ERHVERVSAKADEMI KØBENHAVN

Mod bæredygtig metodeudvikling og identifikation af stoffer i HPLC: Opbygning af database med retentionstider

Projektgruppen ved Laboratorie og miljø:

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1 Forord

Denne rapport omhandler FoU-projektet ”Mod bæredygtig metodeudvikling og identifikation af stoffer i HPLC: Opbygning af en database og maskinlæringsmodel til brug i miljøanalyser”.

Arbejdet er udført i perioden 01.01.2024-31.12.2025 på Cphbusiness Laboratorie og miljø, Hillerød.

Rapporten indeholder valg af materialer, udarbejdede protokoller med risikovurderinger af de benyttede stoffer mm. Rapporten er sat op, så læseren i indholdsfortegnelsen kan klikke sig til de respektive sider fremfor at læse rapporten fra start til slut.

Der er afsnit, som er skrevet på engelsk, så som de udarbejdede protokoller, og der er afsnit som er skrevet på dansk.

> ”*You do the math, you solve one problem, then you solve the next one, and then the next. And if you solve enough problems, you get to come home”.*
>
> Figuren Mark Watney (Matt Damon) i filmen *The Martian* fra 2015

2 Baggrund for projektet

3 Materialer

4 Protokoller

2.1 Introduction

HPLC is one of the most widely used analytical methods in chemical laboratories and is used in almost all chemical sectors, but especially in the pharmaceutical industry, in environmental chemical studies and in food control. It is ismated that approximately 34 million liters of chemical waste are generated worldwide from the use of HPLC equipment (Tobiszewski, 2016) and there is therefore great potential in working towards more sustainable HPLC analyses. According to Ferguson (2022), HPLC can be made more sustainable by, among other things:

1. Reduce organic solvent consumption by scaling down equipment and flow.
2. Replace toxic and environmentally hazardous substances with less problematic alternatives.
3. Eliminate the use of toxic and environmentally harmful substances completely.
4. Reuse the organic solvents that have been used in the analysis.
5. Minimize the number of experiments during method development by using computer simulation.

In addition, we would like to add a point 6:

6. Reduce the acquisition/manufacture of reference substances for identification use.

There is a large consumption of resources in the process of performing an unambiguous identification of the chemical substances, as this requires that the measured retention time of the unknown chemical substance is matched with the retention time of a purchased or synthesized reference substance. Since there can be many possible chemical structures for a given unknown substance, it is not environmentally or economically sustainable to procure/manufacture all the conceivable substances that may be necessary to perform the unambiguous identification, and important knowledge about the content of the sample is therefore lost on this basis.

A knowledge gap has been identified, both in the scientific literature and among users of HPLC methods. This consists partly of a lack of knowledge about the possibility of substituting toxic mobile phases with more sustainable solvents, and partly of being able to predict retention times for chemical substances under several different test conditions such as different stationary and mobile phases.

Recognized needs
Among manufacturers of analysis equipment, there has been a strong focus on point 1. Since 2004, when the first ultra-high performance liquid chromatography equipment came on the market, research and development has been carried out on chromatographic columns, where the standard size used to be 250 mm x 4.6 mm. These had a solvent consumption of 1-2 ml/min, where the most common size is now 100 mm x 2.1 mm, with a solvent consumption of 0.2-0.4 ml/min. There are also so-called nano-scale columns, where the consumption is in the region of 100-1000 nL/min, which is still a rarity, but which can produce a significant reduction in the use of solvents.

Points 3 and 4 have also been researched and developed, e.g. by using high-temperature water or supercritical liquid chromatography, where the solvent is supercritical carbon dioxide. These methods require special equipment, which is not widely used and the areas of application are limited to very specific applications. The specific areas of application also apply to analyses where it is possible to reuse the solvent.

In our pilot study, we therefore chose to take a closer look at points 2, 5 and 6, i.e. replacement with more sustainable solvents, the use of computer simulation to minimize the number of experiments and reduce the need for reference substances.

It has been demonstrated in the feasibility study that the need to replace the use of toxic/environmentally harmful chemicals with less harmful chemicals has been identified by

both academic (Nakov et al., 2022) and industrial parties (Henderson et al., 2011), and the need to work systematically with method development has been described by researchers from Novo Nordisk (Cheung et al., 2022), Which in their case still requires a lot of experiments. It has also been demonstrated in the feasibility study that there is a recognized need in both industry and research circles for a computer-based tool to predict starting conditions and results for method development based only on the structure of the chemical substance and parameters for the test conditions, thereby saving time and resources.

Knowledge gap

The knowledge gap identified in relation to the use of greener solvents consists primarily in the lack of knowledge about the use of these greener solvents, despite the fact that in many cases equally good or even better analytical results are demonstrated compared to the commonly used solvents (Nakov et al., 2022, Funari et al. 2014). The amount of articles on the use of green solvents is small compared to the number of articles where the common solvents are used, and users in companies are therefore not presented with examples where green solvents are used when they seek inspiration to develop new methods.

The knowledge gap identified in relation to the use of computer-based tools for both the development of methods and the identification of substances is that the databases on which the machine learning models are based are not comprehensive enough in terms of the number of substances and the variation in test conditions (Haddad, 2019 and Haddad, 2021). Machine learning models have previously been developed to predict chromatographic results, but often the models are built on databases consisting of 50-150 substances and on a single experimental design (e.g. one stationary phase, one mobile phase, one analysis time and one temperature). This means that the models that have been built previously only work on the system on which they were developed and therefore cannot predict retention times under experimental conditions that have not been used for the development of the model, and the relatively small selection of chemical substances limits the models in what other substances they can make predictions for.

Machine learning as the tool of the future to minimize time and resource consumption in the development of methods and identification of substances

Most chromatography researchers assume that the complexity of HPLC prevents them from being able to predict retention time, which is the time it takes for substances to pass through the chromatography column, based only on the structure of the chemical substance. And it is also true that the molecular structure of a chemical substance and the interactions with the HPLC equipment determine the retention time of the substance and that these interactions are complex. Therefore, the use of HPLC techniques always requires extensive method development, where it is ensured that the method can separate the substances in the sample, so that identification and quantitative determination can be carried out with credible results.

In this process of method development, chemists and laboratory technicians are faced with many decisions that must be considered based on knowledge of the substances that the method is to be used to analyze.

1. What type of chromatography should be chosen?
2. What type of stationary phase and mobile phase should be chosen?
3. What will be the optimal pH and temperature for the separation of the substances?
4. How many samples should be analyzed per day, i.e. what should the analysis time be?

These are just some of the questions a person will ask themselves before and during the work with method development. Often, the literature is consulted to see what others have done with the same or similar substances, and then trial-and-error experiments are carried out in search of a suitable method of analysis. The trial-and-error approach is very time- and resource-consuming, especially if it is not based on a systematic mindset. Larger companies, such as the Danish pharmaceutical manufacturers, have developed more systematic approaches to method

development, one of which is described in Cheung et al. (2022). Here, one's sample is analyzed in an initial screening, where combinations of 5 stationary phases and 6 mobile phases are tested, i.e. 30 trials in total. After this screening, the best starting point can be chosen, and the development can continue from there using chromatographic modelling (Petersson et al. 2014), where 3x3 experiments are performed as input to computer models that can be used to predict the separation of the substances based on the above experiments.
Such a systematic method still requires a lot of resources, including purpose-built HPLC equipment, harmful solvents and time, and there are still a number of tests to be carried out (at least 39) before a final method is developed. The above process must then be repeated for the next sample for which a method is to be developed.

Once developed, analytical methods are often used in targeted methods in which a small number of substances (tens to hundreds) are identified and quantified. These targeted methods, if it is in an environmental or food context, are determined by the authorities in the various areas. The development of analytical equipment and data processing tools has made it possible for chemists and laboratory technicians to go beyond these targeted methods, and there is a lot of research into so-called non-target methods, and they are finding application in areas of authority. In this context, targeted methods are defined as HPLC methods, which only analyse for already known substances, whereas non-targeted methods aim to detect all substances in a given sample. Non-targeted methods are used, among other things, for the analysis of metabolites (metabolomics) and in environmental analysis for contaminants of emerging concern.

Mass spectrometric analysis is often used to identify substances in non-targeted analyses, as a mass spectrum contains information about the mass and structure of a molecule, but unfortunately a substance cannot always be unambiguously identified from the mass spectrum, as there are substances with the same molecular mass but with a different structure. One of the major bottlenecks in non-targeted analyses is therefore sorting out false positive molecular structures, and the traditional method of doing this is to procure (buy or synthesize) reference substances and then measure their retention time by the HPLC analysis. The retention time is specific to the individual substance in interaction with the stationary and the mobile phase. If the retention time of the substance in the sample matches the retention time of the reference substance and there is a match between the mass spectrum of the substance in the sample and that of the reference substance, an unambiguous identification can be obtained. One challenge with the traditional method is that there can be many false positives, perhaps even in the hundreds. Reference substances for all these possible substances often do not exist, they may be unavailable or so expensive that it is economically difficult to procure all the substances that would be necessary to be able to filter out all false positives.

Both the development of HPLC methods and the identification process will benefit greatly from the fact that the retention time of the substances is predicted via a machine learning model. For method development, it will be possible to predict which initial conditions to use only on the basis of molecular structure and stationery/mobile-phase parameters and the number of experiments can therefore be minimized considerably (in the example above, it will be possible to remove the first 30 systematic analyses), which will contribute to a more resource-conscious workflow for method development. For the identification process, it will be possible to predict the retention time for all the possible structures from the molecular weight and then remove the false positives where the predicted retention time does not match the measured retention time. It will then be possible to purchase only fewer reference substances, which in turn will make the final identification process more sustainable.

Recent research has shown that due to the development of machine learning, it is possible to predict the retention time under different test conditions based on the structure of the substance alone.
By using machine learning models, so-called Quantitative Structure Retention Relationships (QSRR), it is possible to predict the retention time, where an accuracy of approx. 5% is demonstrated achievable (Randazzo, 2016, Haddad, 2019) based on the molecular structure alone.

Research within QSRR has so far primarily focused on developing machine-learning models, and there are now several models and tools that can help the user with this part. The development of these machine-learning models has overtaken the development of databases, and the lack of data is an obstacle in the further work to make HPLC method development and identification of unknown substances more sustainable.
The databases used as the basis for the machine-learning models are simply not comprehensive enough in terms of the number of substances and the diversity of the experimental conditions used (Haddad, 2019 and Haddad, 2021). Often, the databases are only built on a single experimental design (e.g. one stationary phase, one mobile phase, one analysis time and one temperature), which means that these models only work on the system on which they were developed and therefore cannot predict retention times under experimental conditions that have not been used for the development of the model, i.e. the model can only be used in the laboratory where it was developed. There is therefore great potential in building new databases that will make the machine learning models generalizable and usable for everyone.

Sustainability in method development and identification
The use of resources is part of the sustainability paradox of chromatographic science (Ferguson, 2023), where the work carried out in the laboratory is considered to be "positively contributing to society". There has therefore been a "carte blanche" not to look at the processes in the laboratory in relation to the green transition (Nikoline Borgerman's presentation at the Laboratory Teacher Seminar, 26 April 2023, Odense). When using HPLC, there is a high consumption of solvents as components in the mobile phase. The most commonly used solvents are methanol and acetonetrile, both of which are harmful with both acute and chronic effects on human health, and thus their use is contrary to the principles of green chemistry of increased safety for personnel (Anastas and Warner, 1998). The life cycle analysis for acetonitrile is also not positive (Henderson et al., 2011) and a replacement with more sustainable solvents would be appropriate. Ferguson (2023) points out that in addition to reducing the use of chemicals, minimising the number of experiments will contribute to the chromatographic method development becoming more sustainable, as it also uses fewer resources. By incorporating more sustainable test conditions, such as sustainable solvents, into the database, future users will be presented with solutions that are sustainable.

2.2 Litteratur liste:

1. Anastas, P. T.; Warner, J. C., 1998, Green Chemistry: Theory and Practice; Oxford University Press.

2. Cheung et al., 2022, Investigation into reversed-phase chromatography peptide separation systems part V: Establishment of a screening strategy for development of methods for assessment of pharmaceutical peptides purity, Journal of Chromatography A, 1668.

3. Ferguson, 2023, The paradox of sustainability in separation science, LCGC, 19, 9, 19-22

4. Funari et al., 2014, A trade off between separation, detection and sustainability in liquid chromatographic fingerprinting, Journal of Chromatography A, 1354, 34-42.

5. Haddad P, (practically) perfect predictions, The analytical scientist, tilgået 2023.10.02, (Practically) Perfect Predictions (theanalyticalscientist.com)

6. Haddad et al., 2021, Prediction of analyte retention time in liquid chromatography, Analytical chemistry, 93, 228-256.

7. Henderson et al., 2011, Expanding GSK's solvent selection guide – embedding sustainability into solvent selection starting at medicinal chemistry, Green chemistry, 13, 854-862.

8. Nakov N, et al., 2023 Green Strategies toward Eco-Friendly HPLC Methods in Pharma Analysis- in High Performance Liquid Chromatography - Recent Advances and Applications. IntechOpen http://dx.doi.org/10.5772/intechopen.110035, tilgået den 25. oktober 2023.

9. Randazzo G, et al., 2016, Prediction of retention time in reversed-phase liquid chromatography as a tool for steroid identification, Analytica Chimica Acta, 916, 8-16.

10. Randazzo G, et al., 2017, Indirect quantitative structure-retention relationship for steroid identification: A chemometric Challenge at "Chimiométrie 2016, Chemometrics and intelligent Laboratory Systems, 160, 52-58.

11. Petersson, et al. 2014, Adaptation of retention models to allow optimization of peptide and protein separations, Chromatography Today, 3, 15-18.

12. Szucs et al., 2021, Structure driven prediction of chromatographic retention times: Applications to pharmaceutical analysis, International Journal of Molecular Science, 22, 3848

13. Taraji et al., 2017, Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structure-Retention Relationships and Design of Experiments, Analytical Chemistry, 89, 1870-1878.

14. Tobiszewski, 2016, Metrics for Green analytical chemistry, Analytical methods, 8, 2993-2999

3.1 Valg af kolonner

Table 1: List of columns used in the study and their characteristics. All columns are manufactured and provided by Agilent.*

Name	Silica type	H	S*	A	B	C (pH 2,8)	C (pH 7,0)	EB retention factor
Zorbax Eclipse PAH	B	1,03	-0,01	0,68	-0,05	0,07	1,4	5,9
Zorbax C18	A	1,08	0,05	0,47	0,06	1,48	1,56	10,7
Zorbax Extend C18	B	1,09	0,05	0,01	-0,04	0,03	0,01	8,4
Polaris Amide-C18	EP	0,84	0,11	-0,33	0,34	-1,65	-0,55	4,2
Zorbax Bonus RP	EP	0,65	0,1	-1,04	0,37	-2,97	-1,1	4,5
Poroshell 120 EC-CN	CN	0,421	-0,06	-0,48	0,002	0,045	0,87	0,95
Zorbax SB-Phenyl	phenyl	0,62	-0,16	0,06	0,03	0,03	1,08	2,7
Poroshell 120 Bonus-RP	EP	0,69	-0,03	-0,57	0,18	-0,67	-0,017	3,98
Poroshell 120 PFP	fluoro	0,63	-0,06	-0,46	0,015	-0,038	0,741	2,88
Zorbax C8	A	0,97	-0,04	0,21	0,17	0,97	1,05	8,3

**H (hydrophobicity), S* (steric), A (acidity), B (alkalinity), C pH 2.8 (charge interactions at pH 2.8), C_pH 7.0 (charge interactions at pH 7.0)*

3.2 PCA analysis of Agilent columns

Purpose:
44 HPLC columns found in the database on www.hplccolumns.org were analyzed using multivariate data analysis in order to find extremes in terms of expanding the area of which we want to test standard compounds.

Dataset:
The data used is the following parameters:

- H (hydrophobicity)
- S* (steric)
- A (acidity)
- B (basicity)
- C_pH 2.8 (charge interactions at pH 2.8)
- C_pH 7.0 (charge interactions at pH 7.0)

All data is autoscaled and full validation is performed using the software LatentiX.

Results:
First, a scatterplot of all 44 objects and 6 variables is obtained (Figure 1).

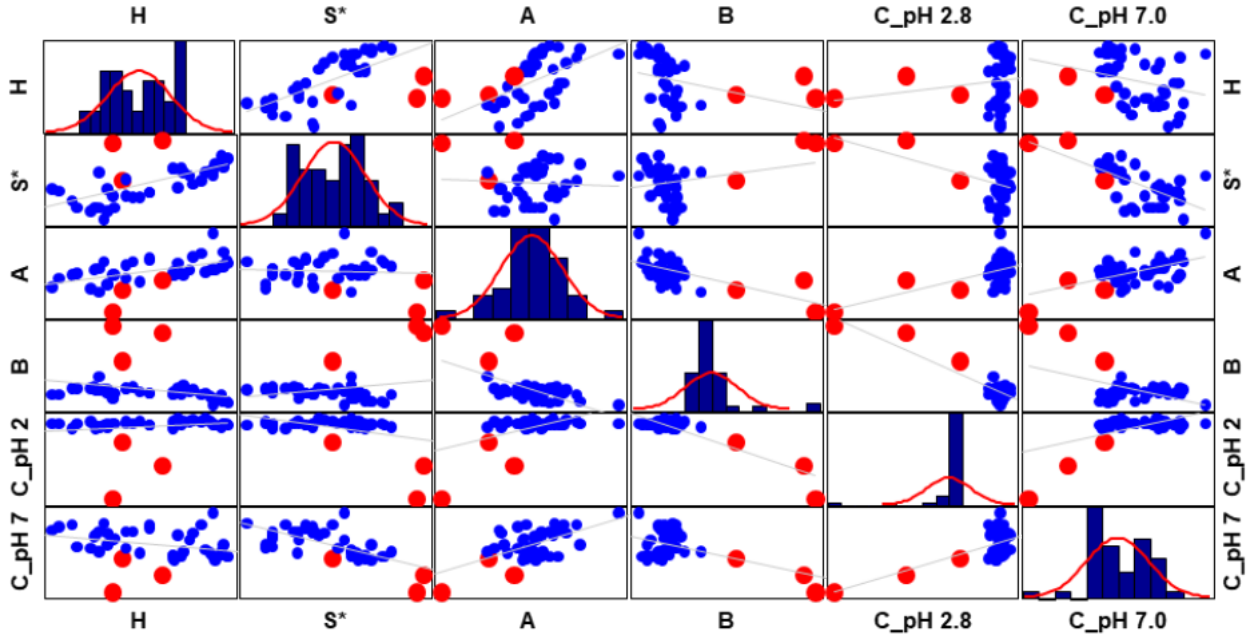

Figure 1: Scatterplot for all objects (44) and six of the seven variables. The red dots are objects (columns) that "disrupt" the correlation between variables.

As seen in Figure 1, there are three columns that disrupt the correlation between variables.

If these three extreme columns are removed from the scatterplot, it is seen that there are more clear correlations between some of the variables (Figure 2). Especially, H and S are highly correlated.

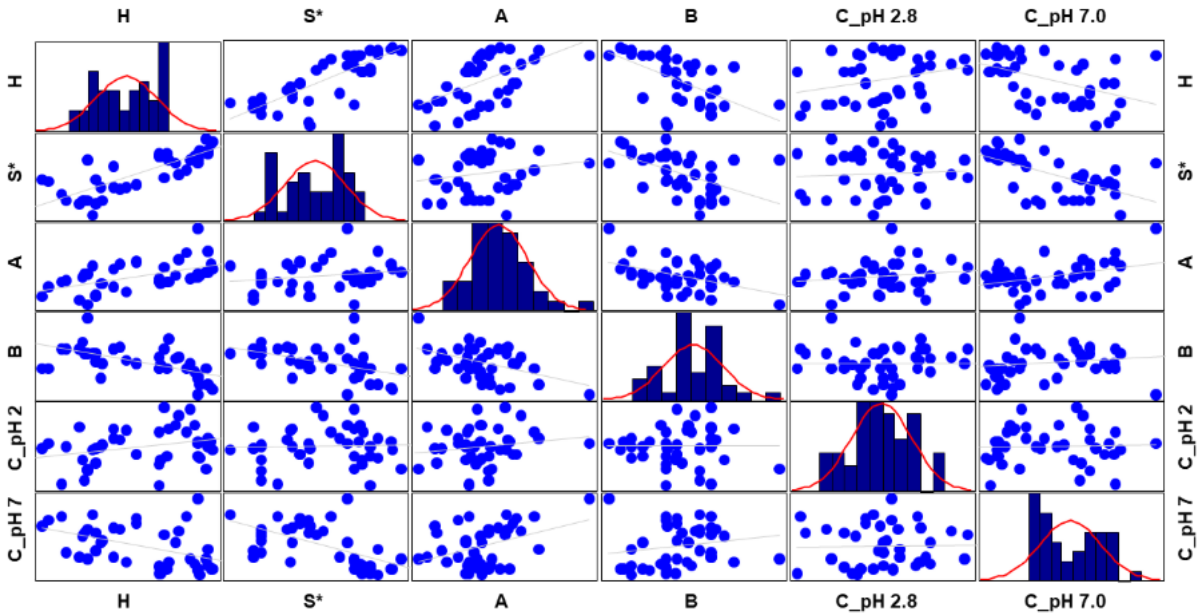

Figure 2: Scatterplot for objects (41) where the "extremes" identified from figure 1 is removed.

Looking at the raw data where the selected columns by “normal” selection is highlighted in green (Figure 3), it is already here clear that especially the parameters A, B and C are of strong importance when expanding the XXXXXXXX.

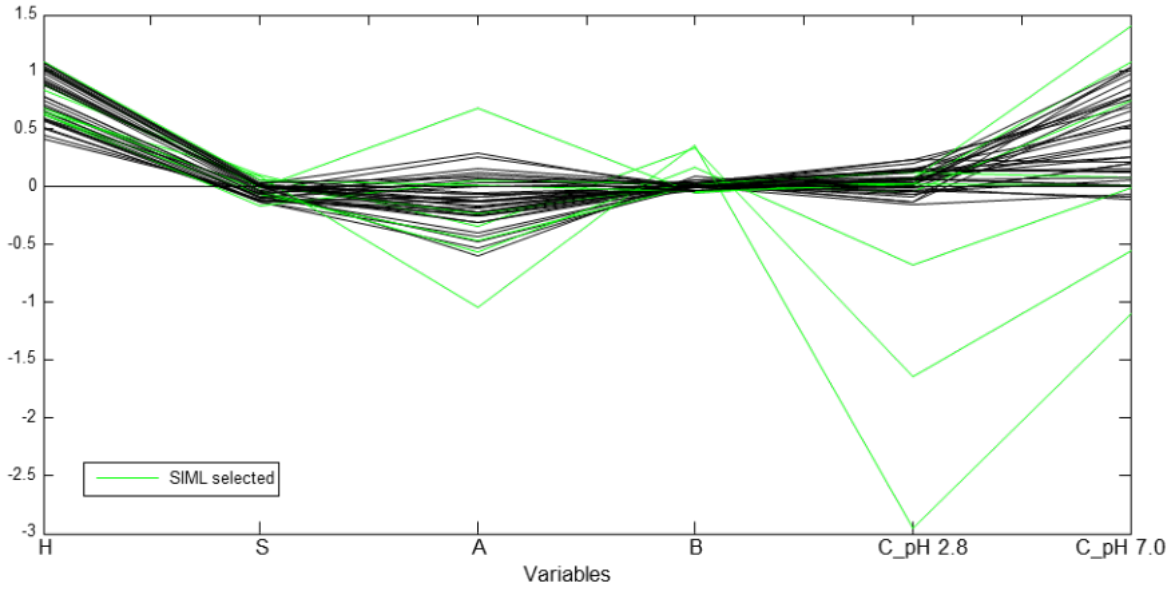

Figure 3: Raw data with selected columns highlighted in green

Running the PCA model with autoscaled data and full validation for all 44 columns, we get the bi-plot seen in figure 4.

