CHEMICAL RISK EVALUATION: PROTECTING HEALTH AND ENVIRONMENT

How to find information using CAS Databases

Dr. Míriam Plana, Senior Customer Success Specialist

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Agenda

Chemical risk evaluation: protecting health and environment

- An introduction to CAS
- What makes CAS different?
- POC’s and POP’s: how to find information using CAS Databases
  - PFAS: brief introduction to these type of compounds
  - How to find relevant information using CAS Databases
- Conclusions

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The ACS mission is to:

- Advance scientific knowledge
- Empower a global community
- Champion scientific integrity

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Chemistry for Life®

CAS is dedicated to the ACS commitment of improving all lives through the transforming power of chemistry.

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Connecting scientific knowledge to accelerate breakthroughs

For over a century, CAS has championed and amplified scientific discovery, innovation, and the individuals and organizations that contribute to breakthroughs big and small.

Today, we continue to connect the world's scientific knowledge to accelerate breakthroughs that improve lives.

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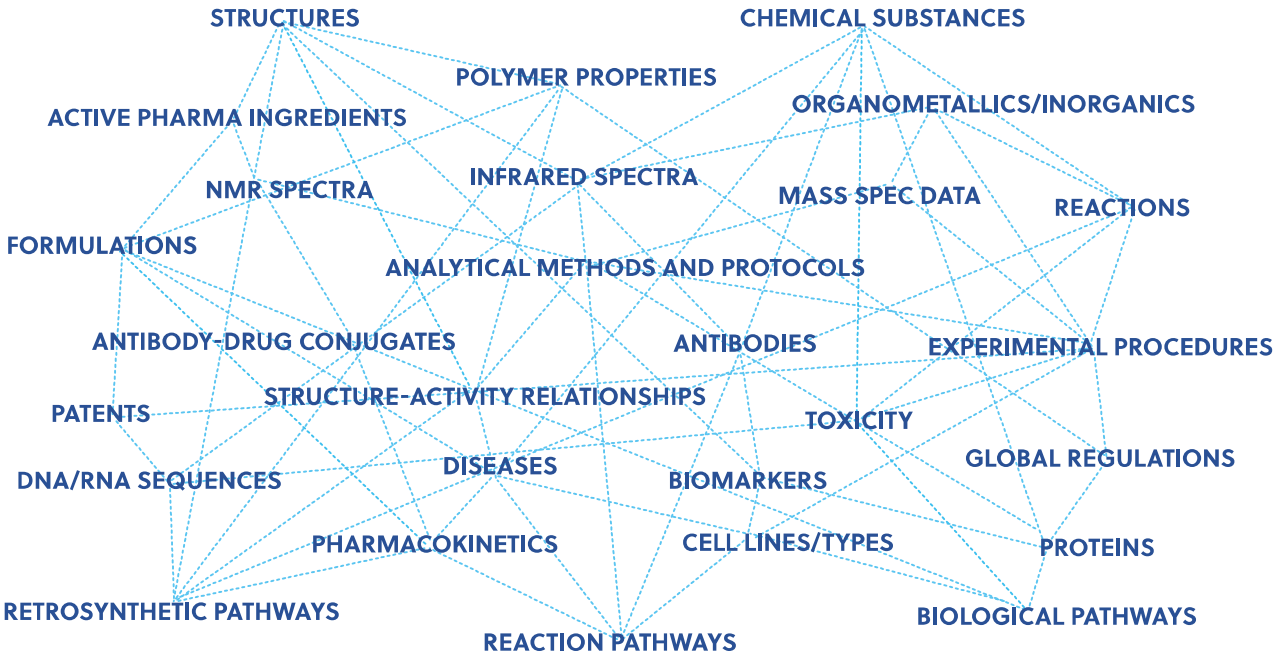
MP1

CAS connects you to the world's published science for better insights



Over
50K
scientific journals and documents

Over
290
million substances

Over
50
languages translated

109
patent authorities worldwide

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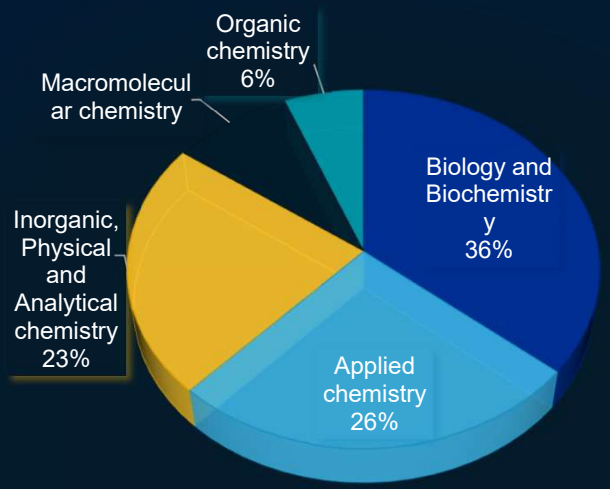
Slide 6

