

Triplos Chemistry Extensions (TCE)





Tripos Chemistry Extensions (TCE)

Brings the Tripos cheminformatics capabilities into the KNIME platform

- read / write and process chemical structures
- perform basic and advanced cheminformatics tasks
- visualize & interpret molecular structures



Tripos Chemistry Extensions (TCE)

Two important things to know about TCE

- No “backend” software required beside the nodes
- Basic cheminformatic nodes are usable at no cost!



Triplos Chemistry Extensions (TCE)

SD Reader



Node 1

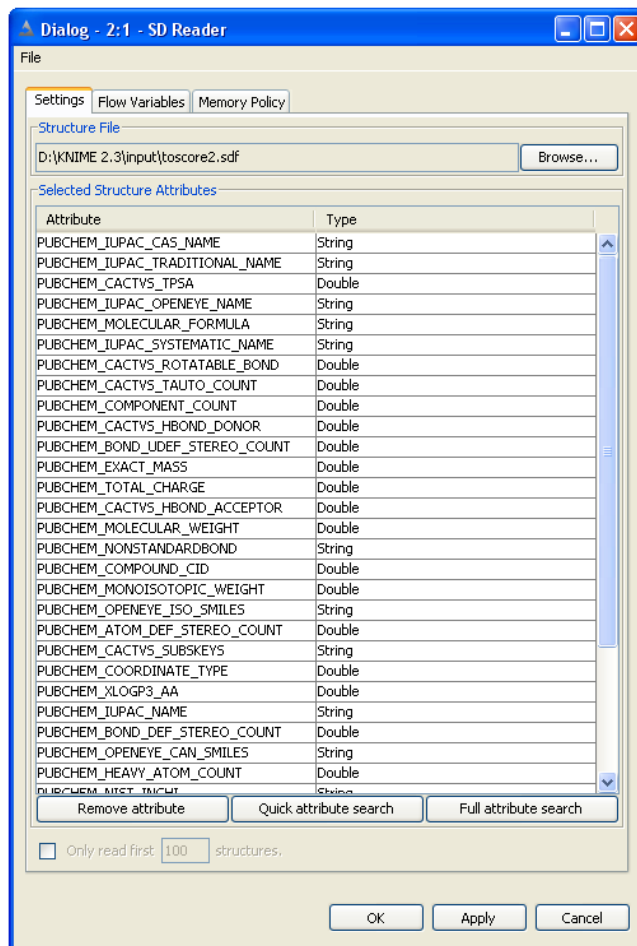


Tripos Chemistry Extensions (TCE)

SD Reader



Node 1





Triplos Chemistry Extensions (TCE)

SD Reader



Node 1



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SLN Reader



Node 2

http://en.wikipedia.org/wiki/SYBYL_Line_Notation



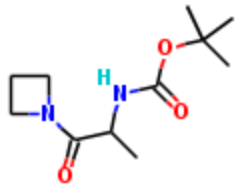
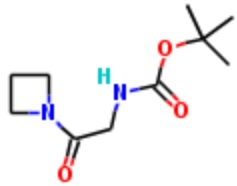
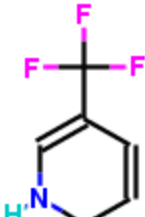
Tripos Chemistry Extensions (TCE)

Table containing the valid structures and ...

File

Spec - Columns: 2 Properties Flow Variables

Table "default" - Rows: 2713

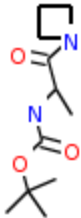
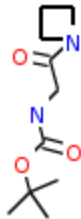
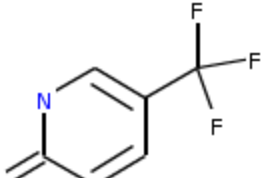
| Row ID | S RegID | sdf SDF structure |
|--------|--------------|---|
| 19 | ZINC42750158 |  |
| 20 | ZINC42750160 |  |
| 21 | ZINC08698270 |  |

