>PINK

Materials Safe (and Sustainable) by Design

How can Informatics Support a Holistic Life Cycle View?

Thomas Exner, Seven Past Nine, Slovenia and Germany

INFRAMES Fall Meeting, Rennes

16 October 2025

THE PINK PROJECT HAS RECEIVED FUNDING FROM THE EUROPEAN UNION'S HORIZON EUROPE RESEARCH AND INNOVATION PROGRAMME UNDER GRANT AGREEMENT NO. 101137809.

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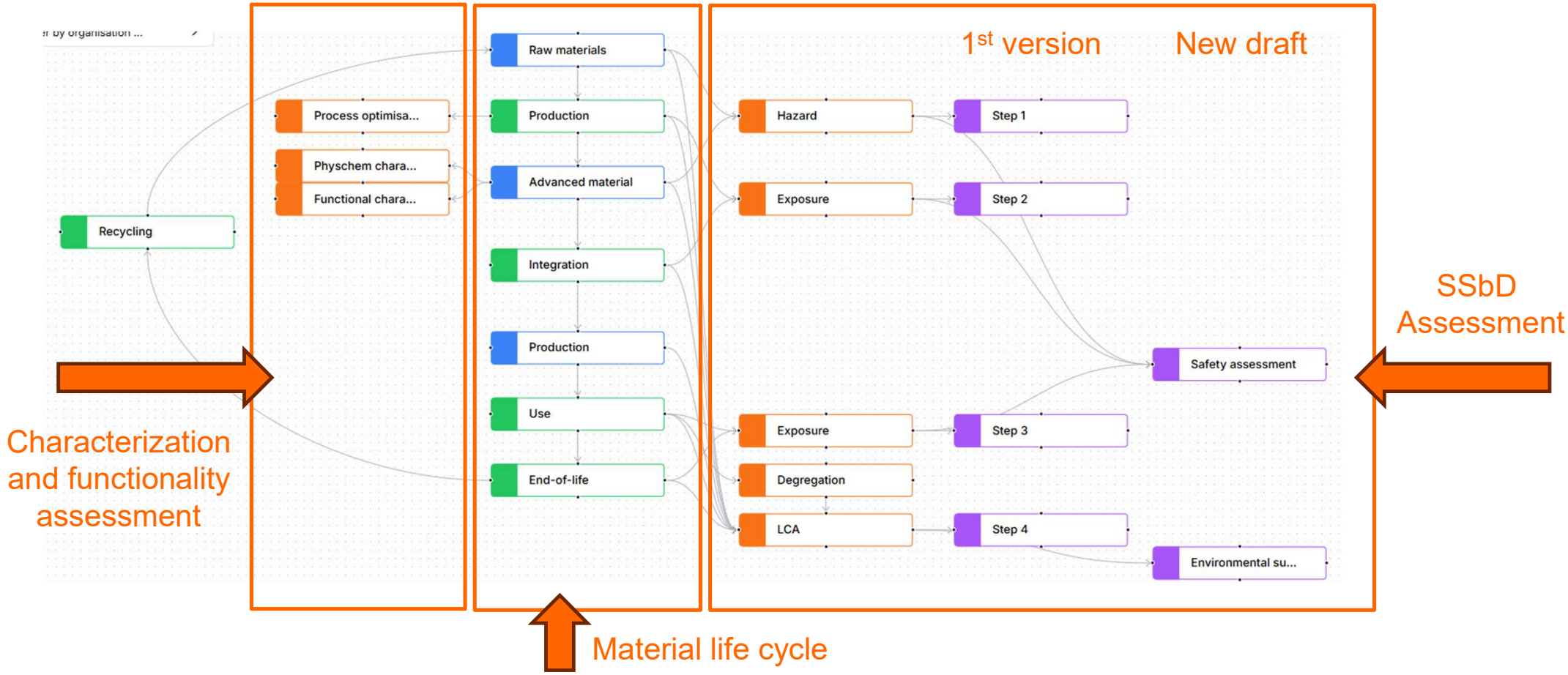
Material Life Cycle

https://green-forum.ec.europa.eu/green-business/environmental-footprint-methods/life-cycle-assessment-ef-methods_en

