



universität  
wien

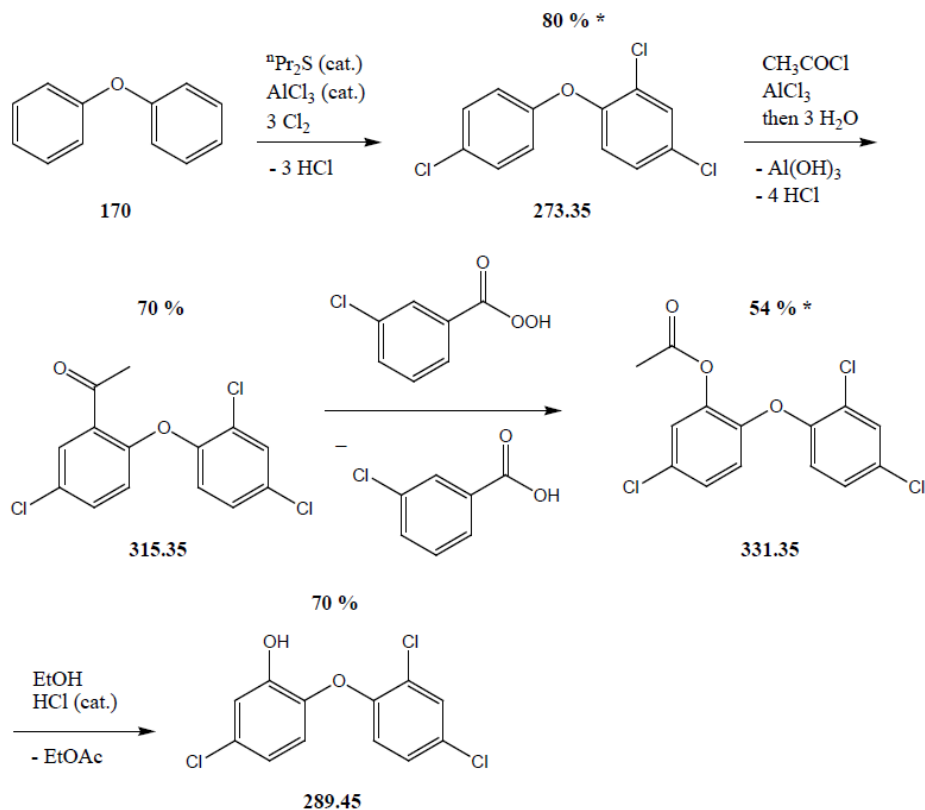
# Synthesis Plans

[ making them machine readable ]

