

## Triplos Chemistry Extensions (TCE)

**Triplos**<sup>™</sup>  
A Certara<sup>™</sup> Company

**Triplos**<sup>™</sup>  
A Certara<sup>™</sup> Company

*Pharsight*  
  
A Certara<sup>™</sup> Company



# 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

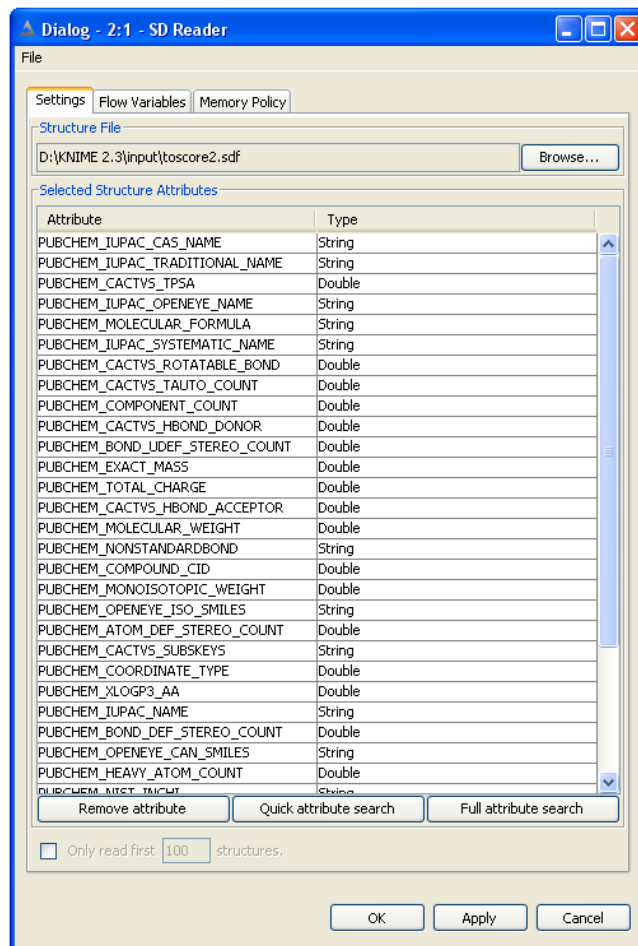


# Tripos Chemistry Extensions (TCE)

SD Reader



Node 1





# Triplos Chemistry Extensions (TCE)

---

SD Reader



Node 1



# Triplos Chemistry Extensions (TCE)

---

## SLN Reader



Node 2

[http://en.wikipedia.org/wiki/SYBYL\\_Line\\_Notation](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