Life Cycle as a Study Design Map

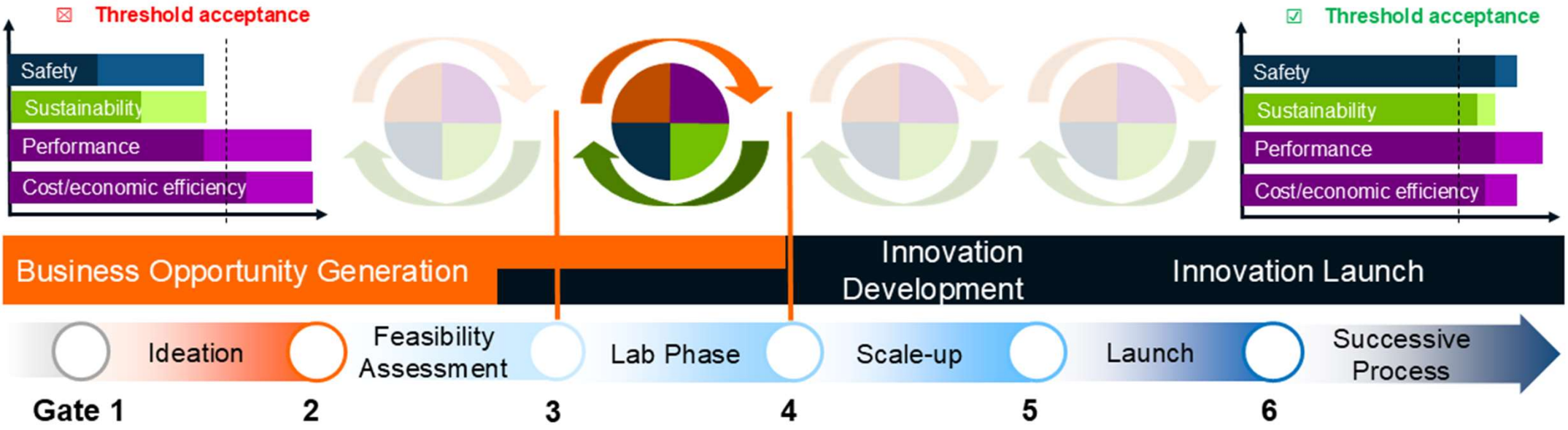


SSbD as a holistic approach

Holistic view on material value chain and life cycle

Tiered list of indicators representing the SSbD dimensions

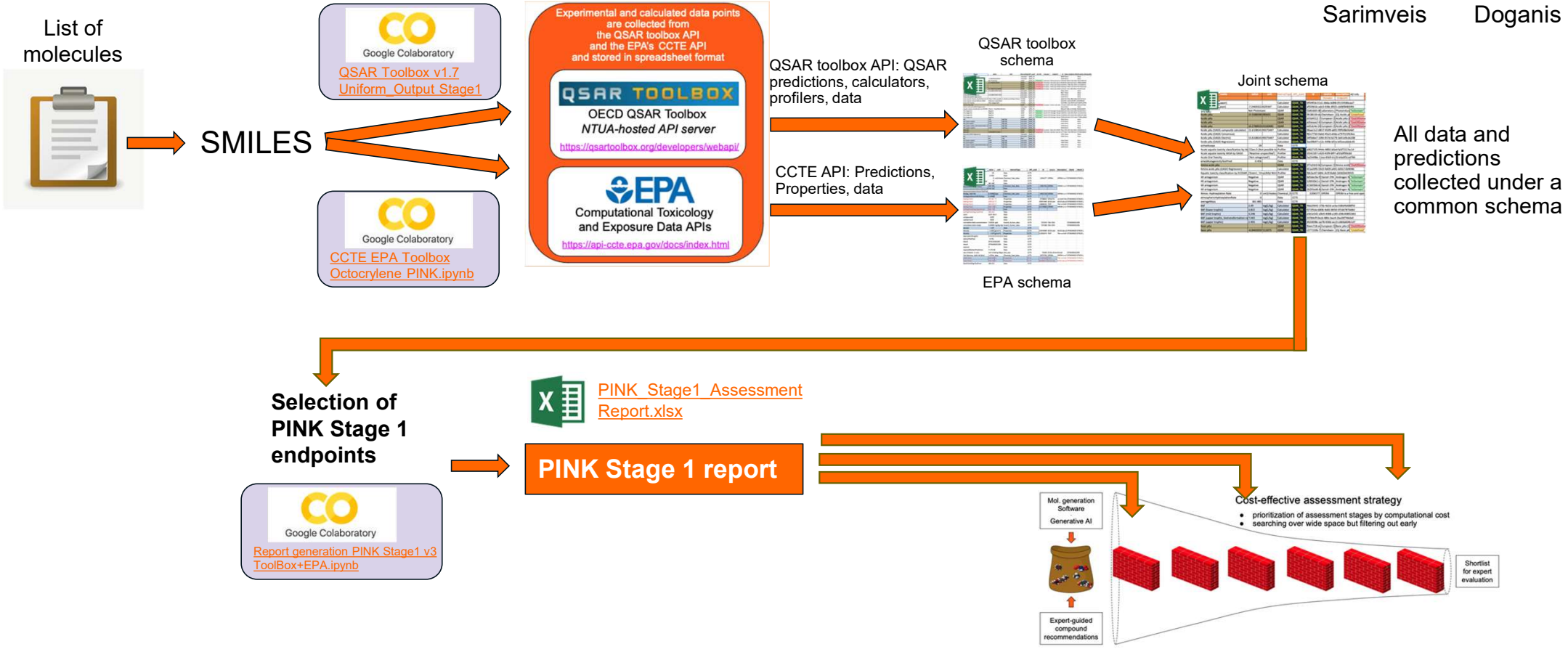
Multi-objective optimization for (re-)design



SAFETY ASSESSMENT

Workflow for candidate selection


Haralambos Sarimveis | Philip Doganis



PINK Hazard Assessment Report

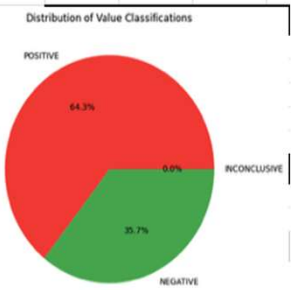
The report provides both Consolidated results for each category for overview and detailed results from multiple models for transparency.

Consolidated results

Carcinogenicity

Summary

Category	Count
POSITIVE	9
NEGATIVE	5
INCONCLU	0



Number of models with verbose output

Count
1

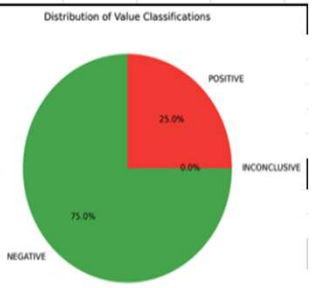
Out of Domain model: 2

Distribution of predictions

Germ Cell Mutagenicity

Summary

Category	Count
POSITIVE	5
NEGATIVE	15
INCONCLU	0



Number of models with verbose output

Count
2

Out of Domain model: 0

Carcinogenicity and Germ Cell Mutagenicity sections

Carcinogenicity

Carcinogenicity Profilers - QSAR Toolbox

Name	Value	Unit	Internaltyp	Api_Used	Id	Source	Descriptior	Ad Info
Carcinogenicity (genotox and nongenot	Structural alert for nongenotoxic (	-	Profiler	TOOLBOX	2256b12d-	-	Endpoint S	-

Carcinogenicity Qualitative QSAR- QSAR Toolbox

Name	Value	Unit	Internaltyp	Api_Used	Id	Source	Descriptior	Ad Info
FDA RCA Cancer Rodent - Danish QSAR D	Positive		QSAR	TOOLBOX	1e7d360f-8	Danish EPA	Carcinogen	InDomain
VEGA - Carcinogenicity model (CAESAR)	NON-Carcinogen		QSAR	TOOLBOX	edaafce9-0	Istituto di F	Carcinogen	OutOfDomain
FDA RCA Cancer Rat - Danish QSAR DB Le	Negative		QSAR	TOOLBOX	7ef3e1a1-d	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Female Rat - Danish QSA	Positive		QSAR	TOOLBOX	eb6861f5-1	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Mouse - Danish QSAR D	Negative		QSAR	TOOLBOX	c11ced21-2	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Female Mouse - Danish	Positive		QSAR	TOOLBOX	12b85d79-	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Female Rat - Danish QSA	Negative		QSAR	TOOLBOX	892add19-	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Male Mouse - Danish QS	Negative		QSAR	TOOLBOX	41b3e7be-	Danish EPA	Carcinogen	InDomain
FDA RCA Cancer Male Mouse - Danish QS	Positive		QSAR	TOOLBOX	adc64575-	Danish EPA	Carcinogen	InDomain
VEGA - Carcinogenicity model (IRFMN-IS	Carcinogen		QSAR	TOOLBOX	1e68bcdf-b	Istituto di F	Carcinogen	InDomain
VEGA - Carcinogenicity inhalation classi	Carcinogen		QSAR	TOOLBOX	494572f1-4	Istituto di F	Carcinogen	InDomain
FDA RCA Cancer Mouse - Danish QSAR D	Positive		QSAR	TOOLBOX	9bb94df1-4	Danish EPA	Carcinogen	InDomain
VEGA - Carcinogenicity model (ISS)	Carcinogen		QSAR	TOOLBOX	e9b1d082-	Istituto di F	Carcinogen	OutOfDomain
FDA RCA Cancer Rodent - Danish QSAR D	Negative		QSAR	TOOLBOX	1d743a96-	Danish EPA	Carcinogen	InDomain
VEGA - Carcinogenicity model (IRFMN-A	Carcinogen		QSAR	TOOLBOX	0665aa46-	Istituto di F	Carcinogen	InDomain
VEGA - Carcinogenicity oral classificatio	Carcinogen		QSAR	TOOLBOX	38cc50db-	Istituto di F	Carcinogen	InDomain

Carcinogenicity Quantitative QSAR - QSAR Toolbox

Name	Value	Unit	Internaltyp	Api_Used	Id	Source	Descriptior	Ad Info
VEGA - Carcinogenicity in male rat (COR	338.8692499661305	mg/kg bdw	QSAR	TOOLBOX	1ce26c1e-9	Istituto di F	Carcinogen	OutOfDomain
VEGA - Carcinogenicity oral Slope Facto	2.634461020253181	mg/kg bdw	QSAR	TOOLBOX	06e49033-	Istituto di F	Carcinogen	OutOfDomain
VEGA - Carcinogenicity inhalation Slope	4.969704075159981	mg/kg bdw	QSAR	TOOLBOX	9dcaa97c-b	Istituto di F	Carcinogen	OutOfDomain
VEGA - Carcinogenicity in female Rat (CC	5922.65914635249	mg/kg bdw	QSAR	TOOLBOX	66f66df4-c	Istituto di F	Carcinogen	OutOfDomain

Carcinogenicity - EPA

Name	Value	Unit	Internaltyp	Api_Used	Id	Source	Descriptior	Ad Info

Carcinogenicity information sheet from the PINK SSbD Stage 1 Hazard Profile Report

