

Reference:

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Using the ESA REACH Tool and AI to identify PFAS and understand REACH

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2 June 2026 | **ESA 7th REACH Workshop** | ESA ESTEC, Noordwijk, The Netherlands | MPTB-RL-HO-0231

Agenda

- You should now know about REACH and PFAS from the previous speakers...
- This presentation is about the tooling you can use to support REACH understanding

01

ESA REACH Tool

Background and benefits



02

General AI

Tips and limitations



03

Targeted AI

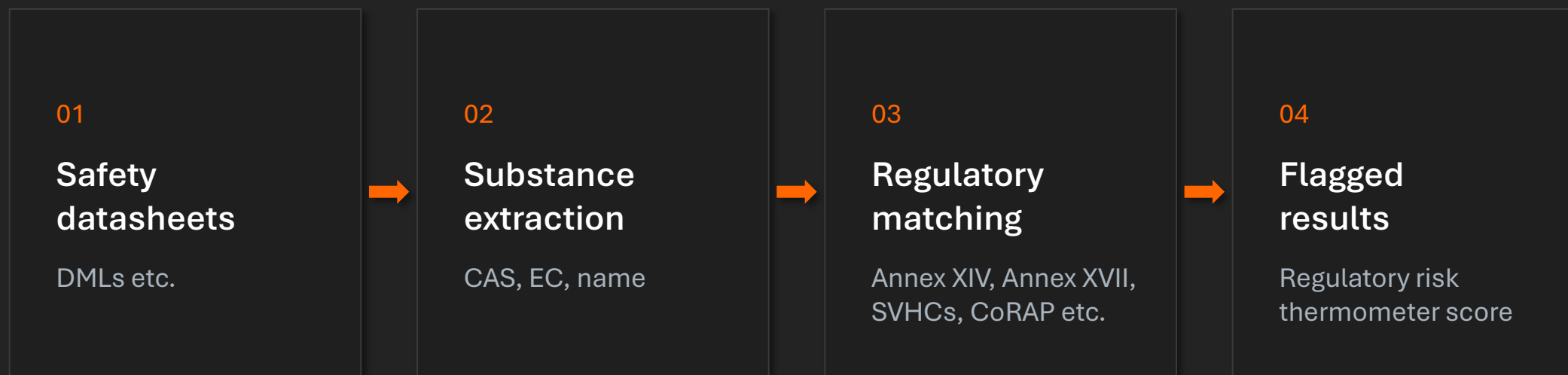
New PFAS identification tool

PHASE 01

The ESA REACH Tool

Built to help space companies see their REACH exposure.

How it works



Cross-references space-relevant materials against REACH Regulatory lists.

The benefits of the ESA REACH Tool

100%

Coverage of REACH lists

Relevant substance lists are updated automatically

Live

Dynamic and real time

Material statuses are instantly updated with regulatory updates

Risk

Obsolescence mitigation

Looks at intentions to help anticipate potential obsolescence

If the substances are fully indexed, the REACH Tool can cross-reference your space materials

Sign up to the ESA REACH Tool

- Space-relevant materials

Displaying only materials used in space, collected by the MPTB and constantly maintained.

- Regulatory risk thermometer

Easy to understand risk score that can be interpreted by non-REACH experts

- PFAS flagging

Flags on materials likely to contain PFAS, to counter their unique obsolescence risk

Substance Name	Risk	EC Numbers	CAS Numbers	CLH	CoRAP	CL	Restr	Auth
Form				▼	▼	▼	▼	▼
titanium dioxide; [in powder form containing 1 % or more of particles with aerodynamic diameter ≤ 10 µm]	1/7	236-675-5	13463-67-7	✓	×	×	×	×
Formaldehyde	1/7	200-001-8	50-00-0	×	✓	×	×	×
formaldehyde ...%	2/7	200-001-8	50-00-0	✓ ⓘ	×	×	×	×
formaldehyde and formaldehyde releasers formaldehyde and formaldehyde releasers	4	200-001-8	50-00-0	×	×	×	✓	×
Formaldehyde, oligomeric reaction products with aniline	6/7	500-036-1	25214-70-4	×	×	✓	×	✓
N,N-dimethylformamide	5/7	200-679-5	68-12-2	×	×	✓	✓	×
N,N-dimethylformamide dimethyl formamide	2/7	200-679-5	68-12-2	✓ ⓘ	×	×	×	×
C ₆ C ₁ -azodi(formamide)	4	204-650-8	123-77-3	✓	×	✓	×	×
Chloroform trichloromethane	6/7	200-663-8	67-66-3	✓	×	×	✓	×
Reaction products of 1,3,4-thiadiazolidine-2,5-dithione, formaldehyde and 4-heptylphenol, branched and linear (RP-HP)	7/7	300-298-5	93925-00-9 1471311-26-8	×	×	✓	×	✓
Formamide	3/7	200-842-0	75-12-7	✓ ⓘ	×	✓	×	×

As a community tool, every material you favourite improves ESA's picture of sector-wide exposure and feeds directly into public consultations.

