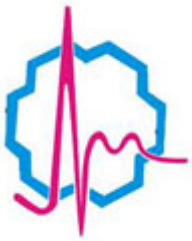
KNIME Workflows LDM and LDM&MLB

Descriptors for nanoparticles based on "Liquid Drop" and Metal–Ligand Binding Models

A Collaborative Project between

University of Gdansk



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LDM and LDM&MLB are KNIME-based workflows, developed in framework of NanoBRIDGES collaborative project (http://nanobridges.eu/) to calculate structural descriptors for nanoparticles. LDM is useful tool to calculate descriptors based on size-dependent “liquid drop” model. LDM&MLB workflow you can calculate also Metal–ligand Binding (MLB) derived descriptors.

Background

In “liquid drop” model (LDM) a nanoparticle is represented as a spherical drop, where elementary particles (molecules) are densely packed and the density of cluster is equal to mass density. The basic equation of LDM is characterized by minimum radius of interactions between elementary particles in cluster and described by the Wigner–Seitz radius:

$$r_W = \left(\frac{3M}{4\pi\rho N_A} \right)^{1/3} \qquad (1)$$

Descriptors, calculated in framework of LDM are size-dependent. More details about LDM can be found in our recent contribution:

Sizochenko, N.; Rasulev, B.; Gajewicz, A.; Kuz'min, V.; Puzyn, T.; Leszczynski, J. From basic physics to mechanisms of toxicity: the "liquid drop" approach applied to develop predictive classification models for toxicity of metal oxide nanoparticles. *Nanoscale* **2014,** *6* (22), 13986-93.

Metal–ligand Binding (MLB) derived descriptors express the properties of single metal cations. Using LDM&MLB workflow you can calculate three MLB-based descriptors: electronegativity, covalent index and cation polarizing power.

Covalent index represents a combination of the electronegativity (χ) and the Pauling radius (r):

$$(CI) = \chi^2 r \qquad (2)$$

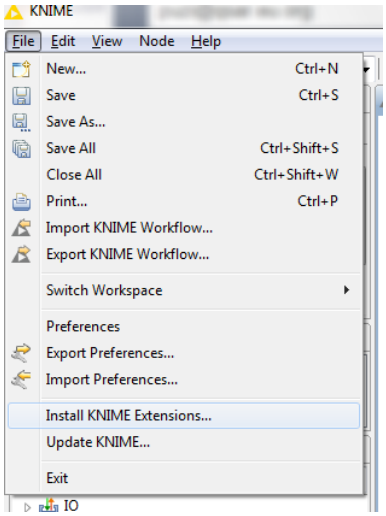
Cation polarizing power encodes represents the combination of the ion charge (Z) and Pauling radius (r):

