

Exploring the use of Artificial Intelligence (AI) for extracting and integrating data obtained through New Approach Methodologies (NAMs) for chemical risk assessment

(AI4NAMs, OC/EFSA/SCER/2021/08)

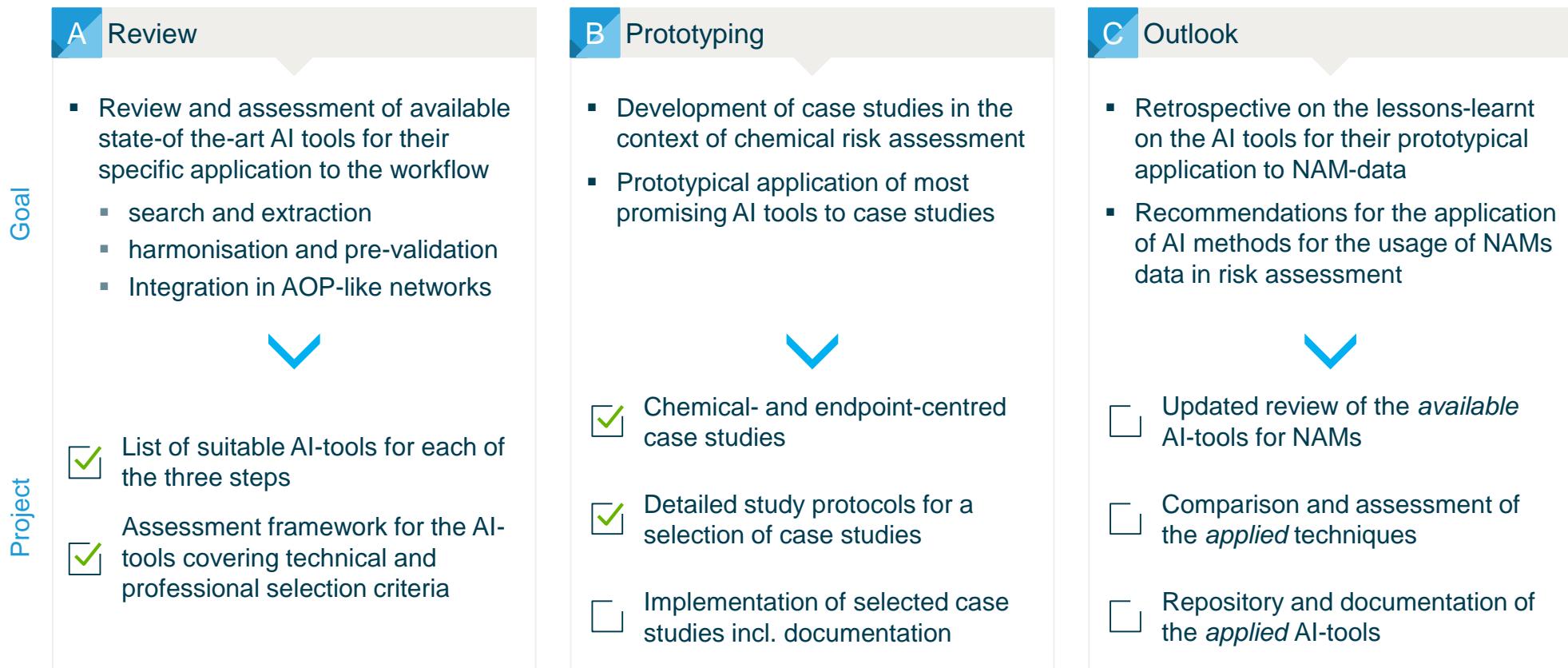
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EFSA Advisory Forum 08/06/2022

The project AI4NAMS, divided into three phases, is currently in the prototyping phase B

