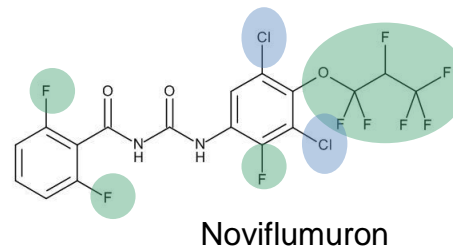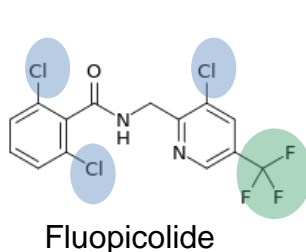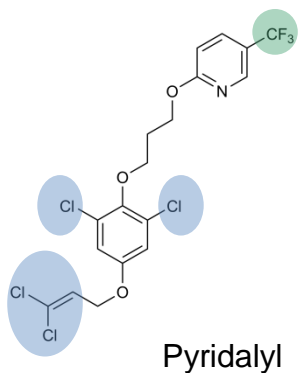# Enamine Agro-like set design

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**
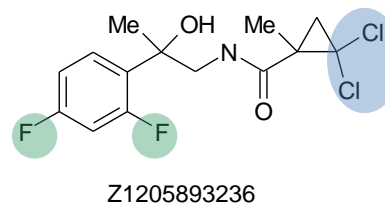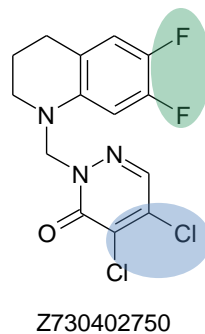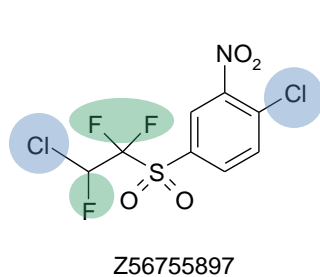
Combination of these clusters represents our Agrolike set of compounds (**51671 cmpds**)

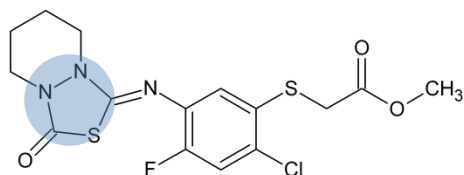**Cluster # 1.** compounds containing >4 atoms of F&Cl

Examples of agrochemicals:

Pyridalyl

Fluopicolide

Noviflumuron

Examples of compounds from the cluster:

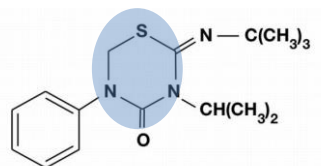Z56755897

Z730402750

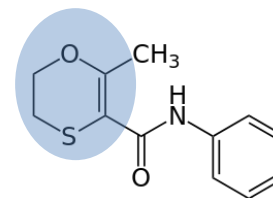Z1205893236

~ 5.5 K cmpds

Cluster # 2. S-containing aliphatic cycles
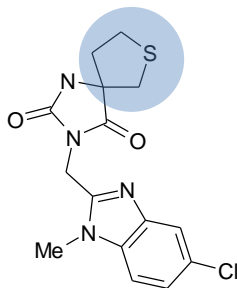
Examples of agrochemicals:
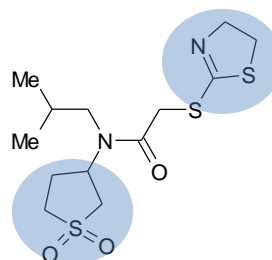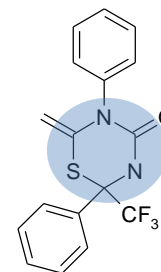
Fluthiacet

Buprofezin

Carboxin

Examples of compounds from the cluster:
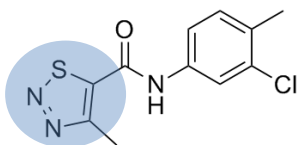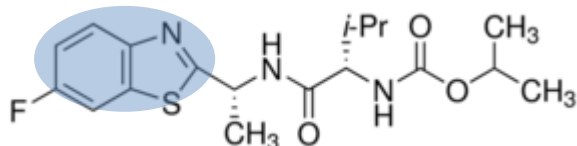
Z427731530

