Green Metrics: Real-Life Tools
& Case Study from Fragrance Industry

A cleaner, greener future for chemicals (science.org)

Green Metrics: Real-Life Tools & Case Study from Fragrance Industry

Goal of the course

Provide a comprehensive perspective of the green metrics developed, used in the chemical industries. The pros/cons and the limitations of all these metrics will be shown as well as the different need between industries. The case of Perfumery industry will be specially emphasized.

Course Syllabus

- Green Chemistry & Sustainability
- Presentation of the different metrics
- Pros/Cons & Limitations
- What is the purpose of these metrics?
- Presentation of different methodologies
- Difference between the pharma industry and Perfumery industry
- Example in the Perfumery industry: Ecoscent Compass, Green Motion or Estée Lauder Companies

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Green Metrics

Mass-Based Metrics for Measuring Greeness

E factor (E)[3]

$$E = \frac{\text{Total mass of waste}}{\text{Mass of final product}}$$

Atom Economy (AE)[6]

$$AE\ (\%) = \frac{\text{Mol wt of product} \times 100}{\text{Sum of mol wts of reactants}}$$

Mass Intensity (MI)[31,32]

$$MI = \frac{\text{Total mass in process}}{\text{Mass of product}}$$

Reaction Mass Efficiency (RME)[31]

$$RME\ (\%) = \frac{\text{Mass of product} \times 100}{\text{Total mass of reactants}}$$

Process Mass Intensity (PMI)[34,35]

$$PMI = \frac{\text{Total mass in process (incl } H_2O\text{)}}{\text{Mass of product}}$$

Mass Productivity (MP)

$$MP\ (\%) = \frac{\text{Mass of product} \times 100}{\text{Total mass (incl solvents)}}$$

Waste Water Intensity (WWI)

$$WWI = \frac{\text{Mass of process water}}{\text{Mass of product}}$$

Effective Mass Yield (EMY)[33]

$$EMY\ (\%) = \frac{\text{Mass of product}}{\text{Mass of hazardous reactants}}$$

Solvent intensity (SI)

$$SI = \frac{\text{Mass of solvents}}{\text{Mass of product}}$$

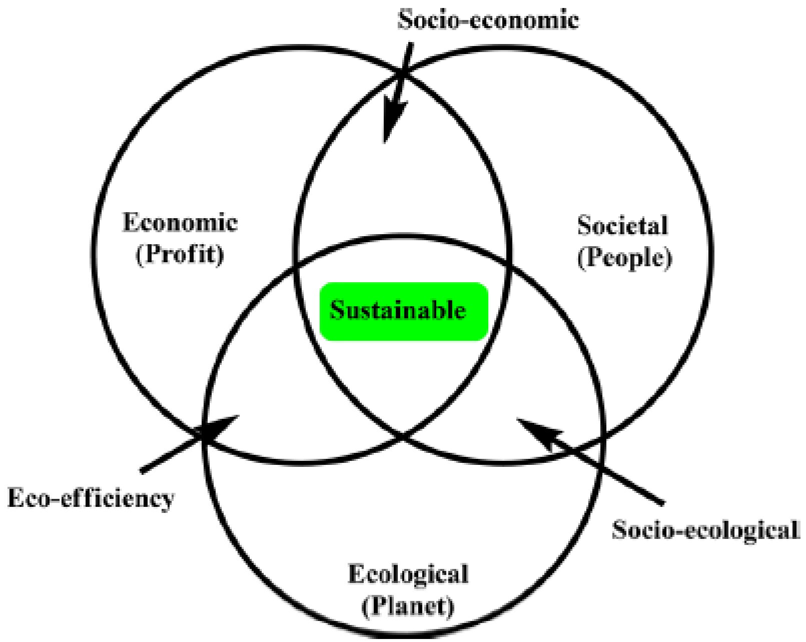
Carbon Economy (CE)[31]

$$CE\ (\%) = \frac{\text{Carbon in product} \times 100}{\text{Total carbon in reactants}}$$

ACS Sustainable Chem. Eng. **2018**, *6*, 32

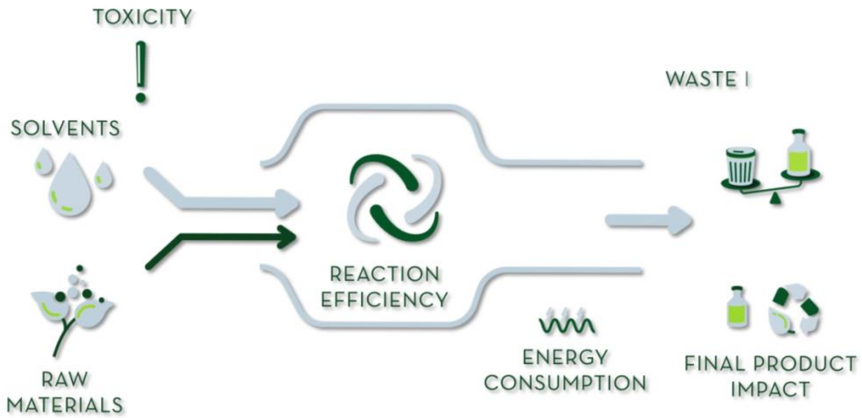
Green Metrics

Sustainability metrics

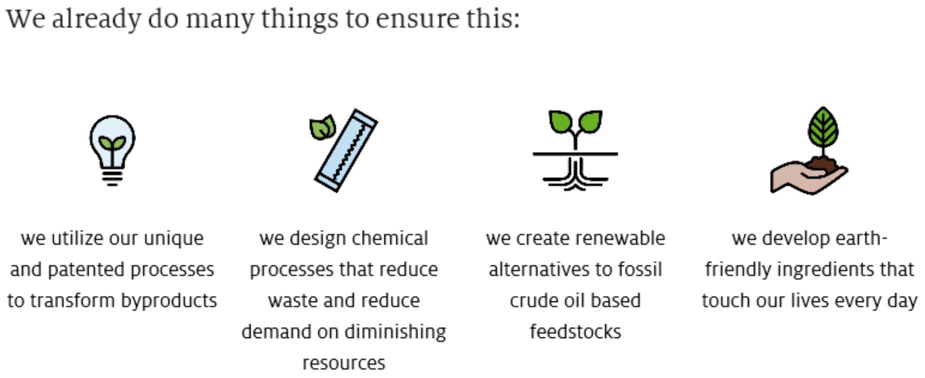


ACS Sustainable Chem. Eng. **2018**, *6*, 32

What are the Different Initiatives in F&F?

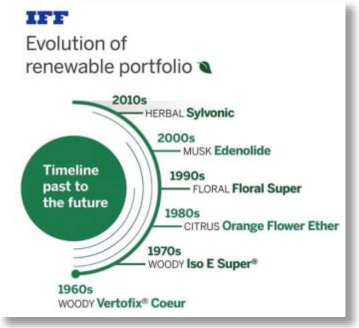


GREEN MOTION™ by Mane
7 concepts, penalty scoring



Symrise

FiveCarbon Path™ by Givaudan
5 concepts (RC, BDG, …)



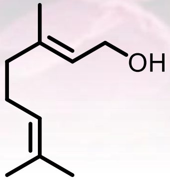
Renewable INGs by IFF
for > 50% RC

But also L'Oreal, Estée Lauder.

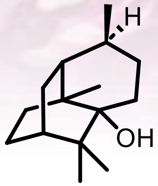
Fragrance – an unique equation

Natural extracts

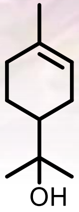
Flower or fruit extraction



Geraniol
(Rose)

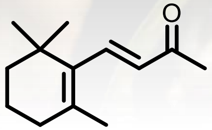


Patchoulol
(Earthy)

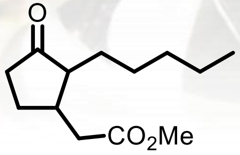


α-Terpineol
(Floral)

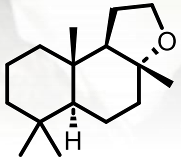
Nature identicals



β-Ionone
(Violet)

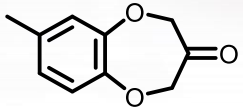


Hedione®
(Jasmine)

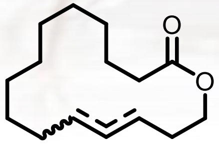


Ambrox® Super
(Amber)

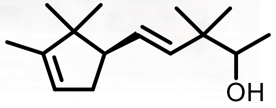
Synthetics



Calone®
(Watery)



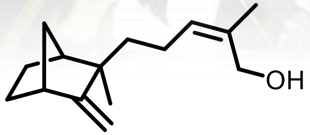
Habanolide®
(Musk)



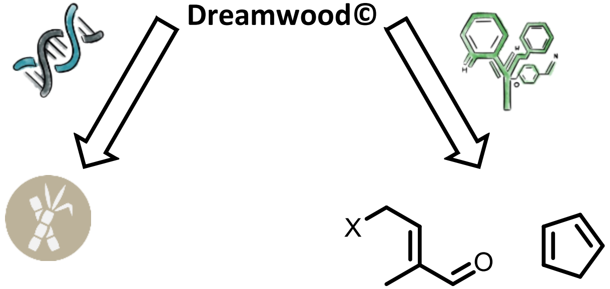
Polysantol®
(Sandalwood)

BIOSYNTHESIS AND CHEMICAL SYNTHESIS

NATURE IDENTICALS

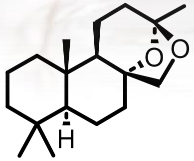


Dreamwood©

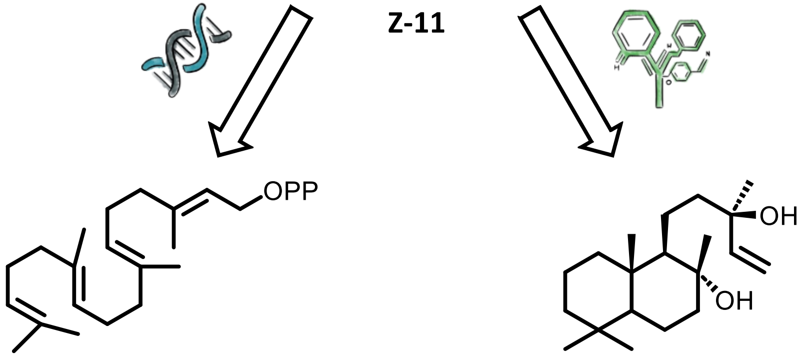


sugar
Renewable carbon
source

SYNTHETICS



Z-11



geranylgeranyl diphosphate

Sclareol

For Clearwood Synthesis: (a) Fehr, C., Vuagnoux, M. Firmenich SA WO 2009141781; (b) Chapuis, C., Firmenich SA WO 2012110375; (c) Birkbeck, A. A. Firmenich SA WO2013001026 .
For Sclareol Synthesis: M. Schalk, L. Pastore, M. A. Mirata, S. Khim, M. Schouwey, F. Deguerry, V. Pineda, L. Rocci, L. Daviet
Toward a Biosynthetic Route to Sclareol and Amber Odorants *J. Am. Chem. Soc.* **2012**, *134*, 18900−18903.

Mass Based Metrics

Chemical Process

$$AE = \frac{MW(Product) \times 100}{\sum MW(Raw\ Materials) + \sum MW(Reagents)}$$

Optimum Value= 100.

$$EFactor = \frac{\sum m(Input\ Materials\ w.o.Water) - m\ (Product)}{m(Product)}$$

Optimum Value= 0.

$$\mathrm{RME} = \frac{m(Product)\times 100}{\sum m(Raw\ Materials)}$$

Optimum Value= 100.

$$cEFactor = \frac{\sum m(Input\ Materials\ incl.Water) - m\ (Product)}{m(Product)}$$

Optimum Value= 0.

$$\mathrm{PMI} = \frac{\sum m(Input\ Materials\ incl.Water)}{m(Product)}$$

Optimum Value= 1.

Roschangar, F; Colberg, J. *Green Chemistry Metrics in Green Techniques for Organic Synthesis and Medicinal Chemistry,* Second Edition. Edited by Wei Zhang and Berkeley W. Cue. (**2018**). Ed. John Wiley & Sons Ltd

Mass Based Metrics

Renewables

Renewables Intensity

$$\mathrm{RI} = \frac{\sum m(Renewably\ Derivable\ Input\ Materials)}{m(Product)}$$

Optimum Value= 1

Renewables Percentage

$$\mathrm{RP} = \frac{\mathrm{RI} \times 100}{\mathrm{PMI}}$$

Optimum Value= 100.

Jiménez-González, C.; Constable, D. J. C.; Ponder, C. S. Evaluating the ‘‘Greenness’’ of chemical processes and products in the pharmaceutical industry—a green metrics primer *Chem. Soc. Rev*., **2012**, *41*, 1485–1498.

Safety and Harzard Metrics

Thermal Hazard
Reagent Hazard
Pressure
Hazardous by-product
Waste: metal, toxicity, upcycling

Solvant Usage: number, recovery
Mass Intensity of Solvent

Biodegradation, Bioaccumulation, Energy use

Curzons, A. D.; Constable, D. J. C.; Mortimera, D. N.; Cunningham, V. L. So you think your process is green, how do you know?—Using principles of sustainability to determine what is green–a corporate perspective *Green Chem.*, **2001**, *3*, 1–6.

Specificity of Perfumery Ingredients

Natural oil extraction
Biotechnology Processes

Metrics should be easy to understand by our clients and final consumers

Our competitors are also our clients: Needs for metrics that could be asked or guessed with the highest accuracy possible

Nowak, P. M. What does it mean that "something is green"? The fundamentals of a Unified Greenness Theory, *Green Chem.*, **2023**, 25, 4625.
https://pubs.rsc.org/en/content/articlelanding/2023/gc/d3gc00800b

Mane: Green Motion^{TM}

Starting Point: 12 Green Chemistry Principles…

Selection ? Which is the most important? Comprehensive?

Some of the principles may be contradictory with each other
Difficult to know what type of action to implement in order to find the optimal overall result.

A yield increase or a reduction of waste may entail higher energy consumption, and this kind of conflicting choice is commonly faced by industrial chemists.

Finding the right balance between being too qualitative and requiring a large amount of information (time and resources consuming)

Green Chem., **2015**, *17*, 2846

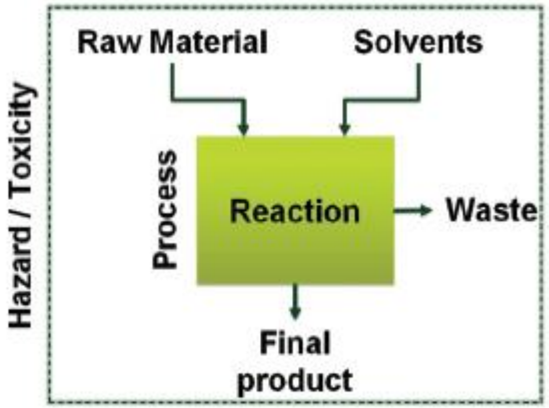
Mane: Green Motion™

Concept	Major criterion		Unit
Raw material	Raw material origin		Category
	Process naturalness		Yes/No
Solvents	Solvent category		Category
Hazard and toxicity of the reagents	GHS pictogram		Pictogram
Reaction	Mass yield		%
	Number of steps		Number
	Number of solvents		Number
	Carbon economy	$\frac{\text{Number of carbons of product}}{\text{Number of carbons of reactants}}$	%
	Number of protection/deprotection step		Number
	Overall processing time		Hour
Process	Most consuming heating process		Category
	Most consuming cooling process		Category
	Vacuum		Category
	Pressure		Category
Hazard and toxicity of the final product	GHS pictogram		Pictogram
Waste	E-Factor	$\frac{\text{Mass waste (kg)}}{\text{Mass desired product (kg)}}$	$kg\ kg^{-1}$

Green Chem., **2015**, *17*, 2846
ACS Sustainable Chem. Eng. **2018**, *6*, 32

Mane: Green Motion^{TM}

The 12 principles of Green Chemistry:
grouped into 7 fundamental concepts



Green Chem., **2015**, *17*, 2846

Mane: Green Motion™

Raw Materials:

Category	Penalties
Synthetic raw materials	10
Raw materials from hemi-synthesis	5
Natural raw materials	0

Solvent categories

Category	Examples	Penalties
CMR and toxic solvent	Methanol, methylene chloride, benzene *etc.*	10
Petrochemical solvent	Toluene, hexane, cyclohexane *etc.*	5
Supercritical fluid	Carbon dioxide *etc.*	2
Ethanol		2
Water		1
No solvent used		0

Green Chem., **2015**, *17*, 2846

Solvents Guide

Solvents Guides:

Family	Solvent	AZ	GCI-PR	GSK	Pfizer	Sanofi[a]	Issues	Overall[b]
Water	Water	—	—	24	Preferred	Recommended	—	Recommended
Alcohols	MeOH	19	14	14	Preferred	Recommended	—	TBC
	EtOH	16	13	17	Preferred	Recommended	—	Recommended
	i-PrOH	16	16	17	Preferred	Recommended	—	Recommended
	n-BuOH	17	13	18	Preferred	Recommended	—	Recommended
	t-BuOH	20	15	15	Preferred	Subst. adv.	—	TBC
	Benzyl alcohol	—	11	20	—	Subst. adv.	—	TBC
	Ethylene glycol	—	13	21	Usable	Subst. adv.	—	TBC
Ketones	Acetone	21	15	15	Preferred	Recommended	—	TBC
	MEK	21	16	15	Preferred	Recommended	—	TBC
	MIBK	22	17	15	—	Recommended	—	TBC
	Cyclohexanone	—	14	20	—	Subst. adv.	—	TBC
Esters	Methyl acetate	—	14	14	—	Subst. adv.	—	TBC
	Ethyl acetate	18	15	16	Preferred	Recommended	—	Recommended
	i-PrOAc	18	13	18	Preferred	Recommended	—	Recommended
	n-BuOAc	13	14	21	—	Recommended	—	Recommended
Ethers	Diethyl ether	27	21	3	Undesirable	Banned	H224	HH
	Diisopropyl ether	—	—	4	Undesirable	Subst. adv.	Perox.	Hazardous
	MTBE	24	21	4	Usable	Subst. adv.	—	TBC
	THF	23	16	4	Usable	Subst. adv.	H351	TBC
	Me-THF	24	15	11	Usable	Recommended	—	Problematic
	1,4-Dioxane	28	21	11	Undesirable	Subst. req.	—	Hazardous
	Anisole	18	13	18	—	Recommended	—	Recommended
	DME	21	23	2	Undesirable	Subst. req.	H360	Hazardous
Hydrocarbons	Pentane	—	—	7	Undesirable	Banned	H224	Hazardous
	Hexane	26	21	1	Undesirable	Subst. req.	—	Hazardous
	Heptane	21	17	14	Usable	Subst. adv.	—	Problematic
	Cyclohexane	25	18	14	Usable	Subst. adv.	—	TBC
	Me-cyclohexane	—	17	16	Usable	Subst. adv.	—	Problematic
	Benzene	—	21	1	Undesirable	Banned	H350	HH
	Toluene	22	18	11	Usable	Subst. adv.	H351	Problematic
	Xylenes	19	15	13	Usable	Subst. adv.	—	Problematic
Halogenated	DCM	20	18	5	Undesirable	Subst. adv.	H351	TBC
	Chloroform	—	18	4	Undesirable	Banned	—	HH
	CCl_4	—	19	3	Undesirable	Banned	H420	HH
	DCE	—	19	4	Undesirable	Banned	H350	HH
	Chlorobenzene	25	16	18	—	Subst. adv.	—	Problematic
Aprotic polar	Acetonitrile	24	14	14	Usable	Recommended	—	Problematic
	DMF	20	17	7	Undesirable	Subst. req.	H360	Hazardous
	DMAc	20	16	4	Undesirable	Subst. req.	H360	Hazardous
	NMP	18	16	7	Undesirable	Subst. req.	H360	Hazardous
	DMPU	—	—	14	—	Subst. adv.	—	Problematic
	DMSO	8	15	14	Usable	Subst. adv.	—	Problematic
	Sulfolane	9	13	21	—	Subst. adv.	—	Recommended
	Nitromethane	—	—	1	—	Banned	Explo.	HH
Miscellaneous	Methoxy-ethanol	21	20	3	—	Subst. req.	H360	Hazardous
Acids	Formic acid	20	15	—	—	Subst. req.	—	TBC
	Acetic acid	17	15	17	Usable	Subst. adv.	—	TBC
	Ac_2O	—	16	15	—	Subst. adv.	—	TBC
Amines	Pyridine	26	16	5	Undesirable	Subst. adv.	—	TBC
	TEA	23	18	3	—	Subst. req.	—	Hazardous

[a] Subst. adv.: substitution advisable; Subst. req.: substitution requested. [b] TBC: to be confirmed; HH: highly hazardous.

Prat, D. *et al. Green Chem.* **2014**, *16*, 4546.
Winterton, N. *Clean Technologies and Environmental Policy* **2021**, *23*, 2499.

Mane: Green Motion^{TM}

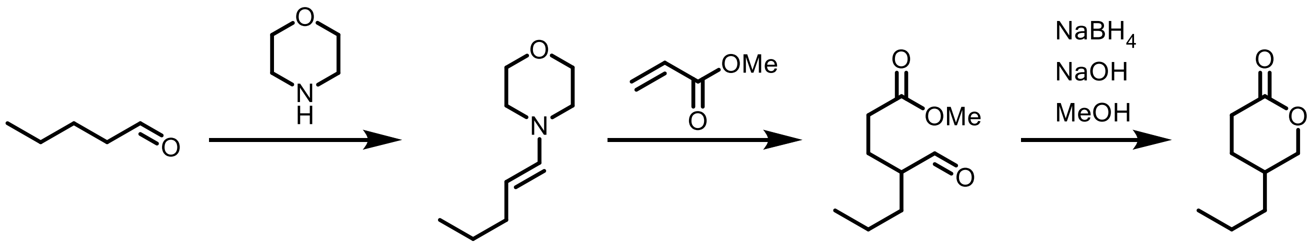
GHS pictogram hierarchy:

Pictogram	Penalties	
	Exploding bomb	4
	Health hazard	3
	Skull & Crossbones	3
	Flame over circle	2
	Corrosion	2
	Environment	1
	Flame	1
	Exclamation mark	1

Green Chem., **2015**, *17*, 2846

Mane: Green Motion™

Reaction efficiency



	1. Activation	2. Addition	3. Reduction	Total
GREEN MOTION™ carbon economy	$\frac{9}{4+5} = 1$	$\frac{9}{4+9} = 0.69$	$\frac{8}{9} = 0.89$	0.61
Trost atom economy	$\frac{155}{87+86} = 0.90$	$\frac{172}{155+86} = 0.71$	$\frac{142}{172} = 0.83$	0.53

Green Chem., **2015**, *17*, 2846

Mane: Green Motion^{TM}

Process efficiency

Focus on the most energy consuming elements:
heating, cooling and pressure variation

But not try to accurately calculate the quantity of heat energy required throughout the process

Penalty points attributed for different heating processes

Green Chem., **2015**, *17*, 2846

Mane: Green Motion^{TM}

Process efficiency

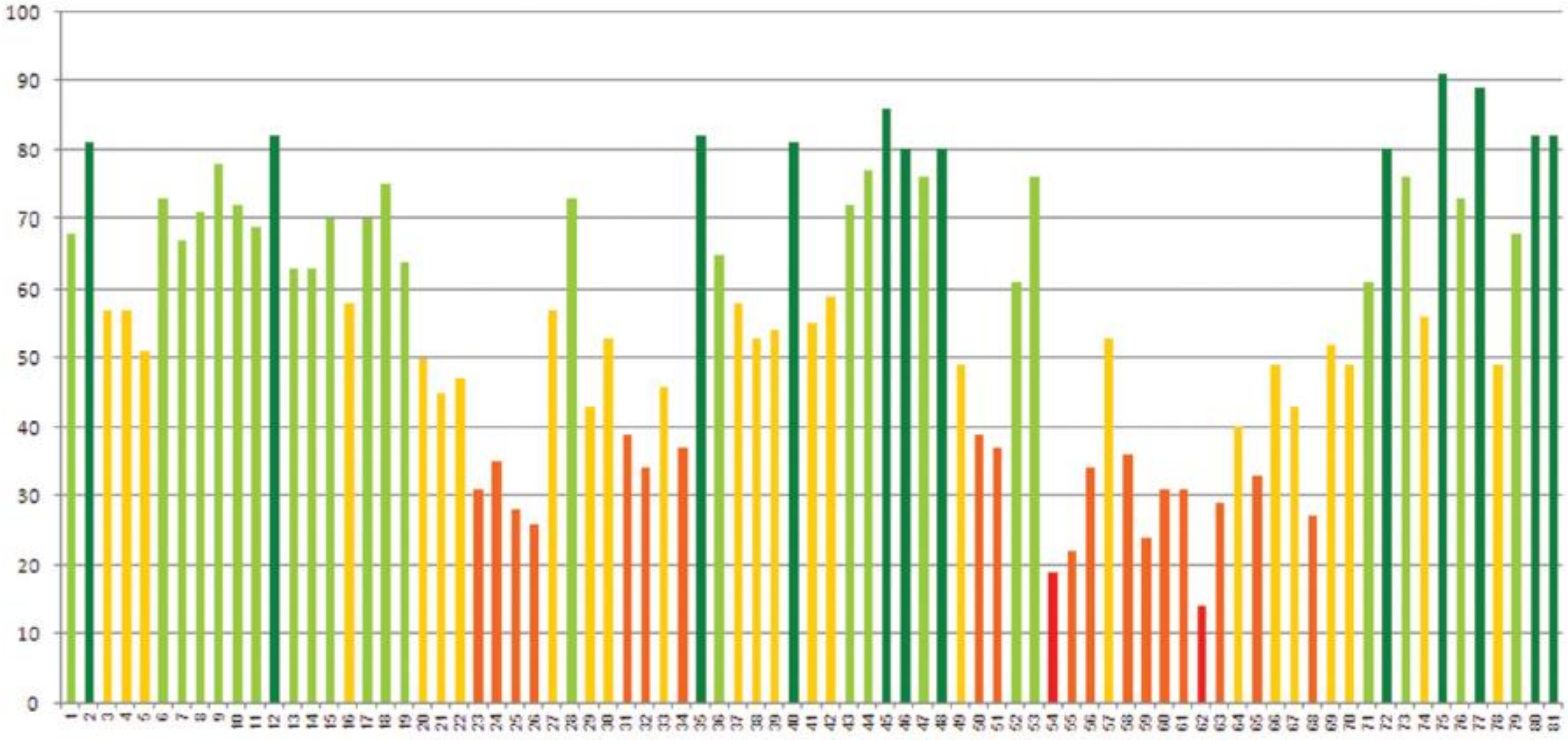
Penalty points attributed for different heating processes

Gas	6	7	8	9	10	11	12	13
Electrical resistance	5	6	7	8	9	10	11	12
Oil	4	5	6	7	8	9	10	11
Steam up to 15b	4	5	6	7	8	9	10	11
Steam up to 6b	3	4	5	6	7	8	9	10
Steam up to 3b	2	3	4	5	6	7	8	9
Steam	1	2	3	4	5	6	7	8
Ambient temperature	0	1	2	3	4	5	6	7
	12 h	24 h	48 h	96 h	144 h	192 h	240 h	288 h

Green Chem., **2015**, *17*, 2846

Mane: Green Motion™

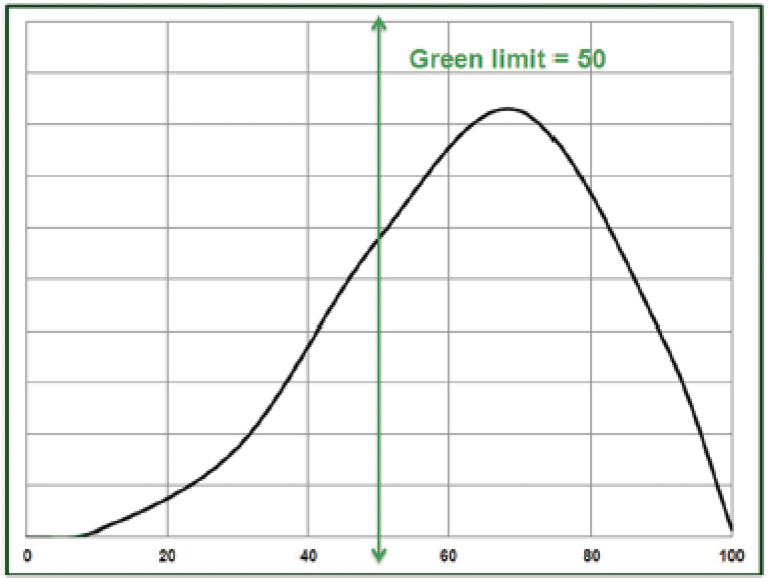
81 products selected to design GREEN MOTION™.:



Green Chem., **2015**, *17*, 2846

Mane: Green Motion™

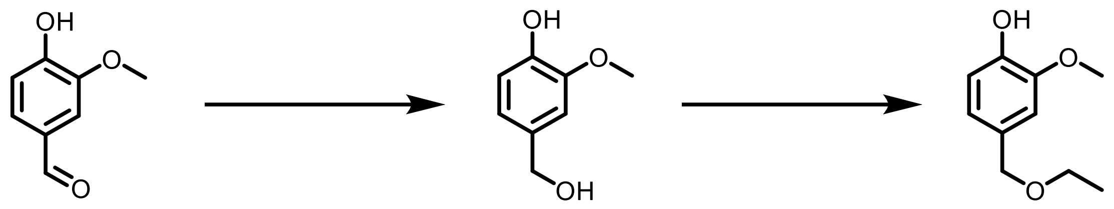
“Green limit” in GREEN MOTION™:



Green Chem., **2015**, *17*, 2846

Mane: Green Motion™

Vanillyl Ethyl Ether:

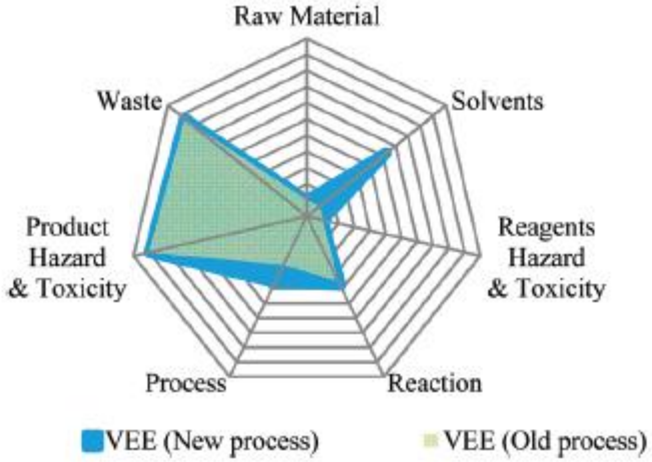


Vanillin

Vanillin Alcohol

Vanillin Ethyl Ether

	Solvent	Solvent toxicity	Yield	Number of steps	Global process length	E-Factor	GREEN MOTION™ rating
1997	1,2-Dichloroethane	Can cause cancer	50%	4	356 h	2.3	23
2002	Dichloromethane	May cause cancer	51%	4	356 h	2.2	24
2012	Toluene	Not carcinogenic	45%	3	182 h	1.2	37



Green Chem., **2015**, *17*, 2846

Mane & L’Oréal: Comparison between Different Tools

Ingredients in Perfume:

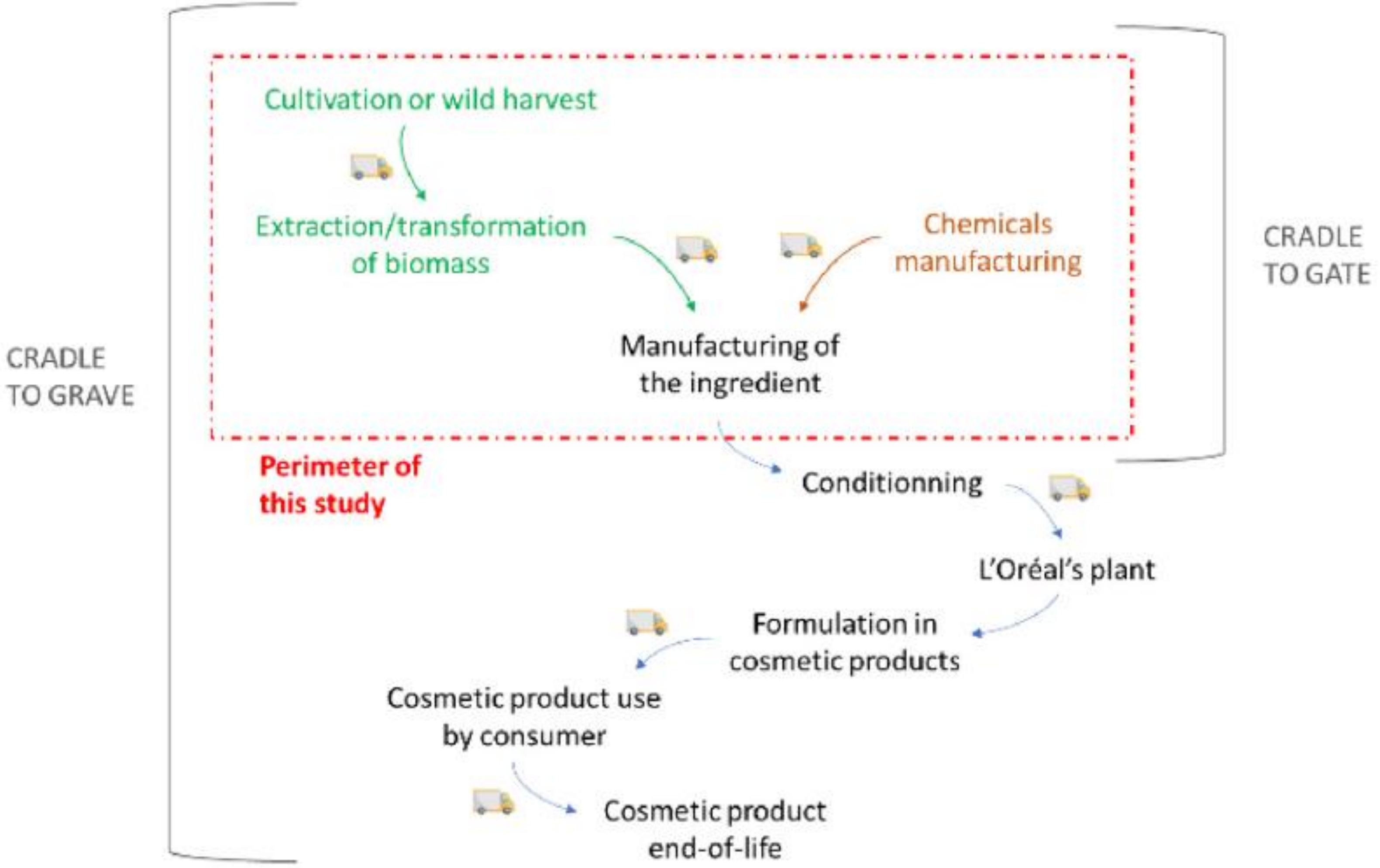
The objective of the present study is to evaluate the environmental
impact of a fragrance and identify eco-design leverages without revealing its **exact composition to preserve confidentiality and industrial knowledge.**

LCA to fragrance can nevertheless appear to be a challenge, due to the numerous ingredients involved and as the composition of a fragrance is one of the best kept secrets of the industry.

Green Chem., **2023**, *25*, 6365.

Mane & L’Oréal: Comparison between Different Tools

Ingredients in Perfume:



Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Ingredients in Perfume:

A representative panel of fragrance ingredients used in cosmetics was evaluated via LCA with the eco-conception tool SPOT, in complementarity with GREEN MOTION™ and the E-factor

Tool	Type of tool	Concept behind	Approach	Perimeter	Complexity
SPOT	Advanced model	Life-cycle assessment	Quantitative	Upstream life cycle including the production process of the ingredient. Downstream life cycle excluded in this study.	High
GREEN MOTION™	Simplified model	Green chemistry principles	Quantitative	Life cycle of the ingredient	Medium
E factor	Metric	Waste measurement	Quantitative	Waste of the production process	Low

Green Chem., **2023**, *25*, 6365.

https://www.loreal.com/en/commitments-and-responsibilities/for-our-products/our-product-eco-design-tool/

Mane & L'Oréal: Comparison between Different Tools

Ingredients in Perfume:

For the production of 1 kg of the material

GREEN MOTION™ impact = 100 – GREEN MOTION™ score

Category	Ingredient	Yield	*E*-Factor	GREEN MOTION™ impact	SPOT single score (mPt)
Essentials oils (EO) and Jungle Essence™ extracts	Lavender EO	1%	100	11	20
	Elemi EO	20%	5	16	1.5
	Orris Butter	0.35%	285	43	46
	Vetiver EO	2%	70	16	4
	Vanilla Pure Jungle Essence™	20%	5	28	14
	Pink Pepper Pure Jungle Essence™	1.5%	33	38	7
Essences by expression	Orange essence	0.01%	4470	24	0.6
Natural extracts with volatile solvent – Absolutes	Orange flower absolute	0.12%	830	64	208
	Jasmine absolute	0.15%	350	64	271
	Narcissus absolute	0.07%	1500	58	209
	Rose absolute	0.16%	600	64	184
Natural extracts with volatile solvent – Resinoids	Benzoin resinoid	85%	3	25	0.3
	Labdanum resinoid	84%	0.3	20	11
	Labdanum absolute	60%	2.5	31	23
	Vanilla absolute	5%	25	49	113
Isolated natural ingredient	*cis*-3-Hexenol (natural)	0.001%	106 680	31	53
Bio-based ingredients with a fossil-based moiety	Iso E super	42% (from myrcene)	3	52	2
	Vetiveryle acetate	0.84%	127	78	9
	Myrcene (from crude sulfate turpentine)	78%	0.4	34	0.6
	Myrcene (from pine)	4%	0.3	29	0.3
Fossil-based ingredients	Hexyl salicylate	99.9%	10	61	1.1
	Ethyl 2-methyl butyrate	87%	1.3	33	0.5
	Hedione	20%	11	72	9
	cis-3-Hexenol (fossil-based)	42%	0.1	57	0.6
Biotechnology ingredients	Antillone	Confidential	11	31	47
	γ-Octalactone		5	27	7
	Tropicalone		27	34	73

Green Chem., **2023**, *25*, 6365
For details see SI: https://www.rsc.org/suppdata/d2/gc/d2gc04860d/d2gc04860d1.pdf.

Mane & L'Oréal: Comparison between Different Tools

Ingredients in Perfume: mPt ??

mPt: dimensionless figure
Unit is milli-point (mPt)……700mPt = 0.7 Pt

The absolute value of the points is not very relevant as the main purpose is to compare relative Differences between products or components.

The scale is chosen in such a way that the value of 1 Pt is representative for 1/1000 of the yearly enviromental load of one average European inhabitant (in some case US…..)

SPOT single score (mPt)
20
1.5
46
4
14
7
0.6
208
271
209
184
0.3
11
23
113
53
2
9
0.6
0.3
1.1
0.5
9
0.6
47
7
73

Green Chem., **2023**, *25*, 6365
For details see SI:
https://www.rsc.org/suppdata/d2/gc/d2gc04860d/d2gc04860d1.pdf.

