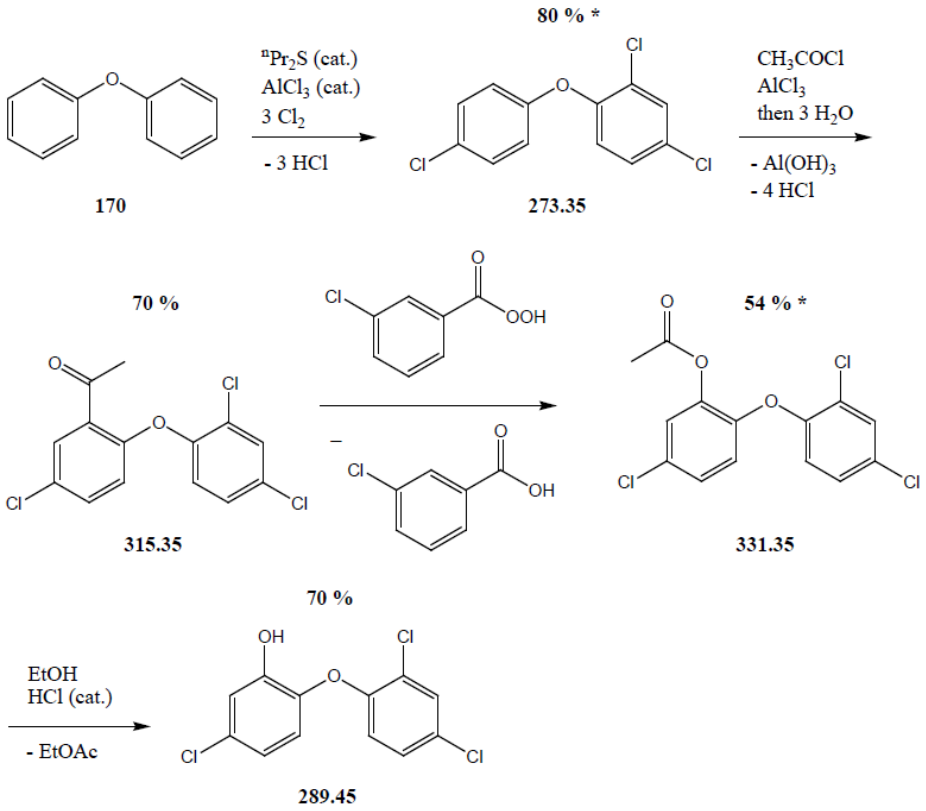
universität wien

Synthesis Plans

[making them machine readable]

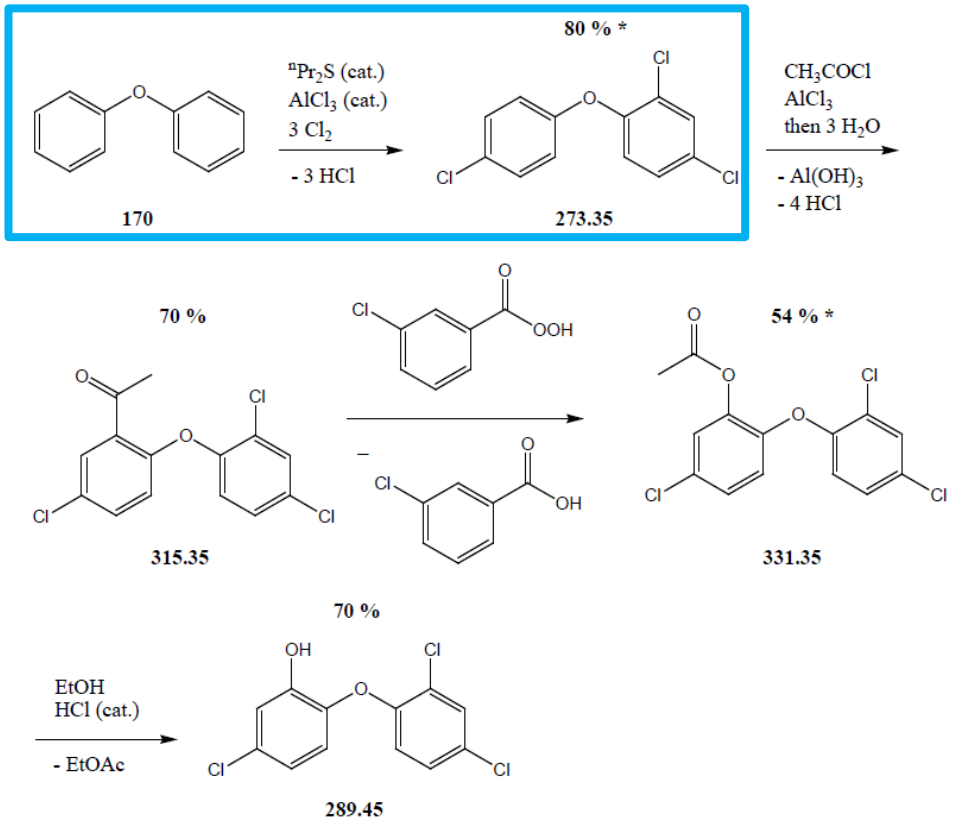
universität wien

What is chemical synthesis?