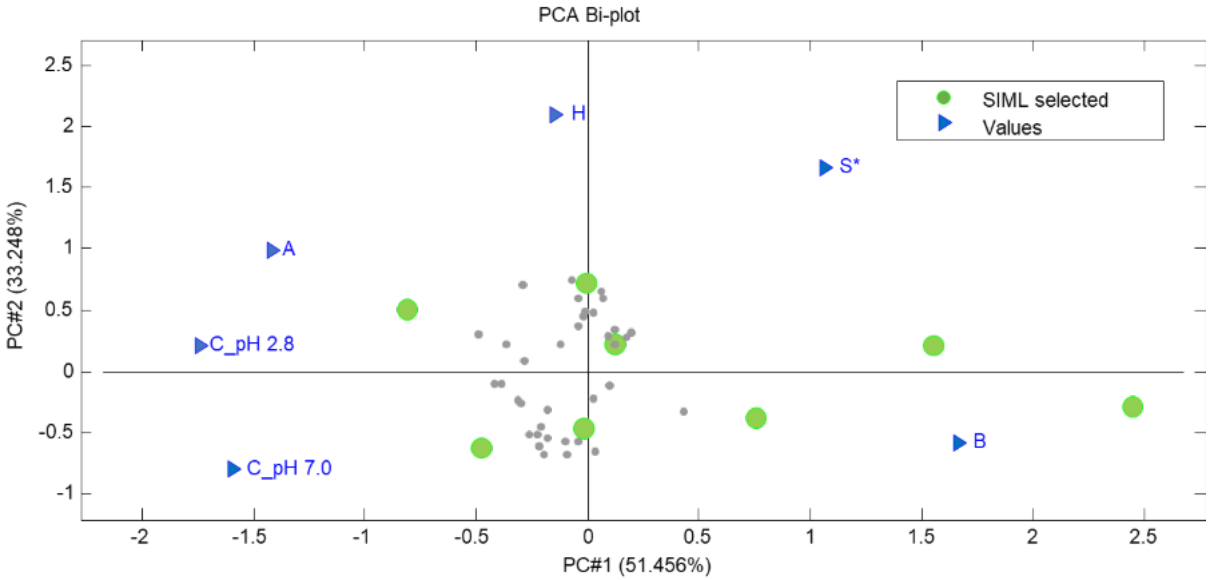

Figure 4: Bi-plot for all objects. The green dots are the columns that is identified as representative columns by SIML.

3.3 Benyttede stof-mix'es

Samtlige stoffer med tilhørende data kan ses i regnearket *Valg af stoffer til FoU projekt* på Sharepoint:

valg af stoffer til FoU projekt.xlsx

Baggrund for kombination af stoffer i de 12 mixes kan ses i regnearket *Kombination af blandinger 2* på Sharepoint:

kombinationer af blandinger2.xlsx

Forventede MZ for de 12 mixes kan ses i regnearket *Expected MZ for the 12 mixes* på Sharepoint: Expected MZ for the 12 mixes.xlsx

Norman Network kalibranter med tilhørende data kan ses i regnearket *Norman Netword Calibrants* på Sharepoint: Norman Network Calibrants.xlsx

3.3.1 Mix A

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 4	50	10
13751-ME5	100	5
13900-0050-100ME5	100	5
18011-MEWS5	100	5
AAR-001-100AN5	100	5
AAR-016-W100ME5	100	5
13900-0080-100ME5	100	5
13900-0100-100ME5	100	5
13900-0105-100ME5	100	5
13900-0185-100ME5	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	75
	Added volume of acetonitrile	25

3.3.2 Mix B

Mix B

Mix B.txt

```
name    smiles
Histamine-2HCl  NCCc1c[nH]cn1
Methomyl    CNC(=O)ON=C(C)SC
Metolcarb   CN=C(O)Oc1cccc(C)c1
Propamocarb free base   CCCOC(=O)NCCCN(C)C
Aldicarb    CNC(=O)ON=CC(C)(C)SC
Carbendazim COC(=O)Nc1nc2ccccc2[nH]1
Isoprocarb  CNC(=O)Oc1ccccc1C(C)C
Carbaryl    CNC(=O)Oc1cccc2ccccc12
Aldicarb-sulfoxide  CNC(=O)ON=CC(C)(C)[S+](C)[O-]
Fenobucarb  CCC(C)c1ccccc1OC(=O)NC
Promecarb   CNC(=O)Oc1cc(C)cc(C(C)C)c1
Propoxur    CNC(=O)Oc1ccccc1OC(C)C
Chlorpropham    CC(C)OC(=O)Nc1cccc(Cl)c1
Oxamyl  CNC(=O)ON=C(SC)C(=O)N(C)C
Carbofuran  CNC(=O)Oc1cccc2c1OC(C)(C)C2
Aldicarb-sulfone    CNC(=O)ON=CC(C)(C)S(C)(=O)=O
Bendiocarb  CNC(=O)Oc1cccc2c1OC(C)(C)O2
Pirimicarb-desmethyl    CNc1nc(C)c(C)c(OC(=O)N(C)C)n1
Methiocarb  CNC(=O)Oc1cc(C)c(SC)c(C)c1
Carbofuran-3-hydroxy    CNC(=O)Oc1cccc2c1OC(C)(C)C2O
Pirimicarb  Cc1nc(N(C)C)nc(OC(=O)N(C)C)c1C
Methiocarb sulfoxide    CNC(=O)Oc1cc(C)c([S+](C)[O-])c(C)c1
Prosulfocarb    CCCN(CCC)C(=O)SCc1ccccc1
Pirimicarb-desmethyl-formamido  Cc1nc(N(C)C=O)nc(OC(=O)N(C)C)c1C
Fenothiocarb    CN(C)C(=O)SCCCCOc1ccccc1
Methiocarb sulfone  CNC(=O)Oc1cc(C)c(S(C)(=O)=O)c(C)c1
Albendazole CCCSc1ccc2[nH]c(NC(=O)OC)nc2c1
Diethofencarb   CCOc1ccc(NC(=O)OC(C)C)cc1OCC
Estrone C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CCC2=O
Benazolin-ethyl ester   CCOC(=O)Cn1c(=O)sc2cccc(Cl)c21
b-Estradiol C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@H]2O
?-Estradiol C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@H]2O
Oxadixyl    COCC(=O)N(c1c(C)cccc1C)N1CCOC1=O
Estriol C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1C[C@@H](O)[C@@H]2O
Testosterone    C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2O
Phenmedipham    COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1
Fenoxycarb  CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1
Triallate   CC(C)N(C(=O)SCC(Cl)=C(Cl)Cl)C(C)C
Progesterone    CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
Iprovalicarb    Cc1ccc(C(C)NC(=O)[C@@H](NC(=O)OC(C)C)C(C)C)cc1
Sethoxydim  CCCC(=NOCC)C1=C(O)CC(CC(C)SCC)CC1=O
Pencycuron  O=C(Nc1ccccc1)N(Cc1ccc(Cl)cc1)C1CCCC1
Tralkoxydim CCON=C(CC)C1=C(O)CC(c2c(C)cc(C)cc2C)CC1=O
Oxadiargyl  C#CCOc1cc(-n2nc(C(C)(C)C)oc2=O)c(Cl)cc1Cl
Pyridaphenthion CCOP(=S)(OCC)Oc1ccc(=O)n(-c2ccccc2)n1
Corticosterone  C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2C(=O)CO
Phosalone   CCOP(=S)(OCC)SCn1c(=O)oc2cc(Cl)ccc21
Famoxadone  CC1(c2ccc(Oc3ccccc3)cc2)OC(=O)N(Nc2ccccc2)C1=O
Pyraclostrobin  COC(=O)N(OC)c1ccccc1COc1ccn(-c2ccc(Cl)cc2)n1
Chlorantraniliprole CNC(=O)c1cc(Cl)cc(C)c1NC(=O)c1cc(Br)nn1-c1ncccc1Cl
Cefoperazone    CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin   CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H]
Emamectin benzoate  CC[C@H](C)[C@H]1O[C@]2(C=C[C@@H]1C)C[C@@H]1C[C@@H](C/C=C(/C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@H](NC)[C@H](C)O4
[C@]34O)O2
```

3.3.3 Mix C

Mix C

Mix C.txt

```
name    smiles
Histamine-2HCl  NCCc1c[nH]cn1
Pyrimethanil    Cc1cc(C)nc(Nc2ccccc2)n1
Thiabendazole   c1ccc2[nH]c(-c3cscn3)nc2c1
Simazine    CCNc1nc(Cl)nc(NCC)n1
Dinotefuran CNC(=N[N+](=O)[O-])NCC1CCOC1
Simetryn    CCNc1nc(NCC)nc(SC)n1
Metribuzin  CSc1nnc(C(C)(C)C)c(=O)n1N
Atrazine    CCNc1nc(Cl)nc(NC(C)C)n1
2-Diethylaminoethyl Hexanoate   CCCCCC(=O)OCCN(CC)CC
Cimaterol   CC(C)NCC(O)c1ccc(N)c(C#N)c1
Acetamiprid C/C(=N\C#N)N(C)Cc1ccc(Cl)nc1
Cyprodinil  Cc1cc(C2CC2)nc(Nc2ccccc2)n1
Terbutaline CC(C)(C)NCC(O)c1cc(O)cc(O)c1
Ametryn CCNc1nc(NC(C)C)nc(SC)n1
Terbuthylazine  CCNc1nc(Cl)nc(NC(C)(C)C)n1
Cimbuterol  CC(C)(C)NCC(O)c1ccc(N)c(C#N)c1
Salbutamol sulfate  CC(C)(C)NCC(O)c1ccc(O)c(CO)c1
Cyanazine   CCNc1nc(Cl)nc(NC(C)(C)C#N)n1
Prometryn   CSc1nc(NC(C)C)nc(NC(C)C)n1
Clothianidin    CN/C(=N\[N+](=O)[O-])NCc1cnc(Cl)s1
Imidacloprid    O=[N+]([O-])/N=C1\NCCN1Cc1ccc(Cl)nc1
Imidaclothiz    O=[N+]([O-])NC1=NCCN1Cc1cnc(Cl)s1
(E)-Nitenpyram  CCN(Cc1ccc(Cl)nc1)/C(=C/[N+](=O)[O-])NC
Ametoctradin    CCCCCCCCc1c(CC)nc2ncnn2c1N
Clenbuterol hydrochloride   CC(C)(C)NCC(O)c1cc(Cl)c(N)c(Cl)c1
Pendimethalin   CCC(CC)Nc1c([N+](=O)[O-])cc(C)c(C)c1[N+](=O)[O-]
Etrimfos    CCOc1cc(OP(=S)(OC)OC)nc(CC)n1
Triflumizole-amino  CCCOCC(=N)Nc1ccc(Cl)cc1C(F)(F)F
Butralin    CCC(C)Nc1c([N+](=O)[O-])cc(C(C)(C)C)cc1[N+](=O)[O-]
Ractopamine hydrochloride   CC(CCc1ccc(O)cc1)NCC(O)c1ccc(O)cc1
Isoxsuprine hydrochloride   CC(COc1ccccc1)NC(C)C(O)c1ccc(O)cc1
Mabuterol   CC(C)(C)NCC(O)c1cc(Cl)c(N)c(C(F)(F)F)c1
Bupirimate  CCCCc1c(C)nc(NCC)nc1OS(=O)(=O)N(C)C
Bromchlorbuterol hydrochloride  CC(C)(C)NCC(O)c1cc(Cl)c(N)c(Br)c1
Mapenterol hydrochloride    CCC(C)(C)NCC(O)c1cc(Cl)c(N)c(C(F)(F)F)c1
Diclobutrazol   CC(C)(C)[C@H](O)[C@H](Cc1ccc(Cl)cc1Cl)n1cncn1
Fenpyrazamine   C=CCSC(=O)n1c(N)c(-c2ccccc2C)c(=O)n1C(C)C
Flurtamone  CNC1=C(c2cccc(C(F)(F)F)c2)C(=O)C(c2ccccc2)O1
Chlorsulfuron   COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2Cl)n1
Brombuterol hydrochloride   CC(C)(C)NCC(O)c1cc(Br)c(N)c(Br)c1
Amidosulfuron   COc1cc(OC)nc(NC(=O)NS(=O)(=O)N(C)S(C)(=O)=O)n1
Metsulfuron-methyl  COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1
Thifensulfuron-methyl   COC(=O)c1sccc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1
Tribenuron-methyl (technical)   COC(=O)c1ccccc1S(=O)(=O)NC(=O)N(C)c1nc(C)nc(OC)n1
Ethoxysulfuron  CCOc1ccccc1OS(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1
Triasulfuron    COc1nc(C)nc(NC(=O)NS(=O)(=O)c2ccccc2OCCCl)n1
Bensulfuron-methyl  COC(=O)c1ccccc1CS(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1
Pyraoxystrobin  CO/C=C(/C(=O)OC)c1ccccc1COc1cc(-c2ccc(Cl)cc2)nn1C
Cinosulfuron    COCCOc1ccccc1S(=O)(=O)NC(=O)Nc1nc(OC)nc(OC)n1
Pyrazosulfuron-ethyl    CCOC(=O)c1cnn(C)c1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1
Fipronil Sulfide    N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1SC(F)(F)F
Halosulfuron-methyl COC(=O)c1c(Cl)nn(C)c1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1
Tritosulfuron   COc1nc(C(F)(F)F)nc(=NC(O)=NS(=O)(=O)c2ccccc2C(F)(F)F)[nH]1
Propyrisulfuron CCCc1ccc2nc(Cl)c(S(=O)(=O)NC(=O)Nc3nc(OC)cc(OC)n3)n2n1
Metazosulfuron  COc1cc(OC)nc(NC(=O)NS(=O)(=O)c2c(C3=NOC(C)CO3)c(Cl)nn2C)n1
Flucetosulfuron COCC(=O)OC(c1ncccc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1)C(C)F
Triflusulfuron-methyl   COC(=O)c1cccc(C)c1S(=O)(=O)NC(=O)Nc1nc(OCC(F)(F)F)nc(N(C)C)n1
tau-Fluvalinate CC(C)[C@@H](Nc1ccc(C(F)(F)F)cc1Cl)C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
Mesosulfuron-methyl COC(=O)c1ccc(CNS(C)(=O)=O)cc1S(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1
Iodosulfuron-methyl sodium  COC(=O)c1ccc(I)cc1S(=O)(=O)NC(=O)Nc1nc(C)nc(OC)n1
Thifluzamide    Cc1nc(C(F)(F)F)c(C(O)=Nc2c(Br)cc(OC(F)(F)F)cc2Br)s1
Cefoperazone    CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Spinosyn A  CC[C@H]1CCC[C@H](O[C@H]2CC[C@H](N(C)C)[C@@H](C)O2)[C@@H](C)C(=O)C2=C[C@@H]3[C@@H](C=C[C@@H]4C[C@@H](O[C@@H]5O[C@@H](C)[C@H](OC)[C@@H](OC)[C@H]5O
Spinosyn D  CC[C@H]1CCC[C@H](O[C@H]2CC[C@H](N(C)C)[C@@H](C)O2)[C@@H](C)C(=O)C2=C[C@@H]3[C@@H](C=C(C)[C@@H]4C[C@@H](O[C@@H]5O[C@@H](C)[C@H](OC)[C@@H](OC)[C@H
Rifaximin   CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)
```

3.3.4 Mix D

Mix D

Mix D.txt

```
name	smiles
o-Toluidine Cc1ccccc1N
Histamine-2HCl	NCCc1c[nH]cn1
2,4-Dimethylaniline Cc1ccc(N)c(C)c1
2,6-Dimethylaniline Cc1cccc(C)c1N
2,4-Diaminotoluene	Cc1ccc(N)cc1N
2-Anisidine (2-Methoxyaniline)	COc1ccccc1N
4-Chloroaniline Nc1ccc(Cl)cc1
2,4,5-Trimethylaniline	Cc1cc(C)c(N)cc1C
2-Methoxy-5-methylaniline	COc1ccc(C)cc1N
4-Methoxy-1,3-phenylenediamine (2,4-Diaminoanisole) COc1ccc(N)cc1N
4-Chloro-2-methylaniline (4-Chloro-o-toluidine) Cc1cc(Cl)ccc1N
2-Aminonaphthalene	Nc1ccc2ccccc2c1
2-Amino-4-nitrotoluene (2-Methyl-5-nitroaniline)	Cc1ccc([N+](=O)[O-])cc1N
4-Aminobiphenyl Nc1ccc(-c2ccccc2)cc1
Acephate	COP(=O)(NC(C)=O)SC
4,4'-Benzidine	Nc1ccc(-c2ccc(N)cc2)cc1
4-Aminoazobenzene	Nc1ccc(N=Nc2ccccc2)cc1
Bis-(4-aminophenyl)methane	Nc1ccc(Cc2ccc(N)cc2)cc1
4-Aminophenylether (4,4'-Oxydianiline)	Nc1ccc(Oc2ccc(N)cc2)cc1
3,3'-Dimethylbenzidine (o-Tolidine) Cc1cc(-c2ccc(N)c(C)c2)ccc1N
Omethoate	CNC(=O)CSP(=O)(OC)OC
4-Aminophenylthioether (4,4?-Diaminodiphenyl sulfide)	Nc1ccc(Sc2ccc(N)cc2)cc1
Thidiazuron O=C(Nc1ccccc1)Nc1cnns1
4-Amino-2,3-dimethylazobenzene (o-Aminoazotoluene)	Cc1cc(N=Nc2ccccc2C)ccc1N
4,4'-Diamino-3,3'-dimethyldiphenyl methane	Cc1cc(Cc2ccc(N)c(C)c2)ccc1N
Dimethoate	CNC(=O)CSP(=S)(OC)OC
Demeton-S-methyl	CCSCCSP(=O)(OC)OC
Methacrifos COC(=O)/C(C)=C/OP(=S)(OC)OC
Ethoprophos CCCSP(=O)(OCC)SCCC
3,3'-Dimethoxybenzidine COc1cc(-c2ccc(N)c(OC)c2)ccc1N
Demeton-S-methyl sulfoxide	CC[S+]([O-])CCSP(=O)(OC)OC
3,3'-Dichlorobenzidine	Nc1ccc(-c2ccc(N)c(Cl)c2)cc1Cl
Formothion	COP(=S)(OC)SCC(=O)N(C)C=O
Demeton (O+S)	CCOP(=O)(OCC)SCCSCC
Demeton (O+S)	CCOP(=S)(OCC)OCCSCC
Phorate CCOP(=S)(OCC)SCSCC
Demeton-S-methyl sulfone	CCS(=O)(=O)CCSP(=O)(OC)OC
4,4'-Methylene-bis(2-chloroaniline) Nc1ccc(Cc2ccc(N)c(Cl)c2)cc1Cl
Cadusafos	CCOP(=O)(SC(C)CC)SC(C)CC
Disulfoton	CCOP(=S)(OCC)SCCSCC
Demeton-S Sulfoxide CCOP(=O)(OCC)SCC[S+]([O-])CC
Phorate-sulfoxide	CCOP(=S)(OCC)SC[S+]([O-])CC
Fenthion	COP(=S)(OC)Oc1ccc(SC)c(C)c1
Vamidothion CNC(=O)C(C)SCCSP(=O)(OC)OC
Terbufos	CCOP(=S)(OCC)SCSC(C)(C)C
Iprobenfos	CC(C)OP(=O)(OC(C)C)SCc1ccccc1
Isocarbofos COP(N)(=S)Oc1ccccc1C(=O)OC(C)C
Disulfoton-sulfoxide	CCOP(=S)(OCC)SCC[S+]([O-])CC
Disulfoton-oxon-sulfon	CCOP(=O)(OCC)SCCS(=O)(=O)CC
Parathion-ethyl CCOP(=S)(OCC)Oc1ccc([N+](=O)[O-])cc1
Phorate-sulfone CCOP(=S)(OCC)SCS(=O)(=O)CC
Fenthion-sulfoxide	COP(=S)(OC)Oc1ccc([S+](C)[O-])c(C)c1
Quinalphos	CCOP(=S)(OCC)Oc1cnc2ccccc2n1
Phoxim	CCOP(=S)(OCC)ON=C(C#N)c1ccccc1
Tolclofos-methyl	COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl
Phosmetoxon COP(=O)(OC)SCN1C(=O)c2ccccc2C1=O
Methidathion	COc1nn(CSP(=S)(OC)OC)c(=O)s1
Terbufos-sulfoxide	CCOP(=S)(OCC)SC[S+]([O-])C(C)(C)C
Diazinon	CCOP(=S)(OCC)Oc1cc(C)nc(C(C)C)n1
Pirimiphos-methyl	CCN(CC)c1nc(C)cc(OP(=S)(OC)OC)n1
Disulfoton-sulfone	CCOP(=S)(OCC)SCCS(=O)(=O)CC
Fenthion-sulfone	COP(=S)(OC)Oc1ccc(S(C)(=O)=O)c(C)c1
Edifenphos	CCOP(=O)(Sc1ccccc1)Sc1ccccc1
Isazofos	CCOP(=S)(OCC)Oc1nc(Cl)n(C(C)C)n1
Triazophos	CCOP(=S)(OCC)Oc1ncn(-c2ccccc2)n1
Malaoxon	CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC
Phosmet COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O
Phenthoate	CCOC(=O)C(SP(=S)(OC)OC)c1ccccc1
Terbufos-sulfone	CCOP(=S)(OCC)SCS(=O)(=O)C(C)(C)C
Chlorpyrifos-methyl COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl
Sulfotep	CCOP(=S)(OCC)OP(=S)(OCC)OCC
EPN CCOP(=S)(Oc1ccc([N+](=O)[O-])cc1)c1ccccc1
Fensulfothion-sulfone	CCOP(=S)(OCC)Oc1ccc(S(C)(=O)=O)cc1
Malathion	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC
Isofenphos-methyl	COP(=S)(NC(C)C)Oc1ccccc1C(=O)OC(C)C
Chlorpyrifos	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
Coumaphos	CCOP(=S)(OCC)Oc1ccc2c(C)c(Cl)c(=O)oc2c1
Anilofos	COP(=S)(OC)SCC(=O)N(c1ccc(Cl)cc1)C(C)C
Profenofos	CCCSP(=O)(OCC)Oc1ccc(Br)cc1Cl
Ethion	CCOP(=S)(OCC)SCSP(=S)(OCC)OCC
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C