Parsed molecules - 2:2 - Molecule to CDK

File

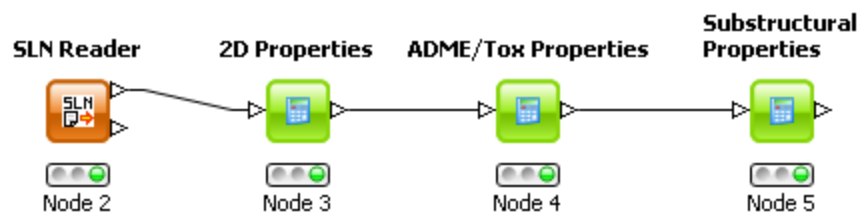
Spec - Columns: 2 Properties Flow Variables

Table "default" - Rows: 2713

| Row ID | S RegID | ox SDF structure |
|--------|--------------|---|
| 19 | ZINC42750158 |  |
| 20 | ZINC42750160 |  |
| 21 | ZINC08698270 |  |

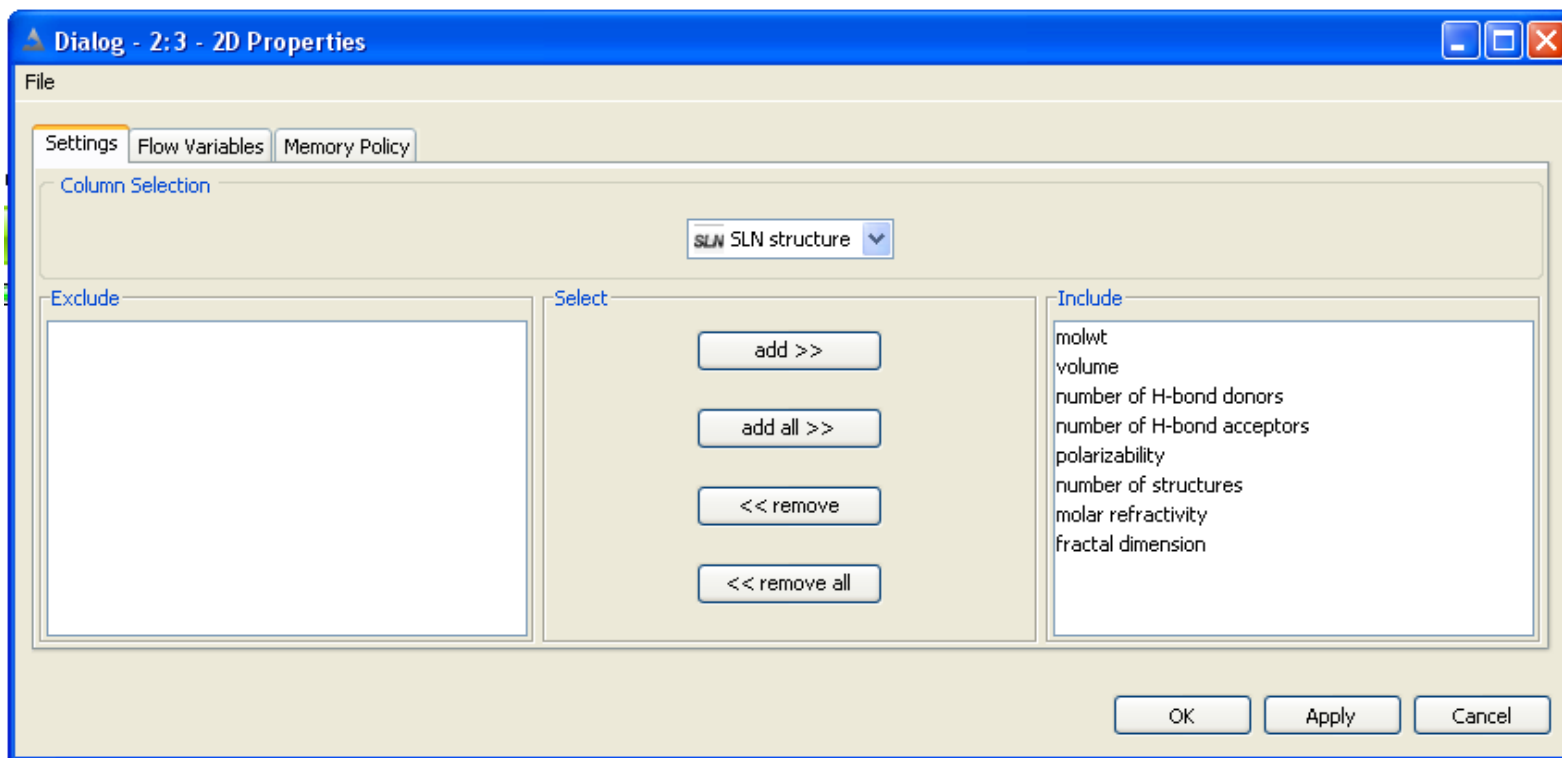


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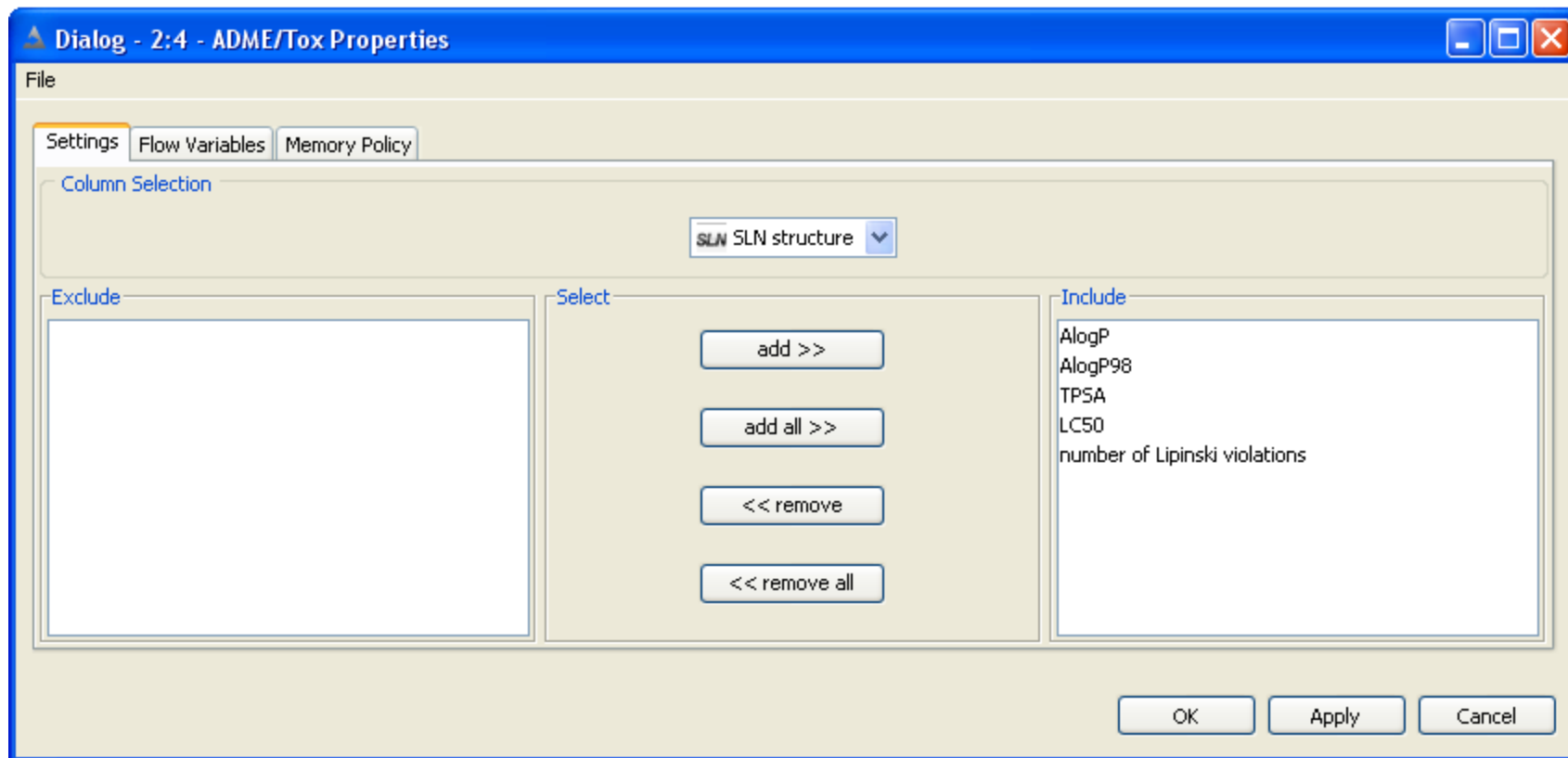