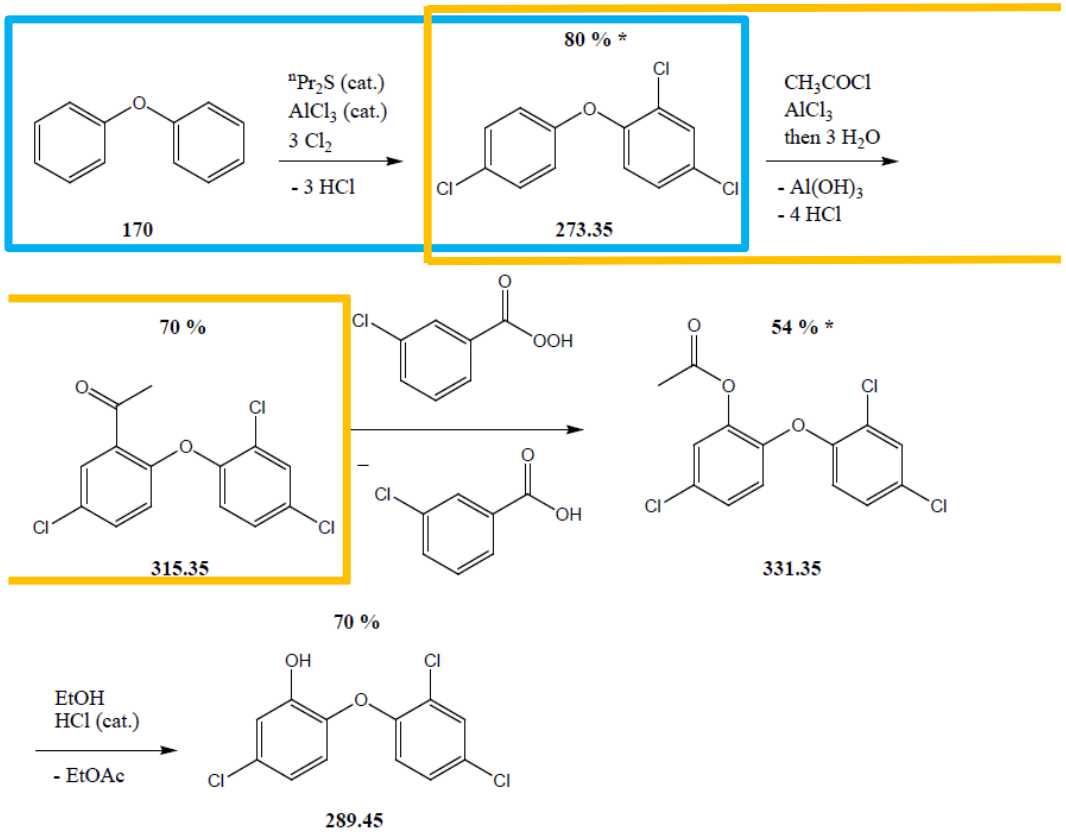
universität wien

Several connected reactions



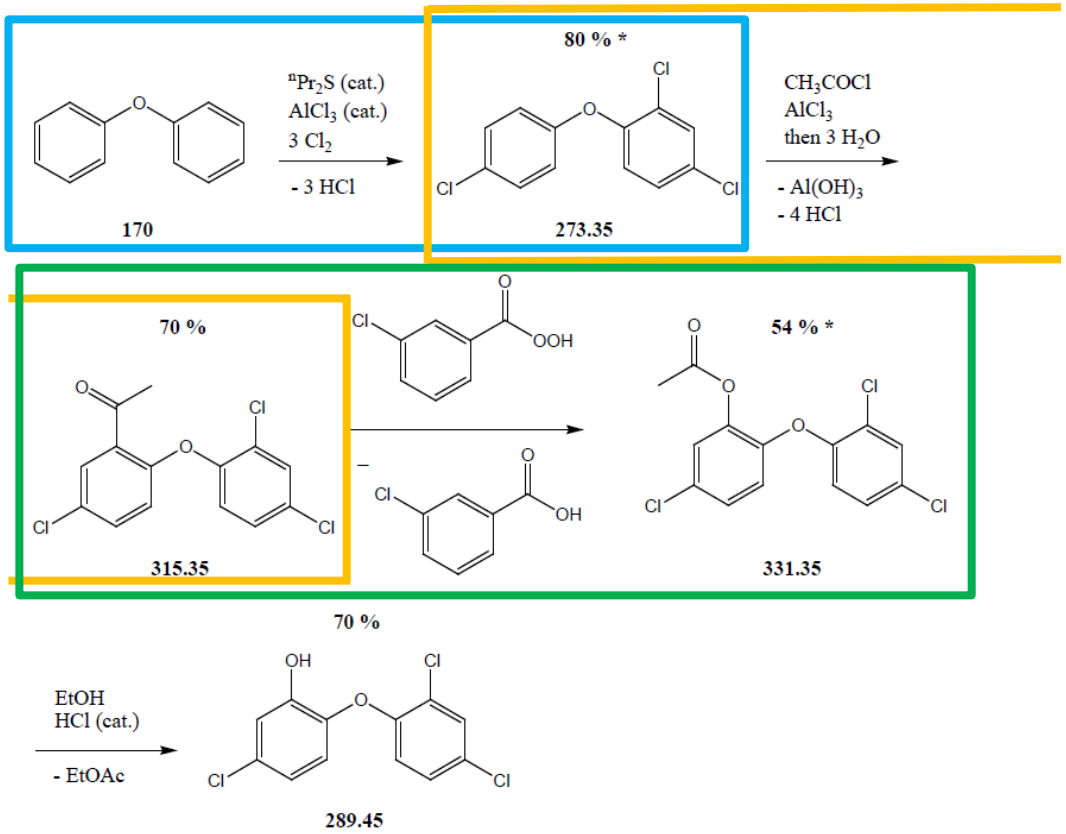
universität wien

Several connected reactions



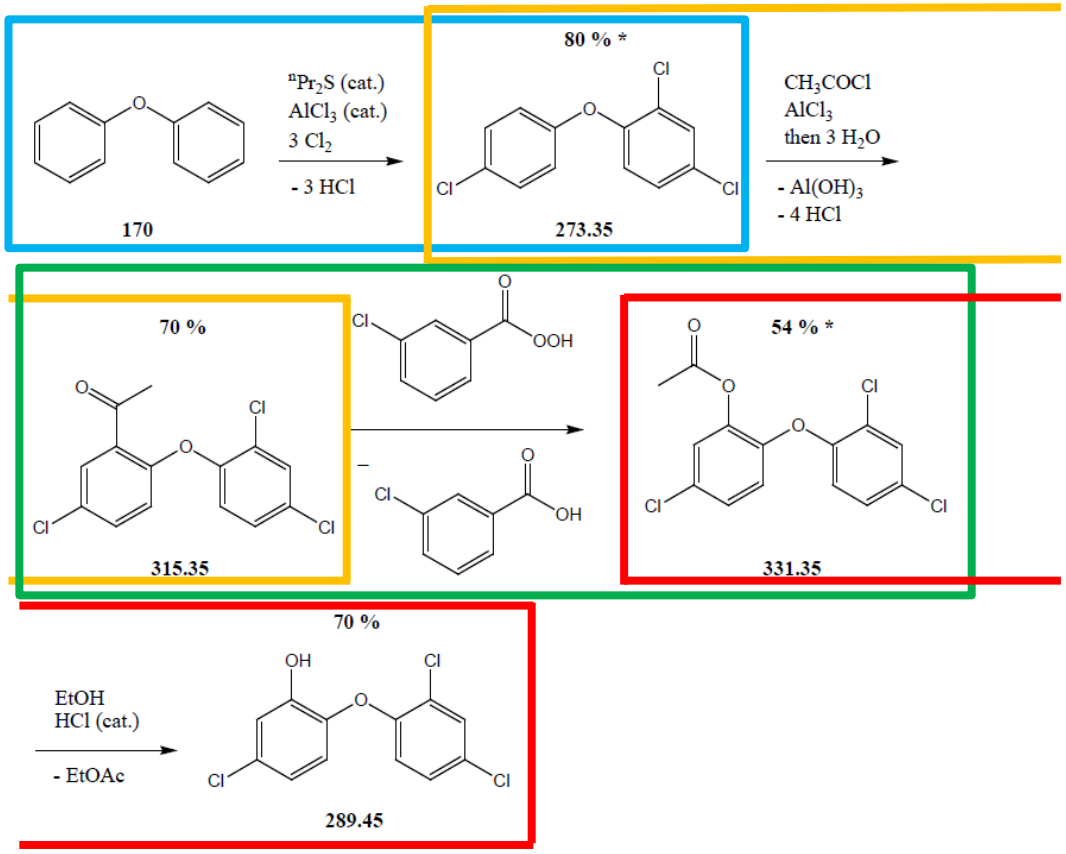
universität wien

Several connected reactions

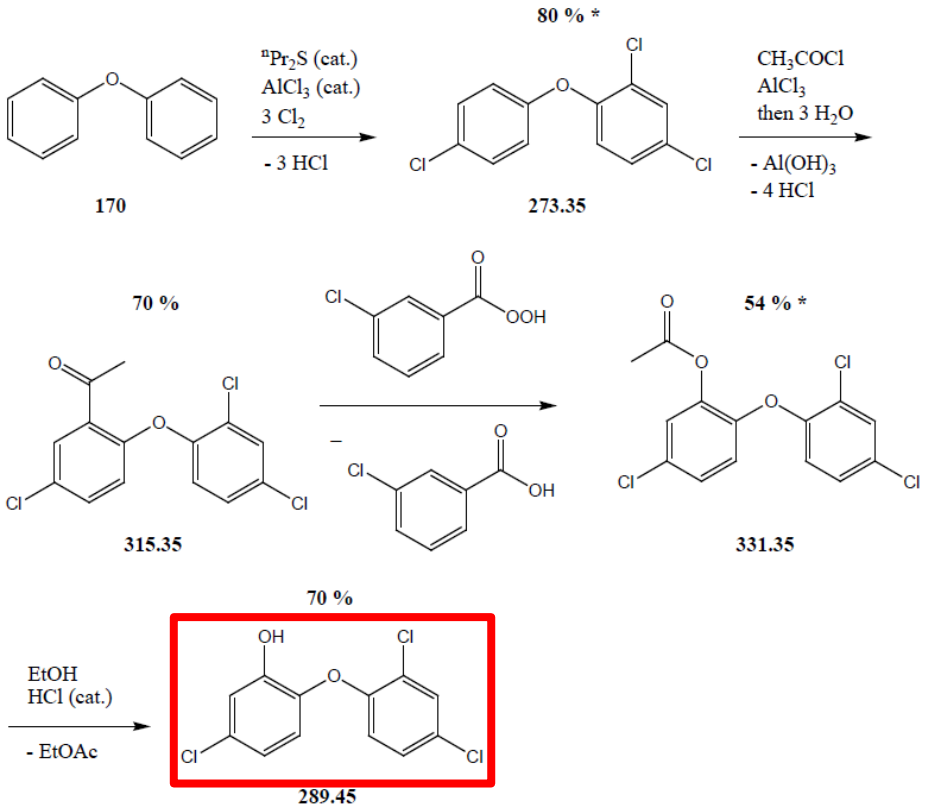


universität wien

Several connected reactions

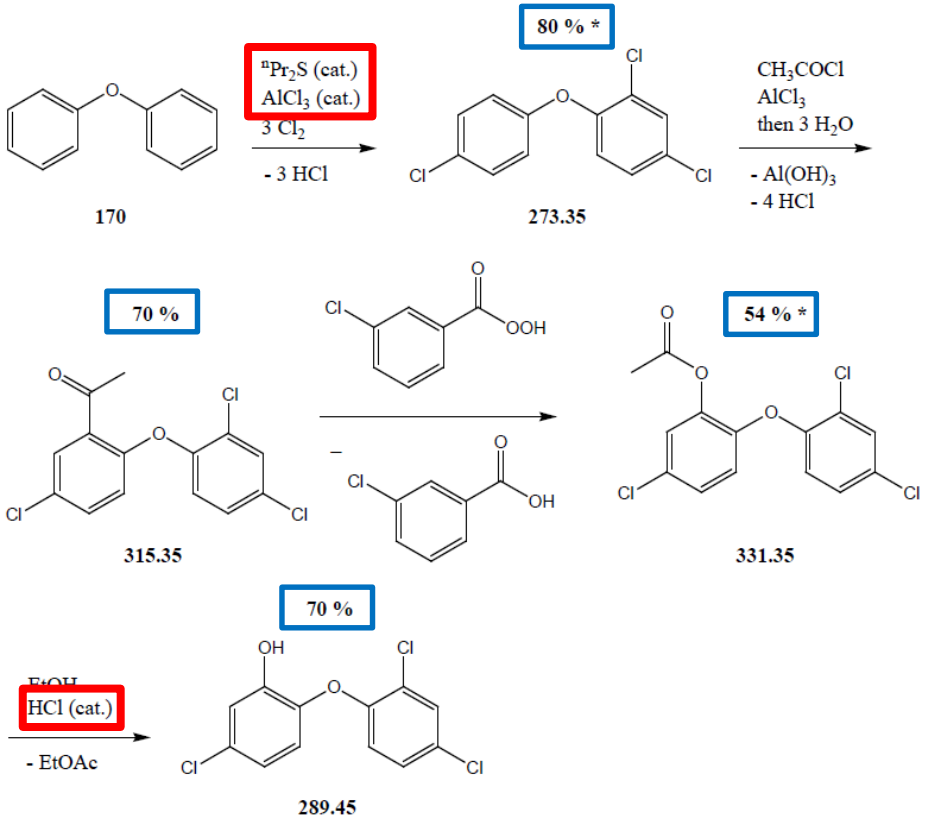


Target molecule



universität wien

Attributes



universität wien

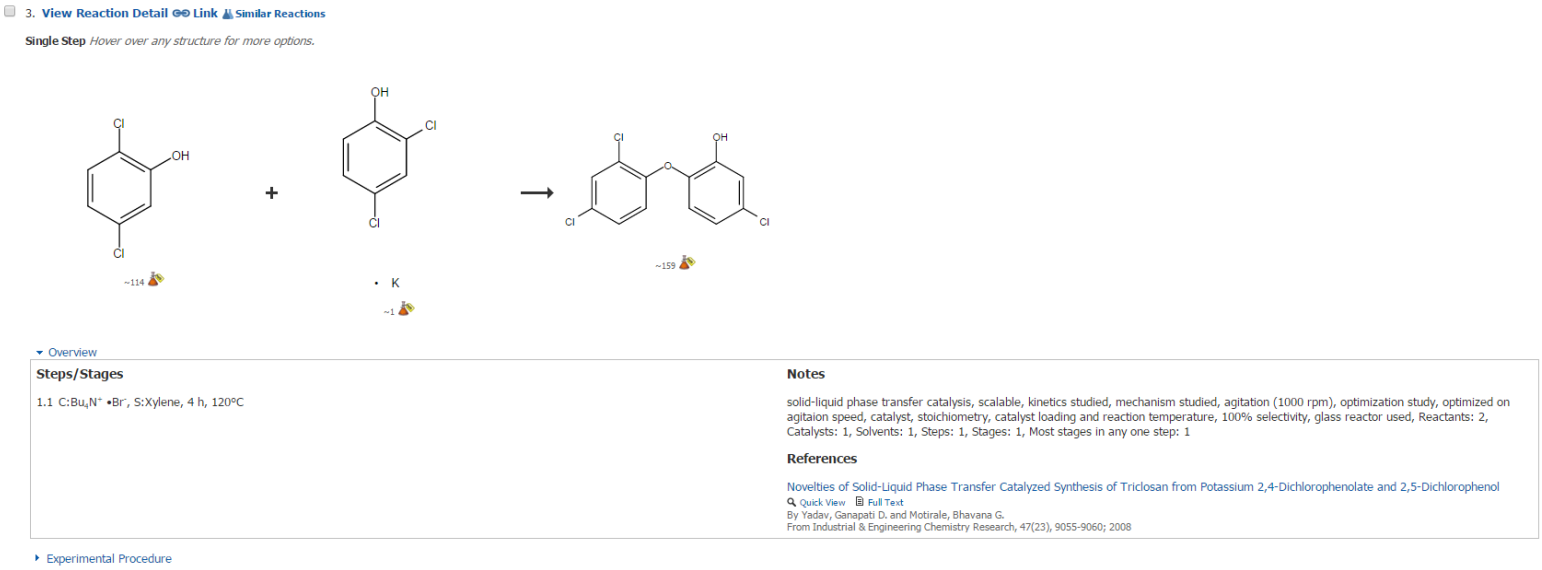
The “classical” way

- Plans published in journals

- Created by chemists using ‘chemical intuition‘

The present