```

3.3.5 Mix E

Mix E

Mix E.txt

```
name	smiles
Trimethylsulfonium (TMS)	C[S+](C)C
Amitrol Nc1nc[nH]n1
Morpholine C1COCCN1
Diethanolamine OCCNCCO
Fosetyl-Al CCO[PH](=O)O
Histamine-2HCl NCCc1c[nH]cn1
N,N-Dimethylsulfamid	CN(C)S(N)(=O)=O
Melamine	Nc1nc(N)nc(N)n1
Cyanuric acid	Oc1nc(O)nc(O)n1
Nereistoxin CN(C)C1CSSC1
Triethanolamine OCCN(CCO)CCO
Methyl-desphenyl chloridazon	Cn1ncc(N)c(Cl)c1=O
Daminozide CN(C)NC(=O)CCC(=O)O
N-alkylpyridinium-3-sulfonate - C1 (1-Methylpyridinium-3-sulfonate) C[n+]1cccc(S(=O)(=O)[O-])c1
Glufosinate CP(=O)(O)CCC(N)C(=O)O
Paraquat dichloride C[n+]1ccc(-c2cc[n+](C)cc2)cc1
N-alkylpyridinium-3-sulfonate - C2 CC[n+]1cccc(S(=O)(=O)[O-])c1
2,6-Dichlorobenzoic acid	O=C(O)c1c(Cl)cccc1Cl
Phthalic acid, bis-methyl ester COC(=O)c1ccccc1C(=O)OC
2-(4-Chlorophenoxy)-propionic acid (4-CPPA) CC(Oc1ccc(Cl)cc1)C(=O)O
N-alkylpyridinium-3-sulfonate - C3 CCC[n+]1cccc(S(=O)(=O)[O-])c1
N-alkylpyridinium-3-sulfonate - C4 CCCC[n+]1cccc(S(=O)(=O)[O-])c1
Diethyl phthalate	CCOC(=O)c1ccccc1C(=O)OCC
N-Acetyl-Glufosinate	CC(=O)NC(CCP(C)(=O)O)C(=O)O
N-alkylpyridinium-3-sulfonate - C5 CCCCC[n+]1cccc(S(=O)(=O)[O-])c1
2,6-Dichlorprop (2,6-DCPP) CC(Oc1c(Cl)cccc1Cl)C(=O)O
N-alkylpyridinium-3-sulfonate - C6 CCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid, bis-allyl ester C=CCOC(=O)c1ccccc1C(=O)OCC=C
Phthalic acid, bis-Isopropylester	CC(C)OC(=O)c1ccccc1C(=O)OC(C)C
Phthalic acid, bis-propyl ester CCCOC(=O)c1ccccc1C(=O)OCCC
Dimethachlor OA COCCN(C(=O)C(=O)O)c1c(C)cccc1C
Propachlor ESA CC(C)N(C(=O)CS(=O)(=O)O)c1ccccc1
N-alkylpyridinium-3-sulfonate - C7 CCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Metalaxyl Metabolite CGA 62826 COCC(=O)N(c1c(C)cccc1C)C(C)C(=O)O
N-alkylpyridinium-3-sulfonate - C8 CCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Metazachlor OA Cc1cccc(C)c1N(Cn1cccn1)C(=O)C(=O)O
Phthalic acid, bis-iso-butyl ester CC(C)COC(=O)c1ccccc1C(=O)OCC(C)C
Dibutyl phthalate	CCCCOC(=O)c1ccccc1C(=O)OCCCC
Phthalic acid, bis-methylglycol ester	COCCOC(=O)c1ccccc1C(=O)OCCOC
N-alkylpyridinium-3-sulfonate - C9 CCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Metalaxyl CGA 108906	COCC(=O)N(c1c(C)cccc1C(=O)O)C(C)C(=O)O
N-alkylpyridinium-3-sulfonate - C10 CCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid, bis-iso-pentyl ester CC(C)CCOC(=O)c1ccccc1C(=O)OCCC(C)C
Phthalic acid, bis-n-pentyl ester	CCCCOC(=O)c1ccccc1C(=O)OCCCCC
Phthalic acid, bis-2-ethoxyethyl ester CCOCCOC(=O)c1ccccc1C(=O)OCCOCC
Phthalic acid, benzylbutyl ester	CCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1
N-alkylpyridinium-3-sulfonate - C11 CCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Alachlor ESA	CCc1cccc(CC)c1N(COC)C(=O)CS(=O)(=O)O
Phthalic acid, bis-phenyl ester O=C(Oc1ccccc1)c1ccccc1C(=O)Oc1ccccc1
Metazachlor ESA Cc1cccc(C)c1N(Cn1cccn1)C(=O)CS(=O)(=O)O
N-alkylpyridinium-3-sulfonate - C12 CCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid, bis-cyclohexyl ester O=C(OC1CCCCC1)c1ccccc1C(=O)OC1CCCCC1
Phthalic acid, bis-4-methyl-2-pentyl ester CC(C)CC(C)OC(=O)c1ccccc1C(=O)OC(C)CC(C)C
Phthalic acid, bis-hexyl ester CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCC
N-alkylpyridinium-3-sulfonate - C13 CCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
N-alkylpyridinium-3-sulfonate - C14 CCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid,bis-n-heptyl ester	CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCC
Phthalic acid,bis-butoxyethyl ester CCCCOCCOC(=O)c1ccccc1C(=O)OCCOCCCC
N-alkylpyridinium-3-sulfonate - C15 CCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
N-alkylpyridinium-3-sulfonate - C16 CCCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid, bis-2-ethylhexyl ester	CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC
Di-n-octyl phthalate	CCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC
N-alkylpyridinium-3-sulfonate - C17 CCCCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
N-alkylpyridinium-3-sulfonate - C18 CCCCCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Diisononyl Phthalate (mixture of branched chain isomers)	CC(C)CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCC(C)C
Phthalic acid, bis-nonyl ester CCCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC
N-alkylpyridinium-3-sulfonate - C19 CCCCCCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
N-alkylpyridinium-3-sulfonate - C20 CCCCCCCCCCCCCCCCCCCC[n+]1cccc(S(=O)(=O)[O-])c1
Phthalic acid, bis-isodecyl ester	CC(C)CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC(C)C
Streptomycin	CN[C@@H]1[C@H](O[C@H]2[C@H](O[C@H]3[C@H](O)[C@@H](O)[C@H](NC(=N)N)[C@@H](O)[C@@H]3NC(=N)N)O[C@@H](C)[C@]2(O)C=O)O[C@@H](CO)[C@H](O)[C@H]1O
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C
```

3.3.6 Mix F

Mix F

Mix F.txt

```
name	smiles
Amitrole	Nc1nc[nH]n1
Guanylurea-HCl	N=C(N)NC(N)=O
HISTAMINE-2HCL	NCCc1c[nH]cn1
Benzoic acid	O=C(O)c1ccccc1
CHLORMEQUAT-CHLORIDE	C[N+](C)(C)CCC1
SALICYLIC ACID	O=C(O)c1ccccc1O
Valproic acid	CCCC(CCC)C(=O)O
BUTOCARBOXIM	CNC(=O)ON=C(C)C(C)SC
MCPA	Cc1cc(Cl)ccc1OCC(=O)O
Ethirimol	CCCCc1c(C)nc(NCC)nc1O
Sulfacetamide	CC(=O)NS(=O)(=O)c1ccc(N)cc1
Sulfaguanidine	N=C(N)NS(=O)(=O)c1ccc(N)cc1
Cyazofamid-dessulfonamide	Cc1ccc(-c2[nH]c(C#N)nc2Cl)cc1
Dichlorvos	COP(=O)(OC)OC=C(Cl)Cl
Chloridazon	Nc1cnn(-c2ccccc2)c(=O)c1Cl
Flonicamid	N#CCNC(=O)c1cncccc1C(F)(F)F
Carboxin	CC1=C(C(=O)Nc2ccccc2)SCCO1
Dicrotophos	COP(=O)(OC)O/C(C)=C/C(=O)N(C)C
Busan (TCMTB)	N#CSCSc1nc2ccccc2s1
Clomazone	CC1(C)CON(Cc2ccccc2Cl)C1=O
DINOTERB	CC(C)(C)c1ccc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Sulfapyridine	Nc1ccc(S(=O)(=O)Nc2ccccn2)cc1
Sulfadiazine	Nc1ccc(S(=O)(=O)Nc2ncccn2)cc1
Phenytoin (5,5-Diphenylhydantoin)	O=C1NC(=O)C(c2ccccc2)(c2ccccc2)N1
Sulfamethoxazole	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)no1
Sulfathiazole	Nc1ccc(S(=O)(=O)Nc2nccs2)cc1
Sulfamerazine	Cc1ccnc(NS(=O)(=O)c2ccc(N)cc2)n1
Sulfamoxol	Cc1nc(NS(=O)(=O)c2ccc(N)cc2)oc1C
Sulfisoxazole	Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C
Acetochlor	CCOCN(C(=O)CCl)c1c(C)cccc1CC
Alachlor	CCc1cccc(CC)c1N(COC)C(=O)CCl
Sulfamethizole	Cc1nnc(NS(=O)(=O)c2ccc(N)cc2)s1
BROMOXYNIL	N#Cc1cc(Br)c(O)c(Br)c1
Dimethenamid	COCC(C)N(CC(=O)CCl)c1c(C)csc1C
Sulfabenzamide	Nc1ccc(S(=O)(=O)NC(=O)c2ccccc2)cc1
Sulfadimidine	Cc1cc(C)nc(NS(=O)(=O)c2ccc(N)cc2)n1
Sulfisomidine	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(C)n1
Sulfameter	COc1cnc(NS(=O)(=O)c2ccc(N)cc2)nc1
Sulfamethoxypyridazine	COc1ccc(NS(=O)(=O)c2ccc(N)cc2)nn1
Sulfamonomethoxine	COc1cc(NS(=O)(=O)c2ccc(N)cc2)ncn1
Sulfachloropyridazine	Nc1ccc(S(=O)(=O)Nc2ccc(Cl)nn2)cc1
TRICLOSAN	Oc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl
Trimethoprim	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC
Fensulfothion-oxon	CCOP(=O)(OCC)Oc1ccc([S+](C)[O-])cc1
Sulfaquinoxaline	Nc1ccc(S(=O)(=O)Nc2cnc3ccccc3n2)cc1
Fenhexamid	CC1(C(=O)Nc2ccc(O)c(Cl)c2Cl)CCCCC1
Fensulfothion	CCOP(=S)(OCC)Oc1ccc([S+](C)[O-])cc1
Fensulfothion-oxon-sulfone	CCOP(=O)(OCC)Oc1ccc(S(C)(=O)=O)cc1
Sulfadimethoxine	COc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(OC)n1
Sulfadoxine	COc1cncnc(NS(=O)(=O)c2ccc(N)cc2)c1OC
Fenamidone	CSC1=N[C@@](C)(c2ccccc2)C(=O)N1Nc1ccccc1
Butachlor	CCCCOCN(C(=O)CCl)c1c(CC)cccc1CC
Sulfaphenazole	Nc1ccc(S(=O)(=O)Nc2ccnn2-c2ccccc2)cc1
Azinphos-methyl	COP(=S)(OC)SCn1nnc2ccccc2c1=O
FLAMPROP	CC(C(=O)O)N(C(=O)c1ccccc1)c1ccc(F)c(Cl)c1
Benodanil	O=C(Nc1ccccc1)c1ccccc1I
Cyazofamid	Cc1ccc(-c2c(Cl)nc(C#N)n2S(=O)(=O)N(C)C)cc1
Flumetsulam	Cc1ccn2nc(S(=O)(=O)Nc3c(F)cccc3F)nc2n1
Benalaxyl	COC(=O)C(C)N(C(=O)Cc1ccccc1)c1c(C)cccc1C
Dimoxystrobin	CNC(=O)/C(=N/OC)c1ccccc1COc1ccc(C)ccc1C
Fenoxanil	CC(Oc1ccc(Cl)cc1Cl)C(O)=NC(C)(C#N)C(C)C
Sulfanitran	CC(=O)Nc1ccc(S(=O)(=O)Nc2ccc([N+](=O)[O-])cc2)cc1
INABENFIDE	O=C(Nc1ccc(Cl)cc1C(O)c1ccccc1)c1ccncc1
TEPRALOXYDIM	CCC(=NOC/C=C/Cl)C1=C(O)CC(C2CCOCC2)CC1=O
Boscalid	O=C(Nc1ccccc1-c1ccc(Cl)cc1)c1ccccnc1Cl
Florasulam	COc1ncc(F)c2nc(S(=O)(=O)Nc3c(F)cccc3F)nn12
Flufenacet	CC(C)N(C(=O)COc1nnc(C(F)(F)F)s1)c1ccc(F)cc1
Benzoximate	CCON=C(OC(=O)c1ccccc1)c1c(OC)ccc(Cl)c1OC
Flumorph	COc1ccc(C(=CC(=O)N2CCOCC2)c2ccc(F)cc2)cc1OC
Fluopicolide	O=C(NCc1ncc(C(F)(F)F)cc1Cl)c1c(Cl)cccc1Cl
Dimethomorph	COc1ccc(C(=CC(=O)N2CCOCC2)c2ccc(Cl)cc2)cc1OC
Clethodim Sulfone	CC/C(=N\OC/C=C/Cl)C1=C(O)CC(CC(C)S(=O)(=O)CC)CC1=O
Diflufenican	O=C(Nc1ccc(F)cc1F)c1cccnc1Oc1cccc(C(F)(F)F)c1
Chromafenozide	Cc1cc(C)cc(C(=O)N(NC(=O)c2ccc3c(c2C)CCCO3)C(C)(C)C)c1
Ethiprole	CC[S+]([O-])c1c(C#N)nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c1N
Fluopyram	O=C(NCCc1ncc(C(F)(F)F)cc1Cl)c1ccccc1C(F)(F)F
Benzovindiflupyr	Cn1cc(C(=O)Nc2cccc3c2C2CCC3C2=C(Cl)Cl)c(C(F)F)n1
Cyflufenamid	O=C(/C(=N\OCC1CC1)c1c(C(F)(F)F)ccc(F)c1F
Fenaminostrobin	CN=C(O)/C(=N/OC)c1ccccc1CO/N=C(/C)/C=C/c1c(Cl)cccc1Cl
Fipronil	N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1[S+]([O-])C(F)(F)F
Fipronil Sulfone	N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1S(=O)(=O)C(F)(F)F
Amisulbrom	Cc1c(Br)c2ccc(F)cc2n1S(=O)(=O)c1ncn(S(=O)(=O)N(C)C)n1
Cyantraniliprole	CNC(=O)c1ccc(C#N)cc(C)c1NC(=O)c1cc(Br)nn1-c1ccccc1Cl
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Flubendiamide	Cc1cc(C(F)(C(F)(F)F)C(F)(F)F)ccc1NC(=O)c1cccc(I)c1C(=O)NC(C)(C)CS(C)(=O)=O
Nigericin sodium salt	CO[C@@H]1C[C@@H](C[C@H]2CC[C@H](C)[C@H]([C@@H](C)C(=O)O)O2)O[C@]2(O[C@](C)([C@H]3CC[C@@](C)([C@@H]4O[C@@H]([C@H]5O[C@@](O)(CO)[C@H](C)C[C@@H]5C)C[C@@H]4C)O3)C[C@H]2C)[C@@H]1C
SALINOMYCIN	CC[C@@H](C(=O)[C@@H](C)[C@@H](O)[C@H](C)[C@@H]1O[C@@H]([C@@H](CC)C(=O)O)CC[C@@H]1C)[C@H]1O[C@]2(C=C[C@@H](O)[C@]3(CC[C@@](C)([C@H]4CC[C@](O)(CC)[C@H](C)O4)O3)O2)[C@H](C)C[C@@H]1C
RIFAXIMIN	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6ccc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
EMAMECTIN	CC[C@H](C)[C@H]1O[C@]2(C=C[C@@H]1C)C[C@@H]1C[C@@H](C/C=C(/C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@H](NC)[C@H](C)O4)[C@H](C)O3)[C@@H](C)/C=C/C=C3/CO[C@@H]4[C@H](O)C(C)=C[C@@H](C(=O)O1)[
TYLOSIN	CC[C@H]1OC(=O)C[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)[C@@H](O[C@H]3C[C@](C)(O)[C@@H](O)[C@H](C)O3)[C@H](N(C)C)[C@H]2O)[C@@H](CC=O)C[C@@H](C)C(=O)/C=C/C(C)=C\[C@H]1CO[C@@H]1O[C@H](C)[C@@H](O)[C@H]
Vancomycin	CN[C@H](CC(C)C)C(=O)N[C@H]1C(=O)N[C@@H](CC(N)=O)C(=O)N[C@H]2C(=O)N[C@H]3C(=O)N[C@H](C(=O)N[C@H](C(=O)O)c4cc(O)cc(O)c4-c4cc3ccc4O)[C@H](O)c3ccc(c(Cl)c3)Oc3cc2cc(c30[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)
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3.3.7 Mix G

Mix G

Mix G.txt

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name	smiles
Histamine-2HCl	NCCc1c[nH]cn1
1H-Benzotriazole	c1ccc2[nH]nnc2c1
5-Methyl-1H-benzotriazole	Cc1ccc2[nH]nnc2c1
4-Methyl-1H-benzotriazole	Cc1cccc2nn[nH]c12
Methamidophos	COP(N)(=O)SC
Oxamyl-oxime	CSC(=NO)C(=O)N(C)C
Acesulfame K	CC1=CC(=O)NS(=O)(=O)O1
Saccharin	O=C1NS(=O)(=O)c2ccccc21
Metamitron	Cc1nnc(-c2ccccc2)c(=O)n1N
4-tert-Octylphenol	CC(C)(C)CC(C)(C)c1ccc(O)cc1
Propachlor	CC(C)N(C(=O)CCl)c1ccccc1
Propanil	CCC(=O)Nc1ccc(Cl)c(Cl)c1
4-nonylphenol	CCCCCCCCCc1ccc(O)cc1
Probenazole	C=CCOC1=NS(=O)(=O)c2ccccc21
Monocrotophos	CNC(=O)/C=C(\C)OP(=O)(OC)OC
Mevinphos	COC(=O)C=C(C)OP(=O)(OC)OC
Bisphenol A	CC(C)(c1ccc(O)cc1)c1ccc(O)cc1
Fonofos	CCOP(=S)(CC)Sc1ccccc1
Heptenophos	COP(=O)(OC)OC1=C(Cl)C2C=CCC12
Hexazinone	CN(C)c1nc(=O)n(C2CCCCC2)c(=O)n1C
Propyzamide	C#CC(C)(C)NC(=O)c1cc(Cl)cc(Cl)c1
Silthiofam	C=CCNC(=O)c1c([Si](C)(C)C)sc(C)c1C
Mepronil	Cc1ccccc1C(=O)Nc1ccccc(OC(C)C)c1
Napropamide	CCN(CC)C(=O)C(C)Oc1cccc2ccccc12
Sulfoxaflor	CC(c1ccc(C(F)(F)F)nc1)S(C)(=O)=NC#N
Metalaxyl	COCC(=O)N(c1c(C)cccc1C)C(C)C(=O)OC
S-Metolachlor	CCc1cccc(C)c1N(C(=O)CCl)[C@@H](C)COC
Propisochlor	CCc1cccc(C)c1N(COC(C)C)C(=O)CCl
Mefenacet	CN(C(=O)COc1nc2ccccc2s1)c1ccccc1
Phosphamidon	CCN(CC)C(=O)C(Cl)=C(C)OP(=O)(OC)OC
Spirotetramat-mono-hydroxy	CO[C@H]1CC[C@]2(CC1)NC(=O)C(c1cc(C)ccc1C)C2O
Pretilachlor	CCCOCCN(C(=O)CCl)c1c(CC)cccc1CC
Spirotetramat-keto-hydroxy	CO[C@H]1CC[C@]2(CC1)NC(=O)C(O)(c1cc(C)ccc1C)C2=O
Penflufen	Cc1nn(C)c(F)c1C(=O)Nc1ccccc1C(C)CC(C)C
Flutolanil	CC(C)Oc1cccc(NC(=O)c2ccccc2C(F)(F)F)c1
Iprodione	CC(C)NC(=O)N1CC(=O)N(c2cc(Cl)cc(Cl)c2)C1=O
Sedaxane	Cn1cc(C(=O)Nc2ccccc2C2CC2C2CC2)c(C(F)F)n1
Zoxamide	CCC(C)(NC(=O)c1ccc(Cl)c(C)c(Cl)c1)C(=O)CCl
Tebufenozide	CCc1ccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)cc1
Isoxaflutole	CS(=O)(=O)c1ccc(C(F)(F)F)ccc1C(=O)c1cnoc1C1CC1
Penthiopyrad	CC(C)CC(C)c1sccc1NC(=O)c1cn(C)nc1C(F)(F)F
Isopyrazam	CC(C)C1C2CCC1c1c(N=C(O)c3cn(C)nc3C(F)F)cccc12
Pyridaben	CC(C)(C)c1ccc(CSc2cnn(C(C)(C)C)c(=O)c2Cl)cc1
Methoxyfenozide	COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C
Proquinazid	CCCOc1nc2ccc(I)cc2c(=O)n1CCC
Spirotetramat	CCOC(=O)OC1=C(c2cc(C)ccc2C)C(=O)N[C@]12CC[C@@H](OC)CC2
Oxaziclomefone	CC1=C(c2ccccc2)C(=O)N(C(C)(C)c2cc(Cl)cc(Cl)c2)CO1
Picolinafen	O=C(Nc1ccc(F)cc1)c1cccc(Oc2cccc(C(F)(F)F)c2)n1
Fluxapyroxad	Cn1cc(C(=O)Nc2ccccc2-c2cc(F)c(F)c(F)c2)c(C(F)F)n1
Tolfenpyrad	CCc1nn(C)c(C(=O)NCc2ccc(Oc3ccc(C)cc3)cc2)c1Cl
Pyrimorph	CC(C)(C)c1cccc(/C(=C\C(=O)C2CNCCO2)c2ccnc(Cl)c2)cc1
Sucralose	OC[C@H]1O[C@H](O[C@]2(CCl)O[C@H](CCl)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1Cl
Fluthiacet-methyl	COC(=O)CSc1cc(N=c2sc(=O)n3n2CCCC3)c(F)cc1Cl
Mandipropamid	C#CCOc1ccc(CCNC(=O)C(OCC#C)c2ccc(Cl)cc2)cc1OC
Metamifop	C[C@H](Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1)C(=O)N(C)c1ccccc1F
Spirotetramat-enol-glucoside	CO[C@H]1CC[C@]2(CC1)NC(=O)C(c1cc(C)ccc1C)=C2O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H](O)[C@H]1O
Penoxsulam	COc1cnc(OC)n2nc(NS(=O)(=O)c3c(OCC(F)F)cccc3C(F)(F)F)nc12
Saflufenacil	CC(C)N(C)S(=O)(=O)NC(=O)c1ccc(-n2c(=O)cc(C(F)(F)F)n(C)c2=O)c(F)cc1Cl
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C

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3.3.8 Mix H:

Mix H

Mix H.txt

	name	smiles
1	Bromomethane	CBr
2	1,2-Dichloroethane	ClCCCl
3	m-Toluidine	Cc1cccc(N)c1
4	3-Methylphenol (m-Cresol)	Cc1cccc(O)c1
5	o-cresol	Cc1ccccc1O
6	1,3-Dichloropropene	ClC=CCCl
7	Histamine-2HCl	NCCc1c[nH]cn1
8	1,2-Dichloropropane	CC(Cl)CCl
9	Chlorobenzene	Clc1ccccc1
10	2,2-Dichloroethanol	OCC(Cl)Cl
11	3,5-dimethylphenol	Cc1cc(C)cc(O)c1
12	3,4-dimethylphenol	Cc1ccc(O)cc1C
13	2,6-dimethylphenol	Cc1cccc(C)c1O
14	2,3-dimethylphenol	Cc1cccc(O)c1C
15	3-chloroaniline	Nc1cccc(Cl)c1
16	Di-n-butylamine	CCCCNCCCC
17	2-Ethyl-6-methylaniline	CCc1cccc(C)c1N
18	4-Amino-2-chlorotoluene	Cc1ccc(N)cc1Cl
19	2-amino-5-chlorophenol	Nc1ccc(Cl)cc1O
20	2-Isopropoxyphenol	CC(C)Oc1ccccc1O
21	3,5-diclorophenol	Oc1cc(Cl)cc(Cl)c1
22	Chlorpicrin	O=[N+]([O-])C(Cl)(Cl)Cl
23	3-methyl-4-nitroanisole	COc1ccc([N+](=O)[O-])c(C)c1
24	4-Phenylphenol	Oc1ccc(-c2ccccc2)cc1
25	2,4-Dichloroanisole	COc1ccc(Cl)cc1Cl
26	1,2,3,5-tetrachlorobenzene	Clc1cc(Cl)c(Cl)c(Cl)c1
27	2,4-dichlorobenzophenone	O=C(c1ccccc1)c1ccc(Cl)cc1Cl
28	Thiacloprid	N#C/N=C1\SCCN1Cc1ccc(Cl)nc1
29	Pentachloroaniline	Nc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
30	Pentachloroanisole	COc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
31	Myclobutanil	CCCCC(C#N)(Cn1cncn1)c1ccc(Cl)cc1
32	Isoprothiolane	CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1
33	Thiamethoxam	CN1COCN(Cc2cnc(Cl)s2)C1=N[N+](=O)[O-]
34	Cyproconazole	CC(C1CC1)C(O)(Cn1cncn1)c1cccc(Cl)cc1
35	Triadimenol	CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n1cncn1
36	Tebuconazole	CC(C)(C)C(O)(CCc1ccc(Cl)cc1)Cn1cncn1
37	Methoprene	COC(C)(C)CCCC(C)C/C=C/C(C)=C/C(=O)OC(C)C
38	Kresoxim-methyl	CO/N=C(/C(=O)OC)c1ccccc1COc1ccccc1C
39	Pyriftalid	COc1cc(OC)nc(Sc2ccccc3c2C(=O)OC3C)n1
40	Pyriproxyfen	CC(COc1ccc(Oc2ccccc2)cc1)Oc1ccccn1
41	Diniconazole	CC(C)(C)C(O)/C(=C\c1ccc(Cl)cc1Cl)n1cncn1
42	Cycloxydim	CCCC(=NOCC)C1=C(O)CC(C2CCCSC2)CC1=O
43	Pyrethrin 1	C=C/C=C\CC1=C(C)[C@@H](OC(=O)[C@@H]2[C@@H](C=C(C)C)C2(C)C)CC1=O
44	Epoxiconazole	Fc1ccc([C@@]2(Cn3cncn3)O[C@@H]2c2ccccc2Cl)cc1
45	Bitertanol	CC(C)(C)C(O)C(Oc1ccc(-c2ccccc2)cc1)n1cncn1
46	Bioresmethrin	CC(C)=C[C@@H]1[C@@H](C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C
47	Piperonyl butoxide	CCCCOCCOCCOCc1cc2c(cc1CCC)OCO2
48	Diclofop methyl	COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1
49	Oxadiazon	CC(C)Oc1cc(-n2nc(C(C)(C)C)oc2=O)c(Cl)cc1Cl
50	Fenpropathrin	CC1(C)C(C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2)C1(C)C
51	Propargite	C#CCOS(=O)OC1CCCCC1Oc1ccc(C(C)(C)C)cc1
52	Etoxazole	CCOc1cc(C(C)(C)C)ccc1C1COC(c2c(F)cccc2F)=N1
53	Dinocap	C/C=C/C(=O)Oc1c(C(C)CCCCCC)cc([N+](=O)[O-])cc1[N+](=O)[O-]
54	Picoxystrobin	CO/C=C(/C(=O)OC)c1ccccc1COc1cccc(C(F)(F)F)n1
55	Spiromesifen	Cc1cc(C)c(C2=C(OC(=O)CC(C)(C)C)C3(CCCC3)OC2=O)c(C)c1
56	Quizalofop-ethyl	CCOC(=O)C(C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1
57	Etofenprox	CCOc1ccc(C(C)(C)COCc2cccc(Oc3ccccc3)c2)cc1
58	Fluazifop-butyl	CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(C(F)(F)F)cn2)cc1
59	Permethrin	CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc1cccc(Oc2ccccc2)c1
60	Rotenone	C=C(C)[C@H]1Cc2c(ccc3c2O[C@@H]2COc4cc(OC)c(OC)cc4[C@@H]2C3=O)O1
61	Enoxastrobin	CO/C=C(/C(=O)OC)c1ccccc1CO/N=C(C)/C=C/c1ccc(Cl)cc1
62	Azoxystrobin	CO/C=C(/C(=O)OC)c1ccccc1Oc1ccc(Oc2ccccc2C#N)ncn1
63	Difenoconazole	CC1COC(C#Cn2cncn2)(c2ccc(Oc3ccc(Cl)cc3)cc2Cl)O1
64	Spirodiclofen	CCC(C)(C)C(=O)OC1=C(c2ccc(Cl)cc2Cl)C(=O)OC12CCCCC2
65	Pyraflufen-ethyl	CCOC(=O)COc1cc(-c2nn(C)c(OC(F)F)c2Cl)c(F)cc1Cl
66	Fenvalerate	CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c1ccc(Cl)cc1
67	(E)-Fenpyroximate	Cc1nn(C)c(Oc2ccccc2)c1/C=N/OCc1ccc(C(=O)OC(C)(C)C)cc1
68	Bifenthrin	Cc1c(COC(=O)[C@@H]2[C@H](/C=C(\Cl)C(F)(F)F)C2(C)C)cccc1-c1ccccc1
69	Coumoxystrobin	CCCCc1c(C)c2ccc(OCc3ccccc3/C(=C\OC)C(=O)OC)cc2oc1=O
70	Propaquizafop	CC(C)=NOCCOC(=O)[C@@H](C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1
71	Fluroglycofen-ethyl	CCOC(=O)C(C)OC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
72	Lactofen	CCOC(=O)C(C)OC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
73	Deltamethrin	CC1(C)[C@H](C(=O)O[C@H](C#N)c2cccc(Oc3ccccc3)c2)[C@@H]1C=C(Br)Br
74	Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
75	Spinetoram	CCO[C@@H]1[C@@H](OC)[C@H](C)O[C@@H](O[C@@H]2C[C@H]3CC[C@@H]4[C@@H](C=CSC(=O)[C@H](C)[C@@H](O[C@H]5CC[C@H](N(C)C)[C@@H](C)O5)CCC[C@H](CC)OC(=O)C[C@H]54)[C@@H]3C2)[C@@H]1OC
76	Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6ccc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
77	Ivermectin	CC[C@H](C)[C@H]1O[C@]2(CC[C@@H]1C)C[C@@H]1C[C@@H](C/C=C(/C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@@H](O)[C@H](C)O4)[C@H](C)O3)[C@@H](C)/C=C/C=C3\CO[C@@H]4[C@H](O)C(C)=C[C@@H](C(=O)O1)[C@]34O)O2
78	2,3-Dimethylphenol	CC1=C(C)C=CC=C1O
79		

3.3.9 Mix I:

Mix I

Mix I.txt