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Dialog - 2:5 - Substructural Properties

File

Settings | Flow Variables | Memory Policy

Column Selection

SLN SLN structure

Exclude

- P atoms
- Se atoms
- bonds
 - total bonds
 - double bonds
 - triple bonds
 - aromatic bonds
 - rotatable bonds
 - non-rotatable bonds
- rings
 - total rings
 - hetero rings
 - largest ring size
- functional groups
 - aldehyde groups
 - amide groups
 - amine (primary) groups
 - amine (secondary) groups
 - amine (tertiary) groups
 - ammonium groups
 - carbonyl groups
 - carboxyl groups
 - ester groups
 - ether groups
 - hydroxyl groups
 - keto groups
 - methyl groups

Select

add >>

add all >>

<< remove

<< remove all

Include

- single bonds



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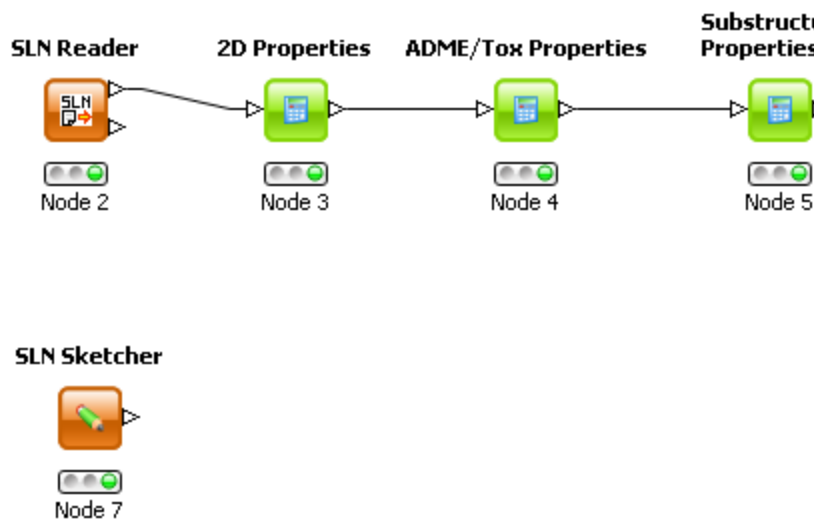
SLN Sketcher