CHARACTERISATION / FUNTIONALITY ASSESSMENT

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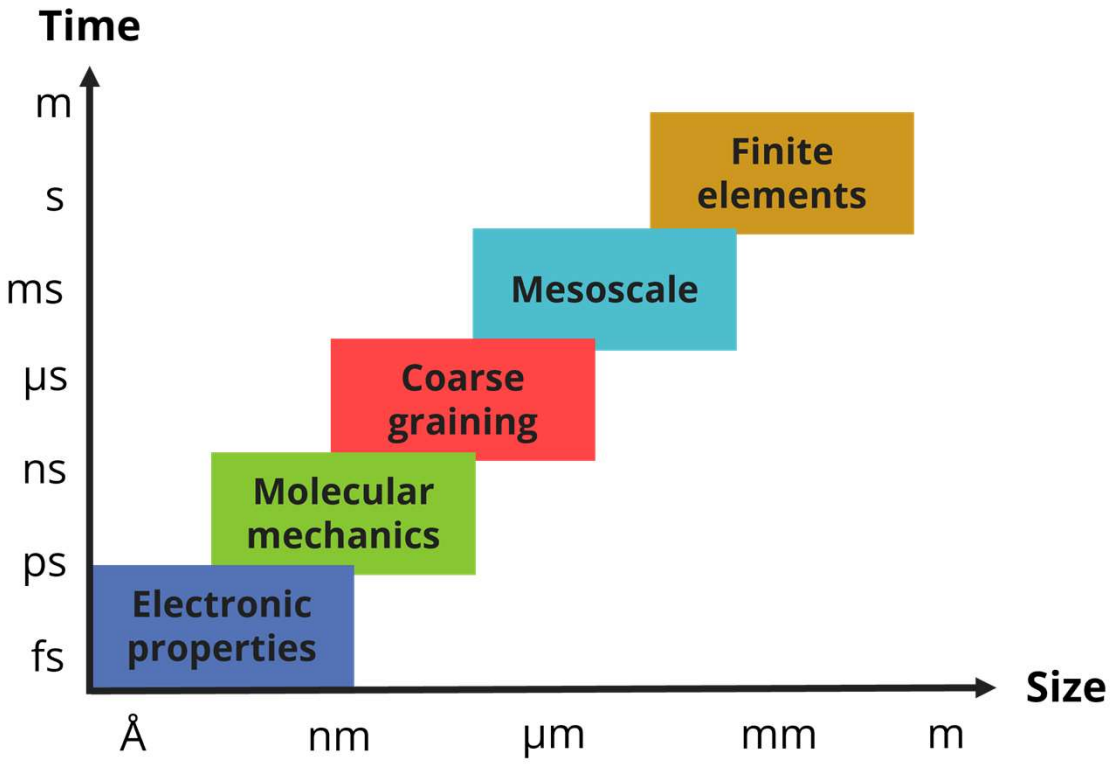
Multiscale modelling for SSbD



- Hydrophobic and oleophobic properties
- Adsorption energies
- Leaching mechanisms
- Toxicity assessment
- Nanoparticle-membrane interfaces

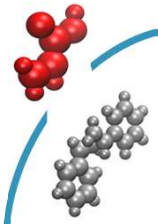

Francesco Mercuri


Andrea Lorenzoni


Fabio Le Piane


Fabio Passi

Modelling workflow for co-polymer analysis



INPUT

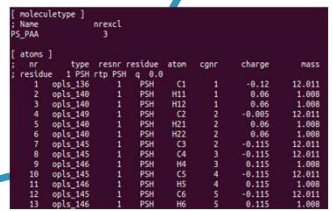
SPECIES::monomers SMILES

POLYMER BUILDER

SPECIES::formula/pdb
RATIO::n_units

FF BUILDER

FF_TYPE::molecular
SPECIES::tags/smiles

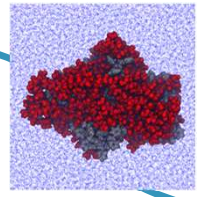


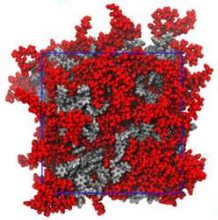
```
[ moleculetype ]
; Name            nrexcl
PS_PAA              3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
; residue   1 PSH rtp PSH  q  0.0
     1    opls_136      1    PSH     C1      1      -0.12     12.011
     2    opls_140      1    PSH    H11      1       0.06      1.008
     3    opls_140      1    PSH    H12      1       0.06      1.008
     4    opls_149      1    PSH     C2      2     -0.005     12.011
     5    opls_140      1    PSH    H21      2       0.06      1.008
     6    opls_140      1    PSH    H22      2       0.06      1.008
     7    opls_145      1    PSH     C3      2     -0.115     12.011
     8    opls_145      1    PSH     C4      3     -0.115     12.011
     9    opls_146      1    PSH     H4      3      0.115      1.008
    10    opls_145      1    PSH     C5      4     -0.115     12.011
    11    opls_146      1    PSH     H5      4      0.115      1.008
    12    opls_145      1    PSH     C6      5     -0.115     12.011
    13    opls_146      1    PSH     H6      5      0.115      1.008
```

