

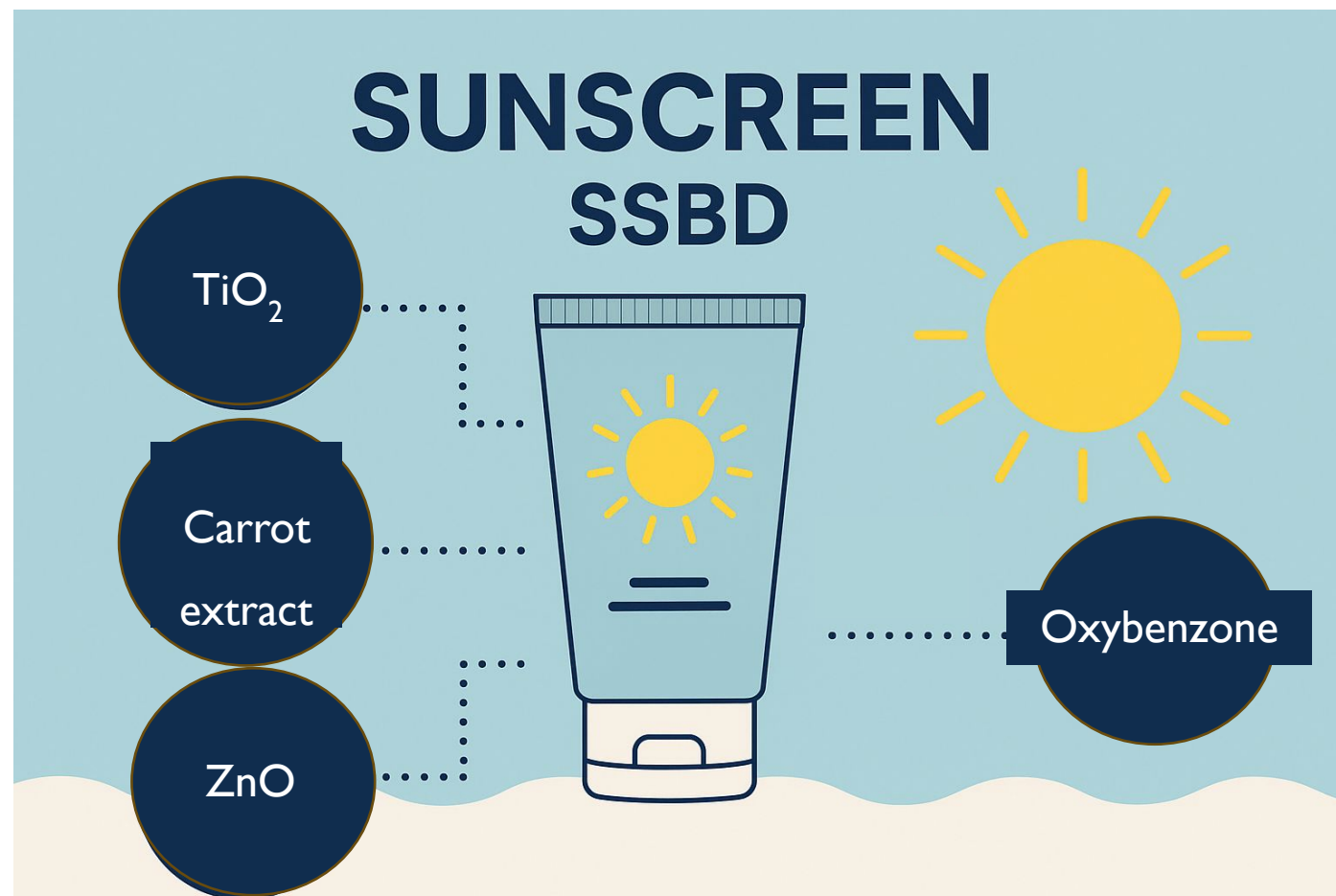
CASE STUDY: SUNSCREEN

GROUP 2

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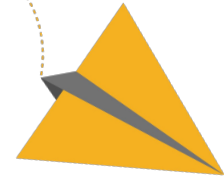