Limitations

The REACH Tool is blind when the regulatory lists are missing index numbers.

- **Group restrictions**
Increasingly regulators are using structural definitions that require looking for specific chemical structures
- **Ambiguous names**
Substance trade names and typos without indexes cannot be cross-referenced
- **List lag**
New substances that meet a structural definition won't be on pre-existing 'exhaustive' lists, and therefore missed

The PFAS problem

10,000+

substances in the PFAS family

Defined by structure, not by a list. The proposed EU restriction spans in the whole family, including substances we rely on in space hardware.

EU REACH STRUCTURAL DEFINITION

Any molecule containing a

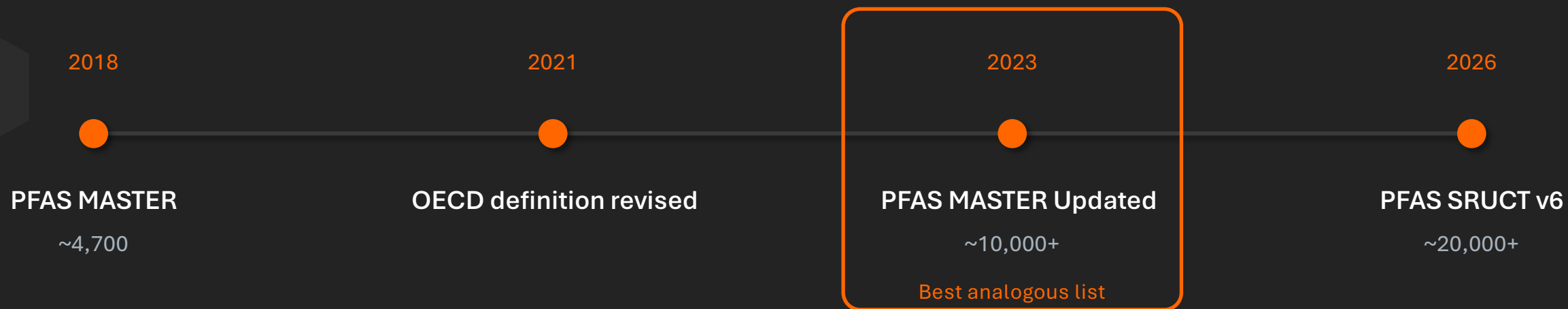
$-\text{CF}_2-$ or $-\text{CF}_3$ group

“Any substance that contains at least one fully fluorinated methyl (CF_3-) or methylene ($-\text{CF}_2-$) carbon atom (without any $\text{H}/\text{Cl}/\text{Br}/\text{I}$ attached to it).”

“A substance that only contains the following structural elements is excluded from the scope of the restriction: CF_3-X or $\text{X}-\text{CF}_2-\text{X}'$, where $\text{X} = -\text{OR}$ or $-\text{NRR}'$ and $\text{X}' = \text{methyl } (-\text{CH}_3)$, methylene ($-\text{CH}_2-$), an aromatic group, a carbonyl group ($-\text{C}(\text{O})-$), $-\text{OR}''$, $-\text{SR}''$ or $-\text{NR}''\text{R}'''$; and where $\text{R}/\text{R}'/\text{R}''/\text{R}'''$ is a hydrogen ($-\text{H}$), methyl ($-\text{CH}_3$), methylene ($-\text{CH}_2-$), an aromatic group or a carbonyl group ($-\text{C}(\text{O})-$).”