- Journals most important medium
- Effort goes to making articles better searchable



universität wien

The downsides

- Searchable only on a molecule basis
- Comparing synthesis plans
- No service for complete synthesis plans

universität wien

File Format

Header

```
# Last changed timestamp: date
# Last changed author: name
# Lit: literature author(s)
#      literature title
#      journal
# DOI: doi
# Aut: name & email
```

universität wien

File Format

Target declaration

skeleton: InChI=1S/C16H16N2O2/c1-18-8-10(16(19)20)5-12-11-3-2-4-13-15(11)9(7-17-13)6-14(12)18/h2-5,7,10,14,17H,6,8H2,1H3,(H,19,20)/t10-,14-/m1/s1

universität wien

File Format

Compound list

compounds:
comp1 InChI=1S/C11H11NO2/c13-11(14)6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7,12H,5-6H2,(H,13,14)
comp2 InChI=1S/C5H9ClO/c1-5(2,3)4(6)7/h1-3H3
comp3 InChI=1S/K.H2O/h;1H2/q+1;/p-1
comp4 InChI=1S/ClH/h1H
[...]

universität wien

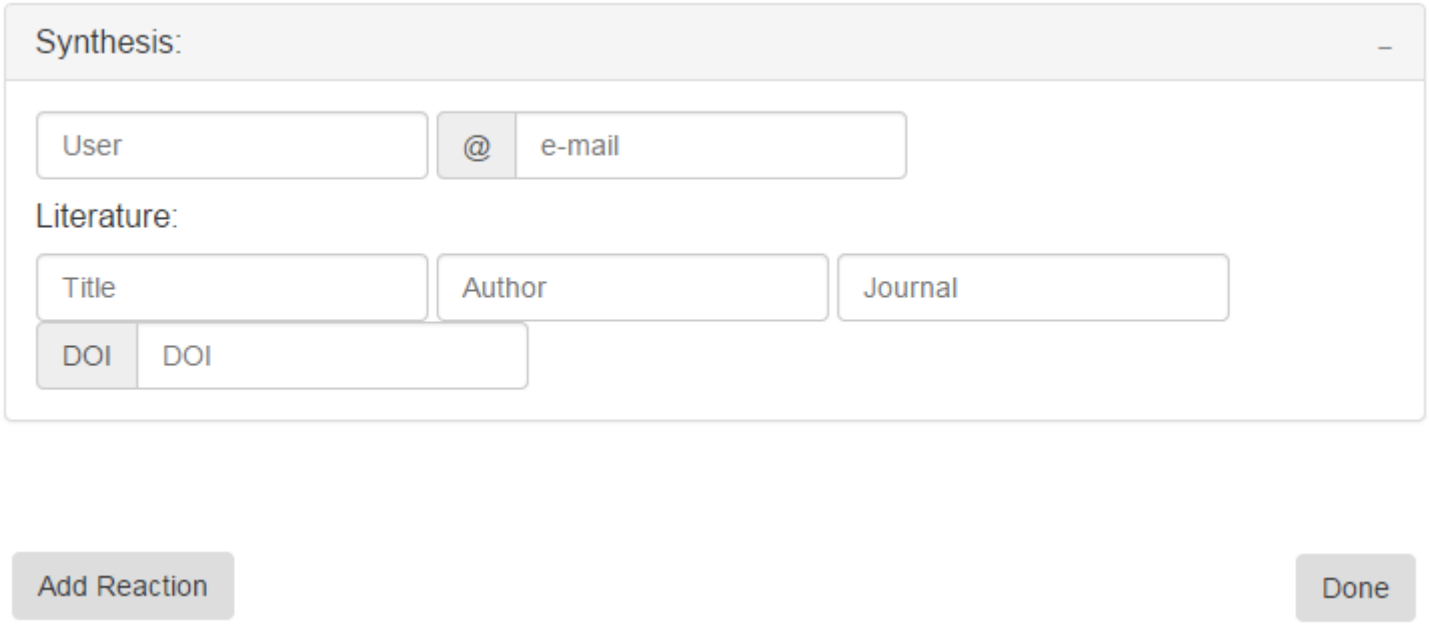
File Format

Reaction definition

```
reactions:
[ ... ]
R04 "Addition of Bromine"
skeletonOut InChI=1S/C16H16BrNO2/c1-16(2,3)15(20)18-8-9-7-
11(17)14(19)10-5-4-6-12(18)13(9)10/h4-6,8,11H,7H2,1-3H3
|comp21| + comp22 -> |comp23| + comp24 + comp25
@yield 85% cat light
```

