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CHEMAXON IN KNIME

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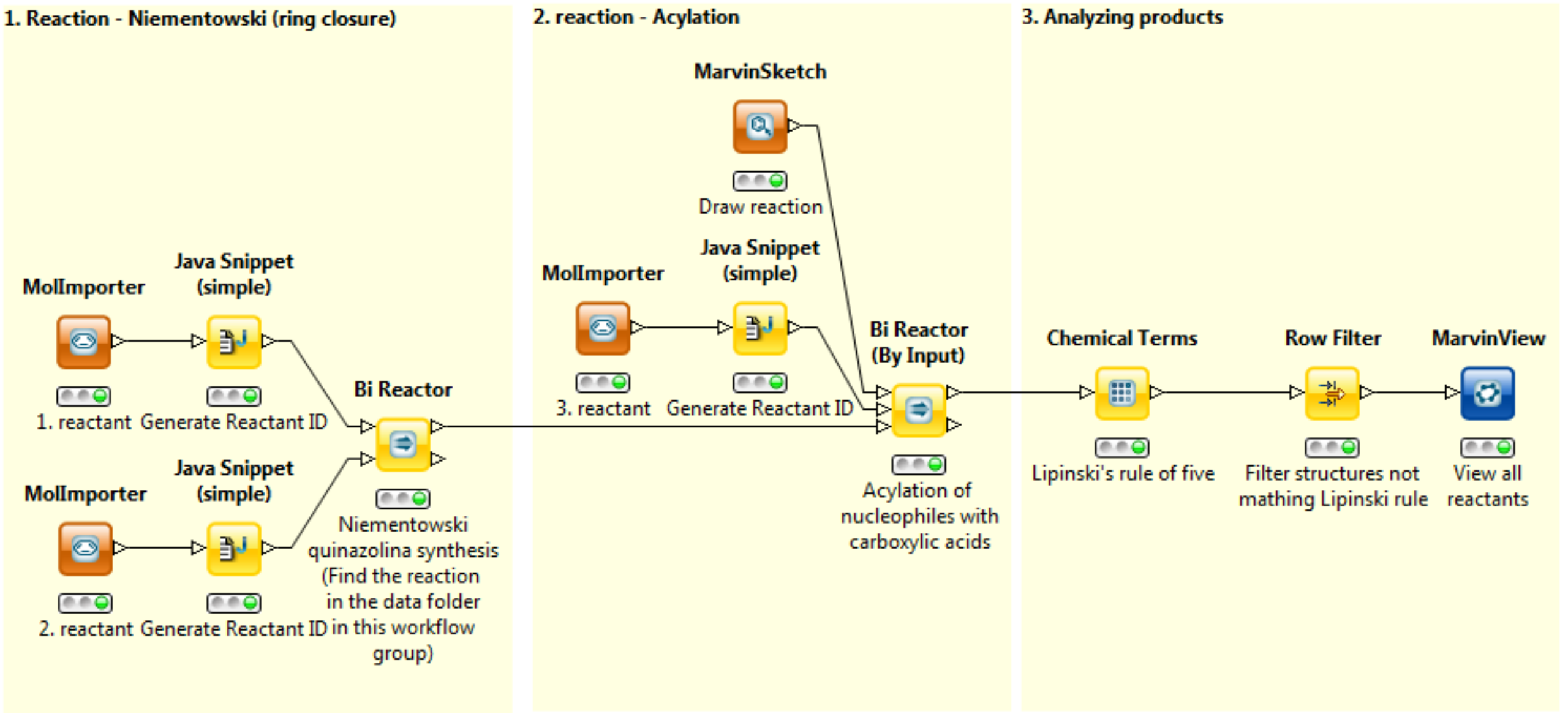
UGM Budapest 2015

