

NICEATM Computational Efforts Update

From curated data to interoperable models for NAM adoption

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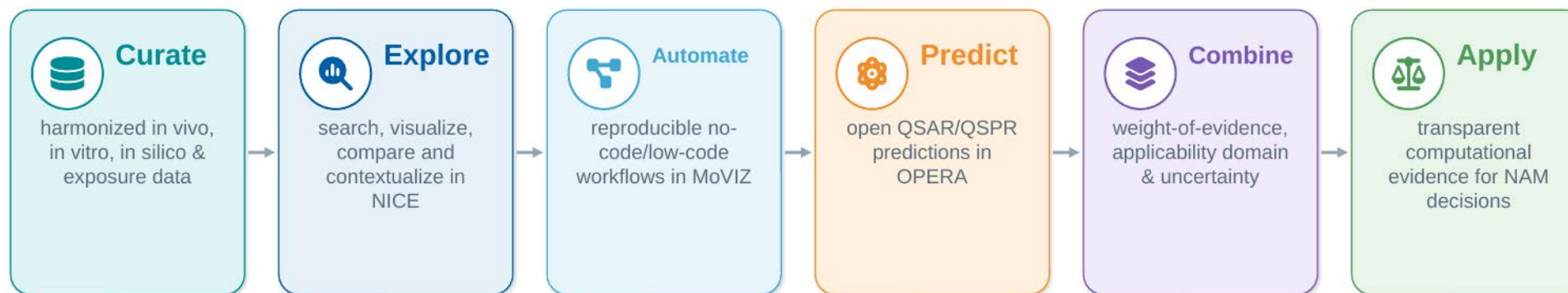
Computational Chemist | NIH/ORIVA/NICEATM

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ECOSYSTEM

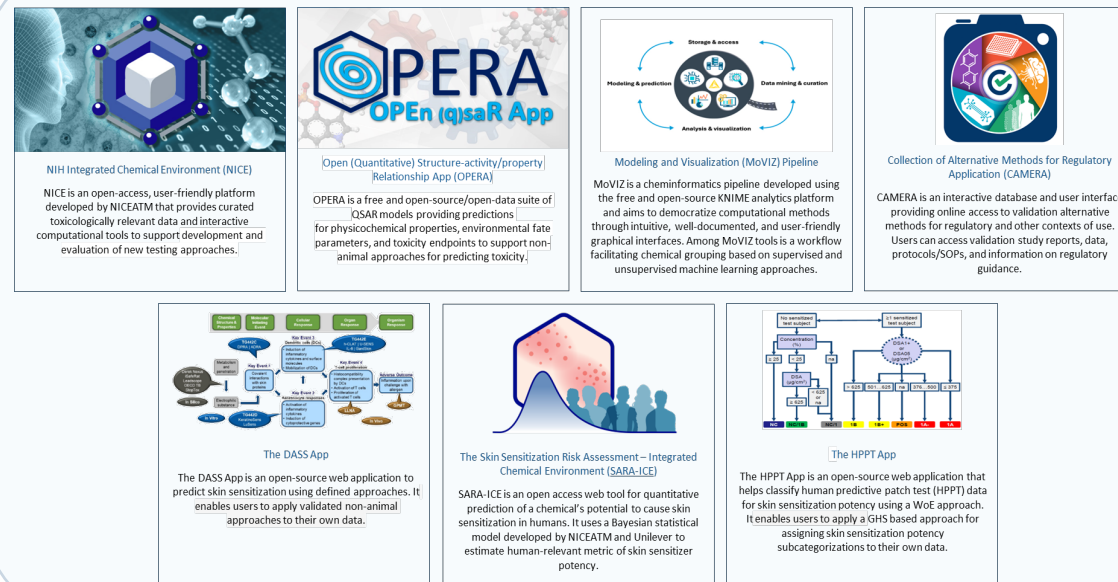
One connected pathway – from evidence to decisions

The portfolio is shifting from **individual tools** toward an **interoperable ecosystem** that makes curated data, automated workflows, and consensus models easier to use in NAM evaluation.



Accessible tools + curated data + interoperability = regulatory-ready computational support.

ECOSYSTEM



Curated data

in vivo, in vitro,
in silico, exposure

Interactive NICE tools

search, PBPK/IVIVE,
Curve Surfer

MoVIZ workflows

no-code/low-code
cheminformatics

OPERA models

QSAR/QSPR
predictions

International collaborations

CATMoS, CoMPAIt

Regulatory support

transparent evidence
for NAM adoption

The ecosystem spans data access, modeling, workflows, and decision support.

