Assessment of QSAR predictions for regulatory purposes with the QSAR Assessment Framework

AIChemist School

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European Chemicals Agency

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Overview

- → *In silico* alternative methods at ECHA
- → (Q)SAR Assessment Framework (QAF)
- → Key assessment elements (AEs)

OUR PURPOSE

We protect health and the environment through our work for chemical safety

OUR VISION

Chemical safety through science, collaboration and knowledge

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Our mandate

Implement EU chemicals laws and policy through technical, scientific, and administrative tasks

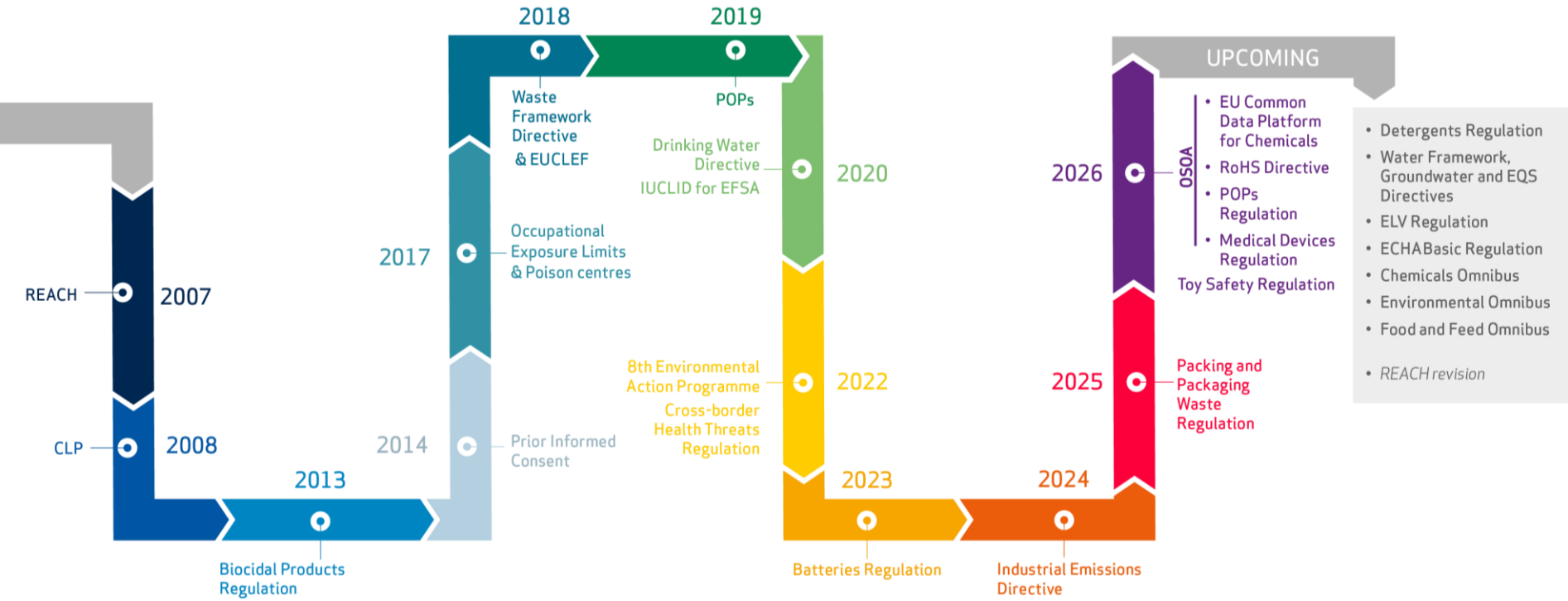
Provide independent, high-quality **scientific opinions** and **decisions** to serve as basis for EU measures

Collaborate with EU institutions, EU countries' authorities, and other bodies

Support companies, particularly smaller ones, in fulfilling their duties

Ensure stakeholders get relevant, reliable and objective **information**

Our tasks


REACH
2007
CLP
2008
2013
Biocidal Products Regulation
2014
Prior Informed Consent
2017
Occupational Exposure Limits & Poison centres
2018
Waste Framework Directive & EUCLEF
2019
POPs
Drinking Water Directive
IUCLID for EFSA
2020
8th Environmental Action Programme
Cross-border Health Threats Regulation
2022
2023
Batteries Regulation
2024
Industrial Emissions Directive
2025
Packing and Packaging Waste Regulation
2026
OSOA
EU Common Data Platform for Chemicals
RoHS Directive
POPs Regulation
Medical Devices Regulation
Toy Safety Regulation
UPCOMING
Detergents Regulation
Water Framework, Groundwater and EQS Directives
ELV Regulation
ECHA Basic Regulation
Chemicals Omnibus
Environmental Omnibus
Food and Feed Omnibus
REACH revision

Our Values

Integrity

We earn trust by being accountable and delivering our mandate in a fair, consistent, and independent manner.

We uphold the highest professional, financial, governance, and ethical standards.

Transparency

We make our opinions and decisions in an open, understandable and accessible way.

We communicate clearly, courteously, and respectfully.

We are open to engaging and embracing diverse perspectives and are inclusive in how we work.

We welcome feedback.

Collaboration

We work closely with our EU and Member State partners and institutions to deliver our shared goals and priorities.

We consult and cooperate with stakeholders.

We listen, engage, and consult with each other.

Innovation

We continuously review and respond to changing circumstances.

We analyse and use data and best available evidence to inform and deliver our mandate.

We exploit synergies and are open to adapting operations using new technologies and ways of working.

ECHA’s commitment to Alternative Methods

→ One of ECHA's strategic objectives is to promote alternative methods

Article 1: The purpose of this Regulation is to ensure a high level of protection of human health and the environment, including the **promotion of alternative methods for assessment of hazards of substances**, as well as the free circulation of substances on the internal market while enhancing competitiveness and innovation.

ECHA’s commitment to Alternative Methods

- → One of ECHA's strategic objectives is to promote alternative methods
- → ECHA supports development and promotion of these methods by:
  - Providing guidance
  - Developing new ways of characterising hazard
  - Contributing to discussion about future regulatory system
- → Our efforts span various processes and legal frameworks within ECHA’s mandate

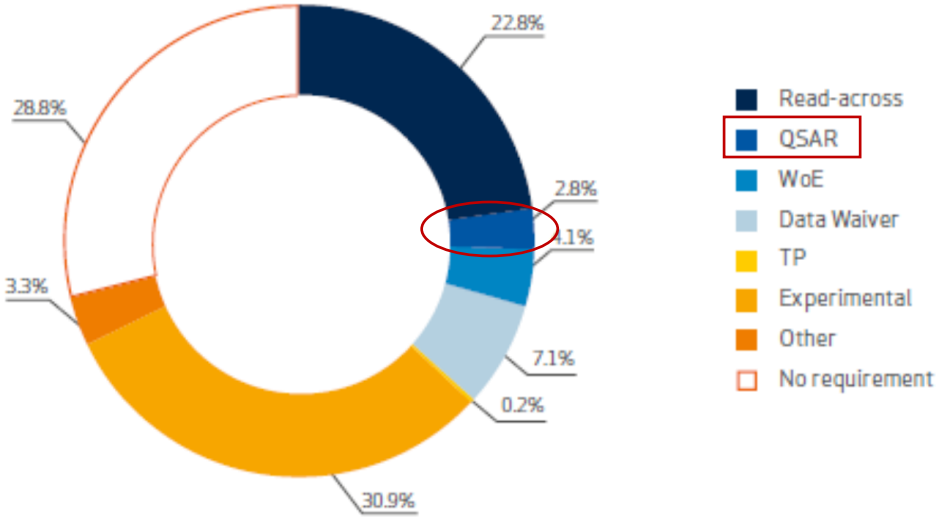
Legal context - REACH

→ REACH registrants can adapt standard information requirements using alternative methods such as *in vitro*, read-across and (Q)SAR studies

