

# Chemical Stripes – Visualizing Chemical Trends of the Past Influencing Today

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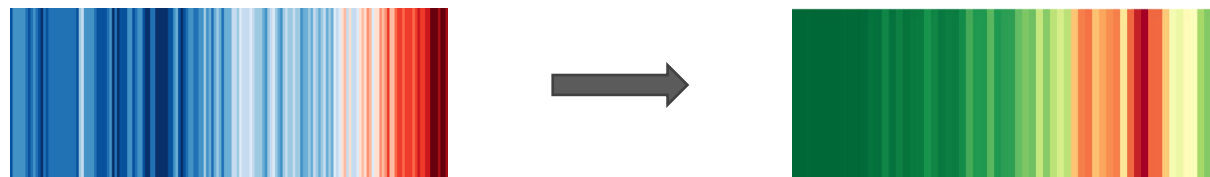
Platform presentation at the SETAC Europe 33rd Annual Meeting, Dublin

Session: 3.20 - PMT/vPvM substances: Assessment, Management and Regulation, 04 May 2023



# Introduction – Today I will talk about...

- The **importance** of investigating **chemical history**
- Why **quick action** is needed
- How **patent data** is a useful resource for this investigation
- How **visualization** can help to raise awareness (**Chemical Stripes**)



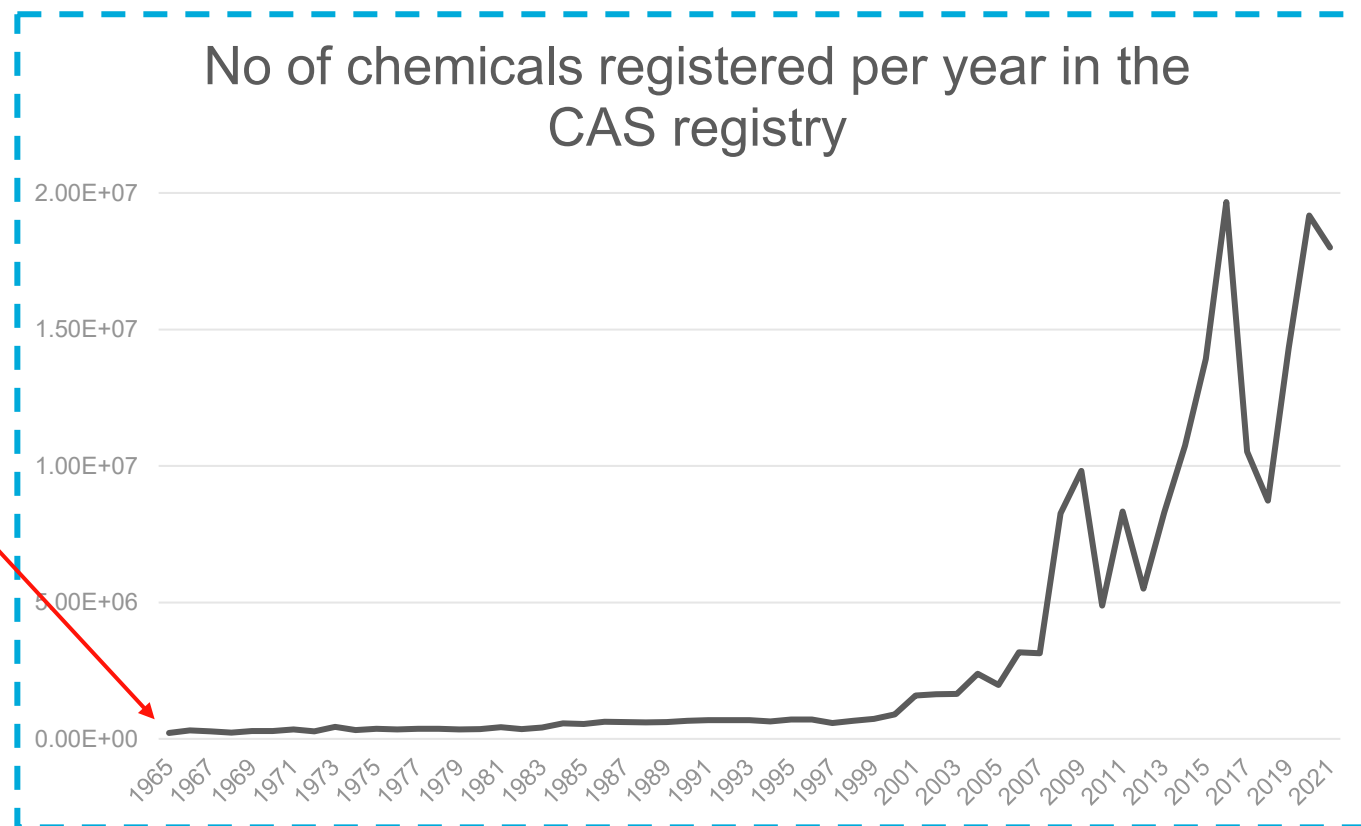
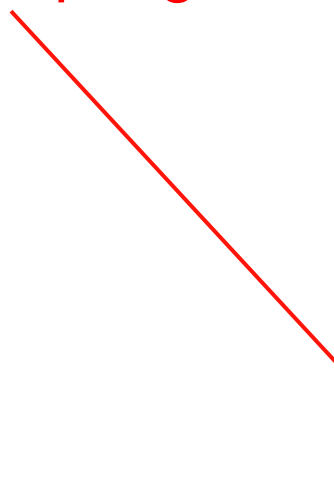
# Introduction – Reconstructing Chemical History

- Investigating **chemical history** for
  - **Health** Risks (long-term)
  - **Environmental** Risks
  - **Legal** Action
  
- Analysing historical **records / data**



# Introduction – Reconstructing Chemical History

- Avoiding new ‘**Silent Springs**’\*



- Can inform policy decisions related to **environmental regulations & public health protection**



# Introduction – The Why and How



- **Quick action** is necessary:
  - Delay makes information **less accurate**
  - **Health impacts** may not (yet) manifest (for) decades after exposure
  - May help **prevent further exposure** & **minimize the risk** of future health impacts

# Introduction – The Why and How

- Patent data as a valuable resource:
  - Detailed record of the development / use of chemicals over time
  - + Information on production methods, uses & safety concerns

CID 74483

## Perfluorooctanesulfonic acid

Depositor-Supplied Patent Identifiers ?