```
name	smiles
Histamine-2HCl	NCCc1c[nH]cn1
4-Nitroimidazole	O=[N+]([O-])c1c[nH]cn1
2-Methyl-4-nitroimidazole	Cc1ncc([N+](=O)[O-])[nH]1
Dimetridazole	Cc1ncc([N+](=O)[O-])n1C
Dimetridazole-2-hydroxy Cn1c(CO)ncc1[N+](=O)[O-]
5-Chloro-1-Methyl-4-Nitroimidazole	Cn1cnc([N+](=O)[O-])c1Cl
5-Nitrobenzimidazole	O=[N+]([O-])c1ccc2[nH]cnc2c1
Ipronidazole	CC(C)c1ncc([N+](=O)[O-])n1C
Metronidazole	Cc1ncc([N+](=O)[O-])n1CCO
Metronidazole-hydroxy	O=[N+]([O-])c1cnc(CO)n1CCO
Phenazone	Cc1cc(=O)n(-c2ccccc2)n1C
Tricyclazole	Cc1cccc2sc3nncn3c12
Chlordimeform free base Cc1ccc(Cl)ccc1N=CN(C)C
Ronidazole (RNZ)	Cn1c([N+](=O)[O-])cnc1COC(N)=O
Ibuprofen	CC(C)Cc1ccc(C(C)C(=O)O)cc1
Clofibric acid	CC(C)(Oc1ccc(Cl)cc1)C(=O)O
Phenamacril CCOC(=O)C(C#N)=C(N)c1ccccc1
Terbutaline CC(C)(C)NCC(O)c1cc(O)cc(O)c1
Naproxene	COc1ccc2cc([C@H](C)C(=O)O)ccc2c1
Propyphenazone	Cc1c(C(C)C)c(=O)n(-c2ccccc2)n1C
Carbamazepine	NC(=O)N1c2ccccc2C=Cc2ccccc21
Salbutamol	CC(C)(C)NCC(O)c1ccc(O)c(CO)c1
Fludioxonil N#Cc1c[nH]cc1-c1cccc2c1OC(F)(F)O2
Ketoprofen	CC(C(=O)O)c1ccccc1C(=O)c2ccccc2)c1
Trichlorphon	COP(=O)(OC)C(O)C(Cl)(Cl)Cl
Propranolol CC(C)NCC(O)COc1cccc2ccccc12
Atenolol	CC(C)NCC(O)COc1ccc(CC(N)=O)cc1
Metoprolol	COCCc1ccc(OCC(O)CNC(C)C)cc1
Sotalol CC(C)NCC(O)c1ccc(NS(C)(=O)=O)cc1
Fenpropidin CC(Cc1ccc(C(C)(C)C)cc1)CN1CCCCC1
Metazachlor Cc1cccc(C)c1N(Cn1cccn1)C(=O)CCl
Penconazole CCCC(Cn1cncn1)c1ccc(Cl)cc1Cl
Ethofumesate	CCOC1Oc2ccc(OS(C)(=O)=O)cc2C1(C)C
Pyrisoxazole	CN1OC(c2ccc(Cl)cc2)CC1(C)c1cccnc1
Uniconazole CC(C)(C)C(O)/C(=C\c1ccc(Cl)cc1)n1cncn1
Triadimefon CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n1cncn1
Paclobutrazol	CC(C)(C)[C@H](O)[C@H](Cc1ccc(Cl)cc1)n1cncn1
Diclofenac	O=C(O)Cc1ccccc1Nc1c(Cl)cccc1Cl
Flutriafol	OC(Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F
Clofentezine	Clc1ccccc1-c1nnc(-c2ccccc2Cl)nn1
Fenpropimorph	CC(Cc1ccc(C(C)(C)C)cc1)CN1C[C@@H](C)O[C@@H](C)C1
Fenazaquin	CC(C)(C)c1ccc(CCOc2ncnc3ccccc23)cc1
Nadolol CC(C)(C)NCC(O)COc1cccc2c1CC(O)C(O)C2
Hexaconazole	CCCCC(O)(Cn1cncn1)c1ccc(Cl)cc1Cl
Flusilazole C[Si](Cn1cncn1)(c1ccc(F)cc1)c1ccc(F)cc1
Triticonazole	CC1(C)CCC(=Cc2ccc(Cl)cc2)C1(O)Cn1cncn1
Metconazole CC1(C)CCC(Cc2ccc(Cl)cc2)C1(O)Cn1cncn1
Bisoprolol	CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1
Fenarimol	OC(c1ccc(Cl)cc1)(c1cncnc1)c1ccccc1Cl
Ipconazole	CC(C)C1CCC(Cc2ccc(Cl)cc2)C1(O)Cn1cncn1
Fenbuconazole	N#CCC(CCc1ccc(Cl)cc1)(Cn1cncn1)c1ccccc1
Bifenox COC(=O)c1cc(Oc2ccc(Cl)cc2Cl)ccc1[N+](=O)[O-]
Propiconazole	CCCC1COC(Cn2cncn2)(c2ccc(Cl)cc2Cl)O1
Triflumizole	CCCOC/C(=N\c1ccc(Cl)cc1C(F)(F)F)n1ccnc1
Chlorfenvinphos CCOP(=O)(OCC)OC(=CCl)c1ccc(Cl)cc1Cl
Isoxaflutole-diketonitrile	CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)C(C#N)C(=O)C1CC1
Oxyfluorfen CCOc1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Fenoxaprop-ethyl	CCOC(=O)C(C)Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1
Bezafibrate CC(C)(Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1)C(=O)O
Tetraconazole	FC(F)C(F)(F)OCC(Cn1cncn1)c1ccc(Cl)cc1Cl
Bromuconazole	Clc1ccc(C2(Cn3cncn3)CC(Br)CO2)c(Cl)c1
Clethodim Sulfoxide CCC(NOC/C=C/Cl)=C1C(=O)CC(CC(C)[S+]([O-])CC)CC1=O
Pyrametostrobin COC(=O)N(OC)c1ccccc1COc1c(C)c(-c2ccccc2)nn1C
Fipronil-desulfinyl N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1C(F)(F)F
Metrafenone COc1cc(C)c(C(=O)c2c(OC)ccc(Br)c2C)c(OC)c1OC
Trifloxystrobin CO/N=C(/C(=O)OC)c1ccccc1CO/N=C(\C)c1cccc(C(F)(F)F)c1
Imibenconazole	Clc1ccc(CSC(Cn2cncn2)=Nc2ccc(Cl)cc2Cl)cc1
Flumetralin CCN(Cc1c(F)cccc1Cl)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Cyflumetofen	COCCOC(=O)C(C#N)(C(=O)c1ccccc1C(F)(F)F)c1ccc(C(C)(C)C)cc1
Flucythrinate	CC(C)C(C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1)c1ccc(OC(F)F)cc1
Fluazinam	O=[N+]([O-])c1cc(C(F)(F)F)c(Cl)c([N+](=O)[O-])c1Nc1ncc(C(F)(F)F)cc1Cl
Pyridalyl	FC(F)(F)c1cccc(OCCCOc2c(Cl)cc(OCC=C(Cl)Cl)cc2Cl)nc1
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6ccc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
Avermectin B1a	CC[C@H](C)[C@H]1O[C@]2(C=C[C@@H]1C)C[C@@H]1C[C@@H](C/C=C(\C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@@H](O)[C@H](C)O4)[C@H](C)O3)[C@@H](C)/C=C/C=C3\CO[C@@H]4[C@H](O)C(C)=C[C@@H](C(=O)O1)[C@]34O)O2
```

3.3.10 Mix J:

Mix J

Mix J.txt

```
name	smiles
Histamine-2HCl	NCCc1c[nH]cn1
Molinate	CCSC(=O)N1CCCCCC1
Cymoxanil	CCNC(=O)NC(=O)C(C#N)=NOC
Isoproturon	CC(C)c1ccc(NC(=O)N(C)C)cc1
Formaldehyde-2,4-dinitrophenylhydrazone (DNPH)	C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Chlorotoluron	Cc1ccc(NC(=O)N(C)C)cc1Cl
Acetaldehyde-2,4-dinitrophenylhydrazone (DNPH)	CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Tebuthiuron	CNC(=O)N(C)c1nnc(C(C)(C)C)s1
Diuron	CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1
Acrolein-2,4-dinitrophenylhydrazone	C=CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Acetone-DNPH	CC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Propionaldehyde-2,4-dinitrophenylhydrazone	CCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Forchlorfenuron	O=C(Nc1ccccc1)Nc1ccnc(Cl)c1
Linuron	CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1
Methacrylaldehyde-2,4-dinitrophenylhydrazone	C=C(C)/C=N/Nc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Crotonaldehyde-2,4-dinitrophenylhydrazone (DNPH)	CC=CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
2-Butanone-2,4-dinitrophenylhydrazone	CCC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Butyraldehyde-2,4-dinitrophenylhydrazone	CCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Dimepiperate	CC(C)(SC(=O)N1CCCCC1)c1ccccc1
Isovaleraldehyde-2,4-dinitrophenylhydrazone	CC(C)CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Pentanal-2,4-dinitrophenylhydrazone	CCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Furfural-2,4-dinitrophenylhydrazone	O=[N+]([O-])c1ccc(NN=Cc2ccco2)c([N+](=O)[O-])c1
Cyclohexanone-2,4-dinitrophenylhydrazone	O=[N+]([O-])c1ccc(NN=C2CCCCC2)c([N+](=O)[O-])c1
Glutaraldehyd-bis(2,4-dinitrophenylhydrazone)	O=CCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
4-Methyl-2-pentanone-2,4-dinitrophenylhydrazone	CC(CC(C)C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Hexanal-2,4-dinitrophenylhydrazone	CCCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Fosthiazate	CCOP(=O)(SC(C)CC)N1CCSC1=O
Benzaldehyde-2,4-dinitrophenylhydrazone	O=[N+]([O-])c1ccc(NN=Cc2ccccc2)c([N+](=O)[O-])c1
Heptanal-2,4-dinitrophenylhydrazone	CCCCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
p-Tolualdehyde-2,4-dinitrophenylhydrazone	Cc1ccc(C=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])cc1
m-Tolualdehyde-2,4-dinitrophenylhydrazone	Cc1cccc(C=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])c1
o-Tolualdehyde-2,4-dinitrophenylhydrazone	Cc1ccccc1C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Buprofezin	CC(C)N1C(=O)N(c2ccccc2)CSC1=NC(C)(C)C
Octanal-2,4-dinitrophenylhydrazone	CCCCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Diflubenzuron	O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(Cl)cc1
2,5-Dimethylbenzaldehyd-2,4-dinitrophenylhydrazone	Cc1ccc(C)c(C=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])c1
Nonanal-2,4-dinitrophenylhydrazone	CCCCCCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Prochloraz desimidazole-amino	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(N)=O
Decanal-2,4-dinitrophenylhydrazone	CCCCCCCCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Thiophanate-methyl	COC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OC
N-(Propyl(2-(2,4,6-trichlorophenoxy)ethyl)carbamoyl)formamide	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)NC=O
Hexythiazox	C[C@H]1[C@H](c2ccc(Cl)cc2)SC(=O)N1C(=O)NC1CCCCC1
Prochloraz	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)n1ccnc1
Sulfentrazone	Cc1nn(-c2cc(NS(C)(=O)=O)c(Cl)cc2Cl)c(=O)n1C(F)F
Carfentrazone-ethyl	CCOC(=O)C(Cl)Cc1cc(-n2nc(C)n(C(F)F)c2=O)c(F)cc1Cl
Chlorimuron-ethyl	CCOC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(Cl)cc(OC)n1
Cyclosulfamuron	COc1cc(OC)nc(NC(=O)NS(=O)(=O)Nc2ccccc2C(=O)C2CC2)n1
Flufenoxuron	O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(Oc2ccc(C(F)(F)F)cc2Cl)cc1F
Metaflumizone	N#Cc1ccc(CC(=NNC(=O)Nc2ccc(OC(F)(F)F)cc2)c2ccc(C(F)(F)F)c2)cc1
Lufenuron	O=C(NC(=O)c1c(F)cccc1F)Nc1cc(Cl)c(OC(F)(F)C(F)C(F)(F)F)cc1Cl
Indoxacarb	COC(=O)N(C(=O)N1COC2(CC(=O)OC)Cc3cc(Cl)ccc3C2=N1)c1ccc(OC(F)(F)F)cc1
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
```

3.3.11 Mix K:

Mix K

Mix K.txt

```
name	smiles
Butanone	CCC(C)=O
Phenol	Oc1ccccc1
Histamine-2HCl	NCCc1c[nH]cn1
4-tert-butylphenol	CC(C)(C)c1ccc(O)cc1
3-Methyl-4-nitrophenol	Cc1cc(O)ccc1[N+](=O)[O-]
Atrazine-desisopropyl-2-hydroxy	CCNc1nc(=O)nc(N)[nH]1
2,6-Dichlorophenol	Oc1c(Cl)cccc1Cl
2,4-Dichlorophenol	Oc1ccc(Cl)cc1Cl
p-(1,1-dimethylpropyl)phenol	CCC(C)(C)c1ccc(O)cc1
4-tert-butylpyrocatechol	CC(C)(C)c1ccc(O)c(O)c1
2,6-Dimethyl- 4-nitrophenol	Cc1cc([N+](=O)[O-])cc(C)c1O
Desethyl-2-hydroxy-atrazin	CC(C)Nc1nc(=O)nc(N)[nH]1
Triethyl phosphate (TEP)	CCOP(=O)(OCC)OCC
Hydroxysimazine	CCNc1nc(O)nc(NCC)n1
2,4-Dinitrophenol	O=[N+]([O-])c1ccc(O)c([N+](=O)[O-])c1
2,6-Dinitrophenol	O=[N+]([O-])c1cccc([N+](=O)[O-])c1O
Atrazine-2-hydroxy	CCNc1nc(O)nc(NC(C)C)n1
Bisphenol F	Oc1ccc(Cc2ccc(O)cc2)cc1
2,4-di-tert-butylphenol	CC(C)(C)c1ccc(O)c(C(C)(C)C)c1
4-octylphenol	CCCCCCCCc1ccc(O)cc1
Dibutyl phosphate	CCCCOP(=O)(O)OCCCC
4-(2,6-Dimethylheptyl)phenol	CC(C)CCCC(C)Cc1ccc(O)cc1
2,6-di-tert-butyl-p-cresol	Cc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Nalidixic acid	CCn1cc(C(=O)O)c(=O)c2ccc(C)nc21
Bisphenol B	CCC(C)(c1ccc(O)cc1)c1ccc(O)cc1
Bisphenol S	O=S(=O)(c1ccc(O)cc1)c1ccc(O)cc1
Daidzein	O=c1c(-c2ccc(O)cc2)coc2cc(O)ccc12
Oxolinic acid	CCn1cc(C(=O)O)c(=O)c2cc3c(cc21)OCO3
Flumequine	CC1CCc2cc(F)cc3c(=O)c(C(=O)O)cn1c23
Cinoxacin	CCn1nc(C(=O)O)c(=O)c2cc3c(cc21)OCO3
Pipemidic acid	CCn1cc(C(=O)O)c(=O)c2cnc(N3CCNCC3)nc21
Norfloxacin	CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCNCC3)cc21
Enoxacin	CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCNCC3)nc21
Trichloropropyl phosphate (TCPP)	O=P(OCCCC1)(OCCCC1)OCCCC1
Triphenyl phosphate (TPP)	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1
Ciprofloxacin	O=C(O)c1cn(C2CC2)c2cc(N3CCNCC3)c(F)cc2c1=O
Pefloxacin	CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCN(C)CC3)cc21
Bisphenol AF	Oc1ccc(C(c2ccc(O)cc2)(C(F)(F)F)C(F)(F)F)cc1
Lomefloxacin hydrochloride	CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCNC(C)C3)c(F)c21
Danofloxacin	CN1C[C@H]2C[C@H]1CN2c1cc2c(cc1F)c(=O)c(C(=O)O)cn2C1CC1
6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	Cc1cc(O)c(C(C)(C)C)cc1Sc1cc(C(C)(C)C)c(O)cc1C
Enrofloxacin	CCN1CCN(c2cc3c(cc2F)c(=O)c(C(=O)O)cn3C2CC2)CC1
Ofloxacin	CC1COc2c(N3CCN(C)CC3)c(F)cc3c(=O)c(C(=O)O)cn1c23
Tricresyl phosphate	Cc1ccc(OP(=O)(Oc2ccc(C)cc2)Oc2ccc(C)cc2)cc1
6,6'-di-tert-butyl-4,4'-butylidenedi-m-cresol	CCCC(c1cc(C(C)(C)C)c(O)cc1C)c1cc(C(C)(C)C)c(O)cc1C
Sarafloxacin hydrochloride	O=C(O)c1cn(-c2ccc(F)cc2)c2cc(N3CCNCC3)c(F)cc2c1=O
Tris(2-butoxyethyl) phosphate	CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC
Tris[2-chloro-1-(chloromethyl)ethyl] phosphate	O=P(OC(CC1)CC1)(OC(CC1)CC1)OC(CC1)CC1
Tetrabromobisphenol A (TBBPA)	CC(C)(c1cc(Br)c(O)c(Br)c1)c1cc(Br)c(O)c(Br)c1
Cefoperazone	CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin	CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
```

3.3.12 Mix L:

Mix L

Mix L.txt

