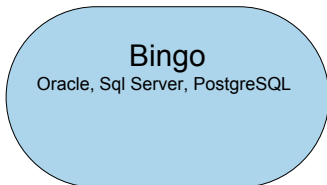


# Indigo KNIME nodes

Mikhail Rybalkin  
Alexander Saveliev

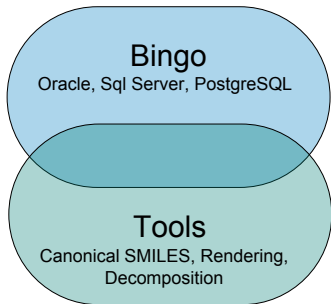
5th KNIME Users Group Meeting and Workshop  
February 2, 2012

## Open-source



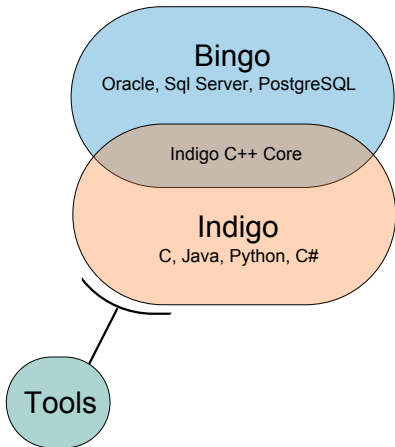
# History of Indigo project

## Open-source



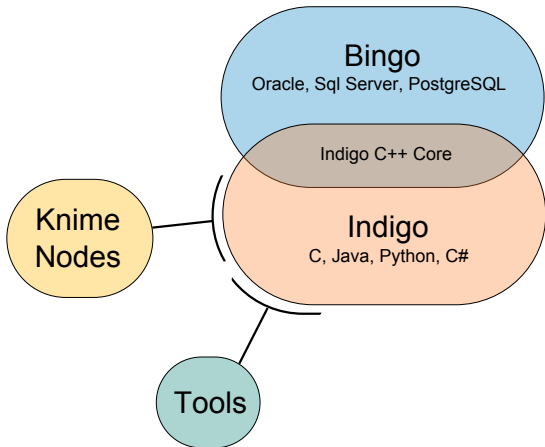
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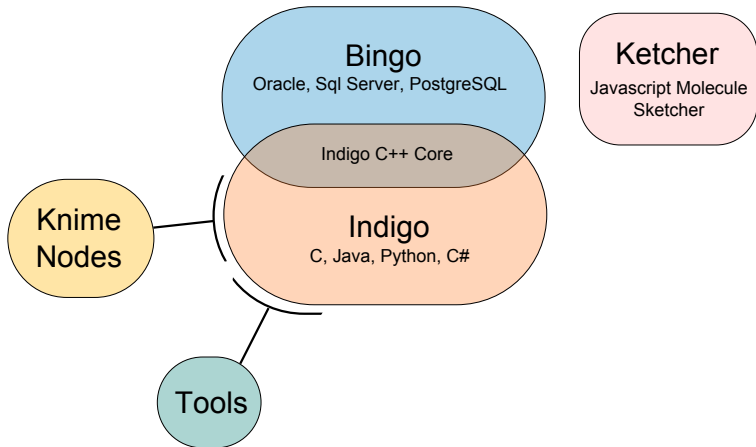
# History of Indigo project

## Open-source



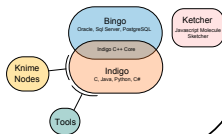
# History of Indigo project

## Open-source



# History of Indigo project

Open-source



## Proprietary projects

- Mass spectrometry
- Molecular dynamics
- Sequence processing
- High-throughput screening
- GPGPU, cluster computing
- Image analysis and recognition

# Why Open Source?

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- ▶ Business model
- ▶ Relationship with the scientific community



# Why Open Source?

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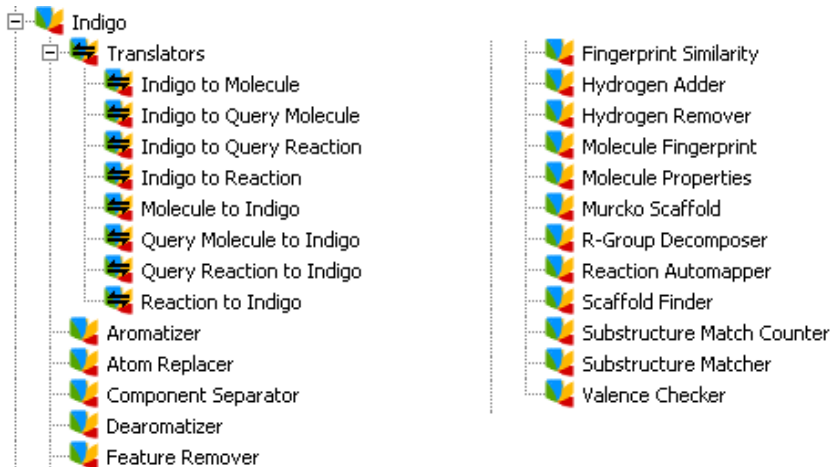
- ▶ Bussiness model
- ▶ Relationship with the scientific commnity
- ▶ Feedback from the commnity
  - ▶ **Suggestions**
  - ▶ Testing