No perfect PFAS list

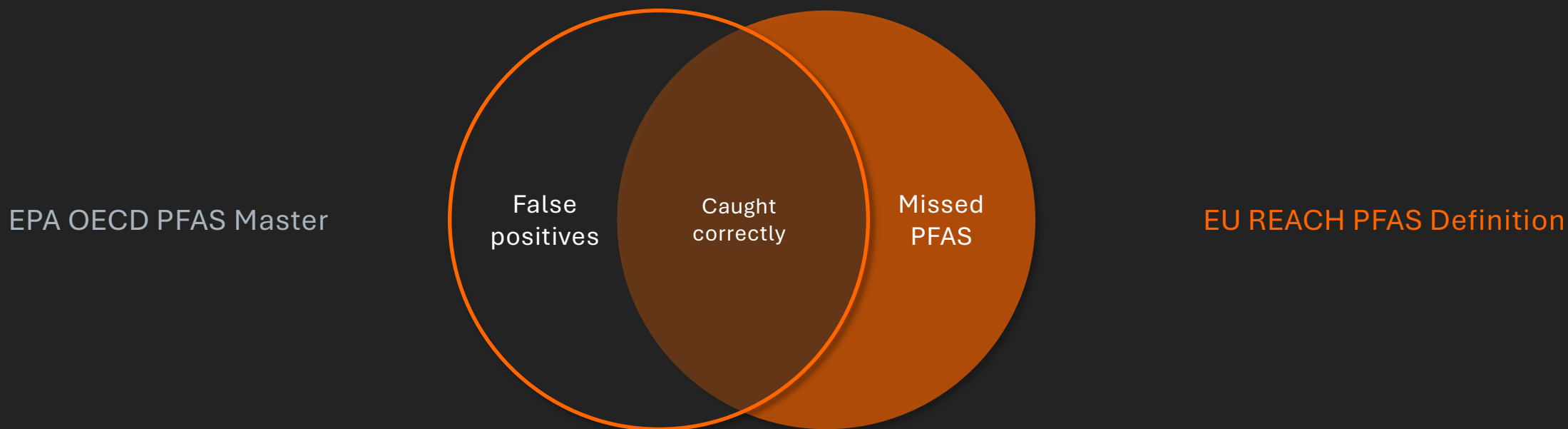
The proposed EU REACH universal PFAS restriction is based on the OECD definition



There's still no exhaustive list for the EU REACH PFAS structural definition

List-based PFAS mapping

EU REACH includes a structural exclusion for certain amines and ethers, not reflected in PFAS Master



Exhaustive lists are essentially impossible for complete PFAS mapping

PHASE 02

Could AI close the gap?

We see more space SMEs using LLMs to help them with REACH, but does it work?

→ **Issues**

Specific to chemical compliance

→ **Nuance**

Small mistakes can have a big impact

→ **Skills**

Methods to overcome shortcomings

Public LLMs still lack REACH understanding

01

AI makes things up

Wrong CAS numbers, wrong regulation, said with full confidence.

02

Lacking legal references

Even when AI is correct, it can fail to cite the correct primary legal text.

03

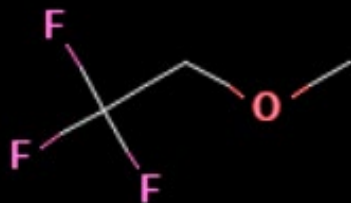
Chemistry knowledge missing

AI focuses on substance names, rather than structures like a chemist.

In chemical compliance, a confident wrong answer is the worst kind.

Spot the difference

2,2,2-Trifluoroethyl methyl ether



EU REACH: PFAS

ASKED: Is this within scope of the EU universal PFAS restriction proposal?

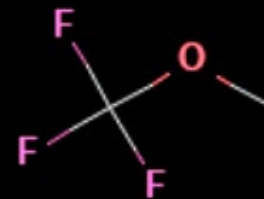
gemini-3.1-pro-preview

Yes, 2,2,2-Trifluoroethyl methyl ether is within the scope of the EU universal PFAS restriction proposal.

gpt-5.2-chat-latest

Yes — 2,2,2-Trifluoroethyl methyl ether is within scope of the EU universal PFAS restriction proposal.

Trifluoromethoxymethane



EU REACH: Not PFAS

ASKED: Is this within scope of the EU universal PFAS restriction proposal?

gemini-3.1-pro-preview

Yes, trifluoromethoxymethane is within the scope of the EU universal PFAS restriction proposal.

gpt-5.2-chat-latest

Short answer: Yes, it is in scope.

Trifluoromethoxymethane has a R-O-CF₃ group. Due to the structural exclusion, it is not in scope of the proposed REACH restriction.

Example of an AI REACH mistake

A real question from a space SME

QUESTION

Are MON-3 and MMH propellants restricted under REACH? Can we use the closed-system fuel exemption?

AI ANSWER

“MMH is regulated under REACH as an SVHC and restricted for certain uses. MON-3 is regulated under REACH as a hazardous mixture.”