AGGREGATOR

SYSTEM::co-polymer
STATUS::amorphous
SIZE::n. chains
ENVIRONMENT::solvent





- **INDICATORS**
- **ACCURACY**

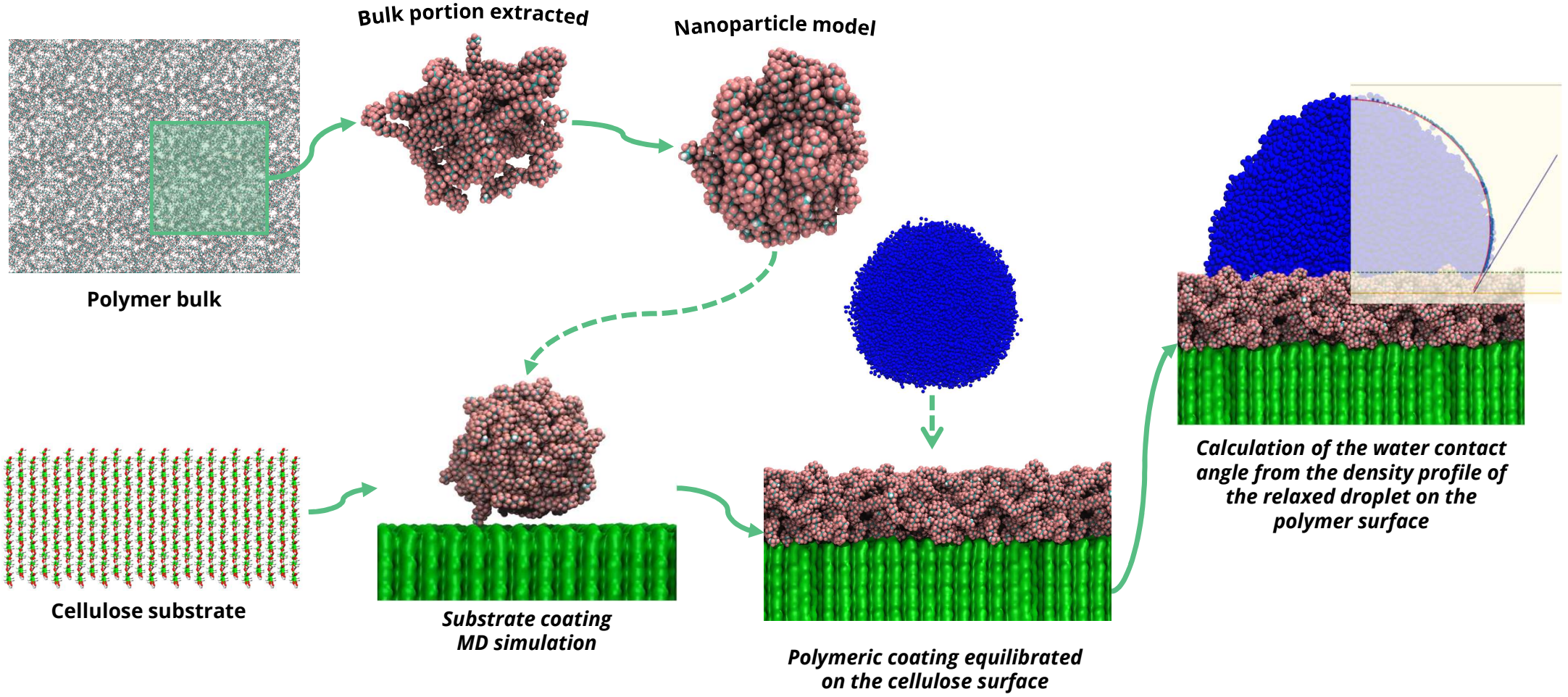
HYDROLITIC DEGRADATION

PROCESS::parameters
CONDITIONS::temperature

MECHANICAL DEGRADATION

PROCESS::parameters
ENVIRONMENT::solvent

Hydrophobicity of a coated surface

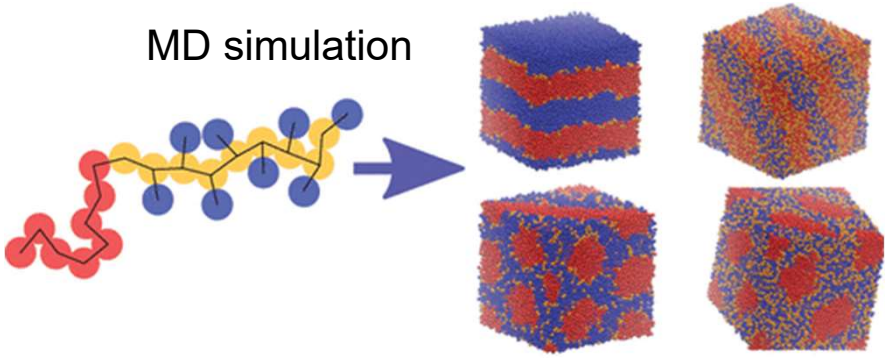


In silico characterization

Vladimir Lobaskin

- Physics-based models relate polymer structure to functionality in an explainable way:
  - Melting point, glass transition point
  - Hydrophilicity (partitioning coefficient), stickiness
  - Mechanical strength (elastic modulus)
  - Solubility and swelling
  - Permeability to gases and liquids
  - Self-assembly

This enables optimization at the stage of material design



Chremos, 2014

Functionality prediction for UV filters

Several python packages were examined for the prediction of UV spectra in terms of implementation efficiency, computational performance and fidelity of results to experimental values.
eChem (https://kthpanor.github.io/echem/docs/title.html) demonstrated the best performance, providing relatively quick results from the following methods:

- ADC(3): Third-order Algebraic Diagrammatic Construction
- TDDFT: Time-Dependent Density Functional Theory
- SA-MCSCF: State-Averaged Multiconfigurational Self-Consistent Field
- MCSCF: Multiconfigurational Self-Consistent Field

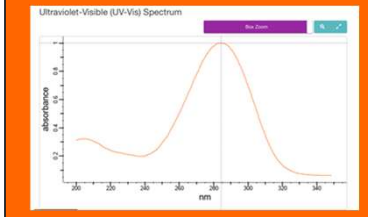
Alternatively, there is https://chemcompute.org/ that allows QM calculations on their servers.


Haralambos Sarimveis


Philip Doganis

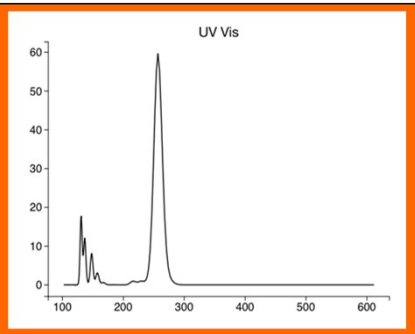
UV case study: **Examination of an alternative UV filter - Urocanic Acid**

- Started from publication on Urocanic acid, a "*novel scaffold for next-gen nature-inspired sunscreens*"
  https://doi.org/10.1039/D4CP02088J ,
  https://doi.org/10.1039/D4CP02087A
- PINK stage 1 report for Urocanic acid prepared

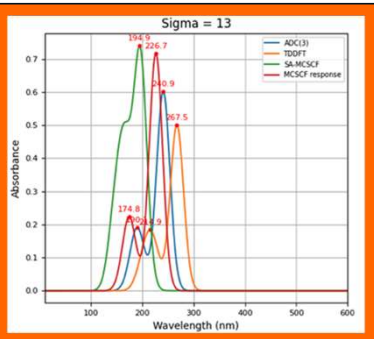


https://spectrabase.com/spectrum/CNRRUcbvaaA

Experimental UV-Vis spectra were retrieved from



https://chemcompute.org/ 3-21G neutral singlet



Computed using QM methods in Python

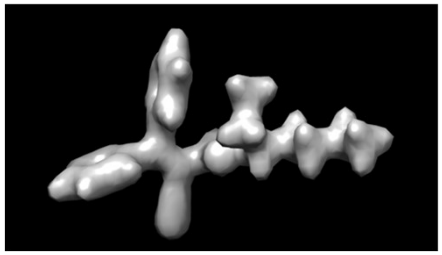
Computationally generated using QM methods used to assess the functionality

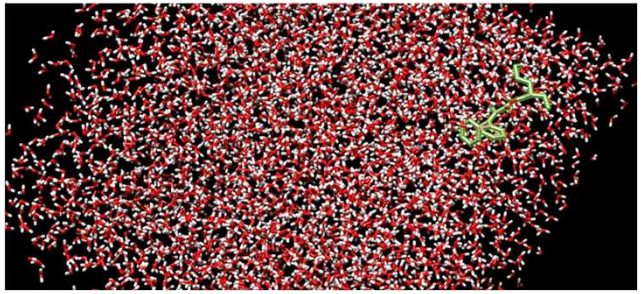
Quantum and molecular simulations to assess solubility, photostability, and encapsulation behavior

Molecular simulations of octocrylene and other chemical UV filters in a water environment in the free state, as well as when complexed with selected cyclodextrins. Cyclodextrins can act as a shield protecting UV filters.

