



Advancing Hazard Assessment and Screening Decisions through AI

Robert Colau, Diana Schramm – 3E

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**Empowering safety. Elevating stewardship.
Enabling sustainability.**

Today's speakers



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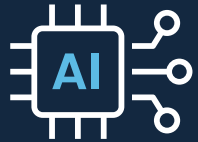
Director, Substance
Compliance & Classification

Introduction

Why AI? Why Now?



Overview



AI Tools



Why AI? Why now?

AI didn't just get better. It got useful—and accessible.

- More computing power + more data + better models
- Chat interfaces made it feel human and approachable
- Generative AI can now produce content – not just data analysis

Traditional Automation

- Follows strict rules
- Does repetitive tasks
- Requires specific inputs
- Output is predictable

Generative AI (e.g., GPT)

- Learns patterns from data
- Creates content & ideas
- Understands natural language
- Output can vary, even creative

Risk of NOT Using AI

- Falling behind competitors
- Manual workload increases
- Missed insights from unstructured data
- Reduced efficiency in complex decision-making

Risk of Using AI

- Inaccurate or biased output
- Overdependence or automation errors
- Data privacy and security issues
- Regulatory uncertainty

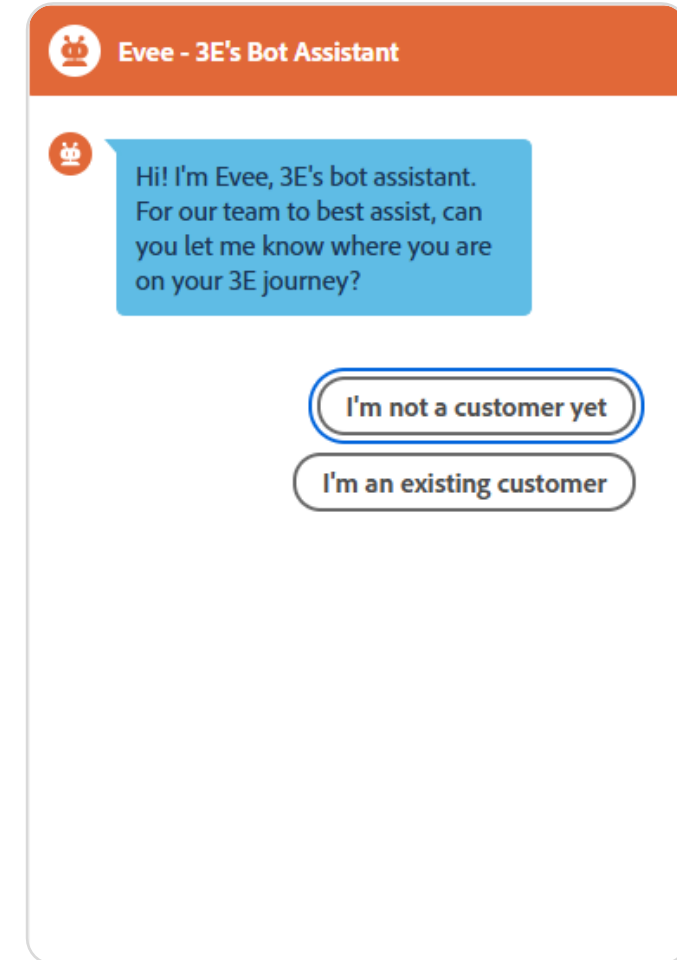
Definition:

- Simple conversational tools for basic interaction

How it Works:

- Simulate human-like conversation, often in a Q&A format.
- Limited to pre-defined topics or trained responses.
- Common in websites for customer support or help desks.

Use case: An AI Chatbot answering SDS questions for customer service.