→ Criteria for adaptations listed in Annex XI of REACH

- a (Q)SAR model whose **scientific validity** has been established
- the substance falls within the **applicability domain** of the model
- results are **adequate for the purpose** of classification and labelling and/or risk assessment
- adequate and **reliable documentation** is provided.

Alternatives used so far



→ Adaptations used more than experimental studies

→ Read-across most used adaptation

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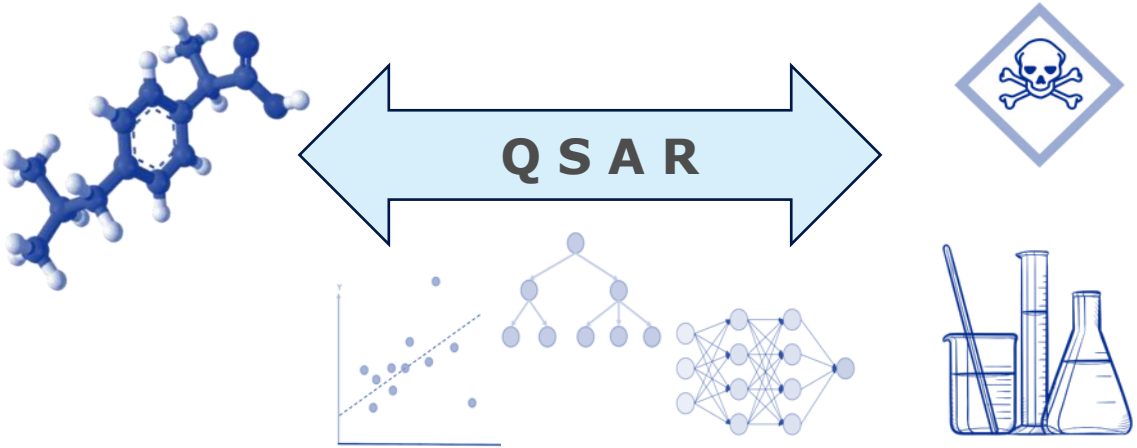
What is a (Q)SAR model?

Quantitative

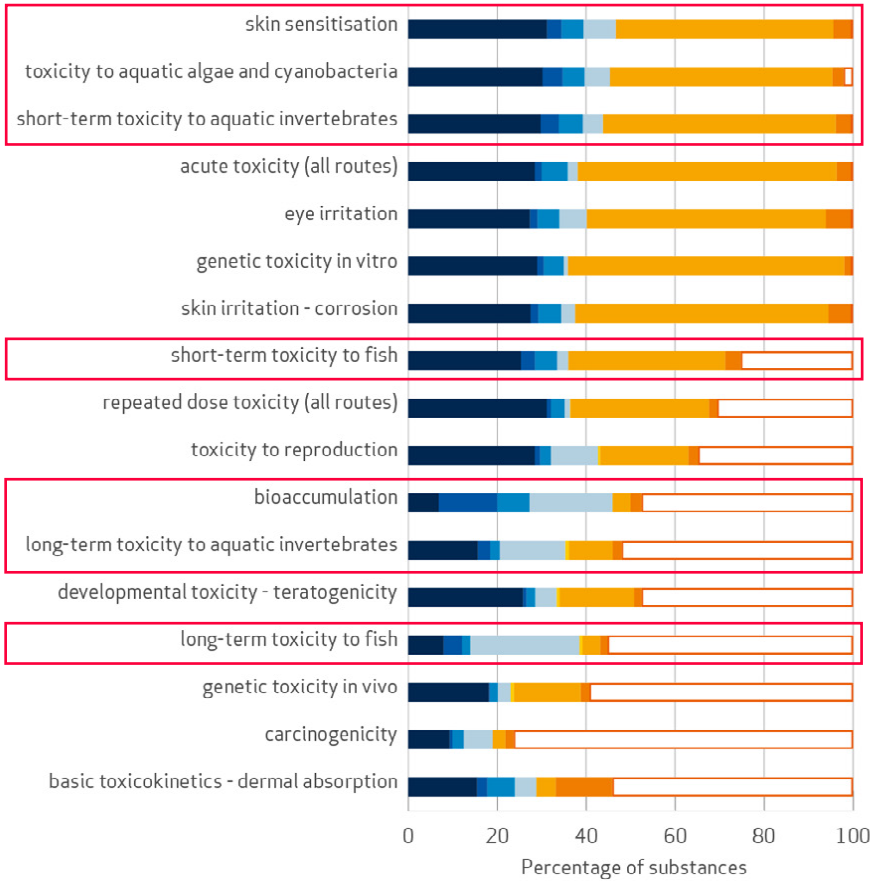
Structural

Activity

Relationships



Use of adaptations in REACH information requirements



REACH information requirements where QSARs most used:

- → Bioaccumulation
- → Aquatic toxicity (all)
- → Skin sensitisation

Room for more effective use of QSARs under REACH

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ECHA approach towards animal-free hazard assessment in three steps:

Step 1. Define

Identify critical needs to transition to animal-free system to steer further development

Step 2. Demonstrate

Apply available tools under current system

Step 3. Re-design

Re-think overall system to enable new approach methodologies and **redefine** main elements

Step 2: Demonstrate

Apply already existing tools under current system to build experience and gain confidence

ECHA focusing on this step, using tools available in following areas:

→ Advancements in *in silico methods*:
- Enhanced predictive capacity and broader applicability from ECHA data efforts
- OECD (Q)SAR Assessment Framework: explicit regulatory acceptance criteria

→ Use of molecular data for read-across and grouping with clear acceptance criteria

→ Establishment of in vitro PBK/TK measurements and modelling for industrial chemicals

→ Integration of 'omics in regulatory toxicological testing for molecular data in relevant biological systems

