

HARMLESS



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 953183



HARMLESS

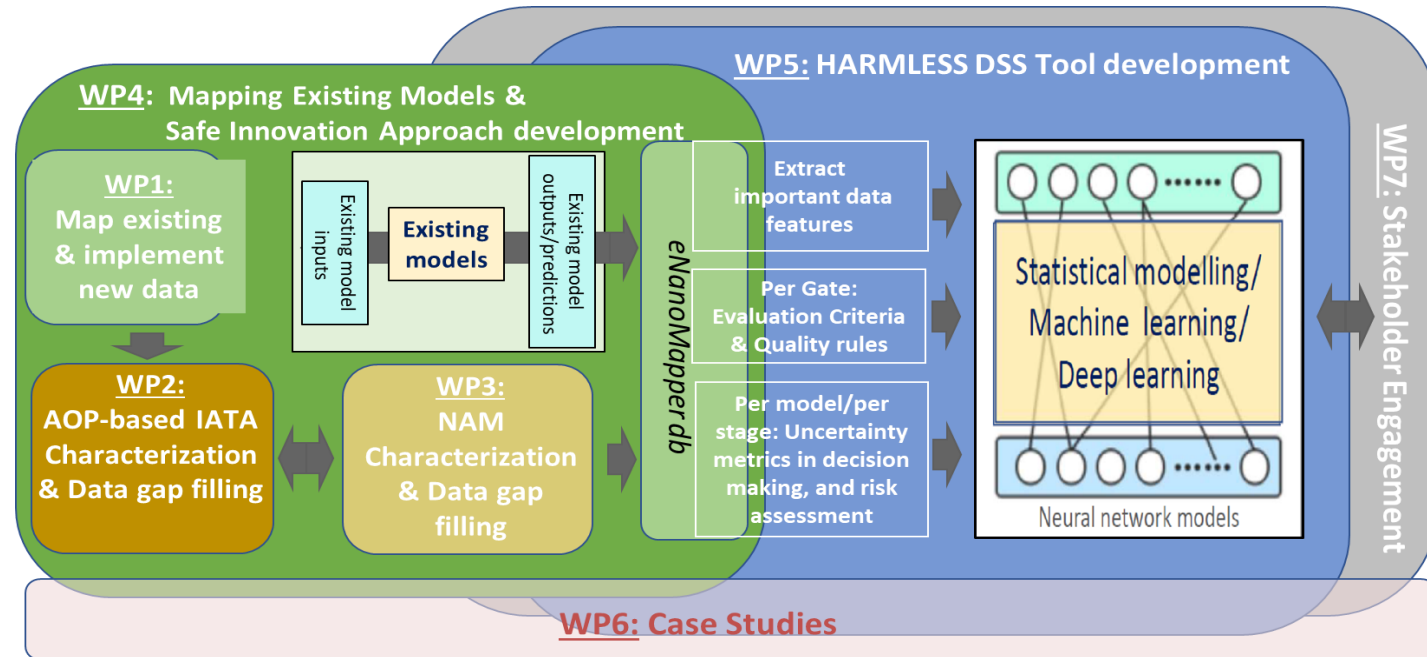
HARMLESS Decision Support System

6th June 2023

NANOSAFE conference, Grenoble

Objectives

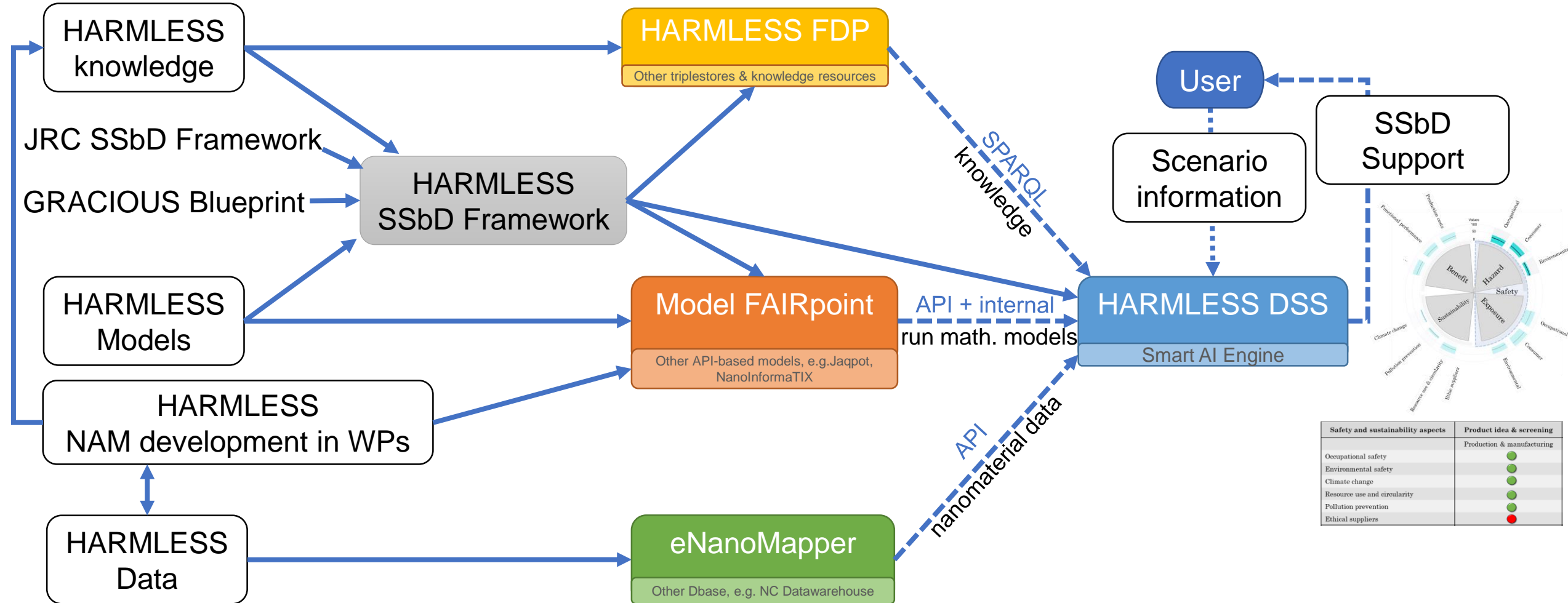
Build a user-friendly Decision Support System based on SSbD Framework



- For complex HARNs and multi-component ENMs
- Using existing and newly generated data, methods and tools
- Integration of data and models
- Use insights from case-studies and stakeholder feedback

Vision: FAIR & Modular Approach
 Data, Knowledge, Models & Interface
 ⇒ stand-alone & interchangeable
 ⇒ exploitable & external view