Mane & L'Oréal: Comparison between Different Tools

Energy and Water consumption:

Energy and water equivalence coefficient: EC

Type of process	Energy and water equivalence coefficient (EC)
Expanded steam (reference)	1
Steam with a pressure of 3 bars	2
Steam with a pressure of 6 bars	3
Steam with a pressure of 15 bars	4
Heating with oil	4
Pyrolysis using gas	6

The global energy and water requirements of a production unit correspond to the energy and water necessary for an average ingredient produced in this unit.
This average ingredient corresponds to an average process duration and process type.

Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Energy and Water consumption:

Type of process	Energy and water equivalence coefficient (EC)
Expanded steam (reference)	1
Steam with a pressure of 3 bars	2
Steam with a pressure of 6 bars	3
Steam with a pressure of 15 bars	4
Heating with oil	4
Pyrolysis using gas	6

To calculate this average, it was assumed that each ingredient is produced in the same proportion as the other ingredients of the same production unit (they were selected to be representative)

$$Average\ Process_{prod\ unit} = \frac{1}{n} * \sum_{i=1}^{n} (Process\ duration_{ing\ i} * EC_{ing\ i})$$

$\sum_{i=1}^{n}(Process\ duration_{ing\ i} * EC_{ing\ i})$: the arithmetic mean of process duration and process type of all ingredients of a given production unit.

n: total number of ingredients in the same production unit

$Process\ duration_{ing}$: the duration of the process of the ingredient,

EC_{ing}: the equivalence coefficient for the ingredient,

Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Energy and Water consumption:

Type of process	Energy and water equivalence coefficient (EC)
Expanded steam (reference)	1
Steam with a pressure of 3 bars	2
Steam with a pressure of 6 bars	3
Steam with a pressure of 15 bars	4
Heating with oil	4
Pyrolysis using gas	6

$$Average\ Process_{prod\ unit} = \frac{1}{n} * \sum_{i=1}^{n} (Process\ duration_{ing\ i} * EC_{ing\ i})$$

$$Energy\ and\ Water\ Requirements_{ing\ x} = \frac{Process\ duration_{ing\ x} * EC_{ing\ x}}{Average\ Process_{prod\ unit}} * Energy\ and\ Water\ requirements_{prod\ unit}$$

Ing_i : all the ingredients produced in the same production unit as ingredient x,
$Energy\ and\ Water\ Requirements_{prod\ unit}$: electricity, gaz and water needs of the production unit per kg of produced ingredient or per kg of starting raw material.

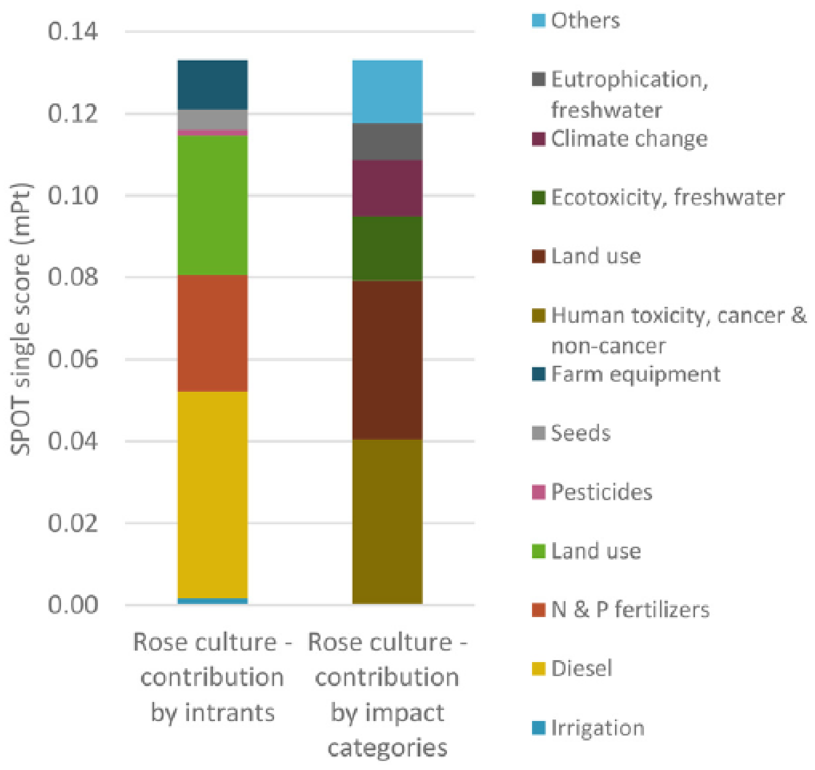
Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Results on different categories:

Rose Culture with extraction

Spot single score (mPt)

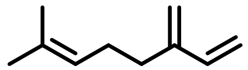


Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

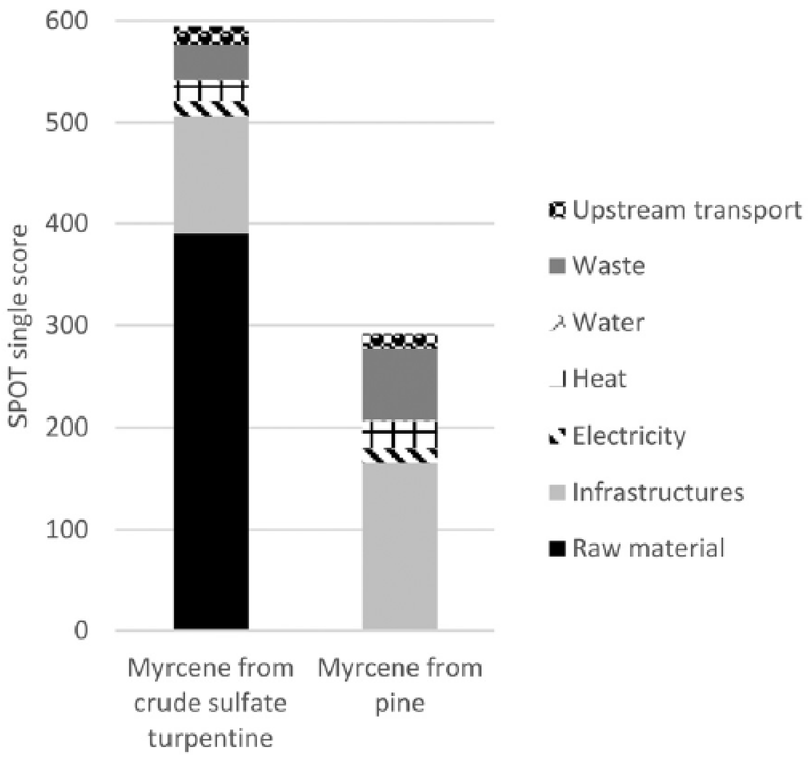
Results on different categories:

Different raw material source of Myrcene



myrcene

Spot single score (mPt)



Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Results on different categories:

(Z)-hex-3-en-1-ol

Different raw materprocess for cis-3-Hexenol:
Extraction from Mint leaves or Chemical Synthesis

Origin	Irrigation	Electricity & infrastructures	Upstream transport	Raw material	Waste	Solvent	Total
Renewable	With	1.846	0.088	59 808	3.794	0	65 536
	Without	1.846	0.088	47 304	3.794	0	53 033
Fossil	—	0.254	0.016	0.165	0.198	3×10^{-3}	0.636

Spot single score (mPt)

Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

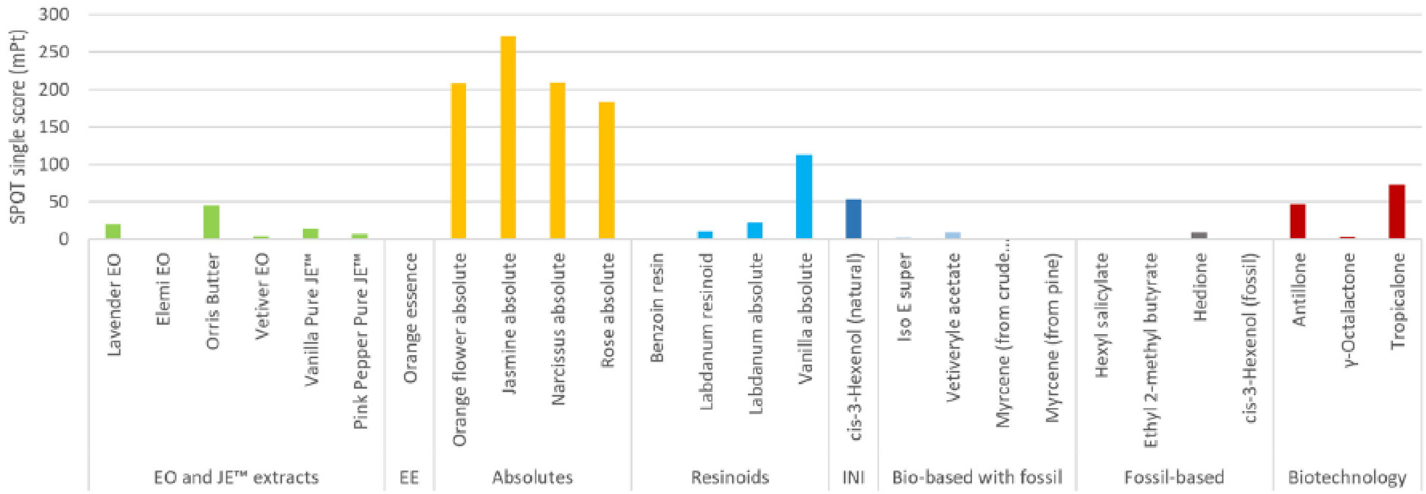
Green Motion Impact™:

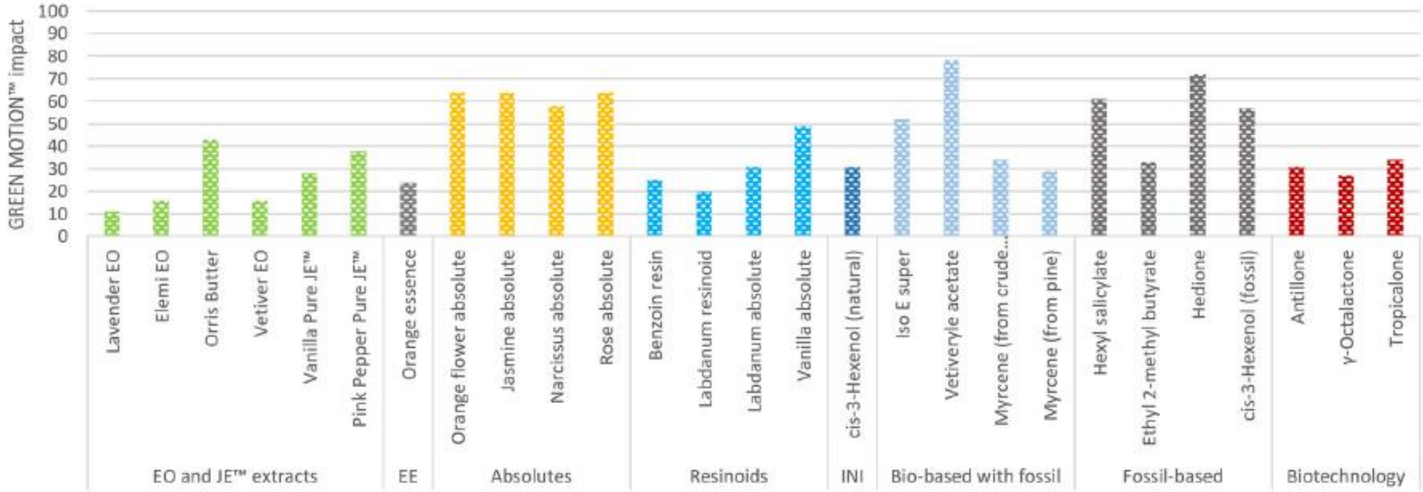
Category	Ingredient	Raw materials	Solvent	Toxicity	Reaction efficiency	Energy consumption	Raw Final product impact	Waste impact *E*-factor	GREEN MOTION™ impact
Essentials oils (EO) and Jungle Essence™ extracts	Lavender EO	A	B	C	C	A	B	A	11
	Elemi EO	A	B	D	C	C	E	B	16
	Orris Butter	A	B	B	D	D	A	F	43
	Vetiver EO	A	A	A	C	B	B	E	16
	Vanilla Pure Jungle Essence™	A	B	B	D	C	B	B	28
	Pink Pepper Pure Jungle Essence™	A	B	B	E	B	E	D	38
Essences by expression	Orange flower absolute	A	B	A	D	B	D	B	24
Natural extracts with volatile solvent – Absolutes	Orange absolute	A	C	D	E	D	D	F	64
	Jasmine absolute	A	D	D	E	D	C	F	64
	Narcissus absolute	A	C	D	E	C	B	F	58
	Rose absolute	A	C	E	E	C	C	F	64
Natural extracts with volatile solvent – Resinoids	Benzoin resinoid	A	C	D	C	C	B	A	25
	Labdanum resinoid	A	B	D	B	D	A	B	20
	Labdanum absolute	A	C	F	C	C	A	B	31
	Vanilla absolute	A	C	E	E	D	B	C	49
Isolated natural ingredients	*cis*-3-Hexenol (natural)	A	C	F	C	C	B	C	31
Bio-based ingredients with a fossil-based moiety	Iso E super	D	C	F	D	C	C	B	52
	Vetiveryle acetate	D	C	E	E	E	C	F	78
	Myrcene (from crude sulfate turpentine)	D	A	D	B	D	D	B	34
	Myrcene (from pine)	D	A	D	D	D	D	B	29
Fossil-based ingredients	Hexyl salicylate	F	D	F	C	D	C	B	61
	Ethyl 2-methyl butyrate	F	B	C	C	C	B	A	33
	Hedione	F	D	F	F	C	A	B	72
	cis-3-Hexenol (fossil-based)	F	C	F	C	E	B	B	57
Biotechnology ingredients	Antillone	A	D	E	C	C	B	C	31
	gamma-Octalactone	A	D	F	B	E	A	A	27
	Tropicalone	A	C	E	C	D	A	D	34

Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Spot vs Green Motion Impact™:





Green Chem., **2023**, *25*, 6365.

Mane & L'Oréal: Comparison between Different Tools

Eco-Design Levers

Ingredient category	Main(s) hotspot(s)	Eco-design levers
Essentials oils (EO) and Jungle Essence™ extracts	Raw material	Yield of culture or extraction More sustainable farming practices More co-products valorization
Essences by expression	Raw material	Yield of culture More sustainable farming practices
Natural extracts with volatile solvent – Absolutes	Raw material and transformation process	Yield of culture More sustainable farming practices More biowaste valorization More efficient extraction processes (yield and energy use)
Natural extracts with volatile solvent – Resinoids	Solvent	Use of more environmentally friendly and less toxic solvents
Isolated natural ingredients	Raw material	Yield of culture More sustainable farming practices More co-products valorization
Bio-based ingredients with a fossil-based moiety	Solvent	More sustainable farming practices More biowaste valorization Yield of manufacturing More efficient extraction processes (yield and energy use) Chemical synthesis optimization (C factor for example[15])
Fossil-based ingredients	Raw material and transformation process	Yield of manufacturing More efficient extraction processes (yield and energy use) Chemical synthesis optimization (C factor for example[15])
Biotechnology ingredients	Confidential	Yield of manufacturing More efficient processes (energy use and downstream processes) Optimization of solvent use

Green Chem., **2023**, *25*,

ECOINGREDIENT COMPASS®

ECOINGREDIENT COMPASS™

RENEWABLE CARBON

100% RC
> 50% RC

BIODEGRADABILITY

Readily biodegradable
Ultimately biodegradable
Partially biodegradable

GREEN CHEMISTRY SCORE

>70% Green Chemistry
50-70% Green Chemistry

DSM-FIRMENICH MOLECULES
concerns synthetic perfumery ingredients

OBJECTIVE
Communicate proactively and transparently on all parameters

CHARACTERIZATION
Based on Fragrance Green properties parameters from **ECO**SCENT **COMPASS™**

RENEWABLE CARBON

BIODEGRADABILITY

GREEN CHEMISTRY SCORE

Fragrance Green Properties

GCP *UNSG*

Renewability

% renewable carbon as parameter

$$\frac{\text{Number of carbon atoms from biogenic source in the finished product}}{\text{Number of carbon atoms in the finished product}}$$

Biodegradation

Ultimately: ≥ 60% biodegradable in 60 days

Biodegradation is the breaking down of chemicals by living organisms such as microbes

cE-factor

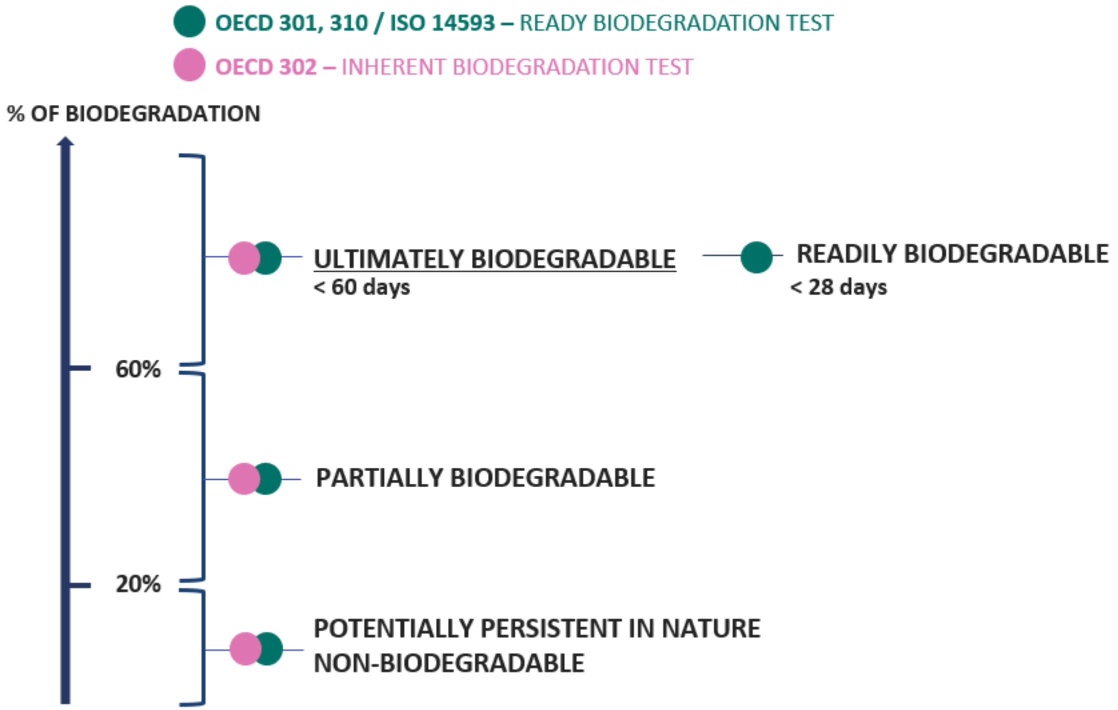
Kilograms of waste generated per kilogram of product *incl.* water

Industry segment	Tonnes per annum	*E* factor (kg waste per kg product)
Oil refining	10^6–10^8	<0.1
Bulk chemicals	10^4–10^6	<1–5
Fine chemicals	10^2–10^4	5–50
Pharmaceuticals	10–10^3	25 – >100

Sheldon, R. A. *Green Chem.* **2007**, *9*, 1273-1283.
Sheldon, R. A. *ACS Sustainable Chem. Eng*. **2018**, *6*, 32–48.

Fragrance Green Properties

Biodegradation, Bioaccumulation,



https://www.oecd.org/chemicalsafety/

Fragrance Green Properties

Additional Green Chemistry principles *GCP* *UNSG*

Atom economy

$$\frac{\text{Number of carbon atoms/finished product}}{\text{Number of carbon atoms/all C-containing reactants \& reagents used}}$$

Catalysis

$$\frac{\text{Number of catalytic steps}}{\text{Total number of steps}}$$

Hazardous reagents

- **List all risk phrases from GHS (5344 phrases)**
- **Clustered by severity**

https://goldbook.iupac.org/terms/view/C00876

Fragrance Green Properties

Atom economy & Catalysis

Ranking between A to E

Up to	E	D	C	B	A	Ranking
	0.4	0.5	0.65	0.8	1	Atom Economy
	0,45	0,65	0,8	0,9	1	Catalysis

Robvieux, F.; Roth, J.; Chapuis, C.; Reiter, M. *Current Opinion in Green and Sustainable Chem*. **2022**, *33*, 100583.

Fragrance Green Properties

Hazardeous reagents

- Clustered by severity (A to E) and occurrence
- Only the most severe categories have been considered (C to E)
- F-Plot have been used to determine frequency
- This was done using an F-plot in order to be sure that more that 98% of the H-phrase for all our reactants/reagents were covered by this methodology
- In case of reactant/reagent having several H-phrase a limit of 11 H-code was set.

	Frequency Risk Phrases										
Cat.	1	2	3	4	5	6	7	8	9	10	11
C	1	1	2	2	3	3	3	4	4	4	5
D	1	2	2	3	3	4	4	5	5	5	5
E	2	3	3	4	5	5	5	5	5	5	5

Final score for Green Chemistry

Average of the 3 sub-scores (A to E) translated in %

Fragrance Green Properties

Hazardeous reagents

As Molecules from Competitors have to be included:

- Solvents are not taken into account
- Temperature of the process is not included
- Steps Economy & Redox Economy not included (*Tetrahedron*, 2014, *69(36)*, 7529; *ACIE* 2009, *48*, 2854; *JOC* 2010, *75*, 4657)

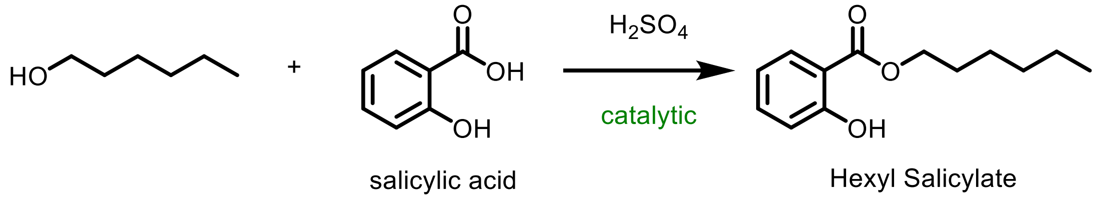
	Frequency Risk Phrases										
Cat.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
C	1	1	2	2	3	3	3	4	4	4	5
D	1	2	2	3	3	4	4	5	5	5	5
E	2	3	3	4	5	5	5	5	5	5	5

Final score for Green Chemistry

Average of the 3 sub-scores (A to E) translated in %

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate



Atom economy

Rank	5	4	3	2	1
Ratio up to	0.4	0.5	0.65	0.8	1

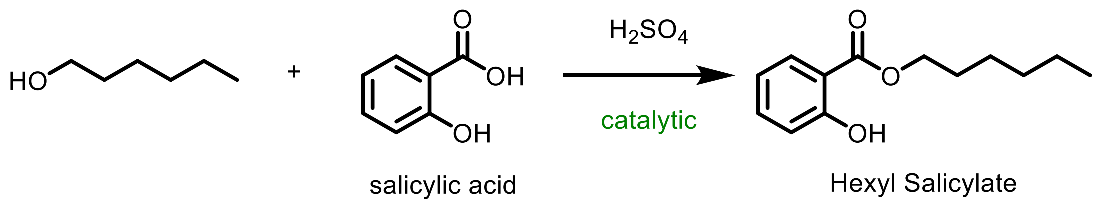
13/13 carbon atoms = 100%

Score 1

Common Fragrance and Flavor Materials: Preparation, Properties and Uses, Horst Surburg, Johannes Panten, **2016** ,Wiley-VCH Verlag GmbH & Co. KGaA.
DOI:10.1002/9783527693153

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate



Catalysis Score

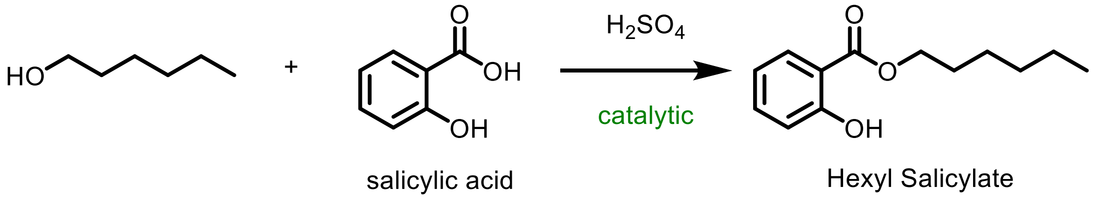
Rank	5	4	3	2	1
Ratio up to	0.45	0.65	0.8	0.9	1

1/1 step = 100%

Score 1

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate



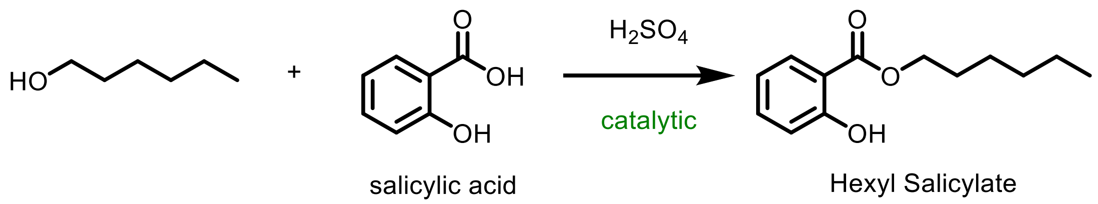
Hazardous Score

All H-code were listed and a score 1 to 5 was given

For Hexyl Salicylate all reactant/reagent and final product were listed and for each the H-code were extracted. Then using our internal classification for each H-phrase, a score (between 1 and 5) was attributed, and this is done for each component.

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate

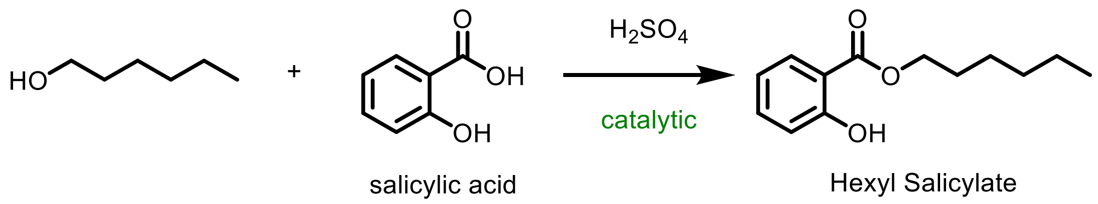


Hazardous Score

Final Ingredient	Reagents/Reactants/Product	1st H code	Score	2nd H code	Score	3rd H code	Score	4th H code	Score
HEXYL SALICYLATE	SALICYLIQUE ACID	H302	2	H318	3				
	HEXANOL	H226	1	H302	2	H312	2	H319	2
	SULFURIC ACIDE 85	H290	2	H314	3				
	HEXYL SALICYLATE	H315	2	H317	2	H400	5	H410	4

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate



Hazardous Score

Final Ingredient	Reagents/Reactants/Product	1st H code	Score	2nd H code	Score	3rd H code	Score	4th H code	Score
HEXYL SALICYLATE	SALICYLIQUE ACID	H302	2	H318	3				
	HEXANOL	H226	1	H302	2	H312	2	H319	2
	SULFURIC ACIDE 85	H290	2	H314	3				
	HEXYL SALICYLATE	H315	2	H317	2	H400	5	H410	4

It has been decided that for the next step of the calculation:
H-code having a score of 1 or 2 are not considered. WHY?
All chemicals have multiple H-code that will be scored of 1 or 2. If they were taken in consideration a huge dilution effect of the more severe H-code will be observed.

Hazardous score should reflect as much as possible the hazardousness or not of the perfumery ingredient.

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate

Hazardous Score

	Frequency Risk Phrases										
Cat.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
3	1	1	2	2	3	3	3	4	4	4	5
4	1	2	2	3	3	4	4	5	5	5	5
5	2	3	3	4	5	5	5	5	5	5	5

- Category 3: 2 times with the decision matrix means a score of 1.
- Category 4: 1 time with the decision matrix means a score of 1.
- Category 5: 1 time with the decision matrix means a score of 2.

Total score: (1+1+2)/3 = 1.

Hexyl Salicylate has a hazardous score of 1

Example of Green Chemistry Score calculation

Synthesis of Hexyl Salicylate

Green Chemistry Score

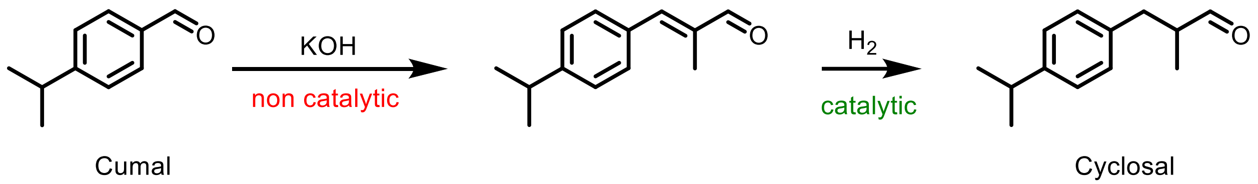
Hexyl Salicylate has:

- Catalysis score of 1
- Atom Economy score of 1
- Hazardous score of 1

overall green chemistry score of 1

Example of Green Chemistry Score calculation

Synthesis of Cyclosal

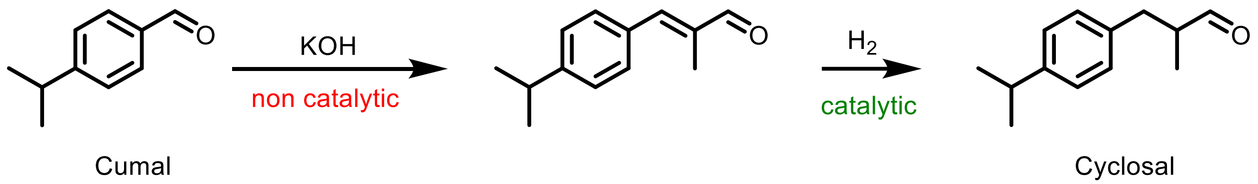


Atom economy?
Catalysis Score?
Hazardous Score?

Common Fragrance and Flavor Materials: Preparation, Properties and Uses, Horst Surburg, Johannes Panten, **2016** ,Wiley-VCH Verlag GmbH & Co. KGaA.
DOI:10.1002/9783527693153

Example of Green Chemistry Score calculation

Synthesis of Cyclosal



Atom economy?
Catalysis Score?
Hazardous Score?

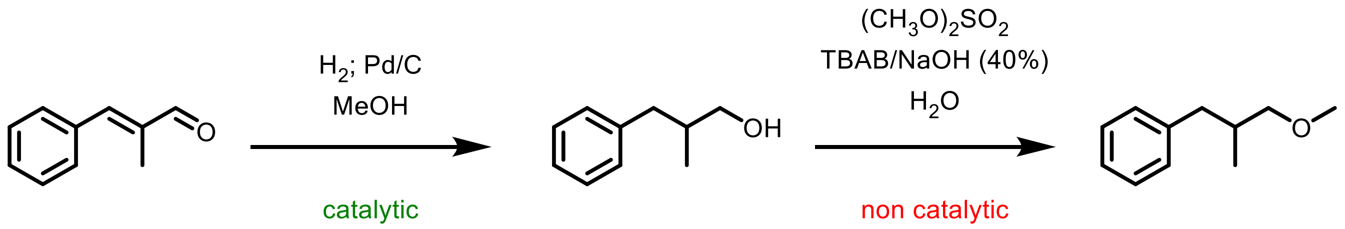
13/13 carbon atoms = 100% — Score 1

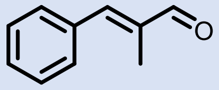
1/2 catalytic steps = 50% — Score 4

Common Fragrance and Flavor Materials: Preparation, Properties and Uses, Horst Surburg, Johannes Panten, **2016** ,Wiley-VCH Verlag GmbH & Co. KGaA.
DOI:10.1002/9783527693153

Example of Green Chemistry Score calculation

Synthesis of Centifol Ether



Reagents	Reagents Carbon	Total Carbon in Final Pdt	Carbon Economy (%)	Total Rewable Carbon	Renewable Carbon (%)	Catalytic Steps	Total Steps	Catalysis (%)
	10	10		0	0	1	2	50
$(CH_3O)_2SO_2$	2	1		0	0			
Total	12	11	0,92	0	0			

Example of Green Chemistry Score calculation

Centifol Ether: E-Factor IN & OUT

	Reactants Reagents	**QTY (kg)**		
Raw Mats	a-Methyl Cinnamic Aldehyde	5012		
	Raney Ni	251		
	Potassium Acetate	21		
	Hydrogen	137		
	Dimethylsulfate	8613		
	Sodium Hydroxide Sol. 40%	13658	5463.2	
	TBAB	205		
	NaHCO3 Sol. 5%	5127	256.5	
	Water	10255	8194.8	4870.7
Product	Centifolether	5129		
Waste	Waste to be burnt	276		
	Water sent to Waster Water Treatment Plant	37551		
	Spent Catalyst	291		

Total of the mass of reactants, reagents and water.
In case of solution the amount of water is re-calculated.

40% NaOH Solution:
13658*0.4 = 5463.2 kg of NaOH and 8194.8 kg of water.
5% $NaHCO_3$ Solution:
5127*.05 = 256.35 kg of $NaHCO_3$ and 4870.65 kg of water.

It is mandatory to extract these figures in order to be able to calculate the Water usage of the final product:

Example of Green Chemistry Score calculation

Centifol Ether: E-Factor IN & OUT

The number indicated are normalized for 1kg of final product
For example:
Dimethylsulfate: 8613/5159 = 1.6695.

Water usage = (8194.8+4870.65+10255)/5159 = 4.52 L/kg of final product.

IN			
Centilfolether	-1	OUT	4.520343
a-Methyl Cinnamic Aldehyde	0.9715	Clean water usage	-0.0535
Raney Ni	0.04865	Waste to be burnt	7.2787
Potassium Acetate	0.00407	Water sent to WWTP	-0.05641
Hydrogen	0.026555	Waste Catalyst	-2.86826
Dimethylsulfate	1.6695		
Sodium Hydroxide	1.05896		
TBAB	0.039736		
$NaHCO_3$	0.04969		
E-Factor IN	2.868661		
E-Factor OUT	2.87		
Waste to be burnt	-0.054 kg/kg		
Water usage in L/Kg of Final Product	4.54		

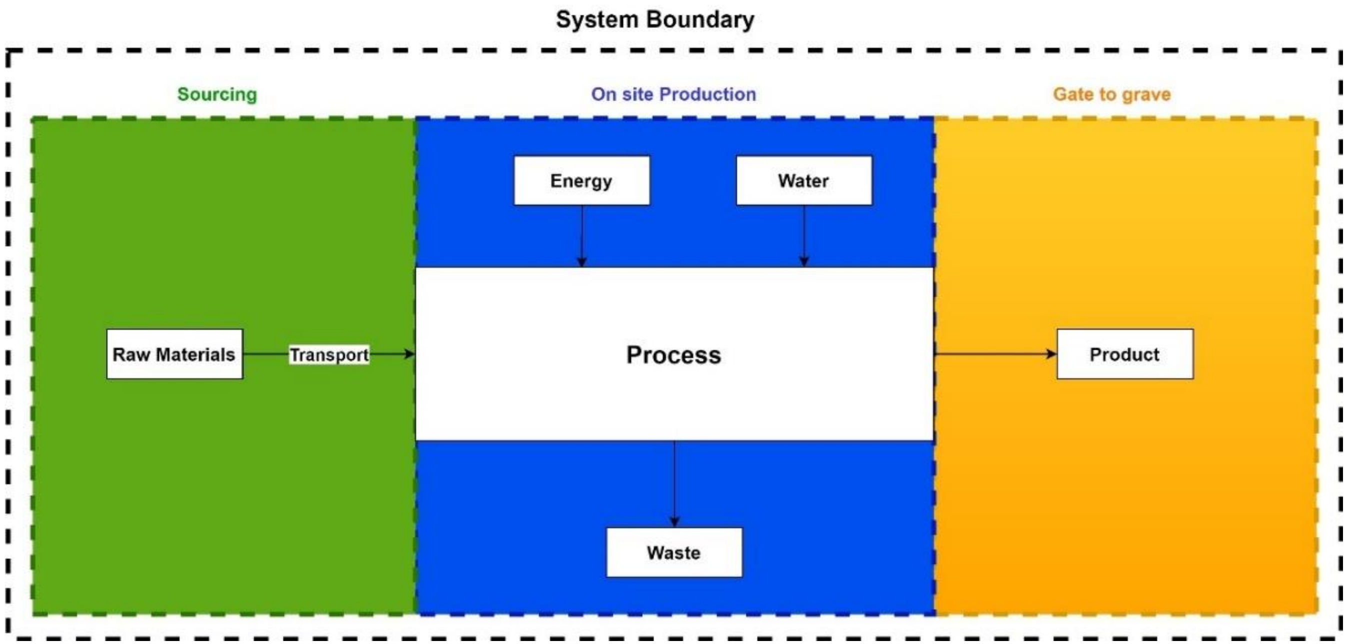
Example of Green Chemistry Score calculation

What could be added next?

Energy by ingredients
Temperature of the process: key criteria ?
Solvent ? Still missing

Product Carbon Footprint (PCF)

Fragrance Green Properties



The considered flow of the analysis shown included:

- Raw materials and their transport (resource extraction to be consumed)
- Energy consumption (resource extraction to provide energy)
- Waste generation and release (impact of waste emission)
- Water consumption (impact of water usage)
- Product properties (impact of the ingredient itself when being used)

Robvieux, F.; Roth, J.; Chapuis, C.; Reiter, M. *Current Opinion in Green and Sustainable Chem*. **2022**, *33*, 100583.