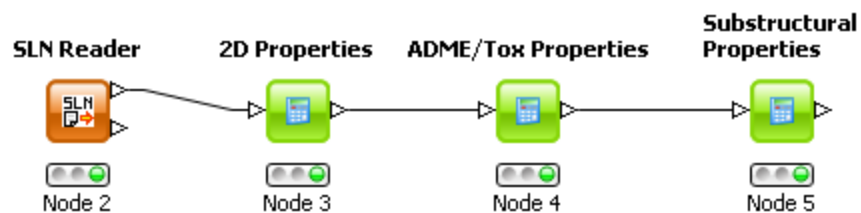
Table "default" - Rows: 2713

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



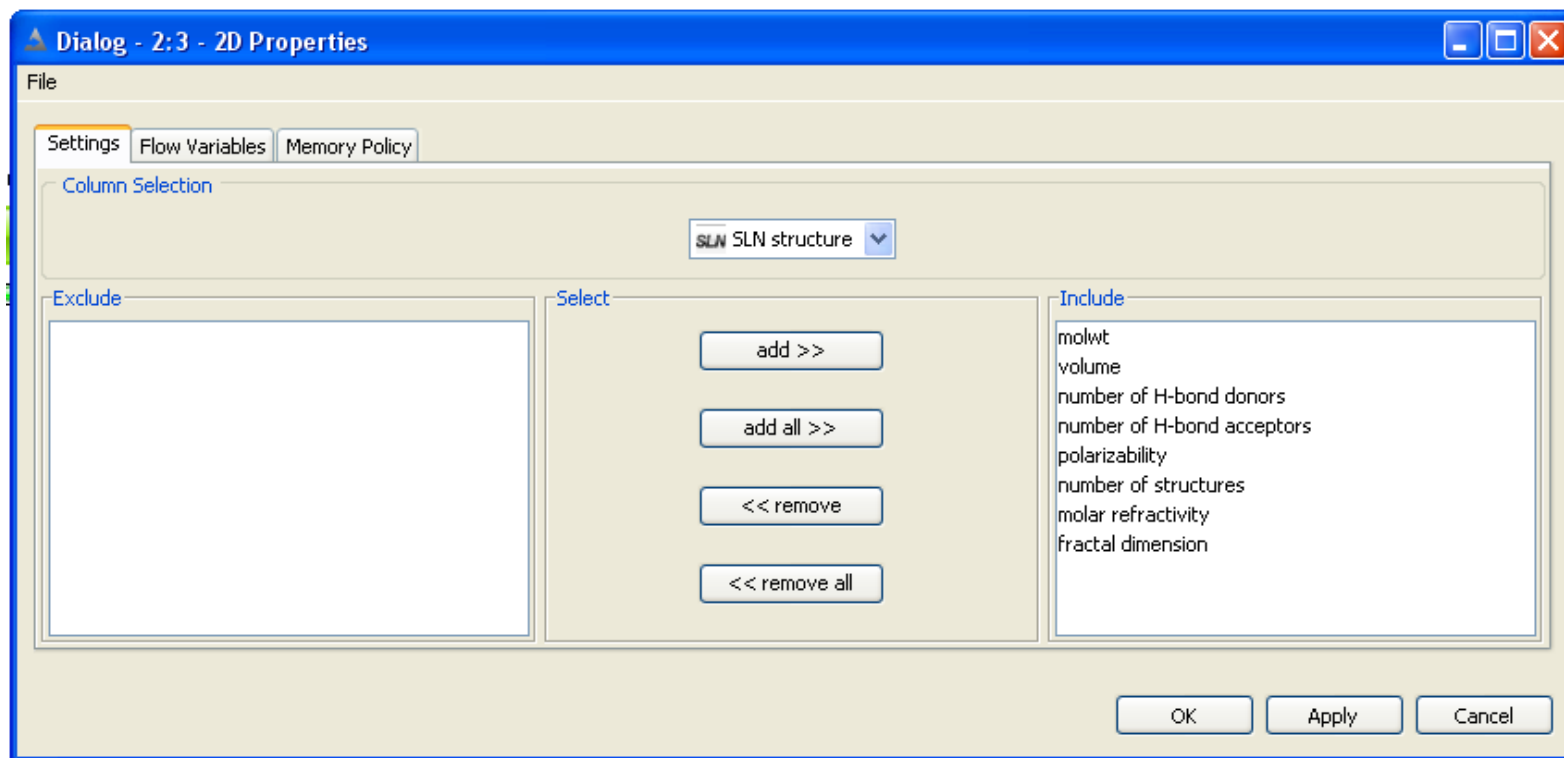
# Tripos Chemistry Extensions (TCE)

