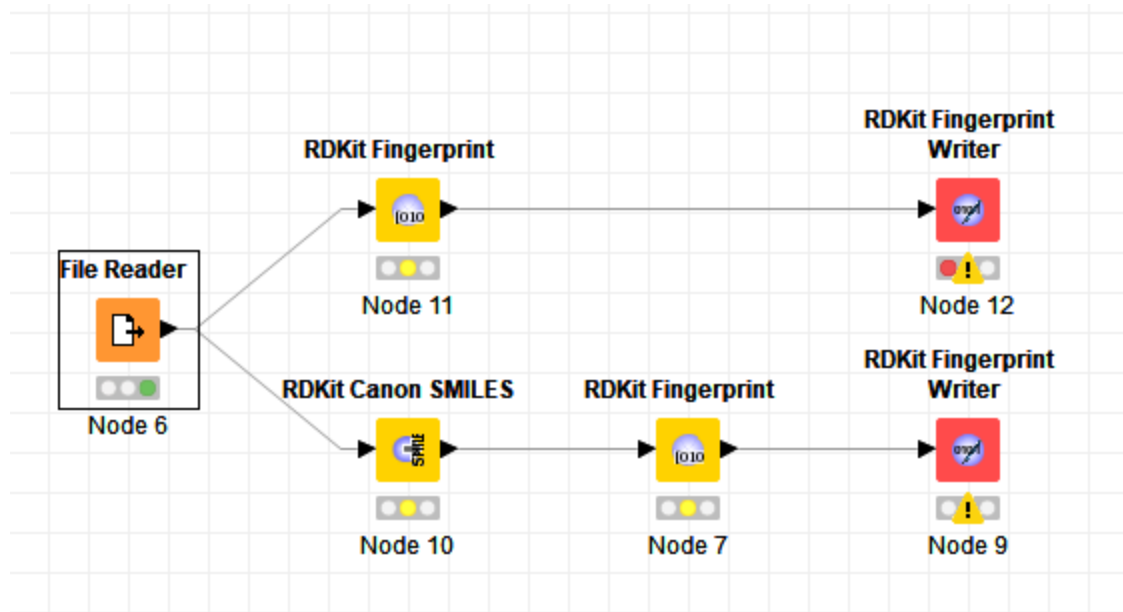


1. Here's my setup.

a. There are two paths because I've tried multiple combinations.



## 2. Downloaded SMILES and read them like this:

Dialog - 2:6 - File Reader



File

Settings | Flow Variables | Job Manager Selection | Memory Policy

Enter ASCII data file location: (press 'Enter' to update preview)

file:/C:/Users/admin/Desktop/smiles/threeb\_p0.smi

Preserve user settings for new location

Basic Settings

read row IDs  ignore spaces and tabs

read column headers  Java-style comments

Column delimiter: <space>

Single line comment:

Preview

Click column header to change column properties (\* = name/type user settings)

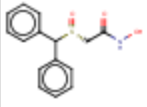
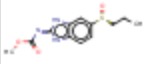
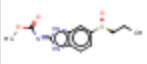
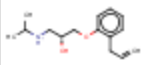
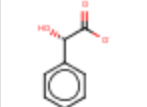
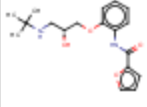

| Row ID | SMI *Col0 | S [SKIP: "...] |
|--------|-----------|----------------|
| Row0   |           | ZINC00000012   |
| Row1   |           | ZINC00000017   |
| Row2   |           | ZINC00000017   |
| Row3   |           | ZINC00000023   |
|        |           |                |

3. This is what I get after reading it.

File Table - 2:6 - File Reader

File [Hilite](#) [Navigation](#) [View](#)

Table "threeb\_p0.sm" - Rows: 74527

| Row ID | SMI Col0  |
|--------|---|
| Row0   |    |
| Row1   |    |
| Row2   |    |
| Row3   |    |
| Row4   |    |
| Row5   |   |
|        |  |

#### 4. This is my RDKit Fingerprint setup:

Dialog - 2:11 - RDKit Fingerprint

File

Options | Advanced | Flow Variables | Job Manager Selection | Memory Policy

Fingerprint type: Morgan

RDKit Mol column: SM Col0

New fingerprint column name: Fingerprint

Remove source column

OK Apply Cancel ?

Options | Advanced | Flow Variables | Job Manager Selection | Memory Policy

Fingerprint Settings

Num Bits: 1024 Radius: 2

Rooted Fingerprints

Create rooted fingerprint

Atom list column for rooted fingerprints: ? <none>

Include atoms (disable to exclude them)