Ingredients Sustainability Index

Developed in partnership with Quantis

Based on 3 environmental indicators

Climate change CO_2
Water depletion
E-toxicity

All stages of the life-cycle of an ingredient considered

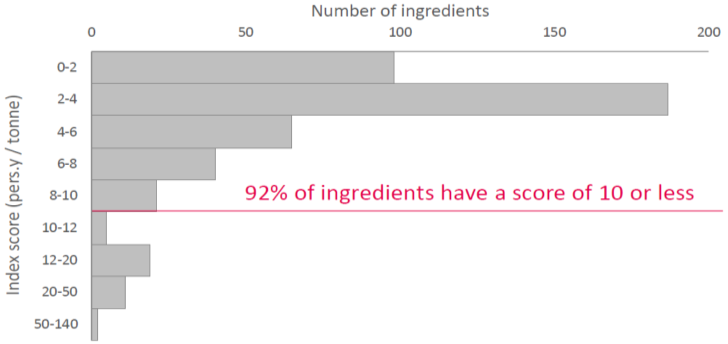
Sourcing & transportation of raw materials
On-site production
Product use and disposal

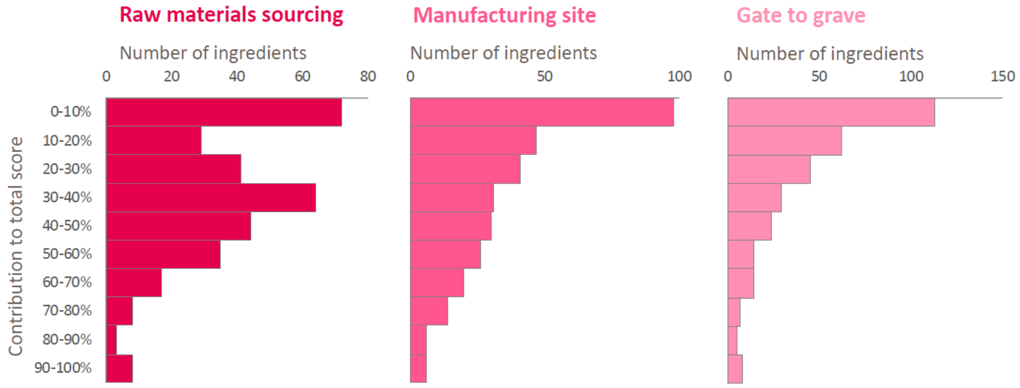
https://quantis.com/

LCA parameters & results

451 unique Perfumery Ingredients modelized in 2017

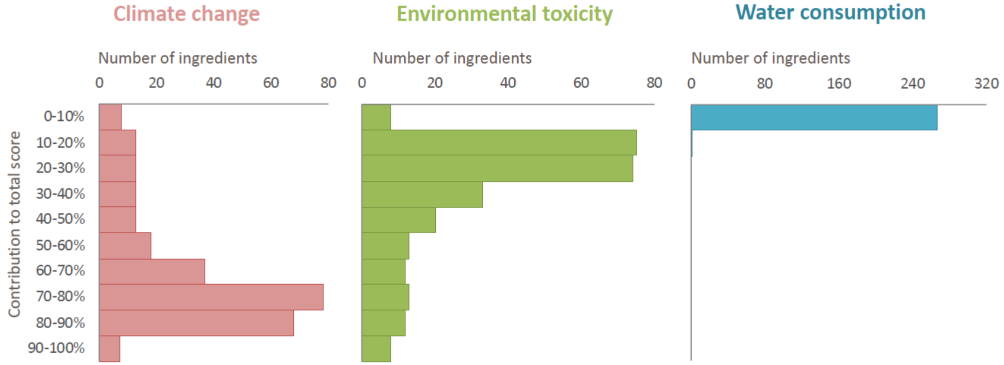
Life cycle stage		Indicators: Climate change	Indicators: Water	Indicators: Environmental toxicity
Sourcing				
	Raw material	✓	✓	✓
	Transport	✓	✓	✓
Onsite production				
	Energy consumption	✓	✓	✓
	Water consumption	0	✓	0
	Waste production	✓	✓	✓
Gate to grave				
	Synthetics properties	Not relevant	Not relevant	✓





Average contributions:

35% 31% 28%



Average contributions:

65% 34% 1%

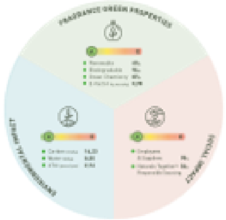
An index score of 1 means that the production of 1 MT of this ingredient has the same impact on the environment as an average global citizen in 1 year.

EcoScent Compass®

ECOSCENT COMPASS®
NEXT GENERATION

2023

2018



	EcoScent Compass® Next Generation	EcoScent Compass® V1
Pillars	**3, advanced & reassigned :** Circular Creation Climate & Nature impact People & Communities impact	3 Fragrance Green Properties Environmental impact Social impact
Life Cycle Analysis	✓	✓
# Sustainability Data	✓ 80	✓ 10
Consumer facing claims, including suitability with retailer labels and third-party certifications	✓ 65	✗
Extended Hero ingredients information for storyproofing, built with an intelligent algo[r] to highlight the most relevant circular ingredients of each creation	✓	✗

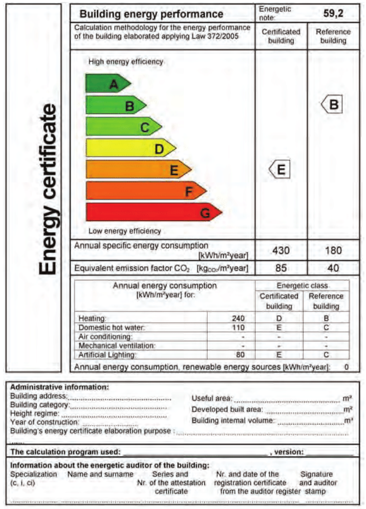
Continuous improvement of the tool, still the same objectives :

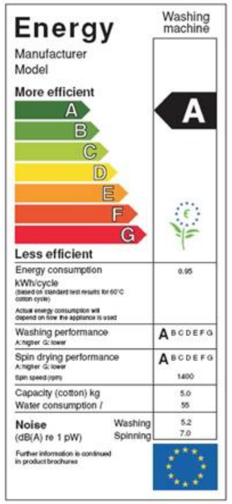
CREATE RESPONSIBLY

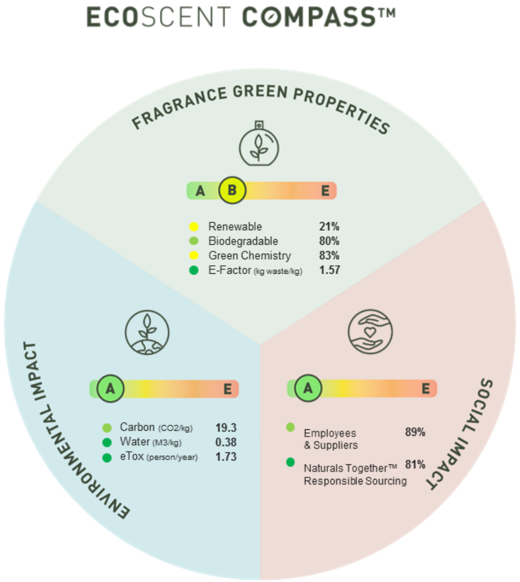
ACT TRANSPARENTLY

INFORM & EMPOWER

EcoScent Compass®: Nutri Score

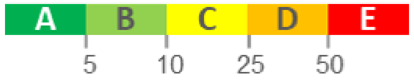






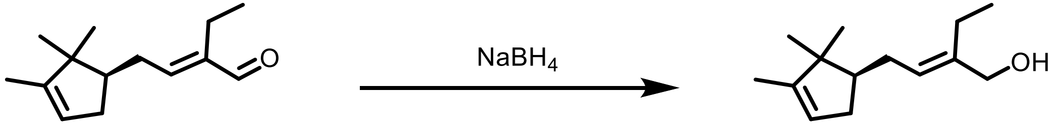
E-factor Nutri- score

Industry segment	Tonnes per annum	*E* factor (kg waste per kg product)
Oil refining	10^6–10^8	<0.1
Bulk chemicals	10^4–10^6	<1–5
Fine chemicals	10^2–10^4	5–50
Pharmaceuticals	10–10^3	25 – >100

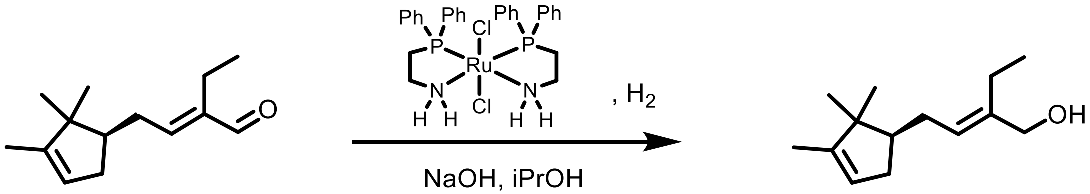


Spearheading in Catalysis: Dartanol®

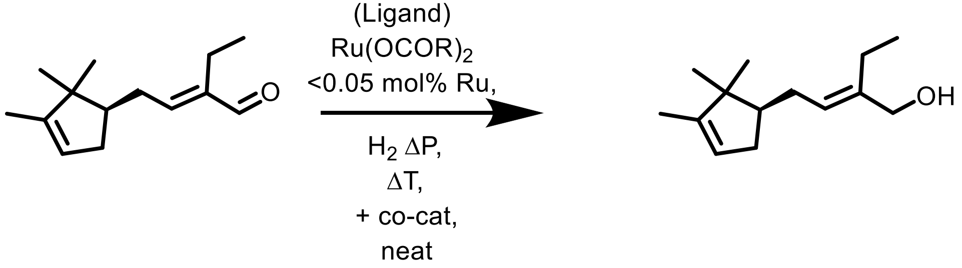
Historical process using sodium borohydride



First Firmenich catalyzed hydrogenation technology



Firmenich latest generation catalyst for hydrogenation

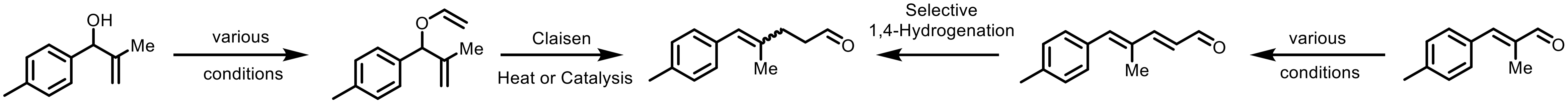


- (2) 100% C use from the raw materials
- (7) 76% green carbon from pine
- (8) No protecting group
- (10) Ultimately biodegradable
- (9) Cutting edge Firmenich hydrogenation technology
- (1) E factor 1.85
- (5) Neat reaction

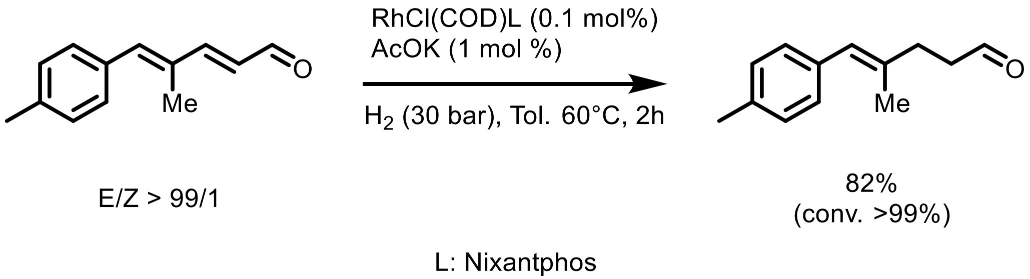
Firmenich, WO2013/050297

Review: Dupau, P. *Helv. Chim. Acta* **2018**, *101*, e1800144.

Spearheading in Catalysis: Mimosal™ Synthesis

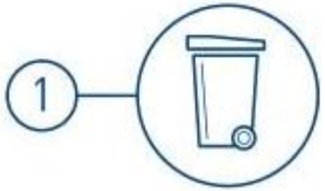


Vinyl ether formation step problematic
Muguet aldehyde product thermally unstable

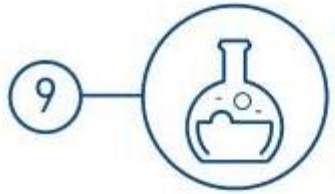


Saudan, L. *et al.* *ChemCatChem* **2022**, *14*, e2022006.
Saudan, L. *et al.* WO2012150053.

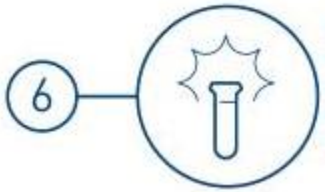
Spearheading in Catalysis: Mimosal™ Synthesis



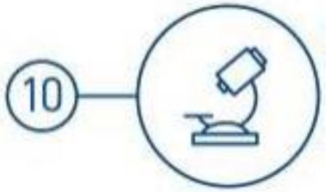
1. Waste Prevention:
E factor = 1.6
vs 12 (Claisen)



9. Catalysis:
Rh cplx (0.005 mol%)



6. Design for Energy Efficiency: t = 60^{o}C vs 185^{o}C (Claisen)

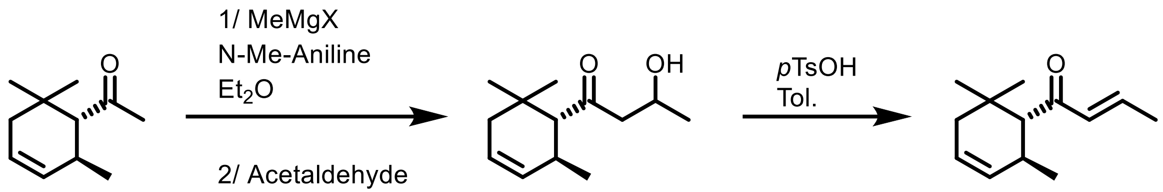


10. Design for Degradation
Muguet aldehyde
64% BDG (28 d)

Saudan, L. *et al. ChemCatChem* **2022**, *14*, e2022006.
Saudan, L. *et al.* WO2012150053.

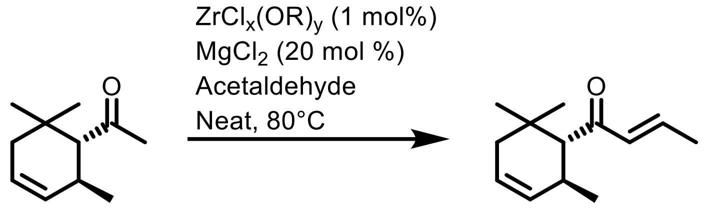
Spearheading in Catalysis: δ-Dasmascone Aldol

Old Process

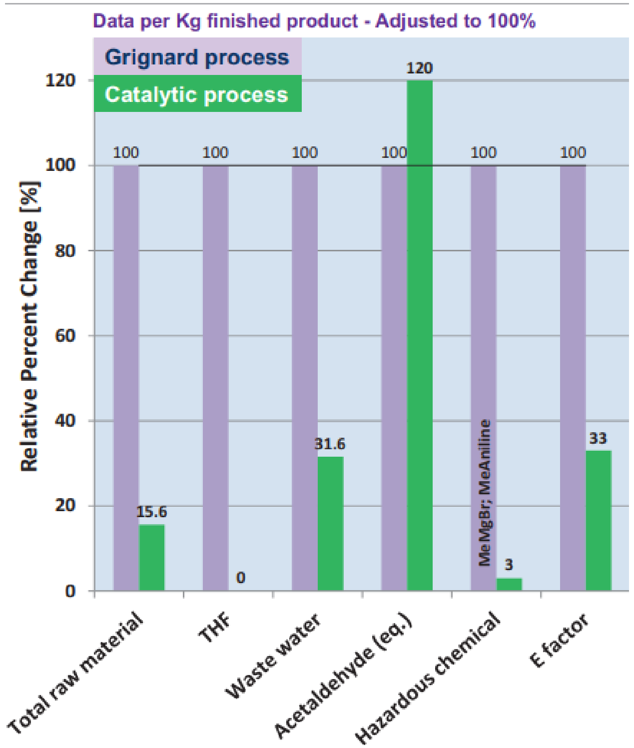


Overall 58%

New Process



Conversion on SM: 32%
Yield on Recycled SM: 88%



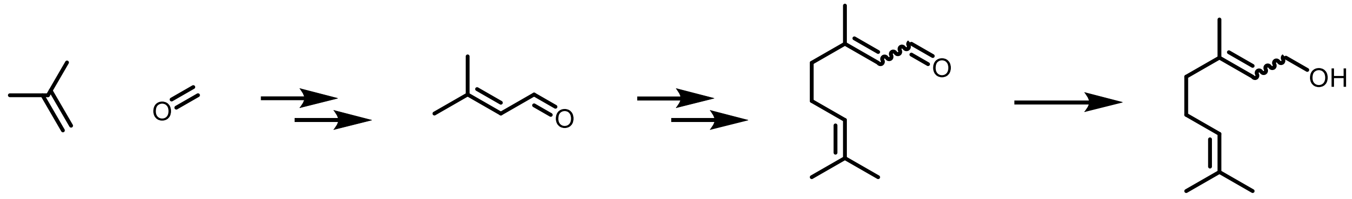
Jacoby, D. *Chimia* **2021**, *75*, 634.

Confidential

From Pine Tree to Perfume

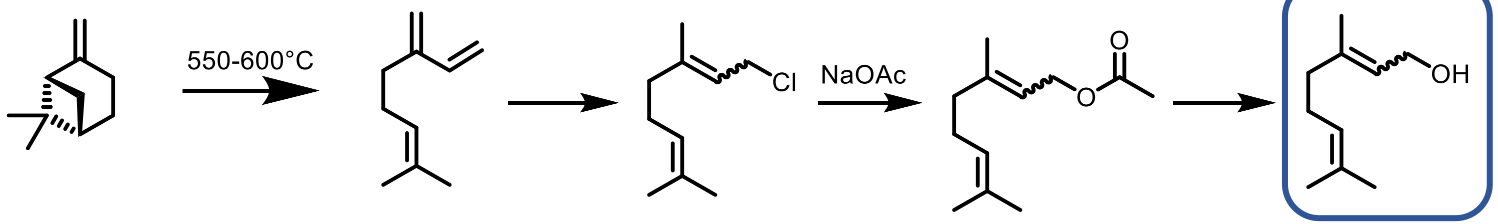
SylverGreen®

CONVERT EXISTING INGREDIENTS GERANIOL



isobutene prenal Citral Geraniol

INTO RC VERSIONS VIA NOVEL CHEMICAL PROCESS FROM MYRCENE



(-)-Beta Pinene

Myrcene
75-80%

Geraniol

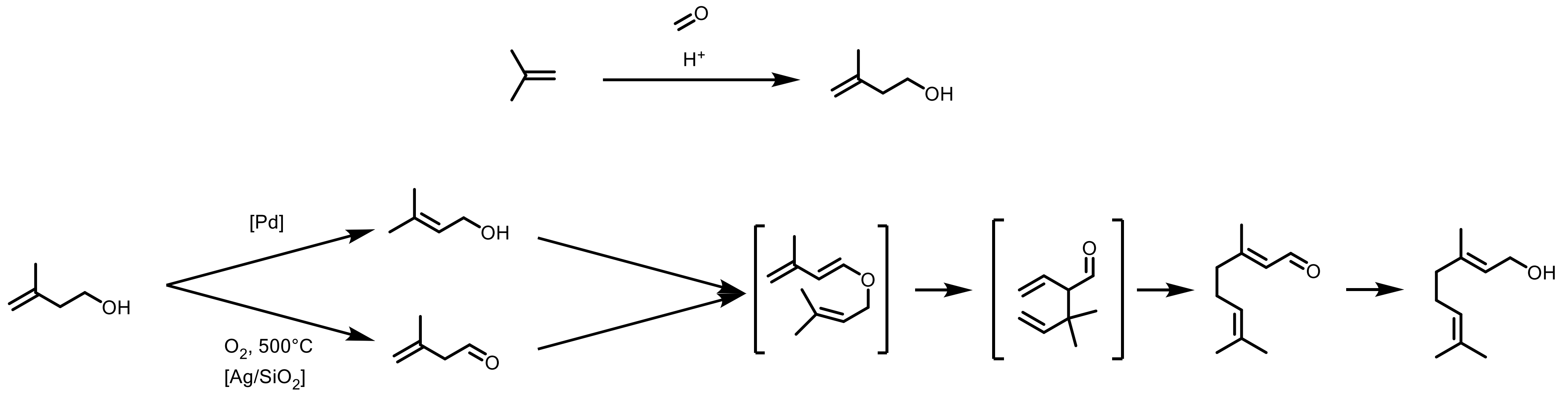
Readily
Biodegradable
100% RC

EXTENSION TO CITRONELLOL & TETRAHYDROGERANIOL

Sagorin, G.; Cazeils, E.; Basset, J.-F.; Reiter, M. *Chimia* **2021**, *75*, 780–787.

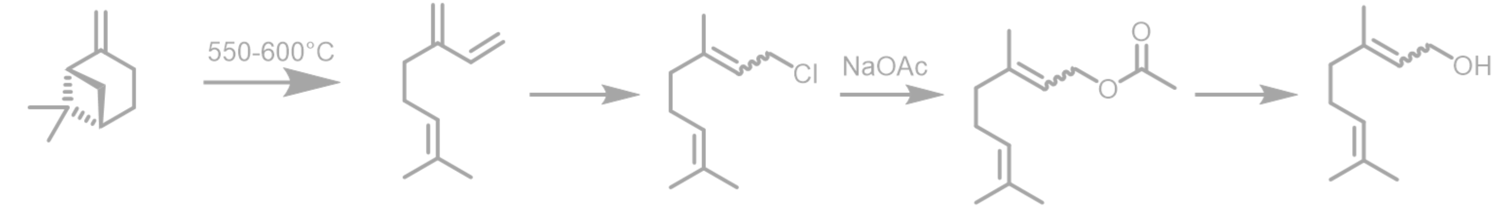
From Pine Tree to Perfume

BASF Synthesis of Citral & Geraniol



Citral

Geraniol



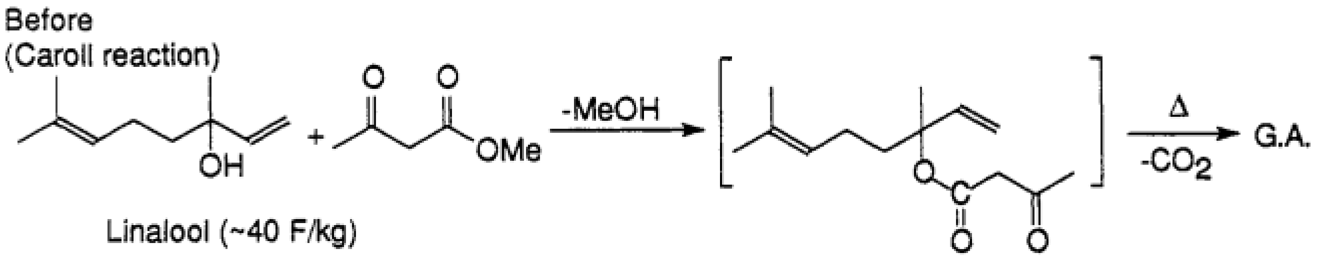
(-)-Beta Pinene

Myrcene
75-80%

Geraniol

Others Examples

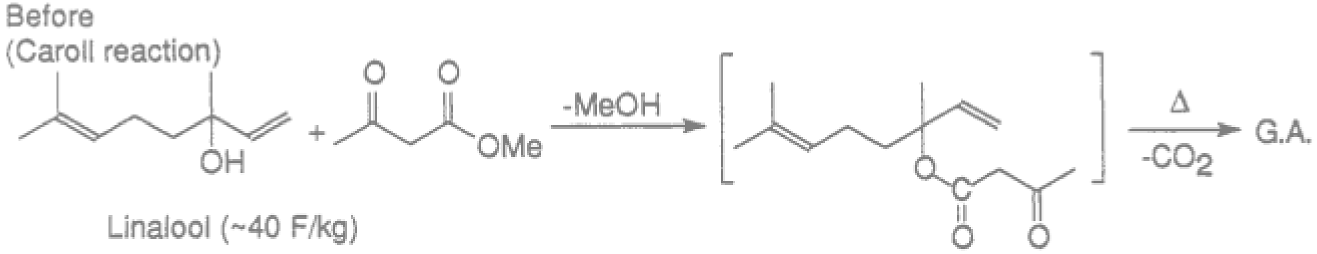
Comparison (ex-Rhodia) ex-Solvay EssentialCo

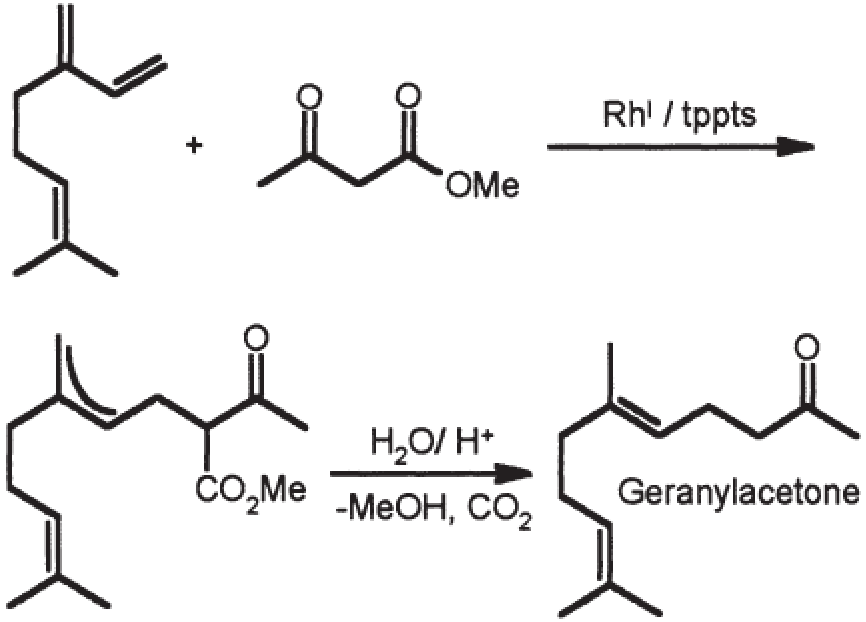


Current Topics in Flavours and Fragrances, **1999**, 59–78.

Others Examples

Comparison (ex-Rhodia) ex-Solvay EssentialCo

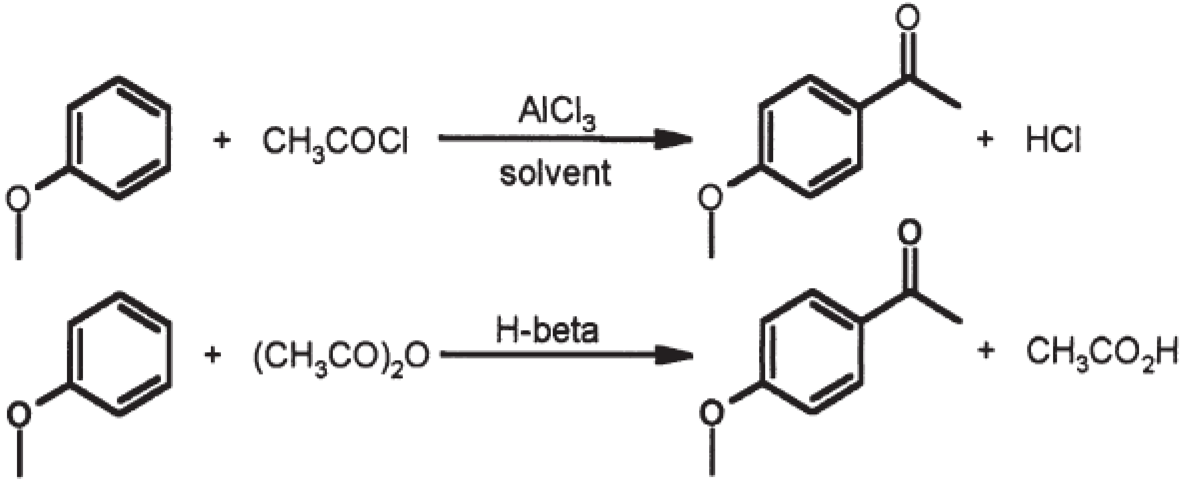




Current Topics in Flavours and Fragrances, **1999**, 59–78.

Others Examples

Comparison



Homogeneous	**Heterogeneous**
$AlCl_3$ > 1 equivalent	H-beta, catalytic & regenerable
Solvent	No solvent
Hydrolysis of products	No water necessary
Phase separation	-
Distillation, organic phase	Distillation, organic phase
Solvent recycle	-
85-95% yield	> 95% yield / higher purity
4.5kg aqueous effluent per kg	0.035kg aqueous effluent per kg

Current Topics in Flavours and Fragrances, **1999**, 59–78.

Example from Chimex

L’Oreal/Chimex: Eco-Footprint Metrics

- H_2O: Water consumption
- iL: Raw materials geographical origin
- eFA: Aqueous waste valorization
- eC: Process carbon footprint
- eVS: Synthetic pathway efficiency
- sIOS: Used organic solvents valorization
- rMP: Raw material of renewable origin
- eF: E-factor
- ieMP: environmental impact of raw materials
- ieD: environmental impact of waste

Green Chem., **2014**, *16*, 1139.

Example from Chimex

L'Oreal/Chimex: Comparison between 3 tools

FLASC™ from GSK
SEEbalance© BASF
EPA's GREENSCOPE

Green metric	Definition	Calculation	Simple interconnections
Atom economy	Efficiency of the reaction stoichiometry	$AE = \frac{M_W(\text{product})}{\sum_i M_w(\text{reactant}_i)}$	
E-factor	Quantity of waste generated to produce 1 unit of product	$E = \frac{\sum_i m(\text{raw material}_i) - m_p}{m_p}$	$MI = E + 1$
Mass intensity/index	Quantity of raw materials needed to produce 1 unit of product	$MI = \frac{\sum_i m(\text{raw material}_i)}{m_p}$	
Reaction mass efficiency	Percentage of product obtained considering the total mass of reactants	$RME = \frac{m_p}{\sum_i m(\text{reactant}_i)}$	$SF = \frac{r \times AE}{RME}$
Stoichiometric factor	Excess of reactants	$SF = \frac{\sum_i m(\text{reactant}_i)}{\sum_i m_s(\text{reactant}_i)}$	
Global material economy	Percentage of product obtained considering the total mass of raw materials	$GME = \frac{m_p}{\sum_i m(\text{raw material}_i)}$	$GME = \frac{1}{MI}$

Where: M_w: molecular weight, m_s: stoichiometric mass, m_p: mass of product, r: reaction yield.

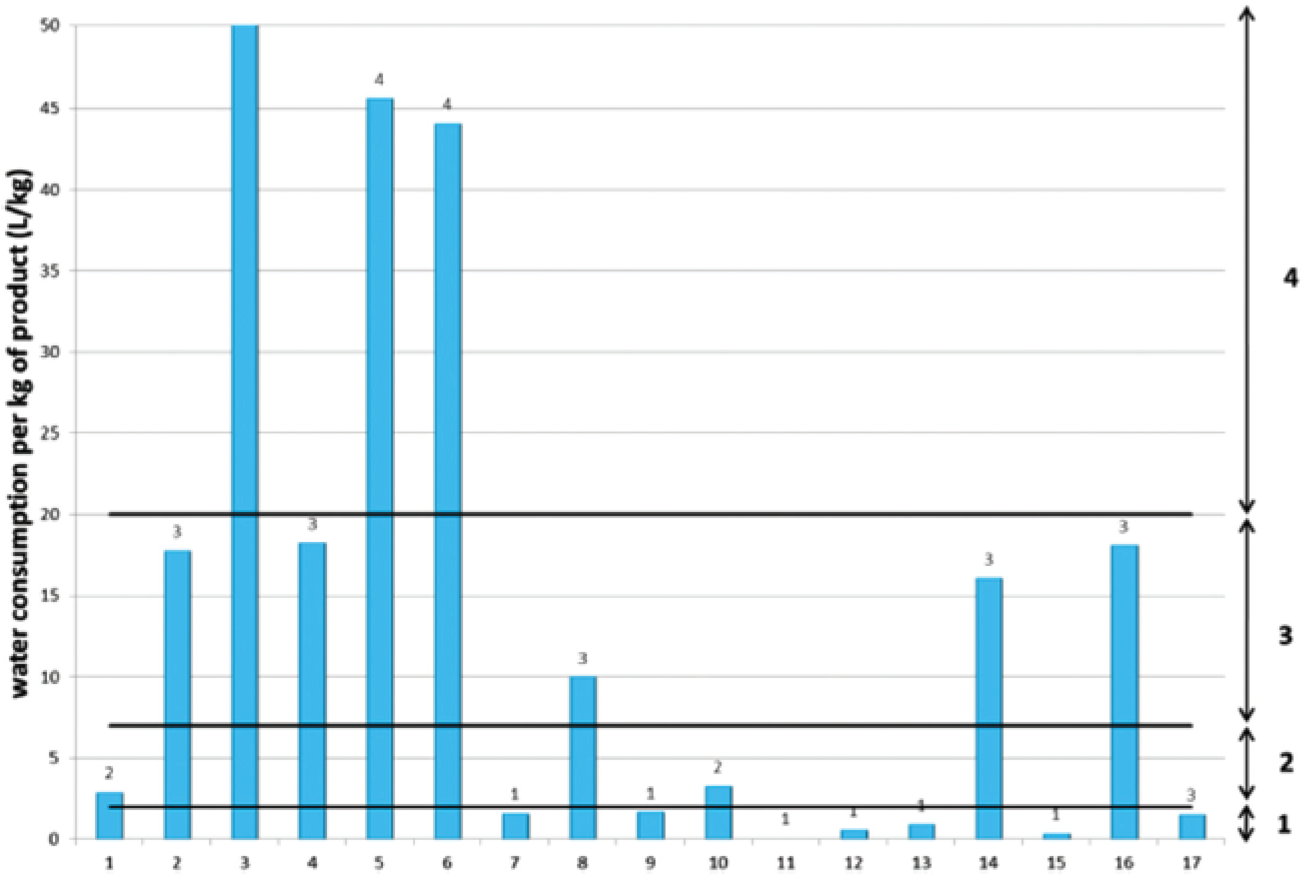
Int. J. LCA, **2007**, *12*, 272.
Int. J. Sustain. Dev., **2008**, *11*, 1.
Ind. Eng. Chem. Res., **2013**, *52*, 6747.

Example from Chimex

Manufacturing footprint:

Cleaning processes, waste treatment (both aqueous & organic), raw materials geographical origin, process carbon footprint

Water usage

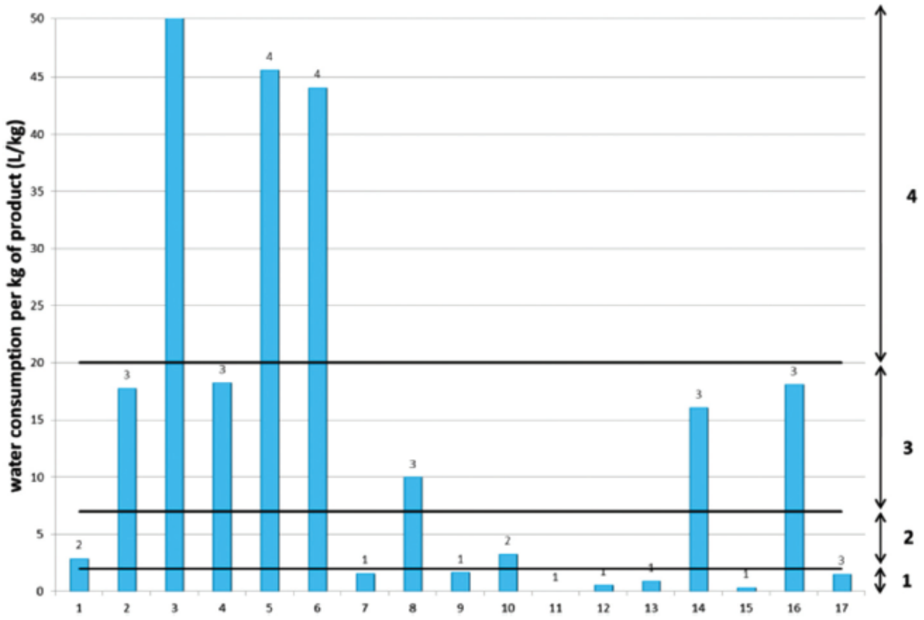


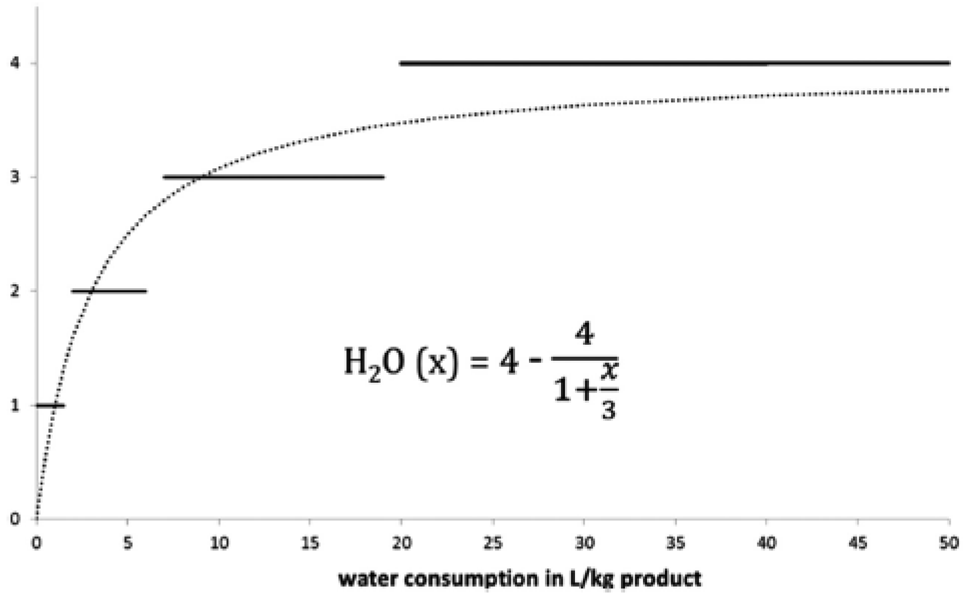
Green Chem., **2014**, *16*, 1139.

Example from Chimex

Manufacturing footprint:

Water usage





Green Chem., **2014**, *16*, 1139.

Example from Chimex

Manufacturing footprint:

Aqueous waste valorization (eFA).

Aqueous waste valorization	eFA
Biological water treatment	1
Partial biological water treatment	2
Aqueous waste burying	3
Absence of valorization	4

Used organic solvents valorization (sIOS).

$$\text{Valorization}(\%) = \frac{\sum_{i=1}^{n} m_{si} \times f_{si}}{\sum_{i=1}^{n} m_{si}}$$

n = number of solvent;
m_{si} = mass of solvent i;
f_{si} = valorization factor for solvent i.

Valorization	sIOS
$90 \leq \text{Valorization} \leq 100$	1
$80 \leq \text{Valorization} < 90$	2
$60 \leq \text{Valorization} < 80$	3
$0 \leq \text{Valorization} < 60$	4

Green Chem., **2014**, *16*, 1139.

Example from Chimex

Manufacturing footprint:

Raw materials geographical origin (iL)

$$EFi = D_{HGV} * EF_{HGV} + D_{rail} * EF_{Rail} + D_{ship} * EF_{Ship} + D_{air} * EF_{Air}$$

EFi = emission factor associated with the transportation of raw material i, in kg of CO2 equivalent per tonne of raw material
D = distance traveled in km by each mean of transportation;
F = emission factor in kilogram of CO_2 equivalent per tonne per kilometer for each mean of transportation

Mean of transportation	Emission factor (kg CO_2e per tonne per km)
HGV	0.234
Rail	0.008
Container ship	0.006
Air	2.090

Green Chem., **2014**, *16*, 1139.

The emission factors used here are set by the official document
Bilan Carbone 5.0 of the French Environment and Energy Management Agency.
It is also possible to refer to GHG Protocol emission factors.

Example from Chimex

Manufacturing footprint:

Raw materials geographical origin (iL)

$$\text{Carbon footprint}_{\text{RMTransportation}} = \frac{\sum_{i=1}^{n} \text{EF}_i \times m_i}{m_\text{p}}$$

EFi = emission factor of raw material i, in kg CO_2e per tonne
n = number of raw material in the process
mi = mass of raw material i used in the process, in tonnes
mp = mass of product, in tonnes

Green Chem., **2014**, *16*, 1139.

Example from Chimex

Manufacturing footprint:

Process carbon footprint (eC).