# Why Open Source?

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- ▶ Business model
- ▶ Relationship with the scientific community
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  - ▶ **Suggestions**
  - ▶ Testing
- ▶ Experience to develop commercial projects

# Indigo Nodes (Stable)



# Indigo Nodes (Nightly)

- Indigo
  - Combinatorial Chemistry
    - Combinatorial Reaction Enumeration
  - Manipulators
    - Aromatizer
    - Atom Replacer
    - Bond Replacer
    - Dearomatizer
    - Feature Remover
    - Hydrogen Adder
    - Hydrogen Remover
  - Molecule Nodes
    - Component Combiner
    - Component Separator
    - Molecule Transformation
    - Murcko Scaffold
    - R-Group Decomposer
    - Scaffold Finder
    - Substructure Match Counter
    - Substructure Matcher
  - Molecule Translators
    - Indigo to Molecule
    - Indigo to Query Molecule
    - Molecule to Indigo
    - Query Molecule to Indigo
  - Properties
    - Fingerprint Similarity
    - Indigo Fingerprint
    - Molecule Properties
    - Valence Checker
  - Reaction Nodes
    - Reaction Automapper
    - Reaction Builder
    - Reaction Splitter
    - Substructure Matcher
  - Reaction Translators
    - Indigo to Reaction
    - Indigo to Query Reaction
    - Reaction to Indigo
    - Query Reaction to Indigo

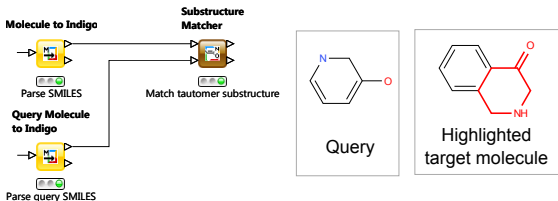
## ► Manipulators



## ▶ Manipulators

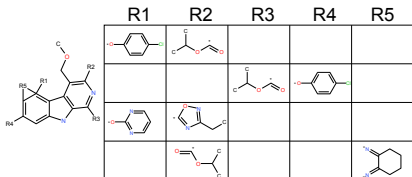
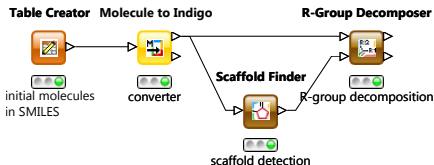


## ▶ Substructure search (Ordinary, Tautomer, Exact)



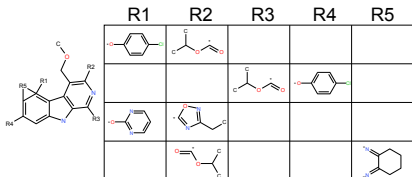
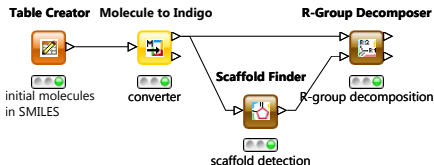
# Functionality (2)

## ► Scaffold finder and R-Group decomposition

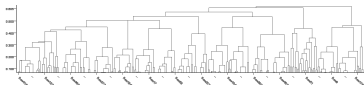
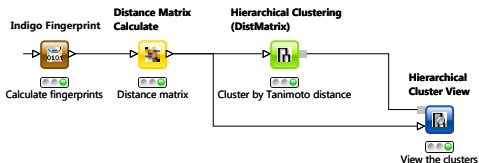


# Functionality (2)

## ▶ Scaffold finder and R-Group decomposition



## ▶ Indigo Fingerprints





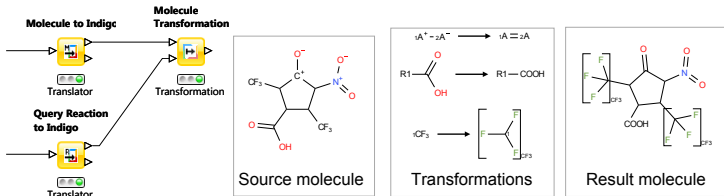
# Whats New?

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- ▶ Reaction Support
- ▶ Library Enumeration

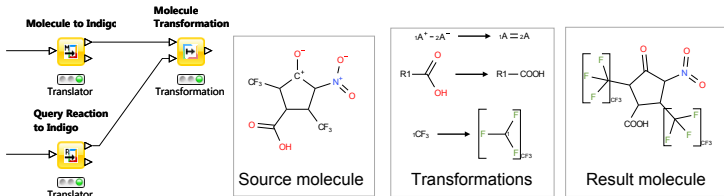
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- ▶ Library Enumeration
- ▶ Molecule Transformations (Standardization)



- ▶ Builder/Splitter Nodes
- ▶ InChI, InChIKey (preliminary)
- ▶ No dependencies on other packages in RHEL, and Mac OS X

- ▶ Real workflow examples (by Simon)
- ▶ Indigo nodes in-depth
- ▶ Planned nodes
- ▶ **Discussion**

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Thank you!