Transparent QSAR criteria: unlocking regulatory potential

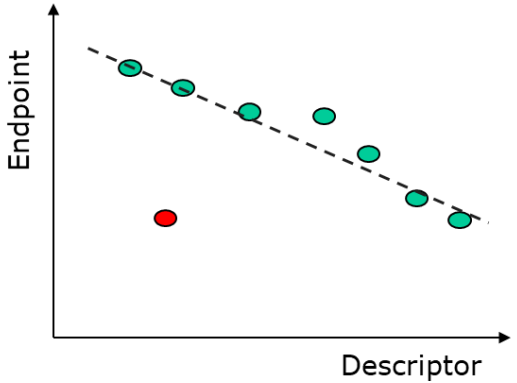
- → Clear and **transparent criteria** key **for wider acceptance** of QSAR models/predictions by users and authorities
- → **Wider acceptance** of QSARs lead to **new regulatory applications** (more adaptation possibilities, broader use in hazard assessment)
- → More **regulatory applications**, significant **reduction potential** for tests needed and costs

Starting point

Valid QSAR model ≠ Valid QSAR result

- → 2004 OECD QSAR principles to assess scientific validity of **QSAR models**
- → Use of valid QSAR model does not guarantee a reliable prediction
- → Need to establish **principles to assess individual results** and a systematic and harmonised **assessment framework** for **QSAR models & predictions**

Why a valid (Q)SAR model alone isn't enough

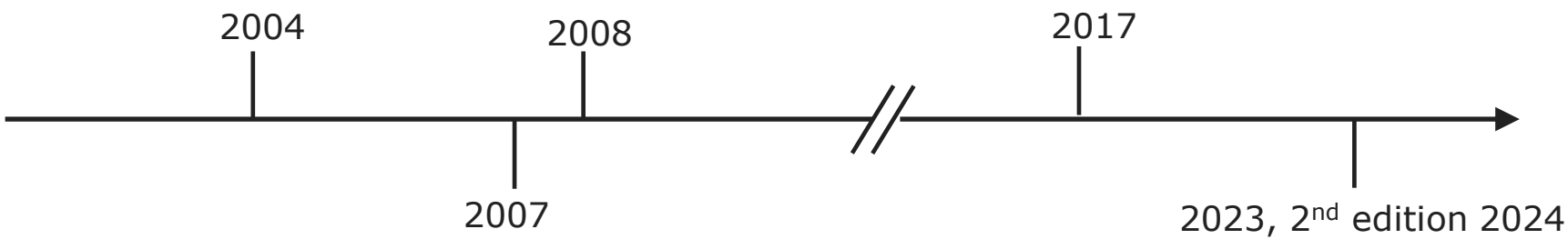


History

OECD principles for validation, regulatory purposes of (Q)SAR Models

ECHA guidance R.6 QSARs and Grouping of Chemicals
QMRF v1.2
QPRF v1.1

JRC
QMRF v2.0



OECD guidance document on validation of (Quantitative) Structure-Activity Relationships [(Q)SAR] models

QSAR Model Reporting Format (QMRF) v1.2
QSAR Prediction Reporting Format (QPRF) v1.1

OECD QSAR Assessment Framework (QAF)
QMRF v2.1
QPRF v2.0
QSAR Results Reporting Format (QRRF) v1.0
Checklists

(Q)SAR Assessment Framework (QAF)

Published in August 2023, second edition Nov 2024

Systematic and harmonised framework for regulatory assessment

Scope

- → QSAR models
- → QSAR predictions
- → Results based on multiple QSAR predictions

Applicability

(Q)SARs, irrespective of:

- → Modelling technique
- → Predicted endpoint
- → Intended regulatory purpose

Audience

- → Regulatory authorities (primarily)
- → Model developers and users (as reference)

QAF guidance document content

Text document

1. Assessment of (Q)SAR Models
2. Assessment of (Q)SAR Predictions
3. Assessment of (Q)SAR Results derived from multiple predictions

Reporting formats

Annex I – (Q)SAR model reporting format (QMRF) v2.1 (minor update)

Annex II – (Q)SAR prediction reporting format (QPRF) v2.0 (major update)

Annex III – (Q)SAR result reporting format (QRRF) v1.0 (Nov 2024)

Support material

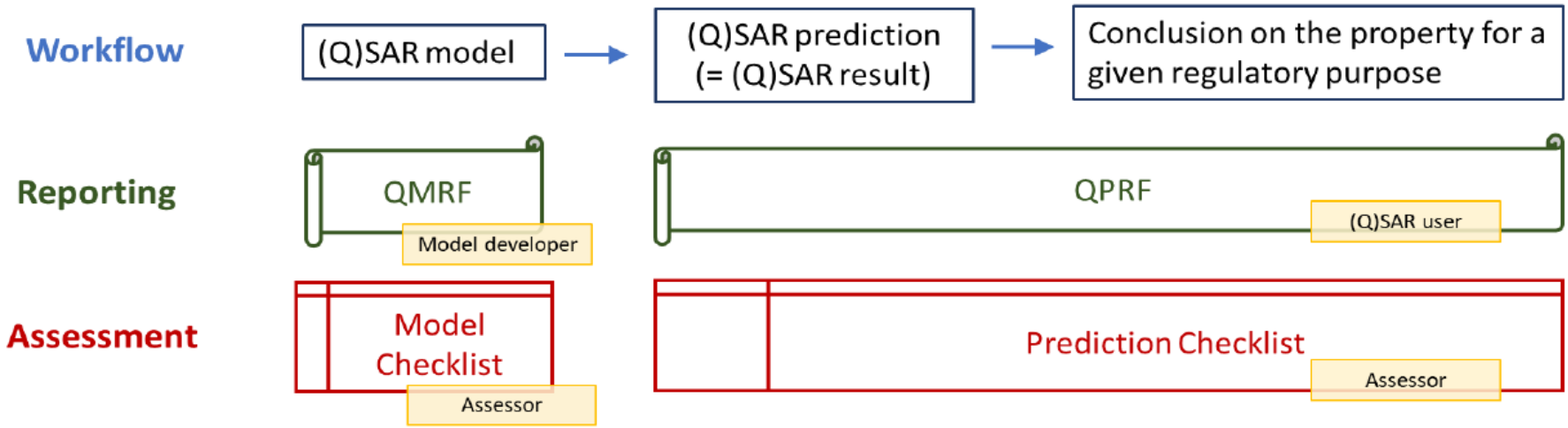
(Q)SAR Assessment Framework checklist (Excel document)

1. Model checklist
2. Prediction checklist
3. Result checklist

+ examples and explanations

Who does what?
Individual prediction

Figure 1. (Q)SAR Assessment Framework (QAF) Result based on an individual prediction