Electricity, steam, fuel, cooling liquids, etc. converted into CO_2 equivalents

$$\text{Global operating time} = \sum_{i=1}^{m} N_i \times d_i$$

m = number of different products on one production plant
N_i = number of batches of product i realized in one year
d_i = global production duration for product i, in hours

The carbon footprint of an operating hour is calculated by dividing energy consumption (in kg CO_2e) by operating time.
The size and duration of a particular product batch give access to the climate change generated by the production of 1 kg of product

$$\mathrm{eC}(x) = 4 - \frac{4}{1 + \frac{x^2}{10}}$$

expressed in kg CO_2e per kg product

Example: 4 kg CO_2e/kg of product: $\mathrm{Ec}(4) = 4 - \frac{4}{1+\frac{4^2}{10}}$ = 2.5

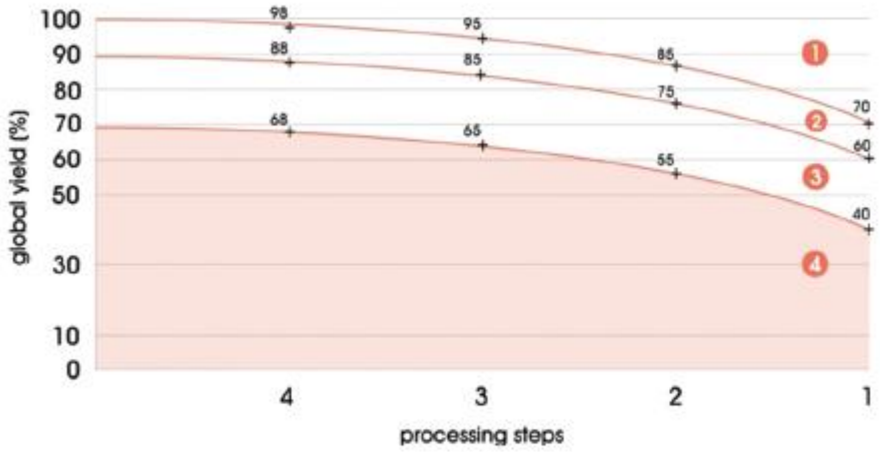
Green Chem., **2014**, *16*, 1139.

Example from Chimex

Eco-design footprint:

Synthetic pathway efficiency (eVS)

More processing steps (with isolation of chemical species): the more consuming for reagents, solvents, time or energy the process is.
Combining both yield and number of steps, is a very visual and simple performance metric.



Green Chem., **2014**, *16*, 1139.

Example from Chimex

Eco-design footprint:

Raw material of renewable origin (rMP)

SOLVENTS \ REAGENTS	<25%	<50%	>50%	>75%
>75%	2	2	1	1
>50%	3	3	2	1
<50%	4	3	3	2
<25%	4	4	3	2

Green Chem., **2014**, *16*, 1139.

Example from Chimex

Eco-design footprint:

Potential environmental impact of raw materials (ieMP)

Potential environmental impact of waste (ieD)

$$\text{ieMP or ieD} = \frac{\sum_{i=1}^{n} \text{Qd}_i \times m_i}{m_\text{P}}$$

Qd_i = hazard quotient for the chemical compound i, which can be a raw material (ieMP) or a waste (ieD)
n = number of raw materials or wastes
m_i = mass of compound i involved in the process
m_P = mass of product formed in the considered synthesis pathway.

Green Chem., **2014**, *16*, 1139.

Example from Chimex

Eco-design footprint:

Potential environmental impact of raw materials (ieMP)

Potential environmental impact of waste (ieD)

$$\text{ieMP or ieD} = \frac{\sum_{i=1}^{n} \text{Qd}_i \times m_i}{m_\text{P}}$$

Qd_i has a value of 1 when a compound has no environmental impact and a maximum at 10

EATOS tool was used to assess the impact: Acute human toxicity, chronic human toxicity, ecotoxicology, ozone creation, air pollution, accumulation, degradability, greenhouse effect, ozone depletion, nitrification and acidification.
Based also on a modified E-Factor called EQ where Q is a factor going from 1 (low impact) to 100 or even 1000 from nasty compounds like Cr, ease of recycling, etc.

Sheldon, R. A. *CHEMTECH*, **1994**, 38.

Eissen, M. Metzger, J. O. *Chem. Eur. J.*, **2002**, *8*, 3580**.**
[http://www.metzger.chemie.uni-oldenburg.de/eatos/eatosmanual.pdf; access 12.10.2023]
ECO Scale: *Beilstein J. Org. Chem.*, **2006**, *2(3)*, 1.

Example from Chimex

Eco-design footprint:

Potential environmental impact of raw materials (ieMP)

Potential environmental impact of waste (ieD)

$$\text{ieMP or ieD} = \frac{\sum_{i=1}^{n} \text{Qd}_i \times m_i}{m_\text{P}}$$

$$\text{Qd}_i = \sum_{j=1}^{p} k_j \times \text{Qcat}_{i,j} \text{ with } \sum_{j=1}^{p} k_j = 1$$

p = number of parameters considered
Qcati, j = regarding the substance i, value of the quotient related to parameter j;
kj = weighting coefficient for parameter j.

Weight the parameters and the same coefficient was applied: kj = 1/5

5 parameters:
Chronic human toxicity: CMR category if existing,
Acute human toxicity: hazard labels, oral LD50 (rat), dermal LD50 (rabbit), inhalation LC50 (rat),
Acute ecotoxicology: LC50 (fish, 96 h), EC50 (daphnia, 48 h), IC50 (algae, 72 h),
Bioaccumulation (log P or log Kow),
Biodegradability (degradation after 28 days).

Sheldon, R. A. *CHEMTECH*, **1994**, 38.

Eissen, M. Metzger, J. O. *Chem. Eur. J.*, **2002**, *8*, 3580.
ECO Scale: *Beilstein J. Org. Chem.*, **2006**, *2(3)*, 1.

Example from Chimex

Eco-design footprint:

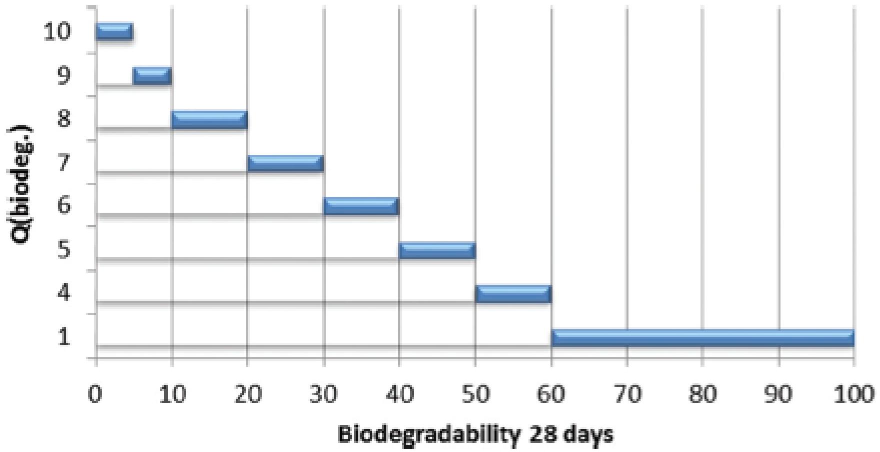
Potential environmental impact of raw materials (ieMP)

Potential environmental impact of waste (ieD)

$$\text{ieMP or ieD} = \frac{\sum_{i=1}^{n} \text{Qd}_i \times m_i}{m_\text{P}}$$

$$\text{Qd}_i = \sum_{j=1}^{p} k_j \times \text{Qcat}_{i,j} \text{ with } \sum_{j=1}^{p} k_j = 1$$

Example for Biodegradation:

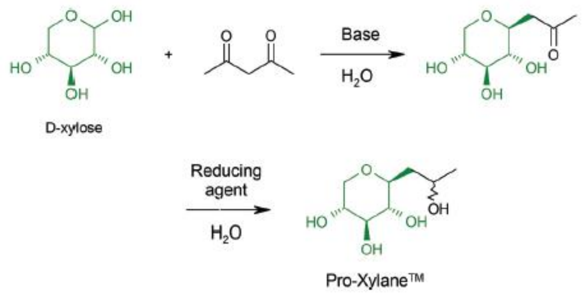


Sheldon, R. A. *CHEMTECH*, **1994**, 38.

Eissen, M. Metzger, J. O. *Chem. Eur. J.*, **2002**, *8*, 3580.
ECO Scale: *Beilstein J. Org. Chem.*, **2006**, *2(3)*, 1.

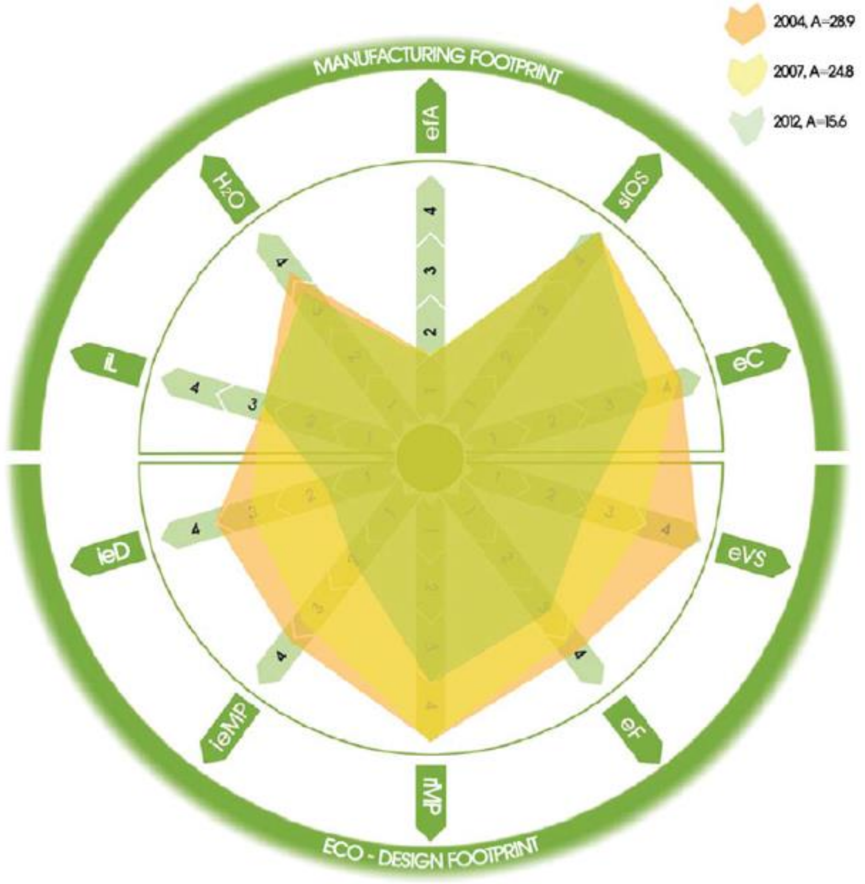
Example from Chimex

Example: Pro-Xylane™



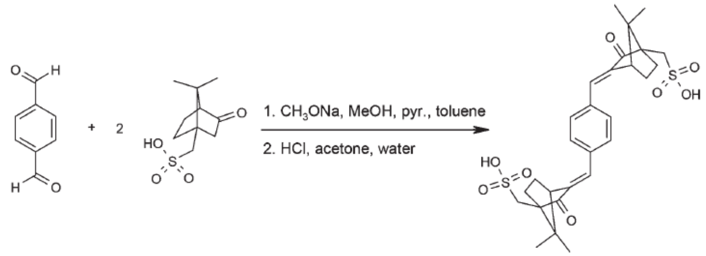
Process	Base	Reducing agent	Global yield	E-factor
2004 (1st pilot scale process)	$NaHCO_3$	$NaBH_4$	43%	14.9
2007 (1st industrial process)	$NaHCO_3$	Metal catalyst	70%	10.4
2012 (Current industrial process)	NaOH	Metal catalyst	85%	5.3

Process	ieMP	ieMP value	ieD	ieD value
2004 (1st pilot scale process)	18.6	3.1	16.9	3.0
2007 (1st industrial process)	15.2	2.8	13.5	2.6
2012 (Current industrial process)	7.9	1.5	6.0	1.1



Example from Chimex

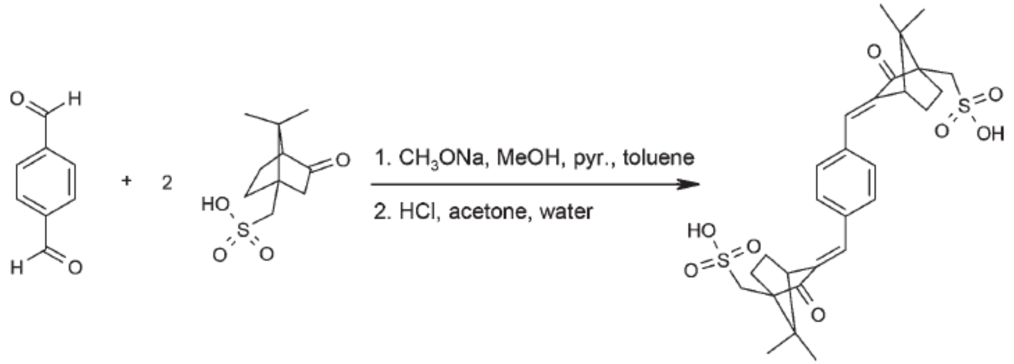
Example: Mexoryl® SX

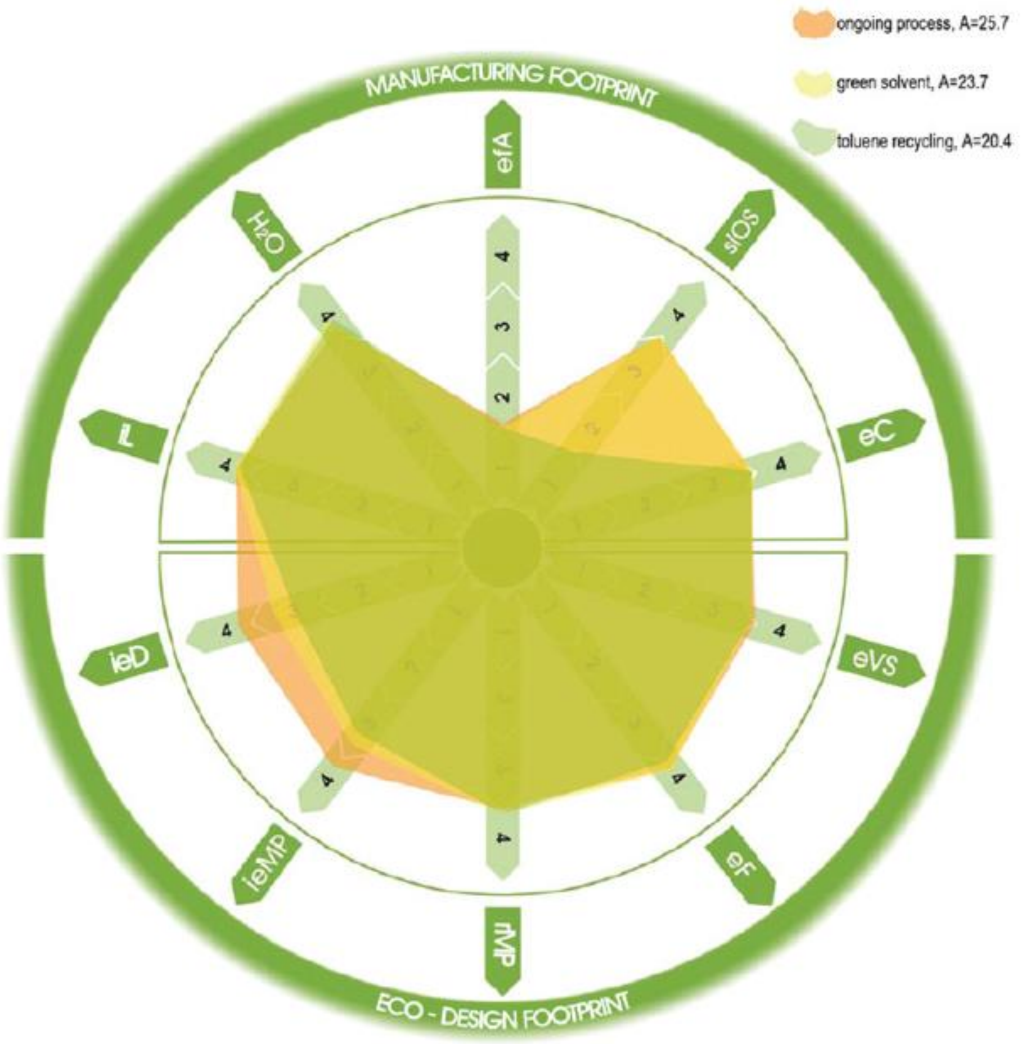


Indicator	Ongoing process		Toluene recycling		Non-toxic solvent of renewable origin	
	Data	Value	Data	Value	Data	Value
iL: raw materials transportation	1.6 kg CO_2e per kg	**3.3**	1.4 kg CO_2e per kg	**3.2**	1.6 kg CO_2e per kg	**3.3**
H_2O: water consumption	17.8 L kg^{-1}	**3.4**	17.8 L kg^{-1}	**3.4**	17.8 L kg^{-1}	**3.4**
eFA: aqueous waste valorization	Water treatment plant	**1**	Water treatment plant	**1**	Water treatment plant	**1**
slOS: organic solvents valorization	Toluene: incineration Pyridine: incineration MeOH: incineration Acetone: recycling	**3**	Toluene: recycling Pyridine: incineration MeOH: incineration Acetone: recycling	**1**	Toluene: incineration Pyridine: incineration MeOH: incineration Acetone: recycling	**3**
eC: energetic carbon footprint	5.4 kg CO_2e per kg	**3**	5.4 kg CO_2e per kg	**3**	5.4 kg CO_2e per kg	**3**
eVS: synthetic pathway efficiency	2 steps, 72%	**3**	2 steps, 72%	**3**	2 steps, 72%	**3**
eF: E-factor	13.7	**3.3**	11.8	**3.2**	13.7	**3.3**
rMP: raw materials of renewable origin	Reagents: 13% Solvents: 59%	**3**	Reagents: 13% Solvents: 68%	**3**	Reagents: 13% Solvents: 73%	**3**
ieMP: environmental impact of raw materials	22.9	**3.4**	14.6	**2.7**	15.9	**2.9**
ieD: environmental impact of waste	21.4	**3.3**	13.1	**2.5**	14.4	**2.7**

Example from Chimex

Example: Mexoryl® SX





Example from Estée Lauder

New «Green Score» Tool for: pharmaceutical and personal care products (PPCPs)

The tool includes several important features:
(1) A balance between assessing inherent chemical and supply chain hazards
(2) a disincentive to use raw materials with low scores or lack of data by weighting their impact to reduce the score further
(3) a certainty score to provide insight on the level of confidence in the Green Score for a given ingredient or chemical component.

3 distinct categories: human health (HH), ecosystem health (ECO), and environmental impact (ENV).

Green Chem., **2022**, *24*, 2397-2408.

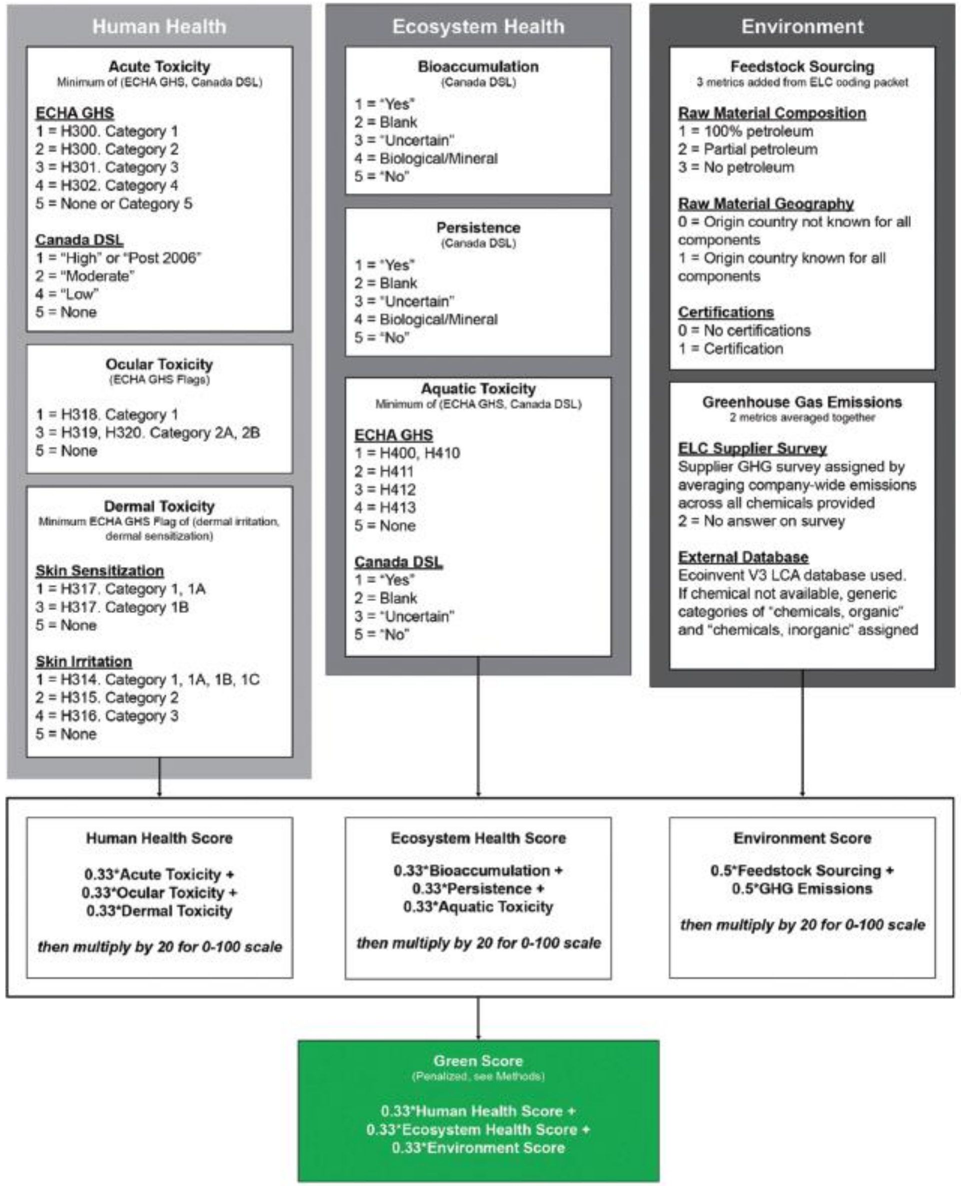
Example from Estée Lauder

New «Green Score» Tool for: pharmaceutical and personal care products (PPCPs)

Key Point: individual chemicals are combined to make ingredients, and ingredients are combined to make formulas.

Step 1:
The chemical composition of each ingredient is established from internal registration records, each of the 2300 + unique components is linked to internal and external chemical data sets, and water components are removed from the scoring.
Step 2:
Each ingredient is scored on metrics covering HH, ECO, and ENV categories. HH and ECO metrics are based on inherent chemical properties and carried out at the component level, while ENV metrics are largely applied at the ingredient level. Each of these metric scores has an associated data quality rating based on a tiered system of data source preferences.
Step 3:
Numeric penalties (i.e., disincentives) are applied to any component or ingredient that receives the lowest score (1) for any metric.
Step 4:
All metric and category scoring is mass averaged up to the ingredient level and a final Green Score is calculated.
Step 5:
Ingredient scores are mass averaged up to the formula level and evaluated against benchmarks.

Example from Estée Lauder



For the classification
GHS and Canadian DSL was used

Example from Estée Lauder

Endpoint description/Source	Score	Score assignment rubric
Acute toxicity: Assesses the inherent lethality hazard via ingestion, inhalation, and dermal absorption exposure routes. The primary data sources are the GHS classification for acute toxicity and the Canada DSL HH priorities classification. If data are present in both the GHS and DSL, the lower (more conservative) score is taken	1	Acute toxicity 1 GHS classification OR DSL HH priorities label is "high" or "post 2006"
	2	Acute toxicity 2 GHS classification OR DSL HH priorities label is "moderate"
	3	Acute toxicity 3 GHS classification
	4	Acute toxicity 4 GHS classification OR DSL HH priorities label is "low"
	5	No acute toxicity GHS classifications AND no DSL HH priorities label is present
Ocular toxicity: Assesses the inherent hazard to cause eye damage and/or irritation. The primary data sources are the GHS classifications for eye irritation and eye damage	1	Eye damage GHS classification
	3	Eye irritation GHS classification
	5	No eye damage or eye irritation GHS classifications present
Dermal toxicity: Assesses the inherent hazard to cause dermal corrosion, irritation, and/or sensitization. The primary data sources are the GHS classifications for skin corrosion, skin irritation, skin mild irritation, and skin sensitization	1	Skin sensitization 1A OR any skin corrosion GHS classification
	2	Any skin irritation GHS classification
	3	Skin sensitization 1B or skin sensitization 1 GHS classification
	4	Skin mild irritation GHS classification
	5	No skin corrosion, skin irritation, skin mild irritation, or skin sensitization GHS classifications present

DSL, Domestic Substance List; GHS, Globally Harmonized System of Classification and Labelling of Chemicals; HH, human health.

HH Scoring

Env. Scoring

Endpoint description/Source	Score	Score assignment rubric
Feedstock sourcing: Assesses for ingredient's environmental impact of sourcing, degree of supply chain transparency, and whether it has a third-party sustainability certification. All data are obtained from ELC suppliers. Three independent submetrics are added to score this metric: - Ingredient composition: Assesses for % of petroleum-derived content - Ingredient geography: Assesses for sourcing transparency - Certifications: Assesses for any RSPO or organic certifications	1	Ingredient source is wholly of petroleum origin
	2	Ingredient source is partially of petroleum origin and partially of biological or mineral origin
	3	Ingredient source is wholly of biological or mineral origin
	+1 Point	All ingredient components have an associated country of origin
	+1 Point	Ingredient is RSPO certified (e.g., mass balance) or certified organic (USDA or COSMOS)
GHG emissions: Assesses ingredient's GHG impact. Calculated by averaging 2 independent submetrics: - GHG supplier emissions: Scopes 1 & 2 emissions effect per kilogram of product, as provided by ELC suppliers - GHG modelled emissions: Scopes 1, 2 & 3 emissions effect of each ingredient component, as obtained from the ecoinvent 3 database, per the component chemical classification. The ingredient GHG modelled emissions score is calculated via the mass-weighted average of its components' scores	1	GHG supplier value/modelled emissions factor is >1000
	2	GHG supplier emissions: No GHG emissions information is provided by the supplier
	$5 - [\log_{10}(x) + 1]$	GHG supplier value/modelled emissions factor (x) is >0.1 but <1000
	5	GHG supplier value/modelled emissions factor is <0.1

COSMOS, COSMetic Organic and Natural Standard; ELC, Estée Lauder Companies; GHG, greenhouse gas; RSPO, Roundtable on Sustainable Palm Oil; USDA, US Department of Agriculture.

Endpoint description/Source	Score	Score assignment rubric
Bioaccumulation: Assesses the propensity to bioaccumulate up the food chain when free in the environment. The primary data source is the Canada DSL bioaccumulation classification. The secondary data source is the component's feedstock sourcing data, as provided by the raw material supplier to ELC	1	DSL bioaccumulation label is "yes"
	2	DSL bioaccumulation label is blank
	3	DSL bioaccumulation label is "uncertain"
	4	Component is not listed in the DSL, and feedstock source is wholly biological or mineral
	5	DSL bioaccumulation label is "no"
Persistence: Assesses the propensity to persist (i.e., not break down or biodegrade) when free in the environment. The primary data source is the Canada DSL persistence classification. The secondary data source is the component's feedstock sourcing data, as provided by the raw material supplier to ELC	1	DSL persistence label is "yes"
	2	DSL persistence label is blank
	3	DSL persistence label is "uncertain"
	4	Component is not listed in the DSL, and feedstock source is wholly biological or mineral
	5	DSL persistence label is "no"
Aquatic toxicity: Assesses the inherent hazard in the aquatic environment, both acutely and chronically. The primary data sources are the GHS classifications for aquatic acute toxicity and aquatic chronic toxicity, along with the DSL inherently toxic to aquatic organisms classification. The more conservative score is taken. If no information is present in the DSL database, it is scored according to the GHS	1	Aquatic acute 1 or aquatic chronic 1 GHS classification OR DSL inherently toxic to aquatic organisms label is "yes"
	2	Aquatic chronic 2 GHS classification OR DSL inherently toxic to aquatic organisms label is blank
	3	Aquatic chronic 3 GHS classification OR DSL inherently toxic to aquatic organisms label is "uncertain"
	4	Aquatic chronic 4 GHS classification
	5	No aquatic acute or aquatic chronic GHS classifications AND DSL inherently toxic to aquatic organisms label is "no"

DSL, Domestic Substance List; ELC, Estée Lauder Companies; GHS, Globally Harmonized System of Classification and Labelling of Chemicals.

Ecosystem Health Scoring

https://www.cosmos-standard.org/en/

Example from Estée Lauder

For HH & ECO: endpoint metrics incomplete or not available

Default type	Acute toxicity	Ocular toxicity	Dermal toxicity	Bioaccumulation	Persistence	Aquatic toxicity
Biological	5	3	3	4	4	5
Mineral	3	3	3	4	4	3
Fluoro compound	2	2	2	3	1	2
Colorant	5	3	3	3	2	2
Polymer	4	3	3	5	1	4
Siloxane/Silicone	4	2	2	5	1	4
Natural metabolite	4	4	4	5	5	4
Petroleum	2	2	2	3	3	2
Unknown	3	3	3	3	3	3

Certainty Score Assignment

Endpoint	Score	Score assignment
All HH and ECO endpoints	2	From default data value
	3	From proxy data value
	5	From GHS or DSL data
ENV feedstock sourcing	3	All raw materials
ENV greenhouse gas emissions	2	From default data value
	4	From individual chemical

DSL, Domestic Substance List; ECO, ecosystem health; ENV, environment; GHS, Globally Harmonized System of Classification and Labelling of Chemicals; HH, human health.

Example from Estée Lauder

Step 1: The chemical composition of each ingredient is established from internal registration records, each of the 2300 + unique components is linked to internal and external chemical data sets, and water components are removed from the scoring

$$P'_{ij} = \frac{P_{ij}}{1 - w_j}$$

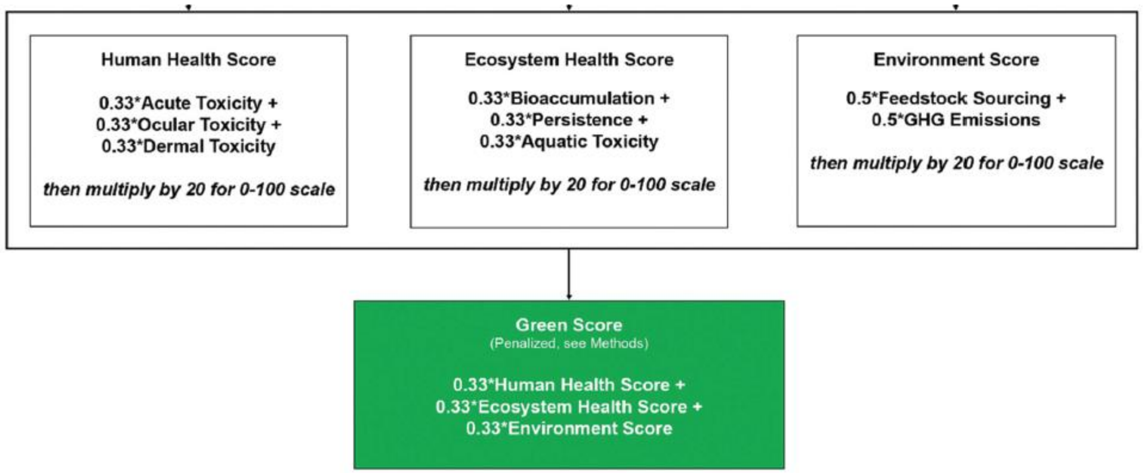
P’ij = adjusted proportion of component i in ingredient j.
Pij = original proportion of component i in ingredient j.
wj = proportion of water in ingredient j.

From suppliers: Scopes 1 and 2 emissions (according to the GHG protocol) per kilogram of manufactured ingredient

Step 4: All metric and category scoring is mass averaged up to the ingredient level and a final Green Score is calculated.

$$I_{jk} = \sum_{i=1}^{n} C_{ijk} \cdot P'_{ij}$$

Ijk = ingredient-level score for ingredient j on metric k.
Cijk = component-level score for component i in ingredient j on metric k.
P’ij = adjusted proportion of component i in ingredient j.
n = number of components in ingredient j.



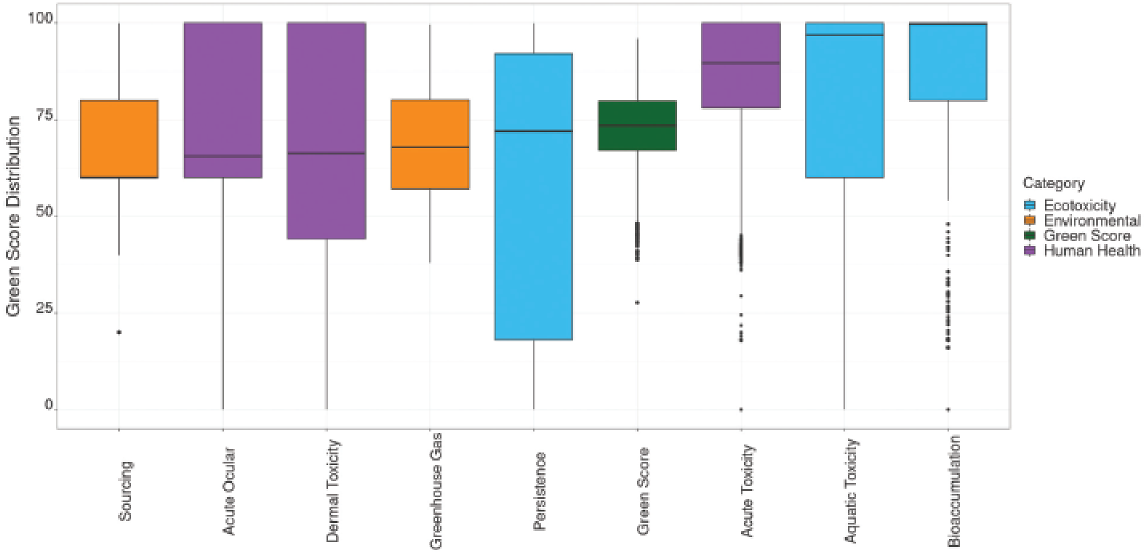
Example from Estée Lauder

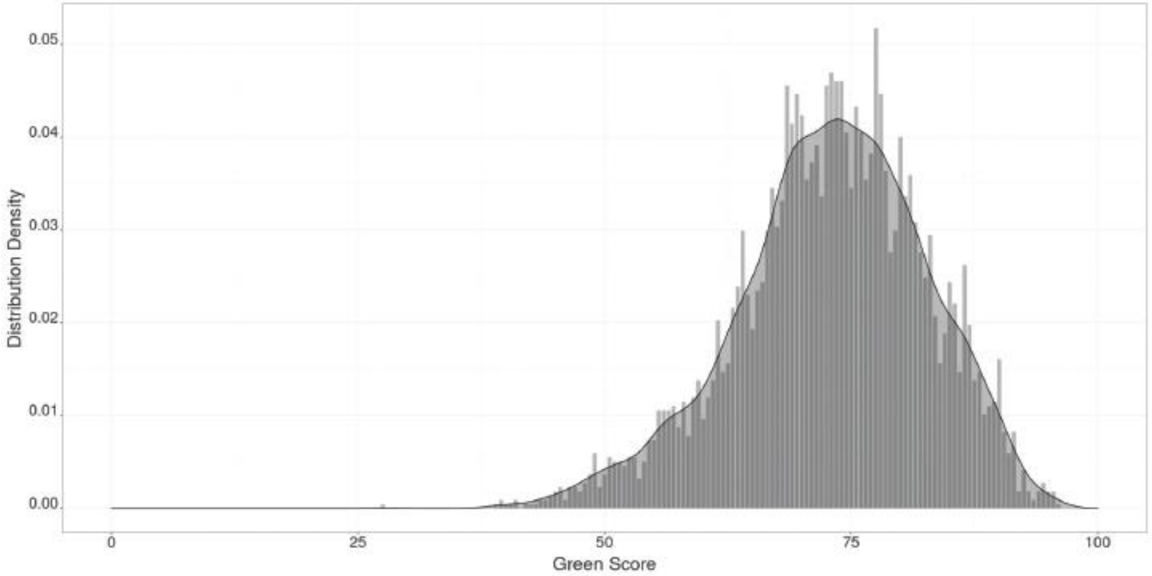
Step 5: Ingredient scores are mass averaged up to the formula level and evaluated against benchmarks

$$F_I = \sum_{j=1}^{r} \frac{I_{jI} \cdot P_{jI}}{100 \cdot \left(1 - \left(\frac{w_I}{100}\right)\right)}$$

FI = formula Green Score for formula I.
IjI = ingredient Green Score for ingredient j in formula I.
PjI = percentage of ingredient j in formula I.
wI = percentage of water in formula I.
r = number of ingredients in formula I.

