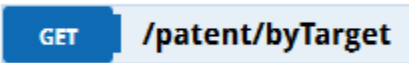



# SureChEMBL API use case example

**Use case:** For a target of interest, find patents that contain (small) molecules that modulate the target and could be used, for example, as tool compounds or to develop an assay.

## Steps in Pipeline Pilot: Target = transthyretin (TTR)

### 1. Get patents for target

- a) Get list:  (11167 patents)
- b) Filter list: e.g.  
relevanceScore = 3,  
frequency > 2,  
exclude “biomarker” in title) (1400 patents remain)
- c) Get patent information: 
- d) Filter list: patent classification = C07D (heterocyclic compounds) (145 patents remain)

## Steps (continued):

### 2. Get compounds for remaining 145 TTR patents

- a) Get list: `GET /patent/entities/pages` (11167 for TTR)
- b) Filter list: e.g. `relevanceScore > 1` (4528 molecules)
- c) Get patent count for compounds: `GET /patent/byCompound/count`

### Further steps (outside of Pipeline Pilot):

1. Addition of MW, HAC, and cLogP to file
2. Addition of link to SureChEMBL page for patents derived from patent number (base URL <https://www.surechembl.org/document/> + SureChEMBL patent ID)
3. File imported into Spotfire for visualisation and analysis