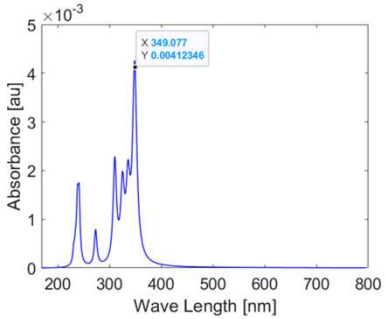
UV filters case study

Octocrylene

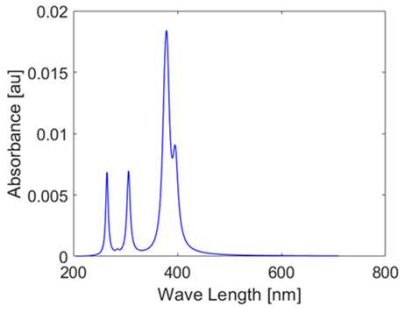




TD-DFT calculations

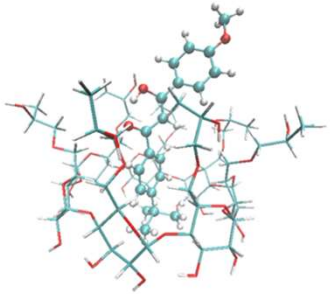


Octocrylene in water

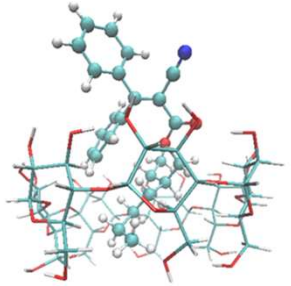


Avobenzone in gas phase

Cyclodextrins



Avobenzone + HP-β-CD



Octocrylene + β-CD

PROCESS OPTIMIZATION

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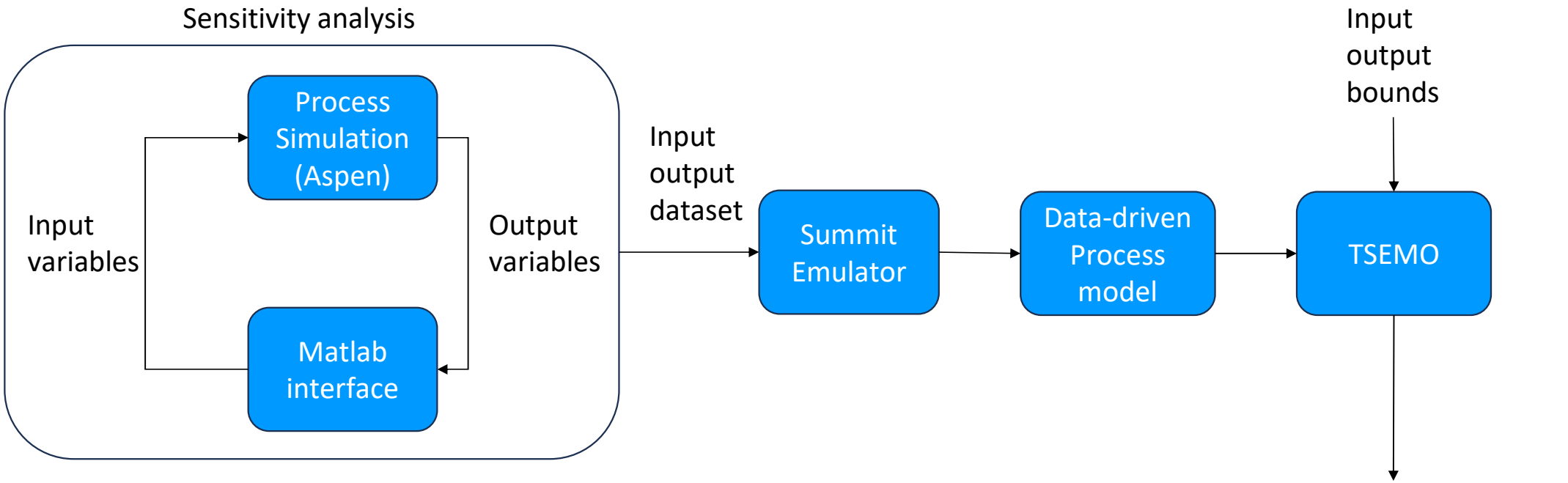
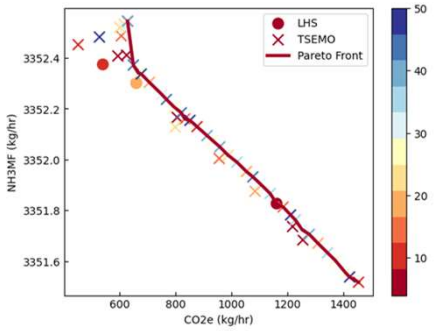
Multi-objective Safe and Sustainable Process Design Optimization



Input: P, T, F_i, C_i (Rv, Recycle, Separation processes)
Output: Yield, CO2e, byproducts (non desirable-potentially toxic)

Haralambos Sarimveis

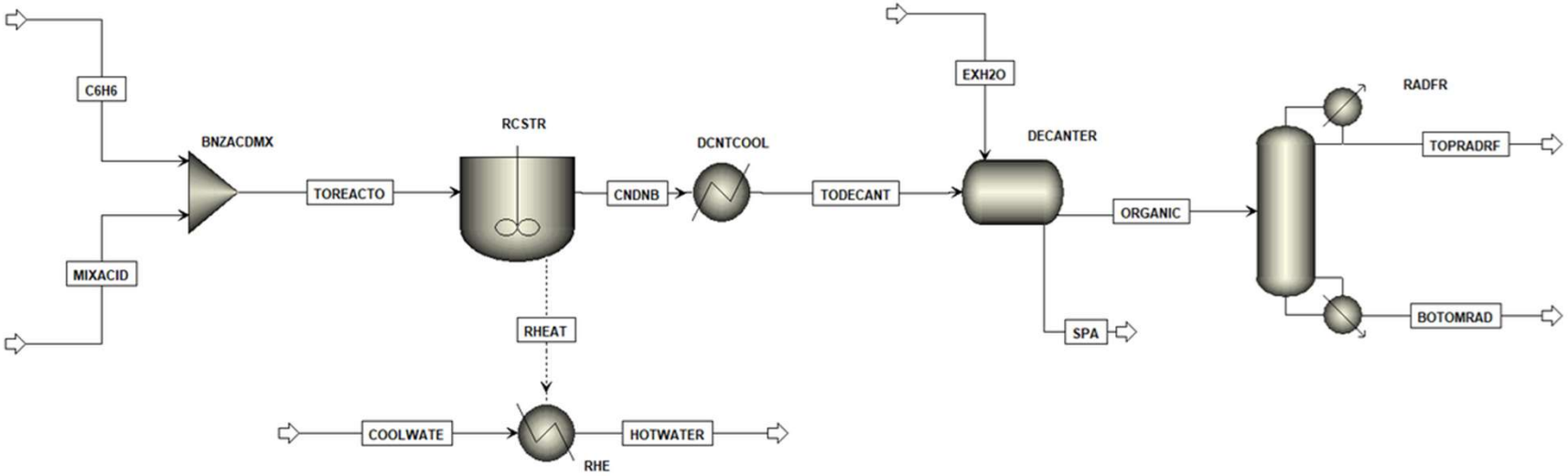
Philip Doganis



Pareto front

Multi-objective optimization of production

Nitration of benzene



Input variables:

Variables	Units	Limits
Reactor Temperature	C	[65.0,95.0]
Residence time	hr	[6.0,13.0]
Benzene to acids ratio	w/w	[0.0,1.0]

4 Objectives:

1. NB_Mol_Percentage_Yield (% mol NB/MOl C6H6) ⇨ Process efficiency (production capacity)
2. DNB_Mol_Yield (mol DNB/hr) ⇨ Safety related (toxic byprod.)
3. CO2e per kg NitroC6h6 (kg CO2/hr) ⇨ LCA related (emissions)
4. TOTALCOST ($) ⇨ LCC related (production costs)