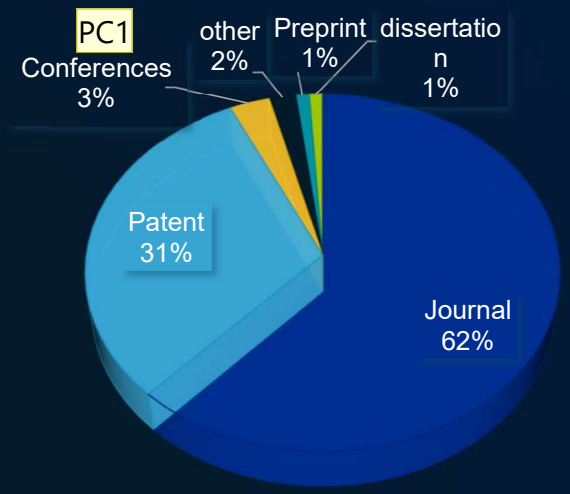
MP1 Slide changed for the one included within the CAS Slide Library: https://iconnect.cas.org/content/80444/presentations

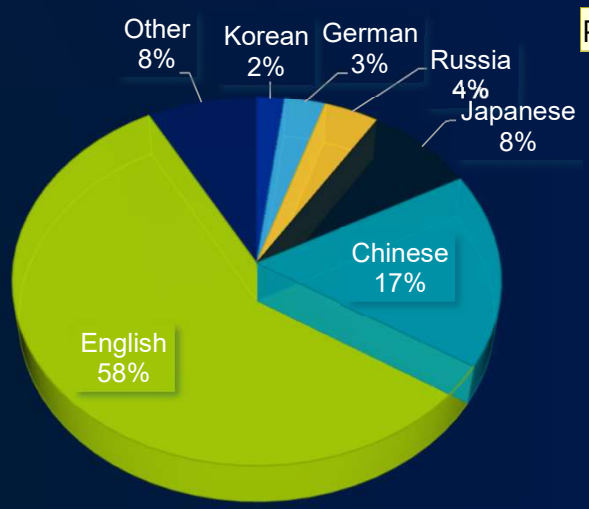
Plana, Miriam, 2025-11-04T08:14:29.495

CAS Content Collection™

Unrivalled coverage beyond chemistry in over 50 languages







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Slide 7

PC1 Graphics and text should be within the slide margins. See the current CAS PowerPoint template to see these margins.
Carlton, Peter, 2025-10-31T17:07:07.440

PC2 We typically advise not to use 3D graphs, but in this case, they are okay. Just something to note for the future.
Carlton, Peter, 2025-10-31T17:07:49.515

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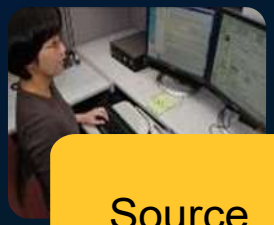
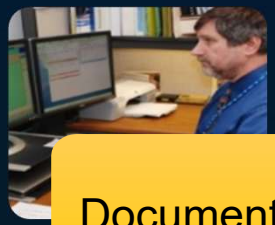
Human analysis by CAS scientists find hidden value in scientific documents

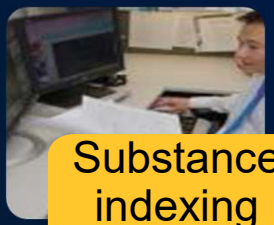


Source selection



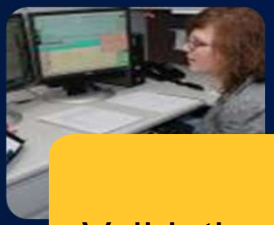
Document indexing

Reaction indexing



Substance indexing

Markush structures



Validation

PC1

Process developed by CAS, standardized for complete, reproducible indexing

Human processing • Multi-disciplinary teams of scientists • Powerful indexing • 50 languages