```
name    smiles
Butanone    CCC(C)=O
Histamine-2HCl  NCCc1c[nH]cn1
2-Methylnaphthalene Cc1ccc2ccccc2c1
Isobutyl paraben    CC(C)COC(=O)c1ccc(O)cc1
Diethyl phthalate   CCOC(=O)c1ccccc1C(=O)OCC
Icaridin    CCC(C)OC(=O)N1CCCCC1CCO
Amiloxate   COc1ccc(C=CC(=O)OCCC(C)C)cc1
2-ethylhexyl salicylate CCCCC(CC)COC(=O)c1ccccc1O
Homosalate  CC1CC(OC(=O)c2ccccc2O)CC(C)(C)C1
Citroflex 2 CCOC(=O)CC(O)(CC(=O)OCC)C(=O)OCC
Octinoxate  CCCCC(CC)COC(=O)C=Cc1ccc(OC)cc1
Dipentyl phthalate  CCCCCOC(=O)c1ccccc1C(=O)OCCCCC
Prednisone  C[C@]12C=CC(=O)C=C1CC[C@@H]1[C@@H]2C(=O)C[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO
Prednisolone    C[C@]12C=CC(=O)C=C1CC[C@@H]1[C@@H]2[C@@H](O)C[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO
Cortisone   C[C@]12CCC(=O)C=C1CC[C@@H]1[C@@H]2C(=O)C[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO
Octocrylene CCCCC(CC)COC(=O)C(C#N)=C(c1ccccc1)c1ccccc1
Hydrocortisone  C[C@]12CCC(=O)C=C1CC[C@@H]1[C@@H]2[C@@H](O)C[C@@]2(C)[C@H]1CC[C@]2(O)C(=O)CO
Di(2-ethylhexyl)adipate (DEHA)  CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC
6?-methylprednisolone   C[C@H]1C[C@@H]2[C@H]([C@@H](O)C[C@@]3(C)[C@H]2CC[C@]3(O)C(=O)CO)[C@@]2(C)C=CC(=O)C=C12
Fluorometholone CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C[C@H](C)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Dexamethasone   C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO
Betamethasone   C[C@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO
Triamcinolone   C[C@]12C=CC(=O)C=C1CC[C@H]1[C@@H]3C[C@@H](O)[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)[C@@]12F
Prednisone-21-acetate   CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3C(=O)C[C@@]21C
Prednisolone-21-acetate CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
Cortisone-21-acetate    CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3C(=O)C[C@@]21C
Hydrocortisone-Acetate  CC(=O)OCC(=O)[C@@]1(O)CCC2C3CCC4=CC(=O)CC[C@]4(C)C3[C@@H](O)C[C@@]21C
Beclomethasone  C[C@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(Cl)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO
Flumethasone    C[C@@H]1C[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO
6?-methyl-Prednisolone-21-acetate   CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C[C@H](C)C4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
Fuorometholone-Acetate  CC(=O)O[C@]1(C(C)=O)CC[C@H]2[C@@H]3C[C@H](C)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Fludrocortisone-Acetate CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Mometasone  C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(Cl)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CC1
Budesonide-(mixOfsomers)    CCCC1O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@]2(C(=O)CO)O1
Hydrocortisone-17-butyrate  CCCC(=O)O[C@]1(C(=O)CO)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
Betamethasone-21-acetate    CC(=O)OCC(=O)[C@@]1(O)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Cexamethasone-21-acetate    CC(=O)OCC(=O)[C@@]1(O)[C@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Triamcinolone-Acetonide CC1(C)O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@@]4(F)[C@@H](O)C[C@]3(C)[C@]2(C(=O)CO)O1
Flurandrenolide CC1(C)O[C@@H]2C[C@H]3[C@@H]4C[C@H](F)C5=CC(=O)CC[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@]2(C(=O)CO)O1
Deflazacort CC(=O)OCC(=O)[C@@]12N=C(C)O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]12C
Hydrocortisone-17-valerate  CCCCC(=O)O[C@]1(C(=O)CO)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
Halcinonide CC1(C)O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)CC[C@]5(C)[C@@]4(F)[C@@H](O)C[C@]3(C)[C@]2(C(=O)CCl)O1
Clobetasol-17-propionate    CCC(=O)O[C@]1(C(=O)CCl)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
21-(acetyloxy)-Triamcinolone-Acetonide  CC(=O)OCC(=O)[C@@]12OC(C)(C)O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]12C
Betamethasone-17-valerate   CCCCC(=O)O[C@]1(C(=O)CO)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Clobetasone-Butyrate    CCCC(=O)O[C@]1(C(=O)CCl)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)C(=O)C[C@@]21C
Triamcinolone-Diacetate CC(=O)OCC(=O)[C@@]1(O)[C@H](OC(C)=O)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Prednicarbate   CCOC(=O)O[C@]1(C(=O)COC(=O)CC)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
Diflorasone-Diacetate   CC(=O)OCC(=O)[C@@]1(OC(C)=O)[C@@H](C)C[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Fluocinonide    CC(=O)OCC(=O)[C@@]12OC(C)(C)O[C@@H]1C[C@H]1[C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]12C
Fluticasone-Propionate  CCC(=O)O[C@]1(C(=O)SCF)[C@H](C)C[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Amcinonide  CC(=O)OCC(=O)[C@@]12OC3(CCCC3)O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]12C
Betamethasone-17,21-dipropionate    CCC(=O)OCC(=O)[C@@]1(OC(=O)CC)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
Beclomethasone-Dipropionate CCC(=O)OCC(=O)[C@@]1(OC(=O)CC)[C@@H](C)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(Cl)[C@@H](O)C[C@@]21C
Alclometasone-17,21-dipropionate    CCC(=O)OCC(=O)[C@@]1(OC(=O)CC)[C@H](C)C[C@H]2[C@H]3[C@H]([C@@H](O)C[C@@]21C)[C@@]1(C)C=CC(=O)C=C1C[C@H]3Cl
Cefoperazone    CCN1CCN(C(=O)N[C@@H](C(=O)N[C@@H]2C(=O)N3C(C(=O)O)=C(CSc4nnnn4C)CS[C@H]23)c2ccc(O)cc2)C(=O)C1=O
Rifaximin   CO[C@H]1/C=C/O[C@@]2(C)Oc3c(C)c(O)c4c(O)c(c5c(nc6cc(C)ccn65)c4c3C2=O)NC(=O)/C(C)=C\C=C\[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(C)=O)[C@@H]1C
2-Ethylhexyl trans-4-methoxycinnamate (OMC) CCCCC(CC)COC(=O)/C=C/C1=CC=C(C=C1)OC
```

3.3.13 RTI opløsning:

	Concentration (µg/mL)	CAS-no.	Final volume (µL)	Final concentration (µg/mL)	Pipetted volume (µL)
Guanylurea-HCl	100 µg/mL		1500	4	60
Amitrole	100 µg/mL	61-82-5	1500	4	60
Histamine-2HCl	100 µg/mL	56-92-8	1500	4	60
Chlormequat-Chloride	100 µg/mL	999-81-5	1500	4	60
Vancomycin	100 µg/mL	1404-90-6	1500	4	60
Butocarboxim	100 µg/mL	34681-10-2	1500	4	60
Tylosin	100 µg/mL	1401-69-0	1500	4	60
Busan (TCMTB)	100 µg/mL	21564-17-0	1500	4	60
Rifaximin	100 µg/mL	80621-81-4	1500	4	60
Emamectin	100 µg/mL	119791-41-2	1500	4	60
Nigericin sodium salt	100 µg/mL	28643-80-3	1500	4	60
Salicylic acid	100 µg/mL	69-72-7	1500	4	60
Tepraloxydim	100 µg/mL	149979-41-9	1500	4	60
Bromoxynil	100 µg/mL	1689-84-5	1500	4	60
MCPA	100 µg/mL	94-74-6	1500	4	60
Valproic acid	100 µg/mL	99-66-1	1500	4	60
Phenytoin	100 µg/mL	57-41-0	1500	4	60
Flamprop	100 µg/mL	58667-63-3	1500	4	60
Benodanil	100 µg/mL	15310-01-7	1500	4	60
Dinoterb	100 µg/mL	1420-07-1	1500	4	60
Inabenfide	100 µg/mL	82211-24-3	1500	4	60
Triclosan	100 µg/mL	3380-34-5	1500	4	60
Salinomycin	100 µg/mL	53003-10-4	1500	4	60
Benzoic acid	100 µg/mL	65-85-0	1500	4	60
Cefoperazone	100 µg/mL	62893-19-0	1500	4	60

4.1 PROTOCOL – column change

The columns need to be cleaned before storage!

CLEANING OF COLUMNS

- Prepare line D with pure ACN (without FA)
  - Degas ACN for 15 min.
  - Add the D-tubes to the flask
  - Set both pumps to 0.800 mL/min
    - Right-click when having the mouse over the pump picture and change the flow rate to 0.800 and press ENTER or click on OK
  - Rinse for 30 min.
  - Stop both pumps (set the flow rate to 0.000 mL/min)

- Disconnect the columns one by one and store them in box (placed in the LCMS cabinet)

- Place some paper towels under the tubes and set both pumps to 0.5000 mL/min and check if the flow of solvent looks "normal" (no air bubbles - splashes)

- If so, stop the pumps
- If not, rinse the system a bit longer – until all air is out of the column tubes

INSTALLATION OF NEW COLUMNS

- The new columns can now be connected with one tube end – REMEMBER TO LOOK CAREFULLY AT THE "LINE NAMES". Start with
  - "1. To column from pump"
  - "2. To column from pump"

- Now check each column one by one by setting the pump flow rate at 0.1000 mL/min and make sure the solvent is passing through the column (hold a paper towel under the outlet) and make sure the pressure is still "low"

- Connect the second tube to the columns and remember to look carefully at the "line names"
  - "1. To column from pump"
  - "2. To column from pump"

- Place the columns on the shelves in the heating cabinet and secure them with the metal fastener

- Set the flow rate to 0.2000 mL/min for both pumps and increase slowly (0.2000 mL/min) to 0.8000 mL/min.

- Make sure the columns don't leak by placing a paper towel at both the inlet and outlet of the columns and see if it gets wet

- If not - close the front
- If yes – tighten the bold slightly more and then close the front

- Prepare the columns by rinsing with 100% ACN (buffer D) at a flow rate of 0.8000 mL/min for 30 min.

- Stop the pumps
- The columns are now ready to go😊

4.2 Protocol - Preparation of mixes

The following procedure describes how to prepare the mixes that will be used for the chromatographic experiments.

There are in total 12 mixes, each containing between 50 and 91 individual compounds.

The 12 mixes are combinations of the bought chemical solutions. There are in total 49 individual solutions (here RTI is taken as 1 solution, which has been prepared beforehand).

10 of the solutions contain exactly one compound and another three individual compounds from the RTI-mix act as the quality control standards. These are spiked into all solutions. This is to be able to monitor the retention time drift for these three compounds across all experiments.

The mixes are prepared to avoid overlapping m/z values for the compounds in the same mix.

The final volume of each mix is 100 µL and the final concentration is approximately 5 µg/L.

The mixes are prepared fresh every day.

The procedure for preparation of the mixes:

With an automatic pipette, transfer the volume specified in the tables below for each of the stock solutions to a HPLC vial with a 200µL insert. Transfer the stated amount of acetonitrile to a total volume of 100 µL. Cap the HPLC vial and store cold.

When the HPLC experiments are done re-cap all vials and store the vials in the freezer for storage until next time.

Preparation of RTI stock solution:
Transfer 60 µL of each of the individual solutions into a HPLC vial. The total volume should end at 1500 µL Cap the vial and store in the freezer.

	Concentration (µg/mL)	CAS-no.	Final volume (µL)	Final concentration (µg/mL)	Pipetted volume (µL)
Guanylurea-HCl	100 µg/mL		1500	4	60
Amitrole	100 µg/mL	61-82-5	1500	4	60
Histamine-2HCl	100 µg/mL	56-92-8	1500	4	60
Chlormequat-Chloride	100 µg/mL	999-81-5	1500	4	60
Vancomycin	100 µg/mL	1404-90-6	1500	4	60
Butocarboxim	100 µg/mL	34681-10-2	1500	4	60
Tylosin	100 µg/mL	1401-69-0	1500	4	60
Busan (TCMTB)	100 µg/mL	21564-17-0	1500	4	60
Rifaximin	100 µg/mL	80621-81-4	1500	4	60
Emamectin	100 µg/mL	119791-41-2	1500	4	60
Nigericin sodium salt	100 µg/mL	28643-80-3	1500	4	60
Salicylic acid	100 µg/mL	69-72-7	1500	4	60
Tepraloxydim	100 µg/mL	149979-41-9	1500	4	60
Bromoxynil	100 µg/mL	1689-84-5	1500	4	60
MCPA	100 µg/mL	94-74-6	1500	4	60
Valproic acid	100 µg/mL	99-66-1	1500	4	60
Phenytoin	100 µg/mL	57-41-0	1500	4	60
Flamprop	100 µg/mL	58667-63-3	1500	4	60
Benodanil	100 µg/mL	15310-01-7	1500	4	60
Dinoterb	100 µg/mL	1420-07-1	1500	4	60
Inabenfide	100 µg/mL	82211-24-3	1500	4	60
Triclosan	100 µg/mL	3380-34-5	1500	4	60
Salinomycin	100 µg/mL	53003-10-4	1500	4	60
Benzoic acid	100 µg/mL	65-85-0	1500	4	60
Cefoperazone	100 µg/mL	62893-19-0	1500	4	60

Mix A

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 4	50	10
13751-ME5	100	5
13900-0050-100ME5	100	5
18011-MEWS5	100	5
AAR-001-100AN5	100	5
AAR-016-W100ME5	100	5
13900-0080-100ME5	100	5
13900-0100-100ME5	100	5
13900-0105-100ME5	100	5
13900-0185-100ME5	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	75
	Added volume of acetonitrile	25

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX A"
*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix B

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 1	50	10
AAR-024-100ME10	100	5
Carbendazim	50	10
Albendazole	50	10
Sethoxydim	50	10
Pencycuron	50	10
Tralkoxydim	50	10
Emamectin benzoate	50	10
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	95
	Added volume of acetonitrile	5

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX B"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix C

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 2	50	10
Pesticide mix 7	50	10
GB/T 22286-2008 11 β-Agonists 100 µg/mL in Methanol	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	45
	Added volume of acetonitrile	55

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX C"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix D

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide 3	50	10
SN/T 3045-2011 Azo Dyes Mixture 120 300 µg/mL in Acetonitrile	300	1,67
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	31,67
	Added volume of acetonitrile	68,33

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX D"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix E

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
NAPS*[2]	100	5
AAR-009-W100ME5	100	5
AAR-011-100MEWS5	100	5
SN/T 3147-2012 Phthalates Mixture 567 1000-5000 µg/mL in Methanol	100 (stock solution is diluted 10x)	5
Histamine*[3]	100	5
Rifaximin*[3]	100	5
Cefoperazone*[4]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	40
	Added volume of acetonitrile	60

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX E"

*[2] NAPS are stored in the refrigerator in HPLC-lab

*[3] Located in "Kemikalie rummet" in the box named "FoU"

*[4] Located in the refrigerator in "HPLC Lab"

Mix F

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 5	50	10
RTI	4	75
Sulfonamides Mixture for GB/T 21316-2007 100 µg/mL in Acetonitrile	100	5
Cefoperazone*[2]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	90
	Added volume of acetonitrile	

In mix F, the three quality control standards are not added. They are already a part of the RTI mix that is included. The concentration of the RTI calibrants are 3 µg/µL

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX F"

*[2] Located in the refrigerator in "HPLC Lab"

Mix G

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 6	50	10
R02192-ME5	100	5
R03125-ME10	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	40
	Added volume of acetonitrile	60

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX G"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix H

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 8	50	10
AAR-029-100ME5	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	35
	Added volume of acetonitrile	65

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX H"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix I

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 9	50	10
18016-ME5	100	5
GB/T 21318-2007, SN/T 1928-2007 10 Nitroimidazoles 100 µg/mL in Methanol	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	40
	Added volume of acetonitrile	60

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX I"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix J

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
Pesticide mix 10	50	10
DNPH-Mix 2 215-700 µg/mL in Acetonitrile*[2]	250	2
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
CDEA mix	xx	xx
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	32
	Added volume of acetonitrile	68 - xx

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX J"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix K

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
AAR-002-100ME5	100	5
AAR-003-100ME5	100	5
AAR-010-100ME5	100	5
GB/T 21312-2007 14 Quinolones 20 µg/mL in Methanol	20	25
PFAS Mixture 151 100 µg/mL in Methanol:Water	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	60
	Added volume of acetonitrile	35

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX K"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

Mix L

Mixture*[1]	Concentration in stock solution (µg/mL)	Volume to pipette from stock (µL)
AAR-004-100AN5	100	5
GB/T 24800.2-2009 41 Glucocorticoids 100 µg/mL in Methanol	100	5
Histamine*[2]	100	5
Rifaximin*[2]	100	5
Cefoperazone*[3]	100	10
	Final concentration in mix (µg/mL)	5
	Final volume of mix (µL)	100
	Pipetted volume from the stock solutions (µL)	30
	Added volume of acetonitrile	70

*[1] All stock solutions are stored in the top drawer in the freezer in "Chemistry lab" in a box named "MIX L"

*[2] Located in "Kemikalie rummet" in the box named "FoU"

*[3] Located in the refrigerator in "HPLC Lab"

4.3
Protocol - Preparation of eluents – ACN and MeOH – pH 2,7

This procedure describes how to prepare eluents for the chromatographic experiments.

Buffer A needs to be freshly prepared before each run!

Buffer A: Water + 0.1% FA:

- Use the 2 L volumetric flask labeled "WATER + FA"
- Rinse the volumetric flask three times with ACN
- Rinse the volumetric flask three times with water
- Add 1950 mL water in the 2 L volumetric flask
- Add 2 mL of conc. formic acid
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as eluent flask
- Degas the solution for 15 min.

Buffer B: ACN + 0.1% FA:

- Use the 1 L volumetric flask labeled "ACN + FA"
- Rinse the volumetric flask three times with ACN
- Add 950 mL ACN in a 1L volumetric flask
- Add 1 mL of conc. formic acid
- Mix well
- Fill up to 1 L with ACN
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

Buffer C: MeOH + 0.1% FA:

- Use the 1 L volumetric flask labeled "MeOH + FA"
- Rinse the volumetric flask three times with MeOH
- Add 950 mL MeOH in a 1L volumetric flask
- Add 1 mL of conc. formic acid
- Mix well
- Fill up to 1 L with MeOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.4
Protocol - Preparation of eluents – ACN and MeOH - pH 4

- Work in the fume hood
- Buffer A needs to be freshly prepared before each run!
- Degassing means place the bottle in the sonication bath
- For all buffers write the batch numbers on the laminated card and hang on the bottle; also write batch numbers in the logbook

Buffer A: Water + 0.1% Formic Acid (FA) + 5 mM Ammonium formate (AmFA):

- Use the 2 L volumetric flask labeled "WATER + FA + AmFA"
- Rinse the volumetric flask three times with ACN
- Rinse the volumetric flask three times with water
- Weigh out 403.44 mg AmFA and add it to the volumetric flask
- Add ~400 mL water in the 2 L volumetric flask
- Add 135.8 µL of conc. FA
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as eluent flask
- Degas the solution for 15 min.

Buffer B: ACN:

- Take an unopened ACN flask
- Degas for 15 min.

Buffer C: MeOH + 0.1% FA + 5 mM Ammonium formate (AmFA):

- Use the 1 L volumetric flask labeled "MeOH + FA + AmFA"
- Rinse the volumetric flask three times with MeOH
- Weigh out 201.7 mg AmFA and add it to the volumetric flask
- Add ~300 mL MeOH in a 1L volumetric flask
- Add 67.9 µL of conc. FA
- Mix well
- Fill up to 1 L with MeOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.5
Protocol - Preparation of eluents – ACN and MeOH – pH 8

- Work in the fume hood
- Buffer A needs to be freshly prepared before each run!
- Degassing means place the bottle in the sonication bath
- For all buffers write the batch numbers on the laminated card and hang on the bottle; also write batch numbers in the logbook

Buffer A: Water + 5 mM Ammonium formate (AmFA)/Ammonium hydroxide (AmOH):

- Use the 2 L volumetric flask labeled "WATER + AmFA/AmOH"
- Rinse the volumetric flask three times with ACN
- Rinse the volumetric flask three times with water
- Weigh out 597,0 mg AmFA and add it to the volumetric flask
- Add ~200 mL water in the 2 L volumetric flask
- Add 46,8 µL NH_4OH
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as eluent flask
- Degas the solution for 15 min.

Buffer B: ACN:

- Take an unopened ACN flask
- Degas for 15 min.

Buffer C: MeOH + 5 mM Ammonium formate (AmFA)/Ammonium hydroxide (AmOH):

- Use the 1 L volumetric flask labeled "MeOH + AmFA/AmOH"
- Rinse the volumetric flask three times with MeOH
- Weigh out 298.5 mg AmFA and add it to the volumetric flask
- Add 200 mL MeOH in a 1L volumetric flask
- Add 23,4 µL NH_4OH
- Mix well
- Fill up to 1 L with MeOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.6
Protocol - Preparation of eluents – Ethanol and 2-propanol - pH 2,7

This procedure describes how to prepare eluents for the chromatographic experiments.

Buffer A needs to be freshly prepared before each run!

Buffer A: Water + 0.1% FA:

- Use the 2 L volumetric flask labeled "WATER + FA"
- Rinse the volumetric flask three times with EtOH
- Rinse the volumetric flask three times with water
- Add 1950 mL water in the 2 L volumetric flask
- Add 2 mL of conc. formic acid
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as eluent flask
- Degas the solution for 15 min.

Buffer B: EtOH + 5,0 % H_2O + 0.1% FA:

- Use the 1 L volumetric flask labeled "EtOH + FA"
- Rinse the volumetric flask three times with EtOH
- Add 900 mL EtOH in a 1L volumetric flask
- Add 50.0 ml H_2O using a volumetric pipette (fuldpipette)
- Add 1 mL of conc. formic acid
- Mix well
- Fill up to 1 L with EtOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

Buffer C: IPA + 5.0% H_2O + 0.1% FA:

- Use the 1 L volumetric flask labeled "IPA + FA"
- Rinse the volumetric flask three times with IPA
- Add 950 mL IPA in a 1L volumetric flask
- Add 50.0 ml H_2O using a volumetric pipette (fuldpipette)
- Add 1 mL of conc. formic acid
- Mix well
- Fill up to 1 L with IPA
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.7
Protocol - Preparation of eluents – Ethanol and 2-propanol - pH 4

Work in the fume hood
Buffer A needs to be freshly prepared before each run!
Degassing means placing the bottle in the sonication bath
For all buffers write the batch numbers on the laminated card and hang them on the bottle; also write batch numbers in the logbook

Buffer A: Water + 5 mM Ammonium formate (AmFA) + FA:

- Use the 2 L volumetric flask labeled "WATER + FA + AmFA"
- Rinse the volumetric flask three times with ACN
- Rinse the volumetric flask three times with water
- Weigh 403.44 mg AmFA and add it to the volumetric flask
- Add ~400 mL water to the 2 L volumetric flask
- Add 135.8 µL of conc. FA
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as an eluent flask
- Degas the solution for 15 min.

Buffer E: EtOH + 5.0 % H_2O + 5 mM Ammonium formate (AmFA) + FA:

- Use the 1 L volumetric flask labeled "EtOH + FA + AmFA"
- Rinse the Volumetric flask three times with EtOH
- Weigh out 201.7 mg AmFA and add it to the volumetric flask
- Add ~300 mL EtOH in a 1L volumetric flask
- Add 50.0 ml H_2O using a volumetric pipette (fuldpipette)
- Add 67.9 µL of conc. FA
- Mix well
- Fill up to 1 L with EtOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

Buffer F: IPA + 5.0% H_2O + 5 mM Ammonium formate (AmFA) + FA:

- Use the 1 L volumetric flask labeled "IPA + FA + AmFA"
- Rinse the volumetric flask three times with IPA
- Weigh out 201.7 mg AmFA and add it to the volumetric flask
- Add ~300 mL IPA in a 1L volumetric flask
- Add 50.0 ml H_2O using a volumetric pipette (fuldpipette)
- Add 67.9 µL of conc. FA
- Mix well
- Fill up to 1 L with IPA
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.8
Protocol - Preparation of eluents - Ethanol and 2-propanol - pH 8

- Work in the fume hood
- Buffer A needs to be freshly prepared before each run!
- Degassing means place the bottle in the sonication bath
- For all buffers write the batch numbers on the laminated card and hang on the bottle; also write batch numbers in the logbook

Buffer A: Water + 5 mM Ammonium formate (AmFA)/Ammonium hydroxide (AmOH):

- Use the 2 L volumetric flask labeled "WATER + AmFA/AmOH"
- Rinse the volumetric flask three times with ACN
- Rinse the volumetric flask three times with water
- Weigh out 597,0 mg AmFA and add it to the volumetric flask
- Add ~200 mL water in the 2 L volumetric flask
- Add 46,8 µL NH_4OH
- Mix well
- Fill up to 2 L with water
- Rinse the original brown flask three times with the prepared solution
- Transfer the solution to the original brown flask and use it as eluent flask
- Degas the solution for 15 min.

Buffer B: EtOH + 5.0% H_2O + 5 mM Ammonium formate (AmFA)/Ammonium hydroxide (AmOH):

- Use the 1 L volumetric flask labeled "MeOH + AmFA/AmOH"
- Rinse the volumetric flask three times with EtOH
- Weigh out 298.5 mg AmFA and add it to the volumetric flask
- Add 200 mL EtOH in a 1L volumetric flask
- Add 50.0 mL of H_2O with a volumetric pipette (fuldpipette)
- Add 23,4 µL NH_4OH
- Mix well
- Fill up to 1 L with EtOH
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

Buffer C: IPA + 5.0% H_2O + 5 mM Ammonium formate (AmFA)/Ammonium hydroxide (AmOH):

- Use the 1 L volumetric flask labeled "MeOH + AmFA/AmOH"
- Rinse the volumetric flask three times with IPA
- Weigh out 298.5 mg AmFA and add it to the volumetric flask
- Add 200 mL IPA in a 1L volumetric flask
- Add 50.0 mL of H_2O with a volumetric pipette (fuldpipette)
- Add 23,4 µL NH_4OH
- Mix well
- Fill up to 1 L with IPA
- Transfer the solution to a blue cap flask (eluent flask)
- Degas the solution for 15 min.

4.9 QUICK GUIDE – sequence list preparation

This is a step-by-step guide for modifying the sequence list

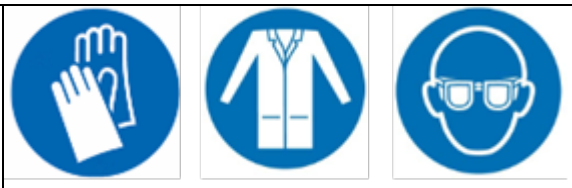
- When it is only the MIX INDEX names that change:
    - Click on SEQUENCE in the upper black line
- Open an old version "Open a sequence" and save it right away with another name! "Save the current Sequence as a new file"
- Change the MIX index name in the column "Sample name"
- Change the column names – ONLY if they have been changed (😉) – in the same line as mix index name ("Sample name")
- Make sure that the "shutdown LS-MS FoU" procedure is at the last line (under "Acq. Method)
- Save the sequence
- When ready to run the sequence - Press RUN

4.10 QUICK GUIDE – start-up

- Prepare BUFFER A – see "Preparation of eluents"
- While degassing the buffer, clean the spray chamber (MS)
    - Make a 50:50 solution of 2-propanol:H_2O (only a small amount)
    - Make sure the MS is STANDBY and that it is not hot!
    - Open the chamber on the right side of the module
    - Use a plastic pipette and add the solution on the front plate of the module – have lens paper under!
    - Close the chamber properly
- Run a CHECKTUNE:
    - Click on METHOD in the upper menu
    - Lock the MS by clicking on the key "Request tune control"
    - Make sure that "Both" are ticked off under "Autotune/Checktune"
    - Click on "Checktune the instrument" (key icon)
    - Now the checktune is running
    - When finished, a checktune report will appear on the screen and hopefully everything is green – passed 😊
    - Click "Release tune control" (key icon)
    - Click on STATUS in the upper menu