IT Architecture & Development Flow

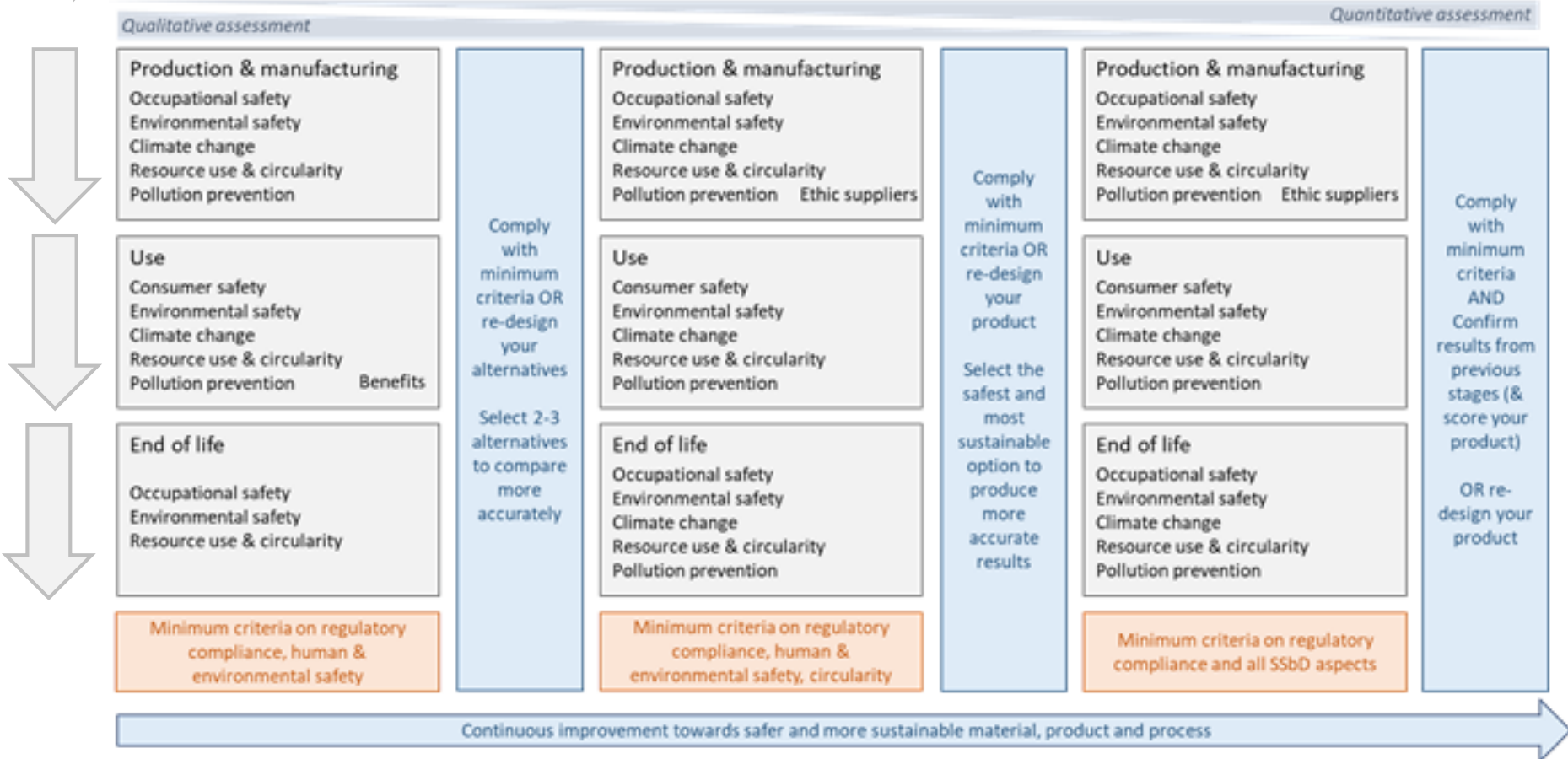


Based on the HARMLESS SSbD Framework

Innovation stages



Life cycle stages











* In line with JRC Framework and GRACIOUS blueprint

Decision Support Approach

*Using existing and newly generated data, methods and tools**

Please perform the following actions to get the most accurate result

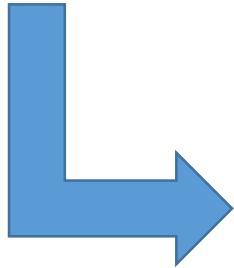
<h3>Advanced Material Early Assessment</h3>  <p>AMEA can be used to guide AdMa SSbD assessment especially in early stages of the innovation cycle by asking if/how the AdMa changes the SSbD benefits and concerns that are typical for conventional materials in the intended use.</p> <p>Start scan run ></p>	<h3>Attach a nano material</h3>  <p>Choose a nano material from Enanomapper and attach it to your scenario</p> <p>Attach nano material ></p>	<h3>StoffenManager Nano Hazard-part</h3>  <p>SMnano Hazard allows a preliminary but swift Tier-1 assessment of the nanomaterial's (occupational) hazard based on hazard banding.</p> <p>Attach existing run > Start scan run ></p>	<h3>LICARA nanoScan</h3>  <p>LICARA nanoScan allows a preliminary but swift assessment of benefits and risks for nano products. This is an excellent Tier-1 tool to start with to gain a simple but broad early view of hazard, exposure and sustainability.</p> <p>Attach existing run > Start scan run ></p>
<h3>Nano Exposure Quantifier (NEQ)</h3>  <p>The NEQ is a complete tool to estimate exposure and related Sbd advice. The NEQ adapts between Tier-1 and Tier-2 questions and thus a good start to get more insight into your exposure situation.</p> <p>Attach existing run > Start scan run ></p>	<h3>Hot Spot Scan - Paints, Coatings, Inks</h3>  <p>Hot Spot Scan - Paints, Coatings, Inks</p> <p>Start scan run ></p>	<h3>Stoffenmanager & NEQ via bayesian network</h3>  <p>Stoffenmanager & NEQ via bayesian network</p> <p>Start scan run ></p>	<h3>QSAR Cytotoxicity Prediction (QCP)</h3>  <p>QCP allows to predict the cytotoxicity of TiO2 nanomaterials based on a QSAR model</p> <p>Start scan run ></p>

** Currently fully integrated elements, more to follow in future ...*

Attach a nanomaterial: Extract data from eNanomapper

Pull existing data from a known (or similar) nanomaterial in eNanomapper

Pull in all measurements about that nanomaterial



Select nanomaterial

Attached nano materials	endpoint_s	effectendpoint_s	reference_owner_s	reference_s	loValue_d	unit_s	E.method_s	effectendpoint_type_s	E.cell_type
	GENOTOX	BREAKS							
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	4	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	2.6	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	3.2	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	7.2	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	4.2	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	6.5	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	5.5	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	2.9	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	3.2	%	COMET	MEAN	Liver cells