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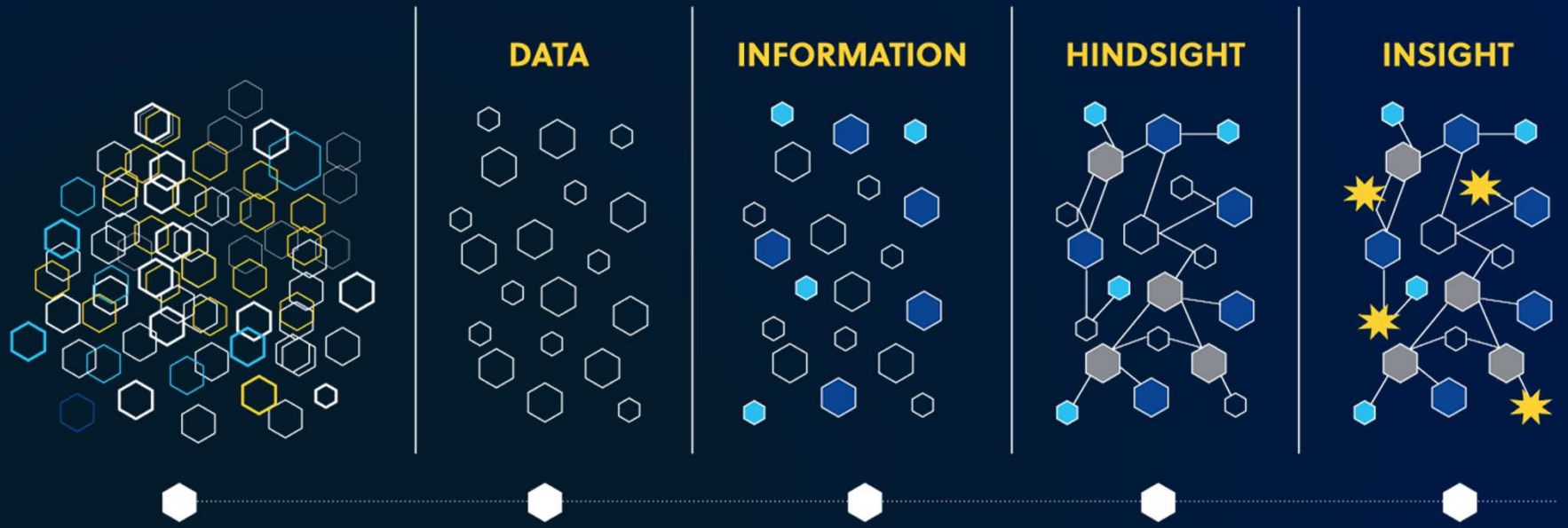
Slide 9

PC1 Resize this to stay within the margins.
Carlton, Peter, 2025-10-31T17:08:26.344

Data is valuable only when it is transformed into insight



CURATE to give data meaning

CONNECT information across disciplines

ANALYZE to reveal insights

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CAS Content Operations workflow