HIGHLIGHTS

Four advances define this year's computational update

LIVE



NICE v5.0

- ✓ Platform rebrand and data updates
- ✓ New Search visualizations
- ✓ PBPK/IVIVE flexibility with httk 2.7.4

EXPANDING



MoVIZ workflows

- ✓ LLM-supported literature extraction
- ✓ QSAR-ready standardization
- ✓ Endpoint-relevant chemical grouping

NEAR RELEASE



CATMoS update

- ✓ Bishop et al. (2024) data added
- ✓ Improved consensus WoE
- ✓ Better counterion/salt/solvent handling

ADVANCING



CoMPAIT

- ✓ International consensus modeling
- ✓ Planned OPERA implementation
- ✓ Manuscript draft to collaborators soon

Supporting work continues in skin sensitization, IVIVE, MPS/QST translation, and AI-assisted NAM discovery.

NICE

NICE v5.0 broadens access and makes PBPK/IVIVE more flexible

ICE v4.2

Jul 2025

chTS v4.2; user
physchem/ADME upload;
updated PCAs

NICE v5.0

Jul 2026

new name, data updates,
endpoint visualizations,
PBPK/IVIVE refinements

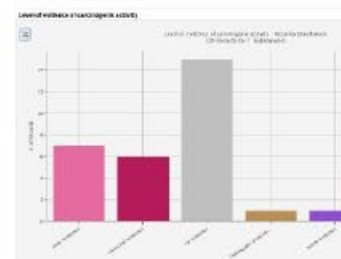
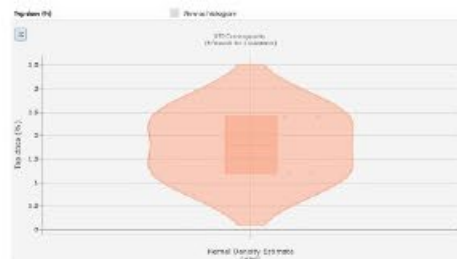
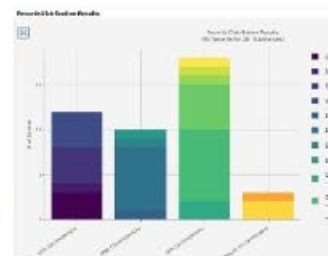
Next

upcoming year

Chemical Quest overhaul; more
endpoint visualizations; further
PBPK/IVIVE refinements



NIH
Integrated
Chemical
Environment



Search & visualization

New cancer and acute-toxicity views;
additional endpoints planned.



PBPK/IVIVE flexibility

httk 2.7.4 plus single-dose and
uneven/custom dosing scenarios.



Next platform step

Chemical Quest overhaul and
continued model refinements.

User value: curated toxicology data and computational models without requiring users to code.

NICE

Modernization turns NICE into a scalable, reproducible scientific platform

What users experience is enabled by a more durable technical foundation.

USER-FACING OUTCOMES

**Faster delivery**

shorter cycles for fixes, data updates, and scientific features

**Interoperability**

APIs and bidirectional exchange with CAMERA and external tools

**Reproducibility**

saved sessions, data versioning, and citable result states

**Reliability**

secure, scalable infrastructure for larger workflows and datasets

ENABLING FOUNDATION

**Cloud-native**

NIH cloud infrastructure and independently scalable services

**DevSecOps**

automated testing, deployment, monitoring, and security

**Modern data pipelines**

more maintainable storage, ETL, APIs, and scientific services

**Future-ready**

architecture for AI-assisted tools and advanced analytics

Foundation

cloud architecture
GitHub/Jira/CI-CD

Migration

database and app
modernization

Modernization

new features
API integrations

Innovation

AI-assisted
scientific tools

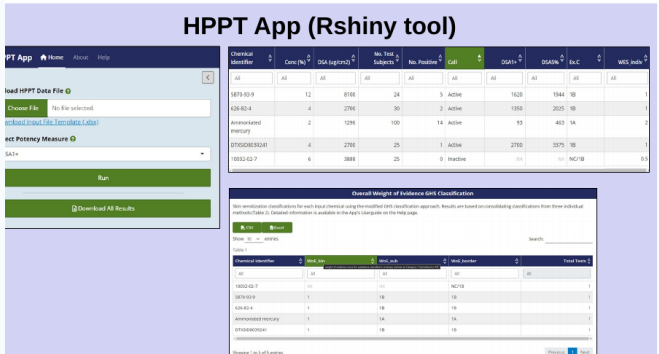
DECISION APPS

Web applications turn curated human and non-animal data into practical decision support.