NRCWE#068, Solid Silica 100 nm - Silica	GENOTOXICITY	DNA STRAND BREAKS	NRCWE	10.1080/17435390.2020.1842932	4.7	%	COMET	MEAN	Liver cells

Showing 1 to 10 of 555 entries

< Previous 1 2 3 4 5 ... 56 Next >



Models,
Status Wheel
& Criteria
Checker

Stoffenmanager nano & Substance Information System

■ SMnano: Tier-1 quick determination of hazard band (based on questions)

Is the Manufactured Nano Object (MNO) soluble in water (biological media)?

This information is generally specified in the SDS or product information sheet.

No (< 0.1 g/L)

Does the MNO consists of persistent nanofibers?

Persistent nanofibers are defined as nanofibers exceeding a length of 5000 nm, with the other two dimensions in the nano-size range (1-100 nm).

No

Is the available toxicological data sufficient to draw conclusions for Hazard banding?

MSDS can provide information on classifications, and in some cases vivo studies might be available.

No

For your product, is Hazard banding based on (limited) data available (by using expert judgment) or based on the hazardous potential of the parental material?

Based on hazardous potential of parental material or other available data (see Table 1 after selecting this option).

Please select the appropriate Hazard band (see Table 1 below):

Hazard band 'D'

Table 1. Classification of MNOs in hazard bands based on insufficient toxicological data.



Type of MNO	Hazard band	Based on
C60 (fullerenes)	D	Particle-specific data
Carbon black	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Ag (nano silver)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Fe (iron)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Au (gold)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Pb (lead)	E	EPA Carc. B2; probable human carcinogen
La (lanthanide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
TiN (titanium nitride)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
TiO ₂ (titanium dioxide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
CeO ₂ (cerium oxide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
ZnO (zinc oxide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
SiO ₂ (silica or silicon dioxide)	Unknown: E; crystalline/quartz: E; amorph, <50 nm: D; amorph, >50 nm: C	Particle-specific data; crystalline silica/quartz has been associated with carcinogenicity (IARC)
Al ₂ O ₃ (aluminum oxide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
FeO (iron oxides)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Sb ₂ O ₃ (antimony oxide)	E	Parent material classified as Carc Cat 3; R40
SnO ₂ (tin oxide)	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
CoO (cobalt oxide)	E	Parent material labeled R43
Nanoclay	>50 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Nano-polystyrene	>30 nm: C; ≤50 nm: D	Parent material and (limited) particle-specific data
Other MNOs	MNOs containing several parent materials: most critical hazard band; parent material unknown: E; parent material classified for C, M, R, or S: E; not classified for C, M, R, or S: D	

EPA = Environmental protection agency; Carc. = carcinogen; IARC = International Agency for Research on Cancer.