AI Assistant



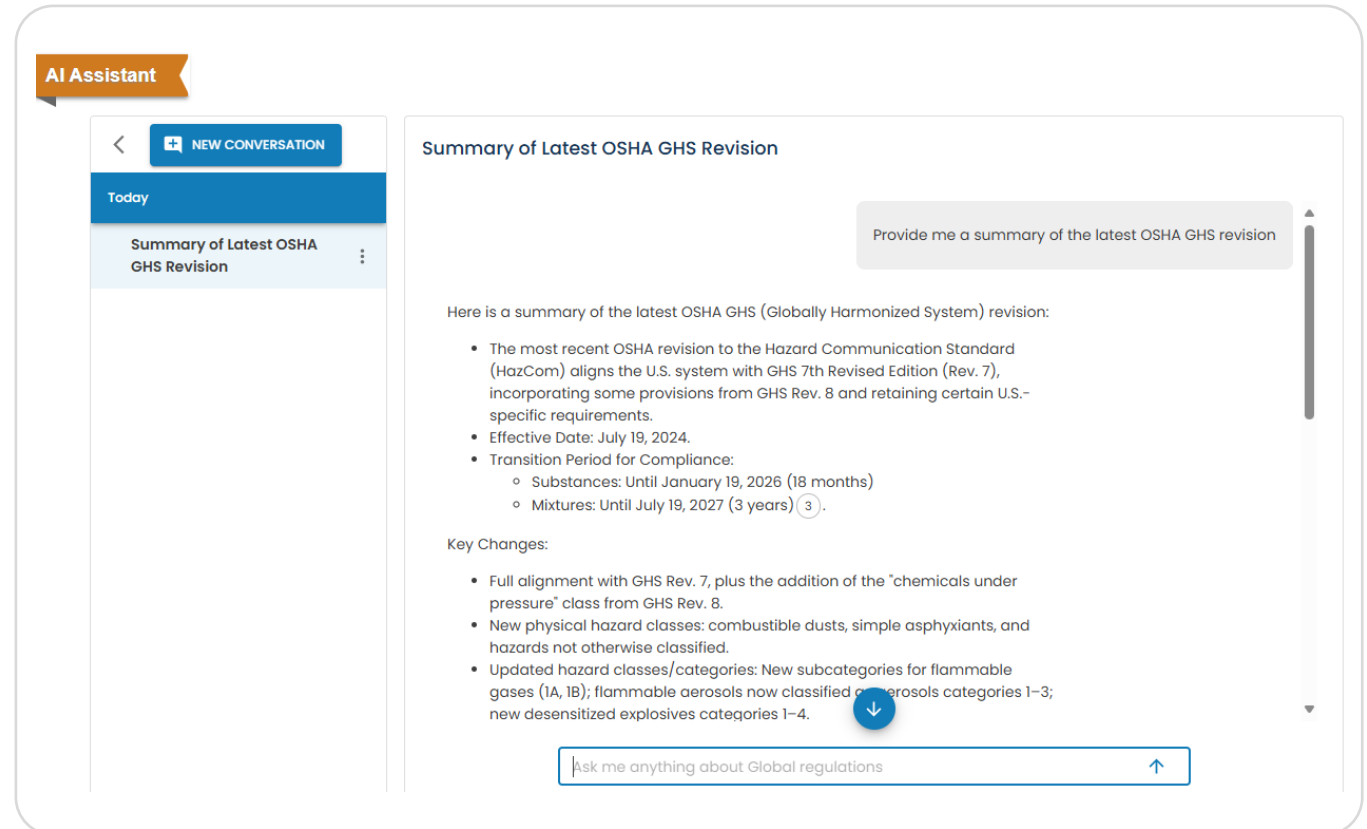
Definition

- Supportive tools for productivity (not fully autonomous)

How it Works:

- Help users complete tasks like summarizing or translating.
- React to instructions but don't act on their own.
- Used in daily work (e.g., drafting emails, organizing notes).

Use Case: An AI assistant that drafts regulatory reports or summarizes regulations.