Plenty of individual modules

Tailor it to your reasearch processes



Multi-step reaction enumeration

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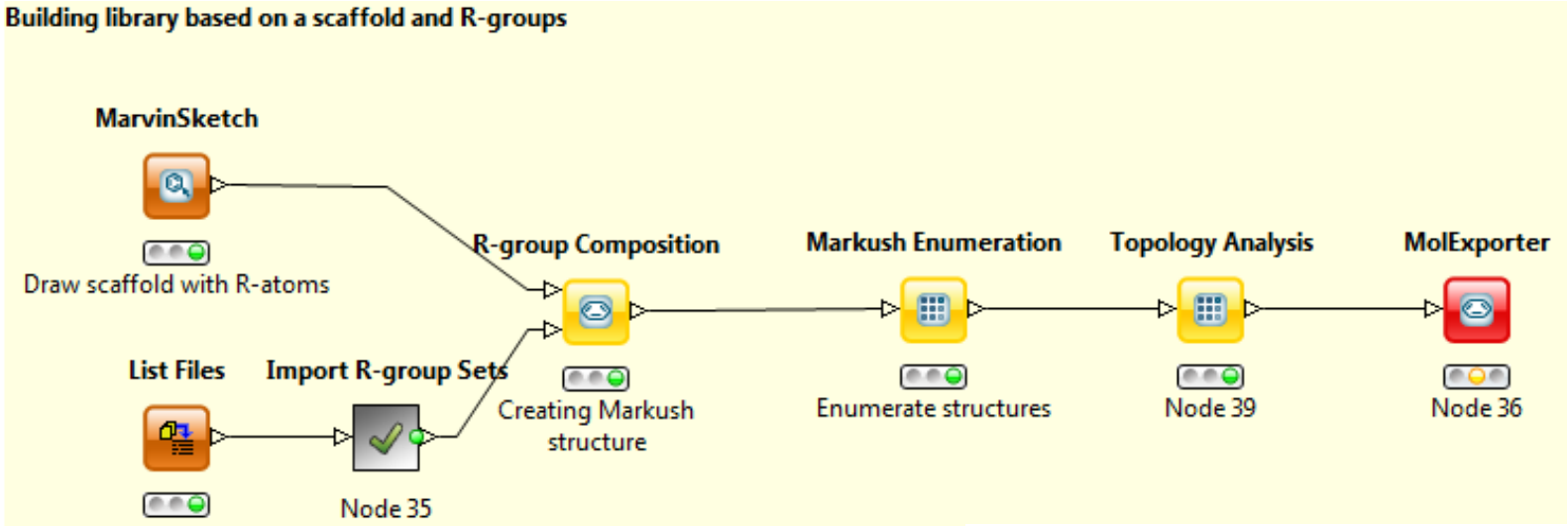
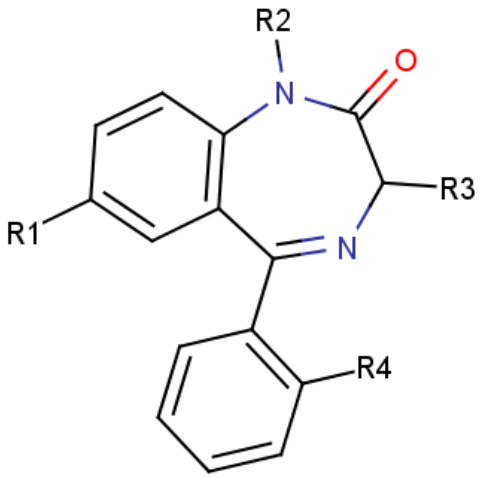
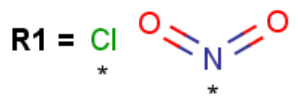
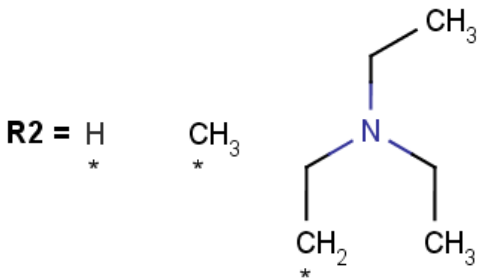
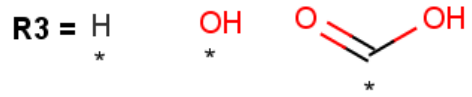