Z19631152

Z57965652

~ 7.5 K cmpds

Cluster # 3. Sulfur containing heteroaromatics

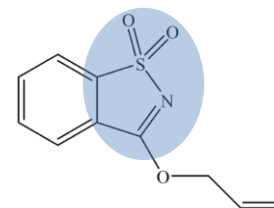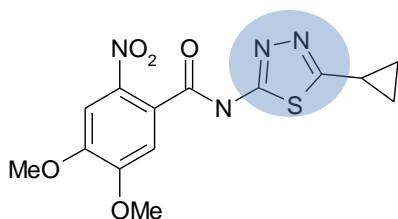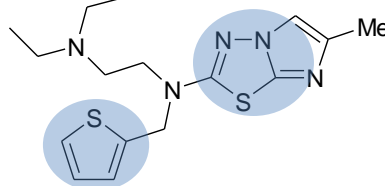## Examples of agrochemicals:

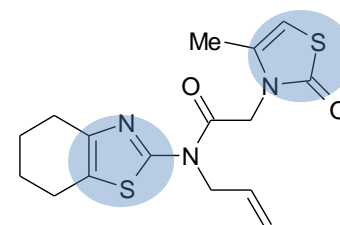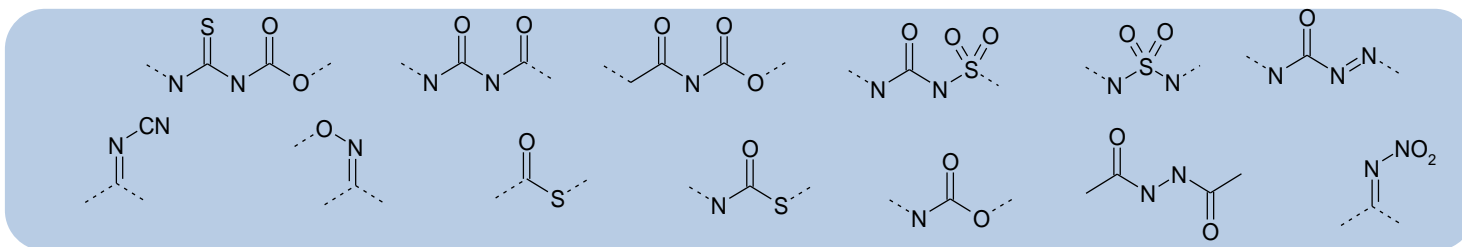

Thiadinil

Benthiavalicarb

Probenazole

Examples of compounds from the cluster:

Z27165731

Z1410210871
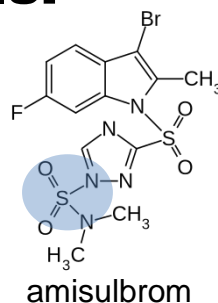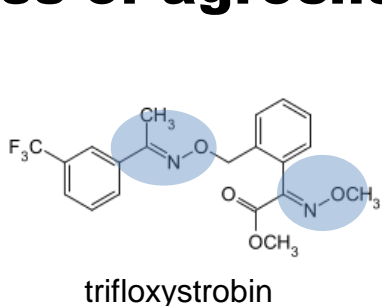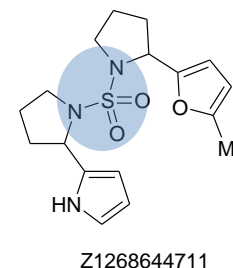
Z90891014

~ 7.5 K cmpds

Cluster # 4. Privileged functional groups: "Not-for-drugs"

Examples of agrochemicals:

trifloxystrobin

amisulbrom

ethoxysulfuron

Examples of compounds from the cluster:

Z961154122

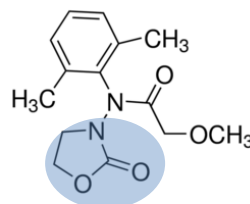Z134724762

Z1268644711
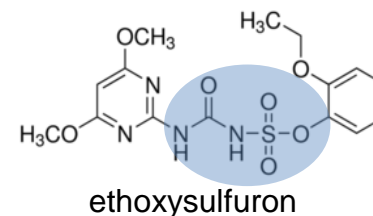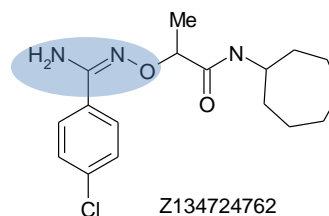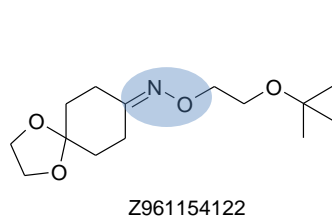
~ 7.3 K cmpds
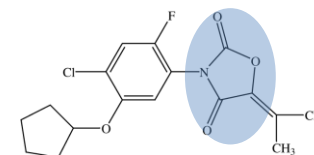
Cluster 5. Oxo-Azoles/azolines

