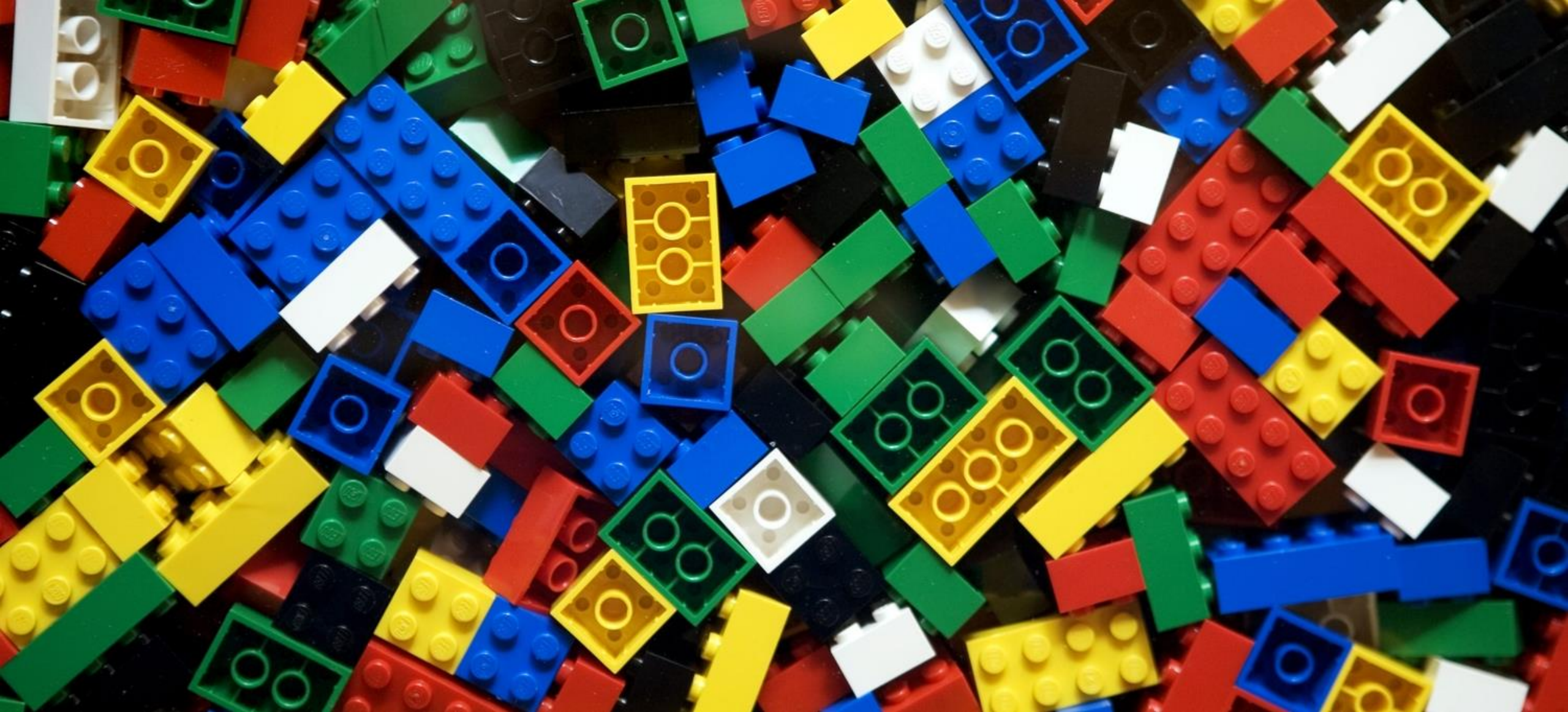


# CHEMAXON IN KNIME

**Attila Szabó**

UGM Budapest 2015



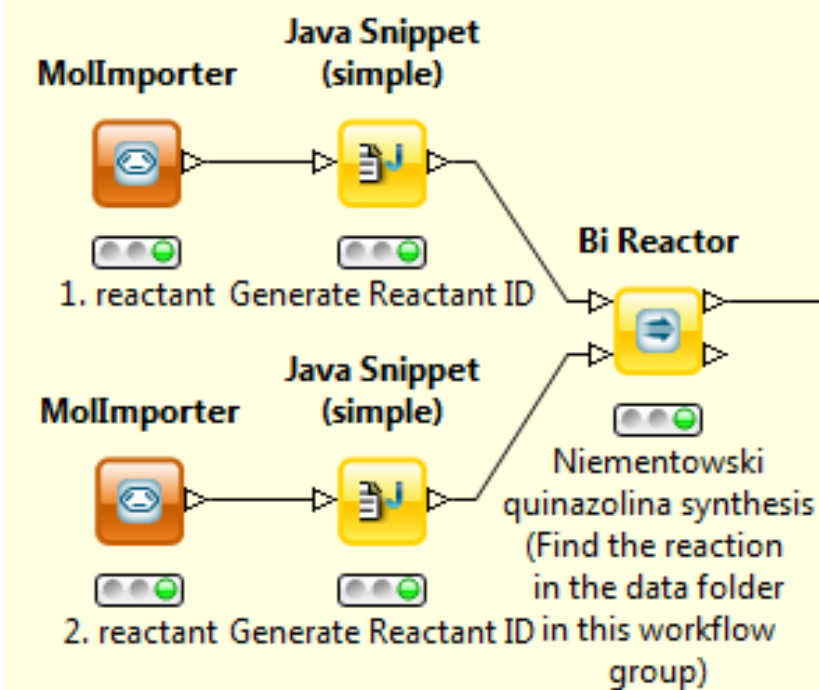
Plenty of individual modules