13th Venice Training School
9. – 13. June 2025

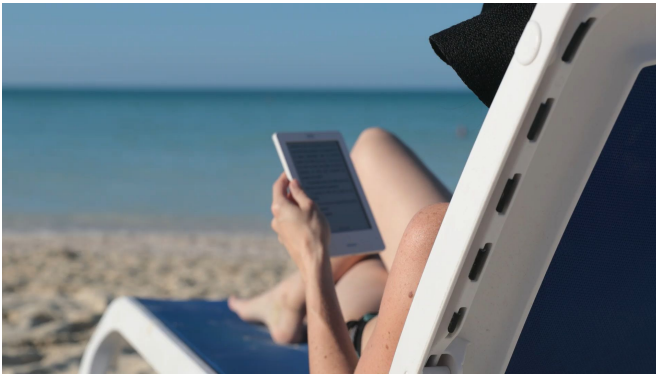


SCOPE

Determine the most suitable alternative to replace oxybenzone in sunscreen formulations, in accordance with the Safe and Sustainable by Design (SSbD) approach, considering options titanium dioxide (TiO_2), zinc oxide (ZnO), and carrot extract.



ROUTE OF EXPOSURE



*Dermal exposure,
Inhalation, Oral ingestion*



*manufacturing facilities, waste
disposal, accidental spills, and
transportation activities, human
utilisation*

STRATEGY

FUNCTIONALITY

- 13 formulations

SAFETY ASSESSMENT

- 3 formulations

HAZARD ASSESSMENT

MCDA

EVALUATION



FUNCTIONALITY

		FORMULATIONS												
Phys-chem properties	ref. values	1	2	3	4	5	6	7	8	9	10	11	12	13
pH	6.9 - 7.9	6.9	6.0	5.3	5.0	4.8	7.2	7.0	6.9	5.9	4.8	7.0	6.0	4.8
viscosity	15000 - 25000 cps	24000	20000	18000	13000	11000	18000	14000	13000	13000	11000	20000	15000	11000
density	1025 - 1040 g/mL	1035	1028	1021	1018	1001	1028	1025	1018	1012	1010	1030	1012	1010
stability	stable	stable	stable	stable	unstable	unstable	stable	stable	stable	stable	stable	stable	unstable	unstable
Microbiological parameters														
total aerobic count	< 10^3 UFC/g o mL	200	800	935	1012	865	10	0	1100	98	0	5	0	0
total molds and yeasts	< 10^3 UFC/g o mL	50	0	0	987	59	15	39	47	36	12	0	0	12
Staphylococcus aureus	negative	negative	negative	negative	negative	negative	negative	negative	positive	negative	negative	negative	negative	negative
Pseudomonas aeruginosa	negative	negative	negative	negative	positive	negative	negative	negative	negative	negative	negative	negative	negative	negative
Candida albicans	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative
Escherichia coli	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative	negative
Organoleptic properties														
colour	off-white	off-white	off-white	true white	true white	blue white	off-white	true white	true white	blue white	blue white	off-white	yellowish	bronwish
scent	fragrance	good	good	not good	not good	not good	good	not good	not good	not good	not good	good	good	good
texture	emulsion	homogeneous	homogeneuos	heterogeneuos	heterogeneuos	heterogeneuos	homogeneous	heterogeneuos	heterogeneuos	heterogeneuos	heterogeneuos	homogeneous	heterogeneuos	heterogeneuos
FPS efficacy														
UVA	80 - 100%	70 %	57 %	49 %	48 %	47 %	98 %	80 %	75 %	74 %	74 %	80 %	74 %	74 %
UVB	80 - 100%	97 %	84 %	78 %	75 %	69 %	69 %	35 %	34 %	34 %	25 %	94 %	34 %	25 %