Over 1,000 scientists

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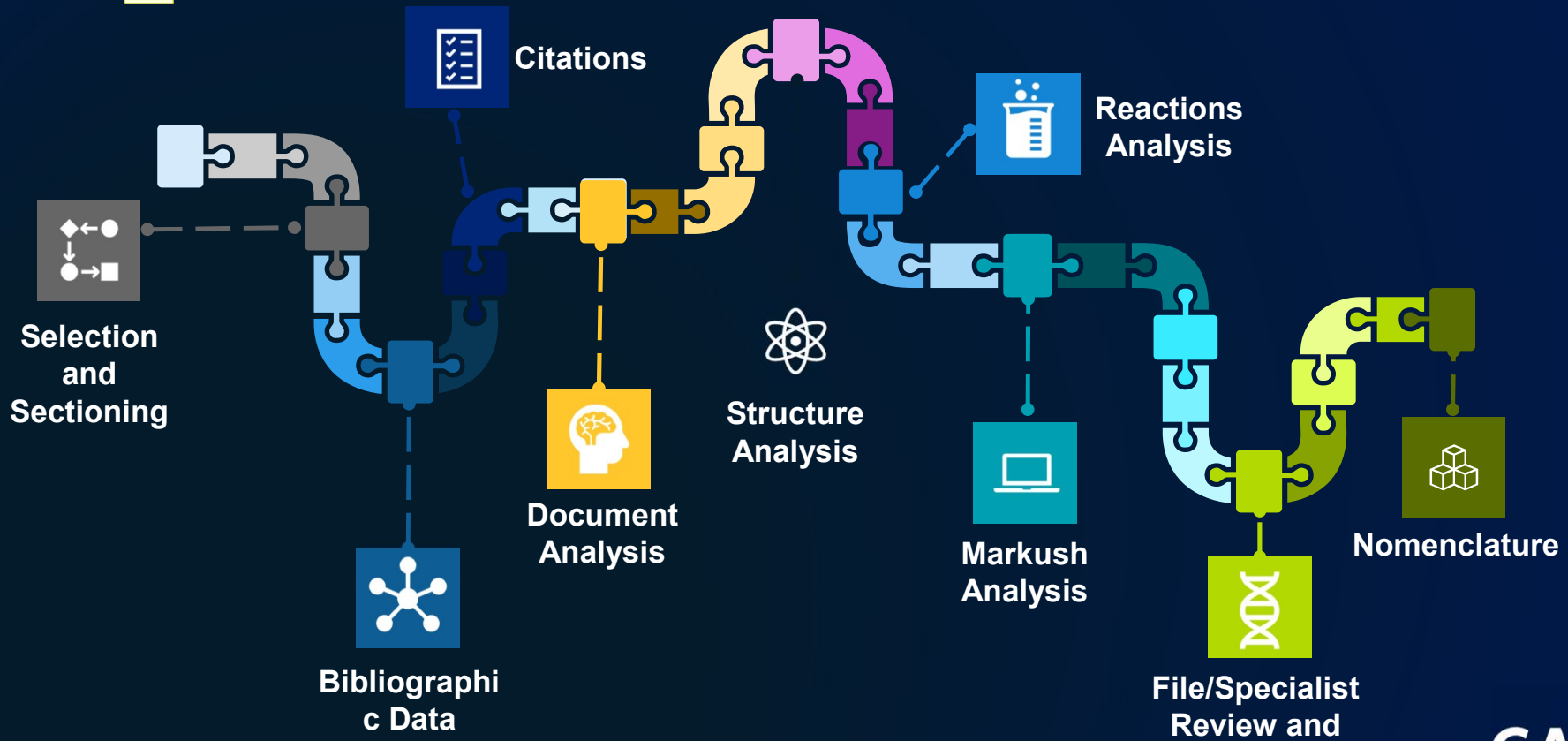

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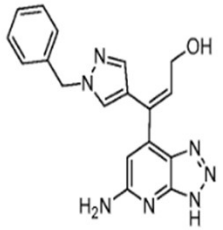
Slide 11

PC1 Delete “a”.
Carlton, Peter, 2025-10-31T17:09:00.867

Author errors identified

16A. (E)-3-(1-Benzyl-1*H*-pyrazol-4-yl)-3-(3-trityl-5-(tritylamino)-3*H*-[1,2,3]triazolo[4,5-b]pyridin-7-yl)prop-2-en-1-ol:



A mixture of Intermediate 2 (127 mg, 0.158 mmol), 1-benzyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-pyrazole (54.0 mg, 0.190 mmol), K_2CO_3 (109 mg, 0.792 mmol) and $PdCl_2$(dppf)-CH_2Cl_2 adduct (12.9 mg, 0.016 mmol) was dissolved in 1:1 THF /water in a pressure-rated vial. The vial was evacuated and backfilled 3x with Ar, then heated behind a blast shield at 80 °C for 2 hours. The reaction mixture was diluted with water and EtOAc. The aq. phase was extracted 3x with EtOAc. The combined organic phases were washed with brine, dried with Na_2SO_4, filtered and concentrated. The product was the purified by silica gel chromatography to provide 16A. (97 mg , 74 %), as a yellow oil. MS (ESI): *m/z* 832.5 (M+H).

Structure and name do not match

- Stereochemistry is inconsistent between name and structure
- Name indicates trityl protecting groups, but none are shown

PC1

CAS experts resolve inconsistencies

- Examine the starting materials and molecular mass
- The structure is correct as named

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Slide 12

PC1 Keep within the margins and use less stylized boxes for the text.
Carlton, Peter, 2025-10-31T17:09:55.501

NI1 0 Margins corrected
Iovine, Nicole M, 2025-10-31T17:33:04.898

CAS by the numbers

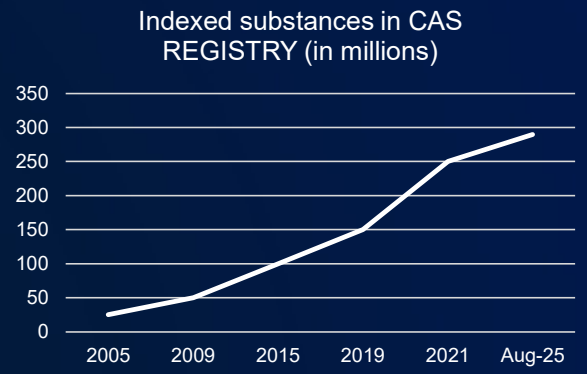
Each Business Day

- 110K Total documents are ingested
- TWO THIRDS of these are JOURNALS and NON-PATENTS
- ONE THIRD of these documents are PATENTS