Example from Estée Lauder





Example from Estée Lauder

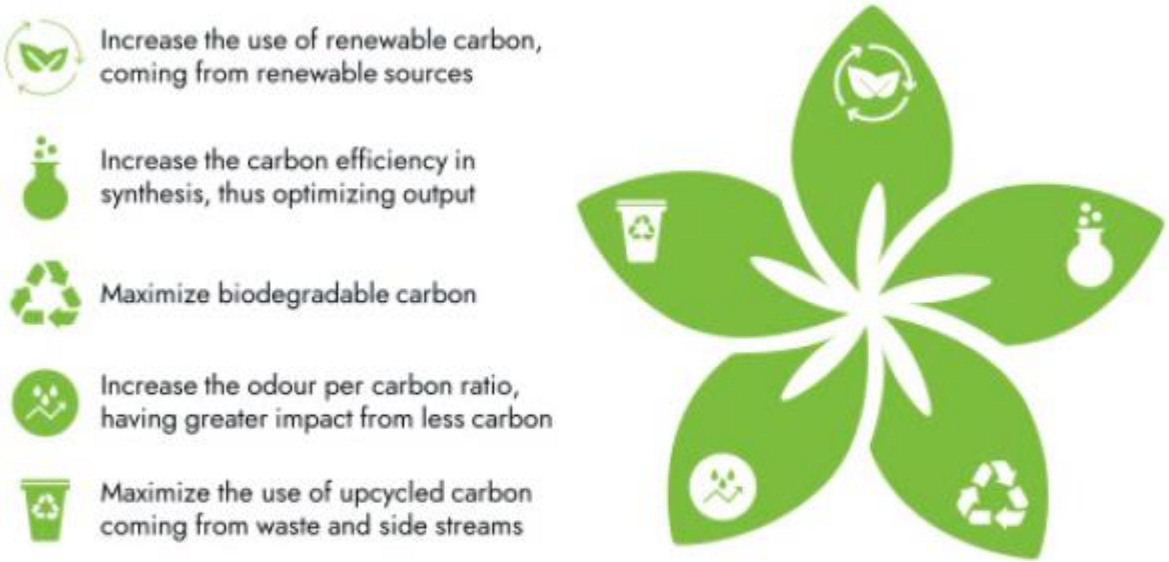
INCI NAME	INGREDIENT FORM	SOURCE	HUMAN HEALTH HAZARDS: HH ACUTE	HH OCULAR	HH DERMAL	ECOSYSTEM HEALTH HAZARDS: ECO BIOACC	ECO PERS	ECO AQTOX	ENVIRONMENTAL HAZARDS: ENV SOURCE	ENV GHG	GREEN SCORE
1. BEESWAX	Solid	Animal related	100	100	100	80	80	100	100	82	93
2. CITRUS AURANTIUM DULCIS (ORANGE) PEEL WAX	Wax	Plant	100	100	100	80	80	100	80	74	88
3. POLYGLYCERYL-3 BEESWAX	Granular	Animal related	100	100	100	80	80	100	80	72	88
4. BEESWAX	Wax	Animal related	100	100	100	80	80	100	80	69	87
5. JOJOBA ESTERS	Powder	Plant	100	100	100	60	60	100	80	83	85
6. SYNTHETIC BEESWAX	Solid	Plant	100	100	100	100	100	18	80	79	84
7. SYNTHETIC WAX	Liquid	Petroleum	80	100	100	100	100	100	40	78	83
8. PARAFFIN	Solid	Petroleum	80	100	100	100	98	100	40	74	83
9. SYNTHETIC BEESWAX	Solid	Plant-Petroleum	100	100	100	100	100	18	80	57	80
10. PARAFFIN	Wax	Petroleum	80	100	100	100	100	98	40	57	80
11. LAVANDULA ANGUSTIFOLIA (LAVENDER) FLOWER WAX	Wax	Plant	100	60	60	80	80	100	60	88	78
12. CARNAUBA	Flakes	Plant	100	60	100	60	60	100	80	65	78
13. ORYZA SATIVA (RICE) BRAN WAX	Solid	Plant	100	60	60	60	60	100	80	88	77
14. OZOKERITE	Solid	Petroleum	100	100	100	60	60	100	40	62	74
15. EUPHORBIA CERIFERA (CANDELILLA) WAX	Granular	Plant	80	60	60	60	60	100	80	65	71
16. POLYETHYLENE/MICROCRYSTALLINE WAX	Solid	Petroleum	70	90	100	100	16	100	40	57	68
17. MICROCRYSTALLINE WAX	Wax	Petroleum	40	60	100	100	18	98	60	68	67
18. MICROCRYSTALLINE WAX	Pellets	Petroleum	40	60	100	100	18	98	40	73	64
19. ROSA CENTIFOLIA/DAMASCENA FLOWER WAX	Wax	Plant	90	16	40	70	70	28	80	65	59
20. CERESIN	Wax	Petroleum	40	40	40	60	60	60	40	55	49

INCI NAME	INGREDIENT FORM	SOURCE	HUMAN HEALTH HAZARDS: DATA CERTAINTY: HH ACUTE	HH OCULAR	HH DERMAL	ECOSYSTEM HEALTH HAZARDS: DATA CERTAINTY: ECO BIOACC	ECO PERS	ECO AQTOX	ENVIRONMENTAL HAZARDS: DATA CERTAINTY: ENV SOURCE	ENV GHG
1. BEESWAX	Solid	Animal related	5	5	5	2	2	5	3	4
2. CITRUS AURANTIUM DULCIS (ORANGE) PEEL WAX	Wax	Plant	5	5	5	2	2	5	3	4
3. POLYGLYCERYL-3 BEESWAX	Granular	Animal related	5	5	5	2	2	5	3	4
4. BEESWAX	Wax	Animal related	5	5	5	2	2	5	3	4
5. JOJOBA ESTERS	Powder	Plant	5	5	5	5	5	5	3	4
6. SYNTHETIC BEESWAX	Solid	Plant	5	3	3	5	5	5	3	3
7. SYNTHETIC WAX	Liquid	Petroleum	5	5	5	5	5	5	3	3
8. PARAFFIN	Solid	Petroleum	5	5	5	5	5	5	3	3
9. SYNTHETIC BEESWAX	Solid	Plant-Petroleum	5	3	3	5	5	5	3	2
10. PARAFFIN	Wax	Petroleum	5	5	5	5	5	5	3	2
11. LAVANDULA ANGUSTIFOLIA (LAVENDER) FLOWER WAX	Wax	Plant	2	2	2	2	2	2	3	4
12. CARNAUBA	Flakes	Plant	5	5	5	5	5	5	3	3
13. ORYZA SATIVA (RICE) BRAN WAX	Solid	Plant	5	2	2	5	5	5	3	4
14. OZOKERITE	Solid	Petroleum	5	5	5	2	2	5	3	3
15. EUPHORBIA CERIFERA (CANDELILLA) WAX	Granular	Plant	5	2	2	5	5	5	3	3
16. POLYETHYLENE/MICROCRYSTALLINE WAX	Solid	Petroleum	5	5	5	5	5	5	3	3
17. MICROCRYSTALLINE WAX	Wax	Petroleum	5	5	5	5	5	5	3	3
18. MICROCRYSTALLINE WAX	Pellets	Petroleum	5	5	5	5	5	5	3	3
19. ROSA CENTIFOLIA/DAMASCENA FLOWER WAX	Wax	Plant	5	5	5	4	4	5	3	3
20. CERESIN	Wax	Petroleum	5	2	2	5	5	5	3	3

Givaudan: FiveCarbon Path (Jan. 2019)

It focuses on:

• Increasing the use of renewable Carbon
• Increasing Carbon efficiency in synthesis
• Maximising biodegradable Carbon
• Increasing the 'odour per Carbon ratio' with high impact material
• Using upcycled Carbon from side streams

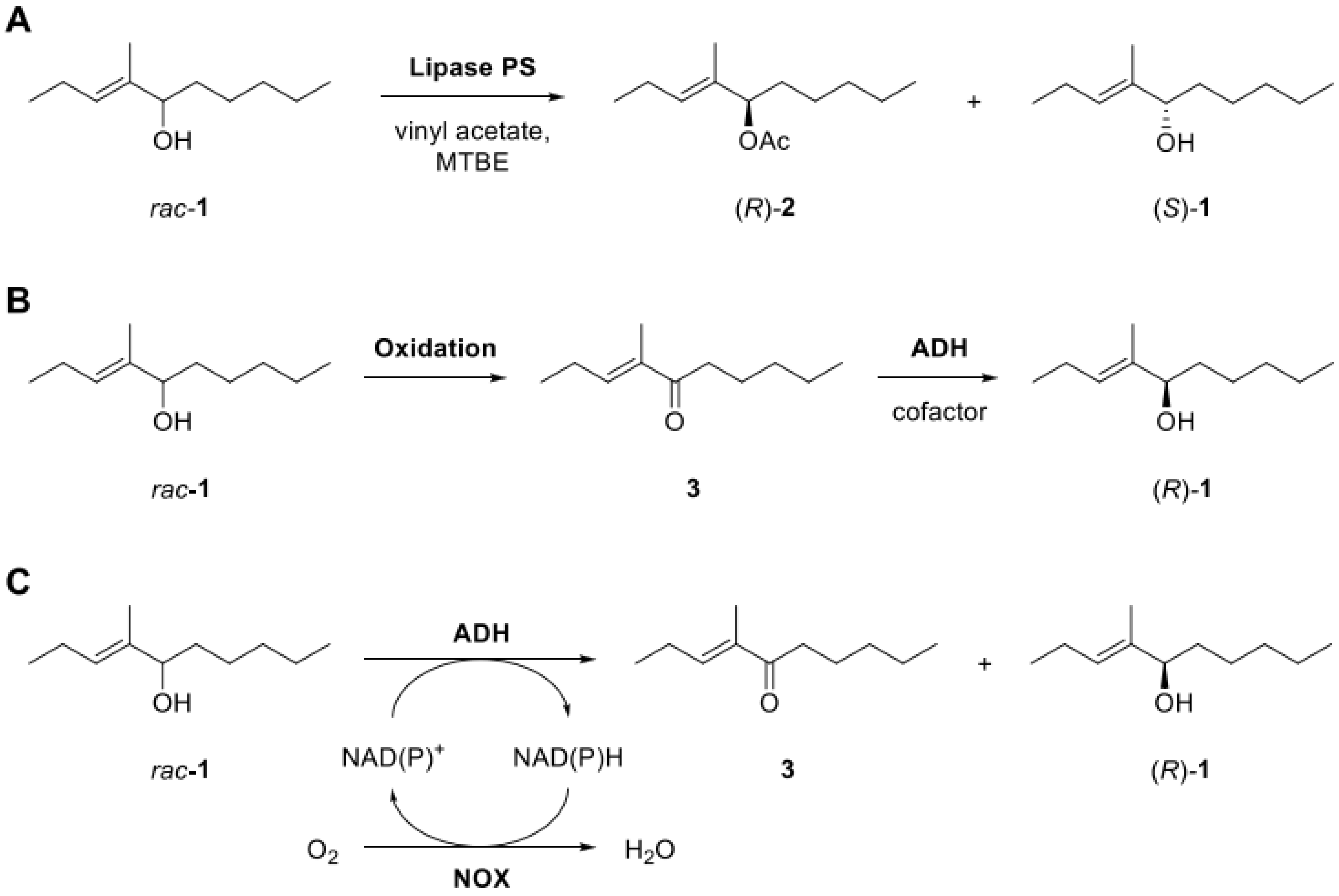


https://www.givaudan.com/media/media-releases/2019/givaudan-fragrances-launches-its-fivecarbon-pathtm
Chimia **2023**, *77*, 384.

Givaudan: FiveCarbon Path (Jan. 2019)

Undecavertol Synthesis

Drawbacks of Route A & B ?
Route C was selected.

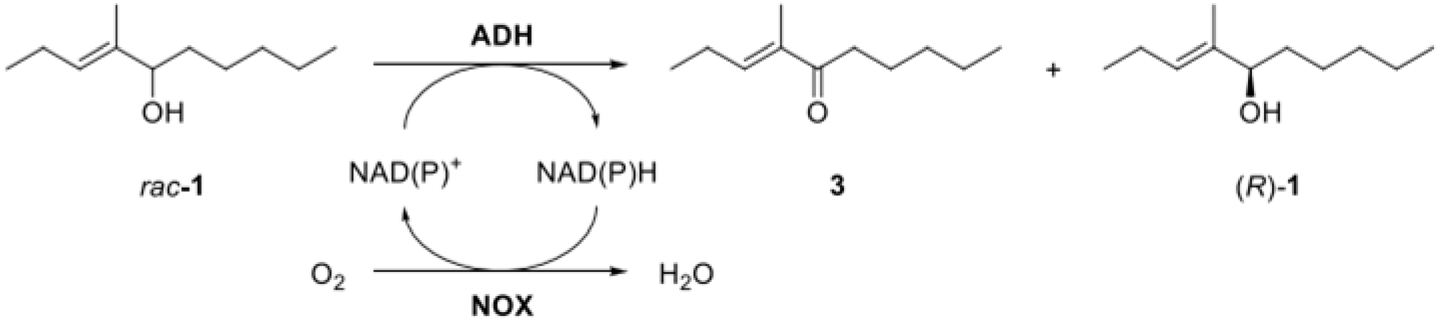


OPRD **2022**, *26*, 2021.
https://doi.org/10.1021/acs.oprd.1c00415?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as

Givaudan: FiveCarbon Path (Jan. 2019)

Undecavertol Synthesis

Optimization of:
- ADH enzyme
- NOX enzyme
- Flow rate of O_2
- Buffer (pH of the mixture)
- Concentration



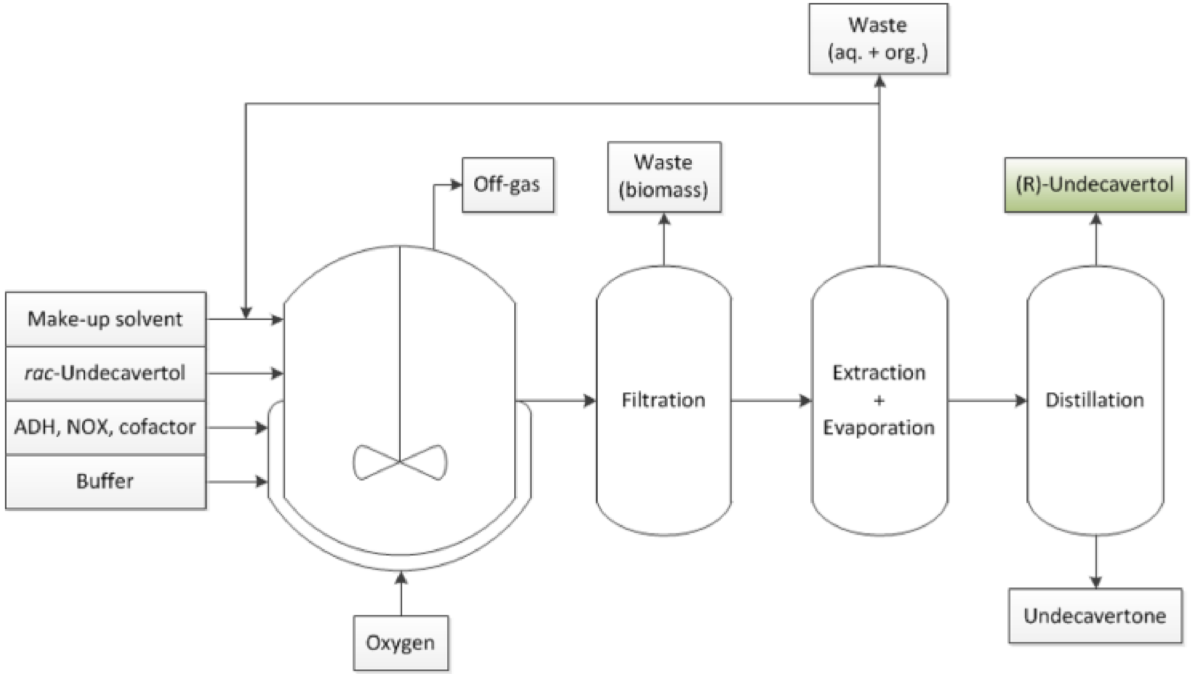
Comparison of the Conditions and Performances of the Three Pilot Runs on the 100 L Scale

batch	substrate mass [kg]	substrate conc. [g L^{-1}]	(*S*)-**1** conv. [%]	ee [%]	ADH conc. [g $kg_{substrate}^{-1}$]	NOX conc. [g $kg_{substrate}^{-1}$]	initial temp. [°C]
1	50	420	99.4 (16 h)	98.8	9.9	2.2	16
2	55	448	99.6 (14 h)	99.1	10.0	2.2	20
3	64	426	99.7 (13 h)	99.5	9.9	2.2	22

OPRD **2022**, *26*, 2021.
https://doi.org/10.1021/acs.oprd.1c00415?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as

Givaudan: FiveCarbon Path (Jan. 2019)

Undecavertol Synthesis

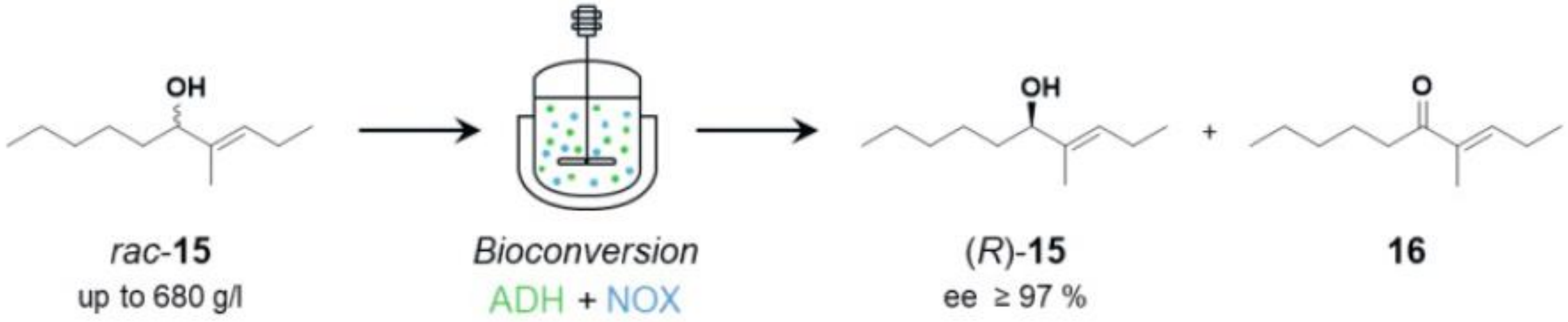


process metric	0.5 L (old enzyme batches)	0.6 L (new enzyme batches)	125 L (second pilot reaction)
conversion [%]	49.9	49.9	49.8
product concentration [$g\ L^{-1}$]	340.6	212.5	224.0
space-time yield [$g\ L^{-1}\ h^{-1}$]	21.3	13.3[a]	14.0

OPRD **2022**, *26*, 2021.
https://doi.org/10.1021/acs.oprd.1c00415?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as

Givaudan: FiveCarbon Path (Jan. 2019)

Undecavertol Synthesis

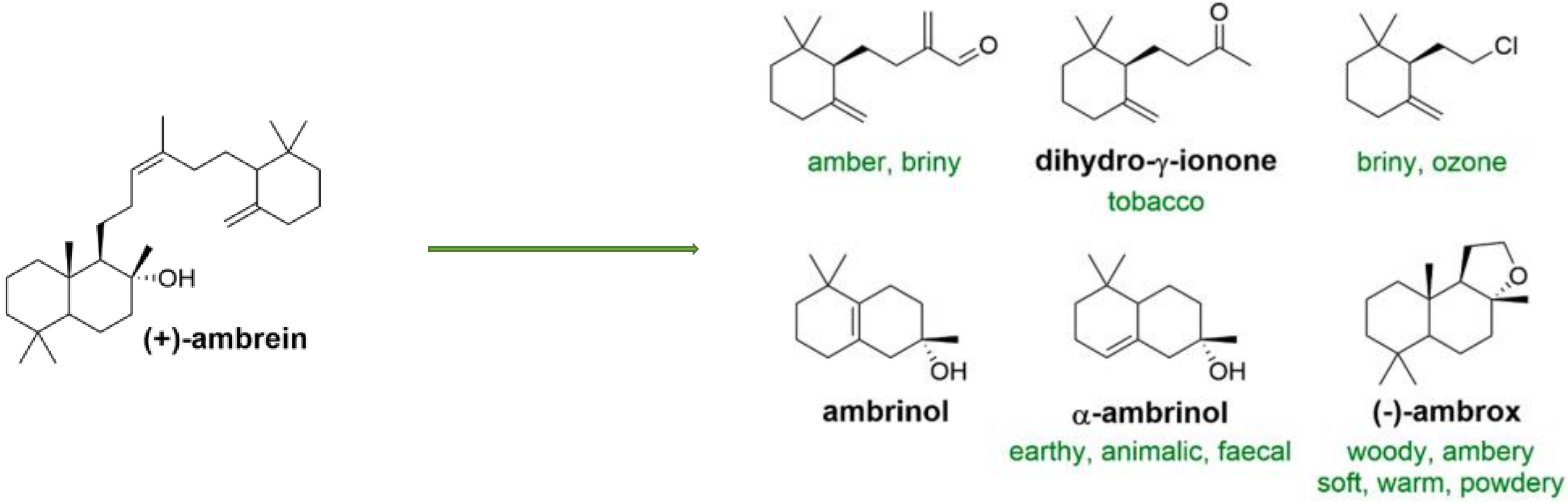


85 kg of (R)-Undecavertol in three batches performed in a 200 L pilot-plant reactor

OPRD **2022**, *26*, 2021.
https://doi.org/10.1021/acs.oprd.1c00415?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as

Givaudan: FiveCarbon Path (Jan. 2019)

(–)-Ambrox©/AmbrofixTM Synthesis

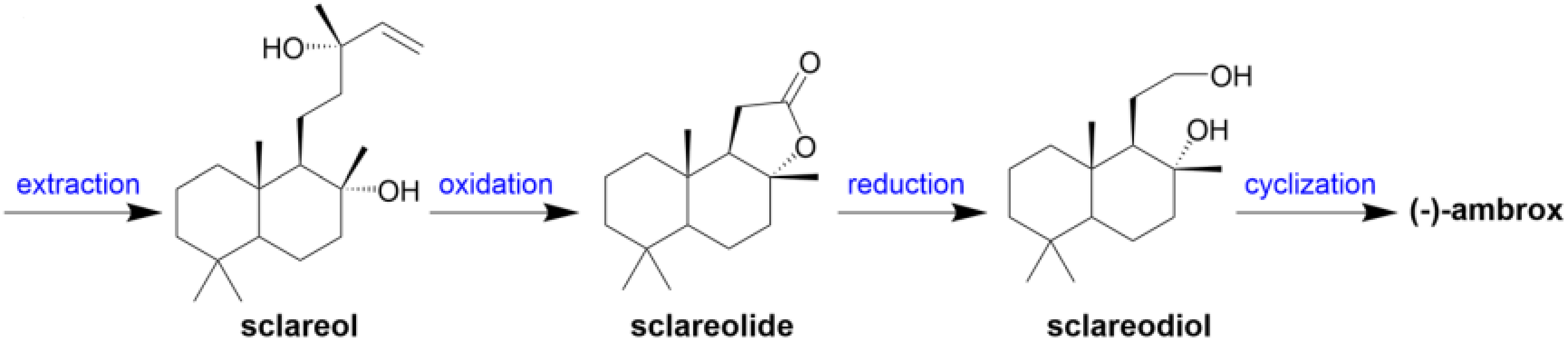


J. Agric. Food Chem. **2023**, *71*, 5042.

Review: https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as

Givaudan: FiveCarbon Path (Jan. 2019)

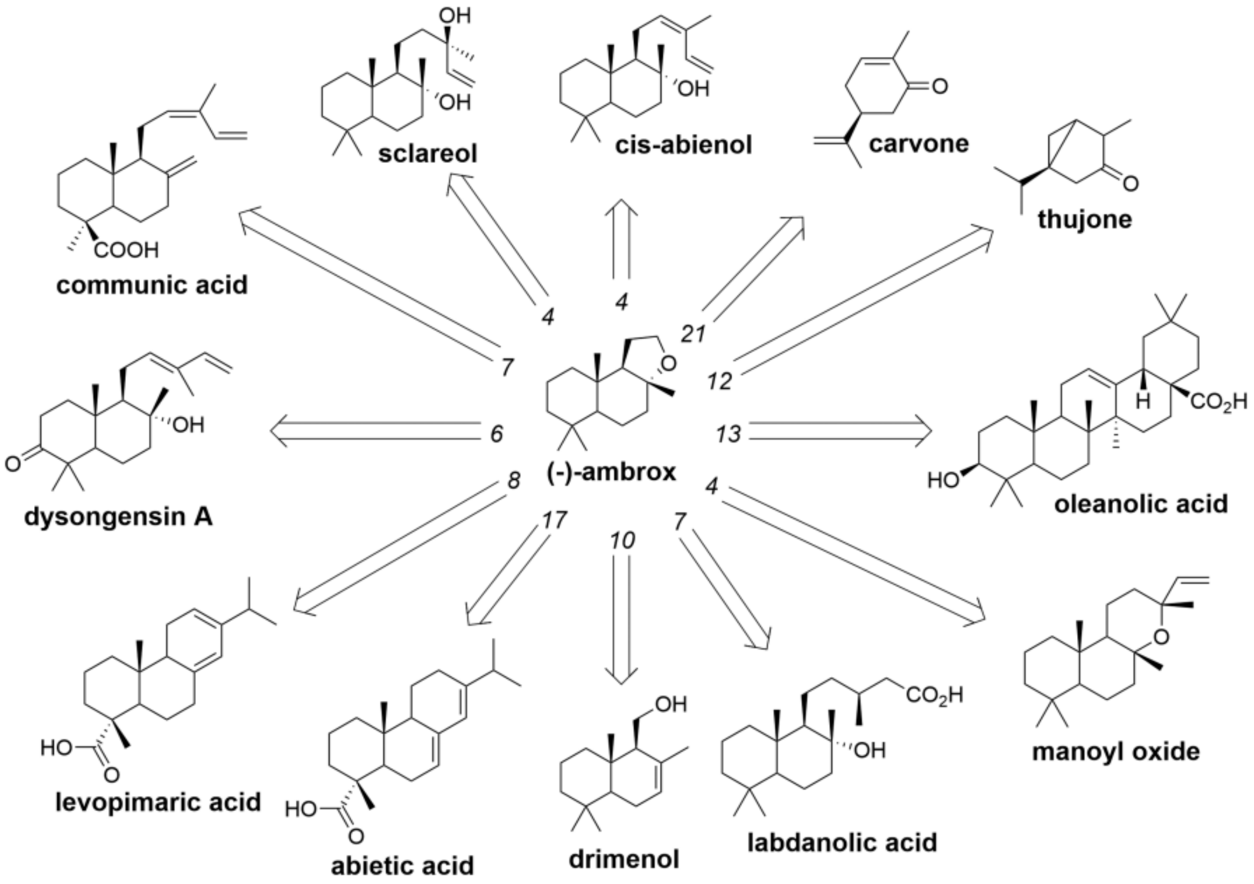
(–)-Ambrox©/Ambrofix™ Current Synthesis

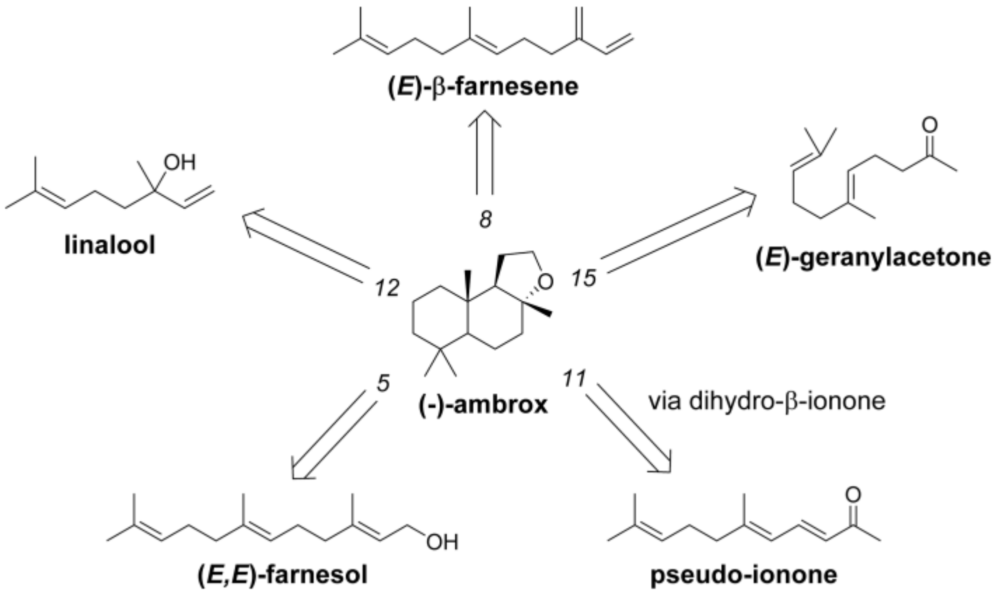


J. Agric. Food Chem. **2023**, *71*, 5042.
Review: https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as
Adv. Synth. Catal. **2018**, *360*, 2339.

Givaudan: FiveCarbon Path (Jan. 2019)

(–)-Ambrox©/AmbrofixTM Known Synthesis





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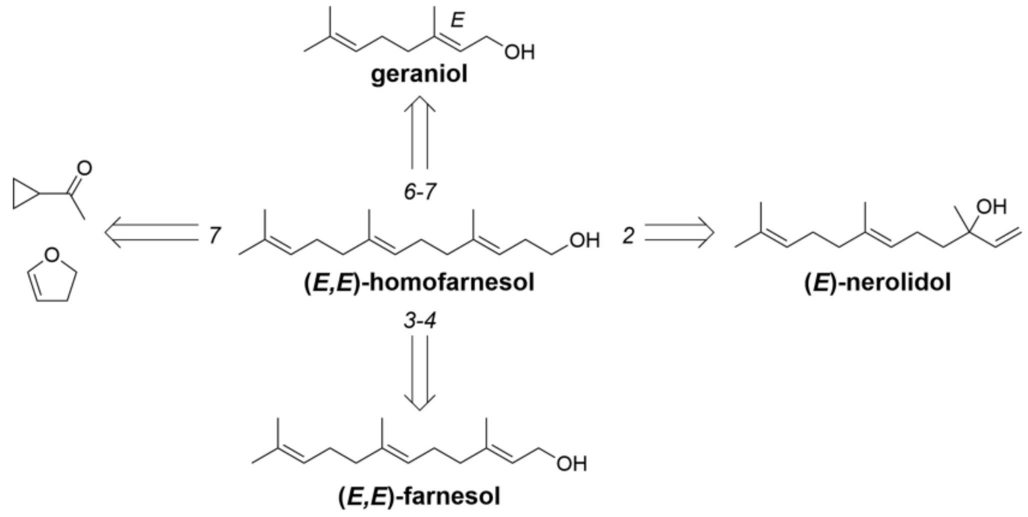
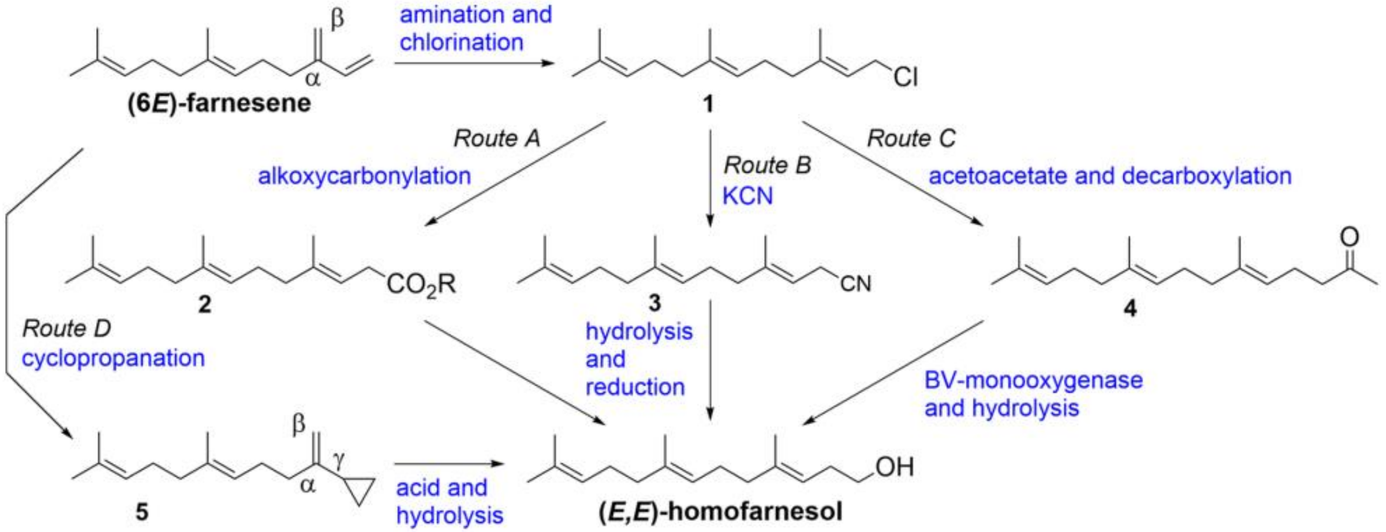
Adv. Synth. Catal. **2018**, *360*, 2339.

Givaudan: FiveCarbon Path (Jan. 2019)

Synthetic and Natural Precursors of (E,E)-Homofarnesol

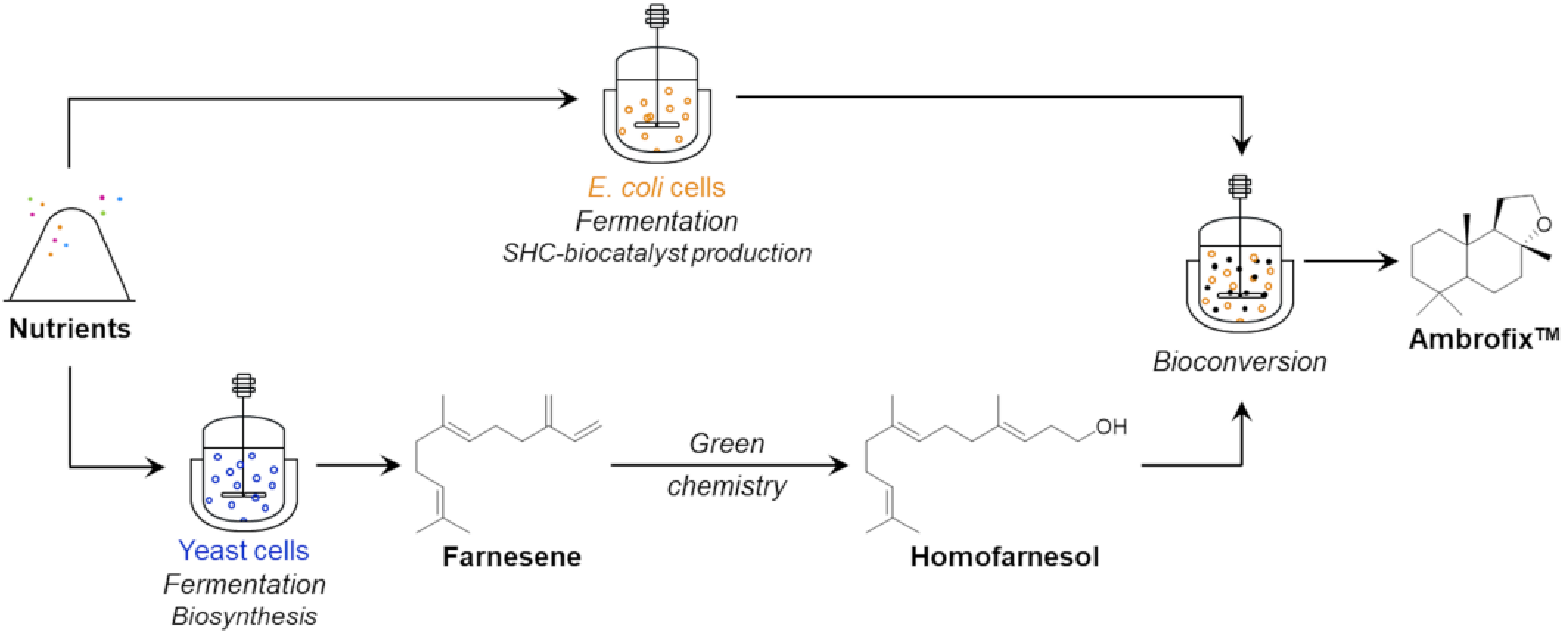




J. Agric. Food Chem. **2023**, *71*, 5042.
[Review: https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as](https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as)
Adv. Synth. Catal. **2018**, *360*, 2339.
See also: *Helv. Chim. Acta* **2014**, *97*, 197.

Givaudan: FiveCarbon Path (Jan. 2019)

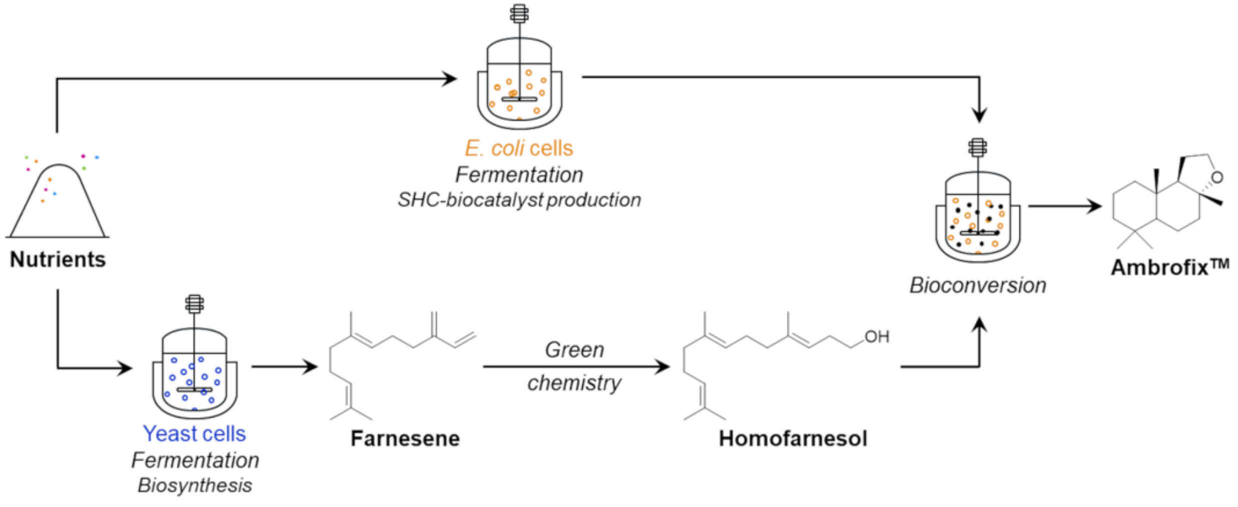
Synthetic and Natural Precursors of (E,E)-Homofarnesol



J. Agric. Food Chem. **2023**, *71*, 5042.
[Review: https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as](https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as)
Adv. Synth. Catal. **2018**, *360*, 2339.

Givaudan: FiveCarbon Path (Jan. 2019)

Synthetic and Natural Precursors of (E,E)-Homofarnesol



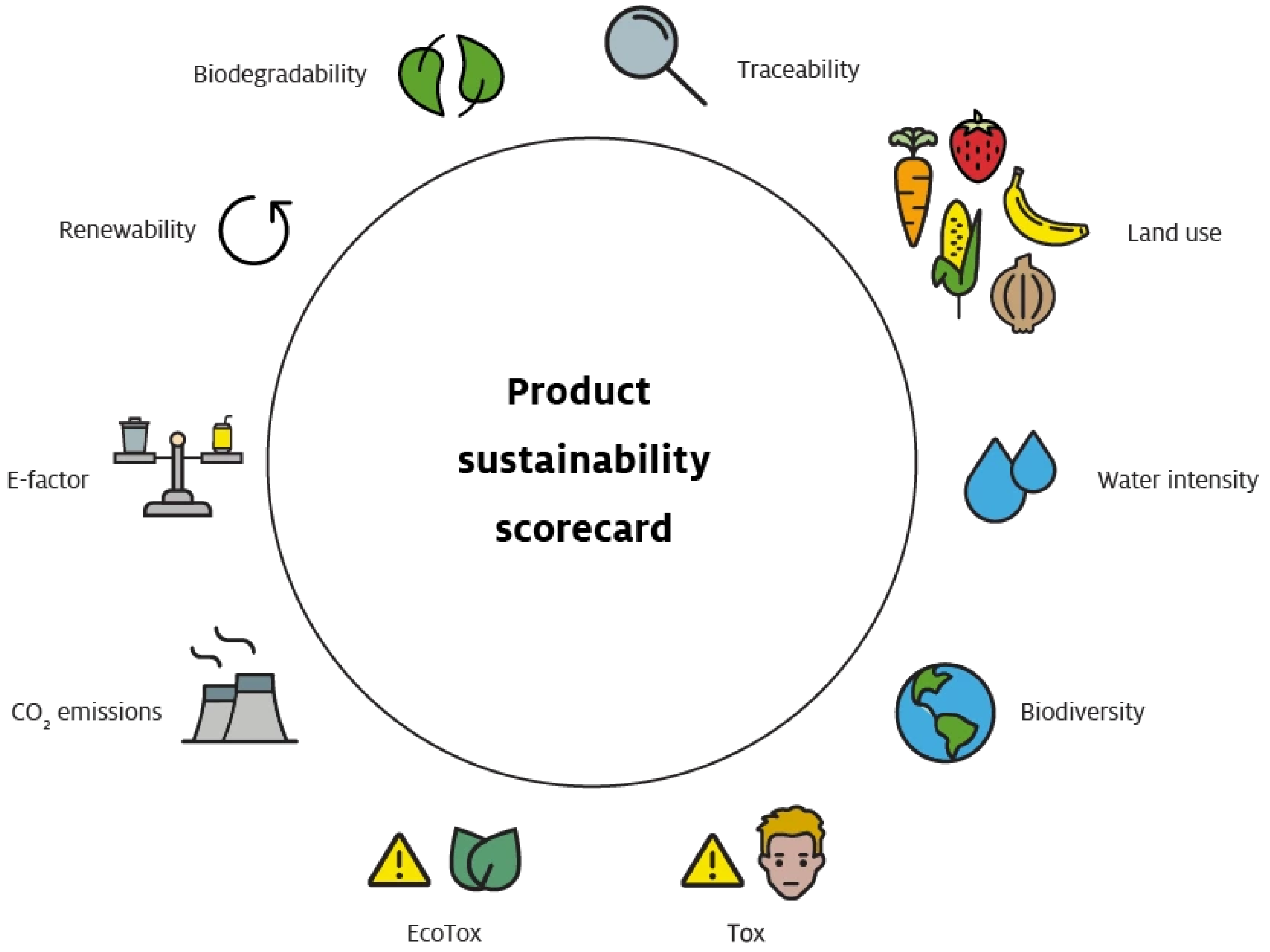
J. Agric. Food Chem. **2023**, *71*, 5042.
Review: https://doi.org/10.1021/acs.jafc.2c09010?urlappend=%3Fref%3DPDF&jav=VoR&rel=cite-as
Adv. Synth. Catal. **2018**, *360*, 2339.

