



INTRODUCTION TO QAF





OECD QSAR Toolbox

❖ initiated in 2006

❖ Developed with the goal of placing substances into chemical **categories** to predict apical outcome of regulatory interest

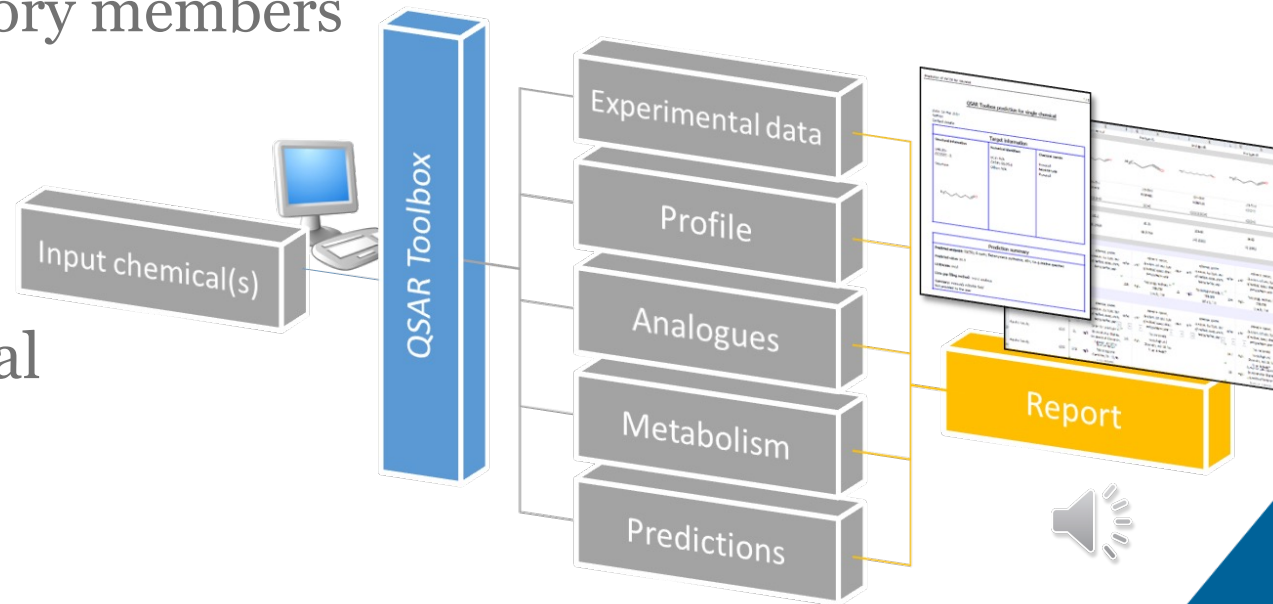
❖ Using data from tested category members [**analogues**] to aid in filling data gaps for untested category members

❖ Now, that and so much more

❖ Experimental data


❖ Profilers for properties of chemical

❖ Metabolism simulators



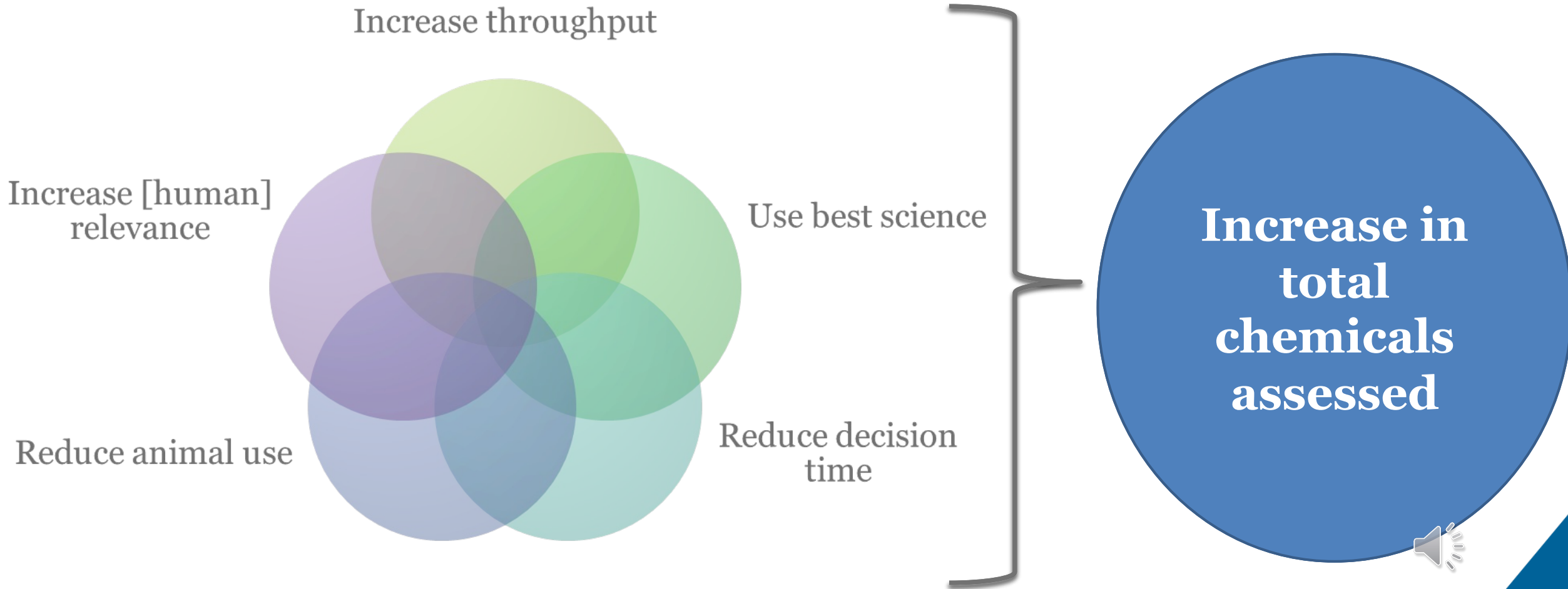


QSAR Toolbox supports alternatives to animal testing

- **Inform testing strategies** - by forming categories and identifying data gaps, intelligent testing strategies can be designed to reduce costs and number of animals required
- **Predict properties** - predictions can replace information requirements (industry) or be used as input to support authorities e.g. prioritisation, substance evaluation
- **Sustainable development and green chemistry** - the toxicity of substances can be predicted even before they are produced 