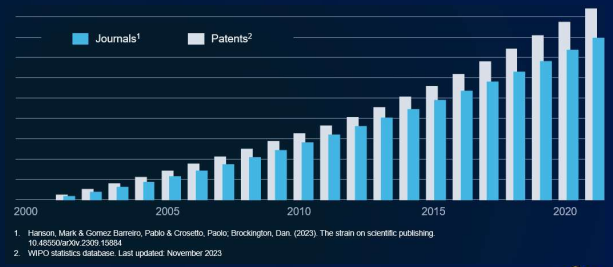
Content coverage

- 94.7M+ publications including
- 290M+ substances and sequences searchable by structure, name, or formula
- 160M+ reactions
- 120.6M commercially available substances
- 1.3M+ Markush structures from 610K patents
- 5.8M+ formulation records with detailed composition and process data

Growth of # indexed substances



Growth of published science



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What are the POCs and POPs?

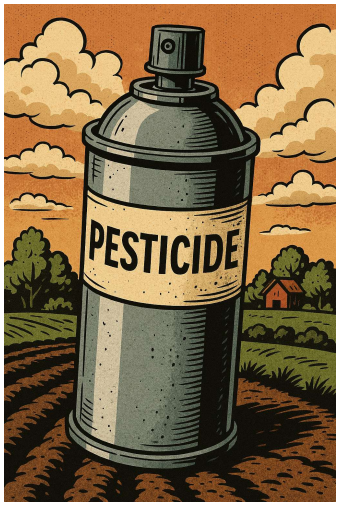
Persistent Organic Contaminants and Pollutants

Persistent Organic Pollutants (POPs) are a group of toxic chemicals that pose serious risks to human health and the environment due to they:

- Persist
- Bioaccumulate
- Biomagnify
- Travel long distances

What kind of substances are they?

- Pesticides
- Industrial Chemicals
- Byproducts



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Why are POPs dangerous?

- **Do not degrade easily**, remaining in soil, water, and air for decades.
- **Accumulate** in animals and humans, especially in fat tissues
- **Cause serious health effects**, including: cancer, immune system suppression, endocrine disruption…

Where can we find these substances?

- Water
- Food
- Air…

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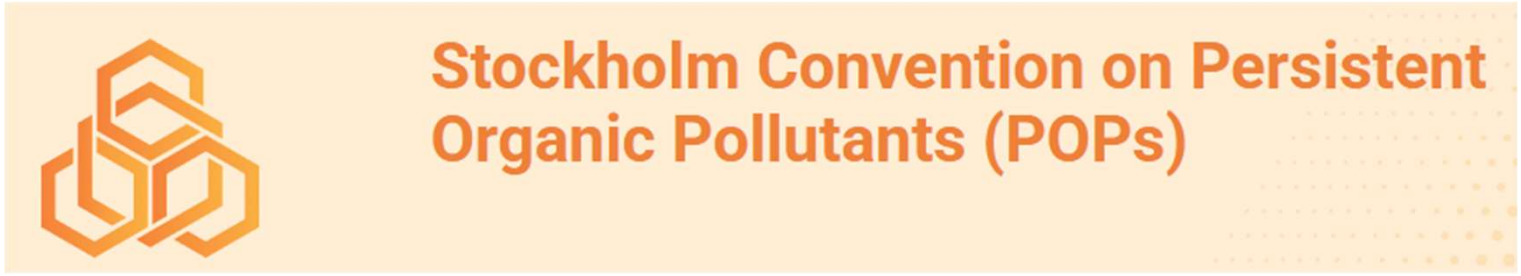
Global action against POPs

Stockholm Convention

Legally binds international agreement aimed:

- **Eliminating** or reducing the release of POPs
- **Monitoring their presence** in the environment and human tissue
- **Supporting** countries in phasing out these substances



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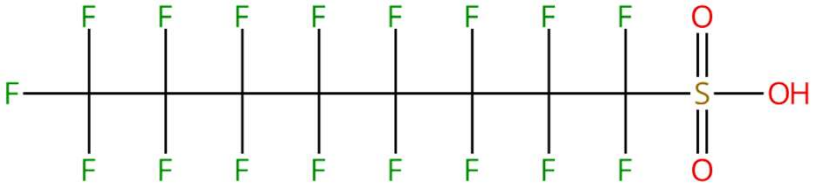
What about the PFAS?