33,291 items Download

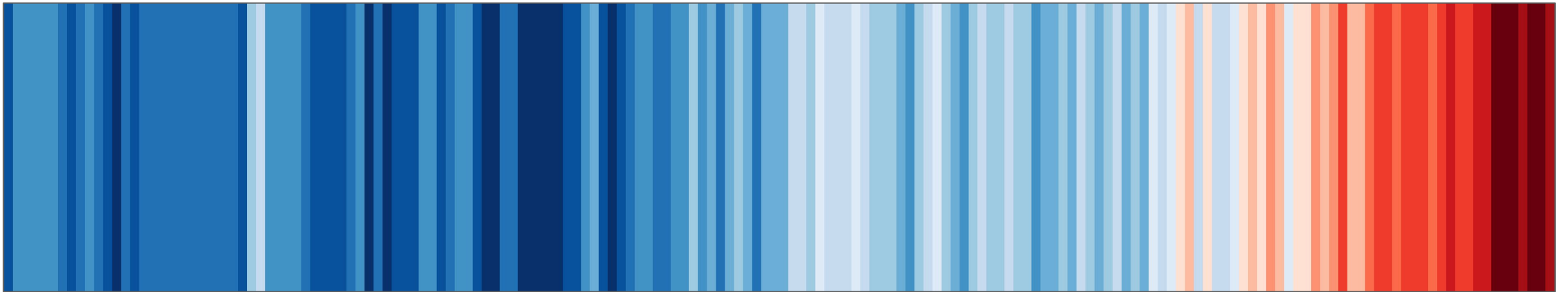
SORT BY Priority Date

#	Publication Number <span>?</span>	Title <span>?</span>	Inventor(s) <span>?</span>	Assignee(s) <span>?</span>	Classification <span>?</span>	Abstract	Priority Date <span>?</span>	Grant Date
1	CN-114035405-A	Composition for preparing top anti-reflection film for photoresist, top anti-reflection film for photoresist and fluorine-containing composition					2022-01-07	
2	CN-114146355-A	Fluorine-free environment-friendly foam extinguishing agent and preparation method thereof					2021-12-27	

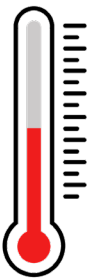
➤ Identify potential sources of exposure & inform risk assessments

# Introduction – The Use of Data Visualisation

- Warming or climate stripes

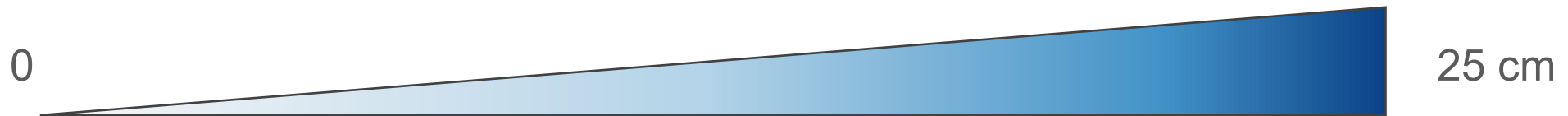
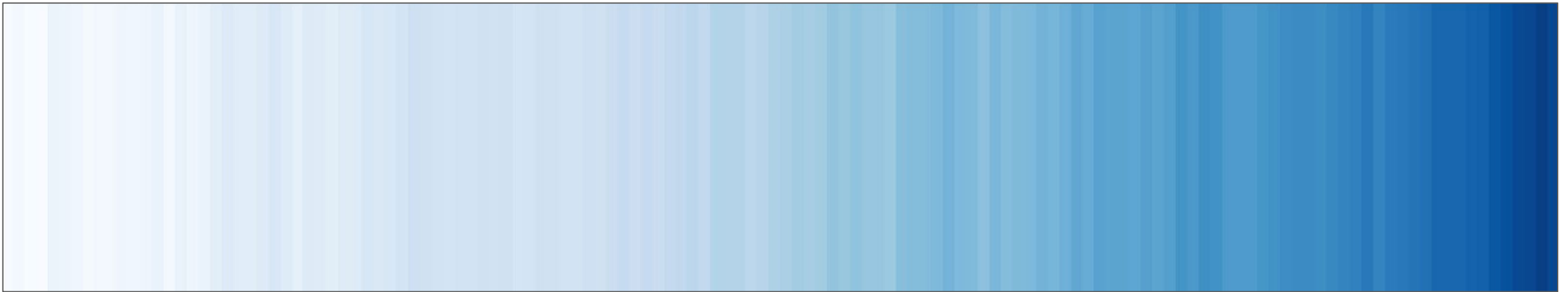


- Communicate complex environmental data in a **simple, intuitive** way
- See **long-term** trends and changes
- Use of colour for quick interpretation (broad audience)



