

Chemspace search KNIME node

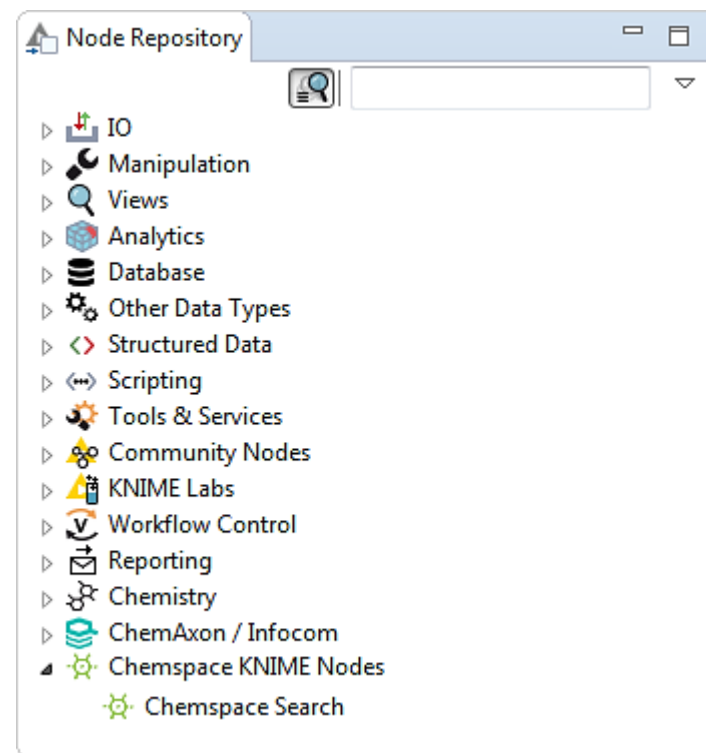
search from your own workflow!

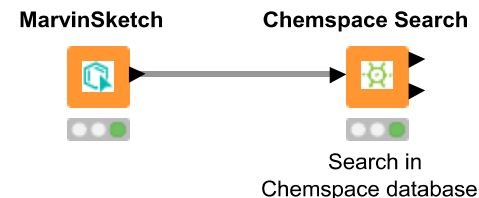
- Source:
 - **Chemspace database**, over 1.6 billion molecules
- Search options:
 - Structure search
(Similarity, Substructure, Exact match)
 - ID search
- Number of hits: up to 2000
- Authentication: API key, requested once via email

Chemspace Search



Search in
Chemspace database





Ask us for the Chemspace API Key!

Access:

Chemspace API Key:

Search options:

SMILES column **SMW Molecule** ▾

Search type:

search by ID

exact search

substructure search

similarity search

Search in categories:

CSSB (In-Stock Building Blocks)

CSSS (In-stock Screening Compounds)

CSMB (Make-On-Demand Building Blocks)

CSMS (Make-On-Demand Screening Compounds)

CSCS (Custom Synthesis)

Maximum hits per query:

show PhysChem parameters for hits

Choose Search type

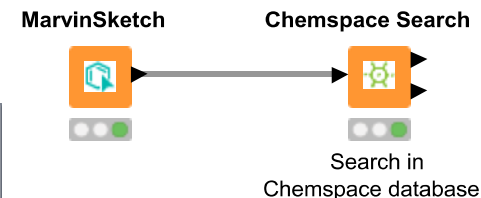
Select query column

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

Precalculated PhysChem

Limit number of hits

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



B) Exact match
with your query

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

C) Perform similarity search

D) Use your query
as **substructure**

For more details, please visit
<https://chem-space.com/search>

Access:

Chemspace API Key:

Search options:

SMILES column

Search type:

search by ID

exact search

substructure search

similarity search

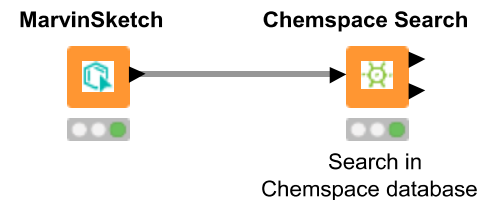
Search in categories:

- CSSB (In-Stock Building Blocks)
- CSSS (In-stock Screening Compounds)
- CSMB (Make-On-Demand Building Blocks)
- CSMS (Make-On-Demand Screening Compounds)
- CSCS (Custom Synthesis)

