



**STRUGGLE, NO SMUGGLE:  
A COMPLIANCE CHECKER  
STORY**

**What are controlled substances?**

○2

**What is Compliance Checker?**

○2

**How does a chemical definition look like?**

○2

**Application study: Controlled substances in ChEMBL**

○7

# WHAT ARE CONTROLLED SUBSTANCES?



”

The term "controlled substance" means a drug or other substance, or immediate precursor, included in schedule I, II, III, IV, or V of part B of this subchapter.

(Source: Title 21 United States Code (USC) Controlled Substances Act)

”

”

A controlled substance is generally a drug or chemical whose manufacture, possession, transport or use is regulated by a government.

[...]

Some precursor chemicals used for the production of illegal drugs are also controlled substances in many countries, even though they may lack the pharmacological effects of the drugs themselves.

(Source: Wikipedia)

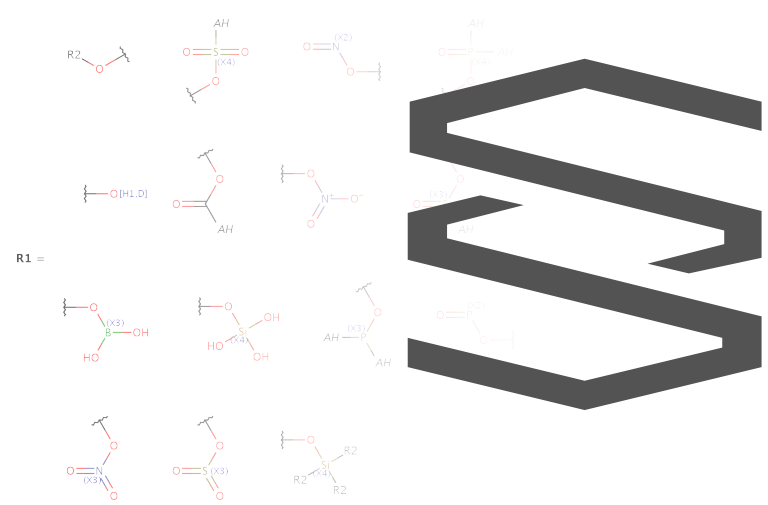
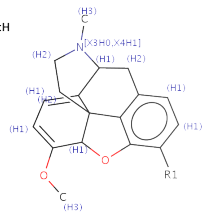
”

# WHAT IS COMPLIANCE CHECKER?

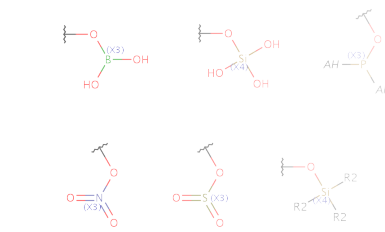


# COMPLIANCE CHECKER

R1 >0  
R2 >0, restH



R1 =



- Alkyl — } Carboaryl — } Carboalcyclyl — }
- F Alkenyl — } Alkynyl — } Heteromonoaryl — }
- Heteromonoalcyclyl — } FusedHetero — }

- Single molecule and batch processing
- Seamless knowledgebase update
- User-defined category groups
- Ready for integration



-  Austria
-  Belgium
-  Canada
-  China
-  Germany
-  Denmark
-  Spain
-  France
-  Ireland

-  India
-  Italy
-  Japan
-  The Netherlands
-  Sweden
-  Singapore
-  Switzerland
-  United Kingdom
-  United States of America

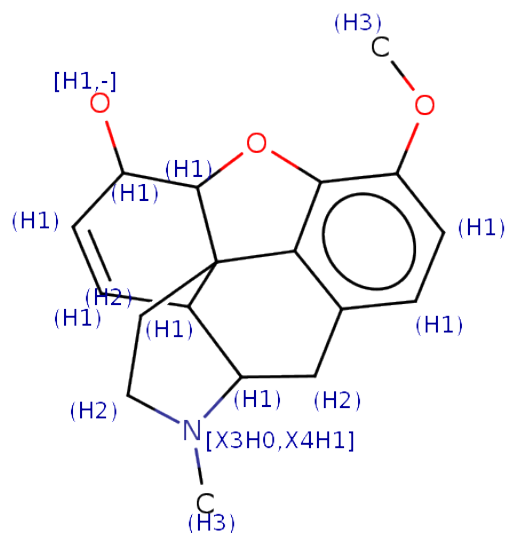
United Nations conventions  
European Union regulations  
Rotterdam Convention  
Montreal Protocol  
Chemical Weapons Convention