SAFETY ASSESSMENT

		Name	Short Name	CAS	MSDS	Carcinogenicity	Mutagenicity	Reproductive Toxicity	Endocrine disruption (humanization)	Respiratory Sensitization	STO-T-RE	Skin Sensitization (oral)	Acute Toxicity (dermal)	Acute Toxicity (inh)	Acute Toxicity (oral)	Skin Corrosion/Irritation	Eye Irritation	Aspiration Hazard	STO-T-SE	PBT/vPvB	PMT/vPvM	Endocrine disruption (environmental)	Ozone Depletion	Chronic Toxicity	Acute Toxicity	Source of information		
																											no	not classified
	SSbD hazard classes																										miss	data missing
Raw Materials																											cat 1	category according to CLP
AdMa		titanium dioxide	TiO2	13463-67-7	YES	cat 2	cat 2	no	miss	cat 1	cat 1	no	cat 4	no	no	no	no	miss	no	no	no	miss	miss	cat 2	no	SDS: EYONIK: Classification (REGULATION (EC) No 1272/2008) as amended by GB-CLP Regulation, UK SI 2019/720, and UK SI 2020/1567; Version 1.21; last revision: 08.03.2024	cat 2	category according to CLP
		Zinc oxide	Zno	1314-13-2	YES	no	no	cat 1	no ≥ 0,1%	no	cat 2	no	cat 4	no	miss	no	no	no	no	no	miss	no ≥ 0,1%	miss	cat 1	cat 1	SDS: ROTH: according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/078/EU; article number: 3549; Version: 4.1 en; Replaces version of: 2024-09-18; Version: (4); last revision: 09.10.2024	cat 3	category according to CLP
		Carrot Extract	Carrot extract	8015-88-1 / 84929-61-3	YES	no	no	no	miss	no	no	cat 1	no	miss	cat 4	cat 2	no	cat 1	no	miss	miss	miss	miss	cat 2	miss	SDS: PRODUCT NAME: Carrot Seed Essential Oil, SUPPLIER: Amphora Aromatics Limited, Airfield House, Western Drive, Bristol, BS14 0AF; PRODUCT NUMBER: 107	cat 4	category according to CLP
Reference Product		Oxybenzone	BP-3	131-57-7	YES	no	no	no	no	no	miss	no	no	miss	miss	no	no	miss	miss	no	miss	no	miss	cat 2	cat 1	SDS: sigma aldrich, version 7.9, de acuerdo el Reglamento (CE) No. 1907/2006, latest revision: 28.8.2023	na	not applicable

Predictive analysis software

5 different UV-Blocker substances for sunscreens to, from their CAS/SMILES, analyse their:

- Chemical properties
- Biodegradability
- Carcinogenicity
- Other properties

How?

Jaqpot

QSAR toolbox

Pink Stage I report

Only substances (e.g., no Nanoparticle data)



Jaqpot

QSAR TOOLBOX



Predictive analysis software - Pros & Cons

Jacpot

Easy to use

Not as comprehensive (access to more models from Episuite, QsarToolbox, VegaHub)

QSAR

Information overload

Very comprehensive

QSAR Toolbox 4.7.1 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition

Data Import Export Delete

Gather Import IUCLID6 IUCLID6 Database Inventory

Documents

Document 1

[C: 1;Md: 0;P: 0] Search chemical (do not ac

[C: 1;Md: 1229;P: 0] Search chemical (do

Databases

Options 63 Selected

f Select All Unselect All Invert

☒ Physical Chemical Properties

☒ Bioconcentration and logKow NITE

☒ Chemical Reactivity COLIPA

☒ ECHA REACH

Organise by: ?