A B C



Project consortium

d-fine

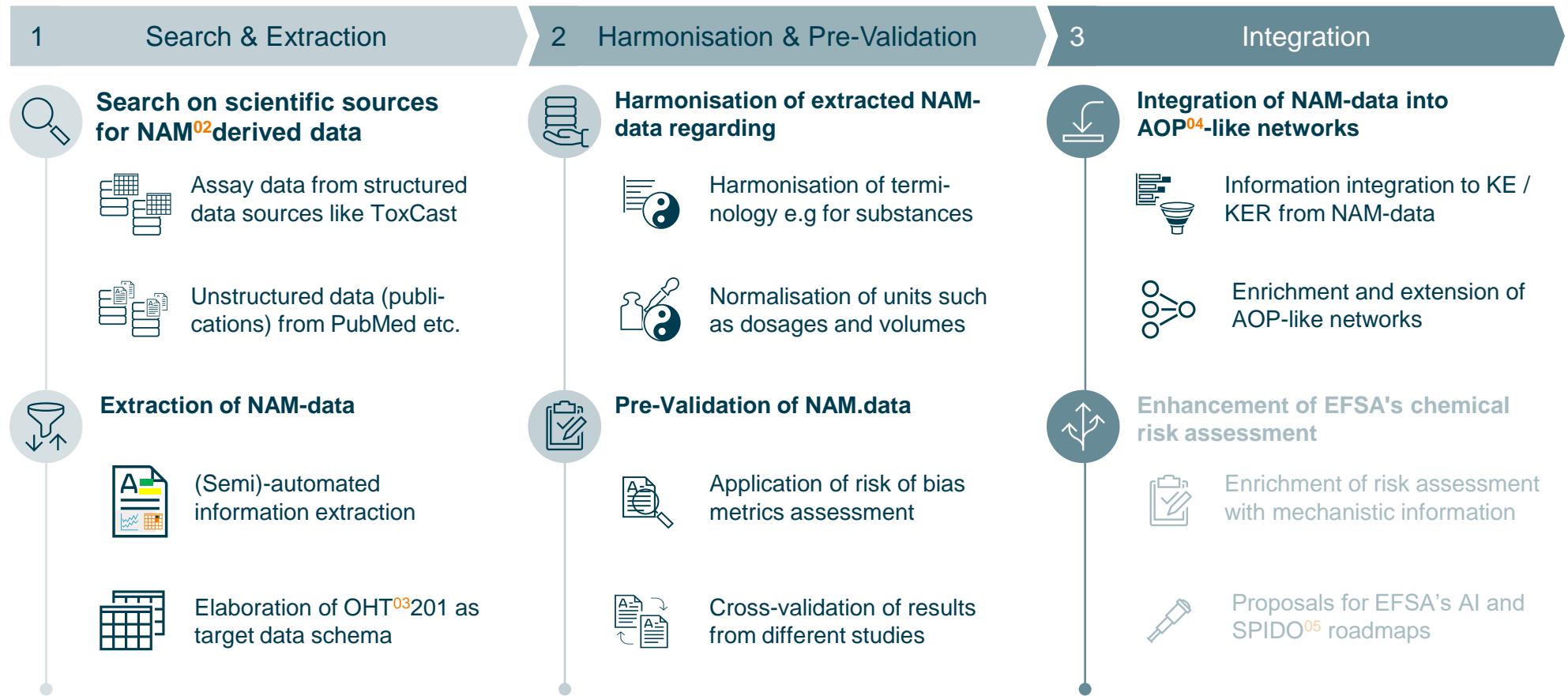
BfR
Bundesinstitut für Risikobewertung

WAGENINGEN
UNIVERSITY & RESEARCH

The ultimate goal of this project is to systematically explore the potential of applying AI-methods to NAM-data collection and integration, supporting better chemical risk assessment while reducing testing in animals.

In this project, selected AI⁰¹ tools and methods are applied on NAM⁰²-data in a three-step workflow