---



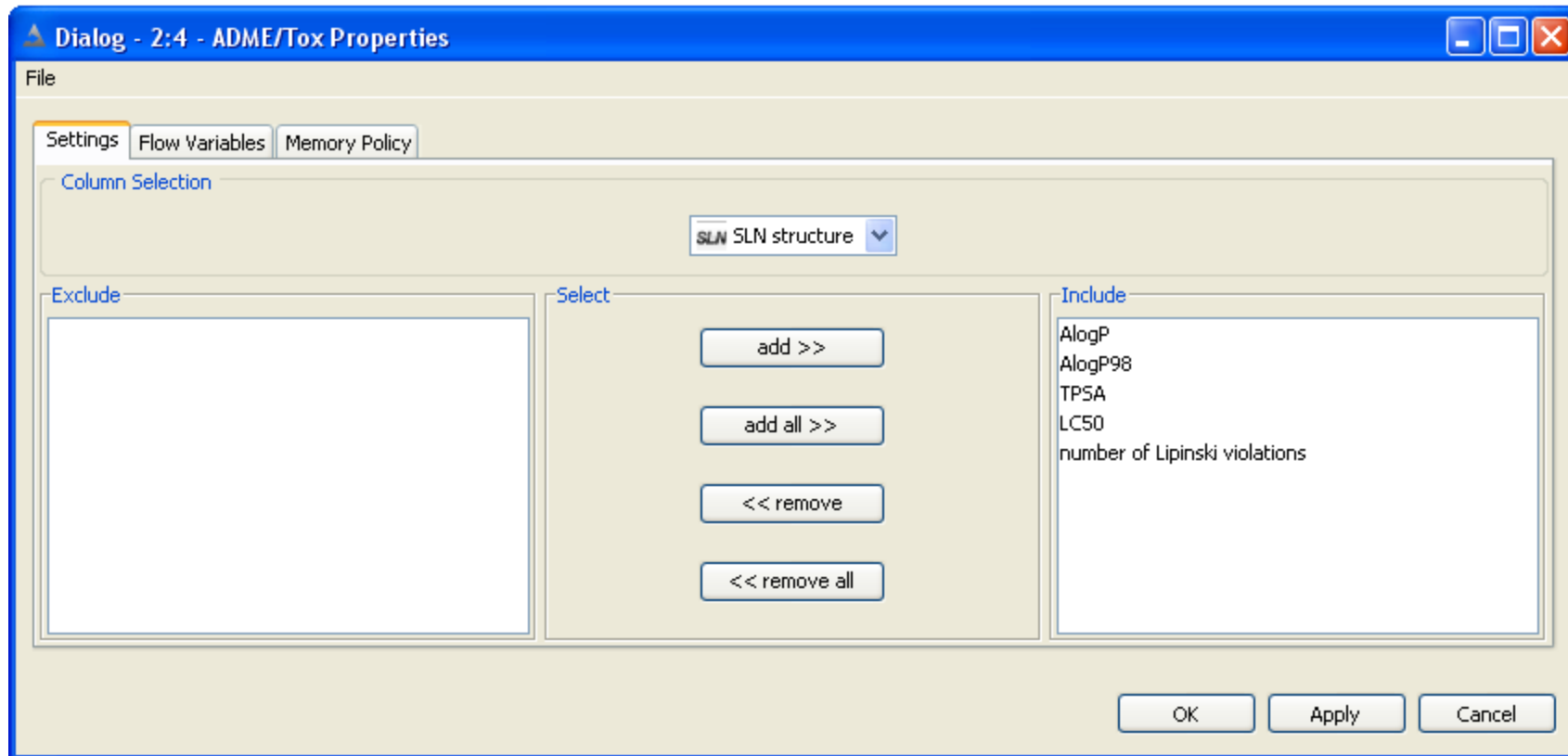


# Triplos Chemistry Extensions (TCE)





# Triplos Chemistry Extensions (TCE)





# Tripos Chemistry Extensions (TCE)

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



# Tripos Chemistry Extensions (TCE)

---





# Tripos Chemistry Extensions (TCE)



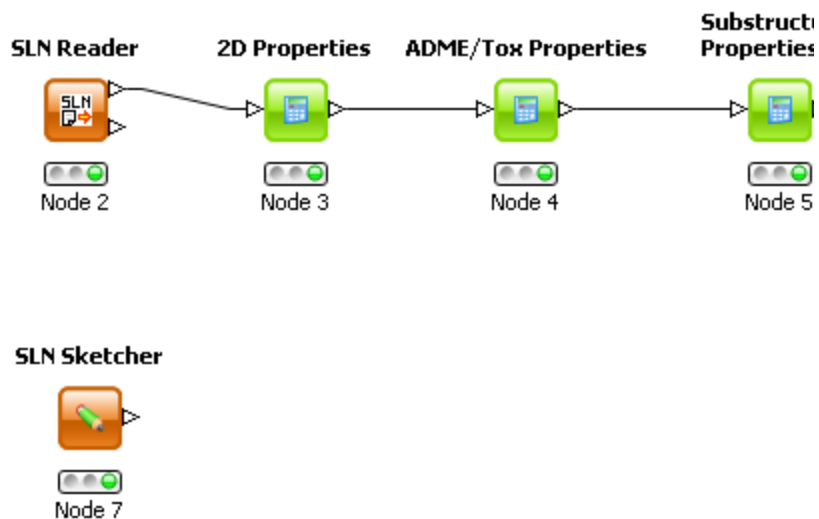
SLN Sketcher



Node 7



# Tripos Chemistry Extensions (TCE)



**Dialog - 2:7 - SLN Sketcher**

File

Settings | Flow Variables | Memory Policy

Query Structure

Structure Name: demo

Sketch... | Browse... | Enter SLN...