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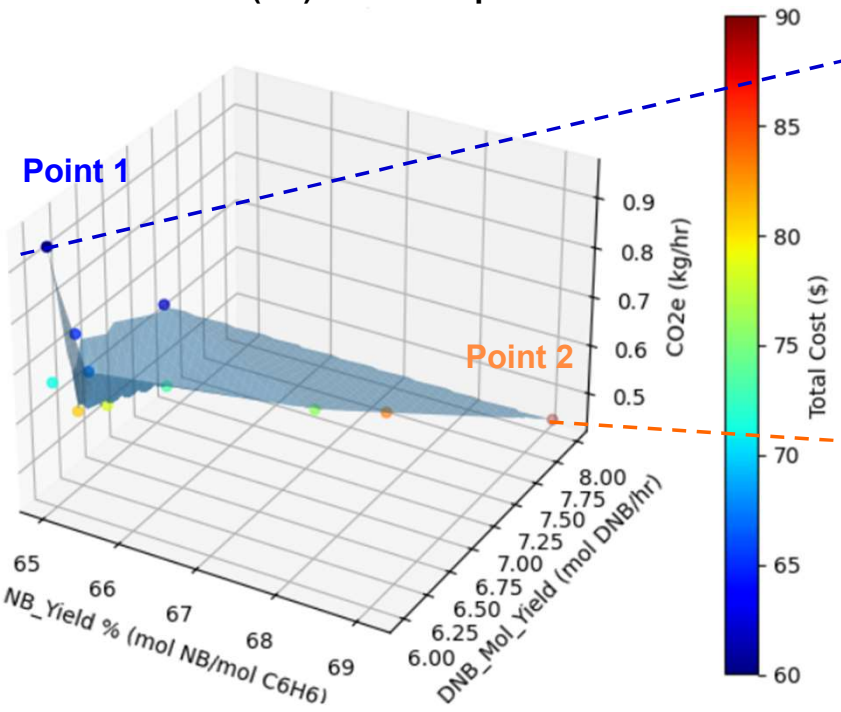
Reading the results – the Pareto front and conflicting objectives

Pareto surface (2D) + heat map for Total cost



Values of the input parameters are decided by the designer

R_T DATA	ResTime DATA	Benz2AcidRatio DATA	NByield DATA	DNByield DATA	CO2e DATA	TOTALCOST DATA
65.0	6.0	0.940553	60.0	0.0	11.0	13811.0
65.724664	6.563721	0.770414	61.987709	0.000173	11.413369	14276.293945
65.030944	6.206928	0.738339	64.898796	0.000194	12.32363	14536.286133
65.480091	6.001707	0.717673	66.898422	0.000226	12.935511	14658.143555
65.0	6.0	0.673955	71.166206	0.000314	14.402148	15174.744141
65.988574	6.371139	0.650601	73.401672	0.000393	15.111883	15502.807617
67.528135	6.660242	0.627405	75.91481	0.000495	15.888021	15788.65918
65.393521	6.229343	0.607747	78.379135	0.000528	16.9161	16062.123047
65.054719	6.189286	0.586421	80.922569	0.000603	17.849514	16366.34668
67.931696	7.095091	0.566099	83.320786	0.000746	18.505066	16815.646484
69.108916	7.980441	0.455444	90.0	0.001396	21.0	18933.447266

Example design options:

Point 1: minimum total cost, CO_2e, DNB **but** also minimum NB

Point 2: maximum total cost, CO_2e, NB **but** also maximum DNB

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USE / END-OF-LIFE

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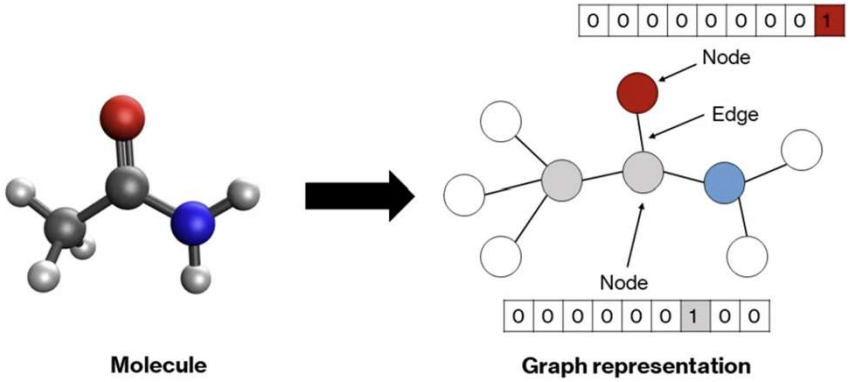
Biodegradability Classification Model


Haralambos Sarimveis


Philip Doganis

- Data sources:
  - https://zenodo.org/records/3540701
  - https://zenodo.org/records/8255910
- Dataset
  - 6849 total labeled molecules
  - Negative/Positive class ratio ~ 55/45
- Graph Neural Networks
  - Use of jaqpotpy library for modelling
  - Graph Attention Network



Biodegradability - Classification Model

Graph Neural Network (GAT) for ReadyBiodegradability Classification

giannis savvas
@john_savvas
about 2 months ago
TORCHSCRIPT

Description | Features | Predict | Metrics | Discussion

Choose Your Prediction Input Method

Fill out the form or Upload a CSV file (max 100 rows)

SMILES *

N#C/C(C(=O)OCC(CC)CCCC)=C(/c1ccccc1)c2cccc

Submit

Result

ID 10584 Success

less than a minute ago less than 5 seconds

Export CSV

Total 1 result

Rows per page
25

SMILES	ReadyBiodegradability	Probabilities
N#C/C(C(=O)OCC(CC)CCCC)=C(/c1ccccc1)c2ccccc2	0	0: 0.867 1: 0.133

Input SMILES to get the prediction

```
[7]: input_data = [{"SMILES": "N#C/C(C(=O)OCC(CC)CCCC)=C(/c1ccccc1)c2ccccc2"}]
```

Get prediction though SDK

```
[8]: prediction = jaqpot.predict_sync(model_id=1928, dataset=input_data)
print(prediction)
```

```
[{'jaqpotMetadata': {'probabilities': [0.867, 0.133], 'jaqpotRowId': '0'}, 'ReadyBiodegradability': 0.0}]
```

https://app.jaqpot.org/dashboard/models/1928/description

LIFE CYCLE ASSESSMENT

THE PINK PROJECT HAS RECEIVED FUNDING FROM THE EUROPEAN UNION'S HORIZON EUROPE RESEARCH AND INNOVATION PROGRAMME UNDER GRANT AGREEMENT NO. 101137809.

ASSOCIATED PARTNERS (I.E. (A) SWISS PARTNERS AND (B) UK PARTNERS) HAVE RECEIVED NATIONAL FUNDING FROM (A) THE SWISS STATE SECRETARIAT FOR EDUCATION, RESEARCH AND INNOVATION (SERI), AND (B) INNOVATE UK.