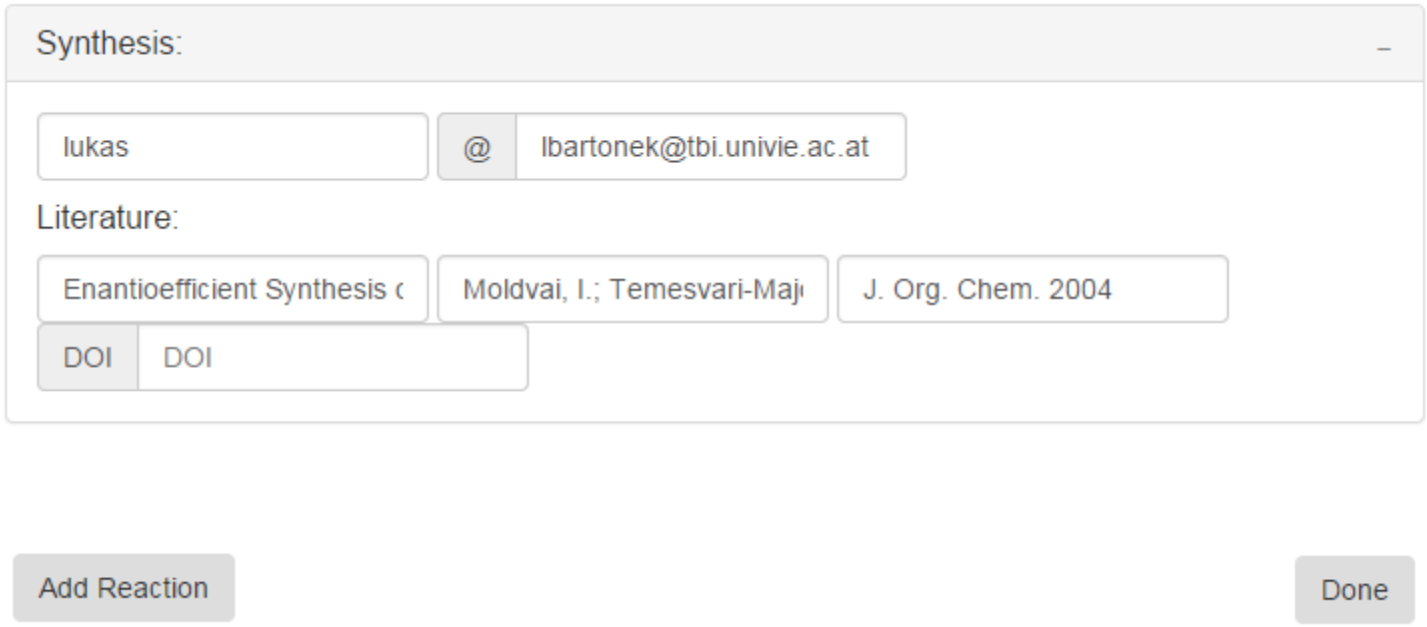
universität wien

Creating new plans



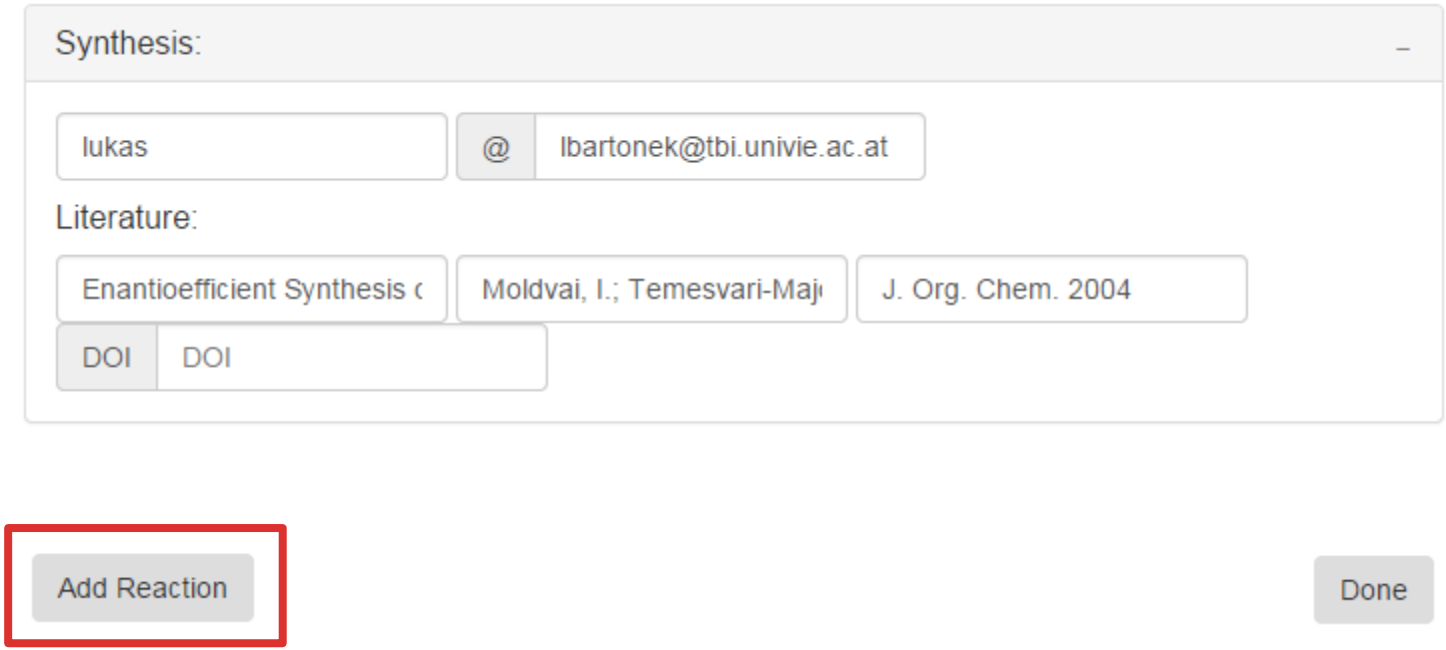
universität wien

Creating new plans



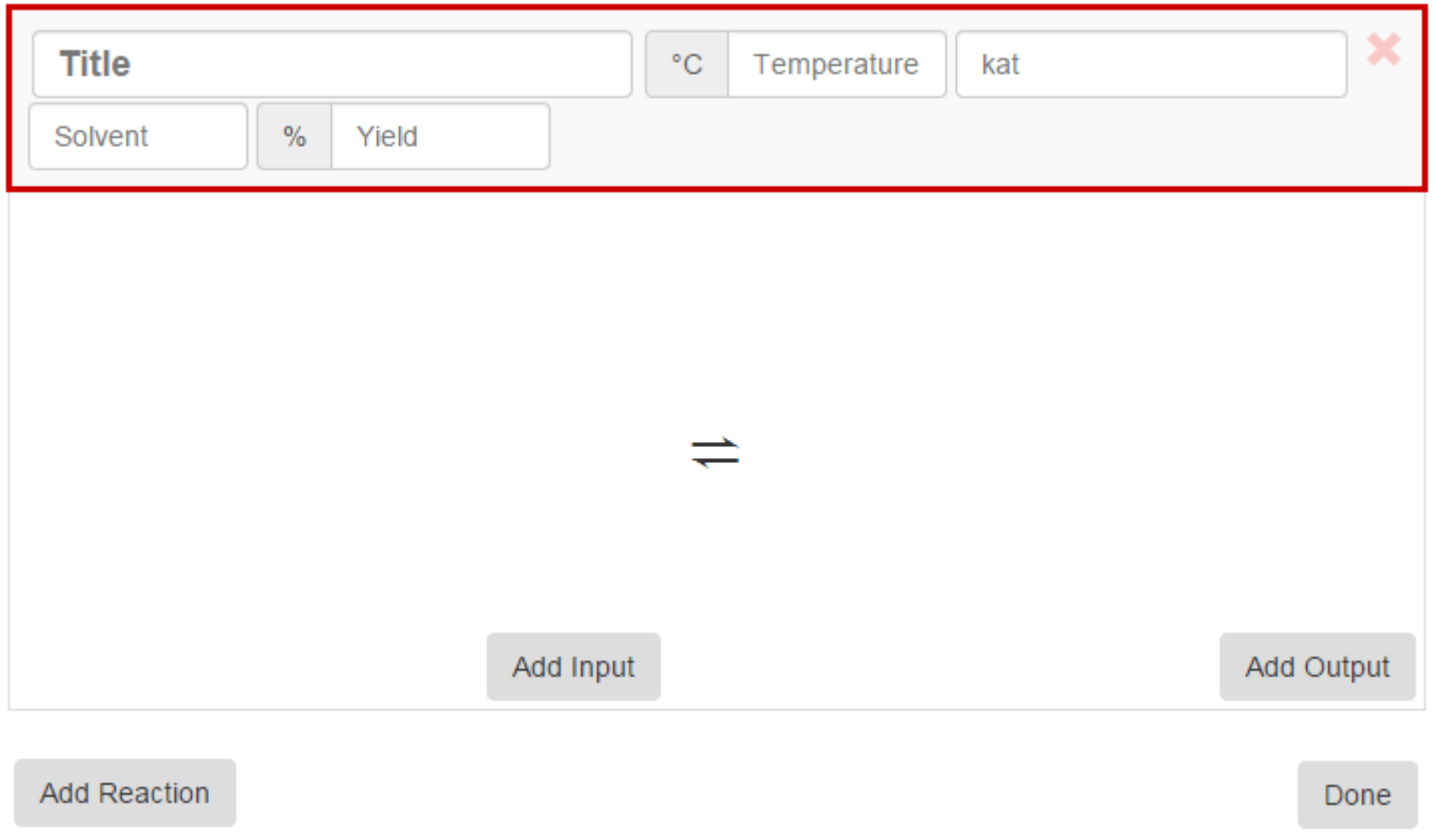
universität wien