Examples of agrochemicals:
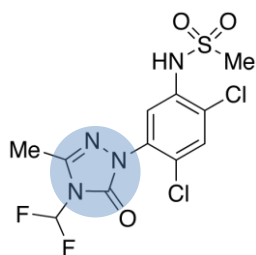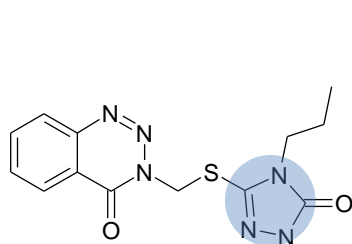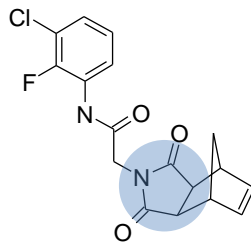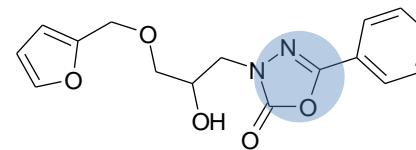

Sulfentrazone

oxadixyl

Pentoxazone

Examples of compounds from the cluster:
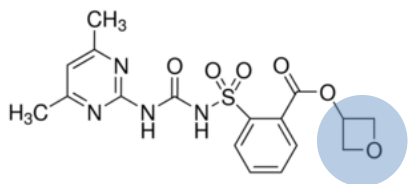

Z24800123

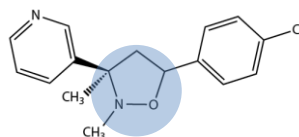Z24800123

Z287299758

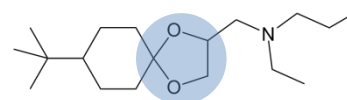# ~4.1 K cmpds

Cluster 6. Aliphatic O-containing heterocycles

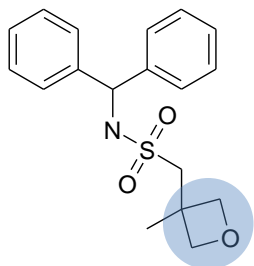**Examples of agrochemicals:**
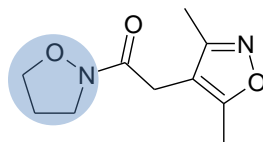

Oxasulfuron

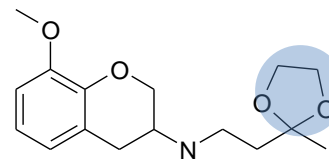Pyrisoxazole

Spiroxamine

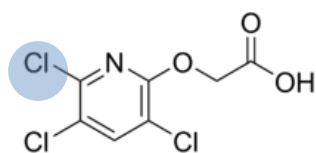**Examples of compounds from the cluster:**
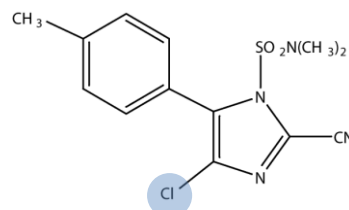

Z1788051306

Z1720336051

Z1823966049
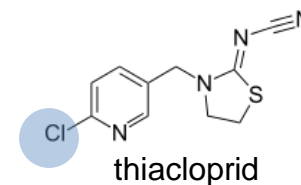
~7.7 K cmpds

Cluster 7. "Active" Cl

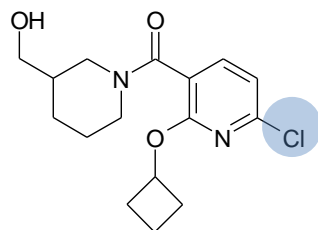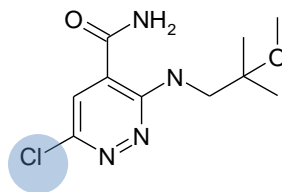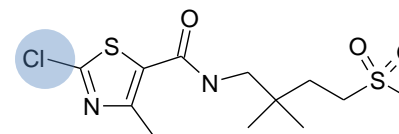**Examples of agrochemicals:**