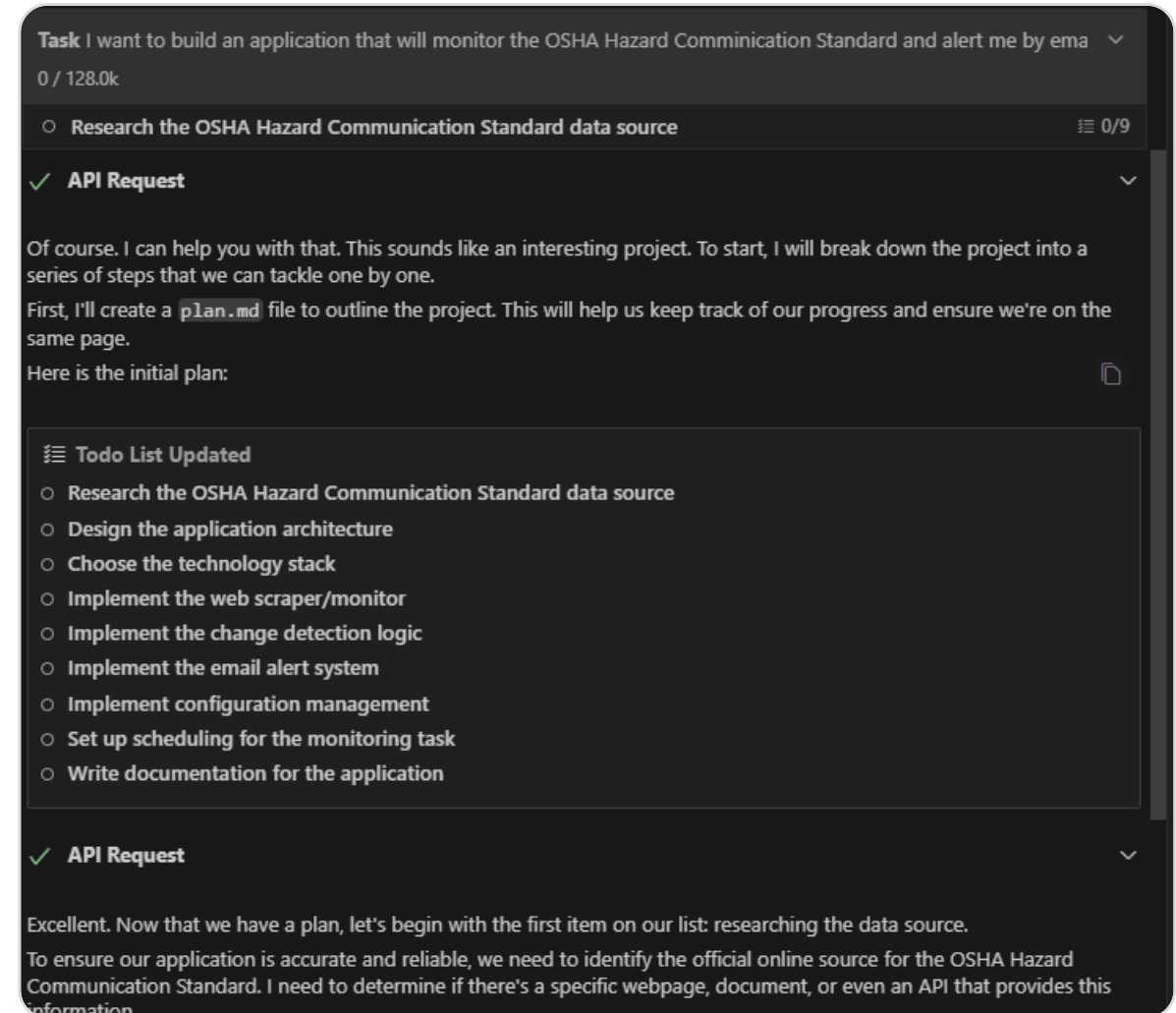
Definition:

- A solution that can reason, plan, and act autonomously to achieve a defined goal.

How it Works:

- Breaks down tasks into manageable steps.
- Learns from results and adjusts plans to succeed.
- Uses tools to achieve goals effectively.

Use Case: An AI agent that monitors new regulations and alerts your team when action is needed.