Chemical Structure: C1=CC=C(C=C1)S2C(=O)N(C(=O)N2)N

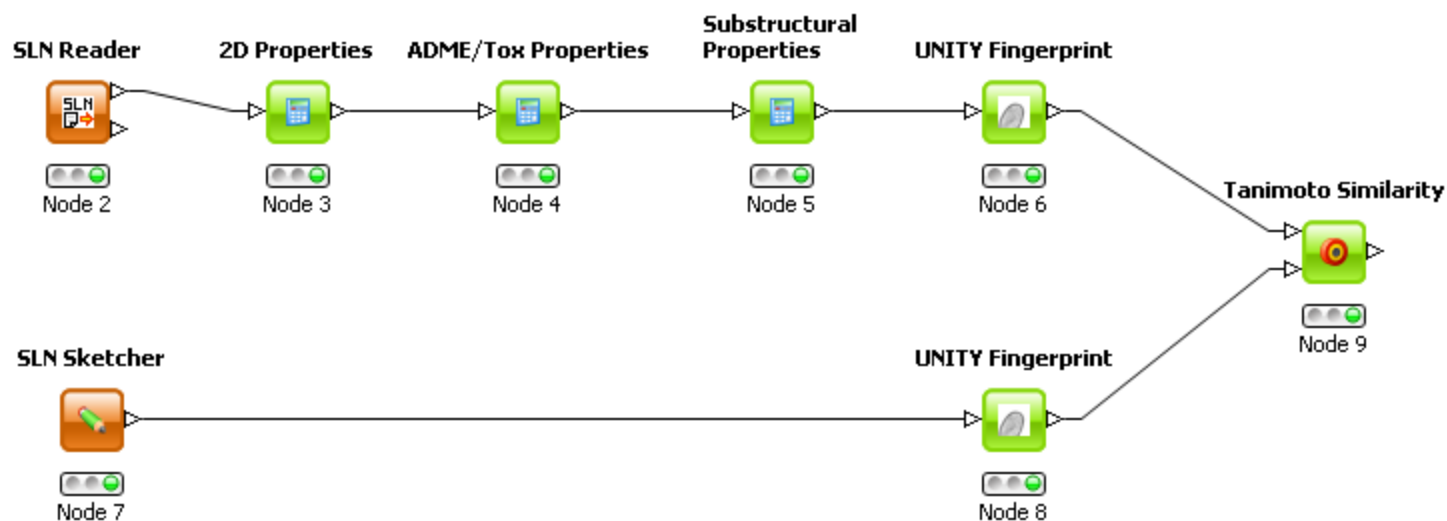
Any

OK | Apply | Cancel



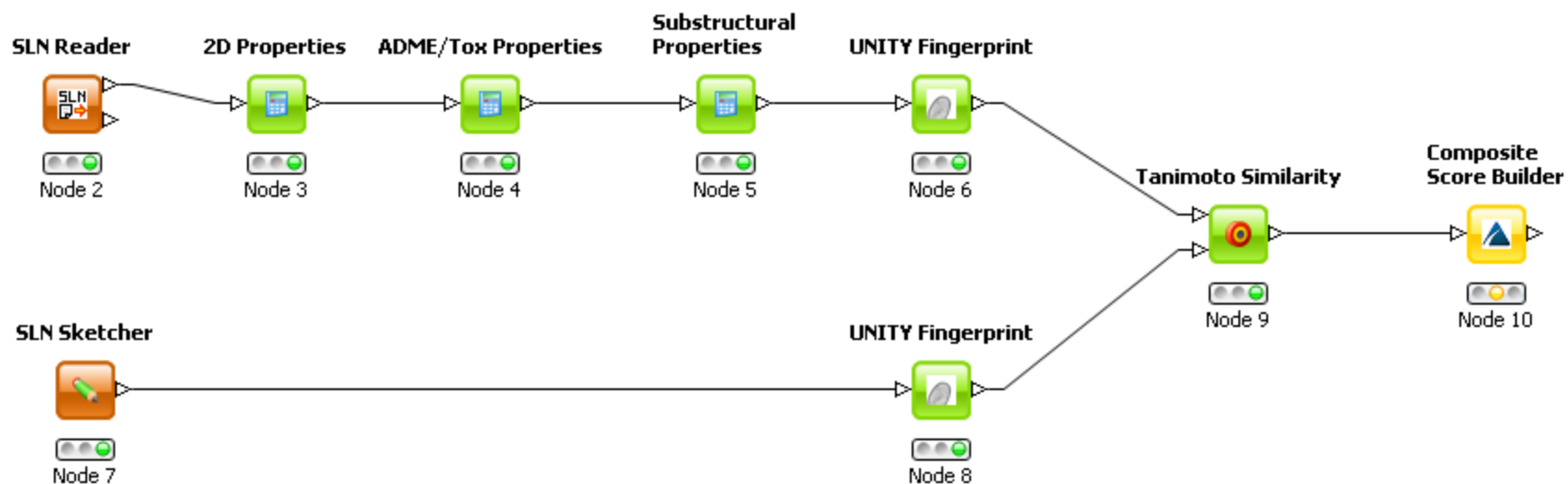


# Tripos Chemistry Extensions (TCE)





# Tripos Chemistry Extensions (TCE)





# Tripos Chemistry Extensions (TCE)

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

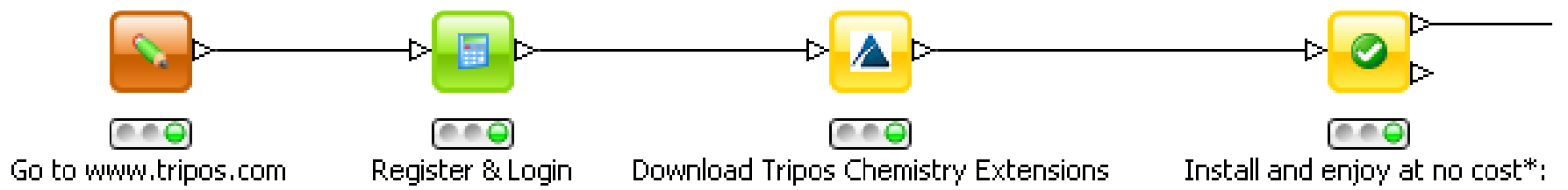
Output normalized scores  
Name (and name prefix) for the output column(s): Score

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    Normalize    Result: 0.7788007830714049



Questions? Comments?

fabian.boes@certara.com