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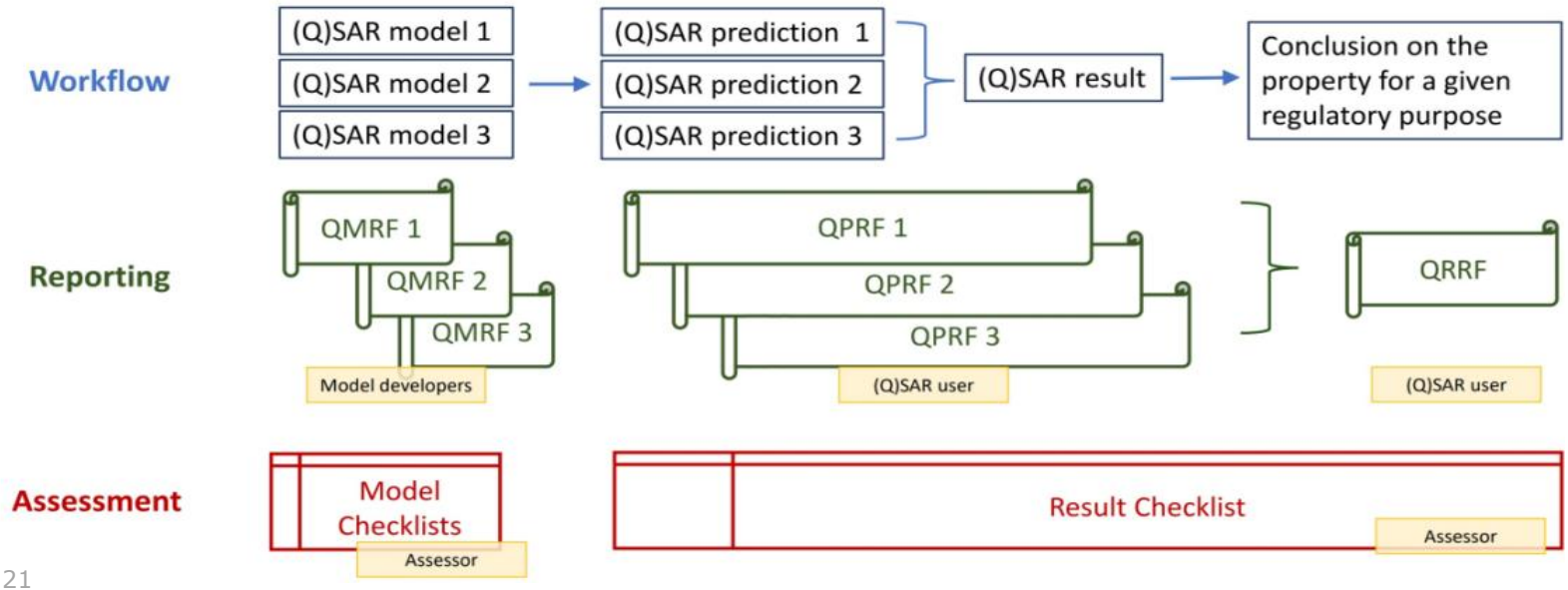
Who does what?
Multiple predictions

Figure 2. (Q)SAR Assessment Framework (QAF) Result based on multiple predictions



OECD principles for (Q)SAR assessment

Five existing OECD principles for evaluating scientific validity of **(Q)SAR models**

Four new OECD principles for evaluating **(Q)SAR predictions**

New principle for evaluating **(Q)SAR results**

OECD principles for (Q)SAR assessment

Five existing OECD principles for evaluating scientific validity of **(Q)SAR models**:

1. Defined endpoint
2. Unambiguous algorithm
3. Defined domain of applicability
4. Appropriate measures of goodness-of-fit, robustness and predictivity
5. Mechanistic interpretation, if possible

OECD principles for (Q)SAR assessment

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1. Defined endpoint
2. Unambiguous algorithm
3. Defined domain of applicability
4. Appropriate measures of goodness-of-fit, robustness and predictivity
5. Mechanistic interpretation, if possible

Defined endpoint	
1.1	Clear scientific and regulatory purpose
1.2	Transparency of the underlying experimental data
1.3	Quality of the underlying experimental data

Unambiguous algorithm	
2.1	Description of the algorithm and/or software
2.2	Inputs and other options
2.3	Model accessibility

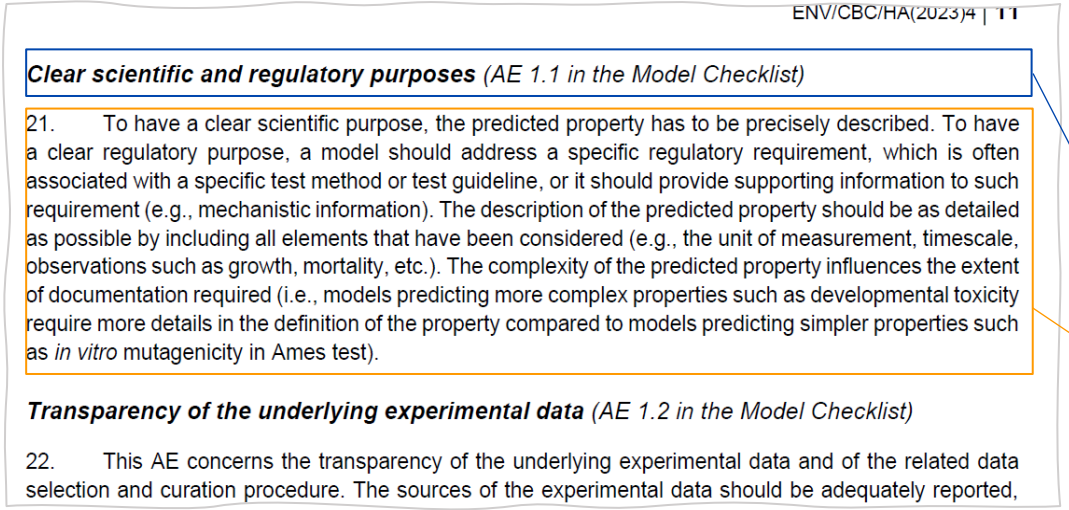
Defined domain of applicability	
3.1	Clear definition of the applicability domain and limitations of the model

Appropriate measures of goodness-of-fit, robustness and predictivity	
4.1	Goodness-of-fit, robustness
4.2	Predictivity

Mechanistic interpretation	
5.1	Plausibility of the mechanistic interpretation

QAF Guidance for the assessment of **models**

Figure: Guidance text with explanation of the Assessment Element (AE) for assessing QSAR Models Principle 1: **a defined endpoint**



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Clear scientific and regulatory purposes *(AE 1.1 in the Model Checklist)*

21. To have a clear scientific purpose, the predicted property has to be precisely described. To have a clear regulatory purpose, a model should address a specific regulatory requirement, which is often associated with a specific test method or test guideline, or it should provide supporting information to such requirement (e.g., mechanistic information). The description of the predicted property should be as detailed as possible by including all elements that have been considered (e.g., the unit of measurement, timescale, observations such as growth, mortality, etc.). The complexity of the predicted property influences the extent of documentation required (i.e., models predicting more complex properties such as developmental toxicity require more details in the definition of the property compared to models predicting simpler properties such as *in vitro* mutagenicity in Ames test).