Human Skin Sensitization Data
 NICESTM and collaborators compiled human data as a resource to evaluate new testing approaches for skin sensitizers.
[Read More](#)

HPPT App (Rshiny tool)



Database and proposed HPPT GHS classification approach

Archives of Toxicology (2023) 99:2823–2837
<https://doi.org/10.1007/s00204-023-03356-3>

REVIEW ARTICLE

A database of human predictive patch test data for skin sensitization

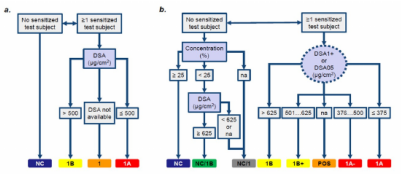
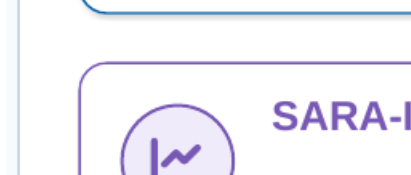
Judy Stockland¹ · Jaleh Abedini² · David G. Allen³ · John Gordon⁴ · Victoria Huff⁵ · Nicole C. Kleinstreuer⁶ · Heon-Sum Ko⁷ · Joanna Matheson⁸ · Hermann-Joachim Thierse⁹ · James Truax¹⁰ · Jens T. Vanselow¹¹ · Matthias Herder¹²

Archives of Toxicology (2024) 98:1233–1245
<https://doi.org/10.1007/s00204-024-03404-4>

REVIEW ARTICLE

Use of human predictive patch test (HPPT) data for the classification of skin sensitization hazard and potency

Matthias Herder¹ · Jaleh Abedini² · David G. Allen³ · Dorit Gernolke⁴ · John Gordon⁵ · Heon-Sum Ko⁶ · Joanna Matheson⁷ · Emily Newell⁸ · Judy Stockland⁹ · Hermann-Joachim Thierse¹⁰ · Kim To¹¹ · James Truax¹² · Jens T. Vanselow¹³ · Nicole Kleinstreuer¹⁴

(a) Standard GHS Classification Approach (b) Modified Classification Approach



HPPT App

Classifies human predictive patch-test data using the modified GHS approach and a weight-of-evidence combination of results.



DASS App

Applies validated defined approaches for skin sensitization to user-provided data in an open-source web application.