Creating new plans



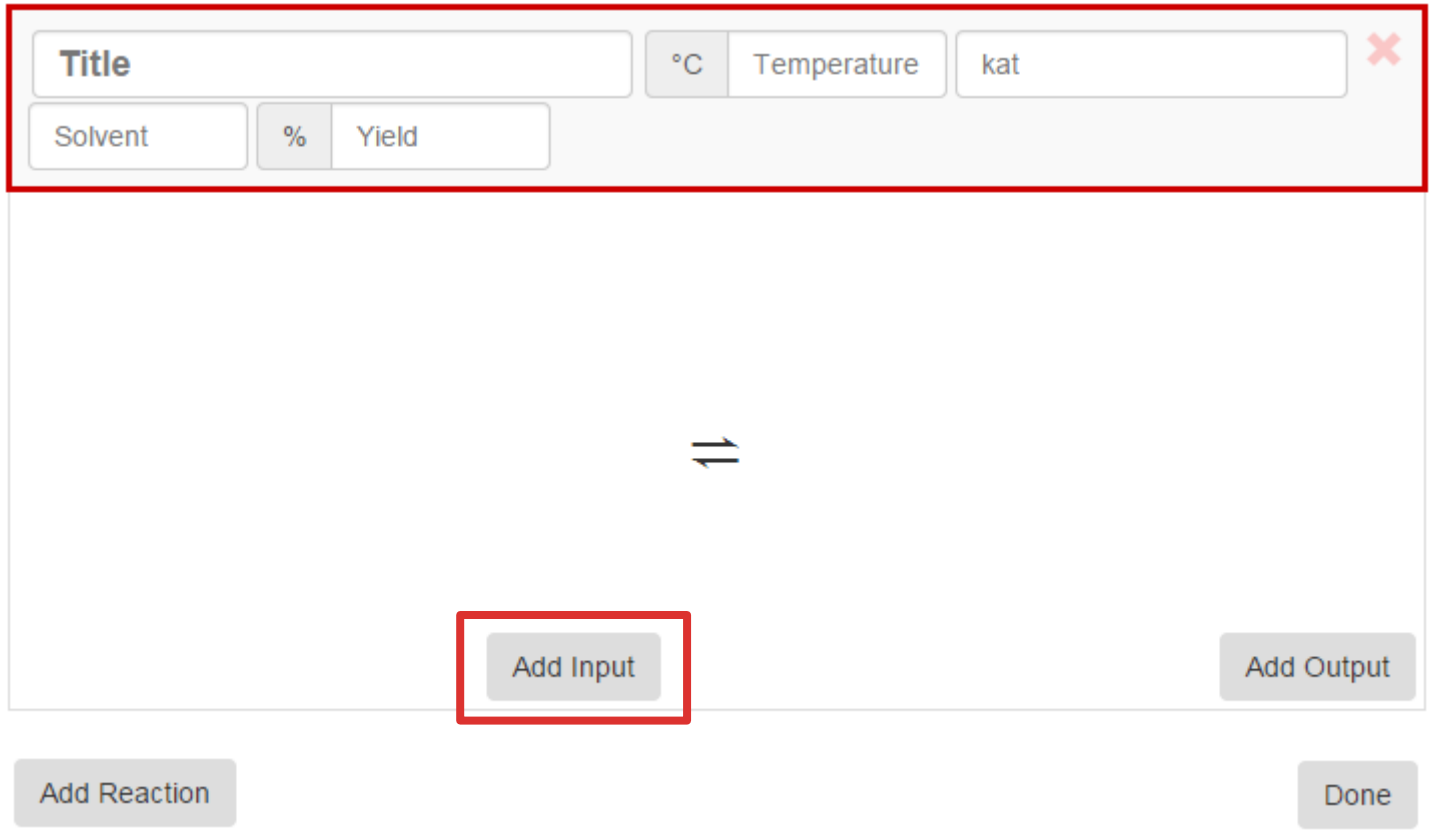
universität wien

Creating new plans



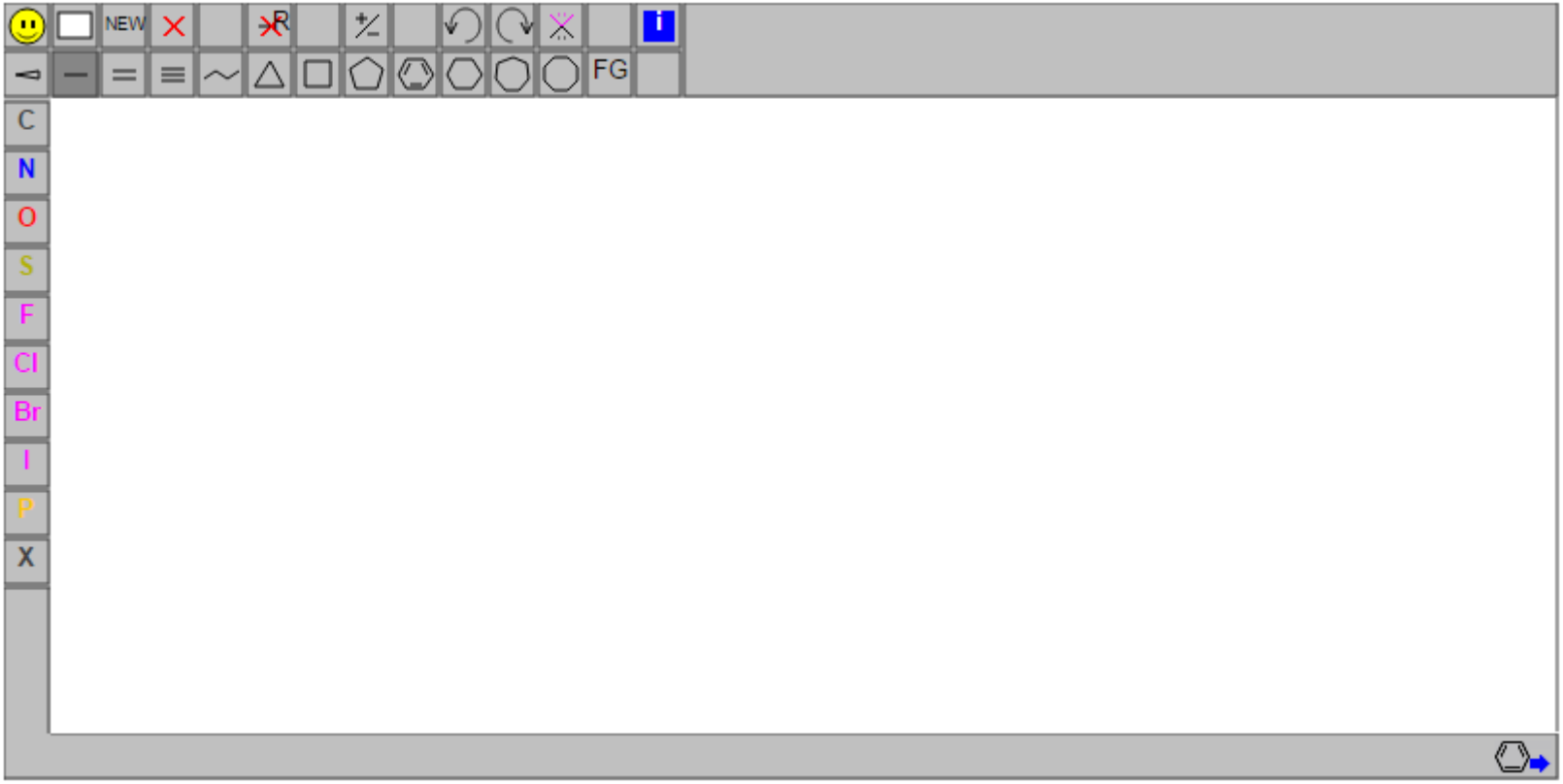
universität wien

Creating new plans



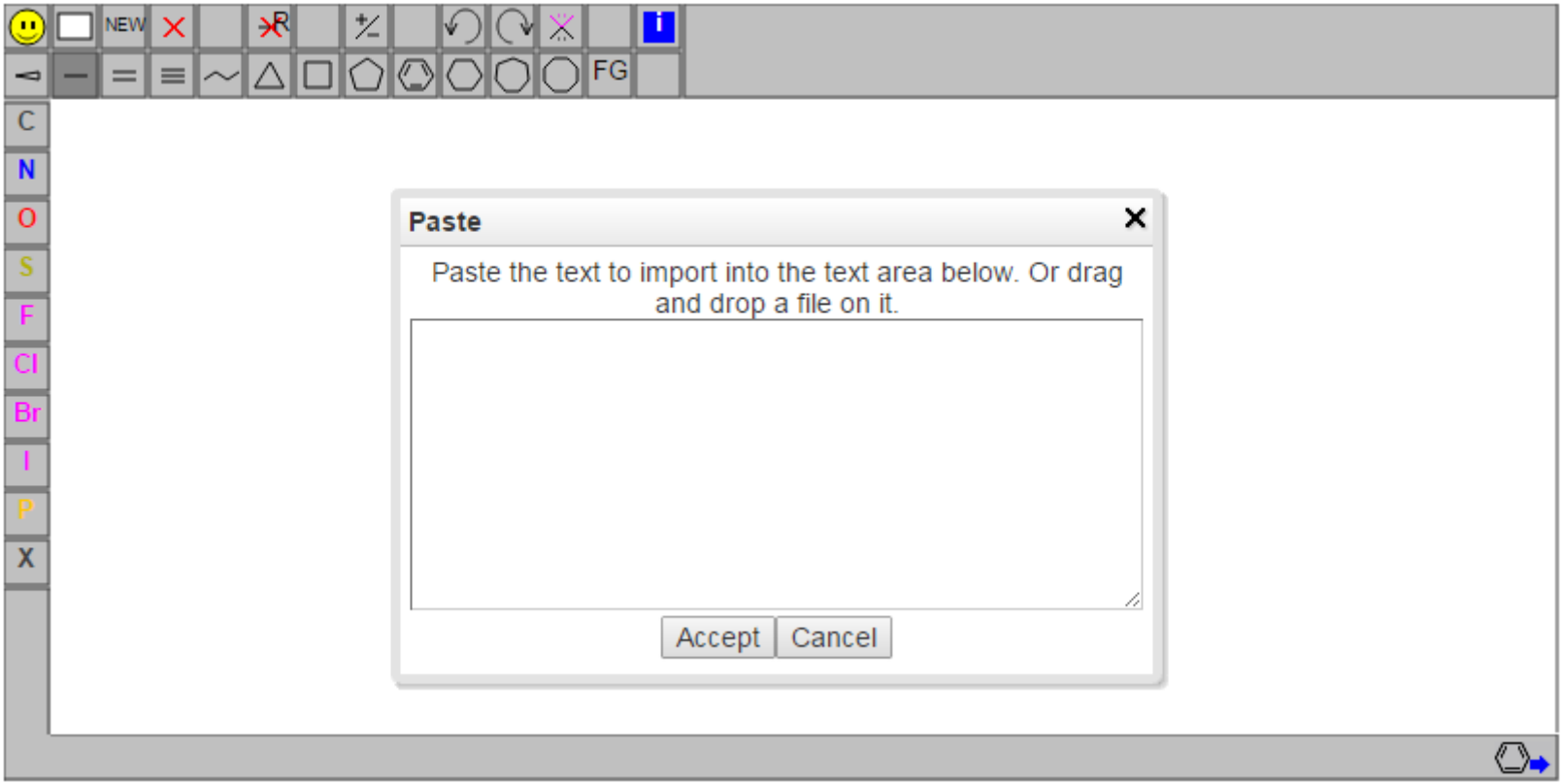