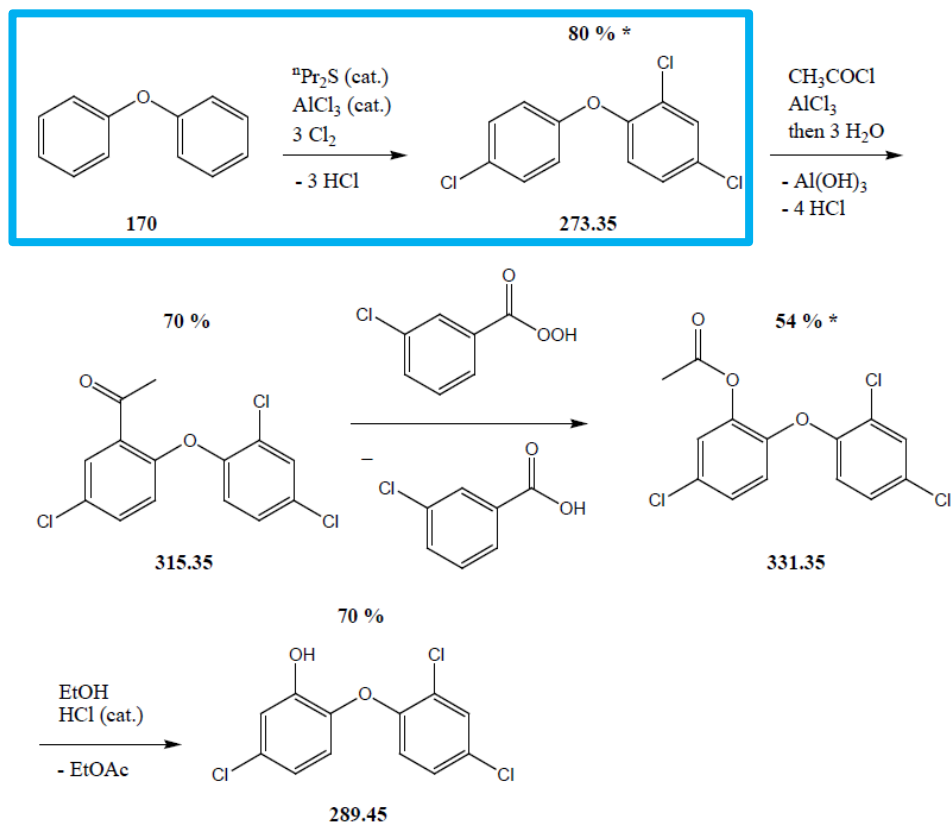




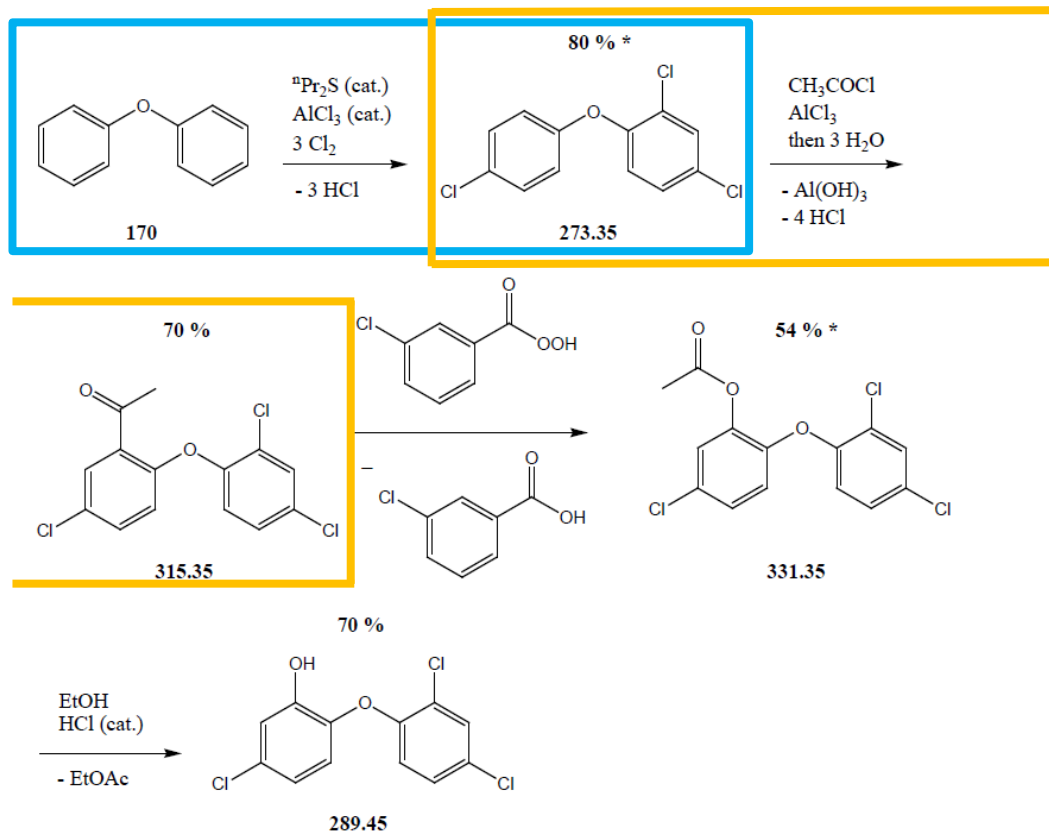
# What is chemical synthesis?