# HOW DOES A DEFINITION LOOK LIKE?



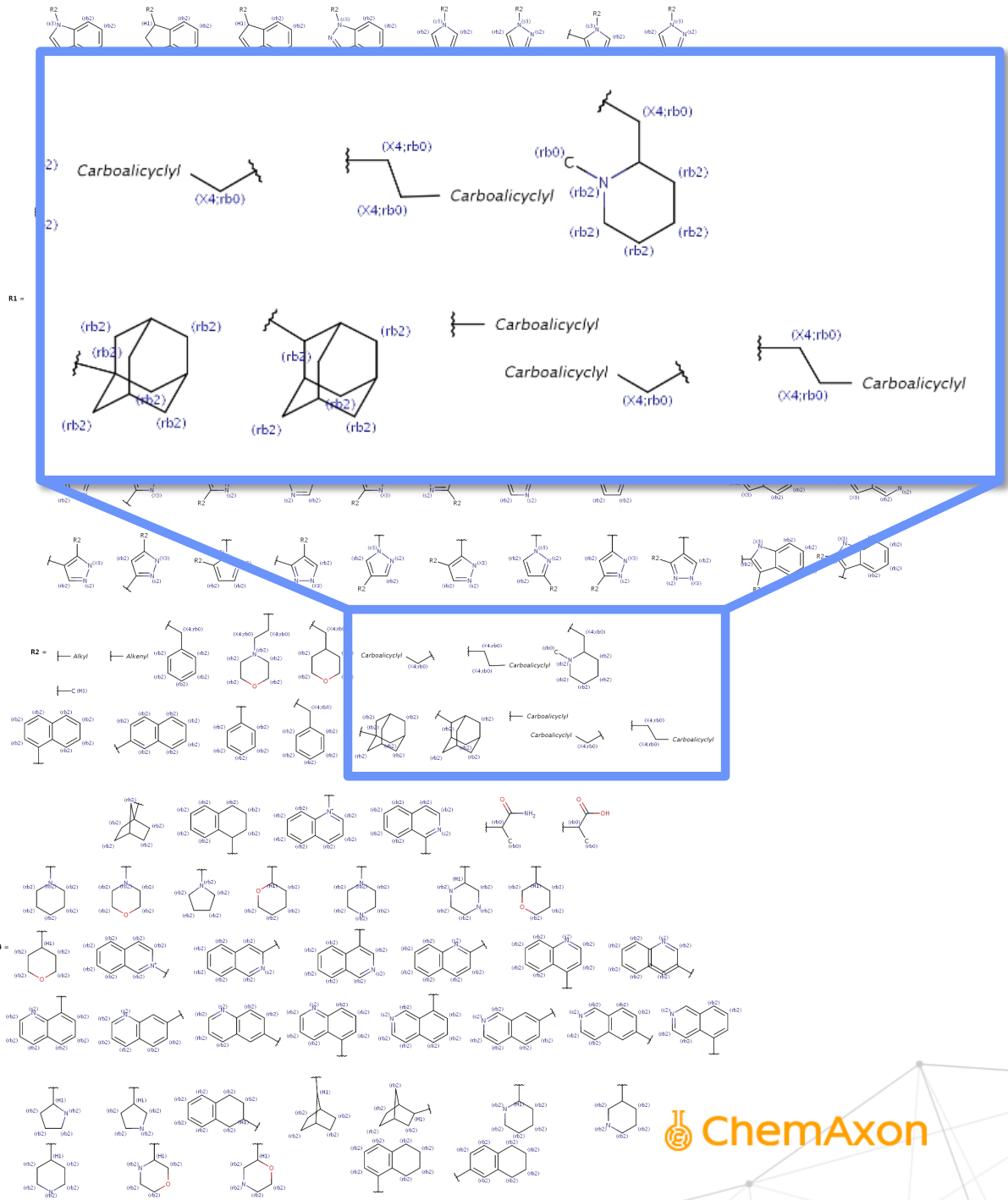
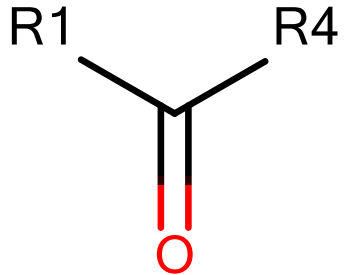
## Controlled Substance Act **Schedule II** (United States)



