

Additional Resources

Computational Toxicology

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NAMs

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Quantitative Structure–Activity Relationships (QSARs)

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oral toxicity data. *J Cheminform.* 2019 Dec;11(1):58. doi: 10.1186/s13321-019-0383-2.

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Read Across

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Physiologically Based Pharmacokinetic (PBPK) Modeling

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In Vitro to In Vivo Extrapolation (IVIVE)

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Quantitative Adverse Outcome Pathways (qAOPs)

- Used as a webinar case study: Foran CM, Rycroft T, Keisler J, Perkins EJ, Linkov I, Garcia-Reyero N. A modular approach for assembly of quantitative adverse outcome pathways. *ALTEX.* **2019**, 36(3):353-362. doi: 10.14573/altex.1810181. Epub 2019 Jan 20. PMID: 30662994.
- Hassan I, El-Masri H, Kosian PA, Ford J, Degitz SJ, Gilbert ME. Neurodevelopment and Thyroid Hormone Synthesis Inhibition in the Rat: Quantitative Understanding Within the Adverse Outcome Pathway Framework. *Toxicol Sci.* **2017** Nov 1;160(1):57-73. doi: 10.1093/toxsci/kfx163. PMID: 28973696; PMCID: PMC10623382.
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Molecular Modeling

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AI / Machine Learning / Deep Learning

- Used as a webinar case study: Bundy, J. L.; Rogers, J. D.; Shah, I.; Judson, R. J.; Everett, L. J.; Harrill, A. J. A Machine Learning Approach to Molecular Initiating Event

Prediction Using High-Throughput Transcriptomic Chemical Screening Data. *J. Chem. Inf. Model.* **2025**, DOI: 10.1021/acs.jcim.5c00699.

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- Lin, Z.; Chou, W.-C. Machine Learning and Artificial Intelligence in Toxicological Sciences. *Toxicol. Sci.* **2022**, 189 (1), 7–19.
- Special Issue: AI Meets Toxicology. *Chem. Res. Toxicol.* **2023**, 36 (8).

Software and Databases

NAMs

- Comprehensive database of available NAMs for hazard characterization: <https://nams.network/>

AOPs

- Adverse Outcome Pathway Database (AOP-DB): <https://catalog.data.gov/dataset/adverse-outcome-pathway-database-aop-db-version-2>
- AOP-Wiki: <https://aopwiki.org/>

Chemical and Bioactivity Data

- CompTox Chemicals Dashboard: <https://comptox.epa.gov/dashboard/>
- Integrated Chemical Environment (ICE): <https://ice.ntp.niehs.nih.gov/>

QSARs

- Dragon version 7.0.4: <https://chm.kode-solutions.net>
- Knime: <https://www.knime.com/>
- Indigo toolkit: <https://lifescience.opensource.epam.com/indigo/>
- istKNN Application version 0.9.3: <https://chm.kode-solutions.net/>
- R Caret Package: <http://www.jstatsoft.org/article/view/v028i05/v28i05.pdf>
- R H2O 3.16.0.3 Package: <https://www.h2o.ai/download/>
- R v. 3.4.0: <https://www.R-project.org>
- SARpy: <https://www.vegahub.eu/portfolio-item/sarpy/>

Read-across

- OECD QSAR Toolbox v. 3.5: <https://www.oecd.org/en/data/tools/oecd-qsar-toolbox.html>
- SQLite v.3: <https://www.sqlite.org/>
- ToxCast/Tox21 (invitrodb_v2): <https://www.epa.gov/chemical-research/toxicity-forecaster-toxcasttmdata>

PBPK Modeling Tools

- ICE PBPK Tool: <https://ice.ntp.niehs.nih.gov/Tools?tool=pbpk>

IVIVE Tools

- ICE IVIVE Tool: <https://ice.ntp.niehs.nih.gov/Tools?tool=ivive>

Molecular Modeling Resources

- AutoDock Vina: <https://github.com/ccsb-scripps/AutoDock-Vina>
- RCSB Protein Data Bank: <https://www.rcsb.org/>

Regulatory Acceptance and Guidelines

General

- EU Tracking System for Alternative methods towards Regulatory acceptance (TSAR): <https://tsar.jrc.ec.europa.eu/document-type/oecd-guidance-document>
- List of alternative methods accepted by US agencies, compiled by the NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM): <https://ntp.niehs.nih.gov/whatwestudy/niceatm/accept-methods>
- Test methods for regulatory use, compiled by PETA Science Consortium International: <https://www.thepsci.eu/test-methods/>

QSAR

- OECD (2024), (Q)SAR Assessment Framework: Guidance for the regulatory assessment of (Quantitative) Structure Activity Relationship models and predictions, Second Edition, OECD Series on Testing and Assessment, No. 405, OECD Publishing, Paris, <https://doi.org/10.1787/bbdac345-en>.
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Read Across

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PBPK

- OECD (2021), *Guidance Document on the Characterisation, Validation and Reporting of Physiologically Based Kinetic (PBK) Models for Regulatory Purposes*, OECD Series on Testing and Assessment, No. 331, OECD Publishing, Paris, <https://doi.org/10.1787/d0de241f-en>.

IVIVE

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- OECD (2014), *The Guidance Document for Using the OECD (Q)SAR Application Toolbox to Develop Chemical Categories According to the OECD Guidance on Grouping Chemicals*, OECD Series on Testing and Assessment, No. 102, OECD Publishing, Paris, <https://doi.org/10.1787/9789264221482-en>.