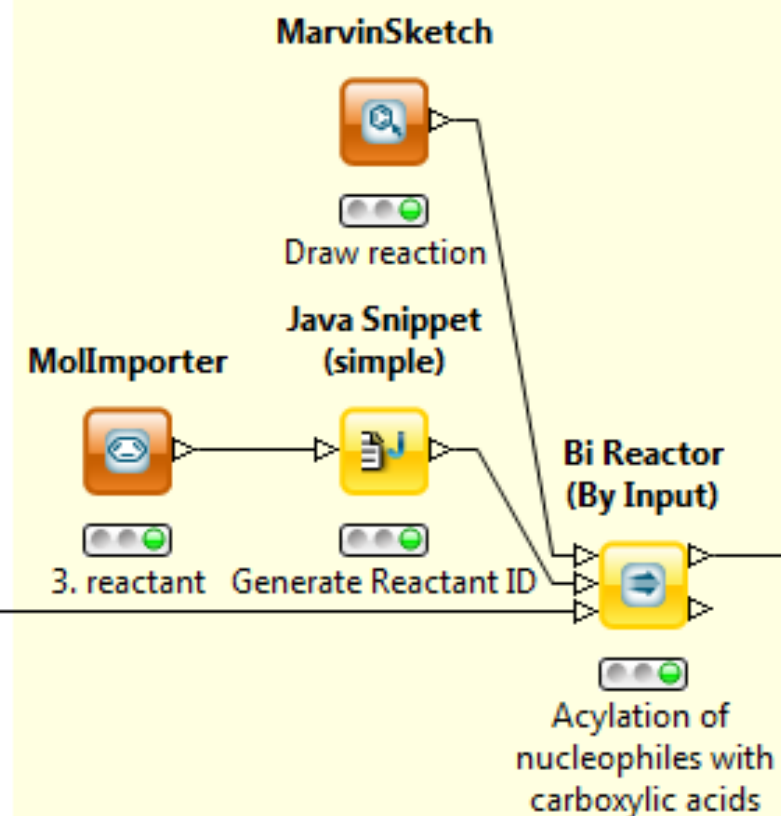


Tailor it to your reasearch processes

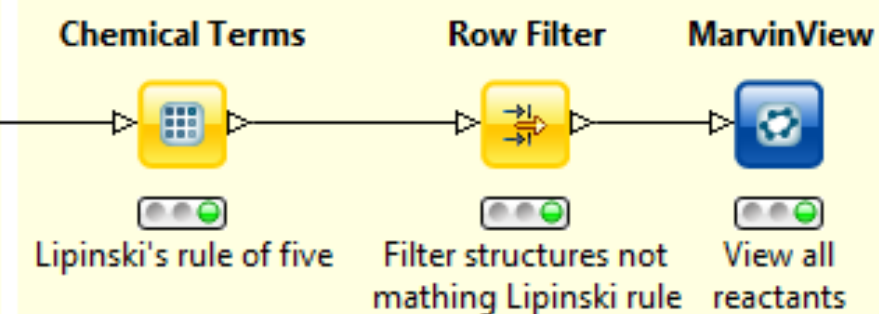
### 1. Reaction - Niementowski (ring closure)



