O-QT: AUDITABLE AI-ASSISTED QSAR TOOLBOX READ-ACROSS WORKFLOWS FOR VHP4SAFETY IMPLEMENTATION

Dr. Ivo Djidrovski[1], Dr. Juliette Legler[1], Dr. Raymond Pieters[1,2], Dr. Marc Teunis [2]

1. Institute for Risk Assessment Sciences, Utrecht University, The Netherlands
2. Innovative testing in life sciences and chemistry, Hogeschool Utrecht, The Netherlands

Background and Aim

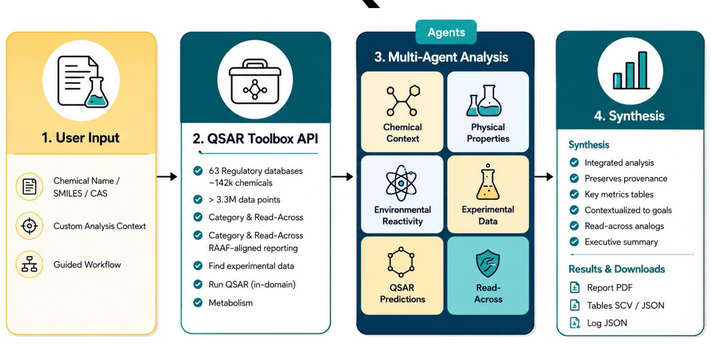
Bottleneck:

Writing justified narratives from complex OECD QSAR Toolbox outputs is expert-intensive, slow, and variable.

Aim:

To help operationalize animal-free, Next Generation Risk Assessment (NGRA) by orchestrating Toolbox data with specialized LLM agents to produce transparent and reproducible *in silico* safety assessments.

What O-QT does:



How O'QT Works

The O-QT workflow delivers auditable and reproducible outputs for animal-free, Next Generation Risk Assessment (NGRA).

User Query & Data Collection: The user initiates an analysis, and the system connects via the official Toolbox Web API to the user's local QSAR Toolbox to retrieve a comprehensive set of chemical data.

Multi-Agent Analysis: A team of specialized AI agents works in parallel to interpret distinct data slices (e.g., Physical Properties, Reactivity, Read-Across), applying expert-level reasoning to each component.

Synthesis & Reporting: A final synthesis agent integrates all specialist analyses into a single, cohesive narrative, creating a justified and evidence-backed New Approach Methodology (NAM)-based assessment.

Output & Review: The system delivers downloadable raw data (JSON/CSV) and a synthesized report designed to accelerate expert review and support the transition to animal-free safety assessment.

User-Friendly Tool

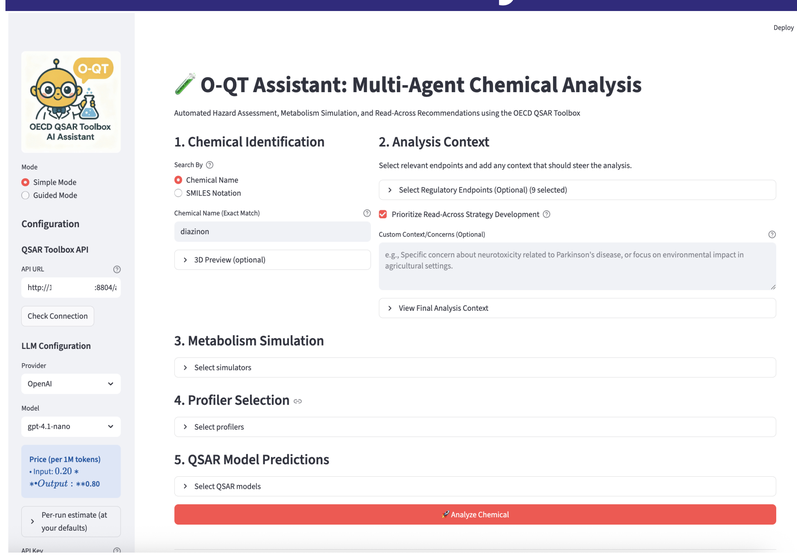


Figure 1: The O'QT Interface for Automated Hazard Reporting

The O-QT interface streamlines hazard assessment. The user provides a chemical identifier and an analysis context (Figure 1). The system then orchestrates a multi-agent workflow, from data collection via the local Toolbox API to final synthesis, delivering a comprehensive report and all underlying data for expert review.