Symrise: Product Sustainability Score Card

- Eco-friendly chemistry
- Resource-efficient production
- New technology and digitalization opportunities

[A positive product impact - Sustainability - Symrise]

Symrise: Product Sustainability Score Card



[A positive product impact - Sustainability - Symrise]

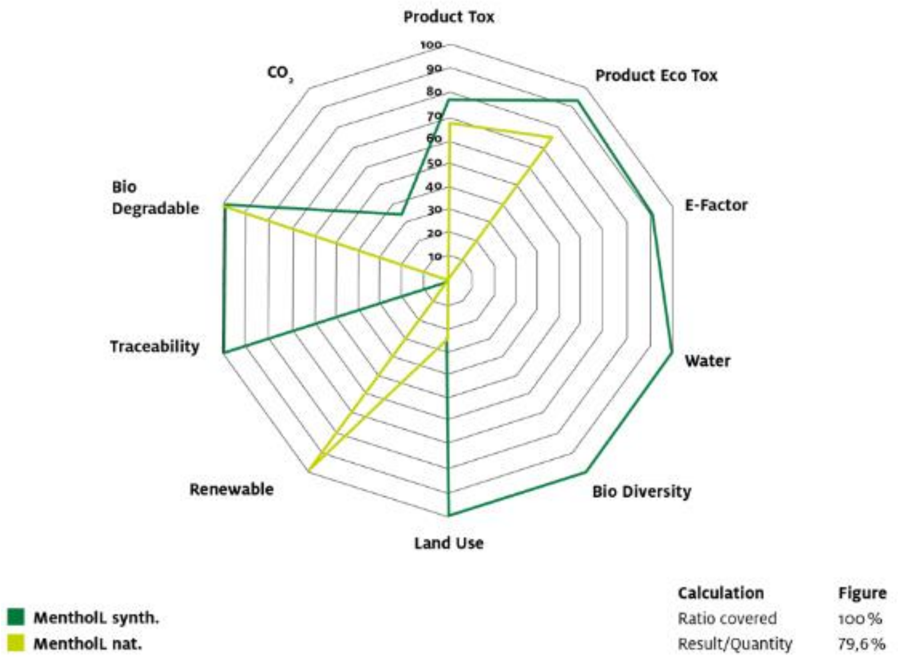
Symrise: Product Sustainability Score Card

Menthol:

The scorecard reveals:
Synthetic variation produced by Symrise offers benefits over the long term:
ranging from a safe, clearly traceable basis of raw materials to comparably energy-efficient, low-waste production and an-end-product of outstanding purity and quality.

The scorecard provides an overview of this information, with synthetic menthol performing better in a variety of categories:

- "water efficiency"
- "traceability"
- "land use"
- "biodiversity"



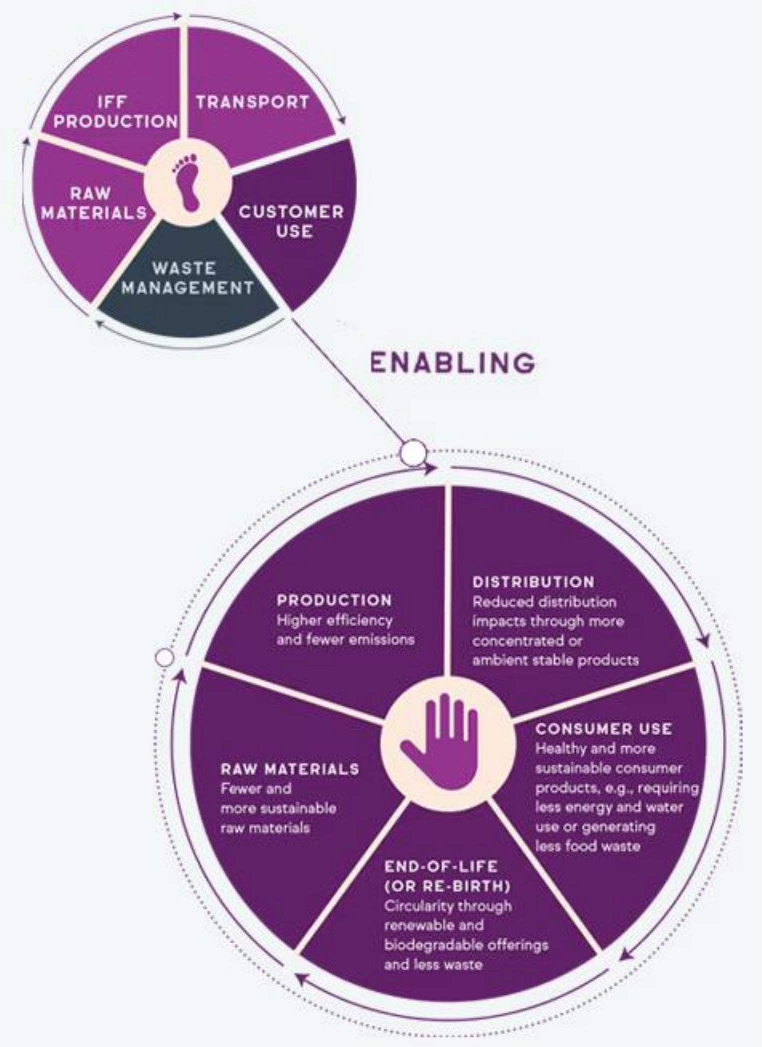
[A positive product impact - Sustainability - Symrise]

IFF

LCA:

Where we believe our products can make one of the biggest differences from a sustainability perspective is through their positive life cycle impacts during the use phase. The scale of benefits we can enable for our customers (IFF's "handprint") far outweighs IFF's manufacturing and operational "footprint".

The scope typically involves all stages of the life cycle, from raw material acquisition until the product leaves the production factory (cradle-to-gate) and ideally also includes distribution, use, and end-of-life scenarios (cradle-to-grave/cradle)



IFF

Green Chemistry Score:

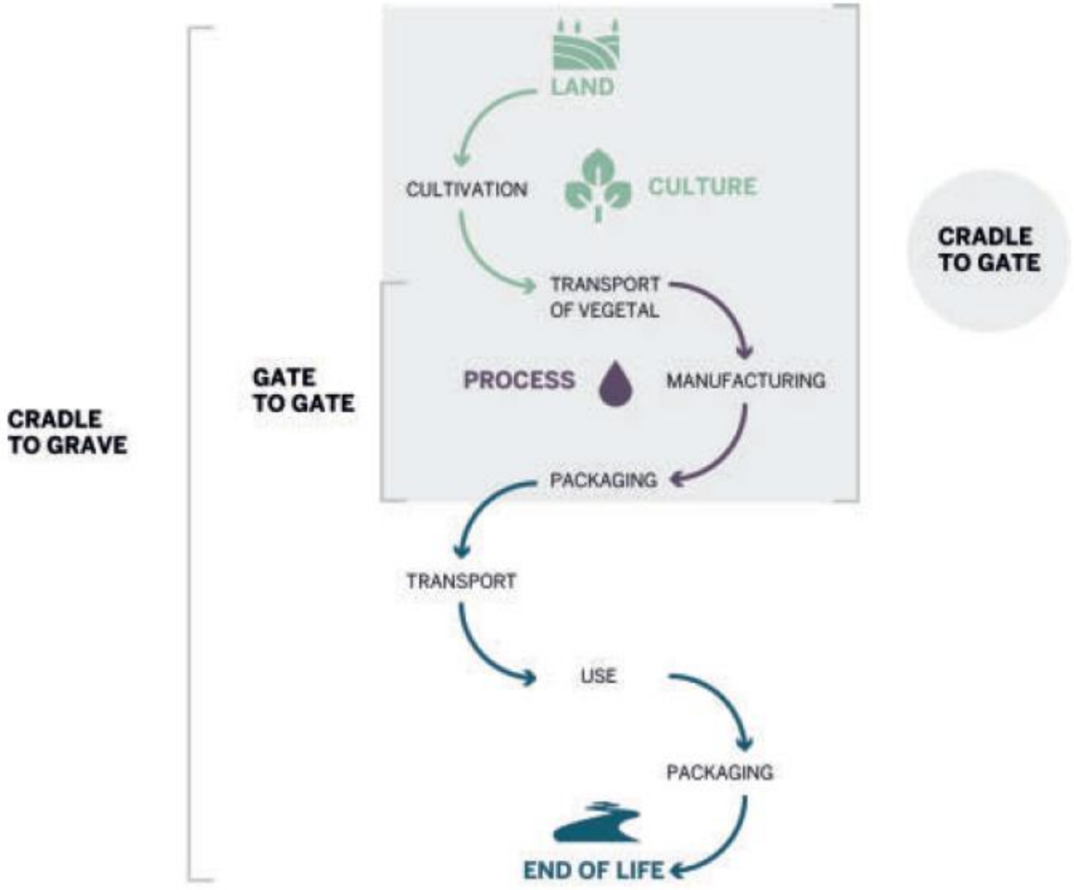
From the R&D phase to commercial production, IFF scientists use our proprietary Green Chemistry Assessment Tool to quantitatively score the overall sustainability of our ingredient catalog, products and processes.

Waste Reduction through Green Chemistry:

This includes converting the byproducts of our natural product processes into useful fragrance ingredients. For example, our terpene-based chemistry utilizes an abundant, readily-available natural raw material – a pine-based side product from the paper industry – to create a number of high-performing fragrance ingredients.

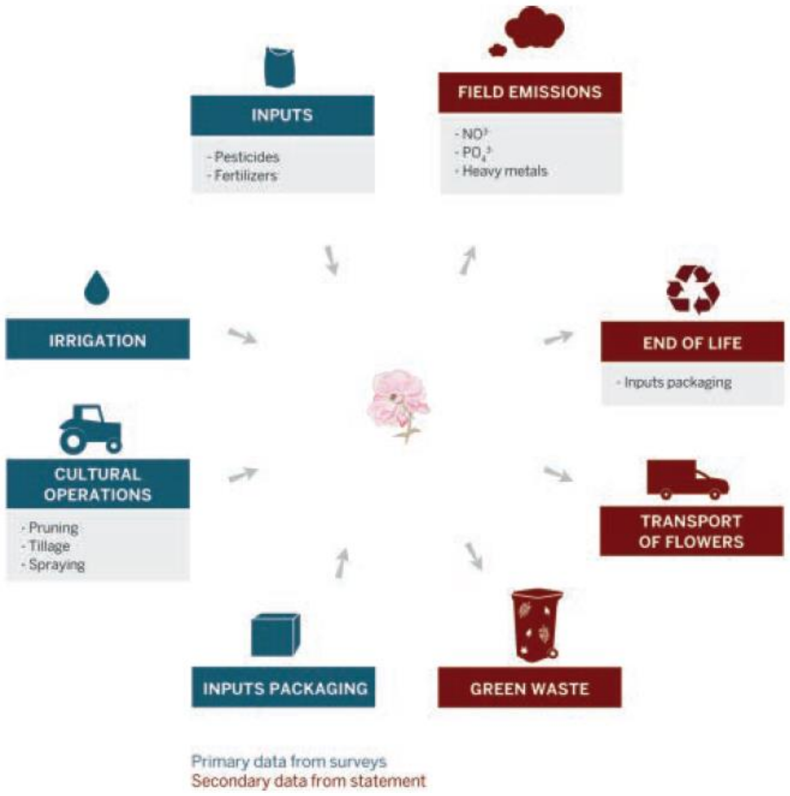
J. H. Amador and S. Palatan, *Perfum. Flavor.*, **2019**, *44*, 38. (April 2019)

LCA of Rose Extracts



J. H. Amador and S. Palatan, *Perfum. Flavor.*, **2019**, *44*, 38. (April 2019)

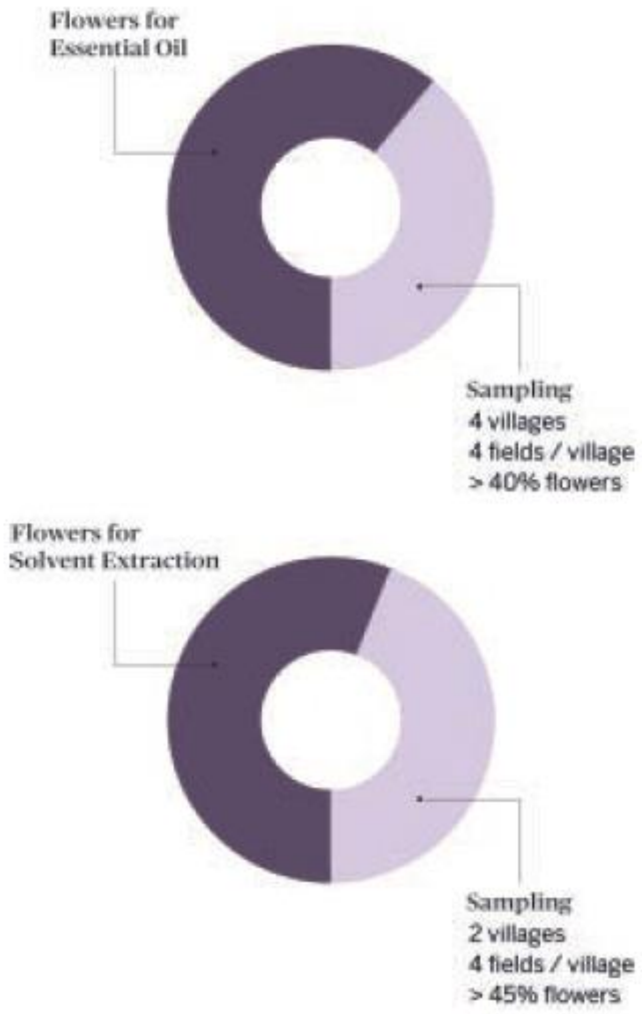
LCA of Rose Extracts



To produce 1kg of rose oil roughly 4 MT of flowers are needed
To produce 4MT of floweres 1ha of rose fields is needed
As the average size of a rose field owned by a Turkish farmer is 0.2 ha,
The production of 100 kg rose oil requires: 500 farmers

J. H. Amador and S. Palatan, *Perfum. Flavor.*, **2019**, *44*, 38. (April 2019)

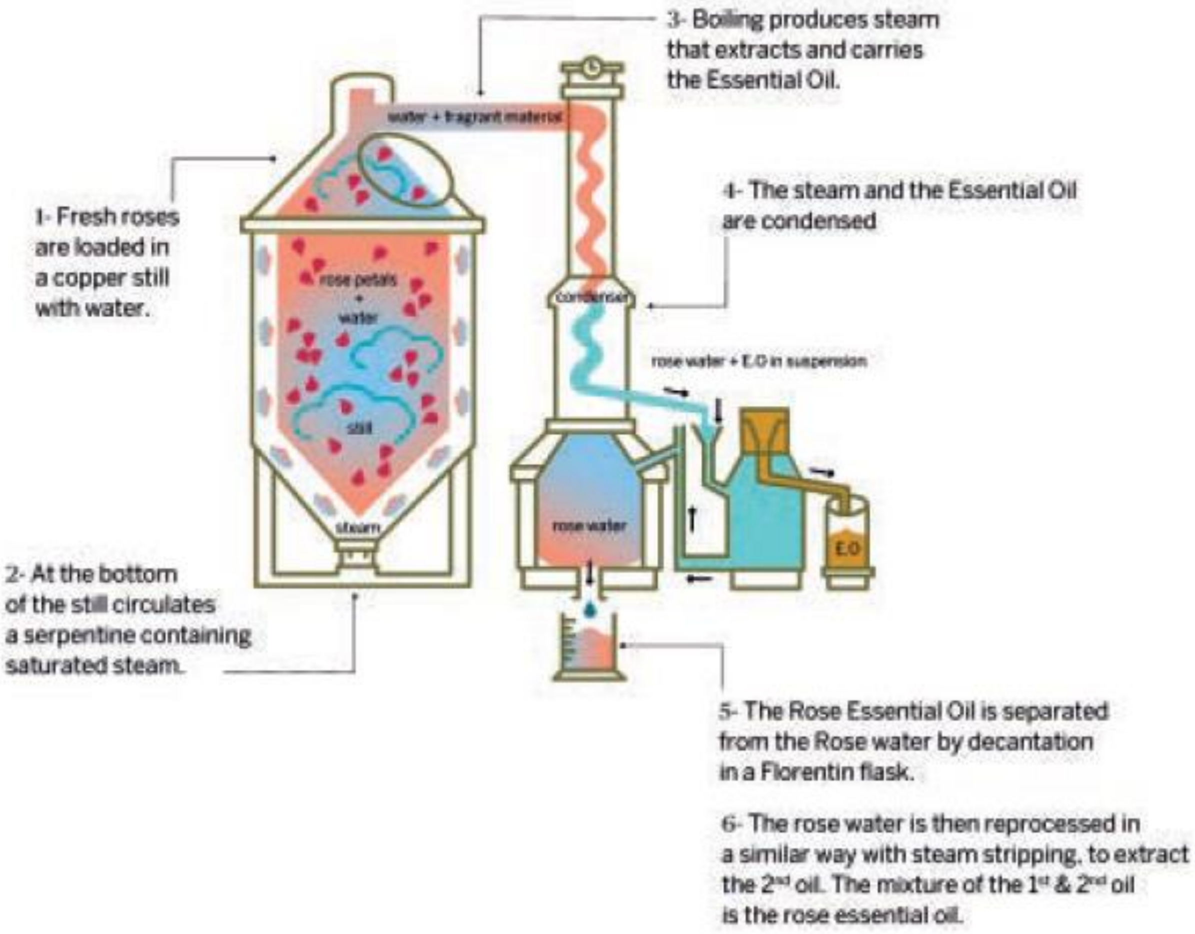
LCA of Rose Extracts

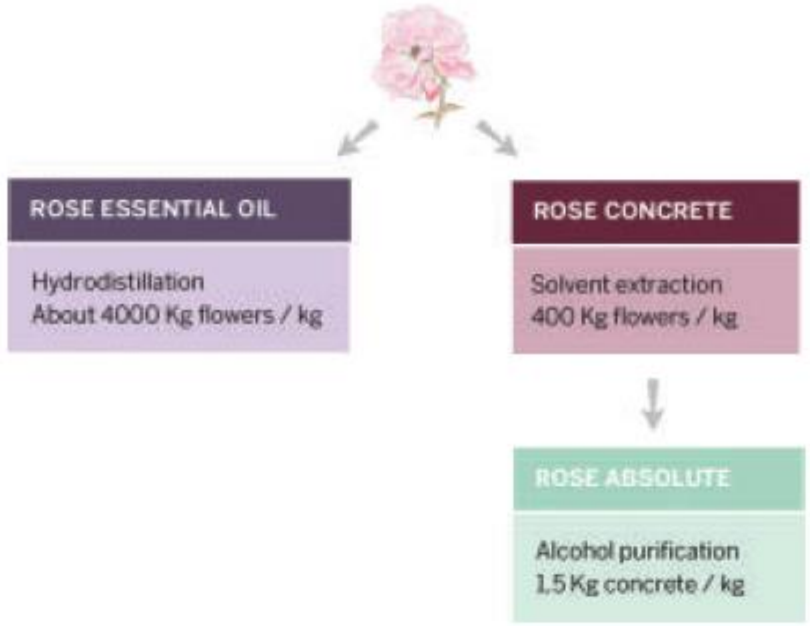


J. H. Amador and S. Palatan, *Perfum. Flavor.*, **2019**, *44*, 38. (April 2019)

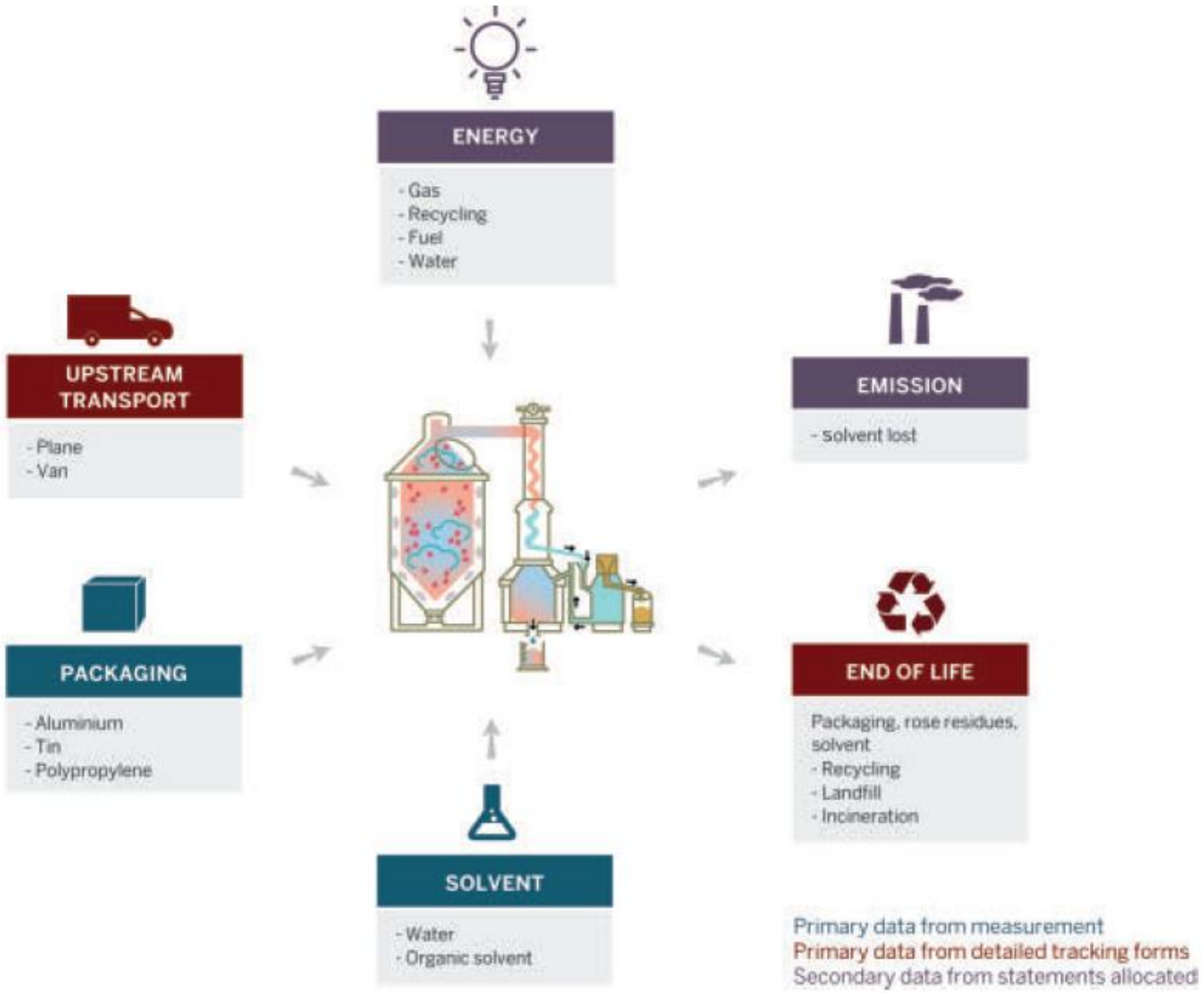
LCA of Rose Extracts

THE DISTILLATION:





LCA of Rose Extracts



LCA of Rose Extracts

Environmental Indicators

CLIMATE CHANGE (Kg CO_2 eq.)

The climate change impact calculation is **based on the global warning potential (GWP)** over 100 years of various greenhouse gas as prescribed by the Intergovernmental Panel on Climate Change (IPCC, 2007).

CONSUMED WATER (m^3)

The consumed water impact represents the **total consumed fresh water**, that is to say the total fresh water withdrawal, less the total water discharged.

ECOSYSTEM QUALITY (PDF*m^2*yr)

The ecosystem quality impact represents the percentage of species that will disappear on a given period of time. It includes the release of substances that cause **acidification** and **eutrophication** of soil and water, the **toxicity affecting wildlife**, **the land use.** Expressed in Percentage of species that will disappear on a given area for a given period of time.

RESOURCES (MJ)

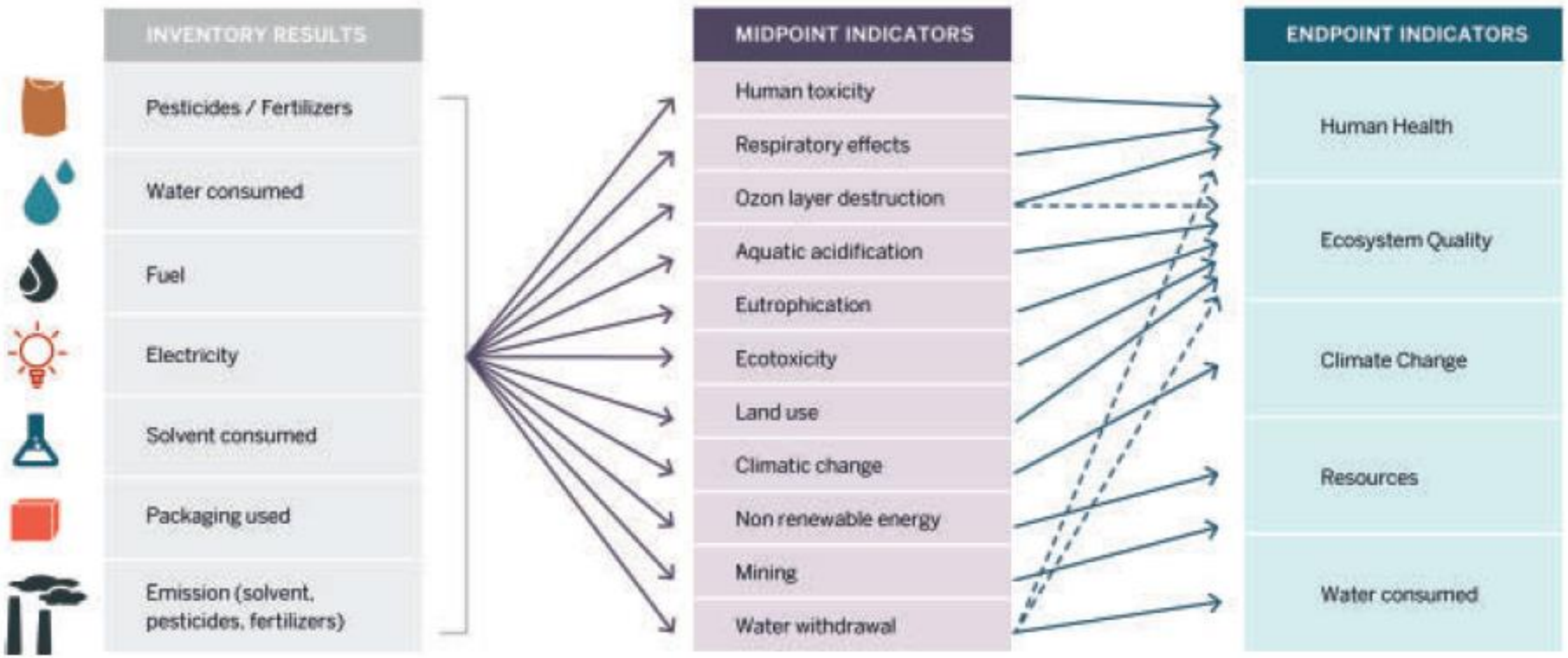
The resources impacts combines the use of primary energy from **non-renewable sources** (fossil and nuclear) and **the extraction of ore.** Expressed in equivalent primary energy i.e. fossil energy (MJ).

HUMAN HEALTH (DALY)

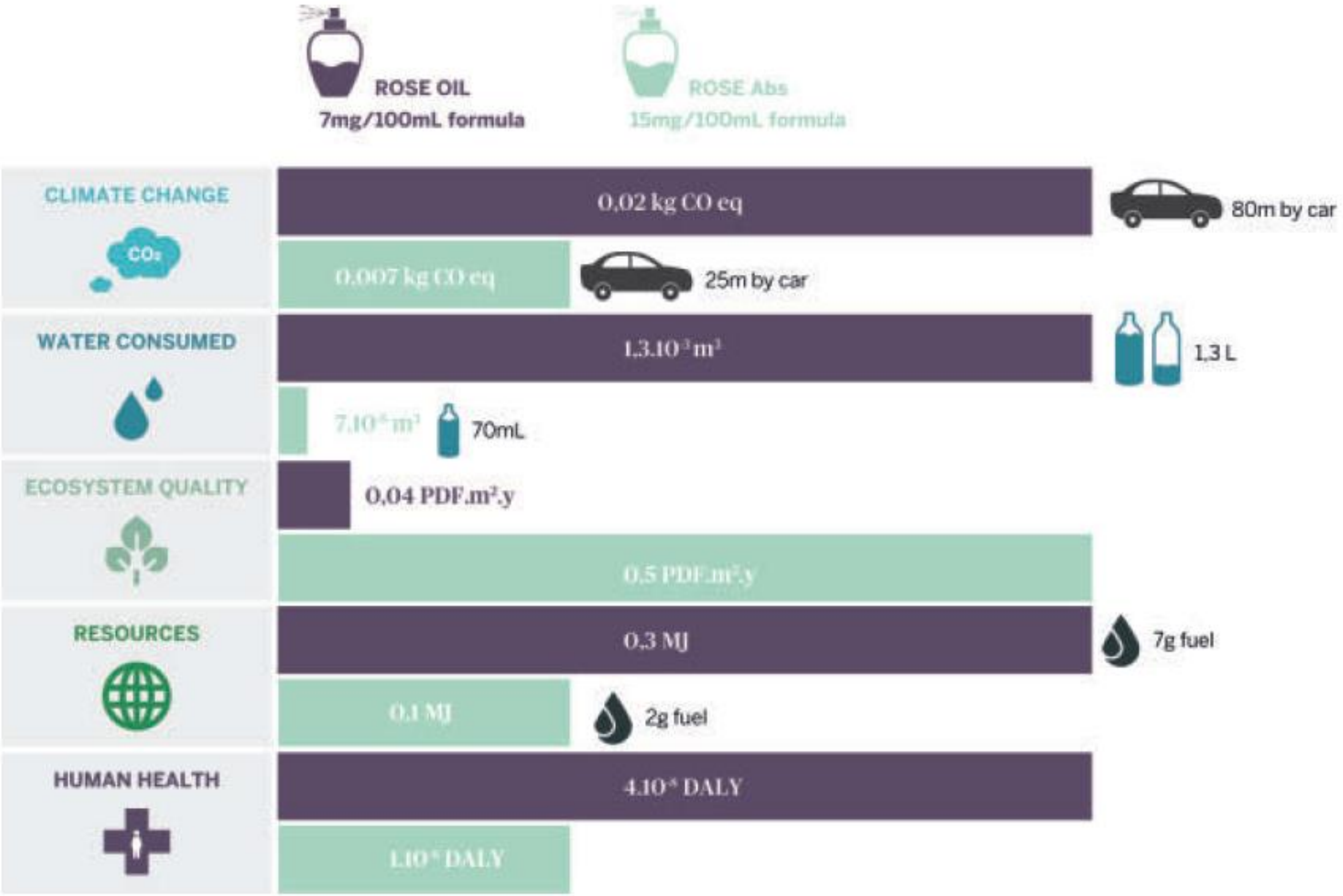
The Human health impact takes into account the substances that affect the human because they are **toxic (carcinogenic and non-carcinogenic)** or they have respiratory effects, or that induce an **increase of UV radiation** from the destruction of the ozone layer. Expressed in Disability Adjusted Life Years.

LCA of Rose Extracts

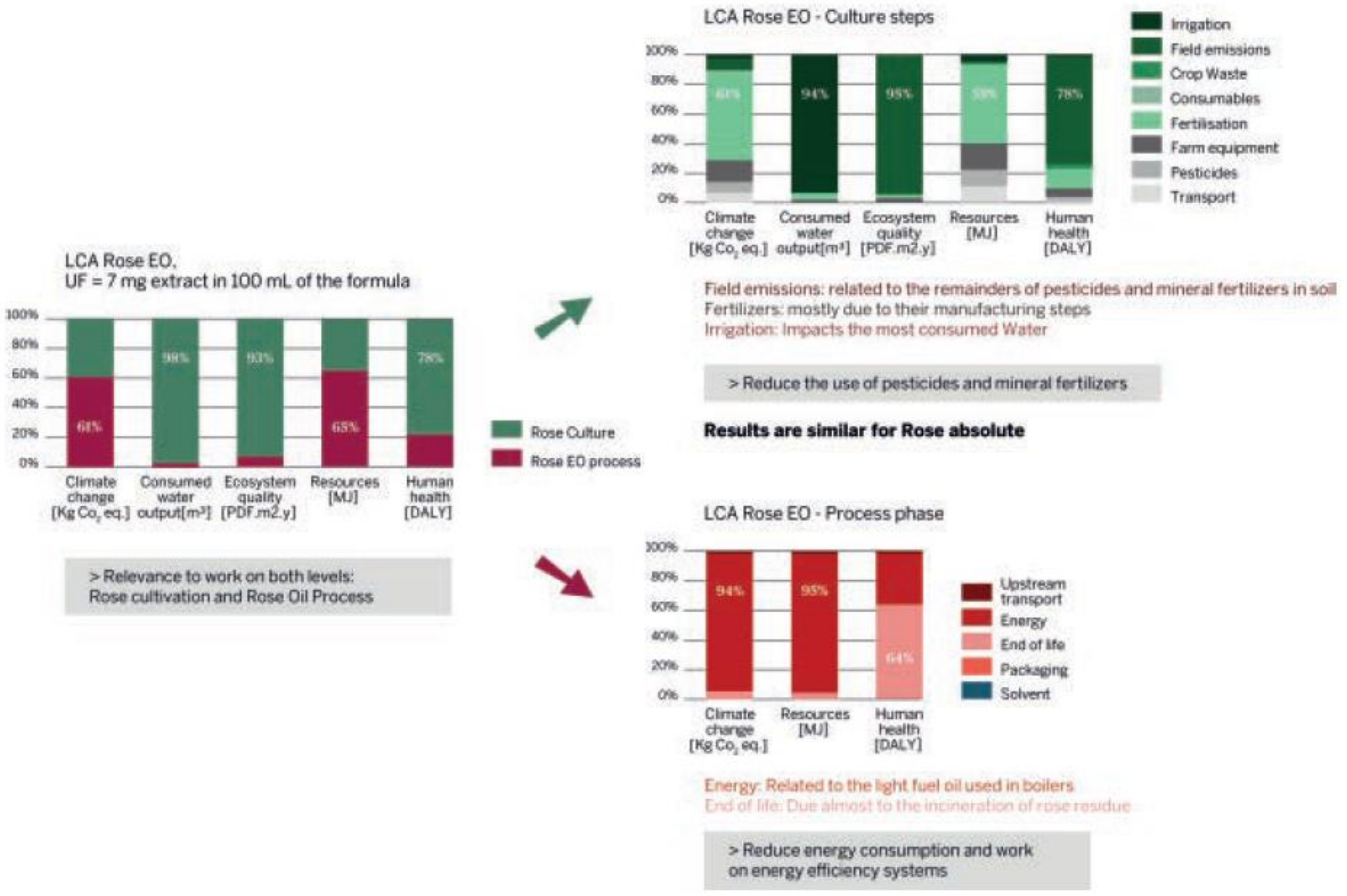
Effect on substances on the Environment



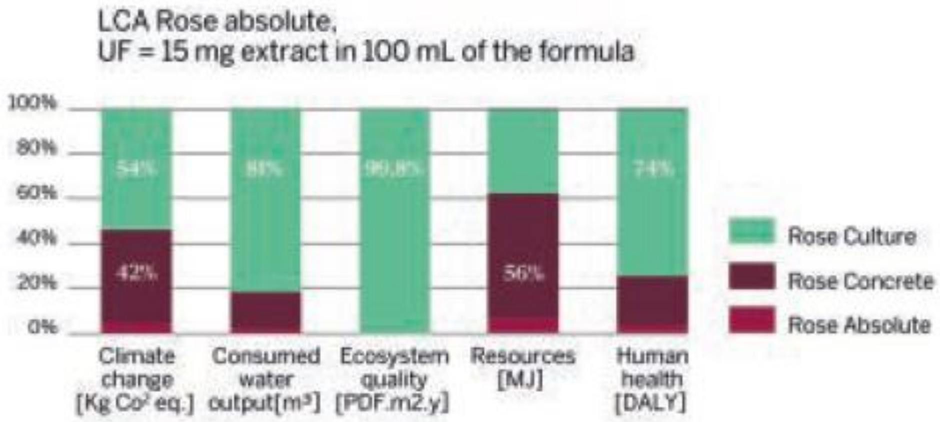
LCA of Rose Extracts

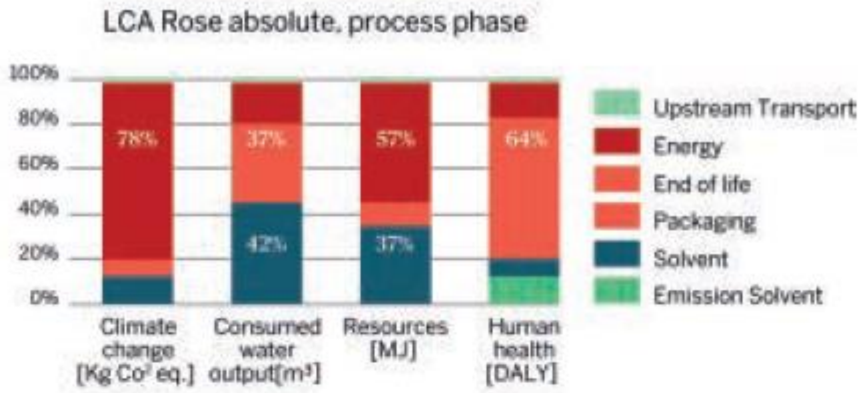


LCA of Rose Essential oil



LCA of Rose Absolute





Energy: Related to the light fuel oil used in boilers
End of life: Due almost to the incineration of rose residue
Solvent: Due to organic solvent lost or waste

> Relevance to work on two levels:
> Rose cultivation and Rose Concrete Process

→

> Reduce energy consumption and
> work on energy efficiency systems

Conclusion?