# Introduction – The Use of Data Visualisation

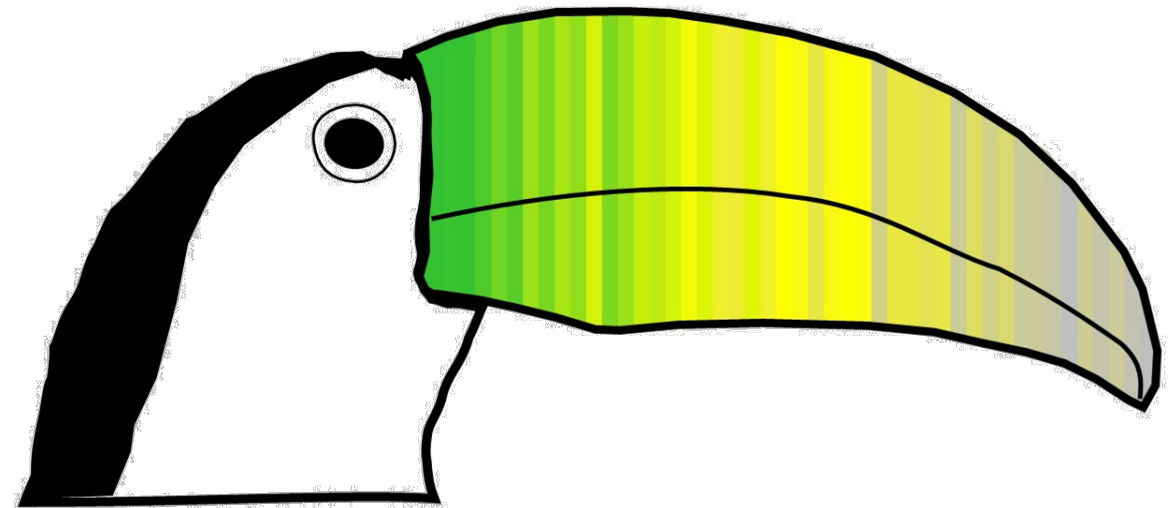
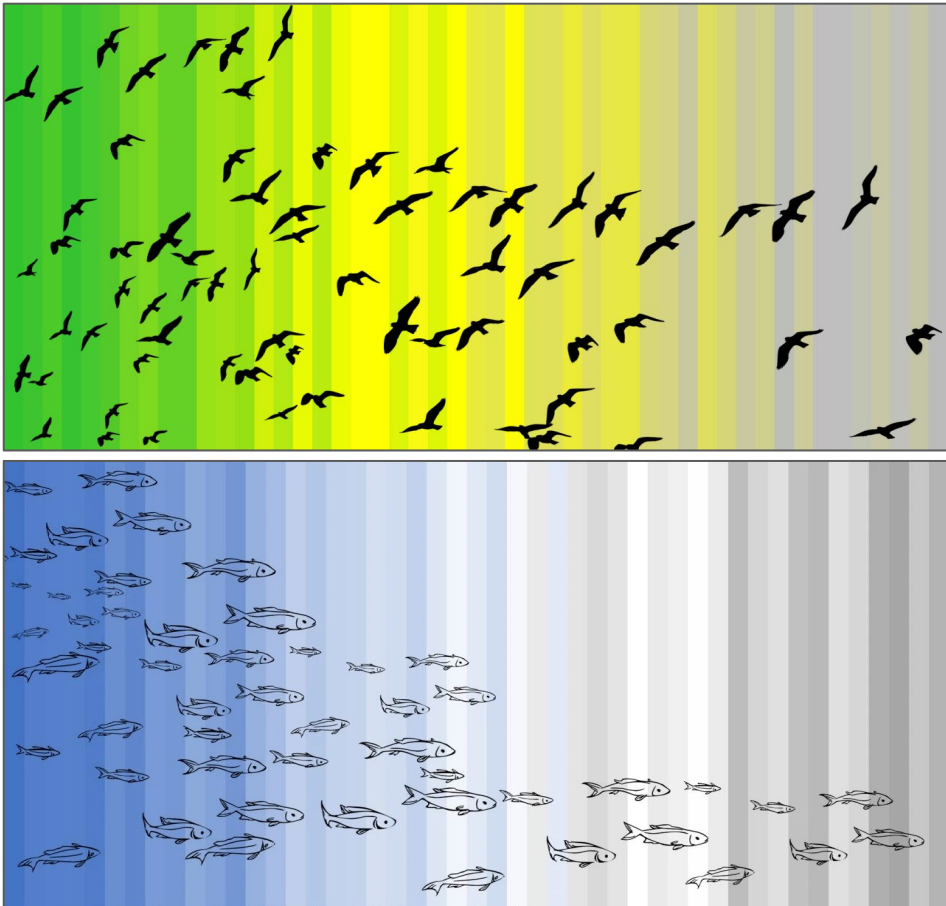
- Extension to other types of **environmental data**
  - Sea level rise