A specific use case for AI



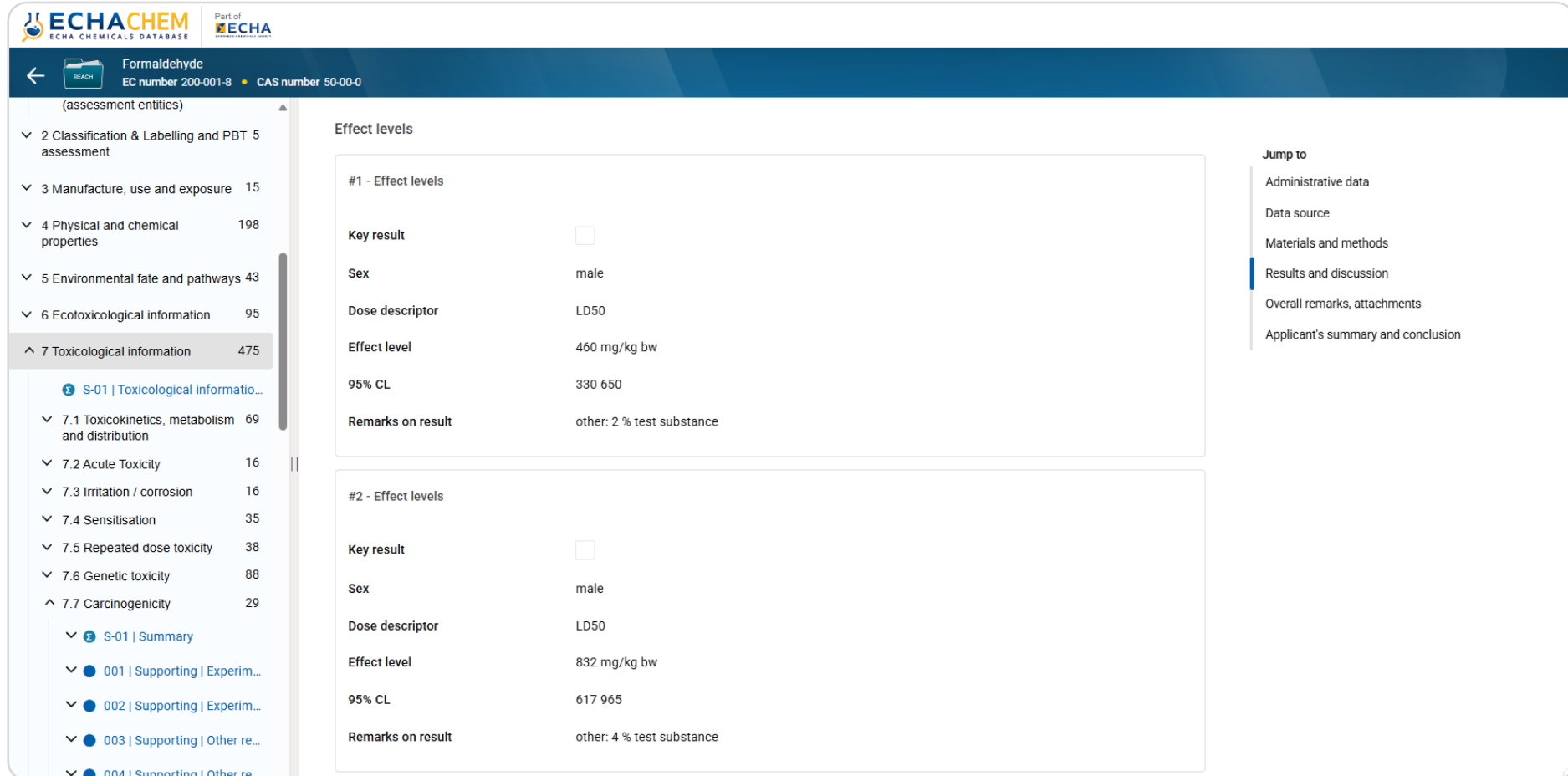
Curating a physical-chemical,
toxicological and ecotoxicological dataset

Why create such a dataset?



Why create such a dataset?

Difficult useability and navigation of the source (ECHA website), as well as occasionally not available



The screenshot displays the ECHA CHEM database interface for Formaldehyde (EC number 200-001-8, CAS number 50-00-0). The interface is divided into three main sections: a left sidebar for navigation, a central content area, and a right sidebar for quick links.

Left Sidebar (Assessment entities):

- 2 Classification & Labelling and PBT 5 assessment
- 3 Manufacture, use and exposure 15
- 4 Physical and chemical properties 198
- 5 Environmental fate and pathways 43
- 6 Ecotoxicological information 95
- 7 Toxicological information 475
 - S-01 | Toxicological information...
 - 7.1 Toxicokinetics, metabolism and distribution 69
 - 7.2 Acute Toxicity 16
 - 7.3 Irritation / corrosion 16
 - 7.4 Sensitisation 35
 - 7.5 Repeated dose toxicity 38
 - 7.6 Genetic toxicity 88
 - 7.7 Carcinogenicity 29
 - S-01 | Summary
 - 001 | Supporting | Experim...
 - 002 | Supporting | Experim...
 - 003 | Supporting | Other re...
 - 004 | Supporting | Other re...

Central Content Area (Effect levels):

#1 - Effect levels

Key result	<input type="checkbox"/>
Sex	male
Dose descriptor	LD50
Effect level	460 mg/kg bw
95% CL	330 650
Remarks on result	other: 2 % test substance

#2 - Effect levels

Key result	<input type="checkbox"/>
Sex	male
Dose descriptor	LD50
Effect level	832 mg/kg bw
95% CL	617 965
Remarks on result	other: 4 % test substance

Right Sidebar (Jump to):

- Administrative data
- Data source
- Materials and methods
- Results and discussion
- Overall remarks, attachments
- Applicant's summary and conclusion

Why create such a dataset?