- They are **per- and polyfluoroalkyl substances** and represent a class of man-made, **highly fluorinated** organic molecules characterized by exceptionally **strong carbon-fluorine bonds**.
- Materials with **remarkable properties**: resistance to chemical and physical degradation, water and oil repellency, emulsification capabilities, and high-temperature stability.

Often referred as “**forever chemicals**”



Perfluorooctanesulfonic acid, CAS RN 1763-23-1

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Why are PFAS concerning?

Scientific studies have linked PFAS exposure to a range of **health issues**:

- Cancer
- Liver damage
- Thyroid disease
- Immune system suppression
- Etc.

PFAS can **bioaccumulate**, meaning they build up in the body over time, and their widespread use makes exposure difficult to avoid.

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Let's review what we know using CAS Content Collection

What do we know about PFAS?

- Following the **Organization for Economic Cooperation and Development (OECD) 2021 definition** guidelines (compounds with even a single CF_2 or CF_3 group):

  Approximately 24 million distinct PFAS molecules were identified

  SEARCH in SciFinder

- Applying the more stringent **United States Environmental Protection Agency (U.S. EPA) definition** (compounds with at least two CF_2 or CF_3 groups):

  Approximately 1.8 million PFAS compounds

  SEARCH in SciFinder

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The reality behind these numbers

10,000-15,000 PFAS compounds estimated to exist

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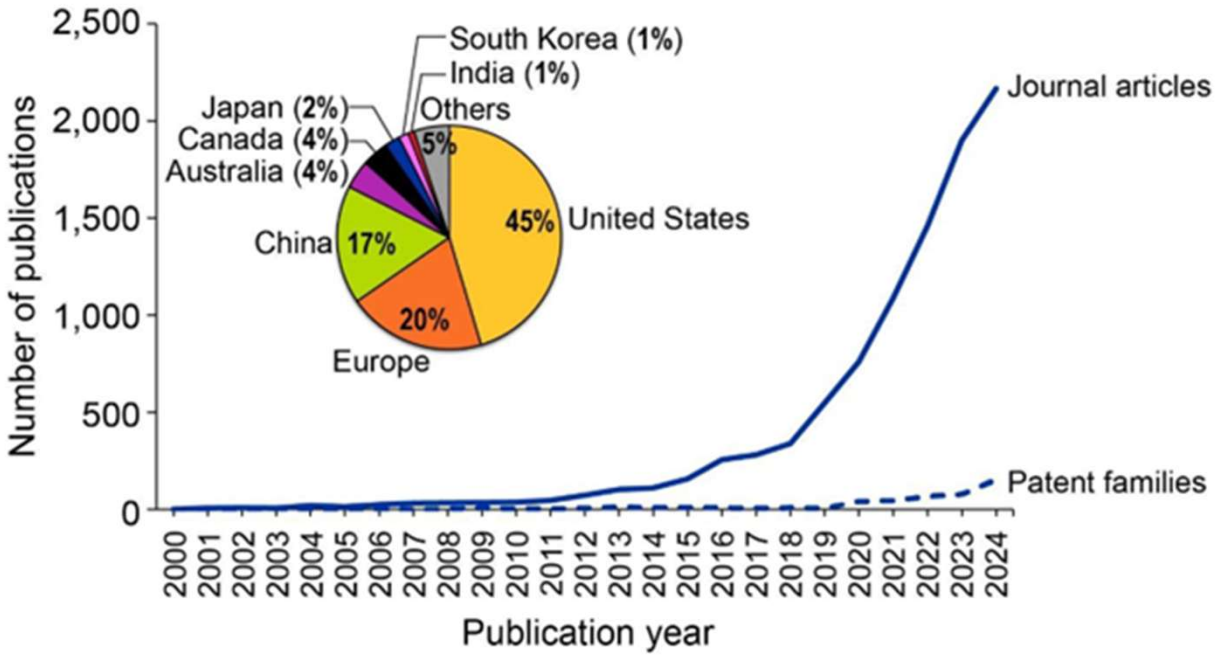
Publications within this topic

PFAS mitigation

- Research on **cleaning PFAS** is growing, but still not enough.