A

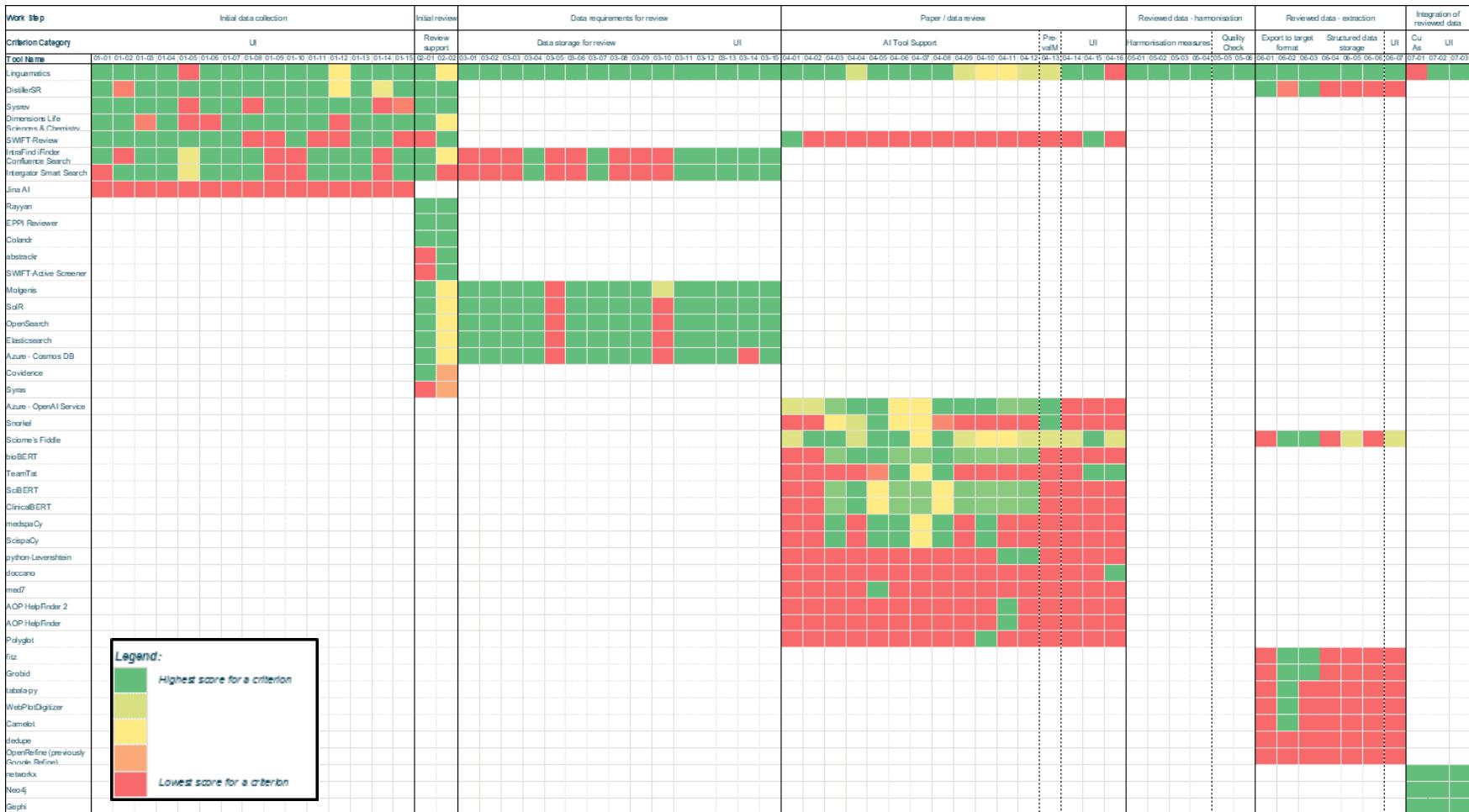


⁰¹ Artificial intelligence ⁰² New Approach Methodologies ⁰³ OECD Harmonisation Template for intermediate effects ⁰⁴ Adverse Outcome Pathway ⁰⁵ Science Studies and Project Identification & Development Office

Overarching goal of work package A was to identify a combination of tools that can jointly accelerate the process. The compatibility of the individual tools with each other is an essential requirement.

To review available state-of the-art AI tools they have been assessed against a set of workflow step specific criteria

A



The expected suitability of the AI tools evaluated varies depending on each step of the workflow and the individual tasks. Thus, tool chains will be implemented for the case studies.

The selection of case studies has been based on the guidelines delineated by EFSA considering the proposals of the consortium

B

Guidelines for the creation of a proposal
(EFSA)



Relevance

12 Case studies (CSs)

Minimum to be proposed



Chemical-centred CSs

6/12

Proposals for chemicals/chemical groups

Including:

- dioxin-like compounds
- phthalates
- pesticides

→ o Endpoint-centred CSs

6/12

Proposals for endpoint(s)

Including:

- endocrine activity
- genotoxicity

Principles for the selection
(Consortium)

Representativeness

Combine chemical-centred and endpoint-centred case studies of different **scientific** as well as **technical complexity levels**

Variety

Include e.g. both case studies with exceptionally **high** and **limited data availability**, also allowing for manageability

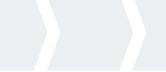
Cover focus areas

Case studies have been designed to allow for in-depth exploration of specific functionalities such as extraction of tabulated data

By combining the guidelines and principles, a balanced selection of case studies is ensured. The broad coverage of different aspects enables the best possible assessment of the capabilities of AI support.