## Additional context in **Schedule III**

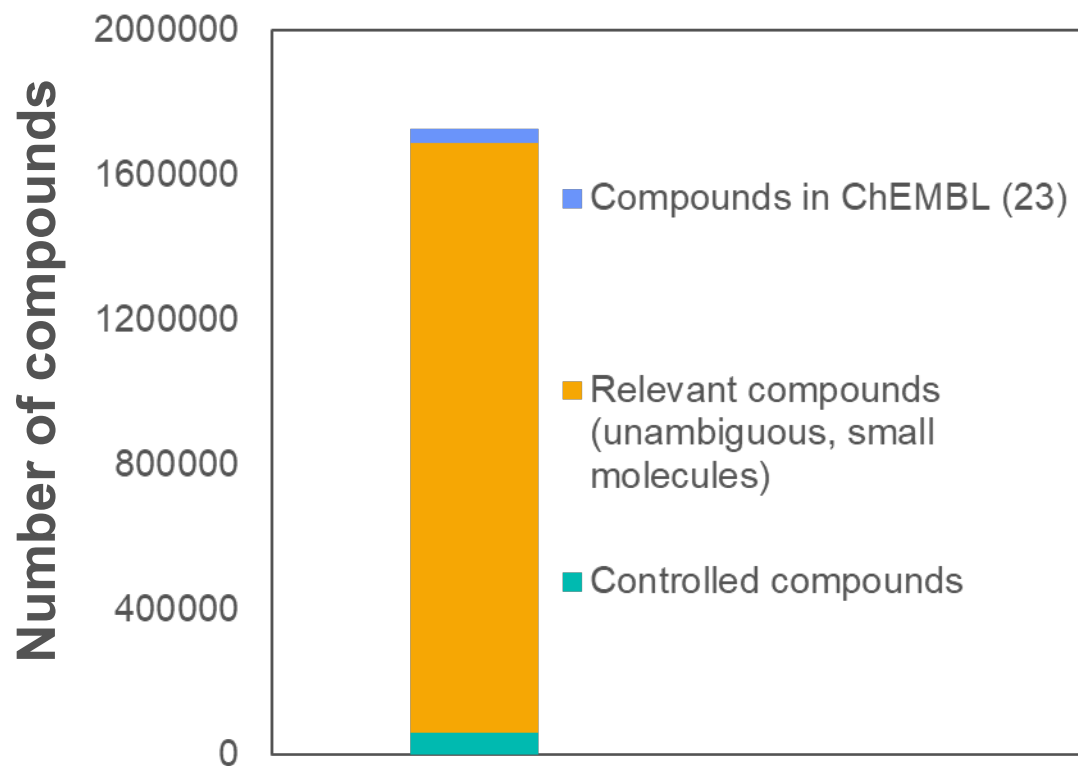
"Not more than 1.8 grams of codeine per 100 milliliters or not more than 90 milligrams per dosage unit, with one or more active, nonnarcotic ingredients in recognized therapeutic amounts"

# Third Generation Synthetic Cannabinoids Act (United Kingdom)



# APPLICATION STUDY: CONTROLLED SUBSTANCES IN CHEMBL





~4% of ChEMBL was controlled on January 25, 2019

## Run details:

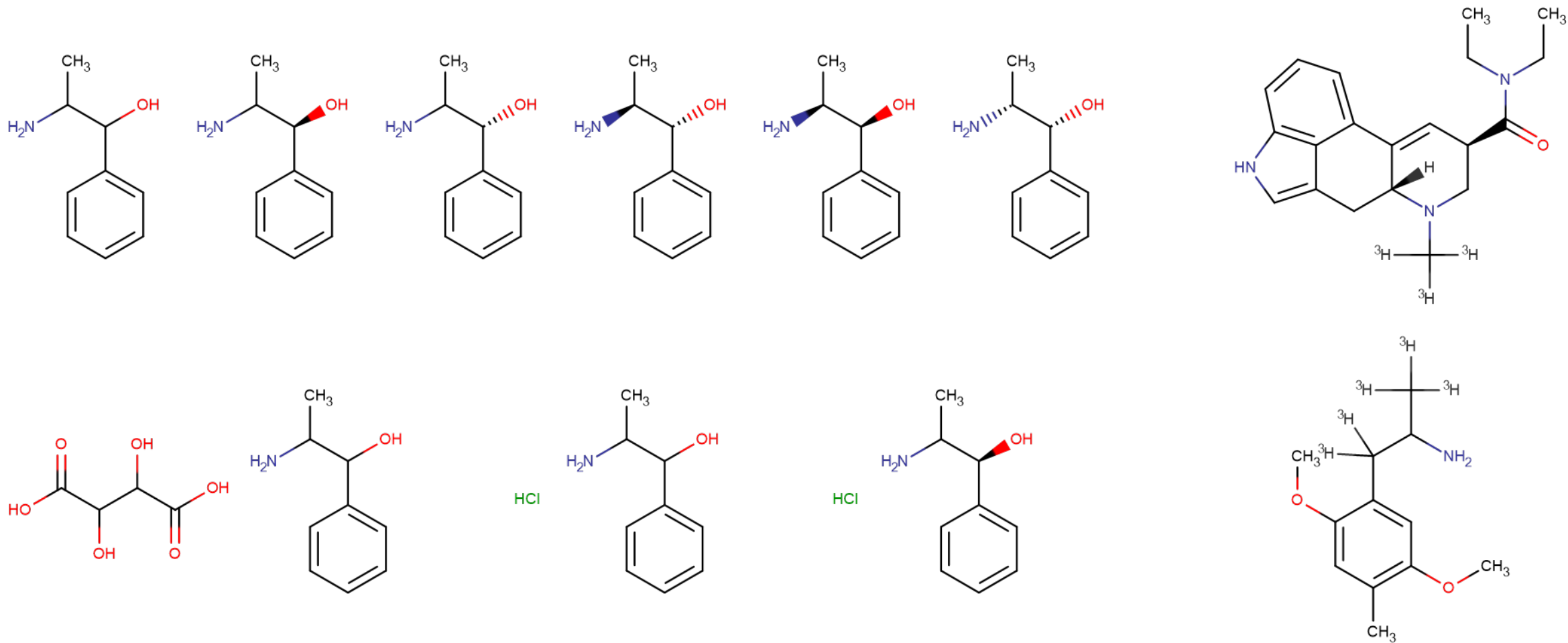
8 logical cores (4 physical) and 32 GB RAM