Transparency of the underlying experimental data *(AE 1.2 in the Model Checklist)*

22. This AE concerns the transparency of the underlying experimental data and of the related data selection and curation procedure. The sources of the experimental data should be adequately reported,

Each principle is broken down to **Assessment Elements** (AEs)

The Guidance gives more details for each AEs

Ideally, an acceptable model should fulfil all AEs. However, depending on the purpose of use, evaluators may accept models where not all AEs are fulfilled

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QAF Guidance for the assessment of models - **Model Checklist**

Model 1			
when more than one model is considered, add a comment here to identify to which model the checklist refers to (e.g. model name)			
Principle	**Assessment element**	**Outcome**	**Comments**
Defined endpoint			
1.1	Clear scientific and regulatory purpose		
1.2	Transparency of the underlying experimental data		
1.3	Quality of the underlying experimental data		
Unambiguous algorithm			
2.1	Description of the algorithm and/or software		
2.2	Inputs and other options		
2.3	Model accessibility		
Defined domain of applicability			
3.1	Clear definition of the applicability domain and limitations of the model		
Appropriate measures of goodness-of-fit, robustness and predictivity			
4.1	Goodness-of-fit, robustness		
4.2	Predictivity		
Mechanistic interpretation			
5.1	Plausibility of the mechanistic interpretation		
Conclusion on the model		The conclusion is based on the outcome of the assessment elements as decided by individual authorities	
Comments			

Outcome (for each Assessment Element (AE)):

- Fulfilled
- Not fulfilled
- Not applicable/assessed, or
- Not documented

Conclusion (for the whole model):

- The model is acceptable for the intended purpose
- The model is not acceptable for the intended purpose
- Documentation insufficient to decide on the acceptance of the model for the intended purpose

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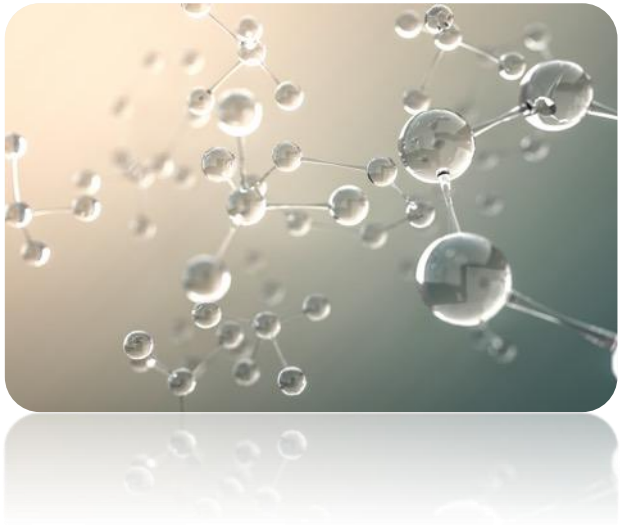
OECD principles for (Q)SAR assessment

Four new OECD principles for evaluating **(Q)SAR predictions**:

1. Correct input
2. Substance within applicability domain
3. Reliable prediction
4. Outcome fit for purpose



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OECD principles for (Q)SAR assessment

Four new OECD principles f
evaluating **(Q)SAR predictio**

1. Correct input
2. Substance within applicability domain
3. Reliable prediction
4. Outcome fit for purpose

Assessment element (AE)		Objective
1.1	Clear and complete description of the input and model settings	All information (input structure and/or parameters, model settings) is available to the assessors, thus making the prediction
1.2	Input representative of the substance under	The structure(s) modelled represent the substance subject to regulatory assessment
1.3	Reliable input (parameters)	Parameters that are input manually (other than the chemical structure) are reliable

Assessment element (AE)		Objective
2.1	Substance within the applicability domain	The substance meets the applicability domain (AD) requirements specified by model developers
2.2	Any other limitation of the model is considered	The substance does not meet any of the criteria for which the model should not be used

Assessment element (AE)		Objective
3.1	Reproducibility	The prediction can be reproduced using the same input and model version
3.2	Overall performance of the model	The model has an overall performance that is considered acceptable for the intended regulatory application
3.3	Fit within the physicochemical, structural and response spaces of the training set of the model	The prediction is result of interpolation in terms of physicochemical, structural and response space
3.4	Performance of the model for similar substances	The model predicts accurately substances similar to the one under analysis
3.5	Mechanistic and/or metabolic considerations	Mechanistic and metabolic considerations support the prediction
3.6	Consistency of information	Additional relevant and reliable information supports the prediction

Outcome is fit for the regulatory purpose		
4.1	Compliance with additional requirements	Regulation specific requirements for the use of computational results are met
4.2	Correspondence between predicted and required property	The modelled property corresponds to the property required by the regulation
4.3	Decidability within the specific framework	The outcome allows to take a regulatory decision in the framework of use

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OECD principles: (Q)SAR predictions

Four new OECD principles for evaluating **(Q)SAR predictions**:

1. Correct input
2. Substance within applicability domain
3. Reliable prediction
4. Outcome fit for purpose

New principle for evaluating **(Q)SAR results**

5. Correct determination of final result from multiple predictions

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OECD principles for (Q)SAR assessment

New principle for evaluating **(Q)SAR results**

5. Correct determination of the final result from multiple predictions

No specific Assessment Elements

A few to be considered as a whole

Correct input(s) to the model		
1.1	settings	High
1.2*	Input representative of the substance under analysis	High
1.3	Reliable input (parameters)	Medium
Substance within the applicability domain of a valid model		
2.1	Substance within the applicability domain	High
2.2	Any other limitation of the model is considered	High
Reliable prediction		
3.1	Reproducibility	High
3.2	Overall performance of the model	Medium
3.3	Fit within the physicochemical, structural and response spaces of the training set of the model	Medium
3.4	Performance of the model for similar substances	High
3.5*	Mechanistic and/or metabolic considerations	High
3.6*	Consistency of information	High
Outcome is fit for the regulatory purpose		
4.1*	Compliance with additional requirements	High
4.2*	Correspondence between predicted property and property required by the regulation	High
4.3*	Decidability within the specific framework	High

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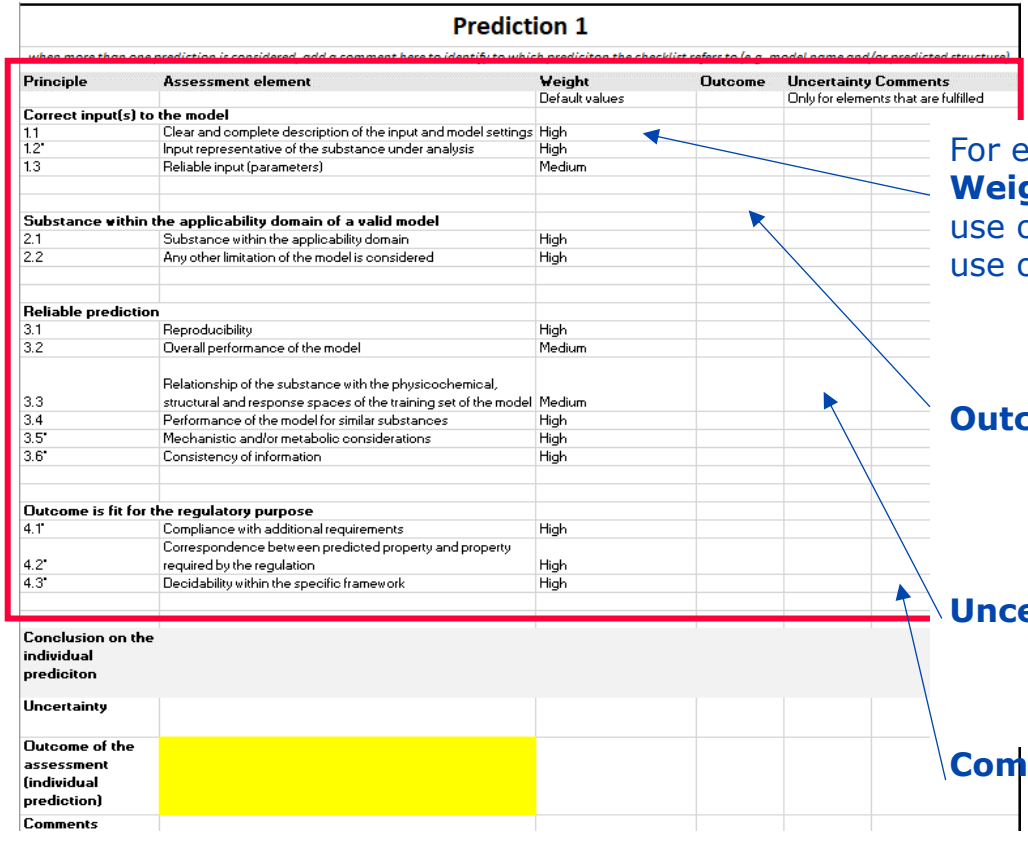
Assessment elements (AE)