# Introduction – The Use of Data Visualisation

- Extension to other types of **environmental data**
  - Biodiversity decrease

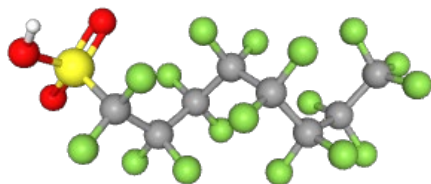


# Introducing Chemical Stripes

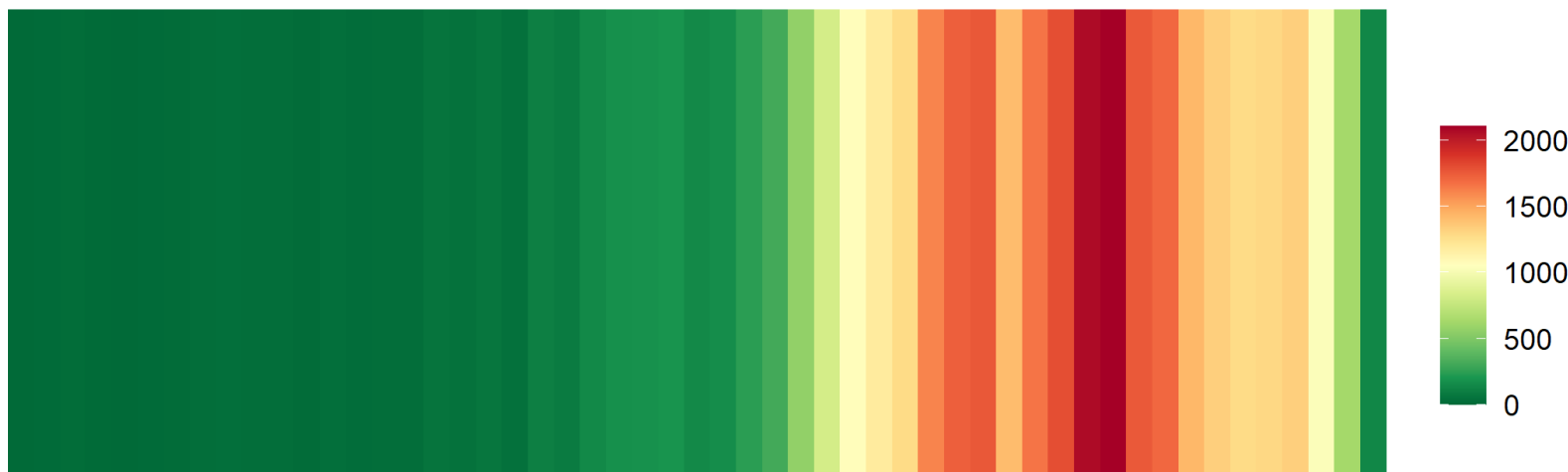
- Use of the **climate stripes concept**
- Use of **patent data** from **PubChem**:
  - Show **trends** and **changes** (estimated) **chemical use** that may have impacted **public health & environment**



Chemical  
Stripes  
Example:

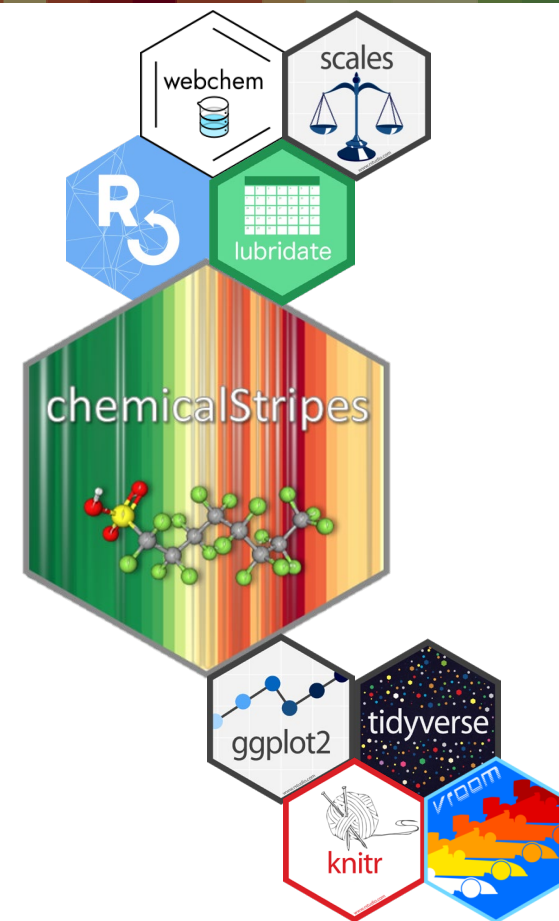


PFOS



# R package

- R package **chemicalStripes** available on GitLab:
  - Input: **PubChem** Chemical Identifier (opt.: date range)
  - Retrieving compound information using **webchem**
  - Automated extraction of patent data from **PubChem**
  - Processing patent data (**big data files**)
  - Creating and saving 'stripes plot'



```
chemical_stripes(pc_id, date_range = c(1960, 2021), colorblind = FALSE)
```

default


# Patent Download

CID 74483

## Perfluorooctanesulfonic acid

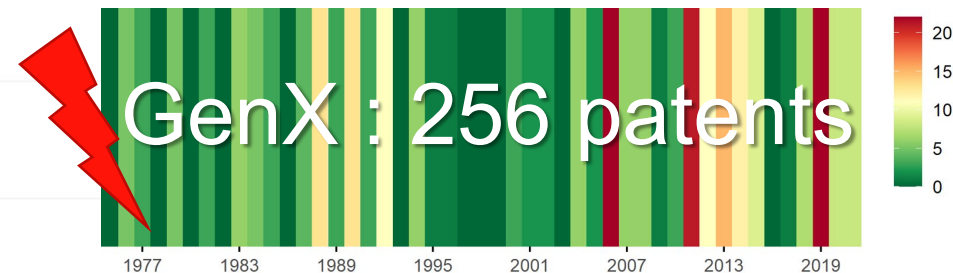
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2	CN-114146355-A	Fluorine-free environment-friendly foam extinguishing agent and preparation method thereof					2021-12-27	
3	CN-114160566-A	Mechanochemical method for decomposing hexachlorobenzene by using natural mineral additive					2021-12-24	
4	CN-114177564-A	Environment-friendly lithium battery extinguishing agent and preparation method and application thereof					2021-12-24	
5	JP-2022037181-A	A method for producing a chemically amplified photosensitive composition, a photosensitive dry film, and a method for producing a patterned resist film.					2021-12-22	
6	CN-114053396-A	Application of INVS protein in preparation of medicine for repairing damage of testicular supporting cells					2021-12-07	



# R package: Example

```
> chemical_stripes(74483)
Getting compound information
A total of 32461 patents were found for CID 74483
[=====] 40% 2s
Downloading patent data...
[=====] 60% 7s
Processing patent data
32460 patents were processed for CID 74483
[=====] 80% 3s
Plotting chemical stripes for the years between 1960 and 2021

Your stripes have been saved as png_74483_1960_2021.png in your folder c:/users/dagny.aurich/Documents/R_stripes/png_74483_1960_2021.png
```