LCA (Antonino, Roland)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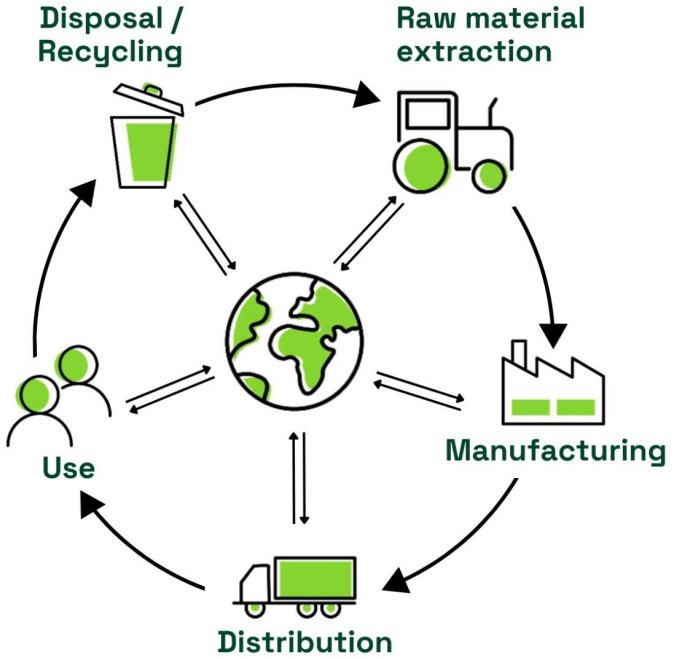
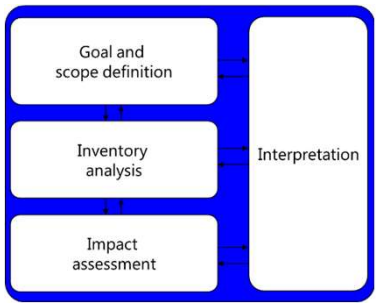
- **LCA is a comprehensive life cycle approach** that quantifies ecological and human health impacts of a product or system over its complete life cycle.
- **LCA uses credible scientific methods** to model steady-state, global environmental and human health impacts.
- **LCA helps decision makers** understand the scale of many environmental and human health impacts of competing products, services, policies, etc.
- **Basic principle** is a 2-step procedure with :
  - (i) **Collection** of the **interactions** of a system with its own environment (Input-Output-Analysis), plus
  - (ii) **Assessment** of each single environmental impact



Picture: https://www.ifco.com/life-cycle-assessment-impact/

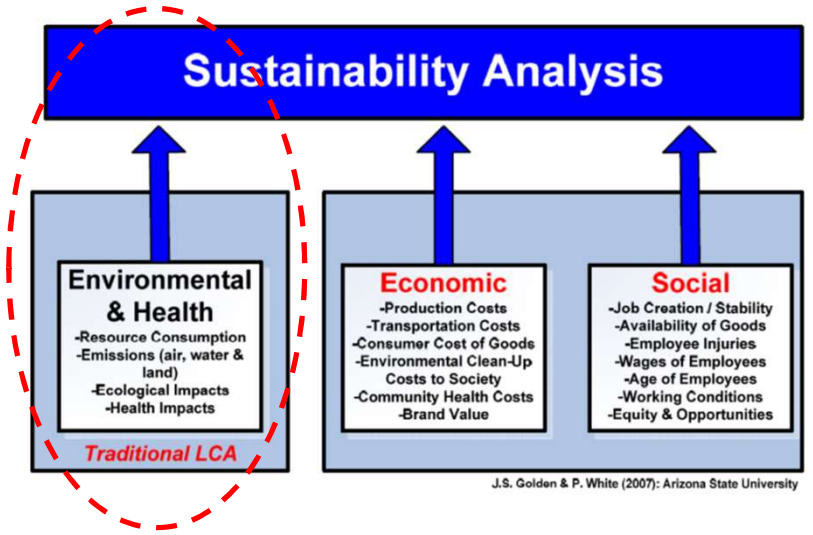
LCA – Possibilities and limitations

- Standardized within the ISO 14‘040 Serie;
- By using this „life cycle perspective“ no (hidden) shift of environmental impacts takes place.



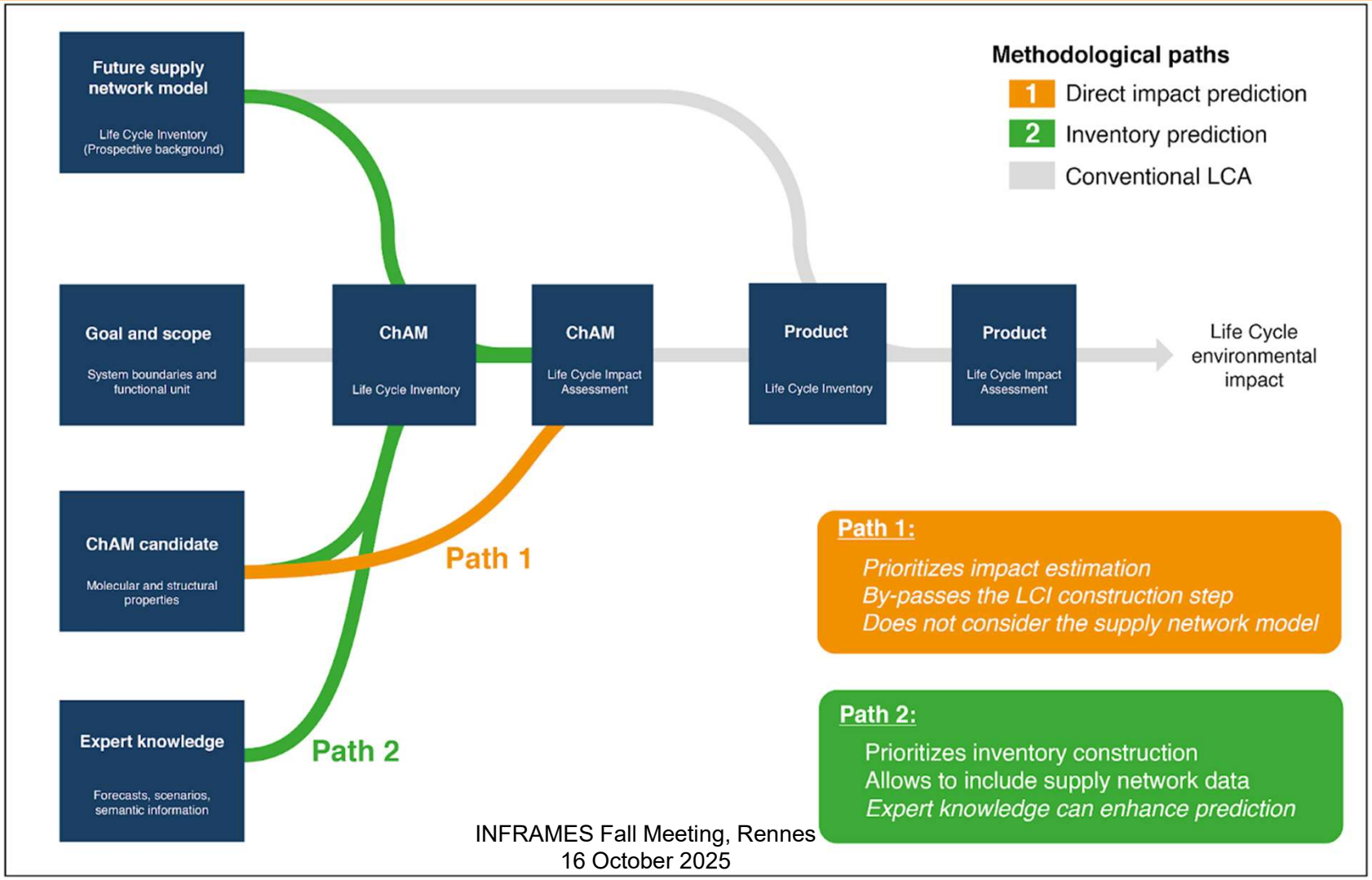
- Allows weak-point analysis ***(hot spots)*** accross the complete product life-cycle ***(from-cradle-to-grave)***
- It is a “**relative approach**” in which all inputs and outputs of the system are **collected in relation to a (specific) function**.
- This perspective on a common function gives a benchmark for comparison of alternatives, that a priori cannot be compared otherwise.