Structured evaluation of OECD principles

- → AEs are specific aspects to inspect
- → Defined in the QAF
- → Associated to different OECD principles
- → AEs have an assigned weight (high, medium, low)
- → Assessed as:
  - Fulfilled (high / medium / low uncertainty)
  - Not fulfilled
  - Not assessed
  - Not documented

Prediction Checklist - for the regulatory assessment of (Q)SAR predictions



Prediction 1

when more than one prediction is considered, add a comment here to identify to which prediciton the checklist refers to (e.g. model name and/or predicted structure)

Principle	Assessment element	Weight	Outcome	Uncertainty Comments
		Default values		Only for elements that are fulfilled
Correct input(s) to the model				
1.1	Clear and complete description of the input and model settings	High		
1.2*	Input representative of the substance under analysis	High		
1.3	Reliable input (parameters)	Medium		
Substance within the applicability domain of a valid model				
2.1	Substance within the applicability domain	High		
2.2	Any other limitation of the model is considered	High		
Reliable prediction				
3.1	Reproducibility	High		
3.2	Overall performance of the model	Medium		
3.3	Relationship of the substance with the physicochemical, structural and response spaces of the training set of the model	Medium		
3.4	Performance of the model for similar substances	High		
3.5*	Mechanistic and/or metabolic considerations	High		
3.6*	Consistency of information	High		
Outcome is fit for the regulatory purpose				
4.1*	Compliance with additional requirements	High		
4.2*	Correspondence between predicted property and property required by the regulation	High		
4.3*	Decidability within the specific framework	High		
Conclusion on the individual prediciton				
Uncertainty				
Outcome of the assessment (individual prediction)				
Comments				

For each assessment element (AE):

Weight - how important is the AE in the context of use of the prediction. It depends on the purpose of use of the prediction (default given)

- High
- Medium
- Low

Outcome:

- Fulfilled
- Not fulfilled
- Not applicable/assessed
- Not documented

Uncertainty:

- High
- Medium
- Low

Comments

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Prediction Checklist - for the regulatory assessment of (Q)SAR predictions

Prediction 1

when more than one prediction is considered, add a comment here to identify to which prediciton the checklist refers to (e.g. model name and/or predicted structure)

Principle	Assessment element	Weight	Outcome	Uncertainty Comments
		Default values		Only for elements that are fulfilled
Correct input(s) to the model				
1.1	Clear and complete description of the input and model settings	High		
1.2*	Input representative of the substance under analysis	High		
1.3	Reliable input (parameters)	Medium		
Substance within the applicability domain of a valid model				
2.1	Substance within the applicability domain	High		
2.2	Any other limitation of the model is considered	High		
Reliable prediction				
3.1	Reproducibility	High		
3.2	Overall performance of the model	Medium		
3.3	Relationship of the substance with the physicochemical, structural and response spaces of the training set of the model	Medium		
3.4	Performance of the model for similar substances	High		
3.5*	Mechanistic and/or metabolic considerations	High		
3.6*	Consistency of information	High		
Outcome is fit for the regulatory purpose				
4.1*	Compliance with additional requirements	High		
4.2*	Correspondence between predicted property and property required by the regulation	High		
4.3*	Decidability within the specific framework	High		
Conclusion on the individual prediciton				
Uncertainty				
Outcome of the assessment (individual prediction)				
Comments				

Conclusion on individual prediction

Uncertainty of the prediction

- High
- Medium
- Low

Based on the highest uncertainty of high weight AEs.

Outcome of the assessment

- Acceptable for the intended purpose;
- Not acceptable for the intended purpose;
- Documentation insufficient to decide on the acceptance for the intended purpose.

The document suggests to accept predictions with low or medium uncertainty

Comments

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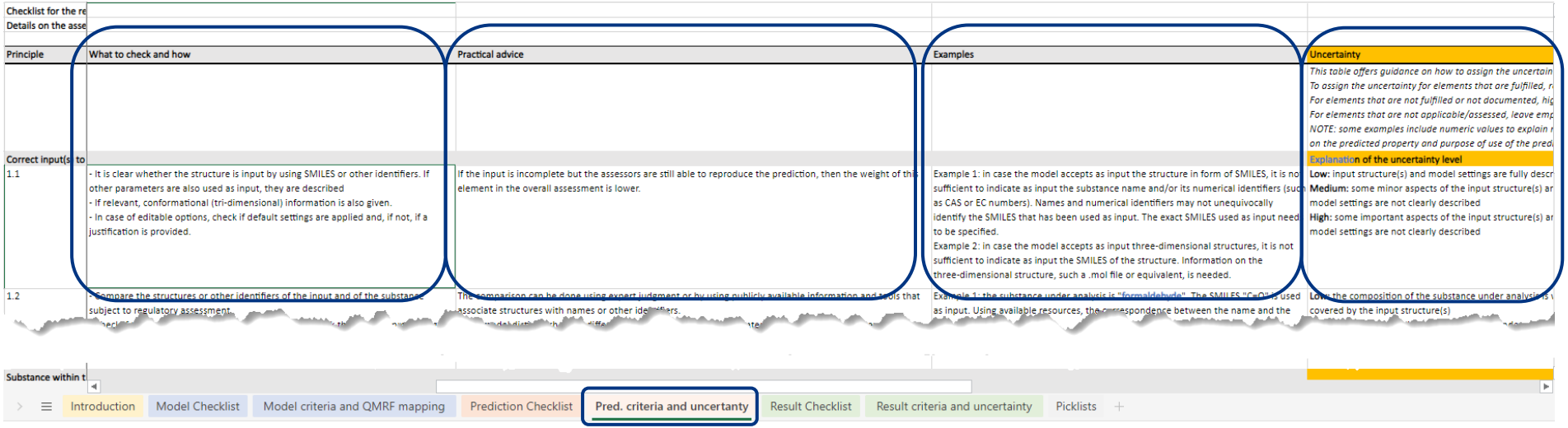
Example for assessment: Correct input