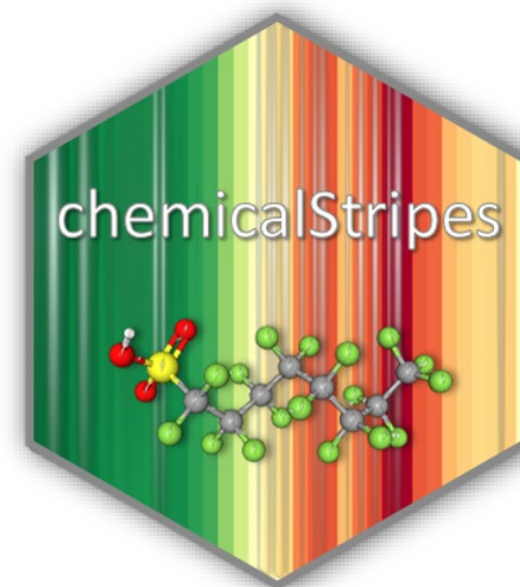
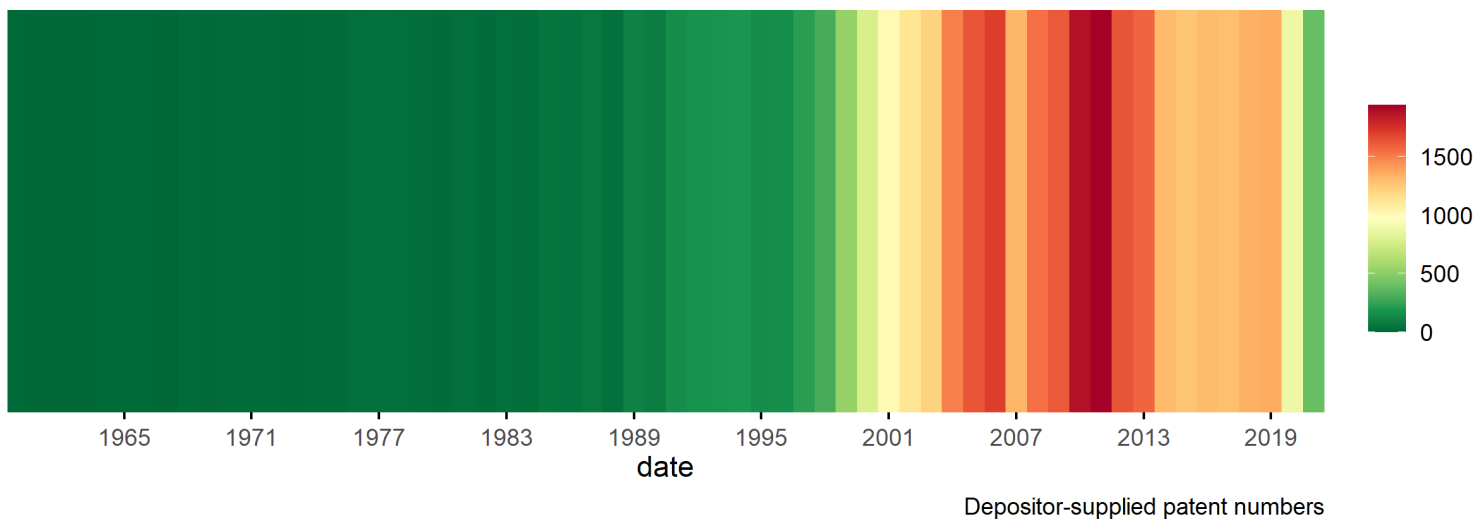
## Chemical Stripes for Perfluorooctanesulfonic acid

PubChem CID: 74483

IUPACName: 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptafluorooctane-1-sulfonic acid