Maximum hits per query:

show PhysChem parameters for hits

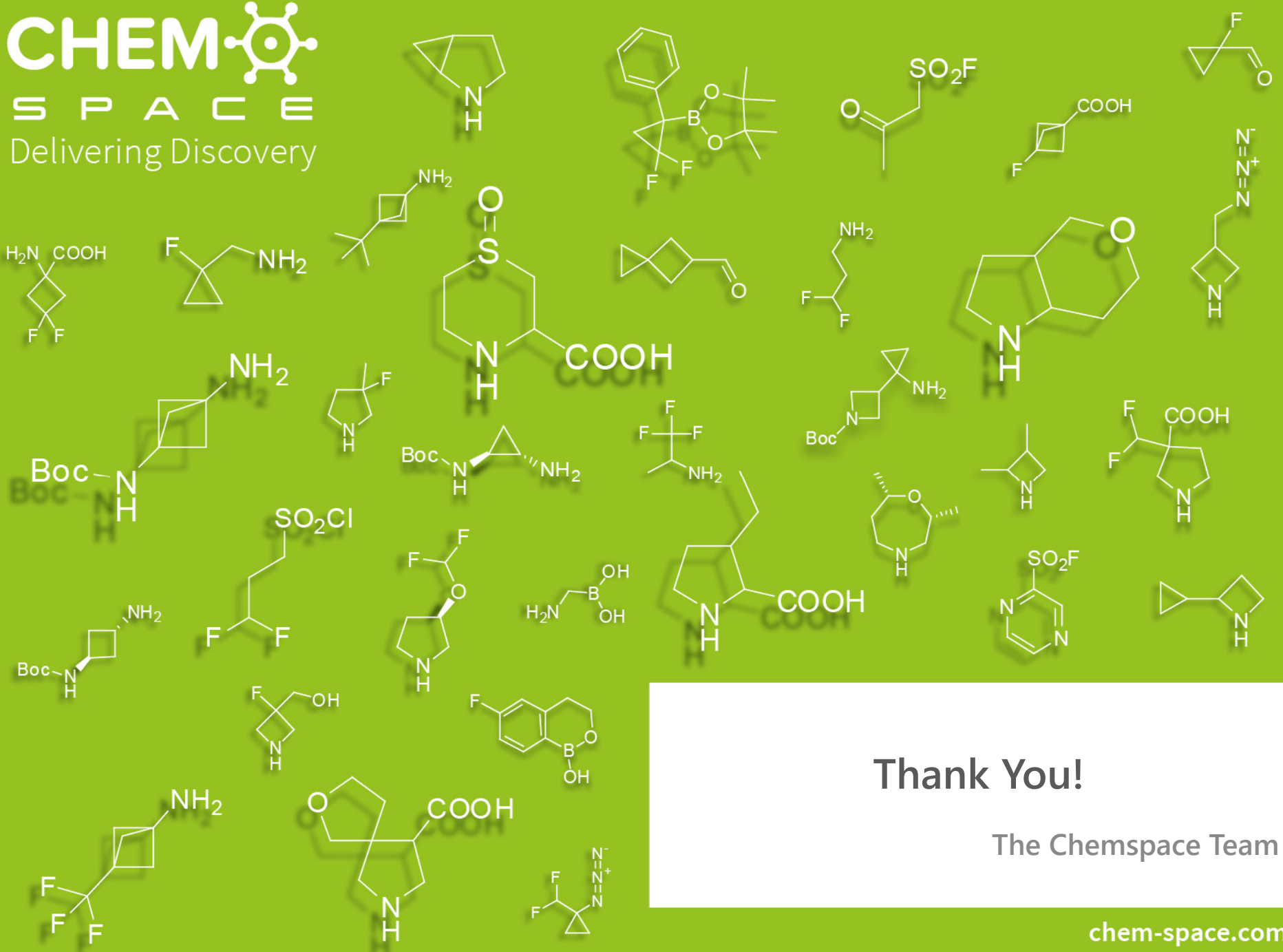
Please contact us at info@chem-space.com to obtain Chemspace API Key



- Paste Chemspace API Key (need to do once)
- Choose search type
 - Select query column
 - Choose sections of the database you wish to search in
 - Run the node and get the results from **Chemspace database!**

Access to Chemspace database 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