Example

→ AE 1.1: Clear and complete description of the **input** and **model settings**



Principle	What to check and how	Practical advice	Examples	Uncertainty
				This table offers guidance on how to assign the uncertain *To assign the uncertainty for elements that are fulfilled, r* *For elements that are not fulfilled or not documented, hig* *For elements that are not applicable/assessed, leave emp* *NOTE: some examples include numeric values to explain r* *on the predicted property and purpose of use of the predi*
Correct input(s) to				Explanation of the uncertainty level
1.1	- It is clear whether the structure is input by using SMILES or other identifiers. If other parameters are also used as input, they are described - If relevant, conformational (tri-dimensional) information is also given. - In case of editable options, check if default settings are applied and, if not, if a justification is provided.	If the input is incomplete but the assessors are still able to reproduce the prediction, then the weight of this element in the overall assessment is lower.	Example 1: in case the model accepts as input the structure in form of SMILES, it is not sufficient to indicate as input the substance name and/or its numerical identifiers (such as CAS or EC numbers). Names and numerical identifiers may not unequivocally identify the SMILES that has been used as input. The exact SMILES used as input need to be specified. Example 2: in case the model accepts as input three-dimensional structures, it is not sufficient to indicate as input the SMILES of the structure. Information on the three-dimensional structure, such a .mol file or equivalent, is needed.	**Low:** input structure(s) and model settings are fully descr **Medium:** some minor aspects of the input structure(s) ar model settings are not clearly described **High:** some important aspects of the input structure(s) ar model settings are not clearly described
1.2	- Compare the structures or other identifiers of the input and of the substance subject to regulatory assessment	The comparison can be done using expert judgment or by using publicly available information and tools that associate structures with names or other identifiers.	Example 1: the substance under analysis is "formaldehyde". The SMILES "C=O" is used as input. Using available resources, the correspondence between the name and the	Low: the composition of the substance under analysis is covered by the input structure(s)
Substance within t				

Introduction | Model Checklist | Model criteria and QMRF mapping | Prediction Checklist | Pred. criteria and uncertainty | Result Checklist | Result criteria and uncertainty | Picklists

What to check and how

Practical advice

Examples

Uncertainty

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1 Correct input(s) to the model

AE 1.1 Clear and complete description of the input and model settings

→ The **complete and unequivocal description** of the model input (not its quality/adequacy):

- **Substance**
  - SMILES, 3D structure, …
- **Input parameters**
  - Partition coefficient, melting point, water solubility, …
- **Editable options**
  - Algorithm options, database selection, applicability criteria, …

1 Correct input(s) to the model

AE 1.2 Input representative of the substance under analysis

→ About chemical **composition**

- Representative of the substance
  - Constituents
  - Isomer
  - Conformation
- Adequate to the model requirements
  - Curation/Ionisation/Salts/Tautomers

1 Correct input(s) to the model

AE 1.3 Reliable input

→ For **input parameters** only

- Information that can be provided to the model
- Required or optional (a default calculation is provided)

→ Reliability of input parameters:

- **Documented** source
- **Reliability** of the experiment/prediction
- Correspondence to model **requirements**
- **Consistency** with other values

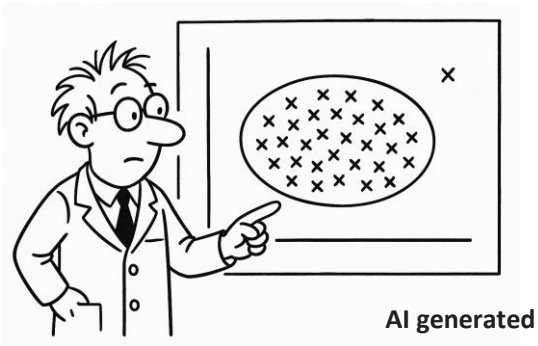
2 Subst. within the applicability domain

AE 2.1 Substance within applicability domain (AD)

→ According to the **model developers**

→ Documented as:
- Automated assessment
- Manual assessment
- Instructions

→ Reported as:
- Within
- Partially/Borderline
- Outside



2 Subst. within the applicability domain

AE 2.2 Any other limitation is considered

→ Some include **limitations**, for example:

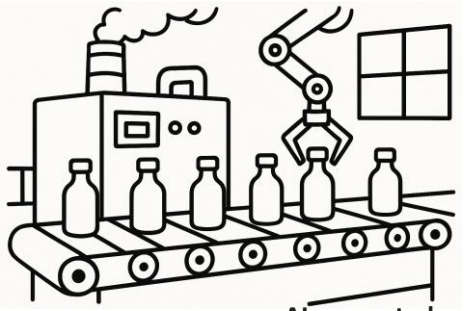
- Not valid for surfactants
- Not valid for organometallics
- Not valid for substances that react in water

3 Reliability of the prediction(s)

AE 3.1 Reproducibility

→ Ability to perform again the prediction with **the same results**

- Ideally with the same version
- Smaller deviations can be justified
- Not always possible

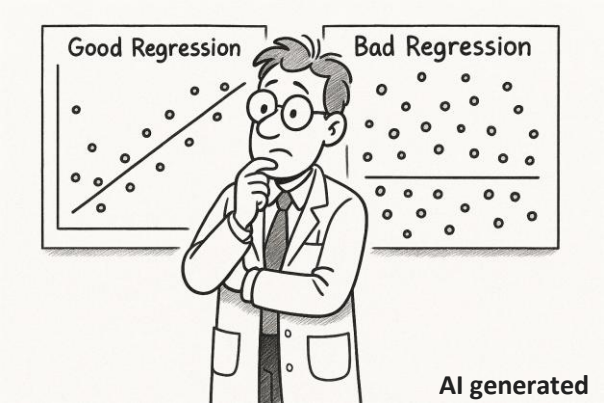


3 Reliability of the prediction(s)

AE 3.2 Overall performance of the model

→ General statistics of the model (QMRF)

- Quality of fit
- Robustness
- Predictiveness



→ Methodology should be well documented

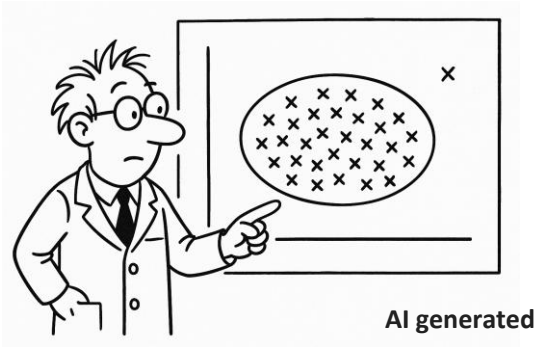
3 Reliability of the prediction(s)

AE 3.3 Fit within the physicochemical, structural and response spaces of the training set of the model

→ According to **assessor** ≠ model developers

→ Spaces

- Physicochemical
- Structural
- Response



3 Reliability of the prediction(s)

AE 3.4 Performance of the model for similar substances

→ Similar substances can be used to support prediction by demonstrating local performance

→ Similarity is:

- Endpoint dependent
- Substance dependent

→ Analogues:

- In the training set
- Out of the training set

3 Reliability of the prediction(s)

AE 3.5 Mechanistic and/or metabolic considerations

→ Mechanism and metabolic consideration

- Is the model trained for a specific expected mechanism?
- Are metabolites taken in account?

