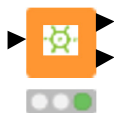


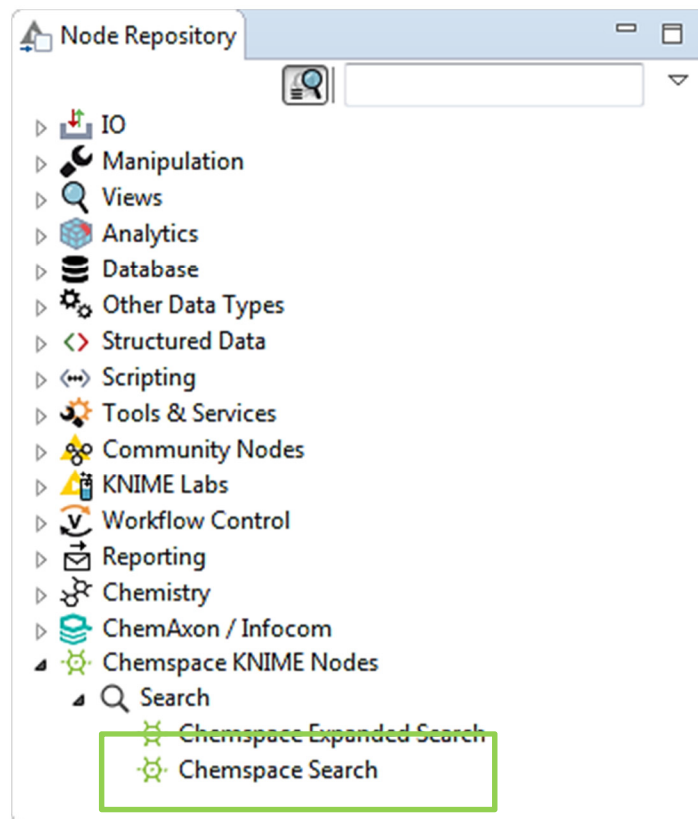
- **Chemspace Search** and **Chemspace Expanded Search** nodes
- Source:
 - **Chemspace database**, 130 million molecules
 - **REAL Database**, 720 million molecules
- Search options:
 - Structure search (Similarity, Substructure, Exact match)
 - ID search
- Number of hits: up to 200
- Authentication: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

- Search in **Chemspace database**:
over **130 million** compounds
- Structure Search:
in Building Blocks and Screening separately
- ID Search:
by Chemspace ID or supplier's code

Chemspace Search



Search in
Chemspace database



Ask us for the Chemspace API Key!

Access:

Chemspace API Key:

Search options:

ID column

Search type:

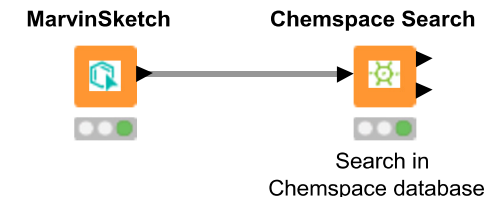
- search by ID
- exact match
- substructure search in Building Blocks
- similarity search in Building Blocks
- substructure search in Screening Compounds
- similarity search in Screening Compounds

Similarity threshold:

Maximum hits per query:

Choose Search type

Please note that Structure search is provided in Building Blocks and Screening Compounds separately

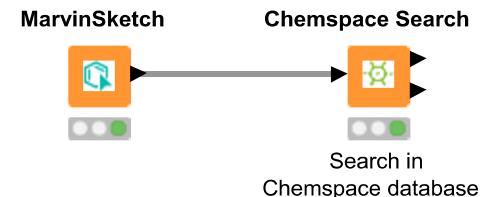


Select query column

- **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:

SMILES column

Search type:

- search by ID
- exact match
- substructure search in Building Blocks
- similarity search in Building Blocks
- substructure search in Screening Compounds
- similarity search in Screening Compounds

Similarity threshold:

Maximum hits per query:

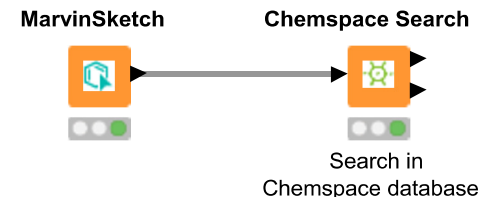
B) Exact match
with your query

C) Perform **similarity search**

Set similarity threshold

A) Find by
Chemspace **ID** or
supplier's **code**

D) Use your query
as **substructure**

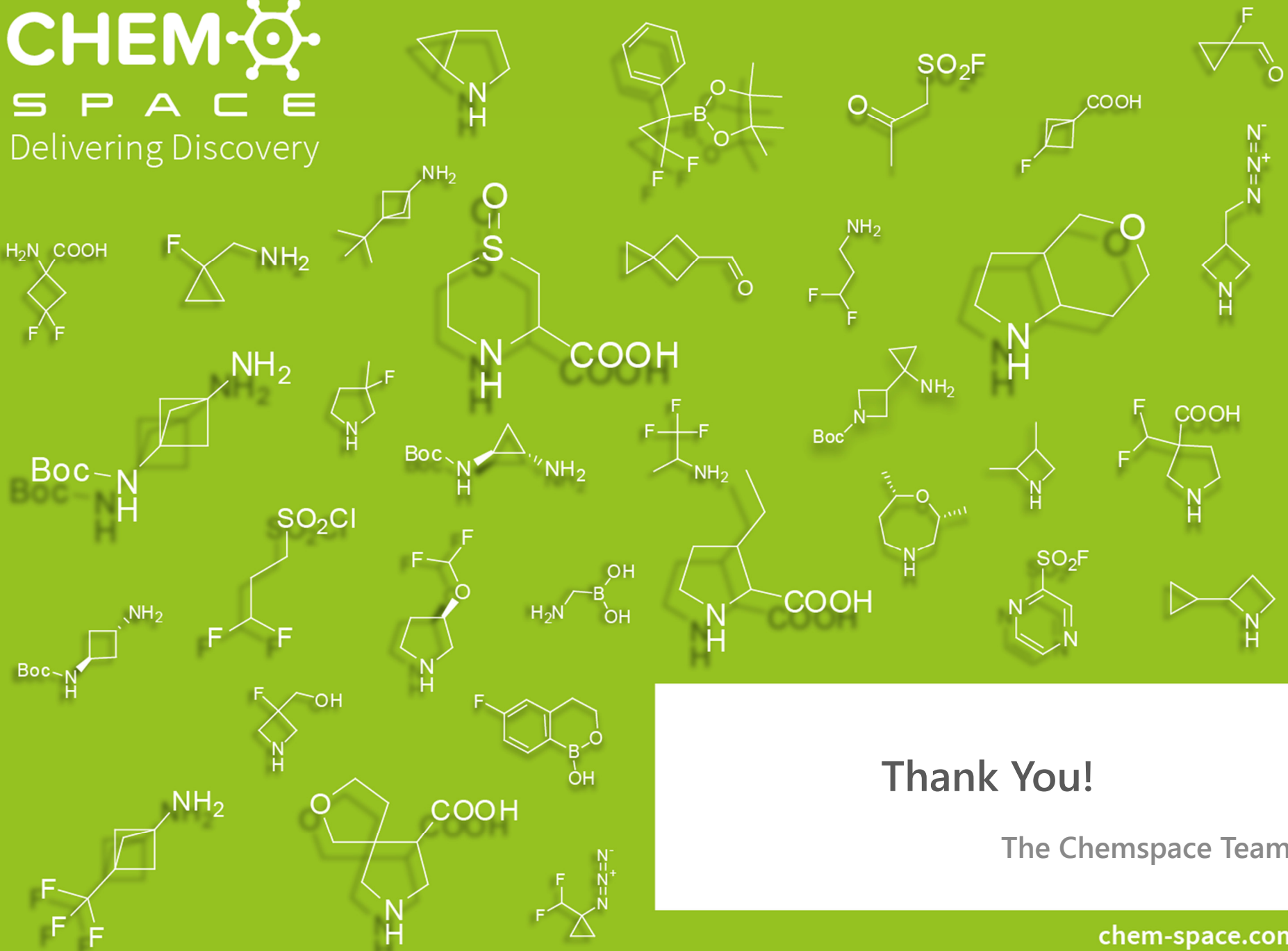


- Paste Chemspace API Key (need to do once)
- Choose search type
 - Select query column
 - Set similarity threshold for Similarity Search
 - Run the node and get the results from **Chemspace database!**

See also our [Chemspace Expanded 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!



Thank You!

The Chemspace Team