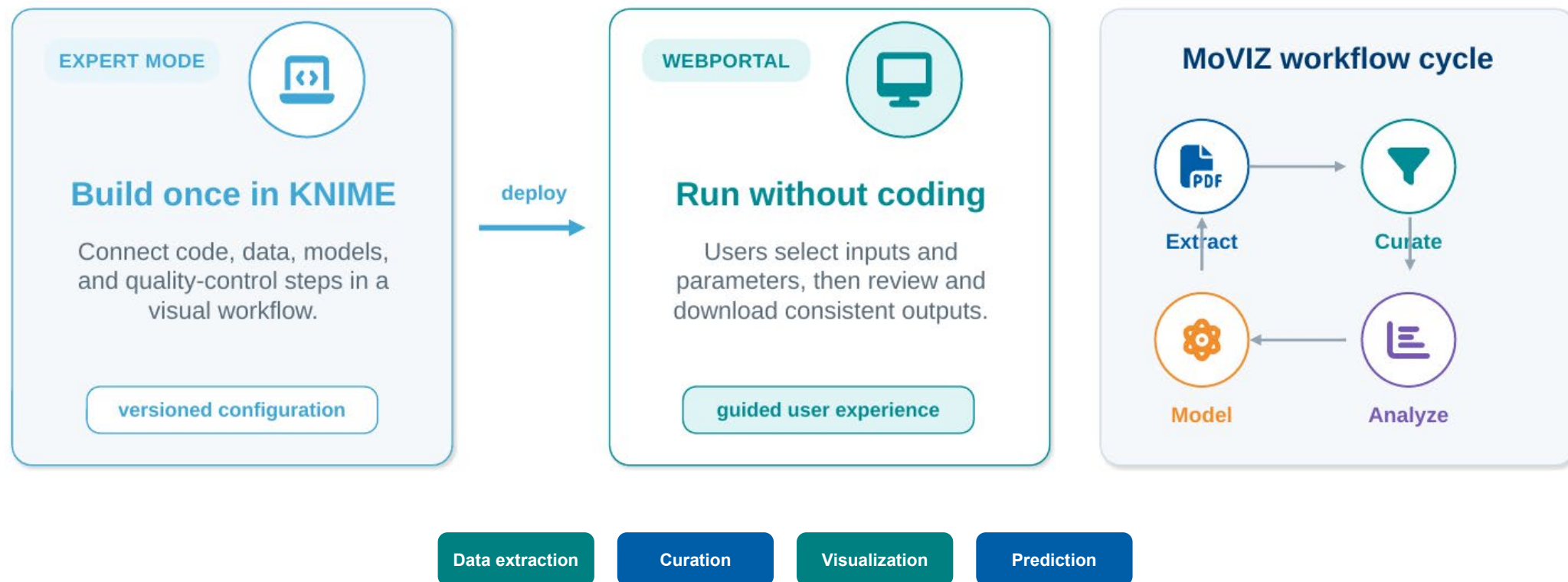
SARA-ICE

Uses a Bayesian model to estimate a human-relevant quantitative metric of skin sensitization potency.

Shared value: open access, documented logic, interactive results, and downloadable outputs.

MOVIZ

MoVIZ packages expert cheminformatics into guided, no-code/low-code workflows.



Democratization means advanced methods are accessible without hiding how they work.

MOVIZ

Modeling and prediction

- AI and machine learning
- QSAR and read across
- Property/activity prediction

Data extraction and access

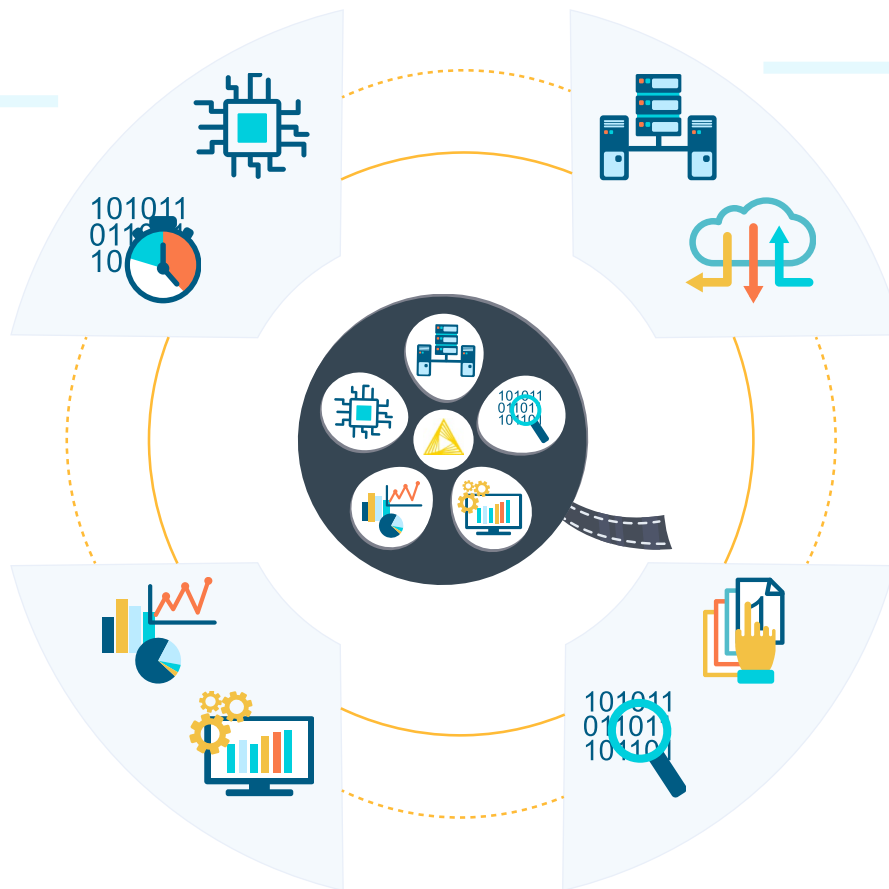
- Literature search and extraction
- Internal database querying
 - Chemical similarity search

Data analysis and visualization

- Data exploration
- Statistical analysis
 - Chemical grouping

Data mining and curation

- Data collection and processing
- Outlier and duplicate detection
- Chemical structure standardization



MOVIZ

Example workflows span extraction, chemical preparation, and endpoint-relevant grouping solving recurring bottlenecks.