$$(CPP) = Z^2/r \quad (3)$$

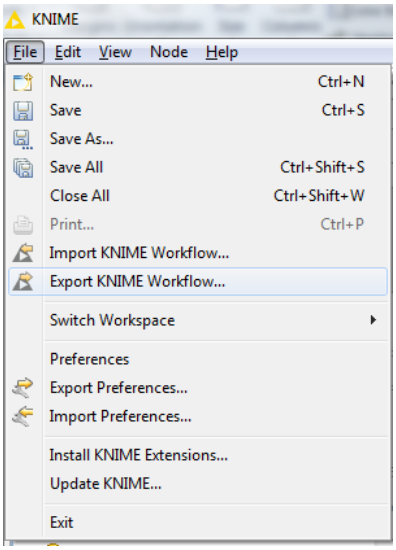
Workflow Installation

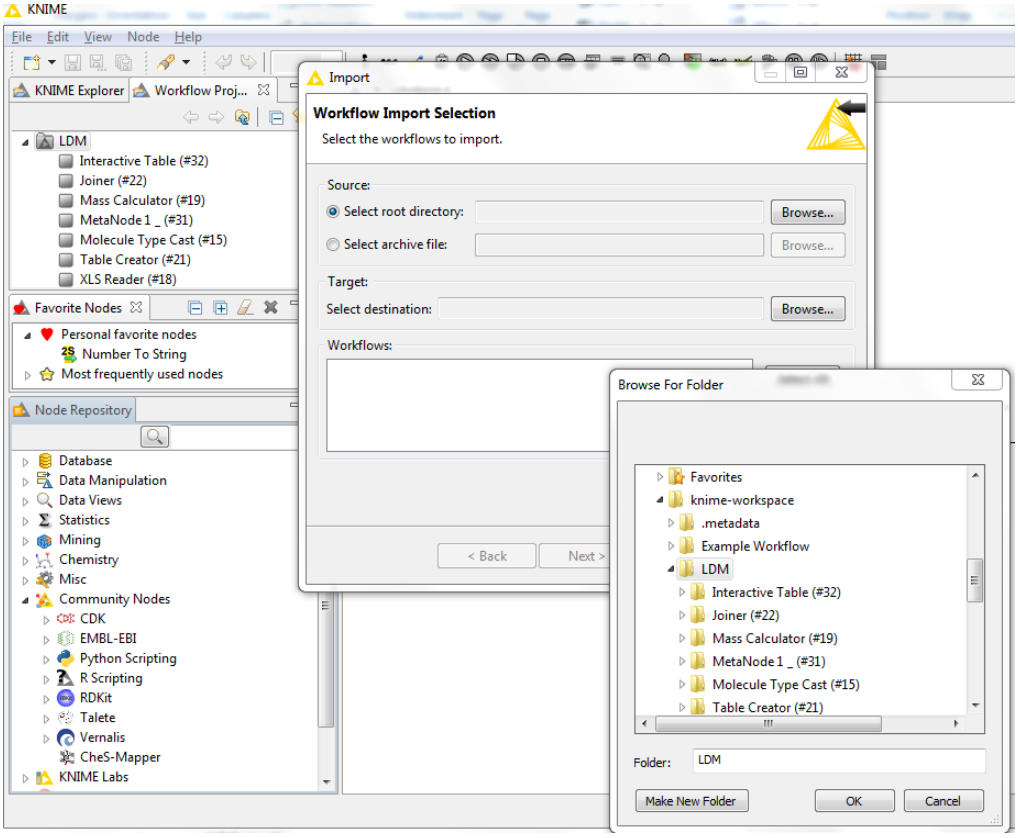
Setup procedures for LDM and LDM&MLB are similar. Thus, we clearly described only the installation for LDM workflow. LDM workflow is working under KNIME Analytics Platform (You can download from here: (https://www.knime.org/knime).

1) To run this tool on KNIME Analytics Platform you have to install CDK Community nodes from KNIME Extensions:

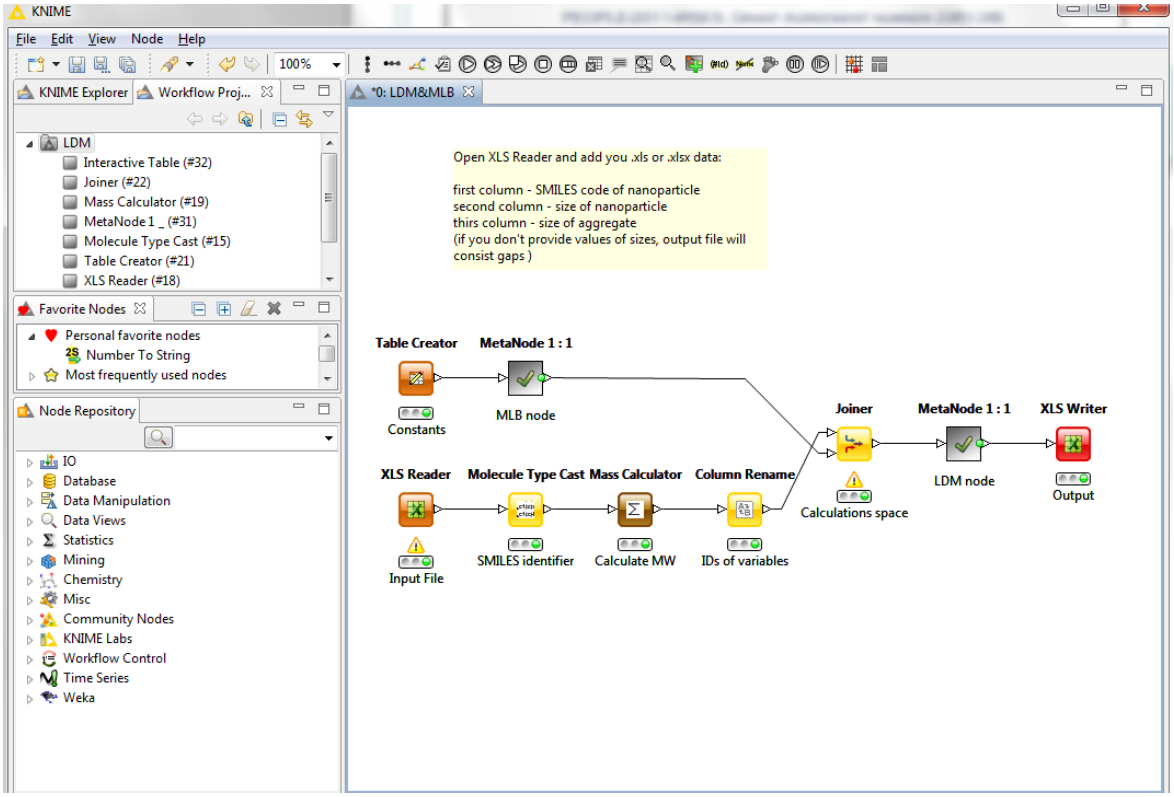


2) To open workflow you should unzip file with workflow and import it to your project:





3) LDM Workflow is ready to use:

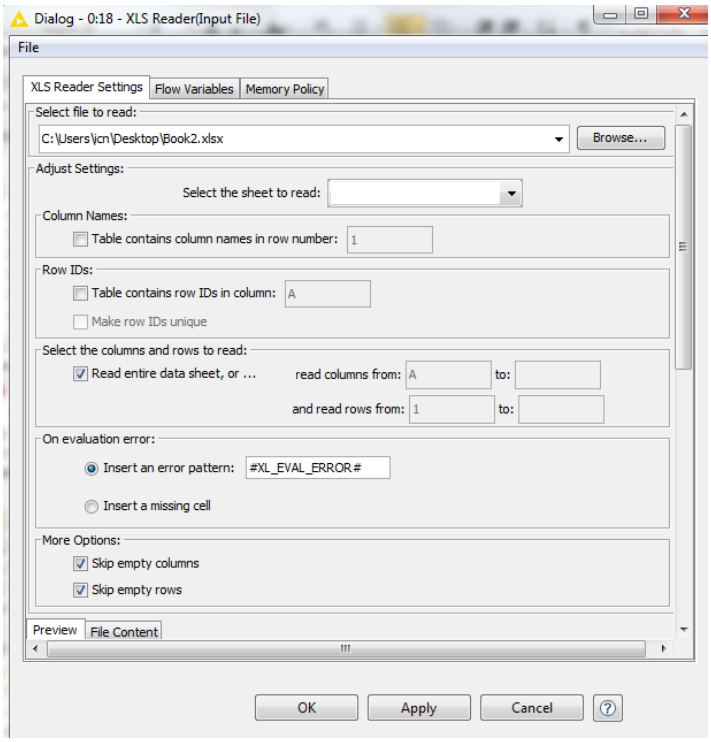


Descriptors Calculation

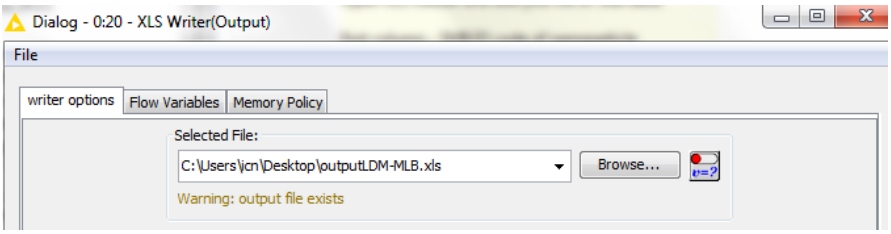
1) To preform calculations please create input-file. Example of input is provided in Input.xls.
2) Let's take a closer. Input file should consist:
   a) SMILES code of nanoparticle at first column;
   b) size of nanoparticles at second column
   c) size of aggregate at third column.

Note: if you don't provide values of sizes for several nanoparticles, output file will have gaps. If you provide only data about chemical composition, output file will consist data about size-independent parameters.

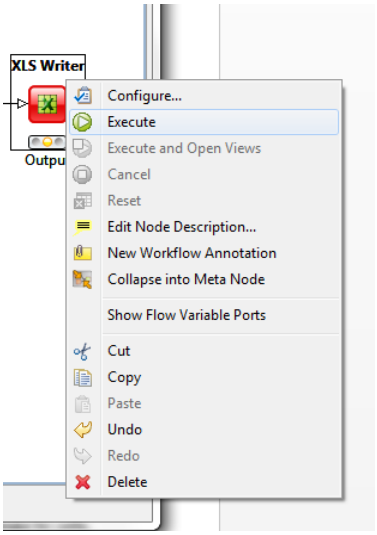
3) To start calculations please double-click the left mouse button on "XLS Reader" node and add your input file:



4) At the next step, please double-click the left mouse button on "XLS Writer" node and add path to your output file:



5) At the last step click the right mouse button on "XLS Writer" node and choose option "Execute":



6) Your output is ready! You can use results of calculations.
   Output has following list of descriptors:
   a) SMILES (copy of input data)
   b) Size of nanoparticle (copy of input data)
   c) Size of aggregate (copy of input data)
   d) molar_weight – molecular weight
   e) Density – mass density
   f) Rw – Wigner–Seitz radius
   g) number of clusters - the number of molecules in a nanocluster
   h) ratio of surface - ratio of surface molecules
   i) surface/volume ratio - ratio of surface molecules to molecules in volume
   j) aggregation size - ratio of particles in aggregate in comparison with the size of a single particle

NOTE: Using LDM&MLB workflow you can calculate also MLB (Metal–ligand Binding) derived descriptors. Procedure of using this workflow is similar. There are only appeared additional descriptors in output file:

   a) Electronegativity
   b) CI - covalent index
   c) CPP – cation polarizing power

Disclaimer

The workflows are provided free of charge. For academic purpose only.

The software is validated on known data sets. Please report for discrepancy of result for any other dataset. Contact us at any of the following addresses:

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