ChEMBL 23 (05/2017)

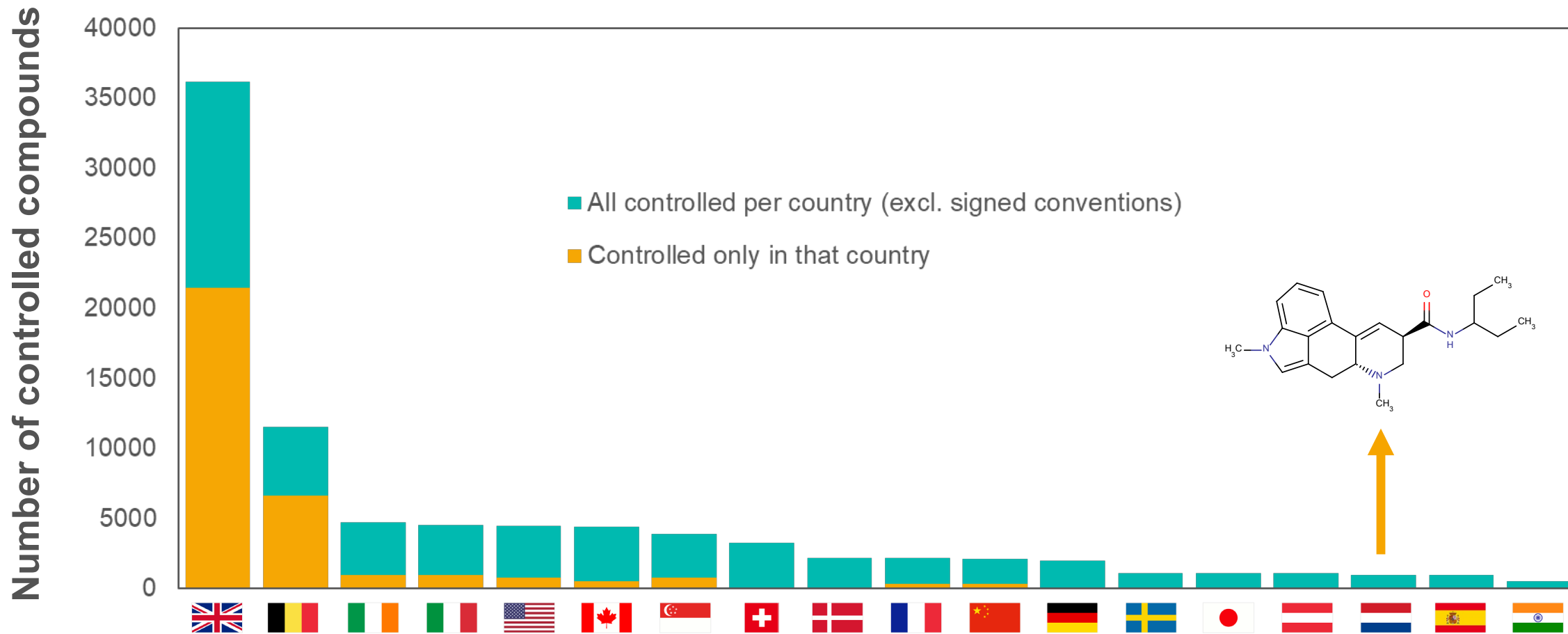
**1,727,111 molecules** in a single SDF

**3.5 h run time** on average\*

\*depending on knowledgebase version

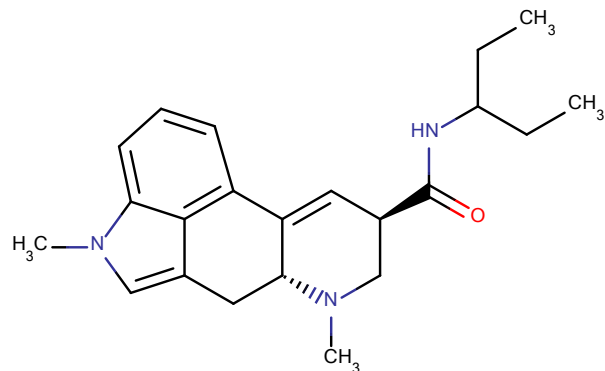


Compounds controlled by  
**all countries**  
 (including EU and UN regulations)