Node 7



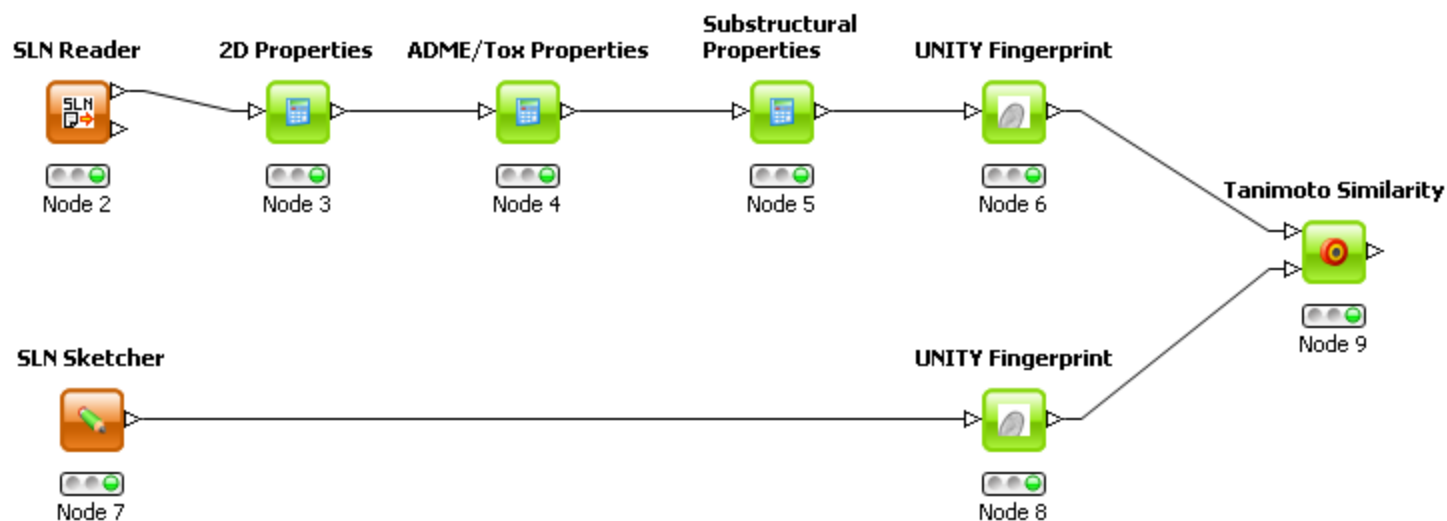
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The screenshot shows a software dialog box titled "Dialog - 2:7 - SLN Sketcher". The window has a blue title bar with standard Windows window controls (minimize, maximize, close). Below the title bar is a "File" menu. The main content area is divided into tabs: "Settings", "Flow Variables", and "Memory Policy". Under the "Settings" tab, there is a section for "Query Structure" with a text input field labeled "Structure Name:" containing the text "demo". Below this input field are three buttons: "Sketch...", "Browse...", and "Enter SLN...". The central part of the dialog displays a chemical structure of a benzothiazine derivative. The structure features a benzene ring with a substituent labeled "Any" in cyan. The benzothiazine core is colored with blue for nitrogen atoms, red for oxygen atoms, and yellow for the sulfur atom. At the bottom of the dialog are three buttons: "OK", "Apply", and "Cancel".