universität wien

Creating new plans



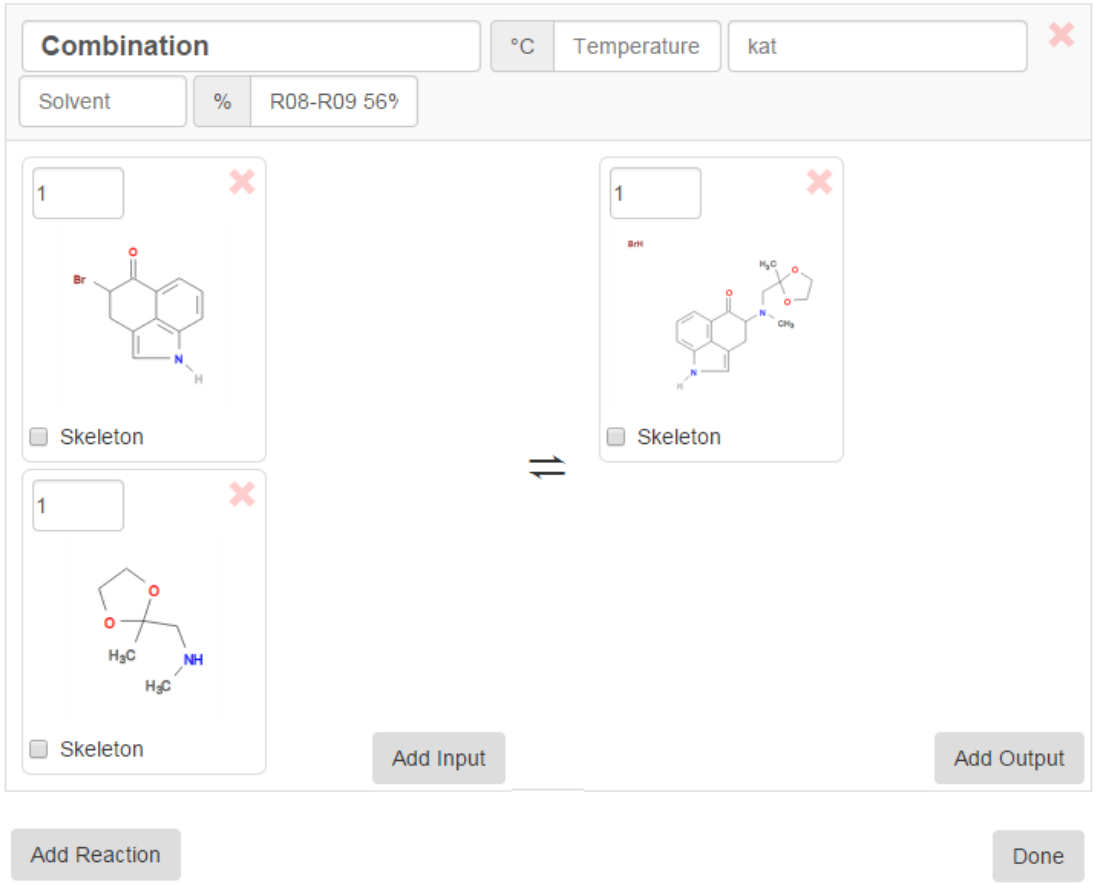
universität wien

Creating new plans

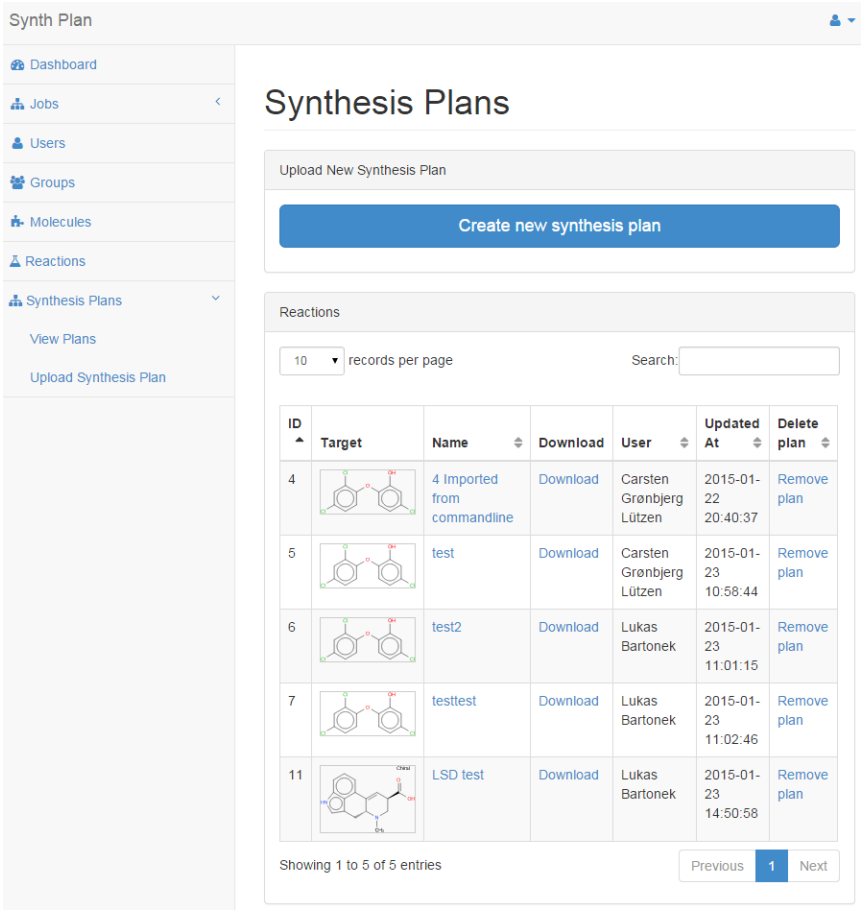


universität wien

Creating new plans



Database



Database created by **Carsten Grønbjerg Lützen** and **Daniel Fentz Johansen** from SDU Odense

Possiblities

- Compare Synthesis Plans
- Compute descriptors
- Generate Graph Rewrite rules

universität
wien

THANK YOU