Confidently wrong

ACTUAL STATUS

- MMH is not on the SVHC Candidate List. The model confused it with hydrazine.
- MMH has no dedicated Annex XVII entry. It is regulated through CLP, workplace and transport rules.
- MON-3 is not a listed REACH substance. Obligations flow from its constituents.

Improve your AI prompts

These tips can reduce but not eliminate hallucinations

01

Give it a role

“You are a REACH compliance officer reviewing a safety data sheet.”

02

Give it context

Paste REACH legal text in the context. Ask for citations to specific annexes or articles.

03

Add chemical knowledge

Ask it to reference a chemical database, such as PubChem for index numbers.

04

Flag what matters

“This is for a regulatory filing. This is important, don’t mess this up. Flag anything uncertain.”

PHASE 03

Targeted AI

Same intelligence, with ground truths hard-coded

01

Grounded in chemistry

Retrieves index data from reputable sources, no guesses

02

Primary sources prioritised

Structural definitions embedded into software to prevent inconsistencies

03

Built for REACH

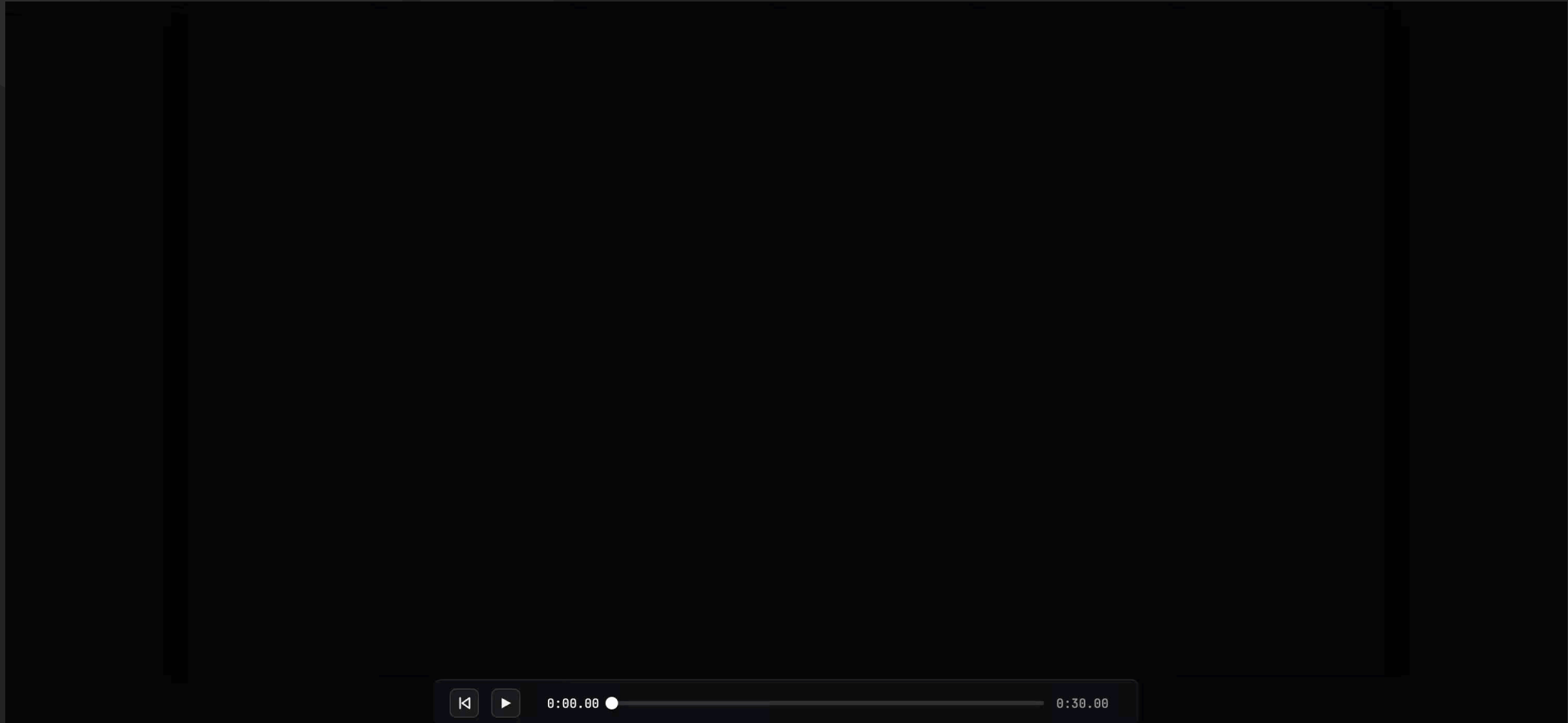
Finely tuned guardrails and minimal generative content