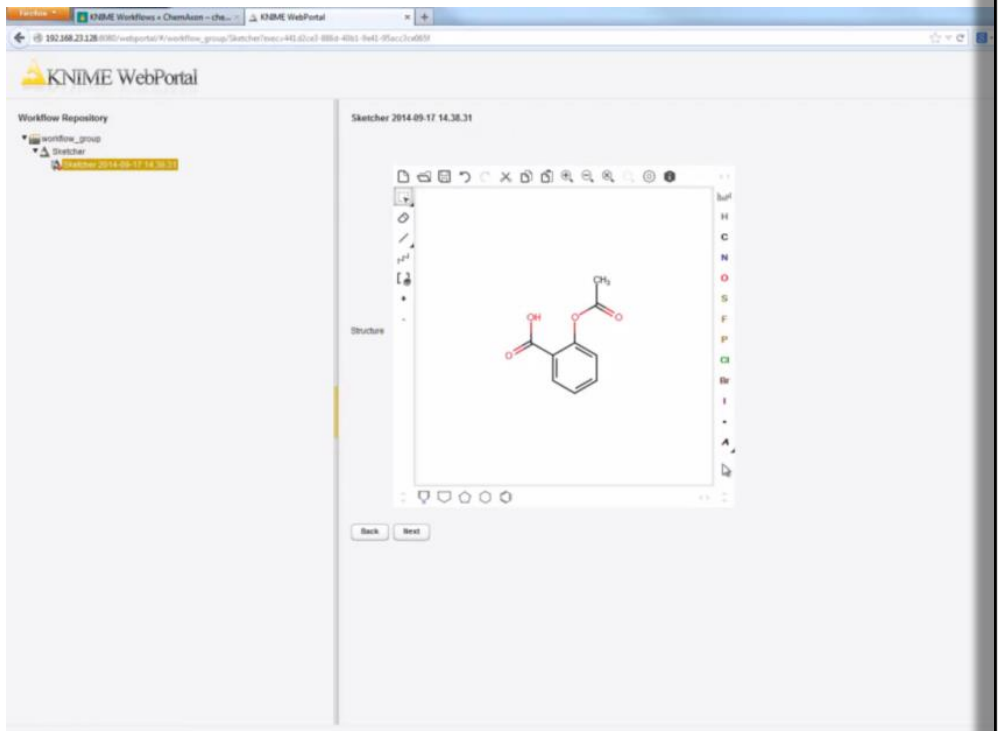




Scaffold-based enumeration

Descriptors

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



KNIME Webportal and Reporting

Compound Report

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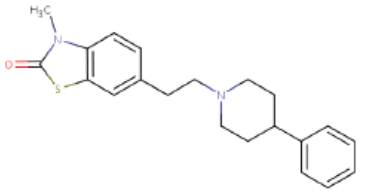
Compound ID	44
IUPAC name	3-methyl-6-[2-(4-phenylpiperidin-1-yl)ethyl]-2,3-dihydro-1,3-benzothiazol-2-one

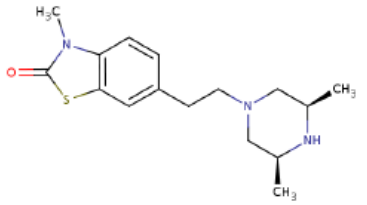
LogP (octanol/water)	4.35
Strongest acidic pKa	
Solubility (pH 7.4)	-1.45