Triclopyr

Cyazofamide

thiacloprid

Examples of compounds from the cluster:
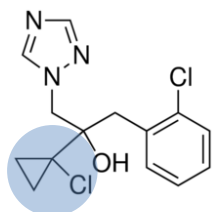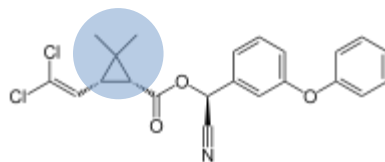
Z1688813223

Z1323999762

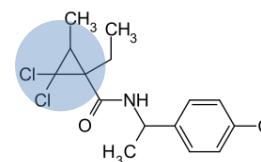Z13335239635

~3.8 K cmpds

Cluster 8. Cyclopropanes

Examples of agrochemicals:
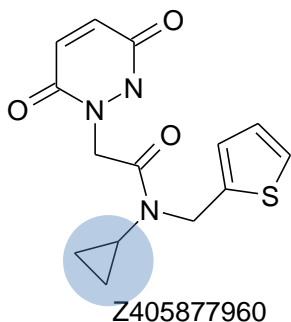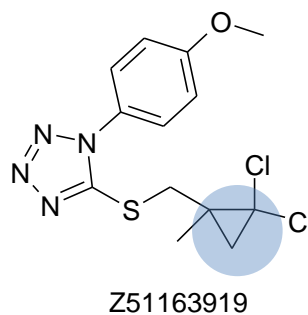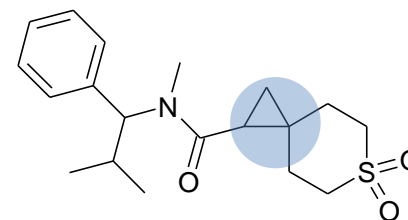

Prothioconazole

Cypermethrine

Carpropamid

Examples of compounds from the cluster:

Z405877960

Z51163919

Z1738962586

~8.4 K cmpds

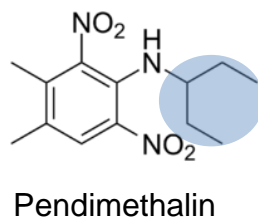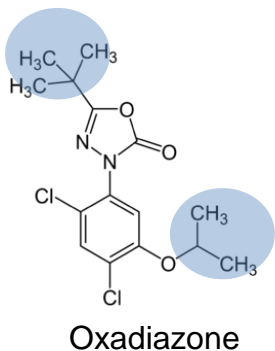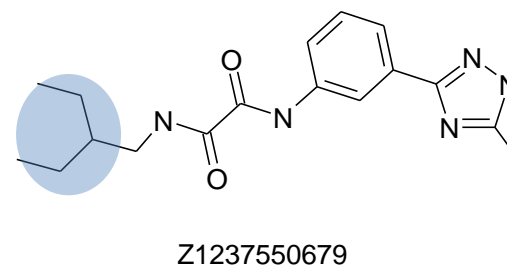# Cluster 9. Branched aliphatic chains

Examples of agrochemicals:

Oxadiazone

Pendimethalin

Thiazopyr

Examples of compounds from the cluster:

Z1228226578

Z9394875050

Z1237550679
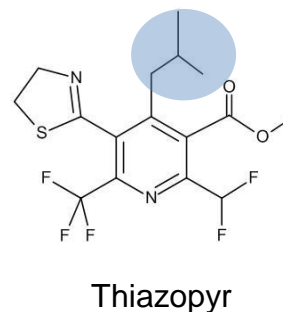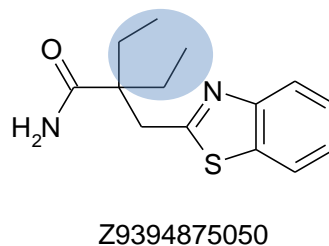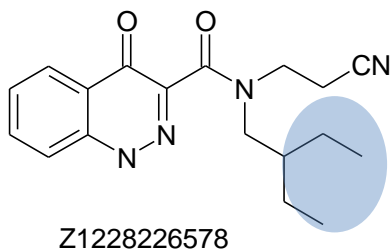
~2.4 K cmpds

Other criteria of selection

1) Abundant **functional groups** (NO_2, CO).

2) Abundant **heterocycles**:
   pyridines, pyrimidines, pyrazoles, triazoles, imidazoles.

3) **Unique** scaffolds/chemotypes
   trivial chemotypes were removed

4) Emphasis on **High Fsp_3**
   lets escape from "agrochemical Flatland"

5) **Physical chemical/structural** limitations
   Mw <350, cLogP <5, # rings < 4, # rotatable bonds <10