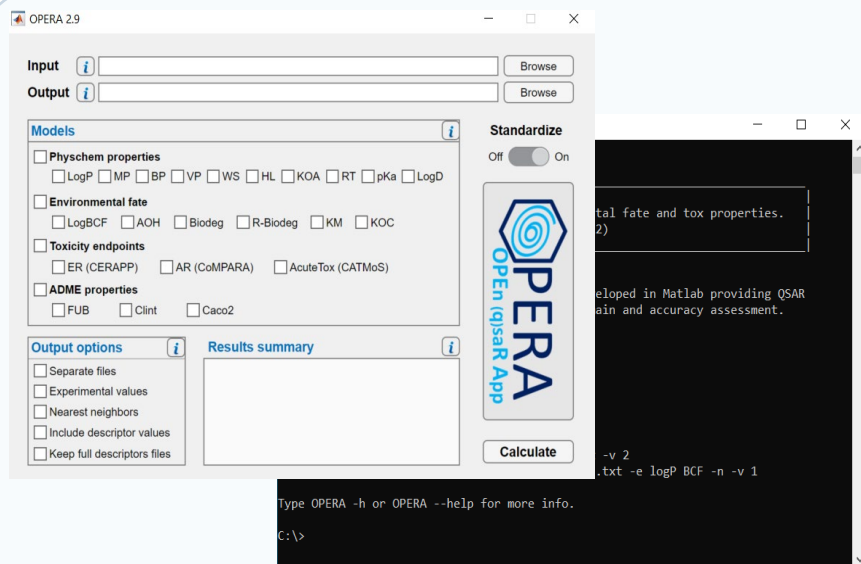


Common output: transparent reports, CSV downloads, reusable configuration files, and human-centered QC

Human review remains in the loop, while inputs, parameters, and outputs are preserved for reuse.

OPERA

OPERA delivers open, documented QSAR predictions for both interactive use and automated workflows.



12,000+ downloads and growing

Four model families



Physchem



Fate



ADME



Toxicity

Three ways to use it



GUI

single or batch



Command line

automated runs



Libraries

Java, C/C++,
Python

Inputs: CAS, DTXSID, InChIKey, SMILES, SDF, Mol → **Outputs:** predictions across multiple endpoints

Open-source + open-data + batch processing—and available through MoVIZ workflows.

OPERA

CATMoS strengthens predictions where the original training data were weakest

NEAR RELEASE

Major CATMoS update scheduled very soon

Bishop et al. (2024) expands coverage in the highly toxic range

Training coverage



Expected impact

More reliable point estimates and category assignments—especially for highly toxic chemicals.

Bishop et al. (2024)



Better training coverage

Incorporates the Bishop et al. (2024) dataset, improving predictive accuracy for highly toxic chemicals in lower GHS/EPA categories.



More consistent consensus WoE

Improves categorical and point estimates for ambiguous cases by refining the consensus weight-of-evidence approach.



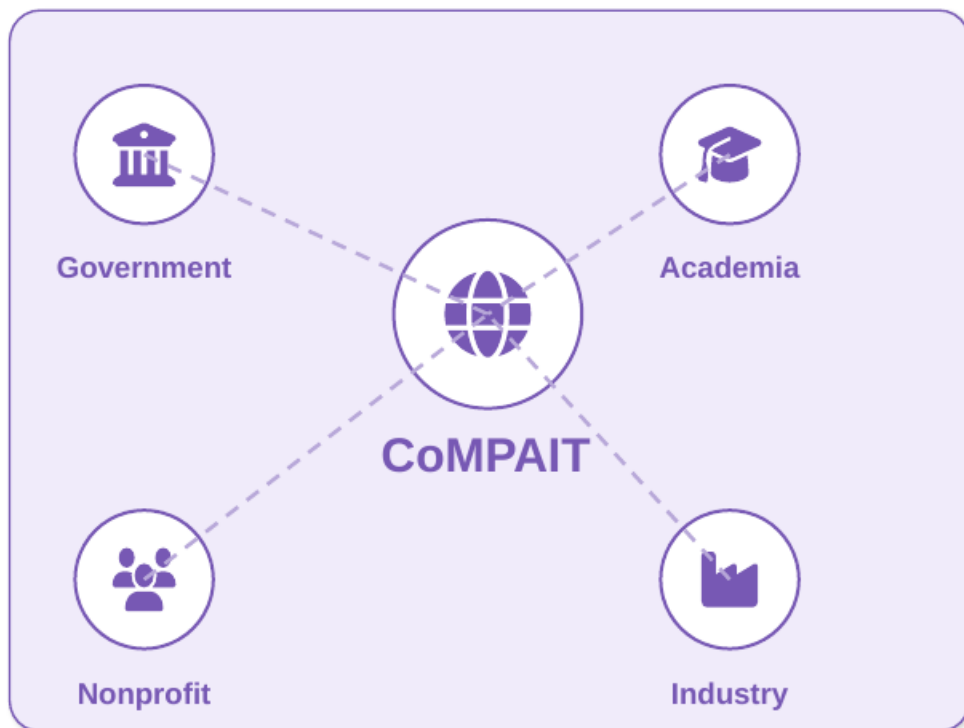
More robust structure handling

Improves processing of compounds containing counterions and common salts or solvents.