Stoffenmanager nano & Substance Information System


- **SMnano: Tier-1 quick determination of hazard band (based on questions)**
- **Substance Information System (SIS)**
 - Automatic hazard score calculation based on H-phrases*

benzene

 Zoek in Nederlandse bronnen  Zoek in Engelse bronnen

Stofinformatie **Gezondheidsgevaaren** Toepassingen Blootstellingsrisico

Deze categorie geeft informatie over mogelijke schadelijke effecten van de stof voor de gezondheid. Gezondheidsgevaaren worden hieronder weergegeven met gevarenaanduidingen (H-zinnen), voorzorgsmaatregelen (P-zinnen) en -symbolen en zinnen binnen de Europese Unie (Verordening (EG) nr. 1272/2008). Health Effect Codes zijn afkomstig uit Pubchem



CLP-pictogrammen [↗](#)

Gevarenaanduiding (H-zinnen)	
H225	Licht ontvlambare vloeistof en damp.
H304	Kan dodelijk zijn als de stof bij inslikken in de luchtwegen terechtkomt.
H315	Veroorzaakt huidirritatie.
H319	Veroorzaakt ernstige oogirritatie.
H340	Kan genetische schade veroorzaken.
H350	Kan kanker veroorzaken.
H372	Veroorzaakt schade aan organen bij langdurige of herhaalde blootstelling.
H401	Giftig voor in het water levende organismen.
H411	Giftig voor in het water levende organismen, met langdurige gevolgen.

Klachten (Health Effect Codes)	
HE7	Zenuwstelselstoornissen, Andere effecten op het zenuwstelsel dan narcose
HE14	Irritatie-ogen, neus, keel, huid, Merkbaar
HE8	Zenuwstelselstoornissen, Narcose
HE12	Hematologische bloedstoornissen, Bloedarmoeden
HE1	kanker, momenteel gereguleerd door OSHA als kankerverwekkend



Project 03-07-2018

Substance Information System

Substance Information System (SIS) is a public tool developed on the TNO DIAMONDS platform that allows users to search and find information on hazardous substances. The tool collects and organizes information from diverse sources to provide an integrative resource on substance properties, safety, health effects, exposure, and application by business sectors.

[Read more](#)