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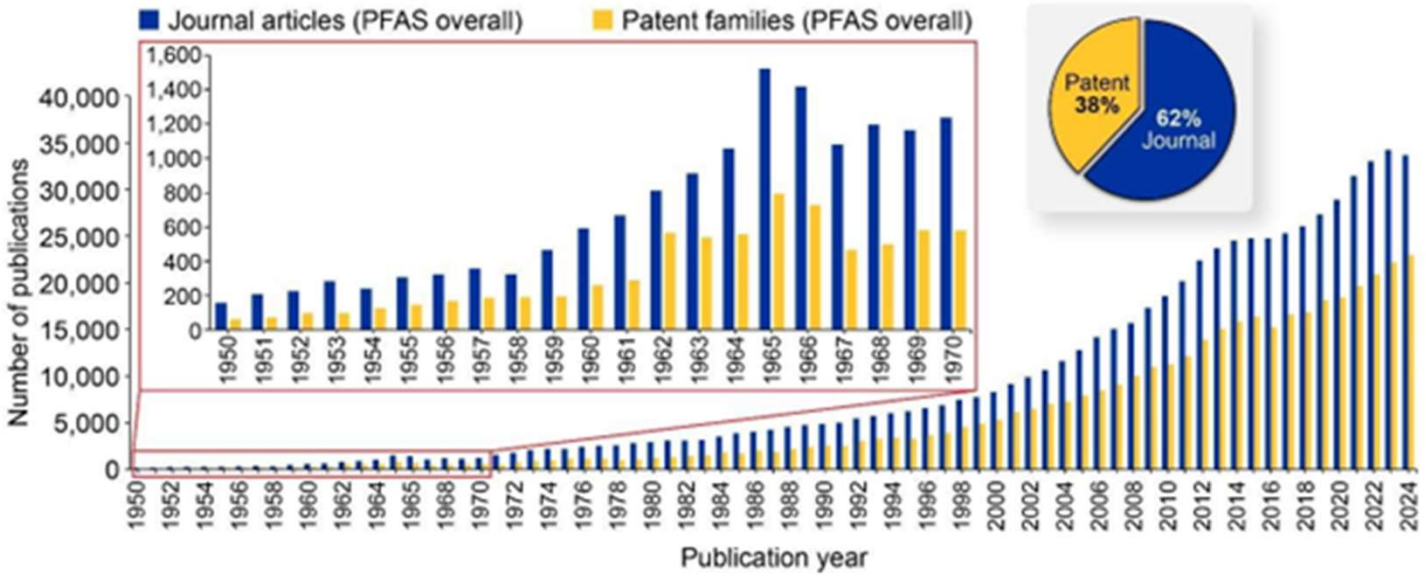
Document types covering PFAS

350,000 unique substances

PFAS compounds remain widely used across various industrial applications.



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Sources of Regulatory Information