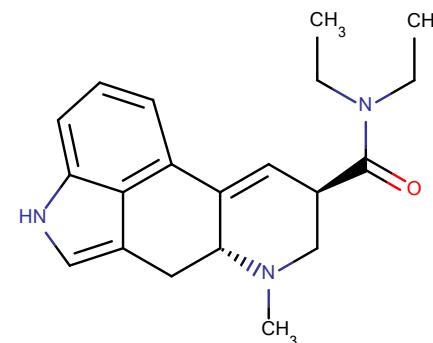
List of controlled substances may vary significantly by country.

## Controlled by the Netherlands



Lysergic acid analog (methysergide)

## Controlled by all 18 countries



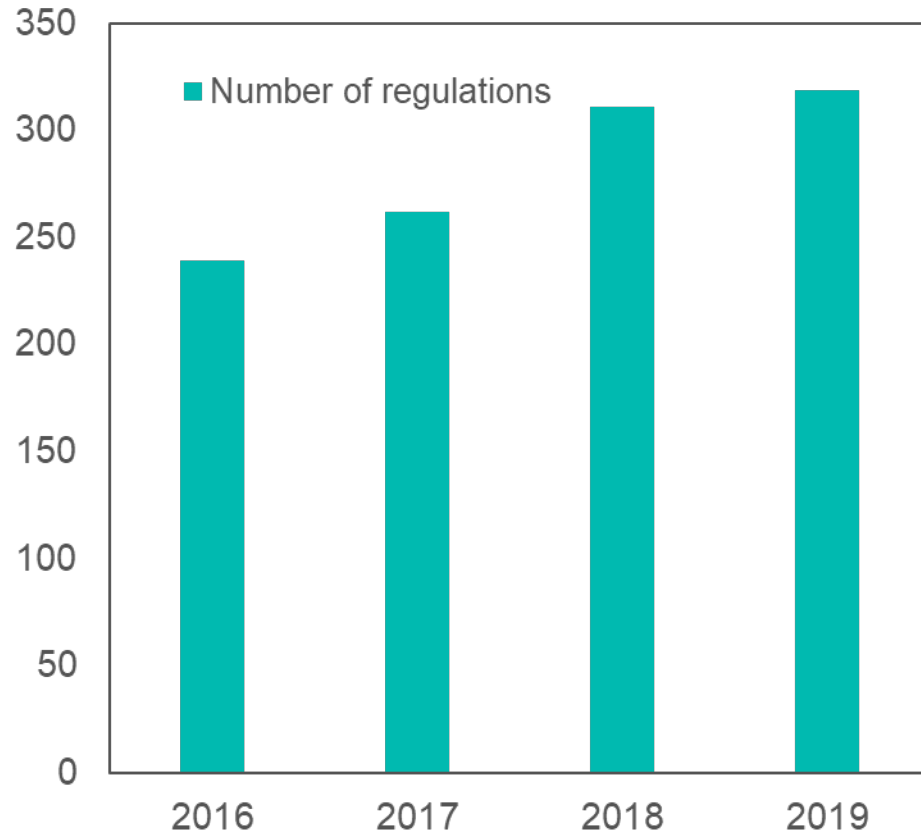
Lysergic acid diethylamide (LSD)

" [...] the mono- and di-alkylamide, pyrrolidine and morpholine derivatives of lysergic acid, and the agents obtained therefrom by introduction of methyl, acetyl or halogen groups. „