Molecular Formula: C<sub>8</sub>H<sub>F</sub><sub>17</sub>O<sub>3</sub>S

Exact Mass: 499.9374938



# R package: Example

```
> chemical_stripes(74483, colorblind=TRUE)
Getting compound information
A total of 32461 patents were found for CID 74483
[=====] 40% 2s
Downloading patent data...
[=====] 60% 44s
Processing patent data
32460 patents were processed for CID 74483
[=====] 80% 17s
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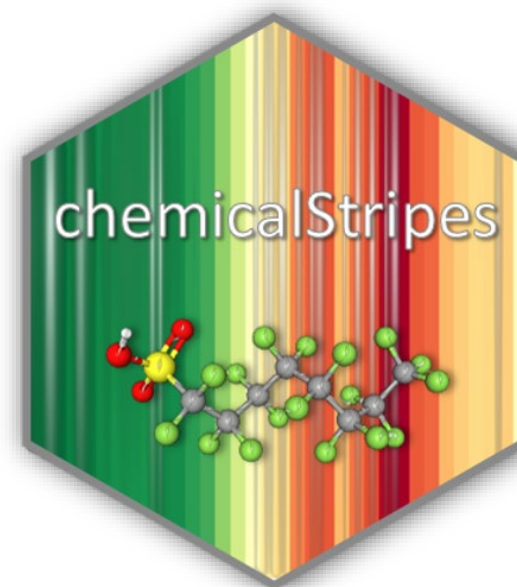
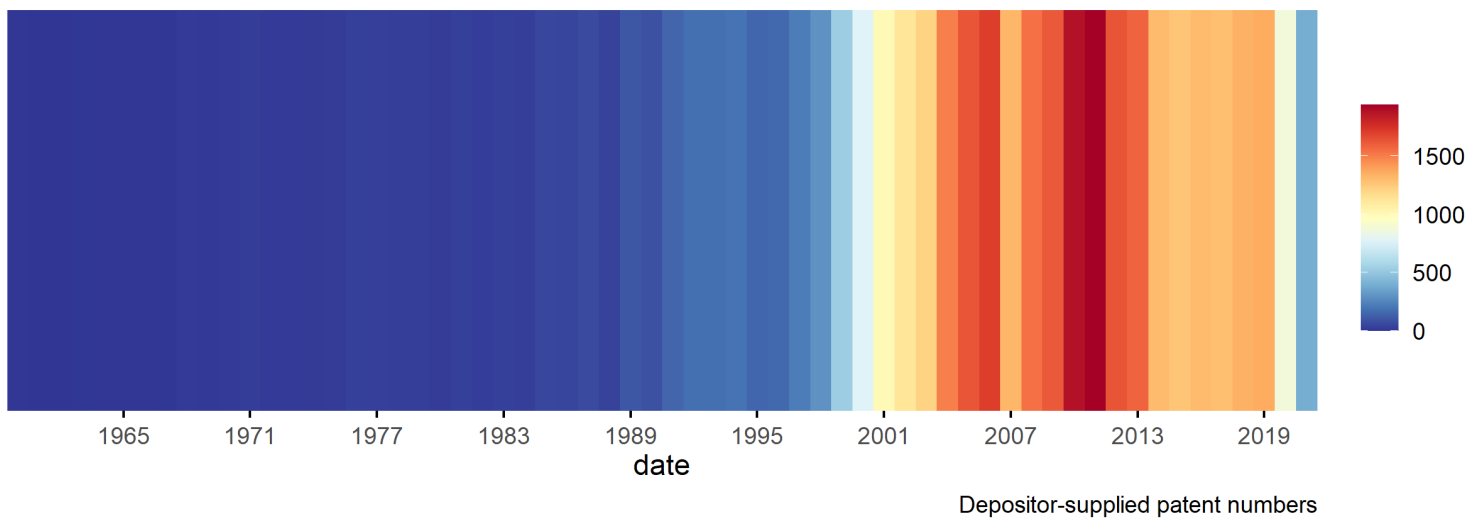
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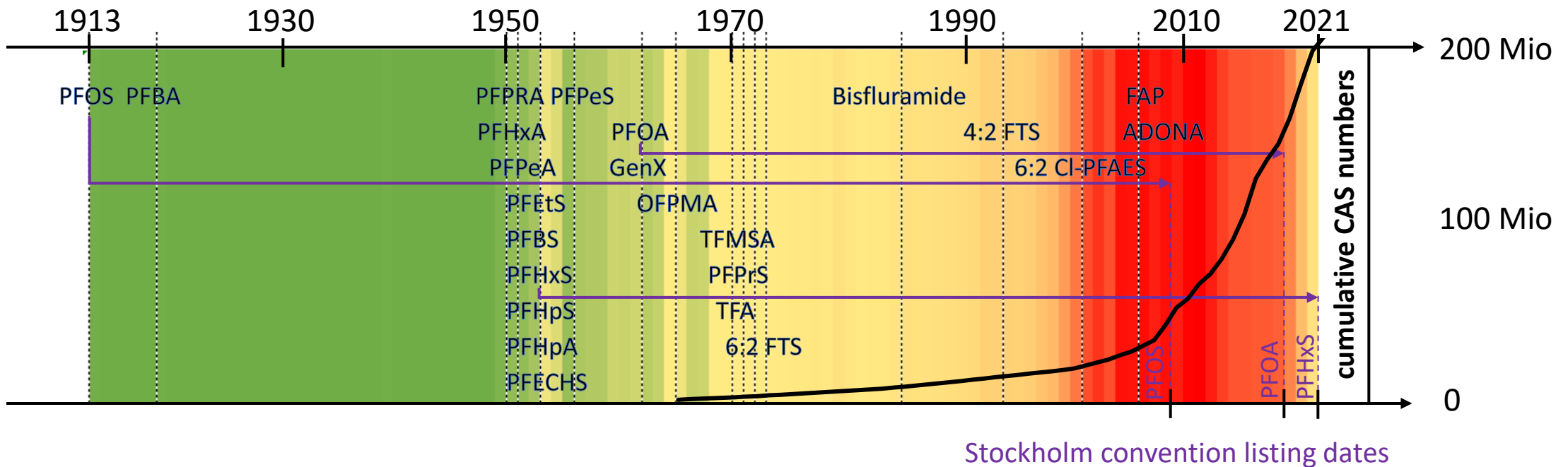
Molecular Formula: C<sub>8</sub>H<sub>F</sub>17O<sub>3</sub>S

Exact Mass: 499.9374938



# Chemical Stripes Visualization - Extended

- Summarized chemical stripes for PFAS with accompanying **regulation dates** and cumulative **Chemical Abstract Service registry numbers**:

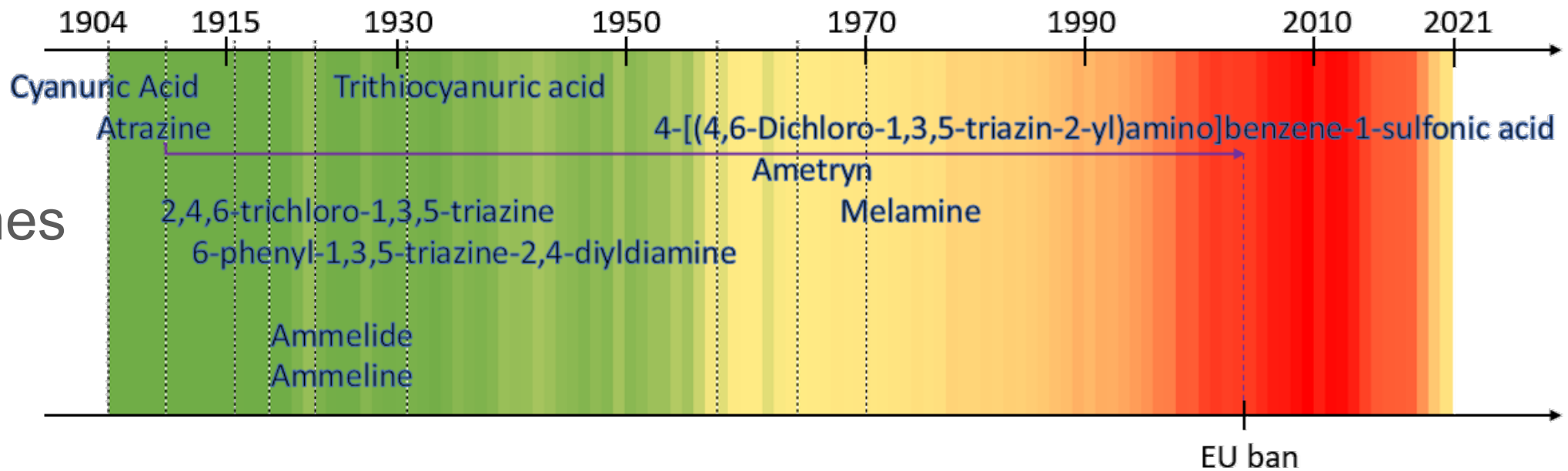


# Chemical Stripes Visualization - Extended

- Many compounds detected in the environment classified as being **persistent and mobile** (often even toxic)
- Can be used for different sets of chemicals



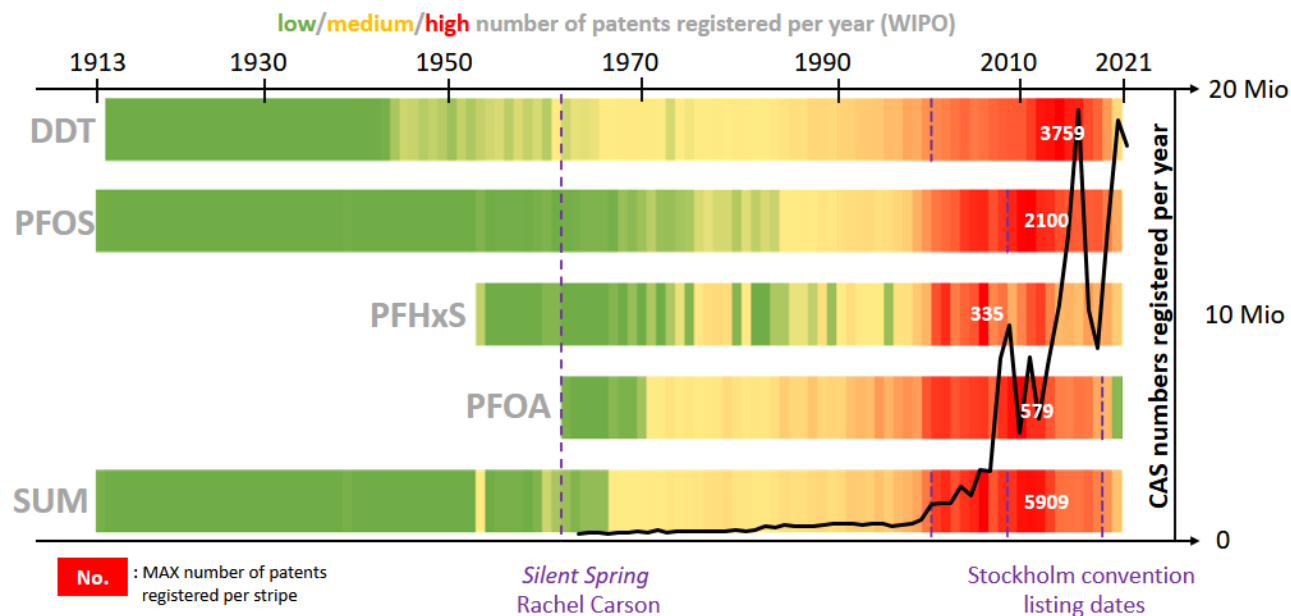
e.g. Triazines





