 but all individual RCRs<1
3	Total RCR <1

Step 2. Production Phase

	Manufacture		Formulation		On-site Use		Average	SSbD level step 2
	Human Health	Environment	Human Health	Environment	Human Health	Environment		
Phenol	0	0	2	0	0	0	0.33	0
Eugenol	1	1	3	1	1	0	1.16	1

Step 3. Use Phase

	Consumer contributing scenario	Environment contributing scenarios		Average	SSbD level step 3
Compounds	AC 11G	ERC 10a	ERC 11a		
Phenol	0	0	0	0	0
Eugenol	0	0	3	1	1

Overall Safety Assessment

Aggregation Formula: Safety Leve l= min (level step 1, level step 2, level step 3).

	Safety			Safety Level
Compounds	Step 1	Step 2	Step 3	
Phenol	1	0	0	0
Eugenol	1	1	1	1

Discussion & Conclusion

Both phenol and eugenol successfully passed Step 1 (Level 1) of the SSbD assessment, allowing continuation to Steps 2 and 3. After completing the evaluation and applying the aggregation formula, eugenol achieved a higher overall safety score (1) compared to phenol (0). This indicates that, theoretically, eugenol could serve as a safer and more sustainable substitute for phenol.

However, since the application context here is wood adhesives, substitution feasibility must also consider performance and functionality. While eugenol shows better safety potential, maintaining equivalent adhesive strength, curing behavior, and material compatibility remains critical. Therefore, achieving both improved safety and preserved functionality represents the key challenge and future focus for successful substitution.

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