### Filtering in Spotfire:

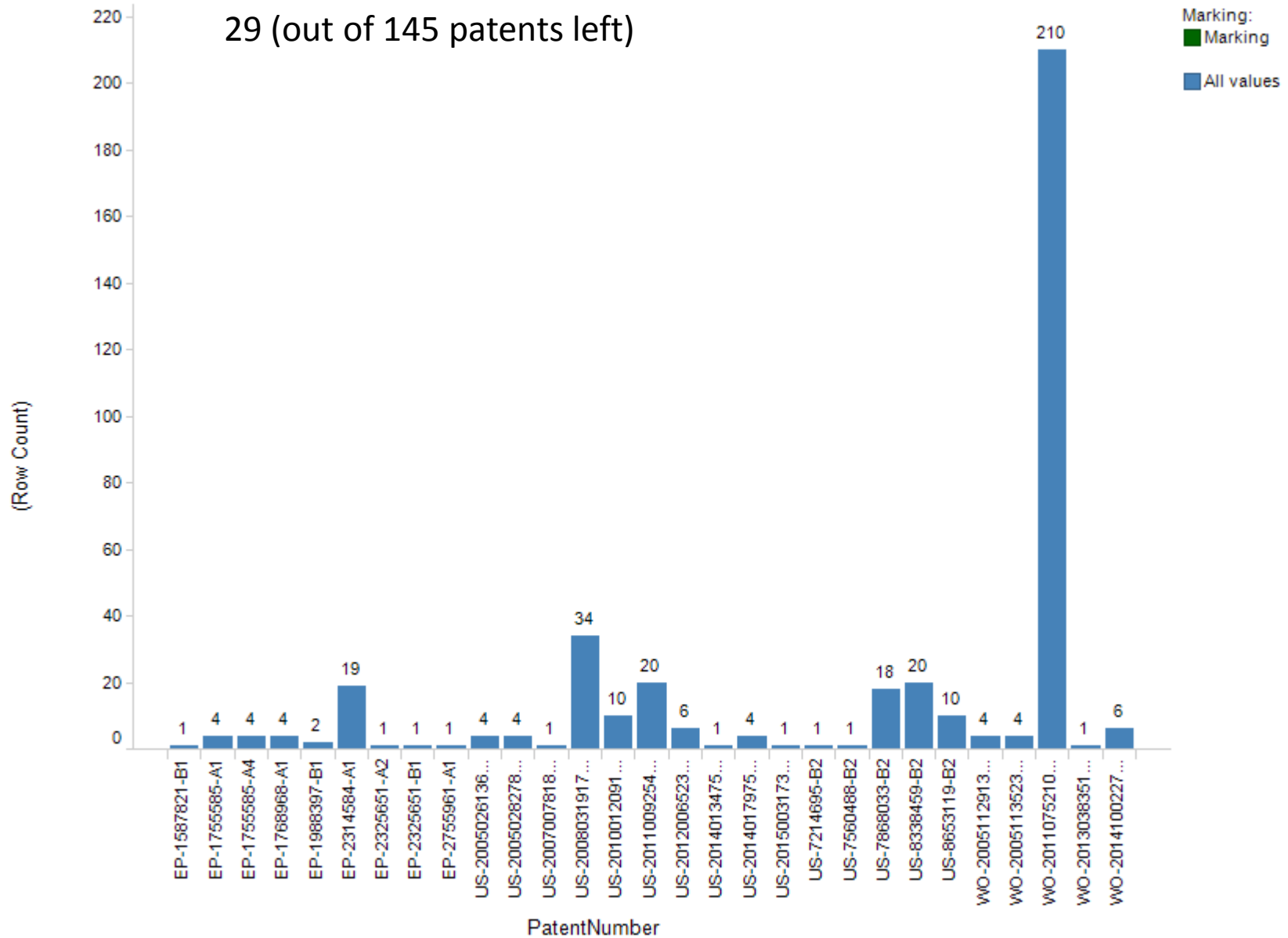
PatentCount = 1-10

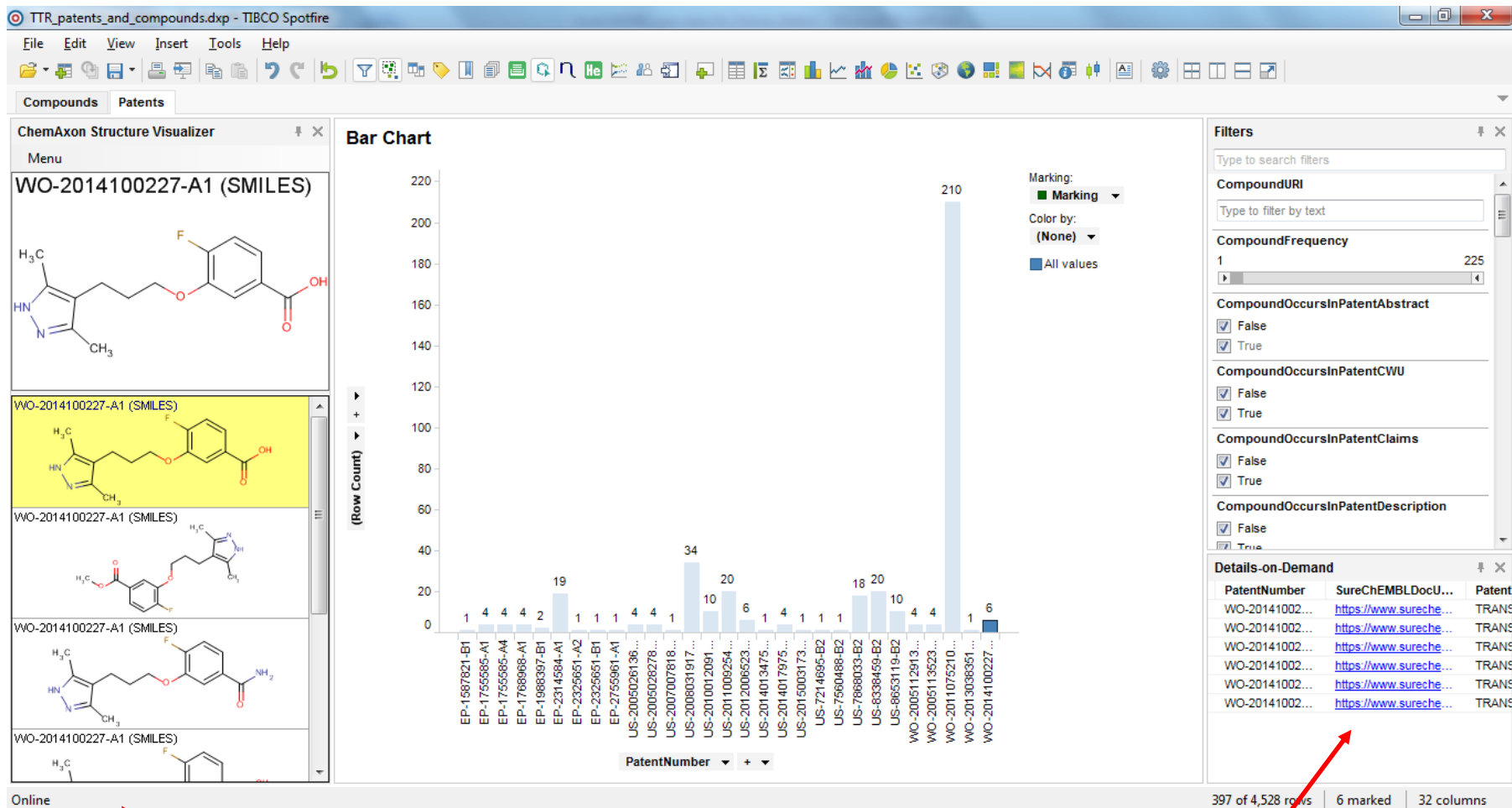
MW = 250-550

TargetOccurInPatentTitle = True

-> 397 compounds (from 4528) left

29 (out of 145 patents left)

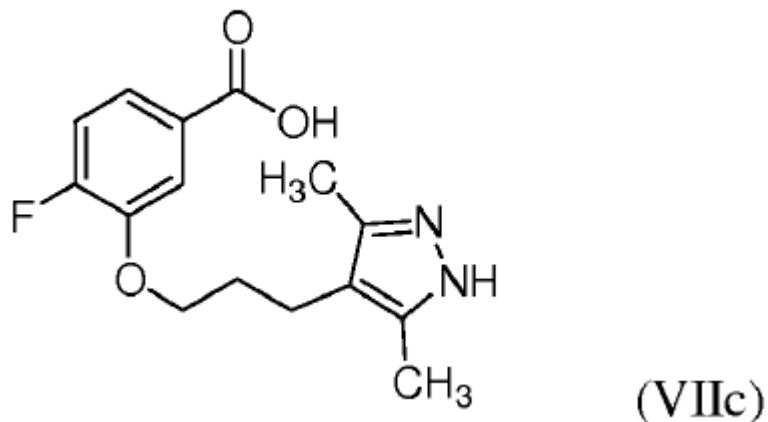




Straightforward to review structures

Clickable links to SureChEMBL patent pages in Spotfire, allowing quick review of relevance of patents

**Most recent patent:** WO-2014100227-A1



In comparison to the clinical candidate tafamidis, we find that Compound VIIc is a highly effective and selective stabilizer of both WT and V122I mutant TTR.

This compound is not in ChEMBL and can only be found in a patent in SciFinder.