Complex datasets

- Substance details
- Methodological considerations
- Results, often multiple at varying conditions
- Review of discussions leading to conclusions
- Study quality determinations

High volume of data = millions of data records

- 55 potentially reported endpoints per substance
- Many studies per endpoint
- Multiple results per study



Why create such a dataset?

Uneven quality of datasets

- Quality of studies themselves (Klimisch = 3 – unreliable)
- Uneven reporting of studies that are of reasonable quality
 - Key details missing from available information
 - Contradictory statements made in varying sections of the reported details

Uneven standardization across reported studies

- E.g., similar results reported in different units
- E.g., multiple studies squeezed into one report
- Result: difficult to ingest as is into a consuming company data management system in its original format

Compound Name	CAS Number	LD ₅₀ (mg/kg)	Species	Test Type
Benzene	71-43-2	930	Rat	unclear
HNA	—	high	Mouse	Subchronic
Acetaminin	123-4	N/A	?	???
Formaldehyde	—	—	Rabbit	negative
Methanol	67-56-1	5630	Guinea pig	Chronic
Methanol	67-56-1	5630	Chronic	good

A specific use case for AI



Curating a physical-chemical,
toxicological and ecotoxicological dataset

How did we create such a dataset?



How did we create such a dataset?

Retrieve raw study data from ECHA website (not AI)

- 19,000 dossiers at the time – focus on Lead Dossiers
- Primarily interested in endpoints supporting GHS classification – up to 55 endpoints per dossier
 - E.g., flash point, acute oral toxicity, acute aquatic toxicity to fish, biodegradation potential
- All told, this resulted in 1.5 million study records retrieved in 3 days



How did we create such a dataset?

Use AI to fulfill quality criteria

- Immediately removes all studies with a Klimisch score of 3
- Removes studies that have been disregarded due to major methodological deficiencies
- Removes endpoints where studies are planned
- Removes QSAR data for certain endpoints
- Removes studies that do not meet completeness criteria
 - E.g. acute toxicity to fish – remove dataset if missing dose descriptor, exposure time, or result value – species and method can be missing
 - E.g., acute oral toxicity – remove dataset if missing dose descriptor or result value – species, sex and method can be missing

Use AI to remove duplicate studies

- If all elements of multiple data records completely match, delete redundancy

How did we create such a dataset?

Use AI to standardize units

- Makes easier to compare study results
- Simple conversions within existing dimensions (e.g., g/kg to mg/kg)
- More complex conversions involving dependencies between data points (e.g., conversion of ml/kg to mg/kg based on reported density)

Use AI to standardize presented data

- Focus on minimal study details needed to make GHS hazard assessment
 - E.g., dose descriptor, study duration, form of exposure, key result, method
- Focus and present only most meaningful results
 - E.g., acute fish toxicity study results presented at 24-, 48-, 72- and 96-hr timepoints. Bring forward only the value most relevant for GHS assessment
 - E.g., water solubility results presented from the temperature closest to room temperature
 - Flag studies where the available data deviate from standard GHS assessment requirements, where additional expert judgment is needed to derive GHS assessment
- Wording used to represent study data often differs → heavy use of AI-based mapping to standard set of phrases

How did we create such a dataset?

Use AI to propose most relevant study per endpoint

- Trained AI to be able to identify the best study per endpoint per substance (study ranking)
 - Adequacy of study: key → supporting → weight of evidence → other
 - Reliability of study: Klimisch 1 → 2 → 4
 - Type of information: Experimental → read-across → mixture rule calc → weight of evidence
 - Method: according to → equivalent to → none required → none available → none followed
 - Endpoint-specific considerations (e.g., acute dermal toxicity)
 - LD50 dose descriptor → other
 - If multiple LD50, select one from most sensitive sex

Other elements to aid in decision-making

- Above criteria don't always result in the best study to use
- Include registrant classification for cross-reference purposes
- Include ECHA summaries, where available, as a hint to values used by registrants

How did we create such a dataset?

Validate, validate, validate:

- AI can get creative, not always welcome
- Important to provide detailed and meticulous instructions to the AI agent
- Important during development to deeply validate the results of the performance against those instructions
- Examples:
 - Phrase mapping hallucinations
 - Unit conversion incorrectly performed
 - Operators (\geq ; $>$; \leq ; $<$) missed
 - Confusion of duration and frequency of treatment



The famous Rodogulous

So what?