Global drivers to use NAMs in chemical risk assessment

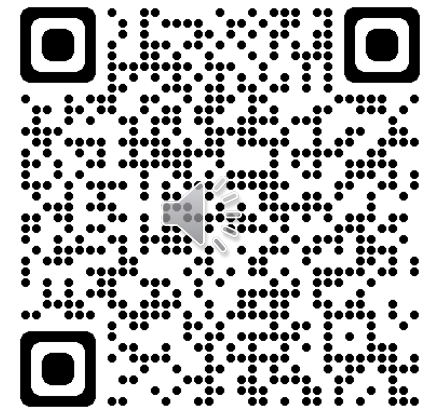




OECD QSAR Assessment Framework (QAF)

Project added to OECD Hazard Assessment Work Programme: Q1 2021

- Co-led by Istituto Superiore di Sanità (ISS) Italy and the European Chemicals Agency (ECHA)
- Supported by QAF Expert Group
 - provided general input on project, feedback on proposed path forward, written comments on drafts
 - met through a series of teleconferences in 2021 - 2023
 - drafting subgroups contribute to writing/review
 - face-to-face meeting of the QAF Expert Group Q4 2022 to help finalise the draft document
 - request for written commenting round to Working Party on Hazard Assessment Q2 2023
 - declassified in Q3 2023





QSAR Assessment Framework: overview

- Objective
 - The aim of the (Quantitative) Structure-Activity Relationship ((Q)SAR) Assessment Framework (QAF) is to develop a systematic and harmonised framework for the regulatory assessment
- Scope
 - (Q)SAR models
 - (Q)SAR predictions and results based on multiple predictions
- Relevance/applicability
 - irrespective of the technique used to build the model, the predicted endpoint, and the intended regulatory purpose
- Audience
 - primarily, regulatory authorities
 - as reference for other stakeholders using (Q)SARs for regulatory purposes





QSAR Assessment Framework

- Based on
 - [GD 49](#): Principles for the validation of QSARs (2004)
 - [GD 69](#): Guidance for Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models (2007)
- Sections on
 - Principles for assessing models
 - Principles for assessing predictions
 - Principles for assessing results from multiple predictions
- For each, development of assessment elements and a checklist of criteria
 - Guidance on how to determine if criteria are met
 - Examples illustrating how to evaluate criteria





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The OECD QSAR Toolbox

To increase the regulatory acceptance of (Q)SAR methods, the OECD is developing a QSAR Toolbox to make (Q)SAR technology readily accessible, transparent, and less demanding in terms of infrastructure costs.

[Download the Toolbox](#) [Guidance Documents and Training Materials](#) [Webinar](#) [Help Desk](#) [Public Discussion Forum](#)

WEBINAR ON THE NEW OECD (Q)SAR ASSESSMENT FRAMEWORK: GUIDANCE FOR ASSESSING (Q)SAR MODELS AND PREDICTIONS



The new OECD (Q)SAR Assessment Framework: guidance for assessing (Q)SAR models and predictions

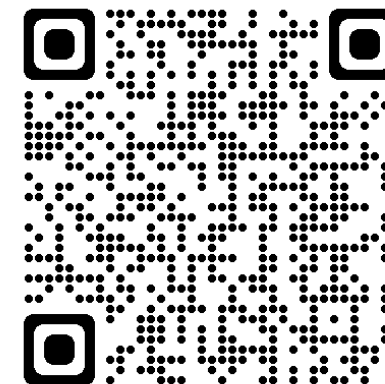
WHEN: 9 November 2023
13:00- 14:30 CET
07:00 - 08:30 EST



WHEN: 9 November 2023 at 13:00 - 14:30 CET / 07:00 - 08:30 EST

The webinar will provide an overview of the [new OECD \(Q\)SAR Assessment Framework](#) for evaluating the scientific validity of (Q)SAR models and introduce new principles for evaluating (Q)SAR predictions: input, applicability domain, reliability, and fitness for purpose.

his new Framework provides regulators with a consistent and transparent approach for reviewing the use of (Q)SAR predictions in a regulatory context and increases the confidence to accept alternative methods for evaluating chemical hazards. The OECD worked closely together with the Istituto Superiore di Sanità (Italy) and the European Chemicals Agency (ECHA), supported by a variety of international experts to develop a checklist of criteria and guidance for evaluating each criterion. The aim of the QAF is to help establish confidence in the use of (Q)SARs in evaluating chemical safety, and was designed to be applicable irrespective of the modelling technique used to build the model, the predicted endpoint, and the intended regulatory purpose. The webinar will begin with an overview of the project and walk through the main aspects of the framework for assessing models and results based on individual or multiple predictions, and provide an opportunity for Q&A.

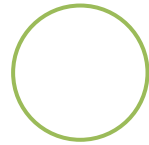


- Links to QAF and background documents
- Registration to upcoming OECD Webinar **9 November**
 - Links to recorded presentations
- Links to examples of how to use QAF
 - Coming soon

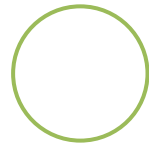


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Thank You For Listening



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