Integration of data and models using Bayesian Approach

Aims

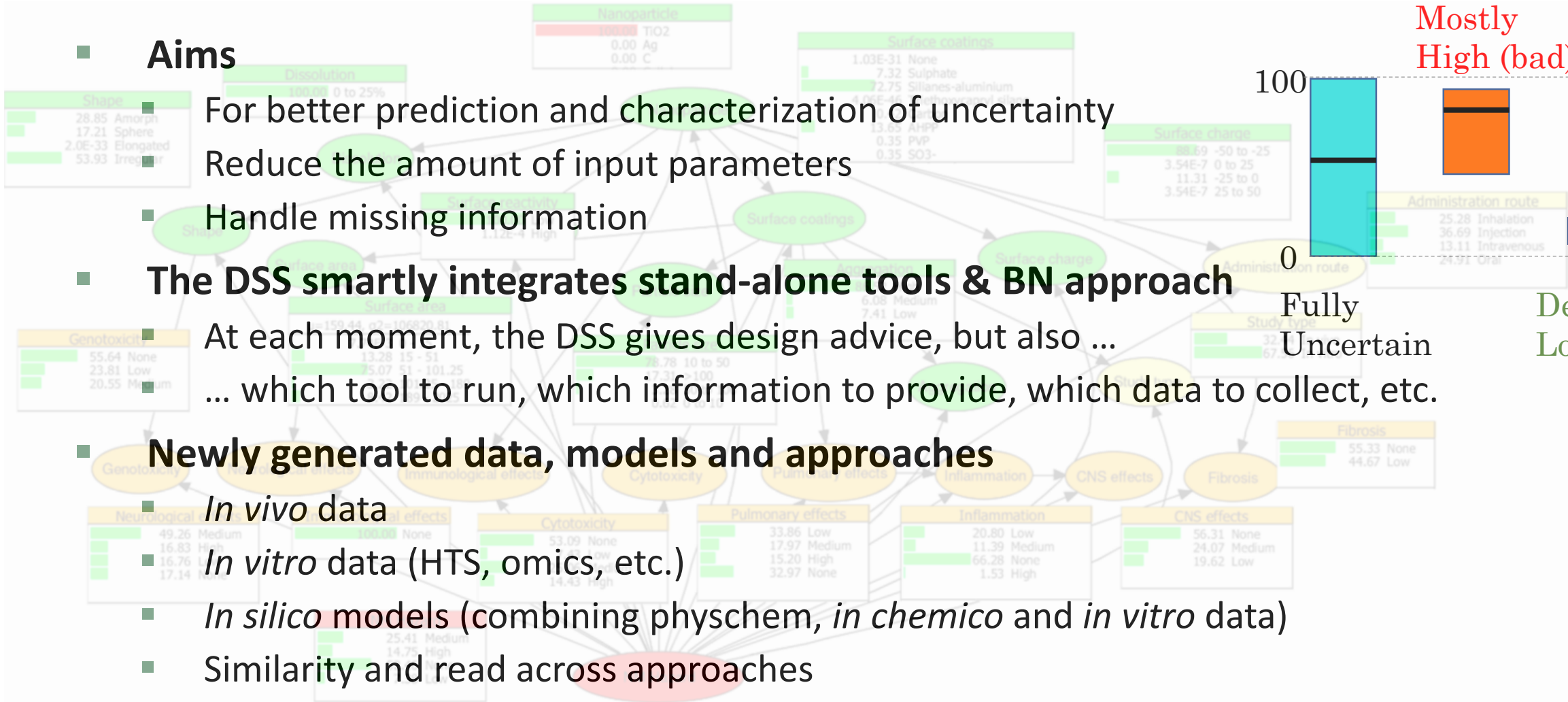
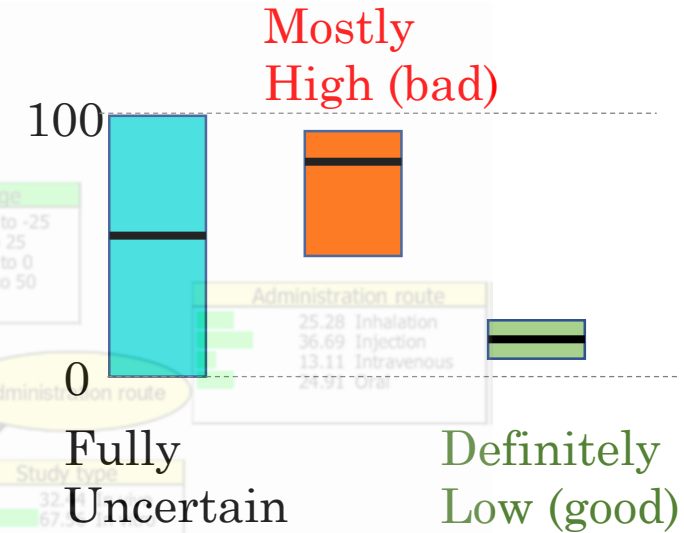
- For better prediction and characterization of uncertainty
- Reduce the amount of input parameters
- Handle missing information

The DSS smartly integrates stand-alone tools & BN approach

- At each moment, the DSS gives design advice, but also ...
- ... which tool to run, which information to provide, which data to collect, etc.