☐ Dossiers/Substances

Inventories

Options 11 Selected

f Select All Unselect All Invert

☒ AIIC

☒ Canada DSL

☒ COSING

☒ DSSTOX

☒ ECHA PR

☒ EINECS

☒ HPVC OECD

Filter endpoint tree... 1 [target]

Structure

Structure info

Parameters

Physical Chemical Properties 1/15 M: > 100 µm

Environmental Fate and Transport

Bioaccumulation 1/8 M: 1.28 log(L/kg)

Biodegradation

in Sewage Treatment Plant

in soil

in water and sediment: simulation tests

in water: screening tests

Ready Biodegradability

% degradation (O2 consumption)

OECD Guideline 301 C (Ready...

28 d 1/1 M: 4 %

Stability 1/10 M: 8.87

Transport and Distribution

Ecotoxicological Information 1/343 M: 8E-07 mg/L

Human Health Hazards 1/815 M: 200 mg/kg bdwt/d

Intermediate effects - mechanistic infor... 1/37 C:2.28E-07 mg/L

Profiling

Predefined

Database Affiliation

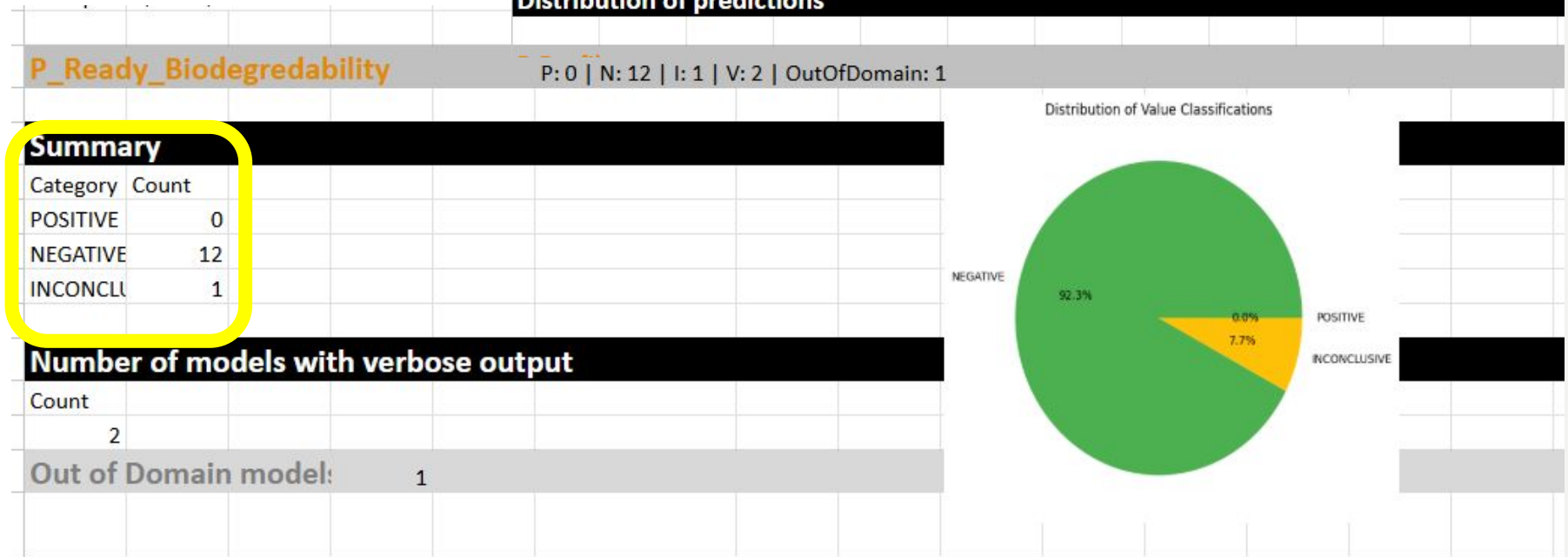
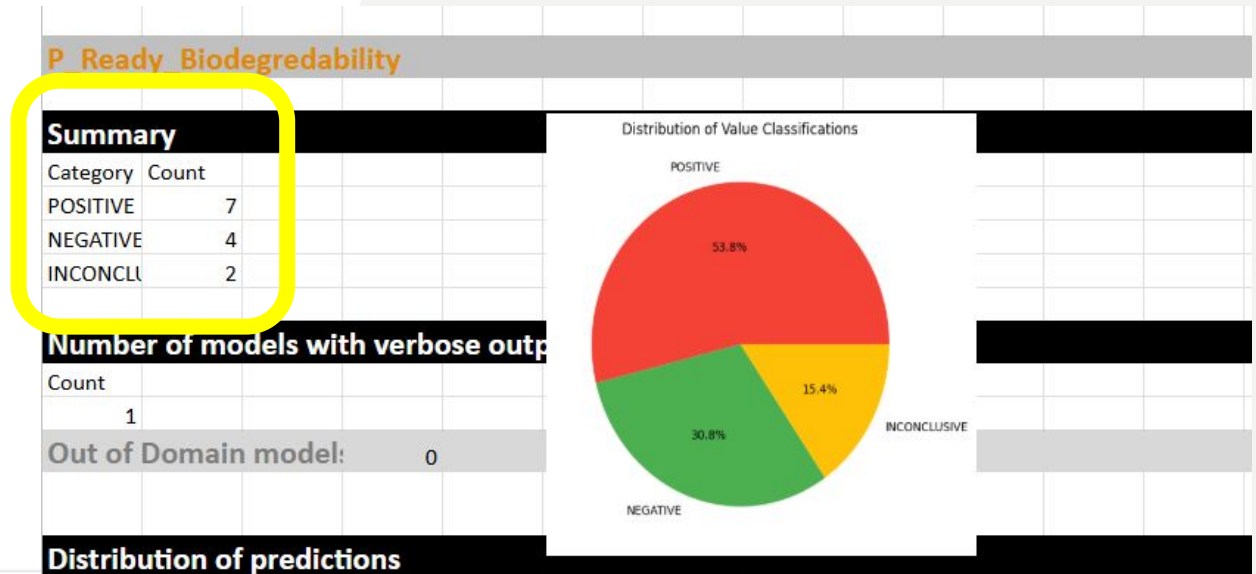
Acute Oral toxicity DB