# Chemical Stripes Visualization - Extended

- Overall trend in **rising** patent and chemical numbers (databases)



## ➤ Alarming:

- Increase of specific chemical classes relevant to **planetary boundary threats**
- Long time frame between **suspecting** a chemical to be a threat and **regulatory action** taking place

?



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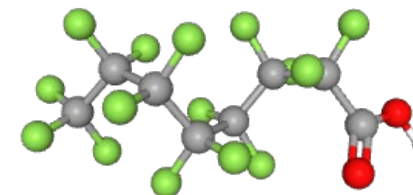
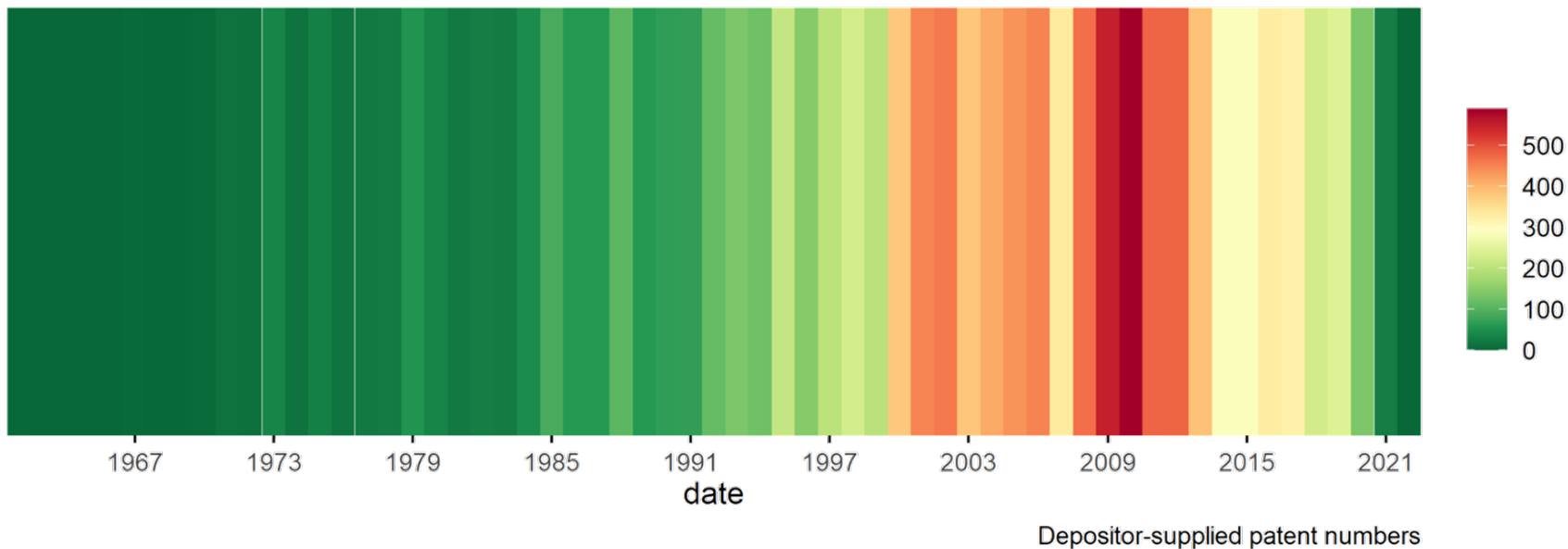
# Use of Chemical Stripes Visualization

- Looking at **specific substance classes** can **raise awareness**:
  - What went **wrong** in the **past**?
  - What actions could have been taken earlier for **better regulation** in the **future**?
- **Need for Action**:
  - Identify **specific hazards** and risks not fully understood/addressed in the past
  - Highlight **regulatory gaps**
  - Promote **effective risk assessment** and **management**
  - Build **public awareness** and support for safer / more sustainable chemical use



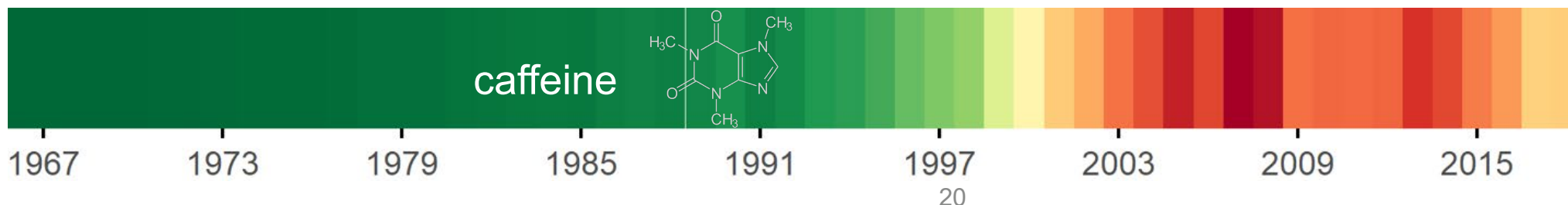
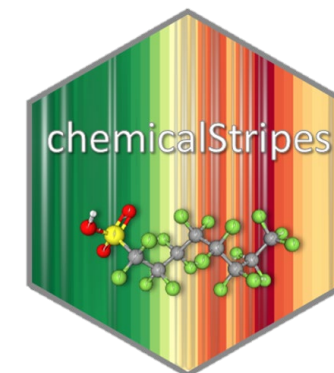
# Use of Chemical Stripes Visualization

- Can support the **interpretation** of (chemical) data