Targeted AI for PFAS identification

- An AI-enhanced PFAS structural analysis tool, built with the space industry in mind
- Designed to help you find unidentified PFAS substances in your portfolio, based on different structural definitions globally

IsItPFAS.com

See it in action



See global PFAS definitions

EU REACH and TSCA have different structural definitions of PFAS

EU / OECD

OECD 2021 · ENV/CBC/MONO(2021)25

“Any chemical with at least one fully fluorinated methyl ($-\text{CF}_3$) or methylene ($-\text{CF}_2-$) carbon atom.”

US TSCA

EPA 2023 · TSCA § 8(a)(7) final rule

Any substance containing one of three sub-structures: $\text{R}-(\text{CF}_2)-\text{CF}(\text{R}')\text{R}''$, $\text{R}-\text{CF}_2\text{OCF}_2-\text{R}'$, or $\text{CF}_3\text{C}(\text{CF}_3)\text{R}'\text{R}''$ — with saturated carbons throughout.

Regulatory Status PFAS Detected

United States (TSCA)

TSCA Reporting Potentially Required

Meets TSCA definition: Contains at least one of the specific sub-structures (e.g., $\text{R}-(\text{CF}_2)-\text{CF}(\text{R}')\text{R}''$, $\text{R}-\text{CF}_2\text{OCF}_2-\text{R}'$, or $\text{CF}_3\text{C}(\text{CF}_3)\text{R}'\text{R}''$).

European Union & EEA (EU REACH)

Universal PFAS Restriction Proposed

Contains at least one fully fluorinated methyl ($-\text{CF}_3$) or methylene ($-\text{CF}_2-$) carbon atom.

United Kingdom (UK REACH)

Indicative PFAS Definition

Contains at least one fully fluorinated methyl ($-\text{CF}_3$) or methylene ($-\text{CF}_2-$) carbon atom.

Canada (CEPA)

Fluoropolymers are expressly excluded from the Canadian PFAS definition.

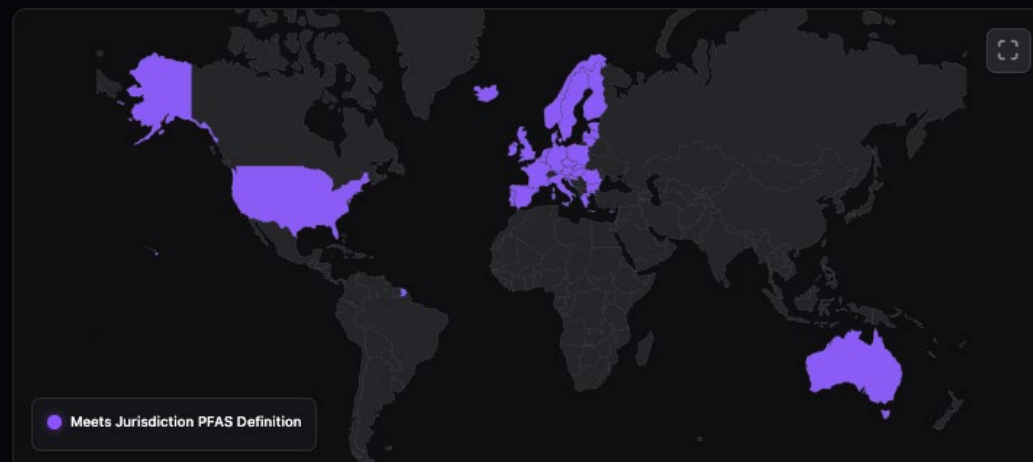
Japan (CSCL)

Not listed as a PFOA, PFOS, or related compound under Japanese regulations.

Australia (AICIS)

Listed as a PFAS under Australian AICIS regulations.

Jurisdictional Map



IsItPFAS features

LAUNCHING SOON

- Check PFAS status of any* substance
- Product level PFAS status and report
- Portfolio tracking and notifications

NEXT

- POPs PFAS integration
- More jurisdictions
- Organisation level portfolios

LATER

- Automated monitoring reports
- Screen novel substances
- API integration

*With a publicly available structure

Thank you, any questions?

Sign up to the IsItPFAS waitlist today for early access.

JOIN THE WAITLIST →

isitpfas.com/pricing

or contact oliver.reiff-musgrove@reachlaw.fi



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