This page goes on, and on, and on, and on (...)

Predictive analysis software - Pros & Cons

Pink Stage I report

- Consolidated information from diff. models
- Visualises discrepancies and alignments in the final results (dependant of substance)
- Good visual cue to fastly screen substances



MCDA - Tier 1 - Carrot extract



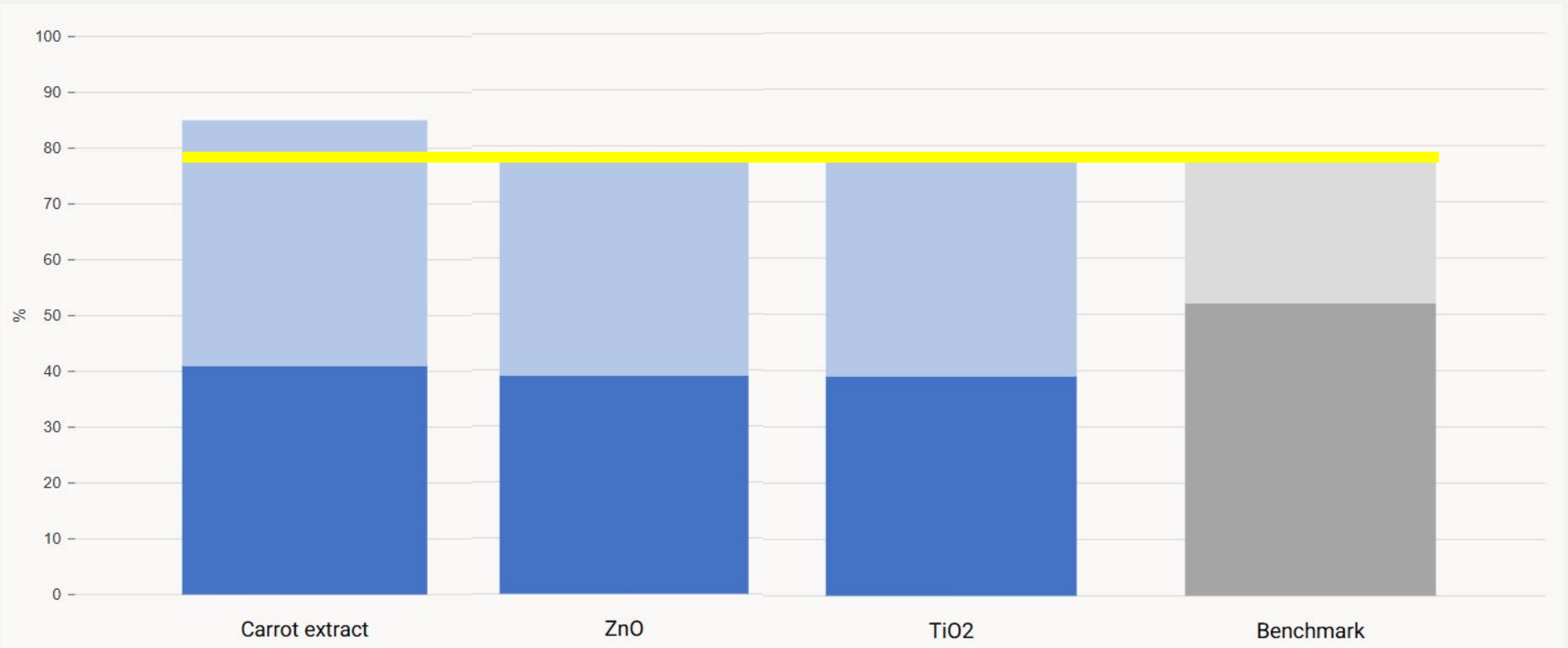
MCDA - Tier 1 - ZnO NPs



MCDA - Tier 1 - TiO2 NPs



MCDA - Tier 1 - General



MCDA - Tier 1 - General

Functionality	Safety	Environment	Social	Economic
★	☆	≡	≡	≡
★	☆	≡	≡	≡
★	☆	≡	≡	≡
SSbD evaluation				
≡ Missing ☆ Low Benefit ★ Medium Benefit ★ High Benefit				