  - Stripes illustrate the **trend of increasing numbers** of potentially threatening chemicals in the environment
- Can help identify possible **changes** due to **regulatory measures**
  - **PFOA** listed in **2019** in the Stockholm Convention (**Elimination**)

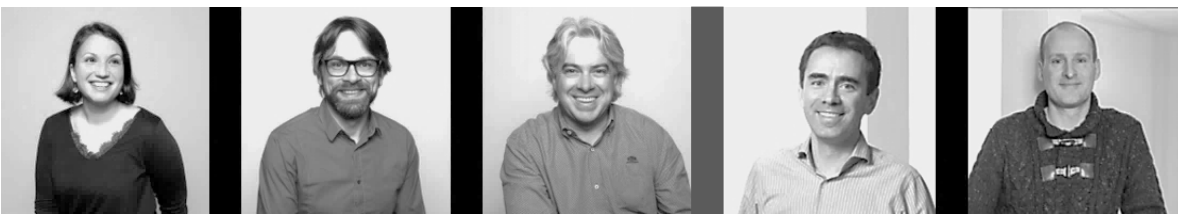


# Conclusion

- Investigating chemical history can help with **environmental regulations** & **public health protection**
- **Quick action** is needed especially regarding **PMT** chemicals
- **Visualizations** are an effective tool to raise **awareness**
- **Chemical Stripes** visualizations (R package) show
  - Trend of **increasing chemical numbers**
  - Possible **regulatory** effects
  - Even for your favourite chemicals....



# Acknowledgements



**SETAC EUROPE 33<sup>RD</sup> ANNUAL MEETING**

30 APRIL - 4 MAY 2023 | DUBLIN, IRELAND + ONLINE

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# THANK YOU!



**CAS**  
A DIVISION OF THE  
AMERICAN CHEMICAL SOCIETY

 U.S. National Library of Medicine  
National Center for Biotechnology Information



**PubChem**

LUXEMBOURG  
INSTITUTE OF SCIENCE  
AND TECHNOLOGY **LIST** 



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