



# **Enamine**

## **Agro-like focused Library**

Focused & Targeted Libraries

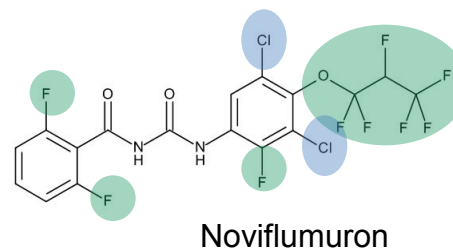
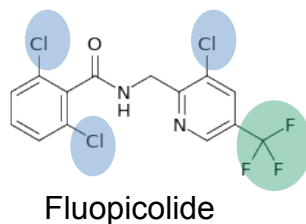
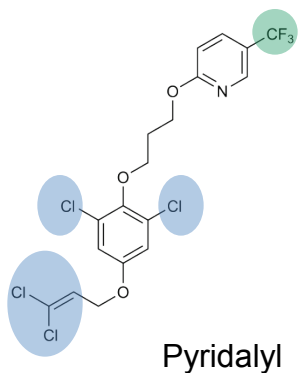
## What makes the molecule agro-like?

Our **analysis** of commercialized agrochemicals identified **9 abundant motifs** which were used for the selection of compounds to **9 clusters**

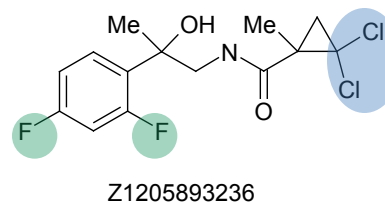
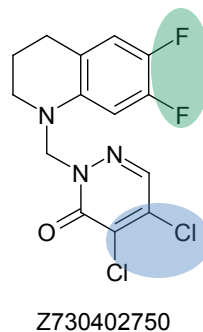
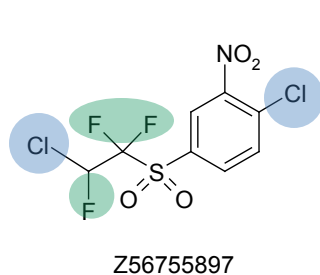
Combination of these clusters and subsequent diversity analysis and careful selection of compounds represents **Agro-like Library** of **10 240 compounds**

## Cluster 1. compounds containing >4 atoms of F&Cl

Examples of agrochemicals:



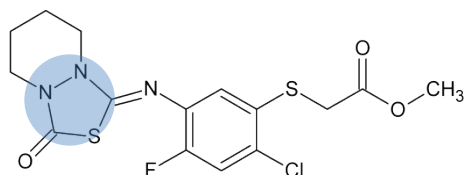
Examples of compounds from the cluster:



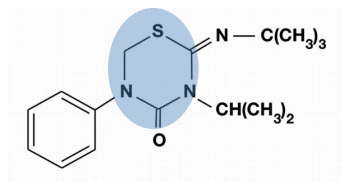
~ 3.5 k compounds

## Cluster 2. S-containing aliphatic cycles

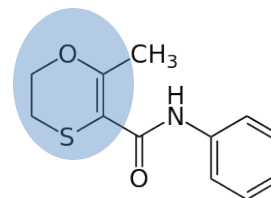
Examples of agrochemicals:



Fluthiacet

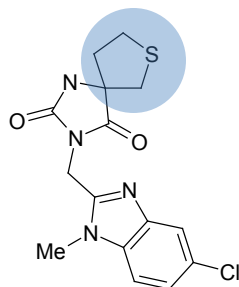


Buprofezin

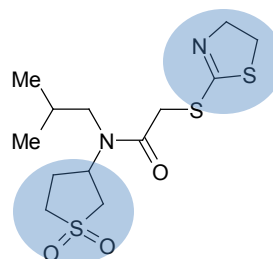


Carboxin

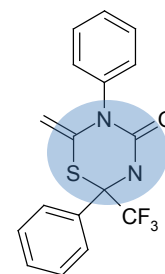
Examples of compounds from the cluster:



Z427731530



Z19631152

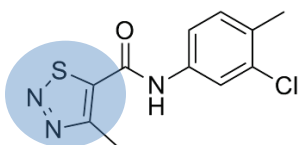


Z57965652

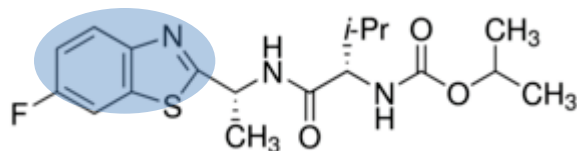
~ 4 k compounds

## Cluster 3. Sulfur containing heteroaromatics

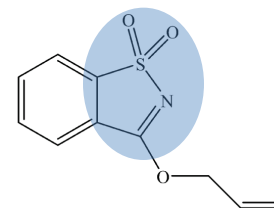
Examples of agrochemicals:



Thiadinil

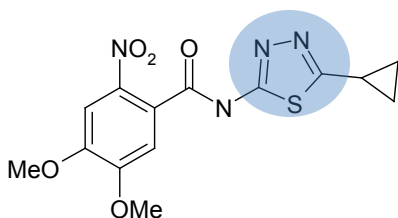


Benthiavalecarb

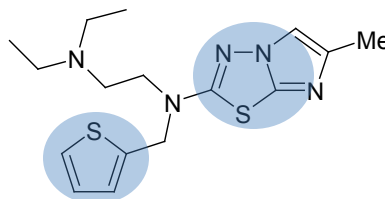


Probenazole

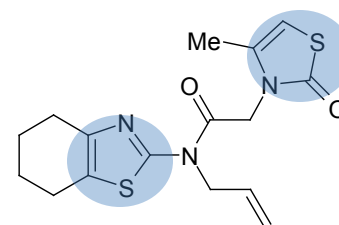
Examples of compounds from the cluster:



Z27165731



Z1410210871



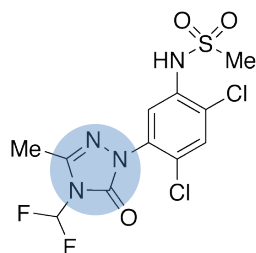
Z90891014

~ 4 k compounds

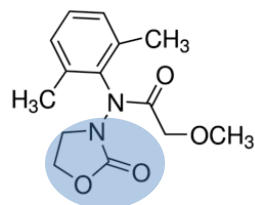


## Cluster 5. Oxo-Azoles/azolines

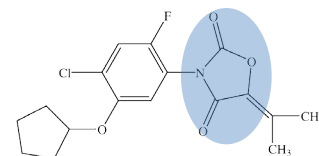
Examples of agrochemicals:



Sulfentrazone

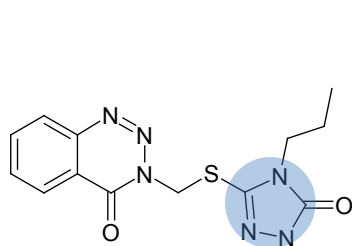


oxadixyl

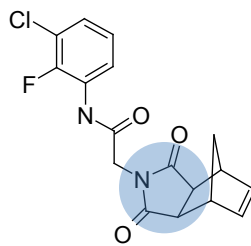


Pentoxazone

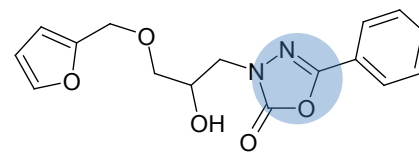
Examples of compounds from the cluster:



Z24800123



Z24800123

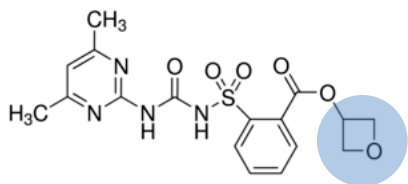


Z287299758

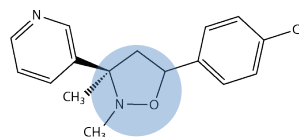
~2.5 k compounds

## Cluster 6. Aliphatic O-containing heterocycles

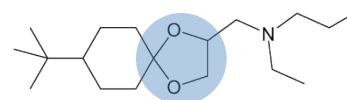
Examples of agrochemicals:



Oxasulfuron

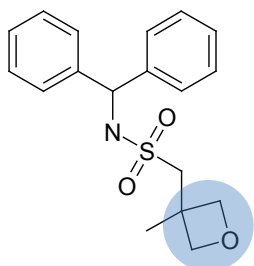


Pyrisoxazole

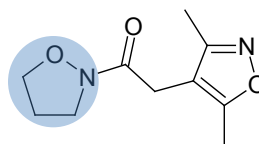


Spiroxamine

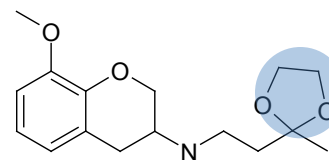
Examples of compounds from the cluster:



Z1788051306



Z1720336051

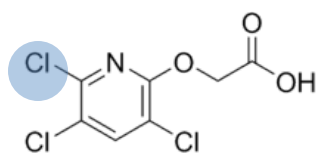


Z1823966049

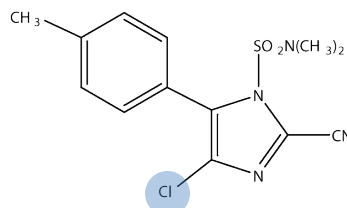
~3.7 k compounds

## Cluster 7. "Active" Cl

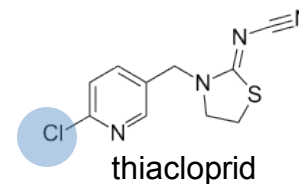
Examples of agrochemicals:



Triclopyr

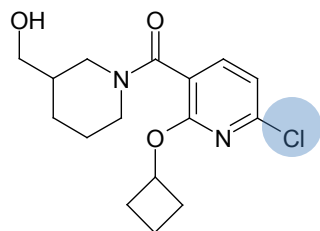


Cyazofamide

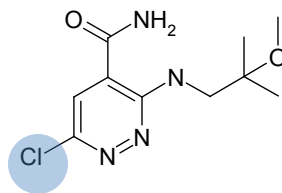


thiacloprid

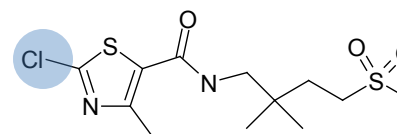
Examples of compounds from the cluster:



Z1688813223



Z1323999762

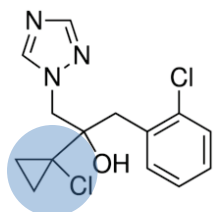


Z13335239635

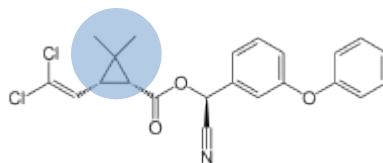
~3.8 K cmpds

## Cluster 8. Cyclopropanes

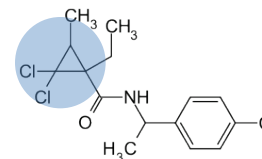
Examples of agrochemicals:



Prothioconazole

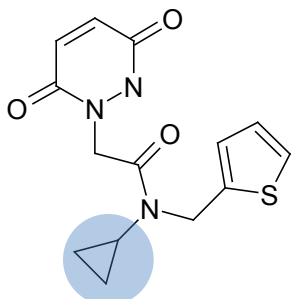


Cypermethrin

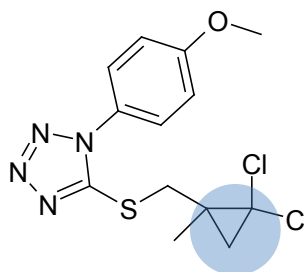


Carpropamid

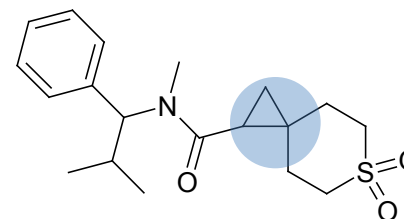
Examples of compounds from the cluster:



Z405877960



Z51163919

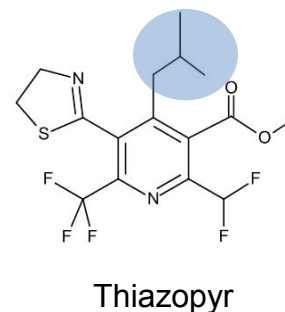
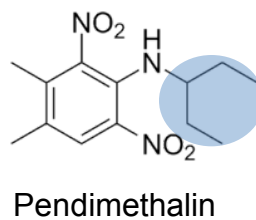
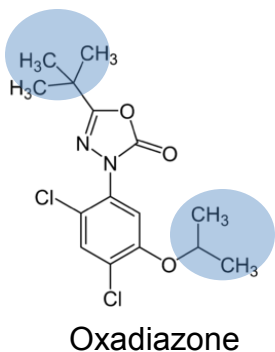


Z1738962586

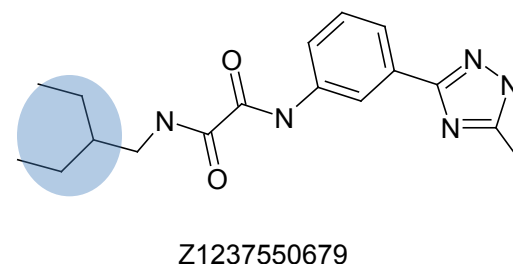
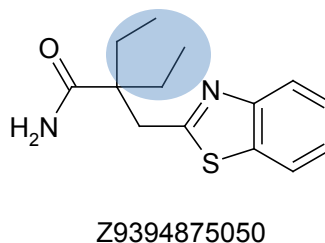
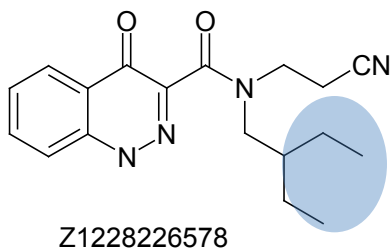
~5.4 k compounds

## Cluster 9. Branched aliphatic chains

Examples of agrochemicals:



Examples of compounds from the cluster:



~2.4 k compounds

## General selection criteria

- Abundant **functional groups** (NO<sub>2</sub>, CO) and privileged chemotypes.
- Abundant **heterocycles**: pyridines, pyrimidines, pyrazoles, triazoles, imidazoles.
- **Unique** scaffolds/chemotypes trivial chemotypes were removed.
- Emphasis on **High Fsp<sup>3</sup>** escape from “agrochemical flatland”
- **Physical chemical/structural** limitations: MW ≤ 400, ClogP ≤ 5, Rings ≤ 4, Rotatable bonds ≤ 10