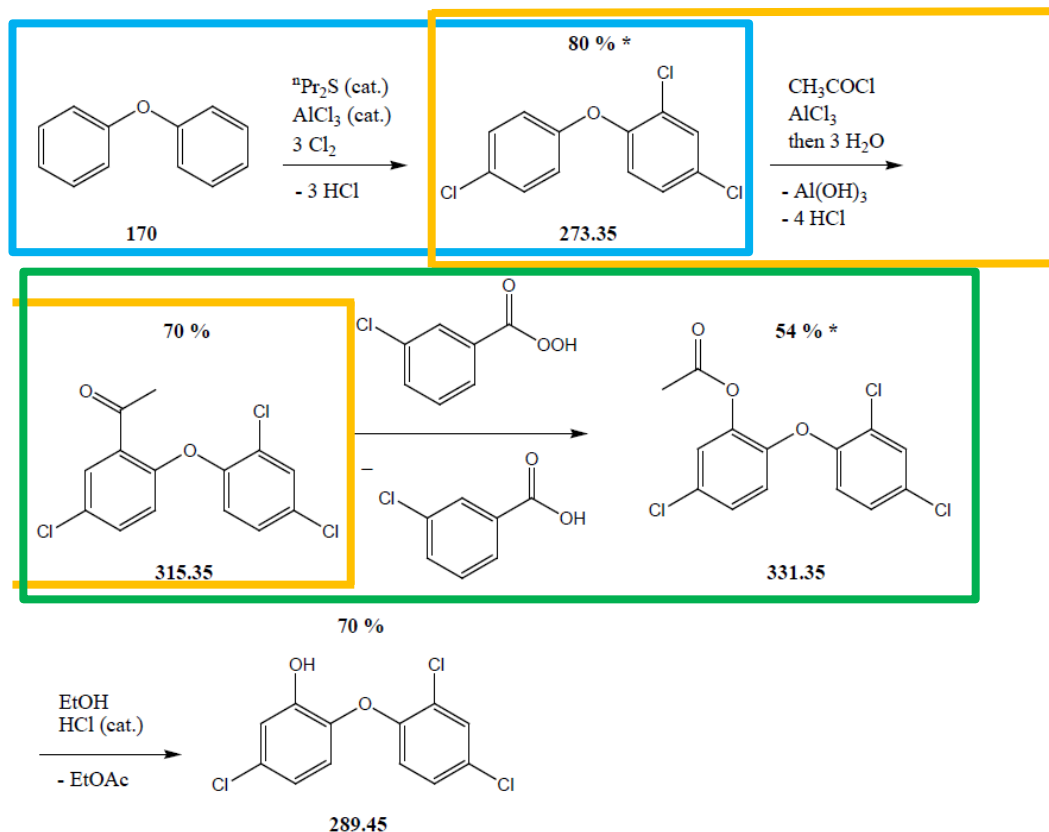
# Several connected reactions



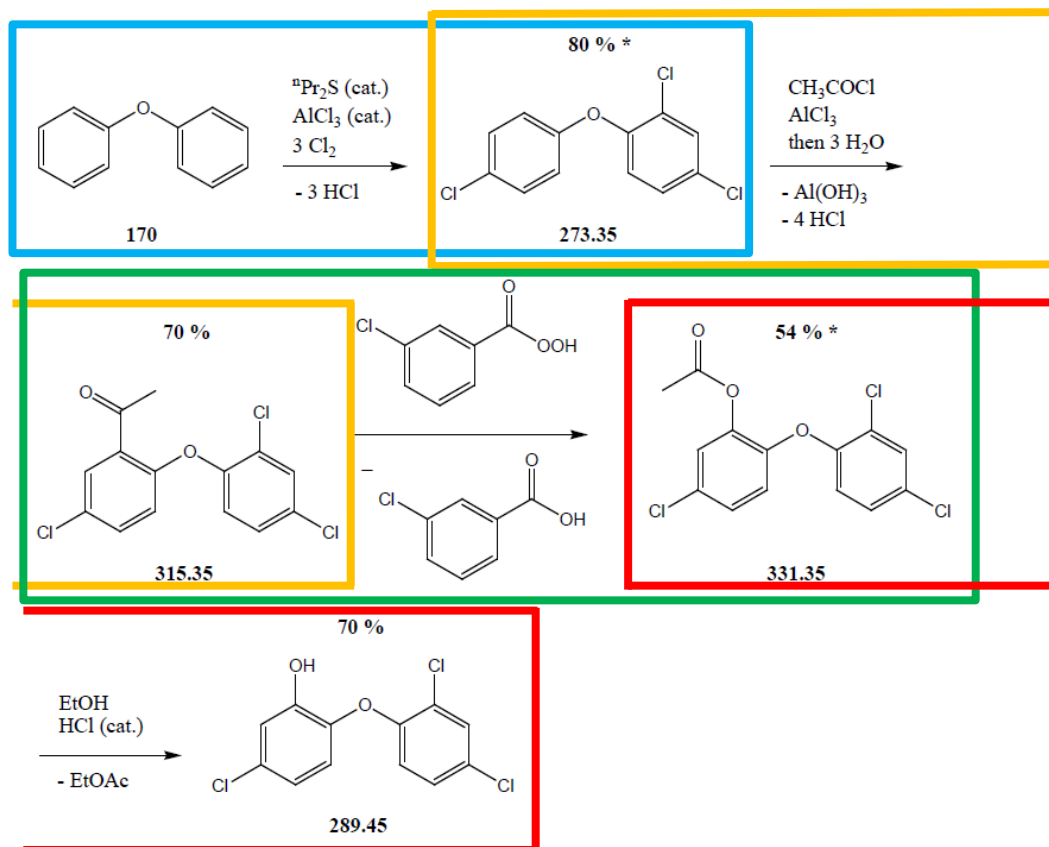
# Several connected reactions



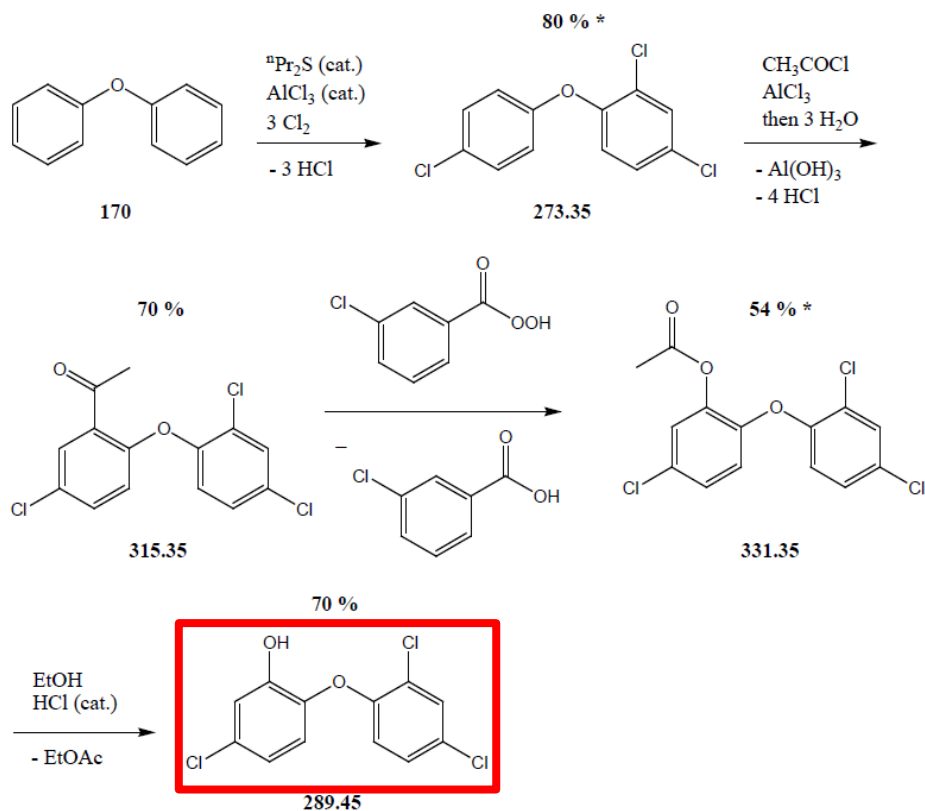