By performing up to 15 LCA on natural extracts:

- Some material or energy flows are recurrently the most impacting.
- The use of mineral fertilizers and pesticides has one of the highest impacts on the resources and climate change
- Crop irrigation has the highest impact on the water consumed. In the case of Turkish rose, these results are overvalued since the sampling selected irrigated fields in higher proportion than the total fields.

- Use fewer pesticides, develop alternatives, favor organic fertilizers with long action, rationalize the use of water through drip irrigation systems and closely monitor the plant's needs.

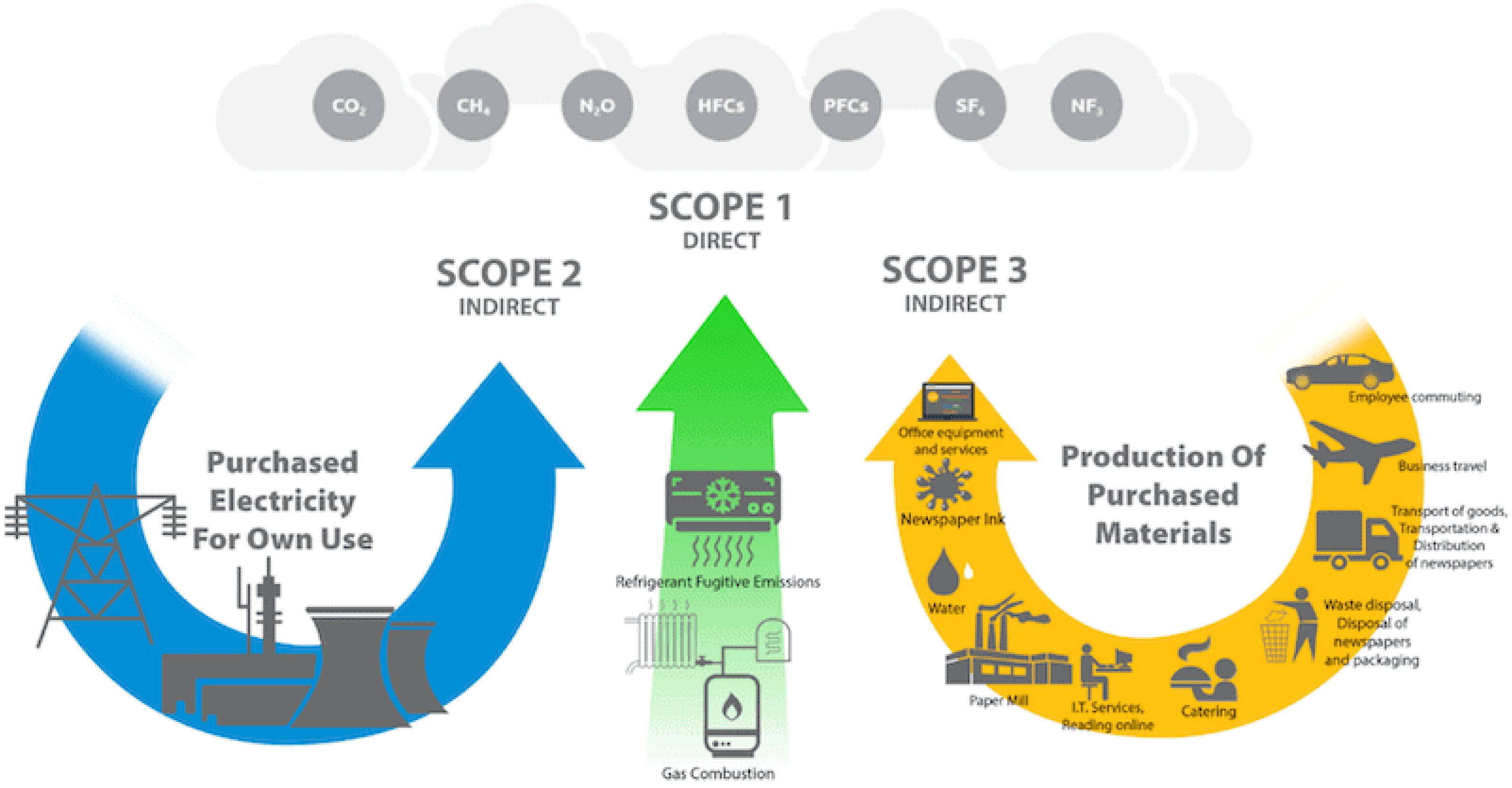
Conclusion?

By performing up to 15 LCA on natural extracts:

- The extraction yield is in general the most impacting factor

- The amount of fuel or gas to generate steam for heating during the extraction or the evaporation is one of the most impacting factors at the process.
- The solvent loss during the evaporation is also one of the most impacting factors at the process stage. New Greener Solvent?
- Transportation by plane is a major impacting factor. As flowers grow worldwide, planes are sometimes used to transport raw materials.

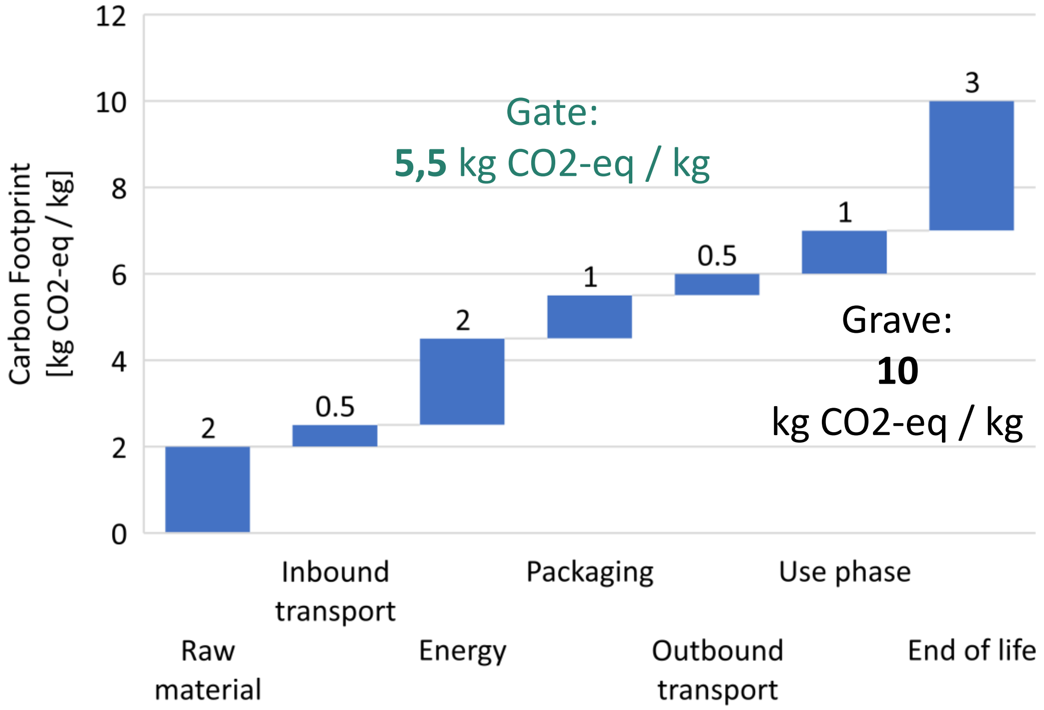
LCA



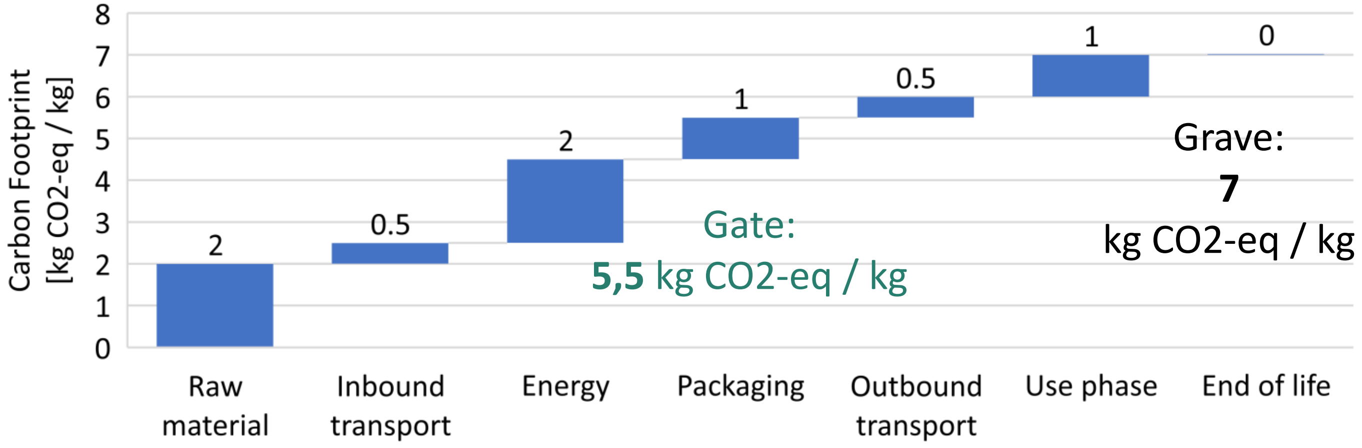
Done with the help: Maud Reiter, Nicolas Habisreutinger & Ulla Leutinois.

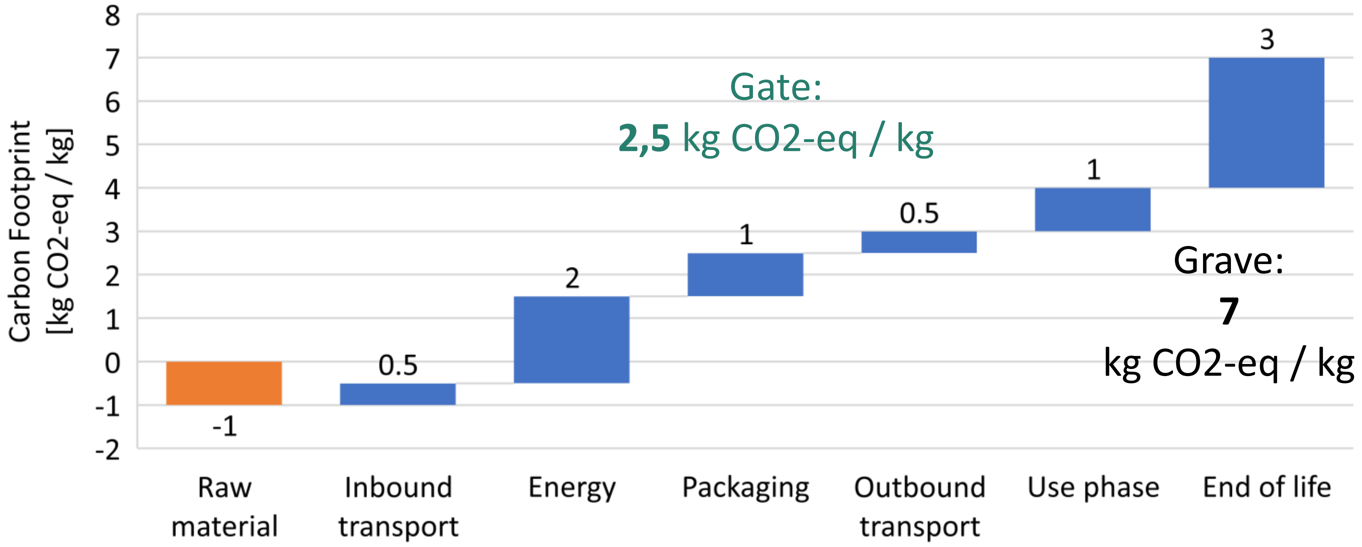
Including Renewable Carbon benefit at gate level

Fossil molecule



Renewable Carbon molecule

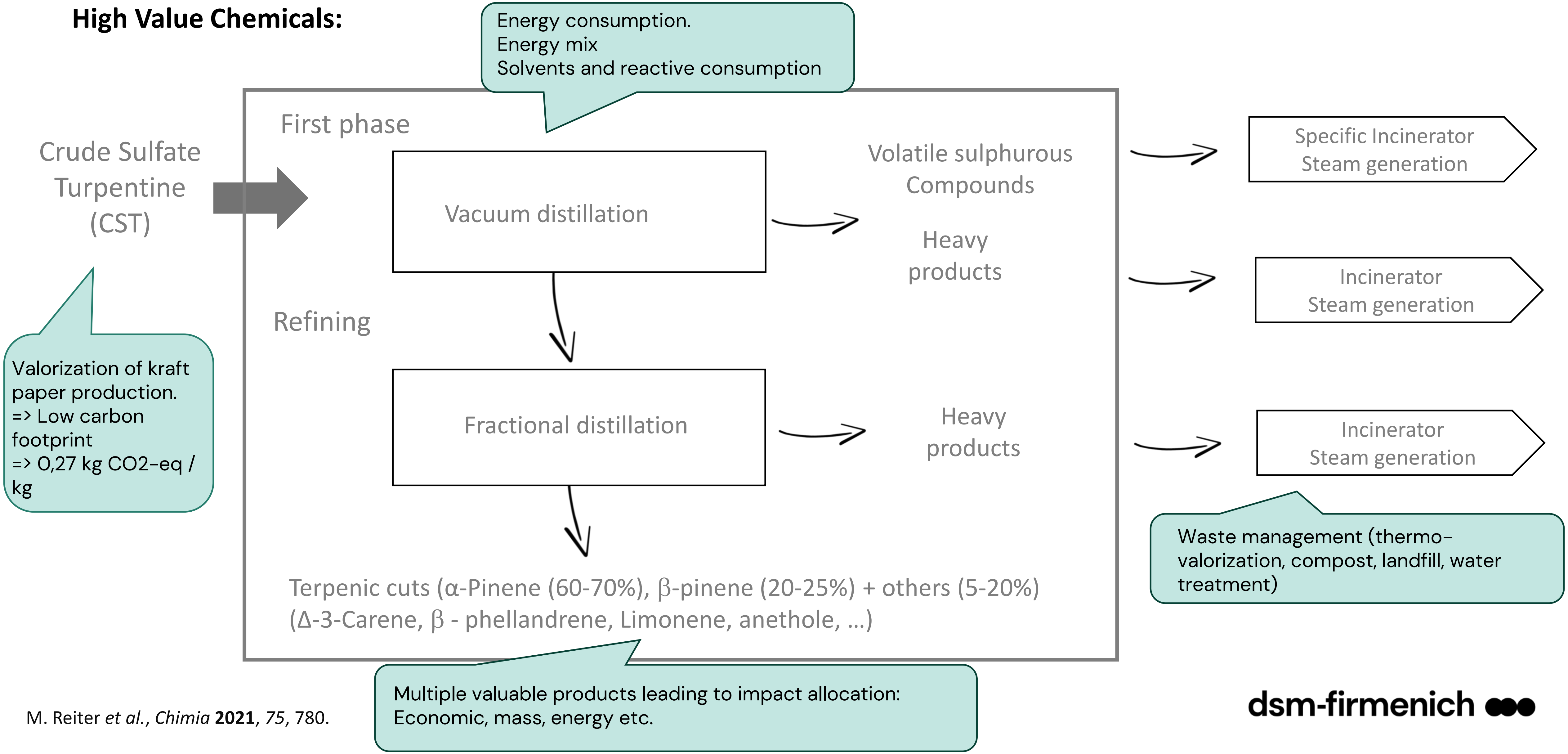




dsm-firmenich

LCA: alpha-Pinene

High Value Chemicals:

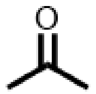


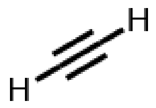
M. Reiter *et al.*, *Chimia* **2021**, *75*, 780.

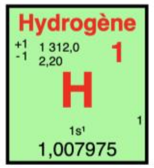
dsm-firmenich

Carbon neutrality; Net-zero Emission

2 Acetone + 2 Acetylene + 2 Hydrogene ⟶ **Linalool**







< 10 kg CO_2-equiv

PRODUCTION

PRODUCTION

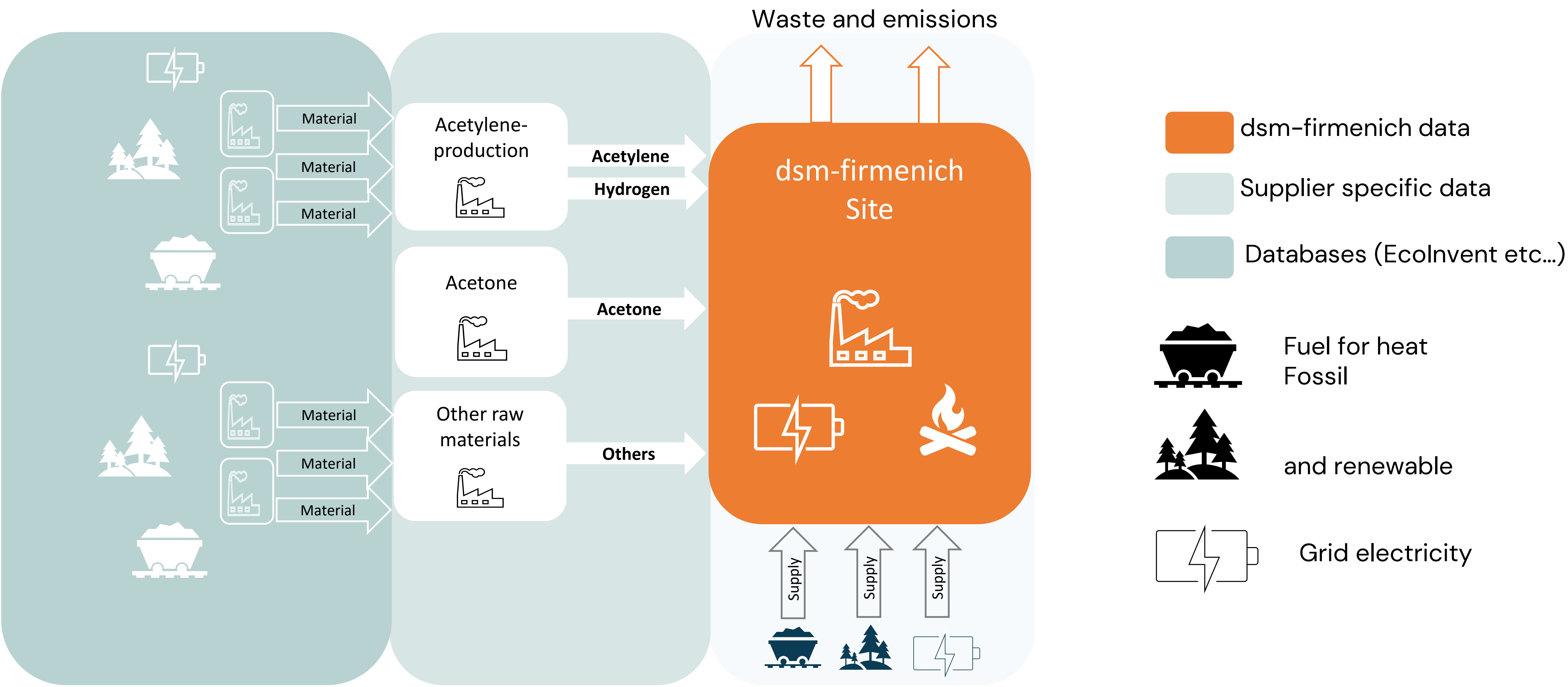
WASTE & EMISSIONS

Net-zero: SBTi requires reduction by 90%. Only 10% can be compensated

Implementing changes in manufacturing processes take several years.
How will the footprint of that process change be in several years?

Creation of LCA models of our own processes

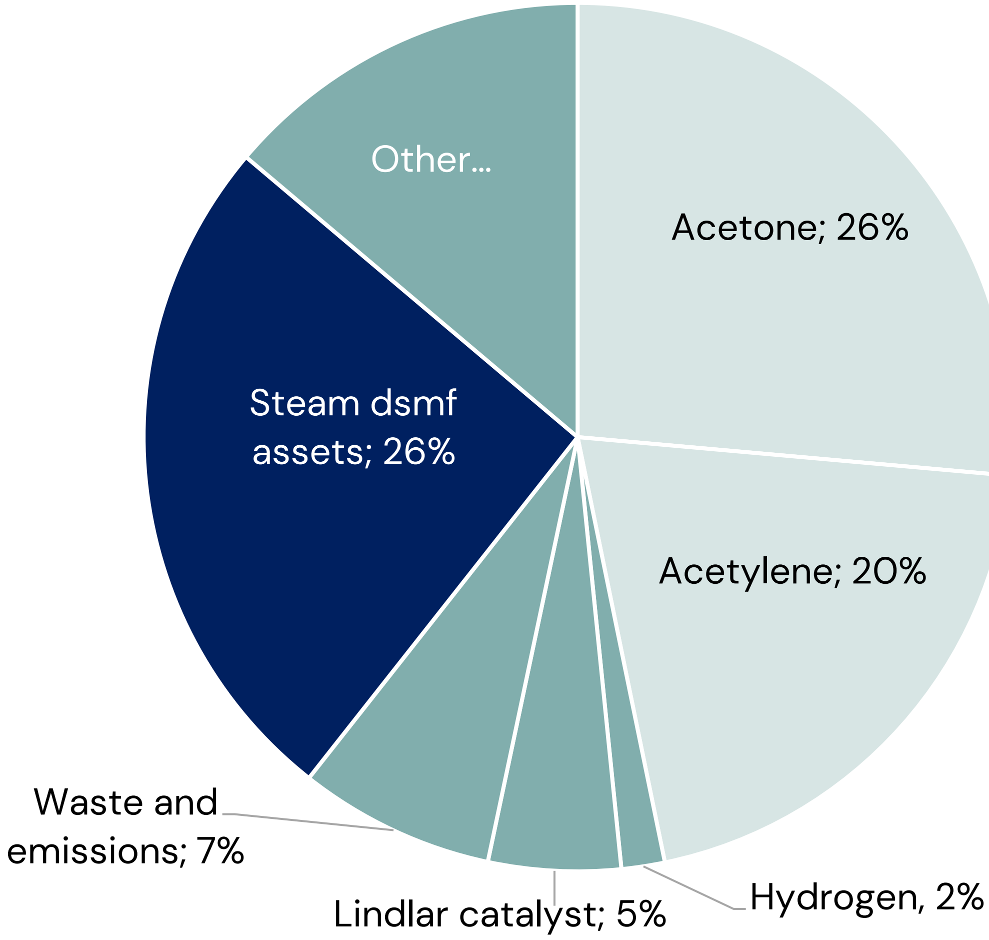
Current footprint is calculated by summing up of consumption data, consisting of foreground and background data



Carbon footprint contribution…

Result from LCA-model based on today's data (own data, supplier specific and Ecoinvent)
Today's footprint of linalool is well below 10 kg CO_2-equiv.

2024

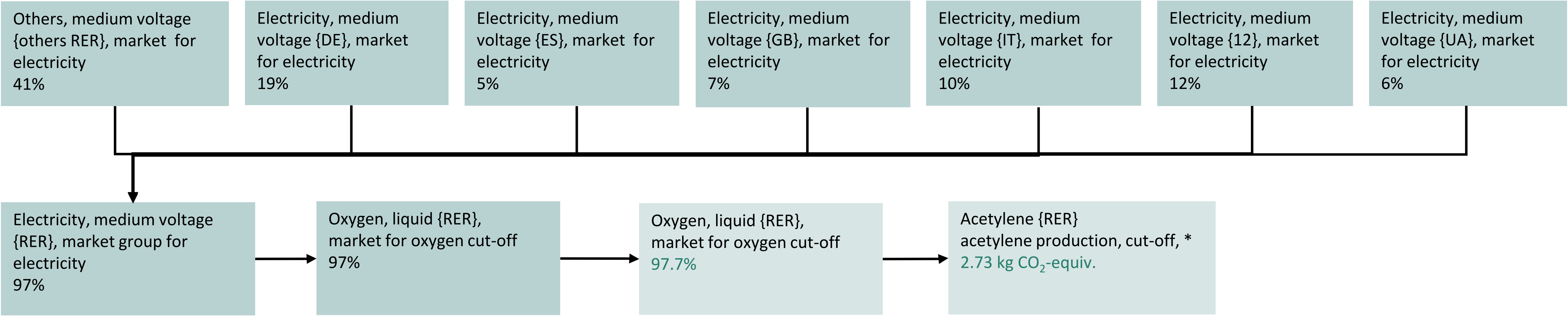


Replacement of natural gas as heat source for steam generation

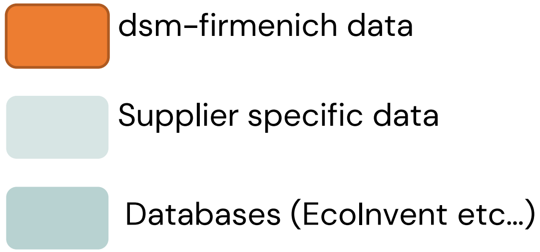
Purchase acetone produced on a different technology, e.g. from CO_2

Acetylene?
From different technology?
Replace acetylene by a different building block?

The main impact from acetylene production is electricity



- Environmental impacts from electricity from the grid are background data
- Appropriate conclusion: Switch to acetylene made by another route?
- Currently also alternative acetylene production processes require a high amount of electricity
- Then rather change to a process without acetylene?

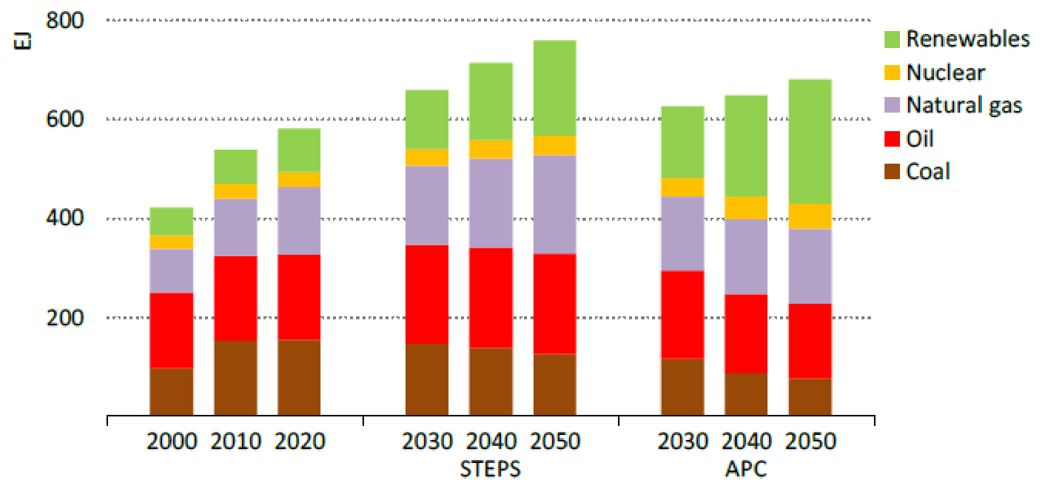


The data shown are from the EcoInvent model.

But the world does not stand still

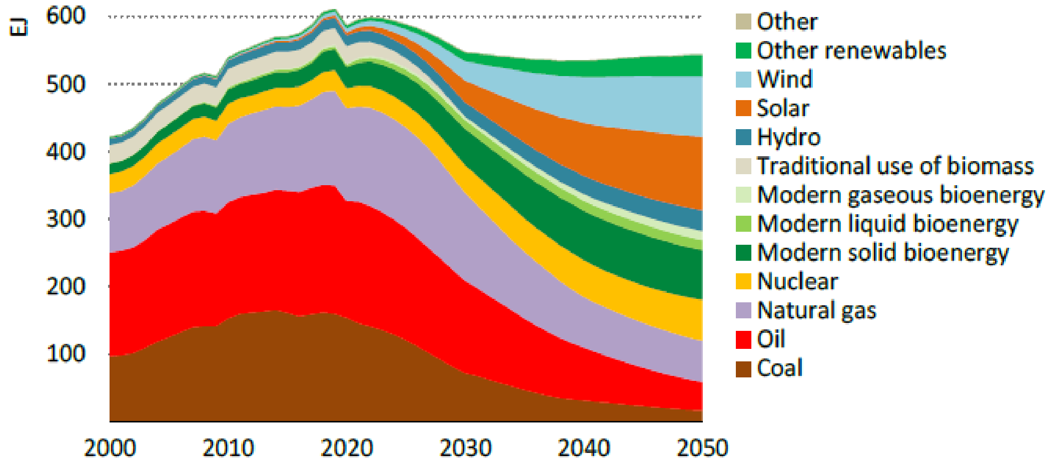
The energy transition will lead to shifts in energy sources ⇨ towards more renewable energy sources.

Figure 1.12 ▷ Total energy supply by source in STEPS and APC



Announced net zero pledges lift renewables in the APC from 12% of total energy supply in 2020 to 35% in 2050, mainly at the expense of coal and oil

Figure 2.5 ▷ Total energy supply in the NZE

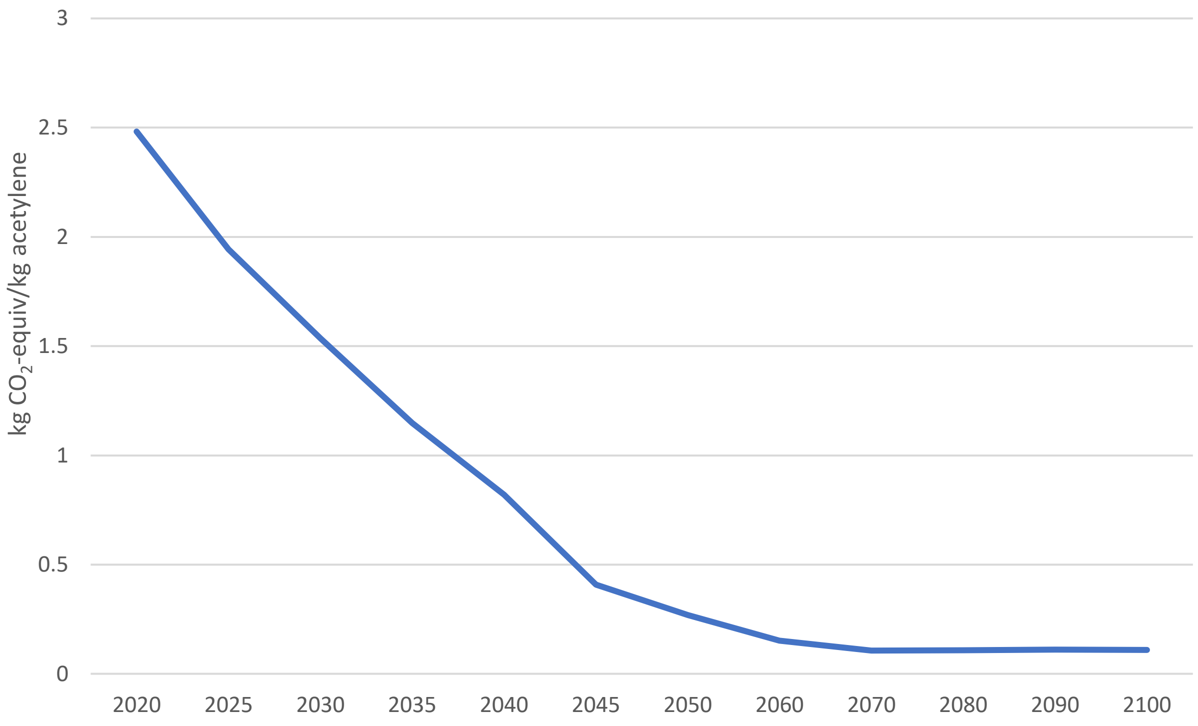


Renewables and nuclear power displace most fossil fuel use in the NZE, and the share of fossil fuels falls from 80% in 2020 to just over 20% in 2050

Will that make a difference to Carbon Footprints?
How to implement that transition into LCA-models?

IEA report "Net Zero by 2050, A Roadmap for the Global Energy Sector" 2021.

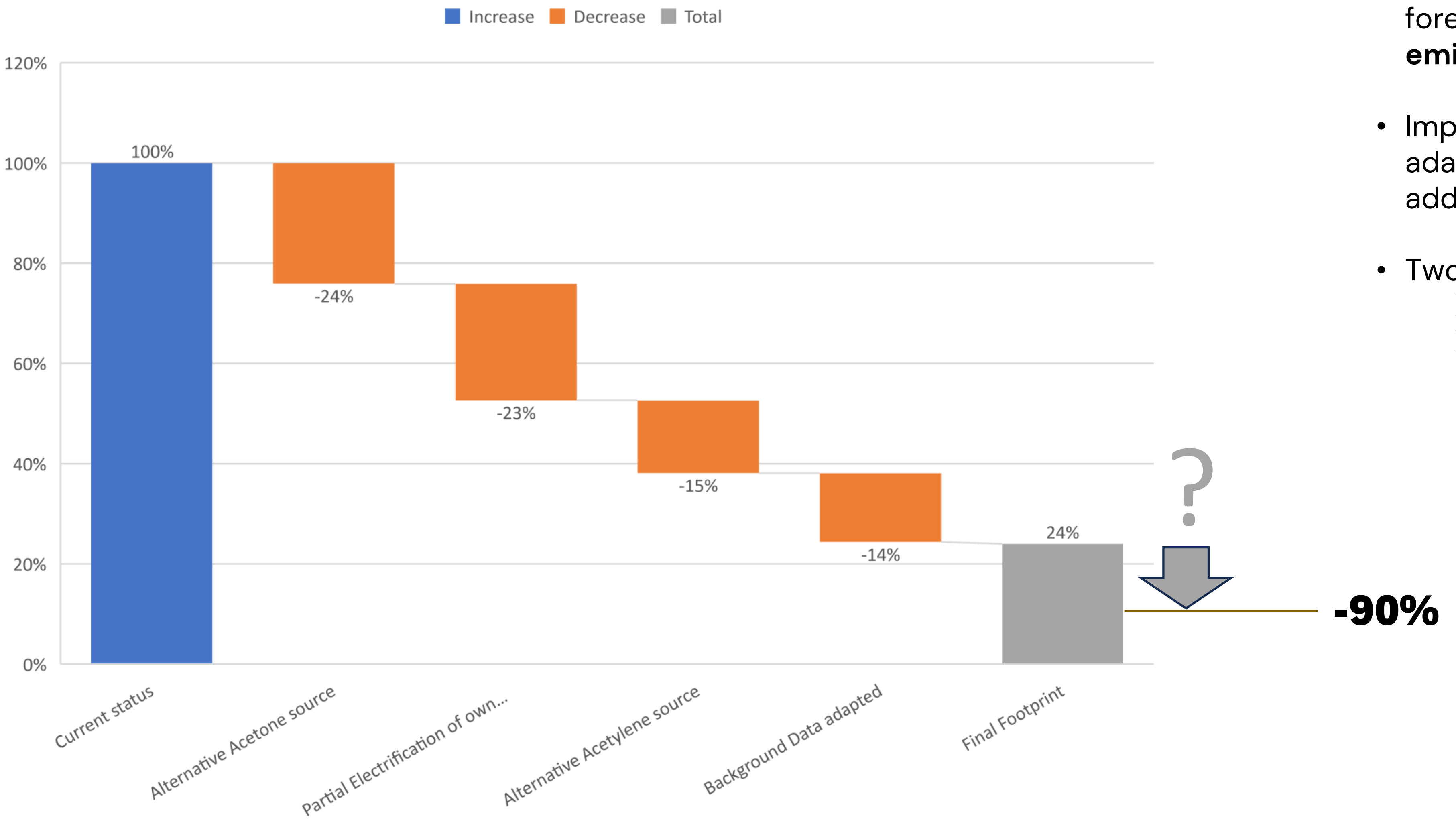
Potential Acetylene Carbon Footprint change



- Acetylene modelled with EcoInvent-REMIND SSP2 Base superstructure
- An example for strong influence of background data on Carbon Footprint
- What does that mean for Linalool's footprint?

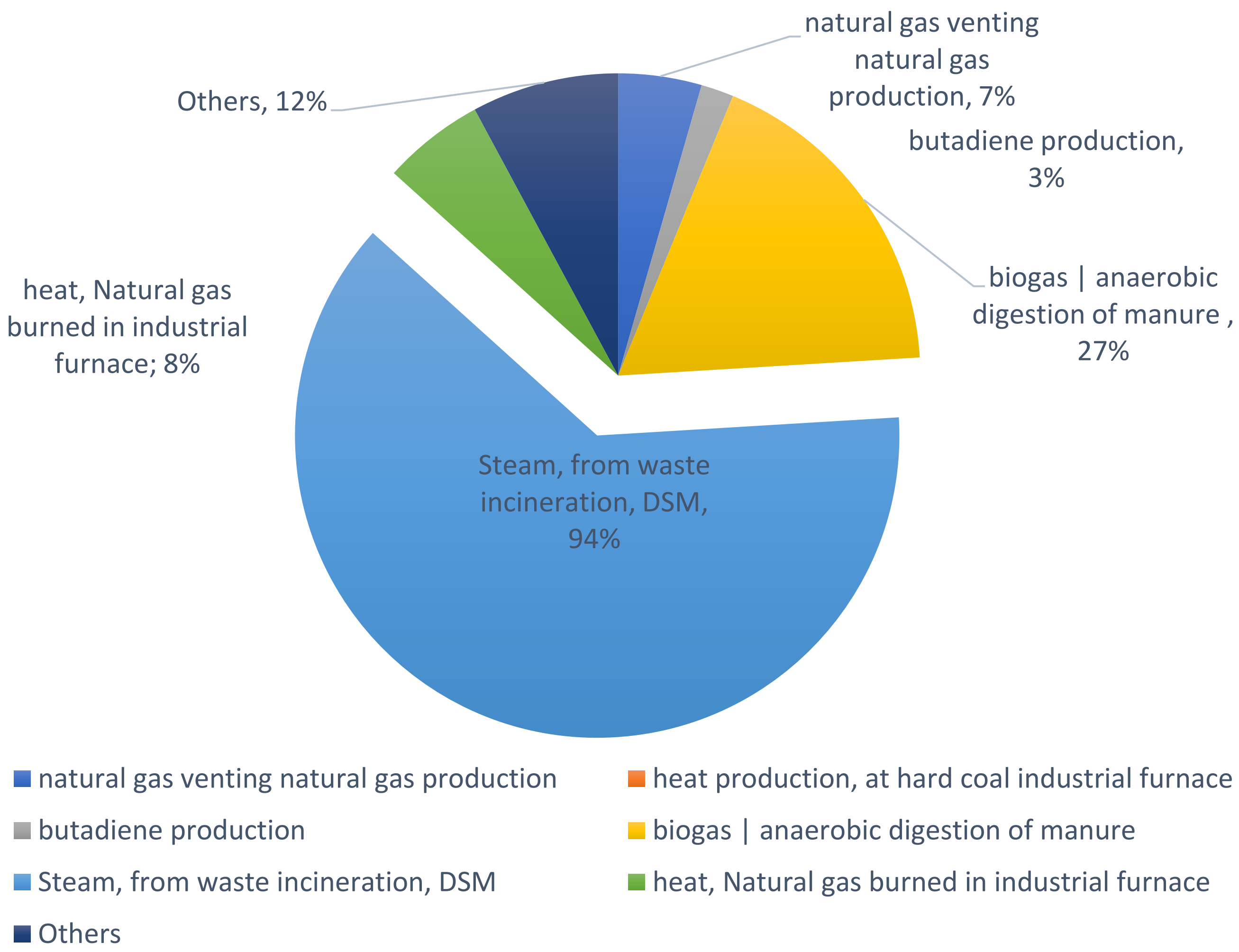
Implementation of various measures

Foreground data could help to lower the footprint by 62 %
Including the background total 76% reduction



- Potential implementation of improvement measures calculated by foreground data changes result in **62% emissions reduction**.
- Implementation of background data adaptation using premise results in additional **14% emissions reduction**.
- Two key questions :
  - ➢ What are the remaining impacts?
  - ➢ How to reduce these to achieve 90% emissions reduction?