### 2. reaction - Acylation

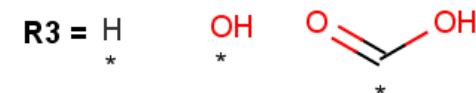
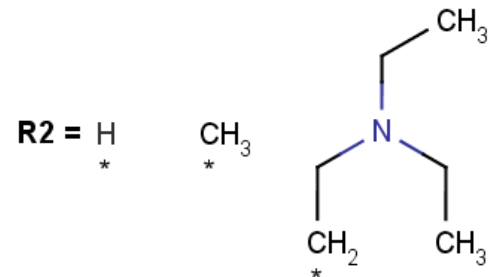
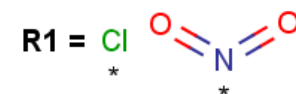
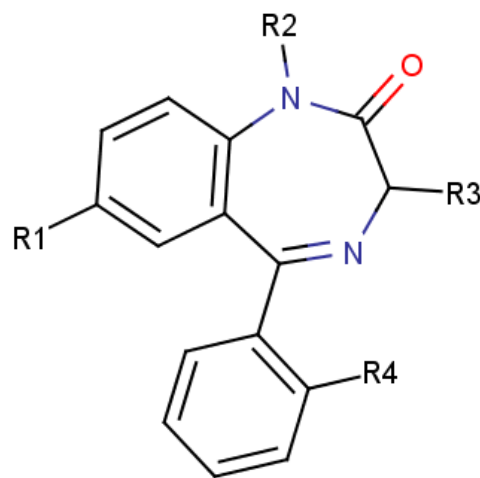
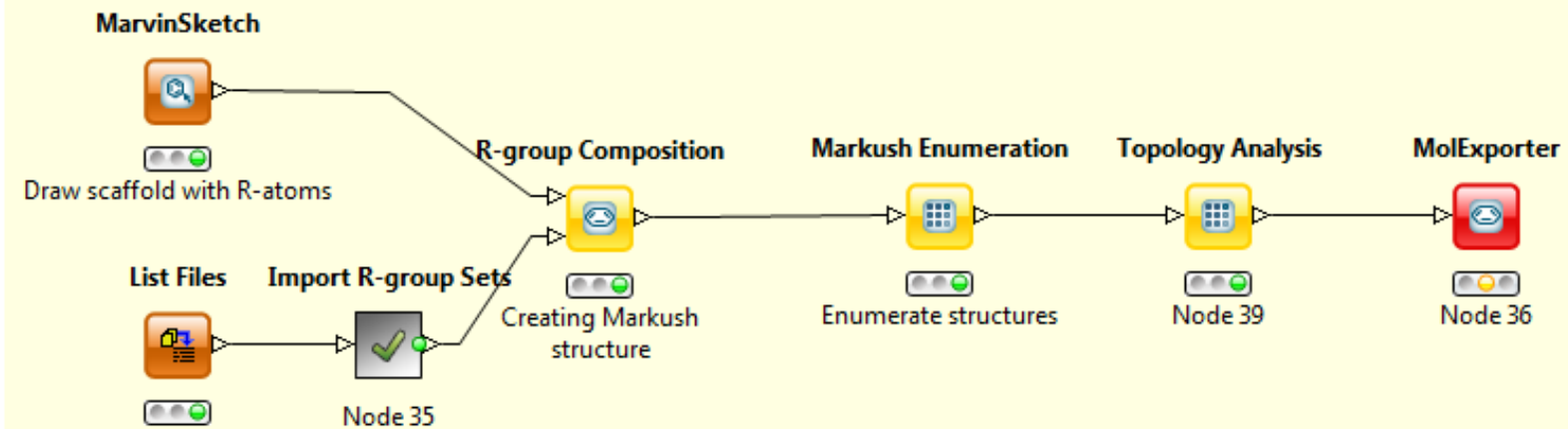


### 3. Analyzing products



## Multi-step reaction enumeration

## Building library based on a scaffold and R-groups



## Scaffold-based enumeration

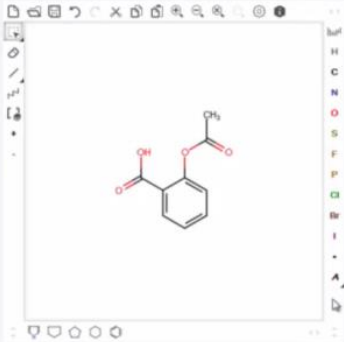
# Descriptors

- pKa
- logP/logD
- Tautomers
- Stereoisomers
- Solubility
- H-bond Donor Acceptor
- Molecular surface area
- Conformation generation
- 3D alignment
- ...