Newly generated data, models and approaches

- In vivo* data
- In vitro* data (HTS, omics, etc.)
- In silico* models (combining physchem, *in chemico* and *in vitro* data)
- Similarity and read across approaches



Decision Support Visualisation

Risk Informed Decision Making

Safety and sustainability aspects	Product idea & screening	Lab Scale	Pilot Scale
	Production & manufacturing	Production & manufacturing	Production & manufacturing
Occupational safety	OK	OK	Warning
Environmental safety	OK	Warning	OK
Climate change	OK	OK	OK
Resource use and circularity	OK	Alert	Warning
Pollution prevention	OK	OK	Alert
Ethical suppliers	Alert	Warning	Alert
	Use	Use	Use
Consumer safety	OK	OK	OK
Environmental safety	OK	Alert	Alert
Climate change	OK	Warning	Warning
Resource use and circularity	OK	OK	Alert
Pollution prevention	OK	OK	Warning
Benefits	OK	OK	Warning
	End of life	End of life	End of life
Occupational safety	OK	OK	OK
Environmental safety	Warning	Warning	Alert
Climate change	OK	Warning	Warning
Resource use and circularity	OK	OK	Alert
Pollution prevention	OK	OK	OK

- **OK** Ready to go to next phase
- **Warning** There are concerns that require attention
- **Alert** There are major concerns blocking progression



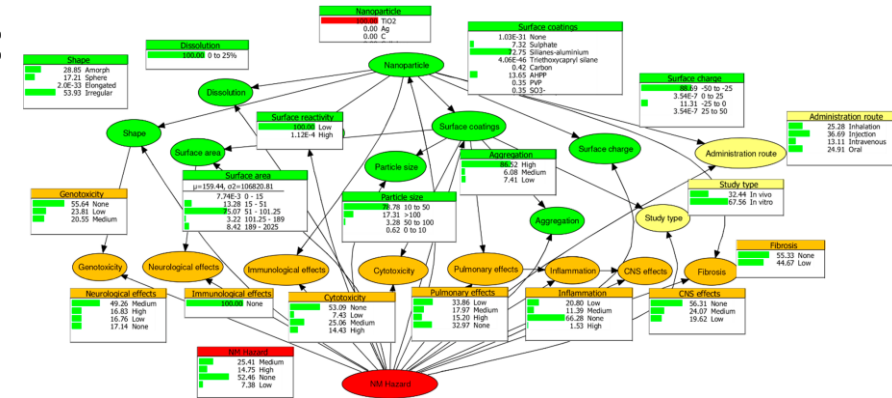
* Fully traceable where value is based on (when click)

Further development of the DSS

- **Simplify:**
 - Reduce the amount of questions to be answered by the user (number of input parameters of the various tools)

- **Further integration of HARMLESS data and models:**

- Newly developed *in silico* models (predictive models)
- *In vitro* high throughput testing scores
- Similarity and read across approaches
- More and smarter SSbD advice



- **Further integration of new data and models from other (sister)projects**

- **Validation in case studies**



Case Study 1
Papermaking



Case Study 2
Paint formulations



Case Study 3
Catalysts



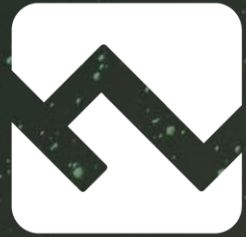
Case Study 4
Facade insulation



Case Study 5
Agriculture

Key points of the decision support system

- Easy to use
 - Follow innovation stages in HARMLESS SSbD framework
 - From limited to more comprehensive data and methods
 - Including uncertainty
 - Use of existing and newly generated data and models
 - Integration of data and knowledge
 - To reduce amount of questions
 - To better characterize the uncertainty
 - To handle missing data (e.g. similarity assessment and read across)
- **Please, reach out to discuss if your data or model can be included**



HARMLESS

FOLLOW US TO NEVER MISS A THING!



LinkedIn



Twitter

www.harmless-project.eu