# Several connected reactions



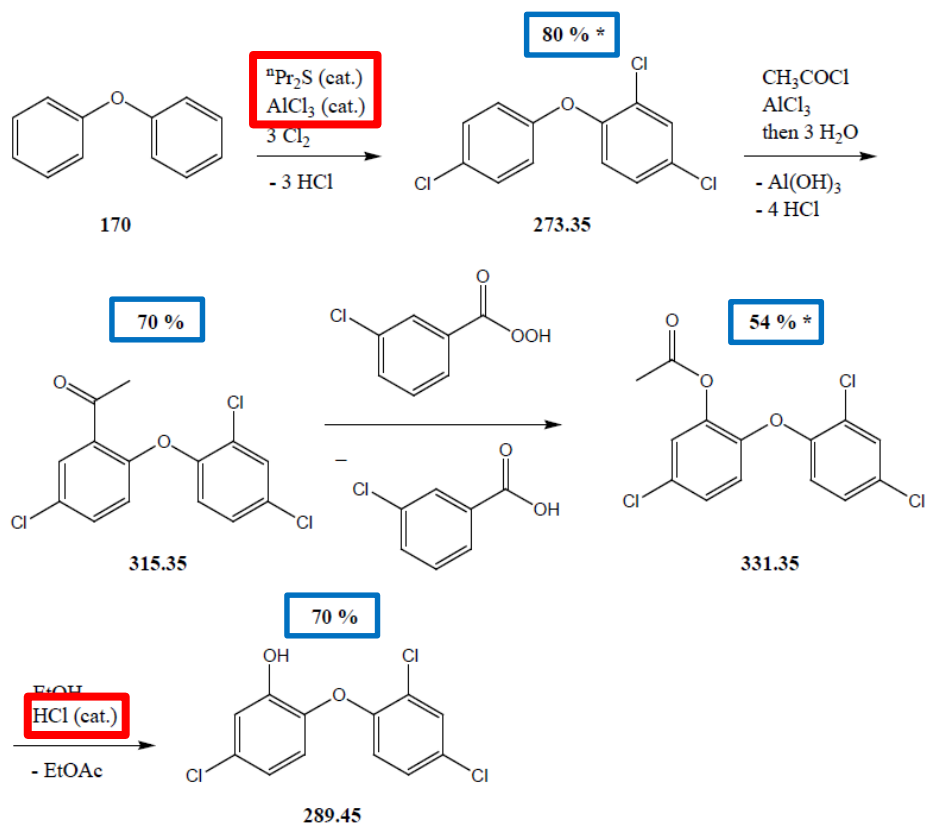
# Several connected reactions



# Target molecule



# Attributes



# The “classical” way

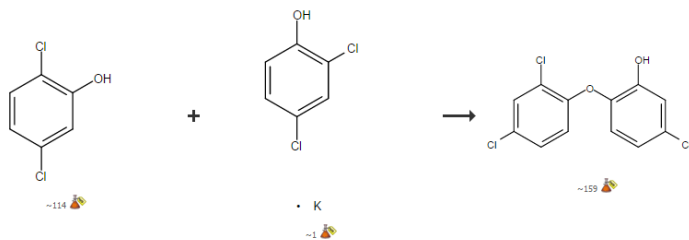
- Plans published in journals
- Created by chemists using ‘chemical intuition’

# The present

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

3. View Reaction Detail [Link](#) [Similar Reactions](#)

Single Step Hover over any structure for more options.