The Agentic Workflow

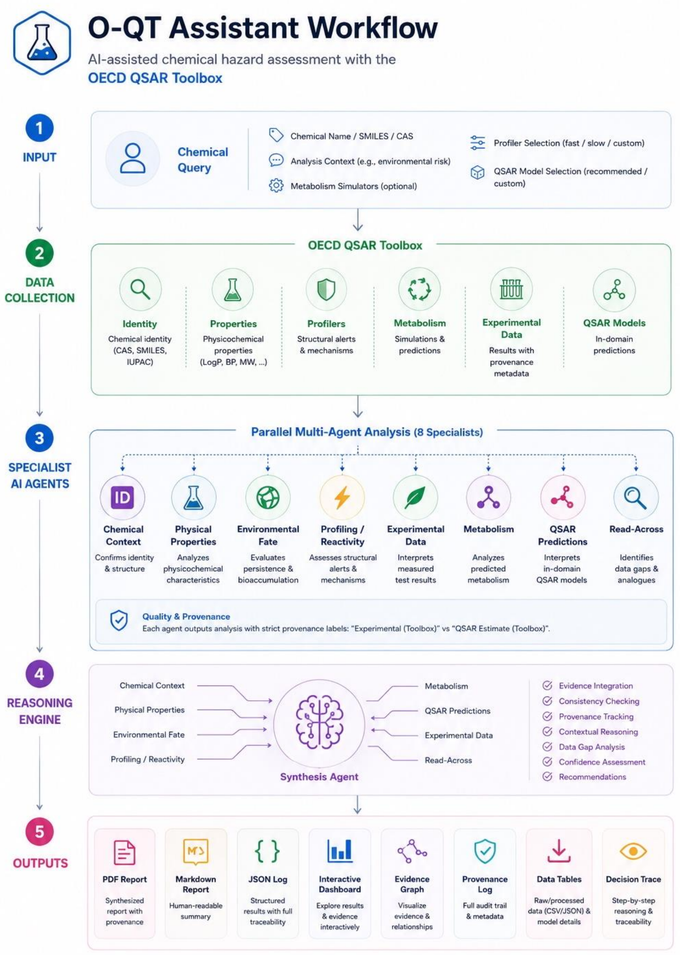
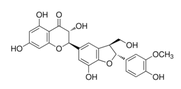


Figure 2: The agentic workflow ensures each data slice is analyzed by a specialized AI, creating a transparent and traceable process.

