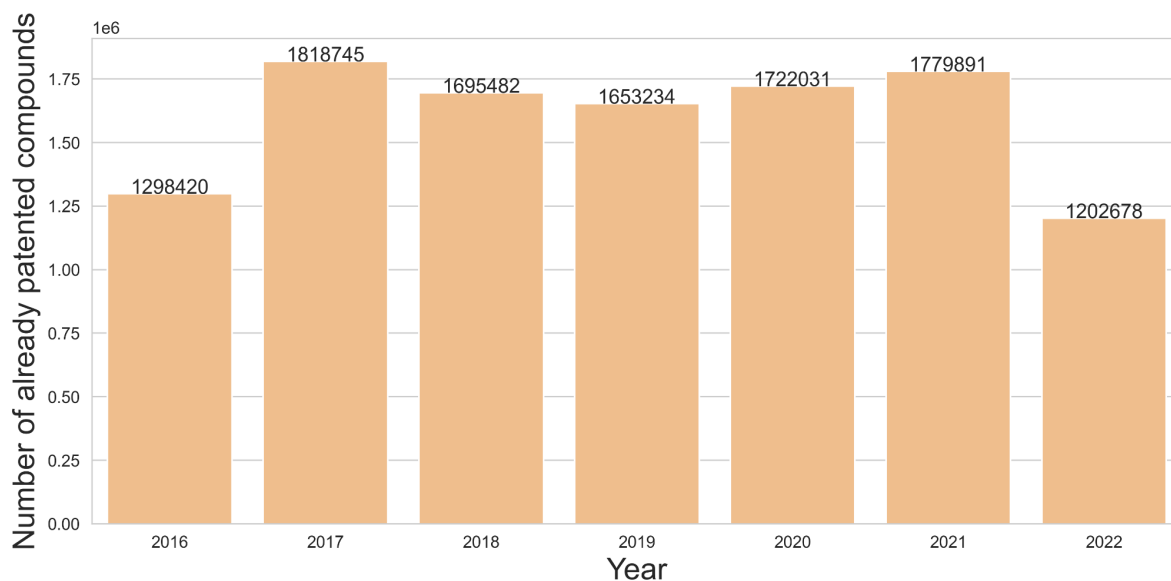
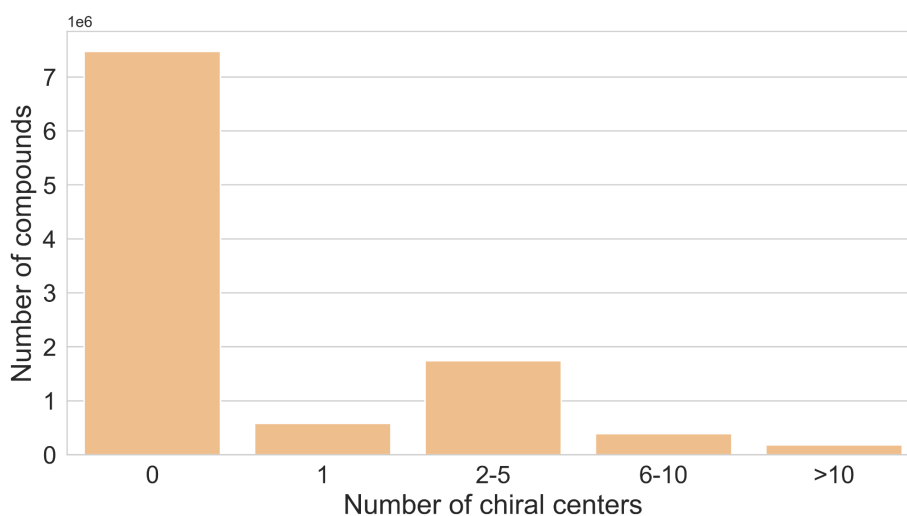


Supplementary Material

Supplementary Figures



Supplementary Figure S1: Repurposed compound distribution over the years. Distribution of compounds that have been found in patent documents from previous years. It is to be noted that the repurposing scenario shown here is only considered from 2015 onwards.



Supplementary Figure S2: Distribution of chiral centers across compounds. Distribution of the number of chiral centers found in the compounds.

Supplementary Tables

Number of patent documents	Number of compounds
< 5	10,148,500
10 - 50	445,227

50 - 100	37,247
100 - 500	37,157
500 - 1000	7,000
> 1000	11,613

Supplementary Table T1: Summary of the number of compounds found associated with patent documents. The compounds were counted based on their unique InChIKey representation in SureChEMBL.

Year	TPSA	# Stereoisomers	# Heteroatoms
2105	79.47	4.40	7.34
2016	83.19	5.05	7.73
2017	81.65	7.01	7.53
2018	80.68	6.57	7.60
2019	82.36	6.52	7.75
2020	83.17	6.47	7.83
2021	82.99	5.78	7.82
2022	81.81	6.37	7.83

Supplementary Table T2: Averaged yearly physicochemical property descriptions for compounds found in patent documents. For each year, we report the topological polar surface area, the number of potential stereoisomers, and the number of heteroatoms.

PAINS	Number of compounds	Percentage of compounds
azo_A(324)	71,539	18.53
anil_di_alk_A(478)	53,902	13.97
indol_3yl_alk(461)	33,103	8.58
catechol_A(92)	23,500	6.09
anil_di_alk_C(246)	22,029	5.71
quinone_A(370)	20,697	5.36
dyes5A(27)	15,780	4.09
mannich_A(296)	15,562	4.03
imine_one_A(321)	14,940	3.87
anil_di_alk_E(186)	12,726	3.29

Supplementary Table T3: Summary of the top PAINS substructures found in patented compounds with molecular weight less than 2000 Daltons.

Patent Field	Number of scaffold	Percentage of scaffold
Abstract	1,7431	0.08
Claims	2,002,898	9.19

Description	9,166,813	42.05
Image (after 2007)	9,391,851	43.08
MOL file (after 2007)	1,215,095	5.57
Title	5,698	0.02

Supplementary Table T4: Summary of the number of unique scaffolds found in the individual patent sections.