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	

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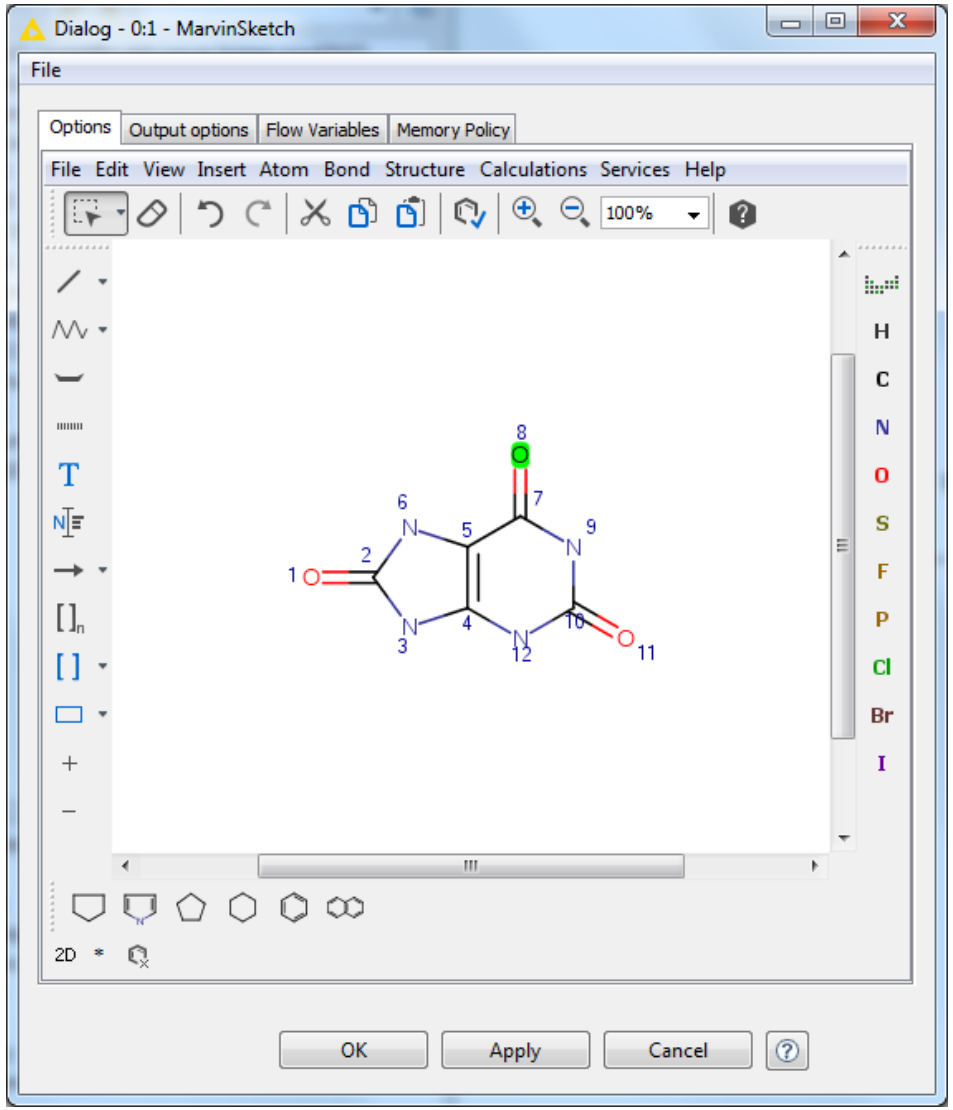
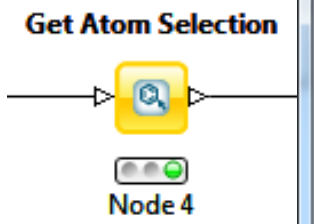
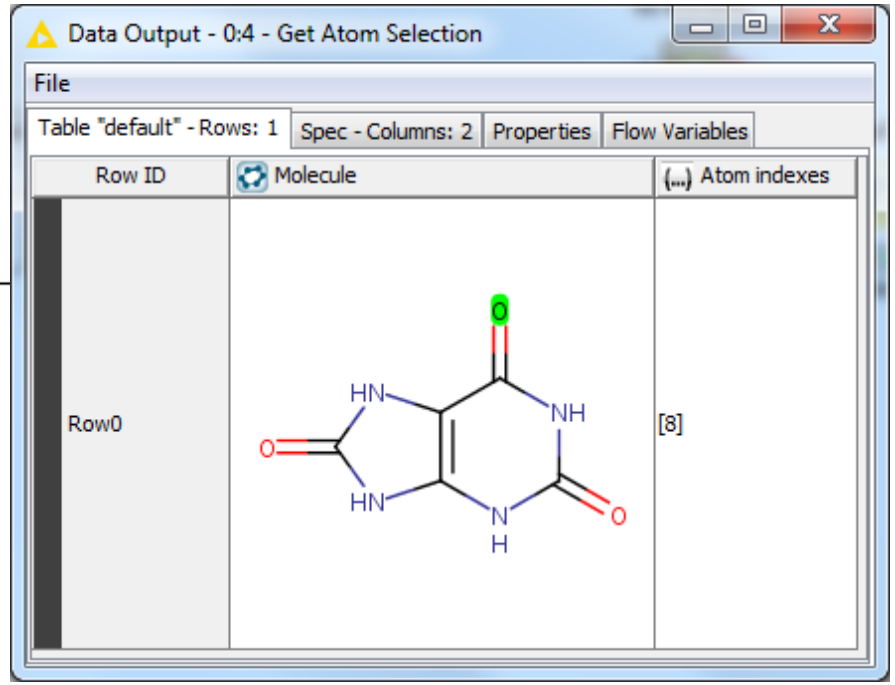
Handle atom selection







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THANK YOU

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