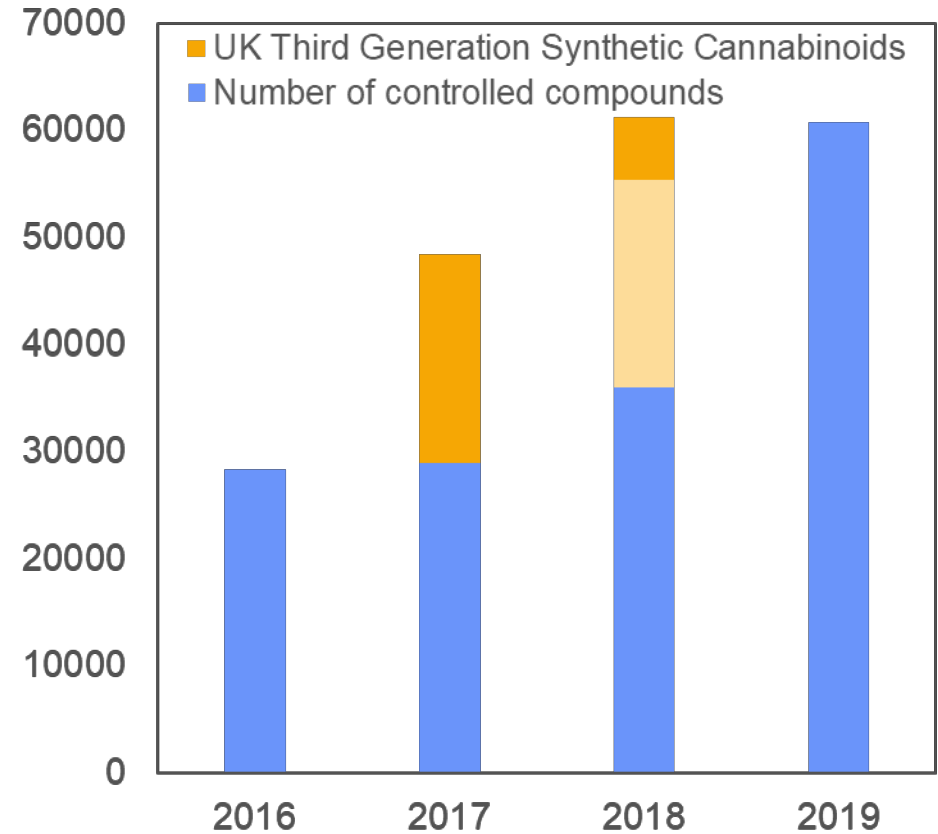
(Opiumwet, List I, 12 May 1928)