3 Reliability of the prediction(s)

AE 3.6 Consistency of information

→ Same or related endpoints

→ Experimental information available
- Has precedence unless well justified

→ Additional predictions

4 Outcome fit for regulatory purposes

AE 4.1 Compliance with additional requirements

→ Regulations can include additional requirements

→ Not identified for REACH

4 Outcome fit for regulatory purposes

AE 4.2 Correspondence between predicted property and property required by the regulation

→ The prediction should reproduce the required information

→ Examples:

- Experimental conditions
- pH dependence
- Identification of adverse effects

4 Outcome fit for regulatory purposes

AE 4.3 Decidability within the specific framework

→ Value corresponds to the requirements

→ Relation with the thresholds

→ Consideration of additional information

ECHA implementation

QAF in line with ECHA's existing QSAR evaluation practices

→ ECHA guidance on information requirements and chemical safety assessment chapter R.6: QSARs and grouping of chemicals (2008)

→ OECD guidance document on validation of QSAR models (2007)

→ Once QAF implemented: reference to OECD (Q)SAR Assessment Framework

For more information (ECHA webinars)

→ Applying the (Q)SAR Assessment Framework at ECHA (2025)

AI generated

→ OECD QSAR Assessment Framework in REACH dossier evaluation: what you need to know (2024)

AI generated

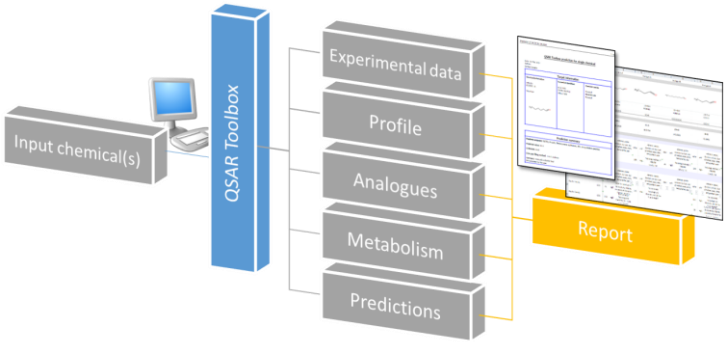
QSAR TOOLBOX

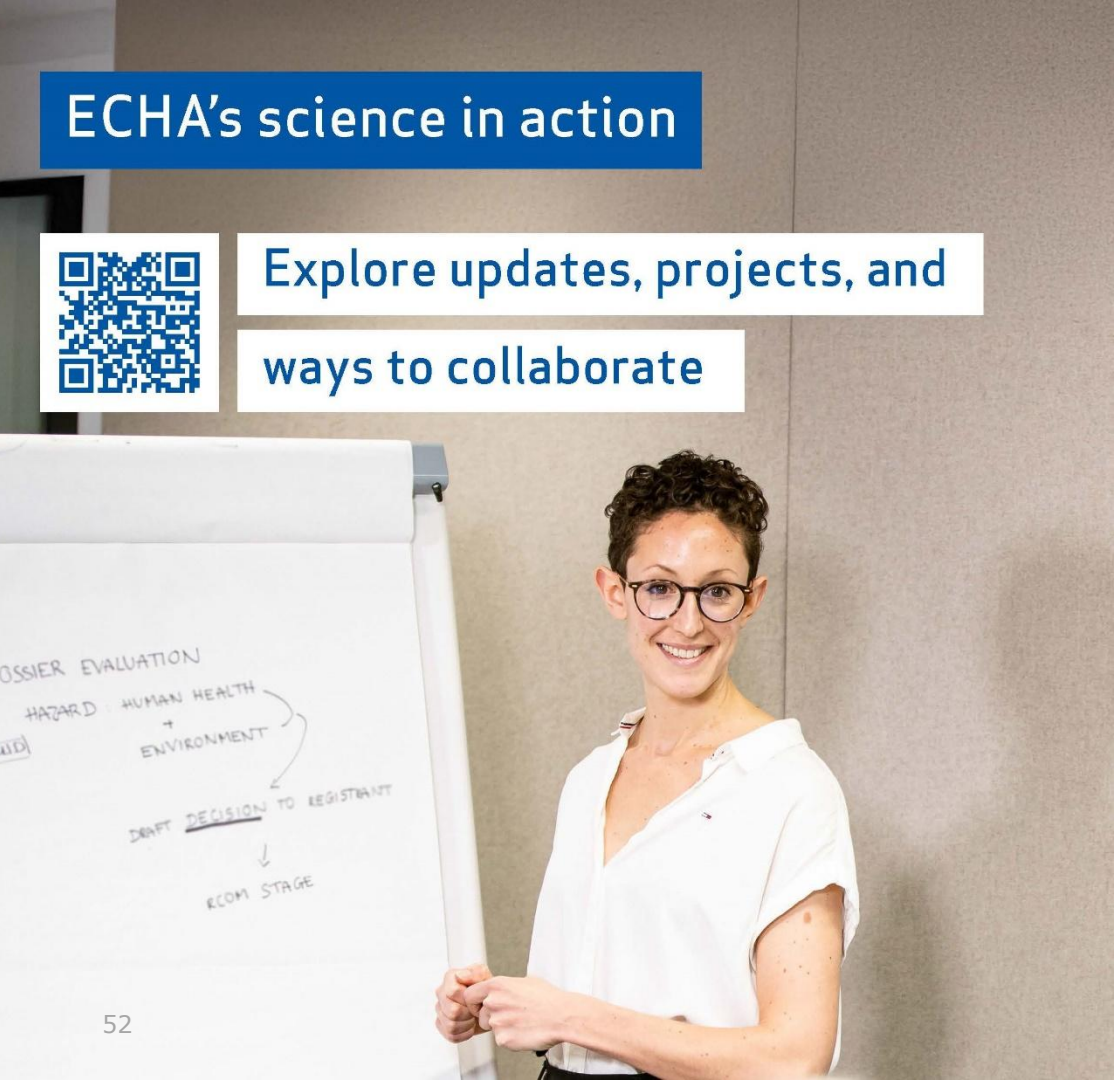
→ **Purpose:**

- Support reproducible and transparent chemical hazard assessment.

→ **Functions**:

- Search/retrieve experimental databases
- Profiling of chemicals
- Simulation of metabolism
- Prediction of properties (QSAR)
- Identification of analogues
- Repository of 3rd party functions
- Customized tools





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- → Our people in science
- → Research needs
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Thank you

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