- Change of BUFFER A
    - Stop both pumps
    - Change the BUFFER A flask and transfer the tubes from the old flask to the new one – remember not to touch the tubes with the gloves (gives a signal in the spectrum 😊)
    - Purge with BUFFER A by opening the purge valves and set the pump rate to 5.000 mL/min with 100% buffer A
    - Purge until there is no air in the tubes (min. 1 minute)
    - Stop the pumps
    - Close the purge valves
    - Set both pumps to 0.400 mL/min with 95:5 (H2O:ACN), while preparing the mixes
- Prepare mix after "Protocol for preparing compound mixes"
- Place the vials in the right order in the autosampler
- Click on SEQUENCE in the upper menu and make sure it is the right sequence
- Click RUN 😊

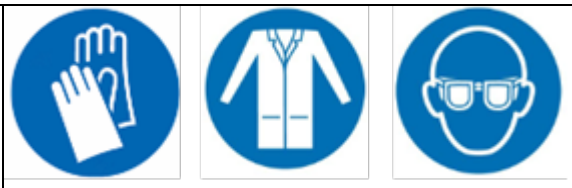
5.1 Kemisk risikovurdering 2-propanol

Risikovurdering	
1. **Stofnavn og koncentration**	**2-propanol**
2. **CAS nr.**	67-63-0
3. **Piktogrammer**	
4. **Signalord**	Fare
5. **H-sætninger**	• **H225:** Meget brandfarlig væske og damp • **H319:** Forårsager alvorlig øjenirritation • **H336:** Kan forårsage sløvhed og svimmelhed • **EUH019:** Kan danne eksplosive peroxider
6. **P-sætninger**	• **P210:** Holdes væk fra varme, varme overflader, gnister, åben ild og andre antændelseskilder. Rygning forbudt. • **P280:** Bær beskyttelseshandsker/øjenbeskyttelse • **P304+P340:** Ved indånding • **P305+P351+P338:** VED KONTAKT MED ØJNENE: Skyl forsigtigt med vand i flere minutter. Fjern eventuelle kontaktlinser, hvis dette kan gøres let. Fortsæt skylning.
7. **Tema**	FoU projekt: Bæredygtig metodeudvikling og identifikation af stoffer – HPLC
8. **Proces hvormed stoffet anvendes**	Rensning af spraykammer på MS og som eluent
9. **Anvendt mængde**	5 mL (50% opløsning) + 1 liter (~100%)

10. **Forholdsregler**	 **Stinkskab:** Ved al arbejde med stoffet **Spild:** C dunk (for det rene stof) – H dunk (opløsningen) **Bortskaffelse af affald:** Produktet må ikke komme i kloakafløb. **Andre forholdsregler:** Opbevar beholderen tætlukket på et tørt. Holdes væk fra varme og antændelseskilder. Arbejd under udsugning. Undgå indånding. Undgå udvikling af dampe.
11. **Risikovurdering og håndtering af stoffet i hele processen**	Der laves en 50:50 opløsning af 2-propanol:H_2O i et bægerglas ved først at afpipettere 5 mL H_2O ned i et bægerglas, og herefter afpipetteres 5 mL 2-propanol ned i samme bægerglas. Blandingen omrøres forsigtigt med en engangspipette. Til fremstilling af eluent skylles målekolben med 2-propanol som hældes i C-dunk og der fyldes herefter halvt op med 2-propanol, tilsættes myresyre og vand. Dernæst fyldes p til stregen med 2-propanol. Al arbejde med at lave opløsningen foregår i stinkskab med engangshandsker på.

5.2 Kemisk risikovurdering Acetonitril

Risikovurdering	
1. **Stofnavn og koncentration**	**Acetonitril**
2. **CAS nr.**	75-05-8
3. **Piktogrammer**	
4. **Signalord**	Fare
5. **H-sætninger**	• **H225:** Meget brandfarlig væske og damp • **H302+H312+H332:** Farlig ved indtagelse, hudkontakt eller indånding • **H319:** Forårsager alvorlig øjenirritation
6. **P-sætninger**	• **P210:** Holdes væk fra varme, varme overflader, gnister, åben ild og andre antændelseskilder. Rygning forbudt. • **P261:** Undgå indånding af dampe og aerosoler. • **P280:** Bær beskyttelseshandsker/øjenbeskyttelse • **P301+P310:** I TILFÆLDE AF INDTAGELSE: Ring omgående til GIFTLINJEN/læge • **P303+P361+P353:** VED KONTAKT MED HUDEN (eller håret): Alt tilsmudset tøj tages straks af. Skyl huden med vand. • **P305+P351+P338:** VED KONTAKT MED ØJNENE: Skyl forsigtigt med vand i flere minutter. Fjern eventuelle kontaktlinser, hvis dette kan gøres let. Fortsæt skylning.
7. **Tema**	FoU projekt: Bæredygtig metodeudvikling og identifikation af stoffer – HPLC
8. **Proces hvormed stoffet anvendes**	Fremstilling af eluent/buffer
9. **Anvendt mængde**	~2000 mL (99,9%)

10. **Forholdsregler**	 **Stinkskab:** Ved al arbejde med stoffet **Spild:** C dunk (rene væske) – H dunk (eluent/buffer) **Bortskaffelse af affald:** Produktet må ikke komme i kloakafløb. **Andre forholdsregler:** Opbevar beholderen tætlukket på et tørt. Holdes væk fra varme og antændelseskilder. Arbejd under udsugning. Undgå indånding.

11. **Risikovurdering og håndtering af stoffet i hele processen**	Acetonitril (ACN) er brandfarligt og farlig ved indånding, så ved fremstilling af eluent/buffer foregår al arbejdet i stinkskab og med engangshandsker, briller og kittel på. Eluent/buffer fremstilles ved at skylles en 1000 mL målekolbe tre gange med ~10 mL ren ACN. Mellem hvert skyl hældes ACN i H-dunken, som står i vasken i stinkskabet. Herefter hældes der ~950 mL ACN i målekolben og der tilsættes 1 mL konc. myresyre (Risikovurdering MYRESYRE) med pipette. Målekolben fyldes op til stregen med ACN. Eluent/buffer overføres til en blue cap flaske og sættes til afgasning i 15 min. Ved overførelsen af eluent/buffer til blue cap flaske tørres eventuelt spild af med et stykke papir som ligges til afdampning i stinkskabet inden det kommes i H spanden. Hvis der spildes større mængder, så skal der anvendes sand og åndedrætsværn! Eluent/buffer skal derefter anvendes ved HPLC'en og da flaskerne med eluent/buffer står ovenpå apparatet er det vigtigt at bruge elefantfoden, hvis man ikke kan være i øjenhøjde med flaskerne. Det er vigtigt, at låget på flasken ikke tages af udenfor sugekassen over apparatet og at slangerne fra den nuværende flaske tages så forsigtigt op, at der ikke kommer sprøjt af ACN. Slangerne anbringes i den nye flaske med lige så stor forsigtighed for at undgå sprøjt. Hvis væsken kommer i øjnene, så skyl øjnene med åbent øjenlåg i flere minutter under rindende vand og søg læge. Hvis væsken kommer i kontakt med huden, så vask med rigelig sæbe og vand.

5.3 Kemisk risikovurdering Methanol

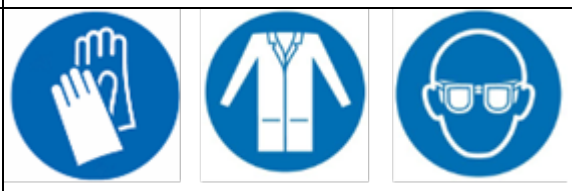
Risikovurdering	
1. **Stofnavn og koncentration**	**Methanol**
2. **CAS nr.**	67-56-1
3. **Piktogrammer**	
4. **Signalord**	Fare
5. **H-sætninger**	• **H225:** Meget brandfarlig væske og damp • **H301+H311+H331:** Giftig ved indtagelse, hudkontakt eller indånding • **H370:** Forårsager organskader
6. **P-sætninger**	• **P210:** Holdes væk fra varme, varme overflader, gnister, åben ild og andre antændelseskilder. Rygning forbudt. • **P280:** Bær beskyttelseshandsker/øjenbeskyttelse. • **P301+P310:** I TILFÆLDE AF INDTAGELSE: Ring omgående til GIFTLINJEN/læge • **P303+P361+P353:** VED KONTAKT MED HUDEN (eller håret): Alt tilsmudset tøj tages straks af. Skyl huden med vand. • **P304+P340:** VED INDÅNDING: Flyt personen til et sted med frisk luft og sørg for, at vedkommende hviler i en stilling som letter vejrtrækningen. Ring omgående til en læge. • **P405:** Opbevares under lås
7. **Tema**	FoU projekt: Bæredygtig metodeudvikling og identifikation af stoffer – HPLC

8. **Proces hvormed stoffet anvendes**	Fremstilling af eluent/buffer
9. **Anvendt mængde**	~1000 mL (99,9%)
10. **Forholdsregler**	   **Stinkskab:** Ved al arbejde med stoffet **Spild:** C dunk (rene væske) – H dunk (eluent/buffer) **Bortskaffelse af affald:** Produktet må ikke komme i kloakafløb. **Andre forholdsregler:** Opbevar beholderen tætlukket på et tørt og godt ventileret sted. Holdes væk fra varme og antændelseskilder. Hold låst inde eller i et område kun med adgang for kvalificeret eller autoriseret personale. Arbejd under udsugning. Undgå indånding. Undgå udvikling af dampe.

11. **Risikovurdering og håndtering af stoffet i hele processen**	Methanol (MeOH)er både brandfarligt og sundhedsskadeligt, så ved fremstilling af eluent/buffer foregår al arbejdet i stinkskab og med engangshandsker, briller og kittel på. Eluent/buffer fremstilles ved at skylles en 1000 mL målekolbe tre gange med ~10 mL ren methanol. Mellem hvert skyl hældes MeOH i H-dunken, som står i vasken i stinkskabet. Herefter hældes der ~950 mL MeOH i målekolben og der tilsættes 1 mL konc. myresyre (Risikovurdering MYRESYRE) med pipette. Målekolben fyldes op til stregen med MeOH. Eluent/buffer overføres til en blue cap flaske og sættes til afgasning i 15 min. Ved overførelsen af eluent/buffer til blue cap flaske tørres eventuelt spild af med et stykke papir som efterfølgende kommes i H dunken. Hvis der spildes større mængder, så skal der anvendes sand og åndedrætsværn! Eluent/buffer skal derefter anvendes ved HPLC'en og da flaskerne med eluent/buffer står ovenpå apparatet er det vigtigt at bruge elefantfoden, hvis man ikke kan være i øjenhøjde med flaskerne. Det er vigtigt at låget på flasken ikke tages af udenfor sugekassen over apparatet og at slangerne som skal ned i flasken tages så forsigtigt op, at der ikke kommer sprøjt af MeOH. Hvis væsken kommer i øjnene, så skyl øjnene med åbent øjenlåg i flere minutter under rindende vand og søg læge. Hvis væsken kommer i kontakt med huden, så vask med rigelig sæbe og vand.

5.4 Kemisk risikovurdering Myresyre

Risikovurdering	
1. **Stofnavn og koncentration**	**Myresyre** (Formic Acid), 98% - 100%
2. **CAS nr.**	64-18-6
3. **Piktogrammer**	
4. **Signalord**	Fare
5. **H-sætninger**	• **H226**: Brandfarlig væske og damp • **H302:** Farlig ved indtagelse • **H314:** Forårsager svære ætsninger på huden og øjenskader • **H331:** Giftig ved indånding
6. **P-sætninger**	• **P210:** Holdes væk fra varme, varme overflader, gnister, åben ild og andre antændelseskilder. Rygning forbudt. • **P280:** Bær beskyttelseshandsker/øjenbeskyttelse. • **P301+P312:** I TILFÆLDE AF INDTAGELSE: Ring til GIFTLINJEN/ læge i tilfælde af ubehag. • **P303+P361+P353:** VED KONTAKT MED HUDEN (eller håret): Tilsmudset tøj tages straks af/fjernes. Skyl huden med vand. • **P304+P340+P310:** VED INDÅNDING: Flyt personen til et sted med frisk luft og sørg for, at vejrtrækningen lettes. Ring omgående til en læge. • **P305+P351+P338:** VED KONTAKT MED ØJNENE: Skyl forsigtigt med vand i flere minutter. Fjern eventuelle kontaktlinser, hvis dette kan gøres let. Fortsæt skylning.
7. **Tema**	FoU projekt: Bæredygtig metodeudvikling og identifikation af stoffer – HPLC
8. **Proces hvormed stoffet anvendes**	Fremstilling af eluent/buffer

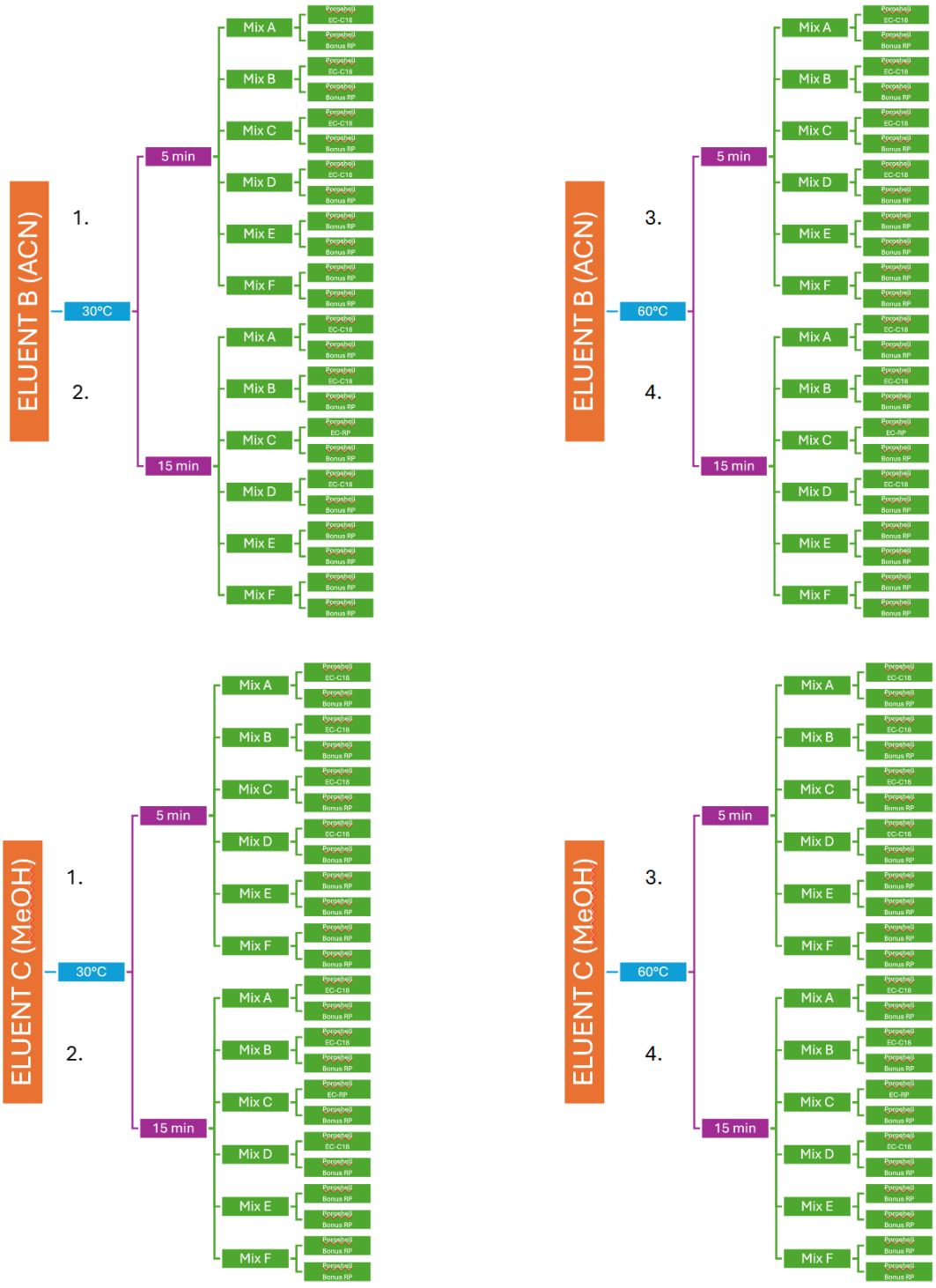
9. **Anvendt mængde**	0,1% (1mL eller 2mL af den konc. myresyre)
10. **Forholdsregler**	 **Stinkskab:** Ved al arbejde med stoffet **Spild:** C dunk (rene væske) – H dunk (eluent/buffer) **Bortskaffelse af affald:** Produktet må ikke komme i kloakafløb. **Andre forholdsregler:** Beskyttet mod lys. Opbevar beholderen tætlukket på et tørt og godt ventileret sted. Holdes væk fra varme og antændelseskilder. Hold låst inde eller i et område kun med adgang for kvalificeret eller autoriseret personale.
11. **Risikovurdering og håndtering af stoffet i hele processen**	Myresyre (FA) er både brandfarligt, ætsende og sundhedsskadeligt, så ved fremstilling af eluent/buffer foregår al arbejdet i stinkskab og med engangshandsker, briller og kittel på. Myresyren anvendes ved fremstilling af eluent/buffer og der henvises derfor til følgende risikovurderinger: Fremstilling af BUFFER B (ACN:FA) Fremstilling af BUFFER C (MeOH:FA) FA står i aflåst skab og skal håndteres under udsug. Håndtering af FA under fremstilling af eluent/buffer foregår med pipette og pipettespidsen kommes i spanden med plastaffald, hvor den afdamper inden udsmidning. Hvis væsken kommer i øjnene, så skyl øjnene med åbent øjenlåg i flere minutter under rindende vand og søg læge. Hvis væsken kommer i kontakt med huden, så vask med rigelig sæbe og vand.

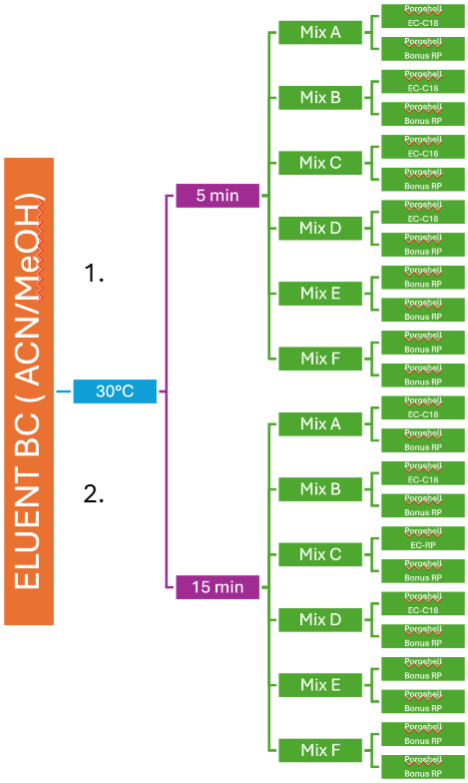
5.5 Kemisk risikovurdering stoffer og mixes

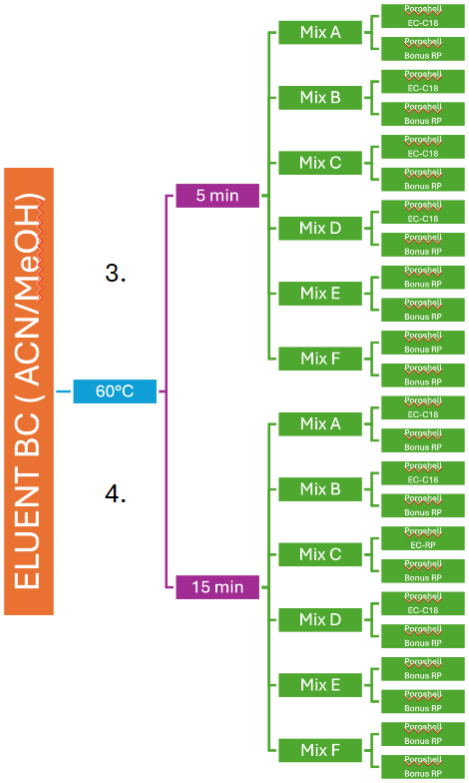
Risikovurdering	
1. Stofnavn og koncentration	Stoffer til brug for F0U-projektet Bæredygtig HPLC Mix A-L Individuelle stoffer
2. Hvilke stoffer og hvad dækker denne risikovurdering	Alle stofferne står i kemikalieoversigten (regneark) på Sharepoint, fanen FOU 2024. Samtlige SDS'er ligger på Sharepoint under. Der er taget udgangspunkt i de værste klassificeringer og lavet en generel risikovurdering ud fra det. Alle stoffer og blandinger er som minimum H225: Meget brandfarlig væske og damp H302: Farlig ved indtagelse H319: Forårsager alvorlig øjenirritation
3. Piktogrammer	
4. Signalord	Fare
5. H-sætninger	H225: Meget brandfarlig væske og damp H301/302/311/312/332: Giftig ved indtagelse, hudkontakt, farlig ved indånding H319: Forårsager alvorlig øjenirritation H350: Kan fremkalde kræft H360: Kan skade forplantningsevnen H370: Forårsager organskader H412. Skadelig for vandlevende organismer, med langvarige virkninger

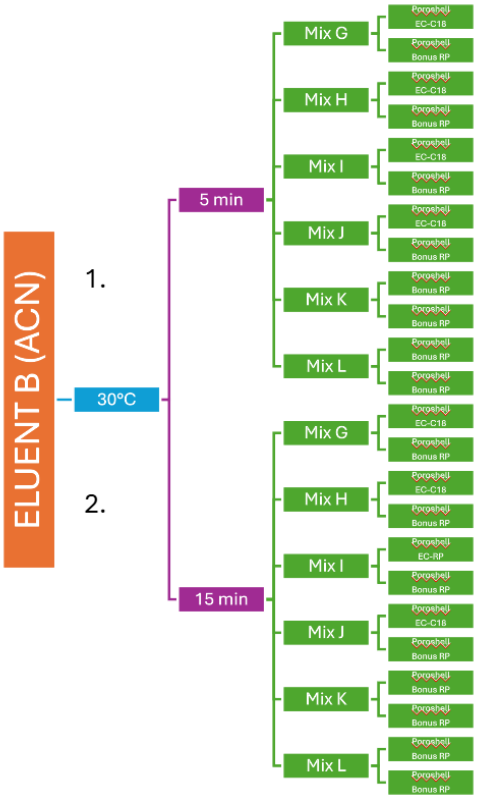
6. P-sætninger	P210: Holdes væk fra varme, varme overflader, gnister, åben ild og andre antændelseskilder. P280: Bær beskyttelseshandsker og briller. P301+P310: I tilfælde af indtagelse, ring omgående til en GIFTINFORMATION eller læge. P201: Indhent særlige anvisninger før brug P308: Ved eksponering eller mistanke om eksponering: Vask, skyl, træk frisk luft
7. Benyttelse	Bruges ved analyse på LC-MS: Ved projektarbejde
8. Beskriv processen og eksponerings-risiko i hele processen	Overførsel af lille mængde fra ampul til vial Håndtering af vials fra fryser til autosampler
9. Anvendt mængde	Slutvolumen af hvert mix er 100 µL og slut koncentrationen er ca. 5 µg/L.
10. Forholdsregler	Der arbejdes med engangshandsker, briller (som altid) og i stinkskab. Spild hældes i H-dunk. Brugte vials tømmes i H-dunk + lægges til afdunstning i stinkskab til glasaffald, låg til plast
11. Risikovurdering og håndtering af stoffet i hele processen	Da risikovurderingen er lavet over denne gruppe af stoffer, der bruges til forsøget, er det lavet ud fra stofferne med de værste iboende stoffer. Fælles for alle er: Stoffer og vials håndteres i stinkskab, med beskyttelsesbriller og handsker. Der arbejdes med små mængder og med lukkede vials.

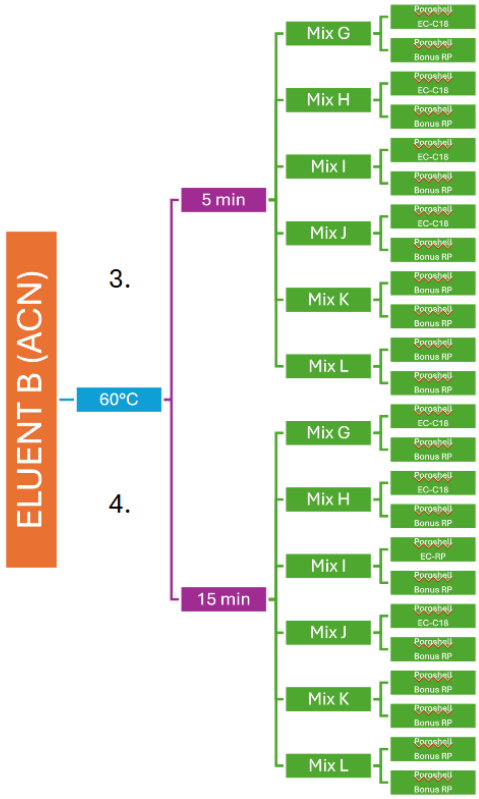
6.1 Eksempel på forsøgsoversigt for 2 kolonner, acetonitril og methanol, 1 pH-værdi

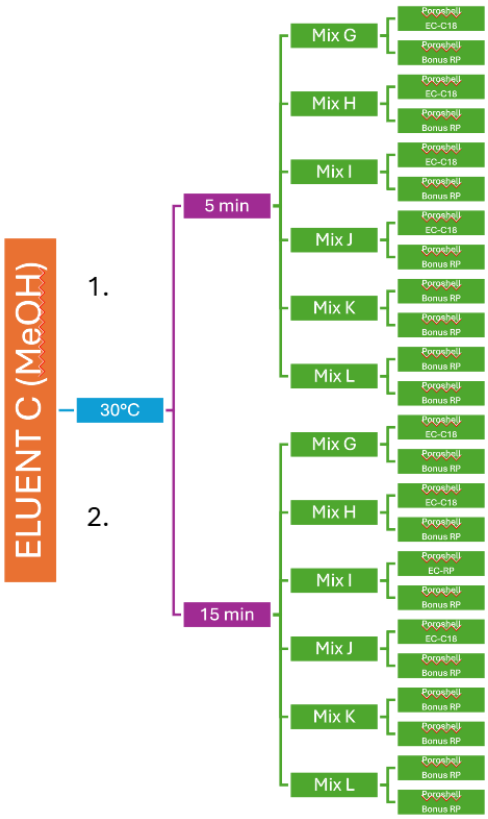


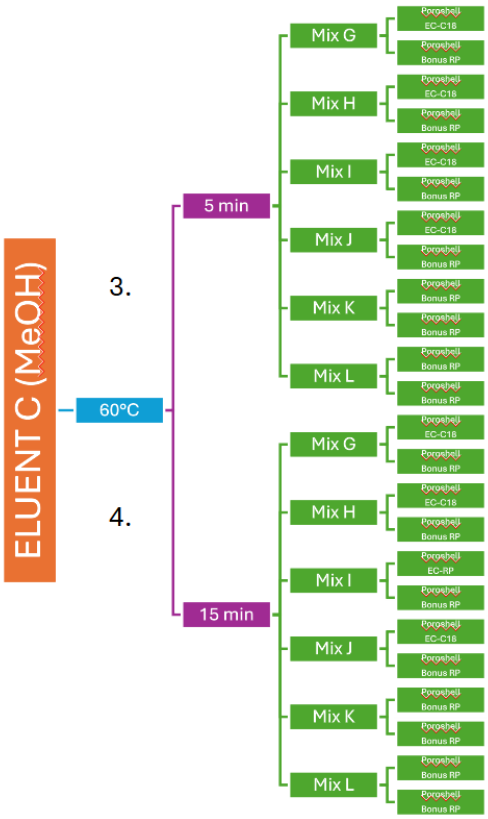

ELUENT BC (ACN/MeOH)
1.
30°C
2.
5 min
15 min
Mix A
Mix B
Mix C
Mix D
Mix E
Mix F
Mix A
Mix B
Mix C
Mix D
Mix E
Mix F

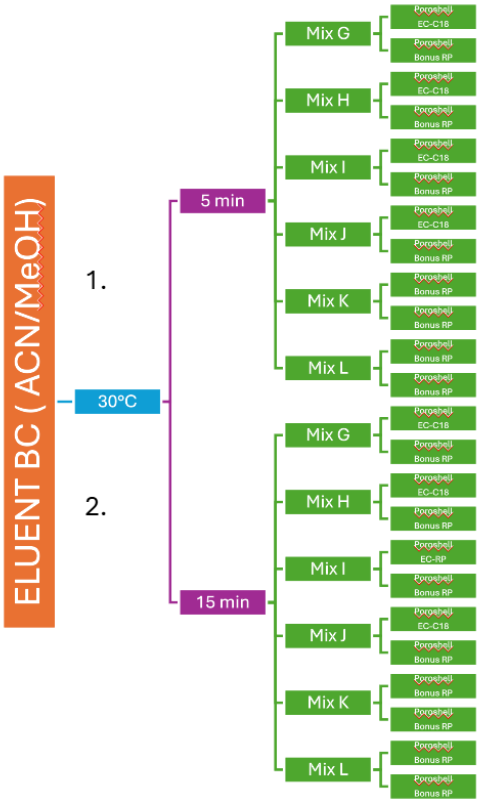

ELUENT BC (ACN/MeOH)
3.
60°C
4.
5 min
15 min
Mix A
Mix B
Mix C
Mix D
Mix E
Mix F
Mix A
Mix B
Mix C
Mix D
Mix E
Mix F

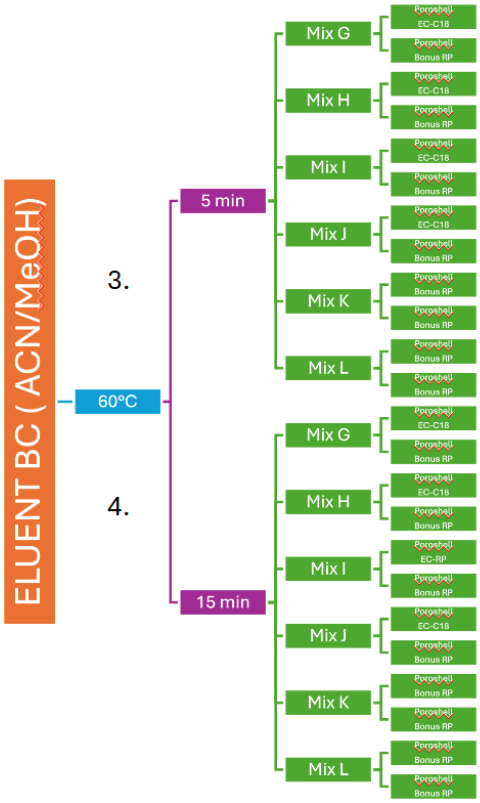

ELUENT B (ACN)
1.
30°C
2.
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L


ELUENT B (ACN)
3.
60°C
4.
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L


ELUENT C (MeOH)
1.
2.
30°C
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Poroshell EC-C18
Poroshell Bonus RP
Poroshell EC-RP


ELUENT C (MeOH)
3.
4.
60°C
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Poroshell EC-C18
Poroshell Bonus RP
Poroshell EC-RP


ELUENT BC (ACN/MeOH)
1.
2.
30°C
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Poroshell EC-C18
Poroshell Bonus RP
Poroshell EC-RP


ELUENT BC (ACN/MeOH)
3.
4.
60°C
5 min
15 min
Mix G
Mix H
Mix I
Mix J
Mix K
Mix L
Poroshell EC-C18
Poroshell Bonus RP
Poroshell EC-RP

6.2 Forsøgsoversigt: ACN og MeOH

						Ansvarlig	Udført
		Mandag		Opstart apparat			
		Onsdag					
ACN MeOH Kombi pH=2,7		Fredag		2 nye kolonner (1+2) - Poroshell	Mix A-F		
		Mandag			Mix G-L		
		Onsdag		2 nye kolonner (3+4 - Poroshell	Mix A-F		
		Fredag			Mix G-L		
ACN MeOH Kombi pH = 4		Mandag		2 nye kolonner (3+4) -- Poroshell	Mix A-F		
		Onsdag			Mix G-L		
		Fredag		2 nye kolonner (1+2) – Poroshell	Mix A-F		
		Mandag			Mix G-L		
ACN MeOH kombi pH = 8		Onsdag		2 nye kolonner (1+2) - Poroshell	Mix A-F		
		Fredag			Mix G-L		
		Mandag		2 nye kolonner (3+4 - Poroshell	Mix A-F		
		Onsdag			Mix G-L		
ACN MeOH Kombi pH=2,7		Fredag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Mandag			Mix G-L		
		Onsdag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Fredag			Mix G-L		
ACN MeOH Kombi pH = 4		Mandag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Onsdag			Mix G-L		
		Fredag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Mandag			Mix G-L		
ACN MeOH Kombi pH=8		Onsdag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Fredag			Mix G-L		
		Mandag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Onsdag			Mix G-L		
		Fredag					
		Mandag					
		Onsdag					
		Fredag					
		Mandag					
		Onsdag					
		Fredag					
		Mandag			-		-
		Onsdag			-		-
		Fredag			-		-
		Mandag			-		-
		Onsdag					
		Fredag					

6.3 Forsøgsoversigt: Ethanol og 2-propanol

						Ansvarlig	Udført
		Mandag		Opstart apparat			
		Onsdag					
Ethanol Propanol Kombi pH=2,7		Fredag		2 nye kolonner (1+2) - Poroshell	Mix A-F		
		Mandag			Mix G-L		
		Onsdag		2 nye kolonner (3+4 - Poroshell	Mix A-F		
		Fredag			Mix G-L		
Ethanol Propanol Kombi pH = 4		Mandag		2 nye kolonner (3+4) -- Poroshell	Mix A-F		
		Onsdag			Mix G-L		
		Fredag		2 nye kolonner (1+2) – Poroshell	Mix A-F		
		Mandag			Mix G-L		
Ethanol Propanol Kombi pH = 8		Onsdag		2 nye kolonner (1+2) - Poroshell	Mix A-F		
		Fredag			Mix G-L		
		Mandag		2 nye kolonner (3+4 - Poroshell	Mix A-F		
		Onsdag			Mix G-L		
Ethanol Propanol Kombi pH=2,7		Fredag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Mandag			Mix G-L		
		Onsdag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Fredag			Mix G-L		
Ethanol Propanol Kombi pH = 4		Mandag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Onsdag			Mix G-L		
		Fredag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Mandag			Mix G-L		
Ethanol Propanol Kombi pH=8		Onsdag		2 nye kolonner (5+6) – Zorba	Mix A-F		
		Fredag			Mix G-L		
		Mandag		2 nye kolonner (7+8) – Zorba	Mix A-F		
		Onsdag			Mix G-L		
		Fredag					
		Mandag					
		Onsdag					
		Fredag					
		Mandag					
		Onsdag					
		Fredag					
		Mandag					
		Onsdag					
		Fredag					
		Mandag					
		Onsdag					
		Fredag					

7.1 Omformatering af signaler

Åbn Python

Hent Chris' fil på Sharepoint, FoU, HPLC, Databehandling, molecular datafile, molecule_consolidator.py

Åbn I appen

Åbn igen

Åbn MestReNova

Download stofliste fra Sharepoint (sds-fil)

Åbn stofliste I MestReNova

Find resultatfil på USB; træk over

Ha' 2 vinduer åbne i Stifinder. USB + "hvor man gemmer"

Molecular mix

Copy

Sæt ind i Chris' fil

Navngiv korrekt

Consolidate and save

Clear area

Input

Ved mix' skift: Slet færdigt mix:

Vælg compounds i bunden

Marker ved klik lille vsntre felt øverst

Delete

7.2 Hjælp til Selektion af retentionstider/stoffer der indgår i databasen

Først fjernes alle ikke-fundne stoffer.

Medtager kun ID med similarity >0,9.

Alle referencer (histamin, cefeporazone og rifaximin) tages med uanset similarity

Oprettes en kolonne der hedder logik:

=TÆL.HVISER($C$2:$C$10000;C5072;$R$2:$R$10000;R5072)

= COUNTIFS($C$2:$C$20000;C2;$R$2:$R$20000;R2)

Hvor kolonne C er isotopoic mass og kolonne R er original filename

Denne funktion tæller hvor mange gange en isotopisk masse indgår i hver kørsel

2 isomere i samme prøve.

1. Hvis der er to isomerer i samme prøve, kan det være to med samme navn.

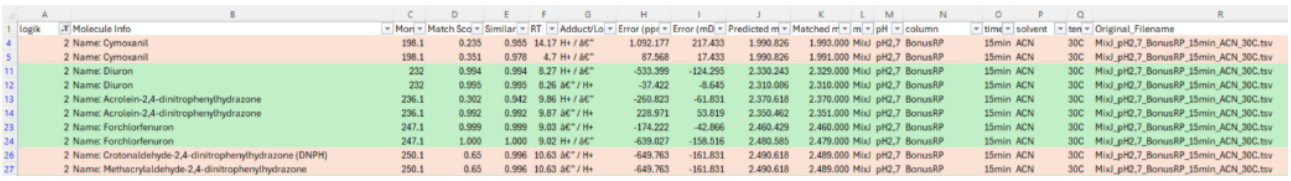
Her vurderes det om de har samme retentionstid og ionisere i både positiv og negativ. Hvis det er tilfældet, markeres begge som identificeret.

Hvis ikke det samme stofnavn i prøven har samme retentionstid (eller begge ioniserer i samme polaritet) markeres de begge som ikke fundet

2. De to isomerer kan også have to forskellige navne og være strukturisomerer.

Her markeres begge som ikke fundet.

Se eksempel på to med samme navn men forskellig retentionstid i den øverste røde. De grønne er samme navn, samme retentionstid og ionisering i både negativ og positiv og sidste røde er to strukturisomerer med samme masse, og hvor det ikke er muligt at skelne.

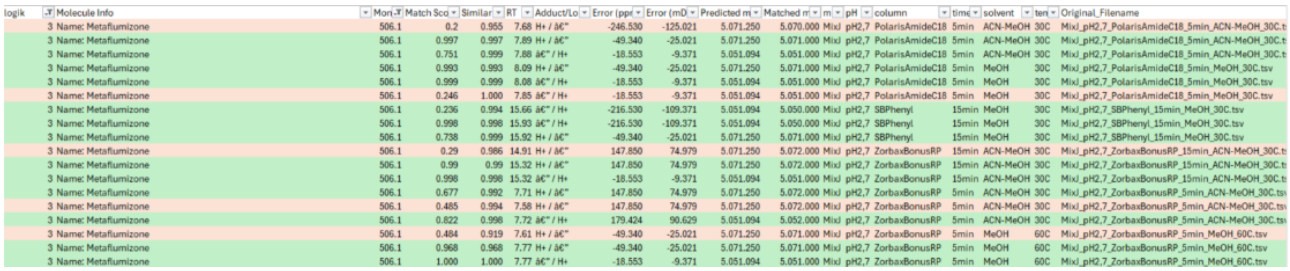


	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	logik	Molecule Info	Mon	Match Sco	Similar	RT	Adduct/Lo	Error (ppr	Error (mD	Predicted m	Matched m	m	pH	column	time	solvent	ten	Original_Filename
4		2 Name: Cymoxanil	198.1	0.235	0.955	14.17	H+ / â€"	1.092.177	217.433	1.990.826	1.993.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
5		2 Name: Cymoxanil	198.1	0.351	0.978	4.7	H+ / â€"	87.568	17.433	1.990.826	1.991.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
11		2 Name: Diuron	232	0.994	0.994	8.27	H+ / â€"	-533.399	-124.295	2.330.243	2.329.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
12		2 Name: Diuron	232	0.995	0.995	8.26	â€" / H+	-37.422	-8.645	2.310.086	2.310.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
13		2 Name: Acrolein-2,4-dinitrophenylhydrazone	236.1	0.302	0.942	9.86	H+ / â€"	-260.823	-61.831	2.370.618	2.370.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
14		2 Name: Acrolein-2,4-dinitrophenylhydrazone	236.1	0.992	0.992	9.87	â€" / H+	228.971	53.819	2.350.462	2.351.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
23		2 Name: Forchlorfenuron	247.1	0.999	0.999	9.03	â€" / H+	-174.222	-42.866	2.460.429	2.460.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
24		2 Name: Forchlorfenuron	247.1	1.000	1.000	9.02	H+ / â€"	-639.027	-158.516	2.480.585	2.479.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
26		2 Name: Crotonaldehyde-2,4-dinitrophenylhydrazone (DNPH)	250.1	0.65	0.996	10.63	â€" / H+	-649.763	-161.831	2.490.618	2.489.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv
27		2 Name: Methacrylaldehyde-2,4-dinitrophenylhydrazone	250.1	0.65	0.996	10.63	â€" / H+	-649.763	-161.831	2.490.618	2.489.000	Mix	pH2,7	BonusRP	15min	ACN	30C	Mix_pH2,7_BonusRP_15min_ACN_30C.tsv

3 Isomere i samme prøve

Hvis der er tre isomerer i samme prøve, vurderes det hvilke der er rigtig ved at se på om to af dem har samme retentionstid og ionisere i både positiv og negativ. Scoren kan også vurderes, men i de fleste tilfælde er scoren høj for alle tre.

Se eksempel:



logik	Molecule Info	Mon	Match Sco	Similar	RT	Adduct/Lo	Error (ppr	Error (mD	Predicted m	Matched m	m	pH	column	time	solvent	ten	Original_Filename
	3 Name: Metaflumizone	506.1	0.2	0.955	7.68	H+ / â€"	-246.530	-125.021	5.071.250	5.070.000	Mix	pH2,7	PolarisAmideC18	5min	ACN-MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.997	0.997	7.89	H+ / â€"	-49.340	-25.021	5.071.250	5.071.000	Mix	pH2,7	PolarisAmideC18	5min	ACN-MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.751	0.999	7.88	â€" / H+	-18.553	-9.371	5.051.094	5.051.000	Mix	pH2,7	PolarisAmideC18	5min	ACN-MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.993	0.993	8.09	H+ / â€"	-49.340	-25.021	5.071.250	5.071.000	Mix	pH2,7	PolarisAmideC18	5min	MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.999	0.999	8.08	â€" / H+	-18.553	-9.371	5.051.094	5.051.000	Mix	pH2,7	PolarisAmideC18	5min	MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.246	1.000	7.85	â€" / H+	-18.553	-9.371	5.051.094	5.051.000	Mix	pH2,7	PolarisAmideC18	5min	MeOH	30C	Mix_pH2,7_PolarisAmideC18_5min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.236	0.994	15.66	â€" / H+	-216.530	-109.371	5.051.094	5.050.000	Mix	pH2,7	SBPhenyl	15min	MeOH	30C	Mix_pH2,7_SBPhenyl_15min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.998	0.998	15.93	â€" / H+	-216.530	-109.371	5.051.094	5.050.000	Mix	pH2,7	SBPhenyl	15min	MeOH	30C	Mix_pH2,7_SBPhenyl_15min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.738	0.999	15.92	H+ / â€"	-49.340	-25.021	5.071.250	5.071.000	Mix	pH2,7	SBPhenyl	15min	MeOH	30C	Mix_pH2,7_SBPhenyl_15min_MeOH_30C.tsv
	3 Name: Metaflumizone	506.1	0.29	0.986	14.91	H+ / â€"	147.850	74.979	5.071.250	5.072.000	Mix	pH2,7	ZorbaxBonusRP	15min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_15min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.99	0.99	15.32	H+ / â€"	147.850	74.979	5.071.250	5.072.000	Mix	pH2,7	ZorbaxBonusRP	15min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_15min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.998	0.998	15.32	â€" / H+	-18.553	-9.371	5.051.094	5.051.000	Mix	pH2,7	ZorbaxBonusRP	15min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_15min_ACN-MeOH_30C.t
	3 Name: Metaflumizone	506.1	0.677	0.992	7.71	H+ / â€"	147.850	74.979	5.071.250	5.072.000	Mix	pH2,7	ZorbaxBonusRP	5min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_5min_ACN-MeOH_30C.ts
	3 Name: Metaflumizone	506.1	0.485	0.994	7.58	H+ / â€"	147.850	74.979	5.071.250	5.072.000	Mix	pH2,7	ZorbaxBonusRP	5min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_5min_ACN-MeOH_30C.ts
	3 Name: Metaflumizone	506.1	0.822	0.998	7.72	â€" / H+	179.424	90.629	5.051.094	5.052.000	Mix	pH2,7	ZorbaxBonusRP	5min	ACN-MeOH	30C	Mix_pH2,7_ZorbaxBonusRP_5min_ACN-MeOH_30C.ts
	3 Name: Metaflumizone	506.1	0.484	0.919	7.61	H+ / â€"	-49.340	-25.021	5.071.250	5.071.000	Mix	pH2,7	ZorbaxBonusRP	5min	MeOH	60C	Mix_pH2,7_ZorbaxBonusRP_5min_MeOH_60C.tsv
	3 Name: Metaflumizone	506.1	0.968	0.968	7.77	H+ / â€"	-49.340	-25.021	5.071.250	5.071.000	Mix	pH2,7	ZorbaxBonusRP	5min	MeOH	60C	Mix_pH2,7_ZorbaxBonusRP_5min_MeOH_60C.tsv
	3 Name: Metaflumizone	506.1	1.000	1.000	7.77	â€" / H+	-18.553	-9.371	5.051.094	5.051.000	Mix	pH2,7	ZorbaxBonusRP	5min	MeOH	60C	Mix_pH2,7_ZorbaxBonusRP_5min_MeOH_60C.tsv

Rød = fejl

Blå = kig mere på til haldor topsøe datasæt i mix J.

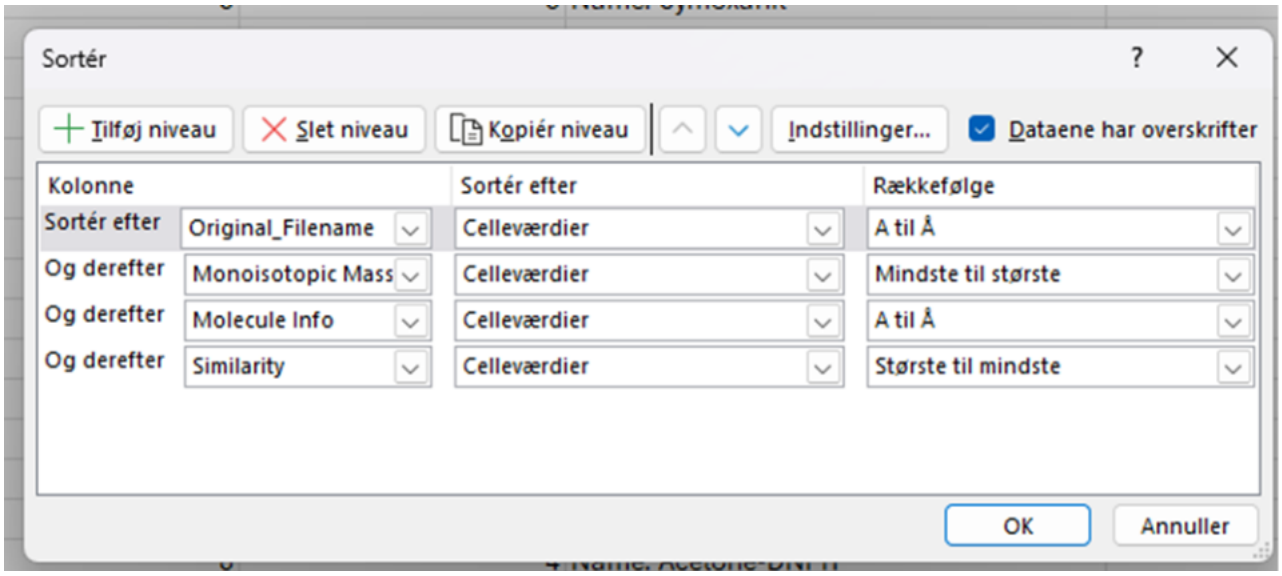
Lys-rød: valgt fra som forkert af mig

Grøn = valgt som korrekt af mig

lilla: similarity under 0,95 skal undersøges nærmere.

Gul – Skal undersøges nærmere

Sorter efter følgende



Mix B

Hydroxyibuprofen med to isomere er farvet gul for isomeren med den laveste retentionstid og den højeste similarity og matchscore

Mix A pH 8

Name: Iomeprol
Name: Iopamidol

Marked red because same chemical structure

Mix F:

Tepraloxydim. In the sorting with three matches per compound, there is a +/- pair with the ame retentiontime and another one in – with a lower retention time. This one does also match the theoretical spectrum well, and it also has a peak in positive, that matches, but are scaled to the same, and therefore dos not score. This low retention time is marked as yellow. In some instances this compound has the highest similarity and match score as well. This compound has both chirality and geometric isomers across two double bonds, giving rise to 4 isomers

Fenoxanil does also have chirl carbons and the same as for tepraloxydim is valid, that two peaks are seen, but only one is scored in both positive and negative. The last one has the correct pattern, but the scaling is off for the theoretical.

The same goes for chletodim sulfone.

For Mix F two datafiles are missing

Mix L.

2-Ethylhexyl trans-4-methoxycinnamate (OMC) and Octinoxate has the same structure and CAS number. They are therefore both green

8.1 Python-fil til omformatering af signal:

Molecular_consolidator.py – ligger på sharepoint: [molecule_consolidator]

molecule_consolidator.py