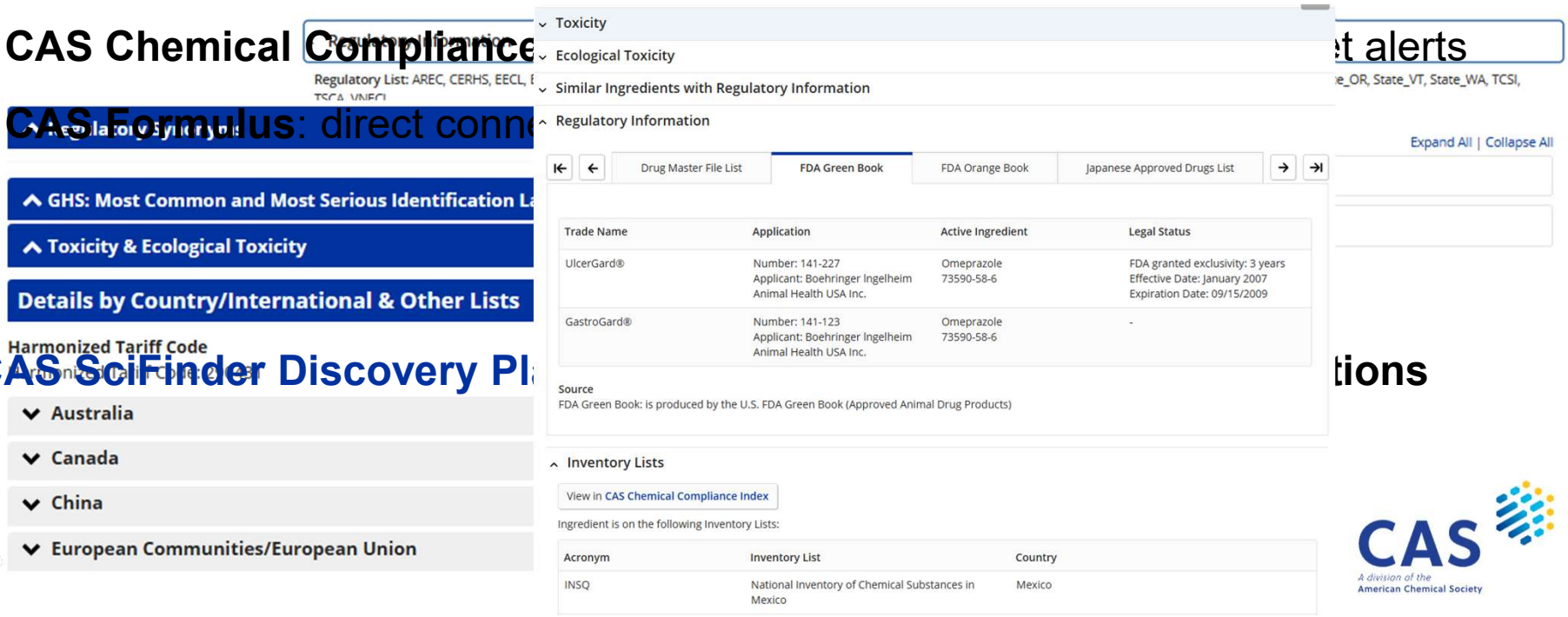
CAS SciFinder, CCI, CAS Formulus

- CAS offers three solutions to find **Regulatory Information.**

  CAS SciFinder: when available, under Substances details

  CAS Chemical Compliance: t alerts

  CAS Formulus: direct conn



CAS SciFinder Discovery Pl tions

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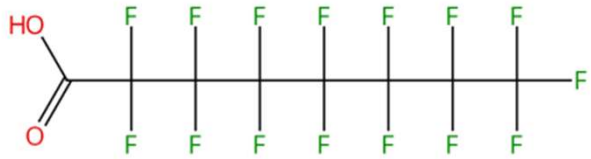
What can be found in CAS Content Collection?

Perfluorooctanoic acid

- Chemical information related to the substance
- Properties information
- Regulatory information
- Toxicology information
- GHS Hazard Statements
- Publications related

335-67-1

Perfluorooctanoic acid



$C_8HF_{15}O_2$

Perfluorooctanoic acid

13K 531 85 View Spectra

Search in SciFinder

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AI Summarization

Summarizes

References search for **"latest enhancements on removing PFAS from the environment"**

AI Summary

Based on the search results, here's a summary of key fin environment:

The removal of per- and polyfluoroalkyl substances (PFAS) to their persistence, bioaccumulation, and toxicity. Various PFAS contamination, including foam fractionation, membr processes, and constructed wetlands. These methods aim with varying degrees of success depending on the specific conditions. Research continues to explore new and improv on cost-effectiveness, sustainability, and the ability to hanc

Key Findings:

1. Treatment Methods:

- Foam Fractionation: Effective for removing PFAS from water, with the use of co-foaming agents enhancing the process. (4)
- Membrane-Based Technologies: Show promise for PFAS removal, particularly in direct filtration, adsorption-based membranes, and hybrid membrane processes. (6)
- Advanced Oxidation Processes (AOPs): Include techniques such as ozonation, photocatalysis, and Fenton processes, demonstrating varying efficiencies in PFAS removal. (8)

2. Environmental Impact and Occurrence:

- PFAS are widely distributed in aquatic environments, with concentrations ranging from low to high levels, depending on the source and location. (5)
- Emerging PFAS alternatives pose similar risks, requiring ongoing monitoring and research into their occurrence and ecological impacts. (1)

3. Challenges and Future Directions:

- The cost and feasibility of PFAS removal from the environment are significant concerns, with estimates suggesting that current removal rates may exceed global GDP. (10)
- Integrated strategies and process modifications are necessary to address the complex nature of PFAS contamination, emphasizing the need for continuous innovation and improvement in treatment technologies. (2)

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Unlocking the future of toxicology with CAS solutions

PC

Manual content curation combined with CAS technology

- CAS Solutions are the **only solutions** that offer **value added content** with far more substance indexing from journals and patents.
- Irrespective on the type of molecular sciences across the current or future research interest, **CAS provides the most comprehensive and highly structured and connection data to answer R&D and IP questions**.
- **Manually curated** journals and patents by **CAS experts** can demonstrate more relations between substances, targets, and other keywords.

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Slide 28

PC1 Sentence case

Carlton, Peter, 2025-10-31T17:20:50.912

Questions?

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the world's science

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