KNIME WebPortal

Workflow Repository

Sketcher 2014-09-17 14:38:31



Structure

Back Next

## Compound Report



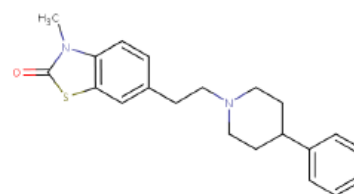
Compound ID 44

IUPAC name 3-methyl-6-[2-(4-phenylpiperidin-1-yl)ethyl]-2,3-dihydro-1,3-benzothiazol-2-one

LogP (octanol/water)  
4.35

Strongest acidic pKa

Solubility (pH 7.4)  
-1.45



Target	IC50
sigma2	8.70
5-HT1A	8.40
5-HT2A	7.00
5-HT3	4.70
D2	6.00
H1	7.70
m1	6.00
sigma1	7.70

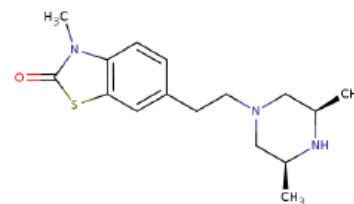
Compound ID 54

IUPAC name 6-[2-[(3R,5S)-3,5-dimethylpiperazin-1-yl]ethyl]-3-methyl-2,3-dihydro-1,3-benzothiazol-2-one

LogP (octanol/water)  
2.38

Strongest acidic pKa

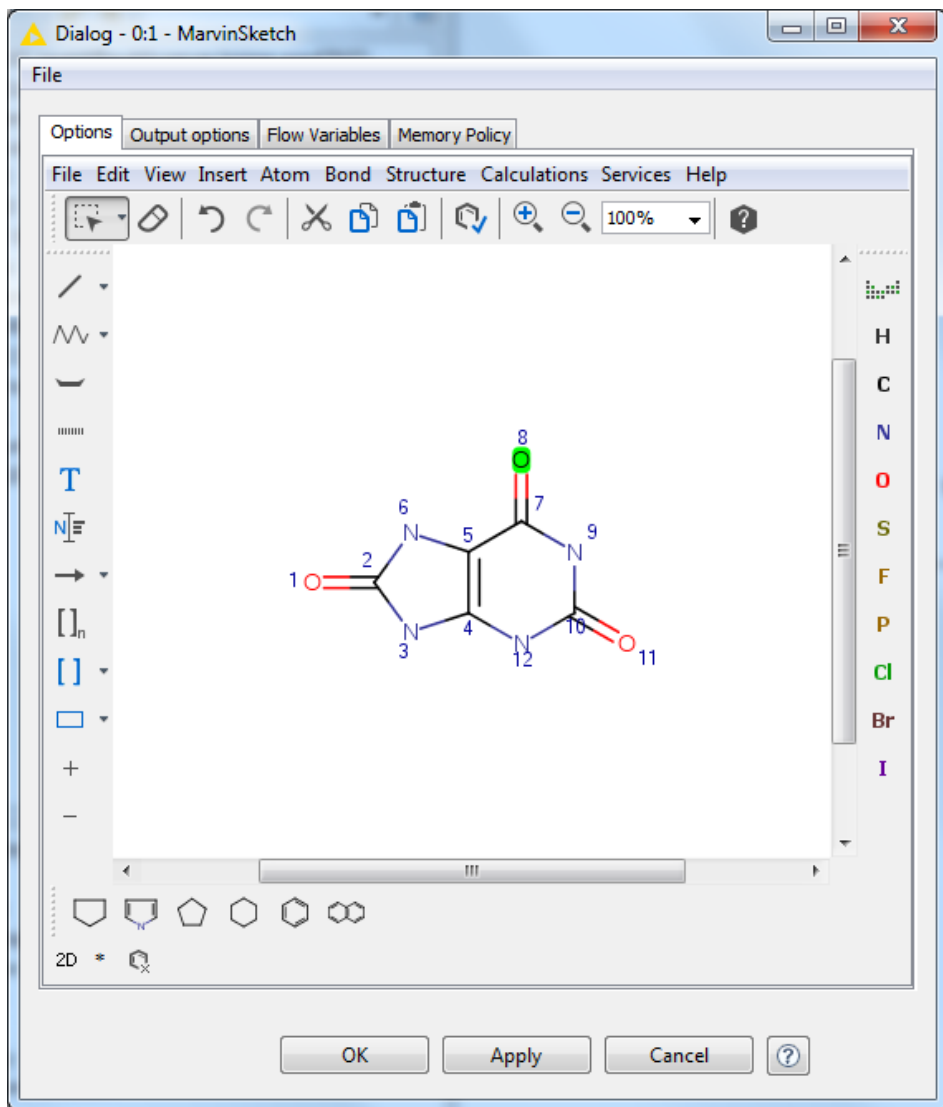
Solubility (pH 7.4)  
0.00



Target	IC50
sigma2	5.70
5-HT1A	
5-HT2A	
5-HT3	
D2	
H1	4.70
m1	

## KNIME Webportal and Reporting

# Handle atom selection



Get Atom Selection



Data Output - 0:4 - Get Atom Selection

File

Table "default" - Rows: 1 Spec - Columns: 2 Properties Flow Variables

Row ID	Molecule	(...) Atom indexes
Row0		[8]



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THANK YOU