```
import tkinter as tk
from tkinter import filedialog, messagebox
import re
import os

# --- Global Constants ---
FILE_TYPES = [("Tab Separated Values", "*.tsv"), ("Text files", "*.txt"), ("All files", "*.*")]
DEFAULT_EXTENSION = ".tsv"
ALLDATA_FILE_PATH = "alldata.tsv"

def _process_molecule_data(text_content):
    """
    Core logic to consolidate molecule data.
    Returns a tuple: (output_lines, messages_to_show, data_lines_consolidated_count, header_processed_flag)
    """
    output_lines = []
    messages_to_show = []
    current_entry_lines = []
    header_processed = False
    data_lines_consolidated_count = 0

    if not text_content:
        messages_to_show.append((messagebox.showwarning, "Empty Text", "There's no text to process."))
        return [], messages_to_show, 0, False

    lines = text_content.split('\n')

    name_pattern = re.compile(r'^\s*\d+\s+(Name:.*)$')
    monoisotopic_data_pattern_simplified = re.compile(
        r'^\s*Monoisotopic Mass:\s*'
        r'('
        r'\S+(?:\s+\S+){4}\s+'
        r'(?:H\+|HCOO-|−)\s*/\s*(?:H\+|[-−])\s+'
        r'[-]?\d+\.?\d*\s+'
        r'[-]?\d+\.?\d*\s+'
        r'\d+\.?\d*\s+'
        r'\d+\.?\d*'
        r'(?:\s+.*)?'
        r')$'
    )
    monoisotopic_data_pattern_fallback = re.compile(
        r'^\s*Monoisotopic Mass:\s*(\S+.*)$'
    )

    for i, line in enumerate(lines):
        if i == 0 and not header_processed:
            modified_header = line.lstrip('\t')
            output_lines.append(modified_header)
            header_processed = True
            continue

        current_line_strip = line.strip()
        if not current_line_strip:
            if current_entry_lines:
                pass
            continue

        if re.match(r'^\s*\d+\s+Name:', current_line_strip):
            if current_entry_lines:
                pass # Discard incomplete previous entry implicitly
            current_entry_lines = [current_line_strip]
        elif current_entry_lines: # Add to current entry only if one has started
            current_entry_lines.append(current_line_strip)

```