CoMPAIT

CoMPAIT aligns 20 international groups around one curated inhalation endpoint

Government, nonprofit, academic, and industry teams contribute independent models to a common evaluation.


20

participating groups

765

chemicals in modeling set

48k+QSAR-ready prediction
structures

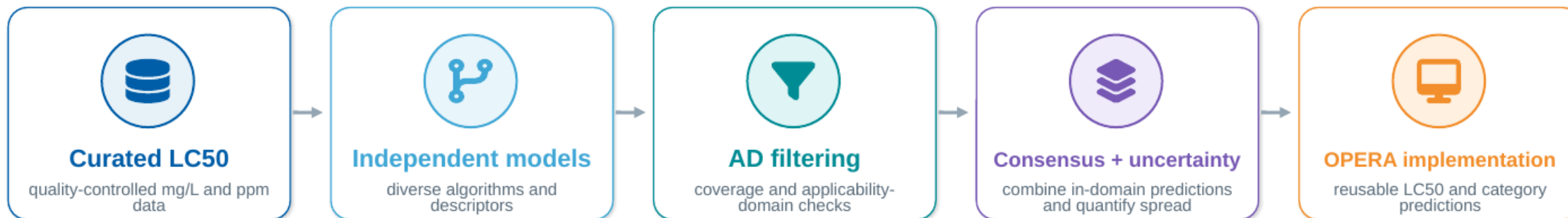
Modeling endpoint and data preparation

- LC50 point estimates in mg/L and ppm
- 612 training chemicals + 153 evaluation chemicals
- Quality flags, unit harmonization, deduplication, and QSAR-ready structures

COMPAIT

Consensus converts diverse models into an implementable OPERA prediction

The approach follows the successful CATMoS and CERAPP/CoMPARA consensus-model pathway.



Interim 2025 evaluation supports the consensus strategy

mg/L
mean $R^2 \approx 0.55$

ppm
mean $R^2 \approx 0.60$

Performance was strongest when multiple models covered the same chemical.



Manuscript and implementation

- Consensus model and uncertainty range will be finalized for OPERA implementation.
- A manuscript draft will be circulated to collaborators soon.

Collaborative science becomes reusable when consensus logic, uncertainty, and implementation are designed together.

EMERGING METHODS

Four parallel efforts extend support beyond current products

GUIDANCE

**OECD in silico tool analysis**

Update Guidance Document 34 to reflect greater use of in silico methodologies, readiness stages, and updated documentation and model-evaluation expectations.

MODEL DEVELOPMENT

**Pubertal IVIVE**

Use htk to model sensitive pubertal stages through physiological distributions, tissue compartments, and relevant mechanisms.

TRANSLATION FRAMEWORK

**MPS/QST inhalation**

Combine PBTK, tissue dosimetry, and toxicodynamics to translate lung-on-chip data into human-relevant inhalation predictions.

PROTOTYPE

**AI-assisted NAM discovery**

Use retrieval-augmented generation over trusted sources to recommend human-relevant methods and evidence-based next steps.

Common goal: translate evidence into human-relevant, decision-ready predictions.

ROADMAP

Near-term priorities focus on interoperability, reproducibility, and trust

Adoption depends on computational evidence that users can find, reproduce, explain, and transfer between systems.



Adoption infrastructure is as important as the model: usable tools, transparent evidence, and interoperable data.

TAKE-HOME

Find it. Run it. Trust it.

NICEATM is building an ecosystem for regulatory-ready computational NAMs.



FIND

Curated evidence

NICE makes data, context, visualizations, and computational tools easier to access.



RUN

Accessible workflows

MoVIZ, OPERA, and decision apps reduce technical barriers while preserving transparency.



TRUST

Consensus & reproducibility

CATMoS and CoMPAIT combine models, applicability domains, uncertainty, and reuse.

Thank you — questions and discussion



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CAMERA Website