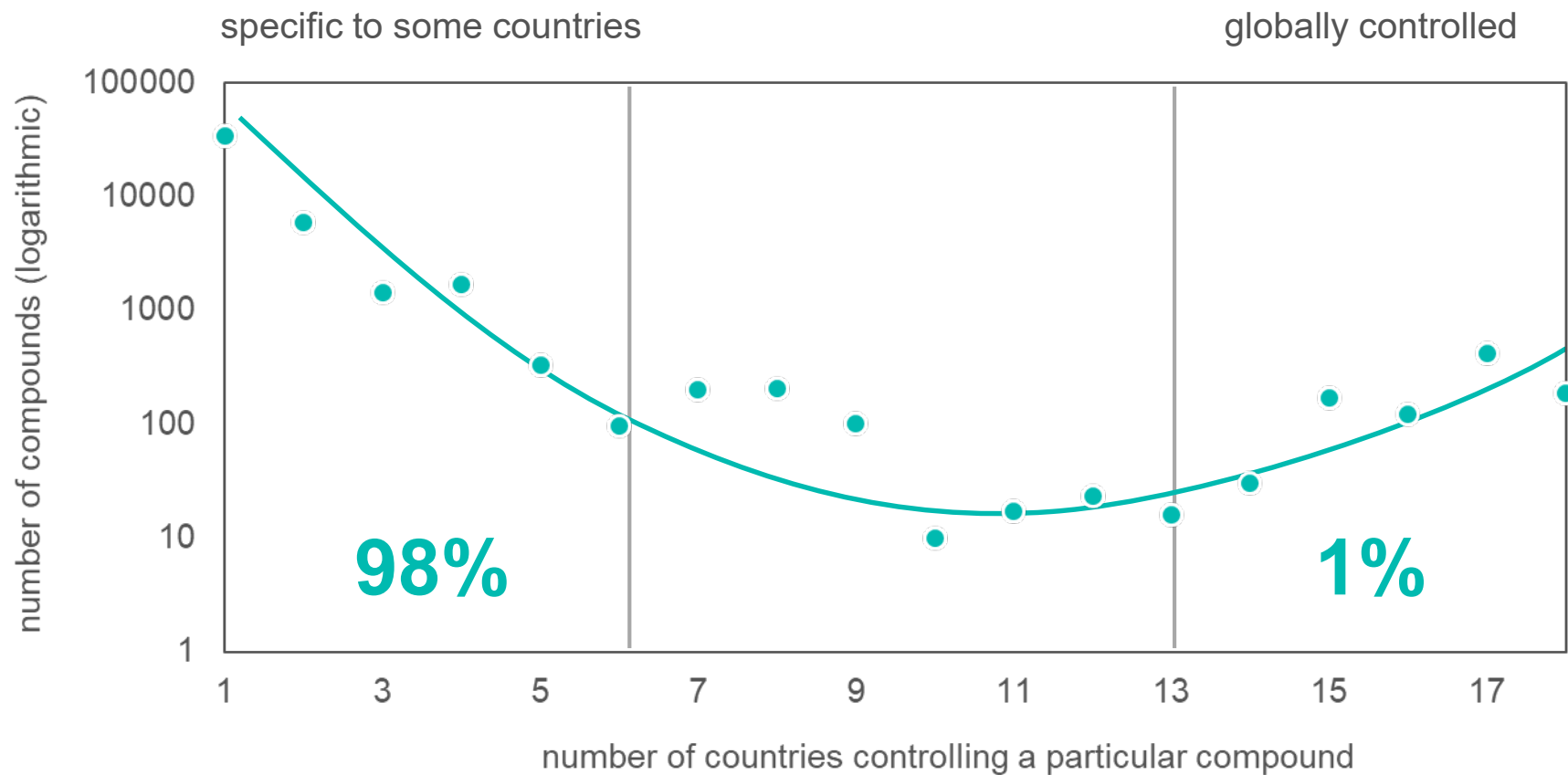
## Regulatory documents



## Controlled substances

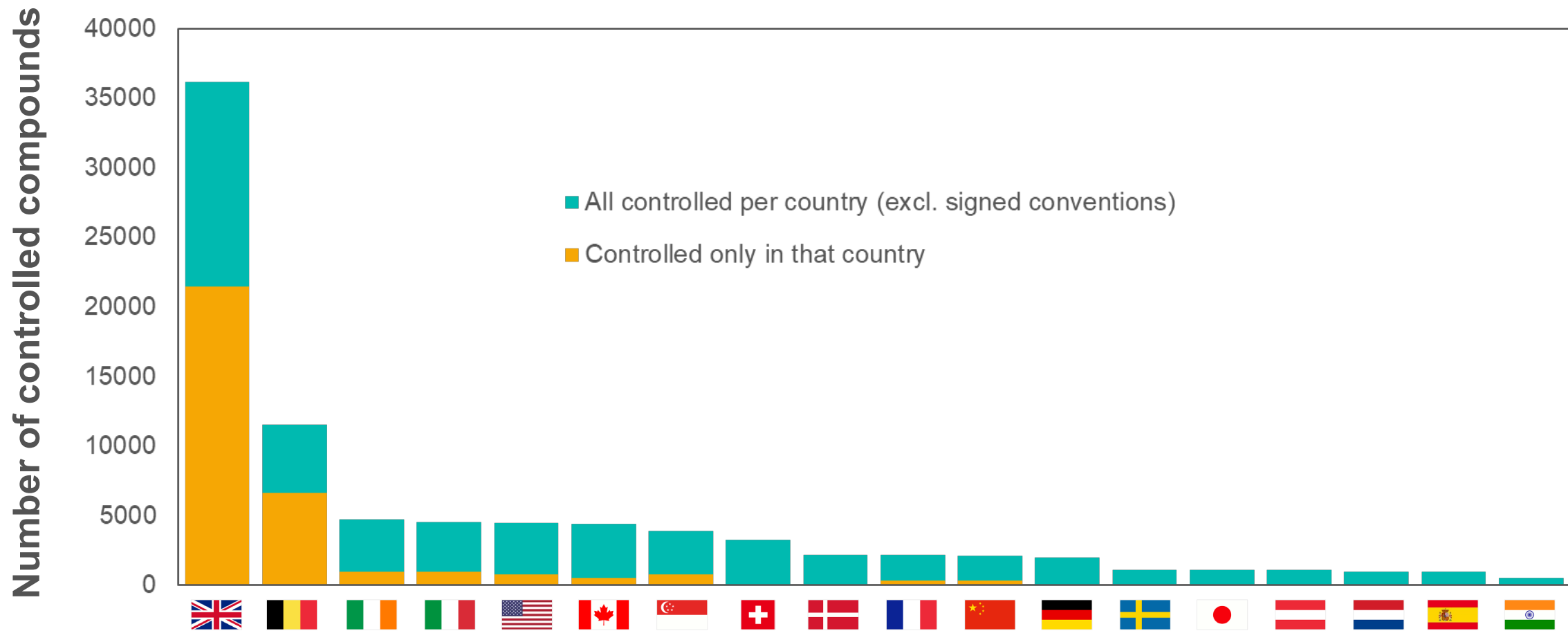


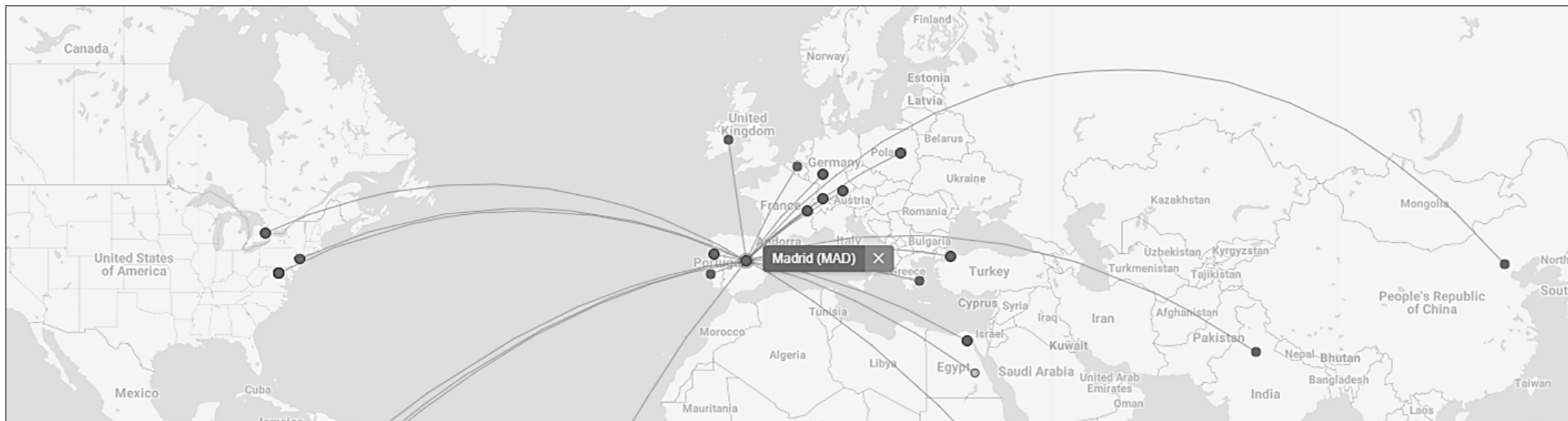
**Number of controlled substances increase rapidly year after year.**



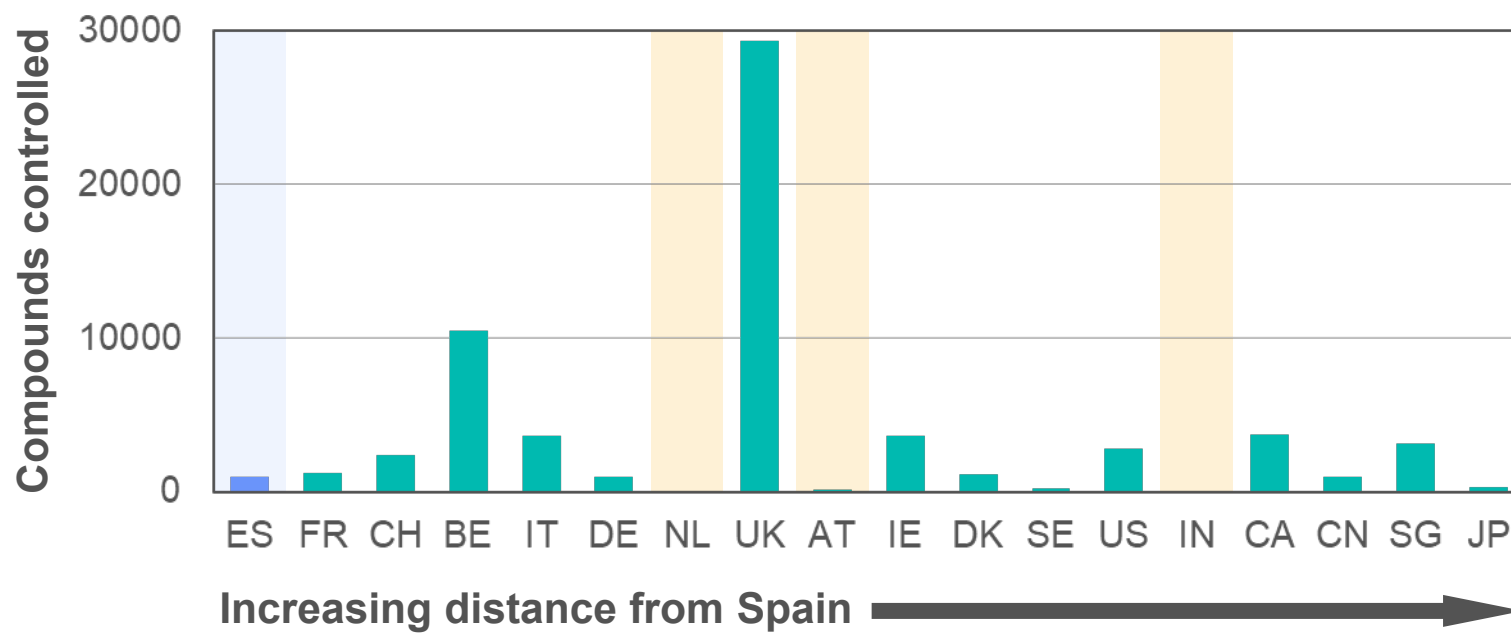
**The vast majority of compounds is only controlled by specific countries.**

**What if we wanted to establish  
a catalog company in Europe?**





<https://www.flightconnections.com/>





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