```
        if len(current_entry_lines) == 4:
            name_line = current_entry_lines[0]
            monoisotopic_line = current_entry_lines[3]
            name_match = name_pattern.match(name_line)
            molecule_name = name_match.group(1).strip() if name_match else ""
            rest_of_data = ""
            monoisotopic_data_match = monoisotopic_data_pattern_simplified.match(monoisotopic_line)

            if monoisotopic_data_match:
                rest_of_data = monoisotopic_data_match.group(1).strip()
                try:
                    first_value_match_re = re.match(r'(\S+)(\s+)(.*)', rest_of_data)
                    if first_value_match_re:
                        first_val = first_value_match_re.group(1)
                        remaining_after_first = first_value_match_re.group(3)
                        second_value_match_re = re.match(r'(\S+)', remaining_after_first)
                        if second_value_match_re:
                            second_val = second_value_match_re.group(1)
                            if first_val == second_val:
                                rest_of_data = remaining_after_first
                except Exception:
                    pass # Keep original rest_of_data if error
            else:
                monoisotopic_data_match_fallback = monoisotopic_data_pattern_fallback.match(monoisotopic_line)
                if monoisotopic_data_match_fallback:
                    rest_of_data = monoisotopic_data_match_fallback.group(1).strip()
                    try:
                        first_value_match_re = re.match(r'(\S+)(\s+)(.*)', rest_of_data)
                        if first_value_match_re:
                            first_val = first_value_match_re.group(1)
                            remaining_after_first = first_value_match_re.group(3)
                            second_value_match_re = re.match(r'(\S+)', remaining_after_first)
                            if second_value_match_re:
                                second_val = second_value_match_re.group(1)
                                if first_val == second_val:
                                    rest_of_data = remaining_after_first
                    except Exception:
                        pass # Keep original rest_of_data if error

            if not (molecule_name or rest_of_data) and name_line: # If parsing failed for a potential entry
                print(f"Warning: Could not parse molecule entry starting with: '{name_line[:50]}...'")

            if molecule_name: # Only add if a name was successfully extracted
                consolidated_line = f"{molecule_name}\t{rest_of_data}"
                output_lines.append(consolidated_line)
                if rest_of_data: # Count only if there was actual data associated with the name
                    data_lines_consolidated_count += 1

            current_entry_lines = [] # Reset for the next block

    if not output_lines: # This means not even a header was processed (e.g. input was only blank lines)
        messages_to_show.append((messagebox.showwarning, "No Content Processed", "The input was empty or no lines were processed."))
    elif data_lines_consolidated_count == 0: # Header might be present, but no actual data consolidated
        if header_processed and len(output_lines) == 1 : # Only header is in output_lines
            messages_to_show.append((messagebox.showinfo, "Header Only", "The header was processed, but no complete 4-line molecule entries with extractable data were found."))
        elif header_processed and len(output_lines) > 1: # Header + names, but no mass data matched
            messages_to_show.append((messagebox.showwarning, "Data Incomplete", "Header and molecule names were processed, but matching mass data was not found for any entries."))
        elif not header_processed and output_lines: # Should be rare if first line is always header
             messages_to_show.append((messagebox.showwarning, "Data Incomplete", "Molecule names were processed, but no header was found and no matching mass data was extracted."))
        else: # Fallback, e.g. header_processed=False, output_lines is empty (covered by "No Content Processed") or contains only things not counted
            messages_to_show.append((messagebox.showwarning, "Processing Issue", "No data was consolidated as expected. Please check input format and script compatibility."))
    elif not header_processed : # data_lines_consolidated_count > 0 but no header was identified
        messages_to_show.append((messagebox.showwarning, "Data Only - Header Issue", "Molecule data was consolidated, but the header was not processed. The data will be saved/displayed."))

    return output_lines, messages_to_show, data_lines_consolidated_count, header_processed


def browse_output_file():
    """Opens a dialog to select a destination file and updates the entry field."""
    file_path = filedialog.asksaveasfilename(
        defaultextension=DEFAULT_EXTENSION, filetypes=FILE_TYPES, title="Select Output File Location"
    )
    if file_path:
        output_file_entry.delete(0, tk.END)
        output_file_entry.insert(0, file_path)

def save_consolidated_molecule_info_action():
    text_content = text_input.get("1.0", tk.END).strip()

    output_lines, messages, data_count, header_present = _process_molecule_data(text_content)

    for msg_func, title, msg_text in messages:
        msg_func(title, msg_text)

    processing_issue_shown = any("Processing Issue" in m[1] for m in messages) # Check title of message

    if not output_lines:
        return
    if processing_issue_shown and not (header_present and len(output_lines) >=1):
        return

    # --- Standard Save Operation ---
    file_path_to_save = output_file_entry.get().strip()
    if not file_path_to_save:
        file_path_to_save = filedialog.asksaveasfilename(
            defaultextension=DEFAULT_EXTENSION, filetypes=FILE_TYPES, title="Save Consolidated Molecule Data As..."
        )
```

```
161
162     main_save_successful = False
163     if file_path_to_save:
164         try:
165             with open(file_path_to_save, 'w', encoding='utf-8') as f:
166                 for out_line in output_lines:
167                     f.write(out_line + '\n')
168             messagebox.showinfo("Success", f"Consolidated molecule data successfully saved to:\n{file_path_to_save}")
169             main_save_successful = True
170         except Exception as e:
171             messagebox.showerror("Error", f"Failed to save file: {e}")
172             main_save_successful = False
173     else:
174         return
175
176     # --- Update "alldata.tsv" ---
177     if main_save_successful and output_lines and len(output_lines) > 0:
178         try:
179             existing_alldata_lines_set = set()
180             alldata_header_from_file = None
181
182             if os.path.exists(ALLDATA_FILE_PATH):
183                 with open(ALLDATA_FILE_PATH, 'r', encoding='utf-8') as f_all_read:
184                     is_first_line = True
185                     for line in f_all_read:
186                         stripped_line = line.strip()
187                         if not stripped_line: continue
188                         if is_first_line:
189                             alldata_header_from_file = stripped_line
190                             is_first_line = False
191                         else: existing_alldata_lines_set.add(stripped_line)
192
193             current_data_header = output_lines[0].strip() if output_lines else None
194             current_new_data_lines = []
195             if len(output_lines) > 1:
196                 for line_idx in range(1, len(output_lines)):
197                     stripped_data_line = output_lines[line_idx].strip()
198                     if stripped_data_line:
199                         current_new_data_lines.append(stripped_data_line)
200
201             final_header_for_alldata = alldata_header_from_file if alldata_header_from_file else current_data_header
202
203             for new_line in current_new_data_lines:
204                 existing_alldata_lines_set.add(new_line)
205
206             if final_header_for_alldata or existing_alldata_lines_set:
207                 with open(ALLDATA_FILE_PATH, 'w', encoding='utf-8') as f_all_write:
208                     if final_header_for_alldata: f_all_write.write(final_header_for_alldata + '\n')
209                     sorted_unique_data_lines = sorted(list(existing_alldata_lines_set))
210                     for unique_line in sorted_unique_data_lines: f_all_write.write(unique_line + '\n')
211                 print(f"'{ALLDATA_FILE_PATH}' updated successfully with unique consolidated data.")
212             else: print(f"No data to write to '{ALLDATA_FILE_PATH}'.")
213         except Exception as e_all:
214             messagebox.showerror("AllData Update Error", f"An error occurred while updating '{ALLDATA_FILE_PATH}':\n{e_all}")
215

216 def display_consolidated_info_action():
217     text_content = text_input.get("1.0", tk.END).strip()
218     output_lines, messages, data_count, header_present = _process_molecule_data(text_content)
219     for msg_func, title, msg_text in messages:
220         msg_func(title, msg_text)
221     processing_issue_shown = any("Processing Issue" in m[1] for m in messages)
222     if not output_lines: return
223     if processing_issue_shown and not (header_present and len(output_lines) >=1): return
224     if output_lines :
225         text_input.delete("1.0", tk.END)
226         text_input.insert("1.0", "\n".join(output_lines))
227         if data_count > 0:
228             messagebox.showinfo("Displayed", "Data consolidated and displayed in the text area.")
229         elif header_present and len(output_lines) == 1 and not data_count:
230             messagebox.showinfo("Displayed", "Header displayed in the text area. No data lines were consolidated.")
231
```

```
231
232 def is_likely_transformed(text_content):
233     lines = text_content.strip().split('\n')
234     if not lines or len(lines) < 2: return False
235     data_lines_checked = 0
236     transformed_indicators = 0
237     start_index = 0
238     if len(lines) > 1 and not (lines[0].startswith("Name:") and "\t" in lines[0]): start_index = 1
239     for i in range(start_index, len(lines)):
240         stripped_line = lines[i].strip()
241         if not stripped_line: continue
242         data_lines_checked += 1
243         if data_lines_checked > 20: break
244         if re.match(r'^\s*Monoisotopic Mass:', stripped_line): return False
245         if re.match(r'^\s*\d+\s+Name:', stripped_line): return False
246         if stripped_line.startswith("Name:") and "\t" in stripped_line: transformed_indicators += 1
247         elif "\t" in stripped_line and not stripped_line.startswith("Name:") and i == 0 and start_index == 0: pass
248     if data_lines_checked > 0 and transformed_indicators > 0: return True
249     return False
250
251 def save_input_as_is_action():
252     current_text_content = text_input.get("1.0", tk.END).strip()
253     if not current_text_content:
254         messagebox.showwarning("Empty Input", "There is no text in the input field to save.")
255         return
256
257     if not is_likely_transformed(current_text_content):
258         messagebox.showinfo(
259             "Action Information",
260             "The 'Save Input As Is...' button is now used for saving content that has been "
261             "processed and displayed in place (i.e., transformed data).\n\n"
262             "The current input does not appear to be transformed. "
263             "Please use 'Consolidate & Display In-Place' first if you wish to save its result this way."
264         )
265         return
266
267     target_file_path = output_file_entry.get().strip()
268     if not target_file_path:
269         messagebox.showwarning(
270             "No Output File Specified",
271             "Please specify a file path in the 'Output File Path' box above the buttons."
272         )
273         return
274
275     try:
276         content_to_save_verbatim = text_input.get("1.0", tk.END)
277         with open(target_file_path, 'w', encoding='utf-8') as f:
278             f.write(content_to_save_verbatim)
279         messagebox.showinfo(
280             "Success",
281             f"Displayed (transformed) content successfully saved to:\n{target_file_path}"
282         )
283     except Exception as e:
284         messagebox.showerror("Error Saving File", f"Failed to save to '{target_file_path}':\n{e}")
285
286 def clear_input_action():
287     """Clears all text from the text_input widget."""
288     if text_input.get("1.0", tk.END).strip(): # Check if there's text to clear
289         if messagebox.askyesno("Confirm Clear", "Are you sure you want to clear the input area?"):
290             text_input.delete("1.0", tk.END)
291     else:
292         messagebox.showinfo("Already Clear", "The input area is already empty.")
293
294
```

```python
def paste_consolidate_save_action():
    """Gets content from clipboard, puts it in text_input, then consolidates and saves."""
    try:
        clipboard_content = root.clipboard_get()
    except tk.TclError: # Handles cases like empty clipboard or non-text content
        messagebox.showwarning("Paste Error", "Could not get text from clipboard, or clipboard is empty.")
        return

    if not clipboard_content.strip():
        messagebox.showwarning("Paste Error", "Clipboard contains no processable text.")
        return

    # Replace content in text_input with clipboard content
    text_input.delete("1.0", tk.END)
    text_input.insert("1.0", clipboard_content)

    # Ensure the UI updates if necessary, though usually not an issue here
    # root.update_idletasks()

    # Now call the main save action which will read from text_input
    save_consolidated_molecule_info_action()


# --- GUI Setup ---
root = tk.Tk()
root.title("Molecule Data Consolidator")
root.geometry("800x700") # Increased height slightly for more buttons if needed

text_input = tk.Text(root, wrap="word", width=90, height=25, undo=True)
text_input.pack(pady=10, padx=10, fill="both", expand=True)

# Frame for file selection (remains the same)
file_selection_frame = tk.Frame(root)
file_selection_frame.pack(pady=(0, 5), padx=10, fill="x")

output_file_label = tk.Label(file_selection_frame, text="Output File Path (for Save buttons):")
output_file_label.pack(side=tk.LEFT, padx=(0, 5))

output_file_entry = tk.Entry(file_selection_frame, width=50)
output_file_entry.pack(side=tk.LEFT, expand=True, fill="x", padx=(0,5))

browse_button = tk.Button(file_selection_frame, text="Browse...", command=browse_output_file)
browse_button.pack(side=tk.LEFT)

# Main action buttons frame
action_button_frame = tk.Frame(root)
action_button_frame.pack(pady=(0,2), padx=10, fill="x") # Use fill="x" to allow wrapping if too many

save_button = tk.Button(action_button_frame, text="Consolidate & Save Data", command=save_consolidated_molecule_info_action)
save_button.pack(side=tk.LEFT, padx=2, pady=2)

display_button = tk.Button(action_button_frame, text="Consolidate & Display In-Place", command=display_consolidated_info_action)
display_button.pack(side=tk.LEFT, padx=2, pady=2)

save_as_is_button = tk.Button(action_button_frame, text="Save Input As Is...", command=save_input_as_is_action)
save_as_is_button.pack(side=tk.LEFT, padx=2, pady=2)

# New row/frame for utility buttons
utility_button_frame = tk.Frame(root)
utility_button_frame.pack(pady=(2,5), padx=10, fill="x")

clear_button = tk.Button(utility_button_frame, text="Clear Input Area", command=clear_input_action)
clear_button.pack(side=tk.LEFT, padx=2, pady=2)

paste_save_button = tk.Button(utility_button_frame, text="Paste, Consolidate & Save", command=paste_consolidate_save_action)
paste_save_button.pack(side=tk.LEFT, padx=2, pady=2)


root.mainloop()
```

8.2 Python-fil til samling af datafiler i excel:

Combine multiple datafiles.py – ligger på Sharepoint [Combine multiple datafiles]

Combine multiple datafiles.py

```python
import tkinter as tk
from tkinter import filedialog, messagebox
import re
import os
import shutil

# --- Global Constants ---
FILE_TYPES = [("Tab Separated Values", "*.tsv"), ("Text files", "*.txt"), ("All files", "*.*")]
DEFAULT_EXTENSION = ".tsv"
ERROR_FOLDER_NAME = "parse_error_files"

# --- Core Processing Function ---
def _process_single_file_data(text_content):
    """
    Parses a TSV file's content where each row is a record.
    Returns a tuple: (header_as_list, data_as_list_of_lists)
    """
    if not text_content.strip():
        return None, []

    lines = text_content.strip().split('\n')
    if not lines:
        return None, []

    # The first line is the header
    header = lines[0].strip().split('\t')

    data_rows = []
    # Process the rest of the lines as data
    for line in lines[1:]:
        if line.strip():
            data_rows.append(line.strip().split('\t'))

    return header, data_rows

# --- Filename Parsing to Metadata ---
def _parse_filename_to_metadata(filename):
    """
    Parses a filename into a dictionary of specific metadata fields.
    Splits gradient time and eluent into separate columns.
    """
    base_name = os.path.splitext(filename)[0]
    parts = base_name.split('_')

    metadata_keys = ["mix", "pH", "column", "time", "solvent", "temp"]
    metadata = {}
    for i, part in enumerate(parts):
        if i < len(metadata_keys):
            metadata[metadata_keys[i]] = part
        else:
            metadata[f"extra_metadata_{i+1}"] = part # For any parts beyond the defined keys

    metadata["Original_Filename"] = filename

    return metadata

# --- GUI Actions ---
def browse_input_folder():
    """Opens a dialog to select an input folder."""
    folder_path = filedialog.askdirectory(title="Select Input Folder Containing Molecule Data Files")
    if folder_path:
        input_folder_entry.delete(0, tk.END)
        input_folder_entry.insert(0, folder_path)

def browse_output_file():
    """Opens a dialog to select a destination file for the consolidated output."""
    file_path = filedialog.asksaveasfilename(
        defaultextension=DEFAULT_EXTENSION, filetypes=FILE_TYPES, title="Select Consolidated Output File Location"
    )
```

```
    if file_path:
        output_file_entry.delete(0, tk.END)
        output_file_entry.insert(0, file_path)

def process_folder_action():
    input_folder = input_folder_entry.get().strip()
    output_file = output_file_entry.get().strip()

    log_output.delete("1.0", tk.END)

    if not input_folder or not os.path.isdir(input_folder):
        messagebox.showwarning("Invalid Input", "Please select a valid input folder.")
        log_output.insert(tk.END, "Error: Invalid input folder.\n")
        return

    if not output_file:
        messagebox.showwarning("Invalid Output", "Please specify an output file path.")
        log_output.insert(tk.END, "Error: Output file not specified.\n")
        return

    error_folder_path = os.path.join(input_folder, ERROR_FOLDER_NAME)
    os.makedirs(error_folder_path, exist_ok=True)
    log_output.insert(tk.END, f"Error files will be moved to: {error_folder_path}\n\n")

    all_consolidated_lines = []
    header_written = False
    processed_file_count = 0
    error_file_count = 0

    log_output.insert(tk.END, f"Starting processing in folder: {input_folder}\n")
    log_output.insert(tk.END, f"Output will be saved to: {output_file}\n\n")

    for filename in os.listdir(input_folder):
        file_path = os.path.join(input_folder, filename)

        if os.path.isdir(file_path) or filename == ERROR_FOLDER_NAME:
            continue

        if not filename.lower().endswith(('.txt', '.tsv')):
            log_output.insert(tk.END, f"   Skipping non-data file: {filename}\n")
            continue

        log_output.insert(tk.END, f"Processing file: {filename}\n")

        try:
            with open(file_path, 'r', encoding='utf-8') as f:
                file_content = f.read()

            original_header_list, data_rows = _process_single_file_data(file_content)
            metadata = _parse_filename_to_metadata(filename)

            if not header_written and data_rows:
                metadata_headers = list(metadata.keys())
                final_header = original_header_list + metadata_headers
                all_consolidated_lines.append("\t".join(final_header))
                header_written = True

            if not data_rows:
                log_output.insert(tk.END, f"   No molecule data extracted from {filename}.\n")
                continue

            for row_list in data_rows:
                metadata_values = [str(metadata[key]) for key in metadata_headers]

                full_row_data = row_list + metadata_values
                all_consolidated_lines.append("\t".join(full_row_data))

```

```
            processed_file_count += 1
            log_output.insert(tk.END, f"   Extracted {len(data_rows)} molecule entries.\n")

        except Exception as e:
            error_file_count += 1
            log_output.insert(tk.END, f"   ERROR processing {filename}: {e}. Moving to '{ERROR_FOLDER_NAME}'.\n")
            try:
                if 'f' in locals() and not f.closed:
                    f.close()
                shutil.move(file_path, os.path.join(error_folder_path, filename))
            except Exception as move_e:
                log_output.insert(tk.END, f"   Could not move file {filename}: {move_e}\n")

    if not all_consolidated_lines:
        messagebox.showwarning("No Data", "No processable data was found in any of the files in the selected folder.")
        log_output.insert(tk.END, "\nCompleted: No data found to consolidate.\n")
        return

    try:
        with open(output_file, 'w', encoding='utf-8') as f_out:
            for line in all_consolidated_lines:
                f_out.write(line + '\n')

        messagebox.showinfo("Success", f"Consolidated data from {processed_file_count} files (Errors: {error_file_count}). Output to:\n{output_file}")
        log_output.insert(tk.END, f"\n--- Processing Complete ---\n")
        log_output.insert(tk.END, f"Consolidated data from {processed_file_count} files.\n")
        log_output.insert(tk.END, f"Files with errors moved: {error_file_count}\n")
        log_output.insert(tk.END, f"Output saved to: {output_file}\n")

    except Exception as e_write:
        messagebox.showerror("File Write Error", f"An error occurred while writing the consolidated output file:\n{e_write}")
        log_output.insert(tk.END, f"\nError writing final output: {e_write}\n")

# --- GUI Setup ---
root = tk.Tk()
root.title("Molecule Data Folder Consolidator with Metadata")
root.geometry("900x700")

# Input Folder Frame
input_folder_frame = tk.Frame(root)
input_folder_frame.pack(pady=(10, 5), padx=10, fill="x")

input_folder_label = tk.Label(input_folder_frame, text="Input Folder:")
input_folder_label.pack(side=tk.LEFT, padx=(0, 5))

input_folder_entry = tk.Entry(input_folder_frame, width=60)
input_folder_entry.pack(side=tk.LEFT, expand=True, fill="x", padx=(0,5))

browse_input_button = tk.Button(input_folder_frame, text="Browse Folder...", command=browse_input_folder)
browse_input_button.pack(side=tk.LEFT)

# Output File Frame
output_file_frame = tk.Frame(root)
output_file_frame.pack(pady=(0, 5), padx=10, fill="x")

output_file_label = tk.Label(output_file_frame, text="Output Consolidated File:")
output_file_label.pack(side=tk.LEFT, padx=(0, 5))

output_file_entry = tk.Entry(output_file_frame, width=60)
output_file_entry.pack(side=tk.LEFT, expand=True, fill="x", padx=(0,5))

browse_output_button = tk.Button(output_file_frame, text="Browse Output...", command=browse_output_file)
browse_output_button.pack(side=tk.LEFT)

# Action Button
process_button = tk.Button(root, text="Process Folder & Consolidate", command=process_folder_action, height=2, font=("Arial", 12, "bold"))
process_button.pack(pady=10, padx=10, fill="x")

# Log Output Area
log_label = tk.Label(root, text="Processing Log:")
log_label.pack(pady=(5,0), padx=10, anchor="w")

log_output = tk.Text(root, wrap="word", width=100, height=15)
log_output.pack(pady=(0,10), padx=10, fill="both", expand=True)

# Main loop
root.mainloop()
```

9 Resultatfiler

Alle resultater findes på Sharepoint:

Signaler fra MS'en Data

Omformateret efter klik-arbejde Datafiles transformed from MSchrom

Databasefiler Combined and colored datafiles

Molecular datafiles Molecular datafiles