

# Pipeline Pilot Integration

**Szilard Dorant**

# The Component Collection: Quick facts

---

- Provides access to ChemAxon tools from Pipeline Pilot
- Developed and Supported by ChemAxon
- Free of charge
- Open source: sources included, may be modified
- Latest version : 1.7
  - Release date: May 2010\*
  - Requires:
    - JChem / Marvin 5.2.5 or newer
    - Pipeline Pilot 7.5 or newer

\*Planned

## Available functionality (1/2)

---

- Standardizer: structure canonicalization
- Chemical Terms expressions for filtering and calculations (including logP, logD, pKa, HBD, HBA, Isoelectric point, PSA and more)
- Reactor : “smart” virtual reaction processing
- Maximum Common Substructure (MCS) based clustering
- IUPAC Name <-> Molecule conversion (both directions)
- JChem Base chemical database: insertion, search and retrieval of structures; create and drop structure tables
- Marvin applets: structure visualization and editing

## Available functionality (2/2)

---

- Major microspecies (major protonation form)
- Microspecies distribution
- Burden eigenvalue descriptor (BCUT)
- MolConverter: conversion of the wide range of structure formats supported by ChemAxon
- Markush (generic structure) enumeration
- Tautomerization: tautomer generation (all, dominant, major, canonical, generic)
- Conformer generation
- Image generation

# Release history - major changes

---

- **Version 1.7, May 2010** (planned)
  - New components: “ChemAxon Image from Molecule“, “ChemAxon Molecular Table Viewer”
  - “JChemSearch” component upgraded
- **Version 1.6, August 2009**
  - New component: "ChemAxon 3D Conformers"
- **Version 1.5, May 2009**
  - New components: "ChemAxon MolConverter", "ChemAxon Tautomerization", "ChemAxon Markush Enumeration"
- **Version 1.4, November 2008**
  - New components: "LibMCS Clustering", "Molecule to IUPAC Name", "Molecule from IUPAC Name“
  - " ChemAxon Reactor" component upgraded
- **Version 1.3, July 2008**
  - New component: “Chemical Terms Calculator”
- **Version 1.2, March 2008**
  - New components: “ChemAxon Reactor”, “Drop JChem Base Table”, “Create JChem Base Table”

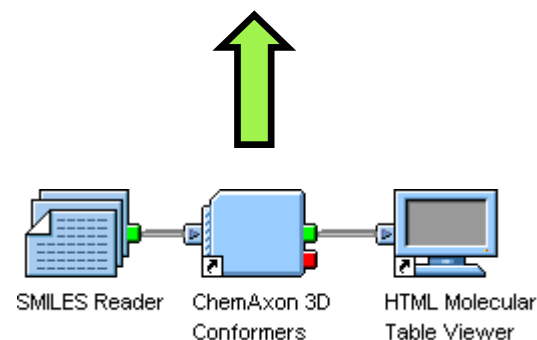
# Conformer generation

## Component for 3D conformer generation

New in 1.6

- Calculation modes:
  - Multiple conformers
  - Lowest energy conformer
- Options:
  - Maximum number of conformers
  - Diversity limit
  - Optimization limit, hyperfine option
  - Time limit
  - Generate with explicit H atoms
  - Energy unit kcal/mol or KJ/mol, into arbitrary property

Parameters	
<input type="checkbox"/> Calculate Lowest Energy Conformer	False
Maximum Number of Conformers	10
Diversity Limit	0.1
Optimization Limit	Normal
Hyperfine	False
Time Limit	900
<input type="checkbox"/> Energy Value Property Name	Energy
Energy Unit	kcal/mol
Prehydrogenize	True



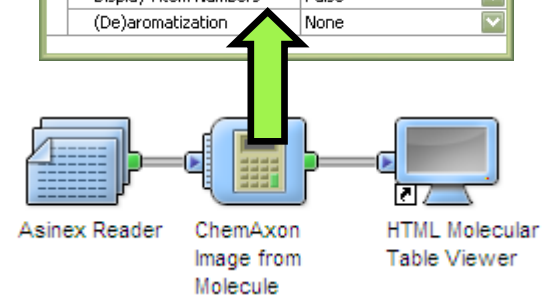
# Image Generation

## High-quality ChemAxon-rendered images

New in 1.7

- Image formats: PNG, BMP, JPEG
- Input either
  - Pipeline Pilot Molecule
  - Structure source (e.g. MRV string)
- Numerous rendering options, for example:
  - Image size, background, transparency
  - Scaling, max scale, atom label size
  - Various aromatization, dearomatization modes
  - R/S label, E/Z label, Absolute label options
  - Mark valence errors
  - Implicit H display, add/remove explicit H
  - etc ...

Parameters	
Output to Property	cxn_image
Import from Property	
Option String	
Image Options	
Image Format	PNG
Width	400
Height	400
Scale	
Max Scale	28
Background Color	
Transparent	False
Rendering	Default
Atom Label Scale Factor	1.0
Chemistry Options	
Implicit Hydrogens	Hetero and Terminal
Explicit Hydrogens	Remove
R/S Labels	All
E/Z Labels	Off
Absolute Labels	On
Mark Valence Errors	True
Labels on Carbon Atoms	Auto
Down Wedge Orientation	Down
Display Atom Maps	True
Display Atom Numbers	False
(De)aromatization	None



# HTML Molecular Spreadsheet

---

Scalable molecule and data display

New in 1.7

- Builds on the architecture of the native Pipeline Pilot component “HTML Molecular Table Viewer” : well tested architecture for paging and data display
- Initial image in table can be Pipeline Pilot or ChemAxon rendered
- On-click of the primary picture various pop-up functions are available:
  - Larger picture (ChemAxon-rendered)
  - Single cell MarvinView applet
  - Structure file: to save or open by desktop application

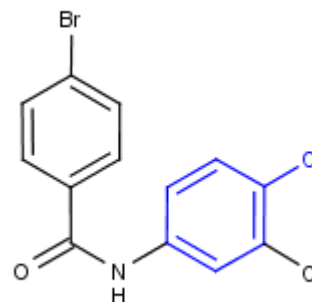


# JChemSearch improvements

## Database search component refurbished

Updated in 1.7

- MRV structure source output option
- Hit coloring (with MRV output)
- Hit alignment
  - Rotate
  - Partial clean
- Flow-trough (“Query filtering”) mode
- Option for fetching data fields from JChem Base structure table
- "Search Type" options "Exact" and "Exact fragment" renamed to "Full Structure" and "Full Fragment" respectively
- New "Search Type" option: "Duplicate"
- Option "Exact Stereo Matching" removed, boolean option "Stereo Search" became 4-state option: "On", "Exact", "Diastereomers", "Off"



# Planned development

---

- Components to ease JChem Cartridge access
- Fragmenter (RECAP), R-group decomposition
- Integration with Instant JChem
- Improvements of several existing components
- Online documentation

*Node release cycle is fast and flexible. Please advise us on priority and additional functionality for future node development.*

# Resources

---

- Download:  
<http://www.chemaxon.com/integration/download.html>
- Technical support forum:  
<http://www.chemaxon.com/forum/forum88.html>
- E-mail:  
[pp@chemaxon.com](mailto:pp@chemaxon.com)
- General presentation:  
[http://www.chemaxon.com/conf/Pipeline\\_Pilot\\_Integration.ppt](http://www.chemaxon.com/conf/Pipeline_Pilot_Integration.ppt)