SME Workflow impacts

Benefits of the resulting data set

Standard application

Flexible application



Benefits of the resulting dataset



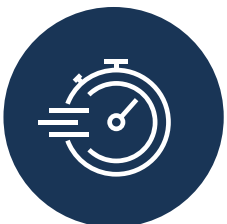
Integration

- Standard integration into data management system, including authoring tool
- MCPs and APIs allow integration in AI tools
- High quality data anywhere



Data quality & consistency

- Built-in completeness checks reduce review cycles
- AI identifies and removes redundant studies automatically
- Expert monitored AI Performance gives high trust in results






Workload reduction

- Speed up assessment process
- SMEs focus on decision-making rather than data cleaning
- Data gathering / conversion removed from process, QA reviews the AI results

Example application – Read Across Support



Category / Parameter	115-84-4 - 2-butyl-2-ethylpropanediol 	144-19-4 - 2,2,4-trimethylpentane-1,3-diol 
▼ Acute Toxicity to Aquatic Invertebrates		
Species	Daphnia magna (Water flea)	Daphnia magna (Water flea)
Duration	48 hrs	48 hrs
ValueType	EC50	EC50
Value	100 mg/l	109.1 mg/l
method of analysis	OECD Test Guideline 202	OECD Test Guideline 202
Remarks	The test was conducted according to guideline	The test was conducted according to guideline
	key study	key study

- Data anywhere
- Fast SME own development for new use cases
- Enhancements available asap
- Inclusion of AI tools without burdensome approval process (no sensitive data exposed)

Example application – Read Across Support



Read across Support Co-pilot

Hello! I'm the Read across Support Co-pilot. How can I help you analyze this data?

Evaluate the read across approach using both source substances to the target substance.

The user is asking me to generate a read-across hypothesis for the target substance 110-03-2, using source substances 115-84-4 and 144-19-4. I need to:

1. Identify what 110-03-2 is from the search results
2. Compare the structures and properties of all three substances
3. Apply ECHA RAAF principles to justify the read-across
4. Use online data for the target substance and cite sources

From the search results, I can see that 110-03-2 is 2,5-Dimethyl-2,5-hexanediol (also called 2,5-dimethylhexane-2,5-diol). The search results provide some safety data sheet information.

Looking at the source substances:

- 115-84-4: 2-butyl-2-ethylpropanediol
- 144-19-4: 2,2,4-trimethylpentane-1,3-diol

And the target:

- 110-03-2: 2,5-Dimethyl-2,5-hexanediol

I need to analyze their structures and properties to establish similarity for read-across.

Benefits

- AI Agent specifically build for an SME Use case
- Tailored result of AI Agents based on business standards
- Same trusted data used as source for AI Agents

Example application – Read Across Support



Read across Support Co-pilot

- **Flash point:** 115–135°C (based on molecular structure)

Predicted Toxicological Endpoints:

- **Acute dermal toxicity:** LD₅₀ > 2,000 mg/kg
- **Skin sensitization:** Non-sensitizing
- **Repeated dose toxicity:** NOAEL likely 50–150 mg/kg bw/day
- **Developmental toxicity:** No developmental effects expected
- **Genotoxicity:** Negative in all standard assays

Uncertainties and Limitations

The target substance shows **slightly enhanced local irritation potential** (H318 eye damage vs. reversible irritation for sources), which may reflect differences in:

- **Hydroxyl group positioning** (2,5-positions vs. other arrangements)
- **Molecular geometry** affecting tissue penetration
- **Purity/impurity profiles** in tested materials

The **absence of comprehensive physical-chemical data** for the target substance limits the precision of property predictions, though the structural similarity strongly supports the read-across approach.

Conclusion

The read-across from both source substances to **2,5-dimethyl-2,5-hexanediol (110-03-2)** is **scientifically justified** based on structural similarity, shared diol functionality, and consistent toxicological patterns. The approach follows ECHA RAAF principles with high confidence for most endpoints, though additional testing may be warranted for local irritation effects given the enhanced classification of the target substance. The **dual-source approach** strengthens the hypothesis by demonstrating consistency across structurally related compounds within the same chemical category.

Possible use cases

- Use AI Agent to support QA Processes
- Use AI Agents to onboard new colleagues
- Impact assessments AI Agent
- Substitution assessment AI Agent
- Etc. etc. etc.

Q&A + Thank you



For more information

Visit us at the 3E booth to
explore our solutions!