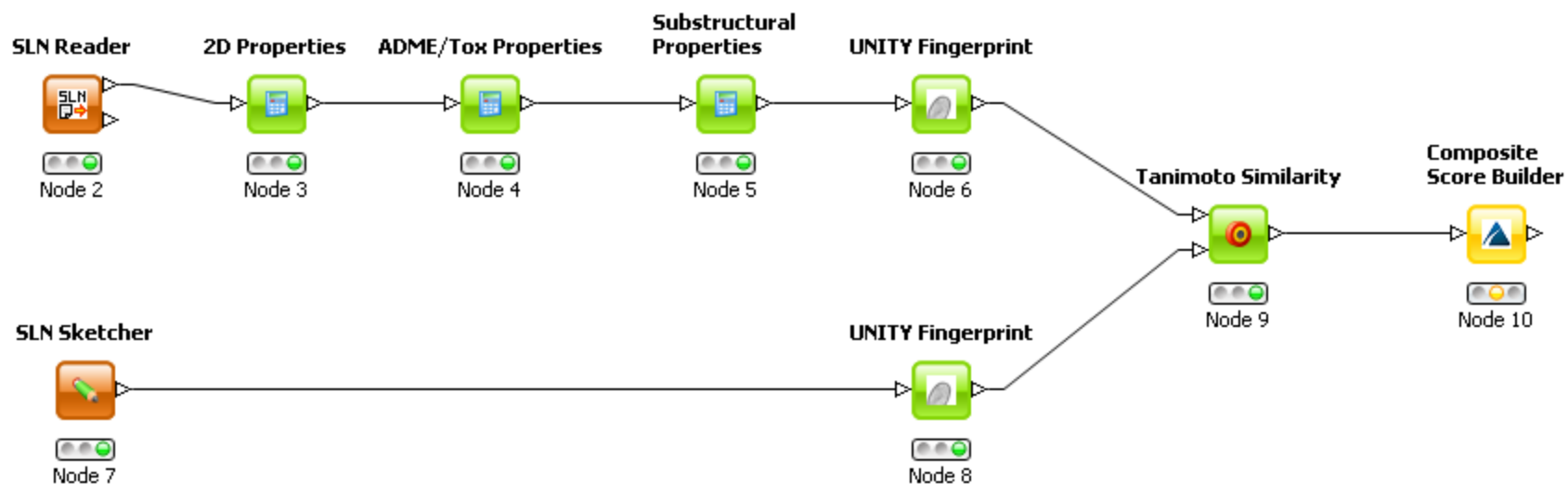


Tripos Chemistry Extensions (TCE)





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Dialog - 2:10 - Composite Score Builder

File

Options | Flow Variables | Memory Policy

Available Columns

- volume
- polarizability
- number of structures
- molar refractivity
- fractal dimension
- AlogP98
- LC50
- single bonds

Add >>
Add All >>
<< Remove
<< Remove All

Selected Columns

| Column Name | Weight | Normalizer |
|-------------------------------|--------|------------|
| molwt | 5 | Gaussian |
| number of H-bond donors | 3 | Two Step |
| number of H-bond acceptors | 3 | Two Step |
| AlogP | 1 | Gaussian |
| TPSA | 1 | Gaussian |
| number of Lipinski violations | 1 | Pass Thru |
| MaxTan | 3 | Pass Thru |

How Should The Overall Score Be Computed?

Sum all normalized scores
 Multiply all normalized scores

Other Options

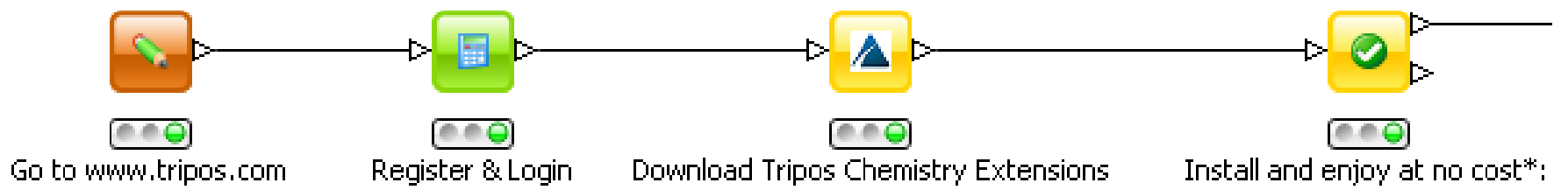
Output normalized scores
Name (and name prefix) for the output column(s): Score

Normalization Rule for molwt

Input values between C1: 200 and C2: 450 return P: 1
Input values less than C1 or greater than C2 return values from a gaussian (bell) curve
with a spread of S: 50 asymptotically approaching B: 0

Test Normalization of Sample Values

Normalize: 475 Result: 0.7788007830714049



Questions? Comments?

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