- Can be used e.g.
  - … for product comparisons;
  - … for (internal) product improvement / DfE;
  - … as basis for (new) legal requirements.
- But

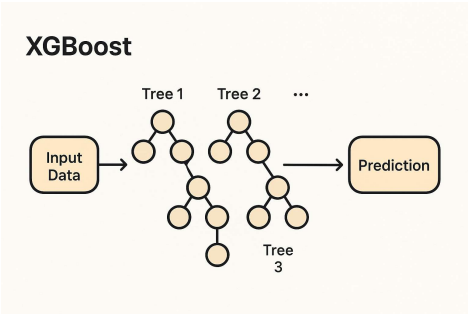


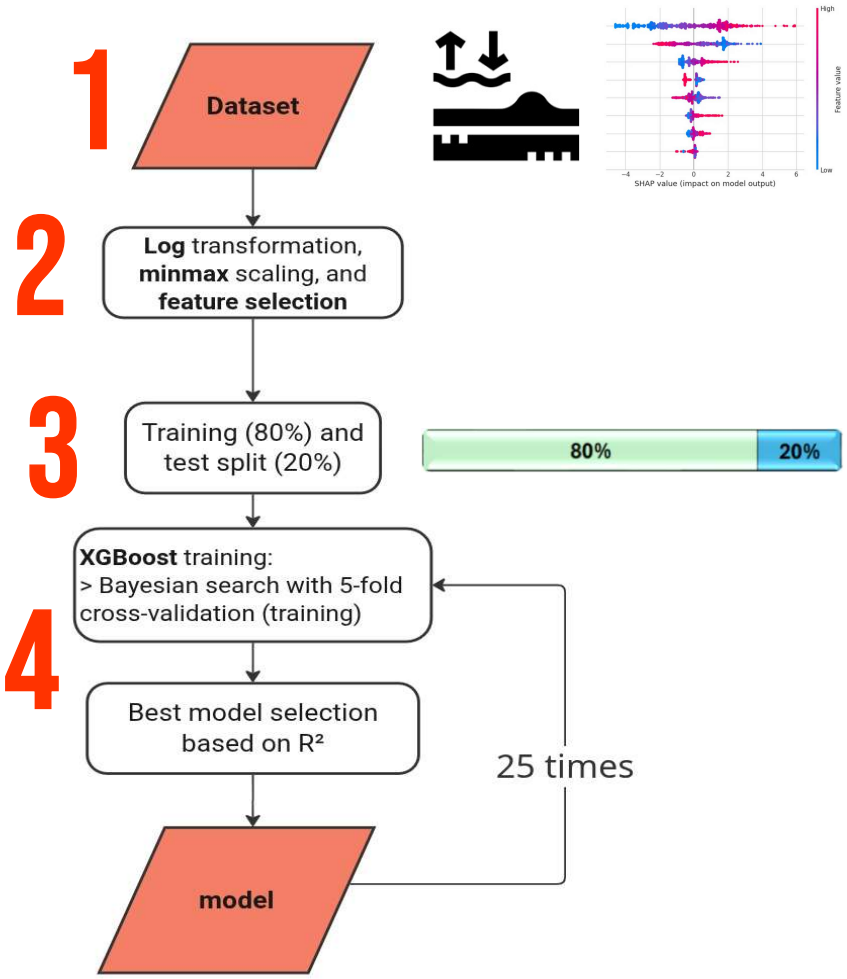
… covers ONE pillar of sustainability only !

Forward-looking LCA

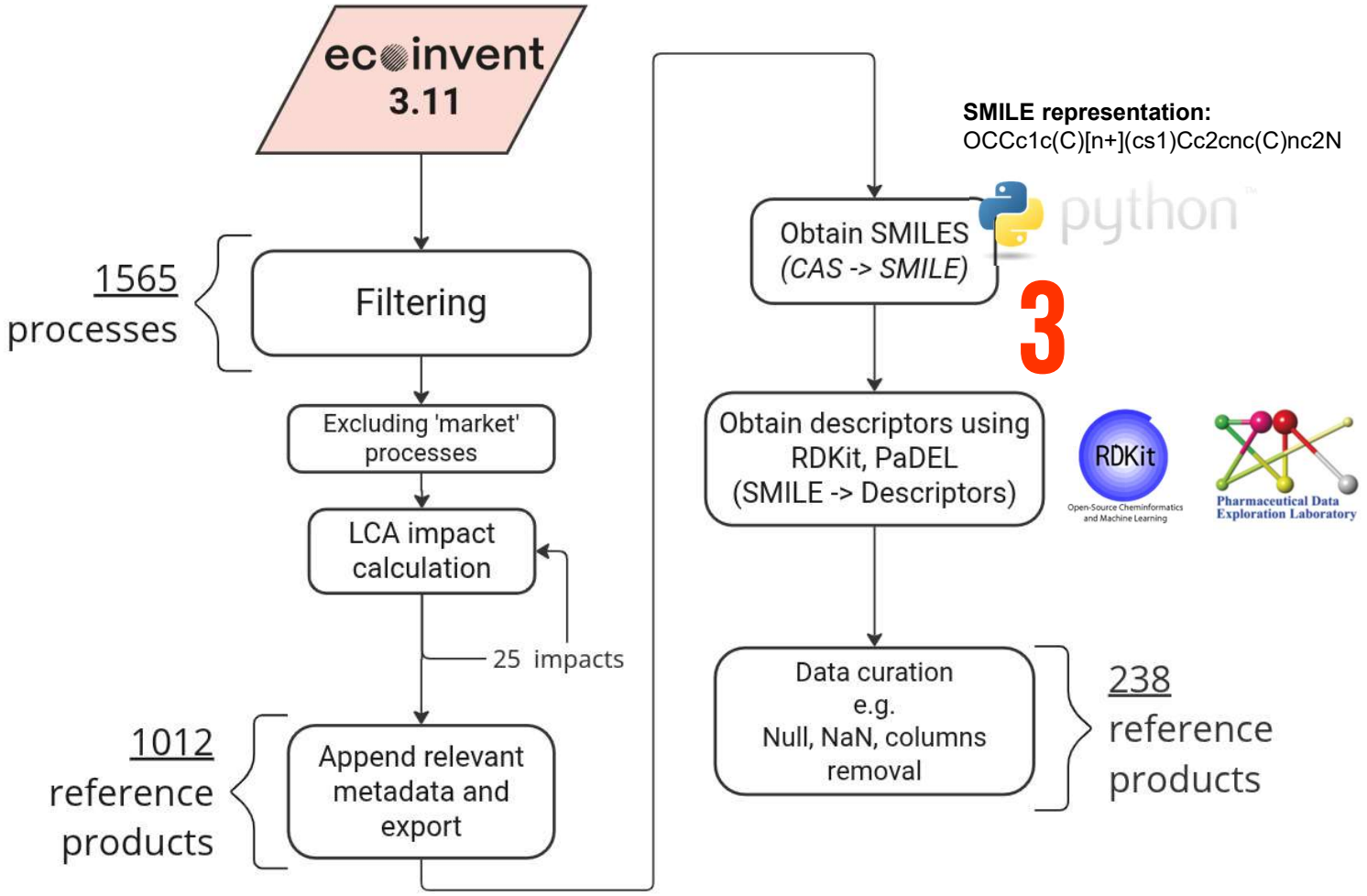


Machine Learning pipeline

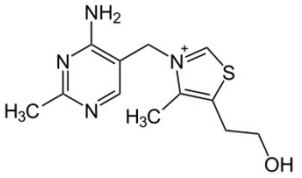




Data preparation



Example of **Thiamine** (vitamin B_1, $C_{12}H_{17}N_4OS^+$)



Summary

- Many different techniques are needed to cover all dimensions of SSbD → functionality, safety, environmental sustainability, socioeconomic sustainability, circularity
- Decisions need to be made based on balancing all this information

1 Thomas Exner

2 Seven Past Nine

>PINK

>THANK YOU!

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