Where is the remaining footprint from ?



Potential carbon footprint:

And after energy transition gives access to a large share of renewable electricity

Linalool's footprint would be reduced by 75%

Main remaining contributor:
Heat generated from fossil-derived distillation/ recycling sludges

These can only be avoided when all materials used come from renewable sources.

Data Exchange Methodology

PACT
PARTNERSHIP FOR CARBON TRANSPARENCY

- Carbon Footprint calculated with IPCC 2021 (AR6)
- Description of the scope (including/excluding etc.)
- Allocation
- Primary / Secondary data share
- Data Quality Rating

Compliant with:

TOGETHER FOR SUSTAINABILITY

Product Environmental Footprint (PEF)

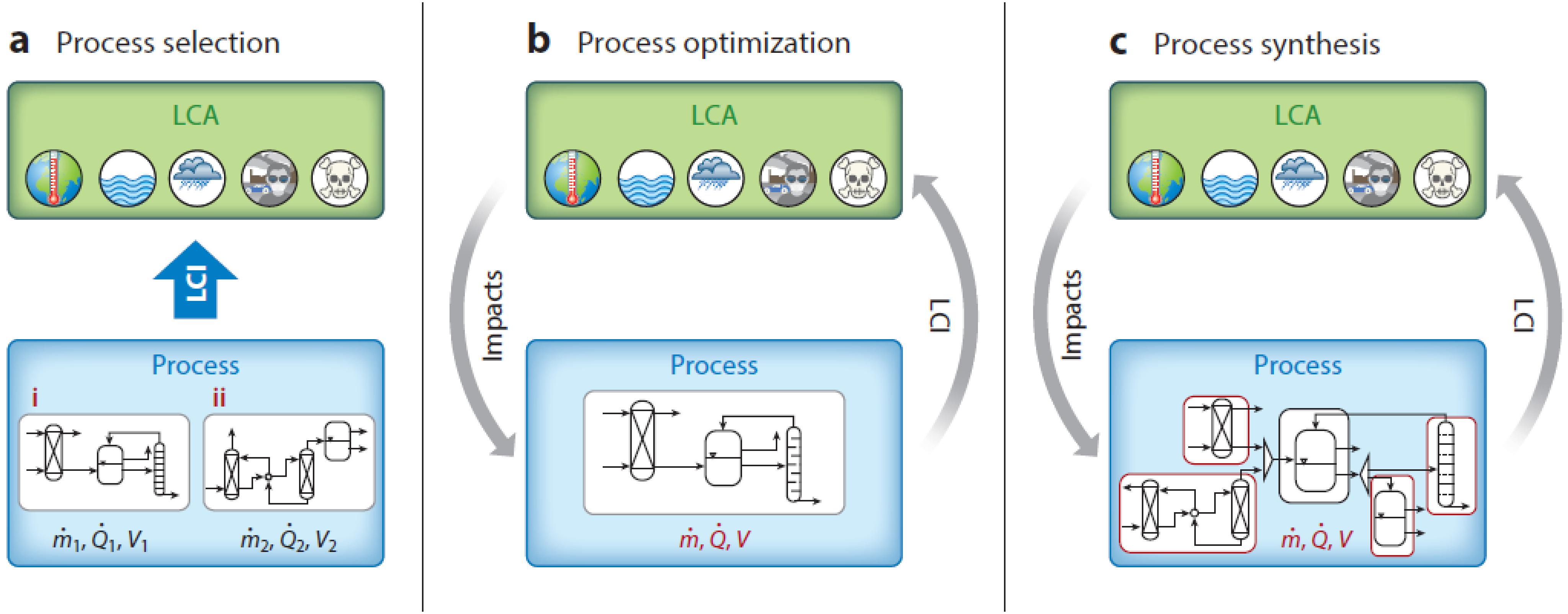
European Commission

Compliant with the PEF v. 3.1 but requiring specific parameters such as:

- Cradle to gate
- Cut-off
- Only carbon footprint
- Possibility to include or exclude renewable carbon benefit.
- Specific DQR

LCA

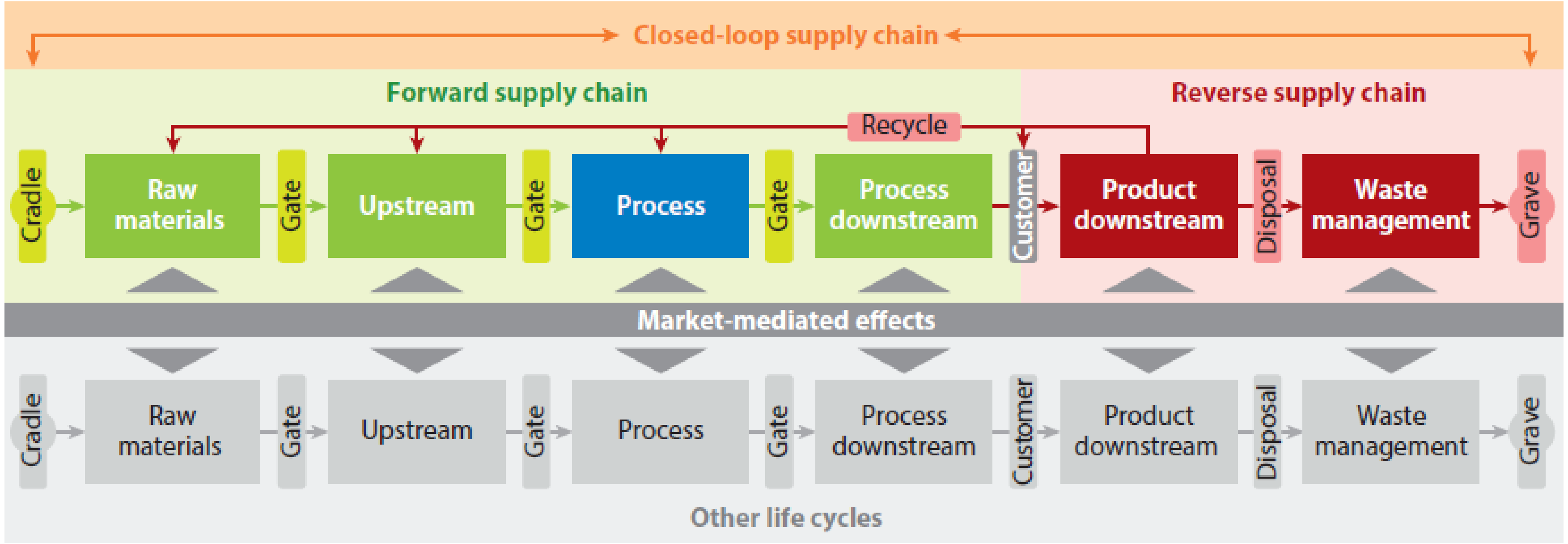
Integration of life cycle assessment (LCA) and process design ranges over various levels



Annu. Rev. Chem. Biomol. Eng. **2020**. 11:20.1–20.31.

LCA

LCA in Supply Chain Management (SCM)



Annu. Rev. Chem. Biomol. Eng. **2020**. 11:20.1–20.31.

IFRA

IFRA: The International Fragrance Association

RESPONSIBLE SOURCING of all raw materials

01

Partnerships with communities

Labor practices & human rights

Sustainable use of ecosystems, biodiversity

ENVIRONMENTAL FOOTPRINT

02

GHG emissions

Energy consumption

Water intake

Waste & circular economy

Green chemistry

We are inspired by Green Chemistry Principles

SAFE, ATTRACTIVE and REWARDING WORKPLACE CULTURE

03

Occupational health & safety

Equal opportunities, diversity & inclusion

Training & development

PRODUCT SAFETY and DESIGN

04

Safe-by-design (for consumers **and the environment**)

Product stewardship

Alternatives to animal testing

TRANSPARENCY

05

Ethics & integrity

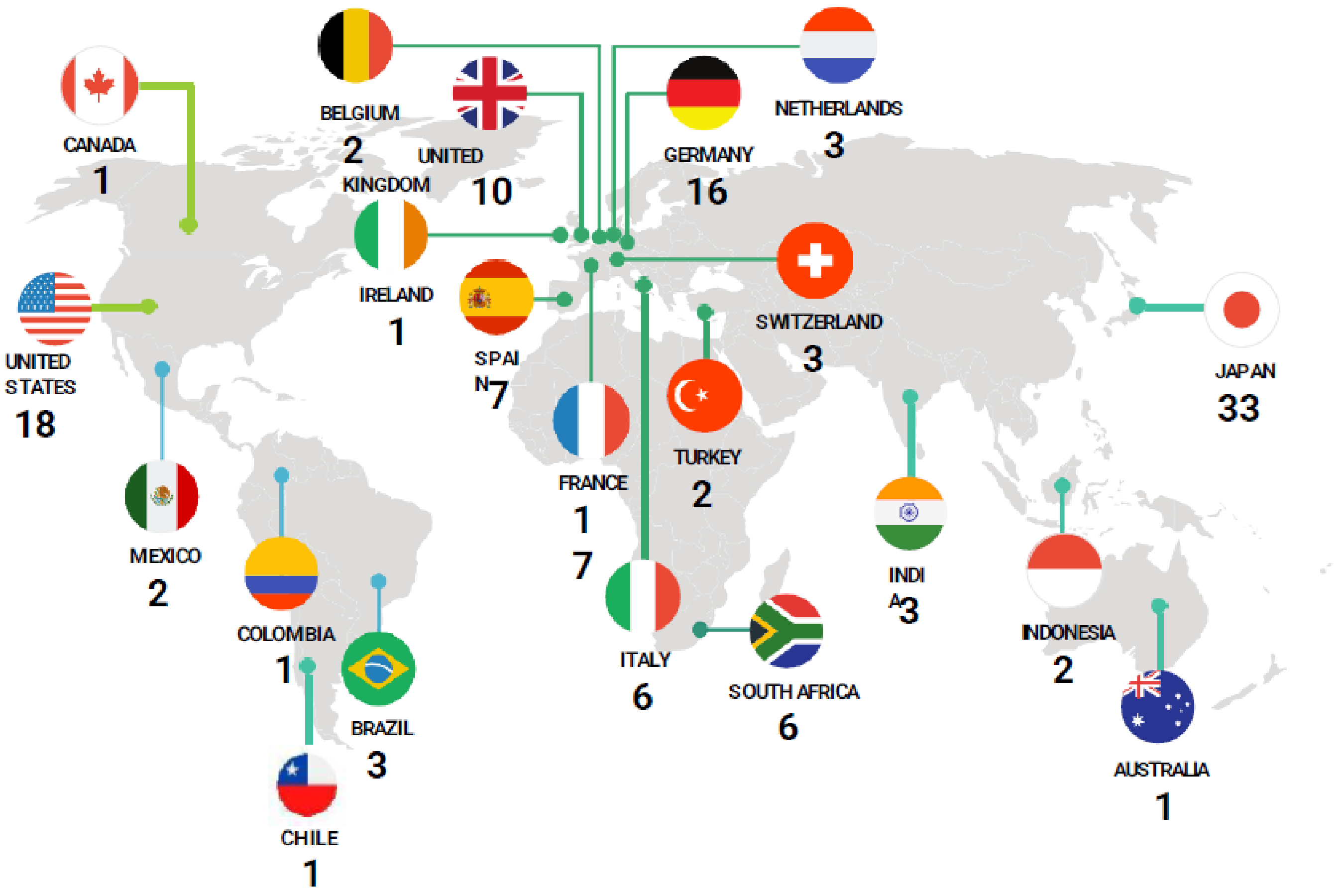
Stakeholder dialogue & collaboration

https://ifrafragrance.org/priorities/sustainability

IFRA

IFRA: The International Fragrance Association

National/regional breakdown by signatory company headquarters



19	NORTH AMERICA
7	LATIN AMERICA
67	EUROPE
6	AFRICA
39	ASIA-PACIFIC

IFRA

IFRA: The International Fragrance Association

- Further developed since its 2020 launch and the first Report in 2021, 'Charter 2.0' reinforces an ambitious approach to sustainability
- Updated text covers alternatives to animal testing, Green Chemistry, workplace culture, 'essentiality' of flavors and fragrances
- Since 2021, more companies have fulfilled or are making progress towards fulfilling the 17 Charter commitments
- The 2023 Report also covers the activities of the new Sustainability Committee, the Sustainability Community, and work on carbon footprint, deforestation, Green Chemistry, and harmonised definitions

- The Compass tool provides direction for scientists and other industry professionals towards the conscious design of greener, safer and more sustainable chemical choices.
- The Compass tool is inclusive, voluntary, global and open to all interested stakeholders through a public consultation.

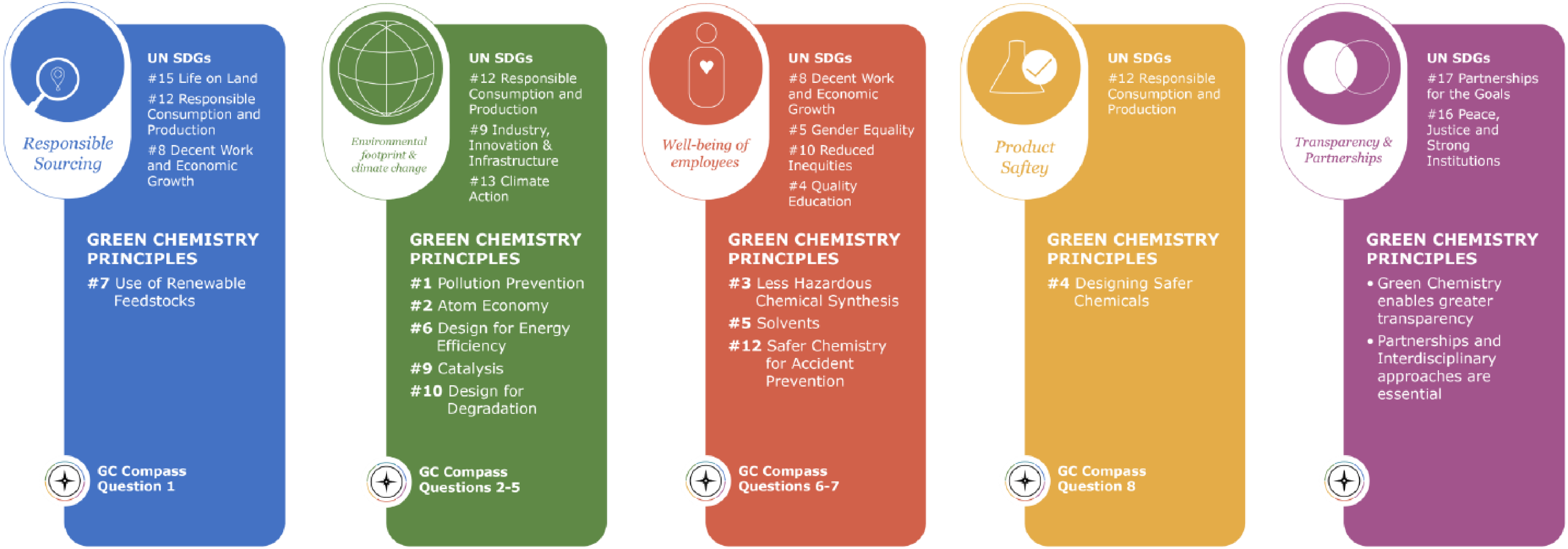
Perfumery & Flavorist - Oct - 2024

IFRA

Scope and Disclaimer: The IFRA Green Chemistry Compass

- Still in development
- General guidance tool for how to consciously design greener, safer and more sustainable chemical choices
- Simplified high-level overview tool looking gate to gate, suitable for in-house assessment; not to be shared externally
- Not meant to determine whether a product meets the EU Safe and Sustainable by Design (SSbD)criteria which are still under development
- Not a substitute for a company's own due diligence on ingredients and processes
- Compliments other tools used by industry
- Helps identify opportunities for improvement

Scope and Disclaimer: The IFRA Green Chemistry Compass



IFRA

9 Green Chemistry Principles were prioritized against the 5 Pillars of the IFRA–IOFI Sustainability Charter

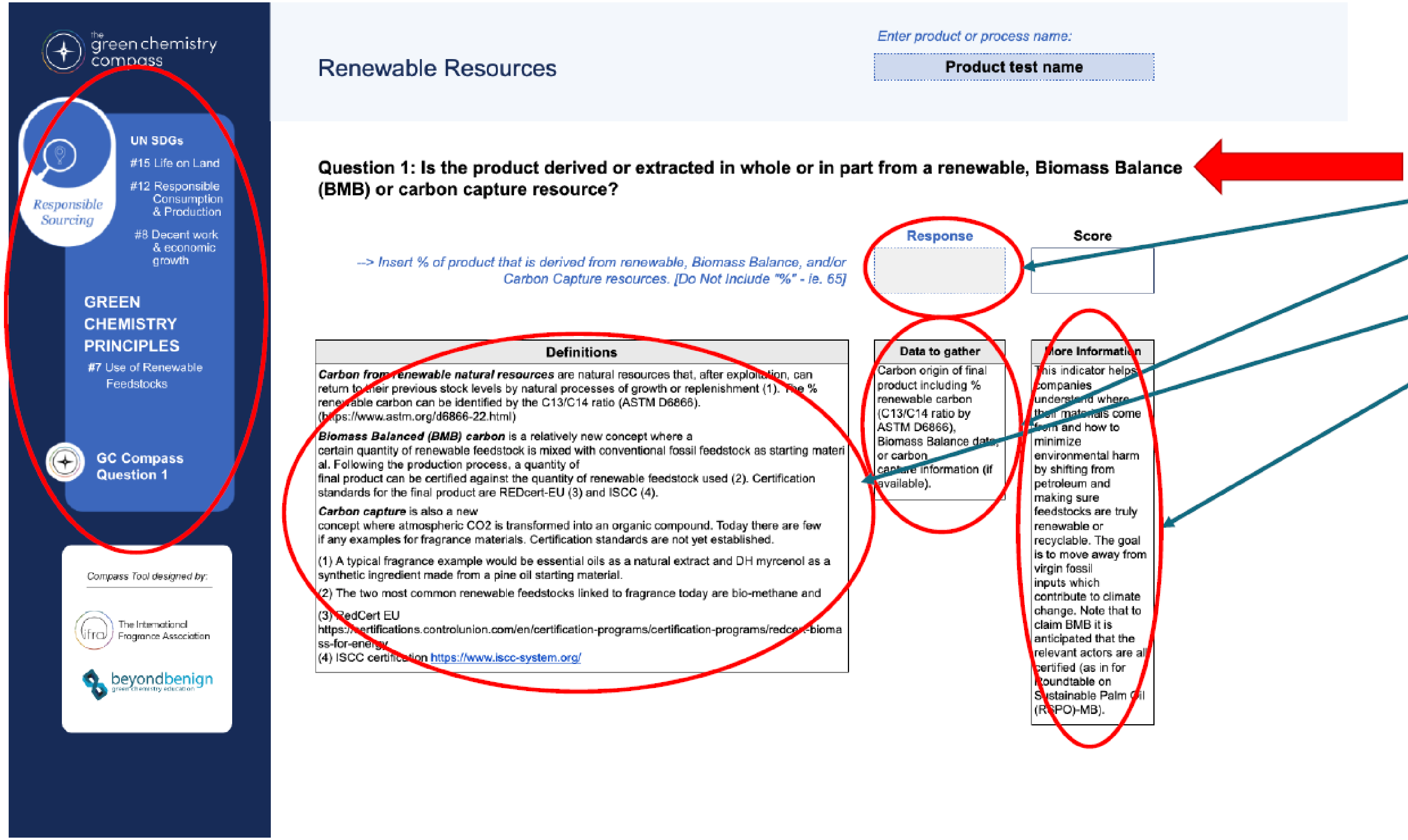
	1.Waste Prevention	2.Atom Economy	3.Less Hazardous Chemical Synthesis	4.Designing Safer Chemicals	5.Safer Solvents & Auxiliaries	6.Design for Energy Efficiency	7.Use of Renewable Feedstocks	8.Reduce Derivatives	9.Catalysis	10.Design for Degradation	11.Real-Time Pollution Prevention	12.Safer Chemistry for Accident Prevention
Responsible Sourcing							Question 1					
Environmental footprint and climate change	Question 4					Question 2			Question 3	Question 5		
Well-Being of Employees			Question 6		Question 7							Question 6
Product Safety				Question 8								
Transparency and Partnerships												

GC Compass: Guiding Questions

Category and Question
Responsible Sourcing
1. Is the product derived or extracted in whole or in part from a renewable, BMB, carbon capture resource?
Environmental footprint & Climate Change
2. a) To what extent is the process for making this product energy intensive? b) Is renewable energy used in whole or in part in the process?
3. a) What type of catalyst, if any, is used in this process? b) What is the mol-recycle number for the catalyst used (if applicable)?
4. How much waste is generated in the process?
5. To what extent is the product or formulation biodegradable?
Well-Being of Employees
6. What type of solvents are used?
7. Do the reagents or raw materials pose any physical, health or environmental hazards?
Product Safety
8. Does the product pose any physical, health or environmental hazards?

IFRA

GC Compass: Guiding Questions



Enter Response

What data is needed?

What does this mean?

Additional Information?

IFRA

GC Compass: Guiding Questions

the green chemistry compass

Responsible Sourcing

UN SDGs
#15 Life on Land
#12 Responsible Consumption & Production
#8 Decent work & economic growth

GREEN CHEMISTRY PRINCIPLES
#7 Use of Renewable Feedstocks

GC Compass Question 1

Compass Tool designed by:
The International Fragrance Association
beyondbenign

Renewable Resources

Enter product or process name:

Product test name

Question 1: Is the product derived or extracted in whole or in part from a renewable, Biomass Balance (BMB) or carbon capture resource?

--> Insert % of product that is derived from renewable, Biomass Balance, and/or Carbon Capture resources. [Do Not Include "%" - ie. 65]

Response	Score
75	Needs Improvement

Score is automatically populated

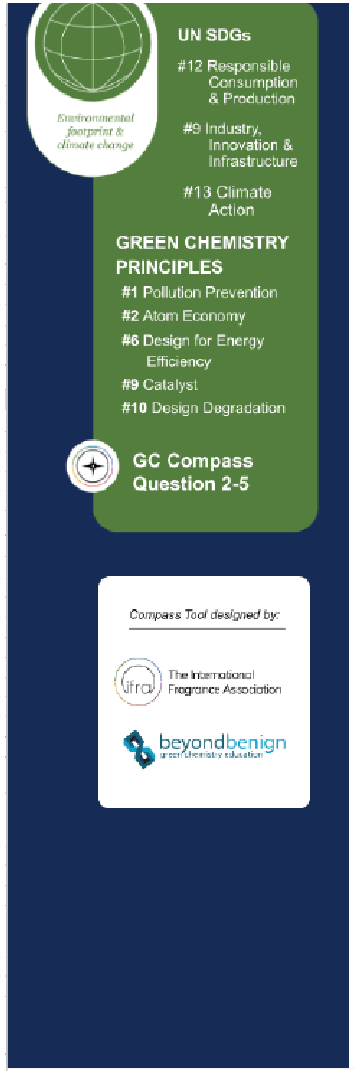
Definitions
Carbon from renewable natural resources are natural resources that, after exploitation, can return to their previous stock levels by natural processes of growth or replenishment (1). The % renewable carbon can be identified by the C13/C14 ratio (ASTM D6866). (https://www.astm.org/d6866-22.html) ***Biomass Balanced (BMB) carbon*** is a relatively new concept where a certain quantity of renewable feedstock is mixed with conventional fossil feedstock as starting materi al. Following the production process, a quantity of final product can be certified against the quantity of renewable feedstock used (2). Certification standards for the final product are REDcert-EU (3) and ISCC (4). ***Carbon capture*** is also a new concept where atmospheric CO2 is transformed into an organic compound. Today there are few if any examples for fragrance materials. Certification standards are not yet established. (1) A typical fragrance example would be essential oils as a natural extract and DH myrcenol as a synthetic ingredient made from a pine oil starting material. (2) The two most common renewable feedstocks linked to fragrance today are bio-methane and (3) RedCert EU https://certifications.controlunion.com/en/certification-programs/certification-programs/redcert-bioma ss-for-energy (4) ISCC certification https://www.iscc-system.org/

Data to gather
Carbon origin of final product including % renewable carbon (C13/C14 ratio by ASTM D6866), Biomass Balance data, or carbon capture information (if available).

More Information
This indicator helps companies understand where their materials come from and how to minimize environmental harm by shifting from petroleum and making sure feedstocks are truly renewable or recyclable. The goal is to move away from virgin fossil inputs which contribute to climate change. Note that to claim BMB it is anticipated that the relevant actors are all certified (as in for Roundtable on Sustainable Palm Oil (RSPO)-MB).

Answers are automatically ranked by Most Preferred, Needs Improvement, or Least Preferred

GC Compass: Guiding Questions



Question 3: a) What type of catalyst, if any, is used in this process? b) What is the mol-recycle number for the catalyst used (if applicable)?

Step 1: What type of catalyst, if any, is used in this process:

--> Mark an "X" to the left of all the catalysts used in the process, or mark an "X" to the left of no catalysts responses or "Do not know".

Response

	Bio-based Catalysts
	Enzymes
	Bio-based catalyst

	No catalysts
	No - we use Stoichiometric reagents
	No - not relevant for this process

	Do not know

	Metal-based Catalysts
	Au
	B
	Bi
	Co
	Cu
	Li
	Mg
	Mn
	Mo
	Nb
	Ni
	P
	Pd
	Sb
	Sc
	Se
	Sn
	Sr
	Ti
	Y
	V
	W
	Y
	Zr

	Scarce (low-moderate hazard) Catalysts
	Ag
	Ge
	Hf
	Ir
	Os
	Pt
	Ru
	Rh
	Ta
	Te
	Zn

	Scarce (high hazard) Catalysts
	As
	Pb
	Cd
	Cr
	Ga
	Hg
	In
	U

Step 1 Score:

Step 2: What is the mol-recycle number for the catalyst used

--> Insert is the mol-recycle number (turnover number (TON)) for the catalyst in this process:

FINAL Score

Check-list of types of catalyst(s) used

Preference to Enzyme/bio-based catalysts and abundant/less hazardous metals

GC Compass: Guiding Questions

the ifra green chemistry compass

Well-being of employees

UN SDGs

#8 Decent Work & Economic Growth

#5 Gender Equality

#10 Reduced Inequalities

#4 Quality Education

GREEN CHEMISTRY PRINCIPLES

#3 Less Hazardous Chemical Synthesis

#5 Solvents

#12 Safer Chemistry for Accident Prevention

GC Compass Question 6-7

Compass Tool designed by:

The International Fragrance Association

beyondbenign green chemistry education

Solvents

Enter product or process name:

Product test name

Question 6: What type of solvents are used?

Score

--> Mark an "X" to the left of all the solvents used in the process, or mark an "X" to the left of no catalysts responses or "Do not know".

Response:

	Most Preferred Solvents
	acetic anhydride
	anisole
	benzyl alcohol
	ethanol
	ethyl acetate
	carbon dioxide (supercritical)
	cyclohexanone
	ethylene glycol
	isopropanol
	isopropyl acetate
	isopropyl myristate
	methyl acetate
	methylethylketone
	n-butylacetate
	n-butylalcohol
	sulfolane
	t-butylalcohol
	water

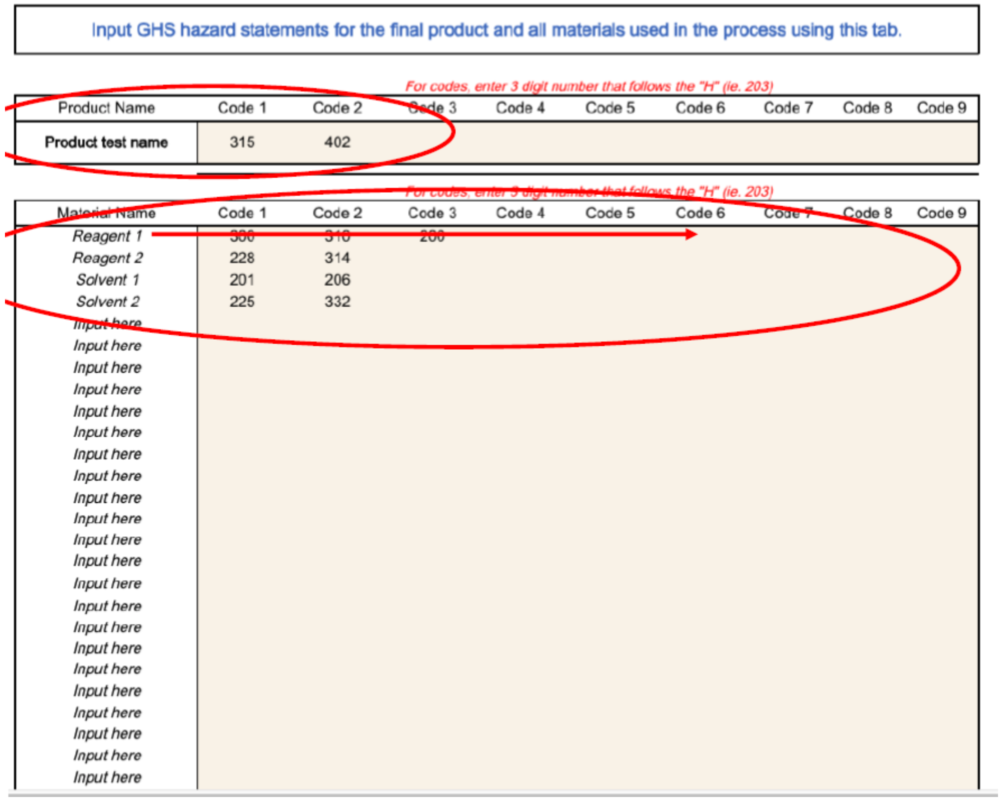
	Needs Improvement Solvents
	acetic acid
	acetone
	acetonitrile
	benzyl benzoate
	chlorobenzene
	dimethyl sulfoxide (DMSO)
	dipropylene glycol
	heptane
	methanol
	methyl-tetrahydrofuran
	methyl-cyclohexane
	N,N'-dimethylpropyleneurea (DMPU)
	toluene
	triethyl citrate
	xylenes

	Least Preferred Solvents
	benzene
	carbon disulfide (CS2)
	carbon tetrachloride (CCl4)
	chloroform
	cyclohexane
	1,2-dichloroethane (DCE)
	dichloromethane (DCM)
	diethyl ether
	diisopropyl ether
	dimethoxyethane (DME)
	dimethylacetamide (DMAc)
	dimethylformamide (DMF)
	1,4-dioxane
	formic acid
	hexamethylphosphoramide
	hexane
	methoxy-ethanol
	methyl isobutyl ketone (MIBK)
	methyl tert-butyl ether (MTBE)
	N-methyl-2-pyrrolidone (NMP)
	nitromethane
	pentane
	pyridine
	tetrahydrofuran (THF)
	triethylamine (TEA)

	No Solvents
	No - Solvents are not used in this process
	Do not know

Definitions
A solvent, typically a liquid, is a substance capable of or used for dissolving a substance. Solvents are used in large volumes in chemical reactions and in purification and extraction techniques. Typical solvents used in chemical reactions and processes can pose physical hazards, such as flammability and explosivity, and a wide range of health hazards.

GC Compass: Guiding Questions



Input GHS hazard statements for the final product and all materials used in the process using this tab.

For codes, enter 3 digit number that follows the "H" (ie. 203)

Product Name	Code 1	Code 2	Code 3	Code 4	Code 5	Code 6	Code 7	Code 8	Code 9
Product test name	315	402							

For codes, enter 3 digit number that follows the "H" (ie. 203)

Material Name	Code 1	Code 2	Code 3	Code 4	Code 5	Code 6	Code 7	Code 8	Code 9
Reagent 1	300	316	200						
Reagent 2	228	314							
Solvent 1	201	206							
Solvent 2	225	332							
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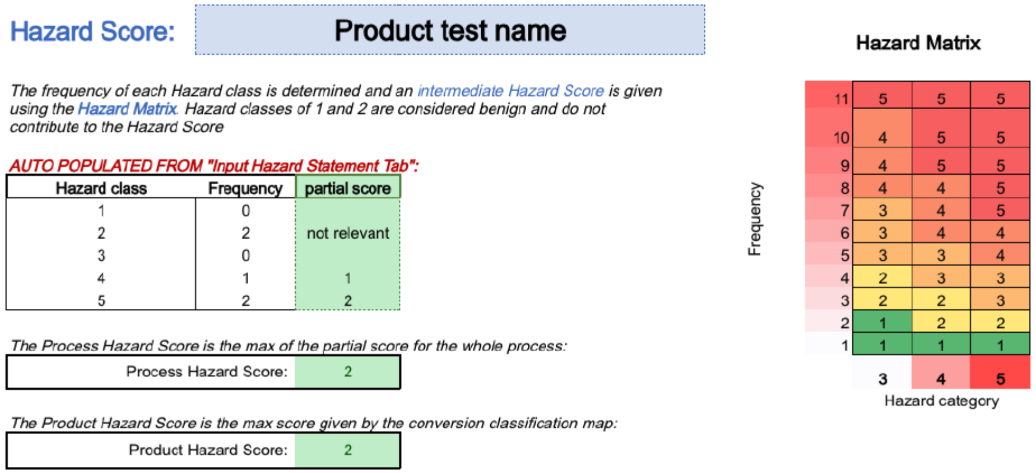

Hazard Score: Product test name

The frequency of each Hazard class is determined and an intermediate Hazard Score is given using the Hazard Matrix. Hazard classes of 1 and 2 are considered benign and do not contribute to the Hazard Score

AUTO POPULATED FROM "Input Hazard Statement Tab":

Hazard class	Frequency	partial score
1	0	not relevant
2	2	not relevant
3	0	
4	1	1
5	2	2

The Process Hazard Score is the max of the partial score for the whole process:

Process Hazard Score:	2

The Product Hazard Score is the max score given by the conversion classification map:

Product Hazard Score:	2

Hazard Matrix

Frequency	3	4	5
11	5	5	5
10	4	5	5
9	4	5	5
8	4	4	5
7	3	4	5
6	3	4	4
5	3	3	4
4	2	3	3
3	2	2	3
2	1	2	2
1	1	1	1

Hazard category

Calculations are based on:

- Severity of hazard (through a weighting of the GHS hazard scores)
- Frequency of hazard category appearance
- Final Hazard Scores ***use worst case*** of Hazard Class and Frequency table

IFRA

GC Compass: Guiding Questions

The following is a summary of indicators for: **My product**

Category and Question	*Result*	*Explanation*	*Most Preferred (target)*
Responsible Sourcing			
1. Is the product derived or extracted in whole or in part from a renewable, BMB, carbon capture resource?	Needs Improvement	75% product derived or extracted in whole or in part from a renewable, Biomass Balance (BMB) or carbon capture resource. Needs Impovement ratings are based on 50% - 99.9% of product being derived from renewable, Biobased Mass Balance, and/or Carbon Capture resources.	100% of product is derived from renewable, Biobased Mass Balance, and/or Carbon Capture resources.
Environmental footprint & Climate Change			
2. a) To what extent is the process for making this product energy intensive? 2. b) Is renewable energy used in whole or in part in the process?	Most Preferred	Temperatures used were between either -10 to 50 degrees Celsius or the pressure was less than 5 ATM. OR The LCA carbon footprint was less than 10 kg CO2/kg material *Note: If 50% or more of the process is renewable energy, the score will be bumped up a level.	Temperatures used are between -10 to 50 degrees Celsius or the pressure was less than 5 ATM. *OR* The LCA carbon footprint is less than 10 kg CO2/kg material "Note: If 50% or more of the process is renewable energy, the score will be bumped up a level."
3. a) What type of catalyst, if any, is used in this process? 3. b) What is the mol-recycle number for the catalyst used (if applicable)?	Needs Improvement	Metal-Based Catalysts were used in the reaction. Consider using a biocatalyst or enzyme or increase the TON.	A biocatalyst or enzyme is used. With the exception of high hazard catalyst, there is preference for catalysts with a mol-recycle number 1,000 or greater, which can improve the score result by one level.
4. How much waste is generated in the process?	Least Preferred	The reported E-factor is 100. Least preferred ratings are when the E-factor is more than 25	The Environmental Impact Factor (E-factor), which is the total mass of waste from the process divided by the total mass of product, is ideally less than 5.
5. To what extent is the product or formulation biodegradable?	Most Preferred	This product or formulation is readily biogradeable, which means, according to the OECD,it is greater than or equal to 60% biodegradable within 28 days	Most preferred is a product or formulation that is readily biodegradable. According to the OECD, readily biodegradable means greater than or equal to 60% biodegradable within 28 days
Well-Being of Employees			
6. What type of solvents are used?	Needs Improvement	One or more of the solvents used in the chemical process or formulation process could use improvement. Check the ACS Pharma Rountable Sovent Tool if looking for a replacement.	The most preferred solvents are ones that have low toxicity, low volatility, and low flammability, The list of most preferred solvents include acetic anhydride, anisole, benzyl alcohol, ethanol, ethyl acetate, carbon dioxide (supercritical), cyclohexanone, ethylene glycol, isopropanol, isopropyl acetate, isopropyl myristate, methyl acetate, methyl ethyl ketone, n-butyl acetate, n-butyl alcohol, sulfolane, t-butyl alcohol, water
7. Do the reagents or raw materials pose any physical, health or environmental hazards?	Most Preferred	The Hazard Score of this process, according to the Hazard Score Calculator, is 2. Most perferred ratings are based on Hazard Scores less than 3.	The most preferred score hazard scores are 1-2, indicating low hazards associated with the reagents and raw materials in the process. Explore the ACS Green Chemistry Institute Pharmaceutical Roundtable's Reagent Guides to find alternative reagents for common chemical transformations: https://reagents.acsgcipr.org/
Product Safety			
8. Does the product pose any physical, health or environmental hazards?	Most Preferred	The Hazard Score of this product, according to the Hazard Score Calculator, is 2. Most perferred ratings are based on Hazard Scores less than 3.	The most preferred score hazard scores are 1-2, indicating low hazards associated with the product.

IFRA

What can the IFRA Green Chemistry Compass help with?

- Target areas for improvement
- Guidance towards best practices
- Where to find additional Green Chemistry Resources (Additional Resources tab included)

Conclusion

Green Metrics & Sustainability in Perfumery

Still an on-going process
Attempt to harmonize different methods of calculation
Definitions of the «best» metrics?

Needs for Renewable Carbons?
Critical environmental factors are still difficult to assess or incompletely characterized by available methods (soil erosion, demographic pressure, …)

LCA Analysis but **Life Cycle Assessment of a product is never set in stone**
Carbon Foot-Print ? Other Foot-Print?

Net-Zero Emission Goal……What is one of the key Problem? What to do ?

Thanks !!