- High functionality improvement
- Low safety benefits

Tier 2 - Carrot extract

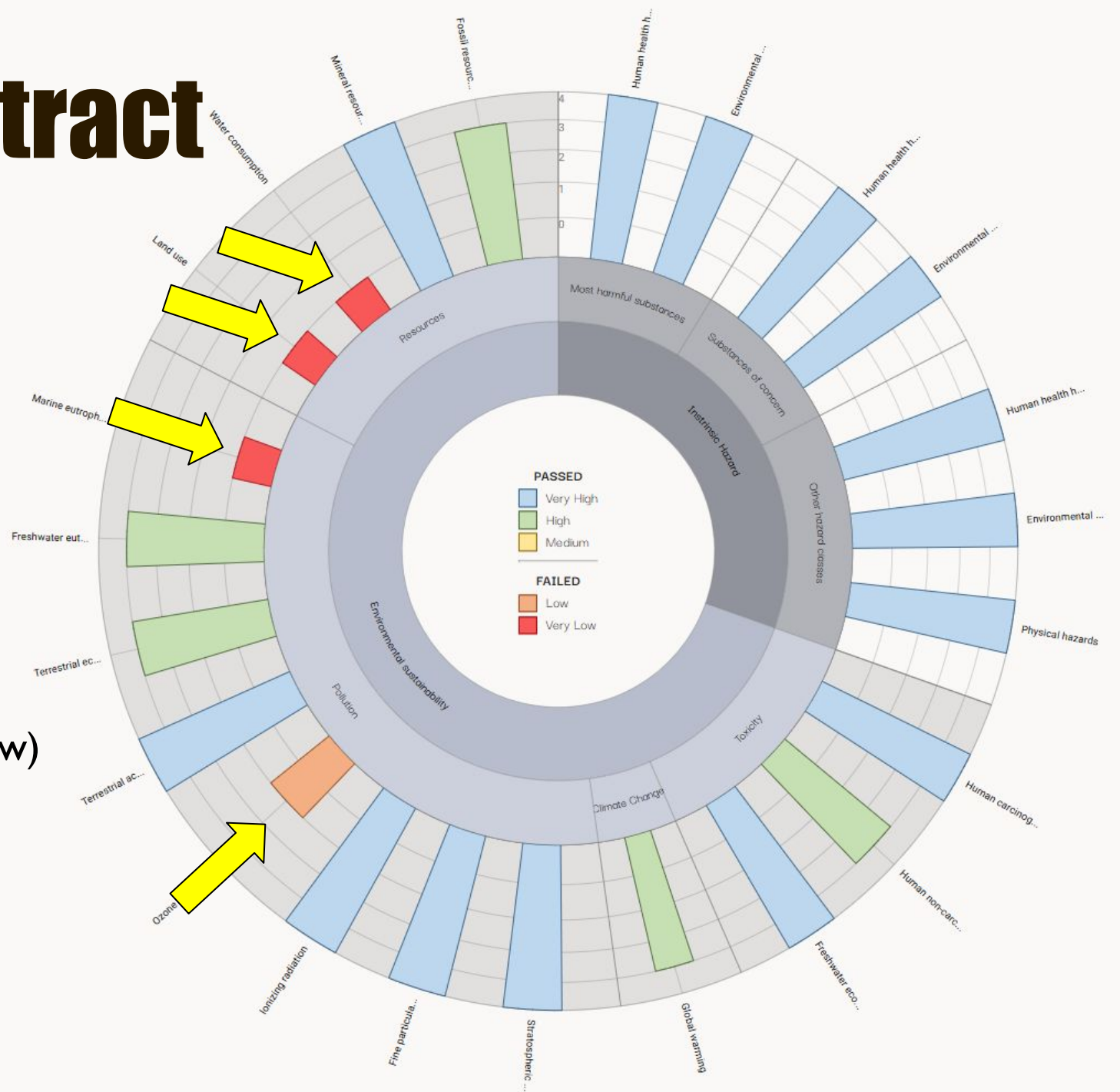
Hazard analysis:

Passed all (very high)

Environmental sustainability:

Failed at:

1. Ozone formation (low)
2. Marine eutrophication (very low)
3. Land use (very low)
4. Water consumption (very low)



MCDA analysis - Tier 2 - Carrot extract

Intrinsic Hazard	Production safety	Application safety	Environmental sustainability	Social sustainability	Economic sustainability
≡	⊘	≡	⊘	≡	≡
SSbD evaluation					
≡	⊘	⚠	⚠	✓	✓+
Missing	Very Low	Low	Medium	High	Very High

- Very Low Production Safety
- Very Low Environmental Sustainability

Dialog with stakeholders

Observations

- Alternatives present higher functionality
- Alternatives present no safety benefits and raise some significant concerns
- Overall, it seems to be no advantage in using alternatives.

However

- Incompleteness of analysis!!
- Lots of missing information → need for research!!
- Discrepancies between SDS and methodology of plant extract preparation
- Nanomaterials: size, coating?
- Ingredient list for «Fragrance» (can be hundreds different components)



THANK YOU FOR YOUR ATTENTION