Overview

## Steps/Stages

1.1 C:Bu<sub>4</sub>N<sup>+</sup> •Br<sup>-</sup>, S:Xylene, 4 h, 120°C

## Notes

solid-liquid phase transfer catalysis, scalable, kinetics studied, mechanism studied, agitation (1000 rpm), optimization study, optimized on agitation speed, catalyst, stoichiometry, catalyst loading and reaction temperature, 100% selectivity, glass reactor used, Reactants: 2, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

## References

Novelties of Solid-Liquid Phase Transfer Catalyzed Synthesis of Triclosan from Potassium 2,4-Dichlorophenolate and 2,5-Dichlorophenol  
[Quick View](#) [Full Text](#)  
 By Yadav, Ganapati D. and Motirale, Bhavana G.  
 From Industrial & Engineering Chemistry Research, 47(23), 9055-9060; 2008

Experimental Procedure

# The downsides

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



# File Format

## Header

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

# 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

# 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

[ ... ]



# 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

# Creating new plans

Synthesis: —

User

@

e-mail

Literature:

Title

Author

Journal

DOI

DOI

Add Reaction

Done

# Creating new plans

Synthesis:

lukas

@

lbartonek@tbi.univie.ac.at

Literature:

Enantioefficient Synthesis c

Moldvai, I.; Temesvari-Majr

J. Org. Chem. 2004

DOI

DOI

Add Reaction

Done

# Creating new plans

Synthesis: —

lukas @ lbartonek@tbi.univie.ac.at

Literature:

Enantioefficient Synthesis c Moldvai, I.; Temesvari-Maj J. Org. Chem. 2004

DOI DOI

Add Reaction

Done

# Creating new plans

Title

°C

Temperature

kat

×

Solvent

%

Yield

⇌

Add Input

Add Output

Add Reaction

Done

# Creating new plans

Title

°C

Temperature

kat

×

Solvent

%

Yield

⇌

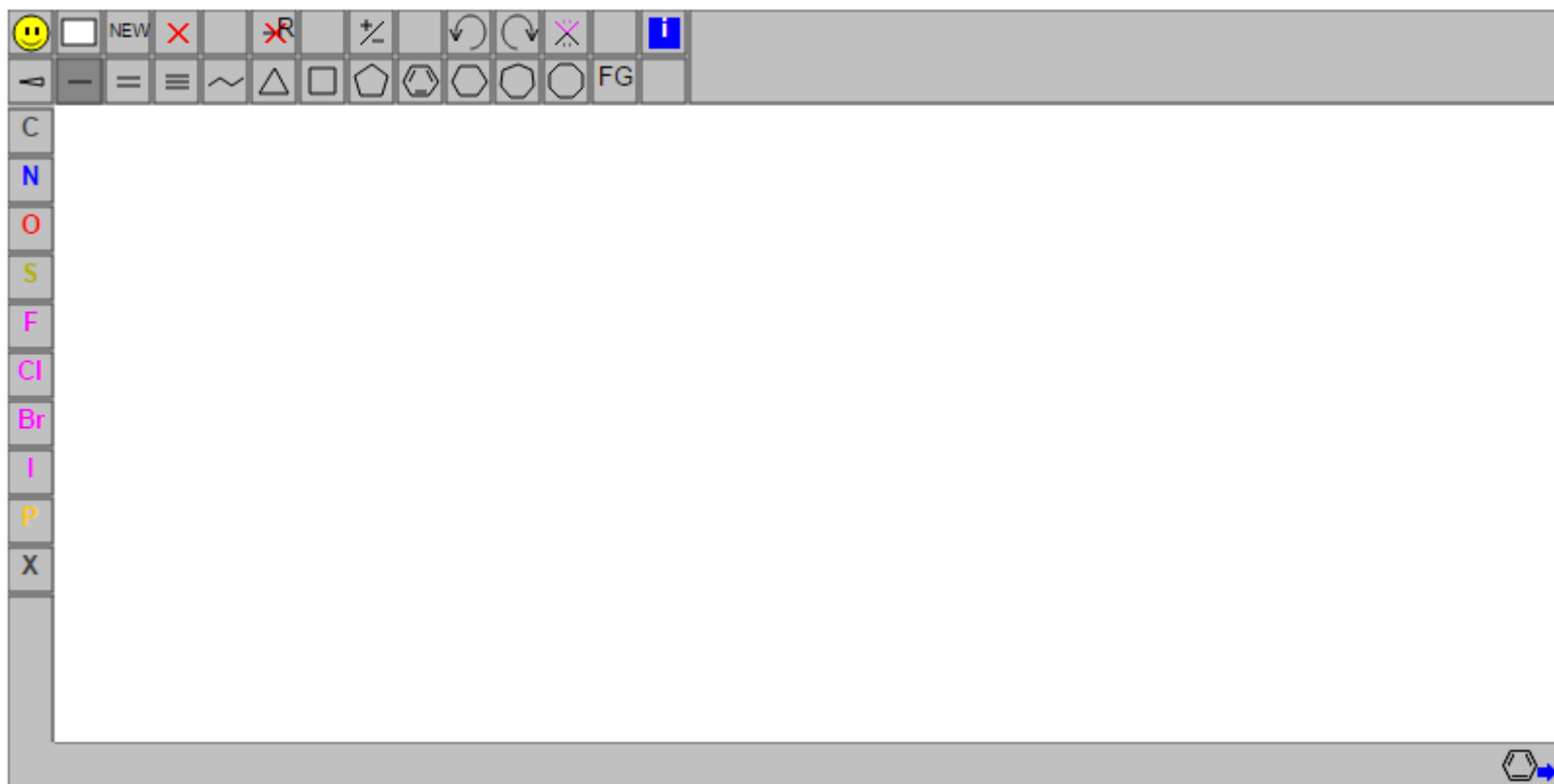
Add Input

Add Output

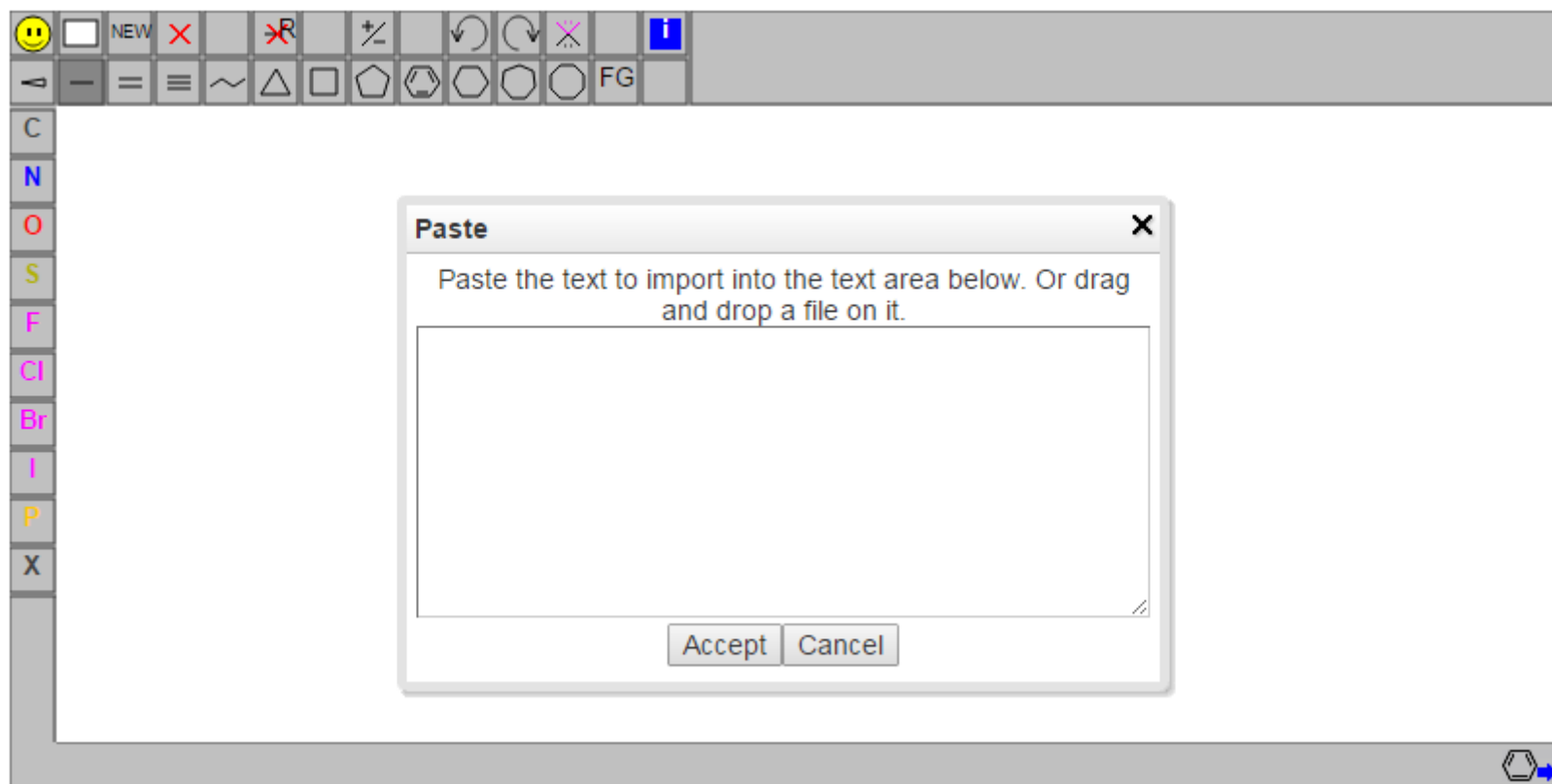
Add Reaction

Done

# Creating new plans



# Creating new plans

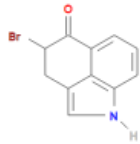


# Creating new plans

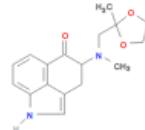
Combination

°C Temperature kat

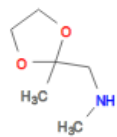
Solvent % R08-R09 56%

1 

☐ Skeleton

1 

☐ Skeleton

1 

☐ Skeleton

Add Input

Add Output

Add Reaction

Done

# Database

Synth Plan

Dashboard

Jobs

Users

Groups

Molecules

Reactions

Synthesis Plans

View Plans

Upload Synthesis Plan

Synthesis Plans






Upload New Synthesis Plan

Create new synthesis plan

Reactions

10 records per page

Search:

ID	Target	Name	Download	User	Updated At	Delete plan
4		4 Imported from commandline	Download	Carsten Grønbjerg Lützen	2015-01-22 20:40:37	Remove plan
5		test	Download	Carsten Grønbjerg Lützen	2015-01-23 10:58:44	Remove plan
6		test2	Download	Lukas Bartonek	2015-01-23 11:01:15	Remove plan
7		testtest	Download	Lukas Bartonek	2015-01-23 11:02:46	Remove plan
11		LSD test	Download	Lukas Bartonek	2015-01-23 14:50:58	Remove plan

Showing 1 to 5 of 5 entries

Previous

1

Next

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

# Possibilities

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



THANK YOU