Six case studies have been selected based on the principals of representativeness, variety and coverage of workflow focus areas

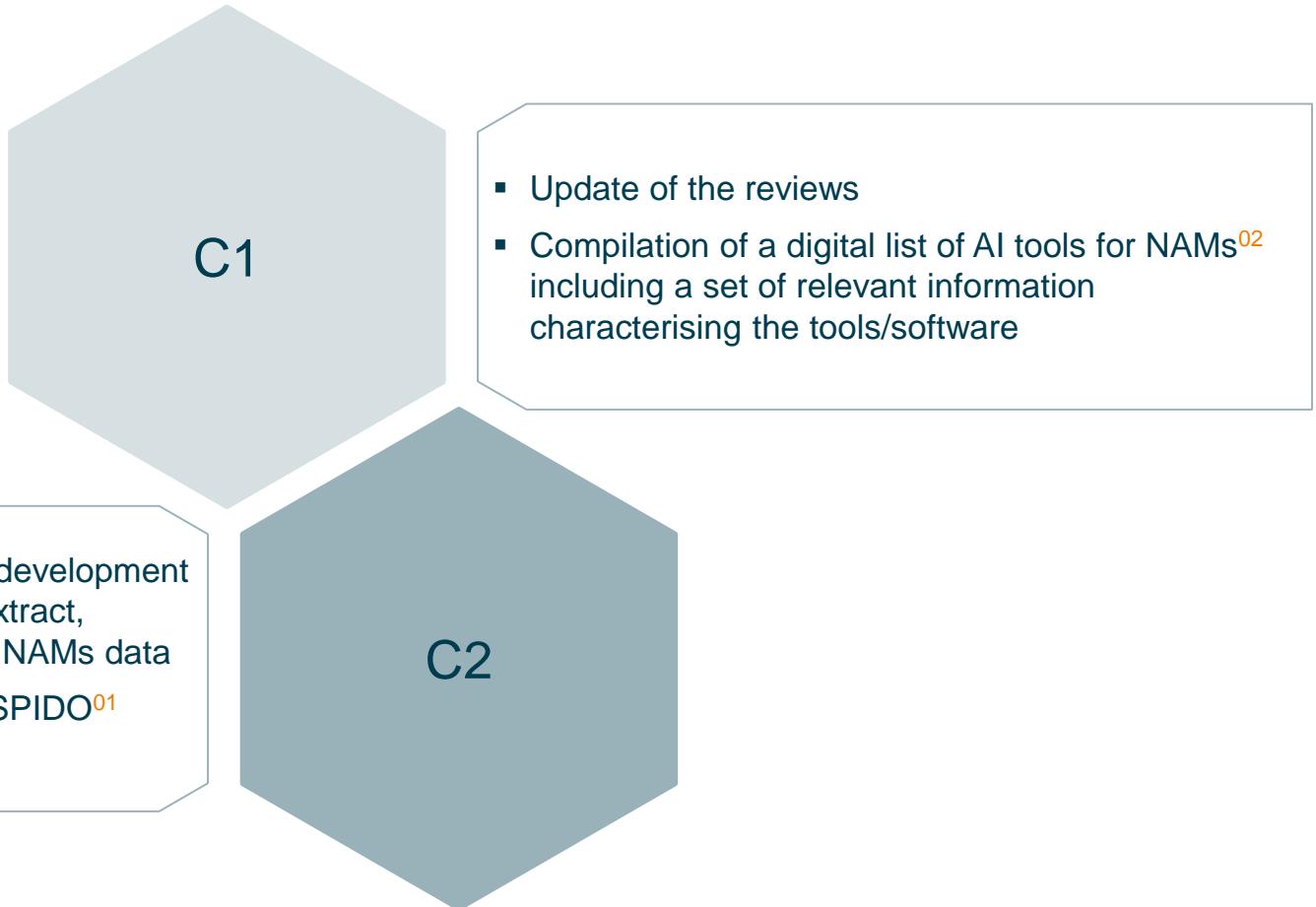
B

Case studies	Stressor group	Scientific complexity	Data richness	Focus workflow steps
 Pyrethroids causing neurotoxicity	▪ Insecticides		  	   
 Bisphenols	▪ Food contact materials	 	  	   
→○ (Cumulative) liver toxicity	▪ Pesticides	  	  	   
 Phthalates	▪ Food contact materials			   
 High potency polychlorinated dibenzodioxins and -furanes	▪ Food contaminants	  	  	   
→○ Hypothyroidism	▪ Pesticides ▪ Food additives ▪ Food contaminants	 	 	   

A balanced selection of scientifically relevant case studies was made to allow an exploration of the capabilities of AI in supporting the target workflow.

In work package C an overall evaluation and proposal of recommendations for EFSA's SPIDO⁰¹ NAMs⁰² & AI roadmaps will be performed

■ ■ ■ c



 The systematic exploration of the potential of applying AI-methods to NAM-data collection and integration facilitates the integration of mechanistic understanding into the chemical risk assessment.

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