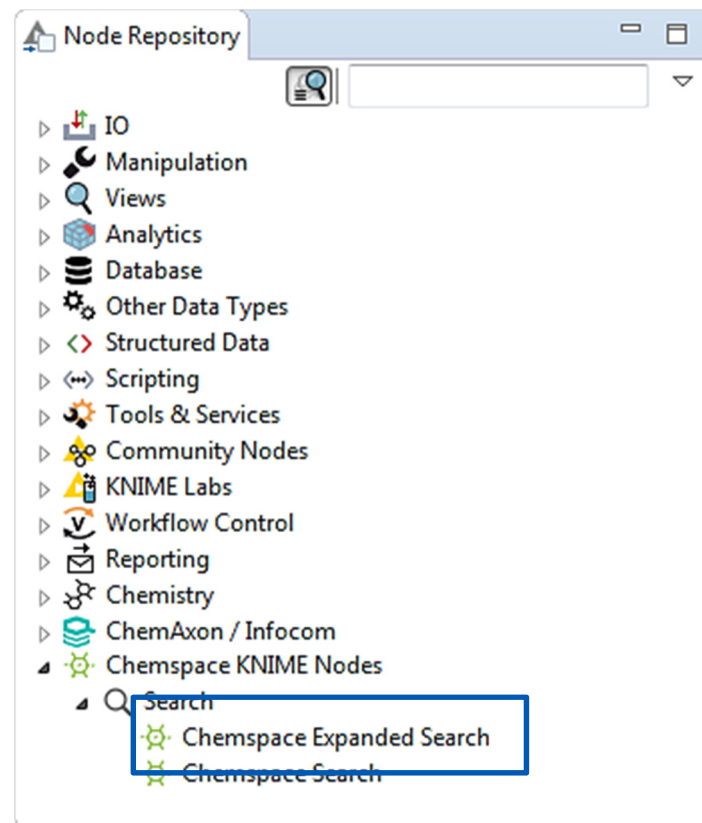
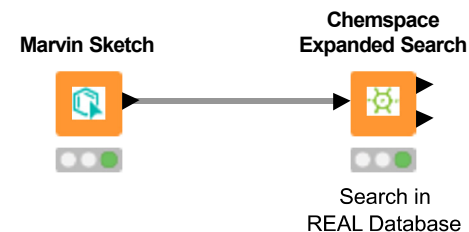


- **Chemspace Search** and **Chemspace Expanded Search** nodes
- Source:
 - **Chemspace database**, 130 million molecules
 - **REAL Database**, 720 million molecules
- Search options:
 - Structure search (Similarity, Substructure, Exact match)
 - ID search
- Number of hits: up to 200
- Authentication: API key, request via email
- **Example KNIME workflow** available

- Search in **REAL Database**:
over **720 million** compounds
- Structure Search
- ID Search:
by REAL id or Chemspace REAL ID





Ask us for the Chemspace API Key!

Access:

Chemspace API Key:

Search options:

ID column

Search type:

- search by ID
- exact search
- substructure search
- similarity search

Similarity threshold:

Maximum hits per query:

show PhysChem parameters for hits

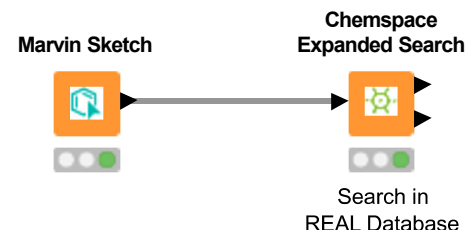
Choose Search type

Select query column

- **ID Search:**
String or Numeric
- **Structure Search:**
SMILES or String

Limit number of hits

Please contact us at info@chem-space.com to obtain Chemspace API Key



Access:
Chemspace API Key:

Search options:

ID column

Search type:

- search by ID
- exact search
- substructure search
- similarity search

Similarity threshold:

Maximum hits per query:

show PhysChem parameters for hits

B) Exact match with your query

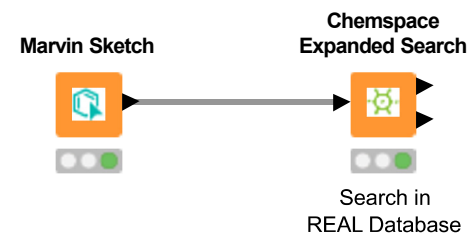
C) Perform similarity search

Set similarity threshold

A) Find by Chemspace ID or supplier's code

D) Use your query as substructure

Display pre-calculated PhysChem for results



- Paste Chemspace API Key (need to do once)
- Choose search type
 - Select query column
 - Set similarity threshold for Similarity Search
 - Run the node and get the results from **REAL Database!**

See also our [Chemspace Search](#) node for KNIME

Access to Chemspace/REAL databases from KNIME interface is provided for free, but the **API Key** is needed. Please follow the instructions below to get the Key:

1. Register on Chemspace website
2. Email us on info@chem-space.com with Key request and provide us with your username or email used for registration
3. Get the Key and explore the chemical universe!