Results & Case studies: 3 Different AI-Generated Hazard Assessments

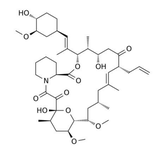
3 Case Studies

Data-poor natural product: endocrine/reactive-alert prioritisation



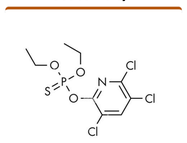
Silychristin

Human-active pharmaceutical: immunotoxicity, metabolism, and persistence



Tacrolimus

Data-rich pesticide benchmark: AChE neurotoxicity and ecotoxicity



Chlorpyrifos

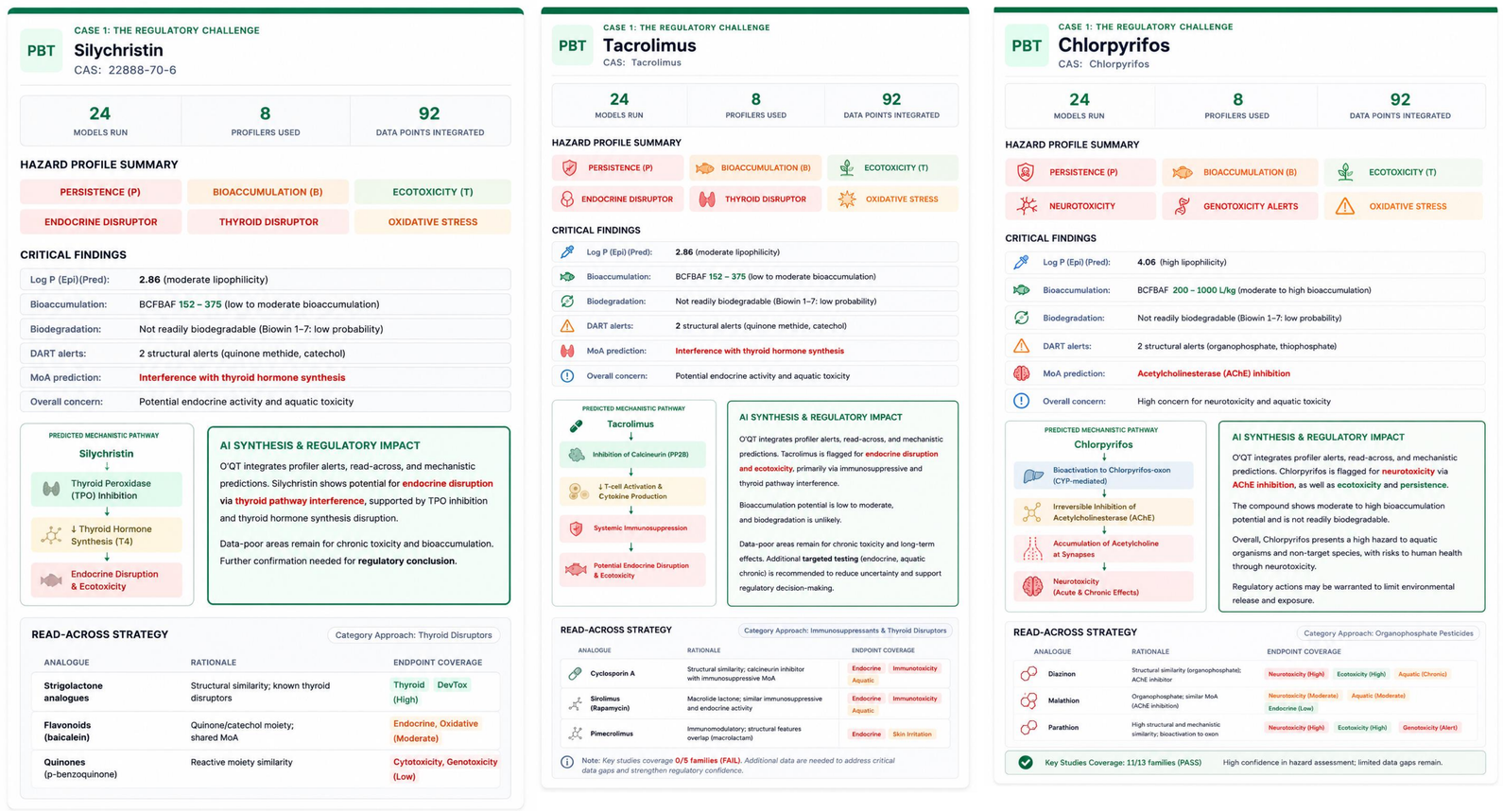


Figure 3: O'QT demonstrates flexibility across **regulatory, mechanistic, and data-poor** scenarios, generating expert-level insights **in minutes**

Trust and transparency

Compliance: Acts as a **client** to the user's local Toolbox; **software not redistributed** (EULA-safe).

Provenance: Every claim ties to **Toolbox-derived evidence**, with downloadable **JSON/CSV**.

Reproducibility: every run **seed / temperature / schema versions** is hashed (e.g., "Run ID: short-hash").

Human-in-the-Loop: **Expert review required**; the system surfaces gaps/uncertainties.

Scan for video demo

Conclusions and next steps

Accelerate Assessment: Automate end-to-end hazard reporting, turning days of work into minutes.

Ensure Compliance: Generate auditable, EULA-compliant read-across proposals where expert review remains central.

Operationalize NAMs: Provide a practical, scalable AI-first approach for both complex and data-poor chemicals.

*VHP4Safety project NWA 1292.19.272 is part of the Netherlands Science Agenda (NWA) research program 'Research along Routes by Consortia (ORC)', which is funded by the Netherlands Organization for Scientific Research (NWO).